

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 0.03_GPa, 0.88_GPa, 1.06_GPa, 1.20_GPa, 1.58_GPa, 1.95_GPa, 2.32_GPa, 2.70_GPa, 3.25_GPa, 4.24_GPa, 4.30_GPa, 4.45_GPa, 4.86_GPa, 5.18_GPa, 5.72_GPa, 6.19_GPa, 6.91_GPa, 7.11_GPa, 8.04_GPa, 8.29_GPa, 8.46_GPa, 8.61_GPa, 9.13_GPa, 9.73_GPa

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 0.88_GPa

Bond precision:	Si- O = 0.0050 A	Wavelength=0.49585	
Cell:	a=9.559 (3)	b=8.743 (5)	c=5.2389 (10)
	alpha=90	beta=106.70 (3)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	419.4 (3)	419.4 (3)	
Space group	P 2/n	P 1 2/n 1	
Hall group	-P 2yac	-P 2yac	
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24	?	
	Si8, 2.305 (Ca), 1.695 (Na)		
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91	Al0.4525 Ca0.5763 Fe0.0695	
	Na1.69 O24 Si8	Mg0.478 Na0.4237 O6 Si2	
Mr	850.92	213.50	
Dx, g cm-3	3.369	3.382	
Z	1	4	
Mu (mm-1)	0.699	0.691	
F000	422.4	422.0	
F000'	423.29		
h, k, lmax	15, 14, 8	14, 9, 8	
Nref	2041	901	
Tmin, Tmax		0.130, 1.000	
Tmin'			

Correction method= # Reported T Limits: Tmin=0.130 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.441

Theta(max)= 24.430

R(reflections)= 0.0758(685)

wR2(reflections)=

wR= 0.1070(901)

S = 3.130

Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing

Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing

Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing

Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low

13.26 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low .

0.570 Why?

Alert level B

PLAT017_ALERT_1_B Check Scattering Type Consistency of AM1

as

AL Error?

PLAT017_ALERT_1_B Check Scattering Type Consistency of FM1

as

FE Error?

PLAT017_ALERT_1_B Check Scattering Type Consistency of AM11

as

AL Error?

PLAT017_ALERT_1_B Check Scattering Type Consistency of MM11

as

MG Error?

PLAT017_ALERT_1_B Check Scattering Type Consistency of FM11

as

FE Error?

PLAT088_ALERT_3_B Poor Data / Parameter Ratio

6.43 Note

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00

Goodness of fit given = 3.130

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ

Please Check

Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8

Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6

Si2

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..

3.08 Check

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...

Please Check

PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...

Please Check

PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...

Please Check

PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms .

Please Check

PLAT213_ALERT_2_C Atom O11A has ADP max/min Ratio

3.9 prolat

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)

2.9 Note

PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare)

O11A Check

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label

MnM1 Check

O11A

MNM1

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label

Cm11 Check

O11A

CM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label

Tm11 Check

O11A

TM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label

MnM1 Check

	O12A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	O12A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	MM11				

PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	FM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA21		
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	1.03Ang From O22A .	0.74	eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please	Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please	Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49585	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1	Constrained at	0.087 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11	Constrained at	0.052 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11	Constrained at	0.86 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1	Constrained at	0.868 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1	Constrained at	0.045 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11	Constrained at	0.088 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21	Constrained at	0.7904 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2	Constrained at	0.3622 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2	Constrained at	0.6378 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21	Constrained at	0.2096 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A .	135.0	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11	Fm11	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.84	Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
	0 1 0, 1 1 0,		
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L= 0.600	375	Report
	0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0,	0 7 0,	
	0 8 0, 0 9 0, 1 2 0, 1 3 0, 1 4 0,	1 5 0,	
	1 6 0, 1 7 0, 1 8 0, 1 9 0, 2 0 0,	2 1 0,	
	2 2 0, 2 3 0, 2 4 0, 2 5 0, 2 6 0,	2 7 0,	
	2 8 0, 2 9 0, 3 1 0, 3 4 0, 3 5 0,	3 6 0,	

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      3 7 0, 3 8 0, 3 9 0, 4 0 0, 4 1 0, 4 3 0,
      4 6 0, 4 7 0, 4 8 0, 4 9 0, 5 1 0, 5 7 0,
      5 8 0, 5 9 0, 6 0 0, 6 1 0, 6 4 0, 6 5 0,
      6 8 0, 7 1 0, 7 2 0, 7 5 0, 7 6 0, 7 7 0,
      7 8 0, 8 0 0, 8 1 0, 8 2 0, 8 3 0, 8 5 0,
      8 6 0, 8 7 0, 9 1 0, 9 2 0, 9 3 0, 9 5 0,
      9 6 0, 10 0 0, 10 1 0, 10 2 0, 10 3 0, 10 4 0,
    -11 0 1, -11 1 1, -11 2 1, -10 1 1, -10 2 1, -10 3 1,
    -10 4 1, -10 5 1, -9 0 1, -9 1 1, -9 2 1, -9 3 1,
     -9 6 1, -8 1 1, -8 2 1, -7 0 1, -7 1 1, -7 8 1,
     -6 6 1, -6 8 1, -5 0 1, -5 6 1, -5 7 1, -5 8 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 708 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 3 Note
      -2 2 1, 5 3 1, 0 0 2,
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked ! Info
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 5 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 5 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of 3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 3.609 Note
      Predicted wR2: Based on SigI**2 5.80 or SHELX Weight 5.80
PLAT985_ALERT_1_G The Ca-f"= 0.1534 Deviates from the B&C-Value 0.1518 Check
PLAT985_ALERT_1_G The Fe-f"= 0.4374 Deviates from the B&C-Value 0.4347 Check

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- 5 **ALERT level A** = Most likely a serious problem - resolve or explain
 6 **ALERT level B** = A potentially serious problem, consider carefully
 50 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 40 **ALERT level G** = General information/check it is not something unexpected
- 61 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 6 ALERT type 2 Indicator that the structure model may be wrong or deficient
 7 ALERT type 3 Indicator that the structure quality may be low
 19 ALERT type 4 Improvement, methodology, query or suggestion
 8 ALERT type 5 Informative message, check
-

Datablock: 1.06_GPa

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Bond precision:   Si- O = 0.0060 A           Wavelength=0.49570

Cell:             a=9.544(3)                b=8.758(5)                c=5.234(1)
                  alpha=90                  beta=106.76(3)              gamma=90
Temperature:      293 K

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	Calculated	Reported
Volume	418.9(3)	418.9(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.373	3.386
Z	1	4
Mu (mm-1)	0.700	0.691
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,9,8
Nref	2041	606
Tmin,Tmax		0.199,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.199 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.297 Theta(max)= 24.430

R(reflections)= 0.0914(477) wR2(reflections)=
wR= 0.1194(606)

S = 3.110 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 13.28 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.560 Why?

PLAT701_ALERT_1_A Bond Calc 2.137(6), Rep 2.115(5), Dev.. 3.67 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.137(6), Rep 2.115(5), Dev.. 3.67 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond Calc 2.000(6), Rep 1.980(5), Dev.. 3.33 Sigma

O12A -MM11 1_555 1_555 # 17 Check

PLAT701_ALERT_1_A Bond Calc 2.000(6), Rep 1.980(5), Dev.. 3.33 Sigma

O12A	-FM11	1_555	1_555		#	18 Check
PLAT701_ALERT_1_A Bond	Calc	3.488(4), Rep	3.473(5), Dev..			3.75 Sigma
AM11	-CA21	1_555	1_555		#	91 Check
PLAT701_ALERT_1_A Bond	Calc	3.488(4), Rep	3.473(5), Dev..			3.75 Sigma
AM11	-NA21	1_555	1_555		#	92 Check
PLAT701_ALERT_1_A Bond	Calc	3.488(4), Rep	3.473(5), Dev..			3.75 Sigma
MM11	-CA21	1_555	1_555		#	113 Check
PLAT701_ALERT_1_A Bond	Calc	3.488(4), Rep	3.473(5), Dev..			3.75 Sigma
MM11	-NA21	1_555	1_555		#	114 Check

Alert level B

PLAT017_ALERT_1_B Check	Scattering Type	Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type	Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B Check	Scattering Type	Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type	Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B Check	Scattering Type	Consistency of FM11	as	FE Error?
PLAT088_ALERT_3_B	Poor Data / Parameter Ratio			6.45 Note
PLAT250_ALERT_2_B	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)			5.1 Note
PLAT701_ALERT_1_B Bond	Calc	3.018(3), Rep	3.025(2), Dev..	2.33 Sigma
SIA1	-CA2	1_555	3_666	 # 38 Check
PLAT701_ALERT_1_B Bond	Calc	3.018(3), Rep	3.025(2), Dev..	2.33 Sigma
SIA1	-NA2	1_555	3_666	 # 39 Check
PLAT701_ALERT_1_B Bond	Calc	3.093(3), Rep	3.086(2), Dev..	2.33 Sigma
MGM1	-AM11	1_555	1_554	 # 48 Check
PLAT701_ALERT_1_B Bond	Calc	3.093(3), Rep	3.086(2), Dev..	2.33 Sigma
MGM1	-AM11	1_555	1_555	 # 49 Check
PLAT701_ALERT_1_B Bond	Calc	3.093(3), Rep	3.086(2), Dev..	2.33 Sigma
MGM1	-MM11	1_555	1_554	 # 52 Check
PLAT701_ALERT_1_B Bond	Calc	3.093(3), Rep	3.086(2), Dev..	2.33 Sigma
MGM1	-MM11	1_555	1_555	 # 53 Check
PLAT701_ALERT_1_B Bond	Calc	3.451(5), Rep	3.436(6), Dev..	3.00 Sigma
MGM1	-CA2	1_555	1_565	 # 54 Check
PLAT701_ALERT_1_B Bond	Calc	3.451(5), Rep	3.436(6), Dev..	3.00 Sigma
MGM1	-NA2	1_555	1_565	 # 55 Check
PLAT701_ALERT_1_B Bond	Calc	3.093(3), Rep	3.086(2), Dev..	2.33 Sigma
AM1	-MM11	1_555	1_554	 # 71 Check
PLAT701_ALERT_1_B Bond	Calc	3.093(3), Rep	3.086(2), Dev..	2.33 Sigma
AM1	-MM11	1_555	1_555	 # 72 Check
PLAT701_ALERT_1_B Bond	Calc	3.451(5), Rep	3.436(6), Dev..	3.00 Sigma
AM1	-CA2	1_555	1_565	 # 73 Check
PLAT701_ALERT_1_B Bond	Calc	3.451(5), Rep	3.436(6), Dev..	3.00 Sigma
AM1	-NA2	1_555	1_565	 # 74 Check

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
 Goodness of fit given = 3.110

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
 Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8
 Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
 Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)
 Rep.: ?

PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight Differ by ..	3.08	Check
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...		Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...		Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...		Please Check
PLAT077_ALERT_4_C	Unit Cell Contains Non-integer Number of Atoms .		Please Check
PLAT213_ALERT_2_C	Atom O12A has ADP max/min Ratio	3.8	prolat
PLAT213_ALERT_2_C	Atom O32A has ADP max/min Ratio	3.2	prolat
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)		O11A Check
PLAT701_ALERT_1_C	Bond Calc 1.615(6), Rep 1.625(5), Dev..	1.67	Sigma
	O11A -SIA1 1_555 1_655	#	1 Check
PLAT701_ALERT_1_C	Bond Calc 1.611(6), Rep 1.622(5), Dev..	1.83	Sigma
	O12A -SIB1 1_555 1_655	#	11 Check
PLAT701_ALERT_1_C	Bond Calc 1.594(6), Rep 1.603(5), Dev..	1.50	Sigma
	O21A -SIA1 1_555 1_545	#	21 Check
PLAT701_ALERT_1_C	Bond Calc 1.650(5), Rep 1.644(5), Dev..	1.20	Sigma
	O31A -SIA1 1_555 1_555	#	34 Check
PLAT701_ALERT_1_C	Bond Calc 1.651(5), Rep 1.644(5), Dev..	1.40	Sigma
	O32A -SIB1 1_555 1_555	#	37 Check
PLAT701_ALERT_1_C	Bond Calc 3.045(3), Rep 3.049(2), Dev..	1.33	Sigma
	SIB1 -CA21 1_555 3_667	#	43 Check
PLAT701_ALERT_1_C	Bond Calc 3.045(3), Rep 3.049(2), Dev..	1.33	Sigma
	SIB1 -NA21 1_555 3_667	#	44 Check
PLAT701_ALERT_1_C	Bond Calc 3.199(3), Rep 3.203(2), Dev..	1.33	Sigma
	MGM1 -CA21 1_555 1_554	#	56 Check
PLAT701_ALERT_1_C	Bond Calc 3.199(3), Rep 3.203(2), Dev..	1.33	Sigma
	MGM1 -CA21 1_555 1_555	#	57 Check
PLAT701_ALERT_1_C	Bond Calc 3.199(3), Rep 3.203(2), Dev..	1.33	Sigma
	MGM1 -NA21 1_555 1_554	#	58 Check
PLAT701_ALERT_1_C	Bond Calc 3.199(3), Rep 3.203(2), Dev..	1.33	Sigma
	MGM1 -NA21 1_555 1_555	#	59 Check
PLAT701_ALERT_1_C	Bond Calc 3.199(3), Rep 3.203(2), Dev..	1.33	Sigma
	AM1 -CA21 1_555 1_554	#	75 Check
PLAT701_ALERT_1_C	Bond Calc 3.199(3), Rep 3.203(2), Dev..	1.33	Sigma
	AM1 -CA21 1_555 1_555	#	76 Check
PLAT701_ALERT_1_C	Bond Calc 3.199(3), Rep 3.203(2), Dev..	1.33	Sigma
	AM1 -NA21 1_555 1_554	#	77 Check
PLAT701_ALERT_1_C	Bond Calc 3.199(3), Rep 3.203(2), Dev..	1.33	Sigma
	AM1 -NA21 1_555 1_555	#	78 Check
PLAT701_ALERT_1_C	Bond Calc 3.199(3), Rep 3.203(2), Dev..	1.33	Sigma
	FM1 -CA21 1_555 1_554	#	79 Check
PLAT701_ALERT_1_C	Bond Calc 3.199(3), Rep 3.203(2), Dev..	1.33	Sigma
	FM1 -CA21 1_555 1_555	#	80 Check
PLAT701_ALERT_1_C	Bond Calc 3.199(3), Rep 3.203(2), Dev..	1.33	Sigma
	FM1 -NA21 1_555 1_554	#	81 Check
PLAT701_ALERT_1_C	Bond Calc 3.199(3), Rep 3.203(2), Dev..	1.33	Sigma
	FM1 -NA21 1_555 1_555	#	82 Check
PLAT711_ALERT_1_C	BOND Unknown or Inconsistent Label		MnM1 Check
	O11A MNM1		
PLAT711_ALERT_1_C	BOND Unknown or Inconsistent Label		Cm11 Check
	O11A CM11		
PLAT711_ALERT_1_C	BOND Unknown or Inconsistent Label		Tm11 Check
	O11A TM11		
PLAT711_ALERT_1_C	BOND Unknown or Inconsistent Label		MnM1 Check
	O12A MNM1		
PLAT711_ALERT_1_C	BOND Unknown or Inconsistent Label		Cm11 Check
	O12A CM11		
PLAT711_ALERT_1_C	BOND Unknown or Inconsistent Label		Tm11 Check

	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	CA2				

PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA21		
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.82Ang From O11A .	-0.73	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.91Ang From O22A .	-0.72	eA-3

● Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please	Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please	Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1	Constrained at	0.087 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11	Constrained at	0.052 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11	Constrained at	0.86 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1	Constrained at	0.868 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1	Constrained at	0.045 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11	Constrained at	0.088 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21	Constrained at	0.7904 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2	Constrained at	0.3622 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2	Constrained at	0.6378 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21	Constrained at	0.2096 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A .	134.5	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A .	139.6	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11	Fm11	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.84	Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
	0 1 0, 1 1 0,		
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L= 0.600	371	Report
	0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,		
	0 8 0, 0 9 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0,		
	1 6 0, 1 7 0, 1 8 0, 1 9 0, 2 0 0, 2 1 0,		
	2 2 0, 2 3 0, 2 4 0, 2 5 0, 2 6 0, 2 7 0,		
	2 8 0, 2 9 0, 3 1 0, 3 4 0, 3 5 0, 3 6 0,		
	3 7 0, 3 8 0, 3 9 0, 4 0 0, 4 1 0, 4 2 0,		
	4 3 0, 4 6 0, 4 7 0, 4 8 0, 4 9 0, 5 1 0,		

```

      5  4  0,   5  7  0,   5  8  0,   5  9  0,   6  0  0,   6  1  0,
      6  2  0,   6  4  0,   6  5  0,   6  8  0,   7  1  0,   7  2  0,
      7  5  0,   7  6  0,   7  7  0,   7  8  0,   8  0  0,   8  1  0,
      8  2  0,   8  3  0,   8  5  0,   8  6  0,   8  7  0,   9  1  0,
      9  2  0,   9  3  0,   9  5  0,   9  6  0,  10  0  0,  10  1  0,
     10  2  0,  10  3  0,  10  4  0, -11  0  1, -11  1  1, -11  2  1,
    -10  1  1, -10  2  1, -10  3  1, -10  4  1,  -9  0  1,  -9  1  1,
     -9  2  1,  -9  6  1,  -8  1  1,  -8  2  1,  -7  0  1,  -7  1  1,
     -7  8  1,  -6  1  1,  -6  6  1,  -6  8  1,  -5  0  1,  -5  6  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      665 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....      3 Note
      -2  2  1,   5  3  1,   0  0  2,
PLAT929_ALERT_5_G No Weight Pars, Obs and Calc R1, wR2, S not Checked      ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ      2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ      5 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ      2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ      5 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of      3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      3.507 Note
      Predicted wR2: Based on SigI**2  7.16 or SHELX Weight  7.16
PLAT985_ALERT_1_G The Ca-f"=      0.1533 Deviates from the B&C-Value  0.1517 Check
PLAT985_ALERT_1_G The Fe-f"=      0.4372 Deviates from the B&C-Value  0.4344 Check

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13 **ALERT level A** = Most likely a serious problem - resolve or explain
 19 **ALERT level B** = A potentially serious problem, consider carefully
 71 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 43 **ALERT level G** = General information/check it is not something unexpected

102 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 9 ALERT type 2 Indicator that the structure model may be wrong or deficient
 7 ALERT type 3 Indicator that the structure quality may be low
 19 ALERT type 4 Improvement, methodology, query or suggestion
 9 ALERT type 5 Informative message, check

Datablock: 1.20_GPa

Bond precision: Si- O = 0.0040 A Wavelength=0.49570

Cell: a=9.546(3) b=8.753(5) c=5.235(1)
 alpha=90 beta=106.74(3) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	418.9(3)	418.9(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.373	3.386
Z	1	4
Mu (mm-1)	0.700	0.691
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,9,8
Nref	2040	609
Tmin,Tmax		0.110,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.110 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.299 Theta(max)= 24.430

R(reflections)= 0.0614(506) wR2(reflections)=
S = 3.020 Npar= 94 wR= 0.0914(609)

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.
GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.
GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.
PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 12.20 Degree
PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.570 Why?

Alert level B

PLAT017_ALERT_1_B Check Scattering Type Consistency of AM1 as AL Error?
PLAT017_ALERT_1_B Check Scattering Type Consistency of FM1 as FE Error?
PLAT017_ALERT_1_B Check Scattering Type Consistency of AM11 as AL Error?

PLAT017_ALERT_1_B	Check Scattering Type Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B	Check Scattering Type Consistency of FM11	as	FE Error?
PLAT088_ALERT_3_B	Poor Data / Parameter Ratio		6.48 Note
PLAT701_ALERT_1_B	Bond Calc 2.124(4), Rep 2.115(5), Dev..		2.25 Sigma
	O11A -MGM1 1_555 1_555	#	2 Check
PLAT701_ALERT_1_B	Bond Calc 2.124(4), Rep 2.115(5), Dev..		2.25 Sigma
	O11A -FM1 1_555 1_555	#	4 Check
PLAT701_ALERT_1_B	Bond Calc 1.991(4), Rep 1.980(5), Dev..		2.75 Sigma
	O12A -MM11 1_555 1_555	#	17 Check
PLAT701_ALERT_1_B	Bond Calc 1.991(4), Rep 1.980(5), Dev..		2.75 Sigma
	O12A -FM11 1_555 1_555	#	18 Check
PLAT701_ALERT_1_B	Bond Calc 3.020(2), Rep 3.025(2), Dev..		2.50 Sigma
	SIA1 -CA2 1_555 3_666	#	38 Check
PLAT701_ALERT_1_B	Bond Calc 3.020(2), Rep 3.025(2), Dev..		2.50 Sigma
	SIA1 -NA2 1_555 3_666	#	39 Check
PLAT701_ALERT_1_B	Bond Calc 3.447(4), Rep 3.436(6), Dev..		2.75 Sigma
	MGM1 -CA2 1_555 1_565	#	54 Check
PLAT701_ALERT_1_B	Bond Calc 3.447(4), Rep 3.436(6), Dev..		2.75 Sigma
	MGM1 -NA2 1_555 1_565	#	55 Check
PLAT701_ALERT_1_B	Bond Calc 3.447(4), Rep 3.436(6), Dev..		2.75 Sigma
	AM1 -CA2 1_555 1_565	#	73 Check
PLAT701_ALERT_1_B	Bond Calc 3.447(4), Rep 3.436(6), Dev..		2.75 Sigma
	AM1 -NA2 1_555 1_565	#	74 Check
PLAT701_ALERT_1_B	Bond Calc 3.481(3), Rep 3.473(5), Dev..		2.67 Sigma
	AM11 -CA21 1_555 1_555	#	91 Check
PLAT701_ALERT_1_B	Bond Calc 3.481(3), Rep 3.473(5), Dev..		2.67 Sigma
	AM11 -NA21 1_555 1_555	#	92 Check
PLAT701_ALERT_1_B	Bond Calc 3.481(3), Rep 3.473(5), Dev..		2.67 Sigma
	MM11 -CA21 1_555 1_555	#	113 Check
PLAT701_ALERT_1_B	Bond Calc 3.481(3), Rep 3.473(5), Dev..		2.67 Sigma
	MM11 -NA21 1_555 1_555	#	114 Check

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
 Goodness of fit given = 3.020

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
 Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8
 Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
 Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)
 Rep.: ?

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.08 Check

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms . Please Check

PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) O11A Check

PLAT701_ALERT_1_C Bond Calc 1.619(4), Rep 1.625(5), Dev.. 1.50 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_C Bond Calc 1.616(4), Rep 1.622(5), Dev.. 1.50 Sigma

O12A -SIB1 1_555 1_655 # 11 Check

PLAT701_ALERT_1_C Bond Calc 2.385(4), Rep 2.391(5), Dev.. 1.50 Sigma

O12A -CA21 1_555 1_555 # 19 Check

PLAT701_ALERT_1_C Bond	Calc	2.385(4), Rep	2.391(5), Dev..	1.50 Sigma
O12A	-NA21	1_555	1_555	# 20 Check
PLAT701_ALERT_1_C Bond	Calc	2.017(4), Rep	2.025(5), Dev..	2.00 Sigma
O22A	-MGM1	1_555	3_666	# 29 Check
PLAT701_ALERT_1_C Bond	Calc	2.017(4), Rep	2.025(5), Dev..	2.00 Sigma
O22A	-FM1	1_555	3_666	# 31 Check
PLAT701_ALERT_1_C Bond	Calc	2.379(3), Rep	2.384(4), Dev..	1.67 Sigma
O22A	-CA21	1_555	3_667	# 32 Check
PLAT701_ALERT_1_C Bond	Calc	2.379(3), Rep	2.384(4), Dev..	1.67 Sigma
O22A	-NA21	1_555	3_667	# 33 Check
PLAT701_ALERT_1_C Bond	Calc	1.651(4), Rep	1.644(5), Dev..	1.75 Sigma
O31A	-SIA1	1_555	1_555	# 34 Check
PLAT701_ALERT_1_C Bond	Calc	1.666(3), Rep	1.670(4), Dev..	1.33 Sigma
O31A	-SIB1	1_555	1_554	# 35 Check
PLAT701_ALERT_1_C Bond	Calc	1.650(4), Rep	1.644(5), Dev..	1.50 Sigma
O32A	-SIB1	1_555	1_555	# 37 Check
PLAT701_ALERT_1_C Bond	Calc	3.046(2), Rep	3.049(2), Dev..	1.50 Sigma
SIB1	-CA21	1_555	3_667	# 43 Check
PLAT701_ALERT_1_C Bond	Calc	3.046(2), Rep	3.049(2), Dev..	1.50 Sigma
SIB1	-NA21	1_555	3_667	# 44 Check
PLAT701_ALERT_1_C Bond	Calc	3.089(2), Rep	3.086(2), Dev..	1.50 Sigma
MGM1	-AM11	1_555	1_554	# 48 Check
PLAT701_ALERT_1_C Bond	Calc	3.089(2), Rep	3.086(2), Dev..	1.50 Sigma
MGM1	-AM11	1_555	1_555	# 49 Check
PLAT701_ALERT_1_C Bond	Calc	3.089(2), Rep	3.086(2), Dev..	1.50 Sigma
MGM1	-MM11	1_555	1_554	# 52 Check
PLAT701_ALERT_1_C Bond	Calc	3.089(2), Rep	3.086(2), Dev..	1.50 Sigma
MGM1	-MM11	1_555	1_555	# 53 Check
PLAT701_ALERT_1_C Bond	Calc	3.089(2), Rep	3.086(2), Dev..	1.50 Sigma
AM1	-MM11	1_555	1_554	# 71 Check
PLAT701_ALERT_1_C Bond	Calc	3.089(2), Rep	3.086(2), Dev..	1.50 Sigma
AM1	-MM11	1_555	1_555	# 72 Check
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label			MnM1 Check
O11A	MNM1			
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label			Cm11 Check
O11A	CM11			
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label			Tm11 Check
O11A	TM11			
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label			MnM1 Check
O12A	MNM1			
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label			Cm11 Check
O12A	CM11			
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label			Tm11 Check
O12A	TM11			
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label			Cm11 Check
O21A	CM11			
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label			Tm11 Check
O21A	TM11			
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label			MnM1 Check
O22A	MNM1			
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label			MnM1 Check
MGM1	MNM1			
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label			Tm11 Check
MGM1	TM11			
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label			Tm11 Check
MGM1	TM11			
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label			MnM1 Check

	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	TM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	TM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	TM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	TM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	TM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	TM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	TM11	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	TM11	NA21				
PLAT918_ALERT_3_C	Reflection(s) with	I(obs) much	Smaller I(calc)	.	1	Check
PLAT939_ALERT_3_C	Large Value of Not	(SHELXL) Weight	Optimized S	.	27.93	Check
PLAT975_ALERT_2_C	Check Calcd Resid.	Dens.	0.72Ang From O12A	.	0.82	eA-3

● **Alert level G**

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.250 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.49570 Ang.
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fm1 Constrained at 0.087 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Fm11 Constrained at 0.052 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Am11 Constrained at 0.86 Check
PLAT300_ALERT_4_G Atom Site Occupancy of MgM1 Constrained at 0.868 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Am1 Constrained at 0.045 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mm11 Constrained at 0.088 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca21 Constrained at 0.7904 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca2 Constrained at 0.3622 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Na2 Constrained at 0.6378 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Na21 Constrained at 0.2096 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 20% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5) 100% Note
PLAT396_ALERT_2_G Deviating Si-O-Si Angle From 150 for O31A . 134.9 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si Angle From 150 for O32A . 139.7 Degree
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 8 Note
SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11 Fm11
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.84 Ratio
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found Please Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
0 1 0, 1 1 0,
PLAT911_ALERT_3_G Missing FCF Refl Between Thmin & STh/L= 0.600 376 Report
0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,
0 8 0, 0 9 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0,
1 6 0, 1 7 0, 1 8 0, 1 9 0, 2 0 0, 2 1 0,
2 2 0, 2 3 0, 2 4 0, 2 5 0, 2 6 0, 2 7 0,
2 8 0, 2 9 0, 3 1 0, 3 4 0, 3 5 0, 3 6 0,
3 7 0, 3 8 0, 3 9 0, 4 0 0, 4 1 0, 4 3 0,
4 6 0, 4 7 0, 4 8 0, 4 9 0, 5 1 0, 5 7 0,
5 8 0, 5 9 0, 6 0 0, 6 1 0, 6 2 0, 6 4 0,
6 5 0, 6 8 0, 7 1 0, 7 2 0, 7 4 0, 7 5 0,
7 6 0, 7 7 0, 7 8 0, 8 0 0, 8 1 0, 8 2 0,
8 3 0, 8 5 0, 8 6 0, 8 7 0, 9 1 0, 9 2 0,
9 3 0, 9 5 0, 9 6 0, 10 0 0, 10 1 0, 10 2 0,
10 3 0, 10 4 0, -11 0 1, -11 1 1, -11 2 1, -10 1 1,
-10 2 1, -10 3 1, -9 0 1, -9 1 1, -9 2 1, -9 6 1,
-8 1 1, -8 2 1, -7 0 1, -7 1 1, -7 5 1, -7 8 1,
-6 1 1, -6 6 1, -6 8 1, -5 0 1, -5 6 1, -5 7 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 657 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 3 Note
-2 2 1, 5 3 1, 0 0 2,
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 2 Units

PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	5 Units
PLAT956_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Hmax Differ	2 Units
PLAT957_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Kmax Differ	5 Units
PLAT966_ALERT_5_G	Note: Non-Standard (i.e. 2.0) OMIT Threshold of	3.0 Sig(I)
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	27.930 Note
	Predicted wR2: Based on SigI**2 5.41 or SHELX Weight	5.41
PLAT985_ALERT_1_G	The Ca-f"= 0.1533 Deviates from the B&C-Value	0.1517 Check
PLAT985_ALERT_1_G	The Fe-f"= 0.4372 Deviates from the B&C-Value	0.4344 Check

5 **ALERT level A** = Most likely a serious problem - resolve or explain
 20 **ALERT level B** = A potentially serious problem, consider carefully
 70 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 43 **ALERT level G** = General information/check it is not something unexpected

96 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 5 ALERT type 2 Indicator that the structure model may be wrong or deficient
 9 ALERT type 3 Indicator that the structure quality may be low
 19 ALERT type 4 Improvement, methodology, query or suggestion
 9 ALERT type 5 Informative message, check

Datablock: 1.58_GPa

Bond precision:	Si- O = 0.0050 A	Wavelength=0.49570
Cell:	a=9.543(3)	b=8.738(5)
	alpha=90	beta=106.72(3)
Temperature:	293 K	c=5.230(1)
		gamma=90
	Calculated	Reported
Volume	417.7(3)	417.7(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24	?
	Si8, 2.305(Ca), 1.695(Na)	
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91	Al0.4525 Ca0.5763 Fe0.0695
	Na1.69 O24 Si8	Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.383	3.396
Z	1	4
Mu (mm-1)	0.702	0.693
F000	422.4	422.0
F000'	423.29	
h, k, lmax	15, 14, 8	13, 9, 8
Nref	2042	605
Tmin, Tmax		0.143, 1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.143 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.296 Theta(max)= 24.460

R(reflections)= 0.0661(495) wR2(reflections)=
wR= 0.0905(605)

S = 2.990 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.
GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.
GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.
PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 12.42 Degree
PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.560 Why?
PLAT701_ALERT_1_A Bond Calc 1.608(4), Rep 1.625(5), Dev.. 4.25 Sigma
O11A -SIA1 1_555 1_655 # 1 Check
PLAT701_ALERT_1_A Bond Calc 1.609(4), Rep 1.622(5), Dev.. 3.25 Sigma
O12A -SIB1 1_555 1_655 # 11 Check

Alert level B

PLAT017_ALERT_1_B Check Scattering Type Consistency of AM1 as AL Error?
PLAT017_ALERT_1_B Check Scattering Type Consistency of FM1 as FE Error?
PLAT017_ALERT_1_B Check Scattering Type Consistency of AM11 as AL Error?
PLAT017_ALERT_1_B Check Scattering Type Consistency of MM11 as MG Error?
PLAT017_ALERT_1_B Check Scattering Type Consistency of FM11 as FE Error?
PLAT088_ALERT_3_B Poor Data / Parameter Ratio 6.44 Note
PLAT701_ALERT_1_B Bond Calc 2.127(4), Rep 2.115(5), Dev.. 3.00 Sigma
O11A -MGM1 1_555 1_555 # 2 Check
PLAT701_ALERT_1_B Bond Calc 2.127(4), Rep 2.115(5), Dev.. 3.00 Sigma
O11A -FM1 1_555 1_555 # 4 Check
PLAT701_ALERT_1_B Bond Calc 1.938(3), Rep 1.931(3), Dev.. 2.33 Sigma
O11A -MM11 1_555 1_554 # 7 Check
PLAT701_ALERT_1_B Bond Calc 1.938(3), Rep 1.931(3), Dev.. 2.33 Sigma
O11A -FM11 1_555 1_554 # 8 Check
PLAT701_ALERT_1_B Bond Calc 1.990(4), Rep 1.980(5), Dev.. 2.50 Sigma
O12A -MM11 1_555 1_555 # 17 Check
PLAT701_ALERT_1_B Bond Calc 1.990(4), Rep 1.980(5), Dev.. 2.50 Sigma
O12A -FM11 1_555 1_555 # 18 Check
PLAT701_ALERT_1_B Bond Calc 2.014(5), Rep 2.025(5), Dev.. 2.20 Sigma
O22A -MGM1 1_555 3_666 # 29 Check
PLAT701_ALERT_1_B Bond Calc 2.014(5), Rep 2.025(5), Dev.. 2.20 Sigma
O22A -FM1 1_555 3_666 # 31 Check
PLAT701_ALERT_1_B Bond Calc 2.375(3), Rep 2.384(4), Dev.. 3.00 Sigma
O22A -CA21 1_555 3_667 # 32 Check

PLAT701_ALERT_1_B Bond	Calc	2.375(3), Rep	2.384(4), Dev..	3.00 Sigma
O22A	-NA21	1_555	3_667	# 33 Check
PLAT701_ALERT_1_B Bond	Calc	3.263(3), Rep	3.270(4), Dev..	2.33 Sigma
SIA1	-CA21	1_555	3_666	# 40 Check

🟡 Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
Goodness of fit given = 2.990

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8
Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)
Rep.: ?

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.08 Check

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms . Please Check

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.5 Note

PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) O11A Check

PLAT701_ALERT_1_C Bond	Calc	2.384(4), Rep	2.391(5), Dev..	1.75 Sigma
O12A	-CA21	1_555	1_555	# 19 Check
PLAT701_ALERT_1_C Bond	Calc	2.384(4), Rep	2.391(5), Dev..	1.75 Sigma
O12A	-NA21	1_555	1_555	# 20 Check
PLAT701_ALERT_1_C Bond	Calc	1.609(5), Rep	1.603(5), Dev..	1.20 Sigma
O21A	-SIA1	1_555	1_545	# 21 Check
PLAT701_ALERT_1_C Bond	Calc	1.596(5), Rep	1.588(5), Dev..	1.60 Sigma
O22A	-SIB1	1_555	1_555	# 28 Check
PLAT701_ALERT_1_C Bond	Calc	1.651(4), Rep	1.644(5), Dev..	1.75 Sigma
O31A	-SIA1	1_555	1_555	# 34 Check
PLAT701_ALERT_1_C Bond	Calc	1.664(3), Rep	1.670(4), Dev..	2.00 Sigma
O31A	-SIB1	1_555	1_554	# 35 Check
PLAT701_ALERT_1_C Bond	Calc	1.649(4), Rep	1.644(5), Dev..	1.25 Sigma
O32A	-SIB1	1_555	1_555	# 37 Check
PLAT701_ALERT_1_C Bond	Calc	3.022(2), Rep	3.025(2), Dev..	1.50 Sigma
SIA1	-CA2	1_555	3_666	# 38 Check
PLAT701_ALERT_1_C Bond	Calc	3.022(2), Rep	3.025(2), Dev..	1.50 Sigma
SIA1	-NA2	1_555	3_666	# 39 Check
PLAT701_ALERT_1_C Bond	Calc	3.194(3), Rep	3.198(4), Dev..	1.33 Sigma
SIB1	-CA2	1_555	3_666	# 41 Check
PLAT701_ALERT_1_C Bond	Calc	3.194(3), Rep	3.198(4), Dev..	1.33 Sigma
SIB1	-NA2	1_555	3_666	# 42 Check
PLAT701_ALERT_1_C Bond	Calc	3.045(2), Rep	3.049(2), Dev..	2.00 Sigma
SIB1	-CA21	1_555	3_667	# 43 Check
PLAT701_ALERT_1_C Bond	Calc	3.045(2), Rep	3.049(2), Dev..	2.00 Sigma
SIB1	-NA21	1_555	3_667	# 44 Check
PLAT701_ALERT_1_C Bond	Calc	3.441(4), Rep	3.436(6), Dev..	1.25 Sigma
MGM1	-CA2	1_555	1_565	# 54 Check
PLAT701_ALERT_1_C Bond	Calc	3.441(4), Rep	3.436(6), Dev..	1.25 Sigma
MGM1	-NA2	1_555	1_565	# 55 Check
PLAT701_ALERT_1_C Bond	Calc	3.198(3), Rep	3.203(2), Dev..	1.67 Sigma
MGM1	-CA21	1_555	1_554	# 56 Check

PLAT701_ALERT_1_C Bond	Calc	3.198(3), Rep	3.203(2), Dev..	1.67 Sigma
MGM1	-CA21	1_555	1_555	# 57 Check
PLAT701_ALERT_1_C Bond	Calc	3.198(3), Rep	3.203(2), Dev..	1.67 Sigma
MGM1	-NA21	1_555	1_554	# 58 Check
PLAT701_ALERT_1_C Bond	Calc	3.198(3), Rep	3.203(2), Dev..	1.67 Sigma
MGM1	-NA21	1_555	1_555	# 59 Check
PLAT701_ALERT_1_C Bond	Calc	3.441(4), Rep	3.436(6), Dev..	1.25 Sigma
AM1	-CA2	1_555	1_565	# 73 Check
PLAT701_ALERT_1_C Bond	Calc	3.441(4), Rep	3.436(6), Dev..	1.25 Sigma
AM1	-NA2	1_555	1_565	# 74 Check
PLAT701_ALERT_1_C Bond	Calc	3.198(3), Rep	3.203(2), Dev..	1.67 Sigma
AM1	-CA21	1_555	1_554	# 75 Check
PLAT701_ALERT_1_C Bond	Calc	3.198(3), Rep	3.203(2), Dev..	1.67 Sigma
AM1	-CA21	1_555	1_555	# 76 Check
PLAT701_ALERT_1_C Bond	Calc	3.198(3), Rep	3.203(2), Dev..	1.67 Sigma
AM1	-NA21	1_555	1_554	# 77 Check
PLAT701_ALERT_1_C Bond	Calc	3.198(3), Rep	3.203(2), Dev..	1.67 Sigma
AM1	-NA21	1_555	1_555	# 78 Check
PLAT701_ALERT_1_C Bond	Calc	3.198(3), Rep	3.203(2), Dev..	1.67 Sigma
FM1	-CA21	1_555	1_554	# 79 Check
PLAT701_ALERT_1_C Bond	Calc	3.198(3), Rep	3.203(2), Dev..	1.67 Sigma
FM1	-CA21	1_555	1_555	# 80 Check
PLAT701_ALERT_1_C Bond	Calc	3.198(3), Rep	3.203(2), Dev..	1.67 Sigma
FM1	-NA21	1_555	1_554	# 81 Check
PLAT701_ALERT_1_C Bond	Calc	3.198(3), Rep	3.203(2), Dev..	1.67 Sigma
FM1	-NA21	1_555	1_555	# 82 Check
PLAT701_ALERT_1_C Bond	Calc	3.177(3), Rep	3.181(3), Dev..	1.33 Sigma
AM11	-CA2	1_555	1_565	# 87 Check
PLAT701_ALERT_1_C Bond	Calc	3.177(3), Rep	3.181(3), Dev..	1.33 Sigma
AM11	-CA2	1_555	1_566	# 88 Check
PLAT701_ALERT_1_C Bond	Calc	3.177(3), Rep	3.181(3), Dev..	1.33 Sigma
AM11	-NA2	1_555	1_565	# 89 Check
PLAT701_ALERT_1_C Bond	Calc	3.177(3), Rep	3.181(3), Dev..	1.33 Sigma
AM11	-NA2	1_555	1_566	# 90 Check
PLAT701_ALERT_1_C Bond	Calc	3.477(3), Rep	3.473(5), Dev..	1.33 Sigma
AM11	-CA21	1_555	1_555	# 91 Check
PLAT701_ALERT_1_C Bond	Calc	3.477(3), Rep	3.473(5), Dev..	1.33 Sigma
AM11	-NA21	1_555	1_555	# 92 Check
PLAT701_ALERT_1_C Bond	Calc	3.177(3), Rep	3.181(3), Dev..	1.33 Sigma
MM11	-CA2	1_555	1_565	# 109 Check
PLAT701_ALERT_1_C Bond	Calc	3.177(3), Rep	3.181(3), Dev..	1.33 Sigma
MM11	-CA2	1_555	1_566	# 110 Check
PLAT701_ALERT_1_C Bond	Calc	3.177(3), Rep	3.181(3), Dev..	1.33 Sigma
MM11	-NA2	1_555	1_565	# 111 Check
PLAT701_ALERT_1_C Bond	Calc	3.177(3), Rep	3.181(3), Dev..	1.33 Sigma
MM11	-NA2	1_555	1_566	# 112 Check
PLAT701_ALERT_1_C Bond	Calc	3.477(3), Rep	3.473(5), Dev..	1.33 Sigma
MM11	-CA21	1_555	1_555	# 113 Check
PLAT701_ALERT_1_C Bond	Calc	3.477(3), Rep	3.473(5), Dev..	1.33 Sigma
MM11	-NA21	1_555	1_555	# 114 Check
PLAT701_ALERT_1_C Bond	Calc	3.177(3), Rep	3.181(3), Dev..	1.33 Sigma
FM11	-CA2	1_555	1_565	# 115 Check
PLAT701_ALERT_1_C Bond	Calc	3.177(3), Rep	3.181(3), Dev..	1.33 Sigma
FM11	-CA2	1_555	1_566	# 116 Check
PLAT701_ALERT_1_C Bond	Calc	3.177(3), Rep	3.181(3), Dev..	1.33 Sigma
FM11	-NA2	1_555	1_565	# 117 Check
PLAT701_ALERT_1_C Bond	Calc	3.177(3), Rep	3.181(3), Dev..	1.33 Sigma

	FM11	-NA2	1_555	1_566		#	118	Check
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			MnM1	Check
	O11A	MNM1						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			Cm11	Check
	O11A	CM11						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			Tm11	Check
	O11A	TM11						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			MnM1	Check
	O12A	MNM1						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			Cm11	Check
	O12A	CM11						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			Tm11	Check
	O12A	TM11						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			Cm11	Check
	O21A	CM11						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			Tm11	Check
	O21A	TM11						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			MnM1	Check
	O22A	MNM1						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			MnM1	Check
	MGM1	MNM1						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			Tm11	Check
	MGM1	TM11						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			Tm11	Check
	MGM1	TM11						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			MnM1	Check
	MNM1	AM1						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			MnM1	Check
	MNM1	FM1						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			MnM1	Check
	MNM1	MM11						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			MnM1	Check
	MNM1	MM11						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			MnM1	Check
	MNM1	CA2						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			MnM1	Check
	MNM1	NA2						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			MnM1	Check
	MNM1	CA21						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			MnM1	Check
	MNM1	CA21						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			MnM1	Check
	MNM1	NA21						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			MnM1	Check
	MNM1	NA21						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			Cm11	Check
	AM11	CM11						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			Tm11	Check
	AM11	TM11						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			Cm11	Check
	CM11	TM11						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			Cm11	Check
	CM11	MM11						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			Cm11	Check
	CM11	FM11						
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label			Cm11	Check
	CM11	CA2						

PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Cm11	Check
	CM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Cm11	Check
	CM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Cm11	Check
	CM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	MM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	FM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA21		
PLAT975_ALERT_2_C	Check	Calcd Resid. Dens. 0.78Ang From O31A .	0.65	eA-3
PLAT975_ALERT_2_C	Check	Calcd Resid. Dens. 0.80Ang From O32A .	0.62	eA-3
PLAT976_ALERT_2_C	Check	Calcd Resid. Dens. 0.78Ang From O12A .	-0.64	eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please	Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please	Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1 Constrained at	0.087	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11 Constrained at	0.052	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11 Constrained at	0.86	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1 Constrained at	0.868	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1 Constrained at	0.045	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11 Constrained at	0.088	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21 Constrained at	0.7904	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2 Constrained at	0.3622	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2 Constrained at	0.6378	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21 Constrained at	0.2096	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A .	134.5	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A .	139.4	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11	Fm11	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.84	Ratio

PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found Please Check
 PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
 PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !
 PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
 0 1 0, 1 1 0,
 PLAT911_ALERT_3_G Missing FCF Refl Between Thmin & STh/L= 0.600 374 Report
 0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,
 0 8 0, 0 9 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0,
 1 6 0, 1 7 0, 1 8 0, 1 9 0, 2 0 0, 2 1 0,
 2 2 0, 2 3 0, 2 4 0, 2 5 0, 2 6 0, 2 7 0,
 2 8 0, 2 9 0, 3 1 0, 3 4 0, 3 5 0, 3 6 0,
 3 7 0, 3 8 0, 3 9 0, 4 0 0, 4 1 0, 4 3 0,
 4 6 0, 4 7 0, 4 8 0, 4 9 0, 5 1 0, 5 7 0,
 5 8 0, 5 9 0, 6 0 0, 6 1 0, 6 2 0, 6 3 0,
 6 4 0, 6 5 0, 6 8 0, 7 1 0, 7 2 0, 7 4 0,
 7 5 0, 7 6 0, 7 7 0, 7 8 0, 8 0 0, 8 1 0,
 8 2 0, 8 3 0, 8 5 0, 8 6 0, 8 7 0, 9 1 0,
 9 2 0, 9 3 0, 9 5 0, 10 0 0, 10 1 0, 10 2 0,
 10 3 0, 10 4 0, -11 0 1, -11 1 1, -11 2 1, -10 1 1,
 -10 2 1, -10 3 1, -9 0 1, -9 1 1, -9 2 1, -9 6 1,
 -8 1 1, -8 2 1, -7 0 1, -7 1 1, -7 5 1, -7 8 1,
 -6 1 1, -6 8 1, -5 0 1, -5 1 1, -5 6 1, -5 7 1,
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 664 Note
 PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 3 Note
 -2 2 1, 5 3 1, 0 0 2,
 PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked ! Info
 PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 2 Units
 PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 5 Units
 PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ 2 Units
 PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 5 Units
 PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of 3.0 Sig(I)
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.346 Note
 Predicted wR2: Based on SigI**2 5.39 or SHELX Weight 5.39
 PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value 0.1517 Check
 PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value 0.4344 Check

-
- 7 **ALERT level A** = Most likely a serious problem - resolve or explain
 17 **ALERT level B** = A potentially serious problem, consider carefully
 97 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 43 **ALERT level G** = General information/check it is not something unexpected
- 121 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 8 ALERT type 2 Indicator that the structure model may be wrong or deficient
 7 ALERT type 3 Indicator that the structure quality may be low
 19 ALERT type 4 Improvement, methodology, query or suggestion
 9 ALERT type 5 Informative message, check
-

Datablock: 1.95_GPa

Bond precision: Si- O = 0.0040 A

Wavelength=0.49570

Cell:	a=9.528(3)	b=8.731(5)	c=5.224(1)
	alpha=90	beta=106.65(3)	gamma=90
Temperature:	293 K		

	Calculated	Reported
Volume	416.4(3)	416.4(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.393	3.407
Z	1	4
Mu (mm-1)	0.704	0.695
F000	422.4	422.0
F000'	423.29	
h, k, lmax	15, 14, 8	13, 9, 8
Nref	2036	597
Tmin, Tmax		0.573, 1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.573 Tmax=1.000
AbsCorr = MULTII-SCAN

Data completeness= 0.293 Theta(max)= 24.460

R(reflections)= 0.0577(480)	wR2(reflections)=
S = 2.370	wR= 0.0733(597)
Npar= 94	

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 10.18 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.550 Why?

PLAT701_ALERT_1_A Bond Calc 1.614(3), Rep 1.625(5), Dev.. 3.67 Sigma

O11A	-SIA1	1_555	1_655		#	1 Check
PLAT701_ALERT_1_A Bond	Calc	1.612(3), Rep	1.622(5), Dev..			3.33 Sigma
O12A	-SIB1	1_555	1_655		#	11 Check
PLAT701_ALERT_1_A Bond	Calc	3.017(2), Rep	3.025(2), Dev..			4.00 Sigma
SIA1	-CA2	1_555	3_666		#	38 Check
PLAT701_ALERT_1_A Bond	Calc	3.017(2), Rep	3.025(2), Dev..			4.00 Sigma
SIA1	-NA2	1_555	3_666		#	39 Check
PLAT701_ALERT_1_A Bond	Calc	3.259(3), Rep	3.270(4), Dev..			3.67 Sigma
SIA1	-CA21	1_555	3_666		#	40 Check
PLAT701_ALERT_1_A Bond	Calc	3.040(2), Rep	3.049(2), Dev..			4.50 Sigma
SIB1	-CA21	1_555	3_667		#	43 Check
PLAT701_ALERT_1_A Bond	Calc	3.040(2), Rep	3.049(2), Dev..			4.50 Sigma
SIB1	-NA21	1_555	3_667		#	44 Check
PLAT701_ALERT_1_A Bond	Calc	3.075(2), Rep	3.086(2), Dev..			5.50 Sigma
MGM1	-AM11	1_555	1_554		#	48 Check
PLAT701_ALERT_1_A Bond	Calc	3.075(2), Rep	3.086(2), Dev..			5.50 Sigma
MGM1	-AM11	1_555	1_555		#	49 Check
PLAT701_ALERT_1_A Bond	Calc	3.075(2), Rep	3.086(2), Dev..			5.50 Sigma
MGM1	-MM11	1_555	1_554		#	52 Check
PLAT701_ALERT_1_A Bond	Calc	3.075(2), Rep	3.086(2), Dev..			5.50 Sigma
MGM1	-MM11	1_555	1_555		#	53 Check
PLAT701_ALERT_1_A Bond	Calc	3.075(2), Rep	3.086(2), Dev..			5.50 Sigma
AM1	-MM11	1_555	1_554		#	71 Check
PLAT701_ALERT_1_A Bond	Calc	3.075(2), Rep	3.086(2), Dev..			5.50 Sigma
AM1	-MM11	1_555	1_555		#	72 Check

🔴 Alert level B

PLAT017_ALERT_1_B	Check	Scattering Type Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B	Check	Scattering Type Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B	Check	Scattering Type Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B	Check	Scattering Type Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B	Check	Scattering Type Consistency of FM11	as	FE Error?
PLAT088_ALERT_3_B	Poor Data / Parameter Ratio			6.35 Note
PLAT701_ALERT_1_B Bond	Calc	3.191(3), Rep	3.198(4), Dev..	2.33 Sigma
SIB1	-CA2	1_555	3_666	 # 41 Check
PLAT701_ALERT_1_B Bond	Calc	3.191(3), Rep	3.198(4), Dev..	2.33 Sigma
SIB1	-NA2	1_555	3_666	 # 42 Check

🟡 Alert level C

GOODF01_ALERT_2_C	The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00			
	Goodness of fit given = 2.370			
PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ		Please Check
	Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8			
	Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2			
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula	Strings Differ		Please Check
	Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)			
	Rep.: ?			
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight Differ by ..		3.08	Check
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...			Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...			Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...			Please Check
PLAT077_ALERT_4_C	Unit Cell Contains Non-integer Number of Atoms .			Please Check

PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd	1)	3.3	Note
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)		O11A	Check
PLAT701_ALERT_1_C	Bond Calc	1.595(4), Rep 1.603(5), Dev..	2.00	Sigma
	O21A -SIA1	1_555 1_545	#	21 Check
PLAT701_ALERT_1_C	Bond Calc	2.019(4), Rep 2.025(5), Dev..	1.50	Sigma
	O22A -MGM1	1_555 3_666	#	29 Check
PLAT701_ALERT_1_C	Bond Calc	2.019(4), Rep 2.025(5), Dev..	1.50	Sigma
	O22A -FM1	1_555 3_666	#	31 Check
PLAT701_ALERT_1_C	Bond Calc	2.379(3), Rep 2.384(4), Dev..	1.67	Sigma
	O22A -CA21	1_555 3_667	#	32 Check
PLAT701_ALERT_1_C	Bond Calc	2.379(3), Rep 2.384(4), Dev..	1.67	Sigma
	O22A -NA21	1_555 3_667	#	33 Check
PLAT701_ALERT_1_C	Bond Calc	1.649(3), Rep 1.644(5), Dev..	1.67	Sigma
	O31A -SIA1	1_555 1_555	#	34 Check
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1	Check
	O11A MNM1			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Cm11	Check
	O11A CM11			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	O11A TM11			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1	Check
	O12A MNM1			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Cm11	Check
	O12A CM11			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	O12A TM11			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Cm11	Check
	O21A CM11			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	O21A TM11			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1	Check
	O22A MNM1			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1	Check
	MGM1 MNM1			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	MGM1 TM11			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	MGM1 TM11			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1	Check
	MNM1 AM1			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1	Check
	MNM1 FM1			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1	Check
	MNM1 MM11			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1	Check
	MNM1 MM11			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1	Check
	MNM1 CA2			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1	Check
	MNM1 NA2			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1	Check
	MNM1 CA21			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1	Check
	MNM1 CA21			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1	Check
	MNM1 NA21			
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1	Check

	MNM1	NA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Cm11 Check
	AM11	CM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	AM11	TM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Cm11 Check
	CM11	TM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Cm11 Check
	CM11	MM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Cm11 Check
	CM11	FM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Cm11 Check
	CM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Cm11 Check
	CM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Cm11 Check
	CM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Cm11 Check
	CM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	MM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	FM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA21		
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF			4 Note
	-2 2 1, 5 3 1, 0 0 2, 4 0 2,			
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	1.01Ang From O31A	.	0.56 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.64Ang From O12A	.	0.53 eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu			
not performed for this radiation type.			
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		3 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570 Ang.	
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	 (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature	 (K)	293 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1	Constrained at	0.087 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11	Constrained at	0.052 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11	Constrained at	0.86 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1	Constrained at	0.868 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1	Constrained at	0.045 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11	Constrained at	0.088 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21	Constrained at	0.7904	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2	Constrained at	0.3622	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2	Constrained at	0.6378	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21	Constrained at	0.2096	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 5)	100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A	.	134.5	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A	.	139.5	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		8	Note
	SiA1 SiB1 MgM1 Aml Fm1 Aml1 Mml1 Fm11			
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	.	1.84	Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		!	Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2	Note
	0 1 0, 1 1 0,			
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L=	0.600	383	Report
	0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,			
	0 8 0, 0 9 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0,			
	1 6 0, 1 7 0, 1 8 0, 1 9 0, 2 0 0, 2 1 0,			
	2 2 0, 2 3 0, 2 4 0, 2 5 0, 2 6 0, 2 7 0,			
	2 8 0, 2 9 0, 3 1 0, 3 2 0, 3 3 0, 3 4 0,			
	3 5 0, 3 6 0, 3 7 0, 3 8 0, 3 9 0, 4 0 0,			
	4 1 0, 4 5 0, 4 6 0, 4 7 0, 4 8 0, 4 9 0,			
	5 1 0, 5 3 0, 5 4 0, 5 5 0, 5 6 0, 5 7 0,			
	5 8 0, 5 9 0, 6 0 0, 6 1 0, 6 2 0, 6 3 0,			
	6 4 0, 6 5 0, 6 8 0, 7 1 0, 7 2 0, 7 5 0,			
	7 6 0, 7 7 0, 7 8 0, 8 0 0, 8 1 0, 8 2 0,			
	8 3 0, 8 5 0, 8 6 0, 8 7 0, 9 1 0, 9 2 0,			
	9 3 0, 9 5 0, 10 0 0, 10 1 0, 10 2 0, 10 3 0,			
	10 4 0, -11 0 1, -11 1 1, -11 2 1, -10 1 1, -10 2 1,			
	-10 3 1, -9 0 1, -9 1 1, -9 2 1, -9 6 1, -8 1 1,			
	-8 2 1, -8 5 1, -7 0 1, -7 1 1, -7 3 1, -7 5 1,			
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	663	Note
PLAT929_ALERT_5_G	No Weight Pars,Obs and Calc R1,wR2,S not Checked		!	Info
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ		2	Units
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ		5	Units
PLAT956_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Hmax Differ		2	Units
PLAT957_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Kmax Differ		5	Units
PLAT966_ALERT_5_G	Note: Non-Standard (i.e. 2.0) OMIT Threshold of		3.0	Sig(I)
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		2.525	Note
	Predicted wR2: Based on SigI**2 5.50 or SHELX Weight	5.50		
PLAT985_ALERT_1_G	The Ca-f"= 0.1533 Deviates from the B&C-Value		0.1517	Check
PLAT985_ALERT_1_G	The Fe-f"= 0.4372 Deviates from the B&C-Value		0.4344	Check

-
- 18 **ALERT level A** = Most likely a serious problem - resolve or explain
8 **ALERT level B** = A potentially serious problem, consider carefully
58 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
42 **ALERT level G** = General information/check it is not something unexpected
- 84 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

7 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
9 ALERT type 5 Informative message, check

Datablock: 2.32_GPa

Bond precision: Si- O = 0.0040 A Wavelength=0.49570

Cell: a=9.516(3) b=8.715(5) c=5.217(1)
 alpha=90 beta=106.62(3) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	414.6(3)	414.6(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.408	3.421
Z	1	4
Mu (mm-1)	0.707	0.698
F000	422.4	422.0
F000'	423.29	
h, k, lmax	15, 14, 8	13, 9, 8
Nref	2031	578
Tmin, Tmax		0.469, 1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.469 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.285 Theta(max)= 24.480

R(reflections)= 0.0498(435) wR2(reflections)=
S = 2.560 Npar= 94 wR= 0.0687(578)

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

