

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 100C, 200C, 25C, 300C, 400C, 500C, 600C

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: 25C

Bond precision: Si- O = 0.0013 A Wavelength=0.71073

Cell: a=9.6458(2) b=9.6521(2) c=12.6206(4)
 alpha=102.458(2) beta=96.225(1) gamma=119.902(1)

Temperature: 293 K

	Calculated	Reported
Volume	961.69(5)	961.69(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	O19 Si8, F, 1.454(O), 2.301(Ca), 0.216(K), 2.588(Na)	Ca2.30 F1 K0.22 Na2.59 O20.45 Si8
Sum formula	Ca2.30 F K0.22 Na2.59 O20.45 Si8	Ca2.30 F1 K0.22 Na2.59 O20.45 Si8
Mr	731.14	731.10
Dx, g cm ⁻³	2.525	2.525
Z	2	2
Mu (mm ⁻¹)	1.392	1.392
F000	726.4	726.4
F000'	729.43	
h, k, lmax	18, 18, 24	18, 18, 22
Nref	15050	13021
Tmin, Tmax	0.451, 0.933	0.790, 1.000
Tmin'	0.417	

Correction method= # Reported T Limits: Tmin=0.790 Tmax=1.000
AbsCorr = MULTII-SCAN

Data completeness= 0.865

Theta(max)= 44.033

R(reflections)= 0.0322(10425)

wR2(reflections)=

wR= 0.0386(9810)

S = 0.965

Npar= 362

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

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low . 0.865 Why?
PLAT992_ALERT_5_A Repd & Actual _reflns_number_gt Values Differ by 615 Check

Alert level B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 14 Note

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent 1 Check
O20
PLAT214_ALERT_2_C Atom Na8 (Anion/Solvent) ADP max/min Ratio 4.6 prolat
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
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
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) O20 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) O21 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) O22 Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) O23 Check

	Calculated	Reported
Volume	962.2(15)	962.3(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	019 Si8, 0.086(O2), F, 0.743(O), 2.301(Ca), 0.216(K), 2.587(Na)	Ca2.30 F1 K0.22 Na2.59 019.92 Si8
Sum formula	Ca2.30 F K0.22 Na2.59 019.92 Si8	Ca2.30 F1 K0.22 Na2.59 019.92 Si8
Mr	722.53	722.47
Dx, g cm ⁻³	2.494	2.493
Z	2	2
Mu (mm ⁻¹)	1.387	1.387
F000	717.8	717.8
F000'	720.81	
h, k, lmax	17, 17, 22	17, 17, 22
Nref	12275	12074
Tmin, Tmax	0.452, 0.933	0.730, 1.000
Tmin'	0.418	

Correction method= # Reported T Limits: Tmin=0.730 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.984 Theta(max)= 40.452

R(reflections)= 0.0340(9620) wR2(reflections)=
S = 0.949 Npar= 353 wR= 0.0409(9026)

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**

PLAT992_ALERT_5_A Repd & Actual _reflns_number_gt Values Differ by 594 Check

 **Alert level B**

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 13 Note
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 2 Check

 **Alert level C**

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT155_ALERT_4_C The Triclinic Unitcell is NOT Reduced Please Do !

PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Na6	0.111	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Na7	0.144	Check

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		3	Info
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 Ca2	Constrained at	0.5702	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca3	Constrained at	0.8407	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca4	Constrained at	0.7518	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1	Constrained at	0.2765	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of K1	Constrained at	0.2162	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1	Constrained at	0.7236	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na5	Constrained at	0.5686	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2	Constrained at	0.4298	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na3	Constrained at	0.1593	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na4	Constrained at	0.2482	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na6	Constrained at	0.2673	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na7	Constrained at	0.2946	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na8	Constrained at	0.2575	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		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
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		020	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		021	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		022	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		024	Check
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O11 .		134.0	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O12 .		135.5	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O13 .		137.8	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O16 .		139.5	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O18 .		138.5	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O19 .		175.6	Degree
PLAT769_ALERT_4_G	CIF Embedded explicitly supplied scattering data		Please	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		385	Note
PLAT882_ALERT_1_G	No Datum for _diffrn_reflns_av_unetI/netI		Please	Do !
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L= 0.600		341	Report
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		2849	Note
PLAT929_ALERT_5_G	No Weight Pars,Obs and Calc R1,wR2,S not Checked			! Info

R(reflections)= 0.0358(9399)

wR2(reflections)=

wR= 0.0412(8772)

