

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Jd43Di57_air

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: Jd43Di57_air

Bond precision:	= 0.0000 A	Wavelength=0.71073	
Cell:	a=9.5882 (2)	b=8.7847 (1)	c=5.2580 (1)
	alpha=90	beta=106.835 (2)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	423.898 (14)	423.898 (14)	
Space group	P 2/n	P 2/n	
Hall group	-P 2yac	-P 2yac	
Moiety formula	0.041 (Al2 O4), 0.375 (Si), 0.979 (O), 0.013 (Fe), 0.11 (Ca), 0.091 (	0.041 (Al2 O4), 0.375 (Si), 0.979 (O), 0.013 (Fe), 0.081 (Na), 0.11 (	
Sum formula	Al0.09 Ca0.11 Fe0.01 Mg0.09 Na0.08 O1.14 Si0.38	Al0.4816 Ca0.5762 Fe0.06925 Mg0.48 Na0.4237 O5 Si1.9709	
Mr	40.51	196.71	
Dx, g cm-3	3.332	3.333	
Z	21	4	
Mu (mm-1)	1.915	1.214	
F000	422.3	428.0	
F000'	424.01		
h, k, lmax	19, 17, 10	19, 17, 10	
Nref	3493	3490	
Tmin, Tmax			
Tmin'			

Correction method= Not given

Data completeness= 0.999

Theta (max)= 44.875

R(reflections)= 0.0218(2919)

wR2(reflections)=
0.0621(3490)

S = 1.120

Npar= 118

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

ABSMU01_ALERT_1_A The ratio of given/expected absorption coefficient lies
outside the range 0.90 <> 1.10

Calculated value of mu = 1.885

Value of mu given = 1.214

PLAT051_ALERT_1_A Mu(calc) and Mu(cif) Ratio Differs from 1.0 by . 57.73 %

Alert level B

DENSD01_ALERT_1_B The ratio of the submitted crystal density and that
calculated from the formula is outside the range 0.95 <> 1.05

Crystal density given = 3.333

Calculated crystal density = 3.082

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 3.04 Check

PLAT046_ALERT_1_B Reported Z, MW and D(calc) are Inconsistent 3.082 Check

PLAT927_ALERT_1_B Reported and Calculated wR2 Differ by -0.0355 Check

PLAT928_ALERT_1_B Reported and Calculated S value Differ by . -0.639 Check

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check

Calc: Al0.09 Ca0.11 Fe0.01 Mg0.09 Na0.08 O1.14 Si0.3
8

Rep.: Al0.4816 Ca0.5762 Fe0.06925 Mg0.48 Na0.4237 O5
Si1.9709

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check

Calc: 0.041(Al2 O4), 0.375(Si), 0.979(O), 0.013(Fe),
0.11(Ca), 0.091(Mg), 0.01(Al), 0.081(Na)

Rep.: 0.041(Al2 O4), 0.375(Si), 0.979(O), 0.013(Fe),
0.081(Na), 0.11(Ca), 0.091(Mg),

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

PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check

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

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.324 Check

PLAT926_ALERT_1_C Reported and Calculated R1 Differ by -0.0016 Check

PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
2 0 0,

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.

Atom count from _chemical_formula_sum: Al0.4816 Ca0.5762 Fe.06925 Mg
 Atom count from _chemical_formula_moiety: Al.082 Ca0.11 Fe.013 Na.081 O
 FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
 _chemical_formula_sum and the formula from the _atom_site* data.
 Atom count from _chemical_formula_sum: Al0.4816 Ca0.5762 Fe.06925 Mg0.4
 Atom count from the _atom_site data: Al0.4816 Ca0.5762 Fe.06925 Mg0.4
 CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
 CELLZ01_ALERT_1_G ALERT: Large difference may be due to a

symmetry error - see SYMMG tests
 From the CIF: _cell_formula_units_Z 4
 From the CIF: _chemical_formula_sum Al0.4816 Ca0.5762 Fe0.06925 Mg0.48
 TEST: Compare cell contents of formula and atom_site data
 WARNING: Unexpected atom type is in site list: O-
 WARNING: Unexpected atom type is in site list: Si+
 WARNING: Unexpected atom type is in site list: Al+
 WARNING: Unexpected atom type is in site list: Fe+
 WARNING: Unexpected atom type is in site list: Mg+
 WARNING: Unexpected atom type is in site list: Ca+
 WARNING: Unexpected atom type is in site list: Na+
 WARNING: Formula and atom_type_symbol element names mismatch.

atom	Z*formula	cif sites	diff
Al	1.93	0.00	1.93
Ca	2.30	0.00	2.30
Fe	0.28	0.00	0.28
Mg	1.92	0.00	1.92
Na	1.69	0.00	1.69
O	20.00	4.88	15.12
Si	7.88	1.92	5.97

