

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C78-I

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: C78-I

Bond precision:	C-C = 0.0082 A	Wavelength=0.68889
Cell:	a=25.450 (7)	b=15.021 (5) c=19.704 (7)
	alpha=90	beta=92.312 (11) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	7526 (4)	7526 (4)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	C78, C36 H44 N4 Ni, C6 H6, 2 (C3 H3)	C78 C36 H44 N4 Ni C6 H6 2 (C3 H3)
Sum formula	C126 H56 N4 Ni	C126 H56 N4 Ni
Mr	1684.44	1684.45
Dx, g cm ⁻³	1.487	1.487
Z	4	4
Mu (mm ⁻¹)	0.299	0.299
F000	3472.0	4044.0
F000'	3474.35	
h, k, lmax		26, 16, 23
Nref		6015
Tmin, Tmax	0.979, 0.982	0.523, 0.745
Tmin'	0.976	

Correction method= # Reported T Limits: Tmin=0.523 Tmax=0.745
AbsCorr = ?

Data completeness= Theta(max)= 26.089

R(reflections)= 0.0760 (5045)	wR2(reflections)= 0.2482 (6015)
S = 1.105	Npar= 944

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 _diffn_measured_fraction_theta_full value Low . 0.818 Why?

Author Response: Our data were obtained at Shanghai Synchrotron Radiation Facility (SSRF), where the measurement method is psi scans, which may cause some angular diffraction points to be lost.

Alert level B

PLAT088_ALERT_3_B Poor Data / Parameter Ratio 6.37 Note
PLAT234_ALERT_4_B Large Hirshfeld Difference C10 --C28 . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C59 --C62 . 0.28 Ang.
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C50 Check
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 1038 Report

24	0	0,	24	10	0,	25	1	0,	25	7	0,	25	9	0,	26	0	0,
26	2	0,	26	4	0,	26	6	0,	26	8	0,	-26	0	1,	-26	2	1,
-26	4	1,	-26	6	1,	-26	8	1,	-25	1	1,	-25	5	1,	-25	7	1,
-25	9	1,	-24	0	1,	-24	2	1,	-24	10	1,	-23	1	1,	-22	0	1,
-21	1	1,	-20	0	1,	-13	13	1,	-6	0	1,	-4	0	1,	-2	0	1,
2	0	1,	2	10	1,	4	10	1,	12	4	1,	25	7	1,	25	9	1,
26	0	1,	26	2	1,	26	4	1,	26	6	1,	26	8	1,	-26	0	2,
-26	2	2,	-26	4	2,	-26	6	2,	-26	8	2,	-25	1	2,	-25	3	2,
-25	5	2,	-25	7	2,	-25	9	2,	-24	0	2,	-24	2	2,	-24	8	2,
-24	10	2,	-23	1	2,	-23	11	2,	-22	0	2,	-22	2	2,	-21	1	2,
-20	0	2,	-19	1	2,	-18	0	2,	-17	1	2,	-16	0	2,	-15	13	2,
-14	0	2,	-12	0	2,	-10	0	2,	-9	1	2,	-9	9	2,	-8	0	2,
-6	0	2,	2	10	2,	12	16	2,	25	9	2,	26	0	2,	26	2	2,
26	4	2,	26	6	2,	26	8	2,	-26	0	3,	-26	2	3,	-26	4	3,
-26	6	3,	-26	8	3,	-25	1	3,	-25	3	3,	-25	5	3,	-25	7	3,
-25	9	3,	-24	0	3,	-24	2	3,	-24	8	3,	-24	10	3,	-23	1	3,

Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C78, C36 H44 N4 Ni, C6 H6, 2(C3 H3)
Rep.: C78 C36 H44 N4 Ni C6 H6 2(C3 H3)

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !

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

PLAT215_ALERT_3_C Disordered C2	has ADP max/min Ratio	3.5 Note
PLAT215_ALERT_3_C Disordered C3	has ADP max/min Ratio	3.9 Note
PLAT215_ALERT_3_C Disordered C13	has ADP max/min Ratio	3.2 Note
PLAT215_ALERT_3_C Disordered C26	has ADP max/min Ratio	3.7 Note
PLAT215_ALERT_3_C Disordered C27	has ADP max/min Ratio	3.1 Note
PLAT215_ALERT_3_C Disordered C30	has ADP max/min Ratio	3.9 Note
PLAT215_ALERT_3_C Disordered C43	has ADP max/min Ratio	3.3 Note
PLAT215_ALERT_3_C Disordered C47	has ADP max/min Ratio	3.8 Note
PLAT215_ALERT_3_C Disordered C51	has ADP max/min Ratio	3.5 Note
PLAT215_ALERT_3_C Disordered C56	has ADP max/min Ratio	3.2 Note

[illegible]

[illegible]

H9DB H9DC

PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	3.15	Ratio
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C15 --C74	1.72	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C15 --C75	1.79	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C15 --C7	1.97	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C19 --C38	1.74	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C14 --C36	1.74	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C14 --C20	1.85	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C14 --C8	1.97	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C14 --C63	2.00	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C6 --C57	1.95	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C4 --C78	1.79	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C4 --C3	1.94	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C1 --C7	1.73	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C2 --C41	2.02	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C3 --C37	1.88	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C3 --C4	1.94	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C28 --C11	1.90	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C28 --C12	2.02	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C7 --C1	1.73	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C7 --C15	1.97	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C8 --C37	1.73	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C8 --C14	1.97	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C9 --C11	1.91	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C11 --C28	1.90	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C11 --C9	1.91	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C12 --C28	2.02	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C13 --C45	1.76	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C13 --C46	1.79	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C13 --C27	2.04	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C16 --C29	1.94	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C16 --C46	2.01	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C18 --C37	1.91	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C18 --C44	1.96	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C20 --C14	1.85	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C21 --C39	1.85	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C21 --C47	2.04	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C22 --C41	1.75	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C22 --C44	1.82	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C23 --C41	2.03	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C24 --C29	1.97	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C29 --C16	1.94	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C30 --C51	1.87	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C30 --C54	1.95	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C30 --C52	2.00	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C31 --C58	1.86	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C31 --C54	1.91	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C31 --C51	1.96	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C33 --C66	1.97	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C34 --C54	1.74	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C34 --C55	1.83	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C34 --C39	1.84	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C36 --C14	1.74	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C37 --C8	1.73	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C37 --C3	1.88	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C37 --C18	1.91	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C38 --C19	1.74	Ang.

PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C38	--C67	1.78 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C38	--C45	1.85 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C38	--C55	1.98 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C39	--C34	1.84 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C39	--C21	1.85 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C41	--C22	1.75 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C41	--C2	2.02 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C41	--C23	2.03 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C44	--C22	1.82 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C44	--C18	1.96 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C45	--C13	1.76 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C45	--C38	1.85 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C46	--C13	1.79 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C46	--C16	2.01 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C47	--C21	2.04 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C51	--C30	1.87 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C51	--C31	1.96 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C52	--C58	1.91 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C52	--C30	2.00 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C52	--C57	2.02 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C54	--C34	1.74 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C54	--C31	1.91 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C54	--C30	1.95 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C55	--C34	1.83 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C55	--C38	1.98 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C56	--C56	1.98 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C56	--C58	1.99 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C57	--C6	1.95 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C57	--C52	2.02 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C58	--C31	1.86 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C58	--C52	1.91 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C58	--C56	1.99 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C61	--C66	1.81 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C63	--C14	2.00 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C64	--C68	1.71 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C64	--C72	1.85 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C64	--C69	1.96 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C65	--C66	1.89 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C65	--C70	1.94 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C60	--C70	1.88 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C66	--C61	1.81 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C66	--C65	1.88 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C66	--C33	1.97 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C67	--C38	1.78 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C68	--C64	1.71 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C68	--C75	1.97 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C69	--C64	1.96 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C70	--C60	1.88 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C70	--C72	1.92 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C70	--C65	1.94 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C71	--C73	1.86 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C72	--C64	1.85 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C72	--C70	1.92 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C73	--C71	1.86 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C74	--C15	1.72 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C75	--C15	1.79 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C75	--C68	1.97 Ang.

PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C78	--C4						1.79 Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							16.00 Deg.
	C8 -C15 -C19	6_565	1_555	1_555		#		8 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							43.50 Deg.
	C1 -C15 -C28	1_555	1_555	6_565		#		14 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							6.70 Deg.
	C12 -C15 -C74	1_555	1_555	6_565		#		18 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							33.20 Deg.
	C19 -C15 -C75	1_555	1_555	6_565		#		26 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							35.00 Deg.
	C8 -C15 -C7	6_565	1_555	6_565		#		30 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							37.90 Deg.
	C75 -C19 -C14	6_565	1_555	1_555		#		39 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							18.00 Deg.
	C8 -C19 -C15	6_565	1_555	1_555		#		43 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							27.40 Deg.
	C7 -C19 -C37	6_565	1_555	1_555		#		50 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							18.40 Deg.
	C14 -C19 -C38	1_555	1_555	6_565		#		54 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							7.00 Deg.
	C38 -C14 -C39	6_565	1_555	1_555		#		64 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							41.00 Deg.
	C38 -C14 -C20	6_565	1_555	6_565		#		73 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							42.30 Deg.
	C39 -C14 -C20	1_555	1_555	6_565		#		77 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							35.00 Deg.
	C75 -C14 -C8	6_565	1_555	6_565		#		80 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							12.20 Deg.
	C19 -C14 -C8	1_555	1_555	6_565		#		81 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							33.00 Deg.
	C75 -C14 -C63	6_565	1_555	6_565		#		87 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							43.40 Deg.
	C67 -C14 -C63	1_555	1_555	6_565		#		89 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							23.00 Deg.
	C69 -C6 -C60	1_555	1_555	6_565		#		106 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							33.00 Deg.
	C56 -C6 -C57	6_565	1_555	6_565		#		109 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							33.20 Deg.
	C53 -C6 -C57	1_555	1_555	6_565		#		113 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							41.50 Deg.
	C78 -C5 -C1	6_565	1_555	1_555		#		122 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							42.10 Deg.
	C17 -C4 -C17	6_565	1_555	1_555		#		133 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							13.40 Deg.
	C43 -C4 -C2	1_555	1_555	6_565		#		144 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							38.80 Deg.
	C43 -C4 -C3	1_555	1_555	6_565		#		155 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							44.30 Deg.
	C2 -C4 -C3	6_565	1_555	6_565		#		156 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							42.70 Deg.
	C78 -C4 -C3	6_565	1_555	6_565		#		157 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							42.20 Deg.
	C28 -C1 -C5	6_565	1_555	1_555		#		165 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							19.30 Deg.
	C3 -C1 -C44	6_565	1_555	1_555		#		170 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...							22.80 Deg.
	C15 -C1 -C9	1_555	1_555	6_565		#		176 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	28.50 Deg.
C15 -C1 -C8	1_555 1_555 6_565	 #	182 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	36.10 Deg.
C44 -C1 -C7	1_555 1_555 6_565	 #	191 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	20.60 Deg.
C44 -C2 -C3	6_565 1_555 1_555	 #	203 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	39.00 Deg.
C17 -C2 -C4	1_555 1_555 6_565	 #	214 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	41.80 Deg.
C42 -C2 -C41	6_565 1_555 6_565	 #	216 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.10 Deg.
C18 -C2 -C41	1_555 1_555 6_565	 #	217 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.30 Deg.
C43 -C3 -C2	6_565 1_555 1_555	 #	226 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.00 Deg.
C44 -C3 -C7	6_565 1_555 1_555	 #	228 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	40.60 Deg.
C78 -C3 -C1	1_555 1_555 6_565	 #	234 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	24.00 Deg.
C44 -C3 -C37	6_565 1_555 6_565	 #	237 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.70 Deg.
C7 -C3 -C37	1_555 1_555 6_565	 #	241 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.70 Deg.
C2 -C17 -C43	1_555 1_555 6_565	 #	255 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.60 Deg.
C56 -C25 -C6	1_555 1_555 6_565	 #	274 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.60 Deg.
C56 -C25 -C6	6_565 1_555 1_555	 #	278 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.30 Deg.
C1 -C28 -C78	6_565 1_555 1_555	 #	285 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	23.10 Deg.
C9 -C28 -C15	1_555 1_555 6_565	 #	293 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	30.50 Deg.
C9 -C28 -C12	1_555 1_555 6_565	 #	304 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	41.70 Deg.
C11 -C28 -C12	6_565 1_555 6_565	 #	308 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.00 Deg.
C37 -C7 -C22	6_565 1_555 1_555	 #	310 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.40 Deg.
C44 -C7 -C3	6_565 1_555 1_555	 #	316 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.50 Deg.
C8 -C7 -C19	1_555 1_555 6_565	 #	322 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	19.80 Deg.
C8 -C7 -C15	1_555 1_555 6_565	 #	333 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.00 Deg.
C19 -C8 -C75	6_565 1_555 1_555	 #	338 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	8.00 Deg.
C15 -C8 -C9	6_565 1_555 1_555	 #	344 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	22.40 Deg.
C7 -C8 -C37	1_555 1_555 6_565	 #	355 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	23.00 Deg.
C19 -C8 -C14	6_565 1_555 6_565	 #	358 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	20.10 Deg.
C75 -C8 -C14	1_555 1_555 6_565	 #	360 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	11.00 Deg.
C15 -C9 -C8	6_565 1_555 1_555	 #	368 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	7.00 Deg.

C12	-C9	-C74	6_565	1_555	1_555		#	372 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		43.80 Deg.
C28	-C9	-C1	1_555	1_555	6_565		#	377 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		40.80 Deg.
C28	-C10	-C5	6_565	1_555	1_555		#	388 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		40.80 Deg.
C28	-C10	-C5	1_555	1_555	6_565		#	389 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		41.00 Deg.
C11	-C10	-C11	6_565	1_555	1_555		#	400 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		12.00 Deg.
C12	-C11	-C74	1_555	1_555	6_565		#	409 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		40.60 Deg.
C73	-C11	-C73	6_565	1_555	1_555		#	412 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		35.80 Deg.
C12	-C11	-C9	1_555	1_555	6_565		#	424 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		39.00 Deg.
C28	-C11	-C9	6_565	1_555	6_565		#	428 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		23.60 Deg.
C9	-C12	-C15	6_565	1_555	1_555		#	433 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		25.50 Deg.
C63	-C12	-C68	6_565	1_555	1_555		#	448 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		35.00 Deg.
C9	-C12	-C28	6_565	1_555	6_565		#	451 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		17.00 Deg.
C47	-C13	-C26	6_565	1_555	1_555		#	458 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		38.50 Deg.
C40	-C13	-C16	6_565	1_555	1_555		#	464 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		28.10 Deg.
C16	-C13	-C41	1_555	1_555	6_565		#	471 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		17.70 Deg.
C21	-C13	-C45	1_555	1_555	6_565		#	481 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		30.30 Deg.
C47	-C13	-C27	6_565	1_555	1_555		#	493 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		43.20 Deg.
C40	-C13	-C27	6_565	1_555	1_555		#	494 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		40.90 Deg.
C26	-C13	-C27	1_555	1_555	1_555		#	495 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		23.00 Deg.
C41	-C16	-C18	6_565	1_555	1_555		#	505 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		27.30 Deg.
C23	-C16	-C29	1_555	1_555	1_555		#	521 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		28.00 Deg.
C41	-C16	-C46	6_565	1_555	6_565		#	523 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		21.00 Deg.
C41	-C18	-C16	6_565	1_555	1_555		#	533 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		31.80 Deg.
C22	-C18	-C46	1_555	1_555	6_565		#	544 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		9.10 Deg.
C2	-C18	-C43	1_555	1_555	6_565		#	547 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		19.30 Deg.
C22	-C18	-C37	1_555	1_555	6_565		#	555 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		43.90 Deg.
C2	-C18	-C44	1_555	1_555	6_565		#	560 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		42.40 Deg.
C43	-C18	-C44	6_565	1_555	6_565		#	564 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		43.70 Deg.
C37	-C18	-C44	6_565	1_555	6_565		#	565 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.00 Deg.
C46 -C20 -C22	6_565 1_555 1_555	 #	570 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	21.00 Deg.
C45 -C20 -C21	6_565 1_555 1_555	 #	572 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	37.70 Deg.
C39 -C20 -C38	6_565 1_555 1_555	 #	578 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	25.60 Deg.
C22 -C20 -C37	1_555 1_555 6_565	 #	584 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.80 Deg.
C38 -C20 -C14	1_555 1_555 6_565	 #	592 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	35.00 Deg.
C49 -C21 -C34	6_565 1_555 1_555	 #	598 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	32.00 Deg.
C45 -C21 -C20	6_565 1_555 1_555	 #	600 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.90 Deg.
C20 -C21 -C46	1_555 1_555 6_565	 #	608 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	22.00 Deg.
C45 -C21 -C39	6_565 1_555 6_565	 #	609 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.50 Deg.
C20 -C21 -C39	1_555 1_555 6_565	 #	613 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.20 Deg.
C49 -C21 -C47	6_565 1_555 6_565	 #	616 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	31.20 Deg.
C13 -C21 -C47	1_555 1_555 6_565	 #	617 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.00 Deg.
C37 -C22 -C7	6_565 1_555 1_555	 #	623 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	26.30 Deg.
C18 -C22 -C41	1_555 1_555 6_565	 #	635 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	33.90 Deg.
C7 -C22 -C44	1_555 1_555 6_565	 #	639 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.50 Deg.
C16 -C23 -C40	1_555 1_555 6_565	 #	652 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	12.50 Deg.
C16 -C23 -C41	1_555 1_555 6_565	 #	661 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.20 Deg.
C42 -C23 -C41	6_565 1_555 6_565	 #	663 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	40.00 Deg.
C17 -C24 -C17	6_565 1_555 1_555	 #	669 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	25.20 Deg.
C23 -C24 -C29	1_555 1_555 1_555	 #	679 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	25.20 Deg.
C23 -C24 -C29	6_565 1_555 1_555	 #	680 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.80 Deg.
C27 -C26 -C51	1_555 1_555 6_565	 #	694 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	35.40 Deg.
C30 -C26 -C49	1_555 1_555 6_565	 #	697 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.40 Deg.
C47 -C27 -C26	6_565 1_555 1_555	 #	711 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.00 Deg.
C51 -C27 -C51	6_565 1_555 1_555	 #	716 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.90 Deg.
C27 -C27 -C51	6_565 1_555 1_555	 #	717 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	28.30 Deg.
C47 -C27 -C13	6_565 1_555 1_555	 #	729 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	39.10 Deg.
C26 -C27 -C13	1_555 1_555 1_555	 #	730 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	33.00 Deg.

C40	-C27	-C13	6_565	1_555	1_555		#	731 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		44.00 Deg.
C27	-C29	-C27	1_555	1_555	6_565		#	739 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		44.00 Deg.
C23	-C29	-C16	1_555	1_555	1_555		#	750 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		25.10 Deg.
C40	-C29	-C16	6_565	1_555	1_555		#	754 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		44.00 Deg.
C23	-C29	-C16	6_565	1_555	6_565		#	755 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		25.10 Deg.
C40	-C29	-C16	1_555	1_555	6_565		#	759 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		38.00 Deg.
C23	-C29	-C24	6_565	1_555	1_555		#	762 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		38.00 Deg.
C23	-C29	-C24	1_555	1_555	1_555		#	763 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		35.00 Deg.
C48	-C30	-C31	6_565	1_555	1_555		#	773 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		33.00 Deg.
C49	-C30	-C34	6_565	1_555	1_555		#	777 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		16.00 Deg.
C26	-C30	-C47	1_555	1_555	6_565		#	782 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		38.00 Deg.
C48	-C30	-C54	6_565	1_555	6_565		#	791 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		37.20 Deg.
C48	-C30	-C52	6_565	1_555	6_565		#	798 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		2.70 Deg.
C31	-C30	-C52	1_555	1_555	6_565		#	801 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		36.00 Deg.
C48	-C31	-C30	6_565	1_555	1_555		#	808 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		38.00 Deg.
C52	-C31	-C58	6_565	1_555	6_565		#	816 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		40.00 Deg.
C48	-C31	-C54	6_565	1_555	6_565		#	822 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		34.20 Deg.
C32	-C31	-C54	1_555	1_555	6_565		#	825 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		43.50 Deg.
C50	-C31	-C51	1_555	1_555	6_565		#	830 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		38.00 Deg.
C54	-C32	-C35	6_565	1_555	1_555		#	841 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		33.50 Deg.
C48	-C32	-C31	6_565	1_555	1_555		#	847 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		28.70 Deg.
C58	-C32	-C57	6_565	1_555	1_555		#	851 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		26.10 Deg.
C31	-C32	-C52	1_555	1_555	6_565		#	860 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		37.20 Deg.
C54	-C33	-C35	6_565	1_555	1_555		#	864 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		28.00 Deg.
C55	-C33	-C36	6_565	1_555	1_555		#	865 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		12.00 Deg.
C55	-C33	-C66	6_565	1_555	6_565		#	877 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		31.10 Deg.
C36	-C33	-C66	1_555	1_555	6_565		#	880 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		36.00 Deg.
C49	-C34	-C30	6_565	1_555	1_555		#	884 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		27.20 Deg.
C21	-C34	-C45	1_555	1_555	6_565		#	887 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	30.80 Deg.
C30 -C34 -C48	1_555 1_555 6_565	 #	895 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	12.00 Deg.
C33 -C34 -C55	1_555 1_555 6_565	 #	908 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.90 Deg.
C45 -C34 -C39	6_565 1_555 6_565	 #	914 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.10 Deg.
C53 -C35 -C32	6_565 1_555 1_555	 #	921 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	20.50 Deg.
C33 -C35 -C55	1_555 1_555 6_565	 #	933 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	27.10 Deg.
C66 -C36 -C76	6_565 1_555 1_555	 #	936 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	14.00 Deg.
C55 -C36 -C33	6_565 1_555 1_555	 #	937 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	35.80 Deg.
C39 -C36 -C38	6_565 1_555 1_555	 #	948 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	20.40 Deg.
C38 -C36 -C14	1_555 1_555 6_565	 #	960 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	41.00 Deg.
C7 -C37 -C44	6_565 1_555 1_555	 #	963 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.00 Deg.
C22 -C37 -C46	6_565 1_555 1_555	 #	969 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	40.20 Deg.
C46 -C37 -C20	1_555 1_555 6_565	 #	976 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	24.50 Deg.
C19 -C37 -C8	1_555 1_555 6_565	 #	980 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	38.00 Deg.
C7 -C37 -C3	6_565 1_555 6_565	 #	983 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	8.00 Deg.
C44 -C37 -C3	1_555 1_555 6_565	 #	985 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	38.00 Deg.
C22 -C37 -C18	6_565 1_555 6_565	 #	991 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	14.00 Deg.
C14 -C38 -C75	6_565 1_555 1_555	 #	999 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.00 Deg.
C14 -C38 -C19	6_565 1_555 6_565	 #	1008 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.20 Deg.
C75 -C38 -C19	1_555 1_555 6_565	 #	1010 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	38.00 Deg.
C39 -C38 -C45	6_565 1_555 6_565	 #	1020 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.30 Deg.
C20 -C38 -C45	1_555 1_555 6_565	 #	1022 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	28.90 Deg.
C36 -C38 -C55	1_555 1_555 6_565	 #	1030 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.00 Deg.
C20 -C39 -C45	6_565 1_555 1_555	 #	1036 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	5.00 Deg.
C38 -C39 -C14	6_565 1_555 1_555	 #	1040 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	39.20 Deg.
C36 -C39 -C55	6_565 1_555 1_555	 #	1047 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	19.10 Deg.
C55 -C39 -C33	1_555 1_555 6_565	 #	1054 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	10.60 Deg.
C45 -C39 -C21	1_555 1_555 6_565	 #	1064 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.50 Deg.
C34 -C39 -C21	6_565 1_555 6_565	 #	1069 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.00 Deg.