```

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
    Label identifying the atom site 2.
GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
    Label identifying the atom site 3.
GEOM008_ALERT_1_A _geom_angle is missing
    Angle between atom sites 1, 2 and 3.
PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low ..... 13.36 Degree
PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.510 Why?
PLAT211_ALERT_2_A ADP of Atom O32A is N.P.D. or (nearly) 2D . Please Check
PLAT701_ALERT_1_A Bond Calc 1.608(4), Rep 1.625(5), Dev.. 4.25 Sigma
    O11A -SIA1 1_555 1_655 ..... # 1 Check
PLAT701_ALERT_1_A Bond Calc 1.607(4), Rep 1.622(5), Dev.. 3.75 Sigma
    O12A -SIB1 1_555 1_655 ..... # 11 Check
PLAT701_ALERT_1_A Bond Calc 2.374(3), Rep 2.384(4), Dev.. 3.33 Sigma
    O22A -CA21 1_555 3_667 ..... # 32 Check
PLAT701_ALERT_1_A Bond Calc 2.374(3), Rep 2.384(4), Dev.. 3.33 Sigma
    O22A -NA21 1_555 3_667 ..... # 33 Check
PLAT701_ALERT_1_A Bond Calc 3.013(2), Rep 3.025(2), Dev.. 6.00 Sigma
    SIA1 -CA2 1_555 3_666 ..... # 38 Check
PLAT701_ALERT_1_A Bond Calc 3.013(2), Rep 3.025(2), Dev.. 6.00 Sigma
    SIA1 -NA2 1_555 3_666 ..... # 39 Check
PLAT701_ALERT_1_A Bond Calc 3.253(3), Rep 3.270(4), Dev.. 5.67 Sigma
    SIA1 -CA21 1_555 3_666 ..... # 40 Check
PLAT701_ALERT_1_A Bond Calc 3.186(3), Rep 3.198(4), Dev.. 4.00 Sigma
    SIB1 -CA2 1_555 3_666 ..... # 41 Check
PLAT701_ALERT_1_A Bond Calc 3.186(3), Rep 3.198(4), Dev.. 4.00 Sigma
    SIB1 -NA2 1_555 3_666 ..... # 42 Check
PLAT701_ALERT_1_A Bond Calc 3.036(2), Rep 3.049(2), Dev.. 6.50 Sigma
    SIB1 -CA21 1_555 3_667 ..... # 43 Check
PLAT701_ALERT_1_A Bond Calc 3.036(2), Rep 3.049(2), Dev.. 6.50 Sigma
    SIB1 -NA21 1_555 3_667 ..... # 44 Check
PLAT701_ALERT_1_A Bond Calc 3.069(2), Rep 3.086(2), Dev.. 8.50 Sigma
    MGM1 -AM11 1_555 1_554 ..... # 48 Check
PLAT701_ALERT_1_A Bond Calc 3.069(2), Rep 3.086(2), Dev.. 8.50 Sigma
    MGM1 -AM11 1_555 1_555 ..... # 49 Check
PLAT701_ALERT_1_A Bond Calc 3.069(2), Rep 3.086(2), Dev.. 8.50 Sigma
    MGM1 -MM11 1_555 1_554 ..... # 52 Check
PLAT701_ALERT_1_A Bond Calc 3.069(2), Rep 3.086(2), Dev.. 8.50 Sigma
    MGM1 -MM11 1_555 1_555 ..... # 53 Check
PLAT701_ALERT_1_A Bond Calc 3.196(2), Rep 3.203(2), Dev.. 3.50 Sigma
    MGM1 -CA21 1_555 1_554 ..... # 56 Check
PLAT701_ALERT_1_A Bond Calc 3.196(2), Rep 3.203(2), Dev.. 3.50 Sigma
    MGM1 -CA21 1_555 1_555 ..... # 57 Check
PLAT701_ALERT_1_A Bond Calc 3.196(2), Rep 3.203(2), Dev.. 3.50 Sigma
    MGM1 -NA21 1_555 1_554 ..... # 58 Check
PLAT701_ALERT_1_A Bond Calc 3.196(2), Rep 3.203(2), Dev.. 3.50 Sigma
    MGM1 -NA21 1_555 1_555 ..... # 59 Check
PLAT701_ALERT_1_A Bond Calc 3.069(2), Rep 3.086(2), Dev.. 8.50 Sigma
    AM1 -MM11 1_555 1_554 ..... # 71 Check
PLAT701_ALERT_1_A Bond Calc 3.069(2), Rep 3.086(2), Dev.. 8.50 Sigma
    AM1 -MM11 1_555 1_555 ..... # 72 Check

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PLAT701_ALERT_1_A	Bond	Calc	3.196(2), Rep	3.203(2), Dev..	3.50 Sigma
AM1	-CA21	1_555	1_554		# 75 Check
PLAT701_ALERT_1_A	Bond	Calc	3.196(2), Rep	3.203(2), Dev..	3.50 Sigma
AM1	-CA21	1_555	1_555		# 76 Check
PLAT701_ALERT_1_A	Bond	Calc	3.196(2), Rep	3.203(2), Dev..	3.50 Sigma
AM1	-NA21	1_555	1_554		# 77 Check
PLAT701_ALERT_1_A	Bond	Calc	3.196(2), Rep	3.203(2), Dev..	3.50 Sigma
AM1	-NA21	1_555	1_555		# 78 Check
PLAT701_ALERT_1_A	Bond	Calc	3.196(2), Rep	3.203(2), Dev..	3.50 Sigma
FM1	-CA21	1_555	1_554		# 79 Check
PLAT701_ALERT_1_A	Bond	Calc	3.196(2), Rep	3.203(2), Dev..	3.50 Sigma
FM1	-CA21	1_555	1_555		# 80 Check
PLAT701_ALERT_1_A	Bond	Calc	3.196(2), Rep	3.203(2), Dev..	3.50 Sigma
FM1	-NA21	1_555	1_554		# 81 Check
PLAT701_ALERT_1_A	Bond	Calc	3.196(2), Rep	3.203(2), Dev..	3.50 Sigma
FM1	-NA21	1_555	1_555		# 82 Check
PLAT701_ALERT_1_A	Bond	Calc	3.463(3), Rep	3.473(5), Dev..	3.33 Sigma
AM11	-CA21	1_555	1_555		# 91 Check
PLAT701_ALERT_1_A	Bond	Calc	3.463(3), Rep	3.473(5), Dev..	3.33 Sigma
AM11	-NA21	1_555	1_555		# 92 Check
PLAT701_ALERT_1_A	Bond	Calc	3.463(3), Rep	3.473(5), Dev..	3.33 Sigma
MM11	-CA21	1_555	1_555		# 113 Check
PLAT701_ALERT_1_A	Bond	Calc	3.463(3), Rep	3.473(5), Dev..	3.33 Sigma
MM11	-NA21	1_555	1_555		# 114 Check

Alert level B

PLAT017_ALERT_1_B	Check	Scattering Type	Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B	Check	Scattering Type	Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B	Check	Scattering Type	Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B	Check	Scattering Type	Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B	Check	Scattering Type	Consistency of FM11	as	FE Error?
PLAT088_ALERT_3_B	Poor Data /	Parameter Ratio			6.15 Note
PLAT701_ALERT_1_B	Bond	Calc	2.381(4), Rep	2.391(5), Dev..	2.50 Sigma
O12A	-CA21	1_555	1_555		# 19 Check
PLAT701_ALERT_1_B	Bond	Calc	2.381(4), Rep	2.391(5), Dev..	2.50 Sigma
O12A	-NA21	1_555	1_555		# 20 Check
PLAT701_ALERT_1_B	Bond	Calc	1.594(4), Rep	1.603(5), Dev..	2.25 Sigma
O21A	-SIA1	1_555	1_545		# 21 Check
PLAT701_ALERT_1_B	Bond	Calc	2.351(3), Rep	2.358(4), Dev..	2.33 Sigma
O21A	-CA2	1_555	3_656		# 26 Check
PLAT701_ALERT_1_B	Bond	Calc	2.351(3), Rep	2.358(4), Dev..	2.33 Sigma
O21A	-NA2	1_555	3_656		# 27 Check
PLAT701_ALERT_1_B	Bond	Calc	2.016(4), Rep	2.025(5), Dev..	2.25 Sigma
O22A	-MGM1	1_555	3_666		# 29 Check
PLAT701_ALERT_1_B	Bond	Calc	2.016(4), Rep	2.025(5), Dev..	2.25 Sigma
O22A	-FM1	1_555	3_666		# 31 Check

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
 Goodness of fit given = 2.560

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
 Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8
 Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
	Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)	
	Rep.: ?	
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight Differ by ..	3.08 Check
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...	Please Check
PLAT077_ALERT_4_C	Unit Cell Contains Non-integer Number of Atoms .	Please Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)	2.3 Note
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)	011A Check
PLAT701_ALERT_1_C	Bond Calc 2.343(4), Rep 2.348(5), Dev..	1.25 Sigma
	O11A -CA2 1_555 1_565	# 9 Check
PLAT701_ALERT_1_C	Bond Calc 2.343(4), Rep 2.348(5), Dev..	1.25 Sigma
	O11A -NA2 1_555 1_565	# 10 Check
PLAT701_ALERT_1_C	Bond Calc 2.052(3), Rep 2.058(3), Dev..	2.00 Sigma
	O12A -MGM1 1_555 1_555	# 12 Check
PLAT701_ALERT_1_C	Bond Calc 2.052(3), Rep 2.058(3), Dev..	2.00 Sigma
	O12A -FM1 1_555 1_555	# 14 Check
PLAT701_ALERT_1_C	Bond Calc 1.649(4), Rep 1.644(5), Dev..	1.25 Sigma
	O31A -SIA1 1_555 1_555	# 34 Check
PLAT701_ALERT_1_C	Bond Calc 1.664(3), Rep 1.670(4), Dev..	2.00 Sigma
	O31A -SIB1 1_555 1_554	# 35 Check
PLAT701_ALERT_1_C	Bond Calc 1.649(4), Rep 1.644(5), Dev..	1.25 Sigma
	O32A -SIB1 1_555 1_555	# 37 Check
PLAT701_ALERT_1_C	Bond Calc 3.428(4), Rep 3.436(6), Dev..	2.00 Sigma
	MGM1 -CA2 1_555 1_565	# 54 Check
PLAT701_ALERT_1_C	Bond Calc 3.428(4), Rep 3.436(6), Dev..	2.00 Sigma
	MGM1 -NA2 1_555 1_565	# 55 Check
PLAT701_ALERT_1_C	Bond Calc 3.428(4), Rep 3.436(6), Dev..	2.00 Sigma
	AM1 -CA2 1_555 1_565	# 73 Check
PLAT701_ALERT_1_C	Bond Calc 3.428(4), Rep 3.436(6), Dev..	2.00 Sigma
	AM1 -NA2 1_555 1_565	# 74 Check
PLAT701_ALERT_1_C	Bond Calc 3.176(3), Rep 3.181(3), Dev..	1.67 Sigma
	AM11 -CA2 1_555 1_565	# 87 Check
PLAT701_ALERT_1_C	Bond Calc 3.176(3), Rep 3.181(3), Dev..	1.67 Sigma
	AM11 -CA2 1_555 1_566	# 88 Check
PLAT701_ALERT_1_C	Bond Calc 3.176(3), Rep 3.181(3), Dev..	1.67 Sigma
	AM11 -NA2 1_555 1_565	# 89 Check
PLAT701_ALERT_1_C	Bond Calc 3.176(3), Rep 3.181(3), Dev..	1.67 Sigma
	AM11 -NA2 1_555 1_566	# 90 Check
PLAT701_ALERT_1_C	Bond Calc 3.176(3), Rep 3.181(3), Dev..	1.67 Sigma
	MM11 -CA2 1_555 1_565	# 109 Check
PLAT701_ALERT_1_C	Bond Calc 3.176(3), Rep 3.181(3), Dev..	1.67 Sigma
	MM11 -CA2 1_555 1_566	# 110 Check
PLAT701_ALERT_1_C	Bond Calc 3.176(3), Rep 3.181(3), Dev..	1.67 Sigma
	MM11 -NA2 1_555 1_565	# 111 Check
PLAT701_ALERT_1_C	Bond Calc 3.176(3), Rep 3.181(3), Dev..	1.67 Sigma
	MM11 -NA2 1_555 1_566	# 112 Check
PLAT701_ALERT_1_C	Bond Calc 3.176(3), Rep 3.181(3), Dev..	1.67 Sigma
	FM11 -CA2 1_555 1_565	# 115 Check
PLAT701_ALERT_1_C	Bond Calc 3.176(3), Rep 3.181(3), Dev..	1.67 Sigma
	FM11 -CA2 1_555 1_566	# 116 Check
PLAT701_ALERT_1_C	Bond Calc 3.176(3), Rep 3.181(3), Dev..	1.67 Sigma
	FM11 -NA2 1_555 1_565	# 117 Check
PLAT701_ALERT_1_C	Bond Calc 3.176(3), Rep 3.181(3), Dev..	1.67 Sigma
	FM11 -NA2 1_555 1_566	# 118 Check

PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O11A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O11A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O11A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O12A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O12A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check

	CM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Cm11	Check
	CM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Cm11	Check
	CM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	MM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	FM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA21		
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF		4	Note
	-2 2 1, 5 3 1, 0 0 2, 4 0 2,			
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.79Ang From O32A .	0.40	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	1.05Ang From O21A .	-0.44	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.96Ang From O22A .	-0.43	eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1 Constrained at	0.087	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11 Constrained at	0.052	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11 Constrained at	0.86	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1 Constrained at	0.868	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1 Constrained at	0.045	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11 Constrained at	0.088	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21 Constrained at	0.7904	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2 Constrained at	0.3622	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2 Constrained at	0.6378	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21 Constrained at	0.2096	Check
PLAT301_ALERT_3_G	Main Residue Disorder (Resd 1)	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A .	134.4	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A .	138.8	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11 Fm11		

PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.84 Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	! Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2 Note
	0 1 0, 1 1 0,	
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L= 0.600	390 Report
	0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,	
	0 8 0, 0 9 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0,	
	1 6 0, 1 7 0, 1 8 0, 1 9 0, 2 0 0, 2 1 0,	
	2 2 0, 2 3 0, 2 4 0, 2 5 0, 2 6 0, 2 7 0,	
	2 8 0, 2 9 0, 3 1 0, 3 4 0, 3 5 0, 3 6 0,	
	3 7 0, 3 8 0, 3 9 0, 4 0 0, 4 1 0, 4 2 0,	
	4 4 0, 4 5 0, 4 6 0, 4 7 0, 4 8 0, 4 9 0,	
	5 1 0, 5 3 0, 5 4 0, 5 5 0, 5 7 0, 5 8 0,	
	5 9 0, 6 0 0, 6 1 0, 6 2 0, 6 3 0, 6 4 0,	
	6 5 0, 6 8 0, 7 1 0, 7 2 0, 7 3 0, 7 5 0,	
	7 6 0, 7 7 0, 7 8 0, 8 0 0, 8 1 0, 8 2 0,	
	8 3 0, 8 4 0, 8 5 0, 8 6 0, 8 7 0, 9 1 0,	
	9 2 0, 9 3 0, 9 5 0, 10 0 0, 10 1 0, 10 2 0,	
	10 3 0, 10 4 0, -11 0 1, -11 1 1, -11 2 1, -10 1 1,	
	-10 2 1, -10 3 1, -10 4 1, -9 0 1, -9 1 1, -9 2 1,	
	-9 6 1, -8 1 1, -8 2 1, -8 5 1, -7 0 1, -7 1 1,	
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	674 Note
PLAT929_ALERT_5_G	No Weight Pars,Obs and Calc R1,wR2,S not Checked	! Info
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	2 Units
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	5 Units
PLAT956_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Hmax Differ	2 Units
PLAT957_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Kmax Differ	5 Units
PLAT966_ALERT_5_G	Note: Non-Standard (i.e. 2.0) OMIT Threshold of	3.0 Sig(I)
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	3.278 Note
	Predicted wR2: Based on SigI**2 3.67 or SHELX Weight	3.67
PLAT985_ALERT_1_G	The Ca-f"= 0.1533 Deviates from the B&C-Value	0.1517 Check
PLAT985_ALERT_1_G	The Fe-f"= 0.4372 Deviates from the B&C-Value	0.4344 Check

39 **ALERT level A** = Most likely a serious problem - resolve or explain
13 **ALERT level B** = A potentially serious problem, consider carefully
76 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
42 **ALERT level G** = General information/check it is not something unexpected

126 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
9 ALERT type 5 Informative message, check

Datablock: 2.70_GPa

Bond precision: Si- O = 0.0050 A

Wavelength=0.49570

Cell: a=9.508(3) b=8.707(5) c=5.213(1)
 alpha=90 beta=106.60(3) gamma=90
 Temperature: 293 K

	Calculated	Reported
Volume	413.6(3)	413.6(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.416	3.429
Z	1	4
Mu (mm-1)	0.709	0.700
F000	422.4	422.0
F000'	423.29	
h, k, lmax	15, 14, 8	13, 9, 8
Nref	2039	578
Tmin, Tmax		0.257, 1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.257 Tmax=1.000
 AbsCorr = MULTII-SCAN

Data completeness= 0.283 Theta(max)= 24.540

R(reflections)= 0.0549(430) wR2(reflections)=
 S = 3.450 Npar= 94 wR= 0.0724(578)

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
 Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
 Label identifying the atom site 2.
 GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
 Label identifying the atom site 3.
 GEOM008_ALERT_1_A _geom_angle is missing
 Angle between atom sites 1, 2 and 3.
 PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 12.24 Degree
 PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.540 Why?
 PLAT701_ALERT_1_A Bond Calc 2.345(4), Rep 2.358(4), Dev.. 3.25 Sigma

	O21A	-CA2	1_555	3_656		#	26	Check
PLAT701_ALERT_1_A	Bond	Calc	2.345(4), Rep	2.358(4), Dev..				3.25 Sigma
	O21A	-NA2	1_555	3_656		#	27	Check
PLAT701_ALERT_1_A	Bond	Calc	2.363(4), Rep	2.384(4), Dev..				5.25 Sigma
	O22A	-CA21	1_555	3_667		#	32	Check
PLAT701_ALERT_1_A	Bond	Calc	2.363(4), Rep	2.384(4), Dev..				5.25 Sigma
	O22A	-NA21	1_555	3_667		#	33	Check
PLAT701_ALERT_1_A	Bond	Calc	3.012(2), Rep	3.025(2), Dev..				6.50 Sigma
	SIA1	-CA2	1_555	3_666		#	38	Check
PLAT701_ALERT_1_A	Bond	Calc	3.012(2), Rep	3.025(2), Dev..				6.50 Sigma
	SIA1	-NA2	1_555	3_666		#	39	Check
PLAT701_ALERT_1_A	Bond	Calc	3.252(3), Rep	3.270(4), Dev..				6.00 Sigma
	SIA1	-CA21	1_555	3_666		#	40	Check
PLAT701_ALERT_1_A	Bond	Calc	3.184(3), Rep	3.198(4), Dev..				4.67 Sigma
	SIB1	-CA2	1_555	3_666		#	41	Check
PLAT701_ALERT_1_A	Bond	Calc	3.184(3), Rep	3.198(4), Dev..				4.67 Sigma
	SIB1	-NA2	1_555	3_666		#	42	Check
PLAT701_ALERT_1_A	Bond	Calc	3.034(3), Rep	3.049(2), Dev..				5.00 Sigma
	SIB1	-CA21	1_555	3_667		#	43	Check
PLAT701_ALERT_1_A	Bond	Calc	3.034(3), Rep	3.049(2), Dev..				5.00 Sigma
	SIB1	-NA21	1_555	3_667		#	44	Check
PLAT701_ALERT_1_A	Bond	Calc	3.066(3), Rep	3.086(2), Dev..				6.67 Sigma
	MGM1	-AM11	1_555	1_554		#	48	Check
PLAT701_ALERT_1_A	Bond	Calc	3.066(3), Rep	3.086(2), Dev..				6.67 Sigma
	MGM1	-AM11	1_555	1_555		#	49	Check
PLAT701_ALERT_1_A	Bond	Calc	3.066(3), Rep	3.086(2), Dev..				6.67 Sigma
	MGM1	-MM11	1_555	1_554		#	52	Check
PLAT701_ALERT_1_A	Bond	Calc	3.066(3), Rep	3.086(2), Dev..				6.67 Sigma
	MGM1	-MM11	1_555	1_555		#	53	Check
PLAT701_ALERT_1_A	Bond	Calc	3.066(3), Rep	3.086(2), Dev..				6.67 Sigma
	AM1	-MM11	1_555	1_554		#	71	Check
PLAT701_ALERT_1_A	Bond	Calc	3.066(3), Rep	3.086(2), Dev..				6.67 Sigma
	AM1	-MM11	1_555	1_555		#	72	Check

Alert level B

PLAT017_ALERT_1_B	Check	Scattering Type	Consistency of AM1	as		AL Error?
PLAT017_ALERT_1_B	Check	Scattering Type	Consistency of FM1	as		FE Error?
PLAT017_ALERT_1_B	Check	Scattering Type	Consistency of AM11	as		AL Error?
PLAT017_ALERT_1_B	Check	Scattering Type	Consistency of MM11	as		MG Error?
PLAT017_ALERT_1_B	Check	Scattering Type	Consistency of FM11	as		FE Error?
PLAT088_ALERT_3_B	Poor	Data / Parameter	Ratio			6.15 Note
PLAT701_ALERT_1_B	Bond	Calc	1.611(5), Rep	1.625(5), Dev..		2.80 Sigma
	O11A	-SIA1	1_555	1_655	#	1 Check
PLAT701_ALERT_1_B	Bond	Calc	2.336(5), Rep	2.348(5), Dev..		2.40 Sigma
	O11A	-CA2	1_555	1_565	#	9 Check
PLAT701_ALERT_1_B	Bond	Calc	2.336(5), Rep	2.348(5), Dev..		2.40 Sigma
	O11A	-NA2	1_555	1_565	#	10 Check
PLAT701_ALERT_1_B	Bond	Calc	1.609(5), Rep	1.622(5), Dev..		2.60 Sigma
	O12A	-SIB1	1_555	1_655	#	11 Check
PLAT701_ALERT_1_B	Bond	Calc	2.049(4), Rep	2.058(3), Dev..		2.25 Sigma
	O12A	-MGM1	1_555	1_555	#	12 Check
PLAT701_ALERT_1_B	Bond	Calc	2.049(4), Rep	2.058(3), Dev..		2.25 Sigma
	O12A	-FM1	1_555	1_555	#	14 Check
PLAT701_ALERT_1_B	Bond	Calc	2.379(5), Rep	2.391(5), Dev..		2.40 Sigma
	O12A	-CA21	1_555	1_555	#	19 Check
PLAT701_ALERT_1_B	Bond	Calc	2.379(5), Rep	2.391(5), Dev..		2.40 Sigma

	O12A	-NA21	1_555	1_555		#	20	Check
PLAT701_ALERT_1_B	Bond	Calc	1.590(5), Rep	1.603(5), Dev..			2.60	Sigma
	O21A	-SIA1	1_555	1_545		#	21	Check
PLAT701_ALERT_1_B	Bond	Calc	3.425(4), Rep	3.436(6), Dev..			2.75	Sigma
	MGM1	-CA2	1_555	1_565		#	54	Check
PLAT701_ALERT_1_B	Bond	Calc	3.425(4), Rep	3.436(6), Dev..			2.75	Sigma
	MGM1	-NA2	1_555	1_565		#	55	Check
PLAT701_ALERT_1_B	Bond	Calc	3.196(3), Rep	3.203(2), Dev..			2.33	Sigma
	MGM1	-CA21	1_555	1_554		#	56	Check
PLAT701_ALERT_1_B	Bond	Calc	3.196(3), Rep	3.203(2), Dev..			2.33	Sigma
	MGM1	-CA21	1_555	1_555		#	57	Check
PLAT701_ALERT_1_B	Bond	Calc	3.196(3), Rep	3.203(2), Dev..			2.33	Sigma
	MGM1	-NA21	1_555	1_554		#	58	Check
PLAT701_ALERT_1_B	Bond	Calc	3.196(3), Rep	3.203(2), Dev..			2.33	Sigma
	MGM1	-NA21	1_555	1_555		#	59	Check
PLAT701_ALERT_1_B	Bond	Calc	3.425(4), Rep	3.436(6), Dev..			2.75	Sigma
	AM1	-CA2	1_555	1_565		#	73	Check
PLAT701_ALERT_1_B	Bond	Calc	3.425(4), Rep	3.436(6), Dev..			2.75	Sigma
	AM1	-NA2	1_555	1_565		#	74	Check
PLAT701_ALERT_1_B	Bond	Calc	3.196(3), Rep	3.203(2), Dev..			2.33	Sigma
	AM1	-CA21	1_555	1_554		#	75	Check
PLAT701_ALERT_1_B	Bond	Calc	3.196(3), Rep	3.203(2), Dev..			2.33	Sigma
	AM1	-CA21	1_555	1_555		#	76	Check
PLAT701_ALERT_1_B	Bond	Calc	3.196(3), Rep	3.203(2), Dev..			2.33	Sigma
	AM1	-NA21	1_555	1_554		#	77	Check
PLAT701_ALERT_1_B	Bond	Calc	3.196(3), Rep	3.203(2), Dev..			2.33	Sigma
	AM1	-NA21	1_555	1_555		#	78	Check
PLAT701_ALERT_1_B	Bond	Calc	3.196(3), Rep	3.203(2), Dev..			2.33	Sigma
	FM1	-CA21	1_555	1_554		#	79	Check
PLAT701_ALERT_1_B	Bond	Calc	3.196(3), Rep	3.203(2), Dev..			2.33	Sigma
	FM1	-CA21	1_555	1_555		#	80	Check
PLAT701_ALERT_1_B	Bond	Calc	3.196(3), Rep	3.203(2), Dev..			2.33	Sigma
	FM1	-NA21	1_555	1_554		#	81	Check
PLAT701_ALERT_1_B	Bond	Calc	3.196(3), Rep	3.203(2), Dev..			2.33	Sigma
	FM1	-NA21	1_555	1_555		#	82	Check
PLAT701_ALERT_1_B	Bond	Calc	3.173(3), Rep	3.181(3), Dev..			2.67	Sigma
	AM11	-CA2	1_555	1_565		#	87	Check
PLAT701_ALERT_1_B	Bond	Calc	3.173(3), Rep	3.181(3), Dev..			2.67	Sigma
	AM11	-CA2	1_555	1_566		#	88	Check
PLAT701_ALERT_1_B	Bond	Calc	3.173(3), Rep	3.181(3), Dev..			2.67	Sigma
	AM11	-NA2	1_555	1_565		#	89	Check
PLAT701_ALERT_1_B	Bond	Calc	3.173(3), Rep	3.181(3), Dev..			2.67	Sigma
	AM11	-NA2	1_555	1_566		#	90	Check
PLAT701_ALERT_1_B	Bond	Calc	3.173(3), Rep	3.181(3), Dev..			2.67	Sigma
	MM11	-CA2	1_555	1_565		#	109	Check
PLAT701_ALERT_1_B	Bond	Calc	3.173(3), Rep	3.181(3), Dev..			2.67	Sigma
	MM11	-CA2	1_555	1_566		#	110	Check
PLAT701_ALERT_1_B	Bond	Calc	3.173(3), Rep	3.181(3), Dev..			2.67	Sigma
	MM11	-NA2	1_555	1_565		#	111	Check
PLAT701_ALERT_1_B	Bond	Calc	3.173(3), Rep	3.181(3), Dev..			2.67	Sigma
	MM11	-NA2	1_555	1_566		#	112	Check
PLAT701_ALERT_1_B	Bond	Calc	3.173(3), Rep	3.181(3), Dev..			2.67	Sigma
	FM11	-CA2	1_555	1_565		#	115	Check
PLAT701_ALERT_1_B	Bond	Calc	3.173(3), Rep	3.181(3), Dev..			2.67	Sigma
	FM11	-CA2	1_555	1_566		#	116	Check
PLAT701_ALERT_1_B	Bond	Calc	3.173(3), Rep	3.181(3), Dev..			2.67	Sigma
	FM11	-NA2	1_555	1_565		#	117	Check

PLAT701_ALERT_1_B Bond	Calc	3.173(3), Rep	3.181(3), Dev..	2.67 Sigma
FM11	-NA2	1_555	1_566	# 118 Check

● Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00

Goodness of fit given = 3.450

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check

Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8

Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)

Rep.: ?

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.08 Check

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms . Please Check

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.6 Note

PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) 011A Check

PLAT701_ALERT_1_C Bond Calc 2.107(5), Rep 2.115(5), Dev.. 1.60 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_C Bond Calc 2.107(5), Rep 2.115(5), Dev.. 1.60 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_C Bond Calc 1.579(5), Rep 1.588(5), Dev.. 1.80 Sigma

O22A -SIB1 1_555 1_555 # 28 Check

PLAT701_ALERT_1_C Bond Calc 2.019(5), Rep 2.025(5), Dev.. 1.20 Sigma

O22A -MGM1 1_555 3_666 # 29 Check

PLAT701_ALERT_1_C Bond Calc 2.019(5), Rep 2.025(5), Dev.. 1.20 Sigma

O22A -FM1 1_555 3_666 # 31 Check

PLAT701_ALERT_1_C Bond Calc 1.664(4), Rep 1.659(4), Dev.. 1.25 Sigma

O32A -SIA1 1_555 1_555 # 36 Check

PLAT701_ALERT_1_C Bond Calc 3.465(4), Rep 3.473(5), Dev.. 2.00 Sigma

AM11 -CA21 1_555 1_555 # 91 Check

PLAT701_ALERT_1_C Bond Calc 3.465(4), Rep 3.473(5), Dev.. 2.00 Sigma

AM11 -NA21 1_555 1_555 # 92 Check

PLAT701_ALERT_1_C Bond Calc 3.465(4), Rep 3.473(5), Dev.. 2.00 Sigma

MM11 -CA21 1_555 1_555 # 113 Check

PLAT701_ALERT_1_C Bond Calc 3.465(4), Rep 3.473(5), Dev.. 2.00 Sigma

MM11 -NA21 1_555 1_555 # 114 Check

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label MnM1 Check

O11A MNM1

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Cm11 Check

O11A CM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Tm11 Check

O11A TM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label MnM1 Check

O12A MNM1

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Cm11 Check

O12A CM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Tm11 Check

O12A TM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Cm11 Check

O21A CM11

PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11	Check
	O21A	TM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	O22A	MNM1					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MGM1	MNM1					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11	Check
	MGM1	TM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11	Check
	MGM1	TM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	AM1					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	FM1					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	MM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	MM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	CA2					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	NA2					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	CA21					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	CA21					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	NA21					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	NA21					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	AM11	CM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11	Check
	AM11	TM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	CM11	TM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	CM11	MM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	CM11	FM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	CM11	CA2					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	CM11	CA2					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	CM11	NA2					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	CM11	NA2					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11	Check
	TM11	MM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11	Check
	TM11	FM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11	Check
	TM11	CA2					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11	Check
	TM11	CA2					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11	Check

	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA21		
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.93Ang From O12A	.	-0.71 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.97Ang From O11A	.	-0.64 eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1	0.087	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11	0.052	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11	0.86	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1	0.868	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1	0.045	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11	0.088	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21	0.7904	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2	0.3622	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2	0.6378	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21	0.2096	Check
PLAT301_ALERT_3_G	Main Residue Disorder	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 1)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A	134.5	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A	138.9	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11		Fm11
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	1.84	Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
	0 1 0, 1 1 0,		
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L=	0.600	383 Report
	0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,		
	0 8 0, 0 9 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0,		
	1 6 0, 1 7 0, 1 8 0, 1 9 0, 2 0 0, 2 1 0,		
	2 2 0, 2 3 0, 2 4 0, 2 5 0, 2 6 0, 2 7 0,		
	2 8 0, 2 9 0, 3 1 0, 3 4 0, 3 5 0, 3 6 0,		
	3 7 0, 3 8 0, 3 9 0, 4 0 0, 4 1 0, 4 2 0,		
	4 6 0, 4 7 0, 4 8 0, 4 9 0, 5 1 0, 5 4 0,		
	5 7 0, 5 8 0, 5 9 0, 6 0 0, 6 1 0, 6 2 0,		
	6 3 0, 6 4 0, 6 5 0, 6 8 0, 7 1 0, 7 2 0,		
	7 4 0, 7 5 0, 7 6 0, 7 7 0, 7 8 0, 8 0 0,		

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      8 1 0,   8 2 0,   8 3 0,   8 4 0,   8 5 0,   8 6 0,
      8 7 0,   9 1 0,   9 2 0,   9 3 0,   9 5 0,  10 0 0,
     10 1 0,  10 2 0,  10 3 0,  10 4 0, -11 0 1, -11 1 1,
    -11 2 1, -10 1 1, -10 2 1, -10 3 1, -10 4 1,  -9 0 1,
     -9 1 1,  -9 2 1,  -9 6 1,  -8 1 1,  -8 2 1,  -8 5 1,
     -7 0 1,  -7 1 1,  -7 5 1,  -7 8 1,  -6 1 1,  -6 6 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      681 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....      3 Note
      -2 2 1,   5 3 1,   0 0 2,
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked      ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ      2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ      5 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ      2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ      5 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of      3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      5.872 Note
      Predicted wR2: Based on SigI**2  2.08 or SHELX Weight  2.08
PLAT985_ALERT_1_G The Ca-f"=      0.1533 Deviates from the B&C-Value  0.1517 Check
PLAT985_ALERT_1_G The Fe-f"=      0.4372 Deviates from the B&C-Value  0.4344 Check

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22 ALERT level A = Most likely a serious problem - resolve or explain
43 ALERT level B = A potentially serious problem, consider carefully
61 ALERT level C = Check. Ensure it is not caused by an omission or oversight
43 ALERT level G = General information/check it is not something unexpected

127 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  7 ALERT type 2 Indicator that the structure model may be wrong or deficient
  7 ALERT type 3 Indicator that the structure quality may be low
 19 ALERT type 4 Improvement, methodology, query or suggestion
  9 ALERT type 5 Informative message, check

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Datablock: 3.25_GPa

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Bond precision:   Si- O = 0.0040 A           Wavelength=0.49570

Cell:             a=9.496(3)           b=8.694(5)           c=5.207(1)
                  alpha=90             beta=106.54(3)        gamma=90
Temperature:      293 K

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	Calculated	Reported
Volume	412.1(3)	412.1(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.429	3.442
Z	1	4
Mu (mm-1)	0.711	0.702
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,9,8
Nref	1990	584
Tmin,Tmax		0.389,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.389 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.293 Theta(max)= 24.330

R(reflections)= 0.0511(481) wR2(reflections)=
wR= 0.0734(584)

S = 2.480 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 13.06 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.550 Why?

PLAT701_ALERT_1_A Bond Calc 2.103(3), Rep 2.115(5), Dev.. 4.00 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.103(3), Rep 2.115(5), Dev.. 4.00 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond Calc 2.336(3), Rep 2.348(5), Dev.. 4.00 Sigma

O11A -CA2 1_555 1_565 # 9 Check

PLAT701_ALERT_1_A Bond Calc 2.336(3), Rep 2.348(5), Dev.. 4.00 Sigma

	O11A	-NA2	1_555	1_565		#	10	Check
PLAT701_ALERT_1_A	Bond	Calc	2.048(2),	Rep	2.058(3),	Dev..		5.00 Sigma
	O12A	-MGM1	1_555	1_555		#	12	Check
PLAT701_ALERT_1_A	Bond	Calc	2.048(2),	Rep	2.058(3),	Dev..		5.00 Sigma
	O12A	-FM1	1_555	1_555		#	14	Check
PLAT701_ALERT_1_A	Bond	Calc	2.376(4),	Rep	2.391(5),	Dev..		3.75 Sigma
	O12A	-CA21	1_555	1_555		#	19	Check
PLAT701_ALERT_1_A	Bond	Calc	2.376(4),	Rep	2.391(5),	Dev..		3.75 Sigma
	O12A	-NA21	1_555	1_555		#	20	Check
PLAT701_ALERT_1_A	Bond	Calc	2.347(3),	Rep	2.358(4),	Dev..		3.67 Sigma
	O21A	-CA2	1_555	3_656		#	26	Check
PLAT701_ALERT_1_A	Bond	Calc	2.347(3),	Rep	2.358(4),	Dev..		3.67 Sigma
	O21A	-NA2	1_555	3_656		#	27	Check
PLAT701_ALERT_1_A	Bond	Calc	2.009(4),	Rep	2.025(5),	Dev..		4.00 Sigma
	O22A	-MGM1	1_555	3_666		#	29	Check
PLAT701_ALERT_1_A	Bond	Calc	2.009(4),	Rep	2.025(5),	Dev..		4.00 Sigma
	O22A	-FM1	1_555	3_666		#	31	Check
PLAT701_ALERT_1_A	Bond	Calc	2.370(3),	Rep	2.384(4),	Dev..		4.67 Sigma
	O22A	-CA21	1_555	3_667		#	32	Check
PLAT701_ALERT_1_A	Bond	Calc	2.370(3),	Rep	2.384(4),	Dev..		4.67 Sigma
	O22A	-NA21	1_555	3_667		#	33	Check
PLAT701_ALERT_1_A	Bond	Calc	3.007(2),	Rep	3.025(2),	Dev..		9.00 Sigma
	SIA1	-CA2	1_555	3_666		#	38	Check
PLAT701_ALERT_1_A	Bond	Calc	3.007(2),	Rep	3.025(2),	Dev..		9.00 Sigma
	SIA1	-NA2	1_555	3_666		#	39	Check
PLAT701_ALERT_1_A	Bond	Calc	3.243(3),	Rep	3.270(4),	Dev..		9.00 Sigma
	SIA1	-CA21	1_555	3_666		#	40	Check
PLAT701_ALERT_1_A	Bond	Calc	3.177(3),	Rep	3.198(4),	Dev..		7.00 Sigma
	SIB1	-CA2	1_555	3_666		#	41	Check
PLAT701_ALERT_1_A	Bond	Calc	3.177(3),	Rep	3.198(4),	Dev..		7.00 Sigma
	SIB1	-NA2	1_555	3_666		#	42	Check
PLAT701_ALERT_1_A	Bond	Calc	3.030(2),	Rep	3.049(2),	Dev..		9.50 Sigma
	SIB1	-CA21	1_555	3_667		#	43	Check
PLAT701_ALERT_1_A	Bond	Calc	3.030(2),	Rep	3.049(2),	Dev..		9.50 Sigma
	SIB1	-NA21	1_555	3_667		#	44	Check
PLAT701_ALERT_1_A	Bond	Calc	3.066(2),	Rep	3.086(2),	Dev..		10.00 Sigma
	MGM1	-AM11	1_555	1_554		#	48	Check
PLAT701_ALERT_1_A	Bond	Calc	3.066(2),	Rep	3.086(2),	Dev..		10.00 Sigma
	MGM1	-AM11	1_555	1_555		#	49	Check
PLAT701_ALERT_1_A	Bond	Calc	3.066(2),	Rep	3.086(2),	Dev..		10.00 Sigma
	MGM1	-MM11	1_555	1_554		#	52	Check
PLAT701_ALERT_1_A	Bond	Calc	3.066(2),	Rep	3.086(2),	Dev..		10.00 Sigma
	MGM1	-MM11	1_555	1_555		#	53	Check
PLAT701_ALERT_1_A	Bond	Calc	3.426(3),	Rep	3.436(6),	Dev..		3.33 Sigma
	MGM1	-CA2	1_555	1_565		#	54	Check
PLAT701_ALERT_1_A	Bond	Calc	3.426(3),	Rep	3.436(6),	Dev..		3.33 Sigma
	MGM1	-NA2	1_555	1_565		#	55	Check
PLAT701_ALERT_1_A	Bond	Calc	3.190(2),	Rep	3.203(2),	Dev..		6.50 Sigma
	MGM1	-CA21	1_555	1_554		#	56	Check
PLAT701_ALERT_1_A	Bond	Calc	3.190(2),	Rep	3.203(2),	Dev..		6.50 Sigma
	MGM1	-CA21	1_555	1_555		#	57	Check
PLAT701_ALERT_1_A	Bond	Calc	3.190(2),	Rep	3.203(2),	Dev..		6.50 Sigma
	MGM1	-NA21	1_555	1_554		#	58	Check
PLAT701_ALERT_1_A	Bond	Calc	3.190(2),	Rep	3.203(2),	Dev..		6.50 Sigma
	MGM1	-NA21	1_555	1_555		#	59	Check
PLAT701_ALERT_1_A	Bond	Calc	3.066(2),	Rep	3.086(2),	Dev..		10.00 Sigma
	AM1	-MM11	1_555	1_554		#	71	Check

PLAT701_ALERT_1_A Bond	Calc	3.066(2), Rep	3.086(2), Dev..	10.00 Sigma
AM1	-MM11	1_555	1_555	# 72 Check
PLAT701_ALERT_1_A Bond	Calc	3.426(3), Rep	3.436(6), Dev..	3.33 Sigma
AM1	-CA2	1_555	1_565	# 73 Check
PLAT701_ALERT_1_A Bond	Calc	3.426(3), Rep	3.436(6), Dev..	3.33 Sigma
AM1	-NA2	1_555	1_565	# 74 Check
PLAT701_ALERT_1_A Bond	Calc	3.190(2), Rep	3.203(2), Dev..	6.50 Sigma
AM1	-CA21	1_555	1_554	# 75 Check
PLAT701_ALERT_1_A Bond	Calc	3.190(2), Rep	3.203(2), Dev..	6.50 Sigma
AM1	-CA21	1_555	1_555	# 76 Check
PLAT701_ALERT_1_A Bond	Calc	3.190(2), Rep	3.203(2), Dev..	6.50 Sigma
AM1	-NA21	1_555	1_554	# 77 Check
PLAT701_ALERT_1_A Bond	Calc	3.190(2), Rep	3.203(2), Dev..	6.50 Sigma
AM1	-NA21	1_555	1_555	# 78 Check
PLAT701_ALERT_1_A Bond	Calc	3.190(2), Rep	3.203(2), Dev..	6.50 Sigma
FM1	-CA21	1_555	1_554	# 79 Check
PLAT701_ALERT_1_A Bond	Calc	3.190(2), Rep	3.203(2), Dev..	6.50 Sigma
FM1	-CA21	1_555	1_555	# 80 Check
PLAT701_ALERT_1_A Bond	Calc	3.190(2), Rep	3.203(2), Dev..	6.50 Sigma
FM1	-NA21	1_555	1_554	# 81 Check
PLAT701_ALERT_1_A Bond	Calc	3.190(2), Rep	3.203(2), Dev..	6.50 Sigma
FM1	-NA21	1_555	1_555	# 82 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
AM11	-CA2	1_555	1_565	# 87 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
AM11	-CA2	1_555	1_566	# 88 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
AM11	-NA2	1_555	1_565	# 89 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
AM11	-NA2	1_555	1_566	# 90 Check
PLAT701_ALERT_1_A Bond	Calc	3.462(3), Rep	3.473(5), Dev..	3.67 Sigma
AM11	-CA21	1_555	1_555	# 91 Check
PLAT701_ALERT_1_A Bond	Calc	3.462(3), Rep	3.473(5), Dev..	3.67 Sigma
AM11	-NA21	1_555	1_555	# 92 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
MM11	-CA2	1_555	1_565	# 109 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
MM11	-CA2	1_555	1_566	# 110 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
MM11	-NA2	1_555	1_565	# 111 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
MM11	-NA2	1_555	1_566	# 112 Check
PLAT701_ALERT_1_A Bond	Calc	3.462(3), Rep	3.473(5), Dev..	3.67 Sigma
MM11	-CA21	1_555	1_555	# 113 Check
PLAT701_ALERT_1_A Bond	Calc	3.462(3), Rep	3.473(5), Dev..	3.67 Sigma
MM11	-NA21	1_555	1_555	# 114 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
FM11	-CA2	1_555	1_565	# 115 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
FM11	-CA2	1_555	1_566	# 116 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
FM11	-NA2	1_555	1_565	# 117 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
FM11	-NA2	1_555	1_566	# 118 Check

PLAT017_ALERT_1_B	Check	Scattering Type Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B	Check	Scattering Type Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B	Check	Scattering Type Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B	Check	Scattering Type Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B	Check	Scattering Type Consistency of FM11	as	FE Error?
PLAT088_ALERT_3_B	Poor Data /	Parameter Ratio		6.21 Note
PLAT701_ALERT_1_B	Bond	Calc 1.616(3), Rep 1.625(5), Dev..		3.00 Sigma
	O11A	-SIA1 1_555 1_655	#	1 Check
PLAT701_ALERT_1_B	Bond	Calc 1.614(3), Rep 1.622(5), Dev..		2.67 Sigma
	O12A	-SIB1 1_555 1_655	#	11 Check
PLAT701_ALERT_1_B	Bond	Calc 1.661(3), Rep 1.670(4), Dev..		3.00 Sigma
	O31A	-SIB1 1_555 1_554	#	35 Check

● Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
 Goodness of fit given = 2.480

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
 Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8
 Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
 Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)
 Rep.: ?

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.08 Check

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms . Please Check

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.4 Note

PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) O11A Check

PLAT701_ALERT_1_C Bond Calc 1.973(4), Rep 1.980(5), Dev.. 1.75 Sigma

O12A -MM11 1_555 1_555 # 17 Check

PLAT701_ALERT_1_C Bond Calc 1.973(4), Rep 1.980(5), Dev.. 1.75 Sigma

O12A -FM11 1_555 1_555 # 18 Check

PLAT701_ALERT_1_C Bond Calc 1.596(4), Rep 1.603(5), Dev.. 1.75 Sigma

O21A -SIA1 1_555 1_545 # 21 Check

PLAT701_ALERT_1_C Bond Calc 1.881(4), Rep 1.887(5), Dev.. 1.50 Sigma

O21A -MM11 1_555 3_666 # 24 Check

PLAT701_ALERT_1_C Bond Calc 1.881(4), Rep 1.887(5), Dev.. 1.50 Sigma

O21A -FM11 1_555 3_666 # 25 Check

PLAT701_ALERT_1_C Bond Calc 1.583(4), Rep 1.588(5), Dev.. 1.25 Sigma

O22A -SIB1 1_555 1_555 # 28 Check

PLAT701_ALERT_1_C Bond Calc 1.650(3), Rep 1.644(5), Dev.. 2.00 Sigma

O31A -SIA1 1_555 1_555 # 34 Check

PLAT701_ALERT_1_C Bond Calc 1.653(3), Rep 1.659(4), Dev.. 2.00 Sigma

O32A -SIA1 1_555 1_555 # 36 Check

PLAT701_ALERT_1_C Bond Calc 1.648(3), Rep 1.644(5), Dev.. 1.33 Sigma

O32A -SIB1 1_555 1_555 # 37 Check

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label MnM1 Check

O11A MNM1

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Cm11 Check

O11A CM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Tm11 Check

O11A TM11

PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	O12A	MNM1					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	O12A	CM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11	Check
	O12A	TM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	O21A	CM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11	Check
	O21A	TM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	O22A	MNM1					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MGM1	MNM1					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11	Check
	MGM1	TM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11	Check
	MGM1	TM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	AM1					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	FM1					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	MM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	MM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	CA2					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	NA2					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	CA21					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	CA21					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	NA21					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1	Check
	MNM1	NA21					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	AM11	CM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11	Check
	AM11	TM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	CM11	TM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	CM11	MM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	CM11	FM11					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	CM11	CA2					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	CM11	CA2					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	CM11	NA2					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11	Check
	CM11	NA2					
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11	Check

	TM11	MM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	FM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA21		
PLAT975_ALERT_2_C	Check	Calcd Resid. Dens.	0.99Ang From O31A .	0.59 eA-3
PLAT975_ALERT_2_C	Check	Calcd Resid. Dens.	0.77Ang From O32A .	0.57 eA-3
PLAT975_ALERT_2_C	Check	Calcd Resid. Dens.	0.52Ang From O12A .	0.42 eA-3
PLAT975_ALERT_2_C	Check	Calcd Resid. Dens.	0.61Ang From O11A .	0.41 eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1 Constrained at	0.087	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11 Constrained at	0.052	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11 Constrained at	0.86	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1 Constrained at	0.868	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1 Constrained at	0.045	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11 Constrained at	0.088	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21 Constrained at	0.7904	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2 Constrained at	0.3622	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2 Constrained at	0.6378	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21 Constrained at	0.2096	Check
PLAT301_ALERT_3_G	Main Residue Disorder (Resd 1)	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A .	134.3	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A .	138.9	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11	Fm11	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.84	Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	4	Note
	0 1 0, 1 1 0, 2 0 0, -1 0 1,		
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L=	0.600	375 Report

```

0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,
0 8 0, 0 9 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0,
1 6 0, 1 7 0, 1 8 0, 1 9 0, 2 1 0, 2 2 0,
2 3 0, 2 4 0, 2 5 0, 2 6 0, 2 7 0, 2 8 0,
2 9 0, 3 1 0, 3 4 0, 3 5 0, 3 6 0, 3 7 0,
3 8 0, 3 9 0, 4 0 0, 4 1 0, 4 2 0, 4 6 0,
4 7 0, 4 8 0, 4 9 0, 5 1 0, 5 4 0, 5 7 0,
5 8 0, 5 9 0, 6 0 0, 6 1 0, 6 2 0, 6 3 0,
6 4 0, 6 5 0, 6 8 0, 7 1 0, 7 2 0, 7 5 0,
7 6 0, 7 7 0, 7 8 0, 8 0 0, 8 1 0, 8 2 0,
8 3 0, 8 4 0, 8 5 0, 8 6 0, 8 7 0, 9 1 0,
9 2 0, 9 3 0, 9 5 0, 10 0 0, 10 1 0, 10 2 0,
10 3 0, 10 4 0, -11 0 1, -11 1 1, -11 2 1, -10 1 1,
-10 2 1, -10 3 1, -10 4 1, -9 0 1, -9 1 1, -9 2 1,
-9 6 1, -8 1 1, -8 2 1, -8 5 1, -7 0 1, -7 1 1,
-7 5 1, -7 8 1, -6 1 1, -6 6 1, -6 8 1, -5 0 1,

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PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 663 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 5 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ 2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 5 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of 3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.624 Note
      Predicted wR2: Based on SigI**2 5.25 or SHELX Weight 5.25
PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value 0.1517 Check
PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value 0.4344 Check

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64 ALERT level A = Most likely a serious problem - resolve or explain
9 ALERT level B = A potentially serious problem, consider carefully
62 ALERT level C = Check. Ensure it is not caused by an omission or oversight
42 ALERT level G = General information/check it is not something unexpected

134 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
9 ALERT type 5 Informative message, check

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Datablock: 4.24_GPa

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Bond precision:  Si- O = 0.0030 A          Wavelength=0.49570

Cell:            a=9.479(3)      b=8.672(5)      c=5.196(1)
                  alpha=90      beta=106.45(3)  gamma=90
Temperature:     293 K

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	Calculated	Reported
Volume	409.6(3)	409.6(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.450	3.462
Z	1	4
Mu (mm-1)	0.716	0.707
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,9,8
Nref	1925	588
Tmin,Tmax		0.234,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.234 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.305 Theta(max)= 24.070

R(reflections)= 0.0578(477) wR2(reflections)=
wR= 0.0717(588)

S = 2.110 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 12.25 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.560 Why?

PLAT701_ALERT_1_A Bond Calc 1.607(3), Rep 1.625(5), Dev.. 6.00 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_A Bond Calc 2.098(3), Rep 2.115(5), Dev.. 5.67 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.098(3), Rep 2.115(5), Dev.. 5.67 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond Calc 2.331(3), Rep 2.348(5), Dev.. 5.67 Sigma

	O11A	-CA2	1_555	1_565		#	9 Check
PLAT701_ALERT_1_A	Bond	Calc	2.331(3), Rep	2.348(5), Dev..			5.67 Sigma
	O11A	-NA2	1_555	1_565		#	10 Check
PLAT701_ALERT_1_A	Bond	Calc	1.609(3), Rep	1.622(5), Dev..			4.33 Sigma
	O12A	-SIB1	1_555	1_655		#	11 Check
PLAT701_ALERT_1_A	Bond	Calc	2.046(2), Rep	2.058(3), Dev..			6.00 Sigma
	O12A	-MGM1	1_555	1_555		#	12 Check
PLAT701_ALERT_1_A	Bond	Calc	2.046(2), Rep	2.058(3), Dev..			6.00 Sigma
	O12A	-FM1	1_555	1_555		#	14 Check
PLAT701_ALERT_1_A	Bond	Calc	1.970(3), Rep	1.980(5), Dev..			3.33 Sigma
	O12A	-MM11	1_555	1_555		#	17 Check
PLAT701_ALERT_1_A	Bond	Calc	1.970(3), Rep	1.980(5), Dev..			3.33 Sigma
	O12A	-FM11	1_555	1_555		#	18 Check
PLAT701_ALERT_1_A	Bond	Calc	2.368(3), Rep	2.391(5), Dev..			7.67 Sigma
	O12A	-CA21	1_555	1_555		#	19 Check
PLAT701_ALERT_1_A	Bond	Calc	2.368(3), Rep	2.391(5), Dev..			7.67 Sigma
	O12A	-NA21	1_555	1_555		#	20 Check
PLAT701_ALERT_1_A	Bond	Calc	2.342(3), Rep	2.358(4), Dev..			5.33 Sigma
	O21A	-CA2	1_555	3_656		#	26 Check
PLAT701_ALERT_1_A	Bond	Calc	2.342(3), Rep	2.358(4), Dev..			5.33 Sigma
	O21A	-NA2	1_555	3_656		#	27 Check
PLAT701_ALERT_1_A	Bond	Calc	2.004(3), Rep	2.025(5), Dev..			7.00 Sigma
	O22A	-MGM1	1_555	3_666		#	29 Check
PLAT701_ALERT_1_A	Bond	Calc	2.004(3), Rep	2.025(5), Dev..			7.00 Sigma
	O22A	-FM1	1_555	3_666		#	31 Check
PLAT701_ALERT_1_A	Bond	Calc	2.364(3), Rep	2.384(4), Dev..			6.67 Sigma
	O22A	-CA21	1_555	3_667		#	32 Check
PLAT701_ALERT_1_A	Bond	Calc	2.364(3), Rep	2.384(4), Dev..			6.67 Sigma
	O22A	-NA21	1_555	3_667		#	33 Check
PLAT701_ALERT_1_A	Bond	Calc	3.004(2), Rep	3.025(2), Dev..			10.50 Sigma
	SIA1	-CA2	1_555	3_666		#	38 Check
PLAT701_ALERT_1_A	Bond	Calc	3.004(2), Rep	3.025(2), Dev..			10.50 Sigma
	SIA1	-NA2	1_555	3_666		#	39 Check
PLAT701_ALERT_1_A	Bond	Calc	3.235(3), Rep	3.270(4), Dev..			11.67 Sigma
	SIA1	-CA21	1_555	3_666		#	40 Check
PLAT701_ALERT_1_A	Bond	Calc	3.169(3), Rep	3.198(4), Dev..			9.67 Sigma
	SIB1	-CA2	1_555	3_666		#	41 Check
PLAT701_ALERT_1_A	Bond	Calc	3.169(3), Rep	3.198(4), Dev..			9.67 Sigma
	SIB1	-NA2	1_555	3_666		#	42 Check
PLAT701_ALERT_1_A	Bond	Calc	3.027(2), Rep	3.049(2), Dev..			11.00 Sigma
	SIB1	-CA21	1_555	3_667		#	43 Check
PLAT701_ALERT_1_A	Bond	Calc	3.027(2), Rep	3.049(2), Dev..			11.00 Sigma
	SIB1	-NA21	1_555	3_667		#	44 Check
PLAT701_ALERT_1_A	Bond	Calc	3.055(2), Rep	3.086(2), Dev..			15.50 Sigma
	MGM1	-AM11	1_555	1_554		#	48 Check
PLAT701_ALERT_1_A	Bond	Calc	3.055(2), Rep	3.086(2), Dev..			15.50 Sigma
	MGM1	-AM11	1_555	1_555		#	49 Check
PLAT701_ALERT_1_A	Bond	Calc	3.055(2), Rep	3.086(2), Dev..			15.50 Sigma
	MGM1	-MM11	1_555	1_554		#	52 Check
PLAT701_ALERT_1_A	Bond	Calc	3.055(2), Rep	3.086(2), Dev..			15.50 Sigma
	MGM1	-MM11	1_555	1_555		#	53 Check
PLAT701_ALERT_1_A	Bond	Calc	3.417(3), Rep	3.436(6), Dev..			6.33 Sigma
	MGM1	-CA2	1_555	1_565		#	54 Check
PLAT701_ALERT_1_A	Bond	Calc	3.417(3), Rep	3.436(6), Dev..			6.33 Sigma
	MGM1	-NA2	1_555	1_565		#	55 Check
PLAT701_ALERT_1_A	Bond	Calc	3.188(2), Rep	3.203(2), Dev..			7.50 Sigma
	MGM1	-CA21	1_555	1_554		#	56 Check

PLAT701_ALERT_1_A Bond	Calc	3.188(2), Rep	3.203(2), Dev..	7.50 Sigma
MGM1	-CA21	1_555	1_555	# 57 Check
PLAT701_ALERT_1_A Bond	Calc	3.188(2), Rep	3.203(2), Dev..	7.50 Sigma
MGM1	-NA21	1_555	1_554	# 58 Check
PLAT701_ALERT_1_A Bond	Calc	3.188(2), Rep	3.203(2), Dev..	7.50 Sigma
MGM1	-NA21	1_555	1_555	# 59 Check
PLAT701_ALERT_1_A Bond	Calc	3.055(2), Rep	3.086(2), Dev..	15.50 Sigma
AM1	-MM11	1_555	1_554	# 71 Check
PLAT701_ALERT_1_A Bond	Calc	3.055(2), Rep	3.086(2), Dev..	15.50 Sigma
AM1	-MM11	1_555	1_555	# 72 Check
PLAT701_ALERT_1_A Bond	Calc	3.417(3), Rep	3.436(6), Dev..	6.33 Sigma
AM1	-CA2	1_555	1_565	# 73 Check
PLAT701_ALERT_1_A Bond	Calc	3.417(3), Rep	3.436(6), Dev..	6.33 Sigma
AM1	-NA2	1_555	1_565	# 74 Check
PLAT701_ALERT_1_A Bond	Calc	3.188(2), Rep	3.203(2), Dev..	7.50 Sigma
AM1	-CA21	1_555	1_554	# 75 Check
PLAT701_ALERT_1_A Bond	Calc	3.188(2), Rep	3.203(2), Dev..	7.50 Sigma
AM1	-CA21	1_555	1_555	# 76 Check
PLAT701_ALERT_1_A Bond	Calc	3.188(2), Rep	3.203(2), Dev..	7.50 Sigma
AM1	-NA21	1_555	1_554	# 77 Check
PLAT701_ALERT_1_A Bond	Calc	3.188(2), Rep	3.203(2), Dev..	7.50 Sigma
AM1	-NA21	1_555	1_555	# 78 Check
PLAT701_ALERT_1_A Bond	Calc	3.188(2), Rep	3.203(2), Dev..	7.50 Sigma
FM1	-CA21	1_555	1_554	# 79 Check
PLAT701_ALERT_1_A Bond	Calc	3.188(2), Rep	3.203(2), Dev..	7.50 Sigma
FM1	-CA21	1_555	1_555	# 80 Check
PLAT701_ALERT_1_A Bond	Calc	3.188(2), Rep	3.203(2), Dev..	7.50 Sigma
FM1	-NA21	1_555	1_554	# 81 Check
PLAT701_ALERT_1_A Bond	Calc	3.188(2), Rep	3.203(2), Dev..	7.50 Sigma
FM1	-NA21	1_555	1_555	# 82 Check
PLAT701_ALERT_1_A Bond	Calc	3.167(2), Rep	3.181(3), Dev..	7.00 Sigma
AM11	-CA2	1_555	1_565	# 87 Check
PLAT701_ALERT_1_A Bond	Calc	3.167(2), Rep	3.181(3), Dev..	7.00 Sigma
AM11	-CA2	1_555	1_566	# 88 Check
PLAT701_ALERT_1_A Bond	Calc	3.167(2), Rep	3.181(3), Dev..	7.00 Sigma
AM11	-NA2	1_555	1_565	# 89 Check
PLAT701_ALERT_1_A Bond	Calc	3.167(2), Rep	3.181(3), Dev..	7.00 Sigma
AM11	-NA2	1_555	1_566	# 90 Check
PLAT701_ALERT_1_A Bond	Calc	3.453(3), Rep	3.473(5), Dev..	6.67 Sigma
AM11	-CA21	1_555	1_555	# 91 Check
PLAT701_ALERT_1_A Bond	Calc	3.453(3), Rep	3.473(5), Dev..	6.67 Sigma
AM11	-NA21	1_555	1_555	# 92 Check
PLAT701_ALERT_1_A Bond	Calc	3.167(2), Rep	3.181(3), Dev..	7.00 Sigma
MM11	-CA2	1_555	1_565	# 109 Check
PLAT701_ALERT_1_A Bond	Calc	3.167(2), Rep	3.181(3), Dev..	7.00 Sigma
MM11	-CA2	1_555	1_566	# 110 Check
PLAT701_ALERT_1_A Bond	Calc	3.167(2), Rep	3.181(3), Dev..	7.00 Sigma
MM11	-NA2	1_555	1_565	# 111 Check
PLAT701_ALERT_1_A Bond	Calc	3.167(2), Rep	3.181(3), Dev..	7.00 Sigma
MM11	-NA2	1_555	1_566	# 112 Check
PLAT701_ALERT_1_A Bond	Calc	3.453(3), Rep	3.473(5), Dev..	6.67 Sigma
MM11	-CA21	1_555	1_555	# 113 Check
PLAT701_ALERT_1_A Bond	Calc	3.453(3), Rep	3.473(5), Dev..	6.67 Sigma
MM11	-NA21	1_555	1_555	# 114 Check
PLAT701_ALERT_1_A Bond	Calc	3.167(2), Rep	3.181(3), Dev..	7.00 Sigma
FM11	-CA2	1_555	1_565	# 115 Check
PLAT701_ALERT_1_A Bond	Calc	3.167(2), Rep	3.181(3), Dev..	7.00 Sigma

FM11	-CA2	1_555	1_566		#	116 Check
PLAT701_ALERT_1_A Bond	Calc	3.167(2), Rep	3.181(3), Dev..			7.00 Sigma
FM11	-NA2	1_555	1_565		#	117 Check
PLAT701_ALERT_1_A Bond	Calc	3.167(2), Rep	3.181(3), Dev..			7.00 Sigma
FM11	-NA2	1_555	1_566		#	118 Check

🔴 Alert level B

PLAT017_ALERT_1_B Check	Scattering Type Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of FM11	as	FE Error?
PLAT088_ALERT_3_B Poor Data / Parameter Ratio			6.26 Note
PLAT701_ALERT_1_B Bond	Calc	1.878(3), Rep	1.887(5), Dev..
O21A	-MM11	1_555	3_666
PLAT701_ALERT_1_B Bond	Calc	1.878(3), Rep	1.887(5), Dev..
O21A	-FM11	1_555	3_666
PLAT701_ALERT_1_B Bond	Calc	1.661(3), Rep	1.670(4), Dev..
O31A	-SIB1	1_555	1_554

🟡 Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
 Goodness of fit given = 2.110

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
 Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8
 Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
 Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)
 Rep.: ?

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.08 Check

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms . Please Check

PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) 011A Check

PLAT701_ALERT_1_C Bond Calc 1.597(3), Rep 1.603(5), Dev.. 2.00 Sigma

O21A -SIA1 1_555 1_545 # 21 Check

PLAT701_ALERT_1_C Bond Calc 1.648(3), Rep 1.644(5), Dev.. 1.33 Sigma

O31A -SIA1 1_555 1_555 # 34 Check

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label MnM1 Check

O11A MNM1

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Cm11 Check

O11A CM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Tm11 Check

O11A TM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label MnM1 Check

O12A MNM1

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Cm11 Check

O12A CM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Tm11 Check

O12A TM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Cm11 Check

	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	CA2				

PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA21		
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.73Ang From O22A		0.61 eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1	0.087	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11	0.052	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11	0.86	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1	0.868	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1	0.045	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11	0.088	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21	0.7904	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2	0.3622	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2	0.6378	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21	0.2096	Check
PLAT301_ALERT_3_G	Main Residue Disorder	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 1)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A	134.0	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A	138.4	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11		Fm11
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	1.84	Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
	0 1 0, 1 1 0,		
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L=	0.600	368 Report
	0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,		
	0 8 0, 0 9 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0,		
	1 6 0, 1 7 0, 1 8 0, 1 9 0, 2 0 0, 2 1 0,		
	2 2 0, 2 3 0, 2 4 0, 2 5 0, 2 6 0, 2 7 0,		
	2 8 0, 2 9 0, 3 1 0, 3 4 0, 3 5 0, 3 6 0,		
	3 7 0, 3 8 0, 3 9 0, 4 0 0, 4 1 0, 4 2 0,		
	4 6 0, 4 7 0, 4 8 0, 4 9 0, 5 1 0, 5 4 0,		
	5 7 0, 5 9 0, 6 0 0, 6 1 0, 6 2 0, 6 3 0,		
	6 4 0, 6 5 0, 6 8 0, 7 1 0, 7 2 0, 7 3 0,		
	7 5 0, 7 6 0, 7 7 0, 8 0 0, 8 1 0, 8 2 0,		