WARNING: Site labels do not match formula elements

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension	1	Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...	5.250	Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records	12	Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records	12	Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K)	293	Check
PLAT301_ALERT_3_G Main 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
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6)	100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 7)	100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 8)	100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 9)	100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10)	100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 11)	100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 12)	100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 13)	100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 14)	100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 15)	100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 16)	100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 17)	100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 18)	100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 19)	100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 20)	100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 21)	100%	Note

PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 22)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 23)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 24)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 25)	100% Note
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		O12B Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		O21B Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		O22B Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		O31B Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		O32B Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		O11A Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		O12A Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		O21A Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		O22A Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		O31A Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		O32A Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiA2 ..O21B .	1.60 Ang.
		x,1+y,z =	1_565 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiA2 ..O11B .	1.62 Ang.
		-1+x,y,z =	1_455 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiA2 ..O31B .	1.65 Ang.
		x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiA2 ..O32B .	1.66 Ang.
		x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiA2 ..O21B .	3.05 Ang.
		-x,1-y,-z =	3_565 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiA2 ..SiB1 .	3.07 Ang.
		x,y,-1+z =	1_554 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiA2 ..SiB1 .	3.11 Ang.
		x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiA2 ..O22B .	3.33 Ang.
		-x,1-y,1-z =	3_566 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiA2 ..O31B .	3.36 Ang.
		1/2-x,y,1/2-z =	2_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiA2 ..O12B .	3.38 Ang.
		-1+x,y,-1+z =	1_454 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiA2 ..SiA2 .	3.52 Ang.
		-x,2-y,-z =	3_575 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiB1 ..O22B .	1.59 Ang.
		x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiB1 ..O12B .	1.62 Ang.
		-1+x,y,z =	1_455 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiB1 ..O32B .	1.65 Ang.
		x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiB1 ..O31B .	1.67 Ang.
		x,y,1+z =	1_556 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiB1 ..O22B .	3.10 Ang.
		-x,1-y,1-z =	3_566 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiB1 ..O21B .	3.21 Ang.
		-x,1-y,1-z =	3_566 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiB1 ..O11B .	3.38 Ang.
		-1+x,y,1+z =	1_456 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiA1 ..O21B .	1.60 Ang.
		x,1+y,z =	1_565 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiA1 ..O11B .	1.62 Ang.
		-1+x,y,z =	1_455 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	SiA1 ..O31B .	1.65 Ang.
		x,y,z =	1_555 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact	SiA1	..032B	.	1.66 Ang.
		x,y,z =		1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	SiA1	..021B	.	3.05 Ang.
		-x,1-y,-z =		3_565 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	SiA1	..022B	.	3.33 Ang.
		-x,1-y,1-z =		3_566 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	SiA1	..031B	.	3.36 Ang.
		1/2-x,y,1/2-z =		2_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	SiA1	..012B	.	3.38 Ang.
		-1+x,y,-1+z =		1_454 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels				16 Note
	O11B	O12B	O21B	O22B
			O31B	O32B
	SiA1			
	SiB1	AlB	Am1	Fm1
			MgM1	Am11
				Mm11
PLAT768_ALERT_4_G RES Embedded Explicitly Supplied Scattering Data				Please Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints				15 Note
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary ..				Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Outdated and Succeeded by SHELXL				2019/3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).				1 Note
	0	1	0,	
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=	0.600			2 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity				4.0 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value				2.381 Note
	Predicted wR2:	Based on SigI**2	2.61	or SHELX Weight
				5.55
PLAT982_ALERT_1_G The Al-f' =	0.0560	Deviates from	IT-Value =	0.0645 Check
PLAT982_ALERT_1_G The Ca-f' =	0.2030	Deviates from	IT-Value =	0.2262 Check
PLAT982_ALERT_1_G The Fe-f' =	0.3010	Deviates from	IT-Value =	0.3463 Check
PLAT982_ALERT_1_G The Mg-f' =	0.0420	Deviates from	IT-Value =	0.0486 Check
PLAT982_ALERT_1_G The Na-f' =	0.0300	Deviates from	IT-Value =	0.0362 Check
PLAT982_ALERT_1_G The Si-f' =	0.0720	Deviates from	IT-Value =	0.0817 Check

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- 2 **ALERT level A** = Most likely a serious problem - resolve or explain
 5 **ALERT level B** = A potentially serious problem, consider carefully
 10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 87 **ALERT level G** = General information/check it is not something unexpected
- 27 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 38 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
 31 ALERT type 4 Improvement, methodology, query or suggestion
 2 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_ABSMU01_Jd43Di57_air
;
PROBLEM: The ratio of given/expected absorption coefficient lies
RESPONSE: ...
;
_vrf_PLAT051_Jd43Di57_air
;
PROBLEM: Mu(calc) and Mu(cif) Ratio Differs from 1.0 by .      57.73 %
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 02/02/2025; check.def file version of 02/02/2025

Datablock Jd43Di57_air - ellipsoid plot