S = 0.968

Npar= 348

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

PLAT992_ALERT_5_A Repd & Actual _reflns_number_gt Values Differ by 627 Check

Alert level B

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 13 Note

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 2 Check

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check

PLAT214_ALERT_2_C Atom Na8 (Anion/Solvent) ADP max/min Ratio 4.1 prolat

PLAT260_ALERT_2_C Large Average Ueq of Residue Including Na6 0.189 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including Na7 0.282 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including Na8 0.184 Check

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info

PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree

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 Ca2 Constrained at 0.5702 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Ca3 Constrained at 0.8408 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Ca4 Constrained at 0.7518 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Ca1 Constrained at 0.2765 Check

PLAT300_ALERT_4_G Atom Site Occupancy of K1 Constrained at 0.2162 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na1 Constrained at 0.7236 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na5 Constrained at 0.5686 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na2 Constrained at 0.4298 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na3 Constrained at 0.1593 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na4 Constrained at 0.2482 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na6 Constrained at 0.2673 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na7 Constrained at 0.2946 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na8 Constrained at 0.2575 Check

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

	Calculated	Reported
Volume	962.31(6)	962.31(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	019 Si8, 0.041(O2), F, 0.312(O), 2.301(Ca), 0.216(K), 2.587(Na)	Ca2.30 F1 K0.22 Na2.59 019.39 Si8
Sum formula	Ca2.30 F K0.22 Na2.59 019.39 Si8	Ca2.30 F1 K0.22 Na2.59 019.39 Si8
Mr	714.19	714.14
Dx, g cm ⁻³	2.465	2.464
Z	2	2
Mu (mm ⁻¹)	1.384	1.384
F000	709.5	709.5
F000'	712.46	
h, k, lmax	17, 17, 22	17, 17, 22
Nref	12151	12058
Tmin, Tmax	0.453, 0.933	0.770, 1.000
Tmin'	0.419	

Correction method= # Reported T Limits: Tmin=0.770 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 40.273

R(reflections)= 0.0372(9145) wR2(reflections)=
S = 0.932 Npar= 348 wR= 0.0497(8443)

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**

PLAT992_ALERT_5_A Repd & Actual _reflns_number_gt Values Differ by 702 Check

 **Alert level B**

PLAT260_ALERT_2_B Large Average Ueq of Residue Including Na7 0.343 Check
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 13 Note
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 2 Check

 **Alert level C**

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check

PLAT214_ALERT_2_C	Atom Na8	(Anion/Solvent) ADP max/min Ratio	4.1	prolat
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	013	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	014	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	017	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	Si1	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Na6	0.237	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Na8	0.217	Check

● Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
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 Ca2	Constrained at	0.5702 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca3	Constrained at	0.8408 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca4	Constrained at	0.7518 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1	Constrained at	0.2765 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of K1	Constrained at	0.2162 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1	Constrained at	0.7236 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na5	Constrained at	0.5686 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2	Constrained at	0.4298 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na3	Constrained at	0.1593 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na4	Constrained at	0.2482 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na6	Constrained at	0.2673 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na7	Constrained at	0.2946 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na8	Constrained at	0.2575 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	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
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	020	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	021	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	024	Check
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O11 .	134.7	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O12 .	135.8	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O13 .	138.2	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O16 .	139.8	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O18 .	138.8	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O19 .	175.7	Degree
PLAT769_ALERT_4_G	CIF Embedded explicitly supplied scattering data		Please Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	380	Note
PLAT882_ALERT_1_G	No Datum for _diffrn_reflns_av_unetI/netI		Please Do !
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L= 0.600	397	Report
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	3296	Note

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

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

Datablock: 400C

Bond precision: Si- O = 0.0018 A

Wavelength=0.71073

Cell: a=9.6767(3) b=9.6795(3) c=12.5673(4)
 alpha=102.396(2) beta=96.262(1) gamma=119.875(1)
 Temperature: 673 K

	Calculated	Reported
Volume	963.94(6)	963.94(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	019 Si8, F, 0.209(O), 2.301(Ca), 0.216(K), 2.587(Na)	Ca2.30 F1 K0.22 Na2.59 019.21 Si8
Sum formula	Ca2.30 F K0.22 Na2.59 019.21 Si8	Ca2.30 F1 K0.22 Na2.59 019.21 Si8
Mr	711.23	711.18
Dx, g cm ⁻³	2.450	2.450
Z	2	2
Mu (mm ⁻¹)	1.380	1.380
F000	706.5	706.5
F000'	709.49	
h, k, lmax	17, 17, 22	17, 17, 22
Nref	12171	12088
Tmin, Tmax	0.454, 0.933	0.770, 1.000
Tmin'	0.420	