```

      8 3 0,   8 4 0,   8 5 0,   8 6 0,   8 7 0,   9 1 0,
      9 2 0,   9 3 0,   9 5 0,  10 0 0,  10 1 0,  10 2 0,
     10 3 0,  10 4 0, -11 0 1, -11 1 1, -11 2 1, -10 1 1,
    -10 2 1, -10 3 1, -10 4 1,  -9 0 1,  -9 1 1,  -9 2 1,
     -9 6 1,  -8 1 1,  -8 2 1,  -8 5 1,  -7 0 1,  -7 1 1,
     -7 5 1,  -7 8 1,  -6 1 1,  -6 8 1,  -5 0 1,  -5 7 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      636 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....      3 Note
      -2 2 1,   5 3 1,   0 0 2,
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked      ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ      2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ      5 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ      2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ      5 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of      3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      2.151 Note
      Predicted wR2: Based on SigI**2  6.26 or SHELX Weight  6.26
PLAT985_ALERT_1_G The Ca-f"=      0.1533 Deviates from the B&C-Value  0.1517 Check
PLAT985_ALERT_1_G The Fe-f"=      0.4372 Deviates from the B&C-Value  0.4344 Check

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68 ALERT level A = Most likely a serious problem - resolve or explain
 9 ALERT level B = A potentially serious problem, consider carefully
51 ALERT level C = Check. Ensure it is not caused by an omission or oversight
43 ALERT level G = General information/check it is not something unexpected

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131 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 5 ALERT type 2 Indicator that the structure model may be wrong or deficient
 7 ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
 9 ALERT type 5 Informative message, check

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Datablock: 4.30_GPa

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Bond precision:   Si- O = 0.0030 A           Wavelength=0.49570

Cell:             a=9.475(3)                b=8.670(5)                c=5.195(1)
                  alpha=90                  beta=106.44(3)              gamma=90
Temperature:      293 K

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	Calculated	Reported
Volume	409.3(3)	409.3(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.452	3.465
Z	1	4
Mu (mm-1)	0.716	0.707
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,9,8
Nref	1935	586
Tmin,Tmax		0.403,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.403 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.303 Theta(max)= 24.120

R(reflections)= 0.0460(471) wR2(reflections)=
wR= 0.0628(586)

S = 2.450 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 12.89 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.560 Why?

PLAT701_ALERT_1_A Bond Calc 1.604(3), Rep 1.625(5), Dev.. 7.00 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_A Bond Calc 2.102(3), Rep 2.115(5), Dev.. 4.33 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.102(3), Rep 2.115(5), Dev.. 4.33 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond Calc 2.331(3), Rep 2.348(5), Dev.. 5.67 Sigma

	O11A	-CA2	1_555	1_565		#	9 Check
PLAT701_ALERT_1_A	Bond	Calc	2.331(3), Rep	2.348(5), Dev..			5.67 Sigma
	O11A	-NA2	1_555	1_565		#	10 Check
PLAT701_ALERT_1_A	Bond	Calc	1.604(3), Rep	1.622(5), Dev..			6.00 Sigma
	O12A	-SIB1	1_555	1_655		#	11 Check
PLAT701_ALERT_1_A	Bond	Calc	2.048(2), Rep	2.058(3), Dev..			5.00 Sigma
	O12A	-MGM1	1_555	1_555		#	12 Check
PLAT701_ALERT_1_A	Bond	Calc	2.048(2), Rep	2.058(3), Dev..			5.00 Sigma
	O12A	-FM1	1_555	1_555		#	14 Check
PLAT701_ALERT_1_A	Bond	Calc	2.367(3), Rep	2.391(5), Dev..			8.00 Sigma
	O12A	-CA21	1_555	1_555		#	19 Check
PLAT701_ALERT_1_A	Bond	Calc	2.367(3), Rep	2.391(5), Dev..			8.00 Sigma
	O12A	-NA21	1_555	1_555		#	20 Check
PLAT701_ALERT_1_A	Bond	Calc	2.341(3), Rep	2.358(4), Dev..			5.67 Sigma
	O21A	-CA2	1_555	3_656		#	26 Check
PLAT701_ALERT_1_A	Bond	Calc	2.341(3), Rep	2.358(4), Dev..			5.67 Sigma
	O21A	-NA2	1_555	3_656		#	27 Check
PLAT701_ALERT_1_A	Bond	Calc	2.005(3), Rep	2.025(5), Dev..			6.67 Sigma
	O22A	-MGM1	1_555	3_666		#	29 Check
PLAT701_ALERT_1_A	Bond	Calc	2.005(3), Rep	2.025(5), Dev..			6.67 Sigma
	O22A	-FM1	1_555	3_666		#	31 Check
PLAT701_ALERT_1_A	Bond	Calc	2.364(3), Rep	2.384(4), Dev..			6.67 Sigma
	O22A	-CA21	1_555	3_667		#	32 Check
PLAT701_ALERT_1_A	Bond	Calc	2.364(3), Rep	2.384(4), Dev..			6.67 Sigma
	O22A	-NA21	1_555	3_667		#	33 Check
PLAT701_ALERT_1_A	Bond	Calc	3.001(2), Rep	3.025(2), Dev..			12.00 Sigma
	SIA1	-CA2	1_555	3_666		#	38 Check
PLAT701_ALERT_1_A	Bond	Calc	3.001(2), Rep	3.025(2), Dev..			12.00 Sigma
	SIA1	-NA2	1_555	3_666		#	39 Check
PLAT701_ALERT_1_A	Bond	Calc	3.234(3), Rep	3.270(4), Dev..			12.00 Sigma
	SIA1	-CA21	1_555	3_666		#	40 Check
PLAT701_ALERT_1_A	Bond	Calc	3.167(3), Rep	3.198(4), Dev..			10.33 Sigma
	SIB1	-CA2	1_555	3_666		#	41 Check
PLAT701_ALERT_1_A	Bond	Calc	3.167(3), Rep	3.198(4), Dev..			10.33 Sigma
	SIB1	-NA2	1_555	3_666		#	42 Check
PLAT701_ALERT_1_A	Bond	Calc	3.025(2), Rep	3.049(2), Dev..			12.00 Sigma
	SIB1	-CA21	1_555	3_667		#	43 Check
PLAT701_ALERT_1_A	Bond	Calc	3.025(2), Rep	3.049(2), Dev..			12.00 Sigma
	SIB1	-NA21	1_555	3_667		#	44 Check
PLAT701_ALERT_1_A	Bond	Calc	3.053(2), Rep	3.086(2), Dev..			16.50 Sigma
	MGM1	-AM11	1_555	1_554		#	48 Check
PLAT701_ALERT_1_A	Bond	Calc	3.053(2), Rep	3.086(2), Dev..			16.50 Sigma
	MGM1	-AM11	1_555	1_555		#	49 Check
PLAT701_ALERT_1_A	Bond	Calc	3.053(2), Rep	3.086(2), Dev..			16.50 Sigma
	MGM1	-MM11	1_555	1_554		#	52 Check
PLAT701_ALERT_1_A	Bond	Calc	3.053(2), Rep	3.086(2), Dev..			16.50 Sigma
	MGM1	-MM11	1_555	1_555		#	53 Check
PLAT701_ALERT_1_A	Bond	Calc	3.419(3), Rep	3.436(6), Dev..			5.67 Sigma
	MGM1	-CA2	1_555	1_565		#	54 Check
PLAT701_ALERT_1_A	Bond	Calc	3.419(3), Rep	3.436(6), Dev..			5.67 Sigma
	MGM1	-NA2	1_555	1_565		#	55 Check
PLAT701_ALERT_1_A	Bond	Calc	3.187(2), Rep	3.203(2), Dev..			8.00 Sigma
	MGM1	-CA21	1_555	1_554		#	56 Check
PLAT701_ALERT_1_A	Bond	Calc	3.187(2), Rep	3.203(2), Dev..			8.00 Sigma
	MGM1	-CA21	1_555	1_555		#	57 Check
PLAT701_ALERT_1_A	Bond	Calc	3.187(2), Rep	3.203(2), Dev..			8.00 Sigma
	MGM1	-NA21	1_555	1_554		#	58 Check

PLAT701_ALERT_1_A Bond	Calc	3.187(2), Rep	3.203(2), Dev..	8.00 Sigma
MGM1	-NA21	1_555	1_555	# 59 Check
PLAT701_ALERT_1_A Bond	Calc	3.053(2), Rep	3.086(2), Dev..	16.50 Sigma
AM1	-MM11	1_555	1_554	# 71 Check
PLAT701_ALERT_1_A Bond	Calc	3.053(2), Rep	3.086(2), Dev..	16.50 Sigma
AM1	-MM11	1_555	1_555	# 72 Check
PLAT701_ALERT_1_A Bond	Calc	3.419(3), Rep	3.436(6), Dev..	5.67 Sigma
AM1	-CA2	1_555	1_565	# 73 Check
PLAT701_ALERT_1_A Bond	Calc	3.419(3), Rep	3.436(6), Dev..	5.67 Sigma
AM1	-NA2	1_555	1_565	# 74 Check
PLAT701_ALERT_1_A Bond	Calc	3.187(2), Rep	3.203(2), Dev..	8.00 Sigma
AM1	-CA21	1_555	1_554	# 75 Check
PLAT701_ALERT_1_A Bond	Calc	3.187(2), Rep	3.203(2), Dev..	8.00 Sigma
AM1	-CA21	1_555	1_555	# 76 Check
PLAT701_ALERT_1_A Bond	Calc	3.187(2), Rep	3.203(2), Dev..	8.00 Sigma
AM1	-NA21	1_555	1_554	# 77 Check
PLAT701_ALERT_1_A Bond	Calc	3.187(2), Rep	3.203(2), Dev..	8.00 Sigma
AM1	-NA21	1_555	1_555	# 78 Check
PLAT701_ALERT_1_A Bond	Calc	3.187(2), Rep	3.203(2), Dev..	8.00 Sigma
FM1	-CA21	1_555	1_554	# 79 Check
PLAT701_ALERT_1_A Bond	Calc	3.187(2), Rep	3.203(2), Dev..	8.00 Sigma
FM1	-CA21	1_555	1_555	# 80 Check
PLAT701_ALERT_1_A Bond	Calc	3.187(2), Rep	3.203(2), Dev..	8.00 Sigma
FM1	-NA21	1_555	1_554	# 81 Check
PLAT701_ALERT_1_A Bond	Calc	3.187(2), Rep	3.203(2), Dev..	8.00 Sigma
FM1	-NA21	1_555	1_555	# 82 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
AM11	-CA2	1_555	1_565	# 87 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
AM11	-CA2	1_555	1_566	# 88 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
AM11	-NA2	1_555	1_565	# 89 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
AM11	-NA2	1_555	1_566	# 90 Check
PLAT701_ALERT_1_A Bond	Calc	3.451(3), Rep	3.473(5), Dev..	7.33 Sigma
AM11	-CA21	1_555	1_555	# 91 Check
PLAT701_ALERT_1_A Bond	Calc	3.451(3), Rep	3.473(5), Dev..	7.33 Sigma
AM11	-NA21	1_555	1_555	# 92 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
MM11	-CA2	1_555	1_565	# 109 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
MM11	-CA2	1_555	1_566	# 110 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
MM11	-NA2	1_555	1_565	# 111 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
MM11	-NA2	1_555	1_566	# 112 Check
PLAT701_ALERT_1_A Bond	Calc	3.451(3), Rep	3.473(5), Dev..	7.33 Sigma
MM11	-CA21	1_555	1_555	# 113 Check
PLAT701_ALERT_1_A Bond	Calc	3.451(3), Rep	3.473(5), Dev..	7.33 Sigma
MM11	-NA21	1_555	1_555	# 114 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
FM11	-CA2	1_555	1_565	# 115 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
FM11	-CA2	1_555	1_566	# 116 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma
FM11	-NA2	1_555	1_565	# 117 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(2), Rep	3.181(3), Dev..	6.00 Sigma

FM11 -NA2 1_555 1_566 # 118 Check

Alert level B

PLAT017_ALERT_1_B Check Scattering Type Consistency of AM1 as AL Error?
 PLAT017_ALERT_1_B Check Scattering Type Consistency of FM1 as FE Error?
 PLAT017_ALERT_1_B Check Scattering Type Consistency of AM11 as AL Error?
 PLAT017_ALERT_1_B Check Scattering Type Consistency of MM11 as MG Error?
 PLAT017_ALERT_1_B Check Scattering Type Consistency of FM11 as FE Error?
 PLAT088_ALERT_3_B Poor Data / Parameter Ratio 6.23 Note
 PLAT701_ALERT_1_B Bond Calc 1.972(3), Rep 1.980(5), Dev.. 2.67 Sigma
 O12A -MM11 1_555 1_555 # 17 Check
 PLAT701_ALERT_1_B Bond Calc 1.972(3), Rep 1.980(5), Dev.. 2.67 Sigma
 O12A -FM11 1_555 1_555 # 18 Check
 PLAT701_ALERT_1_B Bond Calc 1.594(3), Rep 1.603(5), Dev.. 3.00 Sigma
 O21A -SIA1 1_555 1_545 # 21 Check
 PLAT701_ALERT_1_B Bond Calc 1.880(3), Rep 1.887(5), Dev.. 2.33 Sigma
 O21A -MM11 1_555 3_666 # 24 Check
 PLAT701_ALERT_1_B Bond Calc 1.880(3), Rep 1.887(5), Dev.. 2.33 Sigma
 O21A -FM11 1_555 3_666 # 25 Check
 PLAT701_ALERT_1_B Bond Calc 1.663(3), Rep 1.670(4), Dev.. 2.33 Sigma
 O31A -SIB1 1_555 1_554 # 35 Check

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
 outside the range 0.80 <> 2.00
 Goodness of fit given = 2.450
 PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
 Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8
 Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6
 Si2
 PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
 Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695
 (Na)
 Rep.: ?
 PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.08 Check
 PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check
 PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check
 PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check
 PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms . Please Check
 PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) O11A Check
 PLAT701_ALERT_1_C Bond Calc 1.583(3), Rep 1.588(5), Dev.. 1.67 Sigma
 O22A -SIB1 1_555 1_555 # 28 Check
 PLAT701_ALERT_1_C Bond Calc 1.655(3), Rep 1.659(4), Dev.. 1.33 Sigma
 O32A -SIA1 1_555 1_555 # 36 Check
 PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label MnM1 Check
 O11A MNM1
 PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Cm11 Check
 O11A CM11
 PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Tm11 Check
 O11A TM11
 PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label MnM1 Check
 O12A MNM1
 PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Cm11 Check
 O12A CM11
 PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Tm11 Check

	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	CA2				

PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA21		
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.74Ang From O31A	.	0.49 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.78Ang From O32A	.	0.49 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	1.03Ang From O11A	.	0.47 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	1.03Ang From O12A	.	0.44 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.65Ang From O22A	.	0.43 eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1	0.087	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11	0.052	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11	0.86	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1	0.868	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1	0.045	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11	0.088	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21	0.7904	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2	0.3622	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2	0.6378	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21	0.2096	Check
PLAT301_ALERT_3_G	Main Residue Disorder	1	20% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	2)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	3)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	4)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	5)	100% Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A	.	134.1 Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A	.	138.5 Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11	Fm11	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	1.84	Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
	0 1 0, 1 1 0,		
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L=	0.600	367 Report
	0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,		
	0 8 0, 0 9 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0,		
	1 6 0, 1 7 0, 1 8 0, 1 9 0, 2 0 0, 2 1 0,		
	2 2 0, 2 3 0, 2 4 0, 2 5 0, 2 6 0, 2 7 0,		

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      2  8  0,    2  9  0,    3  1  0,    3  4  0,    3  5  0,    3  6  0,
      3  7  0,    3  8  0,    3  9  0,    4  0  0,    4  1  0,    4  6  0,
      4  7  0,    4  8  0,    4  9  0,    5  1  0,    5  4  0,    5  7  0,
      5  9  0,    6  0  0,    6  1  0,    6  2  0,    6  3  0,    6  4  0,
      6  5  0,    6  8  0,    7  1  0,    7  2  0,    7  3  0,    7  4  0,
      7  5  0,    7  6  0,    7  7  0,    8  0  0,    8  1  0,    8  2  0,
      8  3  0,    8  4  0,    8  5  0,    8  6  0,    8  7  0,    9  1  0,
      9  2  0,    9  3  0,    9  5  0,   10  0  0,   10  1  0,   10  2  0,
     10  3  0,   10  4  0,  -11  0  1,  -11  1  1,  -11  2  1,  -10  1  1,
    -10  2  1,  -10  3  1,   -9  0  1,   -9  1  1,   -9  2  1,   -9  5  1,
    -9  6  1,   -8  1  1,   -8  2  1,   -8  5  1,   -7  0  1,   -7  1  1,
    -7  5  1,   -7  8  1,   -6  1  1,   -6  8  1,   -5  0  1,   -5  7  1,

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PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      639 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked      ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ      2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ      5 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ      2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ      5 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of      3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      2.692 Note
      Predicted wR2: Based on SigI**2 4.27 or SHELX Weight 4.27
PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value 0.1517 Check
PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value 0.4344 Check

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66 ALERT level A = Most likely a serious problem - resolve or explain
12 ALERT level B = A potentially serious problem, consider carefully
55 ALERT level C = Check. Ensure it is not caused by an omission or oversight
42 ALERT level G = General information/check it is not something unexpected

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132 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  9 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
19  ALERT type 4 Improvement, methodology, query or suggestion
  9 ALERT type 5 Informative message, check

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Datablock: 4.45_GPa

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Bond precision:   Si- O = 0.0030 A           Wavelength=0.49570

Cell:             a=9.473(3)                b=8.661(5)                c=5.191(1)
                  alpha=90                  beta=106.43(3)              gamma=90
Temperature:      293 K

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	Calculated	Reported
Volume	408.5(3)	408.5(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.459	3.472
Z	1	4
Mu (mm-1)	0.718	0.709
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,9,8
Nref	1933	580
Tmin,Tmax		0.878,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.878 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.300 Theta(max)= 24.130

R(reflections)= 0.0411(482) wR2(reflections)=
wR= 0.0588(580)

S = 2.160 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 12.26 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.560 Why?

PLAT701_ALERT_1_A Bond Calc 1.607(3), Rep 1.625(5), Dev.. 6.00 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_A Bond Calc 2.098(3), Rep 2.115(5), Dev.. 5.67 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.098(3), Rep 2.115(5), Dev.. 5.67 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond Calc 2.327(3), Rep 2.348(5), Dev.. 7.00 Sigma

	O11A	-CA2	1_555	1_565		#	9 Check
PLAT701_ALERT_1_A Bond	Calc		2.327(3), Rep	2.348(5), Dev..			7.00 Sigma
	O11A	-NA2	1_555	1_565		#	10 Check
PLAT701_ALERT_1_A Bond	Calc		1.609(3), Rep	1.622(5), Dev..			4.33 Sigma
	O12A	-SIB1	1_555	1_655		#	11 Check
PLAT701_ALERT_1_A Bond	Calc		2.046(2), Rep	2.058(3), Dev..			6.00 Sigma
	O12A	-MGM1	1_555	1_555		#	12 Check
PLAT701_ALERT_1_A Bond	Calc		2.046(2), Rep	2.058(3), Dev..			6.00 Sigma
	O12A	-FM1	1_555	1_555		#	14 Check
PLAT701_ALERT_1_A Bond	Calc		1.969(3), Rep	1.980(5), Dev..			3.67 Sigma
	O12A	-MM11	1_555	1_555		#	17 Check
PLAT701_ALERT_1_A Bond	Calc		1.969(3), Rep	1.980(5), Dev..			3.67 Sigma
	O12A	-FM11	1_555	1_555		#	18 Check
PLAT701_ALERT_1_A Bond	Calc		2.365(3), Rep	2.391(5), Dev..			8.67 Sigma
	O12A	-CA21	1_555	1_555		#	19 Check
PLAT701_ALERT_1_A Bond	Calc		2.365(3), Rep	2.391(5), Dev..			8.67 Sigma
	O12A	-NA21	1_555	1_555		#	20 Check
PLAT701_ALERT_1_A Bond	Calc		1.592(3), Rep	1.603(5), Dev..			3.67 Sigma
	O21A	-SIA1	1_555	1_545		#	21 Check
PLAT701_ALERT_1_A Bond	Calc		2.344(3), Rep	2.358(4), Dev..			4.67 Sigma
	O21A	-CA2	1_555	3_656		#	26 Check
PLAT701_ALERT_1_A Bond	Calc		2.344(3), Rep	2.358(4), Dev..			4.67 Sigma
	O21A	-NA2	1_555	3_656		#	27 Check
PLAT701_ALERT_1_A Bond	Calc		2.005(3), Rep	2.025(5), Dev..			6.67 Sigma
	O22A	-MGM1	1_555	3_666		#	29 Check
PLAT701_ALERT_1_A Bond	Calc		2.005(3), Rep	2.025(5), Dev..			6.67 Sigma
	O22A	-FM1	1_555	3_666		#	31 Check
PLAT701_ALERT_1_A Bond	Calc		2.364(3), Rep	2.384(4), Dev..			6.67 Sigma
	O22A	-CA21	1_555	3_667		#	32 Check
PLAT701_ALERT_1_A Bond	Calc		2.364(3), Rep	2.384(4), Dev..			6.67 Sigma
	O22A	-NA21	1_555	3_667		#	33 Check
PLAT701_ALERT_1_A Bond	Calc		1.660(2), Rep	1.670(4), Dev..			5.00 Sigma
	O31A	-SIB1	1_555	1_554		#	35 Check
PLAT701_ALERT_1_A Bond	Calc		3.000(2), Rep	3.025(2), Dev..			12.50 Sigma
	SIA1	-CA2	1_555	3_666		#	38 Check
PLAT701_ALERT_1_A Bond	Calc		3.000(2), Rep	3.025(2), Dev..			12.50 Sigma
	SIA1	-NA2	1_555	3_666		#	39 Check
PLAT701_ALERT_1_A Bond	Calc		3.231(2), Rep	3.270(4), Dev..			19.50 Sigma
	SIA1	-CA21	1_555	3_666		#	40 Check
PLAT701_ALERT_1_A Bond	Calc		3.165(2), Rep	3.198(4), Dev..			16.50 Sigma
	SIB1	-CA2	1_555	3_666		#	41 Check
PLAT701_ALERT_1_A Bond	Calc		3.165(2), Rep	3.198(4), Dev..			16.50 Sigma
	SIB1	-NA2	1_555	3_666		#	42 Check
PLAT701_ALERT_1_A Bond	Calc		3.022(2), Rep	3.049(2), Dev..			13.50 Sigma
	SIB1	-CA21	1_555	3_667		#	43 Check
PLAT701_ALERT_1_A Bond	Calc		3.022(2), Rep	3.049(2), Dev..			13.50 Sigma
	SIB1	-NA21	1_555	3_667		#	44 Check
PLAT701_ALERT_1_A Bond	Calc		3.052(2), Rep	3.086(2), Dev..			17.00 Sigma
	MGM1	-AM11	1_555	1_554		#	48 Check
PLAT701_ALERT_1_A Bond	Calc		3.052(2), Rep	3.086(2), Dev..			17.00 Sigma
	MGM1	-AM11	1_555	1_555		#	49 Check
PLAT701_ALERT_1_A Bond	Calc		3.052(2), Rep	3.086(2), Dev..			17.00 Sigma
	MGM1	-MM11	1_555	1_554		#	52 Check
PLAT701_ALERT_1_A Bond	Calc		3.052(2), Rep	3.086(2), Dev..			17.00 Sigma
	MGM1	-MM11	1_555	1_555		#	53 Check
PLAT701_ALERT_1_A Bond	Calc		3.415(3), Rep	3.436(6), Dev..			7.00 Sigma
	MGM1	-CA2	1_555	1_565		#	54 Check

PLAT701_ALERT_1_A Bond	Calc	3.415(3), Rep	3.436(6), Dev..	7.00 Sigma
MGM1	-NA2	1_555	1_565	# 55 Check
PLAT701_ALERT_1_A Bond	Calc	3.184(2), Rep	3.203(2), Dev..	9.50 Sigma
MGM1	-CA21	1_555	1_554	# 56 Check
PLAT701_ALERT_1_A Bond	Calc	3.184(2), Rep	3.203(2), Dev..	9.50 Sigma
MGM1	-CA21	1_555	1_555	# 57 Check
PLAT701_ALERT_1_A Bond	Calc	3.184(2), Rep	3.203(2), Dev..	9.50 Sigma
MGM1	-NA21	1_555	1_554	# 58 Check
PLAT701_ALERT_1_A Bond	Calc	3.184(2), Rep	3.203(2), Dev..	9.50 Sigma
MGM1	-NA21	1_555	1_555	# 59 Check
PLAT701_ALERT_1_A Bond	Calc	3.052(2), Rep	3.086(2), Dev..	17.00 Sigma
AM1	-MM11	1_555	1_554	# 71 Check
PLAT701_ALERT_1_A Bond	Calc	3.052(2), Rep	3.086(2), Dev..	17.00 Sigma
AM1	-MM11	1_555	1_555	# 72 Check
PLAT701_ALERT_1_A Bond	Calc	3.415(3), Rep	3.436(6), Dev..	7.00 Sigma
AM1	-CA2	1_555	1_565	# 73 Check
PLAT701_ALERT_1_A Bond	Calc	3.415(3), Rep	3.436(6), Dev..	7.00 Sigma
AM1	-NA2	1_555	1_565	# 74 Check
PLAT701_ALERT_1_A Bond	Calc	3.184(2), Rep	3.203(2), Dev..	9.50 Sigma
AM1	-CA21	1_555	1_554	# 75 Check
PLAT701_ALERT_1_A Bond	Calc	3.184(2), Rep	3.203(2), Dev..	9.50 Sigma
AM1	-CA21	1_555	1_555	# 76 Check
PLAT701_ALERT_1_A Bond	Calc	3.184(2), Rep	3.203(2), Dev..	9.50 Sigma
AM1	-NA21	1_555	1_554	# 77 Check
PLAT701_ALERT_1_A Bond	Calc	3.184(2), Rep	3.203(2), Dev..	9.50 Sigma
AM1	-NA21	1_555	1_555	# 78 Check
PLAT701_ALERT_1_A Bond	Calc	3.184(2), Rep	3.203(2), Dev..	9.50 Sigma
FM1	-CA21	1_555	1_554	# 79 Check
PLAT701_ALERT_1_A Bond	Calc	3.184(2), Rep	3.203(2), Dev..	9.50 Sigma
FM1	-CA21	1_555	1_555	# 80 Check
PLAT701_ALERT_1_A Bond	Calc	3.184(2), Rep	3.203(2), Dev..	9.50 Sigma
FM1	-NA21	1_555	1_554	# 81 Check
PLAT701_ALERT_1_A Bond	Calc	3.184(2), Rep	3.203(2), Dev..	9.50 Sigma
FM1	-NA21	1_555	1_555	# 82 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
AM11	-CA2	1_555	1_565	# 87 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
AM11	-CA2	1_555	1_566	# 88 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
AM11	-NA2	1_555	1_565	# 89 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
AM11	-NA2	1_555	1_566	# 90 Check
PLAT701_ALERT_1_A Bond	Calc	3.448(3), Rep	3.473(5), Dev..	8.33 Sigma
AM11	-CA21	1_555	1_555	# 91 Check
PLAT701_ALERT_1_A Bond	Calc	3.448(3), Rep	3.473(5), Dev..	8.33 Sigma
AM11	-NA21	1_555	1_555	# 92 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
MM11	-CA2	1_555	1_565	# 109 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
MM11	-CA2	1_555	1_566	# 110 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
MM11	-NA2	1_555	1_565	# 111 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
MM11	-NA2	1_555	1_566	# 112 Check
PLAT701_ALERT_1_A Bond	Calc	3.448(3), Rep	3.473(5), Dev..	8.33 Sigma
MM11	-CA21	1_555	1_555	# 113 Check
PLAT701_ALERT_1_A Bond	Calc	3.448(3), Rep	3.473(5), Dev..	8.33 Sigma

MM11	-NA21	1_555	1_555		#	114 Check
PLAT701_ALERT_1_A	Bond Calc	3.165(2), Rep	3.181(3), Dev..			8.00 Sigma
FM11	-CA2	1_555	1_565		#	115 Check
PLAT701_ALERT_1_A	Bond Calc	3.165(2), Rep	3.181(3), Dev..			8.00 Sigma
FM11	-CA2	1_555	1_566		#	116 Check
PLAT701_ALERT_1_A	Bond Calc	3.165(2), Rep	3.181(3), Dev..			8.00 Sigma
FM11	-NA2	1_555	1_565		#	117 Check
PLAT701_ALERT_1_A	Bond Calc	3.165(2), Rep	3.181(3), Dev..			8.00 Sigma
FM11	-NA2	1_555	1_566		#	118 Check



Alert level B

PLAT017_ALERT_1_B	Check Scattering Type Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B	Check Scattering Type Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B	Check Scattering Type Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B	Check Scattering Type Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B	Check Scattering Type Consistency of FM11	as	FE Error?
PLAT088_ALERT_3_B	Poor Data / Parameter Ratio		6.17 Note
PLAT701_ALERT_1_B	Bond Calc	1.581(3), Rep 1.588(5), Dev..	2.33 Sigma
O22A	-SIB1	1_555 1_555	# 28 Check
PLAT701_ALERT_1_B	Bond Calc	1.653(2), Rep 1.659(4), Dev..	3.00 Sigma
O32A	-SIA1	1_555 1_555	# 36 Check



Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
Goodness of fit given = 2.160

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
	Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8		
	Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2		
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula	Strings Differ	Please Check
	Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)		
	Rep.: ?		
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight Differ by ..		3.08 Check
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...		Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...		Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...		Please Check
PLAT077_ALERT_4_C	Unit Cell Contains Non-integer Number of Atoms .		Please Check
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)		O11A Check
PLAT701_ALERT_1_C	Bond Calc	1.881(3), Rep 1.887(5), Dev..	2.00 Sigma
O21A	-MM11	1_555 3_666	# 24 Check
PLAT701_ALERT_1_C	Bond Calc	1.881(3), Rep 1.887(5), Dev..	2.00 Sigma
O21A	-FM11	1_555 3_666	# 25 Check
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1 Check
O11A	MNM1		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Cm11 Check
O11A	CM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11 Check
O11A	TM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	MnM1 Check
O12A	MNM1		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Cm11 Check
O12A	CM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11 Check

	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	CA2				

PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA21		
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF		4	Note
	-2 2 1, 5 3 1, 0 0 2, 4 0 2,			

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1	0.087	Constrained at Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11	0.052	Constrained at Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11	0.86	Constrained at Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1	0.868	Constrained at Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1	0.045	Constrained at Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11	0.088	Constrained at Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21	0.7904	Constrained at Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2	0.3622	Constrained at Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2	0.6378	Constrained at Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21	0.2096	Constrained at Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A .	134.1	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A .	138.5	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11	Fm11	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.84	Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
	0 1 0, 1 1 0,		
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L=	0.600	372 Report
	0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,		
	0 8 0, 0 9 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0,		
	1 6 0, 1 7 0, 1 8 0, 1 9 0, 2 0 0, 2 1 0,		
	2 2 0, 2 3 0, 2 4 0, 2 5 0, 2 6 0, 2 7 0,		
	2 8 0, 2 9 0, 3 1 0, 3 4 0, 3 5 0, 3 6 0,		
	3 7 0, 3 8 0, 3 9 0, 4 0 0, 4 1 0, 4 6 0,		
	4 7 0, 4 8 0, 4 9 0, 5 1 0, 5 7 0, 5 8 0,		

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      5 9 0, 6 0 0, 6 1 0, 6 2 0, 6 3 0, 6 4 0,
      6 5 0, 6 8 0, 7 1 0, 7 2 0, 7 3 0, 7 5 0,
      7 6 0, 7 7 0, 8 0 0, 8 1 0, 8 2 0, 8 3 0,
      8 4 0, 8 5 0, 8 6 0, 8 7 0, 9 1 0, 9 2 0,
      9 3 0, 9 5 0, 10 0 0, 10 1 0, 10 2 0, 10 3 0,
    -10 4 0, -11 0 1, -11 1 1, -11 2 1, -10 1 1, -10 2 1,
   -10 3 1, -10 4 1, -9 0 1, -9 1 1, -9 2 1, -9 5 1,
    -9 6 1, -8 1 1, -8 2 1, -8 5 1, -7 0 1, -7 1 1,
    -7 5 1, -7 8 1, -6 1 1, -6 8 1, -5 0 1, -5 1 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 642 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 5 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ 2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 5 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of 3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.280 Note
      Predicted wR2: Based on SigI**2 4.70 or SHELX Weight 4.70
PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value 0.1517 Check
PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value 0.4344 Check

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70 ALERT level A = Most likely a serious problem - resolve or explain
8  ALERT level B = A potentially serious problem, consider carefully
51 ALERT level C = Check. Ensure it is not caused by an omission or oversight
42 ALERT level G = General information/check it is not something unexpected

132 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4  ALERT type 2 Indicator that the structure model may be wrong or deficient
7  ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
9  ALERT type 5 Informative message, check

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Datablock: 4.86_GPa

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Bond precision:  Si- O = 0.0030 A           Wavelength=0.49570

Cell:            a=9.462(3)          b=8.649(5)          c=5.186(1)
                  alpha=90           beta=106.39(3)       gamma=90
Temperature:     293 K

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	Calculated	Reported
Volume	407.2(3)	407.2(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.470	3.483
Z	1	4
Mu (mm-1)	0.720	0.711
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,8,8
Nref	1931	582
Tmin,Tmax		0.541,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.541 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.301 Theta(max)= 24.150

R(reflections)= 0.0421(469) wR2(reflections)=
wR= 0.0613(582)

S = 2.290 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 12.27 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.560 Why?

PLAT701_ALERT_1_A Bond Calc 1.605(3), Rep 1.625(5), Dev.. 6.67 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_A Bond Calc 2.094(3), Rep 2.115(5), Dev.. 7.00 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.094(3), Rep 2.115(5), Dev.. 7.00 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond Calc 2.329(3), Rep 2.348(5), Dev.. 6.33 Sigma

	O11A	-CA2	1_555	1_565		#	9 Check
PLAT701_ALERT_1_A Bond	Calc		2.329(3), Rep	2.348(5), Dev..			6.33 Sigma
	O11A	-NA2	1_555	1_565		#	10 Check
PLAT701_ALERT_1_A Bond	Calc		1.605(3), Rep	1.622(5), Dev..			5.67 Sigma
	O12A	-SIB1	1_555	1_655		#	11 Check
PLAT701_ALERT_1_A Bond	Calc		2.045(2), Rep	2.058(3), Dev..			6.50 Sigma
	O12A	-MGM1	1_555	1_555		#	12 Check
PLAT701_ALERT_1_A Bond	Calc		2.045(2), Rep	2.058(3), Dev..			6.50 Sigma
	O12A	-FM1	1_555	1_555		#	14 Check
PLAT701_ALERT_1_A Bond	Calc		1.964(3), Rep	1.980(5), Dev..			5.33 Sigma
	O12A	-MM11	1_555	1_555		#	17 Check
PLAT701_ALERT_1_A Bond	Calc		1.964(3), Rep	1.980(5), Dev..			5.33 Sigma
	O12A	-FM11	1_555	1_555		#	18 Check
PLAT701_ALERT_1_A Bond	Calc		2.365(3), Rep	2.391(5), Dev..			8.67 Sigma
	O12A	-CA21	1_555	1_555		#	19 Check
PLAT701_ALERT_1_A Bond	Calc		2.365(3), Rep	2.391(5), Dev..			8.67 Sigma
	O12A	-NA21	1_555	1_555		#	20 Check
PLAT701_ALERT_1_A Bond	Calc		1.593(3), Rep	1.603(5), Dev..			3.33 Sigma
	O21A	-SIA1	1_555	1_545		#	21 Check
PLAT701_ALERT_1_A Bond	Calc		2.334(3), Rep	2.358(4), Dev..			8.00 Sigma
	O21A	-CA2	1_555	3_656		#	26 Check
PLAT701_ALERT_1_A Bond	Calc		2.334(3), Rep	2.358(4), Dev..			8.00 Sigma
	O21A	-NA2	1_555	3_656		#	27 Check
PLAT701_ALERT_1_A Bond	Calc		2.000(3), Rep	2.025(5), Dev..			8.33 Sigma
	O22A	-MGM1	1_555	3_666		#	29 Check
PLAT701_ALERT_1_A Bond	Calc		2.000(3), Rep	2.025(5), Dev..			8.33 Sigma
	O22A	-FM1	1_555	3_666		#	31 Check
PLAT701_ALERT_1_A Bond	Calc		2.357(3), Rep	2.384(4), Dev..			9.00 Sigma
	O22A	-CA21	1_555	3_667		#	32 Check
PLAT701_ALERT_1_A Bond	Calc		2.357(3), Rep	2.384(4), Dev..			9.00 Sigma
	O22A	-NA21	1_555	3_667		#	33 Check
PLAT701_ALERT_1_A Bond	Calc		2.997(2), Rep	3.025(2), Dev..			14.00 Sigma
	SIA1	-CA2	1_555	3_666		#	38 Check
PLAT701_ALERT_1_A Bond	Calc		2.997(2), Rep	3.025(2), Dev..			14.00 Sigma
	SIA1	-NA2	1_555	3_666		#	39 Check
PLAT701_ALERT_1_A Bond	Calc		3.225(2), Rep	3.270(4), Dev..			22.50 Sigma
	SIA1	-CA21	1_555	3_666		#	40 Check
PLAT701_ALERT_1_A Bond	Calc		3.158(3), Rep	3.198(4), Dev..			13.33 Sigma
	SIB1	-CA2	1_555	3_666		#	41 Check
PLAT701_ALERT_1_A Bond	Calc		3.158(3), Rep	3.198(4), Dev..			13.33 Sigma
	SIB1	-NA2	1_555	3_666		#	42 Check
PLAT701_ALERT_1_A Bond	Calc		3.020(2), Rep	3.049(2), Dev..			14.50 Sigma
	SIB1	-CA21	1_555	3_667		#	43 Check
PLAT701_ALERT_1_A Bond	Calc		3.020(2), Rep	3.049(2), Dev..			14.50 Sigma
	SIB1	-NA21	1_555	3_667		#	44 Check
PLAT701_ALERT_1_A Bond	Calc		3.046(2), Rep	3.086(2), Dev..			20.00 Sigma
	MGM1	-AM11	1_555	1_554		#	48 Check
PLAT701_ALERT_1_A Bond	Calc		3.046(2), Rep	3.086(2), Dev..			20.00 Sigma
	MGM1	-AM11	1_555	1_555		#	49 Check
PLAT701_ALERT_1_A Bond	Calc		3.046(2), Rep	3.086(2), Dev..			20.00 Sigma
	MGM1	-MM11	1_555	1_554		#	52 Check
PLAT701_ALERT_1_A Bond	Calc		3.046(2), Rep	3.086(2), Dev..			20.00 Sigma
	MGM1	-MM11	1_555	1_555		#	53 Check
PLAT701_ALERT_1_A Bond	Calc		3.412(3), Rep	3.436(6), Dev..			8.00 Sigma
	MGM1	-CA2	1_555	1_565		#	54 Check
PLAT701_ALERT_1_A Bond	Calc		3.412(3), Rep	3.436(6), Dev..			8.00 Sigma
	MGM1	-NA2	1_555	1_565		#	55 Check

PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
MGM1	-CA21	1_555	1_554	# 56 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
MGM1	-CA21	1_555	1_555	# 57 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
MGM1	-NA21	1_555	1_554	# 58 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
MGM1	-NA21	1_555	1_555	# 59 Check
PLAT701_ALERT_1_A Bond	Calc	3.046(2), Rep	3.086(2), Dev..	20.00 Sigma
AM1	-MM11	1_555	1_554	# 71 Check
PLAT701_ALERT_1_A Bond	Calc	3.046(2), Rep	3.086(2), Dev..	20.00 Sigma
AM1	-MM11	1_555	1_555	# 72 Check
PLAT701_ALERT_1_A Bond	Calc	3.412(3), Rep	3.436(6), Dev..	8.00 Sigma
AM1	-CA2	1_555	1_565	# 73 Check
PLAT701_ALERT_1_A Bond	Calc	3.412(3), Rep	3.436(6), Dev..	8.00 Sigma
AM1	-NA2	1_555	1_565	# 74 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
AM1	-CA21	1_555	1_554	# 75 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
AM1	-CA21	1_555	1_555	# 76 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
AM1	-NA21	1_555	1_554	# 77 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
AM1	-NA21	1_555	1_555	# 78 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
FM1	-CA21	1_555	1_554	# 79 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
FM1	-CA21	1_555	1_555	# 80 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
FM1	-NA21	1_555	1_554	# 81 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
FM1	-NA21	1_555	1_555	# 82 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
AM11	-CA2	1_555	1_565	# 87 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
AM11	-CA2	1_555	1_566	# 88 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
AM11	-NA2	1_555	1_565	# 89 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
AM11	-NA2	1_555	1_566	# 90 Check
PLAT701_ALERT_1_A Bond	Calc	3.444(3), Rep	3.473(5), Dev..	9.67 Sigma
AM11	-CA21	1_555	1_555	# 91 Check
PLAT701_ALERT_1_A Bond	Calc	3.444(3), Rep	3.473(5), Dev..	9.67 Sigma
AM11	-NA21	1_555	1_555	# 92 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
MM11	-CA2	1_555	1_565	# 109 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
MM11	-CA2	1_555	1_566	# 110 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
MM11	-NA2	1_555	1_565	# 111 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma
MM11	-NA2	1_555	1_566	# 112 Check
PLAT701_ALERT_1_A Bond	Calc	3.444(3), Rep	3.473(5), Dev..	9.67 Sigma
MM11	-CA21	1_555	1_555	# 113 Check
PLAT701_ALERT_1_A Bond	Calc	3.444(3), Rep	3.473(5), Dev..	9.67 Sigma
MM11	-NA21	1_555	1_555	# 114 Check
PLAT701_ALERT_1_A Bond	Calc	3.165(2), Rep	3.181(3), Dev..	8.00 Sigma

	FM11	-CA2		1_555	1_565		#	115	Check
PLAT701_ALERT_1_A	Bond	Calc	3.165(2),	Rep	3.181(3),	Dev..			8.00 Sigma
	FM11	-CA2		1_555	1_566		#	116	Check
PLAT701_ALERT_1_A	Bond	Calc	3.165(2),	Rep	3.181(3),	Dev..			8.00 Sigma
	FM11	-NA2		1_555	1_565		#	117	Check
PLAT701_ALERT_1_A	Bond	Calc	3.165(2),	Rep	3.181(3),	Dev..			8.00 Sigma
	FM11	-NA2		1_555	1_566		#	118	Check

● Alert level B

PLAT017_ALERT_1_B	Check	Scattering Type	Consistency of AM1	as		AL Error?	
PLAT017_ALERT_1_B	Check	Scattering Type	Consistency of FM1	as		FE Error?	
PLAT017_ALERT_1_B	Check	Scattering Type	Consistency of AM11	as		AL Error?	
PLAT017_ALERT_1_B	Check	Scattering Type	Consistency of MM11	as		MG Error?	
PLAT017_ALERT_1_B	Check	Scattering Type	Consistency of FM11	as		FE Error?	
PLAT088_ALERT_3_B	Poor	Data / Parameter Ratio				6.19 Note	
PLAT701_ALERT_1_B	Bond	Calc	1.878(3),	Rep	1.887(5),	Dev..	
	O21A	-MM11		1_555	3_666		#
PLAT701_ALERT_1_B	Bond	Calc	1.878(3),	Rep	1.887(5),	Dev..	
	O21A	-FM11		1_555	3_666		#
PLAT701_ALERT_1_B	Bond	Calc	1.662(3),	Rep	1.670(4),	Dev..	
	O31A	-SIB1		1_555	1_554		#
PLAT701_ALERT_1_B	Bond	Calc	1.654(2),	Rep	1.659(4),	Dev..	
	O32A	-SIA1		1_555	1_555		#

● Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
Goodness of fit given = 2.290

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8
Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)
Rep.: ?

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.08 Check

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms . Please Check

PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) 011A Check

PLAT701_ALERT_1_C Bond Calc 1.928(2), Rep 1.931(3), Dev.. 1.50 Sigma

O11A -MM11 1_555 1_554 # 7 Check

PLAT701_ALERT_1_C Bond Calc 1.928(2), Rep 1.931(3), Dev.. 1.50 Sigma

O11A -FM11 1_555 1_554 # 8 Check

PLAT701_ALERT_1_C Bond Calc 1.584(3), Rep 1.588(5), Dev.. 1.33 Sigma

O22A -SIB1 1_555 1_555 # 28 Check

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label MnM1 Check

O11A MNM1

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Cm11 Check

O11A CM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Tm11 Check

O11A TM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label MnM1 Check

	O12A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	O12A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	MM11				

PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	FM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA21		
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.74Ang From O31A .	0.48	eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please	Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please	Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1 Constrained at	0.087	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11 Constrained at	0.052	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11 Constrained at	0.86	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1 Constrained at	0.868	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1 Constrained at	0.045	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11 Constrained at	0.088	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21 Constrained at	0.7904	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2 Constrained at	0.3622	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2 Constrained at	0.6378	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21 Constrained at	0.2096	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A .	133.8	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A .	138.2	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11	Fm11	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.84	Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
	0 1 0, 1 1 0,		
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L= 0.600	340	Report
	0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,		
	0 8 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0, 1 6 0,		
	1 7 0, 1 8 0, 2 0 0, 2 1 0, 2 2 0, 2 3 0,		
	2 4 0, 2 5 0, 2 6 0, 2 7 0, 2 8 0, 3 1 0,		

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      3  4  0,    3  5  0,    3  6  0,    3  7  0,    3  8  0,    4  0  0,
      4  1  0,    4  6  0,    4  7  0,    4  8  0,    5  1  0,    5  7  0,
      5  8  0,    6  0  0,    6  1  0,    6  2  0,    6  3  0,    6  4  0,
      6  5  0,    6  8  0,    7  1  0,    7  2  0,    7  3  0,    7  5  0,
      7  6  0,    7  7  0,    8  0  0,    8  1  0,    8  2  0,    8  3  0,
      8  4  0,    8  5  0,    8  6  0,    8  7  0,    9  1  0,    9  2  0,
      9  3  0,    9  4  0,    9  5  0,   10  0  0,   10  1  0,   10  2  0,
     10  3  0,   10  4  0,  -11  0  1,  -11  1  1,  -11  2  1,  -10  1  1,
    -10  2  1,  -10  3  1,   -9  0  1,   -9  1  1,   -9  2  1,   -9  4  1,
    -9  5  1,   -9  6  1,   -8  1  1,   -8  2  1,   -8  7  1,   -7  0  1,
    -7  1  1,   -7  5  1,   -7  8  1,   -6  1  1,   -6  8  1,   -5  0  1,
    -5  1  1,   -5  7  1,   -5  8  1,   -4  5  1,   -4  6  1,   -4  7  1,

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PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      547 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked      ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ      2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ      6 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ      2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ      6 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of      3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      2.383 Note
      Predicted wR2: Based on SigI**2 4.58 or SHELX Weight 4.58
PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value 0.1517 Check
PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value 0.4344 Check

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69 ALERT level A = Most likely a serious problem - resolve or explain
10 ALERT level B = A potentially serious problem, consider carefully
52 ALERT level C = Check. Ensure it is not caused by an omission or oversight
42 ALERT level G = General information/check it is not something unexpected

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134 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  5 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
19  ALERT type 4 Improvement, methodology, query or suggestion
  9 ALERT type 5 Informative message, check

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Datablock: 5.18_GPa

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Bond precision:   Si- O = 0.0030 A           Wavelength=0.49570

Cell:             a=9.458(3)           b=8.642(5)           c=5.185(1)
                  alpha=90             beta=106.35(3)        gamma=90
Temperature:      293 K

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	Calculated	Reported
Volume	406.7(3)	406.7(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.474	3.488
Z	1	4
Mu (mm-1)	0.721	0.712
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,8,8
Nref	1933	888
Tmin,Tmax		0.693,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.693 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.459 Theta(max)= 24.170

R(reflections)= 0.0555(676) wR2(reflections)=
wR= 0.0692(888)

S = 1.570 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 13.21 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.550 Why?

