

checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: upyropnnmcif

Bond precision: C-C = 0.0106 Å

Wavelength=0.71069

Cell: a=13.198(2)
 alpha=90

b=14.852(2)
beta=90

c=23.407(4)
gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	4588.2(12)	4588.1(12)
Space group	P n n m	P n n m
Hall group	-P 2 2n	-P -2xabc;-
Moiety formula	C15 H3 O3O U6, 2(00.50), 2(00.50), 3(0), 2(N)	2(N H4 1+). 6(U O2 2+). 1.5(C10 O8 H2 4-). 4(O H 1-). 2(O 2
Sum formula	C15 H3 N2 O35 U6	C15 H3 N2 O35 U6
Mr	2199.37	2199.30
Dx, g cm-3	3.184	3.183
Z	4	4
Mu (mm-1)	21.198	21.198
F000	3756.0	3756.0
F000'	3532.27	
h, k, lmax	20, 22, 36	20, 22, 35
Nref	8997	8983
Tmin, Tmax	0.142, 0.529	0.100, 0.599
Tmin'	0.013	

Correction method= EMPIRICAL

Data completeness= 0.998

Theta(max)= 33.210

R(reflections)= 0.0444(6688)

wR2(reflections)= wR= 0.0747(
8983)

S = 2.940

Npar= 139

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)		24
PLAT306_ALERT_2_A	Isolated Oxygen Atom (H-atoms Missing ?)		03W
PLAT306_ALERT_2_A	Isolated Oxygen Atom (H-atoms Missing ?)		04W
PLAT601_ALERT_2_A	Structure Contains Solvent Accessible Voids of	.	338 A**3
PLAT770_ALERT_2_A	Suspect C-H Bond in CIF:	C7B -- H1C6B ..	2.65 Ang.
PLAT770_ALERT_2_A	Suspect C-H Bond in CIF:	C7A -- H1C3A ..	2.63 Ang.
PLAT770_ALERT_2_A	Suspect C-H Bond in CIF:	C1A -- H1C3A ..	2.05 Ang.
PLAT770_ALERT_2_A	Suspect C-H Bond in CIF:	C1B -- H1C6B ..	2.06 Ang.
PLAT770_ALERT_2_A	Suspect C-H Bond in CIF:	C2B -- H1C3B ..	2.05 Ang.
PLAT770_ALERT_2_A	Suspect C-H Bond in CIF:	C8B -- H1C3B ..	2.61 Ang.
PLAT772_ALERT_2_A	Suspect O-H Bond in CIF:	081B -- H1C3B ..	2.65 Ang.
PLAT772_ALERT_2_A	Suspect O-H Bond in CIF:	072B -- H1C6B ..	2.67 Ang.
PLAT772_ALERT_2_A	Suspect O-H Bond in CIF:	072A -- H1C3A ..	2.62 Ang.

Alert level B

PLAT430_ALERT_2_B	Short Inter D...A Contact	01H .. 04W ..	2.72 Ang.
PLAT430_ALERT_2_B	Short Inter D...A Contact	02H .. N1 ..	2.74 Ang.

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 = 2.940

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	?
PLAT127_ALERT_1_C	Implicit Hall Symbol Inconsistent with Explicit	-P -2xabc;-2y
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	3
PLAT311_ALERT_2_C	Isolated Disordered Oxygen Atom (No H's ?)	*01W
PLAT311_ALERT_2_C	Isolated Disordered Oxygen Atom (No H's ?)	*02W
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0106 Ang
PLAT430_ALERT_2_C	Short Inter D...A Contact	04W .. 022U .. 2.88 Ang.

