

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: dendoraite

Bond precision:	C-C = 0.0080 A	Wavelength=0.71073
Cell:	a=10.695(6)	b=6.285(4) c=19.227(12)
	alpha=90	beta=90.933(10) gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	1292.2(14)	1292.2(14)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C2 H4 Al0.92 Fe0.08 K0.69 Na O14 P2, 1.314(N)	?
Sum formula	C2 H4 Al0.92 Fe0.08 K0.69 N1.31 Na O14 P2	C2 H4 Al0.90 Fe0.10 K0.69 N1.31 Na O14 P2
Mr	411.62	412.06
Dx, g cm-3	2.116	2.118
Z	4	4
Mu (mm-1)	0.825	0.841
F000	821.3	822.0
F000'	823.68	
h,k,lmax	11,6,20	11,6,20
Nref	1728	1695
Tmin,Tmax	0.980,0.997	
Tmin'	0.959	

Correction method= Not given

Data completeness= 0.981 Theta(max)= 22.671

R(reflections)= 0.0467(1322) wR2(reflections)= 0.1207(1695)

S = 1.066 Npar= 215

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

THETM01_ALERT_3_A The value of $\sin(\theta_{\max})/\lambda$ is less than 0.550
Calculated $\sin(\theta_{\max})/\lambda = 0.5423$

Alert level B

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) Ow2 Check
PLAT780_ALERT_1_B Coordinates do not Form a Properly Connected Set Please Do !

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 0.44 Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT088_ALERT_3_C Poor Data / Parameter Ratio 8.04 Note
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 5.1 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Oh1 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.008 Ang.

Alert level G

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: C2 H4 Al0.9 Fe.1 K0.69 N1.31 Na1
Atom count from the _atom_site data: C2 H4 Al0.916 Fe.084 K0.686 N1.3
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C2 H4 Al0.90 Fe0.10 K0.69 N1.31 Na
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	8.00	8.00	0.00
H	16.00	16.00	0.00
Al	3.60	3.66	-0.06
Fe	0.40	0.34	0.06
K	2.76	2.74	0.02
N	5.24	5.26	-0.02
Na	4.00	4.00	0.00
O	56.00	56.00	0.00
P	8.00	8.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 7 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 3 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 3 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 4 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) 8% 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
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 4 Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 3.41 Ratio
PLAT774_ALERT_1_G Check X-Y Bond in CIF: K1 --Ow1 .. 4.08 Ang.
PLAT774_ALERT_1_G Check X-Y Bond in CIF: K1 --Ow1 .. 4.28 Ang.

PLAT774_ALERT_1_G	Check	X-Y Bond in CIF: K2	--09	..	4.16 Ang.
PLAT774_ALERT_1_G	Check	X-Y Bond in CIF: K2	--06	..	4.25 Ang.
PLAT774_ALERT_1_G	Check	X-Y Bond in CIF: K2	--04	..	4.28 Ang.
PLAT774_ALERT_1_G	Check	X-Y Bond in CIF: K2	--Ow2	..	4.38 Ang.
PLAT774_ALERT_1_G	Check	X-Y Bond in CIF: K2	--08	..	4.45 Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			77 Check
	NA -P1 -O12	4.565 1.555 4.565			41.57 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			111 Check
	O6 -P2 -NA	1.555 1.555 3.766			36.33 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			114 Check
	O4 -P2 -NA	2.655 1.555 3.766			40.52 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			118 Check
	O8 -P2 -K1	1.555 1.555 1.565			43.07 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			132 Check
	C2 -C1 -O11	1.555 1.555 1.555			29.40 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			135 Check
	C2 -C1 -O12	1.555 1.555 1.555			26.30 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			153 Check
	C1 -C2 -O9	1.555 1.555 1.555			29.30 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			156 Check
	C1 -C2 -O10	1.555 1.555 1.555			26.60 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			163 Check
	O12 -C2 -NA	1.555 1.555 1.555			42.70 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			631 Check
	P1 -OH1 -O4	1.555 1.555 1.555			35.90 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			632 Check
	P1 -OH1 -O3	1.555 1.555 1.555			34.72 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			634 Check
	P1 -OH1 -O2	1.555 1.555 1.555			34.17 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			680 Check
	O8 -OH1 -H1	1.555 1.555 1.555			6.00 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			683 Check
	O7 -OH1 -H1	1.555 1.555 1.555			43.00 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			687 Check
	P1 -O2 -O4	1.555 1.555 1.555			35.65 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			689 Check
	P1 -O2 -O3	1.555 1.555 1.555			34.50 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			692 Check
	P1 -O2 -OH1	1.555 1.555 1.555			35.71 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			715 Check
	AL -O2 -O3	2.655 1.555 2.655			41.96 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			738 Check
	O9 -O2 -C1	3.666 1.555 3.666			22.84 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			747 Check
	O11 -O2 -C2	3.666 1.555 3.666			22.68 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			751 Check
	C1 -O2 -C2	3.666 1.555 3.666			27.84 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			753 Check
	P1 -O3 -O2	1.555 1.555 1.555			34.48 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			755 Check
	P1 -O3 -O4	1.555 1.555 1.555			33.87 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			758 Check
	P1 -O3 -OH1	1.555 1.555 1.555			36.28 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			774 Check
	AL -O3 -O2	1.555 1.555 2.645			44.30 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			781 Check
	AL -O3 -O7	1.555 1.555 1.555			40.32 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			810 Check
	P1 -O4 -O2	1.555 1.555 1.555			35.96 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			813 Check
	P1 -O4 -OH1	1.555 1.555 1.555			37.87 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF . #			817 Check