PLAT701_ALERT_1_A Bond Calc 1.607(3), Rep 1.625(5), Dev.. 6.00 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_A Bond Calc 2.093(3), Rep 2.115(5), Dev.. 7.33 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.093(3), Rep 2.115(5), Dev.. 7.33 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond Calc 2.324(3), Rep 2.348(5), Dev.. 8.00 Sigma

	O11A	-CA2	1_555	1_565		#	9 Check
PLAT701_ALERT_1_A Bond	Calc	2.324(3), Rep	2.348(5), Dev..				8.00 Sigma
	O11A	-NA2	1_555	1_565		#	10 Check
PLAT701_ALERT_1_A Bond	Calc	1.608(3), Rep	1.622(5), Dev..				4.67 Sigma
	O12A	-SIB1	1_555	1_655		#	11 Check
PLAT701_ALERT_1_A Bond	Calc	2.045(2), Rep	2.058(3), Dev..				6.50 Sigma
	O12A	-MGM1	1_555	1_555		#	12 Check
PLAT701_ALERT_1_A Bond	Calc	2.045(2), Rep	2.058(3), Dev..				6.50 Sigma
	O12A	-FM1	1_555	1_555		#	14 Check
PLAT701_ALERT_1_A Bond	Calc	1.964(3), Rep	1.980(5), Dev..				5.33 Sigma
	O12A	-MM11	1_555	1_555		#	17 Check
PLAT701_ALERT_1_A Bond	Calc	1.964(3), Rep	1.980(5), Dev..				5.33 Sigma
	O12A	-FM11	1_555	1_555		#	18 Check
PLAT701_ALERT_1_A Bond	Calc	2.359(3), Rep	2.391(5), Dev..				10.67 Sigma
	O12A	-CA21	1_555	1_555		#	19 Check
PLAT701_ALERT_1_A Bond	Calc	2.359(3), Rep	2.391(5), Dev..				10.67 Sigma
	O12A	-NA21	1_555	1_555		#	20 Check
PLAT701_ALERT_1_A Bond	Calc	1.591(3), Rep	1.603(5), Dev..				4.00 Sigma
	O21A	-SIA1	1_555	1_545		#	21 Check
PLAT701_ALERT_1_A Bond	Calc	1.876(3), Rep	1.887(5), Dev..				3.67 Sigma
	O21A	-MM11	1_555	3_666		#	24 Check
PLAT701_ALERT_1_A Bond	Calc	1.876(3), Rep	1.887(5), Dev..				3.67 Sigma
	O21A	-FM11	1_555	3_666		#	25 Check
PLAT701_ALERT_1_A Bond	Calc	2.339(2), Rep	2.358(4), Dev..				9.50 Sigma
	O21A	-CA2	1_555	3_656		#	26 Check
PLAT701_ALERT_1_A Bond	Calc	2.339(2), Rep	2.358(4), Dev..				9.50 Sigma
	O21A	-NA2	1_555	3_656		#	27 Check
PLAT701_ALERT_1_A Bond	Calc	1.999(3), Rep	2.025(5), Dev..				8.67 Sigma
	O22A	-MGM1	1_555	3_666		#	29 Check
PLAT701_ALERT_1_A Bond	Calc	1.999(3), Rep	2.025(5), Dev..				8.67 Sigma
	O22A	-FM1	1_555	3_666		#	31 Check
PLAT701_ALERT_1_A Bond	Calc	2.363(2), Rep	2.384(4), Dev..				10.50 Sigma
	O22A	-CA21	1_555	3_667		#	32 Check
PLAT701_ALERT_1_A Bond	Calc	2.363(2), Rep	2.384(4), Dev..				10.50 Sigma
	O22A	-NA21	1_555	3_667		#	33 Check
PLAT701_ALERT_1_A Bond	Calc	1.661(2), Rep	1.670(4), Dev..				4.50 Sigma
	O31A	-SIB1	1_555	1_554		#	35 Check
PLAT701_ALERT_1_A Bond	Calc	1.651(2), Rep	1.659(4), Dev..				4.00 Sigma
	O32A	-SIA1	1_555	1_555		#	36 Check
PLAT701_ALERT_1_A Bond	Calc	2.9967(19), Rep	3.025(2), Dev..				14.89 Sigma
	SIA1	-CA2	1_555	3_666		#	38 Check
PLAT701_ALERT_1_A Bond	Calc	2.9967(19), Rep	3.025(2), Dev..				14.89 Sigma
	SIA1	-NA2	1_555	3_666		#	39 Check
PLAT701_ALERT_1_A Bond	Calc	3.223(2), Rep	3.270(4), Dev..				23.50 Sigma
	SIA1	-CA21	1_555	3_666		#	40 Check
PLAT701_ALERT_1_A Bond	Calc	3.156(2), Rep	3.198(4), Dev..				21.00 Sigma
	SIB1	-CA2	1_555	3_666		#	41 Check
PLAT701_ALERT_1_A Bond	Calc	3.156(2), Rep	3.198(4), Dev..				21.00 Sigma
	SIB1	-NA2	1_555	3_666		#	42 Check
PLAT701_ALERT_1_A Bond	Calc	3.0198(19), Rep	3.049(2), Dev..				15.37 Sigma
	SIB1	-CA21	1_555	3_667		#	43 Check
PLAT701_ALERT_1_A Bond	Calc	3.0198(19), Rep	3.049(2), Dev..				15.37 Sigma
	SIB1	-NA21	1_555	3_667		#	44 Check
PLAT701_ALERT_1_A Bond	Calc	3.045(2), Rep	3.086(2), Dev..				20.50 Sigma
	MGM1	-AM11	1_555	1_554		#	48 Check
PLAT701_ALERT_1_A Bond	Calc	3.045(2), Rep	3.086(2), Dev..				20.50 Sigma
	MGM1	-AM11	1_555	1_555		#	49 Check

PLAT701_ALERT_1_A Bond	Calc	3.045(2), Rep	3.086(2), Dev..	20.50 Sigma
MGM1	-MM11	1_555	1_554	# 52 Check
PLAT701_ALERT_1_A Bond	Calc	3.045(2), Rep	3.086(2), Dev..	20.50 Sigma
MGM1	-MM11	1_555	1_555	# 53 Check
PLAT701_ALERT_1_A Bond	Calc	3.411(3), Rep	3.436(6), Dev..	8.33 Sigma
MGM1	-CA2	1_555	1_565	# 54 Check
PLAT701_ALERT_1_A Bond	Calc	3.411(3), Rep	3.436(6), Dev..	8.33 Sigma
MGM1	-NA2	1_555	1_565	# 55 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
MGM1	-CA21	1_555	1_554	# 56 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
MGM1	-CA21	1_555	1_555	# 57 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
MGM1	-NA21	1_555	1_554	# 58 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
MGM1	-NA21	1_555	1_555	# 59 Check
PLAT701_ALERT_1_A Bond	Calc	3.045(2), Rep	3.086(2), Dev..	20.50 Sigma
AM1	-MM11	1_555	1_554	# 71 Check
PLAT701_ALERT_1_A Bond	Calc	3.045(2), Rep	3.086(2), Dev..	20.50 Sigma
AM1	-MM11	1_555	1_555	# 72 Check
PLAT701_ALERT_1_A Bond	Calc	3.411(3), Rep	3.436(6), Dev..	8.33 Sigma
AM1	-CA2	1_555	1_565	# 73 Check
PLAT701_ALERT_1_A Bond	Calc	3.411(3), Rep	3.436(6), Dev..	8.33 Sigma
AM1	-NA2	1_555	1_565	# 74 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
AM1	-CA21	1_555	1_554	# 75 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
AM1	-CA21	1_555	1_555	# 76 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
AM1	-NA21	1_555	1_554	# 77 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
AM1	-NA21	1_555	1_555	# 78 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
FM1	-CA21	1_555	1_554	# 79 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
FM1	-CA21	1_555	1_555	# 80 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
FM1	-NA21	1_555	1_554	# 81 Check
PLAT701_ALERT_1_A Bond	Calc	3.183(2), Rep	3.203(2), Dev..	10.00 Sigma
FM1	-NA21	1_555	1_555	# 82 Check
PLAT701_ALERT_1_A Bond	Calc	3.164(2), Rep	3.181(3), Dev..	8.50 Sigma
AM11	-CA2	1_555	1_565	# 87 Check
PLAT701_ALERT_1_A Bond	Calc	3.164(2), Rep	3.181(3), Dev..	8.50 Sigma
AM11	-CA2	1_555	1_566	# 88 Check
PLAT701_ALERT_1_A Bond	Calc	3.164(2), Rep	3.181(3), Dev..	8.50 Sigma
AM11	-NA2	1_555	1_565	# 89 Check
PLAT701_ALERT_1_A Bond	Calc	3.164(2), Rep	3.181(3), Dev..	8.50 Sigma
AM11	-NA2	1_555	1_566	# 90 Check
PLAT701_ALERT_1_A Bond	Calc	3.444(3), Rep	3.473(5), Dev..	9.67 Sigma
AM11	-CA21	1_555	1_555	# 91 Check
PLAT701_ALERT_1_A Bond	Calc	3.444(3), Rep	3.473(5), Dev..	9.67 Sigma
AM11	-NA21	1_555	1_555	# 92 Check
PLAT701_ALERT_1_A Bond	Calc	3.164(2), Rep	3.181(3), Dev..	8.50 Sigma
MM11	-CA2	1_555	1_565	# 109 Check
PLAT701_ALERT_1_A Bond	Calc	3.164(2), Rep	3.181(3), Dev..	8.50 Sigma
MM11	-CA2	1_555	1_566	# 110 Check
PLAT701_ALERT_1_A Bond	Calc	3.164(2), Rep	3.181(3), Dev..	8.50 Sigma

MM11	-NA2	1_555	1_565		#	111 Check
PLAT701_ALERT_1_A Bond	Calc	3.164(2), Rep	3.181(3), Dev..			8.50 Sigma
MM11	-NA2	1_555	1_566		#	112 Check
PLAT701_ALERT_1_A Bond	Calc	3.444(3), Rep	3.473(5), Dev..			9.67 Sigma
MM11	-CA21	1_555	1_555		#	113 Check
PLAT701_ALERT_1_A Bond	Calc	3.444(3), Rep	3.473(5), Dev..			9.67 Sigma
MM11	-NA21	1_555	1_555		#	114 Check
PLAT701_ALERT_1_A Bond	Calc	3.164(2), Rep	3.181(3), Dev..			8.50 Sigma
FM11	-CA2	1_555	1_565		#	115 Check
PLAT701_ALERT_1_A Bond	Calc	3.164(2), Rep	3.181(3), Dev..			8.50 Sigma
FM11	-CA2	1_555	1_566		#	116 Check
PLAT701_ALERT_1_A Bond	Calc	3.164(2), Rep	3.181(3), Dev..			8.50 Sigma
FM11	-NA2	1_555	1_565		#	117 Check
PLAT701_ALERT_1_A Bond	Calc	3.164(2), Rep	3.181(3), Dev..			8.50 Sigma
FM11	-NA2	1_555	1_566		#	118 Check

Alert level B

PLAT017_ALERT_1_B Check	Scattering Type Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of FM11	as	FE Error?
PLAT088_ALERT_3_B Poor Data / Parameter Ratio			6.20 Note
PLAT701_ALERT_1_B Bond	Calc 1.581(3), Rep 1.588(5), Dev..		2.33 Sigma
O22A	-SIB1 1_555 1_555		# 28 Check

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula	Strings Differ	Please Check
Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8		
Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2		
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula	Strings Differ	Please Check
Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)		
Rep.: ?		
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..	3.08 Check	
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...	Please Check	
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...	Please Check	
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...	Please Check	
PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms .	Please Check	
PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare)	O11A Check	
PLAT701_ALERT_1_C Bond	Calc 1.928(2), Rep 1.931(3), Dev..	1.50 Sigma
O11A -MM11 1_555 1_554		# 7 Check
PLAT701_ALERT_1_C Bond	Calc 1.928(2), Rep 1.931(3), Dev..	1.50 Sigma
O11A -FM11 1_555 1_554		# 8 Check
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	MnM1 Check
O11A MNM1		
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	Cm11 Check
O11A CM11		
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	Tm11 Check
O11A TM11		
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	MnM1 Check
O12A MNM1		
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	Cm11 Check
O12A CM11		

PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	TM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	TM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check

	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA21		
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF			4 Note
	-2 2 1, 5 3 1, 0 0 2, 4 0 2,			
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.75Ang From O22A .			0.63 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.87Ang From O12A .			0.61 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.04Ang From O11A .			0.60 eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		3 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		0.250 Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka		0.49570 Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)		293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)		293 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1 Constrained at		0.087 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11 Constrained at		0.052 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11 Constrained at		0.86 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1 Constrained at		0.868 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1 Constrained at		0.045 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11 Constrained at		0.088 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21 Constrained at		0.7904 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2 Constrained at		0.3622 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2 Constrained at		0.6378 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21 Constrained at		0.2096 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		20% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)		100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)		100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)		100% Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A .		133.8 Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A .		138.3 Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		8 Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11	Fm11	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .		1.84 Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2 Note
	0 1 0, 1 1 0,		
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L= 0.600		339 Report
	0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,		
	0 8 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0, 1 6 0,		
	1 7 0, 1 8 0, 2 0 0, 2 1 0, 2 2 0, 2 3 0,		

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2 4 0, 2 5 0, 2 6 0, 2 7 0, 2 8 0, 3 1 0,
3 4 0, 3 5 0, 3 6 0, 3 7 0, 3 8 0, 4 0 0,
4 1 0, 4 6 0, 4 7 0, 4 8 0, 5 1 0, 5 7 0,
6 0 0, 6 1 0, 6 2 0, 6 3 0, 6 4 0, 6 5 0,
6 8 0, 7 1 0, 7 2 0, 7 3 0, 7 5 0, 7 6 0,
7 7 0, 8 0 0, 8 1 0, 8 2 0, 8 3 0, 8 4 0,
8 5 0, 8 6 0, 8 7 0, 9 1 0, 9 2 0, 9 3 0,
9 4 0, 9 5 0, 10 0 0, 10 1 0, 10 2 0, 10 3 0,
10 4 0, -11 0 1, -11 1 1, -11 2 1, -10 1 1, -10 2 1,
-10 3 1, -10 4 1, -9 0 1, -9 1 1, -9 2 1, -9 4 1,
-9 6 1, -8 1 1, -8 2 1, -8 7 1, -7 0 1, -7 1 1,
-7 5 1, -7 8 1, -6 1 1, -6 8 1, -5 0 1, -5 1 1,
-5 7 1, -5 8 1, -4 5 1, -4 6 1, -4 7 1, -4 8 1,

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PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 548 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 6 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ 2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 6 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of 3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 1.551 Note
      Predicted wR2: Based on SigI**2 8.24 or SHELX Weight 8.24
PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value 0.1517 Check
PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value 0.4344 Check

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73 ALERT level A = Most likely a serious problem - resolve or explain
7  ALERT level B = A potentially serious problem, consider carefully
53 ALERT level C = Check. Ensure it is not caused by an omission or oversight
42 ALERT level G = General information/check it is not something unexpected

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134 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
9 ALERT type 5 Informative message, check

```

Datablock: 5.72_GPa

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Bond precision:  Si- O = 0.0040 A          Wavelength=0.49570

Cell:            a=9.449(3)          b=8.635(5)          c=5.178(1)
                  alpha=90           beta=106.31(3)       gamma=90
Temperature:     293 K

```

	Calculated	Reported
Volume	405.5(3)	405.5(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.485	3.498
Z	1	4
Mu (mm-1)	0.723	0.714
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,8,8
Nref	1933	581
Tmin,Tmax		0.598,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.598 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.301 Theta(max)= 24.190

R(reflections)= 0.0384(412) wR2(reflections)=
wR= 0.0544(581)

S = 2.310 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 13.36 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.560 Why?

PLAT701_ALERT_1_A Bond Calc 1.600(4), Rep 1.625(5), Dev.. 6.25 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_A Bond Calc 2.089(4), Rep 2.115(5), Dev.. 6.50 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.089(4), Rep 2.115(5), Dev.. 6.50 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond Calc 2.324(4), Rep 2.348(5), Dev.. 6.00 Sigma

	O11A	-CA2	1_555	1_565		#	9 Check
PLAT701_ALERT_1_A Bond	Calc	2.324(4), Rep	2.348(5), Dev..				6.00 Sigma
	O11A	-NA2	1_555	1_565		#	10 Check
PLAT701_ALERT_1_A Bond	Calc	1.601(3), Rep	1.622(5), Dev..				7.00 Sigma
	O12A	-SIB1	1_555	1_655		#	11 Check
PLAT701_ALERT_1_A Bond	Calc	2.045(3), Rep	2.058(3), Dev..				4.33 Sigma
	O12A	-MGM1	1_555	1_555		#	12 Check
PLAT701_ALERT_1_A Bond	Calc	2.045(3), Rep	2.058(3), Dev..				4.33 Sigma
	O12A	-FM1	1_555	1_555		#	14 Check
PLAT701_ALERT_1_A Bond	Calc	1.964(4), Rep	1.980(5), Dev..				4.00 Sigma
	O12A	-MM11	1_555	1_555		#	17 Check
PLAT701_ALERT_1_A Bond	Calc	1.964(4), Rep	1.980(5), Dev..				4.00 Sigma
	O12A	-FM11	1_555	1_555		#	18 Check
PLAT701_ALERT_1_A Bond	Calc	2.359(4), Rep	2.391(5), Dev..				8.00 Sigma
	O12A	-CA21	1_555	1_555		#	19 Check
PLAT701_ALERT_1_A Bond	Calc	2.359(4), Rep	2.391(5), Dev..				8.00 Sigma
	O12A	-NA21	1_555	1_555		#	20 Check
PLAT701_ALERT_1_A Bond	Calc	1.590(4), Rep	1.603(5), Dev..				3.25 Sigma
	O21A	-SIA1	1_555	1_545		#	21 Check
PLAT701_ALERT_1_A Bond	Calc	2.332(3), Rep	2.358(4), Dev..				8.67 Sigma
	O21A	-CA2	1_555	3_656		#	26 Check
PLAT701_ALERT_1_A Bond	Calc	2.332(3), Rep	2.358(4), Dev..				8.67 Sigma
	O21A	-NA2	1_555	3_656		#	27 Check
PLAT701_ALERT_1_A Bond	Calc	2.002(4), Rep	2.025(5), Dev..				5.75 Sigma
	O22A	-MGM1	1_555	3_666		#	29 Check
PLAT701_ALERT_1_A Bond	Calc	2.002(4), Rep	2.025(5), Dev..				5.75 Sigma
	O22A	-FM1	1_555	3_666		#	31 Check
PLAT701_ALERT_1_A Bond	Calc	2.354(3), Rep	2.384(4), Dev..				10.00 Sigma
	O22A	-CA21	1_555	3_667		#	32 Check
PLAT701_ALERT_1_A Bond	Calc	2.354(3), Rep	2.384(4), Dev..				10.00 Sigma
	O22A	-NA21	1_555	3_667		#	33 Check
PLAT701_ALERT_1_A Bond	Calc	2.995(2), Rep	3.025(2), Dev..				15.00 Sigma
	SIA1	-CA2	1_555	3_666		#	38 Check
PLAT701_ALERT_1_A Bond	Calc	2.995(2), Rep	3.025(2), Dev..				15.00 Sigma
	SIA1	-NA2	1_555	3_666		#	39 Check
PLAT701_ALERT_1_A Bond	Calc	3.218(3), Rep	3.270(4), Dev..				17.33 Sigma
	SIA1	-CA21	1_555	3_666		#	40 Check
PLAT701_ALERT_1_A Bond	Calc	3.156(3), Rep	3.198(4), Dev..				14.00 Sigma
	SIB1	-CA2	1_555	3_666		#	41 Check
PLAT701_ALERT_1_A Bond	Calc	3.156(3), Rep	3.198(4), Dev..				14.00 Sigma
	SIB1	-NA2	1_555	3_666		#	42 Check
PLAT701_ALERT_1_A Bond	Calc	3.016(2), Rep	3.049(2), Dev..				16.50 Sigma
	SIB1	-CA21	1_555	3_667		#	43 Check
PLAT701_ALERT_1_A Bond	Calc	3.016(2), Rep	3.049(2), Dev..				16.50 Sigma
	SIB1	-NA21	1_555	3_667		#	44 Check
PLAT701_ALERT_1_A Bond	Calc	3.039(2), Rep	3.086(2), Dev..				23.50 Sigma
	MGM1	-AM11	1_555	1_554		#	48 Check
PLAT701_ALERT_1_A Bond	Calc	3.039(2), Rep	3.086(2), Dev..				23.50 Sigma
	MGM1	-AM11	1_555	1_555		#	49 Check
PLAT701_ALERT_1_A Bond	Calc	3.039(2), Rep	3.086(2), Dev..				23.50 Sigma
	MGM1	-MM11	1_555	1_554		#	52 Check
PLAT701_ALERT_1_A Bond	Calc	3.039(2), Rep	3.086(2), Dev..				23.50 Sigma
	MGM1	-MM11	1_555	1_555		#	53 Check
PLAT701_ALERT_1_A Bond	Calc	3.407(4), Rep	3.436(6), Dev..				7.25 Sigma
	MGM1	-CA2	1_555	1_565		#	54 Check
PLAT701_ALERT_1_A Bond	Calc	3.407(4), Rep	3.436(6), Dev..				7.25 Sigma
	MGM1	-NA2	1_555	1_565		#	55 Check

PLAT701_ALERT_1_A Bond	Calc	3.182(2), Rep	3.203(2), Dev..	10.50 Sigma
MGM1	-CA21	1_555	1_554	# 56 Check
PLAT701_ALERT_1_A Bond	Calc	3.182(2), Rep	3.203(2), Dev..	10.50 Sigma
MGM1	-CA21	1_555	1_555	# 57 Check
PLAT701_ALERT_1_A Bond	Calc	3.182(2), Rep	3.203(2), Dev..	10.50 Sigma
MGM1	-NA21	1_555	1_554	# 58 Check
PLAT701_ALERT_1_A Bond	Calc	3.182(2), Rep	3.203(2), Dev..	10.50 Sigma
MGM1	-NA21	1_555	1_555	# 59 Check
PLAT701_ALERT_1_A Bond	Calc	3.039(2), Rep	3.086(2), Dev..	23.50 Sigma
AM1	-MM11	1_555	1_554	# 71 Check
PLAT701_ALERT_1_A Bond	Calc	3.039(2), Rep	3.086(2), Dev..	23.50 Sigma
AM1	-MM11	1_555	1_555	# 72 Check
PLAT701_ALERT_1_A Bond	Calc	3.407(4), Rep	3.436(6), Dev..	7.25 Sigma
AM1	-CA2	1_555	1_565	# 73 Check
PLAT701_ALERT_1_A Bond	Calc	3.407(4), Rep	3.436(6), Dev..	7.25 Sigma
AM1	-NA2	1_555	1_565	# 74 Check
PLAT701_ALERT_1_A Bond	Calc	3.182(2), Rep	3.203(2), Dev..	10.50 Sigma
AM1	-CA21	1_555	1_554	# 75 Check
PLAT701_ALERT_1_A Bond	Calc	3.182(2), Rep	3.203(2), Dev..	10.50 Sigma
AM1	-CA21	1_555	1_555	# 76 Check
PLAT701_ALERT_1_A Bond	Calc	3.182(2), Rep	3.203(2), Dev..	10.50 Sigma
AM1	-NA21	1_555	1_554	# 77 Check
PLAT701_ALERT_1_A Bond	Calc	3.182(2), Rep	3.203(2), Dev..	10.50 Sigma
AM1	-NA21	1_555	1_555	# 78 Check
PLAT701_ALERT_1_A Bond	Calc	3.182(2), Rep	3.203(2), Dev..	10.50 Sigma
FM1	-CA21	1_555	1_554	# 79 Check
PLAT701_ALERT_1_A Bond	Calc	3.182(2), Rep	3.203(2), Dev..	10.50 Sigma
FM1	-CA21	1_555	1_555	# 80 Check
PLAT701_ALERT_1_A Bond	Calc	3.182(2), Rep	3.203(2), Dev..	10.50 Sigma
FM1	-NA21	1_555	1_554	# 81 Check
PLAT701_ALERT_1_A Bond	Calc	3.182(2), Rep	3.203(2), Dev..	10.50 Sigma
FM1	-NA21	1_555	1_555	# 82 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.181(3), Dev..	6.33 Sigma
AM11	-CA2	1_555	1_565	# 87 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.181(3), Dev..	6.33 Sigma
AM11	-CA2	1_555	1_566	# 88 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.181(3), Dev..	6.33 Sigma
AM11	-NA2	1_555	1_565	# 89 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.181(3), Dev..	6.33 Sigma
AM11	-NA2	1_555	1_566	# 90 Check
PLAT701_ALERT_1_A Bond	Calc	3.440(3), Rep	3.473(5), Dev..	11.00 Sigma
AM11	-CA21	1_555	1_555	# 91 Check
PLAT701_ALERT_1_A Bond	Calc	3.440(3), Rep	3.473(5), Dev..	11.00 Sigma
AM11	-NA21	1_555	1_555	# 92 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.181(3), Dev..	6.33 Sigma
MM11	-CA2	1_555	1_565	# 109 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.181(3), Dev..	6.33 Sigma
MM11	-CA2	1_555	1_566	# 110 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.181(3), Dev..	6.33 Sigma
MM11	-NA2	1_555	1_565	# 111 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.181(3), Dev..	6.33 Sigma
MM11	-NA2	1_555	1_566	# 112 Check
PLAT701_ALERT_1_A Bond	Calc	3.440(3), Rep	3.473(5), Dev..	11.00 Sigma
MM11	-CA21	1_555	1_555	# 113 Check
PLAT701_ALERT_1_A Bond	Calc	3.440(3), Rep	3.473(5), Dev..	11.00 Sigma
MM11	-NA21	1_555	1_555	# 114 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.181(3), Dev..	6.33 Sigma

FM11	-CA2	1_555	1_565		#	115	Check
PLAT701_ALERT_1_A	Bond	Calc	3.162(3), Rep	3.181(3), Dev..			6.33 Sigma
FM11	-CA2	1_555	1_566		#	116	Check
PLAT701_ALERT_1_A	Bond	Calc	3.162(3), Rep	3.181(3), Dev..			6.33 Sigma
FM11	-NA2	1_555	1_565		#	117	Check
PLAT701_ALERT_1_A	Bond	Calc	3.162(3), Rep	3.181(3), Dev..			6.33 Sigma
FM11	-NA2	1_555	1_566		#	118	Check

🔴 Alert level B

PLAT017_ALERT_1_B	Check	Scattering Type Consistency of AM1	as	AL Error?		
PLAT017_ALERT_1_B	Check	Scattering Type Consistency of FM1	as	FE Error?		
PLAT017_ALERT_1_B	Check	Scattering Type Consistency of AM11	as	AL Error?		
PLAT017_ALERT_1_B	Check	Scattering Type Consistency of MM11	as	MG Error?		
PLAT017_ALERT_1_B	Check	Scattering Type Consistency of FM11	as	FE Error?		
PLAT088_ALERT_3_B	Poor Data / Parameter Ratio			6.18 Note		
PLAT701_ALERT_1_B	Bond	Calc	1.577(4), Rep	1.588(5), Dev..		
O22A	-SIB1	1_555	1_555			
				#	28	Check

🟡 Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
 Goodness of fit given = 2.310

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
 Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8
 Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
 Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)
 Rep.: ?

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.08 Check

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms . Please Check

PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) O11A Check

PLAT701_ALERT_1_C Bond Calc 1.881(4), Rep 1.887(5), Dev.. 1.50 Sigma

O21A -MM11 1_555 3_666 # 24 Check

PLAT701_ALERT_1_C Bond Calc 1.881(4), Rep 1.887(5), Dev.. 1.50 Sigma

O21A -FM11 1_555 3_666 # 25 Check

PLAT701_ALERT_1_C Bond Calc 1.664(3), Rep 1.670(4), Dev.. 2.00 Sigma

O31A -SIB1 1_555 1_554 # 35 Check

PLAT701_ALERT_1_C Bond Calc 1.655(3), Rep 1.659(4), Dev.. 1.33 Sigma

O32A -SIA1 1_555 1_555 # 36 Check

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label MnM1 Check

O11A MNM1

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Cm11 Check

O11A CM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Tm11 Check

O11A TM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label MnM1 Check

O12A MNM1

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Cm11 Check

O12A CM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Tm11 Check

	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	CA2				

PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA21		

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info

PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !

PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.250 Check

PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check

PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.49570 Ang.

PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check

PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Fm1 Constrained at 0.087 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Fm11 Constrained at 0.052 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Am11 Constrained at 0.86 Check

PLAT300_ALERT_4_G Atom Site Occupancy of MgM1 Constrained at 0.868 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Am1 Constrained at 0.045 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Mm11 Constrained at 0.088 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Ca21 Constrained at 0.7904 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Ca2 Constrained at 0.3622 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na2 Constrained at 0.6378 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na21 Constrained at 0.2096 Check

PLAT301_ALERT_3_G Main Residue Disorder (Resd 1) 20% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 100% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5) 100% Note

PLAT396_ALERT_2_G Deviating Si-O-Si Angle From 150 for O31A . 133.7 Degree

PLAT396_ALERT_2_G Deviating Si-O-Si Angle From 150 for O32A . 138.0 Degree

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 8 Note

SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11 Fm11

PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.84 Ratio

PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found Please Check

PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info

PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !

PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note

0 1 0, 1 1 0,

PLAT911_ALERT_3_G Missing FCF Refl Between Thmin & STh/L= 0.600 338 Report

0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,

0 8 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0, 1 6 0,

1 7 0, 1 8 0, 2 0 0, 2 1 0, 2 2 0, 2 3 0,

2 4 0, 2 5 0, 2 6 0, 2 7 0, 2 8 0, 3 1 0,

3 4 0, 3 5 0, 3 6 0, 3 7 0, 3 8 0, 4 0 0,

4 1 0, 4 6 0, 4 7 0, 4 8 0, 5 1 0, 5 7 0,

5 8 0, 6 0 0, 6 1 0, 6 2 0, 6 3 0, 6 4 0,

6 5 0, 6 8 0, 7 1 0, 7 2 0, 7 5 0, 7 6 0,

7 7 0, 8 0 0, 8 1 0, 8 2 0, 8 3 0, 8 4 0,

8	5	0,	8	6	0,	8	7	0,	9	1	0,	9	2	0,	9	3	0,
9	4	0,	9	5	0,	10	0	0,	10	1	0,	10	2	0,	10	3	0,
10	4	0,	-11	0	1,	-11	1	1,	-11	2	1,	-10	1	1,	-10	2	1,
-10	3	1,	-9	0	1,	-9	1	1,	-9	2	1,	-9	4	1,	-9	5	1,
-9	6	1,	-8	1	1,	-8	2	1,	-8	5	1,	-8	7	1,	-7	0	1,
-7	1	1,	-7	5	1,	-7	8	1,	-6	1	1,	-6	8	1,	-5	0	1,
-5	1	1,	-5	7	1,	-5	8	1,	-4	5	1,	-4	6	1,	-4	7	1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600															552	Note	
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked															!	Info	
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ															2	Units	
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ															6	Units	
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ															2	Units	
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ															6	Units	
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of															3.0	Sig(I)	
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value															2.935	Note	
Predicted wR2: Based on SigI**2 2.92 or SHELX Weight															2.92		
PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value															0.1517	Check	
PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value															0.4344	Check	

69 **ALERT level A** = Most likely a serious problem - resolve or explain
 7 **ALERT level B** = A potentially serious problem, consider carefully
 52 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 42 **ALERT level G** = General information/check it is not something unexpected

132 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 4 ALERT type 2 Indicator that the structure model may be wrong or deficient
 6 ALERT type 3 Indicator that the structure quality may be low
 19 ALERT type 4 Improvement, methodology, query or suggestion
 9 ALERT type 5 Informative message, check

Datablock: 6.19_GPa

Bond precision:	Si- O = 0.0040 A	Wavelength=0.49570	
Cell:	a=9.432(3)	b=8.618(5)	c=5.170(1)
	alpha=90	beta=106.26(3)	gamma=90
Temperature:	293 K		

	Calculated	Reported
Volume	403.4(3)	403.4(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.503	3.516
Z	1	4
Mu (mm-1)	0.727	0.718
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,8,8
Nref	1930	577
Tmin,Tmax		0.497,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.497 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.299 Theta(max)= 24.220

R(reflections)= 0.0417(420) wR2(reflections)=
wR= 0.0609(577)

S = 2.120 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 13.37 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.550 Why?

PLAT701_ALERT_1_A Bond Calc 1.608(4), Rep 1.625(5), Dev.. 4.25 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_A Bond Calc 2.080(4), Rep 2.115(5), Dev.. 8.75 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.080(4), Rep 2.115(5), Dev.. 8.75 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond Calc 2.321(4), Rep 2.348(5), Dev.. 6.75 Sigma

	O11A	-CA2	1_555	1_565		#	9 Check
PLAT701_ALERT_1_A Bond	Calc	2.321(4), Rep	2.348(5), Dev..				6.75 Sigma
	O11A	-NA2	1_555	1_565		#	10 Check
PLAT701_ALERT_1_A Bond	Calc	1.607(4), Rep	1.622(5), Dev..				3.75 Sigma
	O12A	-SIB1	1_555	1_655		#	11 Check
PLAT701_ALERT_1_A Bond	Calc	2.041(3), Rep	2.058(3), Dev..				5.67 Sigma
	O12A	-MGM1	1_555	1_555		#	12 Check
PLAT701_ALERT_1_A Bond	Calc	2.041(3), Rep	2.058(3), Dev..				5.67 Sigma
	O12A	-FM1	1_555	1_555		#	14 Check
PLAT701_ALERT_1_A Bond	Calc	1.953(4), Rep	1.980(5), Dev..				6.75 Sigma
	O12A	-MM11	1_555	1_555		#	17 Check
PLAT701_ALERT_1_A Bond	Calc	1.953(4), Rep	1.980(5), Dev..				6.75 Sigma
	O12A	-FM11	1_555	1_555		#	18 Check
PLAT701_ALERT_1_A Bond	Calc	2.358(4), Rep	2.391(5), Dev..				8.25 Sigma
	O12A	-CA21	1_555	1_555		#	19 Check
PLAT701_ALERT_1_A Bond	Calc	2.358(4), Rep	2.391(5), Dev..				8.25 Sigma
	O12A	-NA21	1_555	1_555		#	20 Check
PLAT701_ALERT_1_A Bond	Calc	1.586(4), Rep	1.603(5), Dev..				4.25 Sigma
	O21A	-SIA1	1_555	1_545		#	21 Check
PLAT701_ALERT_1_A Bond	Calc	2.332(3), Rep	2.358(4), Dev..				8.67 Sigma
	O21A	-CA2	1_555	3_656		#	26 Check
PLAT701_ALERT_1_A Bond	Calc	2.332(3), Rep	2.358(4), Dev..				8.67 Sigma
	O21A	-NA2	1_555	3_656		#	27 Check
PLAT701_ALERT_1_A Bond	Calc	1.995(4), Rep	2.025(5), Dev..				7.50 Sigma
	O22A	-MGM1	1_555	3_666		#	29 Check
PLAT701_ALERT_1_A Bond	Calc	1.995(4), Rep	2.025(5), Dev..				7.50 Sigma
	O22A	-FM1	1_555	3_666		#	31 Check
PLAT701_ALERT_1_A Bond	Calc	2.355(3), Rep	2.384(4), Dev..				9.67 Sigma
	O22A	-CA21	1_555	3_667		#	32 Check
PLAT701_ALERT_1_A Bond	Calc	2.355(3), Rep	2.384(4), Dev..				9.67 Sigma
	O22A	-NA21	1_555	3_667		#	33 Check
PLAT701_ALERT_1_A Bond	Calc	1.660(3), Rep	1.670(4), Dev..				3.33 Sigma
	O31A	-SIB1	1_555	1_554		#	35 Check
PLAT701_ALERT_1_A Bond	Calc	2.987(2), Rep	3.025(2), Dev..				19.00 Sigma
	SIA1	-CA2	1_555	3_666		#	38 Check
PLAT701_ALERT_1_A Bond	Calc	2.987(2), Rep	3.025(2), Dev..				19.00 Sigma
	SIA1	-NA2	1_555	3_666		#	39 Check
PLAT701_ALERT_1_A Bond	Calc	3.209(3), Rep	3.270(4), Dev..				20.33 Sigma
	SIA1	-CA21	1_555	3_666		#	40 Check
PLAT701_ALERT_1_A Bond	Calc	3.143(3), Rep	3.198(4), Dev..				18.33 Sigma
	SIB1	-CA2	1_555	3_666		#	41 Check
PLAT701_ALERT_1_A Bond	Calc	3.143(3), Rep	3.198(4), Dev..				18.33 Sigma
	SIB1	-NA2	1_555	3_666		#	42 Check
PLAT701_ALERT_1_A Bond	Calc	3.010(2), Rep	3.049(2), Dev..				19.50 Sigma
	SIB1	-CA21	1_555	3_667		#	43 Check
PLAT701_ALERT_1_A Bond	Calc	3.010(2), Rep	3.049(2), Dev..				19.50 Sigma
	SIB1	-NA21	1_555	3_667		#	44 Check
PLAT701_ALERT_1_A Bond	Calc	3.033(2), Rep	3.086(2), Dev..				26.50 Sigma
	MGM1	-AM11	1_555	1_554		#	48 Check
PLAT701_ALERT_1_A Bond	Calc	3.033(2), Rep	3.086(2), Dev..				26.50 Sigma
	MGM1	-AM11	1_555	1_555		#	49 Check
PLAT701_ALERT_1_A Bond	Calc	3.033(2), Rep	3.086(2), Dev..				26.50 Sigma
	MGM1	-MM11	1_555	1_554		#	52 Check
PLAT701_ALERT_1_A Bond	Calc	3.033(2), Rep	3.086(2), Dev..				26.50 Sigma
	MGM1	-MM11	1_555	1_555		#	53 Check
PLAT701_ALERT_1_A Bond	Calc	3.407(3), Rep	3.436(6), Dev..				9.67 Sigma
	MGM1	-CA2	1_555	1_565		#	54 Check

PLAT701_ALERT_1_A Bond	Calc	3.407(3), Rep	3.436(6), Dev..	9.67 Sigma
MGM1	-NA2	1_555	1_565	# 55 Check
PLAT701_ALERT_1_A Bond	Calc	3.180(2), Rep	3.203(2), Dev..	11.50 Sigma
MGM1	-CA21	1_555	1_554	# 56 Check
PLAT701_ALERT_1_A Bond	Calc	3.180(2), Rep	3.203(2), Dev..	11.50 Sigma
MGM1	-CA21	1_555	1_555	# 57 Check
PLAT701_ALERT_1_A Bond	Calc	3.180(2), Rep	3.203(2), Dev..	11.50 Sigma
MGM1	-NA21	1_555	1_554	# 58 Check
PLAT701_ALERT_1_A Bond	Calc	3.180(2), Rep	3.203(2), Dev..	11.50 Sigma
MGM1	-NA21	1_555	1_555	# 59 Check
PLAT701_ALERT_1_A Bond	Calc	3.033(2), Rep	3.086(2), Dev..	26.50 Sigma
AM1	-MM11	1_555	1_554	# 71 Check
PLAT701_ALERT_1_A Bond	Calc	3.033(2), Rep	3.086(2), Dev..	26.50 Sigma
AM1	-MM11	1_555	1_555	# 72 Check
PLAT701_ALERT_1_A Bond	Calc	3.407(3), Rep	3.436(6), Dev..	9.67 Sigma
AM1	-CA2	1_555	1_565	# 73 Check
PLAT701_ALERT_1_A Bond	Calc	3.407(3), Rep	3.436(6), Dev..	9.67 Sigma
AM1	-NA2	1_555	1_565	# 74 Check
PLAT701_ALERT_1_A Bond	Calc	3.180(2), Rep	3.203(2), Dev..	11.50 Sigma
AM1	-CA21	1_555	1_554	# 75 Check
PLAT701_ALERT_1_A Bond	Calc	3.180(2), Rep	3.203(2), Dev..	11.50 Sigma
AM1	-CA21	1_555	1_555	# 76 Check
PLAT701_ALERT_1_A Bond	Calc	3.180(2), Rep	3.203(2), Dev..	11.50 Sigma
AM1	-NA21	1_555	1_554	# 77 Check
PLAT701_ALERT_1_A Bond	Calc	3.180(2), Rep	3.203(2), Dev..	11.50 Sigma
AM1	-NA21	1_555	1_555	# 78 Check
PLAT701_ALERT_1_A Bond	Calc	3.180(2), Rep	3.203(2), Dev..	11.50 Sigma
FM1	-CA21	1_555	1_554	# 79 Check
PLAT701_ALERT_1_A Bond	Calc	3.180(2), Rep	3.203(2), Dev..	11.50 Sigma
FM1	-CA21	1_555	1_555	# 80 Check
PLAT701_ALERT_1_A Bond	Calc	3.180(2), Rep	3.203(2), Dev..	11.50 Sigma
FM1	-NA21	1_555	1_554	# 81 Check
PLAT701_ALERT_1_A Bond	Calc	3.180(2), Rep	3.203(2), Dev..	11.50 Sigma
FM1	-NA21	1_555	1_555	# 82 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(2), Rep	3.181(3), Dev..	9.50 Sigma
AM11	-CA2	1_555	1_565	# 87 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(2), Rep	3.181(3), Dev..	9.50 Sigma
AM11	-CA2	1_555	1_566	# 88 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(2), Rep	3.181(3), Dev..	9.50 Sigma
AM11	-NA2	1_555	1_565	# 89 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(2), Rep	3.181(3), Dev..	9.50 Sigma
AM11	-NA2	1_555	1_566	# 90 Check
PLAT701_ALERT_1_A Bond	Calc	3.437(3), Rep	3.473(5), Dev..	12.00 Sigma
AM11	-CA21	1_555	1_555	# 91 Check
PLAT701_ALERT_1_A Bond	Calc	3.437(3), Rep	3.473(5), Dev..	12.00 Sigma
AM11	-NA21	1_555	1_555	# 92 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(2), Rep	3.181(3), Dev..	9.50 Sigma
MM11	-CA2	1_555	1_565	# 109 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(2), Rep	3.181(3), Dev..	9.50 Sigma
MM11	-CA2	1_555	1_566	# 110 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(2), Rep	3.181(3), Dev..	9.50 Sigma
MM11	-NA2	1_555	1_565	# 111 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(2), Rep	3.181(3), Dev..	9.50 Sigma
MM11	-NA2	1_555	1_566	# 112 Check
PLAT701_ALERT_1_A Bond	Calc	3.437(3), Rep	3.473(5), Dev..	12.00 Sigma
MM11	-CA21	1_555	1_555	# 113 Check
PLAT701_ALERT_1_A Bond	Calc	3.437(3), Rep	3.473(5), Dev..	12.00 Sigma

MM11	-NA21	1_555	1_555		#	114 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(2), Rep	3.181(3), Dev..			9.50 Sigma
FM11	-CA2	1_555	1_565		#	115 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(2), Rep	3.181(3), Dev..			9.50 Sigma
FM11	-CA2	1_555	1_566		#	116 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(2), Rep	3.181(3), Dev..			9.50 Sigma
FM11	-NA2	1_555	1_565		#	117 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(2), Rep	3.181(3), Dev..			9.50 Sigma
FM11	-NA2	1_555	1_566		#	118 Check

🟡 Alert level B

PLAT017_ALERT_1_B Check	Scattering Type Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of FM11	as	FE Error?
PLAT088_ALERT_3_B Poor Data / Parameter Ratio			6.14 Note
PLAT701_ALERT_1_B Bond	Calc	1.877(4), Rep	1.887(5), Dev..
O21A	-MM11	1_555	3_666
PLAT701_ALERT_1_B Bond	Calc	1.877(4), Rep	1.887(5), Dev..
O21A	-FM11	1_555	3_666
PLAT701_ALERT_1_B Bond	Calc	1.577(4), Rep	1.588(5), Dev..
O22A	-SIB1	1_555	1_555

🟡 Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
Goodness of fit given = 2.120

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8
Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)
Rep.: ?

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.08 Check

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms . Please Check

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.3 Note

PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) 011A Check

PLAT701_ALERT_1_C Bond	Calc	1.925(3), Rep	1.931(3), Dev..			2.00 Sigma
O11A	-MM11	1_555	1_554		#	7 Check
PLAT701_ALERT_1_C Bond	Calc	1.925(3), Rep	1.931(3), Dev..			2.00 Sigma
O11A	-FM11	1_555	1_554		#	8 Check
PLAT701_ALERT_1_C Bond	Calc	1.653(3), Rep	1.659(4), Dev..			2.00 Sigma
O32A	-SIA1	1_555	1_555		#	36 Check
PLAT701_ALERT_1_C Bond	Calc	1.639(3), Rep	1.644(5), Dev..			1.67 Sigma
O32A	-SIB1	1_555	1_555		#	37 Check
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label					MnM1 Check
O11A	MNM1					
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label					Cm11 Check
O11A	CM11					

PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O11A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O12A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O12A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check

	CM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	MM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	FM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA21		

● Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu			
	not performed for this radiation type.			
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please	Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check	
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please	Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.	
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check	
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1	Constrained at	0.087	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11	Constrained at	0.052	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11	Constrained at	0.86	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1	Constrained at	0.868	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1	Constrained at	0.045	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11	Constrained at	0.088	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21	Constrained at	0.7904	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2	Constrained at	0.3622	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2	Constrained at	0.6378	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21	Constrained at	0.2096	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	5)	100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A	.	133.6	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A	.	138.0	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		8	Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11		Fm11	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	.	1.84	Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		!	Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2	Note
	0 1 0, 1 1 0,			
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L=	0.600	337	Report
	0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0,		0 7 0,	
	0 8 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0,		1 6 0,	

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1 7 0, 1 8 0, 2 0 0, 2 1 0, 2 2 0, 2 3 0,
2 4 0, 2 5 0, 2 6 0, 2 7 0, 2 8 0, 3 1 0,
3 4 0, 3 5 0, 3 6 0, 3 7 0, 3 8 0, 4 0 0,
4 1 0, 4 2 0, 4 6 0, 4 7 0, 4 8 0, 5 1 0,
5 4 0, 5 7 0, 5 8 0, 6 0 0, 6 1 0, 6 2 0,
6 3 0, 6 4 0, 6 5 0, 6 8 0, 7 1 0, 7 2 0,
7 5 0, 7 6 0, 7 7 0, 8 0 0, 8 1 0, 8 2 0,
8 3 0, 8 4 0, 8 5 0, 8 6 0, 9 1 0, 9 2 0,
9 3 0, 9 4 0, 9 5 0, 10 0 0, 10 1 0, 10 2 0,
10 3 0, 10 4 0, -11 0 1, -11 1 1, -11 2 1, -10 1 1,
-10 2 1, -10 3 1, -10 4 1, -9 0 1, -9 1 1, -9 2 1,
-9 4 1, -9 6 1, -8 1 1, -8 2 1, -8 5 1, -8 7 1,
-7 0 1, -7 1 1, -7 5 1, -7 8 1, -6 1 1, -6 8 1,
-5 0 1, -5 1 1, -5 7 1, -5 8 1, -4 5 1, -4 6 1,

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PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 560 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 6 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ 2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 6 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of 3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.249 Note
                Predicted wR2: Based on SigI**2 4.82 or SHELX Weight 4.82
PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value 0.1517 Check
PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value 0.4344 Check

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70 ALERT level A = Most likely a serious problem - resolve or explain
9 ALERT level B = A potentially serious problem, consider carefully
53 ALERT level C = Check. Ensure it is not caused by an omission or oversight
42 ALERT level G = General information/check it is not something unexpected

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135 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
9 ALERT type 5 Informative message, check

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Datablock: 7.11_GPa

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Bond precision:  Si- O = 0.0050 A          Wavelength=0.49570

Cell:            a=9.417(3)          b=8.600(5)          c=5.160(1)
                  alpha=90           beta=106.17(3)       gamma=90
Temperature:     293 K

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	Calculated	Reported
Volume	401.4(3)	401.4(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.520	3.534
Z	1	4
Mu (mm-1)	0.730	0.721
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,8,8
Nref	1997	577
Tmin,Tmax		0.497,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.497 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.289 Theta(max)= 24.600

R(reflections)= 0.0454(437) wR2(reflections)=
wR= 0.0930(577)

S = 2.920 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 12.88 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.550 Why?

PLAT211_ALERT_2_A ADP of Atom O11A is N.P.D. or (nearly) 2D . Please Check

PLAT211_ALERT_2_A ADP of Atom O21A is N.P.D. or (nearly) 2D . Please Check

PLAT701_ALERT_1_A Bond Calc 1.588(5), Rep 1.625(5), Dev.. 7.40 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_A Bond Calc 2.089(5), Rep 2.115(5), Dev.. 5.20 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.089(5), Rep 2.115(5), Dev.. 5.20 Sigma

	O11A	-FM1	1_555	1_555	#	4 Check
PLAT701_ALERT_1_A Bond	Calc	2.319(5), Rep	2.348(5), Dev..			5.80 Sigma
	O11A	-CA2	1_555	1_565	#	9 Check
PLAT701_ALERT_1_A Bond	Calc	2.319(5), Rep	2.348(5), Dev..			5.80 Sigma
	O11A	-NA2	1_555	1_565	#	10 Check
PLAT701_ALERT_1_A Bond	Calc	2.031(3), Rep	2.058(3), Dev..			9.00 Sigma
	O12A	-MGM1	1_555	1_555	#	12 Check
PLAT701_ALERT_1_A Bond	Calc	2.031(3), Rep	2.058(3), Dev..			9.00 Sigma
	O12A	-FM1	1_555	1_555	#	14 Check
PLAT701_ALERT_1_A Bond	Calc	1.946(5), Rep	1.980(5), Dev..			6.80 Sigma
	O12A	-MM11	1_555	1_555	#	17 Check
PLAT701_ALERT_1_A Bond	Calc	1.946(5), Rep	1.980(5), Dev..			6.80 Sigma
	O12A	-FM11	1_555	1_555	#	18 Check
PLAT701_ALERT_1_A Bond	Calc	2.354(5), Rep	2.391(5), Dev..			7.40 Sigma
	O12A	-CA21	1_555	1_555	#	19 Check
PLAT701_ALERT_1_A Bond	Calc	2.354(5), Rep	2.391(5), Dev..			7.40 Sigma
	O12A	-NA21	1_555	1_555	#	20 Check
PLAT701_ALERT_1_A Bond	Calc	1.871(5), Rep	1.887(5), Dev..			3.20 Sigma
	O21A	-MM11	1_555	3_666	#	24 Check
PLAT701_ALERT_1_A Bond	Calc	1.871(5), Rep	1.887(5), Dev..			3.20 Sigma
	O21A	-FM11	1_555	3_666	#	25 Check
PLAT701_ALERT_1_A Bond	Calc	2.329(4), Rep	2.358(4), Dev..			7.25 Sigma
	O21A	-CA2	1_555	3_656	#	26 Check
PLAT701_ALERT_1_A Bond	Calc	2.329(4), Rep	2.358(4), Dev..			7.25 Sigma
	O21A	-NA2	1_555	3_656	#	27 Check
PLAT701_ALERT_1_A Bond	Calc	1.990(5), Rep	2.025(5), Dev..			7.00 Sigma
	O22A	-MGM1	1_555	3_666	#	29 Check
PLAT701_ALERT_1_A Bond	Calc	1.990(5), Rep	2.025(5), Dev..			7.00 Sigma
	O22A	-FM1	1_555	3_666	#	31 Check
PLAT701_ALERT_1_A Bond	Calc	2.334(4), Rep	2.384(4), Dev..			12.50 Sigma
	O22A	-CA21	1_555	3_667	#	32 Check
PLAT701_ALERT_1_A Bond	Calc	2.334(4), Rep	2.384(4), Dev..			12.50 Sigma
	O22A	-NA21	1_555	3_667	#	33 Check
PLAT701_ALERT_1_A Bond	Calc	1.645(4), Rep	1.670(4), Dev..			6.25 Sigma
	O31A	-SIB1	1_555	1_554	#	35 Check
PLAT701_ALERT_1_A Bond	Calc	2.988(2), Rep	3.025(2), Dev..			18.50 Sigma
	SIA1	-CA2	1_555	3_666	#	38 Check
PLAT701_ALERT_1_A Bond	Calc	2.988(2), Rep	3.025(2), Dev..			18.50 Sigma
	SIA1	-NA2	1_555	3_666	#	39 Check
PLAT701_ALERT_1_A Bond	Calc	3.204(3), Rep	3.270(4), Dev..			22.00 Sigma
	SIA1	-CA21	1_555	3_666	#	40 Check
PLAT701_ALERT_1_A Bond	Calc	3.131(3), Rep	3.198(4), Dev..			22.33 Sigma
	SIB1	-CA2	1_555	3_666	#	41 Check
PLAT701_ALERT_1_A Bond	Calc	3.131(3), Rep	3.198(4), Dev..			22.33 Sigma
	SIB1	-NA2	1_555	3_666	#	42 Check
PLAT701_ALERT_1_A Bond	Calc	3.005(2), Rep	3.049(2), Dev..			22.00 Sigma
	SIB1	-CA21	1_555	3_667	#	43 Check
PLAT701_ALERT_1_A Bond	Calc	3.005(2), Rep	3.049(2), Dev..			22.00 Sigma
	SIB1	-NA21	1_555	3_667	#	44 Check
PLAT701_ALERT_1_A Bond	Calc	3.027(3), Rep	3.086(2), Dev..			19.67 Sigma
	MGM1	-AM11	1_555	1_554	#	48 Check
PLAT701_ALERT_1_A Bond	Calc	3.027(3), Rep	3.086(2), Dev..			19.67 Sigma
	MGM1	-AM11	1_555	1_555	#	49 Check
PLAT701_ALERT_1_A Bond	Calc	3.027(3), Rep	3.086(2), Dev..			19.67 Sigma
	MGM1	-MM11	1_555	1_554	#	52 Check
PLAT701_ALERT_1_A Bond	Calc	3.027(3), Rep	3.086(2), Dev..			19.67 Sigma
	MGM1	-MM11	1_555	1_555	#	53 Check

PLAT701_ALERT_1_A Bond	Calc	3.408(4), Rep	3.436(6), Dev..	7.00 Sigma
MGM1	-CA2	1_555	1_565	# 54 Check
PLAT701_ALERT_1_A Bond	Calc	3.408(4), Rep	3.436(6), Dev..	7.00 Sigma
MGM1	-NA2	1_555	1_565	# 55 Check
PLAT701_ALERT_1_A Bond	Calc	3.173(3), Rep	3.203(2), Dev..	10.00 Sigma
MGM1	-CA21	1_555	1_554	# 56 Check
PLAT701_ALERT_1_A Bond	Calc	3.173(3), Rep	3.203(2), Dev..	10.00 Sigma
MGM1	-CA21	1_555	1_555	# 57 Check
PLAT701_ALERT_1_A Bond	Calc	3.173(3), Rep	3.203(2), Dev..	10.00 Sigma
MGM1	-NA21	1_555	1_554	# 58 Check
PLAT701_ALERT_1_A Bond	Calc	3.173(3), Rep	3.203(2), Dev..	10.00 Sigma
MGM1	-NA21	1_555	1_555	# 59 Check
PLAT701_ALERT_1_A Bond	Calc	3.027(3), Rep	3.086(2), Dev..	19.67 Sigma
AM1	-MM11	1_555	1_554	# 71 Check
PLAT701_ALERT_1_A Bond	Calc	3.027(3), Rep	3.086(2), Dev..	19.67 Sigma
AM1	-MM11	1_555	1_555	# 72 Check
PLAT701_ALERT_1_A Bond	Calc	3.408(4), Rep	3.436(6), Dev..	7.00 Sigma
AM1	-CA2	1_555	1_565	# 73 Check
PLAT701_ALERT_1_A Bond	Calc	3.408(4), Rep	3.436(6), Dev..	7.00 Sigma
AM1	-NA2	1_555	1_565	# 74 Check
PLAT701_ALERT_1_A Bond	Calc	3.173(3), Rep	3.203(2), Dev..	10.00 Sigma
AM1	-CA21	1_555	1_554	# 75 Check
PLAT701_ALERT_1_A Bond	Calc	3.173(3), Rep	3.203(2), Dev..	10.00 Sigma
AM1	-CA21	1_555	1_555	# 76 Check
PLAT701_ALERT_1_A Bond	Calc	3.173(3), Rep	3.203(2), Dev..	10.00 Sigma
AM1	-NA21	1_555	1_554	# 77 Check
PLAT701_ALERT_1_A Bond	Calc	3.173(3), Rep	3.203(2), Dev..	10.00 Sigma
AM1	-NA21	1_555	1_555	# 78 Check
PLAT701_ALERT_1_A Bond	Calc	3.173(3), Rep	3.203(2), Dev..	10.00 Sigma
FM1	-CA21	1_555	1_554	# 79 Check
PLAT701_ALERT_1_A Bond	Calc	3.173(3), Rep	3.203(2), Dev..	10.00 Sigma
FM1	-CA21	1_555	1_555	# 80 Check
PLAT701_ALERT_1_A Bond	Calc	3.173(3), Rep	3.203(2), Dev..	10.00 Sigma
FM1	-NA21	1_555	1_554	# 81 Check
PLAT701_ALERT_1_A Bond	Calc	3.173(3), Rep	3.203(2), Dev..	10.00 Sigma
FM1	-NA21	1_555	1_555	# 82 Check
PLAT701_ALERT_1_A Bond	Calc	3.160(3), Rep	3.181(3), Dev..	7.00 Sigma
AM11	-CA2	1_555	1_565	# 87 Check
PLAT701_ALERT_1_A Bond	Calc	3.160(3), Rep	3.181(3), Dev..	7.00 Sigma
AM11	-CA2	1_555	1_566	# 88 Check
PLAT701_ALERT_1_A Bond	Calc	3.160(3), Rep	3.181(3), Dev..	7.00 Sigma
AM11	-NA2	1_555	1_565	# 89 Check
PLAT701_ALERT_1_A Bond	Calc	3.160(3), Rep	3.181(3), Dev..	7.00 Sigma
AM11	-NA2	1_555	1_566	# 90 Check
PLAT701_ALERT_1_A Bond	Calc	3.431(4), Rep	3.473(5), Dev..	10.50 Sigma
AM11	-CA21	1_555	1_555	# 91 Check
PLAT701_ALERT_1_A Bond	Calc	3.431(4), Rep	3.473(5), Dev..	10.50 Sigma
AM11	-NA21	1_555	1_555	# 92 Check
PLAT701_ALERT_1_A Bond	Calc	3.160(3), Rep	3.181(3), Dev..	7.00 Sigma
MM11	-CA2	1_555	1_565	# 109 Check
PLAT701_ALERT_1_A Bond	Calc	3.160(3), Rep	3.181(3), Dev..	7.00 Sigma
MM11	-CA2	1_555	1_566	# 110 Check
PLAT701_ALERT_1_A Bond	Calc	3.160(3), Rep	3.181(3), Dev..	7.00 Sigma
MM11	-NA2	1_555	1_565	# 111 Check
PLAT701_ALERT_1_A Bond	Calc	3.160(3), Rep	3.181(3), Dev..	7.00 Sigma
MM11	-NA2	1_555	1_566	# 112 Check
PLAT701_ALERT_1_A Bond	Calc	3.431(4), Rep	3.473(5), Dev..	10.50 Sigma

MM11	-CA21	1_555	1_555		#	113 Check
PLAT701_ALERT_1_A	Bond Calc	3.431(4), Rep	3.473(5), Dev..			10.50 Sigma
MM11	-NA21	1_555	1_555		#	114 Check
PLAT701_ALERT_1_A	Bond Calc	3.160(3), Rep	3.181(3), Dev..			7.00 Sigma
FM11	-CA2	1_555	1_565		#	115 Check
PLAT701_ALERT_1_A	Bond Calc	3.160(3), Rep	3.181(3), Dev..			7.00 Sigma
FM11	-CA2	1_555	1_566		#	116 Check
PLAT701_ALERT_1_A	Bond Calc	3.160(3), Rep	3.181(3), Dev..			7.00 Sigma
FM11	-NA2	1_555	1_565		#	117 Check
PLAT701_ALERT_1_A	Bond Calc	3.160(3), Rep	3.181(3), Dev..			7.00 Sigma
FM11	-NA2	1_555	1_566		#	118 Check

🔴 Alert level B

PLAT017_ALERT_1_B	Check Scattering Type Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B	Check Scattering Type Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B	Check Scattering Type Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B	Check Scattering Type Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B	Check Scattering Type Consistency of FM11	as	FE Error?
PLAT088_ALERT_3_B	Poor Data / Parameter Ratio		6.14 Note
PLAT212_ALERT_2_B	ADP of Atom Ca21 is N.P.D. or (nearly) 2D .		Please Check
PLAT212_ALERT_2_B	ADP of Atom Na21 is N.P.D. or (nearly) 2D .		Please Check
PLAT213_ALERT_2_B	Atom SiB1 has ADP max/min Ratio		4.3 prolat
PLAT701_ALERT_1_B	Bond Calc 1.577(5), Rep 1.588(5), Dev..		2.20 Sigma
O22A	-SIB1 1_555 1_555	#	28 Check
PLAT701_ALERT_1_B	Bond Calc 1.656(4), Rep 1.644(5), Dev..		3.00 Sigma
O31A	-SIA1 1_555 1_555	#	34 Check

🟡 Alert level C

GOODF01_ALERT_2_C	The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00		
	Goodness of fit given = 2.920		
PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ		Please Check
	Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8		
	Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2		
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ		Please Check
	Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)		
	Rep.: ?		
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight Differ by ..		3.08 Check
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...		Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...		Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...		Please Check
PLAT077_ALERT_4_C	Unit Cell Contains Non-integer Number of Atoms .		Please Check
PLAT213_ALERT_2_C	Atom O22A has ADP max/min Ratio		4.0 oblate
PLAT213_ALERT_2_C	Atom O31A has ADP max/min Ratio		3.4 oblate
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)		O11A Check
PLAT701_ALERT_1_C	Bond Calc 1.613(5), Rep 1.622(5), Dev..		1.80 Sigma
O12A	-SIB1 1_555 1_655	#	11 Check
PLAT701_ALERT_1_C	Bond Calc 1.596(5), Rep 1.603(5), Dev..		1.40 Sigma
O21A	-SIA1 1_555 1_545	#	21 Check
PLAT701_ALERT_1_C	Bond Calc 1.639(4), Rep 1.644(5), Dev..		1.25 Sigma
O32A	-SIB1 1_555 1_555	#	37 Check
PLAT711_ALERT_1_C	BOND Unknown or Inconsistent Label		MnM1 Check
O11A	MNM1		

PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O11A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O11A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O12A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O12A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check

	CM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	CM11	Check
	CM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	MM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	FM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA21		

Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu			
	not performed for this radiation type.			
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please	Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check	
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please	Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.	
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check	
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature	293	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1	0.087	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11	0.052	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11	0.86	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1	0.868	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1	0.045	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11	0.088	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21	0.7904	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2	0.3622	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2	0.6378	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21	0.2096	Check	
PLAT301_ALERT_3_G	Main Residue Disorder	1)	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	5)	100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A	133.0	Degree	
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A	137.2	Degree	
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note	
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11	Fm11		
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	1.84	Ratio	
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		!	Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note	
	0 1 0, 1 1 0,			
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L=	0.600	335	Report

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0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,
0 8 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0, 1 6 0,
1 7 0, 1 8 0, 2 0 0, 2 1 0, 2 2 0, 2 3 0,
2 4 0, 2 5 0, 2 6 0, 2 7 0, 2 8 0, 3 1 0,
3 4 0, 3 5 0, 3 6 0, 3 7 0, 3 8 0, 4 0 0,
4 1 0, 4 6 0, 4 7 0, 4 8 0, 5 1 0, 5 4 0,
5 7 0, 6 0 0, 6 1 0, 6 2 0, 6 3 0, 6 4 0,
6 5 0, 6 6 0, 6 8 0, 7 1 0, 7 2 0, 7 3 0,
7 4 0, 7 5 0, 7 6 0, 7 7 0, 8 0 0, 8 1 0,
8 2 0, 8 3 0, 8 4 0, 8 5 0, 8 6 0, 9 1 0,
9 2 0, 9 3 0, 9 4 0, 9 5 0, 10 0 0, 10 1 0,
10 2 0, 10 3 0, 10 4 0, -11 0 1, -11 1 1, -11 2 1,
-10 1 1, -10 2 1, -10 3 1, -10 4 1, -9 0 1, -9 1 1,
-9 2 1, -9 4 1, -9 5 1, -9 6 1, -8 1 1, -8 2 1,
-8 6 1, -8 7 1, -7 0 1, -7 1 1, -7 5 1, -7 8 1,
-6 1 1, -6 8 1, -5 0 1, -5 4 1, -5 7 1, -5 8 1,

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PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 591 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 6 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ 2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 6 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of 3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.830 Note
Predicted wR2: Based on SigI**2 5.69 or SHELX Weight 5.69
PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value 0.1517 Check
PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value 0.4344 Check

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72 ALERT level A = Most likely a serious problem - resolve or explain
11 ALERT level B = A potentially serious problem, consider carefully
53 ALERT level C = Check. Ensure it is not caused by an omission or oversight
42 ALERT level G = General information/check it is not something unexpected

133 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
9 ALERT type 5 Informative message, check

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Datablock: 8.04_GPa

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Bond precision:  Si- O = 0.0030 A          Wavelength=0.49570

Cell:            a=9.397(3)      b=8.577(5)      c=5.149(1)
                  alpha=90       beta=106.11(3)   gamma=90
Temperature:     293 K

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	Calculated	Reported
Volume	398.7(3)	398.7(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.544	3.557
Z	1	4
Mu (mm-1)	0.735	0.726
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,8,8
Nref	1923	573
Tmin,Tmax		0.696,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.696 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.298 Theta(max)= 24.290

R(reflections)= 0.0396(410) wR2(reflections)=
wR= 0.0579(573)

S = 1.730 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 12.36 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.560 Why?