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: C15 H3 N2 O35 U6
 Atom count from _chemical_formula_moiety: C0.12 H0.5304 N.012 O0.12

PLAT004_ALERT_5_G	Info: Polymeric Structure Found with Dimension	.	1
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in CIF		?
PLAT199_ALERT_1_G	Check the Reported _cell_measurement_temperature		293 K
PLAT200_ALERT_1_G	Check the Reported _diffn_ambient_temperature		293 K
PLAT302_ALERT_4_G	Note: Anion/Solvent Disorder		25 Perc.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		3
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	.	3.23 Ratio
PLAT773_ALERT_2_G	Check long C-C Bond in CIF:	C7B -- C6B .	2.49 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF:	C7B -- C2B .	2.51 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF:	C7B -- C8B .	2.95 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF:	C6B -- C3B .	2.79 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF:	C6B -- C2B .	2.42 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF:	C6B -- C2B .	2.42 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF:	C7A -- C7A .	2.97 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF:	C7A -- C1A .	2.53 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF:	C7A -- C3A .	2.47 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF:	C1A -- C1A .	2.82 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF:	C1A -- C1A .	2.43 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF:	C1A -- C3A .	2.44 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF:	C1B -- C1B .	2.41 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF:	C1B -- C3B .	2.41 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF:	C1B -- C2B .	2.79 Ang.

PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C1B	--	C8B	.	2.52	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C3B	--	C8B	.	2.47	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C3B	--	C8B	.	2.47	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C2B	--	C2B	.	2.42	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C3A	--	C3A	.	2.82	Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				68	
	U1 -01H -012U	1.555	1.555	1.555	37.01	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				77	
	U2 -01H -021U	1.555	1.555	1.555	36.66	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				85	
	U3 -01H -031U	1.555	1.555	1.555	37.05	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				111	
	U2 -081B -021U	2.555	1.555	2.555	38.44	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				128	
	082B -081B -C8B	1.555	1.555	1.555	28.60	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				139	
	C3B -081B -C2B	1.555	1.555	1.555	29.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				141	
	C3B -081B -H1C3B	1.555	1.555	1.555	19.57	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				142	
	C2B -081B -C8B	1.555	1.555	1.555	33.90	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				149	
	U3 -071A -032U	4.555	1.555	4.555	36.40	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				159	
	071A -071A -C7A	2.655	1.555	2.655	24.20	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				176	
	072A -071A -C7A	1.555	1.555	1.555	28.60	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				185	
	C7A -071A -C1A	1.555	1.555	1.555	32.70	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				188	
	C7A -071A -C1A	2.655	1.555	2.655	29.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				189	
	C1A -071A -C1A	1.555	1.555	2.655	28.20	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				192	
	U2 -071B -022U	1.555	1.555	1.555	38.56	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				216	
	072B -071B -C7B	1.555	1.555	1.555	28.60	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				220	
	C7B -071B -C1B	1.555	1.555	1.555	34.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				223	
	C1B -071B -C2B	1.555	1.555	1.555	28.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				225	
	C2B -071B -C8B	1.555	1.555	1.555	29.40	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				228	
	U3 -082B -031U	3.545	1.555	3.545	37.62	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				230	
	U3 -082B -032U	3.545	1.555	3.545	36.54	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				240	
	081B -082B -C8B	1.555	1.555	1.555	28.40	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				259	
	C1B -082B -C2B	1.555	1.555	1.555	26.90	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				261	
	C2B -082B -C8B	1.555	1.555	1.555	33.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				266	
	U1 -01 -011U	1.555	1.555	1.555	36.78	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				267	
	U1 -01 -012U	1.555	1.555	1.555	37.97	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				279	
	U2 -01 -021U	4.555	1.555	4.555	37.67	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				281	
	U2 -01 -022U	4.555	1.555	4.555	37.98	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #				290	