C16	-C40	-C41	6_565	1_555	1_555		# 1080 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	36.60 Deg.
C23	-C40	-C29	6_565	1_555	1_555		# 1089 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	12.30 Deg.
C47	-C40	-C26	1_555	1_555	6_565		# 1093 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	21.00 Deg.
C16	-C41	-C40	6_565	1_555	1_555		# 1104 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	26.20 Deg.
C46	-C41	-C22	1_555	1_555	6_565		# 1116 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	27.00 Deg.
C18	-C41	-C2	6_565	1_555	6_565		# 1120 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	32.80 Deg.
C42	-C41	-C2	1_555	1_555	6_565		# 1121 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	26.00 Deg.
C16	-C41	-C23	6_565	1_555	6_565		# 1126 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	34.60 Deg.
C18	-C42	-C41	6_565	1_555	1_555		# 1136 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	11.00 Deg.
C2	-C42	-C43	6_565	1_555	1_555		# 1137 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	28.50 Deg.
C41	-C42	-C16	1_555	1_555	6_565		# 1142 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	21.40 Deg.
C3	-C43	-C44	6_565	1_555	1_555		# 1164 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	34.00 Deg.
C2	-C43	-C42	6_565	1_555	1_555		# 1168 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	42.60 Deg.
C17	-C43	-C4	6_565	1_555	1_555		# 1175 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	33.00 Deg.
C2	-C43	-C18	6_565	1_555	6_565		# 1177 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	42.80 Deg.
C42	-C43	-C18	1_555	1_555	6_565		# 1181 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	17.10 Deg.
C43	-C44	-C2	1_555	1_555	6_565		# 1188 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	26.30 Deg.
C7	-C44	-C37	6_565	1_555	1_555		# 1190 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	36.60 Deg.
C1	-C44	-C78	1_555	1_555	6_565		# 1203 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	23.00 Deg.
C37	-C44	-C22	1_555	1_555	6_565		# 1208 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	43.80 Deg.
C2	-C44	-C18	6_565	1_555	6_565		# 1214 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	43.10 Deg.
C22	-C44	-C18	6_565	1_555	6_565		# 1218 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	31.30 Deg.
C34	-C45	-C49	6_565	1_555	1_555		# 1232 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	40.00 Deg.
C21	-C45	-C13	6_565	1_555	6_565		# 1234 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	24.90 Deg.
C39	-C45	-C38	1_555	1_555	6_565		# 1242 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	40.30 Deg.
C20	-C46	-C45	6_565	1_555	1_555		# 1251 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	31.90 Deg.
C41	-C46	-C18	1_555	1_555	6_565		# 1255 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	14.00 Deg.
C22	-C46	-C37	6_565	1_555	1_555		# 1257 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	25.00 Deg.
C45	-C46	-C21	1_555	1_555	6_565		# 1265 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	13.50 Deg.
C41 -C46 -C16	1_555 1_555 6_565		# 1277 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.90 Deg.
C18 -C46 -C16	6_565 1_555 6_565		# 1279 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	41.70 Deg.
C13 -C46 -C16	6_565 1_555 6_565		# 1282 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.60 Deg.
C30 -C47 -C49	6_565 1_555 1_555		# 1303 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	37.70 Deg.
C13 -C47 -C21	6_565 1_555 6_565		# 1305 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	37.70 Deg.
C49 -C47 -C21	1_555 1_555 6_565		# 1310 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	13.40 Deg.
C31 -C48 -C52	6_565 1_555 1_555		# 1317 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	28.00 Deg.
C30 -C48 -C49	6_565 1_555 1_555		# 1322 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	28.40 Deg.
C49 -C48 -C34	1_555 1_555 6_565		# 1331 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.70 Deg.
C47 -C49 -C26	1_555 1_555 6_565		# 1341 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	25.00 Deg.
C21 -C49 -C45	6_565 1_555 1_555		# 1344 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	28.00 Deg.
C30 -C49 -C48	6_565 1_555 1_555		# 1348 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.60 Deg.
C47 -C49 -C13	1_555 1_555 6_565		# 1356 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	27.40 Deg.
C52 -C50 -C31	6_565 1_555 1_555		# 1366 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	27.40 Deg.
C52 -C50 -C31	1_555 1_555 6_565		# 1371 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.90 Deg.
C47 -C51 -C26	1_555 1_555 6_565		# 1384 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.90 Deg.
C51 -C51 -C27	6_565 1_555 1_555		# 1385 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	41.30 Deg.
C30 -C51 -C31	6_565 1_555 6_565		# 1402 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.00 Deg.
C31 -C52 -C48	6_565 1_555 1_555		# 1406 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	30.50 Deg.
C58 -C52 -C58	1_555 1_555 6_565		# 1420 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	6.00 Deg.
C31 -C52 -C30	6_565 1_555 6_565		# 1424 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	21.00 Deg.
C48 -C52 -C30	1_555 1_555 6_565		# 1427 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	11.60 Deg.
C58 -C52 -C57	1_555 1_555 6_565		# 1433 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.00 Deg.
C58 -C52 -C57	6_565 1_555 6_565		# 1437 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	28.00 Deg.
C57 -C53 -C58	6_565 1_555 1_555		# 1450 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	36.40 Deg.
C35 -C53 -C54	6_565 1_555 1_555		# 1456 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.40 Deg.
C56 -C53 -C6	6_565 1_555 1_555		# 1463 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	38.30 Deg.
C61 -C53 -C6	6_565 1_555 1_555		# 1464 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	20.00 Deg.

C33	-C54	-C55	6_565	1_555	1_555		# 1475 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	43.70 Deg.
C32	-C54	-C53	6_565	1_555	1_555		# 1478 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	22.40 Deg.
C48	-C54	-C31	1_555	1_555	6_565		# 1491 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	22.00 Deg.
C48	-C54	-C30	1_555	1_555	6_565		# 1498 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	42.60 Deg.
C34	-C54	-C30	6_565	1_555	6_565		# 1501 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	41.10 Deg.
C31	-C54	-C30	6_565	1_555	6_565		# 1502 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	34.40 Deg.
C54	-C55	-C35	1_555	1_555	6_565		# 1511 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	35.00 Deg.
C33	-C55	-C34	6_565	1_555	6_565		# 1518 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	44.00 Deg.
C36	-C55	-C38	6_565	1_555	6_565		# 1525 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	25.30 Deg.
C39	-C55	-C38	1_555	1_555	6_565		# 1529 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	38.00 Deg.
C6	-C56	-C61	6_565	1_555	1_555		# 1537 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	42.10 Deg.
C25	-C56	-C56	1_555	1_555	6_565		# 1543 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	13.00 Deg.
C57	-C56	-C58	1_555	1_555	6_565		# 1549 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	41.00 Deg.
C58	-C57	-C58	6_565	1_555	1_555		# 1555 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	44.40 Deg.
C53	-C57	-C32	6_565	1_555	1_555		# 1559 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	27.40 Deg.
C58	-C57	-C57	1_555	1_555	6_565		# 1565 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	16.40 Deg.
C56	-C57	-C6	1_555	1_555	6_565		# 1569 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	24.00 Deg.
C58	-C57	-C52	6_565	1_555	6_565		# 1573 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	27.40 Deg.
C58	-C58	-C57	6_565	1_555	1_555		# 1587 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	42.40 Deg.
C32	-C58	-C53	6_565	1_555	1_555		# 1592 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	16.80 Deg.
C52	-C58	-C31	1_555	1_555	6_565		# 1598 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	27.00 Deg.
C57	-C58	-C56	6_565	1_555	6_565		# 1608 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	41.40 Deg.
C53	-C58	-C56	1_555	1_555	6_565		# 1613 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	27.90 Deg.
C6	-C61	-C56	6_565	1_555	1_555		# 1619 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	26.30 Deg.
C60	-C61	-C69	1_555	1_555	6_565		# 1627 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	28.00 Deg.
C59	-C62	-C70	6_565	1_555	1_555		# 1640 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	28.10 Deg.
C59	-C62	-C70	1_555	1_555	6_565		# 1644 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	37.00 Deg.
C68	-C63	-C65	6_565	1_555	1_555		# 1647 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	11.50 Deg.
C74	-C63	-C12	1_555	1_555	6_565		# 1661 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.90 Deg.
C75 -C63 -C14	1_555 1_555 6_565		# 1665 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.00 Deg.
C71 -C64 -C72	6_565 1_555 1_555		# 1669 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.00 Deg.
C70 -C64 -C59	6_565 1_555 1_555		# 1672 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	28.90 Deg.
C65 -C64 -C68	1_555 1_555 6_565		# 1682 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	12.10 Deg.
C72 -C64 -C72	1_555 1_555 6_565		# 1685 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	36.20 Deg.
C59 -C64 -C69	1_555 1_555 6_565		# 1692 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	32.00 Deg.
C68 -C65 -C63	6_565 1_555 1_555		# 1697 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	26.20 Deg.
C64 -C65 -C71	1_555 1_555 6_565		# 1710 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.60 Deg.
C76 -C65 -C66	1_555 1_555 6_565		# 1714 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	20.70 Deg.
C64 -C65 -C70	1_555 1_555 6_565		# 1721 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	25.10 Deg.
C60 -C76 -C69	1_555 1_555 6_565		# 1738 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	27.20 Deg.
C66 -C60 -C76	6_565 1_555 1_555		# 1747 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	36.10 Deg.
C61 -C60 -C6	1_555 1_555 6_565		# 1750 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.30 Deg.
C59 -C60 -C70	1_555 1_555 6_565		# 1757 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	19.00 Deg.
C70 -C59 -C64	6_565 1_555 1_555		# 1763 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	26.70 Deg.
C69 -C59 -C60	6_565 1_555 1_555		# 1767 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	26.60 Deg.
C60 -C66 -C69	6_565 1_555 1_555		# 1775 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.70 Deg.
C36 -C66 -C55	6_565 1_555 1_555		# 1777 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	38.00 Deg.
C76 -C66 -C65	6_565 1_555 6_565		# 1791 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	33.00 Deg.
C67 -C66 -C65	1_555 1_555 6_565		# 1796 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.30 Deg.
C36 -C66 -C33	6_565 1_555 6_565		# 1799 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	4.00 Deg.
C55 -C66 -C33	1_555 1_555 6_565		# 1802 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.00 Deg.
C65 -C67 -C68	6_565 1_555 1_555		# 1809 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.60 Deg.
C63 -C67 -C68	6_565 1_555 1_555		# 1811 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	25.00 Deg.
C76 -C67 -C66	6_565 1_555 1_555		# 1817 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	31.50 Deg.
C14 -C67 -C75	1_555 1_555 6_565		# 1825 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	40.50 Deg.
C66 -C67 -C36	1_555 1_555 6_565		# 1832 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	20.10 Deg.
C14 -C67 -C38	1_555 1_555 6_565		# 1838 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	9.10 Deg.

C74	-C68	-C12	6_565	1_555	1_555		# 1856 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	21.80 Deg.
C71	-C68	-C64	1_555	1_555	6_565		# 1859 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	29.00 Deg.
C63	-C68	-C75	6_565	1_555	6_565		# 1863 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	38.80 Deg.
C6	-C69	-C61	1_555	1_555	6_565		# 1878 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	26.00 Deg.
C59	-C69	-C70	6_565	1_555	1_555		# 1881 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	26.00 Deg.
C66	-C69	-C76	1_555	1_555	6_565		# 1888 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	21.90 Deg.
C70	-C69	-C64	1_555	1_555	6_565		# 1896 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	9.00 Deg.
C64	-C70	-C71	6_565	1_555	1_555		# 1900 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	40.00 Deg.
C59	-C70	-C60	6_565	1_555	6_565		# 1908 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	18.00 Deg.
C69	-C70	-C60	1_555	1_555	6_565		# 1912 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	41.00 Deg.
C64	-C70	-C72	6_565	1_555	6_565		# 1914 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	32.60 Deg.
C71	-C70	-C72	1_555	1_555	6_565		# 1915 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	39.00 Deg.
C64	-C70	-C65	6_565	1_555	6_565		# 1920 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	11.00 Deg.
C64	-C71	-C70	6_565	1_555	1_555		# 1927 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	33.00 Deg.
C68	-C71	-C65	1_555	1_555	6_565		# 1935 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	6.60 Deg.
C72	-C71	-C72	6_565	1_555	1_555		# 1937 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	25.70 Deg.
C71	-C72	-C64	6_565	1_555	1_555		# 1951 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	12.70 Deg.
C72	-C72	-C71	6_565	1_555	1_555		# 1953 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	41.60 Deg.
C73	-C72	-C73	1_555	1_555	6_565		# 1959 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	32.80 Deg.
C72	-C72	-C64	6_565	1_555	6_565		# 1962 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	20.20 Deg.
C71	-C72	-C64	1_555	1_555	6_565		# 1966 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	21.50 Deg.
C64	-C72	-C70	1_555	1_555	6_565		# 1971 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	11.10 Deg.
C74	-C73	-C12	1_555	1_555	6_565		# 1984 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	19.50 Deg.
C72	-C73	-C72	1_555	1_555	6_565		# 1987 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	36.40 Deg.
C11	-C73	-C11	6_565	1_555	1_555		# 1991 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	34.10 Deg.
C72	-C73	-C71	1_555	1_555	6_565		# 1998 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	26.00 Deg.
C12	-C74	-C9	6_565	1_555	1_555		# 2004 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	29.10 Deg.
C63	-C74	-C68	1_555	1_555	6_565		# 2010 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	32.00 Deg.
C12	-C74	-C15	6_565	1_555	6_565		# 2018 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	19.80 Deg.
C9 -C74 -C15	1_555 1_555 6_565	# 2020 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	29.90 Deg.
C19 -C75 -C8	6_565 1_555 1_555	# 2026 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	11.00 Deg.
C14 -C75 -C38	6_565 1_555 1_555	# 2030 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	25.80 Deg.
C8 -C75 -C15	1_555 1_555 6_565	# 2041 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	14.70 Deg.
C63 -C75 -C68	1_555 1_555 6_565	# 2048 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	44.00 Deg.
C4 -C77 -C4	6_565 1_555 1_555	# 2057 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	43.80 Deg.
C5 -C77 -C78	1_555 1_555 6_565	# 2059 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	43.80 Deg.
C5 -C77 -C78	6_565 1_555 1_555	# 2062 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	44.20 Deg.
C5 -C78 -C28	6_565 1_555 1_555	# 2071 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	16.70 Deg.
C3 -C78 -C44	1_555 1_555 6_565	# 2079 Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	12 Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	! Info
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers	1 Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	5109 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3 Note
1 1 0, 2 0 0, 0 0 1,		
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	761 Note
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	6 Units
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	3 Units
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	2 Units
PLAT956_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Hmax Differ	6 Units
PLAT957_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Kmax Differ	3 Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.	2 Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	5 Info
PLAT984_ALERT_1_G	The Ni-f' = 0.3453 Deviates from the B&C-Value	0.3428 Check
PLAT985_ALERT_1_G	The Ni-f" = 1.0604 Deviates from the B&C-Value	1.0569 Check

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

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

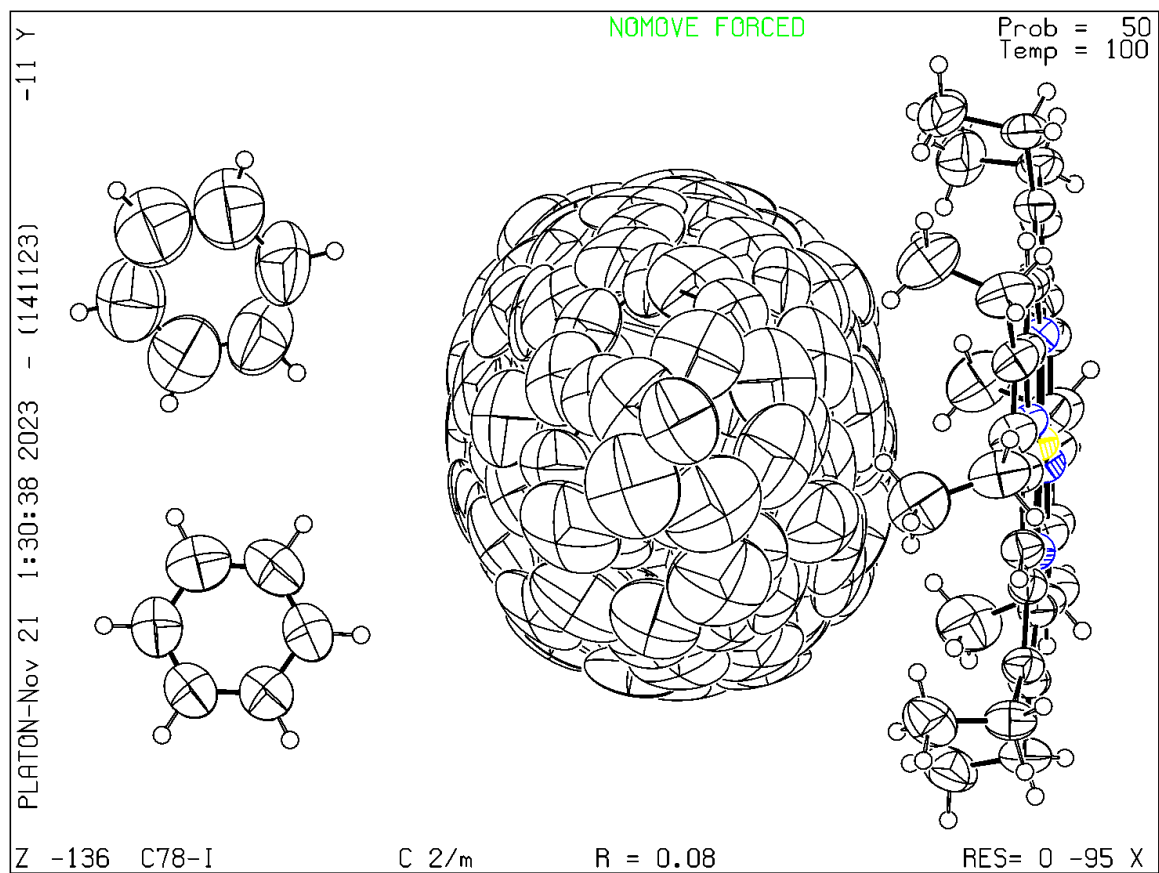
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C78-II

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: C78-II

Bond precision: C-C = 0.0073 Å Wavelength=0.68889

Cell: a=25.412 (4) b=15.089 (3) c=19.729 (4)
 alpha=90 beta=93.213 (4) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	7553 (2)	7553 (2)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	C78, C36 H44 N4 Ni, C6 H6, 2 (C3 H3)	C78 C36 H44 N4 Ni C6 H6 2 (C3 H3)
Sum formula	C126 H56 N4 Ni	C126 H56 N4 Ni
Mr	1684.44	1684.45
Dx, g cm ⁻³	1.481	1.481
Z	4	4
Mu (mm ⁻¹)	0.298	0.298
F000	3472.0	3472.0
F000'	3474.35	
h, k, lmax		30, 17, 22
Nref		6408
Tmin, Tmax	0.976, 0.982	0.520, 0.745
Tmin'	0.976	

Correction method= # Reported T Limits: Tmin=0.520 Tmax=0.745
AbsCorr = ?

Data completeness= Theta(max)= 24.550

R(reflections)= 0.0950 (5509)

wR2(reflections)=
0.2832 (6408)

S = 1.045

Npar= 957

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 _diffn_measured_fraction_theta_full value Low . 0.894 Why?

Author Response: Our data were obtained at Shanghai Synchrotron Radiation Facility (SSRF), where the measurement method is psi scans, which may cause some angular diffraction points to be lost.

Alert level B

PLAT088_ALERT_3_B Poor Data / Parameter Ratio 6.70 Note
PLAT215_ALERT_3_B Disordered C29 has ADP max/min Ratio 4.2 Note
PLAT215_ALERT_3_B Disordered C49 has ADP max/min Ratio 4.1 Note
PLAT215_ALERT_3_B Disordered C50 has ADP max/min Ratio 4.4 Note
PLAT215_ALERT_3_B Disordered C64 has ADP max/min Ratio 4.3 Note
PLAT234_ALERT_4_B Large Hirshfeld Difference C2 --C65 . 0.26 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference C15 --C32 . 0.30 Ang.
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C15 Check
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 717 Report

0	8	0,	0	16	0,	1	17	0,	14	16	0,	16	4	0,	17	15	0,
18	14	0,	19	7	0,	19	13	0,	20	12	0,	21	11	0,	21	13	0,
22	12	0,	23	11	0,	24	10	0,	25	9	0,	26	0	0,	26	8	0,
27	7	0,	28	6	0,	29	5	0,	-29	5	1,	-28	6	1,	-27	7	1,
-26	8	1,	-25	9	1,	-24	10	1,	-23	11	1,	-22	12	1,	-21	11	1,
-21	13	1,	-20	12	1,	-19	13	1,	-18	14	1,	-17	15	1,	-14	12	1,
-14	16	1,	-11	7	1,	-6	6	1,	-1	17	1,	0	8	1,	0	16	1,
1	17	1,	2	2	1,	2	6	1,	14	16	1,	18	14	1,	19	13	1,
20	12	1,	21	11	1,	21	13	1,	22	10	1,	22	12	1,	23	3	1,
23	11	1,	24	10	1,	25	9	1,	26	0	1,	26	8	1,	27	7	1,
28	6	1,	29	5	1,	-29	5	2,	-28	6	2,	-27	7	2,	-26	8	2,
-25	9	2,	-24	10	2,	-23	11	2,	-22	10	2,	-22	12	2,	-21	11	2,
-21	13	2,	-20	6	2,	-20	12	2,	-19	13	2,	-18	14	2,	-17	15	2,
-16	8	2,	-14	16	2,	-7	11	2,	-1	17	2,	1	17	2,	11	13	2,
18	14	2,	19	13	2,	20	12	2,	21	11	2,	22	10	2,	22	12	2,
23	9	2,	23	11	2,	24	8	2,	24	10	2,	25	9	2,	26	6	2,

Alert level C

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc.: C78, C36 H44 N4 Ni, C6 H6, 2(C3 H3)
Rep.: C78 C36 H44 N4 Ni C6 H6 2(C3 H3)

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.28 Report

PLAT213_ALERT_2_C Atom C76 has ADP max/min Ratio 3.1 oblate

PLAT215_ALERT_3_C Disordered C3 has ADP max/min Ratio 3.5 Note

PLAT215_ALERT_3_C Disordered C9 has ADP max/min Ratio 3.2 Note

PLAT215_ALERT_3_C Disordered C30 has ADP max/min Ratio 3.5 Note

PLAT215_ALERT_3_C Disordered C33 has ADP max/min Ratio 3.1 Note

PLAT215_ALERT_3_C Disordered C35 has ADP max/min Ratio 3.2 Note

[illegible]

[illegible]

PLAT300_ALERT_4_G	Atom Site Occupancy of H2B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6B	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		92%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)		100%	Note
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		10	Note
	H1DA H1DB H1DC H2DA H2DB H8DA H8DB H9DA			
	H9DB H9DC			
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .		3.20	Ratio
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C4	--C13	1.76	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C4	--C8	2.04	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C5	--C8	1.81	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C5	--C19	1.87	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C17	--C77	1.79	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C10	--C51	1.81	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C10	--C19	1.91	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C21	--C12	1.72	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C21	--C1	1.96	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C21	--C50	1.98	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C21	--C53	2.03	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C20	--C62	1.83	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C19	--C5	1.87	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C19	--C10	1.91	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C1	--C21	1.96	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C1	--C31	1.97	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C7	--C3	1.80	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C7	--C7	1.94	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C8	--C5	1.81	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C8	--C4	2.04	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C3	--C75	1.72	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C3	--C9	1.75	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C3	--C7	1.80	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C3	--C6	1.92	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C6	--C3	1.92	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C23	--C18	1.79	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C9	--C3	1.75	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C9	--C70	1.95	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C11	--C73	1.78	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C11	--C69	1.94	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C12	--C21	1.72	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C12	--C70	1.90	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C12	--C67	2.05	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C13	--C73	1.73	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C13	--C4	1.76	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C13	--C67	1.98	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C18	--C31	1.72	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C18	--C23	1.79	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C24	--C25	1.73	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C24	--C25	1.99	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C25	--C24	1.99	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C26	--C33	1.78	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C26	--C34	1.84	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C28	--C78	1.83	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C28	--C51	1.91	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C28	--C45	1.97	Ang.

PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C29	--C45	1.88 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C30	--C33	1.80 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C30	--C36	1.92 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C31	--C18	1.72 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C31	--C1	1.97 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C33	--C30	1.80 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C33	--C26	1.78 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C34	--C26	1.84 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C35	--C59	1.90 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C35	--C55	1.99 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C36	--C30	1.92 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C36	--C37	1.88 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C37	--C59	1.83 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C37	--C36	1.88 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C38	--C56	1.85 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C39	--C55	1.71 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C40	--C45	1.74 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C40	--C47	1.97 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C41	--C51	1.88 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C42	--C55	1.80 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C42	--C46	2.04 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C45	--C40	1.74 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C45	--C29	1.88 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C45	--C28	1.97 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C46	--C42	2.04 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C47	--C40	1.97 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C50	--C21	1.98 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C51	--C67	1.74 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C51	--C10	1.81 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C51	--C41	1.88 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C51	--C28	1.91 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C52	--C66	1.93 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C53	--C69	1.80 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C53	--C21	2.02 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C55	--C39	1.71 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C55	--C58	1.91 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C55	--C42	1.80 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C55	--C35	1.99 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C56	--C38	1.85 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C56	--C58	1.88 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C58	--C55	1.91 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C58	--C56	1.88 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C59	--C37	1.83 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C59	--C35	1.90 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C62	--C69	1.76 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C62	--C68	1.75 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C62	--C64	1.79 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C62	--C20	1.83 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C63	--C71	2.01 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C64	--C62	1.79 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C66	--C72	1.84 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C66	--C52	1.93 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C67	--C51	1.74 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C67	--C13	1.98 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C67	--C12	2.05 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C68	--C62	1.75 Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF: C69	--C62	1.76 Ang.

PLAT773_ALERT_2_G	Check	long	C-C Bond	in	CIF: C69	--C53	1.80 Ang.
PLAT773_ALERT_2_G	Check	long	C-C Bond	in	CIF: C69	--C72	1.81 Ang.
PLAT773_ALERT_2_G	Check	long	C-C Bond	in	CIF: C69	--C11	1.94 Ang.
PLAT773_ALERT_2_G	Check	long	C-C Bond	in	CIF: C70	--C12	1.90 Ang.
PLAT773_ALERT_2_G	Check	long	C-C Bond	in	CIF: C70	--C9	1.95 Ang.
PLAT773_ALERT_2_G	Check	long	C-C Bond	in	CIF: C71	--C72	1.91 Ang.
PLAT773_ALERT_2_G	Check	long	C-C Bond	in	CIF: C71	--C63	2.01 Ang.
PLAT773_ALERT_2_G	Check	long	C-C Bond	in	CIF: C72	--C69	1.81 Ang.
PLAT773_ALERT_2_G	Check	long	C-C Bond	in	CIF: C72	--C66	1.84 Ang.
PLAT773_ALERT_2_G	Check	long	C-C Bond	in	CIF: C72	--C71	1.91 Ang.
PLAT773_ALERT_2_G	Check	long	C-C Bond	in	CIF: C73	--C13	1.73 Ang.
PLAT773_ALERT_2_G	Check	long	C-C Bond	in	CIF: C73	--C11	1.78 Ang.
PLAT773_ALERT_2_G	Check	long	C-C Bond	in	CIF: C75	--C3	1.72 Ang.
PLAT773_ALERT_2_G	Check	long	C-C Bond	in	CIF: C77	--C17	1.79 Ang.
PLAT773_ALERT_2_G	Check	long	C-C Bond	in	CIF: C78	--C28	1.83 Ang.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		32.90 Deg.
	C12	-C4	-C5	6_565	1_555 1_555	 #	14 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		24.70 Deg.
	C70	-C4	-C13	1_555	1_555 6_565	 #	18 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		14.00 Deg.
	C9	-C4	-C8	6_565	1_555 6_565	 #	22 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		23.70 Deg.
	C10	-C5	-C1	1_555	1_555 6_565	 #	34 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		25.60 Deg.
	C9	-C5	-C4	6_565	1_555 1_555	 #	40 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		31.40 Deg.
	C6	-C5	-C8	1_555	1_555 6_565	 #	48 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		25.50 Deg.
	C47	-C17	-C28	6_565	1_555 1_555	 #	65 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		23.30 Deg.
	C1	-C17	-C10	6_565	1_555 1_555	 #	68 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		4.90 Deg.
	C31	-C17	-C77	1_555	1_555 6_565	 #	88 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		34.80 Deg.
	C12	-C10	-C5	6_565	1_555 1_555	 #	100 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		30.40 Deg.
	C21	-C10	-C54	1_555	1_555 6_565	 #	111 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		17.50 Deg.
	C21	-C10	-C51	1_555	1_555 6_565	 #	117 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		22.00 Deg.
	C1	-C10	-C19	6_565	1_555 6_565	 #	121 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		36.00 Deg.
	C54	-C21	-C67	6_565	1_555 1_555	 #	131 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		15.00 Deg.
	C51	-C21	-C40	6_565	1_555 1_555	 #	132 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		37.90 Deg.
	C10	-C21	-C12	1_555	1_555 6_565	 #	148 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		6.30 Deg.
	C10	-C21	-C1	1_555	1_555 6_565	 #	154 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		44.20 Deg.
	C12	-C21	-C1	6_565	1_555 6_565	 #	156 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		24.00 Deg.
	C51	-C21	-C50	6_565	1_555 6_565	 #	157 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		29.60 Deg.
	C40	-C21	-C50	1_555	1_555 6_565	 #	160 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond) Angle(s)	in CIF ...		27.00 Deg.
	C54	-C21	-C53	6_565	1_555 6_565	 #	166 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	8.80 Deg.
C67 -C21 -C53	1_555 1_555 6_565	 #	167 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	21.00 Deg.
C72 -C20 -C72	6_565 1_555 1_555	 #	182 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	32.90 Deg.
C66 -C20 -C71	1_555 1_555 6_565	 #	187 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.30 Deg.
C66 -C20 -C62	1_555 1_555 6_565	 #	198 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.90 Deg.
C31 -C19 -C77	6_565 1_555 1_555	 #	206 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	25.00 Deg.
C23 -C19 -C7	6_565 1_555 1_555	 #	208 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.40 Deg.
C7 -C19 -C6	1_555 1_555 6_565	 #	216 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.50 Deg.
C1 -C19 -C17	1_555 1_555 6_565	 #	219 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	9.10 Deg.
C1 -C19 -C10	1_555 1_555 6_565	 #	232 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.70 Deg.
C5 -C19 -C10	6_565 1_555 6_565	 #	237 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.60 Deg.
C65 -C2 -C61	6_565 1_555 1_555	 #	247 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.60 Deg.
C65 -C2 -C61	1_555 1_555 6_565	 #	250 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.00 Deg.
C10 -C1 -C12	6_565 1_555 1_555	 #	259 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	33.20 Deg.
C12 -C1 -C5	1_555 1_555 6_565	 #	267 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.00 Deg.
C10 -C1 -C21	6_565 1_555 6_565	 #	268 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.80 Deg.
C17 -C1 -C31	6_565 1_555 6_565	 #	275 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	36.40 Deg.
C19 -C1 -C31	1_555 1_555 6_565	 #	276 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	36.00 Deg.
C23 -C7 -C19	6_565 1_555 1_555	 #	284 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	37.00 Deg.
C6 -C7 -C8	6_565 1_555 1_555	 #	288 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	14.40 Deg.
C8 -C7 -C3	1_555 1_555 6_565	 #	295 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.00 Deg.
C3 -C8 -C3	6_565 1_555 1_555	 #	303 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.00 Deg.
C6 -C8 -C7	6_565 1_555 1_555	 #	309 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	33.00 Deg.
C3 -C8 -C8	6_565 1_555 6_565	 #	312 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.00 Deg.
C3 -C8 -C8	1_555 1_555 6_565	 #	314 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	37.80 Deg.
C9 -C8 -C5	1_555 1_555 6_565	 #	326 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	6.60 Deg.
C9 -C8 -C4	1_555 1_555 6_565	 #	333 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.40 Deg.
C75 -C8 -C4	6_565 1_555 6_565	 #	336 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.40 Deg.
C5 -C8 -C4	6_565 1_555 6_565	 #	337 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.00 Deg.

	C3	-C3	-C8	6_565	1_555	1_555		#	340 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		19.00 Deg.
	C8	-C3	-C6	6_565	1_555	1_555		#	344 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		41.00 Deg.
	C8	-C3	-C7	6_565	1_555	6_565		#	359 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		24.00 Deg.
	C6	-C3	-C7	1_555	1_555	6_565		#	363 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		31.80 Deg.
	C3	-C3	-C6	6_565	1_555	6_565		#	367 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		19.00 Deg.
	C8	-C3	-C6	1_555	1_555	6_565		#	368 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		29.00 Deg.
	C7	-C6	-C23	6_565	1_555	1_555		#	375 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		11.00 Deg.
	C8	-C6	-C3	6_565	1_555	1_555		#	381 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		38.00 Deg.
	C23	-C6	-C19	1_555	1_555	6_565		#	386 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		40.30 Deg.
	C5	-C6	-C9	1_555	1_555	6_565		#	392 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		21.00 Deg.
	C8	-C6	-C3	6_565	1_555	6_565		#	396 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		12.40 Deg.
	C3	-C6	-C3	1_555	1_555	6_565		#	399 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		32.00 Deg.
	C7	-C23	-C6	6_565	1_555	1_555		#	403 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		15.70 Deg.
	C31	-C23	-C77	1_555	1_555	6_565		#	416 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		28.60 Deg.
	C23	-C22	-C7	1_555	1_555	6_565		#	430 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		28.60 Deg.
	C23	-C22	-C7	6_565	1_555	1_555		#	433 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		43.90 Deg.
	C75	-C9	-C11	6_565	1_555	1_555		#	446 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		34.00 Deg.
	C5	-C9	-C12	6_565	1_555	1_555		#	449 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		34.00 Deg.
	C8	-C9	-C6	1_555	1_555	6_565		#	456 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		15.90 Deg.
	C8	-C9	-C3	1_555	1_555	6_565		#	462 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		18.00 Deg.
	C4	-C9	-C70	6_565	1_555	6_565		#	466 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		25.70 Deg.
	C4	-C11	-C9	6_565	1_555	1_555		#	478 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		30.70 Deg.
	C13	-C11	-C70	1_555	1_555	6_565		#	486 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		20.20 Deg.
	C13	-C11	-C69	1_555	1_555	6_565		#	497 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		44.70 Deg.
	C73	-C11	-C69	6_565	1_555	6_565		#	501 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		22.20 Deg.
	C10	-C12	-C1	6_565	1_555	1_555		#	506 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		26.40 Deg.
	C4	-C12	-C9	6_565	1_555	1_555		#	516 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		28.60 Deg.
	C54	-C12	-C21	1_555	1_555	6_565		#	519 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF	...		44.90 Deg.
	C4	-C12	-C70	6_565	1_555	6_565		#	527 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.60 Deg.
C54 -C12 -C67	1_555 1_555 6_565	 #	532 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	41.80 Deg.
C21 -C12 -C67	6_565 1_555 6_565	 #	536 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.40 Deg.
C70 -C12 -C67	6_565 1_555 6_565	 #	537 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	11.00 Deg.
C69 -C13 -C71	6_565 1_555 1_555	 #	540 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.00 Deg.
C70 -C13 -C53	6_565 1_555 1_555	 #	541 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	38.50 Deg.
C11 -C13 -C4	1_555 1_555 6_565	 #	557 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	37.00 Deg.
C70 -C13 -C67	6_565 1_555 6_565	 #	559 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	12.30 Deg.
C53 -C13 -C67	1_555 1_555 6_565	 #	562 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.00 Deg.
C27 -C14 -C16	6_565 1_555 1_555	 #	574 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	41.50 Deg.
C14 -C15 -C14	6_565 1_555 1_555	 #	592 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	38.50 Deg.
C34 -C16 -C29	1_555 1_555 6_565	 #	614 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	40.10 Deg.
C14 -C16 -C26	1_555 1_555 6_565	 #	620 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	11.70 Deg.
C77 -C18 -C31	1_555 1_555 6_565	 #	636 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.00 Deg.
C36 -C24 -C35	6_565 1_555 1_555	 #	645 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	26.00 Deg.
C33 -C24 -C25	6_565 1_555 1_555	 #	655 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	31.00 Deg.
C33 -C24 -C25	6_565 1_555 6_565	 #	666 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	5.80 Deg.
C25 -C24 -C25	1_555 1_555 6_565	 #	670 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.50 Deg.
C25 -C25 -C33	6_565 1_555 1_555	 #	675 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	41.30 Deg.
C26 -C25 -C26	1_555 1_555 6_565	 #	680 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.00 Deg.
C33 -C25 -C24	6_565 1_555 1_555	 #	683 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.00 Deg.
C25 -C25 -C24	6_565 1_555 6_565	 #	687 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.60 Deg.
C33 -C25 -C24	1_555 1_555 6_565	 #	690 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.00 Deg.
C14 -C26 -C14	6_565 1_555 1_555	 #	697 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	12.00 Deg.
C25 -C26 -C25	1_555 1_555 6_565	 #	705 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	13.90 Deg.
C27 -C26 -C16	1_555 1_555 6_565	 #	712 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	38.00 Deg.
C25 -C26 -C33	1_555 1_555 6_565	 #	716 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.30 Deg.
C27 -C26 -C34	1_555 1_555 6_565	 #	725 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.40 Deg.
C33 -C26 -C34	6_565 1_555 6_565	 #	728 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.10 Deg.

C34	-C27	-C29	6_565	1_555	1_555		#	736 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		41.90 Deg.
C14	-C27	-C26	6_565	1_555	1_555		#	747 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		31.60 Deg.
C46	-C28	-C29	6_565	1_555	1_555		#	755 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		37.00 Deg.
C47	-C28	-C78	6_565	1_555	6_565		#	765 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		21.70 Deg.
C40	-C28	-C51	1_555	1_555	6_565		#	775 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		44.10 Deg.
C46	-C28	-C45	6_565	1_555	6_565		#	780 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		25.70 Deg.
C47	-C29	-C28	6_565	1_555	1_555		#	791 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		13.00 Deg.
C27	-C29	-C16	1_555	1_555	6_565		#	805 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		37.00 Deg.
C46	-C29	-C45	6_565	1_555	6_565		#	814 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		34.60 Deg.
C30	-C29	-C45	1_555	1_555	6_565		#	819 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		32.80 Deg.
C45	-C30	-C42	6_565	1_555	1_555		#	826 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		31.10 Deg.
C46	-C30	-C29	6_565	1_555	1_555		#	828 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		40.60 Deg.
C29	-C30	-C34	1_555	1_555	6_565		#	836 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		39.40 Deg.
C42	-C30	-C44	1_555	1_555	6_565		#	840 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		23.40 Deg.
C24	-C30	-C33	1_555	1_555	6_565		#	845 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		21.10 Deg.
C24	-C30	-C36	1_555	1_555	6_565		#	852 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		44.20 Deg.
C33	-C30	-C36	6_565	1_555	6_565		#	857 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		36.00 Deg.
C19	-C31	-C23	6_565	1_555	1_555		#	869 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		41.00 Deg.
C77	-C31	-C18	6_565	1_555	6_565		#	873 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		44.00 Deg.
C19	-C31	-C1	6_565	1_555	6_565		#	880 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		34.10 Deg.
C17	-C31	-C1	1_555	1_555	6_565		#	882 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		15.00 Deg.
C27	-C32	-C16	1_555	1_555	6_565		#	891 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		16.70 Deg.
C77	-C32	-C31	6_565	1_555	1_555		#	902 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		4.90 Deg.
C25	-C33	-C25	6_565	1_555	1_555		#	918 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		27.00 Deg.
C24	-C33	-C36	6_565	1_555	1_555		#	920 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		15.00 Deg.
C27	-C34	-C16	6_565	1_555	1_555		#	939 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		29.80 Deg.
C29	-C34	-C46	6_565	1_555	1_555		#	941 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		27.00 Deg.
C33	-C34	-C24	1_555	1_555	6_565		#	952 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		20.00 Deg.
C36	-C35	-C24	6_565	1_555	1_555		#	966 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.40 Deg.
C44 -C35 -C37	6_565 1_555 1_555	 #	970 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.80 Deg.
C37 -C35 -C55	1_555 1_555 6_565	 #	982 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	26.00 Deg.
C24 -C36 -C33	6_565 1_555 1_555	 #	986 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	39.00 Deg.
C24 -C36 -C30	6_565 1_555 6_565	 #	995 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.00 Deg.
C35 -C36 -C37	6_565 1_555 6_565	 #	999 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	23.50 Deg.
C44 -C36 -C37	1_555 1_555 6_565	 #	1002 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.00 Deg.
C44 -C37 -C42	6_565 1_555 1_555	 #	1009 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	10.00 Deg.
C55 -C37 -C38	6_565 1_555 1_555	 #	1011 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.40 Deg.
C35 -C37 -C36	1_555 1_555 6_565	 #	1022 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	10.00 Deg.
C57 -C38 -C39	6_565 1_555 1_555	 #	1030 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	11.00 Deg.
C55 -C38 -C37	6_565 1_555 1_555	 #	1032 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	39.20 Deg.
C64 -C39 -C56	1_555 1_555 6_565	 #	1049 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	38.00 Deg.
C57 -C39 -C38	6_565 1_555 1_555	 #	1050 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	13.00 Deg.
C43 -C39 -C49	1_555 1_555 6_565	 #	1061 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	30.00 Deg.
C57 -C39 -C55	6_565 1_555 6_565	 #	1062 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	23.40 Deg.
C38 -C39 -C55	1_555 1_555 6_565	 #	1065 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	11.00 Deg.
C51 -C40 -C21	6_565 1_555 1_555	 #	1071 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.70 Deg.
C50 -C40 -C41	6_565 1_555 1_555	 #	1075 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	6.90 Deg.
C28 -C40 -C47	1_555 1_555 6_565	 #	1091 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	32.20 Deg.
C45 -C41 -C42	6_565 1_555 1_555	 #	1100 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	33.00 Deg.
C50 -C41 -C40	6_565 1_555 1_555	 #	1102 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	12.00 Deg.
C43 -C41 -C49	1_555 1_555 6_565	 #	1108 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	22.00 Deg.
C50 -C41 -C51	6_565 1_555 6_565	 #	1111 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	23.10 Deg.
C40 -C41 -C51	1_555 1_555 6_565	 #	1115 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.00 Deg.
C44 -C42 -C37	6_565 1_555 1_555	 #	1121 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.30 Deg.
C41 -C42 -C50	1_555 1_555 6_565	 #	1131 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	23.10 Deg.
C37 -C42 -C55	1_555 1_555 6_565	 #	1135 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	22.00 Deg.
C45 -C42 -C46	6_565 1_555 6_565	 #	1138 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	30.50 Deg.

C30 -C42 -C46	1_555	1_555	6_565		# 1140 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	20.70 Deg.
C41 -C43 -C50	1_555	1_555	6_565		# 1152 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	12.60 Deg.
C39 -C43 -C57	1_555	1_555	6_565		# 1157 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	40.00 Deg.
C49 -C43 -C52	6_565	1_555	6_565		# 1160 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	11.80 Deg.
C68 -C43 -C52	1_555	1_555	6_565		# 1163 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	18.00 Deg.
C37 -C44 -C55	6_565	1_555	1_555		# 1172 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	26.20 Deg.
C35 -C44 -C36	6_565	1_555	1_555		# 1178 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	27.00 Deg.
C42 -C44 -C45	6_565	1_555	1_555		# 1182 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	43.00 Deg.
C30 -C44 -C45	6_565	1_555	1_555		# 1184 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	29.20 Deg.
C36 -C44 -C24	1_555	1_555	6_565		# 1192 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	20.40 Deg.
C41 -C45 -C50	6_565	1_555	1_555		# 1202 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	35.00 Deg.
C42 -C45 -C44	6_565	1_555	1_555		# 1204 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	36.10 Deg.
C50 -C45 -C40	1_555	1_555	6_565		# 1213 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	19.00 Deg.
C46 -C45 -C29	1_555	1_555	6_565		# 1218 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	41.00 Deg.
C46 -C45 -C28	1_555	1_555	6_565		# 1225 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	43.60 Deg.
C40 -C45 -C28	6_565	1_555	6_565		# 1228 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	42.30 Deg.
C29 -C45 -C28	6_565	1_555	6_565		# 1229 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	25.90 Deg.
C28 -C46 -C47	6_565	1_555	1_555		# 1238 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	42.00 Deg.
C29 -C46 -C34	6_565	1_555	1_555		# 1240 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	39.60 Deg.
C30 -C46 -C42	6_565	1_555	6_565		# 1246 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	12.00 Deg.
C45 -C46 -C42	1_555	1_555	6_565		# 1248 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	31.30 Deg.
C29 -C47 -C46	6_565	1_555	1_555		# 1263 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	16.00 Deg.
C28 -C47 -C40	6_565	1_555	6_565		# 1266 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	25.40 Deg.
C28 -C48 -C47	6_565	1_555	1_555		# 1276 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	24.60 Deg.
C10 -C48 -C1	6_565	1_555	1_555		# 1280 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	32.90 Deg.
C51 -C48 -C40	1_555	1_555	6_565		# 1292 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	25.00 Deg.
C51 -C48 -C21	1_555	1_555	6_565		# 1298 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	15.30 Deg.
C68 -C49 -C52	6_565	1_555	1_555		# 1307 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	12.60 Deg.
C39 -C49 -C57	6_565	1_555	1_555		# 1313 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	19.90 Deg.
C50 -C49 -C41	1_555 1_555 6_565		# 1317 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	33.60 Deg.
C40 -C50 -C51	6_565 1_555 1_555		# 1323 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	13.00 Deg.
C49 -C50 -C43	1_555 1_555 6_565		# 1330 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	26.50 Deg.
C45 -C50 -C42	1_555 1_555 6_565		# 1341 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.30 Deg.
C40 -C50 -C21	6_565 1_555 6_565		# 1343 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	10.50 Deg.
C51 -C50 -C21	1_555 1_555 6_565		# 1344 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.00 Deg.
C21 -C51 -C54	6_565 1_555 1_555		# 1350 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.30 Deg.
C54 -C51 -C67	1_555 1_555 6_565		# 1361 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.00 Deg.
C21 -C51 -C10	6_565 1_555 6_565		# 1364 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.10 Deg.
C48 -C51 -C10	1_555 1_555 6_565		# 1367 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.00 Deg.
C40 -C51 -C41	6_565 1_555 6_565		# 1371 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	7.70 Deg.
C50 -C51 -C41	1_555 1_555 6_565		# 1374 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	39.90 Deg.
C40 -C51 -C28	6_565 1_555 6_565		# 1378 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	36.50 Deg.
C48 -C51 -C28	1_555 1_555 6_565		# 1380 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.10 Deg.
C53 -C52 -C67	1_555 1_555 6_565		# 1390 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	27.60 Deg.
C63 -C52 -C62	6_565 1_555 1_555		# 1392 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.00 Deg.
C68 -C52 -C43	6_565 1_555 6_565		# 1400 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	8.20 Deg.
C49 -C52 -C43	1_555 1_555 6_565		# 1405 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	38.50 Deg.
C63 -C52 -C66	6_565 1_555 6_565		# 1407 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	12.70 Deg.
C62 -C52 -C66	1_555 1_555 6_565		# 1410 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.00 Deg.
C67 -C53 -C54	6_565 1_555 1_555		# 1414 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	33.00 Deg.
C70 -C53 -C13	6_565 1_555 1_555		# 1420 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	14.70 Deg.
C52 -C53 -C68	1_555 1_555 6_565		# 1426 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	24.80 Deg.
C13 -C53 -C69	1_555 1_555 6_565		# 1432 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.00 Deg.
C67 -C53 -C21	6_565 1_555 6_565		# 1434 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.40 Deg.
C54 -C53 -C21	1_555 1_555 6_565		# 1436 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	27.00 Deg.
C67 -C54 -C53	6_565 1_555 1_555		# 1443 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	14.00 Deg.
C21 -C54 -C51	6_565 1_555 1_555		# 1447 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	39.80 Deg.