PLAT701_ALERT_1_A Bond Calc 1.604(3), Rep 1.625(5), Dev.. 7.00 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_A Bond Calc 2.070(3), Rep 2.115(5), Dev.. 15.00 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.070(3), Rep 2.115(5), Dev.. 15.00 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond Calc 1.918(2), Rep 1.931(3), Dev.. 6.50 Sigma

	O11A	-MM11	1_555	1_554		#	7 Check
PLAT701_ALERT_1_A Bond	Calc		1.918(2), Rep	1.931(3), Dev..			6.50 Sigma
	O11A	-FM11	1_555	1_554		#	8 Check
PLAT701_ALERT_1_A Bond	Calc		2.310(3), Rep	2.348(5), Dev..			12.67 Sigma
	O11A	-CA2	1_555	1_565		#	9 Check
PLAT701_ALERT_1_A Bond	Calc		2.310(3), Rep	2.348(5), Dev..			12.67 Sigma
	O11A	-NA2	1_555	1_565		#	10 Check
PLAT701_ALERT_1_A Bond	Calc		1.602(3), Rep	1.622(5), Dev..			6.67 Sigma
	O12A	-SIB1	1_555	1_655		#	11 Check
PLAT701_ALERT_1_A Bond	Calc		2.033(2), Rep	2.058(3), Dev..			12.50 Sigma
	O12A	-MGM1	1_555	1_555		#	12 Check
PLAT701_ALERT_1_A Bond	Calc		2.033(2), Rep	2.058(3), Dev..			12.50 Sigma
	O12A	-FM1	1_555	1_555		#	14 Check
PLAT701_ALERT_1_A Bond	Calc		1.950(3), Rep	1.980(5), Dev..			10.00 Sigma
	O12A	-MM11	1_555	1_555		#	17 Check
PLAT701_ALERT_1_A Bond	Calc		1.950(3), Rep	1.980(5), Dev..			10.00 Sigma
	O12A	-FM11	1_555	1_555		#	18 Check
PLAT701_ALERT_1_A Bond	Calc		2.347(3), Rep	2.391(5), Dev..			14.67 Sigma
	O12A	-CA21	1_555	1_555		#	19 Check
PLAT701_ALERT_1_A Bond	Calc		2.347(3), Rep	2.391(5), Dev..			14.67 Sigma
	O12A	-NA21	1_555	1_555		#	20 Check
PLAT701_ALERT_1_A Bond	Calc		1.584(3), Rep	1.603(5), Dev..			6.33 Sigma
	O21A	-SIA1	1_555	1_545		#	21 Check
PLAT701_ALERT_1_A Bond	Calc		1.872(3), Rep	1.887(5), Dev..			5.00 Sigma
	O21A	-MM11	1_555	3_666		#	24 Check
PLAT701_ALERT_1_A Bond	Calc		1.872(3), Rep	1.887(5), Dev..			5.00 Sigma
	O21A	-FM11	1_555	3_666		#	25 Check
PLAT701_ALERT_1_A Bond	Calc		2.326(3), Rep	2.358(4), Dev..			10.67 Sigma
	O21A	-CA2	1_555	3_656		#	26 Check
PLAT701_ALERT_1_A Bond	Calc		2.326(3), Rep	2.358(4), Dev..			10.67 Sigma
	O21A	-NA2	1_555	3_656		#	27 Check
PLAT701_ALERT_1_A Bond	Calc		1.575(3), Rep	1.588(5), Dev..			4.33 Sigma
	O22A	-SIB1	1_555	1_555		#	28 Check
PLAT701_ALERT_1_A Bond	Calc		1.989(3), Rep	2.025(5), Dev..			12.00 Sigma
	O22A	-MGM1	1_555	3_666		#	29 Check
PLAT701_ALERT_1_A Bond	Calc		1.989(3), Rep	2.025(5), Dev..			12.00 Sigma
	O22A	-FM1	1_555	3_666		#	31 Check
PLAT701_ALERT_1_A Bond	Calc		2.349(3), Rep	2.384(4), Dev..			11.67 Sigma
	O22A	-CA21	1_555	3_667		#	32 Check
PLAT701_ALERT_1_A Bond	Calc		2.349(3), Rep	2.384(4), Dev..			11.67 Sigma
	O22A	-NA21	1_555	3_667		#	33 Check
PLAT701_ALERT_1_A Bond	Calc		1.653(3), Rep	1.670(4), Dev..			5.67 Sigma
	O31A	-SIB1	1_555	1_554		#	35 Check
PLAT701_ALERT_1_A Bond	Calc		1.646(3), Rep	1.659(4), Dev..			4.33 Sigma
	O32A	-SIA1	1_555	1_555		#	36 Check
PLAT701_ALERT_1_A Bond	Calc		2.978(2), Rep	3.025(2), Dev..			23.50 Sigma
	SIA1	-CA2	1_555	3_666		#	38 Check
PLAT701_ALERT_1_A Bond	Calc		2.978(2), Rep	3.025(2), Dev..			23.50 Sigma
	SIA1	-NA2	1_555	3_666		#	39 Check
PLAT701_ALERT_1_A Bond	Calc		3.192(3), Rep	3.270(4), Dev..			26.00 Sigma
	SIA1	-CA21	1_555	3_666		#	40 Check
PLAT701_ALERT_1_A Bond	Calc		3.130(3), Rep	3.198(4), Dev..			22.67 Sigma
	SIB1	-CA2	1_555	3_666		#	41 Check
PLAT701_ALERT_1_A Bond	Calc		3.130(3), Rep	3.198(4), Dev..			22.67 Sigma
	SIB1	-NA2	1_555	3_666		#	42 Check
PLAT701_ALERT_1_A Bond	Calc		2.999(2), Rep	3.049(2), Dev..			25.00 Sigma
	SIB1	-CA21	1_555	3_667		#	43 Check

PLAT701_ALERT_1_A Bond	Calc	2.999(2), Rep	3.049(2), Dev..	25.00 Sigma
SIB1	-NA21	1_555	3_667	# 44 Check
PLAT701_ALERT_1_A Bond	Calc	3.018(2), Rep	3.086(2), Dev..	34.00 Sigma
MGM1	-AM11	1_555	1_554	# 48 Check
PLAT701_ALERT_1_A Bond	Calc	3.018(2), Rep	3.086(2), Dev..	34.00 Sigma
MGM1	-AM11	1_555	1_555	# 49 Check
PLAT701_ALERT_1_A Bond	Calc	3.018(2), Rep	3.086(2), Dev..	34.00 Sigma
MGM1	-MM11	1_555	1_554	# 52 Check
PLAT701_ALERT_1_A Bond	Calc	3.018(2), Rep	3.086(2), Dev..	34.00 Sigma
MGM1	-MM11	1_555	1_555	# 53 Check
PLAT701_ALERT_1_A Bond	Calc	3.390(3), Rep	3.436(6), Dev..	15.33 Sigma
MGM1	-CA2	1_555	1_565	# 54 Check
PLAT701_ALERT_1_A Bond	Calc	3.390(3), Rep	3.436(6), Dev..	15.33 Sigma
MGM1	-NA2	1_555	1_565	# 55 Check
PLAT701_ALERT_1_A Bond	Calc	3.171(2), Rep	3.203(2), Dev..	16.00 Sigma
MGM1	-CA21	1_555	1_554	# 56 Check
PLAT701_ALERT_1_A Bond	Calc	3.171(2), Rep	3.203(2), Dev..	16.00 Sigma
MGM1	-CA21	1_555	1_555	# 57 Check
PLAT701_ALERT_1_A Bond	Calc	3.171(2), Rep	3.203(2), Dev..	16.00 Sigma
MGM1	-NA21	1_555	1_554	# 58 Check
PLAT701_ALERT_1_A Bond	Calc	3.171(2), Rep	3.203(2), Dev..	16.00 Sigma
MGM1	-NA21	1_555	1_555	# 59 Check
PLAT701_ALERT_1_A Bond	Calc	3.018(2), Rep	3.086(2), Dev..	34.00 Sigma
AM1	-MM11	1_555	1_554	# 71 Check
PLAT701_ALERT_1_A Bond	Calc	3.018(2), Rep	3.086(2), Dev..	34.00 Sigma
AM1	-MM11	1_555	1_555	# 72 Check
PLAT701_ALERT_1_A Bond	Calc	3.390(3), Rep	3.436(6), Dev..	15.33 Sigma
AM1	-CA2	1_555	1_565	# 73 Check
PLAT701_ALERT_1_A Bond	Calc	3.390(3), Rep	3.436(6), Dev..	15.33 Sigma
AM1	-NA2	1_555	1_565	# 74 Check
PLAT701_ALERT_1_A Bond	Calc	3.171(2), Rep	3.203(2), Dev..	16.00 Sigma
AM1	-CA21	1_555	1_554	# 75 Check
PLAT701_ALERT_1_A Bond	Calc	3.171(2), Rep	3.203(2), Dev..	16.00 Sigma
AM1	-CA21	1_555	1_555	# 76 Check
PLAT701_ALERT_1_A Bond	Calc	3.171(2), Rep	3.203(2), Dev..	16.00 Sigma
AM1	-NA21	1_555	1_554	# 77 Check
PLAT701_ALERT_1_A Bond	Calc	3.171(2), Rep	3.203(2), Dev..	16.00 Sigma
AM1	-NA21	1_555	1_555	# 78 Check
PLAT701_ALERT_1_A Bond	Calc	3.171(2), Rep	3.203(2), Dev..	16.00 Sigma
FM1	-CA21	1_555	1_554	# 79 Check
PLAT701_ALERT_1_A Bond	Calc	3.171(2), Rep	3.203(2), Dev..	16.00 Sigma
FM1	-CA21	1_555	1_555	# 80 Check
PLAT701_ALERT_1_A Bond	Calc	3.171(2), Rep	3.203(2), Dev..	16.00 Sigma
FM1	-NA21	1_555	1_554	# 81 Check
PLAT701_ALERT_1_A Bond	Calc	3.171(2), Rep	3.203(2), Dev..	16.00 Sigma
FM1	-NA21	1_555	1_555	# 82 Check
PLAT701_ALERT_1_A Bond	Calc	3.150(2), Rep	3.181(3), Dev..	15.50 Sigma
AM11	-CA2	1_555	1_565	# 87 Check
PLAT701_ALERT_1_A Bond	Calc	3.150(2), Rep	3.181(3), Dev..	15.50 Sigma
AM11	-CA2	1_555	1_566	# 88 Check
PLAT701_ALERT_1_A Bond	Calc	3.150(2), Rep	3.181(3), Dev..	15.50 Sigma
AM11	-NA2	1_555	1_565	# 89 Check
PLAT701_ALERT_1_A Bond	Calc	3.150(2), Rep	3.181(3), Dev..	15.50 Sigma
AM11	-NA2	1_555	1_566	# 90 Check
PLAT701_ALERT_1_A Bond	Calc	3.426(3), Rep	3.473(5), Dev..	15.67 Sigma
AM11	-CA21	1_555	1_555	# 91 Check
PLAT701_ALERT_1_A Bond	Calc	3.426(3), Rep	3.473(5), Dev..	15.67 Sigma

AM11	-NA21	1_555	1_555		#	92 Check
PLAT701_ALERT_1_A Bond	Calc	3.150(2), Rep	3.181(3), Dev..			15.50 Sigma
MM11	-CA2	1_555	1_565		#	109 Check
PLAT701_ALERT_1_A Bond	Calc	3.150(2), Rep	3.181(3), Dev..			15.50 Sigma
MM11	-CA2	1_555	1_566		#	110 Check
PLAT701_ALERT_1_A Bond	Calc	3.150(2), Rep	3.181(3), Dev..			15.50 Sigma
MM11	-NA2	1_555	1_565		#	111 Check
PLAT701_ALERT_1_A Bond	Calc	3.150(2), Rep	3.181(3), Dev..			15.50 Sigma
MM11	-NA2	1_555	1_566		#	112 Check
PLAT701_ALERT_1_A Bond	Calc	3.426(3), Rep	3.473(5), Dev..			15.67 Sigma
MM11	-CA21	1_555	1_555		#	113 Check
PLAT701_ALERT_1_A Bond	Calc	3.426(3), Rep	3.473(5), Dev..			15.67 Sigma
MM11	-NA21	1_555	1_555		#	114 Check
PLAT701_ALERT_1_A Bond	Calc	3.150(2), Rep	3.181(3), Dev..			15.50 Sigma
FM11	-CA2	1_555	1_565		#	115 Check
PLAT701_ALERT_1_A Bond	Calc	3.150(2), Rep	3.181(3), Dev..			15.50 Sigma
FM11	-CA2	1_555	1_566		#	116 Check
PLAT701_ALERT_1_A Bond	Calc	3.150(2), Rep	3.181(3), Dev..			15.50 Sigma
FM11	-NA2	1_555	1_565		#	117 Check
PLAT701_ALERT_1_A Bond	Calc	3.150(2), Rep	3.181(3), Dev..			15.50 Sigma
FM11	-NA2	1_555	1_566		#	118 Check

Alert level B

PLAT017_ALERT_1_B Check Scattering Type Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B Check Scattering Type Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B Check Scattering Type Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B Check Scattering Type Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B Check Scattering Type Consistency of FM11	as	FE Error?
PLAT088_ALERT_3_B Poor Data / Parameter Ratio		6.10 Note

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula	Strings Differ	Please Check
Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8		
Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6		
Si2		
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula	Strings Differ	Please Check
Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695		
(Na)		
Rep.: ?		
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..	3.08 Check	
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...	Please Check	
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...	Please Check	
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...	Please Check	
PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms .	Please Check	
PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare)	O11A Check	
PLAT701_ALERT_1_C Bond Calc 1.639(3), Rep 1.644(5), Dev..	1.67 Sigma	
O32A -SIB1 1_555 1_555	# 37 Check	
PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label	MnM1 Check	
O11A MNM1		
PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label	Cm11 Check	
O11A CM11		
PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label	Tm11 Check	
O11A TM11		
PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label	MnM1 Check	
O12A MNM1		

PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O12A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	TM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check

	TM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	NA21				

- Alert level G

[illegible]

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        6 0 0,    6 1 0,    6 2 0,    6 3 0,    6 4 0,    6 5 0,
        6 8 0,    7 1 0,    7 2 0,    7 4 0,    7 5 0,    7 6 0,
        7 7 0,    8 0 0,    8 1 0,    8 2 0,    8 3 0,    8 4 0,
        8 5 0,    8 6 0,    9 1 0,    9 2 0,    9 3 0,    9 5 0,
       10 0 0,   10 1 0,   10 2 0,   10 3 0,  -11 0 1, -11 1 1,
      -10 1 1, -10 2 1, -10 3 1,  -9 0 1,  -9 1 1,  -9 2 1,
      -9 4 1,  -9 6 1,  -8 1 1,  -8 2 1,  -8 5 1,  -8 6 1,
      -8 7 1,  -7 0 1,  -7 1 1,  -7 3 1,  -7 5 1,  -7 8 1,
      -6 1 1,  -6 8 1,  -5 0 1,  -5 7 1,  -5 8 1,  -4 5 1,
      -4 6 1,  -4 7 1,  -4 8 1,  -3 4 1,  -3 5 1,  -3 6 1,

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PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      570 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked      ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ      2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ      6 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ      2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ      6 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of      3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      1.769 Note
      Predicted wR2: Based on SigI**2 5.98 or SHELX Weight 5.98
PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value 0.1517 Check
PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value 0.4344 Check

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76 ALERT level A = Most likely a serious problem - resolve or explain
 6 ALERT level B = A potentially serious problem, consider carefully
48 ALERT level C = Check. Ensure it is not caused by an omission or oversight
42 ALERT level G = General information/check it is not something unexpected

135 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 3 ALERT type 2 Indicator that the structure model may be wrong or deficient
 6 ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
 9 ALERT type 5 Informative message, check

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Datablock: 8.46_GPa

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Bond precision:   Si- O = 0.0040 A           Wavelength=0.49570

Cell:             a=9.389(3)           b=8.571(5)           c=5.141(1)
                  alpha=90             beta=106.05(3)        gamma=90
Temperature:      293 K

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	Calculated	Reported
Volume	397.6(3)	397.6(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.554	3.567
Z	1	4
Mu (mm-1)	0.737	0.728
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,8,8
Nref	1932	580
Tmin,Tmax		0.941,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.941 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.300 Theta(max)= 24.350

R(reflections)= 0.0430(391) wR2(reflections)=
wR= 0.0722(580)

S = 1.780 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 13.33 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.550 Why?

PLAT701_ALERT_1_A Bond Calc 1.605(4), Rep 1.625(5), Dev.. 5.00 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_A Bond Calc 2.063(4), Rep 2.115(5), Dev.. 13.00 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.063(4), Rep 2.115(5), Dev.. 13.00 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond Calc 1.916(3), Rep 1.931(3), Dev.. 5.00 Sigma

	O11A	-MM11	1_555	1_554		#	7 Check
PLAT701_ALERT_1_A Bond	Calc		1.916(3), Rep	1.931(3), Dev..			5.00 Sigma
	O11A	-FM11	1_555	1_554		#	8 Check
PLAT701_ALERT_1_A Bond	Calc		2.310(4), Rep	2.348(5), Dev..			9.50 Sigma
	O11A	-CA2	1_555	1_565		#	9 Check
PLAT701_ALERT_1_A Bond	Calc		2.310(4), Rep	2.348(5), Dev..			9.50 Sigma
	O11A	-NA2	1_555	1_565		#	10 Check
PLAT701_ALERT_1_A Bond	Calc		1.603(4), Rep	1.622(5), Dev..			4.75 Sigma
	O12A	-SIB1	1_555	1_655		#	11 Check
PLAT701_ALERT_1_A Bond	Calc		2.026(3), Rep	2.058(3), Dev..			10.67 Sigma
	O12A	-MGM1	1_555	1_555		#	12 Check
PLAT701_ALERT_1_A Bond	Calc		2.026(3), Rep	2.058(3), Dev..			10.67 Sigma
	O12A	-FM1	1_555	1_555		#	14 Check
PLAT701_ALERT_1_A Bond	Calc		1.943(4), Rep	1.980(5), Dev..			9.25 Sigma
	O12A	-MM11	1_555	1_555		#	17 Check
PLAT701_ALERT_1_A Bond	Calc		1.943(4), Rep	1.980(5), Dev..			9.25 Sigma
	O12A	-FM11	1_555	1_555		#	18 Check
PLAT701_ALERT_1_A Bond	Calc		2.349(4), Rep	2.391(5), Dev..			10.50 Sigma
	O12A	-CA21	1_555	1_555		#	19 Check
PLAT701_ALERT_1_A Bond	Calc		2.349(4), Rep	2.391(5), Dev..			10.50 Sigma
	O12A	-NA21	1_555	1_555		#	20 Check
PLAT701_ALERT_1_A Bond	Calc		1.582(4), Rep	1.603(5), Dev..			5.25 Sigma
	O21A	-SIA1	1_555	1_545		#	21 Check
PLAT701_ALERT_1_A Bond	Calc		1.873(4), Rep	1.887(5), Dev..			3.50 Sigma
	O21A	-MM11	1_555	3_666		#	24 Check
PLAT701_ALERT_1_A Bond	Calc		1.873(4), Rep	1.887(5), Dev..			3.50 Sigma
	O21A	-FM11	1_555	3_666		#	25 Check
PLAT701_ALERT_1_A Bond	Calc		2.312(3), Rep	2.358(4), Dev..			15.33 Sigma
	O21A	-CA2	1_555	3_656		#	26 Check
PLAT701_ALERT_1_A Bond	Calc		2.312(3), Rep	2.358(4), Dev..			15.33 Sigma
	O21A	-NA2	1_555	3_656		#	27 Check
PLAT701_ALERT_1_A Bond	Calc		1.566(4), Rep	1.588(5), Dev..			5.50 Sigma
	O22A	-SIB1	1_555	1_555		#	28 Check
PLAT701_ALERT_1_A Bond	Calc		1.990(4), Rep	2.025(5), Dev..			8.75 Sigma
	O22A	-MGM1	1_555	3_666		#	29 Check
PLAT701_ALERT_1_A Bond	Calc		1.990(4), Rep	2.025(5), Dev..			8.75 Sigma
	O22A	-FM1	1_555	3_666		#	31 Check
PLAT701_ALERT_1_A Bond	Calc		2.342(3), Rep	2.384(4), Dev..			14.00 Sigma
	O22A	-CA21	1_555	3_667		#	32 Check
PLAT701_ALERT_1_A Bond	Calc		2.342(3), Rep	2.384(4), Dev..			14.00 Sigma
	O22A	-NA21	1_555	3_667		#	33 Check
PLAT701_ALERT_1_A Bond	Calc		1.653(3), Rep	1.670(4), Dev..			5.67 Sigma
	O31A	-SIB1	1_555	1_554		#	35 Check
PLAT701_ALERT_1_A Bond	Calc		1.645(3), Rep	1.659(4), Dev..			4.67 Sigma
	O32A	-SIA1	1_555	1_555		#	36 Check
PLAT701_ALERT_1_A Bond	Calc		2.975(2), Rep	3.025(2), Dev..			25.00 Sigma
	SIA1	-CA2	1_555	3_666		#	38 Check
PLAT701_ALERT_1_A Bond	Calc		2.975(2), Rep	3.025(2), Dev..			25.00 Sigma
	SIA1	-NA2	1_555	3_666		#	39 Check
PLAT701_ALERT_1_A Bond	Calc		3.192(3), Rep	3.270(4), Dev..			26.00 Sigma
	SIA1	-CA21	1_555	3_666		#	40 Check
PLAT701_ALERT_1_A Bond	Calc		3.133(3), Rep	3.198(4), Dev..			21.67 Sigma
	SIB1	-CA2	1_555	3_666		#	41 Check
PLAT701_ALERT_1_A Bond	Calc		3.133(3), Rep	3.198(4), Dev..			21.67 Sigma
	SIB1	-NA2	1_555	3_666		#	42 Check
PLAT701_ALERT_1_A Bond	Calc		2.996(2), Rep	3.049(2), Dev..			26.50 Sigma
	SIB1	-CA21	1_555	3_667		#	43 Check

PLAT701_ALERT_1_A Bond	Calc	2.996(2), Rep	3.049(2), Dev..		26.50 Sigma
SIB1	-NA21	1_555	3_667	#	44 Check
PLAT701_ALERT_1_A Bond	Calc	3.012(3), Rep	3.086(2), Dev..		24.67 Sigma
MGM1	-AM11	1_555	1_554	#	48 Check
PLAT701_ALERT_1_A Bond	Calc	3.012(3), Rep	3.086(2), Dev..		24.67 Sigma
MGM1	-AM11	1_555	1_555	#	49 Check
PLAT701_ALERT_1_A Bond	Calc	3.012(3), Rep	3.086(2), Dev..		24.67 Sigma
MGM1	-MM11	1_555	1_554	#	52 Check
PLAT701_ALERT_1_A Bond	Calc	3.012(3), Rep	3.086(2), Dev..		24.67 Sigma
MGM1	-MM11	1_555	1_555	#	53 Check
PLAT701_ALERT_1_A Bond	Calc	3.389(4), Rep	3.436(6), Dev..		11.75 Sigma
MGM1	-CA2	1_555	1_565	#	54 Check
PLAT701_ALERT_1_A Bond	Calc	3.389(4), Rep	3.436(6), Dev..		11.75 Sigma
MGM1	-NA2	1_555	1_565	#	55 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(3), Rep	3.203(2), Dev..		11.33 Sigma
MGM1	-CA21	1_555	1_554	#	56 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(3), Rep	3.203(2), Dev..		11.33 Sigma
MGM1	-CA21	1_555	1_555	#	57 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(3), Rep	3.203(2), Dev..		11.33 Sigma
MGM1	-NA21	1_555	1_554	#	58 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(3), Rep	3.203(2), Dev..		11.33 Sigma
MGM1	-NA21	1_555	1_555	#	59 Check
PLAT701_ALERT_1_A Bond	Calc	3.012(3), Rep	3.086(2), Dev..		24.67 Sigma
AM1	-MM11	1_555	1_554	#	71 Check
PLAT701_ALERT_1_A Bond	Calc	3.012(3), Rep	3.086(2), Dev..		24.67 Sigma
AM1	-MM11	1_555	1_555	#	72 Check
PLAT701_ALERT_1_A Bond	Calc	3.389(4), Rep	3.436(6), Dev..		11.75 Sigma
AM1	-CA2	1_555	1_565	#	73 Check
PLAT701_ALERT_1_A Bond	Calc	3.389(4), Rep	3.436(6), Dev..		11.75 Sigma
AM1	-NA2	1_555	1_565	#	74 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(3), Rep	3.203(2), Dev..		11.33 Sigma
AM1	-CA21	1_555	1_554	#	75 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(3), Rep	3.203(2), Dev..		11.33 Sigma
AM1	-CA21	1_555	1_555	#	76 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(3), Rep	3.203(2), Dev..		11.33 Sigma
AM1	-NA21	1_555	1_554	#	77 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(3), Rep	3.203(2), Dev..		11.33 Sigma
AM1	-NA21	1_555	1_555	#	78 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(3), Rep	3.203(2), Dev..		11.33 Sigma
FM1	-CA21	1_555	1_554	#	79 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(3), Rep	3.203(2), Dev..		11.33 Sigma
FM1	-CA21	1_555	1_555	#	80 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(3), Rep	3.203(2), Dev..		11.33 Sigma
FM1	-NA21	1_555	1_554	#	81 Check
PLAT701_ALERT_1_A Bond	Calc	3.169(3), Rep	3.203(2), Dev..		11.33 Sigma
FM1	-NA21	1_555	1_555	#	82 Check
PLAT701_ALERT_1_A Bond	Calc	3.149(3), Rep	3.181(3), Dev..		10.67 Sigma
AM11	-CA2	1_555	1_565	#	87 Check
PLAT701_ALERT_1_A Bond	Calc	3.149(3), Rep	3.181(3), Dev..		10.67 Sigma
AM11	-CA2	1_555	1_566	#	88 Check
PLAT701_ALERT_1_A Bond	Calc	3.149(3), Rep	3.181(3), Dev..		10.67 Sigma
AM11	-NA2	1_555	1_565	#	89 Check
PLAT701_ALERT_1_A Bond	Calc	3.149(3), Rep	3.181(3), Dev..		10.67 Sigma
AM11	-NA2	1_555	1_566	#	90 Check
PLAT701_ALERT_1_A Bond	Calc	3.422(4), Rep	3.473(5), Dev..		12.75 Sigma
AM11	-CA21	1_555	1_555	#	91 Check
PLAT701_ALERT_1_A Bond	Calc	3.422(4), Rep	3.473(5), Dev..		12.75 Sigma

AM11	-NA21	1_555	1_555		#	92 Check
PLAT701_ALERT_1_A Bond	Calc	3.149(3), Rep	3.181(3), Dev..			10.67 Sigma
MM11	-CA2	1_555	1_565		#	109 Check
PLAT701_ALERT_1_A Bond	Calc	3.149(3), Rep	3.181(3), Dev..			10.67 Sigma
MM11	-CA2	1_555	1_566		#	110 Check
PLAT701_ALERT_1_A Bond	Calc	3.149(3), Rep	3.181(3), Dev..			10.67 Sigma
MM11	-NA2	1_555	1_565		#	111 Check
PLAT701_ALERT_1_A Bond	Calc	3.149(3), Rep	3.181(3), Dev..			10.67 Sigma
MM11	-NA2	1_555	1_566		#	112 Check
PLAT701_ALERT_1_A Bond	Calc	3.422(4), Rep	3.473(5), Dev..			12.75 Sigma
MM11	-CA21	1_555	1_555		#	113 Check
PLAT701_ALERT_1_A Bond	Calc	3.422(4), Rep	3.473(5), Dev..			12.75 Sigma
MM11	-NA21	1_555	1_555		#	114 Check
PLAT701_ALERT_1_A Bond	Calc	3.149(3), Rep	3.181(3), Dev..			10.67 Sigma
FM11	-CA2	1_555	1_565		#	115 Check
PLAT701_ALERT_1_A Bond	Calc	3.149(3), Rep	3.181(3), Dev..			10.67 Sigma
FM11	-CA2	1_555	1_566		#	116 Check
PLAT701_ALERT_1_A Bond	Calc	3.149(3), Rep	3.181(3), Dev..			10.67 Sigma
FM11	-NA2	1_555	1_565		#	117 Check
PLAT701_ALERT_1_A Bond	Calc	3.149(3), Rep	3.181(3), Dev..			10.67 Sigma
FM11	-NA2	1_555	1_566		#	118 Check

Alert level B

PLAT017_ALERT_1_B Check Scattering Type Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B Check Scattering Type Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B Check Scattering Type Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B Check Scattering Type Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B Check Scattering Type Consistency of FM11	as	FE Error?
PLAT088_ALERT_3_B Poor Data / Parameter Ratio		6.17 Note

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula	Strings Differ	Please Check
Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8		
Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6		
Si2		
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula	Strings Differ	Please Check
Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695		
(Na)		
Rep.: ?		
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..	3.08 Check	
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...	Please Check	
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...	Please Check	
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...	Please Check	
PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms .	Please Check	
PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare)	O11A Check	
PLAT701_ALERT_1_C Bond Calc 1.648(3), Rep 1.644(5), Dev..	1.33 Sigma	
O31A -SIA1 1_555 1_555	# 34 Check	
PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label	MnM1 Check	
O11A MNM1		
PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label	Cm11 Check	
O11A CM11		
PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label	Tm11 Check	
O11A TM11		
PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label	MnM1 Check	
O12A MNM1		

PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O12A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	TM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check

	TM11	FM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	TM11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	TM11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	TM11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	TM11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	TM11	Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	TM11	Check
	TM11	NA21		
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.41Ang From O12A	.	0.41 eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please	Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please	Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1	0.087	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11	0.052	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11	0.86	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1	0.868	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1	0.045	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11	0.088	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21	0.7904	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2	0.3622	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2	0.6378	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21	0.2096	Check
PLAT301_ALERT_3_G	Main Residue Disorder	1	20% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	2)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	3)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	4)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	5)	100% Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A	.	133.3 Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A	.	137.3 Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11	Fm11	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	1.84	Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
	0 1 0, 1 1 0,		
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L=	0.600	328 Report
	0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0,	0 7 0,	
	0 8 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0,	1 6 0,	
	1 7 0, 1 8 0, 2 0 0, 2 1 0, 2 2 0,	2 3 0,	
	2 4 0, 2 5 0, 2 6 0, 2 7 0, 2 8 0,	3 1 0,	
	3 4 0, 3 5 0, 3 6 0, 3 7 0, 3 8 0,	4 0 0,	

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      4 1 0,    4 6 0,    4 7 0,    4 8 0,    5 1 0,    5 7 0,
      5 8 0,    6 0 0,    6 1 0,    6 2 0,    6 4 0,    6 5 0,
      6 8 0,    7 1 0,    7 2 0,    7 5 0,    7 6 0,    7 7 0,
      8 0 0,    8 1 0,    8 2 0,    8 3 0,    8 4 0,    8 5 0,
      8 6 0,    9 1 0,    9 2 0,    9 3 0,    9 5 0,   10 0 0,
     10 1 0,   10 2 0,   10 3 0,  -11 0 1,  -11 1 1,  -10 1 1,
    -10 2 1,  -10 3 1,  -10 4 1,   -9 0 1,   -9 1 1,   -9 2 1,
     -9 4 1,   -9 6 1,   -8 1 1,   -8 2 1,   -8 5 1,   -8 6 1,
     -8 7 1,   -7 0 1,   -7 1 1,   -7 3 1,   -7 5 1,   -7 8 1,
     -6 1 1,   -6 8 1,   -5 0 1,   -5 7 1,   -5 8 1,   -4 5 1,
     -4 6 1,   -4 7 1,   -4 8 1,   -3 4 1,   -3 5 1,   -3 6 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      564 Note
PLAT929_ALERT_5_G No Weight Pars, Obs and Calc R1, wR2, S not Checked      ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ      2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ      6 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ      2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ      6 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of      3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      1.876 Note
      Predicted wR2: Based on SigI**2 7.52 or SHELX Weight 7.52
PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value 0.1517 Check
PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value 0.4344 Check

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76 ALERT level A = Most likely a serious problem - resolve or explain
 6 ALERT level B = A potentially serious problem, consider carefully
49 ALERT level C = Check. Ensure it is not caused by an omission or oversight
42 ALERT level G = General information/check it is not something unexpected

135 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 4 ALERT type 2 Indicator that the structure model may be wrong or deficient
 6 ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
 9 ALERT type 5 Informative message, check

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Datablock: 8.61_GPa

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Bond precision:   Si- O = 0.0040 A           Wavelength=0.49570

Cell:             a=9.386(3)                b=8.561(5)                c=5.141(1)
                  alpha=90                  beta=106.07(3)              gamma=90
Temperature:      293 K

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	Calculated	Reported
Volume	397.0(3)	397.0(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.559	3.573
Z	1	4
Mu (mm-1)	0.738	0.729
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,8,8
Nref	1939	557
Tmin,Tmax		0.907,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.907 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.287 Theta(max)= 24.390

R(reflections)= 0.0386(406) wR2(reflections)=
wR= 0.0601(557)

S = 2.400 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 12.25 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.540 Why?

PLAT088_ALERT_3_A Poor Data / Parameter Ratio 5.93 Note

PLAT701_ALERT_1_A Bond Calc 1.599(4), Rep 1.625(5), Dev.. 6.50 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_A Bond Calc 2.066(4), Rep 2.115(5), Dev.. 12.25 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.066(4), Rep 2.115(5), Dev.. 12.25 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond	Calc	1.919(3), Rep	1.931(3), Dev..	4.00 Sigma
O11A	-MM11	1_555	1_554	# 7 Check
PLAT701_ALERT_1_A Bond	Calc	1.919(3), Rep	1.931(3), Dev..	4.00 Sigma
O11A	-FM11	1_555	1_554	# 8 Check
PLAT701_ALERT_1_A Bond	Calc	2.306(4), Rep	2.348(5), Dev..	10.50 Sigma
O11A	-CA2	1_555	1_565	# 9 Check
PLAT701_ALERT_1_A Bond	Calc	2.306(4), Rep	2.348(5), Dev..	10.50 Sigma
O11A	-NA2	1_555	1_565	# 10 Check
PLAT701_ALERT_1_A Bond	Calc	1.600(4), Rep	1.622(5), Dev..	5.50 Sigma
O12A	-SIB1	1_555	1_655	# 11 Check
PLAT701_ALERT_1_A Bond	Calc	2.032(3), Rep	2.058(3), Dev..	8.67 Sigma
O12A	-MGM1	1_555	1_555	# 12 Check
PLAT701_ALERT_1_A Bond	Calc	2.032(3), Rep	2.058(3), Dev..	8.67 Sigma
O12A	-FM1	1_555	1_555	# 14 Check
PLAT701_ALERT_1_A Bond	Calc	1.941(4), Rep	1.980(5), Dev..	9.75 Sigma
O12A	-MM11	1_555	1_555	# 17 Check
PLAT701_ALERT_1_A Bond	Calc	1.941(4), Rep	1.980(5), Dev..	9.75 Sigma
O12A	-FM11	1_555	1_555	# 18 Check
PLAT701_ALERT_1_A Bond	Calc	2.345(4), Rep	2.391(5), Dev..	11.50 Sigma
O12A	-CA21	1_555	1_555	# 19 Check
PLAT701_ALERT_1_A Bond	Calc	2.345(4), Rep	2.391(5), Dev..	11.50 Sigma
O12A	-NA21	1_555	1_555	# 20 Check
PLAT701_ALERT_1_A Bond	Calc	1.585(4), Rep	1.603(5), Dev..	4.50 Sigma
O21A	-SIA1	1_555	1_545	# 21 Check
PLAT701_ALERT_1_A Bond	Calc	1.867(4), Rep	1.887(5), Dev..	5.00 Sigma
O21A	-MM11	1_555	3_666	# 24 Check
PLAT701_ALERT_1_A Bond	Calc	1.867(4), Rep	1.887(5), Dev..	5.00 Sigma
O21A	-FM11	1_555	3_666	# 25 Check
PLAT701_ALERT_1_A Bond	Calc	2.320(3), Rep	2.358(4), Dev..	12.67 Sigma
O21A	-CA2	1_555	3_656	# 26 Check
PLAT701_ALERT_1_A Bond	Calc	2.320(3), Rep	2.358(4), Dev..	12.67 Sigma
O21A	-NA2	1_555	3_656	# 27 Check
PLAT701_ALERT_1_A Bond	Calc	1.575(4), Rep	1.588(5), Dev..	3.25 Sigma
O22A	-SIB1	1_555	1_555	# 28 Check
PLAT701_ALERT_1_A Bond	Calc	1.983(4), Rep	2.025(5), Dev..	10.50 Sigma
O22A	-MGM1	1_555	3_666	# 29 Check
PLAT701_ALERT_1_A Bond	Calc	1.983(4), Rep	2.025(5), Dev..	10.50 Sigma
O22A	-FM1	1_555	3_666	# 31 Check
PLAT701_ALERT_1_A Bond	Calc	2.347(3), Rep	2.384(4), Dev..	12.33 Sigma
O22A	-CA21	1_555	3_667	# 32 Check
PLAT701_ALERT_1_A Bond	Calc	2.347(3), Rep	2.384(4), Dev..	12.33 Sigma
O22A	-NA21	1_555	3_667	# 33 Check
PLAT701_ALERT_1_A Bond	Calc	1.654(3), Rep	1.670(4), Dev..	5.33 Sigma
O31A	-SIB1	1_555	1_554	# 35 Check
PLAT701_ALERT_1_A Bond	Calc	2.975(2), Rep	3.025(2), Dev..	25.00 Sigma
SIA1	-CA2	1_555	3_666	# 38 Check
PLAT701_ALERT_1_A Bond	Calc	2.975(2), Rep	3.025(2), Dev..	25.00 Sigma
SIA1	-NA2	1_555	3_666	# 39 Check
PLAT701_ALERT_1_A Bond	Calc	3.186(3), Rep	3.270(4), Dev..	28.00 Sigma
SIA1	-CA21	1_555	3_666	# 40 Check
PLAT701_ALERT_1_A Bond	Calc	3.126(3), Rep	3.198(4), Dev..	24.00 Sigma
SIB1	-CA2	1_555	3_666	# 41 Check
PLAT701_ALERT_1_A Bond	Calc	3.126(3), Rep	3.198(4), Dev..	24.00 Sigma
SIB1	-NA2	1_555	3_666	# 42 Check
PLAT701_ALERT_1_A Bond	Calc	2.996(2), Rep	3.049(2), Dev..	26.50 Sigma
SIB1	-CA21	1_555	3_667	# 43 Check
PLAT701_ALERT_1_A Bond	Calc	2.996(2), Rep	3.049(2), Dev..	26.50 Sigma

SIB1	-NA21	1_555	3_667		#	44 Check
PLAT701_ALERT_1_A Bond	Calc	3.011(2), Rep	3.086(2), Dev..			37.50 Sigma
MGM1	-AM11	1_555	1_554		#	48 Check
PLAT701_ALERT_1_A Bond	Calc	3.011(2), Rep	3.086(2), Dev..			37.50 Sigma
MGM1	-AM11	1_555	1_555		#	49 Check
PLAT701_ALERT_1_A Bond	Calc	3.011(2), Rep	3.086(2), Dev..			37.50 Sigma
MGM1	-MM11	1_555	1_554		#	52 Check
PLAT701_ALERT_1_A Bond	Calc	3.011(2), Rep	3.086(2), Dev..			37.50 Sigma
MGM1	-MM11	1_555	1_555		#	53 Check
PLAT701_ALERT_1_A Bond	Calc	3.383(4), Rep	3.436(6), Dev..			13.25 Sigma
MGM1	-CA2	1_555	1_565		#	54 Check
PLAT701_ALERT_1_A Bond	Calc	3.383(4), Rep	3.436(6), Dev..			13.25 Sigma
MGM1	-NA2	1_555	1_565		#	55 Check
PLAT701_ALERT_1_A Bond	Calc	3.168(2), Rep	3.203(2), Dev..			17.50 Sigma
MGM1	-CA21	1_555	1_554		#	56 Check
PLAT701_ALERT_1_A Bond	Calc	3.168(2), Rep	3.203(2), Dev..			17.50 Sigma
MGM1	-CA21	1_555	1_555		#	57 Check
PLAT701_ALERT_1_A Bond	Calc	3.168(2), Rep	3.203(2), Dev..			17.50 Sigma
MGM1	-NA21	1_555	1_554		#	58 Check
PLAT701_ALERT_1_A Bond	Calc	3.168(2), Rep	3.203(2), Dev..			17.50 Sigma
MGM1	-NA21	1_555	1_555		#	59 Check
PLAT701_ALERT_1_A Bond	Calc	3.011(2), Rep	3.086(2), Dev..			37.50 Sigma
AM1	-MM11	1_555	1_554		#	71 Check
PLAT701_ALERT_1_A Bond	Calc	3.011(2), Rep	3.086(2), Dev..			37.50 Sigma
AM1	-MM11	1_555	1_555		#	72 Check
PLAT701_ALERT_1_A Bond	Calc	3.383(4), Rep	3.436(6), Dev..			13.25 Sigma
AM1	-CA2	1_555	1_565		#	73 Check
PLAT701_ALERT_1_A Bond	Calc	3.383(4), Rep	3.436(6), Dev..			13.25 Sigma
AM1	-NA2	1_555	1_565		#	74 Check
PLAT701_ALERT_1_A Bond	Calc	3.168(2), Rep	3.203(2), Dev..			17.50 Sigma
AM1	-CA21	1_555	1_554		#	75 Check
PLAT701_ALERT_1_A Bond	Calc	3.168(2), Rep	3.203(2), Dev..			17.50 Sigma
AM1	-CA21	1_555	1_555		#	76 Check
PLAT701_ALERT_1_A Bond	Calc	3.168(2), Rep	3.203(2), Dev..			17.50 Sigma
AM1	-NA21	1_555	1_554		#	77 Check
PLAT701_ALERT_1_A Bond	Calc	3.168(2), Rep	3.203(2), Dev..			17.50 Sigma
AM1	-NA21	1_555	1_555		#	78 Check
PLAT701_ALERT_1_A Bond	Calc	3.168(2), Rep	3.203(2), Dev..			17.50 Sigma
FM1	-CA21	1_555	1_554		#	79 Check
PLAT701_ALERT_1_A Bond	Calc	3.168(2), Rep	3.203(2), Dev..			17.50 Sigma
FM1	-CA21	1_555	1_555		#	80 Check
PLAT701_ALERT_1_A Bond	Calc	3.168(2), Rep	3.203(2), Dev..			17.50 Sigma
FM1	-NA21	1_555	1_554		#	81 Check
PLAT701_ALERT_1_A Bond	Calc	3.168(2), Rep	3.203(2), Dev..			17.50 Sigma
FM1	-NA21	1_555	1_555		#	82 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..			11.33 Sigma
AM11	-CA2	1_555	1_565		#	87 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..			11.33 Sigma
AM11	-CA2	1_555	1_566		#	88 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..			11.33 Sigma
AM11	-NA2	1_555	1_565		#	89 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..			11.33 Sigma
AM11	-NA2	1_555	1_566		#	90 Check
PLAT701_ALERT_1_A Bond	Calc	3.418(3), Rep	3.473(5), Dev..			18.33 Sigma
AM11	-CA21	1_555	1_555		#	91 Check
PLAT701_ALERT_1_A Bond	Calc	3.418(3), Rep	3.473(5), Dev..			18.33 Sigma
AM11	-NA21	1_555	1_555		#	92 Check

PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..	11.33 Sigma
MM11	-CA2	1_555	1_565	# 109 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..	11.33 Sigma
MM11	-CA2	1_555	1_566	# 110 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..	11.33 Sigma
MM11	-NA2	1_555	1_565	# 111 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..	11.33 Sigma
MM11	-NA2	1_555	1_566	# 112 Check
PLAT701_ALERT_1_A Bond	Calc	3.418(3), Rep	3.473(5), Dev..	18.33 Sigma
MM11	-CA21	1_555	1_555	# 113 Check
PLAT701_ALERT_1_A Bond	Calc	3.418(3), Rep	3.473(5), Dev..	18.33 Sigma
MM11	-NA21	1_555	1_555	# 114 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..	11.33 Sigma
FM11	-CA2	1_555	1_565	# 115 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..	11.33 Sigma
FM11	-CA2	1_555	1_566	# 116 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..	11.33 Sigma
FM11	-NA2	1_555	1_565	# 117 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..	11.33 Sigma
FM11	-NA2	1_555	1_566	# 118 Check

Alert level B

PLAT017_ALERT_1_B Check	Scattering Type Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of FM11	as	FE Error?
PLAT701_ALERT_1_B Bond	Calc	1.650(3), Rep	1.659(4), Dev..
O32A	-SIA1	1_555	1_555
			# 36 Check
PLAT701_ALERT_1_B Bond	Calc	1.636(3), Rep	1.644(5), Dev..
O32A	-SIB1	1_555	1_555
			# 37 Check

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
Goodness of fit given = 2.400

PLAT041_ALERT_1_C Calc. and Reported SumFormula	Strings Differ	Please Check
Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8		
Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2		
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula	Strings Differ	Please Check
Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)		
Rep.: ?		
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..	3.08 Check	
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...	Please Check	
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...	Please Check	
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...	Please Check	
PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms .	Please Check	
PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare)	O11A Check	
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	MnM1 Check
O11A	MNM1	
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	Cm11 Check
O11A	CM11	
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	Tm11 Check

	O11A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O12A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O12A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				

PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	MM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	FM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA21		

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1 Constrained at	0.087	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11 Constrained at	0.052	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11 Constrained at	0.86	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1 Constrained at	0.868	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1 Constrained at	0.045	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11 Constrained at	0.088	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21 Constrained at	0.7904	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2 Constrained at	0.3622	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2 Constrained at	0.6378	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21 Constrained at	0.2096	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A .	133.0	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A .	137.0	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11	Fm11	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.84	Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
	0 1 0, 1 1 0,		
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L= 0.600	340	Report
	0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,		
	0 8 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0, 1 6 0,		
	1 7 0, 1 8 0, 2 0 0, 2 1 0, 2 2 0, 2 3 0,		

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      2  4  0,    2  5  0,    2  6  0,    2  7  0,    2  8  0,    3  1  0,
      3  4  0,    3  5  0,    3  6  0,    3  7  0,    3  8  0,    4  0  0,
      4  1  0,    4  6  0,    4  7  0,    4  8  0,    5  1  0,    5  4  0,
      5  7  0,    5  8  0,    6  0  0,    6  1  0,    6  2  0,    6  3  0,
      6  4  0,    6  5  0,    6  8  0,    7  1  0,    7  2  0,    7  4  0,
      7  5  0,    7  6  0,    7  7  0,    8  0  0,    8  1  0,    8  2  0,
      8  3  0,    8  4  0,    8  5  0,    8  6  0,    9  1  0,    9  2  0,
      9  3  0,    9  5  0,   10  0  0,   10  1  0,   10  2  0,   10  3  0,
     -11  0  1,  -11  1  1,  -10  1  1,  -10  2  1,  -10  3  1,   -9  0  1,
     -9  1  1,   -9  2  1,   -9  4  1,   -9  6  1,   -8  1  1,   -8  2  1,
     -8  5  1,   -8  6  1,   -8  7  1,   -7  0  1,   -7  1  1,   -7  3  1,
     -7  5  1,   -7  8  1,   -6  1  1,   -6  8  1,   -5  0  1,   -5  1  1,
     -5  7  1,   -5  8  1,   -4  5  1,   -4  6  1,   -4  7  1,   -4  8  1,

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PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      575 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked      ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ      2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ      6 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ      2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ      6 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of      3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      2.761 Note
      Predicted wR2: Based on SigI**2 3.87 or SHELX Weight 3.87
PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value 0.1517 Check
PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value 0.4344 Check

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76 ALERT level A = Most likely a serious problem - resolve or explain
7  ALERT level B = A potentially serious problem, consider carefully
48 ALERT level C = Check. Ensure it is not caused by an omission or oversight
42 ALERT level G = General information/check it is not something unexpected

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135 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4  ALERT type 2 Indicator that the structure model may be wrong or deficient
6  ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
9  ALERT type 5 Informative message, check

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Datablock: 9.13_GPa

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Bond precision:   Si- O = 0.0040 A           Wavelength=0.49570

Cell:             a=9.388(3)                b=8.536(5)                c=5.138(1)
                  alpha=90                  beta=105.93(3)              gamma=90

Temperature:      293 K

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	Calculated	Reported
Volume	395.9(3)	395.9(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.569	3.582
Z	1	4
Mu (mm-1)	0.740	0.731
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,13,8	13,7,8
Nref	1802	424
Tmin,Tmax		0.798,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.798 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.235 Theta(max)= 23.810

R(reflections)= 0.0346(322) wR2(reflections)=
wR= 0.0531(424)

S = 1.990 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 10.66 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.460 Why?

