

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cs6-185

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: cs6-185

Bond precision:	C-C = 0.0074 Å	Wavelength=0.82641
Cell:	a=25.3712 (6) alpha=90	b=15.0697 (3) beta=94.686 (1) c=19.9969 (5) gamma=90
Temperature:	185 K	
	Calculated	Reported
Volume	7620.0 (3)	7620.0 (3)
Space group	C 2/m	C 1 2/m 1
Hall group	-C 2y	-C 2y
Moiety formula	C82 N U, C36 H44 N4 Ni, 2(C3 H3), 0.775(C6 H6), C0.45 S0.45	C82 N U1, C36 H44 N4 Ni, 1.78(C6 H6), 0.22(C2 S2)
Sum formula	C129.10 H54.65 N5 Ni S0.45 U	C129.10 H54.65 N5 Ni S0.45 U
Mr	1986.35	1986.82
Dx, g cm ⁻³	1.732	1.732
Z	4	4
Mu (mm ⁻¹)	1.814	1.848
F000	3965.1	3966.0
F000'	3943.91	
h, k, lmax	31, 18, 24	31, 18, 24
Nref	7815	7664
Tmin, Tmax		0.766, 0.831
Tmin'		

Correction method= # Reported T Limits: Tmin=0.766 Tmax=0.831
AbsCorr = MULTII-SCAN

Data completeness= 0.981

Theta(max)= 30.670

R(reflections)= 0.0831(7127)

wR2(reflections)=
0.2342(7664)

S = 1.041

Npar= 1048

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

PLAT088_ALERT_3_B Poor Data / Parameter Ratio 7.31 Note

 Alert level C

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT215_ALERT_3_C Disordered C19 has ADP max/min Ratio 3.7 Note
PLAT215_ALERT_3_C Disordered C20 has ADP max/min Ratio 3.3 Note
PLAT215_ALERT_3_C Disordered C28 has ADP max/min Ratio 3.2 Note
PLAT215_ALERT_3_C Disordered C33 has ADP max/min Ratio 3.3 Note
PLAT215_ALERT_3_C Disordered C53 has ADP max/min Ratio 3.2 Note
PLAT215_ALERT_3_C Disordered C54 has ADP max/min Ratio 3.5 Note
PLAT234_ALERT_4_C Large Hirshfeld Difference C13 --C31 . 0.16 Ang.
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C7S 0.147 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including S1S 0.153 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.113 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 46 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 15 Note
PLAT977_ALERT_2_C Check Negative Difference Density on H5S -0.32 eA-3

 Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C129.1 H54.65 N5 Ni1 S0.45 U1
Atom count from _chemical_formula_moiety:C129.1199 H54.68 N5 Ni1 S0.44
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 85 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 92 Report
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.15 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 54.04 Why ?
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.82641 Ang.
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 5 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 12 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 74 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 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) U1 --N1 . 7.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) U2 --C63 . 5.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) U4 --N1 . 5.4 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of C2 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4 Constrained at 0.5 Check

[illegible]

PLAT300_ALERT_4_G	Atom Site Occupancy of C64	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C65	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C66	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C67	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C68	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C69	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C70	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C71	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C72	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C74	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C75	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C76	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C77	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C78	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C79	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C80	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C82	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		93%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 4)		9.30	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 5)		0.90	Check
PLAT315_ALERT_2_G	Singly Bonded Carbon Detected (H-atoms Missing).		C10S	Check
PLAT333_ALERT_2_G	Large Aver C6-Ring C-C Dist C3 -C14 .		1.43	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C15 ..C33		3.19	Ang.
	3/2-x,1/2-y,-z =	7_655	Check	
PLAT432_ALERT_2_G	Short Inter X...Y Contact C28 ..C33		3.19	Ang.
	3/2-x,-1/2+y,-z =	4_645	Check	
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .		2.38	Ratio
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C2 --C10		2.01	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C2 --C11		1.83	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C4 --C8		2.00	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C5 --C7		2.03	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C5 --C10		1.92	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C7 --C8		1.78	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C8 --C20		1.96	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C10 --C14		1.78	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C11 --C15		1.72	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C13 --C29		1.85	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C13 --C30		1.86	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C15 --C27		1.70	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C16 --C47		1.77	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C20 --C21		1.88	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C22 --C41		1.84	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C22 --C42		1.74	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C23 --C39		1.89	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C28 --C34		1.85	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C28 --C36		1.91	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C29 --C32		1.96	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C30 --C53		2.03	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C32 --C51		1.89	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C32 --C53		1.79	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C34 --C70		1.99	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C34 --C71		1.95	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C35 --C47		1.98	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C35 --C70		1.97	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C36 --C49		1.94	Ang.

PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C37	--C66	2.04	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C38	--C44	1.97	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C38	--C47	1.94	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C39	--C43	1.94	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C39	--C46	1.87	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C39	--C66	2.03	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C40	--C42	1.70	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C41	--C41	1.83	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C41	--C44	1.83	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C41	--C64	1.83	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C43	--C61	1.95	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C44	--C60	1.91	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C48	--C59	1.74	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C49	--C55	1.77	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C49	--C56	1.71	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C50	--C55	1.77	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C51	--C53	1.76	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C52	--C54	1.74	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C53	--C54	1.74	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C55	--C72	2.03	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C57	--C68	1.86	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C57	--C69	1.71	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C58	--C66	1.79	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C58	--C69	2.00	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C61	--C80	1.99	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C62	--C65	1.90	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C64	--C77	1.91	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C65	--C76	2.00	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C67	--C76	1.84	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C69	--C76	1.82	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C71	--C72	1.90	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C75	--C79	1.91	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C75	--C80	1.88	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C76	--C79	1.97	Ang.
PLAT773_ALERT_2_G	Check	long	C-C	Bond	in	CIF:	C78	--C80	1.76	Ang.
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in	CIF ...		42.40	Deg.
	C2	-C1	-C2	1_555	1_555	6_555		#	1	Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in	CIF ...		19.80	Deg.
	C3	-C2	-C10	1_555	1_555	6_555		#	29	Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in	CIF ...		30.90	Deg.
	C3	-C2	-C11	1_555	1_555	6_555		#	30	Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in	CIF ...		43.30	Deg.
	C11	-C2	-C10	6_555	1_555	6_555		#	33	Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in	CIF ...		27.30	Deg.
	C12	-C2	-C12	6_555	1_555	1_555		#	43	Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in	CIF ...		42.10	Deg.
	C2	-C3	-C12	1_555	1_555	6_555		#	46	Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in	CIF ...		21.60	Deg.
	C10	-C3	-C4	6_555	1_555	1_555		#	51	Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in	CIF ...		8.60	Deg.
	C11	-C3	-C14	6_555	1_555	1_555		#	60	Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in	CIF ...		10.50	Deg.
	C5	-C4	-C8	1_555	1_555	6_555		#	67	Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in	CIF ...		43.60	Deg.
	C9	-C4	-C8	6_555	1_555	6_555		#	70	Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in	CIF ...		25.40	Deg.
	C10	-C4	-C3	6_555	1_555	1_555		#	73	Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.30 Deg.
C26 -C4 -C17	6_555 1_555 1_555	 #	85 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.10 Deg.
C4 -C5 -C10	1_555 1_555 6_555	 #	87 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	33.40 Deg.
C6 -C5 -C7	1_555 1_555 6_555	 #	91 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.80 Deg.
C8 -C5 -C7	6_555 1_555 6_555	 #	99 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	5.00 Deg.
C19 -C5 -C24	1_555 1_555 6_555	 #	117 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.70 Deg.
C7 -C6 -C7	6_555 1_555 1_555	 #	131 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.50 Deg.
C8 -C6 -C5	6_555 1_555 1_555	 #	134 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	39.80 Deg.
C6 -C7 -C5	6_555 1_555 6_555	 #	144 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	37.00 Deg.
C6 -C7 -C8	1_555 1_555 6_555	 #	146 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.40 Deg.
C7 -C7 -C8	6_555 1_555 6_555	 #	156 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	8.50 Deg.
C8 -C7 -C5	1_555 1_555 6_555	 #	160 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	21.30 Deg.
C21 -C7 -C21	6_555 1_555 1_555	 #	170 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	22.00 Deg.
C5 -C8 -C4	6_555 1_555 6_555	 #	172 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	5.30 Deg.
C7 -C8 -C7	1_555 1_555 6_555	 #	191 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	40.50 Deg.
C9 -C8 -C4	1_555 1_555 6_555	 #	197 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	6.60 Deg.
C19 -C8 -C24	6_555 1_555 1_555	 #	208 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.30 Deg.
C24 -C8 -C20	1_555 1_555 6_555	 #	214 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.70 Deg.
C4 -C9 -C10	6_555 1_555 1_555	 #	226 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	28.60 Deg.
C5 -C9 -C8	6_555 1_555 1_555	 #	233 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	31.10 Deg.
C10 -C9 -C3	1_555 1_555 6_555	 #	250 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.40 Deg.
C3 -C10 -C2	6_555 1_555 6_555	 #	253 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	40.40 Deg.
C3 -C10 -C11	6_555 1_555 1_555	 #	256 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.70 Deg.
C4 -C10 -C5	6_555 1_555 6_555	 #	263 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	33.80 Deg.
C9 -C10 -C5	1_555 1_555 6_555	 #	273 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	9.90 Deg.
C11 -C10 -C14	1_555 1_555 6_555	 #	280 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	11.10 Deg.
C26 -C10 -C17	1_555 1_555 6_555	 #	295 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.60 Deg.
C3 -C11 -C10	6_555 1_555 1_555	 #	298 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	38.80 Deg.
C12 -C11 -C2	1_555 1_555 6_555	 #	307 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.00 Deg.