C12	-C54	-C10	1_555	1_555	6_565		# 1454 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	35.90 Deg.
C53	-C54	-C70	1_555	1_555	6_565		# 1458 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	19.00 Deg.
C37	-C55	-C44	6_565	1_555	1_555		# 1466 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	6.00 Deg.
C57	-C55	-C39	1_555	1_555	6_565		# 1474 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	33.00 Deg.
C38	-C55	-C58	6_565	1_555	6_565		# 1477 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	35.80 Deg.
C59	-C55	-C58	1_555	1_555	6_565		# 1481 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	32.40 Deg.
C44	-C55	-C42	1_555	1_555	6_565		# 1486 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	30.00 Deg.
C37	-C55	-C35	6_565	1_555	6_565		# 1491 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	38.60 Deg.
C44	-C55	-C35	1_555	1_555	6_565		# 1493 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	13.00 Deg.
C39	-C56	-C57	6_565	1_555	1_555		# 1503 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	39.40 Deg.
C57	-C56	-C38	1_555	1_555	6_565		# 1516 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	43.60 Deg.
C38	-C56	-C58	6_565	1_555	6_565		# 1525 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	29.00 Deg.
C38	-C57	-C55	6_565	1_555	1_555		# 1528 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	13.00 Deg.
C49	-C57	-C43	1_555	1_555	6_565		# 1540 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	35.80 Deg.
C56	-C57	-C64	1_555	1_555	6_565		# 1544 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	44.00 Deg.
C59	-C58	-C59	6_565	1_555	1_555		# 1554 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	16.00 Deg.
C38	-C58	-C55	1_555	1_555	6_565		# 1560 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	37.00 Deg.
C58	-C59	-C58	6_565	1_555	1_555		# 1572 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	24.90 Deg.
C38	-C59	-C55	6_565	1_555	1_555		# 1582 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	24.30 Deg.
C55	-C59	-C37	1_555	1_555	6_565		# 1588 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	44.00 Deg.
C76	-C59	-C35	1_555	1_555	6_565		# 1591 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	43.70 Deg.
C37	-C59	-C35	6_565	1_555	6_565		# 1595 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	38.00 Deg.
C58	-C60	-C58	1_555	1_555	6_565		# 1596 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	44.70 Deg.
C65	-C60	-C56	6_565	1_555	1_555		# 1605 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	44.70 Deg.
C65	-C60	-C56	1_555	1_555	6_565		# 1608 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	27.00 Deg.
C62	-C61	-C63	1_555	1_555	6_565		# 1616 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	39.80 Deg.
C64	-C61	-C56	6_565	1_555	1_555		# 1621 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	22.60 Deg.
C62	-C61	-C66	1_555	1_555	6_565		# 1628 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	44.50 Deg.
C2	-C61	-C20	1_555	1_555	6_565		# 1636 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	32.00 Deg.
C66 -C62 -C71	6_565 1_555 1_555		# 1640 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.50 Deg.
C71 -C62 -C69	1_555 1_555 6_565		# 1651 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	9.20 Deg.
C52 -C62 -C68	1_555 1_555 6_565		# 1658 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.00 Deg.
C63 -C62 -C64	6_565 1_555 6_565		# 1661 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	36.30 Deg.
C61 -C62 -C64	1_555 1_555 6_565		# 1663 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.00 Deg.
C66 -C62 -C20	6_565 1_555 6_565		# 1667 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.00 Deg.
C62 -C63 -C66	6_565 1_555 1_555		# 1676 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.30 Deg.
C52 -C63 -C68	6_565 1_555 1_555		# 1682 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.40 Deg.
C64 -C63 -C61	1_555 1_555 6_565		# 1688 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	14.00 Deg.
C62 -C63 -C71	6_565 1_555 6_565		# 1690 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.60 Deg.
C66 -C63 -C71	1_555 1_555 6_565		# 1692 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	10.00 Deg.
C39 -C64 -C57	1_555 1_555 6_565		# 1708 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	19.00 Deg.
C63 -C64 -C62	1_555 1_555 6_565		# 1714 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	41.50 Deg.
C56 -C65 -C64	6_565 1_555 1_555		# 1719 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.00 Deg.
C62 -C66 -C63	6_565 1_555 1_555		# 1733 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.00 Deg.
C71 -C66 -C69	6_565 1_555 1_555		# 1739 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	41.80 Deg.
C20 -C66 -C72	1_555 1_555 6_565		# 1750 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.00 Deg.
C62 -C66 -C52	6_565 1_555 6_565		# 1753 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	36.70 Deg.
C63 -C66 -C52	1_555 1_555 6_565		# 1755 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.00 Deg.
C54 -C67 -C21	6_565 1_555 1_555		# 1762 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.40 Deg.
C52 -C67 -C68	6_565 1_555 1_555		# 1769 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	37.00 Deg.
C53 -C67 -C70	6_565 1_555 1_555		# 1770 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	19.50 Deg.
C21 -C67 -C51	1_555 1_555 6_565		# 1777 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	25.00 Deg.
C53 -C67 -C13	6_565 1_555 6_565		# 1781 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	19.20 Deg.
C70 -C67 -C13	1_555 1_555 6_565		# 1786 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	31.00 Deg.
C54 -C67 -C12	6_565 1_555 6_565		# 1789 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	12.00 Deg.
C49 -C68 -C43	6_565 1_555 1_555		# 1803 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	25.90 Deg.
C67 -C68 -C53	1_555 1_555 6_565		# 1809 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	32.00 Deg.

C52	-C68	-C62	6_565	1_555	6_565		# 1811 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	20.40 Deg.
C63	-C68	-C62	1_555	1_555	6_565		# 1813 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	27.00 Deg.
C71	-C69	-C66	6_565	1_555	1_555		# 1818 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	14.00 Deg.
C13	-C69	-C70	6_565	1_555	1_555		# 1824 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	44.00 Deg.
C71	-C69	-C62	6_565	1_555	6_565		# 1827 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	19.40 Deg.
C66	-C69	-C62	1_555	1_555	6_565		# 1829 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	33.00 Deg.
C70	-C69	-C53	1_555	1_555	6_565		# 1836 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	42.00 Deg.
C71	-C69	-C72	6_565	1_555	6_565		# 1838 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	40.60 Deg.
C73	-C69	-C72	1_555	1_555	6_565		# 1841 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	37.00 Deg.
C13	-C69	-C11	6_565	1_555	6_565		# 1846 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	25.30 Deg.
C53	-C70	-C67	6_565	1_555	1_555		# 1857 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	44.50 Deg.
C4	-C70	-C11	1_555	1_555	6_565		# 1861 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	14.00 Deg.
C13	-C70	-C69	6_565	1_555	1_555		# 1863 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	30.80 Deg.
C67	-C70	-C54	1_555	1_555	6_565		# 1871 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	8.50 Deg.
C4	-C70	-C9	1_555	1_555	6_565		# 1883 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	43.90 Deg.
C12	-C70	-C9	6_565	1_555	6_565		# 1888 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	14.00 Deg.
C69	-C71	-C13	6_565	1_555	1_555		# 1890 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	21.00 Deg.
C66	-C71	-C62	6_565	1_555	1_555		# 1893 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	4.40 Deg.
C72	-C71	-C72	1_555	1_555	6_565		# 1914 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	24.00 Deg.
C66	-C71	-C63	6_565	1_555	6_565		# 1918 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	6.60 Deg.
C62	-C71	-C63	1_555	1_555	6_565		# 1920 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	17.30 Deg.
C71	-C72	-C69	1_555	1_555	6_565		# 1943 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	28.70 Deg.
C71	-C72	-C66	1_555	1_555	6_565		# 1949 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	11.90 Deg.
C72	-C72	-C71	6_565	1_555	6_565		# 1953 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	21.00 Deg.
C72	-C73	-C72	6_565	1_555	1_555		# 1963 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	24.90 Deg.
C69	-C73	-C71	1_555	1_555	6_565		# 1975 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	27.00 Deg.
C69	-C73	-C13	1_555	1_555	6_565		# 1980 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	42.10 Deg.
C75	-C74	-C11	6_565	1_555	1_555		# 1996 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	42.10 Deg.
C75	-C74	-C11	1_555	1_555	6_565		# 1999 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	27.10 Deg.
C9 -C75 -C4	6_565 1_555 1_555	# 2008 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	20.70 Deg.
C3 -C75 -C8	1_555 1_555 6_565	# 2023 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	19.00 Deg.
C3 -C75 -C3	1_555 1_555 6_565	# 2029 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	38.50 Deg.
C8 -C75 -C3	6_565 1_555 6_565	# 2031 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	42.00 Deg.
C59 -C76 -C59	1_555 1_555 6_565	# 2037 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	23.40 Deg.
C35 -C76 -C36	6_565 1_555 1_555	# 2039 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	23.40 Deg.
C35 -C76 -C36	1_555 1_555 6_565	# 2042 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	35.40 Deg.
C19 -C77 -C23	1_555 1_555 6_565	# 2060 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	15.00 Deg.
C31 -C77 -C17	6_565 1_555 6_565	# 2062 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	16.00 Deg.
C27 -C78 -C16	6_565 1_555 1_555	# 2073 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	18.30 Deg.
C31 -C78 -C77	6_565 1_555 1_555	# 2079 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	15.30 Deg.
C47 -C78 -C28	1_555 1_555 6_565	# 2100 Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	12 Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	! Info
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers	1 Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	3088 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min). 0 0 1,	1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	54 Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 Info
PLAT984_ALERT_1_G	The Ni-f' = 0.3453 Deviates from the B&C-Value	0.3428 Check
PLAT985_ALERT_1_G	The Ni-f" = 1.0604 Deviates from the B&C-Value	1.0569 Check

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

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

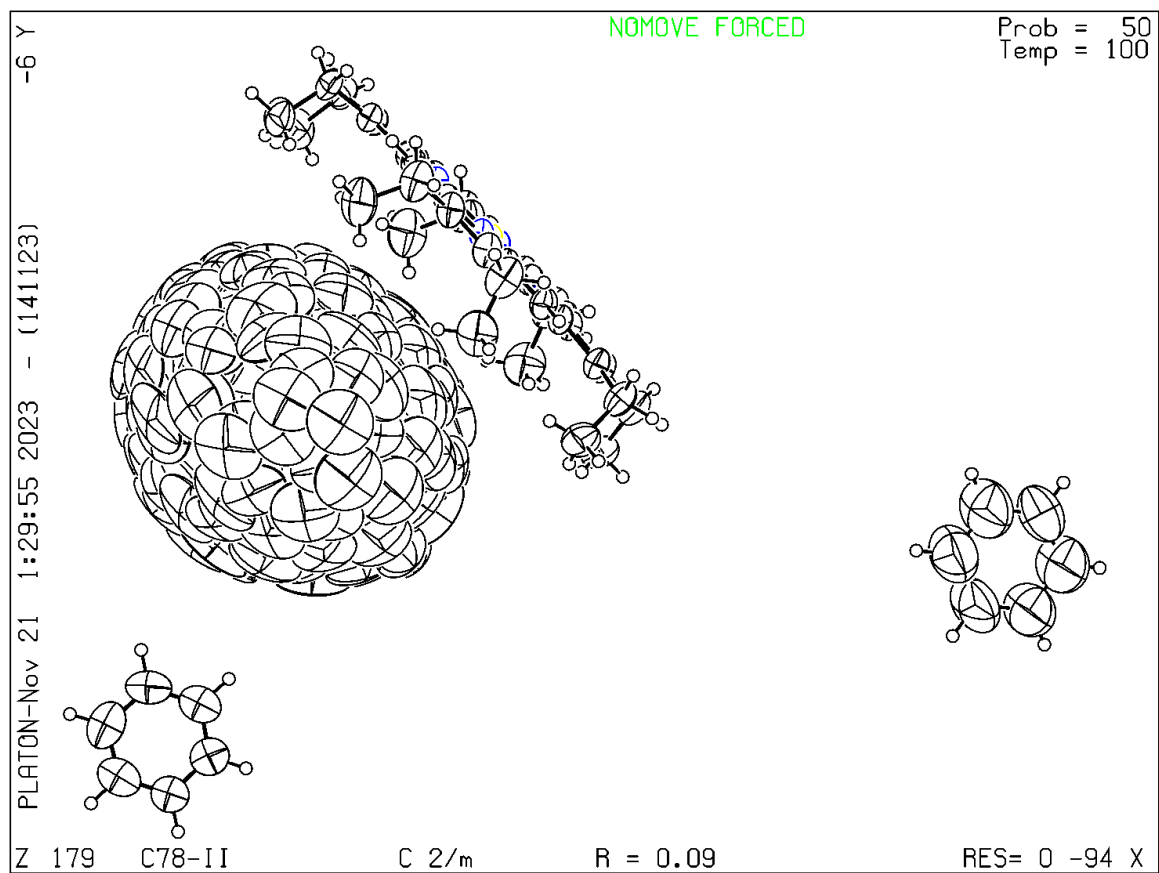
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C3-1

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: C3-1

Bond precision: C-C = 0.0078 Å Wavelength=0.71073

Cell: a=9.276(4) b=17.092(7) c=20.259(8)
 alpha=102.897(12) beta=90.871(12) gamma=105.056(12)
Temperature: 140 K

	Calculated	Reported
Volume	3014(2)	3014(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C59 H56 N15 O3, 2(O) [+ solvent]	C59 H56 N15 O3, 2(O)
Sum formula	C59 H56 N15 O5 [+ solvent]	C59 H56 N15 O5
Mr	1055.19	1055.19
Dx, g cm ⁻³	1.163	1.163
Z	2	2
Mu (mm ⁻¹)	0.078	0.078
F000	1110.0	1110.0
F000'	1110.41	
h, k, lmax		11, 20, 24
Nref		10645
Tmin, Tmax	0.986, 0.992	
Tmin'	0.985	

Correction method= Not given

Data completeness= Theta(max)= 25.027

R(reflections)= 0.0942(5830)	wR2(reflections)=
S = 1.104	0.3390(10613)
Npar= 722	

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 B

PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)		01_2	Check
PLAT306_ALERT_2_B	Isolated Oxygen Atom (H-atoms Missing ?)		02_2	Check



Alert level C

DIFMX02_ALERT_1_C	The maximum difference density is > 0.1*ZMAX*0.75			
	The relevant atom site should be identified.			
RINTA01_ALERT_3_C	The value of Rint is greater than 0.12			
	Rint given	0.152		
PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12		0.152	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)		0.34	Report
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density		0.80	eA-3
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range		3.4	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range		4.1	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C75_1 --C77_1	.	0.17	Ang.
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	01_2	0.136	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	02_2	0.113	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds		0.00784	Ang.
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4			Please Check
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...		-6.432	Report
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).		7	Note
	1 0 0, 0 1 0, 0 -1 1, 0 0 1, 0 1 1,		0 -1 2,	
	0 0 2,			
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595	26	Report
	1 1 0, -1 2 0, 0 2 0, -1 3 0, 0 -2 1,		1 -2 1,	
	-1 -1 1, 1 0 1, -1 1 1, 1 1 1, 0 2 1,		0 -2 2,	
	1 -2 2, 1 -1 2, -1 0 2, 1 0 2, -1 1 2,		0 1 2,	
	1 1 2, 0 2 2, -2 3 2, 0 -2 3, -1 -1 3,		0 0 3,	
	1 0 3, -2 3 3,			
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..		1	Check
	-1 -3 2,			
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.96Ang From 01_2	.	-0.42	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H30C_1	.	-0.32	eA-3



Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		80	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		3	Report
	H20# H32# H47#			
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.012	Degree
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records		1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		1	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		1%	Note
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C75_1	Check	
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C75_1 - C76_1	.	1.53	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C75_1 - C77_1	.	1.55	Ang.
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H29_1 ..H31B_1	.	2.12	Ang.
	x,y,z =		1_555	Check

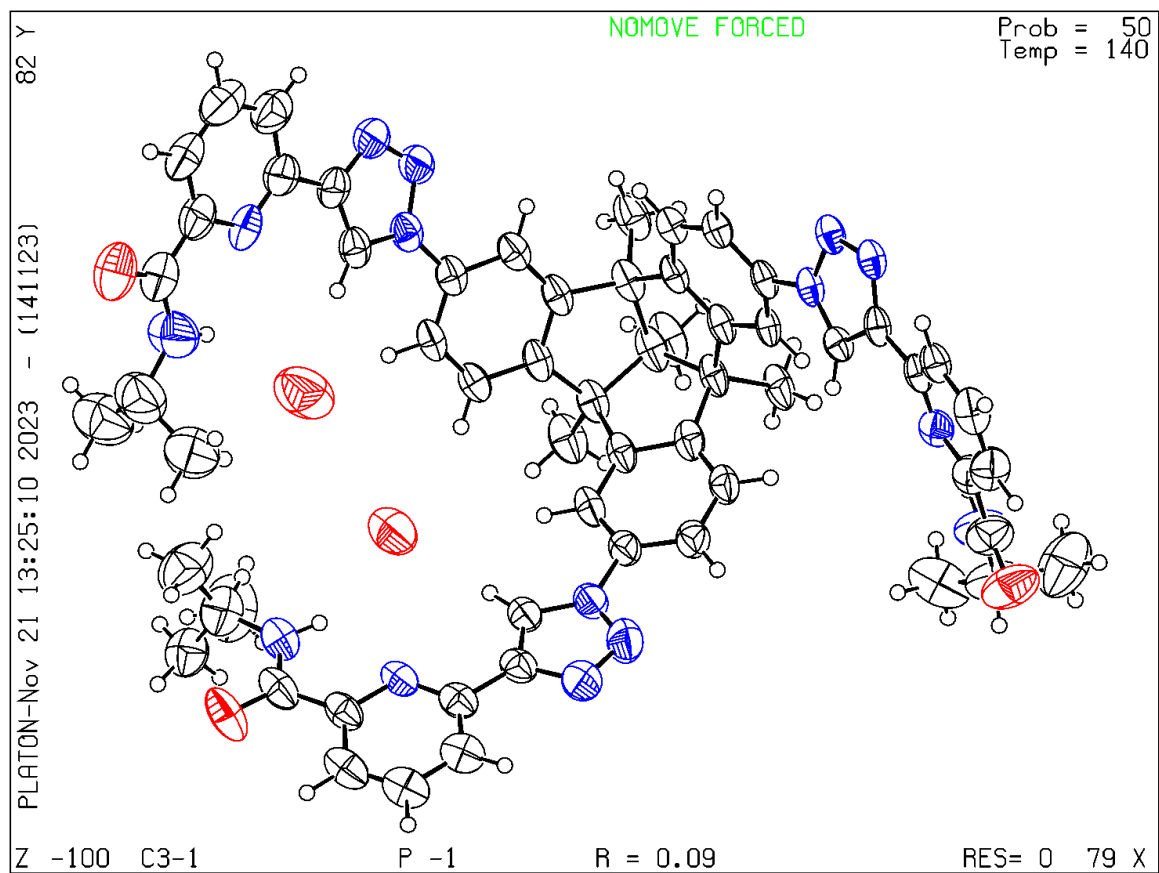
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C3-P-1

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: C3-P-1

Bond precision:	C-C = 0.0210 A	Wavelength=1.34139
Cell:	a=23.5481 (9)	b=23.5481 (9) c=12.9841 (5)
	alpha=90	beta=90 gamma=120
Temperature:	293 K	
	Calculated	Reported
Volume	6235.3 (5)	6235.3 (5)
Space group	R 3	R 3 :H
Hall group	R 3	R 3
Moiety formula	C59 H57 N15 O3, 7 (C H Cl3)	?
Sum formula	C66 H64 Cl21 N15 O3	C198 H192 Cl163 N45 O9
Mr	1859.77	5579.30
Dx, g cm ⁻³	1.486	1.486
Z	3	1
Mu (mm ⁻¹)	4.496	4.496
F000	2838.0	2838.0
F000'	2862.66	
h, k, lmax		26, 26, 14
Nref		4155
Tmin, Tmax	0.298, 0.487	0.415, 1.000
Tmin'	0.206	

Correction method= # Reported T Limits: Tmin=0.415 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= Theta (max)= 49.558

R(reflections)= 0.1572 (2980)	wR2(reflections)=
S = 1.468	0.3883 (4155)
Npar= 316	

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 B

THETM01_ALERT_3_B The value of sine(theta_max)/wavelength is less than 0.575

Calculated sin(theta_max)/wavelength = 0.5674

PLAT082_ALERT_2_B	High R1 Value	0.16	Report
PLAT084_ALERT_3_B	High wR2 Value (i.e. > 0.25)	0.39	Report
PLAT260_ALERT_2_B	Large Average Ueq of Residue Including C12	0.401	Check
PLAT260_ALERT_2_B	Large Average Ueq of Residue Including C114	0.372	Check
PLAT260_ALERT_2_B	Large Average Ueq of Residue Including C115	0.498	Check
PLAT340_ALERT_3_B	Low Bond Precision on C-C Bonds	0.021	Ang.