Correction method= # Reported T Limits: Tmin=0.770 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.993

Theta(max)= 40.265

R(reflections)= 0.0375(8920)

wR2(reflections)=

wR= 0.0524(8215)

S = 0.907

Npar= 333

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

PLAT992_ALERT_5_A Repd & Actual _reflns_number_gt Values Differ by 705 Check

Alert level B

PLAT260_ALERT_2_B Large Average Ueq of Residue Including Na7 0.359 Check

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 13 Note

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check

PLAT214_ALERT_2_C Atom Na8 (Anion/Solvent) ADP max/min Ratio 4.3 prolat

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 013 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 014 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 016 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 017 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si1 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si5 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si8 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including Na6 0.260 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including Na8 0.266 Check

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

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info

PLAT300_ALERT_4_G Atom Site Occupancy of Ca2 Constrained at 0.5702 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Ca3 Constrained at 0.8408 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Ca4 Constrained at 0.7518 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Ca1 Constrained at 0.2765 Check

PLAT300_ALERT_4_G Atom Site Occupancy of K1 Constrained at 0.2162 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na1 Constrained at 0.7236 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na5 Constrained at 0.5686 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na2 Constrained at 0.4298 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na3 Constrained at 0.1593 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na4 Constrained at 0.2482 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na6 Constrained at 0.2673 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na7 Constrained at 0.2946 Check

PLAT300_ALERT_4_G Atom Site Occupancy of Na8 Constrained at 0.2575 Check

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
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	020	Check
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O11 .	134.9	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O12 .	136.2	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O13 .	138.4	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O16 .	139.9	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O18 .	139.1	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O19 .	175.5	Degree
PLAT769_ALERT_4_G	CIF Embedded explicitly supplied scattering data		Please Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	365	Note
PLAT882_ALERT_1_G	No Datum for _diffrn_reflms_av_unetI/netI		Please Do !
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L= 0.600	394	Report
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	3546	Note
PLAT929_ALERT_5_G	No Weight Pars,Obs and Calc R1,wR2,S not Checked		! Info

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

Datablock: 500C

Bond precision: Si- O = 0.0017 A Wavelength=0.71073

Cell: a=9.6821(2) b=9.6863(2) c=12.5643(3)

 alpha=102.421(1) beta=96.268(1) gamma=119.855(1)

Temperature: 293 K

	Calculated	Reported
Volume	964.95(4)	964.95(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	O19 Si8, F, 0.176(O), 2.301(Ca), 0.216(K), 2.587(Na)	Ca2.30 F1 K0.22 Na2.59 O19.18 Si8
Sum formula	Ca2.30 F K0.22 Na2.59 O19.18 Si8	Ca2.30 F1 K0.22 Na2.59 O19.18 Si8
Mr	710.70	710.65
Dx, g cm ⁻³	2.446	2.446
Z	2	2
Mu (mm ⁻¹)	1.378	1.378
F000	706.0	706.0
F000'	708.97	
h, k, lmax	17, 17, 22	17, 17, 22
Nref	12208	12119
Tmin, Tmax	0.455, 0.933	0.800, 1.000
Tmin'	0.421	

Correction method= # Reported T Limits: Tmin=0.800 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 40.303

R(reflections)= 0.0368(8847) wR2(reflections)=
S = 0.982 Npar= 333 wR= 0.0432(8189)

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**

PLAT992_ALERT_5_A Repd & Actual _reflns_number_gt Values Differ by 658 Check

 **Alert level B**

PLAT260_ALERT_2_B Large Average Ueq of Residue Including Na6 0.301 Check
 PLAT260_ALERT_2_B Large Average Ueq of Residue Including Na7 0.400 Check
 PLAT260_ALERT_2_B Large Average Ueq of Residue Including Na8 0.338 Check
 PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 13 Note

 **Alert level C**

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
 PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check

PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..		Please	Check
PLAT214_ALERT_2_C	Atom Na8 (Anion/Solvent) ADP max/min Ratio	4.2	prolat	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	013	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	014	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	016	Check	
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	017	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Si1	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Si2	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Si4	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Si5	Check	
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Si8	Check	
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including K1	0.134	Check	