PLAT088_ALERT_3_A Poor Data / Parameter Ratio 4.51 Note

PLAT701_ALERT_1_A Bond Calc 1.607(4), Rep 1.625(5), Dev.. 4.50 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_A Bond Calc 2.056(4), Rep 2.115(5), Dev.. 14.75 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.056(4), Rep 2.115(5), Dev.. 14.75 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond	Calc	1.919(3), Rep	1.931(3), Dev..	4.00 Sigma
O11A	-MM11	1_555	1_554	# 7 Check
PLAT701_ALERT_1_A Bond	Calc	1.919(3), Rep	1.931(3), Dev..	4.00 Sigma
O11A	-FM11	1_555	1_554	# 8 Check
PLAT701_ALERT_1_A Bond	Calc	2.309(4), Rep	2.348(5), Dev..	9.75 Sigma
O11A	-CA2	1_555	1_565	# 9 Check
PLAT701_ALERT_1_A Bond	Calc	2.309(4), Rep	2.348(5), Dev..	9.75 Sigma
O11A	-NA2	1_555	1_565	# 10 Check
PLAT701_ALERT_1_A Bond	Calc	1.606(3), Rep	1.622(5), Dev..	5.33 Sigma
O12A	-SIB1	1_555	1_655	# 11 Check
PLAT701_ALERT_1_A Bond	Calc	2.029(3), Rep	2.058(3), Dev..	9.67 Sigma
O12A	-MGM1	1_555	1_555	# 12 Check
PLAT701_ALERT_1_A Bond	Calc	2.029(3), Rep	2.058(3), Dev..	9.67 Sigma
O12A	-FM1	1_555	1_555	# 14 Check
PLAT701_ALERT_1_A Bond	Calc	1.938(4), Rep	1.980(5), Dev..	10.50 Sigma
O12A	-MM11	1_555	1_555	# 17 Check
PLAT701_ALERT_1_A Bond	Calc	1.938(4), Rep	1.980(5), Dev..	10.50 Sigma
O12A	-FM11	1_555	1_555	# 18 Check
PLAT701_ALERT_1_A Bond	Calc	2.339(4), Rep	2.391(5), Dev..	13.00 Sigma
O12A	-CA21	1_555	1_555	# 19 Check
PLAT701_ALERT_1_A Bond	Calc	2.339(4), Rep	2.391(5), Dev..	13.00 Sigma
O12A	-NA21	1_555	1_555	# 20 Check
PLAT701_ALERT_1_A Bond	Calc	1.583(4), Rep	1.603(5), Dev..	5.00 Sigma
O21A	-SIA1	1_555	1_545	# 21 Check
PLAT701_ALERT_1_A Bond	Calc	1.867(4), Rep	1.887(5), Dev..	5.00 Sigma
O21A	-MM11	1_555	3_666	# 24 Check
PLAT701_ALERT_1_A Bond	Calc	1.867(4), Rep	1.887(5), Dev..	5.00 Sigma
O21A	-FM11	1_555	3_666	# 25 Check
PLAT701_ALERT_1_A Bond	Calc	2.320(3), Rep	2.358(4), Dev..	12.67 Sigma
O21A	-CA2	1_555	3_656	# 26 Check
PLAT701_ALERT_1_A Bond	Calc	2.320(3), Rep	2.358(4), Dev..	12.67 Sigma
O21A	-NA2	1_555	3_656	# 27 Check
PLAT701_ALERT_1_A Bond	Calc	1.565(4), Rep	1.588(5), Dev..	5.75 Sigma
O22A	-SIB1	1_555	1_555	# 28 Check
PLAT701_ALERT_1_A Bond	Calc	1.985(4), Rep	2.025(5), Dev..	10.00 Sigma
O22A	-MGM1	1_555	3_666	# 29 Check
PLAT701_ALERT_1_A Bond	Calc	1.985(4), Rep	2.025(5), Dev..	10.00 Sigma
O22A	-FM1	1_555	3_666	# 31 Check
PLAT701_ALERT_1_A Bond	Calc	2.345(3), Rep	2.384(4), Dev..	13.00 Sigma
O22A	-CA21	1_555	3_667	# 32 Check
PLAT701_ALERT_1_A Bond	Calc	2.345(3), Rep	2.384(4), Dev..	13.00 Sigma
O22A	-NA21	1_555	3_667	# 33 Check
PLAT701_ALERT_1_A Bond	Calc	1.658(3), Rep	1.670(4), Dev..	4.00 Sigma
O31A	-SIB1	1_555	1_554	# 35 Check
PLAT701_ALERT_1_A Bond	Calc	1.646(3), Rep	1.659(4), Dev..	4.33 Sigma
O32A	-SIA1	1_555	1_555	# 36 Check
PLAT701_ALERT_1_A Bond	Calc	2.975(2), Rep	3.025(2), Dev..	25.00 Sigma
SIA1	-CA2	1_555	3_666	# 38 Check
PLAT701_ALERT_1_A Bond	Calc	2.975(2), Rep	3.025(2), Dev..	25.00 Sigma
SIA1	-NA2	1_555	3_666	# 39 Check
PLAT701_ALERT_1_A Bond	Calc	3.180(3), Rep	3.270(4), Dev..	30.00 Sigma
SIA1	-CA21	1_555	3_666	# 40 Check
PLAT701_ALERT_1_A Bond	Calc	3.120(3), Rep	3.198(4), Dev..	26.00 Sigma
SIB1	-CA2	1_555	3_666	# 41 Check
PLAT701_ALERT_1_A Bond	Calc	3.120(3), Rep	3.198(4), Dev..	26.00 Sigma
SIB1	-NA2	1_555	3_666	# 42 Check
PLAT701_ALERT_1_A Bond	Calc	2.996(2), Rep	3.049(2), Dev..	26.50 Sigma

	SIB1	-CA21	1_555	3_667		#	43 Check
PLAT701_ALERT_1_A	Bond	Calc	2.996(2), Rep	3.049(2), Dev..			26.50 Sigma
	SIB1	-NA21	1_555	3_667		#	44 Check
PLAT701_ALERT_1_A	Bond	Calc	3.008(2), Rep	3.086(2), Dev..			39.00 Sigma
	MGM1	-AM11	1_555	1_554		#	48 Check
PLAT701_ALERT_1_A	Bond	Calc	3.008(2), Rep	3.086(2), Dev..			39.00 Sigma
	MGM1	-AM11	1_555	1_555		#	49 Check
PLAT701_ALERT_1_A	Bond	Calc	3.008(2), Rep	3.086(2), Dev..			39.00 Sigma
	MGM1	-MM11	1_555	1_554		#	52 Check
PLAT701_ALERT_1_A	Bond	Calc	3.008(2), Rep	3.086(2), Dev..			39.00 Sigma
	MGM1	-MM11	1_555	1_555		#	53 Check
PLAT701_ALERT_1_A	Bond	Calc	3.380(4), Rep	3.436(6), Dev..			14.00 Sigma
	MGM1	-CA2	1_555	1_565		#	54 Check
PLAT701_ALERT_1_A	Bond	Calc	3.380(4), Rep	3.436(6), Dev..			14.00 Sigma
	MGM1	-NA2	1_555	1_565		#	55 Check
PLAT701_ALERT_1_A	Bond	Calc	3.163(3), Rep	3.203(2), Dev..			13.33 Sigma
	MGM1	-CA21	1_555	1_554		#	56 Check
PLAT701_ALERT_1_A	Bond	Calc	3.163(3), Rep	3.203(2), Dev..			13.33 Sigma
	MGM1	-CA21	1_555	1_555		#	57 Check
PLAT701_ALERT_1_A	Bond	Calc	3.163(3), Rep	3.203(2), Dev..			13.33 Sigma
	MGM1	-NA21	1_555	1_554		#	58 Check
PLAT701_ALERT_1_A	Bond	Calc	3.163(3), Rep	3.203(2), Dev..			13.33 Sigma
	MGM1	-NA21	1_555	1_555		#	59 Check
PLAT701_ALERT_1_A	Bond	Calc	3.008(2), Rep	3.086(2), Dev..			39.00 Sigma
	AM1	-MM11	1_555	1_554		#	71 Check
PLAT701_ALERT_1_A	Bond	Calc	3.008(2), Rep	3.086(2), Dev..			39.00 Sigma
	AM1	-MM11	1_555	1_555		#	72 Check
PLAT701_ALERT_1_A	Bond	Calc	3.380(4), Rep	3.436(6), Dev..			14.00 Sigma
	AM1	-CA2	1_555	1_565		#	73 Check
PLAT701_ALERT_1_A	Bond	Calc	3.380(4), Rep	3.436(6), Dev..			14.00 Sigma
	AM1	-NA2	1_555	1_565		#	74 Check
PLAT701_ALERT_1_A	Bond	Calc	3.163(3), Rep	3.203(2), Dev..			13.33 Sigma
	AM1	-CA21	1_555	1_554		#	75 Check
PLAT701_ALERT_1_A	Bond	Calc	3.163(3), Rep	3.203(2), Dev..			13.33 Sigma
	AM1	-CA21	1_555	1_555		#	76 Check
PLAT701_ALERT_1_A	Bond	Calc	3.163(3), Rep	3.203(2), Dev..			13.33 Sigma
	AM1	-NA21	1_555	1_554		#	77 Check
PLAT701_ALERT_1_A	Bond	Calc	3.163(3), Rep	3.203(2), Dev..			13.33 Sigma
	AM1	-NA21	1_555	1_555		#	78 Check
PLAT701_ALERT_1_A	Bond	Calc	3.163(3), Rep	3.203(2), Dev..			13.33 Sigma
	FM1	-CA21	1_555	1_554		#	79 Check
PLAT701_ALERT_1_A	Bond	Calc	3.163(3), Rep	3.203(2), Dev..			13.33 Sigma
	FM1	-CA21	1_555	1_555		#	80 Check
PLAT701_ALERT_1_A	Bond	Calc	3.163(3), Rep	3.203(2), Dev..			13.33 Sigma
	FM1	-NA21	1_555	1_554		#	81 Check
PLAT701_ALERT_1_A	Bond	Calc	3.163(3), Rep	3.203(2), Dev..			13.33 Sigma
	FM1	-NA21	1_555	1_555		#	82 Check
PLAT701_ALERT_1_A	Bond	Calc	3.146(3), Rep	3.181(3), Dev..			11.67 Sigma
	AM11	-CA2	1_555	1_565		#	87 Check
PLAT701_ALERT_1_A	Bond	Calc	3.146(3), Rep	3.181(3), Dev..			11.67 Sigma
	AM11	-CA2	1_555	1_566		#	88 Check
PLAT701_ALERT_1_A	Bond	Calc	3.146(3), Rep	3.181(3), Dev..			11.67 Sigma
	AM11	-NA2	1_555	1_565		#	89 Check
PLAT701_ALERT_1_A	Bond	Calc	3.146(3), Rep	3.181(3), Dev..			11.67 Sigma
	AM11	-NA2	1_555	1_566		#	90 Check
PLAT701_ALERT_1_A	Bond	Calc	3.408(3), Rep	3.473(5), Dev..			21.67 Sigma
	AM11	-CA21	1_555	1_555		#	91 Check

PLAT701_ALERT_1_A Bond	Calc	3.408(3), Rep	3.473(5), Dev..	21.67 Sigma
AM11	-NA21	1_555	1_555	# 92 Check
PLAT701_ALERT_1_A Bond	Calc	3.146(3), Rep	3.181(3), Dev..	11.67 Sigma
MM11	-CA2	1_555	1_565	# 109 Check
PLAT701_ALERT_1_A Bond	Calc	3.146(3), Rep	3.181(3), Dev..	11.67 Sigma
MM11	-CA2	1_555	1_566	# 110 Check
PLAT701_ALERT_1_A Bond	Calc	3.146(3), Rep	3.181(3), Dev..	11.67 Sigma
MM11	-NA2	1_555	1_565	# 111 Check
PLAT701_ALERT_1_A Bond	Calc	3.146(3), Rep	3.181(3), Dev..	11.67 Sigma
MM11	-NA2	1_555	1_566	# 112 Check
PLAT701_ALERT_1_A Bond	Calc	3.408(3), Rep	3.473(5), Dev..	21.67 Sigma
MM11	-CA21	1_555	1_555	# 113 Check
PLAT701_ALERT_1_A Bond	Calc	3.408(3), Rep	3.473(5), Dev..	21.67 Sigma
MM11	-NA21	1_555	1_555	# 114 Check
PLAT701_ALERT_1_A Bond	Calc	3.146(3), Rep	3.181(3), Dev..	11.67 Sigma
FM11	-CA2	1_555	1_565	# 115 Check
PLAT701_ALERT_1_A Bond	Calc	3.146(3), Rep	3.181(3), Dev..	11.67 Sigma
FM11	-CA2	1_555	1_566	# 116 Check
PLAT701_ALERT_1_A Bond	Calc	3.146(3), Rep	3.181(3), Dev..	11.67 Sigma
FM11	-NA2	1_555	1_565	# 117 Check
PLAT701_ALERT_1_A Bond	Calc	3.146(3), Rep	3.181(3), Dev..	11.67 Sigma
FM11	-NA2	1_555	1_566	# 118 Check

🔴 Alert level B

PLAT017_ALERT_1_B Check	Scattering Type Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of FM11	as	FE Error?

🟡 Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula	Strings Differ	Please Check
Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8		
Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6		
Si2		
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula	Strings Differ	Please Check
Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695		
(Na)		
Rep.: ?		
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..	3.08 Check	
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...	Please Check	
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...	Please Check	
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...	Please Check	
PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms .	Please Check	
PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare)	O11A Check	
PLAT701_ALERT_1_C Bond	Calc 1.640(3), Rep 1.644(5), Dev..	1.33 Sigma
O31A	-SIA1 1_555 1_555	# 34 Check
PLAT701_ALERT_1_C Bond	Calc 1.638(3), Rep 1.644(5), Dev..	2.00 Sigma
O32A	-SIB1 1_555 1_555	# 37 Check
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	MnM1 Check
O11A	MNM1	
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	Cm11 Check
O11A	CM11	
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	Tm11 Check
O11A	TM11	

PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O12A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O12A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check

	TM11	MM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	FM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA21		

Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.			
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !	
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check	
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka		0.49570	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	(K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature	(K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1	Constrained at	0.087	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11	Constrained at	0.052	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11	Constrained at	0.86	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1	Constrained at	0.868	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1	Constrained at	0.045	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11	Constrained at	0.088	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21	Constrained at	0.7904	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2	Constrained at	0.3622	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2	Constrained at	0.6378	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21	Constrained at	0.2096	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)		100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A		132.9	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A		137.1	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		8	Note
	SiA1	SiB1	MgM1	Am1
	Fm1	Am11	Mm11	Fm11
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)		1.84	Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please Check	
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info	
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !	
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2	Note
	0	1	0,	1
	1	1	0,	0,
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L=	0.600	369	Report
	0	2	0,	0
	0	3	0,	0
	0	4	0,	0
	0	5	0,	0
	0	6	0,	0
	0	7	0,	0
	1	2	0,	1
	1	3	0,	1
	1	4	0,	1
	1	5	0,	1
	1	6	0,	1
	1	7	0,	1
	2	0	0,	2
	2	1	0,	2
	2	2	0,	2
	2	3	0,	2
	2	4	0,	2
	2	5	0,	2
	2	6	0,	2
	2	7	0,	2
	3	1	0,	3
	3	4	0,	3
	3	5	0,	3
	3	6	0,	3

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      3  7  0,   4  0  0,   4  1  0,   4  6  0,   4  7  0,   5  1  0,
      5  7  0,   6  0  0,   6  1  0,   6  2  0,   6  3  0,   6  4  0,
      6  5  0,   7  1  0,   7  2  0,   7  4  0,   7  5  0,   7  6  0,
      7  7  0,   8  0  0,   8  1  0,   8  2  0,   8  3  0,   8  4  0,
      8  5  0,   8  6  0,   9  1  0,   9  2  0,   9  3  0,   9  5  0,
     10  0  0,  10  1  0,  10  2  0,  10  3  0, -11  0  1, -11  1  1,
    -10  1  1, -10  2  1, -10  3  1, -10  4  1,  -9  0  1,  -9  1  1,
     -9  2  1,  -9  4  1,  -9  6  1,  -8  1  1,  -8  2  1,  -8  5  1,
     -8  6  1,  -8  7  1,  -7  0  1,  -7  1  1,  -7  3  1,  -7  5  1,
     -6  1  1,  -5  0  1,  -5  7  1,  -4  4  1,  -4  5  1,  -4  6  1,
     -4  7  1,  -3  3  1,  -3  4  1,  -3  5  1,  -3  6  1,  -3  7  1,
     -2  2  1,  -2  3  1,  -2  4  1,  -2  5  1,  -2  6  1,  -2  7  1,

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PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 493 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 6 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ 2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 6 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of 3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.108 Note
      Predicted wR2: Based on SigI**2 4.61 or SHELX Weight 4.61
PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value 0.1517 Check
PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value 0.4344 Check

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77 ALERT level A = Most likely a serious problem - resolve or explain
 5 ALERT level B = A potentially serious problem, consider carefully
49 ALERT level C = Check. Ensure it is not caused by an omission or oversight
42 ALERT level G = General information/check it is not something unexpected

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136 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 3 ALERT type 2 Indicator that the structure model may be wrong or deficient
 6 ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
 9 ALERT type 5 Informative message, check

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Datablock: 9.73_GPa

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Bond precision:   Si- O = 0.0060 A           Wavelength=0.49570

Cell:             a=9.361(3)           b=8.555(5)           c=5.123(1)
                  alpha=90             beta=106.07(3)        gamma=90
Temperature:      293 K

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	Calculated	Reported
Volume	394.2(3)	394.2(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.585	3.598
Z	1	4
Mu (mm-1)	0.744	0.734
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,8,8
Nref	1830	571
Tmin,Tmax		0.428,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.428 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.312 Theta(max)= 23.990

R(reflections)= 0.0529(323) wR2(reflections)=
wR= 0.0837(571)

S = 1.660 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 12.69 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.550 Why?

PLAT701_ALERT_1_A Bond Calc 1.598(5), Rep 1.625(5), Dev.. 5.40 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_A Bond Calc 2.058(6), Rep 2.115(5), Dev.. 9.50 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.058(6), Rep 2.115(5), Dev.. 9.50 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond Calc 1.912(4), Rep 1.931(3), Dev.. 4.75 Sigma

	O11A	-MM11	1_555	1_554		#	7 Check
PLAT701_ALERT_1_A Bond	Calc	1.912(4), Rep	1.931(3), Dev..				4.75 Sigma
	O11A	-FM11	1_555	1_554		#	8 Check
PLAT701_ALERT_1_A Bond	Calc	2.304(6), Rep	2.348(5), Dev..				7.33 Sigma
	O11A	-CA2	1_555	1_565		#	9 Check
PLAT701_ALERT_1_A Bond	Calc	2.304(6), Rep	2.348(5), Dev..				7.33 Sigma
	O11A	-NA2	1_555	1_565		#	10 Check
PLAT701_ALERT_1_A Bond	Calc	1.597(5), Rep	1.622(5), Dev..				5.00 Sigma
	O12A	-SIB1	1_555	1_655		#	11 Check
PLAT701_ALERT_1_A Bond	Calc	2.021(4), Rep	2.058(3), Dev..				9.25 Sigma
	O12A	-MGM1	1_555	1_555		#	12 Check
PLAT701_ALERT_1_A Bond	Calc	2.021(4), Rep	2.058(3), Dev..				9.25 Sigma
	O12A	-FM1	1_555	1_555		#	14 Check
PLAT701_ALERT_1_A Bond	Calc	1.936(5), Rep	1.980(5), Dev..				8.80 Sigma
	O12A	-MM11	1_555	1_555		#	17 Check
PLAT701_ALERT_1_A Bond	Calc	1.936(5), Rep	1.980(5), Dev..				8.80 Sigma
	O12A	-FM11	1_555	1_555		#	18 Check
PLAT701_ALERT_1_A Bond	Calc	2.346(6), Rep	2.391(5), Dev..				7.50 Sigma
	O12A	-CA21	1_555	1_555		#	19 Check
PLAT701_ALERT_1_A Bond	Calc	2.346(6), Rep	2.391(5), Dev..				7.50 Sigma
	O12A	-NA21	1_555	1_555		#	20 Check
PLAT701_ALERT_1_A Bond	Calc	1.863(5), Rep	1.887(5), Dev..				4.80 Sigma
	O21A	-MM11	1_555	3_666		#	24 Check
PLAT701_ALERT_1_A Bond	Calc	1.863(5), Rep	1.887(5), Dev..				4.80 Sigma
	O21A	-FM11	1_555	3_666		#	25 Check
PLAT701_ALERT_1_A Bond	Calc	2.310(4), Rep	2.358(4), Dev..				12.00 Sigma
	O21A	-CA2	1_555	3_656		#	26 Check
PLAT701_ALERT_1_A Bond	Calc	2.310(4), Rep	2.358(4), Dev..				12.00 Sigma
	O21A	-NA2	1_555	3_656		#	27 Check
PLAT701_ALERT_1_A Bond	Calc	1.564(6), Rep	1.588(5), Dev..				4.00 Sigma
	O22A	-SIB1	1_555	1_555		#	28 Check
PLAT701_ALERT_1_A Bond	Calc	1.994(6), Rep	2.025(5), Dev..				5.17 Sigma
	O22A	-MGM1	1_555	3_666		#	29 Check
PLAT701_ALERT_1_A Bond	Calc	1.994(6), Rep	2.025(5), Dev..				5.17 Sigma
	O22A	-FM1	1_555	3_666		#	31 Check
PLAT701_ALERT_1_A Bond	Calc	2.342(4), Rep	2.384(4), Dev..				10.50 Sigma
	O22A	-CA21	1_555	3_667		#	32 Check
PLAT701_ALERT_1_A Bond	Calc	2.342(4), Rep	2.384(4), Dev..				10.50 Sigma
	O22A	-NA21	1_555	3_667		#	33 Check
PLAT701_ALERT_1_A Bond	Calc	1.651(4), Rep	1.670(4), Dev..				4.75 Sigma
	O31A	-SIB1	1_555	1_554		#	35 Check
PLAT701_ALERT_1_A Bond	Calc	1.646(4), Rep	1.659(4), Dev..				3.25 Sigma
	O32A	-SIA1	1_555	1_555		#	36 Check
PLAT701_ALERT_1_A Bond	Calc	2.965(3), Rep	3.025(2), Dev..				20.00 Sigma
	SIA1	-CA2	1_555	3_666		#	38 Check
PLAT701_ALERT_1_A Bond	Calc	2.965(3), Rep	3.025(2), Dev..				20.00 Sigma
	SIA1	-NA2	1_555	3_666		#	39 Check
PLAT701_ALERT_1_A Bond	Calc	3.179(4), Rep	3.270(4), Dev..				22.75 Sigma
	SIA1	-CA21	1_555	3_666		#	40 Check
PLAT701_ALERT_1_A Bond	Calc	3.123(4), Rep	3.198(4), Dev..				18.75 Sigma
	SIB1	-CA2	1_555	3_666		#	41 Check
PLAT701_ALERT_1_A Bond	Calc	3.123(4), Rep	3.198(4), Dev..				18.75 Sigma
	SIB1	-NA2	1_555	3_666		#	42 Check
PLAT701_ALERT_1_A Bond	Calc	2.987(3), Rep	3.049(2), Dev..				20.67 Sigma
	SIB1	-CA21	1_555	3_667		#	43 Check
PLAT701_ALERT_1_A Bond	Calc	2.987(3), Rep	3.049(2), Dev..				20.67 Sigma
	SIB1	-NA21	1_555	3_667		#	44 Check

PLAT701_ALERT_1_A Bond	Calc	3.000(3), Rep	3.086(2), Dev..		28.67 Sigma
MGM1	-AM11	1_555	1_554	#	48 Check
PLAT701_ALERT_1_A Bond	Calc	3.000(3), Rep	3.086(2), Dev..		28.67 Sigma
MGM1	-AM11	1_555	1_555	#	49 Check
PLAT701_ALERT_1_A Bond	Calc	3.000(3), Rep	3.086(2), Dev..		28.67 Sigma
MGM1	-MM11	1_555	1_554	#	52 Check
PLAT701_ALERT_1_A Bond	Calc	3.000(3), Rep	3.086(2), Dev..		28.67 Sigma
MGM1	-MM11	1_555	1_555	#	53 Check
PLAT701_ALERT_1_A Bond	Calc	3.380(5), Rep	3.436(6), Dev..		11.20 Sigma
MGM1	-CA2	1_555	1_565	#	54 Check
PLAT701_ALERT_1_A Bond	Calc	3.380(5), Rep	3.436(6), Dev..		11.20 Sigma
MGM1	-NA2	1_555	1_565	#	55 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.203(2), Dev..		13.67 Sigma
MGM1	-CA21	1_555	1_554	#	56 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.203(2), Dev..		13.67 Sigma
MGM1	-CA21	1_555	1_555	#	57 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.203(2), Dev..		13.67 Sigma
MGM1	-NA21	1_555	1_554	#	58 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.203(2), Dev..		13.67 Sigma
MGM1	-NA21	1_555	1_555	#	59 Check
PLAT701_ALERT_1_A Bond	Calc	3.000(3), Rep	3.086(2), Dev..		28.67 Sigma
AM1	-MM11	1_555	1_554	#	71 Check
PLAT701_ALERT_1_A Bond	Calc	3.000(3), Rep	3.086(2), Dev..		28.67 Sigma
AM1	-MM11	1_555	1_555	#	72 Check
PLAT701_ALERT_1_A Bond	Calc	3.380(5), Rep	3.436(6), Dev..		11.20 Sigma
AM1	-CA2	1_555	1_565	#	73 Check
PLAT701_ALERT_1_A Bond	Calc	3.380(5), Rep	3.436(6), Dev..		11.20 Sigma
AM1	-NA2	1_555	1_565	#	74 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.203(2), Dev..		13.67 Sigma
AM1	-CA21	1_555	1_554	#	75 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.203(2), Dev..		13.67 Sigma
AM1	-CA21	1_555	1_555	#	76 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.203(2), Dev..		13.67 Sigma
AM1	-NA21	1_555	1_554	#	77 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.203(2), Dev..		13.67 Sigma
AM1	-NA21	1_555	1_555	#	78 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.203(2), Dev..		13.67 Sigma
FM1	-CA21	1_555	1_554	#	79 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.203(2), Dev..		13.67 Sigma
FM1	-CA21	1_555	1_555	#	80 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.203(2), Dev..		13.67 Sigma
FM1	-NA21	1_555	1_554	#	81 Check
PLAT701_ALERT_1_A Bond	Calc	3.162(3), Rep	3.203(2), Dev..		13.67 Sigma
FM1	-NA21	1_555	1_555	#	82 Check
PLAT701_ALERT_1_A Bond	Calc	3.141(3), Rep	3.181(3), Dev..		13.33 Sigma
AM11	-CA2	1_555	1_565	#	87 Check
PLAT701_ALERT_1_A Bond	Calc	3.141(3), Rep	3.181(3), Dev..		13.33 Sigma
AM11	-CA2	1_555	1_566	#	88 Check
PLAT701_ALERT_1_A Bond	Calc	3.141(3), Rep	3.181(3), Dev..		13.33 Sigma
AM11	-NA2	1_555	1_565	#	89 Check
PLAT701_ALERT_1_A Bond	Calc	3.141(3), Rep	3.181(3), Dev..		13.33 Sigma
AM11	-NA2	1_555	1_566	#	90 Check
PLAT701_ALERT_1_A Bond	Calc	3.416(4), Rep	3.473(5), Dev..		14.25 Sigma
AM11	-CA21	1_555	1_555	#	91 Check
PLAT701_ALERT_1_A Bond	Calc	3.416(4), Rep	3.473(5), Dev..		14.25 Sigma
AM11	-NA21	1_555	1_555	#	92 Check
PLAT701_ALERT_1_A Bond	Calc	3.141(3), Rep	3.181(3), Dev..		13.33 Sigma

MM11	-CA2	1_555	1_565		#	109	Check
PLAT701_ALERT_1_A	Bond Calc	3.141(3), Rep	3.181(3), Dev..			13.33	Sigma
MM11	-CA2	1_555	1_566		#	110	Check
PLAT701_ALERT_1_A	Bond Calc	3.141(3), Rep	3.181(3), Dev..			13.33	Sigma
MM11	-NA2	1_555	1_565		#	111	Check
PLAT701_ALERT_1_A	Bond Calc	3.141(3), Rep	3.181(3), Dev..			13.33	Sigma
MM11	-NA2	1_555	1_566		#	112	Check
PLAT701_ALERT_1_A	Bond Calc	3.416(4), Rep	3.473(5), Dev..			14.25	Sigma
MM11	-CA21	1_555	1_555		#	113	Check
PLAT701_ALERT_1_A	Bond Calc	3.416(4), Rep	3.473(5), Dev..			14.25	Sigma
MM11	-NA21	1_555	1_555		#	114	Check
PLAT701_ALERT_1_A	Bond Calc	3.141(3), Rep	3.181(3), Dev..			13.33	Sigma
FM11	-CA2	1_555	1_565		#	115	Check
PLAT701_ALERT_1_A	Bond Calc	3.141(3), Rep	3.181(3), Dev..			13.33	Sigma
FM11	-CA2	1_555	1_566		#	116	Check
PLAT701_ALERT_1_A	Bond Calc	3.141(3), Rep	3.181(3), Dev..			13.33	Sigma
FM11	-NA2	1_555	1_565		#	117	Check
PLAT701_ALERT_1_A	Bond Calc	3.141(3), Rep	3.181(3), Dev..			13.33	Sigma
FM11	-NA2	1_555	1_566		#	118	Check

Alert level B

PLAT017_ALERT_1_B	Check Scattering Type Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B	Check Scattering Type Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B	Check Scattering Type Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B	Check Scattering Type Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B	Check Scattering Type Consistency of FM11	as	FE Error?
PLAT088_ALERT_3_B	Poor Data / Parameter Ratio		6.07 Note
PLAT701_ALERT_1_B	Bond Calc 1.589(6), Rep 1.603(5), Dev..		2.33 Sigma
O21A	-SIA1 1_555 1_545	#	21 Check
PLAT701_ALERT_1_B	Bond Calc 1.634(4), Rep 1.644(5), Dev..		2.50 Sigma
O32A	-SIB1 1_555 1_555	#	37 Check

Alert level C

PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ	Please Check
	Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	
	Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2	
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
	Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)	
	Rep.: ?	
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight Differ by ..	3.08 Check
PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...	Please Check
PLAT077_ALERT_4_C	Unit Cell Contains Non-integer Number of Atoms .	Please Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)	2.2 Note
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)	O11A Check
PLAT711_ALERT_1_C	BOND Unknown or Inconsistent Label	MnM1 Check
O11A	MNM1	
PLAT711_ALERT_1_C	BOND Unknown or Inconsistent Label	Cm11 Check
O11A	CM11	
PLAT711_ALERT_1_C	BOND Unknown or Inconsistent Label	Tm11 Check
O11A	TM11	
PLAT711_ALERT_1_C	BOND Unknown or Inconsistent Label	MnM1 Check

	O12A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	O12A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		MnM1 Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Cm11 Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	MM11				

PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	FM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label	Tm11	Check
	TM11	NA21		
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.76Ang From O31A .	0.52	eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please	Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please	Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1 Constrained at	0.087	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11 Constrained at	0.052	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11 Constrained at	0.86	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1 Constrained at	0.868	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1 Constrained at	0.045	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11 Constrained at	0.088	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21 Constrained at	0.7904	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2 Constrained at	0.3622	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2 Constrained at	0.6378	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21 Constrained at	0.2096	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A .	132.9	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A .	136.7	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11	Fm11	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.84	Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..	Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
	0 1 0, 1 1 0,		
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L= 0.600	330	Report
	0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,		
	0 8 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0, 1 6 0,		
	1 7 0, 1 8 0, 2 0 0, 2 1 0, 2 2 0, 2 3 0,		
	2 4 0, 2 5 0, 2 6 0, 2 7 0, 2 8 0, 3 1 0,		

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3 4 0, 3 5 0, 3 6 0, 3 7 0, 3 8 0, 4 0 0,
4 1 0, 4 6 0, 4 7 0, 4 8 0, 5 1 0, 5 7 0,
5 8 0, 6 0 0, 6 1 0, 6 2 0, 6 4 0, 6 5 0,
6 8 0, 7 1 0, 7 2 0, 7 4 0, 7 5 0, 7 6 0,
7 7 0, 8 0 0, 8 1 0, 8 2 0, 8 3 0, 8 4 0,
8 5 0, 8 6 0, 9 1 0, 9 2 0, 9 3 0, 9 5 0,
10 0 0, 10 1 0, 10 2 0, 10 3 0, -11 0 1, -11 1 1,
-10 1 1, -10 2 1, -10 3 1, -9 0 1, -9 1 1, -9 2 1,
-9 4 1, -9 6 1, -8 1 1, -8 2 1, -8 5 1, -8 6 1,
-8 7 1, -7 0 1, -7 1 1, -7 3 1, -7 5 1, -7 8 1,
-6 1 1, -6 8 1, -5 0 1, -5 7 1, -5 8 1, -4 5 1,
-4 6 1, -4 7 1, -4 8 1, -3 3 1, -3 4 1, -3 5 1,

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PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 520 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 6 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ 2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 6 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of 3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 1.799 Note
Predicted wR2: Based on SigI**2 9.46 or SHELX Weight 9.46
PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value 0.1517 Check
PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value 0.4344 Check

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75 ALERT level A = Most likely a serious problem - resolve or explain
8 ALERT level B = A potentially serious problem, consider carefully
49 ALERT level C = Check. Ensure it is not caused by an omission or oversight
42 ALERT level G = General information/check it is not something unexpected

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135 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
9 ALERT type 5 Informative message, check

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Datablock: 8.29_GPa

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Bond precision:  Si- O = 0.0043 A          Wavelength=0.49570

Cell:            a=9.385(3)          b=8.571(5)          c=5.145(1)
                  alpha=90           beta=106.11(3)       gamma=90
Temperature:     293 K

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	Calculated	Reported
Volume	397.6(3)	397.6(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.554	3.567
Z	1	4
Mu (mm-1)	0.737	0.728
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,8,8
Nref	1990	557
Tmin,Tmax		0.912,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.912 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.280 Theta(max)= 24.650

R(reflections)= 0.0422(376) wR2(reflections)=
wR= 0.0611(557)

S = 1.960 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 10.42 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.560 Why?

PLAT088_ALERT_3_A Poor Data / Parameter Ratio 5.93 Note

PLAT701_ALERT_1_A Bond Calc 1.598(4), Rep 1.625(5), Dev.. 6.75 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_A Bond Calc 2.068(4), Rep 2.115(5), Dev.. 11.75 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.068(4), Rep 2.115(5), Dev.. 11.75 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond	Calc	2.308(4), Rep	2.348(5), Dev..	10.00 Sigma
O11A	-CA2	1_555	1_565	# 9 Check
PLAT701_ALERT_1_A Bond	Calc	2.308(4), Rep	2.348(5), Dev..	10.00 Sigma
O11A	-NA2	1_555	1_565	# 10 Check
PLAT701_ALERT_1_A Bond	Calc	1.597(4), Rep	1.622(5), Dev..	6.25 Sigma
O12A	-SIB1	1_555	1_655	# 11 Check
PLAT701_ALERT_1_A Bond	Calc	2.036(3), Rep	2.058(3), Dev..	7.33 Sigma
O12A	-MGM1	1_555	1_555	# 12 Check
PLAT701_ALERT_1_A Bond	Calc	2.036(3), Rep	2.058(3), Dev..	7.33 Sigma
O12A	-FM1	1_555	1_555	# 14 Check
PLAT701_ALERT_1_A Bond	Calc	1.944(4), Rep	1.980(5), Dev..	9.00 Sigma
O12A	-MM11	1_555	1_555	# 17 Check
PLAT701_ALERT_1_A Bond	Calc	1.944(4), Rep	1.980(5), Dev..	9.00 Sigma
O12A	-FM11	1_555	1_555	# 18 Check
PLAT701_ALERT_1_A Bond	Calc	2.347(4), Rep	2.391(5), Dev..	11.00 Sigma
O12A	-CA21	1_555	1_555	# 19 Check
PLAT701_ALERT_1_A Bond	Calc	2.347(4), Rep	2.391(5), Dev..	11.00 Sigma
O12A	-NA21	1_555	1_555	# 20 Check
PLAT701_ALERT_1_A Bond	Calc	1.586(4), Rep	1.603(5), Dev..	4.25 Sigma
O21A	-SIA1	1_555	1_545	# 21 Check
PLAT701_ALERT_1_A Bond	Calc	1.866(4), Rep	1.887(5), Dev..	5.25 Sigma
O21A	-MM11	1_555	3_666	# 24 Check
PLAT701_ALERT_1_A Bond	Calc	1.866(4), Rep	1.887(5), Dev..	5.25 Sigma
O21A	-FM11	1_555	3_666	# 25 Check
PLAT701_ALERT_1_A Bond	Calc	2.319(3), Rep	2.358(4), Dev..	13.00 Sigma
O21A	-CA2	1_555	3_656	# 26 Check
PLAT701_ALERT_1_A Bond	Calc	2.319(3), Rep	2.358(4), Dev..	13.00 Sigma
O21A	-NA2	1_555	3_656	# 27 Check
PLAT701_ALERT_1_A Bond	Calc	1.567(5), Rep	1.588(5), Dev..	4.20 Sigma
O22A	-SIB1	1_555	1_555	# 28 Check
PLAT701_ALERT_1_A Bond	Calc	1.991(5), Rep	2.025(5), Dev..	6.80 Sigma
O22A	-MGM1	1_555	3_666	# 29 Check
PLAT701_ALERT_1_A Bond	Calc	1.991(5), Rep	2.025(5), Dev..	6.80 Sigma
O22A	-FM1	1_555	3_666	# 31 Check
PLAT701_ALERT_1_A Bond	Calc	2.343(3), Rep	2.384(4), Dev..	13.67 Sigma
O22A	-CA21	1_555	3_667	# 32 Check
PLAT701_ALERT_1_A Bond	Calc	2.343(3), Rep	2.384(4), Dev..	13.67 Sigma
O22A	-NA21	1_555	3_667	# 33 Check
PLAT701_ALERT_1_A Bond	Calc	1.655(3), Rep	1.670(4), Dev..	5.00 Sigma
O31A	-SIB1	1_555	1_554	# 35 Check
PLAT701_ALERT_1_A Bond	Calc	1.649(3), Rep	1.659(4), Dev..	3.33 Sigma
O32A	-SIA1	1_555	1_555	# 36 Check
PLAT701_ALERT_1_A Bond	Calc	2.976(2), Rep	3.025(2), Dev..	24.50 Sigma
SIA1	-CA2	1_555	3_666	# 38 Check
PLAT701_ALERT_1_A Bond	Calc	2.976(2), Rep	3.025(2), Dev..	24.50 Sigma
SIA1	-NA2	1_555	3_666	# 39 Check
PLAT701_ALERT_1_A Bond	Calc	3.192(3), Rep	3.270(4), Dev..	26.00 Sigma
SIA1	-CA21	1_555	3_666	# 40 Check
PLAT701_ALERT_1_A Bond	Calc	3.131(3), Rep	3.198(4), Dev..	22.33 Sigma
SIB1	-CA2	1_555	3_666	# 41 Check
PLAT701_ALERT_1_A Bond	Calc	3.131(3), Rep	3.198(4), Dev..	22.33 Sigma
SIB1	-NA2	1_555	3_666	# 42 Check
PLAT701_ALERT_1_A Bond	Calc	2.996(2), Rep	3.049(2), Dev..	26.50 Sigma
SIB1	-CA21	1_555	3_667	# 43 Check
PLAT701_ALERT_1_A Bond	Calc	2.996(2), Rep	3.049(2), Dev..	26.50 Sigma
SIB1	-NA21	1_555	3_667	# 44 Check
PLAT701_ALERT_1_A Bond	Calc	3.016(2), Rep	3.086(2), Dev..	35.00 Sigma

	MGM1	-AM11	1_555	1_554		#	48 Check
PLAT701_ALERT_1_A Bond	Calc		3.016(2), Rep	3.086(2), Dev..			35.00 Sigma
	MGM1	-AM11	1_555	1_555		#	49 Check
PLAT701_ALERT_1_A Bond	Calc		3.016(2), Rep	3.086(2), Dev..			35.00 Sigma
	MGM1	-MM11	1_555	1_554		#	52 Check
PLAT701_ALERT_1_A Bond	Calc		3.016(2), Rep	3.086(2), Dev..			35.00 Sigma
	MGM1	-MM11	1_555	1_555		#	53 Check
PLAT701_ALERT_1_A Bond	Calc		3.387(4), Rep	3.436(6), Dev..			12.25 Sigma
	MGM1	-CA2	1_555	1_565		#	54 Check
PLAT701_ALERT_1_A Bond	Calc		3.387(4), Rep	3.436(6), Dev..			12.25 Sigma
	MGM1	-NA2	1_555	1_565		#	55 Check
PLAT701_ALERT_1_A Bond	Calc		3.165(3), Rep	3.203(2), Dev..			12.67 Sigma
	MGM1	-CA21	1_555	1_554		#	56 Check
PLAT701_ALERT_1_A Bond	Calc		3.165(3), Rep	3.203(2), Dev..			12.67 Sigma
	MGM1	-CA21	1_555	1_555		#	57 Check
PLAT701_ALERT_1_A Bond	Calc		3.165(3), Rep	3.203(2), Dev..			12.67 Sigma
	MGM1	-NA21	1_555	1_554		#	58 Check
PLAT701_ALERT_1_A Bond	Calc		3.165(3), Rep	3.203(2), Dev..			12.67 Sigma
	MGM1	-NA21	1_555	1_555		#	59 Check
PLAT701_ALERT_1_A Bond	Calc		3.016(2), Rep	3.086(2), Dev..			35.00 Sigma
	AM1	-MM11	1_555	1_554		#	71 Check
PLAT701_ALERT_1_A Bond	Calc		3.016(2), Rep	3.086(2), Dev..			35.00 Sigma
	AM1	-MM11	1_555	1_555		#	72 Check
PLAT701_ALERT_1_A Bond	Calc		3.387(4), Rep	3.436(6), Dev..			12.25 Sigma
	AM1	-CA2	1_555	1_565		#	73 Check
PLAT701_ALERT_1_A Bond	Calc		3.387(4), Rep	3.436(6), Dev..			12.25 Sigma
	AM1	-NA2	1_555	1_565		#	74 Check
PLAT701_ALERT_1_A Bond	Calc		3.165(3), Rep	3.203(2), Dev..			12.67 Sigma
	AM1	-CA21	1_555	1_554		#	75 Check
PLAT701_ALERT_1_A Bond	Calc		3.165(3), Rep	3.203(2), Dev..			12.67 Sigma
	AM1	-CA21	1_555	1_555		#	76 Check
PLAT701_ALERT_1_A Bond	Calc		3.165(3), Rep	3.203(2), Dev..			12.67 Sigma
	AM1	-NA21	1_555	1_554		#	77 Check
PLAT701_ALERT_1_A Bond	Calc		3.165(3), Rep	3.203(2), Dev..			12.67 Sigma
	AM1	-NA21	1_555	1_555		#	78 Check
PLAT701_ALERT_1_A Bond	Calc		3.165(3), Rep	3.203(2), Dev..			12.67 Sigma
	FM1	-CA21	1_555	1_554		#	79 Check
PLAT701_ALERT_1_A Bond	Calc		3.165(3), Rep	3.203(2), Dev..			12.67 Sigma
	FM1	-CA21	1_555	1_555		#	80 Check
PLAT701_ALERT_1_A Bond	Calc		3.165(3), Rep	3.203(2), Dev..			12.67 Sigma
	FM1	-NA21	1_555	1_554		#	81 Check
PLAT701_ALERT_1_A Bond	Calc		3.165(3), Rep	3.203(2), Dev..			12.67 Sigma
	FM1	-NA21	1_555	1_555		#	82 Check
PLAT701_ALERT_1_A Bond	Calc		3.147(3), Rep	3.181(3), Dev..			11.33 Sigma
	AM11	-CA2	1_555	1_565		#	87 Check
PLAT701_ALERT_1_A Bond	Calc		3.147(3), Rep	3.181(3), Dev..			11.33 Sigma
	AM11	-CA2	1_555	1_566		#	88 Check
PLAT701_ALERT_1_A Bond	Calc		3.147(3), Rep	3.181(3), Dev..			11.33 Sigma
	AM11	-NA2	1_555	1_565		#	89 Check
PLAT701_ALERT_1_A Bond	Calc		3.147(3), Rep	3.181(3), Dev..			11.33 Sigma
	AM11	-NA2	1_555	1_566		#	90 Check
PLAT701_ALERT_1_A Bond	Calc		3.418(3), Rep	3.473(5), Dev..			18.33 Sigma
	AM11	-CA21	1_555	1_555		#	91 Check
PLAT701_ALERT_1_A Bond	Calc		3.418(3), Rep	3.473(5), Dev..			18.33 Sigma
	AM11	-NA21	1_555	1_555		#	92 Check
PLAT701_ALERT_1_A Bond	Calc		3.147(3), Rep	3.181(3), Dev..			11.33 Sigma
	MM11	-CA2	1_555	1_565		#	109 Check

PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..	11.33 Sigma
MM11	-CA2	1_555	1_566	# 110 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..	11.33 Sigma
MM11	-NA2	1_555	1_565	# 111 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..	11.33 Sigma
MM11	-NA2	1_555	1_566	# 112 Check
PLAT701_ALERT_1_A Bond	Calc	3.418(3), Rep	3.473(5), Dev..	18.33 Sigma
MM11	-CA21	1_555	1_555	# 113 Check
PLAT701_ALERT_1_A Bond	Calc	3.418(3), Rep	3.473(5), Dev..	18.33 Sigma
MM11	-NA21	1_555	1_555	# 114 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..	11.33 Sigma
FM11	-CA2	1_555	1_565	# 115 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..	11.33 Sigma
FM11	-CA2	1_555	1_566	# 116 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..	11.33 Sigma
FM11	-NA2	1_555	1_565	# 117 Check
PLAT701_ALERT_1_A Bond	Calc	3.147(3), Rep	3.181(3), Dev..	11.33 Sigma
FM11	-NA2	1_555	1_566	# 118 Check

🔴 Alert level B

PLAT017_ALERT_1_B Check	Scattering Type Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of FM11	as	FE Error?
PLAT701_ALERT_1_B Bond	Calc	1.922(3), Rep	1.931(3), Dev..
O11A	-MM11	1_555	1_554
PLAT701_ALERT_1_B Bond	Calc	1.922(3), Rep	1.931(3), Dev..
O11A	-FM11	1_555	1_554

🟡 Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula	Strings Differ	Please Check
Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8		
Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2		
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula	Strings Differ	Please Check
Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)		
Rep.: ?		
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..	3.08 Check	
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...	Please Check	
PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ...	Please Check	
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...	Please Check	
PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms .	Please Check	
PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare)	O11A Check	
PLAT701_ALERT_1_C Bond	Calc	1.640(3), Rep
O32A	-SIB1	1_555
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	MnM1 Check
O11A	MNM1	
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	Cm11 Check
O11A	CM11	
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	Tm11 Check
O11A	TM11	
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	MnM1 Check
O12A	MNM1	

PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O12A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	TM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check

	TM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label		Tm11 Check
	TM11	NA21				

- Alert level G

0	1	0,	1	1	0,													
PLAT911_ALERT_3_G	Missing	FCF	Refl	Between	Thmin	&	STh/L=	0.600									340	Report
0	2	0,	0	3	0,	0	4	0,	0	5	0,	0	6	0,	0	7	0,	
0	8	0,	1	2	0,	1	3	0,	1	4	0,	1	5	0,	1	6	0,	
1	7	0,	1	8	0,	2	0	0,	2	1	0,	2	2	0,	2	3	0,	
2	4	0,	2	5	0,	2	6	0,	2	7	0,	2	8	0,	3	1	0,	
3	4	0,	3	5	0,	3	6	0,	3	7	0,	3	8	0,	4	0	0,	
4	1	0,	4	6	0,	4	7	0,	4	8	0,	5	1	0,	5	4	0,	

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      5 7 0,   5 8 0,   6 0 0,   6 1 0,   6 2 0,   6 3 0,
      6 4 0,   6 5 0,   6 6 0,   6 8 0,   7 1 0,   7 2 0,
      7 3 0,   7 4 0,   7 5 0,   7 6 0,   7 7 0,   8 0 0,
      8 1 0,   8 2 0,   8 3 0,   8 4 0,   8 5 0,   8 6 0,
      9 1 0,   9 2 0,   9 3 0,   9 5 0,  10 0 0,  10 1 0,
     10 2 0,  10 3 0, -11 0 1, -11 1 1, -10 1 1, -10 2 1,
    -10 3 1,  -9 0 1,  -9 1 1,  -9 2 1,  -9 4 1,  -9 6 1,
     -8 1 1,  -8 2 1,  -8 5 1,  -8 6 1,  -8 7 1,  -7 0 1,
     -7 1 1,  -7 8 1,  -6 1 1,  -6 8 1,  -5 0 1,  -5 1 1,
     -5 7 1,  -5 8 1,  -4 5 1,  -4 6 1,  -4 7 1,  -4 8 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      592 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked      ! Info
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ      2 Units
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ      6 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ      2 Units
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ      6 Units
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of      3.0 Sig(I)
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      2.019 Note
      Predicted wR2: Based on SigI**2 5.33 or SHELX Weight 5.33
PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value 0.1517 Check
PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value 0.4344 Check

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75 ALERT level A = Most likely a serious problem - resolve or explain
 7 ALERT level B = A potentially serious problem, consider carefully
48 ALERT level C = Check. Ensure it is not caused by an omission or oversight
42 ALERT level G = General information/check it is not something unexpected

135 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 3 ALERT type 2 Indicator that the structure model may be wrong or deficient
 6 ALERT type 3 Indicator that the structure quality may be low
19 ALERT type 4 Improvement, methodology, query or suggestion
 9 ALERT type 5 Informative message, check

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Datablock: 6.91_GPa

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Bond precision:   Si- O = 0.0050 A           Wavelength=0.49570

Cell:             a=9.417(3)                b=8.610(5)                c=5.165(1)
                  alpha=90                  beta=106.24(3)              gamma=90
Temperature:      293 K

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	Calculated	Reported
Volume	402.1(3)	402.1(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.514	3.527
Z	1	4
Mu (mm-1)	0.729	0.720
F000	422.4	422.0
F000'	423.29	
h,k,lmax	15,14,8	13,9,8
Nref	1958	539
Tmin,Tmax		0.849,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.849 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.275 Theta(max)= 24.370

R(reflections)= 0.0578(366) wR2(reflections)=
wR= 0.0653(539)

S = 2.420 Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.

GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.

GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

PLAT027_ALERT_3_A _diffn_refl_theta_full value (too) Low 10.12 Degree

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.530 Why?

PLAT088_ALERT_3_A Poor Data / Parameter Ratio 5.73 Note

PLAT701_ALERT_1_A Bond Calc 1.603(5), Rep 1.625(5), Dev.. 4.40 Sigma

O11A -SIA1 1_555 1_655 # 1 Check

PLAT701_ALERT_1_A Bond Calc 2.077(5), Rep 2.115(5), Dev.. 7.60 Sigma

O11A -MGM1 1_555 1_555 # 2 Check

PLAT701_ALERT_1_A Bond Calc 2.077(5), Rep 2.115(5), Dev.. 7.60 Sigma

O11A -FM1 1_555 1_555 # 4 Check

PLAT701_ALERT_1_A Bond	Calc	2.320(5), Rep	2.348(5), Dev..	5.60 Sigma
O11A	-CA2	1_555	1_565	# 9 Check
PLAT701_ALERT_1_A Bond	Calc	2.320(5), Rep	2.348(5), Dev..	5.60 Sigma
O11A	-NA2	1_555	1_565	# 10 Check
PLAT701_ALERT_1_A Bond	Calc	1.604(5), Rep	1.622(5), Dev..	3.60 Sigma
O12A	-SIB1	1_555	1_655	# 11 Check
PLAT701_ALERT_1_A Bond	Calc	2.040(3), Rep	2.058(3), Dev..	6.00 Sigma
O12A	-MGM1	1_555	1_555	# 12 Check
PLAT701_ALERT_1_A Bond	Calc	2.040(3), Rep	2.058(3), Dev..	6.00 Sigma
O12A	-FM1	1_555	1_555	# 14 Check
PLAT701_ALERT_1_A Bond	Calc	1.944(5), Rep	1.980(5), Dev..	7.20 Sigma
O12A	-MM11	1_555	1_555	# 17 Check
PLAT701_ALERT_1_A Bond	Calc	1.944(5), Rep	1.980(5), Dev..	7.20 Sigma
O12A	-FM11	1_555	1_555	# 18 Check
PLAT701_ALERT_1_A Bond	Calc	2.366(5), Rep	2.391(5), Dev..	5.00 Sigma
O12A	-CA21	1_555	1_555	# 19 Check
PLAT701_ALERT_1_A Bond	Calc	2.366(5), Rep	2.391(5), Dev..	5.00 Sigma
O12A	-NA21	1_555	1_555	# 20 Check
PLAT701_ALERT_1_A Bond	Calc	1.869(5), Rep	1.887(5), Dev..	3.60 Sigma
O21A	-MM11	1_555	3_666	# 24 Check
PLAT701_ALERT_1_A Bond	Calc	1.869(5), Rep	1.887(5), Dev..	3.60 Sigma
O21A	-FM11	1_555	3_666	# 25 Check
PLAT701_ALERT_1_A Bond	Calc	2.324(4), Rep	2.358(4), Dev..	8.50 Sigma
O21A	-CA2	1_555	3_656	# 26 Check
PLAT701_ALERT_1_A Bond	Calc	2.324(4), Rep	2.358(4), Dev..	8.50 Sigma
O21A	-NA2	1_555	3_656	# 27 Check
PLAT701_ALERT_1_A Bond	Calc	1.996(5), Rep	2.025(5), Dev..	5.80 Sigma
O22A	-MGM1	1_555	3_666	# 29 Check
PLAT701_ALERT_1_A Bond	Calc	1.996(5), Rep	2.025(5), Dev..	5.80 Sigma
O22A	-FM1	1_555	3_666	# 31 Check
PLAT701_ALERT_1_A Bond	Calc	2.352(4), Rep	2.384(4), Dev..	8.00 Sigma
O22A	-CA21	1_555	3_667	# 32 Check
PLAT701_ALERT_1_A Bond	Calc	2.352(4), Rep	2.384(4), Dev..	8.00 Sigma
O22A	-NA21	1_555	3_667	# 33 Check
PLAT701_ALERT_1_A Bond	Calc	1.657(4), Rep	1.670(4), Dev..	3.25 Sigma
O31A	-SIB1	1_555	1_554	# 35 Check
PLAT701_ALERT_1_A Bond	Calc	2.987(2), Rep	3.025(2), Dev..	19.00 Sigma
SIA1	-CA2	1_555	3_666	# 38 Check
PLAT701_ALERT_1_A Bond	Calc	2.987(2), Rep	3.025(2), Dev..	19.00 Sigma
SIA1	-NA2	1_555	3_666	# 39 Check
PLAT701_ALERT_1_A Bond	Calc	3.206(3), Rep	3.270(4), Dev..	21.33 Sigma
SIA1	-CA21	1_555	3_666	# 40 Check
PLAT701_ALERT_1_A Bond	Calc	3.144(3), Rep	3.198(4), Dev..	18.00 Sigma
SIB1	-CA2	1_555	3_666	# 41 Check
PLAT701_ALERT_1_A Bond	Calc	3.144(3), Rep	3.198(4), Dev..	18.00 Sigma
SIB1	-NA2	1_555	3_666	# 42 Check
PLAT701_ALERT_1_A Bond	Calc	3.007(2), Rep	3.049(2), Dev..	21.00 Sigma
SIB1	-CA21	1_555	3_667	# 43 Check
PLAT701_ALERT_1_A Bond	Calc	3.007(2), Rep	3.049(2), Dev..	21.00 Sigma
SIB1	-NA21	1_555	3_667	# 44 Check
PLAT701_ALERT_1_A Bond	Calc	3.032(3), Rep	3.086(2), Dev..	18.00 Sigma
MGM1	-AM11	1_555	1_554	# 48 Check
PLAT701_ALERT_1_A Bond	Calc	3.032(3), Rep	3.086(2), Dev..	18.00 Sigma
MGM1	-AM11	1_555	1_555	# 49 Check
PLAT701_ALERT_1_A Bond	Calc	3.032(3), Rep	3.086(2), Dev..	18.00 Sigma
MGM1	-MM11	1_555	1_554	# 52 Check
PLAT701_ALERT_1_A Bond	Calc	3.032(3), Rep	3.086(2), Dev..	18.00 Sigma

	MGM1	-MM11	1_555	1_555		#	53 Check
PLAT701_ALERT_1_A Bond	Calc		3.398(4), Rep	3.436(6), Dev..			9.50 Sigma
	MGM1	-CA2	1_555	1_565		#	54 Check
PLAT701_ALERT_1_A Bond	Calc		3.398(4), Rep	3.436(6), Dev..			9.50 Sigma
	MGM1	-NA2	1_555	1_565		#	55 Check
PLAT701_ALERT_1_A Bond	Calc		3.175(3), Rep	3.203(2), Dev..			9.33 Sigma
	MGM1	-CA21	1_555	1_554		#	56 Check
PLAT701_ALERT_1_A Bond	Calc		3.175(3), Rep	3.203(2), Dev..			9.33 Sigma
	MGM1	-CA21	1_555	1_555		#	57 Check
PLAT701_ALERT_1_A Bond	Calc		3.175(3), Rep	3.203(2), Dev..			9.33 Sigma
	MGM1	-NA21	1_555	1_554		#	58 Check
PLAT701_ALERT_1_A Bond	Calc		3.175(3), Rep	3.203(2), Dev..			9.33 Sigma
	MGM1	-NA21	1_555	1_555		#	59 Check
PLAT701_ALERT_1_A Bond	Calc		3.032(3), Rep	3.086(2), Dev..			18.00 Sigma
	AM1	-MM11	1_555	1_554		#	71 Check
PLAT701_ALERT_1_A Bond	Calc		3.032(3), Rep	3.086(2), Dev..			18.00 Sigma
	AM1	-MM11	1_555	1_555		#	72 Check
PLAT701_ALERT_1_A Bond	Calc		3.398(4), Rep	3.436(6), Dev..			9.50 Sigma
	AM1	-CA2	1_555	1_565		#	73 Check
PLAT701_ALERT_1_A Bond	Calc		3.398(4), Rep	3.436(6), Dev..			9.50 Sigma
	AM1	-NA2	1_555	1_565		#	74 Check
PLAT701_ALERT_1_A Bond	Calc		3.175(3), Rep	3.203(2), Dev..			9.33 Sigma
	AM1	-CA21	1_555	1_554		#	75 Check
PLAT701_ALERT_1_A Bond	Calc		3.175(3), Rep	3.203(2), Dev..			9.33 Sigma
	AM1	-CA21	1_555	1_555		#	76 Check
PLAT701_ALERT_1_A Bond	Calc		3.175(3), Rep	3.203(2), Dev..			9.33 Sigma
	AM1	-NA21	1_555	1_554		#	77 Check
PLAT701_ALERT_1_A Bond	Calc		3.175(3), Rep	3.203(2), Dev..			9.33 Sigma
	AM1	-NA21	1_555	1_555		#	78 Check
PLAT701_ALERT_1_A Bond	Calc		3.175(3), Rep	3.203(2), Dev..			9.33 Sigma
	FM1	-CA21	1_555	1_554		#	79 Check
PLAT701_ALERT_1_A Bond	Calc		3.175(3), Rep	3.203(2), Dev..			9.33 Sigma
	FM1	-CA21	1_555	1_555		#	80 Check
PLAT701_ALERT_1_A Bond	Calc		3.175(3), Rep	3.203(2), Dev..			9.33 Sigma
	FM1	-NA21	1_555	1_554		#	81 Check
PLAT701_ALERT_1_A Bond	Calc		3.175(3), Rep	3.203(2), Dev..			9.33 Sigma
	FM1	-NA21	1_555	1_555		#	82 Check
PLAT701_ALERT_1_A Bond	Calc		3.154(3), Rep	3.181(3), Dev..			9.00 Sigma
	AM11	-CA2	1_555	1_565		#	87 Check
PLAT701_ALERT_1_A Bond	Calc		3.154(3), Rep	3.181(3), Dev..			9.00 Sigma
	AM11	-CA2	1_555	1_566		#	88 Check
PLAT701_ALERT_1_A Bond	Calc		3.154(3), Rep	3.181(3), Dev..			9.00 Sigma
	AM11	-NA2	1_555	1_565		#	89 Check
PLAT701_ALERT_1_A Bond	Calc		3.154(3), Rep	3.181(3), Dev..			9.00 Sigma
	AM11	-NA2	1_555	1_566		#	90 Check
PLAT701_ALERT_1_A Bond	Calc		3.436(4), Rep	3.473(5), Dev..			9.25 Sigma
	AM11	-CA21	1_555	1_555		#	91 Check
PLAT701_ALERT_1_A Bond	Calc		3.436(4), Rep	3.473(5), Dev..			9.25 Sigma
	AM11	-NA21	1_555	1_555		#	92 Check
PLAT701_ALERT_1_A Bond	Calc		3.154(3), Rep	3.181(3), Dev..			9.00 Sigma
	MM11	-CA2	1_555	1_565		#	109 Check
PLAT701_ALERT_1_A Bond	Calc		3.154(3), Rep	3.181(3), Dev..			9.00 Sigma
	MM11	-CA2	1_555	1_566		#	110 Check
PLAT701_ALERT_1_A Bond	Calc		3.154(3), Rep	3.181(3), Dev..			9.00 Sigma
	MM11	-NA2	1_555	1_565		#	111 Check
PLAT701_ALERT_1_A Bond	Calc		3.154(3), Rep	3.181(3), Dev..			9.00 Sigma
	MM11	-NA2	1_555	1_566		#	112 Check

PLAT701_ALERT_1_A Bond	Calc	3.436(4), Rep	3.473(5), Dev..	9.25 Sigma
MM11	-CA21	1_555	1_555	# 113 Check
PLAT701_ALERT_1_A Bond	Calc	3.436(4), Rep	3.473(5), Dev..	9.25 Sigma
MM11	-NA21	1_555	1_555	# 114 Check
PLAT701_ALERT_1_A Bond	Calc	3.154(3), Rep	3.181(3), Dev..	9.00 Sigma
FM11	-CA2	1_555	1_565	# 115 Check
PLAT701_ALERT_1_A Bond	Calc	3.154(3), Rep	3.181(3), Dev..	9.00 Sigma
FM11	-CA2	1_555	1_566	# 116 Check
PLAT701_ALERT_1_A Bond	Calc	3.154(3), Rep	3.181(3), Dev..	9.00 Sigma
FM11	-NA2	1_555	1_565	# 117 Check
PLAT701_ALERT_1_A Bond	Calc	3.154(3), Rep	3.181(3), Dev..	9.00 Sigma
FM11	-NA2	1_555	1_566	# 118 Check

Alert level B

PLAT017_ALERT_1_B Check	Scattering Type Consistency of AM1	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of FM1	as	FE Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of AM11	as	AL Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of MM11	as	MG Error?
PLAT017_ALERT_1_B Check	Scattering Type Consistency of FM11	as	FE Error?
PLAT701_ALERT_1_B Bond	Calc	1.922(3), Rep	1.931(3), Dev..
O11A	-MM11	1_555	1_554
PLAT701_ALERT_1_B Bond	Calc	1.922(3), Rep	1.931(3), Dev..
O11A	-FM11	1_555	1_554
PLAT701_ALERT_1_B Bond	Calc	1.592(5), Rep	1.603(5), Dev..
O21A	-SIA1	1_555	1_545
PLAT701_ALERT_1_B Bond	Calc	1.575(5), Rep	1.588(5), Dev..
O22A	-SIB1	1_555	1_555

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.80 <> 2.00
Goodness of fit given = 2.420

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8
Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)
Rep.: ?