U3	-01	-031U	4.555	1.555	4.555	38.64	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	294	
U3	-01	-032U	4.555	1.555	4.555	37.18	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	309	
071A	-01	-072A	1.555	1.555	1.555	43.88	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	383	
U1	-072B	-011U	1.555	1.555	1.555	37.31	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	384	
U1	-072B	-012U	1.555	1.555	1.555	35.66	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	393	
071B	-072B	-C7B	1.555	1.555	1.555	27.90	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	413	
C7B	-072B	-C1B	1.555	1.555	1.555	33.70	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	415	
C6B	-072B	-C1B	1.555	1.555	1.555	28.50	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	416	
C6B	-072B	-H1C6B	1.555	1.555	1.555	19.26	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	420	
U1	-072A	-011U	1.555	1.555	1.555	36.83	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	429	
071A	-072A	-C7A	1.555	1.555	1.555	27.40	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	448	
C7A	-072A	-C1A	1.555	1.555	1.555	34.90	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	451	
C1A	-072A	-C3A	1.555	1.555	1.555	29.30	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	453	
C3A	-072A	-H1C3A	1.555	1.555	1.555	19.68	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	468	
U2	-02H	-022U	4.555	1.555	4.555	37.66	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	476	
U3	-02H	-032U	1.555	1.555	1.555	37.08	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	484	
081B	-02H	-082B	3.555	1.555	3.555	44.65	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	525	
C6B	-C7B	-C1B	1.555	1.555	1.555	29.60	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	528	
C6B	-C7B	-H1C6B	1.555	1.555	1.555	21.28	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	529	
C1B	-C7B	-C2B	1.555	1.555	1.555	28.50	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	532	
C2B	-C7B	-C8B	1.555	1.555	1.555	30.10	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	536	
072B	-C6B	-C7B	1.555	1.555	1.555	26.10	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	545	
072B	-C6B	-C7B	6.555	1.555	6.555	26.10	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	553	
C7B	-C6B	-C1B	1.555	1.555	1.555	32.00	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	560	
C7B	-C6B	-C1B	6.555	1.555	6.555	32.00	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	567	
C1B	-C6B	-C2B	1.555	1.555	1.555	29.60	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	572	
C1B	-C6B	-C2B	6.555	1.555	6.555	29.60	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	574	
C3B	-C6B	-C2B	1.555	1.555	1.555	30.00	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	575	
C3B	-C6B	-C2B	1.555	1.555	6.555	30.00	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	588	
071A	-C7A	-C7A	2.655	1.555	2.655	24.10	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	599	
C7A	-C7A	-C1A	2.655	1.555	2.655	29.80	Deg.
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle in	CIF #	602	

	C1A -C7A -C1A	1.555	1.555	2.655		28.80	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			603	
	C1A -C7A -C3A	1.555	1.555	1.555		29.80	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			607	
	C3A -C7A -H1C3A	1.555	1.555	1.555		21.42	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			610	
	071A -C1A -C7A	1.555	1.555	1.555		26.80	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			620	
	071A -C1A -C7A	2.655	1.555	2.655		24.40	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			627	
	072A -C1A -C7A	1.555	1.555	1.555		29.80	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			642	
	C7A -C1A -C1A	2.655	1.555	2.655		30.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			651	
	C1A -C1A -C3A	2.655	1.555	2.655		29.80	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			653	
	C1A -C1A -C1A	5.655	1.555	6.555		30.40	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			655	
	C1A -C1A -C3A	5.655	1.555	2.655		29.80	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			657	
	C1A -C1A -C3A	6.555	1.555	1.555		29.80	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			661	
	C3A -C1A -H1C3A	1.555	1.555	1.555		23.92	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			665	
	071B -C1B -C7B	1.555	1.555	1.555		27.90	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			680	
	082B -C1B -C8B	1.555	1.555	1.555		24.90	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			682	
	072B -C1B -C7B	1.555	1.555	1.555		28.30	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			697	
	C6B -C1B -C1B	1.555	1.555	6.555		30.40	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			702	
	C6B -C1B -H1C6B	1.555	1.555	1.555		23.76	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			705	
	C1B -C1B -C2B	6.555	1.555	6.555		29.90	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			708	
	C3B -C1B -C2B	1.555	1.555	1.555		30.30	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			709	
	C3B -C1B -C2B	1.555	1.555	6.555		30.10	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			713	
	C2B -C1B -C8B	1.555	1.555	1.555		29.80	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			724	
	081B -C3B -C8B	1.555	1.555	1.555		26.30	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			733	
	081B -C3B -C8B	6.555	1.555	6.555		26.30	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			735	
	C6B -C3B -C1B	1.555	1.555	1.555		30.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			736	
	C6B -C3B -C1B	1.555	1.555	6.555		30.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			743	
	C1B -C3B -C2B	1.555	1.555	1.555		30.10	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			749	
	C1B -C3B -C2B	6.555	1.555	6.555		30.10	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			754	
	C2B -C3B -C8B	1.555	1.555	1.555		32.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			758	
	C2B -C3B -C8B	6.555	1.555	6.555		32.00	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			771	
	081B -C2B -C8B	1.555	1.555	1.555		28.60	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			774	
	071B -C2B -C7B	1.555	1.555	1.555		25.20	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		#			788	