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info	
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.001	Degree	
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 Ca2 Constrained at	0.5702	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca3 Constrained at	0.8408	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca4 Constrained at	0.7518	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca1 Constrained at	0.2765	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of K1 Constrained at	0.2162	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Na1 Constrained at	0.7236	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Na5 Constrained at	0.5686	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2 Constrained at	0.4298	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Na3 Constrained at	0.1593	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Na4 Constrained at	0.2482	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Na6 Constrained at	0.2673	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Na7 Constrained at	0.2946	Check	
PLAT300_ALERT_4_G	Atom Site Occupancy of Na8 Constrained at	0.2575	Check	
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	
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	020	Check	
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O11	135.0	Degree	
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O12	136.5	Degree	
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O13	138.7	Degree	
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O18	139.4	Degree	
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O19	175.5	Degree	
PLAT769_ALERT_4_G	CIF Embedded explicitly supplied scattering data		Please	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	365	Note	
PLAT882_ALERT_1_G	No Datum for _diffrn_reflms_av_unetI/netI		Please	Do !
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L= 0.600	369	Report	
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	3597	Note	

1 **ALERT level A** = Most likely a serious problem - resolve or explain
 4 **ALERT level B** = A potentially serious problem, consider carefully
 14 **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

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

Datablock: 600C

Bond precision: Si- O = 0.0019 A

Wavelength=0.71073

Cell: a=9.6878(2) b=9.6888(3) c=12.5606(3)
 alpha=102.446(1) beta=96.279(1) gamma=119.850(1)
 Temperature: 293 K

	Calculated	Reported
Volume	965.32(5)	965.32(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	O19 Si8, F, 0.175(O), 2.301(Ca), 0.216(K), 2.587(Na)	Ca2.30 F1 K0.22 Na2.59 O19.17 Si8
Sum formula	Ca2.30 F K0.22 Na2.59 O19.17 Si8	Ca2.30 F1 K0.22 Na2.59 O19.17 Si8
Mr	710.67	710.62
Dx, g cm ⁻³	2.445	2.445
Z	2	2
Mu (mm ⁻¹)	1.378	1.378
F000	706.0	706.0
F000'	708.93	
h, k, lmax	17, 17, 22	17, 17, 22
Nref	12207	12121
Tmin, Tmax	0.455, 0.933	0.760, 1.000
Tmin'	0.421	

Correction method= # Reported T Limits: Tmin=0.760 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.993

Theta(max)= 40.299

R(reflections)= 0.0378(8514)

wR2(reflections)=

wR= 0.0460(7834)

S = 0.947

Npar= 333

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

PLAT992_ALERT_5_A Repd & Actual _reflns_number_gt Values Differ by 680 Check

Alert level B

PLAT260_ALERT_2_B Large Average Ueq of Residue Including Na6 0.319 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including Na7 0.466 Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including Na8 0.401 Check
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 13 Note

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT214_ALERT_2_C Atom Na8 (Anion/Solvent) ADP max/min Ratio 4.5 prolat
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 08 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 013 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 014 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 016 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 017 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si3 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si4 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si5 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Si8 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including K1 0.212 Check

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
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 Ca2 Constrained at 0.5702 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca3 Constrained at 0.8408 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca4 Constrained at 0.7518 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ca1 Constrained at 0.2765 Check
PLAT300_ALERT_4_G Atom Site Occupancy of K1 Constrained at 0.2162 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Na1 Constrained at 0.7236 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Na5 Constrained at 0.5686 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Na2 Constrained at 0.4298 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of Na3	Constrained at	0.1593	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na4	Constrained at	0.2482	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na6	Constrained at	0.2673	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na7	Constrained at	0.2946	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na8	Constrained at	0.2575	Check
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
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)		020	Check
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O11	.	135.2	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O12	.	136.8	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O13	.	138.7	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O18	.	139.5	Degree
PLAT396_ALERT_2_G	Deviating Si-O-Si Angle From 150 for O19	.	175.4	Degree
PLAT769_ALERT_4_G	CIF Embedded explicitly supplied scattering data			Please Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		365	Note
PLAT882_ALERT_1_G	No Datum for _diffrn_reflms_av_unetI/netI			Please Do !
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L= 0.600		392	Report
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		3929	Note
PLAT929_ALERT_5_G	No Weight Pars,Obs and Calc R1,wR2,S not Checked			! Info

-
- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
 4 **ALERT level B** = A potentially serious problem, consider carefully
 16 **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
- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 22 ALERT type 2 Indicator that the structure model may be wrong or deficient
 3 ALERT type 3 Indicator that the structure quality may be low
 30 ALERT type 4 Improvement, methodology, query or suggestion
 3 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.

PLATON version of 28/11/2022; check.def file version of 28/11/2022