P1	-O4	-O3	1.555	1.555	1.555	34.17 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	829 Check
AL	-O4	-O3	2.645	1.555	2.645	43.00 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	844 Check
AL	-O4	-O7	2.645	1.555	2.645	42.55 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	873 Check
P2	-OH5	-O8	1.555	1.555	1.555	36.25 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	874 Check
P2	-OH5	-O7	1.555	1.555	1.555	36.26 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	876 Check
P2	-OH5	-O6	1.555	1.555	1.555	34.41 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	908 Check
NA	-OH5	-O10	1.554	1.555	1.554	44.32 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	932 Check
O6	-OH5	-H2	3.765	1.555	1.555	7.00 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	940 Check
P2	-O6	-O7	1.555	1.555	1.555	34.38 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	942 Check
P2	-O6	-OH5	1.555	1.555	1.555	36.74 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	945 Check
P2	-O6	-O8	1.555	1.555	1.555	32.71 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	989 Check
OH5	-O6	-O6	3.765	1.555	3.765	44.92 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1002 Check
O4	-O6	-O11	2.655	1.555	4.665	44.65 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1006 Check
P2	-O7	-OH5	1.555	1.555	1.555	38.34 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1008 Check
P2	-O7	-O8	1.555	1.555	1.555	34.13 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1011 Check
P2	-O7	-O6	1.555	1.555	1.555	34.03 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1027 Check
AL	-O7	-O4	1.555	1.555	2.655	44.15 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1034 Check
AL	-O7	-O3	1.555	1.555	1.555	39.71 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1050 Check
P2	-O8	-OH5	1.555	1.555	1.555	38.98 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1051 Check
P2	-O8	-O7	1.555	1.555	1.555	34.69 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1053 Check
P2	-O8	-O6	1.555	1.555	1.555	32.90 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1094 Check
O9	-O8	-O3	3.666	1.555	2.655	43.72 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1114 Check
O3	-O8	-O4	2.655	1.555	2.655	40.48 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1117 Check
C1	-O9	-O10	1.555	1.555	1.555	26.50 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1119 Check
C1	-O9	-C2	1.555	1.555	1.555	36.80 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1125 Check
C2	-O9	-O11	1.555	1.555	1.555	29.44 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1127 Check
AL	-O9	-O3	4.566	1.555	4.566	43.54 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1132 Check
AL	-O9	-O2	4.566	1.555	3.666	44.89 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1138 Check
AL	-O9	-O4	4.566	1.555	3.656	44.51 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1182 Check
C1	-O10	-O9	1.555	1.555	1.555	26.90 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1183 Check
C1	-O10	-C2	1.555	1.555	1.555	33.90 Deg.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s) in CIF . #	1190 Check

C2	-O10	-O12	1.555	1.555	1.555	26.39 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1227 Check
C1	-O10	-O11	1.555	1.555	1.555	20.60 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1229 Check
C2	-O10	-O11	1.555	1.555	1.555	13.42 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1231 Check
O12	-O10	-O11	1.555	1.555	1.555	39.81 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1249 Check
C2	-O11	-O12	1.555	1.555	1.555	26.70 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1251 Check
C2	-O11	-C1	1.555	1.555	1.555	36.70 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1257 Check
C1	-O11	-O9	1.555	1.555	1.555	29.25 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1264 Check
AL	-O11	-O7	4.566	1.555	4.566	44.20 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1314 Check
C2	-O12	-O11	1.555	1.555	1.555	27.40 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1315 Check
C2	-O12	-C1	1.555	1.555	1.555	33.50 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1322 Check
C1	-O12	-O10	1.555	1.555	1.555	26.48 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1358 Check
C2	-O12	-O12	2.646	1.555	2.646	21.90 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1365 Check
C2	-O12	-O12	2.656	1.555	2.656	22.10 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1376 Check
O4	-O12	-O2	4.666	1.555	4.666	44.30 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1417 Check
O6	-OW1	-P2	3.665	1.555	3.665	25.01 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1424 Check
OH5	-OW1	-P2	3.665	1.555	3.665	26.99 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1430 Check
O7	-OW1	-OH5	1.455	1.555	1.455	42.31 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1436 Check
O6	-OW1	-H3	3.665	1.555	1.555	12.00 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1444 Check
P2	-OW1	-H3	3.665	1.555	1.555	34.00 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1449 Check
O11	-OW1	-H4	4.565	1.555	1.555	44.00 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1451 Check
O7	-OW1	-H4	1.455	1.555	1.555	16.00 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1453 Check
O2	-OW1	-H4	2.545	1.555	1.555	33.00 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1479 Check
O10	-OW2	-O9	1.555	1.555	1.555	40.52 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1511 Check
OH5	-OW2	-O8	1.556	1.555	1.556	40.37 Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF . #					1523 Check
O8	-OW2	-OH1	1.556	1.555	1.556	42.20 Deg.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints					4 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .					Please Do !
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...					1 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity					3.7 Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged					Please Check

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

16 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
6 ALERT type 3 Indicator that the structure quality may be low
92 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

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