

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ar192b3

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: ar192b3

Bond precision: N- C = 0.0370 Å

Wavelength=0.71073

Cell: a=37.3679(17) b=26.2614(17) c=35.8129(14)
 alpha=90 beta=118.486(7) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	30890(3)	30890(3)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	2(K Na2 O126.80 W36), C2 N2, 10(C2 H8 N), 2(C1.40 H6.20 N), 1.2	?
Sum formula	C32.20 H102.60 K2 N16 Na4 O280.60 W72	C18 H128 K N9 Na2 O142 W36
Mr	18610.54	9446.97
Dx, g cm-3	4.002	4.063
Z	4	8
Mu (mm-1)	26.826	26.830
F000	32250.4	33120.0
F000'	32067.39	
h, k, lmax	46, 32, 44	46, 32, 44
Nref	30370	30320
Tmin, Tmax	0.158, 0.261	0.080, 0.347
Tmin'	0.006	

Correction method= # Reported T Limits: Tmin=0.080 Tmax=0.347
AbsCorr = ANALYTICAL

Data completeness= 0.998

Theta(max)= 26.000

R(reflections)= 0.0539(19312)

wR2(reflections)= 0.1241(30320)

S = 1.021

Npar= 1682

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

PLAT201_ALERT_2_A	Isotropic non-H Atoms in Main Residue(s)	18	Report
PLAT602_ALERT_2_A	VERY LARGE Solvent Accessible VOID(S) in Structure	!	Info
PLAT973_ALERT_2_A	Check Calcd Positive Residual Density on W3	2.21	eA-3
PLAT973_ALERT_2_A	Check Calcd Positive Residual Density on W32	2.21	eA-3
PLAT975_ALERT_2_A	Check Calcd Residual Density 1.04A From 0142	2.85	eA-3
PLAT975_ALERT_2_A	Check Calcd Residual Density 0.55A From 0124	2.36	eA-3
PLAT975_ALERT_2_A	Check Calcd Residual Density 0.98A From 085	2.20	eA-3

Alert level B

PLAT043_ALERT_1_B	Calculated and Reported Mol. Weight Differ by ..	283.40	Check
PLAT213_ALERT_2_B	Atom 070 has ADP max/min Ratio	4.2	oblate
PLAT213_ALERT_2_B	Atom 092 has ADP max/min Ratio	4.2	prolat
PLAT213_ALERT_2_B	Atom 0111 has ADP max/min Ratio	4.5	oblate
PLAT220_ALERT_2_B	Non-Solvent Resd 1 0 Ueq(max)/Ueq(min) Range	8.7	Ratio
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	0122	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	0130	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	0131	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	0132	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	0133	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)	0135	Check
PLAT413_ALERT_2_B	Short Inter XH3 .. XHn H10A .. H18C ..	1.99	Ang.
PLAT415_ALERT_2_B	Short Inter D-H..H-X H5D .. H18C ..	1.93	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 02 .. 0145 ..	2.76	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 010 .. 0139 ..	2.74	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 010 .. 095 ..	2.76	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 027 .. 0138 ..	2.84	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 033 .. 0116 ..	2.72	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 047 .. 0130 ..	2.66	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 073 .. 0144 ..	2.80	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 086 .. 0133 ..	2.78	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 089 .. 0124 ..	2.73	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 094 .. 0146 ..	2.80	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 0111 .. 0135 ..	2.79	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 0112 .. 0133 ..	2.67	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 0112 .. 0142 ..	2.73	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 0115 .. 0142 ..	2.74	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 0116 .. 0122 ..	2.65	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 0121 .. 0133 ..	2.83	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 0124 .. 0132 ..	2.63	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 0125 .. 0131 ..	2.63	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 0131 .. 0135 ..	2.77	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 0133 .. 0139 ..	2.84	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 0134 .. 0145 ..	2.59	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 0134 .. 0135 ..	2.71	Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact 0135 .. 0138 ..	2.67	Ang.
PLAT910_ALERT_3_B	Missing # of FCF Reflection(s) Below Theta(Min)	41	Note
PLAT971_ALERT_2_B	Check Calcd Residual Density 2.63A From 052	2.86	eA-3
PLAT971_ALERT_2_B	Check Calcd Residual Density 1.04A From 0142	2.85	eA-3
PLAT971_ALERT_2_B	Check Calcd Residual Density 3.00A From 0143	2.70	eA-3
PLAT971_ALERT_2_B	Check Calcd Residual Density 2.50A From 0140	2.70	eA-3
PLAT971_ALERT_2_B	Check Calcd Residual Density 2.35A From C16	2.56	eA-3
PLAT971_ALERT_2_B	Check Calcd Residual Density 1.26A From 0124	2.53	eA-3
PLAT972_ALERT_2_B	Check Calcd Residual Density 1.78A From 0107	-2.70	eA-3