C12	-C11	-C13	1_555	1_555	6_555		#	308 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		27.00 Deg.
C14	-C11	-C29	6_555	1_555	1_555		#	318 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		28.60 Deg.
C29	-C11	-C15	1_555	1_555	6_555		#	324 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		41.60 Deg.
C2	-C12	-C2	6_555	1_555	1_555		#	325 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		34.20 Deg.
C11	-C12	-C3	1_555	1_555	6_555		#	333 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		14.70 Deg.
C11	-C12	-C14	1_555	1_555	6_555		#	334 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		27.40 Deg.
C12	-C13	-C12	6_555	1_555	1_555		#	357 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		17.30 Deg.
C14	-C13	-C11	1_555	1_555	6_555		#	373 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		33.60 Deg.
C14	-C13	-C29	1_555	1_555	6_555		#	374 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		44.60 Deg.
C31	-C13	-C30	1_555	1_555	6_555		#	380 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		27.00 Deg.
C3	-C14	-C10	1_555	1_555	6_555		#	381 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		19.00 Deg.
C11	-C14	-C3	6_555	1_555	1_555		#	385 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		33.00 Deg.
C11	-C14	-C10	6_555	1_555	6_555		#	386 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		40.40 Deg.
C13	-C14	-C12	1_555	1_555	6_555		#	393 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		33.40 Deg.
C29	-C14	-C15	6_555	1_555	1_555		#	401 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		13.40 Deg.
C14	-C15	-C11	1_555	1_555	6_555		#	402 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		8.20 Deg.
C16	-C15	-C27	1_555	1_555	6_555		#	407 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		43.30 Deg.
C29	-C15	-C14	6_555	1_555	1_555		#	417 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		11.00 Deg.
C26	-C16	-C17	6_555	1_555	1_555		#	431 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		16.00 Deg.
C27	-C16	-C36	6_555	1_555	1_555		#	440 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		11.00 Deg.
C27	-C16	-C47	6_555	1_555	6_555		#	441 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		35.10 Deg.
C28	-C16	-C15	6_555	1_555	1_555		#	443 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		22.60 Deg.
C36	-C16	-C47	1_555	1_555	6_555		#	448 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		25.60 Deg.
C4	-C17	-C10	1_555	1_555	6_555		#	451 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		12.70 Deg.
C16	-C17	-C27	1_555	1_555	6_555		#	460 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		7.30 Deg.
C25	-C17	-C18	6_555	1_555	1_555		#	471 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		41.00 Deg.
C26	-C17	-C16	6_555	1_555	1_555		#	477 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		19.00 Deg.
U5	-C17	-U4	1_555	1_555	1_555		#	486 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		8.30 Deg.
C17	-C18	-C26	1_555	1_555	6_555		#	487 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	8.10 Deg.
C24 -C18 -C19	6_555 1_555 1_555	 #	499 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	28.00 Deg.
C25 -C18 -C17	6_555 1_555 1_555	 #	505 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	20.00 Deg.
C25 -C18 -C26	6_555 1_555 6_555	 #	508 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	24.30 Deg.
C38 -C18 -C46	1_555 1_555 6_555	 #	521 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.90 Deg.
U4 -C18 -U1	1_555 1_555 1_555	 #	529 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	20.40 Deg.
U4 -C18 -U5	1_555 1_555 1_555	 #	530 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.00 Deg.
U5 -C18 -U1	1_555 1_555 1_555	 #	531 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.40 Deg.
C8 -C19 -C5	6_555 1_555 1_555	 #	539 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	11.50 Deg.
C18 -C19 -C25	1_555 1_555 6_555	 #	549 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	26.50 Deg.
C20 -C19 -C23	1_555 1_555 6_555	 #	553 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	36.00 Deg.
C24 -C19 -C23	6_555 1_555 6_555	 #	565 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	36.00 Deg.
C24 -C19 -U1	6_555 1_555 1_555	 #	567 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.70 Deg.
U1 -C19 -U5	1_555 1_555 1_555	 #	574 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	13.80 Deg.
U4 -C19 -U1	1_555 1_555 1_555	 #	575 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.30 Deg.
U4 -C19 -U5	1_555 1_555 1_555	 #	576 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	41.10 Deg.
C19 -C20 -C8	1_555 1_555 6_555	 #	579 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	5.10 Deg.
C21 -C20 -C21	1_555 1_555 6_555	 #	587 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	31.40 Deg.
C23 -C20 -C40	6_555 1_555 1_555	 #	607 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	7.20 Deg.
C24 -C20 -C19	6_555 1_555 1_555	 #	611 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.20 Deg.
U4 -C20 -U1	1_555 1_555 1_555	 #	621 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.00 Deg.
C7 -C21 -C7	6_555 1_555 1_555	 #	622 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	14.30 Deg.
C21 -C21 -C20	6_555 1_555 6_555	 #	638 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	35.30 Deg.
C22 -C21 -C20	1_555 1_555 6_555	 #	646 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.70 Deg.
C20 -C22 -C23	6_555 1_555 1_555	 #	653 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.20 Deg.
C21 -C22 -C21	6_555 1_555 1_555	 #	660 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	38.00 Deg.
C23 -C22 -C40	1_555 1_555 6_555	 #	681 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	21.90 Deg.
C42 -C22 -C41	1_555 1_555 6_555	 #	698 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	24.40 Deg.
C42 -C22 -C42	1_555 1_555 6_555	 #	699 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.70 Deg.