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.08 Check

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms . Please Check

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 2.3 Note

PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) O11A Check

PLAT701_ALERT_1_C Bond	Calc	1.638(4), Rep	1.644(5), Dev..	1.50 Sigma
O32A	-SIB1	1_555	1_555	# 37 Check
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	MnM1	Check	
O11A	MNM1			
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	Cm11	Check	
O11A	CM11			
PLAT711_ALERT_1_C BOND	Unknown or Inconsistent Label	Tm11	Check	
O11A	TM11			

PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O12A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O12A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O12A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	O21A	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	O21A	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	O22A	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MGM1	MNM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	MGM1	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	AM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	FM1				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	CA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	MnM1	Check
	MNM1	NA21				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	AM11	CM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check
	AM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	TM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	MM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	FM11				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	CA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Cm11	Check
	CM11	NA2				
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent	Label	Tm11	Check

	TM11	MM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	FM11		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA21		
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc)		.	1 Check
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.83Ang From O31A	.	0.67 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.91Ang From O32A	.	0.57 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.53Ang From O31A	.	0.50 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.47Ang From O32A	.	0.46 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.88Ang From O21A	.	0.45 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.81Ang From O32A	.	0.42 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	1.09Ang From O32A	.	-0.44 eA-3

● Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please	Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please	Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1	Constrained at	0.087 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11	Constrained at	0.052 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11	Constrained at	0.86 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1	Constrained at	0.868 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1	Constrained at	0.045 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11	Constrained at	0.088 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21	Constrained at	0.7904 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2	Constrained at	0.3622 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2	Constrained at	0.6378 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21	Constrained at	0.2096 Check
PLAT301_ALERT_3_G	Main Residue Disorder (Resd	1)	20% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	2)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	3)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	4)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd	5)	100% Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A	.	133.5 Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A	.	137.5 Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
	SiA1	SiB1	MgM1
	Am1	Fm1	Am11
	Mm11	Fm11	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	.	1.84 Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info

PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !
 PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
 0 1 0, 1 1 0,
 PLAT911_ALERT_3_G Missing FCF Refl Between Thmin & STh/L= 0.600 391 Report
 0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,
 0 8 0, 0 9 0, 1 2 0, 1 3 0, 1 4 0, 1 5 0,
 1 6 0, 1 7 0, 1 8 0, 1 9 0, 2 0 0, 2 1 0,
 2 2 0, 2 3 0, 2 4 0, 2 5 0, 2 6 0, 2 7 0,
 2 8 0, 2 9 0, 3 1 0, 3 4 0, 3 5 0, 3 6 0,
 3 7 0, 3 8 0, 3 9 0, 4 0 0, 4 1 0, 4 2 0,
 4 6 0, 4 7 0, 4 8 0, 4 9 0, 5 1 0, 5 4 0,
 5 7 0, 5 8 0, 5 9 0, 6 0 0, 6 1 0, 6 2 0,
 6 3 0, 6 4 0, 6 5 0, 6 6 0, 6 8 0, 7 1 0,
 7 2 0, 7 4 0, 7 5 0, 7 6 0, 7 7 0, 8 0 0,
 8 1 0, 8 2 0, 8 3 0, 8 4 0, 8 5 0, 8 6 0,
 9 1 0, 9 2 0, 9 3 0, 9 5 0, 10 0 0, 10 1 0,
 10 2 0, 10 3 0, 10 4 0, -11 0 1, -11 1 1, -11 2 1,
 -10 1 1, -10 2 1, -10 3 1, -10 4 1, -9 0 1, -9 1 1,
 -9 2 1, -9 4 1, -9 6 1, -8 1 1, -8 2 1, -8 6 1,
 -8 7 1, -7 0 1, -7 1 1, -7 3 1, -7 5 1, -7 8 1,
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 662 Note
 PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked ! Info
 PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ 2 Units
 PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ 5 Units
 PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ 2 Units
 PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ 5 Units
 PLAT960_ALERT_3_G Number of Intensities with I < - 2*Sigma(I) 1 Check
 PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of 3.0 Sig(I)
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 6.452 Note
 Predicted wR2: Based on SigI**2 2.44 or SHELX Weight 2.44
 PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value 0.1517 Check
 PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value 0.4344 Check

72 **ALERT level A** = Most likely a serious problem - resolve or explain
 9 **ALERT level B** = A potentially serious problem, consider carefully
 58 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 43 **ALERT level G** = General information/check it is not something unexpected

134 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 12 ALERT type 2 Indicator that the structure model may be wrong or deficient
 8 ALERT type 3 Indicator that the structure quality may be low
 19 ALERT type 4 Improvement, methodology, query or suggestion
 9 ALERT type 5 Informative message, check

Datablock: 0.03_GPa

Bond precision: Si- O = 0.0070 A Wavelength=0.49570

Cell: a=9.567(3) b=8.788(5) c=5.252(1)
 alpha=90 beta=106.94(3) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	422.4(3)	422.4(3)
Space group	P 2/n	P 1 2/n 1
Hall group	-P 2yac	-P 2yac
Moiety formula	Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695(Na)	?
Sum formula	Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8	Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2
Mr	850.92	213.50
Dx, g cm-3	3.345	3.358
Z	1	4
Mu (mm-1)	0.694	0.685
F000	422.4	422.0
F000'	423.29	
h,k,lmax	16,14,8	11,10,8
Nref	2180	479
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.220

Theta(max)= 24.930

R(reflections)= 0.0600(332)

wR2(reflections)=
wR= 0.0948(479)

S = 1.810

Npar= 94

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

Alert level A

```

EXPT005_ALERT_1_A _exptl_crystal_description is missing
    Crystal habit description.
    The following tests will not be performed.
    CRYSR_01
GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
    Label identifying the atom site 2.
GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
    Label identifying the atom site 3.
GEOM008_ALERT_1_A _geom_angle is missing
    Angle between atom sites 1, 2 and 3.
PLAT027_ALERT_3_A _diffrn_reflths_theta_full value (too) Low ..... 12.19 Degree
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.460 Why?
PLAT088_ALERT_3_A Poor Data / Parameter Ratio ..... 5.10 Note
PLAT699_ALERT_1_A Missing _exptl_crystal_description Value ..... Please Do !
PLAT701_ALERT_1_A Bond Calc 1.591(8), Rep 1.625(5), Dev.. 4.25 Sigma
    O11A -SIA1 1_555 1_655 ..... # 1 Check

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PLAT701_ALERT_1_A Bond	Calc	1.957(5), Rep	1.931(3), Dev..	5.20 Sigma
O11A	-MM11	1_555	1_554	# 7 Check
PLAT701_ALERT_1_A Bond	Calc	1.957(5), Rep	1.931(3), Dev..	5.20 Sigma
O11A	-FM11	1_555	1_554	# 8 Check
PLAT701_ALERT_1_A Bond	Calc	2.368(6), Rep	2.348(5), Dev..	3.33 Sigma
O11A	-CA2	1_555	1_565	# 9 Check
PLAT701_ALERT_1_A Bond	Calc	2.368(6), Rep	2.348(5), Dev..	3.33 Sigma
O11A	-NA2	1_555	1_565	# 10 Check
PLAT701_ALERT_1_A Bond	Calc	1.598(7), Rep	1.622(5), Dev..	3.43 Sigma
O12A	-SIB1	1_555	1_655	# 11 Check
PLAT701_ALERT_1_A Bond	Calc	2.006(6), Rep	1.980(5), Dev..	4.33 Sigma
O12A	-MM11	1_555	1_555	# 17 Check
PLAT701_ALERT_1_A Bond	Calc	2.006(6), Rep	1.980(5), Dev..	4.33 Sigma
O12A	-FM11	1_555	1_555	# 18 Check
PLAT701_ALERT_1_A Bond	Calc	2.358(5), Rep	2.384(4), Dev..	5.20 Sigma
O22A	-CA21	1_555	3_667	# 32 Check
PLAT701_ALERT_1_A Bond	Calc	2.358(5), Rep	2.384(4), Dev..	5.20 Sigma
O22A	-NA21	1_555	3_667	# 33 Check
PLAT701_ALERT_1_A Bond	Calc	3.287(4), Rep	3.270(4), Dev..	4.25 Sigma
SIA1	-CA21	1_555	3_666	# 40 Check
PLAT701_ALERT_1_A Bond	Calc	3.217(4), Rep	3.198(4), Dev..	4.75 Sigma
SIB1	-CA2	1_555	3_666	# 41 Check
PLAT701_ALERT_1_A Bond	Calc	3.217(4), Rep	3.198(4), Dev..	4.75 Sigma
SIB1	-NA2	1_555	3_666	# 42 Check
PLAT701_ALERT_1_A Bond	Calc	3.096(3), Rep	3.086(2), Dev..	3.33 Sigma
MGM1	-AM11	1_555	1_554	# 48 Check
PLAT701_ALERT_1_A Bond	Calc	3.096(3), Rep	3.086(2), Dev..	3.33 Sigma
MGM1	-AM11	1_555	1_555	# 49 Check
PLAT701_ALERT_1_A Bond	Calc	3.096(3), Rep	3.086(2), Dev..	3.33 Sigma
MGM1	-MM11	1_555	1_554	# 52 Check
PLAT701_ALERT_1_A Bond	Calc	3.096(3), Rep	3.086(2), Dev..	3.33 Sigma
MGM1	-MM11	1_555	1_555	# 53 Check
PLAT701_ALERT_1_A Bond	Calc	3.455(4), Rep	3.436(6), Dev..	4.75 Sigma
MGM1	-CA2	1_555	1_565	# 54 Check
PLAT701_ALERT_1_A Bond	Calc	3.455(4), Rep	3.436(6), Dev..	4.75 Sigma
MGM1	-NA2	1_555	1_565	# 55 Check
PLAT701_ALERT_1_A Bond	Calc	3.096(3), Rep	3.086(2), Dev..	3.33 Sigma
AM1	-MM11	1_555	1_554	# 71 Check
PLAT701_ALERT_1_A Bond	Calc	3.096(3), Rep	3.086(2), Dev..	3.33 Sigma
AM1	-MM11	1_555	1_555	# 72 Check
PLAT701_ALERT_1_A Bond	Calc	3.455(4), Rep	3.436(6), Dev..	4.75 Sigma
AM1	-CA2	1_555	1_565	# 73 Check
PLAT701_ALERT_1_A Bond	Calc	3.455(4), Rep	3.436(6), Dev..	4.75 Sigma
AM1	-NA2	1_555	1_565	# 74 Check
PLAT701_ALERT_1_A Bond	Calc	3.193(3), Rep	3.181(3), Dev..	4.00 Sigma
AM11	-CA2	1_555	1_565	# 87 Check
PLAT701_ALERT_1_A Bond	Calc	3.193(3), Rep	3.181(3), Dev..	4.00 Sigma
AM11	-CA2	1_555	1_566	# 88 Check
PLAT701_ALERT_1_A Bond	Calc	3.193(3), Rep	3.181(3), Dev..	4.00 Sigma
AM11	-NA2	1_555	1_565	# 89 Check
PLAT701_ALERT_1_A Bond	Calc	3.193(3), Rep	3.181(3), Dev..	4.00 Sigma
AM11	-NA2	1_555	1_566	# 90 Check
PLAT701_ALERT_1_A Bond	Calc	3.193(3), Rep	3.181(3), Dev..	4.00 Sigma
MM11	-CA2	1_555	1_565	# 109 Check
PLAT701_ALERT_1_A Bond	Calc	3.193(3), Rep	3.181(3), Dev..	4.00 Sigma
MM11	-CA2	1_555	1_566	# 110 Check
PLAT701_ALERT_1_A Bond	Calc	3.193(3), Rep	3.181(3), Dev..	4.00 Sigma

MM11	-NA2	1_555	1_565		#	111 Check
PLAT701_ALERT_1_A Bond	Calc	3.193(3), Rep	3.181(3), Dev..			4.00 Sigma
MM11	-NA2	1_555	1_566		#	112 Check
PLAT701_ALERT_1_A Bond	Calc	3.193(3), Rep	3.181(3), Dev..			4.00 Sigma
FM11	-CA2	1_555	1_565		#	115 Check
PLAT701_ALERT_1_A Bond	Calc	3.193(3), Rep	3.181(3), Dev..			4.00 Sigma
FM11	-CA2	1_555	1_566		#	116 Check
PLAT701_ALERT_1_A Bond	Calc	3.193(3), Rep	3.181(3), Dev..			4.00 Sigma
FM11	-NA2	1_555	1_565		#	117 Check
PLAT701_ALERT_1_A Bond	Calc	3.193(3), Rep	3.181(3), Dev..			4.00 Sigma
FM11	-NA2	1_555	1_566		#	118 Check

Alert level B

PLAT017_ALERT_1_B Check	Scattering Type	Consistency of AM1	as			AL Error?
PLAT017_ALERT_1_B Check	Scattering Type	Consistency of FM1	as			FE Error?
PLAT017_ALERT_1_B Check	Scattering Type	Consistency of AM11	as			AL Error?
PLAT017_ALERT_1_B Check	Scattering Type	Consistency of MM11	as			MG Error?
PLAT017_ALERT_1_B Check	Scattering Type	Consistency of FM11	as			FE Error?
PLAT701_ALERT_1_B Bond	Calc	2.133(6), Rep	2.115(5), Dev..			3.00 Sigma
O11A	-MGM1	1_555	1_555		#	2 Check
PLAT701_ALERT_1_B Bond	Calc	2.133(6), Rep	2.115(5), Dev..			3.00 Sigma
O11A	-FM1	1_555	1_555		#	4 Check
PLAT701_ALERT_1_B Bond	Calc	2.343(5), Rep	2.358(4), Dev..			3.00 Sigma
O21A	-CA2	1_555	3_656		#	26 Check
PLAT701_ALERT_1_B Bond	Calc	2.343(5), Rep	2.358(4), Dev..			3.00 Sigma
O21A	-NA2	1_555	3_656		#	27 Check
PLAT701_ALERT_1_B Bond	Calc	1.669(4), Rep	1.659(4), Dev..			2.50 Sigma
O32A	-SIA1	1_555	1_555		#	36 Check
PLAT701_ALERT_1_B Bond	Calc	3.210(3), Rep	3.203(2), Dev..			2.33 Sigma
MGM1	-CA21	1_555	1_554		#	56 Check
PLAT701_ALERT_1_B Bond	Calc	3.210(3), Rep	3.203(2), Dev..			2.33 Sigma
MGM1	-CA21	1_555	1_555		#	57 Check
PLAT701_ALERT_1_B Bond	Calc	3.210(3), Rep	3.203(2), Dev..			2.33 Sigma
MGM1	-NA21	1_555	1_554		#	58 Check
PLAT701_ALERT_1_B Bond	Calc	3.210(3), Rep	3.203(2), Dev..			2.33 Sigma
MGM1	-NA21	1_555	1_555		#	59 Check
PLAT701_ALERT_1_B Bond	Calc	3.210(3), Rep	3.203(2), Dev..			2.33 Sigma
AM1	-CA21	1_555	1_554		#	75 Check
PLAT701_ALERT_1_B Bond	Calc	3.210(3), Rep	3.203(2), Dev..			2.33 Sigma
AM1	-CA21	1_555	1_555		#	76 Check
PLAT701_ALERT_1_B Bond	Calc	3.210(3), Rep	3.203(2), Dev..			2.33 Sigma
AM1	-NA21	1_555	1_554		#	77 Check
PLAT701_ALERT_1_B Bond	Calc	3.210(3), Rep	3.203(2), Dev..			2.33 Sigma
AM1	-NA21	1_555	1_555		#	78 Check
PLAT701_ALERT_1_B Bond	Calc	3.210(3), Rep	3.203(2), Dev..			2.33 Sigma
FM1	-CA21	1_555	1_554		#	79 Check
PLAT701_ALERT_1_B Bond	Calc	3.210(3), Rep	3.203(2), Dev..			2.33 Sigma
FM1	-CA21	1_555	1_555		#	80 Check
PLAT701_ALERT_1_B Bond	Calc	3.210(3), Rep	3.203(2), Dev..			2.33 Sigma
FM1	-NA21	1_555	1_554		#	81 Check
PLAT701_ALERT_1_B Bond	Calc	3.210(3), Rep	3.203(2), Dev..			2.33 Sigma
FM1	-NA21	1_555	1_555		#	82 Check
PLAT701_ALERT_1_B Bond	Calc	3.485(4), Rep	3.473(5), Dev..			3.00 Sigma
AM11	-CA21	1_555	1_555		#	91 Check
PLAT701_ALERT_1_B Bond	Calc	3.485(4), Rep	3.473(5), Dev..			3.00 Sigma
AM11	-NA21	1_555	1_555		#	92 Check

PLAT701_ALERT_1_B Bond	Calc	3.485(4), Rep	3.473(5), Dev..	3.00 Sigma
MM11	-CA21	1_555	1_555	# 113 Check
PLAT701_ALERT_1_B Bond	Calc	3.485(4), Rep	3.473(5), Dev..	3.00 Sigma
MM11	-NA21	1_555	1_555	# 114 Check

Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.132

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: Al1.81 Ca2.31 Fe0.28 Mg1.91 Na1.69 O24 Si8
Rep.: Al0.4525 Ca0.5763 Fe0.0695 Mg0.478 Na0.4237 O6 Si2

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: Al1.81 Fe0.28 Mg1.91 O24 Si8, 2.305(Ca), 1.695 (Na)
Rep.: ?

PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.08 Check

PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ... Please Check

PLAT054_ALERT_1_C Medium Crystal Dimension Missing (or Error) ... Please Check

PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ... Please Check

PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms . Please Check

PLAT213_ALERT_2_C Atom O11A has ADP max/min Ratio 3.1 prolat

PLAT213_ALERT_2_C Atom O31A has ADP max/min Ratio 3.8 prolat

PLAT313_ALERT_2_C Oxygen with Three Covalent Bonds (rare) O11A Check

PLAT701_ALERT_1_C Bond Calc 2.068(5), Rep 2.058(3), Dev.. 2.00 Sigma

O12A -MGM1 1_555 1_555 # 12 Check

PLAT701_ALERT_1_C Bond Calc 2.068(5), Rep 2.058(3), Dev.. 2.00 Sigma

O12A -FM1 1_555 1_555 # 14 Check

PLAT701_ALERT_1_C Bond Calc 1.597(6), Rep 1.588(5), Dev.. 1.50 Sigma

O22A -SIB1 1_555 1_555 # 28 Check

PLAT701_ALERT_1_C Bond Calc 2.015(6), Rep 2.025(5), Dev.. 1.67 Sigma

O22A -MGM1 1_555 3_666 # 29 Check

PLAT701_ALERT_1_C Bond Calc 2.015(6), Rep 2.025(5), Dev.. 1.67 Sigma

O22A -FM1 1_555 3_666 # 31 Check

PLAT701_ALERT_1_C Bond Calc 1.652(5), Rep 1.644(5), Dev.. 1.60 Sigma

O31A -SIA1 1_555 1_555 # 34 Check

PLAT701_ALERT_1_C Bond Calc 1.678(4), Rep 1.670(4), Dev.. 2.00 Sigma

O31A -SIB1 1_555 1_554 # 35 Check

PLAT701_ALERT_1_C Bond Calc 3.053(3), Rep 3.049(2), Dev.. 1.33 Sigma

SIB1 -CA21 1_555 3_667 # 43 Check

PLAT701_ALERT_1_C Bond Calc 3.053(3), Rep 3.049(2), Dev.. 1.33 Sigma

SIB1 -NA21 1_555 3_667 # 44 Check

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label MnM1 Check

O11A MNM1

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Cm11 Check

O11A CM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Tm11 Check

O11A TM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label MnM1 Check

O12A MNM1

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Cm11 Check

O12A CM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Tm11 Check

O12A TM11

PLAT711_ALERT_1_C BOND Unknown or Inconsistent Label Cm11 Check

O21A CM11

PLAT711_ALERT_1_C	BOND O21A	Unknown or TM11	Inconsistent Label	Tm11 Check
PLAT711_ALERT_1_C	BOND O22A	Unknown or MNM1	Inconsistent Label	MnM1 Check
PLAT711_ALERT_1_C	BOND MGM1	Unknown or MNM1	Inconsistent Label	MnM1 Check
PLAT711_ALERT_1_C	BOND MGM1	Unknown or TM11	Inconsistent Label	Tm11 Check
PLAT711_ALERT_1_C	BOND MGM1	Unknown or TM11	Inconsistent Label	Tm11 Check
PLAT711_ALERT_1_C	BOND MNM1	Unknown or AM1	Inconsistent Label	MnM1 Check
PLAT711_ALERT_1_C	BOND MNM1	Unknown or FM1	Inconsistent Label	MnM1 Check
PLAT711_ALERT_1_C	BOND MNM1	Unknown or MM11	Inconsistent Label	MnM1 Check
PLAT711_ALERT_1_C	BOND MNM1	Unknown or MM11	Inconsistent Label	MnM1 Check
PLAT711_ALERT_1_C	BOND MNM1	Unknown or CA2	Inconsistent Label	MnM1 Check
PLAT711_ALERT_1_C	BOND MNM1	Unknown or NA2	Inconsistent Label	MnM1 Check
PLAT711_ALERT_1_C	BOND MNM1	Unknown or CA21	Inconsistent Label	MnM1 Check
PLAT711_ALERT_1_C	BOND MNM1	Unknown or CA21	Inconsistent Label	MnM1 Check
PLAT711_ALERT_1_C	BOND MNM1	Unknown or NA21	Inconsistent Label	MnM1 Check
PLAT711_ALERT_1_C	BOND MNM1	Unknown or NA21	Inconsistent Label	MnM1 Check
PLAT711_ALERT_1_C	BOND AM11	Unknown or CM11	Inconsistent Label	Cm11 Check
PLAT711_ALERT_1_C	BOND AM11	Unknown or TM11	Inconsistent Label	Tm11 Check
PLAT711_ALERT_1_C	BOND CM11	Unknown or TM11	Inconsistent Label	Cm11 Check
PLAT711_ALERT_1_C	BOND CM11	Unknown or MM11	Inconsistent Label	Cm11 Check
PLAT711_ALERT_1_C	BOND CM11	Unknown or FM11	Inconsistent Label	Cm11 Check
PLAT711_ALERT_1_C	BOND CM11	Unknown or CA2	Inconsistent Label	Cm11 Check
PLAT711_ALERT_1_C	BOND CM11	Unknown or CA2	Inconsistent Label	Cm11 Check
PLAT711_ALERT_1_C	BOND CM11	Unknown or NA2	Inconsistent Label	Cm11 Check
PLAT711_ALERT_1_C	BOND CM11	Unknown or NA2	Inconsistent Label	Cm11 Check
PLAT711_ALERT_1_C	BOND TM11	Unknown or MM11	Inconsistent Label	Tm11 Check
PLAT711_ALERT_1_C	BOND TM11	Unknown or FM11	Inconsistent Label	Tm11 Check
PLAT711_ALERT_1_C	BOND TM11	Unknown or CA2	Inconsistent Label	Tm11 Check
PLAT711_ALERT_1_C	BOND TM11	Unknown or CA2	Inconsistent Label	Tm11 Check
PLAT711_ALERT_1_C	BOND	Unknown or	Inconsistent Label	Tm11 Check

	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA2		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	CA21		
PLAT711_ALERT_1_C	BOND	Unknown or Inconsistent Label		Tm11 Check
	TM11	NA21		
PLAT920_ALERT_1_C	Theta(Max)	in CIF and FCF Differ by		0.38 Degree

● Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT020_ALERT_3_G	The Value of Rint is Greater Than 0.12	0.132	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.49570	Ang.
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm1 Constrained at	0.087	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fm11 Constrained at	0.052	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am11 Constrained at	0.86	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of MgM1 Constrained at	0.868	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Am1 Constrained at	0.045	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mm11 Constrained at	0.088	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca21 Constrained at	0.7904	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2 Constrained at	0.3622	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2 Constrained at	0.6378	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na21 Constrained at	0.2096	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O31A .	135.3	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O32A .	139.9	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	8	Note
	SiA1 SiB1 MgM1 Am1 Fm1 Am11 Mm11 Fm11		
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.84	Ratio
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found		Please Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		! Info
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	2	Note
	0 1 0, 1 1 0,		
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L=	0.600	461 Report
	0 2 0, 0 3 0, 0 4 0, 0 5 0, 0 6 0, 0 7 0,		
	0 8 0, 0 9 0, 0 10 0, 1 2 0, 1 3 0, 1 4 0,		
	1 5 0, 1 6 0, 1 7 0, 1 8 0, 1 9 0, 1 10 0,		
	2 0 0, 2 1 0, 2 2 0, 2 4 0, 2 5 0, 2 6 0,		
	2 7 0, 2 8 0, 2 9 0, 2 10 0, 3 1 0, 3 2 0,		
	3 3 0, 3 6 0, 3 7 0, 3 8 0, 3 9 0, 3 10 0,		
	4 0 0, 4 1 0, 4 2 0, 4 3 0, 4 4 0, 4 5 0,		
	4 8 0, 4 9 0, 5 1 0, 5 2 0, 5 3 0, 5 4 0,		
	5 5 0, 5 6 0, 5 7 0, 5 9 0, 6 0 0, 6 1 0,		
	6 2 0, 6 3 0, 6 4 0, 6 5 0, 6 6 0, 6 7 0,		

6	8	0,	7	1	0,	7	2	0,	7	3	0,	7	4	0,	7	5	0,		
7	6	0,	7	7	0,	7	8	0,	8	0	0,	8	1	0,	8	2	0,		
8	3	0,	8	4	0,	8	5	0,	8	6	0,	8	7	0,	9	1	0,		
9	2	0,	9	3	0,	9	4	0,	9	5	0,	9	6	0,	10	0	0,		
10	1	0,	10	2	0,	10	3	0,	10	4	0,	-11	0	1,	-11	1	1,		
-11	2	1,	-10	1	1,	-10	2	1,	-10	3	1,	-10	4	1,	-10	5	1,		
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600															687	Note			
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF															3	Note			
-2	2	1,	5	3	1,	0	0	2,											
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked															!	Info			
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ															5	Units			
PLAT951_ALERT_5_G Calculated (ThMax) and CIF-Reported Kmax Differ															4	Units			
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ															5	Units			
PLAT957_ALERT_1_G Calculated (ThMax) and Actual (FCF) Kmax Differ															4	Units			
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of															3.0	Sig(I)			
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value															1.799	Note			
Predicted wR2: Based on SigI**2 9.97 or SHELX Weight 9.97																			
PLAT985_ALERT_1_G The Ca-f"= 0.1533 Deviates from the B&C-Value															0.1517	Check			
PLAT985_ALERT_1_G The Fe-f"= 0.4372 Deviates from the B&C-Value															0.4344	Check			

43 **ALERT level A** = Most likely a serious problem - resolve or explain
 26 **ALERT level B** = A potentially serious problem, consider carefully
 60 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 44 **ALERT level G** = General information/check it is not something unexpected

131 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 5 ALERT type 2 Indicator that the structure model may be wrong or deficient
 9 ALERT type 3 Indicator that the structure quality may be low
 19 ALERT type 4 Improvement, methodology, query or suggestion
 9 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_GEOM006_0.88_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_0.88_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_0.88_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_0.88_GPa
;
PROBLEM: _diffrn_reflns_theta_full value (too) Low .....      13.26 Degree
RESPONSE: ...
;
_vrf_PLAT029_0.88_GPa
```

```

;
PROBLEM: _diffn_measured_fraction_theta_full value Low .      0.570 Why?
RESPONSE: ...
;
_vrf_GEOM006_1.06_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_1.06_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_1.06_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_1.06_GPa
;
PROBLEM: _diffn_refl_theta_full value (too) Low .....      13.28 Degree
RESPONSE: ...
;
_vrf_PLAT029_1.06_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low .      0.560 Why?
RESPONSE: ...
;
_vrf_PLAT701_1.06_GPa
;
PROBLEM: Bond      Calc      2.137(6), Rep      2.115(5), Dev..      3.67 Sigma
RESPONSE: ...
;
_vrf_GEOM006_1.20_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_1.20_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_1.20_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_1.20_GPa
;
PROBLEM: _diffn_refl_theta_full value (too) Low .....      12.20 Degree
RESPONSE: ...
;
_vrf_PLAT029_1.20_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low .      0.570 Why?

```

```

RESPONSE: ...
;
_vrf_GEOM006_1.58_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_1.58_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_1.58_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_1.58_GPa
;
PROBLEM: _diffrn_reflns_theta_full value (too) Low ..... 12.42 Degree
RESPONSE: ...
;
_vrf_PLAT029_1.58_GPa
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low . 0.560 Why?
RESPONSE: ...
;
_vrf_PLAT701_1.58_GPa
;
PROBLEM: Bond      Calc      1.608(4), Rep      1.625(5), Dev.. 4.25 Sigma
RESPONSE: ...
;
_vrf_GEOM006_1.95_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_1.95_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_1.95_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_1.95_GPa
;
PROBLEM: _diffrn_reflns_theta_full value (too) Low ..... 10.18 Degree
RESPONSE: ...
;
_vrf_PLAT029_1.95_GPa
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low . 0.550 Why?
RESPONSE: ...
;

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```

_vrf_PLAT701_1.95_GPa
;
PROBLEM: Bond      Calc      1.614(3), Rep      1.625(5), Dev..      3.67 Sigma
RESPONSE: ...
;
_vrf_GEOM006_2.32_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_2.32_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_2.32_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_2.32_GPa
;
PROBLEM: _diffn_refl_theta_full value (too) Low .....      13.36 Degree
RESPONSE: ...
;
_vrf_PLAT029_2.32_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low .      0.510 Why?
RESPONSE: ...
;
_vrf_PLAT211_2.32_GPa
;
PROBLEM: ADP of Atom O32A      is N.P.D. or (nearly) 2D .      Please Check
RESPONSE: ...
;
_vrf_PLAT701_2.32_GPa
;
PROBLEM: Bond      Calc      1.608(4), Rep      1.625(5), Dev..      4.25 Sigma
RESPONSE: ...
;
_vrf_GEOM006_2.70_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_2.70_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_2.70_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_2.70_GPa
;

```

```

PROBLEM: _diffn_refl_theta_full value (too) Low ..... 12.24 Degree
RESPONSE: ...
;
_vrf_PLAT029_2.70_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low . 0.540 Why?
RESPONSE: ...
;
_vrf_PLAT701_2.70_GPa
;
PROBLEM: Bond      Calc      2.345(4), Rep      2.358(4), Dev.. 3.25 Sigma
RESPONSE: ...
;
_vrf_GEOM006_3.25_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_3.25_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_3.25_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_3.25_GPa
;
PROBLEM: _diffn_refl_theta_full value (too) Low ..... 13.06 Degree
RESPONSE: ...
;
_vrf_PLAT029_3.25_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low . 0.550 Why?
RESPONSE: ...
;
_vrf_PLAT701_3.25_GPa
;
PROBLEM: Bond      Calc      2.103(3), Rep      2.115(5), Dev.. 4.00 Sigma
RESPONSE: ...
;
_vrf_GEOM006_4.24_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_4.24_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_4.24_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...

```

```

;
_vrf_PLAT027_4.24_GPa
;
PROBLEM: _diffn_refl_theta_full value (too) Low ..... 12.25 Degree
RESPONSE: ...
;
_vrf_PLAT029_4.24_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low . 0.560 Why?
RESPONSE: ...
;
_vrf_PLAT701_4.24_GPa
;
PROBLEM: Bond      Calc      1.607(3), Rep      1.625(5), Dev..      6.00 Sigma
RESPONSE: ...
;
_vrf_GEOM006_4.30_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_4.30_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_4.30_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_4.30_GPa
;
PROBLEM: _diffn_refl_theta_full value (too) Low ..... 12.89 Degree
RESPONSE: ...
;
_vrf_PLAT029_4.30_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low . 0.560 Why?
RESPONSE: ...
;
_vrf_PLAT701_4.30_GPa
;
PROBLEM: Bond      Calc      1.604(3), Rep      1.625(5), Dev..      7.00 Sigma
RESPONSE: ...
;
_vrf_GEOM006_4.45_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_4.45_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_4.45_GPa

```

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;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_4.45_GPa
;
PROBLEM: _diffn_refl_theta_full value (too) Low ..... 12.26 Degree
RESPONSE: ...
;
_vrf_PLAT029_4.45_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low . 0.560 Why?
RESPONSE: ...
;
_vrf_PLAT701_4.45_GPa
;
PROBLEM: Bond      Calc      1.607(3), Rep      1.625(5), Dev..      6.00 Sigma
RESPONSE: ...
;
_vrf_GEOM006_4.86_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_4.86_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_4.86_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_4.86_GPa
;
PROBLEM: _diffn_refl_theta_full value (too) Low ..... 12.27 Degree
RESPONSE: ...
;
_vrf_PLAT029_4.86_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low . 0.560 Why?
RESPONSE: ...
;
_vrf_PLAT701_4.86_GPa
;
PROBLEM: Bond      Calc      1.605(3), Rep      1.625(5), Dev..      6.67 Sigma
RESPONSE: ...
;
_vrf_GEOM006_5.18_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_5.18_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing

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RESPONSE: ...
;
_vrf_GEOM008_5.18_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_5.18_GPa
;
PROBLEM: _diffrn_reflns_theta_full value (too) Low ..... 13.21 Degree
RESPONSE: ...
;
_vrf_PLAT029_5.18_GPa
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low . 0.550 Why?
RESPONSE: ...
;
_vrf_PLAT701_5.18_GPa
;
PROBLEM: Bond      Calc      1.607(3), Rep      1.625(5), Dev..      6.00 Sigma
RESPONSE: ...
;
_vrf_GEOM006_5.72_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_5.72_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_5.72_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_5.72_GPa
;
PROBLEM: _diffrn_reflns_theta_full value (too) Low ..... 13.36 Degree
RESPONSE: ...
;
_vrf_PLAT029_5.72_GPa
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low . 0.560 Why?
RESPONSE: ...
;
_vrf_PLAT701_5.72_GPa
;
PROBLEM: Bond      Calc      1.600(4), Rep      1.625(5), Dev..      6.25 Sigma
RESPONSE: ...
;
_vrf_GEOM006_6.19_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;

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_vrf_GEOM007_6.19_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_6.19_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_6.19_GPa
;
PROBLEM: _diffn_refl_theta_full value (too) Low ..... 13.37 Degree
RESPONSE: ...
;
_vrf_PLAT029_6.19_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low . 0.550 Why?
RESPONSE: ...
;
_vrf_PLAT701_6.19_GPa
;
PROBLEM: Bond      Calc      1.608(4), Rep      1.625(5), Dev.. 4.25 Sigma
RESPONSE: ...
;
_vrf_GEOM006_7.11_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_7.11_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_7.11_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_7.11_GPa
;
PROBLEM: _diffn_refl_theta_full value (too) Low ..... 12.88 Degree
RESPONSE: ...
;
_vrf_PLAT029_7.11_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low . 0.550 Why?
RESPONSE: ...
;
_vrf_PLAT211_7.11_GPa
;
PROBLEM: ADP of Atom O11A      is N.P.D. or (nearly) 2D . Please Check
RESPONSE: ...
;
_vrf_PLAT701_7.11_GPa
;

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```

PROBLEM: Bond      Calc      1.588(5), Rep      1.625(5), Dev..      7.40 Sigma
RESPONSE: ...
;
_vrf_GEOM006_8.04_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_8.04_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_8.04_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_8.04_GPa
;
PROBLEM: _diffn_refl_theta_full value (too) Low .....      12.36 Degree
RESPONSE: ...
;
_vrf_PLAT029_8.04_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low .      0.560 Why?
RESPONSE: ...
;
_vrf_PLAT701_8.04_GPa
;
PROBLEM: Bond      Calc      1.604(3), Rep      1.625(5), Dev..      7.00 Sigma
RESPONSE: ...
;
_vrf_GEOM006_8.46_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_8.46_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_8.46_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_8.46_GPa
;
PROBLEM: _diffn_refl_theta_full value (too) Low .....      13.33 Degree
RESPONSE: ...
;
_vrf_PLAT029_8.46_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low .      0.550 Why?
RESPONSE: ...

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;
_vrf_PLAT701_8.46_GPa
;
PROBLEM: Bond      Calc      1.605(4), Rep      1.625(5), Dev..      5.00 Sigma
RESPONSE: ...
;
_vrf_GEOM006_8.61_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_8.61_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_8.61_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_8.61_GPa
;
PROBLEM: _diffn_refl_theta_full value (too) Low .....      12.25 Degree
RESPONSE: ...
;
_vrf_PLAT029_8.61_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low .      0.540 Why?
RESPONSE: ...
;
_vrf_PLAT088_8.61_GPa
;
PROBLEM: Poor Data / Parameter Ratio .....      5.93 Note
RESPONSE: ...
;
_vrf_PLAT701_8.61_GPa
;
PROBLEM: Bond      Calc      1.599(4), Rep      1.625(5), Dev..      6.50 Sigma
RESPONSE: ...
;
_vrf_GEOM006_9.13_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_9.13_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_9.13_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_9.13_GPa

```

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;
PROBLEM: _diffn_refl_theta_full value (too) Low ..... 10.66 Degree
RESPONSE: ...
;
_vrf_PLAT029_9.13_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low . 0.460 Why?
RESPONSE: ...
;
_vrf_PLAT088_9.13_GPa
;
PROBLEM: Poor Data / Parameter Ratio ..... 4.51 Note
RESPONSE: ...
;
_vrf_PLAT701_9.13_GPa
;
PROBLEM: Bond      Calc      1.607(4), Rep      1.625(5), Dev.. 4.50 Sigma
RESPONSE: ...
;
_vrf_GEOM006_9.73_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_9.73_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_9.73_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_9.73_GPa
;
PROBLEM: _diffn_refl_theta_full value (too) Low ..... 12.69 Degree
RESPONSE: ...
;
_vrf_PLAT029_9.73_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low . 0.550 Why?
RESPONSE: ...
;
_vrf_PLAT701_9.73_GPa
;
PROBLEM: Bond      Calc      1.598(5), Rep      1.625(5), Dev.. 5.40 Sigma
RESPONSE: ...
;
_vrf_GEOM006_8.29_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_8.29_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing

```

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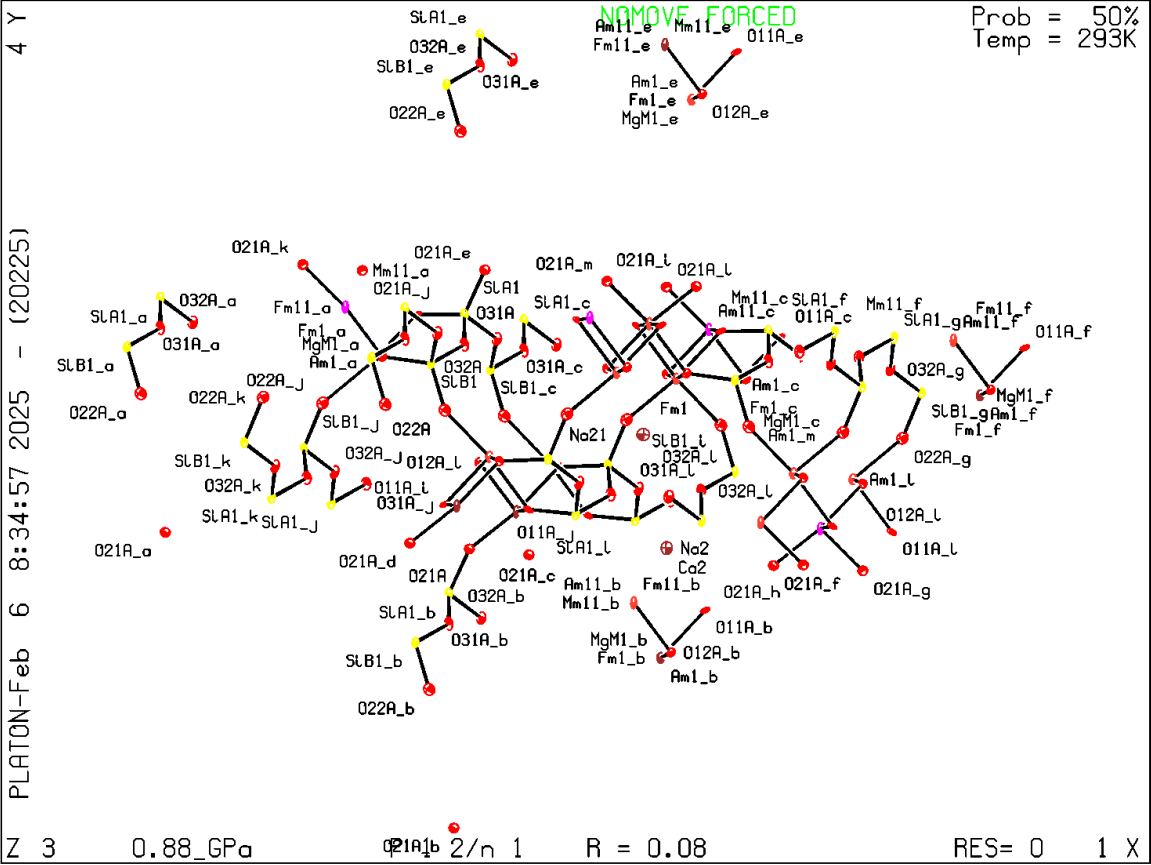
RESPONSE: ...
;
_vrf_GEOM008_8.29_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_8.29_GPa
;
PROBLEM: _diffrn_reflns_theta_full value (too) Low ..... 10.42 Degree
RESPONSE: ...
;
_vrf_PLAT029_8.29_GPa
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low . 0.560 Why?
RESPONSE: ...
;
_vrf_PLAT088_8.29_GPa
;
PROBLEM: Poor Data / Parameter Ratio ..... 5.93 Note
RESPONSE: ...
;
_vrf_PLAT701_8.29_GPa
;
PROBLEM: Bond      Calc      1.598(4), Rep      1.625(5), Dev.. 6.75 Sigma
RESPONSE: ...
;
_vrf_GEOM006_6.91_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_6.91_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_6.91_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_6.91_GPa
;
PROBLEM: _diffrn_reflns_theta_full value (too) Low ..... 10.12 Degree
RESPONSE: ...
;
_vrf_PLAT029_6.91_GPa
;
PROBLEM: _diffrn_measured_fraction_theta_full value Low . 0.530 Why?
RESPONSE: ...
;
_vrf_PLAT088_6.91_GPa
;
PROBLEM: Poor Data / Parameter Ratio ..... 5.73 Note
RESPONSE: ...
;

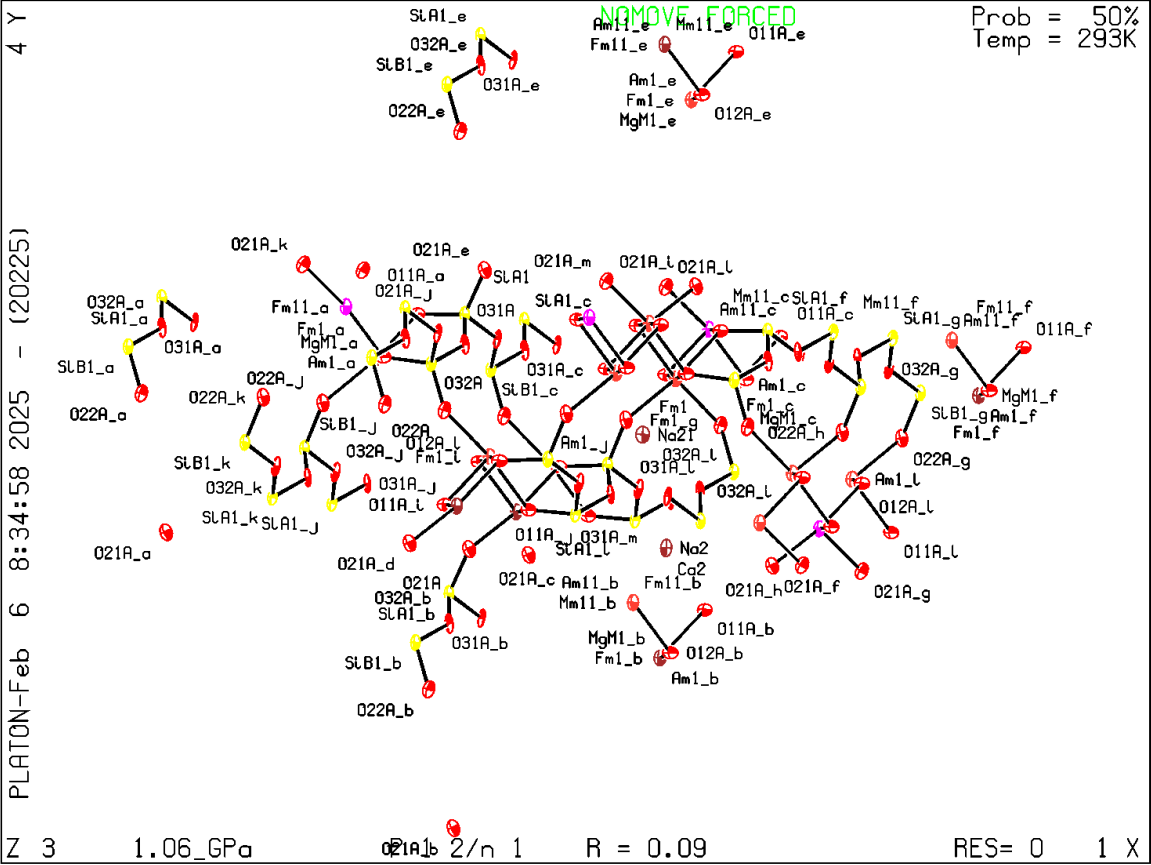
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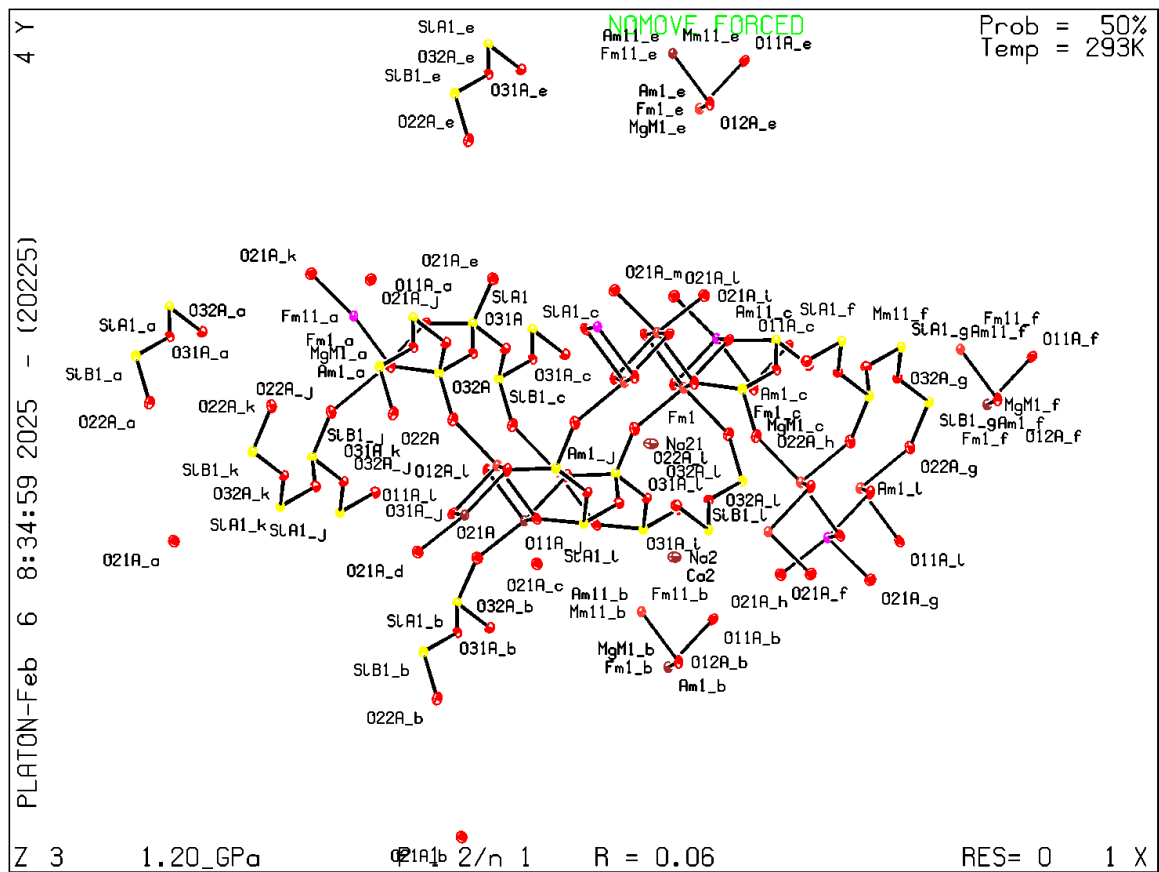
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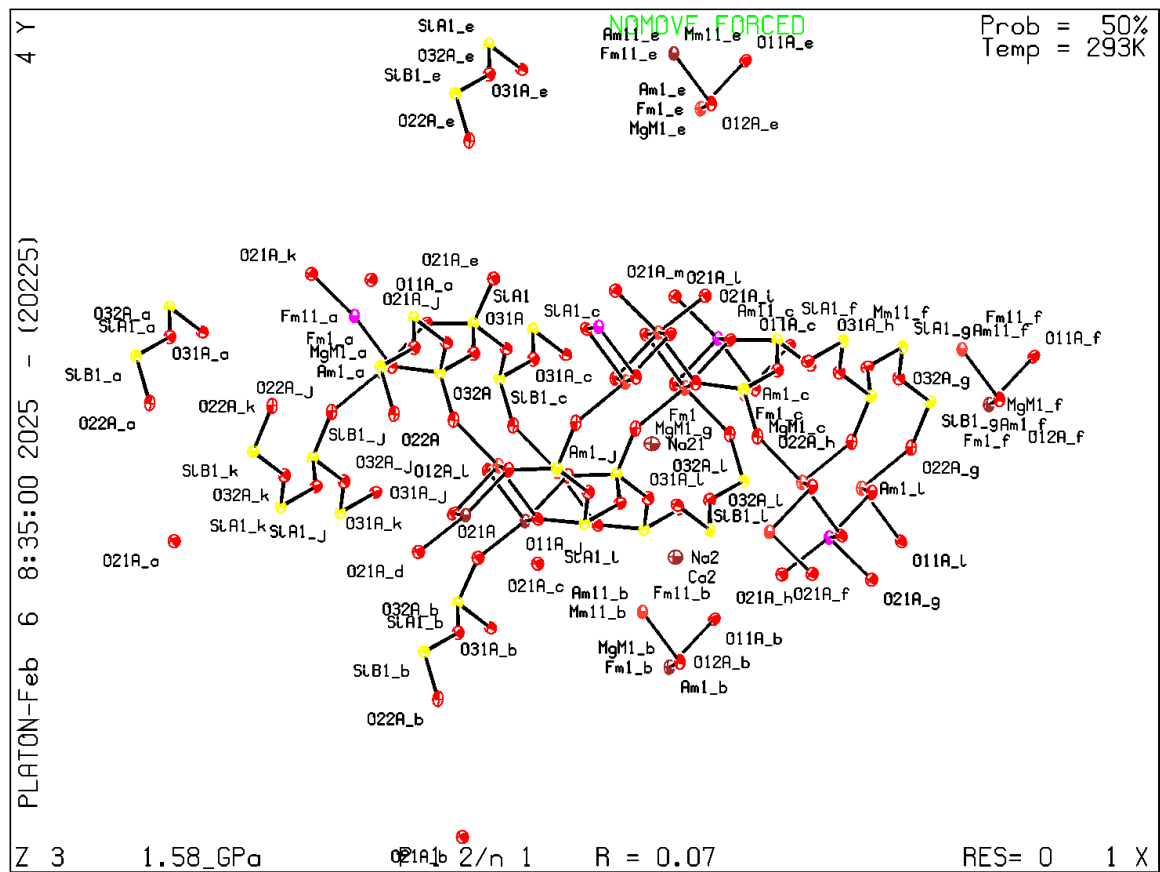
_vrf_PLAT701_6.91_GPa
;
PROBLEM: Bond      Calc      1.603(5), Rep      1.625(5), Dev..      4.40 Sigma
RESPONSE: ...
;
_vrf_EXPT005_0.03_GPa
;
PROBLEM: _exptl_crystal_description is missing
RESPONSE: ...
;
_vrf_GEOM006_0.03_GPa
;
PROBLEM: _geom_angle_atom_site_label_2 is missing
RESPONSE: ...
;
_vrf_GEOM007_0.03_GPa
;
PROBLEM: _geom_angle_atom_site_label_3 is missing
RESPONSE: ...
;
_vrf_GEOM008_0.03_GPa
;
PROBLEM: _geom_angle is missing
RESPONSE: ...
;
_vrf_PLAT027_0.03_GPa
;
PROBLEM: _diffn_reflths_theta_full value (too) Low .....      12.19 Degree
RESPONSE: ...
;
_vrf_PLAT029_0.03_GPa
;
PROBLEM: _diffn_measured_fraction_theta_full value Low .      0.460 Why?
RESPONSE: ...
;
_vrf_PLAT088_0.03_GPa
;
PROBLEM: Poor Data / Parameter Ratio .....      5.10 Note
RESPONSE: ...
;
_vrf_PLAT699_0.03_GPa
;
PROBLEM: Missing _exptl_crystal_description Value .....      Please Do !
RESPONSE: ...
;
_vrf_PLAT701_0.03_GPa
;
PROBLEM: Bond      Calc      1.591(8), Rep      1.625(5), Dev..      4.25 Sigma
RESPONSE: ...
;
# end Validation Reply Form