PLAT972_ALERT_2_B	Check Calcd Residual Density	0.73A	From W16	-2.51 eA-3
PLAT976_ALERT_2_B	Check Calcd Residual Density	0.65A	From 0143	-2.00 eA-3

● Alert level C

CHEMW03_ALERT_2_C The ratio of given/expected molecular weight as calculated from the _atom_site* data lies outside the range 0.99 <> 1.01

From the CIF: _cell_formula_units_Z 8

From the CIF: _chemical_formula_weight 9446.97

TEST: Calculate formula weight from _atom_site_*

atom	mass	num	sum
W	183.85	36.00	6618.60
K	39.10	1.00	39.10
Na	22.99	2.00	45.98
O	16.00	140.30	2244.66
N	14.01	8.00	112.06
C	12.01	16.10	193.38
H	1.01	51.30	51.71

Calculated formula weight 9305.48

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.125

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	25	Check
PLAT213_ALERT_2_C	Atom 016	has ADP max/min Ratio	3.8 prolat
PLAT213_ALERT_2_C	Atom 031	has ADP max/min Ratio	3.3 prolat
PLAT213_ALERT_2_C	Atom 079	has ADP max/min Ratio	3.1 prolat
PLAT213_ALERT_2_C	Atom 091	has ADP max/min Ratio	3.3 prolat
PLAT213_ALERT_2_C	Atom 097	has ADP max/min Ratio	3.6 oblate
PLAT213_ALERT_2_C	Atom 0104	has ADP max/min Ratio	3.8 prolat
PLAT213_ALERT_2_C	Atom 0114	has ADP max/min Ratio	3.1 prolat
PLAT213_ALERT_2_C	Atom 0126	has ADP max/min Ratio	3.3 oblate
PLAT234_ALERT_4_C	Large Hirshfeld Difference W31 -- 097 ..	0.16	Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Na1	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	N7	Check
PLAT430_ALERT_2_C	Short Inter D...A Contact 07 .. 0122 ..	2.88	Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact 013 .. 0128 ..	2.89	Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact 019 .. 0124 ..	2.89	Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact 022 .. 0130 ..	2.90	Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact 041 .. 0130 ..	2.89	Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact 0107 .. 0125 ..	2.89	Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact 0137 .. 0141 ..	2.88	Ang.
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.600	9 Report
PLAT971_ALERT_2_C	Check Calcd Residual Density	2.70A	From 0145 2.50 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	2.90A	From 063 2.49 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	1.09A	From W2 2.41 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	0.55A	From 0124 2.36 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	1.14A	From W22 2.32 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	0.91A	From C12' 2.32 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	1.16A	From 04 2.31 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	1.10A	From W19 2.30 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	2.82A	From 036 2.28 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	0.90A	From 089 2.27 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	2.63A	From 0146 2.26 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	0.83A	From 09 2.26 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	1.10A	From W12 2.25 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	1.52A	From C13 2.25 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	1.21A	From 081 2.22 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	1.08A	From W18 2.20 eA-3
PLAT971_ALERT_2_C	Check Calcd Residual Density	0.98A	From 085 2.20 eA-3

PLAT972_ALERT_2_C	Check	Calcd	Residual Density	0.80A	From	W23	-2.34	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	2.46A	From	094	-2.26	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	1.81A	From	0140	-2.24	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	0.85A	From	012	-2.24	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	0.88A	From	W32	-2.23	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	0.77A	From	W16	-2.23	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	2.50A	From	073	-2.21	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	1.56A	From	0126	-2.21	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	2.68A	From	089	-2.18	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	0.86A	From	K1	-2.17	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	0.75A	From	W1	-2.15	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	2.06A	From	075	-2.11	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	0.73A	From	W10	-2.10	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	0.99A	From	W27	-2.08	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	0.61A	From	W13	-2.07	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	0.78A	From	W25	-2.03	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	1.17A	From	023	-2.01	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	0.65A	From	0143	-2.00	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	0.70A	From	W12	-1.99	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	1.96A	From	0118	-1.98	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	0.69A	From	W32	-1.96	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	0.86A	From	W5	-1.94	eA-3
PLAT972_ALERT_2_C	Check	Calcd	Residual Density	0.77A	From	W36	-1.91	eA-3
PLAT977_ALERT_2_C	Check	the	Negative Difference Density on			H1A	-0.58	eA-3
PLAT977_ALERT_2_C	Check	the	Negative Difference Density on			H4D	-0.62	eA-3
PLAT977_ALERT_2_C	Check	the	Negative Difference Density on			H5B	-0.59	eA-3
PLAT977_ALERT_2_C	Check	the	Negative Difference Density on			H5E	-1.17	eA-3
PLAT977_ALERT_2_C	Check	the	Negative Difference Density on			H7D	-0.55	eA-3
PLAT977_ALERT_2_C	Check	the	Negative Difference Density on			H7E	-0.56	eA-3
PLAT977_ALERT_2_C	Check	the	Negative Difference Density on			H8A	-0.39	eA-3
PLAT977_ALERT_2_C	Check	the	Negative Difference Density on			H9C	-0.80	eA-3
PLAT977_ALERT_2_C	Check	the	Negative Difference Density on			H13A	-0.69	eA-3
PLAT977_ALERT_2_C	Check	the	Negative Difference Density on			H18B	-0.37	eA-3
PLAT978_ALERT_2_C	Number	C-C Bonds with Positive Residual Density.					0	Note