U4	-C22	-U1	6_555	1_555	6_555		#	704 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		4.80 Deg.
C24	-C23	-C19	1_555	1_555	6_555		#	722 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		30.50 Deg.
C40	-C23	-C44	6_555	1_555	1_555		#	733 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		21.30 Deg.
C44	-C23	-C39	1_555	1_555	6_555		#	737 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		17.50 Deg.
U4	-C23	-U1	6_555	1_555	6_555		#	740 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		26.30 Deg.
C8	-C24	-C5	1_555	1_555	6_555		#	744 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		11.90 Deg.
C18	-C24	-C25	6_555	1_555	1_555		#	753 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		36.00 Deg.
C19	-C24	-C5	6_555	1_555	6_555		#	757 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		29.40 Deg.
C20	-C24	-C23	6_555	1_555	1_555		#	768 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		17.60 Deg.
U1	-C24	-U5	6_555	1_555	6_555		#	783 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		15.00 Deg.
U4	-C24	-U1	6_555	1_555	6_555		#	784 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		17.20 Deg.
U4	-C24	-U5	6_555	1_555	6_555		#	785 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		11.40 Deg.
C17	-C25	-C26	6_555	1_555	1_555		#	788 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		7.50 Deg.
C24	-C25	-C19	1_555	1_555	6_555		#	806 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		23.90 Deg.
C38	-C25	-C46	6_555	1_555	1_555		#	819 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		16.50 Deg.
U4	-C25	-U1	6_555	1_555	6_555		#	828 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		21.80 Deg.
U4	-C25	-U5	6_555	1_555	6_555		#	829 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		18.60 Deg.
U5	-C25	-U1	6_555	1_555	6_555		#	830 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		29.70 Deg.
C4	-C26	-C10	6_555	1_555	1_555		#	831 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		14.00 Deg.
C16	-C26	-C27	6_555	1_555	1_555		#	844 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		34.00 Deg.
C17	-C26	-C18	6_555	1_555	6_555		#	850 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		39.00 Deg.
C17	-C26	-C25	6_555	1_555	1_555		#	851 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		4.30 Deg.
C25	-C26	-C18	1_555	1_555	6_555		#	858 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		19.60 Deg.
U5	-C26	-U4	6_555	1_555	6_555		#	866 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		35.00 Deg.
C16	-C27	-C15	6_555	1_555	6_555		#	868 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		11.70 Deg.
C26	-C27	-C17	1_555	1_555	6_555		#	878 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		28.70 Deg.
C28	-C27	-C15	1_555	1_555	6_555		#	881 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		28.80 Deg.
C36	-C27	-C47	6_555	1_555	1_555		#	890 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...		27.10 Deg.
C15	-C28	-C29	6_555	1_555	1_555		#	897 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	14.50 Deg.
C16 -C28 -C27	6_555 1_555 1_555	 #	903 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	37.70 Deg.
C27 -C28 -C36	1_555 1_555 6_555	 #	912 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	4.40 Deg.
C50 -C28 -C34	1_555 1_555 6_555	 #	928 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	11.60 Deg.
C14 -C29 -C11	6_555 1_555 1_555	 #	937 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	27.00 Deg.
C15 -C29 -C28	6_555 1_555 1_555	 #	946 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	10.80 Deg.
C30 -C29 -C32	1_555 1_555 6_555	 #	954 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	14.40 Deg.
C32 -C30 -C52	6_555 1_555 1_555	 #	973 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	11.40 Deg.
C32 -C30 -C53	6_555 1_555 6_555	 #	974 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	22.40 Deg.
C52 -C30 -C53	1_555 1_555 6_555	 #	979 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.20 Deg.
C13 -C31 -C13	6_555 1_555 1_555	 #	980 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	24.20 Deg.
C30 -C31 -C32	6_555 1_555 1_555	 #	992 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	24.20 Deg.
C30 -C31 -C32	1_555 1_555 6_555	 #	993 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	26.50 Deg.
C30 -C32 -C29	6_555 1_555 6_555	 #	995 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	30.90 Deg.
C52 -C32 -C51	6_555 1_555 6_555	 #	1013 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	35.20 Deg.
C52 -C32 -C53	6_555 1_555 1_555	 #	1014 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.50 Deg.
C53 -C32 -C53	1_555 1_555 6_555	 #	1022 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	32.80 Deg.
C28 -C33 -C15	6_555 1_555 1_555	 #	1025 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	32.30 Deg.
C29 -C33 -C15	6_555 1_555 1_555	 #	1032 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	23.50 Deg.
C30 -C33 -C32	6_555 1_555 1_555	 #	1039 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	31.50 Deg.
C32 -C33 -C52	1_555 1_555 6_555	 #	1045 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	14.90 Deg.
C50 -C33 -C34	6_555 1_555 1_555	 #	1055 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.10 Deg.
C51 -C33 -C52	6_555 1_555 6_555	 #	1058 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.50 Deg.
C33 -C34 -C28	1_555 1_555 6_555	 #	1061 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	22.70 Deg.
C49 -C34 -C35	6_555 1_555 1_555	 #	1070 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.00 Deg.
C50 -C34 -C28	6_555 1_555 6_555	 #	1074 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	38.40 Deg.
C55 -C34 -C70	1_555 1_555 6_555	 #	1092 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	5.70 Deg.
C55 -C34 -C71	1_555 1_555 6_555	 #	1093 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.10 Deg.
C71 -C34 -C70	6_555 1_555 6_555	 #	1094 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.90 Deg.

C34	-C35	-C50	1_555	1_555	6_555		# 1097 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	14.50 Deg.
C36	-C35	-C47	1_555	1_555	6_555		# 1100 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	44.30 Deg.
C49	-C35	-C57	6_555	1_555	1_555		# 1116 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	11.00 Deg.
C49	-C35	-C70	6_555	1_555	6_555		# 1117 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	38.70 Deg.
C57	-C35	-C70	1_555	1_555	6_555		# 1127 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	41.30 Deg.
C16	-C36	-C28	1_555	1_555	6_555		# 1131 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	4.70 Deg.
C27	-C36	-C16	6_555	1_555	1_555		# 1134 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	4.80 Deg.
C35	-C36	-C49	1_555	1_555	6_555		# 1146 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	14.70 Deg.
C47	-C36	-C37	6_555	1_555	1_555		# 1156 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	43.40 Deg.
C38	-C37	-C45	1_555	1_555	6_555		# 1174 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	18.20 Deg.
C46	-C37	-C38	6_555	1_555	1_555		# 1186 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	12.20 Deg.
C47	-C37	-C36	6_555	1_555	1_555		# 1194 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	17.70 Deg.
C59	-C37	-C66	1_555	1_555	6_555		# 1212 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	15.30 Deg.
U1	-C37	-U3	1_555	1_555	1_555		# 1219 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	17.90 Deg.
U5	-C37	-U1	1_555	1_555	1_555		# 1220 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	28.00 Deg.
U5	-C37	-U3	1_555	1_555	1_555		# 1221 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	12.60 Deg.
C18	-C38	-C25	1_555	1_555	6_555		# 1222 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	23.00 Deg.
C37	-C38	-C47	1_555	1_555	6_555		# 1239 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	16.10 Deg.
C39	-C38	-C44	1_555	1_555	6_555		# 1246 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	34.60 Deg.
C45	-C38	-C39	6_555	1_555	1_555		# 1259 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	32.40 Deg.
C46	-C38	-C37	6_555	1_555	1_555		# 1268 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	15.00 Deg.
C46	-C38	-C47	6_555	1_555	6_555		# 1272 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	14.50 Deg.
U1	-C38	-U3	1_555	1_555	1_555		# 1282 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	16.90 Deg.
U1	-C38	-U4	1_555	1_555	1_555		# 1283 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	31.40 Deg.
U4	-C38	-U3	1_555	1_555	1_555		# 1284 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	19.90 Deg.
U5	-C38	-U1	1_555	1_555	1_555		# 1285 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	28.70 Deg.
U5	-C38	-U3	1_555	1_555	1_555		# 1286 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	20.20 Deg.
U5	-C38	-U4	1_555	1_555	1_555		# 1287 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	11.00 Deg.
C38	-C39	-C46	1_555	1_555	6_555		# 1296 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.40 Deg.
C40 -C39 -C23	1_555 1_555 6_555		# 1302 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.60 Deg.
C40 -C39 -C43	1_555 1_555 6_555		# 1303 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.10 Deg.
C44 -C39 -C23	6_555 1_555 6_555		# 1313 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.60 Deg.
C44 -C39 -C40	6_555 1_555 1_555		# 1315 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.10 Deg.
C44 -C39 -C43	6_555 1_555 6_555		# 1316 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	36.00 Deg.
C45 -C39 -C66	6_555 1_555 6_555		# 1330 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.50 Deg.
C60 -C39 -C66	1_555 1_555 6_555		# 1344 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.70 Deg.
U1 -C39 -U3	1_555 1_555 1_555		# 1351 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.10 Deg.
U1 -C39 -U4	1_555 1_555 1_555		# 1352 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	32.70 Deg.
U3 -C39 -U4	1_555 1_555 1_555		# 1353 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.20 Deg.
C20 -C40 -C22	1_555 1_555 6_555		# 1354 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	22.80 Deg.
C23 -C40 -C20	6_555 1_555 1_555		# 1364 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	26.40 Deg.
C41 -C40 -C42	1_555 1_555 6_555		# 1381 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.60 Deg.
C43 -C40 -C41	6_555 1_555 1_555		# 1391 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.70 Deg.
C44 -C40 -C39	6_555 1_555 1_555		# 1399 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.70 Deg.
U1 -C40 -U3	1_555 1_555 1_555		# 1406 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.30 Deg.
U1 -C40 -U4	1_555 1_555 1_555		# 1407 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	33.40 Deg.
U4 -C40 -U3	1_555 1_555 1_555		# 1408 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	25.00 Deg.
C40 -C41 -C44	1_555 1_555 6_555		# 1414 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.70 Deg.
C42 -C41 -C22	6_555 1_555 6_555		# 1424 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.50 Deg.
C42 -C41 -C41	6_555 1_555 6_555		# 1428 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	22.50 Deg.
C42 -C41 -C41	1_555 1_555 6_555		# 1429 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	22.00 Deg.
C42 -C41 -C42	6_555 1_555 1_555		# 1430 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.00 Deg.
C43 -C41 -C44	6_555 1_555 6_555		# 1448 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	7.80 Deg.
C62 -C41 -C64	1_555 1_555 6_555		# 1464 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	36.50 Deg.
U2 -C41 -U1	1_555 1_555 1_555		# 1472 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	26.30 Deg.
U2 -C41 -U3	1_555 1_555 1_555		# 1473 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.20 Deg.
U3 -C41 -U1	1_555 1_555 1_555		# 1474 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	8.70 Deg.