082B -C2B -C8B	1.555	1.555	1.555	28.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				791
C7B -C2B -C1B	1.555	1.555	1.555	31.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				797
C6B -C2B -C1B	1.555	1.555	1.555	29.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				798
C6B -C2B -C1B	1.555	1.555	6.555	30.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				809
C1B -C2B -C2B	6.555	1.555	6.555	29.90 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				812
C3B -C2B -C2B	1.555	1.555	6.555	29.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				814
C3B -C2B -H1C3B	1.555	1.555	1.555	23.97 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				826
071B -C8B -C7B	1.555	1.555	1.555	24.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				836
C7B -C8B -C1B	1.555	1.555	1.555	30.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				841
C1B -C8B -C2B	1.555	1.555	1.555	27.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				843
C3B -C8B -C2B	1.555	1.555	1.555	30.00 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				844
C3B -C8B -H1C3B	1.555	1.555	1.555	21.55 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				847
072A -C3A -C7A	1.555	1.555	1.555	26.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				856
072A -C3A -C7A	6.555	1.555	6.555	26.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				864
C7A -C3A -C1A	1.555	1.555	1.555	31.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				873
C7A -C3A -C1A	6.555	1.555	6.555	31.70 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				876
C1A -C3A -C1A	1.555	1.555	2.655	30.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				883
C1A -C3A -C3A	2.655	1.555	2.655	29.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				885
C1A -C3A -C1A	5.655	1.555	6.555	30.40 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				886
C1A -C3A -C3A	5.655	1.555	2.655	29.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				902
072B -H1C6B-C7B	1.555	1.555	1.555	27.92 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				908
072B -H1C6B-C7B	6.555	1.555	6.555	27.92 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				914
C7B -H1C6B-C1B	1.555	1.555	1.555	34.35 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				918
C7B -H1C6B-C1B	6.555	1.555	6.555	34.35 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				919
C6B -H1C6B-C1B	1.555	1.555	1.555	35.85 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				920
C6B -H1C6B-C1B	1.555	1.555	6.555	35.85 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				926
081B -H1C3B-C8B	1.555	1.555	1.555	27.95 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				932
081B -H1C3B-C8B	6.555	1.555	6.555	27.95 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				933
C3B -H1C3B-C2B	1.555	1.555	1.555	36.19 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				934
C3B -H1C3B-C2B	1.555	1.555	6.555	36.19 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				938
C2B -H1C3B-C8B	1.555	1.555	1.555	34.41 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				941

C2B -H1C3B-C8B	6.555	1.555	6.555	34.41	Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				944	
072A -H1C3A-C7A	1.555	1.555	1.555	28.36	Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				950	
072A -H1C3A-C7A	6.555	1.555	6.555	28.36	Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				955	
C7A -H1C3A-C1A	1.555	1.555	1.555	34.12	Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				959	
C7A -H1C3A-C1A	6.555	1.555	6.555	34.12	Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				962	
C1A -H1C3A-C3A	1.555	1.555	1.555	36.25	Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF #				963	
C1A -H1C3A-C3A	6.555	1.555	1.555	36.25	Deg.
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found					!

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 39 ALERT type 2 Indicator that the structure model may be wrong or deficient
 2 ALERT type 3 Indicator that the structure quality may be low
 131 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*, 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.