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.153

PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12	0.153	Report
PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18)	6.64	Note
PLAT234_ALERT_4_C	Large Hirshfeld Difference C8_1 --C9_1 .	0.18	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of N12_1	Check	
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of C11	Check	
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of C20	Check	
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C25_1 - C26_1 .	1.42	Ang.
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4	Please	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	8.758	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.079	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.809	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.268	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.208	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.567	28	Report
	-26 18 1, 2 22 1, 0 23 1, -2 24 1, -18 26 1, -17 26 2,		
	-24 21 3, 3 21 3, 1 22 3, -21 24 3, -3 24 3, -20 24 4,		
	-20 23 5, -12 25 5, -22 20 6, 2 20 6, 0 21 6, -20 22 6,		
	-2 22 6, 4 18 7, -4 22 7, -15 23 7, -4 21 8, -21 12 9,		
	-9 21 9, -19 13 10, -8 5 14, 0 7 14,		

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	10	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	2	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms H14#	1	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	3	Check
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	6	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	2	Report

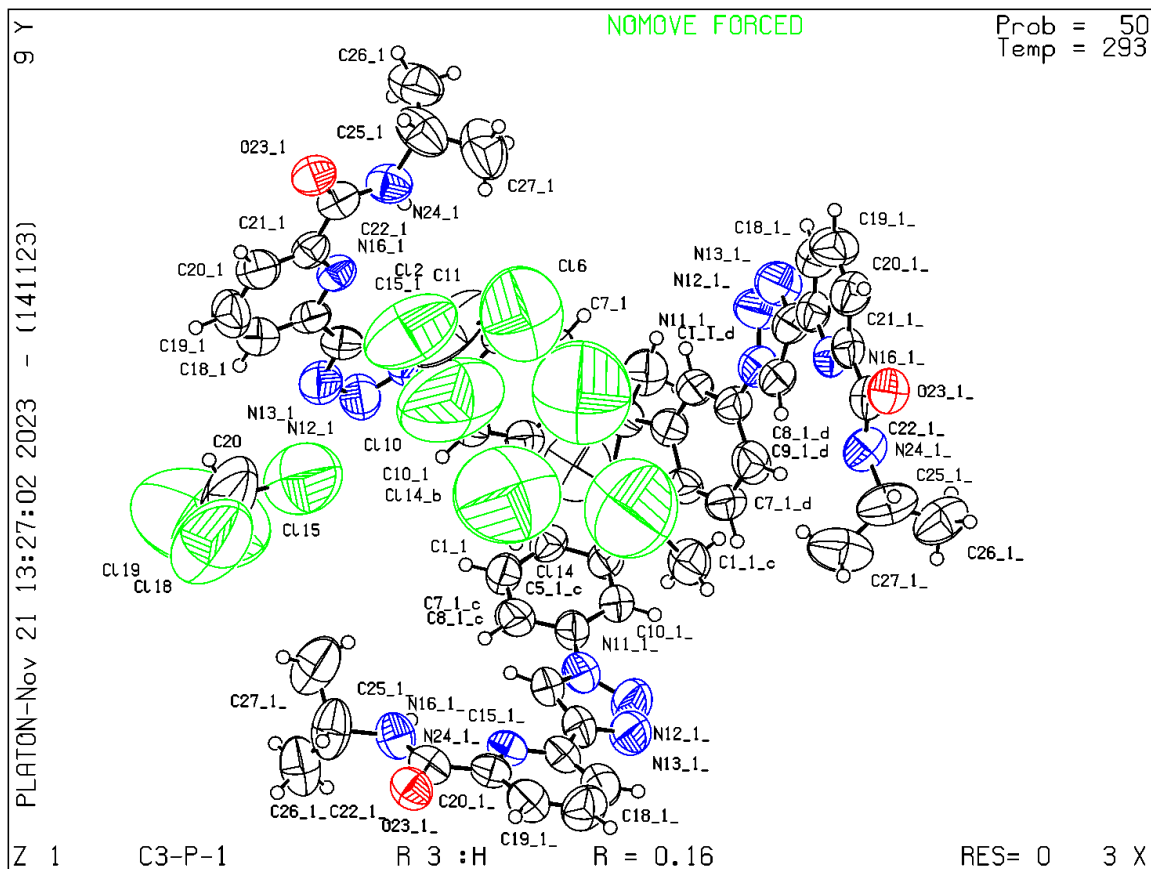
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) T-3

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: T-3

Bond precision:	C-C = 0.0164 Å	Wavelength=0.71073	
Cell:	a=22.156 (2)	b=23.722 (3)	c=80.692 (9)
	alpha=90	beta=90	gamma=90
Temperature:	273 K		
	Calculated	Reported	
Volume	42411 (8)	42411 (8)	
Space group	P c c n	P c c n	
Hall group	-P 2ab 2ac	-P 2ab 2ac	
Moiety formula	C236 H226 La4 N60 O14, 4 (C F3 O3 S) [+ solvent]	C236 H226 La4 N60 O14, 4 (C F3 O3 S)	
Sum formula	C240 H226 F12 La4 N60 O26 S4 [+ solvent]	C240 H226 F12 La4 N60 O26 S4	
Mr	5278.70	5278.70	
Dx, g cm ⁻³	0.827	0.827	
Z	4	4	
Mu (mm ⁻¹)	0.465	0.465	
F000	10776.0	10776.0	
F000'	10777.58		
h, k, lmax		22, 23, 80	
Nref		21539	
Tmin, Tmax	0.823, 0.878		
Tmin'	0.823		

Correction method= Not given

Data completeness= Theta(max)= 20.810

R(reflections)= 0.1056 (10971)

wR2(reflections)=
0.3254 (21539)

S = 0.970

Npar= 1375

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 $\sin(\theta_{\max})/\lambda = 0.4999$

Author Response: The crystals of this giant supramolecular assembly diffract very weakly in nature, possibly due to a large amount of amorphous solvents and highly-disordered counterions existing in the unit cell, which occupy as much as 52.6% of the unit cell based on PLATON calculation.

PLAT910_ALERT_3_A Missing # of FCF Reflection(s) Below $\theta(\text{Min})$. 549 Note

2	0	0,	4	0	0,	6	0	0,	1	1	0,	3	1	0,	5	1	0,
0	2	0,	2	2	0,	4	2	0,	6	2	0,	1	3	0,	3	3	0,
5	3	0,	0	4	0,	2	4	0,	4	4	0,	1	5	0,	3	5	0,
0	6	0,	2	6	0,	1	1	1,	2	1	1,	3	1	1,	4	1	1,

Author Response: The missing FCF reflections below $\theta(\text{Min})$ may be caused by the high beamstop $\theta(\text{min})$ limit set.

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18

Rint given 0.222

PLAT020_ALERT_3_B The Value of Rint is Greater Than 0.12 0.222 Report

PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 7.1 Ratio

PLAT260_ALERT_2_B Large Average Ueq of Residue Including S1_5 0.329 Check

PLAT413_ALERT_2_B Short Inter XH3 .. XHn H31C_2 ..H31C_2 . 1.90 Ang.
3/2-x,-1/2-y,z = 2_645 Check

Alert level C

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low . 0.970 Why?

PLAT082_ALERT_2_C High R1 Value 0.11 Report

PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.33 Report

PLAT220_ALERT_2_C NonSolvent Resd 1 N Ueq(max)/Ueq(min) Range 3.6 Ratio

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 8.5 Ratio

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O27_2 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C11_1 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C46_1 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C69_1 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of La02 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C29_1 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C52_1 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C29_2 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C75_2 Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S1_4 Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S1_5 Check

PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	La01	0.138	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Si_4	0.125	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds		0.0164	Ang.
PLAT412_ALERT_2_C	Short Intra XH3 .. XHn	H1A_1 ..H7AC_1	1.84	Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_C	Short Intra XH3 .. XHn	H29_1 ..H30B_1	1.86	Ang.
		x,y,z =	1_555	Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N28_1 --H28_1		Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N51_1 --H51_1		Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N28_2 --H28_2		Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N74_2 --H74_2		Please Check
PLAT430_ALERT_2_C	Short Inter D...A Contact	O1_3 ..O4_4	2.88	Ang.
		x,y,z =	1_555	Check
PLAT430_ALERT_2_C	Short Inter D...A Contact	O1_3 ..O4_5	2.89	Ang.
		1-x,1/2+y,3/2-z =	3_656	Check
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4			Please Check
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...		-3.580	Report
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & Sth/L=	0.500	126	Report
	22 0 0, 7 1 0, 6 6 0, 1 7 0, 5 7 0, 0 8 0,			
	6 6 1, 1 7 1, 1 8 1, 7 0 2, 22 0 2, 0 7 2,			
	1 7 2, 2 7 2, 0 8 2, 1 8 2, 0 9 2, 1 7 3,			
	2 7 3, 7 0 4, 22 0 4, 0 7 4, 1 7 4, 2 7 4,			
	0 8 4, 0 9 4, 6 2 5, 3 6 5, 1 7 5, 2 7 5,			
	7 0 6, 8 0 6, 22 0 6, 0 7 6, 1 7 6, 2 7 6,			
	0 8 6, 1 7 7, 9 9 7, 16 15 7, 7 0 8, 8 0 8,			
	22 0 8, 6 1 8, 0 7 8, 1 7 8, 0 8 8, 11 11 8,			
	15 16 8, 2 6 9, 1 7 9, 15 16 9, 6 0 10, 7 0 10,			
	8 0 10, 6 1 10, 7 1 10, 2 6 10, 0 7 10, 1 7 10,			
	0 8 10, 15 16 10, 6 1 11, 7 1 11, 5 3 11, 1 6 11,			
	2 6 11, 1 7 11, 6 0 12, 7 0 12, 6 1 12, 3 5 12,			
	0 6 12, 1 6 12, 0 7 12, 6 1 13, 1 6 13, 6 0 14,			
	7 0 14, 6 1 14, 0 6 14, 1 6 14, 0 7 14, 5 1 15,			
	5 2 15, 2 5 15, 1 6 15, 5 0 16, 6 0 16, 5 1 16,			
	1 5 16, 0 6 16, 5 1 17, 1 5 17, 5 0 18, 4 1 18,			
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF		33	Note
	2 0 0, 1 1 0, 0 2 0, 5 3 0, 1 1 1, 2 1 1,			
	4 1 1, 1 2 1, 0 0 2, 1 2 2, 1 1 3, 1 2 3,			
	0 0 4, 1 0 4, 2 0 4, 0 0 6, 0 0 8, 2 0 8,			
	5 0 8, 0 2 8, 0 4 8, 1 1 9, 4 1 9, 2 4 9,			
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.18Ang From La01	-1.57	eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on	La01	1.11	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H1AB_1		-0.41	eA-3

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	170	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	170	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	6	Report
	H20# H35# H50# H77# H92# H107#		
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as	mixed	Check
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	22	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	2	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	5	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	273	Check

PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 273 Check
 PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C5_4 Check
 PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C5_5 Check
 PLAT432_ALERT_2_G Short Inter X...Y Contact C31_2 ..C31_2 . 2.82 Ang.
 3/2-x, -1/2-y, z = 2_645 Check
 PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info
 PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 286 Note

La01	La02	C1_1	H1A_1	H1AB_1	H1AC_1	C2_1	C3_1
C4_1	C5_1	C6_1	H6A_1	H6AB_1	H6AC_1	C7_1	H7A_1
H7AB_1	H7AC_1	C8_1	H8A_1	H8AB_1	H8AC_1	C9_1	C10_1
H10_1	C11_1	H11_1	C12_1	C13_1	H13_1	C14_1	N15_1
N16_1	N17_1	C18_1	C19_1	H19_1	N20_1	C21_1	C22_1
H22_1	C23_1	H23_1	C24_1	H24_1	C25_1	C26_1	O27_1
N28_1	H28_1	C29_1	H29_1	C30_1	H30A_1	H30B_1	H30C_1
C31_1	H31A_1	H31B_1	H31C_1	C32_1	C33_1	H33_1	C34_1
H34_1	C35_1	C36_1	H36_1	C37_1	N38_1	N39_1	N40_1
C41_1	C42_1	H42_1	N43_1	C44_1	C45_1	H45_1	C46_1
H46_1	C47_1	H47_1	C48_1	C49_1	O50_1	N51_1	H51_1
C52_1	H52_1	C53_1	H53A_1	H53B_1	H53C_1	C54_1	H54A_1
H54B_1	H54C_1	C55_1	C56_1	H56_1	C57_1	H57_1	C58_1
C59_1	H59_1	C60_1	N61_1	N62_1	N63_1	C64_1	C65_1
H65_1	N66_1	C67_1	C68_1	H68_1	C69_1	H69_1	C70_1
H70_1	C71_1	C72_1	O73_1	N74_1	H74_1	C75_1	H75_1
C76_1	H76A_1	H76B_1	H76C_1	C77_1	H77A_1	H77B_1	H77C_1
C1_2	H1A_2	H1AB_2	H1AC_2	C2_2	C3_2	C4_2	C5_2
C6_2	H6A_2	H6AB_2	H6AC_2	C7_2	H7A_2	H7B_2	H7C_2
C8_2	H8A_2	H8B_2	H8C_2	C9_2	C10_2	H10_2	C11_2
H11_2	C12_2	C13_2	H13_2	C14_2	N15_2	N16_2	N17_2
C18_2	C19_2	H19_2	N20_2	C21_2	C22_2	H22_2	C23_2
H23_2	C24_2	H24_2	C25_2	C26_2	O27_2	N28_2	H28_2
C29_2	H29_2	C30_2	H30A_2	H30B_2	H30C_2	C31_2	H31A_2
H31B_2	H31C_2	C32_2	C33_2	H33_2	C34_2	H34_2	C35_2
C36_2	H36_2	C37_2	N38_2	N39_2	N40_2	C41_2	C42_2
H42_2	N43_2	C44_2	C45_2	H45_2	C46_2	H46_2	C47_2
H47_2	C48_2	C49_2	O50_2	N51_2	H51_2	C52_2	H52_2
C53_2	H53A_2	H53B_2	H53C_2	C54_2	H54A_2	H54B_2	H54C_2
C55_2	C56_2	H56_2	C57_2	H57_2	C58_2	C59_2	H59_2
C60_2	N61_2	N62_2	N63_2	C64_2	C65_2	H65_2	N66_2
C67_2	C68_2	H68_2	C69_2	H69_2	C70_2	H70_2	C71_2
C72_2	O73_2	N74_2	H74_2	C75_2	C76_2	H76A_2	H76B_2
H76C_2	C77_2	H77A_2	H77B_2	H77C_2	O1_3	S1_4	O2_4
O3_4	O4_4	C5_4	F6_4	F7_4	F8_4	S1_5	O2_5
O3_5	O4_5	C5_5	F6_5	F7_5	F8_5		

PLAT794_ALERT_5_G Tentative Bond Valency for La01 (III) . 3.94 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for La02 (III) . 3.98 Info
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 1945 Note
 PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
 PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
 PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.6 Low
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

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

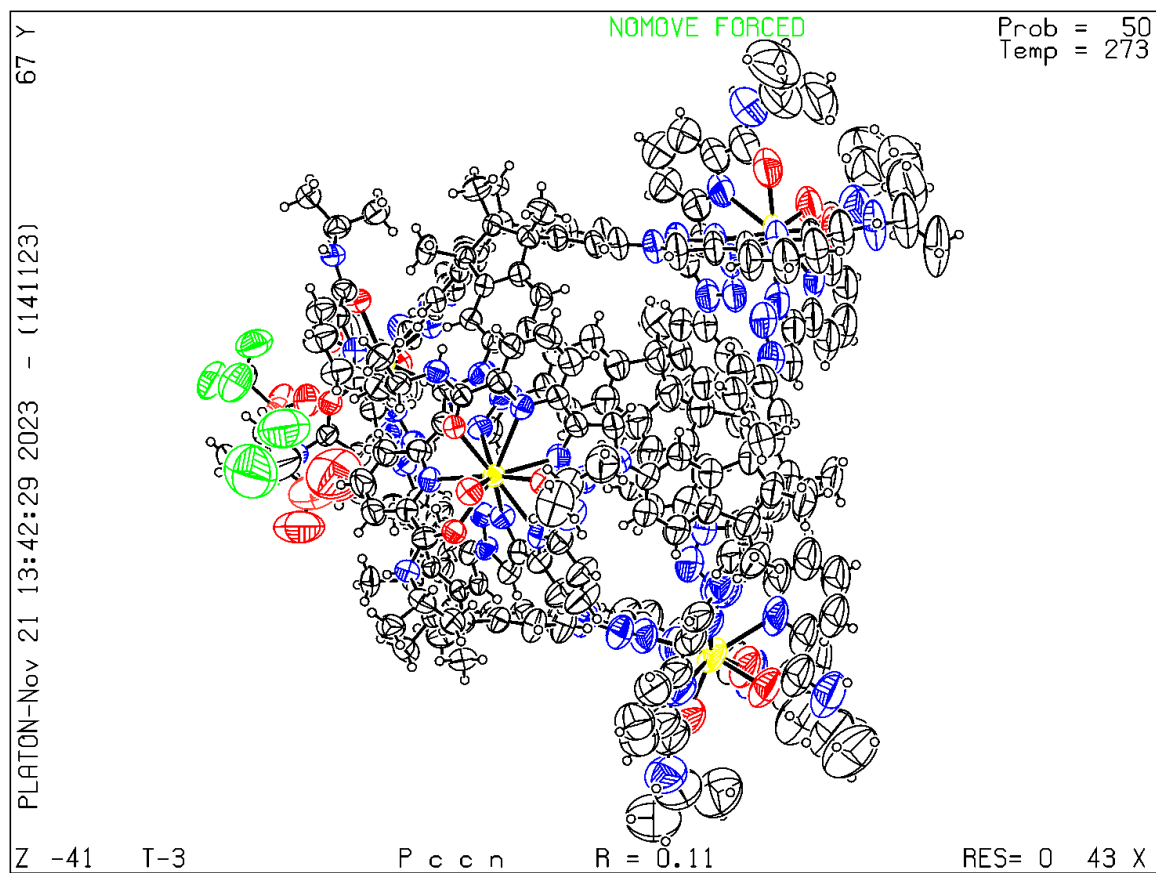
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) S4-4

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: S4-4

Bond precision:	C-C = 0.0501 Å	Wavelength=0.71073	
Cell:	a=62.91(1)	b=36.326(6)	c=36.322(5)
	alpha=90	beta=125.2600	gamma=90
Temperature:	278 K		
	Calculated	Reported	
Volume	67777(18)	67780(18)	
Space group	C 2/m	C 2/m	
Hall group	-C 2y	-C 2y	
Moiety formula	C236 H176 La4 N60 O12, 2(C2 H3) [+ solvent]	C240H182La4 N60 O12 [+ solvent]	
Sum formula	C240 H182 La4 N60 O12 [+ solvent]	C240 H182 La4 N60 O12	
Mr	4654.09	4654.09	
Dx, g cm ⁻³	0.456	0.456	
Z	4	4	
Mu (mm ⁻¹)	0.272	0.272	
F000	9464.0	9464.0	
F000'	9462.25		
h, k, lmax		45, 25, 25	
Nref		13201	
Tmin, Tmax	0.901, 0.934		
Tmin'	0.894		

Correction method= Not given

Data completeness= Theta(max)= 14.737

R(reflections)= 0.1580(6363)

wR2(reflections)=
0.4720(13201)

S = 1.568

Npar= 1613

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

RINTA01_ALERT_3_A The value of Rint is greater than 0.25
Rint given 0.327

Author Response: (1) The highest resolution of the crystal can only reach about 1.5 angstrom, whether utilizing the Bruker D8 VENTURE photon II diffractometer with Is 3.0 microfocus X-ray source or the Shanghai Synchrotron Radiation Facility (SSRF). (2) Because of the large number of amorphous solvents and highly-disordered counterions existing in the unit cell, which occupy as much as 75.1% of the unit cell based on PLATON/SOLV calculation. (3) The inherent weak diffraction ability of crystal also might be attributed to the presence of isomers.

THETM01_ALERT_3_A The value of $\sin(\theta_{\max})/\lambda$ is less than 0.550
Calculated $\sin(\theta_{\max})/\lambda = 0.3579$

Author Response: The crystals of this giant supramolecular assembly diffract very weakly in nature, possibly due to a large amount of amorphous solvents and highly-disordered counterions existing in the unit cell, which occupy as much as 75.1% of the unit cell based on PLATON calculation.

PLAT020_ALERT_3_A The Value of Rint is Greater Than 0.12 0.327 Report

Author Response: The explanation of this problem is the same as the first one.

PLAT084_ALERT_3_A High wR2 Value (i.e. > 0.25) 0.47 Report

Author Response: The inherent diffraction ability of the crystal is very weak. Although we have tried to cultivate the crystal repeatedly and test using different diffraction instruments, even the SSRF, the highest resolution of the data can only reach 1.5 angstrom. The weak data diffraction ability is mainly attributed to the large cavity containing a large number of amorphous solvents and highly -disordered counterions, as well as the existence of isomers.