C41	-C42	-C43	6_555	1_555	1_555		# 1496 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	22.50 Deg.
C42	-C42	-C41	6_555	1_555	1_555		# 1506 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	15.10 Deg.
U1	-C42	-U3	6_555	1_555	6_555		# 1517 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	34.60 Deg.
U2	-C42	-U1	1_555	1_555	6_555		# 1518 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	24.20 Deg.
U2	-C42	-U3	1_555	1_555	6_555		# 1519 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	33.60 Deg.
C40	-C43	-C44	6_555	1_555	1_555		# 1526 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	9.00 Deg.
C41	-C43	-C42	6_555	1_555	1_555		# 1534 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	17.80 Deg.
C44	-C43	-C39	1_555	1_555	6_555		# 1547 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	16.40 Deg.
C62	-C43	-C64	6_555	1_555	1_555		# 1562 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	32.00 Deg.
C64	-C43	-C61	1_555	1_555	6_555		# 1568 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	37.00 Deg.
U1	-C43	-U2	6_555	1_555	1_555		# 1572 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	16.90 Deg.
U3	-C43	-U1	6_555	1_555	6_555		# 1573 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	26.50 Deg.
U3	-C43	-U2	6_555	1_555	1_555		# 1574 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	30.20 Deg.
C39	-C44	-C38	6_555	1_555	6_555		# 1586 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	10.00 Deg.
C39	-C44	-C45	6_555	1_555	1_555		# 1590 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	44.90 Deg.
C39	-C44	-C60	6_555	1_555	6_555		# 1591 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	37.00 Deg.
C40	-C44	-C23	6_555	1_555	1_555		# 1595 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	21.10 Deg.
C43	-C44	-C41	1_555	1_555	6_555		# 1611 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	35.70 Deg.
C45	-C44	-C38	1_555	1_555	6_555		# 1617 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	36.60 Deg.
C45	-C44	-C60	1_555	1_555	6_555		# 1619 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	17.40 Deg.
U1	-C44	-U3	6_555	1_555	6_555		# 1627 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	15.59 Deg.
U1	-C44	-U4	6_555	1_555	6_555		# 1628 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	32.70 Deg.
U3	-C44	-U4	6_555	1_555	6_555		# 1629 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	22.30 Deg.
C38	-C45	-C46	6_555	1_555	1_555		# 1636 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	9.70 Deg.
C39	-C45	-C44	6_555	1_555	1_555		# 1645 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	37.40 Deg.
C46	-C45	-C37	1_555	1_555	6_555		# 1660 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	28.80 Deg.
C60	-C45	-C66	6_555	1_555	1_555		# 1678 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	29.50 Deg.
C66	-C45	-C59	1_555	1_555	6_555		# 1685 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	17.90 Deg.
U1	-C45	-U3	6_555	1_555	6_555		# 1690 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	13.76 Deg.
U1 -C45 -U4	6_555 1_555 6_555	# 1691 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.80 Deg.
U1 -C45 -U5	6_555 1_555 6_555	# 1692 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	31.70 Deg.
U3 -C45 -U4	6_555 1_555 6_555	# 1693 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	30.80 Deg.
U3 -C45 -U5	6_555 1_555 6_555	# 1694 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.60 Deg.
U5 -C45 -U4	6_555 1_555 6_555	# 1695 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	12.70 Deg.
C25 -C46 -C18	1_555 1_555 6_555	# 1702 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	36.40 Deg.
C37 -C46 -C47	6_555 1_555 1_555	# 1713 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	26.50 Deg.
C38 -C46 -C39	6_555 1_555 6_555	# 1721 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	23.10 Deg.
C45 -C46 -C39	1_555 1_555 6_555	# 1732 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	14.10 Deg.
U1 -C46 -U3	6_555 1_555 6_555	# 1745 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.40 Deg.
U1 -C46 -U4	6_555 1_555 6_555	# 1746 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	30.40 Deg.
U4 -C46 -U3	6_555 1_555 6_555	# 1747 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	19.30 Deg.
U5 -C46 -U1	6_555 1_555 6_555	# 1748 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	27.20 Deg.
U5 -C46 -U3	6_555 1_555 6_555	# 1749 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	19.10 Deg.
U5 -C46 -U4	6_555 1_555 6_555	# 1750 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	2.80 Deg.
C27 -C47 -C16	1_555 1_555 6_555	# 1755 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	31.10 Deg.
C36 -C47 -C35	6_555 1_555 6_555	# 1765 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.00 Deg.
C37 -C47 -C38	6_555 1_555 6_555	# 1775 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	6.30 Deg.
C46 -C47 -C38	1_555 1_555 6_555	# 1786 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.60 Deg.
C48 -C47 -C35	1_555 1_555 6_555	# 1791 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.00 Deg.
U5 -C47 -U1	6_555 1_555 6_555	# 1795 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	21.50 Deg.
C35 -C48 -C49	6_555 1_555 1_555	# 1799 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	28.90 Deg.
C36 -C48 -C47	6_555 1_555 1_555	# 1806 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	30.40 Deg.
C47 -C48 -C37	1_555 1_555 6_555	# 1816 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.90 Deg.
C67 -C48 -C58	1_555 1_555 6_555	# 1838 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	35.50 Deg.
C67 -C48 -C59	1_555 1_555 6_555	# 1839 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.60 Deg.
C34 -C49 -C50	6_555 1_555 1_555	# 1843 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	13.00 Deg.
C35 -C49 -C36	6_555 1_555 6_555	# 1848 Check	
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	41.90 Deg.