● 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: C18 H128 K1 N9 Na2 O142 W36
 Atom count from the _atom_site data: C16.1 H51.3 K1 N8 Na2 O140.3 W
 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 8
 From the CIF: _chemical_formula_sum C18 H128 K N9 Na2 O142 W36
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	144.00	128.80	15.20
H	1024.00	410.40	613.60
K	8.00	8.00	0.00
N	72.00	64.00	8.00
Na	16.00	16.00	0.00
O	1136.00	1122.40	13.60
W	288.00	288.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	18	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	14	Report
PLAT020_ALERT_3_G	The value of Rint is greater than 0.12	0.125	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50	Check
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3	Report

[illegible]

PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 32)..	100 %	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 33)..	100 %	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (165.80) in Resd. #	1	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (8.60) in Resd. #	8	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (1.20) in Resd. #	9	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (3.30) in Resd. #	10	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.70) in Resd. #	12	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.80) in Resd. #	13	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.80) in Resd. #	19	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.50) in Resd. #	20	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.60) in Resd. #	21	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.60) in Resd. #	22	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.60) in Resd. #	23	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.50) in Resd. #	24	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.60) in Resd. #	25	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.60) in Resd. #	26	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.70) in Resd. #	27	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.40) in Resd. #	28	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.40) in Resd. #	29	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.40) in Resd. #	30	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.80) in Resd. #	31	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (3.60) in Resd. #	32	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (0.20) in Resd. #	33	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	0124	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	0125	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	0137	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	0138	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	0139	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	0140	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	0141	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	0142	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	0143	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	0144	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	0145	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	0146	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	0147	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact 028 .. C17 ..	2.98	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact 060 .. C16 ..	2.85	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact 060 .. C15 ..	3.01	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact 062 .. C11' ..	3.01	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact 077 .. C11' ..	2.87	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact 098 .. C17 ..	2.80	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact 0107 .. C4 ..	2.93	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact 0118 .. C12' ..	2.37	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact 0132 .. C11' ..	2.76	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact N5 .. C18 ..	2.93	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact N6 .. C12 ..	1.50	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact N6' .. C12 ..	0.90	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact N8 .. C16 ..	1.50	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact N8 .. C15 ..	1.50	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C9 .. C18 ..	3.15	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C10 .. C18 ..	3.14	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C11 .. C12 ..	2.76	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C11' .. C12 ..	2.16	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C17 .. C18 ..	2.81	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C11' -- C12' .	1.94	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C12 -- C12' .	1.85	Ang.
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: W2 -- K1 ..	4.06	Ang.
PLAT774_ALERT_1_G	Suspect X-Y Bond in CIF: W5 -- K1 ..	4.07	Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	862	Check
	N6' -N6 -C12 1.555 1.555 1.555	31.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #	871	Check

N6	-N6'	-C11'	1.555	1.555	1.555	10.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					883	Check
C11'	-C11	-N6	1.555	1.555	1.555	29.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					885	Check
N6	-C11	-N6'	1.555	1.555	1.555	25.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					887	Check
N6	-C11'	-N6'	1.555	1.555	1.555	11.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					892	Check
N6'	-C12	-N6	1.555	1.555	1.555	26.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					895	Check
N6'	-C12'	-N6	1.555	1.555	1.555	28.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					896	Check
N6'	-C12'	-C12	1.555	1.555	1.555	29.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #					899	Check
N6	-C12'	-C11'	1.555	1.555	1.555	22.00	Deg.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #					2	Note
C2	N2						
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #					10	Note
C0.60	H2.40	N0.30					
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #					18	Note
0							
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #					20	Note
0							
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #					21	Note
0							
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #					22	Note
0							
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #					23	Note
0							
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #					25	Note
0							
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #					26	Note
0							
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #					28	Note
0							
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #					29	Note
0							
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #					30	Note
0							
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #					32	Note
C	H3						
PLAT794_ALERT_5_G	Tentative Bond Valency for W11 (VI)					6.16	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints					12	Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...					14	Check

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

8 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
 155 **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
 109 **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.