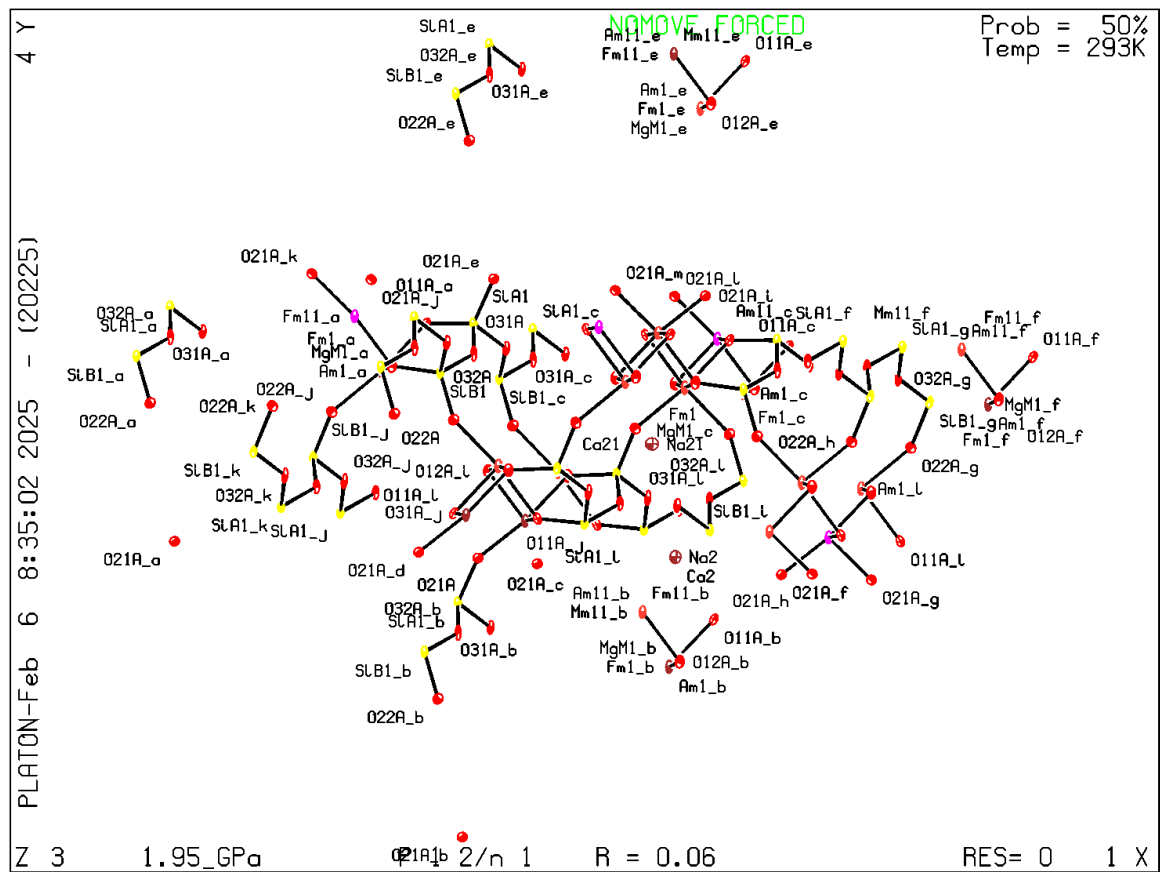
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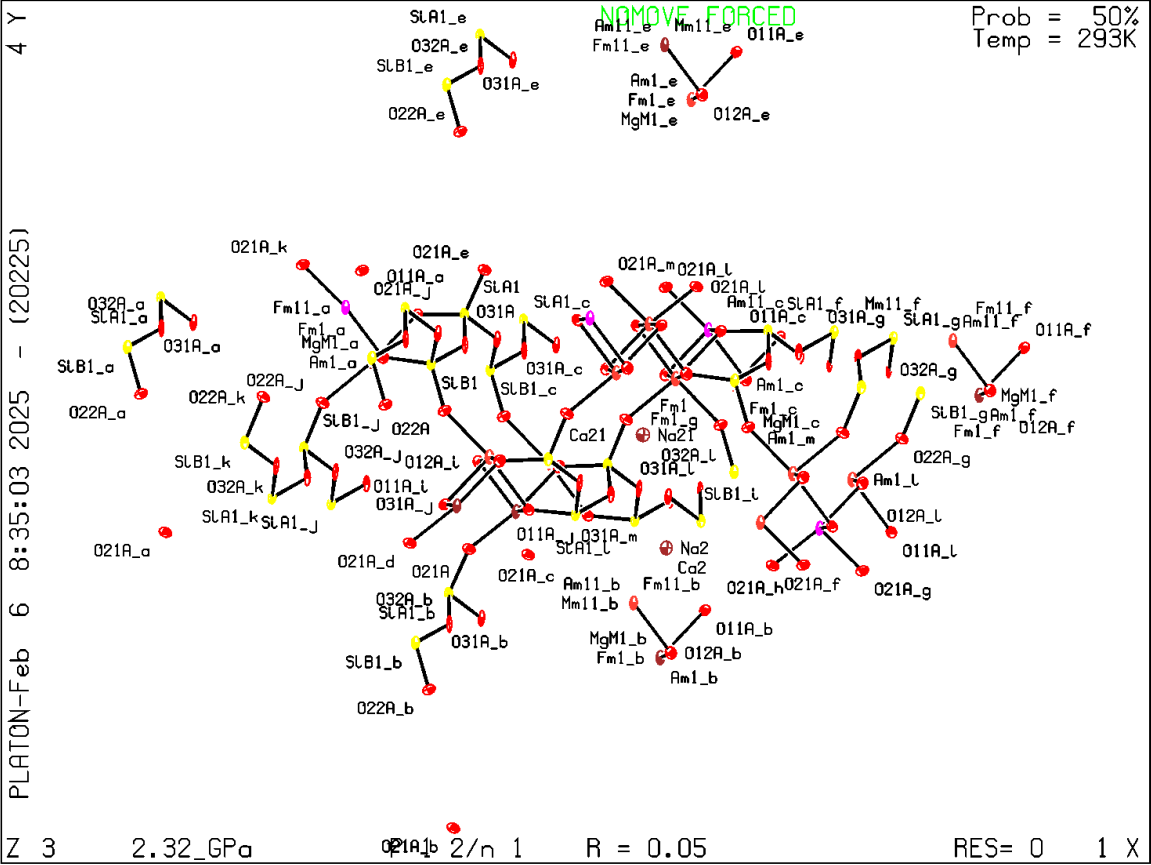


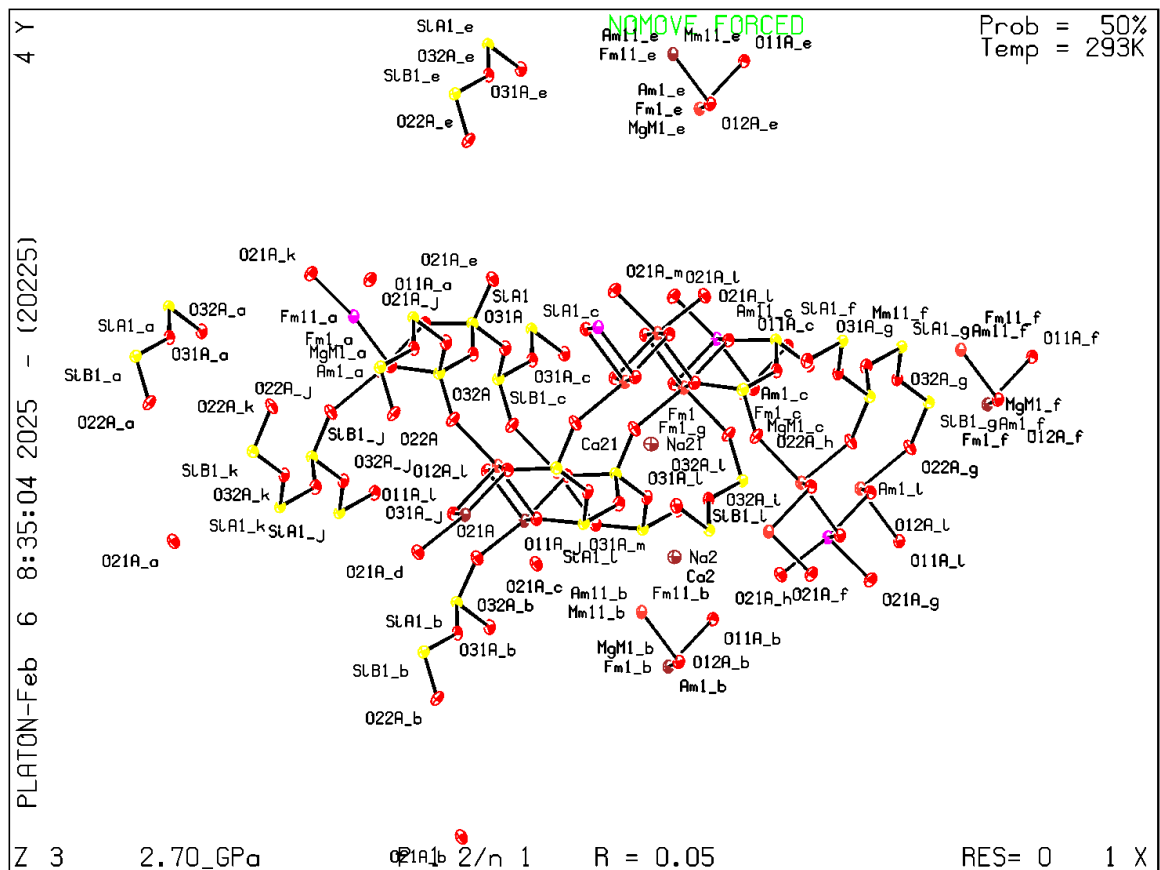


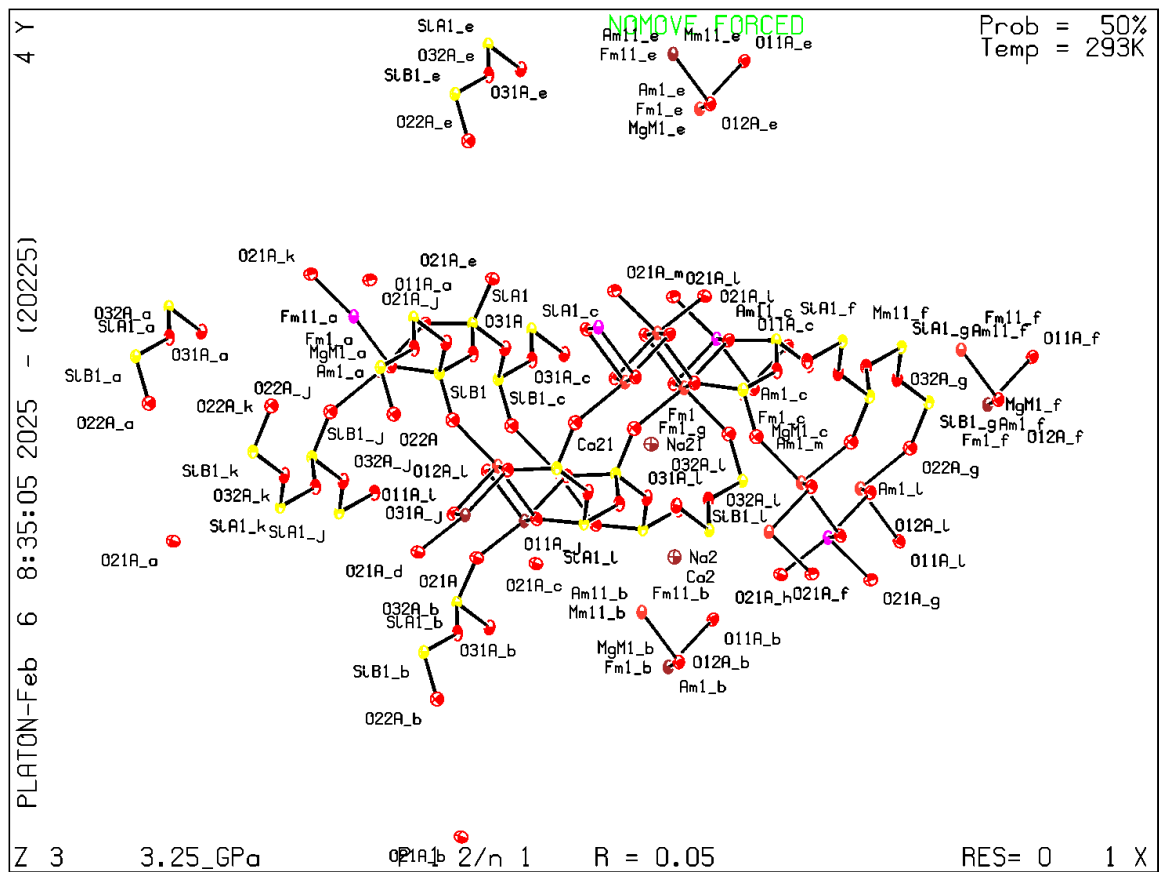


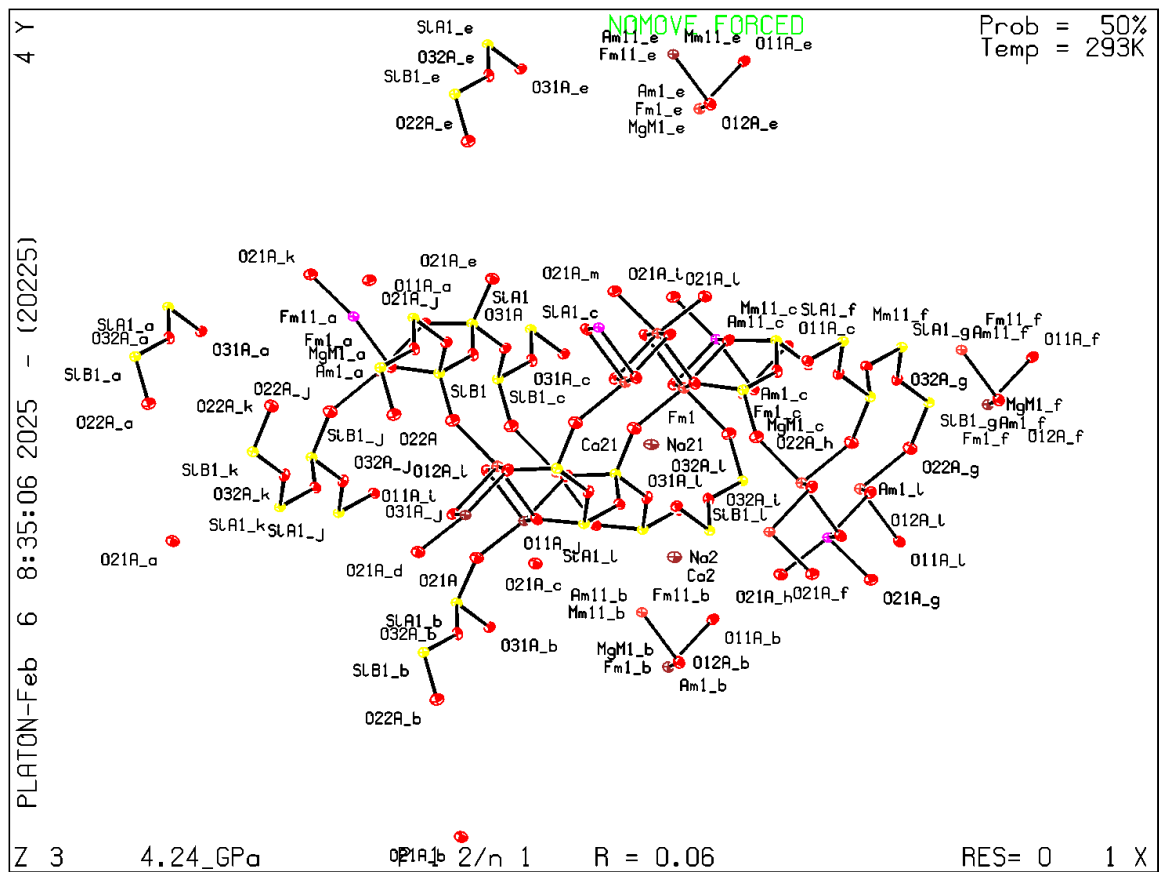


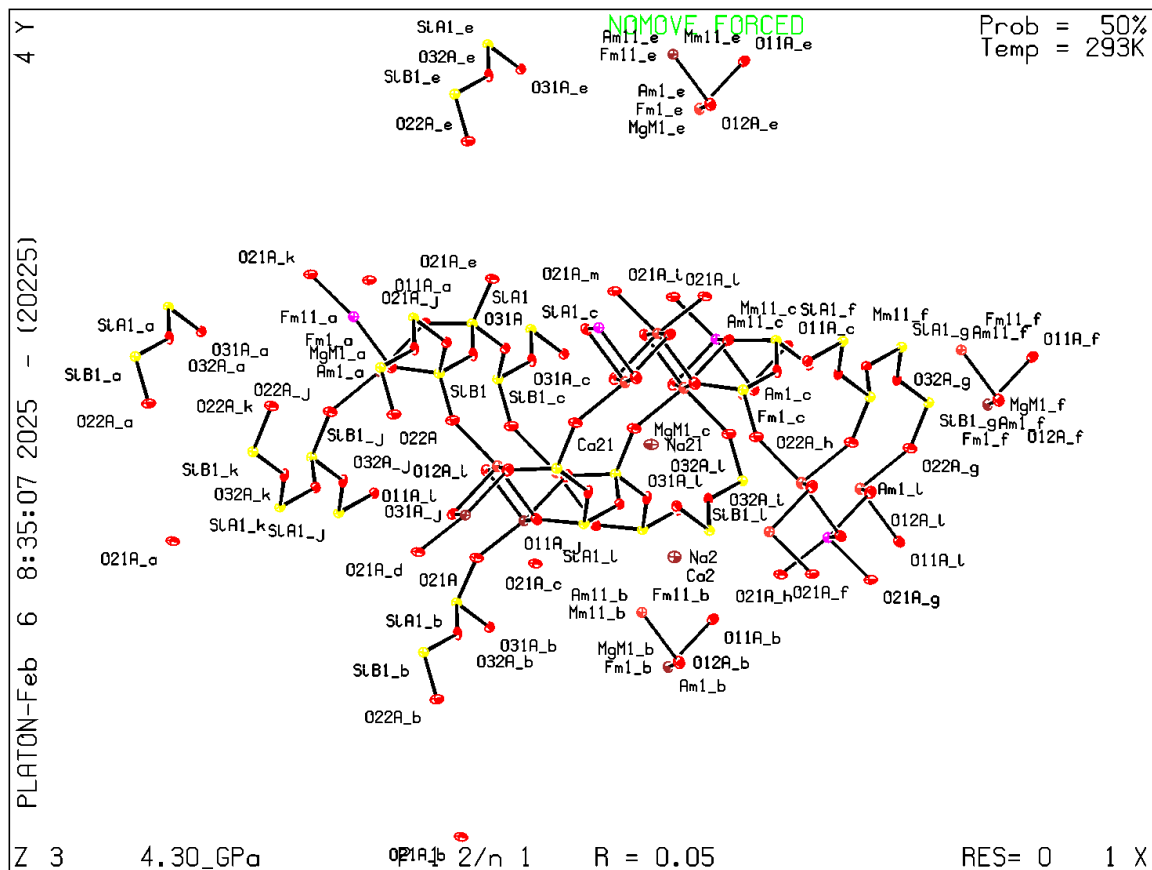
Datablock 2.32_GPa - ellipsoid plot

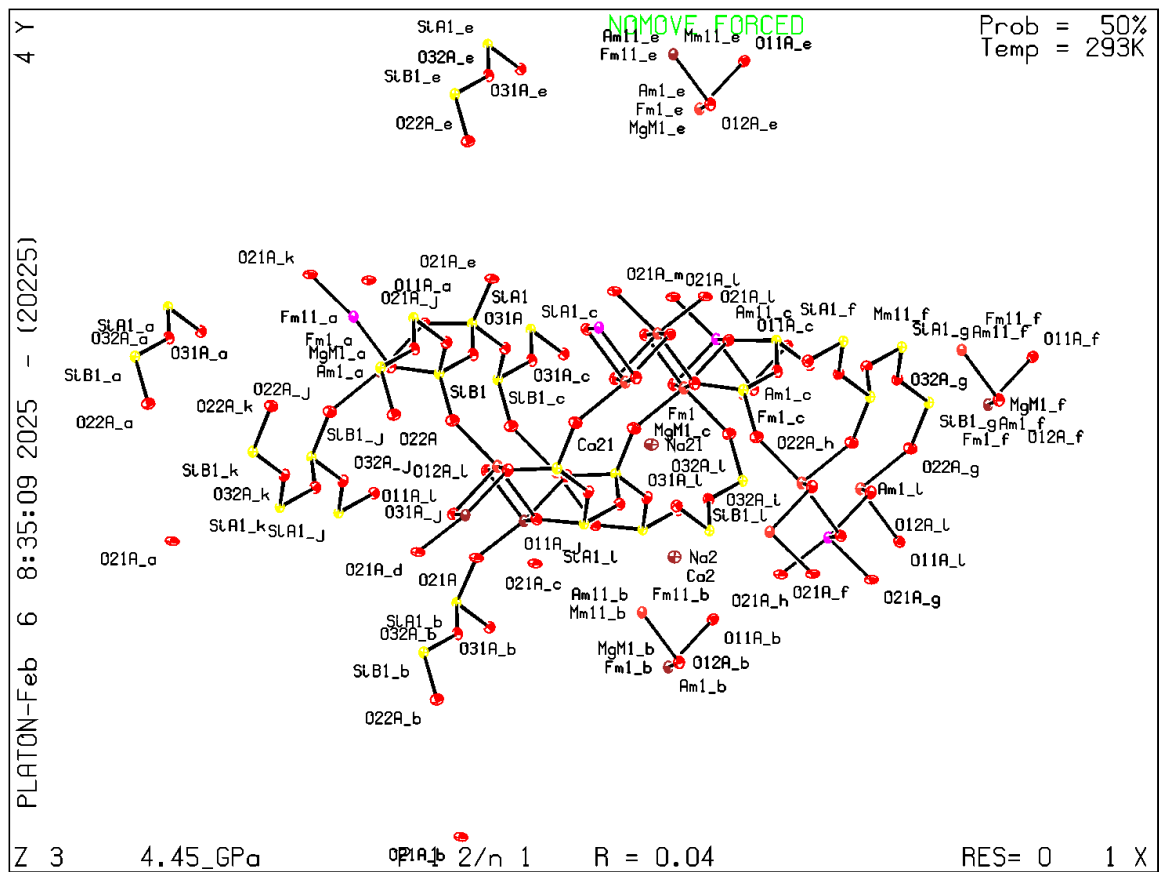


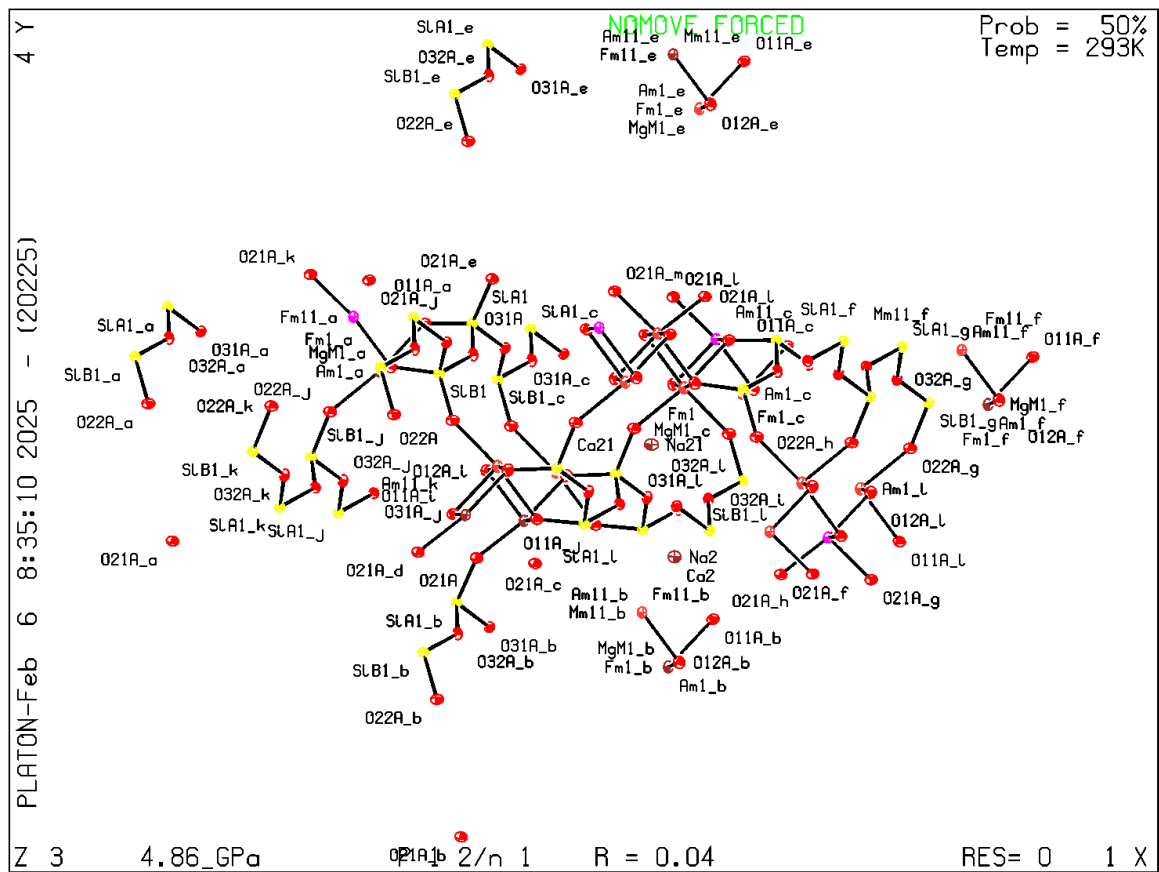




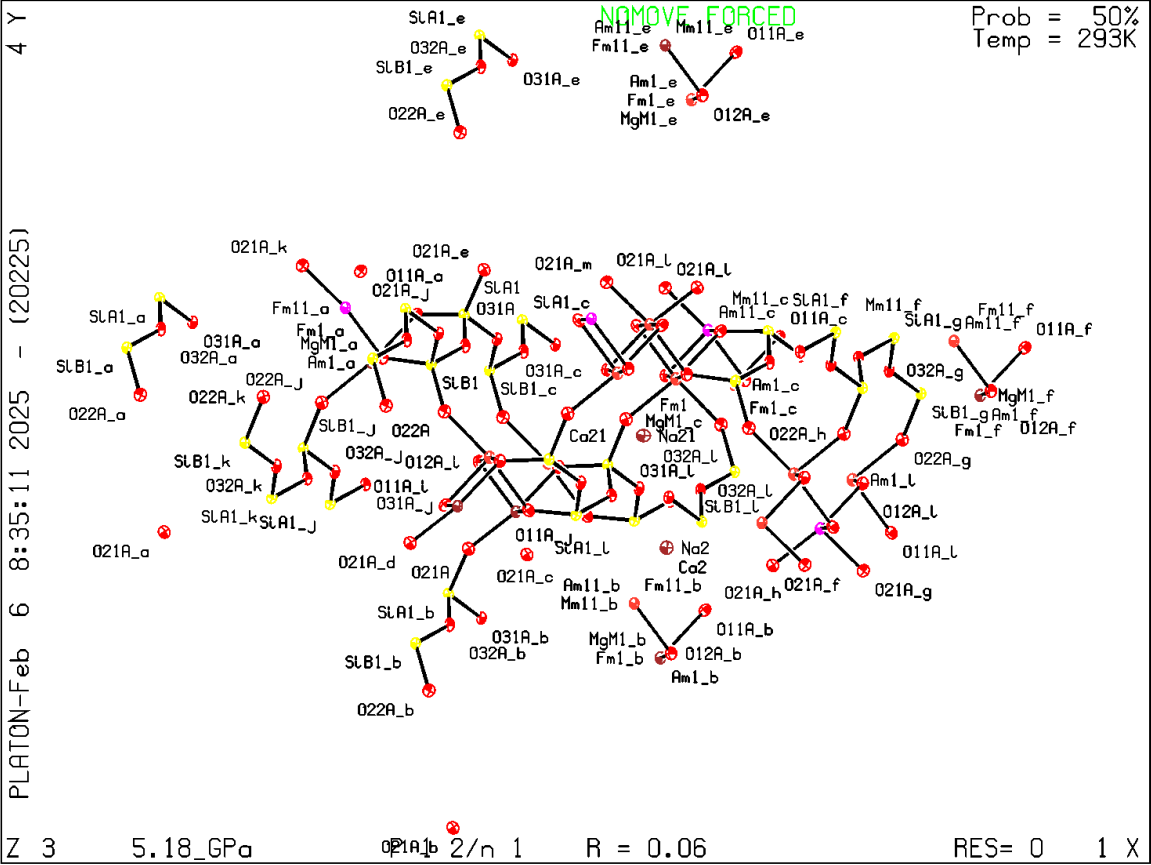


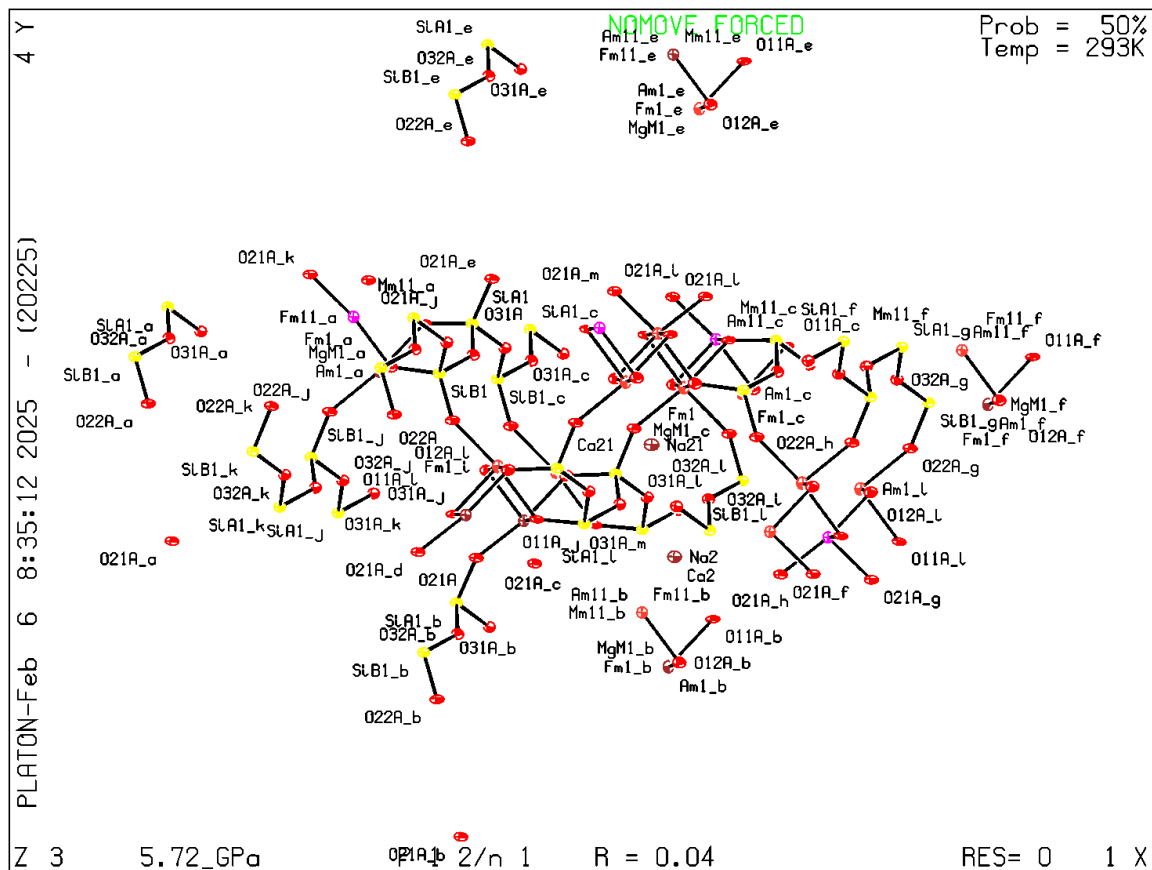


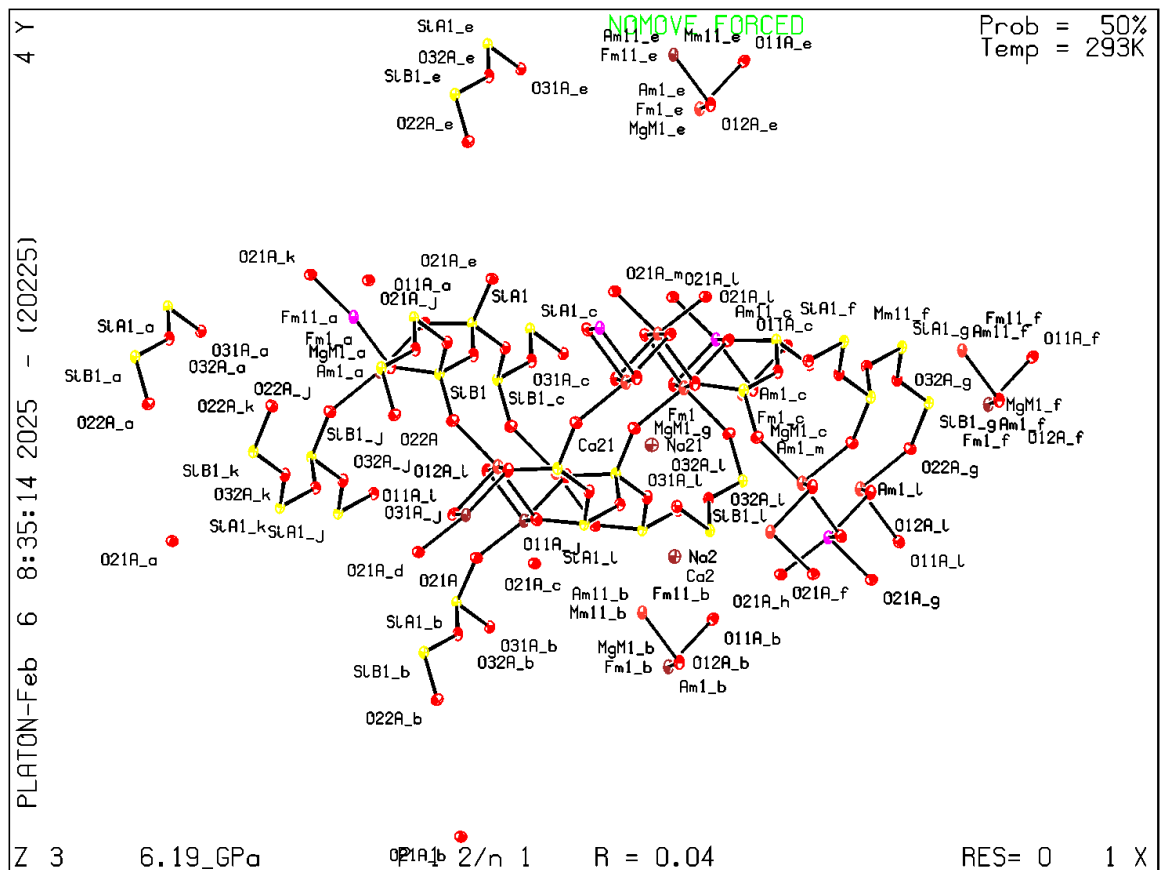


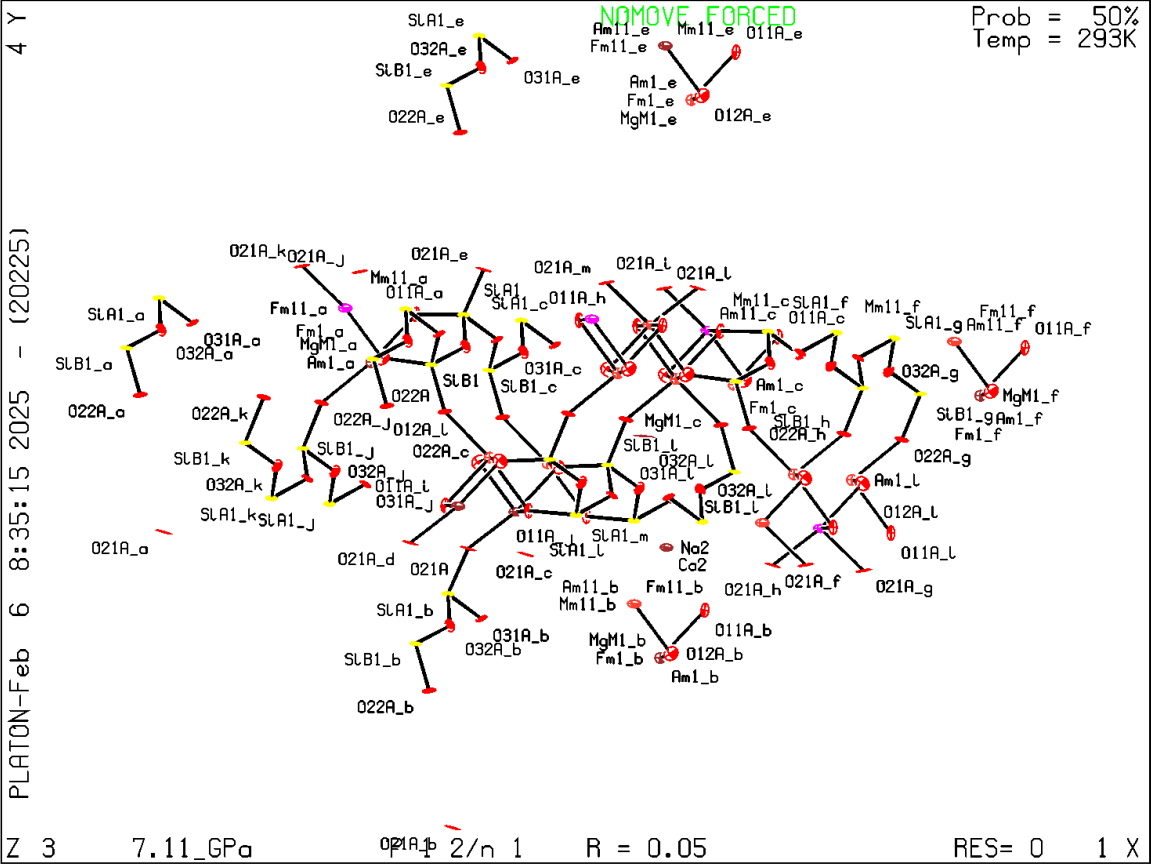


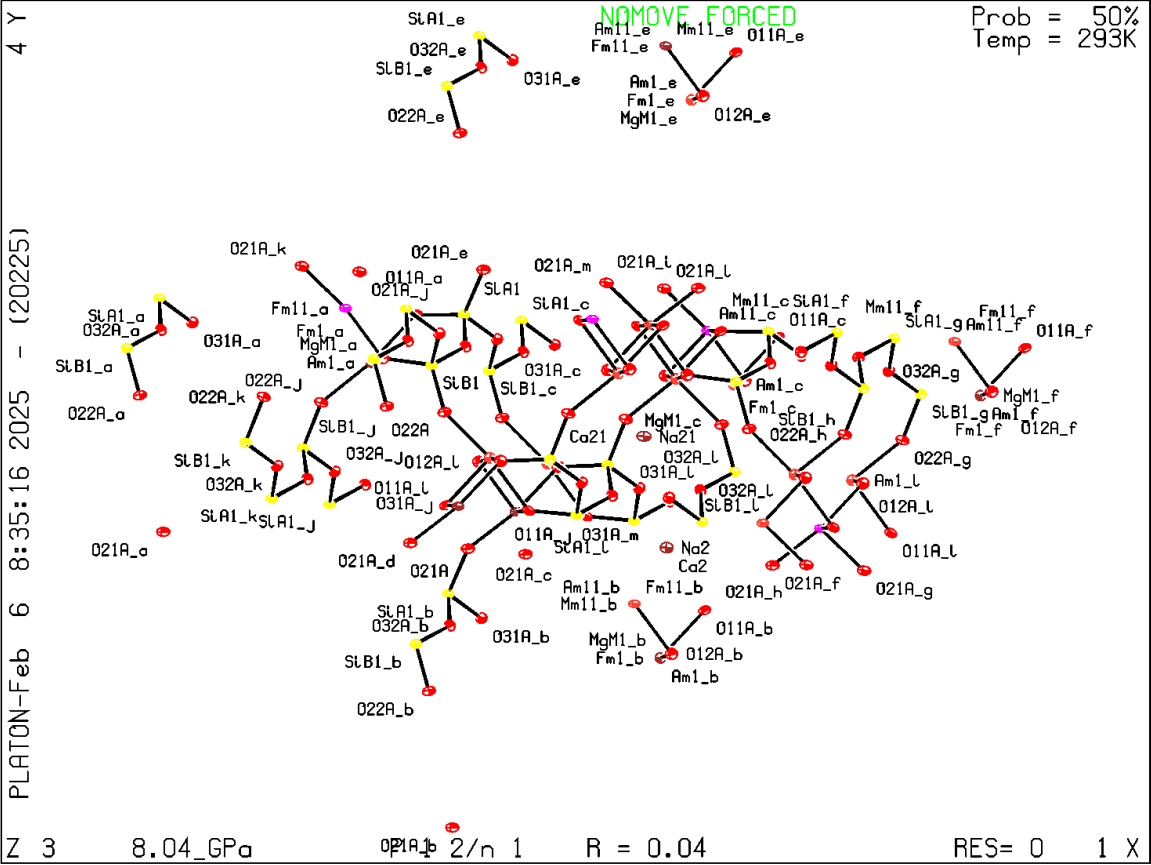
Datablock 5.18_GPa - ellipsoid plot

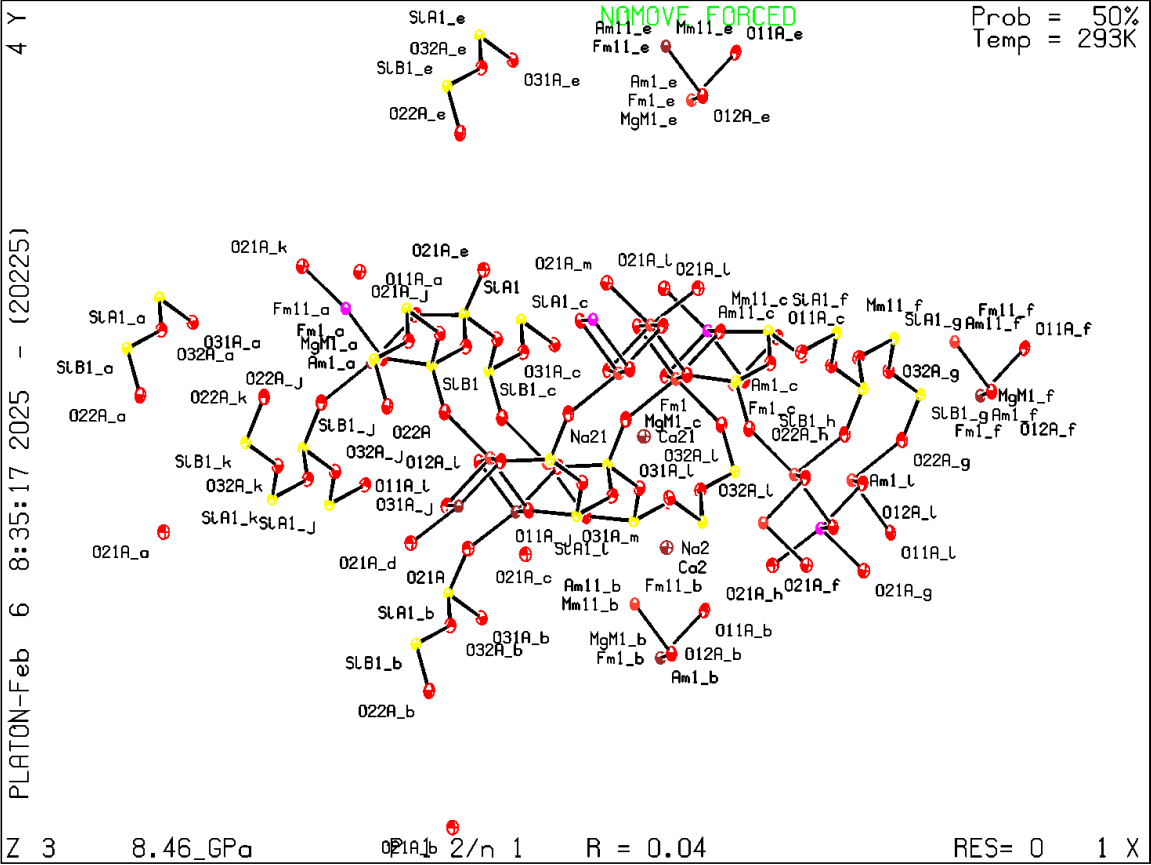


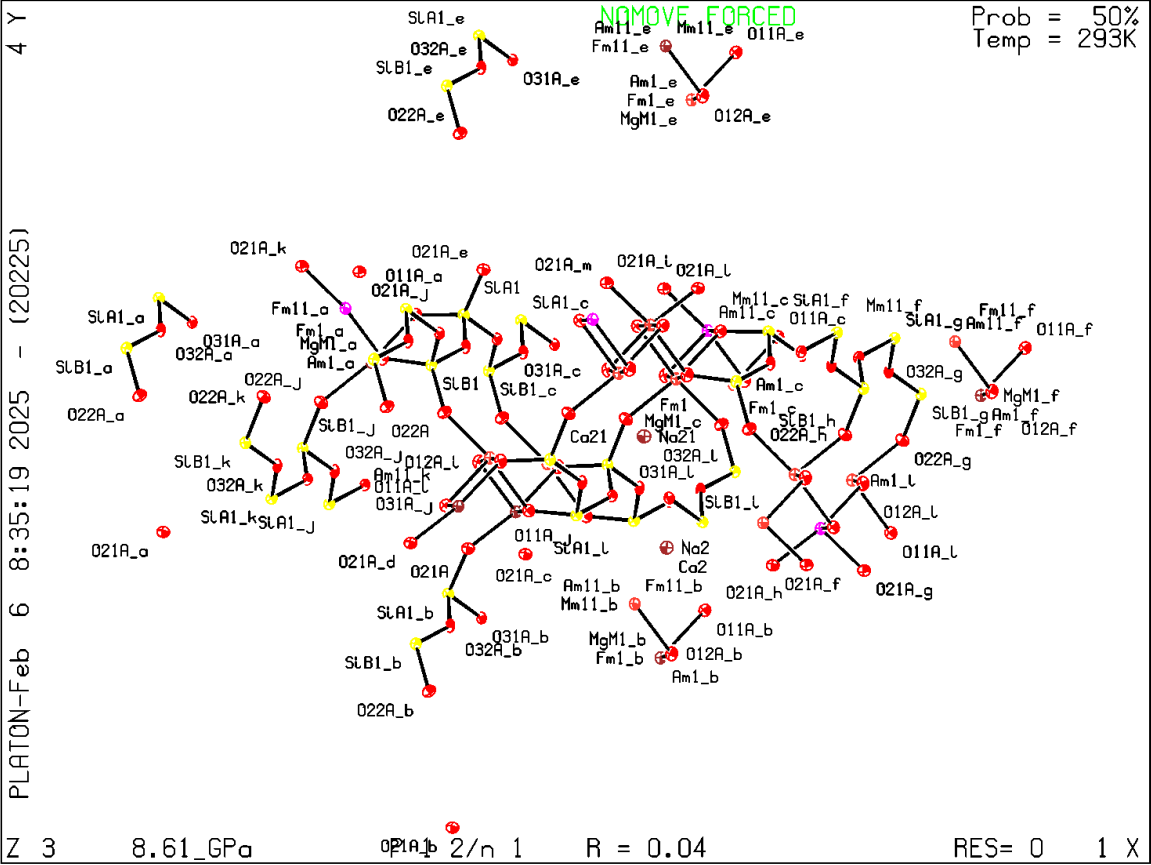


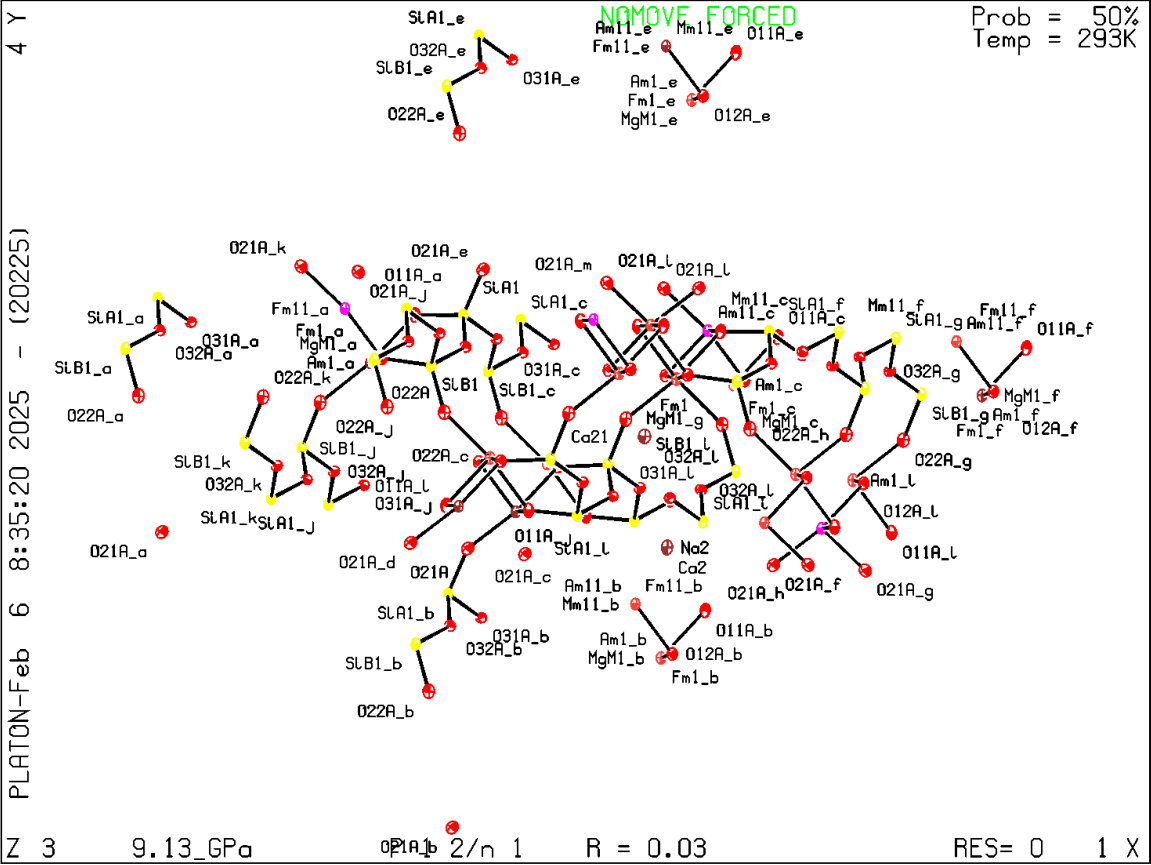


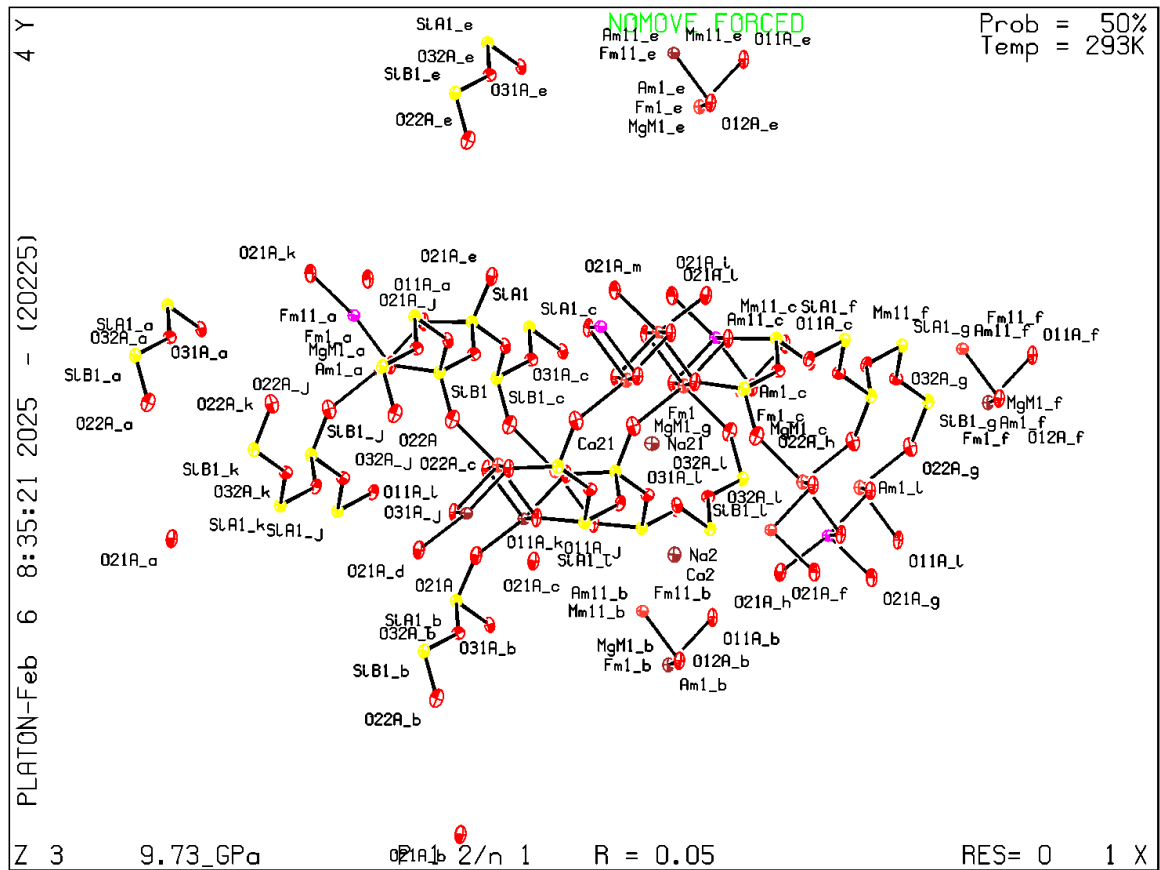












Datablock 8.29_GPa - ellipsoid plot