C48 -C49 -C36	1_555	1_555	6_555		# 1855 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	44.40 Deg.
C70 -C49 -C55	1_555	1_555	6_555		# 1875 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	2.30 Deg.
C70 -C49 -C56	1_555	1_555	6_555		# 1876 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	11.00 Deg.
C34 -C50 -C55	6_555	1_555	6_555		# 1890 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	21.40 Deg.
C35 -C50 -C49	6_555	1_555	1_555		# 1892 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	38.50 Deg.
C51 -C50 -C55	1_555	1_555	6_555		# 1897 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	15.50 Deg.
C34 -C51 -C50	6_555	1_555	1_555		# 1902 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	21.70 Deg.
C52 -C51 -C32	1_555	1_555	6_555		# 1910 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	27.60 Deg.
C52 -C51 -C53	1_555	1_555	6_555		# 1913 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	25.00 Deg.
C55 -C51 -C71	6_555	1_555	1_555		# 1928 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	42.10 Deg.
C71 -C51 -C54	1_555	1_555	6_555		# 1933 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	9.90 Deg.
C32 -C52 -C30	6_555	1_555	1_555		# 1936 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	9.30 Deg.
C53 -C52 -C53	6_555	1_555	1_555		# 1952 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	4.80 Deg.
C32 -C53 -C30	1_555	1_555	6_555		# 1955 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	38.90 Deg.
C52 -C53 -C30	6_555	1_555	6_555		# 1964 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	28.80 Deg.
C52 -C53 -C32	1_555	1_555	6_555		# 1965 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	35.00 Deg.
C52 -C53 -C32	6_555	1_555	1_555		# 1966 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	39.90 Deg.
C52 -C53 -C51	6_555	1_555	6_555		# 1969 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	43.60 Deg.
C53 -C53 -C32	6_555	1_555	6_555		# 1977 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	14.80 Deg.
C53 -C53 -C52	6_555	1_555	1_555		# 1981 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	43.90 Deg.
C51 -C54 -C52	6_555	1_555	6_555		# 1991 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	30.50 Deg.
C53 -C54 -C52	1_555	1_555	6_555		# 1996 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	17.70 Deg.
C53 -C54 -C53	1_555	1_555	6_555		# 1998 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	22.40 Deg.
C71 -C54 -C55	6_555	1_555	1_555		# 2013 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	17.20 Deg.
C72 -C54 -C72	6_555	1_555	1_555		# 2026 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	3.60 Deg.
C34 -C55 -C50	1_555	1_555	6_555		# 2028 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	34.80 Deg.
C54 -C55 -C72	1_555	1_555	6_555		# 2044 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	10.50 Deg.
C70 -C55 -C56	6_555	1_555	1_555		# 2053 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	39.10 Deg.
C71 -C55 -C54	6_555	1_555	1_555		# 2059 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.80 Deg.
C71 -C55 -C72	6_555 1_555 6_555		# 2062 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	25.10 Deg.
C55 -C56 -C71	1_555 1_555 6_555		# 2065 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	37.50 Deg.
C57 -C56 -C49	1_555 1_555 6_555		# 2066 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	40.90 Deg.
C69 -C56 -C74	6_555 1_555 1_555		# 2072 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	12.00 Deg.
C70 -C56 -C49	6_555 1_555 6_555		# 2073 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	20.90 Deg.
C49 -C57 -C35	6_555 1_555 1_555		# 2095 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.40 Deg.
C56 -C57 -C69	1_555 1_555 6_555		# 2106 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.70 Deg.
C58 -C57 -C67	1_555 1_555 6_555		# 2107 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	31.70 Deg.
C58 -C57 -C68	1_555 1_555 6_555		# 2108 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	9.40 Deg.
C70 -C57 -C56	6_555 1_555 1_555		# 2115 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	26.00 Deg.
C59 -C58 -C66	1_555 1_555 6_555		# 2130 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.00 Deg.
C67 -C58 -C59	6_555 1_555 1_555		# 2138 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	40.90 Deg.
C67 -C58 -C66	6_555 1_555 6_555		# 2139 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	40.90 Deg.
C68 -C58 -C69	6_555 1_555 6_555		# 2148 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	20.70 Deg.
C68 -C58 -C76	6_555 1_555 1_555		# 2149 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.60 Deg.
C60 -C59 -C45	1_555 1_555 6_555		# 2175 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	22.10 Deg.
C66 -C59 -C60	6_555 1_555 1_555		# 2185 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	7.00 Deg.
C67 -C59 -C58	6_555 1_555 1_555		# 2193 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.60 Deg.
U3 -C59 -U1	1_555 1_555 1_555		# 2198 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.00 Deg.
U3 -C59 -U5	1_555 1_555 1_555		# 2199 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	17.50 Deg.
U5 -C59 -U1	1_555 1_555 1_555		# 2200 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	21.20 Deg.
C39 -C60 -C44	1_555 1_555 6_555		# 2201 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	31.50 Deg.
C45 -C60 -C39	6_555 1_555 1_555		# 2206 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	22.30 Deg.
C61 -C60 -C65	1_555 1_555 6_555		# 2221 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	24.30 Deg.
C66 -C60 -C59	6_555 1_555 1_555		# 2231 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.50 Deg.
U3 -C60 -U1	1_555 1_555 1_555		# 2236 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	27.50 Deg.
C60 -C61 -C66	1_555 1_555 6_555		# 2243 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.10 Deg.
C62 -C61 -C43	1_555 1_555 6_555		# 2249 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	44.90 Deg.