Alert level B

PLAT082_ALERT_2_B	High R1 Value	0.16	Report
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of	O56_9	Check
PLAT241_ALERT_2_B	High 'MainMol' Ueq as Compared to Neighbors of	O56_13	Check
PLAT242_ALERT_2_B	Low 'MainMol' Ueq as Compared to Neighbors of	La1	Check
PLAT242_ALERT_2_B	Low 'MainMol' Ueq as Compared to Neighbors of	La02	Check
PLAT242_ALERT_2_B	Low 'MainMol' Ueq as Compared to Neighbors of	La2	Check

PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	C62	Check
PLAT260_ALERT_2_B	Large Average	Ueq of Residue Including	Lal	0.304	Check
PLAT260_ALERT_2_B	Large Average	Ueq of Residue Including	Cl_5	0.309	Check
PLAT315_ALERT_2_B	Singly Bonded Carbon Detected (H-atoms Missing).			C59_1	Check
PLAT315_ALERT_2_B	Singly Bonded Carbon Detected (H-atoms Missing).			C60_1	Check
PLAT315_ALERT_2_B	Singly Bonded Carbon Detected (H-atoms Missing).			C59_8	Check
PLAT315_ALERT_2_B	Singly Bonded Carbon Detected (H-atoms Missing).			C2_5	Check
PLAT342_ALERT_3_B	Low Bond Precision on	C-C Bonds		0.05006	Ang.
PLAT910_ALERT_3_B	Missing # of FCF Reflection(s) Below Theta(Min).			41	Note
	0	2	0,	1	1
	4	0	0,	4	2
	-3	3	1,	-2	0
	0	2	1,	1	1
	1	3	0,	2	0
	0	0,	2	0	0,
	2	2	0,	3	1
	0,	3	1	0,	
	-3	1,	-4	0	1,
	-4	2	1,	-3	1
	1,	-3	1,	0	0
	0	1,	-1	1	1,
	-1	1	1,	-1	3
	1,	-1	3	1,	0
	0	0	1,	0	1,
	3	1	1,	3	1
	1,	3	1,	2	0
	2	0	1,	2	2
	1,	2	2	1,	3
	3	1	1,		

Alert level C

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	48%	Check
PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	8.18	Note
PLAT193_ALERT_1_C	Cell and Diffraction Temperatures Differ by	5	Degree
PLAT199_ALERT_1_C	Reported _cell_measurement_temperature	273	Check
PLAT218_ALERT_3_C	Constrained U(ij) Components(s) for N7#	2	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	O56_7	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	O56_11	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	N44_7	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	N46_7	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	N49_7	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	N46_9	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	N49_9	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C6	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C12_5	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C17_5	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C5	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C48	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C49	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C53	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C55	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C56	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C58_7	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C103	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C58_13	Check
PLAT329_ALERT_4_C	Carbon Atom Hybridisation Unclear for	C17	Check
PLAT329_ALERT_4_C	Carbon Atom Hybridisation Unclear for	C51	Check
PLAT361_ALERT_2_C	Long C(sp3)-C(sp3) Bond C53 - C55	1.65	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C47_5 - C50_5	1.56	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C47_7 - C50_7	1.55	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C54_7 - C55_7	1.55	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C47_9 - C50_9	1.56	Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C54_9 - C55_9	1.55	Ang.
PLAT412_ALERT_2_C	Short Intra XH3 .. XHn H7A_5 ..H23_5	1.83	Ang.
	x,y,z =	1_555	Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N57_5 --H57_5		Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N57_7 --H57_7		Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N57_9 --H57_9		Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N57_11 --H57_11		Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N57_13 --H57_13		Please Check
PLAT701_ALERT_1_C	Bond Calc 2.55(3), Rep 2.6(4), Dev..	1.67	Sigma
LA02	-N46_5	1_555	6_565
		#	20 Check

PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
 PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -27.889 Report
 PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -4.328 Report
 PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.342 Report
 PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.358 116 Report

0	4	0,	3	3	0,	5	1	0,	6	0	0,	6	2	0,	7	1	0,
7	5	0,	7	7	0,	8	0	0,	10	0	0,	15	5	0,	-37	5	1,
-31	15	1,	-11	25	1,	-9	1	1,	-8	0	1,	-8	2	1,	-7	1	1,
-6	0	1,	-6	2	1,	-4	10	1,	-1	5	1,	1	9	1,	4	0	1,
6	0	1,	7	1	1,	9	25	1,	29	15	1,	35	5	1,	-13	3	2,
-9	1	2,	-8	0	2,	-8	2	2,	-6	2	2,	-4	4	2,	-3	3	2,
2	2	2,	3	1	2,	3	3	2,	4	0	2,	4	2	2,	-18	4	3,
-13	9	3,	-7	3	3,	-6	0	3,	-4	2	3,	-3	3	3,	-3	13	3,
-2	2	3,	-1	9	3,	0	0	3,	1	7	3,	4	2	3,	6	0	3,
-14	0	4,	-5	1	4,	-4	0	4,	-2	14	4,	4	2	4,	6	0	4,
-41	1	5,	-40	6	5,	-5	1	5,	8	6	5,	19	19	5,	31	1	5,
-41	5	6,	-3	5	6,	-41	7	7,	-33	17	7,	-21	23	7,	-14	0	7,
-9	25	7,	-5	25	7,	-3	3	7,	-2	4	7,	0	0	7,	3	3	7,
7	23	7,	19	17	7,	27	7	7,	-40	10	8,	-32	18	8,	-24	22	8,
-10	0	8,	8	22	8,	16	18	8,	24	10	8,	-17	1	9,	23	9	9,
-42	8	10,	-20	2	10,	-10	2	10,	-10	24	10,	22	8	10,	-9	3	12,

PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 13 Note

0	4	0,	1	1	0,	2	0	0,	4	0	0,	6	0	0,	-5	1	1,
-1	1	1,	0	0	1,	-6	2	2,	-2	2	2,	2	2	2,	-3	3	3,
-4	0	4,															

PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on La02 1.35 eA-3
 PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on La1 1.26 eA-3
 PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on La2 1.11 eA-3
 PLAT977_ALERT_2_C Check Negative Difference Density on H60C_7 . -0.31 eA-3

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: C240 H182 La4 N60 O12
 Atom count from the _atom_site data: C240 H183 La4 N60 O12
 CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
 CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
 symmetry error - see SYMMG tests
 From the CIF: _cell_formula_units_Z 4
 From the CIF: _chemical_formula_sum C240 H182 La4 N60 O12
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	960.00	960.00	0.00
H	728.00	732.00	-4.00
La	16.00	16.00	0.00
N	240.00	240.00	0.00
O	48.00	48.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 207 Note
 PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 212 Report
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 5 Report
 H25# H43# H60# H76# H92#
 PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
 Calc: C236 H176 La4 N60 O12, 2(C2 H3)
 Rep.: C240H182La4 N60 O12
 PLAT128_ALERT_4_G Alternate Setting for Input Space Group C2/m I2/m Note

PLAT145_ALERT_4_G	s.u. on beta	Small or Missing	0.0000	Degree
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains	DFIX Records	65	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains	DANG Records	6	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains	FLAT Records	24	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains	SAME Records	8	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains	SADI Records	32	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains	DELU Records	14	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains	SIMU Records	14	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains	ISOR Records	3	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		0.0300	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		0.0300	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par		0.0050	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par		0.0050	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of O56_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O56_8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O56_10	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O56_12	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N44_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N45_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N46_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N49_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N57_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N44_8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N45_8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N46_8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N49_8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N57_8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N44_10	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N45_10	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N46_10	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N49_10	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N57_10	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N44_11	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N45_11	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N46_11	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N49_11	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N44_12	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N45_12	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N46_12	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N49_12	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N57_12	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N44_13	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N45_13	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N46_13	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N49_13	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C51_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C52_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C53_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C54_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C55_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C58_1	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C47_8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C48_8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C50_8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C51_8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C52_8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C53_8	Constrained at	0.5	Check

[illegible]

PLAT300_ALERT_4_G	Atom Site Occupancy of H60A_8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60B_8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H54A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H54B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H54C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60C_8	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H57A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H57C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48_10	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52_10	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H53_10	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59A_10	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59B_10	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59C_10	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48_11	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52_11	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H53_11	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59A_11	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59B_11	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59C_11	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60A_11	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60B_11	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60C_11	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48_12	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52_12	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H53_12	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59A_12	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59B_12	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59C_12	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48_13	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52_13	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H53_13	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59A_13	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59B_13	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H59C_13	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60A_13	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60B_13	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H60C_13	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		27%	Note
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C3_5	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C4_5	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C5_5	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for		C47	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for		C48	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for		C49	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C58_7	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for		C58_9	Check
PLAT344_ALERT_2_G	Unusual sp? Angle Range in Solvent/Ion for		C2_5	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C47_1 - C50_1 .		1.58	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C48 - C51 .		1.51	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C54 - C55 .		1.60	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C58_7 - C59_7 .		1.60	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C58_7 - C60_7 .		1.57	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C58_9 - C59_9 .		1.58	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C58_9 - C60_9 .		1.57	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C58_11 - C60_11 .		1.57	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C58_13 - C60_13 .		1.58	Ang.

PLAT410_ALERT_2_G Short Intra H...H Contact	H3	..H51B	.	1.87 Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn	H6	..H46A	.	1.93 Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn	H17B	..H57B	.	1.99 Ang.
		x,y,z =	1_555	Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn	H17C	..H57B	.	2.00 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C1_5	..C4_5	.	2.69 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C1_5	..C5_5	.	2.73 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C1_5	..C3_5	.	2.73 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C2_5	..C4_5	.	1.77 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C2_5	..C5_5	.	1.78 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C2_5	..C3_5	.	1.78 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C2_5	..C22_5	.	2.38 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C2_5	..C21_5	.	2.40 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C2_5	..C10_5	.	2.41 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C2_5	..C9_5	.	2.41 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C2_5	..C20_5	.	2.45 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C2_5	..C15_5	.	2.46 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C2_5	..C6_5	.	2.91 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C2_5	..C8_5	.	2.91 Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C2_5	..C7_5	.	2.95 Ang.
		x,y,z =	1_555	Check

PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 284 Note

La02	H02	C1_5	H1A_5	H1B_5	H1C_5	C2_5	C3_5
C4_5	C5_5	C6_5	H6A_5	H6B_5	H6C_5	C7_5	H7A_5
H7B_5	H7C_5	C8_5	H8A_5	H8B_5	H8C_5	C9_5	C10_5
C11_5	H11_5	C12_5	C13_5	C14_5	H14_5	C15_5	C16_5
H16_5	C17_5	C18_5	C19_5	H19_5	C20_5	C21_5	C22_5
C23_5	H23_5	C24_5	H24_5	C25_5	C26_5	H26_5	N44_5
N45_5	N46_5	C47_5	C48_5	H48_5	N49_5	C50_5	C51_5
H51_5	C52_5	H52_5	C53_5	H53_5	C54_5	C55_5	O56_5
N57_5	H57_5	C58_5	H58_5	C59_5	H59A_5	H59B_5	H59C_5
C60_5	H60A_5	H60B_5	H60C_5	C1_2	C2_2	H2_2	C3_2
H3_2	C4_2	C5_2	C6_2	H6_2	N44_1	N45_1	N46_1
C47_1	C48_1	H48_1	N49_1	C50_1	C51_1	C52_1	H52_1
C53_1	H53_1	C54_1	C55_1	O56_1	N57_1	C58_1	C59_1
C60_1	N44_7	N45_7	N46_7	C47_7	C48_7	H48_7	N49_7
C50_7	C51_7	H51_7	C52_7	H52_7	C53_7	H53_7	C54_7
C55_7	O56_7	N57_7	H57_7	C58_7	C59_7	H59A_7	H59B_7
H59C_7	C60_7	H60A_7	H60B_7	H60C_7	N44_8	N45_8	N46_8

C47_8	C48_8	H48_8	N49_8	C50_8	C51_8	C52_8	H52_8
C53_8	H53_8	C54_8	C55_8	O56_8	N57_8	C58_8	C59_8
C60_8	H60A_8	H60B_8	H60C_8	N44_9	N45_9	N46_9	C47_9
C48_9	H48_9	N49_9	C50_9	C51_9	H51_9	C52_9	H52_9
C53_9	H53_9	C54_9	C55_9	O56_9	N57_9	H57_9	C58_9
C59_9	H59A_9	H59B_9	H59C_9	C60_9	H60A_9	H60B_9	H60C_9
N44_10	N45_10	N46_10	C47_10	C48_10	H48_10	N49_10	C50_10
C51_10	C52_10	H52_10	C53_10	H53_10	C54_10	C55_10	O56_10
N57_10	C58_10	C59_10	H59A_10	H59B_10	H59C_10	C60_10	N44_11
N45_11	N46_11	C47_11	C48_11	H48_11	N49_11	C50_11	C51_11
C52_11	H52_11	C53_11	H53_11	C54_11	C55_11	O56_11	N57_11
H57_11	C58_11	C59_11	H59A_11	H59B_11	H59C_11	C60_11	H60A_11
H60B_11	H60C_11	N44_12	N45_12	N46_12	C47_12	C48_12	H48_12
N49_12	C50_12	C51_12	C52_12	H52_12	C53_12	H53_12	C54_12
C55_12	O56_12	N57_12	C58_12	C59_12	H59A_12	H59B_12	H59C_12
C60_12	N44_13	N45_13	N46_13	C47_13	C48_13	H48_13	N49_13
C50_13	C51_13	C52_13	H52_13	C53_13	H53_13	C54_13	C55_13
O56_13	N57_13	H57_13	C58_13	C59_13	H59A_13	H59B_13	H59C_13
C60_13	H60A_13	H60B_13	H60C_13				
PLAT721_ALERT_1_G Bond	Calc	0.97000, Rep	0.96000 Dev...				0.01 Ang.
C60_8	-H60A_8	1_555	1_555		#	329	Check
PLAT721_ALERT_1_G Bond	Calc	0.97000, Rep	0.96000 Dev...				0.01 Ang.
C59_10	-H59B_10	1_555	1_555		#	396	Check
PLAT721_ALERT_1_G Bond	Calc	0.97000, Rep	0.96000 Dev...				0.01 Ang.
C59_13	-H59B_13	1_555	1_555		#	491	Check
PLAT722_ALERT_1_G Angle	Calc	115.00, Rep	109.50 Dev...				5.50 Degree
H57A	-C57	-H57B	1_555	1_555 1_555	#	261	Check
PLAT722_ALERT_1_G Angle	Calc	106.00, Rep	109.50 Dev...				3.50 Degree
H57B	-C57	-H57C	1_555	1_555 1_555	#	264	Check
PLAT722_ALERT_1_G Angle	Calc	115.00, Rep	117.70 Dev...				2.70 Degree
H57B	-C57	-H57A	1_555	1_555 6_565	#	267	Check
PLAT722_ALERT_1_G Angle	Calc	115.00, Rep	117.70 Dev...				2.70 Degree
H57A	-C57	-H57B	1_555	1_555 6_565	#	270	Check
PLAT722_ALERT_1_G Angle	Calc	106.00, Rep	100.80 Dev...				5.20 Degree
H57C	-C57	-H57B	1_555	1_555 6_565	#	272	Check
PLAT722_ALERT_1_G Angle	Calc	115.00, Rep	109.50 Dev...				5.50 Degree
H57A	-C57	-H57B	6_565	1_555 6_565	#	273	Check
PLAT722_ALERT_1_G Angle	Calc	106.00, Rep	100.80 Dev...				5.20 Degree
H57B	-C57	-H57C	1_555	1_555 6_565	#	276	Check
PLAT722_ALERT_1_G Angle	Calc	106.00, Rep	109.50 Dev...				3.50 Degree
H57B	-C57	-H57C	6_565	1_555 6_565	#	279	Check
PLAT722_ALERT_1_G Angle	Calc	111.00, Rep	109.50 Dev...				1.50 Degree
H60B_8	-C60_8	-H60C_8	1_555	1_555 1_555	#	875	Check
PLAT722_ALERT_1_G Angle	Calc	108.00, Rep	109.50 Dev...				1.50 Degree
H59A_10	-C59_10	-H59B_10	1_555	1_555 1_555	#	1069	Check
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)						1.15 Ratio
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C2_5	--C4_5					1.77 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C2_5	--C5_5					1.78 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C2_5	--C3_5					1.78 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C47_1	--C47_11					1.84 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C47_1	--C51_11					1.93 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C51_1	--C51_11					1.73 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C51_1	--C47_11					2.08 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C54_1	--C55_10					1.80 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C55_1	--C58_10					2.00 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C58_1	--C58_1					1.90 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C47_8	--C47_13					1.83 Ang.

PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C50_8	--C51_13	1.79 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C51_8	--C47_13	1.87 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C54_8	--C55_12	1.95 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C55_8	--C58_12	2.07 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C58_8	--C60_12	1.91 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C47_10	--C47_10	1.78 Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C47_12	--C47_12	1.90 Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		29.70 Deg.
	H54C -C54 -H54A 1_555 1_555 6_565	# 235	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		29.70 Deg.
	H54B -C54 -H54B 1_555 1_555 6_565	# 238	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		29.70 Deg.
	H54A -C54 -H54C 1_555 1_555 6_565	# 242	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		9.80 Deg.
	H57C -C57 -H57A 1_555 1_555 6_565	# 268	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		9.80 Deg.
	H57B -C57 -H57B 1_555 1_555 6_565	# 271	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		9.80 Deg.
	H57A -C57 -H57C 1_555 1_555 6_565	# 275	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		5.10 Deg.
	N45_1-N44_1-N45_1 1_555 1_555 6_565	# 506	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		26.00 Deg.
	N45_1-N45_1-N44_1 6_565 1_555 6_565	# 513	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		10.00 Deg.
	N45_1-N46_1-N45_1 1_555 1_555 6_565	# 521	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		9.00 Deg.
	C50_1-C47_1-C50_1 6_565 1_555 1_555	# 530	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		13.10 Deg.
	C50_1-N49_1-C50_1 1_555 1_555 6_565	# 556	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		21.00 Deg.
	C50_1-C50_1-C47_1 6_565 1_555 1_555	# 576	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		17.00 Deg.
	C50_1-C51_1-C50_1 1_555 1_555 6_565	# 583	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		39.00 Deg.
	C55_1-C54_1-O56_1 1_555 1_555 1_555	# 603	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		42.00 Deg.
	C55_1-C54_1-C55_1 1_555 1_555 1_555	# 606	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		37.40 Deg.
	O56_1-C54_1-C55_1 1_555 1_555 1_555	# 607	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		41.30 Deg.
	N57_1-C55_1-C58_1 1_555 1_555 1_555	# 628	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		27.00 Deg.
	O56_1-O56_1-C55_1 1_555 1_555 1_555	# 630	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		38.00 Deg.
	C55_1-O56_1-C55_1 1_555 1_555 1_555	# 631	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		40.00 Deg.
	C55_1-N57_1-C55_1 1_555 1_555 1_555	# 651	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		34.30 Deg.
	O56_1-C60_1-O56_1 6_565 1_555 1_555	# 666	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		7.00 Deg.
	N45_8-N44_8-N45_8 6_565 1_555 1_555	# 723	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		30.00 Deg.
	N46_8-N45_8-N46_8 6_565 1_555 1_555	# 731	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		38.27 Deg.
	N45_8-N45_8-N44_8 6_565 1_555 1_555	# 732	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		10.00 Deg.
	N45_8-N46_8-N45_8 6_565 1_555 1_555	# 738	Check

PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.00 Deg.
C50_1-C47_8-C50_8 6_565 1_555 1_555	# 749 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.00 Deg.
C50_8-C47_8-C47_1 1_555 1_555 6_565	# 759 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	12.00 Deg.
C50_8-N49_8-C50_1 1_555 1_555 6_565	# 767 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	33.00 Deg.
C50_1-C50_8-C51_1 6_565 1_555 6_565	# 789 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	20.00 Deg.
C50_8-C51_8-C50_1 1_555 1_555 6_565	# 796 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.00 Deg.
C50_8-C51_8-C47_1 1_555 1_555 6_565	# 801 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	27.70 Deg.
C55_8-C54_8-O56_1 1_555 1_555 1_555	# 816 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	27.00 Deg.
C55_8-C54_8-C55_1 1_555 1_555 1_555	# 819 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.90 Deg.
O56_1-C54_8-C55_1 1_555 1_555 1_555	# 820 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	28.00 Deg.
O56_1-C55_8-O56_8 1_555 1_555 1_555	# 822 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	32.00 Deg.
N57_8-C55_8-N57_1 1_555 1_555 1_555	# 834 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	40.90 Deg.
N57_1-C55_8-C58_1 1_555 1_555 1_555	# 841 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	40.00 Deg.
O56_1-O56_8-C55_8 1_555 1_555 1_555	# 842 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	28.00 Deg.
O56_1-O56_8-C55_1 1_555 1_555 1_555	# 843 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.00 Deg.
C55_8-O56_8-C55_1 1_555 1_555 1_555	# 844 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	39.00 Deg.
C55_1-N57_8-C55_8 1_555 1_555 1_555	# 853 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	10.00 Deg.
N45_1-N44_1-N45_1 1_555 1_555 1_555	# 933 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.00 Deg.
N46_1-N45_1-N46_1 1_555 1_555 1_555	# 938 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	10.00 Deg.
N45_1-N46_1-N45_1 1_555 1_555 1_555	# 943 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.00 Deg.
C50_1-C47_1-C50_1 6_565 1_555 1_555	# 954 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.40 Deg.
C50_1-C47_1-C47_1 1_555 1_555 6_565	# 960 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.00 Deg.
C50_1-N49_1-C50_1 1_555 1_555 6_565	# 972 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.10 Deg.
C50_1-N49_1-C47_1 1_555 1_555 6_565	# 975 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.00 Deg.
C50_1-C50_1-C47_1 6_565 1_555 1_555	# 990 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.90 Deg.
C50_1-C51_1-C50_1 1_555 1_555 6_565	# 1009 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	23.00 Deg.
O56_1-C55_1-O56_1 1_555 1_555 1_555	# 1026 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	35.00 Deg.
C55_1-C55_1-O56_1 1_555 1_555 1_555	# 1027 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.00 Deg.
C55_1-N57_1-C55_1 1_555 1_555 1_555	# 1055 Check	
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.40 Deg.

N57_1-C58_1-C55_1	1_555	1_555	1_555		# 1066 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	10.00 Deg.	
N45_1-N44_1-N45_1	1_555	1_555	1_555		# 1079 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	44.00 Deg.	
N46_1-N45_1-N46_1	1_555	1_555	1_555		# 1080 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	10.00 Deg.	
N45_1-N46_1-N45_1	1_555	1_555	1_555		# 1091 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	19.00 Deg.	
C50_1-C47_1-C50_1	6_565	1_555	1_555		# 1101 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	37.00 Deg.	
C50_1-C47_1-C47_1	1_555	1_555	6_565		# 1105 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	42.00 Deg.	
C50_1-C47_1-C51_1	6_565	1_555	6_565		# 1108 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	21.00 Deg.	
C50_1-N49_1-C50_1	1_555	1_555	6_565		# 1118 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	42.10 Deg.	
C50_1-N49_1-C47_1	1_555	1_555	6_565		# 1121 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	39.00 Deg.	
C50_1-C50_1-N49_1	6_565	1_555	6_565		# 1144 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	42.80 Deg.	
N49_1-C50_1-N49_1	1_555	1_555	6_565		# 1147 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	17.00 Deg.	
C50_1-C51_1-C50_1	1_555	1_555	6_565		# 1151 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	35.00 Deg.	
C50_1-C51_1-C47_1	1_555	1_555	6_565		# 1156 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	9.00 Deg.	
N45_1-N44_1-N45_1	1_555	1_555	1_555		# 1215 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	10.00 Deg.	
N45_1-N46_1-N45_1	1_555	1_555	1_555		# 1233 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	8.60 Deg.	
C50_1-C47_1-C50_1	6_565	1_555	1_555		# 1241 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	9.90 Deg.	
C50_1-N49_1-C50_1	1_555	1_555	6_565		# 1259 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	10.00 Deg.	
C50_1-C51_1-C50_1	1_555	1_555	6_565		# 1297 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	44.00 Deg.	
C55_8-C55_1-O56_1	1_555	1_555	1_555		# 1307 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	38.00 Deg.	
N57_8-C55_1-N57_1	1_555	1_555	1_555		# 1312 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	44.00 Deg.	
C55_8-C55_1-O56_8	1_555	1_555	1_555		# 1317 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	14.00 Deg.	
O56_1-C55_1-O56_8	1_555	1_555	1_555		# 1318 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	33.00 Deg.	
C55_1-N57_1-C55_8	1_555	1_555	1_555		# 1343 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	36.00 Deg.	
N57_1-C58_1-N57_8	1_555	1_555	1_555		# 1344 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	41.20 Deg.	
N57_8-C58_1-C55_8	1_555	1_555	1_555		# 1351 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	43.00 Deg.	
N57_8-C60_1-C58_8	1_555	1_555	1_555		# 1362 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	11.00 Deg.	
N45_1-N44_1-N45_1	1_555	1_555	1_555		# 1367 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	42.00 Deg.	
N46_1-N45_1-N46_1	1_555	1_555	1_555		# 1374 Check
PLAT779_ALERT_4_G Suspect or Irrelevant	(Bond) Angle(s)	in CIF	...	10.00 Deg.	
N45_1-N46_1-N45_1	1_555	1_555	1_555		# 1379 Check

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 17.00 Deg.
 C50_8-C47_1-C50_1 6_565 1_555 1_555 # 1388 Check
 PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 44.00 Deg.
 C50_1-C47_1-C47_8 1_555 1_555 6_565 # 1394 Check
 PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 21.00 Deg.
 C50_1-N49_1-C50_8 1_555 1_555 6_565 # 1406 Check
 PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 35.00 Deg.
 C50_8-C50_1-N49_8 6_565 1_555 6_565 # 1433 Check
 PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 11.00 Deg.
 C50_1-C51_1-C50_8 1_555 1_555 6_565 # 1442 Check
 PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 38.90 Deg.
 H60A_-C60_1-H60A_ 1_555 1_555 6_565 # 1483 Check
 PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 38.90 Deg.
 H60C_-C60_1-H60B_ 1_555 1_555 6_565 # 1489 Check
 PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 38.90 Deg.
 H60B_-C60_1-H60C_ 1_555 1_555 6_565 # 1493 Check
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 5187 Note
 PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
 PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
 PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
 PLAT908_ALERT_2_G Max. Perc. Data with I > 2*s(I) per Res.Shell . 55.31% Note
 PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 38% Note
 PLAT930_ALERT_2_G FCF-based Twin Law (3 1-1) Est.d BASF 0.41 Check
 PLAT930_ALERT_2_G FCF-based Twin Law (3-1-1) Est.d BASF 0.32 Check
 PLAT930_ALERT_2_G FCF-based Twin Law (1-1 1) Est.d BASF 0.32 Check
 PLAT930_ALERT_2_G FCF-based Twin Law (1 0 0) Est.d BASF 0.33 Check
 PLAT931_ALERT_5_G CIFcalcFCF Twin Law (3-1-1) Est.d BASF 0.45 Check
 PLAT931_ALERT_5_G CIFcalcFCF Twin Law (1 1 1) Est.d BASF 0.44 Check
 PLAT931_ALERT_5_G CIFcalcFCF Twin Law (1 0 0) Est.d BASF 0.43 Check
 PLAT931_ALERT_5_G CIFcalcFCF Twin Law (3 1-1) Est.d BASF 0.46 Check
 PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 30 Note
 -2 4 7, 3 1 2, -10 2 10, -5 1 4, -10 0 8, 3 3 2,
 -13 9 3, 15 5 0, 4 2 2, -6 2 2, -8 2 2, 7 5 0,
 -3 3 7, -14 0 4, 3 3 7, -13 3 2, 8 6 5, -3 13 3,
 1 7 3, -20 2 10, -1 9 3, 6 0 4, -18 4 3, 1 9 1,
 -2 14 4, 4 2 4, -4 10 1, -3 5 6, -9 3 12, -17 1 9,
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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

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

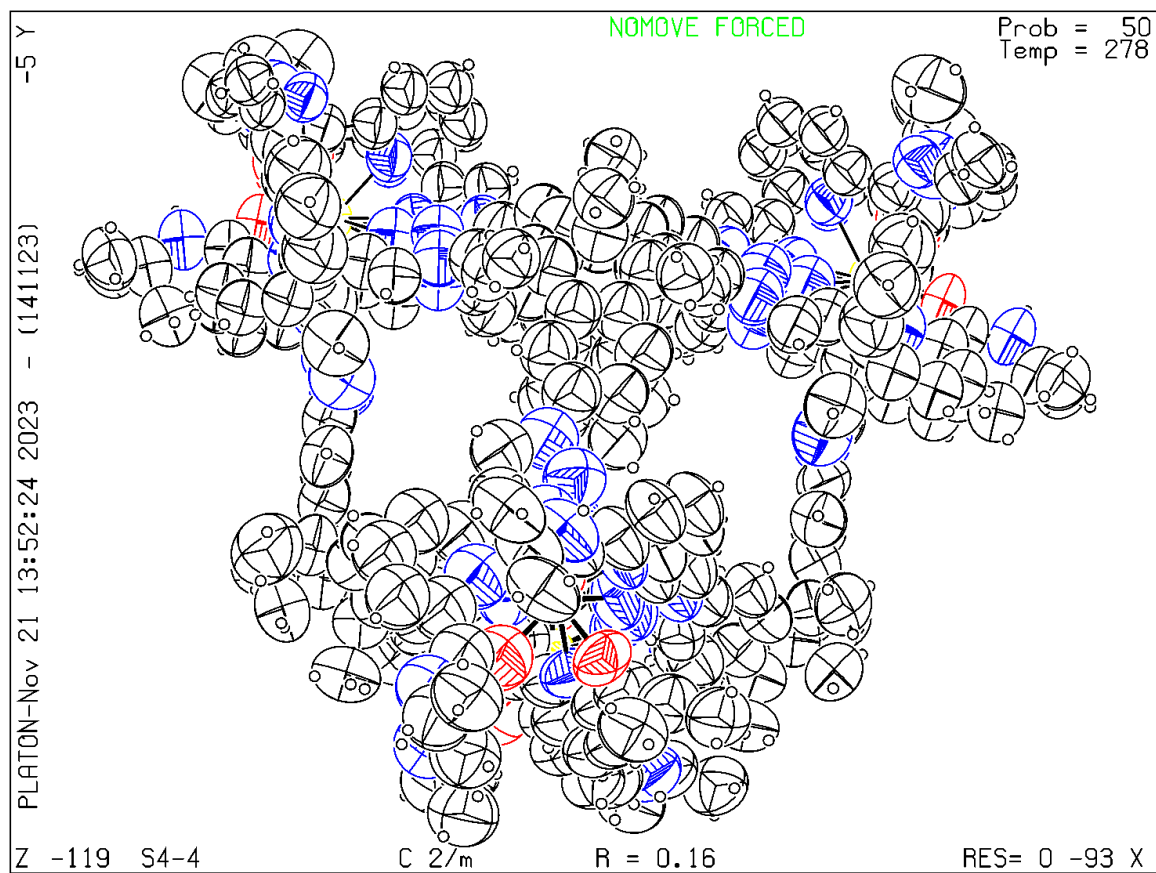
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C60@S4-4

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: C60@S4-4

Bond precision: C-C = 0.0164 Å Wavelength=0.71073

Cell: a=39.925 (8) b=41.557 (8) c=41.117 (8)
 alpha=90 beta=95.23 (3) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	67936 (23)	67935 (24)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C236 H228 La4 N60 O14, C60, 8(C F3 O3 S) [+ solvent]	C236 H228 La4 N60 O14, C60, 8(C F3 O3 S)
Sum formula	C304 H228 F24 La4 N60 O38 S8 [+ solvent]	C304 H228 F24 La4 N60 O38 S8
Mr	6597.54	6597.54
Dx, g cm ⁻³	1.290	1.290
Z	8	8
Mu (mm ⁻¹)	0.626	0.626
F000	26784.0	26784.0
F000'	26794.94	
h, k, lmax		43, 45, 45
Nref		47409
Tmin, Tmax	0.928, 0.939	
Tmin'	0.778	

Correction method= Not given

Data completeness= Theta(max)= 23.019

R(reflections)= 0.1210 (28575)

wR2(reflections)=
0.3921 (47013)

S = 1.353

Npar= 3548

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 B

THETM01_ALERT_3_B The value of $\sin(\theta_{\max})/\lambda$ is less than 0.575

Calculated $\sin(\theta_{\max})/\lambda = 0.5502$

PLAT084_ALERT_3_B	High	wR2 Value (i.e. > 0.25)		0.39	Report
PLAT242_ALERT_2_B	Low	'MainMol' Ueq as Compared to Neighbors of		C52_2	Check
PLAT973_ALERT_2_B	Check	Calcd Positive Resid. Density on	La2_5	1.56	eA-3

Alert level C

PLAT082_ALERT_2_C	High	R1 Value		0.12	Report
PLAT220_ALERT_2_C	NonSolvent	Resd 1 C	Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1 H	Uiso(max)/Uiso(min) Range	4.2	Ratio
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of		O27_3	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of		O73_3	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of		O27_4	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of		C19_1	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of		C19_2	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of		C45_3	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of		C46_3	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of		C47_3	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of		C70_3	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of		C57_4	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of		La1_5	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of		La4_5	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of		C41_1	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of		C58_1	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of		C29_2	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of		C75_2	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of		C29_3	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of		C49_3	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of		C75_3	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of		C29_4	Check
PLAT243_ALERT_4_C	High	'Solvent' Ueq as Compared to Neighbors of		S1_10	Check
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of		S1_6	Check
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of		S1_7	Check
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of		S1_8	Check
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of		S1_9	Check
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of		S1_11	Check
PLAT244_ALERT_4_C	Low	'Solvent' Ueq as Compared to Neighbors of		S1_13	Check
PLAT250_ALERT_2_C	Large	U3/U1 Ratio for Average U(i,j) Tensor		2.6	Note
PLAT250_ALERT_2_C	Large	U3/U1 Ratio for Average U(i,j) Tensor		2.7	Note
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	La1_5	0.143	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	C1_15	0.259	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_6	0.130	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_7	0.196	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_8	0.223	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_9	0.190	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_10	0.239	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_11	0.271	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_12	0.255	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_13	0.272	Check

PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01639 Ang.
PLAT361_ALERT_2_C	Long C(sp3)-C(sp3) Bond C2_1 - C3_1 .	1.68 Ang.
PLAT361_ALERT_2_C	Long C(sp3)-C(sp3) Bond C2_3 - C4_3 .	1.64 Ang.
PLAT361_ALERT_2_C	Long C(sp3)-C(sp3) Bond C2_4 - C3_4 .	1.65 Ang.
PLAT412_ALERT_2_C	Short Intra XH3 .. XHn H1AB_3 ..H6A_3 .	1.80 Ang.
	x,y,z =	1_555 Check
PLAT412_ALERT_2_C	Short Intra XH3 .. XHn H1AB_4 ..H8A_4 .	1.86 Ang.
	x,y,z =	1_555 Check
PLAT413_ALERT_2_C	Short Inter XH3 .. XHn H76C_3 ..H7A_4 .	2.06 Ang.
	-x,y,1/2-z =	2_555 Check
PLAT413_ALERT_2_C	Short Inter XH3 .. XHn H31C_4 ..H31C_4 .	2.03 Ang.
	1-x,y,1/2-z =	2_655 Check
PLAT414_ALERT_2_C	Short Intra D-H..H-X H24_4 ..H28_4 .	1.99 Ang.
	x,y,z =	1_555 Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N40_1 --H40_1 .	Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N74_1 --H74_1 .	Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N28_2 --H28_2 .	Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N51_3 --H51_3 .	Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N74_3 --H74_3 .	Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N28_4 --H28_4 .	Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N51_4 --H51_4 .	Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor N74_4 --H74_4 .	Please Check
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4	Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.626 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & Sth/L= 0.550	391 Report
	2 0 0, 0 2 0, 0 44 0, 1 45 0, 3 45 0, 5 45 0,	
	7 45 0, 2 2 1, -8 20 1, 10 44 1, -7 45 1, -5 45 1,	
	-3 45 1, -1 45 1, 1 45 1, 3 45 1, 0 0 2, 43 7 2,	
	-43 9 2, 24 38 2, 19 41 2, -13 43 2, -7 45 2, -5 45 2,	
	-3 45 2, -1 45 2, 1 45 2, 7 45 2, -43 9 3, -39 21 3,	
	-14 42 3, -13 43 3, 9 43 3, -4 44 3, -7 45 3, -5 45 3,	
	-3 45 3, -1 45 3, 1 45 3, -20 0 4, -39 21 4, 34 28 4,	
	25 37 4, 9 41 4, -14 42 4, -8 44 4, -6 44 4, -7 45 4,	
	-5 45 4, -3 45 4, -1 45 4, 43 1 5, -14 4 5, -43 9 5,	
	-3 13 5, -39 21 5, 33 29 5, 26 36 5, 8 40 5, 16 42 5,	
	-10 44 5, -8 44 5, -5 45 5, -3 45 5, 1 45 5, 15 5 6,	
	-43 9 6, 15 9 6, 41 13 6, 40 16 6, 4 20 6, -36 26 6,	
	31 31 6, 27 35 6, 8 38 6, -19 41 6, 13 43 6, -10 44 6,	
	-8 44 6, -5 45 6, -3 45 6, 2 20 7, 2 24 7, 12 26 7,	
	8 38 7, -16 42 7, -10 44 7, -3 45 7, 3 45 7, 41 11 8,	
	-3 15 8, 2 22 8, 35 25 8, 5 33 8, 17 41 8, -16 42 8,	
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	2 Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.96Ang From La3_5	1.72 eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.60Ang From F7_11	1.61 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.21Ang From S1_10	-1.55 eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on La1_5	1.44 eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on La4_5	1.37 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.05Ang From O2_15 .	0.89 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 1.08Ang From O4_10 .	0.76 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.70Ang From N17_4 .	-0.61 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.95Ang From O3_10 .	-0.52 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H54A_2 .	-0.44 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H54B_2 .	-0.42 eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu

not performed for this radiation type.

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	171	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	432	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	12	Report
H26# H38# H50# H77# H92# H107# H134# H149# H164# H191# H206#			
H221#			
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	18	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	34	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	8	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	16	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	3	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	C5_6	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	C5_7	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	C5_8	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	C5_9	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	C5_10	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	C5_11	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	C5_12	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	C5_13	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C1_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C5_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C8_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C10_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C12_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C15_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C17_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C20_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C24_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C25_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C27_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C28_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C30_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C32_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C35_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C36_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C37_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C39_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C40_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C43_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C45_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C46_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C47_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C51_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C54_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C56_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C59_15	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C60_15	Check
PLAT344_ALERT_2_G	Unusual sp3 Angle Range in Solvent/Ion for	C5_13	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F7_13 ..C42_3 .	2.93	Ang.
	1-x,y,1/2-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F8_13 ..C42_3 .	2.69	Ang.
	1-x,y,1/2-z =	2_655	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C42_3 ..C5_13 .	3.12	Ang.

1-x,y,1/2-z = 2_655 Check
 PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure ! Info
 PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 666 Note

C1_1	H1A_1	H1AB_1	H1AC_1	C2_1	C3_1	C4_1	C5_1
C6_1	H6A_1	H6AB_1	H6AC_1	C7_1	H7A_1	H7AB_1	H7AC_1
C8_1	H8A_1	H8AB_1	H8AC_1	C9_1	C10_1	C11_1	H11_1
C12_1	C13_1	H13_1	C14_1	H14_1	C15_1	C16_1	H16_1
C17_1	C18_1	H18_1	C19_1	H19_1	C20_1	C21_1	C22_1
H22_1	C23_1	C24_1	H24_1	C25_1	H25_1	C26_1	N27_1
N28_1	N29_1	C30_1	C31_1	H31_1	N32_1	C33_1	C34_1
H34_1	C35_1	H35_1	C36_1	H36_1	C37_1	C38_1	O39_1
N40_1	H40_1	C41_1	H41_1	C42_1	H42A_1	H42B_1	H42C_1
C43_1	H43A_1	H43B_1	H43C_1	N44_1	N45_1	N46_1	C47_1
C48_1	H48_1	N49_1	C50_1	C51_1	H51_1	C52_1	H52_1
C53_1	H53_1	C54_1	C55_1	O56_1	N57_1	H57_1	C58_1
H58_1	C59_1	H59A_1	H59B_1	H59C_1	C60_1	H60A_1	H60B_1
H60C_1	N61_1	N62_1	N63_1	C64_1	C65_1	H65_1	N66_1
C67_1	C68_1	H68_1	C69_1	H69_1	C70_1	H70_1	C71_1
C72_1	O73_1	N74_1	H74_1	C75_1	H75_1	C76_1	H76A_1
H76B_1	H76C_1	C77_1	H77A_1	H77B_1	H77C_1	C1_2	H1A_2
H1AB_2	H1AC_2	C2_2	C3_2	C4_2	C5_2	C6_2	H6A_2
H6AB_2	H6AC_2	C7_2	H7A_2	H7AB_2	H7AC_2	C8_2	H8A_2
H8AB_2	H8AC_2	C9_2	C10_2	C11_2	H11_2	C12_2	H12_2
C13_2	C14_2	H14_2	N15_2	N16_2	N17_2	C18_2	C19_2
H19_2	N20_2	C21_2	C22_2	H22_2	C23_2	H23_2	C24_2
H24_2	C25_2	C26_2	O27_2	N28_2	H28_2	C29_2	H29_2
C30_2	H30A_2	H30B_2	H30C_2	C31_2	H31A_2	H31B_2	H31C_2
C32_2	C33_2	C34_2	H34_2	C35_2	H35_2	C36_2	C37_2
H37_2	N38_2	N39_2	N40_2	C41_2	C42_2	H42_2	N43_2
C44_2	C45_2	H45_2	C46_2	H46_2	C47_2	H47_2	C48_2
C49_2	O50_2	N51_2	H51_2	C52_2	H52_2	C53_2	H53A_2
H53B_2	H53C_2	C54_2	H54A_2	H54B_2	H54C_2	C55_2	C56_2
H56_2	C57_2	C58_2	H58_2	C59_2	H59_2	C60_2	N61_2
N62_2	N63_2	C64_2	C65_2	H65_2	N66_2	C67_2	C68_2
H68_2	C69_2	H69_2	C70_2	H70_2	C71_2	C72_2	O73_2
N74_2	H74_2	C75_2	H75_2	C76_2	H76A_2	H76B_2	H76C_2
C77_2	H77A_2	H77B_2	H77C_2	C1_3	H1A_3	H1AB_3	H1AC_3
C2_3	C3_3	C4_3	C5_3	C6_3	H6A_3	H6AB_3	H6AC_3
C7_3	H7A_3	H7AB_3	H7AC_3	C8_3	H8A_3	H8AB_3	H8AC_3
C9_3	C10_3	C11_3	H11_3	C12_3	H12_3	C13_3	C14_3
H14_3	N15_3	N16_3	N17_3	C18_3	C19_3	H19_3	N20_3
C21_3	C22_3	H22_3	C23_3	H23_3	C24_3	H24_3	C25_3
C26_3	O27_3	N28_3	H28_3	C29_3	H29_3	C30_3	H30A_3
H30B_3	H30C_3	C31_3	H31A_3	H31B_3	H31C_3	C32_3	C33_3
H33_3	C34_3	C35_3	H35_3	C36_3	H36_3	C37_3	N38_3
N39_3	N40_3	C41_3	C42_3	H42_3	N43_3	C44_3	C45_3
H45_3	C46_3	H46_3	C47_3	H47_3	C48_3	C49_3	O50_3
N51_3	H51_3	C52_3	H52_3	C53_3	H53A_3	H53B_3	H53C_3
C54_3	H54A_3	H54B_3	H54C_3	C55_3	C56_3	C57_3	H57_3
C58_3	C59_3	H59_3	C60_3	H60_3	N61_3	N62_3	N63_3
C64_3	C65_3	H65_3	N66_3	C67_3	C68_3	H68_3	C69_3
H69_3	C70_3	H70_3	C71_3	C72_3	O73_3	N74_3	H74_3
C75_3	H75_3	C76_3	H76A_3	H76B_3	H76C_3	C77_3	H77A_3
H77B_3	H77C_3	C1_4	H1A_4	H1AB_4	H1AC_4	C2_4	C3_4
C4_4	C5_4	C6_4	H6A_4	H6AB_4	H6AC_4	C7_4	H7A_4
H7AB_4	H7AC_4	C8_4	H8A_4	H8AB_4	H8AC_4	C9_4	C10_4
C11_4	H11_4	C12_4	H12_4	C13_4	C14_4	H14_4	N15_4

N16_4	N17_4	C18_4	C19_4	H19_4	N20_4	C21_4	C22_4
H22_4	C23_4	H23_4	C24_4	H24_4	C25_4	C26_4	O27_4
N28_4	H28_4	C29_4	H29_4	C30_4	H30A_4	H30B_4	H30C_4
C31_4	H31A_4	H31B_4	H31C_4	C32_4	C33_4	H33_4	C34_4
C35_4	H35_4	C36_4	H36_4	C37_4	N38_4	N39_4	N40_4
C41_4	C42_4	H42_4	N43_4	C44_4	C45_4	H45_4	C46_4
H46_4	C47_4	H47_4	C48_4	C49_4	O50_4	N51_4	H51_4
C52_4	H52_4	C53_4	H53A_4	H53B_4	H53C_4	C54_4	H54A_4
H54B_4	H54C_4	C55_4	C56_4	C57_4	H57_4	C58_4	H58_4
C59_4	C60_4	H60_4	N61_4	N62_4	N63_4	C64_4	C65_4
H65_4	N66_4	C67_4	C68_4	H68_4	C69_4	H69_4	C70_4
H70_4	C71_4	C72_4	O73_4	N74_4	H74_4	C75_4	H75_4
C76_4	H76A_4	H76B_4	H76C_4	C77_4	H77A_4	H77B_4	H77C_4
La1_5	La2_5	La3_5	La4_5	S1_6	O2_6	O3_6	O4_6
C5_6	F6_6	F7_6	F8_6	S1_7	O2_7	O3_7	O4_7
C5_7	F6_7	F7_7	F8_7	S1_8	O2_8	O3_8	O4_8
C5_8	F6_8	F7_8	F8_8	S1_9	O2_9	O3_9	O4_9
C5_9	F6_9	F7_9	F8_9	S1_10	O2_10	O3_10	O4_10
C5_10	F6_10	F7_10	F8_10	S1_11	O2_11	O3_11	O4_11
C5_11	F6_11	F7_11	F8_11	S1_12	O2_12	O3_12	O4_12
C5_12	F6_12	F7_12	F8_12	S1_13	O2_13	O3_13	O4_13
C5_13	F6_13	F7_13	F8_13	C1_15	O1_15	C2_15	O2_15
C3_15	C4_15	C5_15	C6_15	C7_15	C8_15	C9_15	C10_15
C11_15	C12_15	C13_15	C14_15	C15_15	C16_15	C17_15	C18_15
C19_15	C20_15	C21_15	C22_15	C23_15	C24_15	C25_15	C26_15
C27_15	C28_15	C29_15	C30_15	C31_15	C32_15	C33_15	C34_15
C35_15	C36_15	C37_15	C38_15	C39_15	C40_15	C41_15	C42_15
C43_15	C44_15	C45_15	C46_15	C47_15	C48_15	C49_15	C50_15
C51_15	C52_15	C53_15	C54_15	C55_15	C56_15	C57_15	C58_15
C59_15	C60_15						

```

PLAT794_ALERT_5_G Tentative Bond Valency for La1_5      (III)      .      3.93 Info
PLAT794_ALERT_5_G Tentative Bond Valency for La4_5      (III)      .      3.89 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 17225 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE   Suppressed      ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .      Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL      2019/3 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....      2 Note
                2  0  0,    0  0  2,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File      7 Note
                -5  7 10,  -3 15  8, -14  4  5,  -3 13  5, -14  4 14, 15  5  6,
                -10  8 22,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....      1.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.      0 Info
PLAT982_ALERT_1_G The La-f' =    -0.2345 Deviates from IT-value =    -0.2871 Check
PLAT982_ALERT_1_G The S-f' =     0.1265 Deviates from IT-value =     0.1246 Check
PLAT983_ALERT_1_G The La-f" =     2.4853 Deviates from IT-Value =     2.4523 Check
PLAT983_ALERT_1_G The S-f" =     0.1256 Deviates from IT-Value =     0.1234 Check

```

-
- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
 4 **ALERT level B** = A potentially serious problem, consider carefully
 74 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 69 **ALERT level G** = General information/check it is not something unexpected
- 8 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data

99 ALERT type 2 Indicator that the structure model may be wrong or deficient
10 ALERT type 3 Indicator that the structure quality may be low
27 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.