C64	-C61	-C43	6_555	1_555	6_555		# 2255 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	11.00 Deg.
C64	-C61	-C62	6_555	1_555	1_555		# 2257 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	27.70 Deg.
C65	-C61	-C77	6_555	1_555	1_555		# 2269 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	16.20 Deg.
C65	-C61	-C80	6_555	1_555	6_555		# 2270 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	13.20 Deg.
C77	-C61	-C80	1_555	1_555	6_555		# 2282 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	34.10 Deg.
U2	-C61	-U1	1_555	1_555	1_555		# 2289 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	12.10 Deg.
U3	-C61	-U1	1_555	1_555	1_555		# 2290 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	25.00 Deg.
U3	-C61	-U2	1_555	1_555	1_555		# 2291 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	30.70 Deg.
C43	-C62	-C41	6_555	1_555	1_555		# 2298 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	11.90 Deg.
C61	-C62	-C65	1_555	1_555	6_555		# 2305 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	25.00 Deg.
C64	-C62	-C61	6_555	1_555	1_555		# 2316 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	16.00 Deg.
C64	-C62	-C65	6_555	1_555	6_555		# 2318 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	34.70 Deg.
U2	-C62	-U1	1_555	1_555	1_555		# 2325 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	27.80 Deg.
U2	-C62	-U3	1_555	1_555	1_555		# 2326 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	13.20 Deg.
U3	-C62	-U1	1_555	1_555	1_555		# 2327 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	18.80 Deg.
C62	-C63	-C64	6_555	1_555	1_555		# 2329 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	18.80 Deg.
C62	-C63	-C64	1_555	1_555	6_555		# 2332 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	30.20 Deg.
C78	-C63	-C78	6_555	1_555	1_555		# 2354 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	22.67 Deg.
U2	-C63	-U3	1_555	1_555	6_555		# 2361 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	22.67 Deg.
U2	-C63	-U3	1_555	1_555	1_555		# 2362 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	21.40 Deg.
C43	-C64	-C41	1_555	1_555	6_555		# 2368 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	18.20 Deg.
C61	-C64	-C65	6_555	1_555	1_555		# 2378 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	24.00 Deg.
C62	-C64	-C41	6_555	1_555	6_555		# 2383 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	41.00 Deg.
C62	-C64	-C43	6_555	1_555	1_555		# 2384 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	30.40 Deg.
C65	-C64	-C77	1_555	1_555	6_555		# 2399 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	34.70 Deg.
U2	-C64	-U1	1_555	1_555	6_555		# 2406 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	12.10 Deg.
U3	-C64	-U1	6_555	1_555	6_555		# 2407 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	28.30 Deg.
U3	-C64	-U2	6_555	1_555	1_555		# 2408 Check
PLAT779_ALERT_4_G	Suspect	or Irrelevant	(Bond)	Angle(s)	in CIF	...	29.10 Deg.
C60	-C65	-C66	6_555	1_555	1_555		# 2411 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	33.30 Deg.
C61 -C65 -C62	6_555 1_555 6_555		# 2417 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	37.00 Deg.
C61 -C65 -C64	6_555 1_555 1_555		# 2418 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	5.10 Deg.
C64 -C65 -C62	1_555 1_555 6_555		# 2428 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	22.60 Deg.
C77 -C65 -C80	6_555 1_555 1_555		# 2446 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	23.00 Deg.
C80 -C65 -C76	1_555 1_555 6_555		# 2450 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	24.70 Deg.
U3 -C65 -U2	6_555 1_555 1_555		# 2453 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.00 Deg.
C45 -C66 -C39	1_555 1_555 6_555		# 2462 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	33.20 Deg.
C59 -C66 -C37	6_555 1_555 6_555		# 2473 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	41.30 Deg.
C59 -C66 -C67	6_555 1_555 1_555		# 2479 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	32.70 Deg.
C60 -C66 -C39	6_555 1_555 6_555		# 2484 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	20.70 Deg.
C65 -C66 -C61	1_555 1_555 6_555		# 2504 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	12.50 Deg.
C67 -C66 -C58	1_555 1_555 6_555		# 2512 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.80 Deg.
U1 -C66 -U5	6_555 1_555 6_555		# 2517 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.60 Deg.
U3 -C66 -U1	6_555 1_555 6_555		# 2518 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	27.30 Deg.
U3 -C66 -U5	6_555 1_555 6_555		# 2519 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.00 Deg.
C58 -C67 -C68	6_555 1_555 1_555		# 2531 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	36.00 Deg.
C58 -C67 -C76	6_555 1_555 6_555		# 2532 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	31.50 Deg.
C59 -C67 -C66	6_555 1_555 1_555		# 2536 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.20 Deg.
C68 -C67 -C76	1_555 1_555 6_555		# 2545 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	8.90 Deg.
C58 -C68 -C67	6_555 1_555 1_555		# 2549 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	13.60 Deg.
C76 -C68 -C80	6_555 1_555 1_555		# 2566 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	8.50 Deg.
C56 -C69 -C70	6_555 1_555 1_555		# 2572 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	27.30 Deg.
C68 -C69 -C58	1_555 1_555 6_555		# 2579 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	18.40 Deg.
C68 -C69 -C76	1_555 1_555 6_555		# 2580 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	38.80 Deg.
C74 -C69 -C82	6_555 1_555 1_555		# 2592 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.10 Deg.
C75 -C69 -C82	6_555 1_555 1_555		# 2598 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	40.80 Deg.
C35 -C70 -C34	6_555 1_555 6_555		# 2605 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	39.60 Deg.
C49 -C70 -C34	1_555 1_555 6_555		# 2606 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	4.10 Deg.