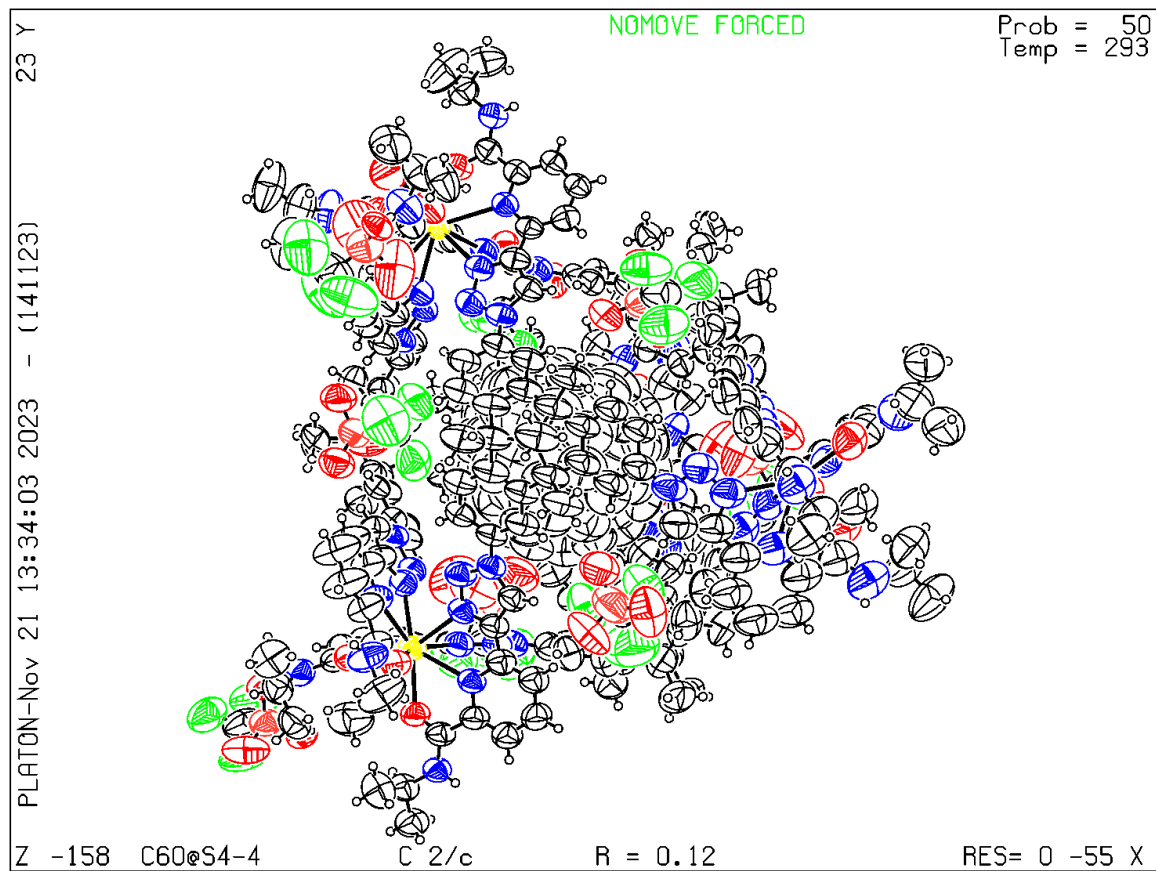
Publication of your CIF in IUCr journals

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 14/11/2023; check.def file version of 14/09/2023



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C70@S4-4

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: C70@S4-4

Bond precision: C-C = 0.0145 Å Wavelength=0.71073

Cell: a=40.408 (8) b=42.122 (8) c=41.136 (8)
 alpha=90 beta=96.44 (3) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	69574 (24)	69574 (24)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C236 H227 La4 N60 O12, C70, 11 (C F3 O3 S) [+ solvent]	C236 H227 La4 N60 O12, C70, 11 (C F3 O3 S)
Sum formula	C317 H227 F33 La4 N60 O45 S11 [+ solvent]	C317 H227 F33 La4 N60 O45 S11
Mr	7131.84	7131.84
Dx, g cm ⁻³	1.362	1.362
Z	8	8
Mu (mm ⁻¹)	0.639	0.639
F000	28880.0	28880.0
F000'	28895.93	
h, k, lmax		44, 46, 45
Nref		48416
Tmin, Tmax	0.858, 0.909	
Tmin'	0.852	

Correction method= Not given

Data completeness= Theta (max)= 22.996

R(reflections)= 0.1224 (33359)

wR2(reflections)=
0.3877 (47685)

S = 1.575

Npar= 3835

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 $\sin(\theta_{\max})/\lambda = 0.5497$

Author Response: The crystals of this giant supramolecular assembly diffract very weakly in nature, possibly due to a large amount of amorphous solvents and highly-disordered counterions existing in the unit cell, which occupy as much as 37.8% of the unit cell based on PLATON calculation.

Alert level B

REFLT01_ALERT_1_B The number of symmetry-independent reflections cannot exceed the total number of reflections measured

Number of symmetry-independent reflections = 48416

Total number of reflections = 47685

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) 0.39 Report

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C58_2 Check

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of C41_3 Check

PLAT260_ALERT_2_B Large Average Ueq of Residue Including S1_16 0.384 Check

PLAT260_ALERT_2_B Large Average Ueq of Residue Including S1_17 0.347 Check

PLAT412_ALERT_2_B Short Intra XH3 .. XHn H1A_2 ..H8AC_2 . 1.75 Ang.

x, y, z = 1_555 Check

PLAT413_ALERT_2_B Short Inter XH3 .. XHn H75_1 ..H76A_1 . 1.90 Ang.

-x, 1-y, -z = 5_565 Check

PLAT430_ALERT_2_B Short Inter D...A Contact O3 ..O3 . 2.63 Ang.

1-x, y, 1/2-z = 2_655 Check

PLAT430_ALERT_2_B Short Inter D...A Contact O3_16 ..O3_16 . 2.58 Ang.

-x, y, 1/2-z = 2_555 Check

Alert level C

PLAT030_ALERT_1_C _diffn_reflms_number < _reflms_number_total Please Check

PLAT052_ALERT_1_C Info on Absorption Correction Method Not Given Please Do !

PLAT082_ALERT_2_C High R1 Value 0.12 Report

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O56_1 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O39_2 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O39_4 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O73_4 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C69_2 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C35_3 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C69_3 Check

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C70_3 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N57_3 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C41_1 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C58_1 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C75_2 Check

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C58_3 Check

PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C75_4	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C37_18	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	S1	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	S1_5	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	S1_6	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	S1_7	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	S1_9	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	S1_10	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	S1_11	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	S1_13	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	S1_16	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	S1_17	Check
PLAT250_ALERT_2_C	Large	U3/U1 Ratio for Average U(i,j) Tensor		2.3	Note
PLAT250_ALERT_2_C	Large	U3/U1 Ratio for Average U(i,j) Tensor		2.3	Note
PLAT250_ALERT_2_C	Large	U3/U1 Ratio for Average U(i,j) Tensor		3.0	Note
PLAT250_ALERT_2_C	Large	U3/U1 Ratio for Average U(i,j) Tensor		2.6	Note
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	La01	0.122	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	C1_18	0.246	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1	0.250	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_5	0.126	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_6	0.132	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_7	0.172	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_8	0.147	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_9	0.250	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_10	0.178	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_11	0.239	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	S1_13	0.218	Check
PLAT342_ALERT_3_C	Low	Bond Precision on C-C Bonds		0.0145	Ang.
PLAT361_ALERT_2_C	Long	C(sp3)-C(sp3) Bond	C2_4 - C5_4	1.66	Ang.
PLAT369_ALERT_2_C	Long	C(sp2)-C(sp2) Bond	C37_3 - C38_3	1.53	Ang.
PLAT413_ALERT_2_C	Short	Inter XH3 .. XHn	H7AB_3 ..H59A_4	2.10	Ang.
			1/2-x, 3/2-y, -z =	7_565	Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N74_3	--H74_3		Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N57_4	--H57_4		Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N74_4	--H74_4		Please Check
PLAT431_ALERT_2_C	Short Inter HL..A Contact	F6_17	..N61_3	2.76	Ang.
			1/2-x, -1/2+y, 1/2-z =	4_545	Check
PLAT906_ALERT_3_C	Large	K Value in the Analysis of Variance		2.040	Check
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & Sth/L=	0.550	730	Report
		2 0 0, 8 0 0, 22 0 0, 24 0 0, 15 1 0, 27 1 0,			
		0 2 0, 8 2 0, 10 2 0, 5 3 0, 19 3 0, 23 5 0,			
		20 6 0, 19 7 0, 6 8 0, 8 8 0, 7 9 0, 13 11 0,			
		16 12 0, 18 14 0, 22 14 0, 9 15 0, 23 17 0, 14 18 0,			
		5 19 0, 8 24 0, 10 26 0, -17 1 1, -22 2 1, 2 2 1,			
		10 2 1, -19 3 1, -7 3 1, 15 3 1, -24 4 1, -16 4 1,			
		-4 4 1, -2 4 1, 12 4 1, -17 5 1, -14 6 1, -6 6 1,			
		6 6 1, 18 6 1, 26 6 1, -19 7 1, 13 7 1, -8 8 1,			
		28 8 1, 9 9 1, -6 10 1, 8 10 1, 14 10 1, 18 10 1,			
		-13 11 1, 13 11 1, 20 12 1, 24 12 1, -11 13 1, 11 13 1,			
		15 13 1, 25 13 1, -9 15 1, 20 16 1, -1 17 1, 9 17 1,			
		-6 18 1, 2 18 1, 21 19 1, -8 20 1, 1 21 1, -14 22 1,			
		10 22 1, -5 23 1, -32 32 1, -28 0 2, -20 0 2, -12 0 2,			
		-10 0 2, -4 0 2, 4 0 2, 8 0 2, 12 0 2, 20 0 2,			
		29 1 2, -22 2 2, -8 2 2, -2 2 2, 10 2 2, 20 2 2,			
		22 2 2, 24 4 2, -27 5 2, -21 5 2, -17 5 2, -3 5 2,			
PLAT913_ALERT_3_C	Missing	# of Very Strong Reflections in FCF		13	Note
		2 0 0, 0 2 0, 2 2 1, -4 4 1, -2 2 2, -3 5 2,			

0 0 4, 8 0 4, 8 4 4, 2 4 7, -3 7 7, -4 0 10,
-8 0 12,
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 15 Check
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.58Ang From O3_17 . 1.00 eA-3

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 193 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 458 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 12 Report
H26# H38# H50# H83# H95# H106# H139# H151# H163# H196# H208#
H220#

PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 8 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 43 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 10 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 30 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 9 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C5_5 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C5_6 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C5_7 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C6_8 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C5_9 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C5_10 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C5_11 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C6_13 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C5_16 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of C5_17 Check
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C2_18 -C12_18 0.18 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C7_18 -C22_18 0.16 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C8_18 -C25_18 0.18 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C14_18 -C33_18 0.19 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C23_18 -C42_18 0.20 Ang.
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C1_18 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C4_18 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C18_18 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C21_18 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C29_18 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C39_18 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C41_18 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C46_18 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C47_18 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C50_18 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C54_18 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C68_18 Check
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C70_18 Check
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C47_18 - C63_18 . 1.52 Ang.
PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C65_18 - C70_18 . 1.51 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact F8_16 ..C58_1 . 2.69 Ang.
-1/2+x,1/2+y,z = 3_455 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact F6_17 ..C18_3 . 2.84 Ang.

		$1/2-x, -1/2+y, 1/2-z =$	4_545	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F6_17 ..C53_4 .	2.91	Ang.
		$1/2-x, -1/2+y, 1/2-z =$	4_545	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F8_17 ..C53_4 .	2.54	Ang.
		$1/2-x, -1/2+y, 1/2-z =$	4_545	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O2_11 ..C48_4 .	2.99	Ang.
		$x, y, z =$	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O3_11 ..C48_3 .	3.01	Ang.
		$x, y, z =$	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C12_1 ..C16_18 .	3.19	Ang.
		$x, y, z =$	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C18_4 ..C59_18 .	3.10	Ang.
		$x, y, z =$	1_555	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact	F8_17 ..F8_17 .	2.80	Ang.
		$1/2-x, 1/2-y, 1-z =$	7_556	Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure		!	Info
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		689	Note

La01	La02	La03	La04	C1_1	H1A_1	H1AB_1	H1AC_1
C2_1	C3_1	C4_1	C5_1	C6_1	H6A_1	H6AB_1	H6AC_1
C7_1	H7A_1	H7AB_1	H7AC_1	C8_1	H8A_1	H8AB_1	H8AC_1
C9_1	C10_1	C11_1	H11_1	C12_1	C13_1	H13_1	C14_1
H14_1	C15_1	C16_1	C17_1	H17_1	C18_1	C19_1	H19_1
C20_1	H20_1	C21_1	C22_1	C23_1	H23_1	C24_1	H24_1
C25_1	C26_1	H26_1	N27_1	N28_1	N29_1	C30_1	C31_1
H31_1	N32_1	C33_1	C34_1	H34_1	C35_1	H35_1	C36_1
H36_1	C37_1	C38_1	O39_1	N40_1	H40_1	C41_1	H41_1
C42_1	H42A_1	H42B_1	H42C_1	N44_1	N45_1	N46_1	C47_1
C48_1	H48_1	N49_1	C50_1	C51_1	H51_1	C52_1	H52_1
C53_1	H53_1	C54_1	C43_1	H43A_1	H43B_1	H43C_1	C55_1
O56_1	N57_1	H57_1	C58_1	H58_1	C59_1	H59A_1	H59B_1
H59C_1	N61_1	N62_1	N63_1	C64_1	C65_1	H65_1	N66_1
C67_1	C68_1	H68_1	C69_1	H69_1	C70_1	H70_1	C71_1
C60_1	H60A_1	H60B_1	H60C_1	C72_1	O73_1	N74_1	H74_1
C75_1	H75_1	C76_1	H76A_1	H76B_1	H76C_1	C77_1	H77A_1
H77B_1	H77C_1	C1_2	H1A_2	H1AB_2	H1AC_2	C2_2	C3_2
C4_2	C5_2	C6_2	H6A_2	H6AB_2	H6AC_2	C7_2	H7A_2
H7AB_2	H7AC_2	C8_2	H8A_2	H8AB_2	H8AC_2	C9_2	C10_2
C11_2	H11_2	C12_2	C13_2	H13_2	C14_2	H14_2	C15_2
C16_2	C17_2	H17_2	C18_2	C19_2	H19_2	C20_2	H20_2
C21_2	C22_2	C23_2	H23_2	C24_2	H24_2	C25_2	C26_2
H26_2	N27_2	N28_2	N29_2	C30_2	C31_2	H31_2	N32_2
C33_2	C34_2	H34_2	C35_2	H35_2	C36_2	H36_2	C37_2
C38_2	O39_2	N40_2	H40_2	C41_2	H41_2	C42_2	H42A_2
H42B_2	H42C_2	C43_2	H43A_2	H43B_2	H43C_2	N44_2	N45_2
N46_2	C47_2	C48_2	H48_2	N49_2	C50_2	C51_2	H51_2
C52_2	H52_2	C53_2	H53_2	C54_2	C55_2	O56_2	N57_2
H57_2	C58_2	C59_2	H59A_2	H59B_2	H59C_2	N61_2	N62_2
N63_2	C64_2	C65_2	H65_2	N66_2	C67_2	C68_2	H68_2
C69_2	H69_2	C70_2	H70_2	C71_2	C60_2	H60A_2	H60B_2
H60C_2	C72_2	O73_2	N74_2	H74_2	C75_2	H75_2	C76_2
H76A_2	H76B_2	H76C_2	C77_2	H77A_2	H77B_2	H77C_2	C1_3
H1A_3	H1AB_3	H1AC_3	C2_3	C3_3	C4_3	C5_3	C6_3
H6A_3	H6AB_3	H6AC_3	C7_3	H7A_3	H7AB_3	H7AC_3	C8_3
H8A_3	H8AB_3	H8AC_3	C9_3	C10_3	C11_3	H11_3	C12_3
C13_3	H13_3	C14_3	H14_3	C15_3	C16_3	C17_3	H17_3
C18_3	C19_3	H19_3	C20_3	H20_3	C21_3	C22_3	C23_3
H23_3	C24_3	C25_3	H25_3	C26_3	H26_3	N27_3	N28_3

N29_3	C30_3	C31_3	H31_3	N32_3	C33_3	C34_3	H34_3
C35_3	H35_3	C36_3	H36_3	C37_3	C38_3	O39_3	N40_3
H40_3	C41_3	H41_3	C42_3	H42A_3	H42B_3	H42C_3	N44_3
N45_3	N46_3	C47_3	C48_3	H48_3	N49_3	C50_3	C51_3
H51_3	C52_3	H52_3	C53_3	H53_3	C54_3	C43_3	H43A_3
H43B_3	H43C_3	C55_3	O56_3	N57_3	H57_3	C58_3	H58_3
C59_3	H59A_3	H59B_3	H59C_3	N61_3	N62_3	N63_3	C64_3
C65_3	H65_3	N66_3	C67_3	C68_3	H68_3	C69_3	H69_3
C70_3	H70_3	C71_3	C60_3	H60A_3	H60B_3	H60C_3	C72_3
O73_3	N74_3	H74_3	C75_3	H75_3	C76_3	H76A_3	H76B_3
H76C_3	C77_3	H77A_3	H77B_3	H77C_3	C1_4	H1A_4	H1AB_4
H1AC_4	C2_4	C3_4	C4_4	C5_4	C6_4	H6A_4	H6AB_4
H6AC_4	C7_4	H7A_4	H7AB_4	H7AC_4	C8_4	H8A_4	H8AB_4
H8AC_4	C9_4	C10_4	C11_4	H11_4	C12_4	C13_4	H13_4
C14_4	H14_4	C15_4	C16_4	C17_4	H17_4	C18_4	C19_4
H19_4	C20_4	H20_4	C21_4	C22_4	C23_4	H23_4	C24_4
C25_4	H25_4	C26_4	H26_4	N27_4	N28_4	N29_4	C30_4
C31_4	H31_4	N32_4	C33_4	C34_4	H34_4	C35_4	H35_4
C36_4	H36_4	C37_4	C38_4	O39_4	N40_4	H40_4	C41_4
H41_4	C42_4	H42A_4	H42B_4	H42C_4	C43_4	H43A_4	H43B_4
H43C_4	N44_4	N45_4	N46_4	C47_4	C48_4	H48_4	N49_4
C50_4	C51_4	H51_4	C52_4	H52_4	C53_4	H53_4	C54_4
C55_4	O56_4	N57_4	H57_4	C58_4	H58_4	C59_4	H59A_4
H59B_4	H59C_4	C60_4	H60A_4	H60B_4	H60C_4	N61_4	N62_4
N63_4	C64_4	C65_4	H65_4	N66_4	C67_4	C68_4	H68_4
C69_4	H69_4	C70_4	H70_4	C71_4	C72_4	O73_4	N74_4
H74_4	C75_4	H75_4	C76_4	H76A_4	H76B_4	H76C_4	C77_4
H77A_4	H77B_4	H77C_4	S1_5	O2_5	O3_5	O4_5	C5_5
F6_5	F7_5	F8_5	S1_6	O2_6	O3_6	O4_6	C5_6
F6_6	F7_6	F8_6	S1_7	O2_7	O3_7	O4_7	C5_7
F6_7	F7_7	F8_7	S1_8	O3_8	O4_8	O5_8	C6_8
F7_8	F8_8	F9_8	S1_9	O2_9	O3_9	O4_9	C5_9
F6_9	F7_9	F8_9	S1_10	O2_10	O3_10	O4_10	C5_10
F6_10	F7_10	F8_10	S1_11	O2_11	O3_11	O4_11	C5_11
F6_11	F7_11	F8_11	S1_13	O2_13	O3_13	O4_13	C6_13
F7_13	F8_13	F9_13	S1_16	O2_16	O3_16	O4_16	C5_16
F6_16	F7_16	F8_16	S1_17	O2_17	O3_17	O4_17	C5_17
F6_17	F7_17	F8_17	C1_18	C2_18	C3_18	C4_18	C5_18
C6_18	C7_18	C8_18	C9_18	C10_18	C11_18	C12_18	C13_18
C14_18	C15_18	C16_18	C17_18	C18_18	C19_18	C20_18	C21_18
C22_18	C23_18	C24_18	C25_18	C26_18	C27_18	C28_18	C29_18
C30_18	C31_18	C32_18	C33_18	C34_18	C35_18	C36_18	C37_18
C38_18	C39_18	C40_18	C41_18	C42_18	C43_18	C44_18	C45_18
C46_18	C47_18	C48_18	C49_18	C50_18	C51_18	C52_18	C53_18
C54_18	C55_18	C56_18	C57_18	C58_18	C59_18	C60_18	C61_18
C62_18	C63_18	C64_18	C65_18	C66_18	C67_18	C68_18	C69_18
C70_18							

PLAT773_ALERT_2_G Check long C-C Bond in CIF: C11_18 --C13_18 1.96 Ang.
 PLAT773_ALERT_2_G Check long C-C Bond in CIF: C29_18 --C31_18 1.97 Ang.
 PLAT773_ALERT_2_G Check long C-C Bond in CIF: C58_18 --C60_18 1.98 Ang.
 PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 42.40 Deg.
 C12_1-C11_1-C13_1 1_555 1_555 1_555 # 1375 Check
 PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 43.10 Deg.
 C12_1-C13_1-C11_1 1_555 1_555 1_555 # 1384 Check
 PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 42.90 Deg.
 C30_1-C29_1-C31_1 1_555 1_555 1_555 # 1435 Check
 PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 42.20 Deg.

```

C30_1-C31_1-C29_1  1_555  1_555  1_555  .....  # 1444 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 41.70 Deg.
C59_1-C58_1-C60_1  1_555  1_555  1_555  .....  # 1528 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 41.20 Deg.
C59_1-C60_1-C58_1  1_555  1_555  1_555  .....  # 1537 Check
PLAT794_ALERT_5_G Tentative Bond Valency for La01 (III) . 3.88 Info
PLAT794_ALERT_5_G Tentative Bond Valency for La02 (III) . 3.96 Info
PLAT794_ALERT_5_G Tentative Bond Valency for La03 (III) . 3.82 Info
PLAT794_ALERT_5_G Tentative Bond Valency for La04 (III) . 3.92 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 13065 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL 2019/3 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 50 Note
12 6 13, -1 17 7, 10 4 7, 5 15 17, -5 1 6, -17 5 3,
-7 3 1, -11 5 9, 11 9 5, 2 10 5, -1 1 14, -4 2 21,
-6 4 17, 10 2 0, 4 6 13, -3 7 18, 1 11 21, -17 5 1,
4 6 3, 5 1 7, -22 4 10, -4 0 2, 2 8 6, 9 7 21,
2 12 3, -3 7 14, 8 6 12, 12 0 2, -5 3 4, -11 13 10,
16 10 13, -2 4 7, -21 7 8, 3 3 3, 17 3 6, 20 6 0,
-1 17 1, 18 6 1, 1 3 9, -7 11 11, -2 4 1, -9 5 15,
10 8 4, 13 13 13, -14 2 15, -10 0 20, 9 9 1, 13 11 12,
-6 8 7, 3 1 7,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 1.0 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info
PLAT982_ALERT_1_G The La-f' = -0.2345 Deviates from IT-value = -0.2871 Check
PLAT982_ALERT_1_G The S-f' = 0.1265 Deviates from IT-value = 0.1246 Check
PLAT983_ALERT_1_G The La-f" = 2.4853 Deviates from IT-Value = 2.4523 Check
PLAT983_ALERT_1_G The S-f" = 0.1256 Deviates from IT-Value = 0.1234 Check
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 10 Check

```

-
- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
10 **ALERT level B** = A potentially serious problem, consider carefully
56 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
80 **ALERT level G** = General information/check it is not something unexpected
- 11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
83 ALERT type 2 Indicator that the structure model may be wrong or deficient
9 ALERT type 3 Indicator that the structure quality may be low
38 ALERT type 4 Improvement, methodology, query or suggestion
6 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.