C49 -C70 -C35	1_555	1_555	6_555		# 2607 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	42.10 Deg.
C55 -C70 -C34	6_555	1_555	6_555		# 2609 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	25.20 Deg.
C55 -C70 -C71	6_555	1_555	1_555		# 2613 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	42.00 Deg.
C56 -C70 -C69	6_555	1_555	1_555		# 2620 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	14.00 Deg.
C56 -C70 -C74	6_555	1_555	6_555		# 2622 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	42.90 Deg.
C57 -C70 -C35	6_555	1_555	6_555		# 2624 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	44.70 Deg.
C57 -C70 -C49	6_555	1_555	1_555		# 2625 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	34.10 Deg.
C69 -C70 -C74	1_555	1_555	6_555		# 2634 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	37.90 Deg.
C51 -C71 -C34	1_555	1_555	6_555		# 2641 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	12.60 Deg.
C55 -C71 -C34	6_555	1_555	6_555		# 2652 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	10.70 Deg.
C70 -C71 -C56	1_555	1_555	6_555		# 2662 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	5.20 Deg.
C72 -C71 -C72	1_555	1_555	6_555		# 2668 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	43.60 Deg.
C54 -C72 -C55	6_555	1_555	6_555		# 2670 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	44.60 Deg.
C54 -C72 -C71	6_555	1_555	1_555		# 2672 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	32.20 Deg.
C54 -C72 -C71	1_555	1_555	6_555		# 2674 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	6.70 Deg.
C71 -C72 -C55	1_555	1_555	6_555		# 2678 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	15.80 Deg.
C72 -C72 -C71	6_555	1_555	6_555		# 2683 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	19.70 Deg.
C72 -C73 -C72	6_555	1_555	1_555		# 2690 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	36.40 Deg.
C82 -C73 -C74	6_555	1_555	1_555		# 2700 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	36.40 Deg.
C82 -C73 -C74	1_555	1_555	6_555		# 2702 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	2.80 Deg.
C56 -C74 -C70	1_555	1_555	6_555		# 2705 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	42.40 Deg.
C82 -C74 -C75	6_555	1_555	1_555		# 2719 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	38.60 Deg.
C69 -C75 -C74	6_555	1_555	1_555		# 2723 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	25.20 Deg.
C76 -C75 -C68	1_555	1_555	6_555		# 2732 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	26.10 Deg.
C76 -C75 -C80	1_555	1_555	6_555		# 2734 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	44.60 Deg.
C80 -C75 -C79	6_555	1_555	6_555		# 2735 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	37.80 Deg.
C82 -C75 -C74	6_555	1_555	1_555		# 2743 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	11.00 Deg.
C58 -C76 -C67	1_555	1_555	6_555		# 2749 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond)	Angle(s)	in CIF ...	32.00 Deg.
C68 -C76 -C58	6_555	1_555	1_555		# 2755 Check

PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.80 Deg.
C68 -C76 -C67	6_555 1_555 6_555		# 2757 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	42.60 Deg.
C68 -C76 -C69	6_555 1_555 6_555		# 2758 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.20 Deg.
C75 -C76 -C69	1_555 1_555 6_555		# 2769 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	28.30 Deg.
C77 -C76 -C65	1_555 1_555 6_555		# 2772 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	41.30 Deg.
C80 -C76 -C65	6_555 1_555 6_555		# 2778 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	13.00 Deg.
C80 -C76 -C77	6_555 1_555 1_555		# 2782 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	41.10 Deg.
C80 -C76 -C79	6_555 1_555 6_555		# 2783 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	33.40 Deg.
C61 -C77 -C64	1_555 1_555 6_555		# 2784 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	15.10 Deg.
C65 -C77 -C61	6_555 1_555 1_555		# 2792 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.60 Deg.
C78 -C77 -C79	1_555 1_555 6_555		# 2805 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	16.90 Deg.
C80 -C77 -C76	6_555 1_555 1_555		# 2814 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	24.60 Deg.
U3 -C77 -U2	1_555 1_555 1_555		# 2819 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	21.30 Deg.
C77 -C78 -C80	1_555 1_555 6_555		# 2823 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.40 Deg.
C79 -C78 -C79	6_555 1_555 1_555		# 2835 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	43.60 Deg.
C75 -C79 -C76	6_555 1_555 6_555		# 2841 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	32.00 Deg.
C78 -C79 -C78	6_555 1_555 1_555		# 2853 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	23.30 Deg.
C80 -C79 -C76	1_555 1_555 6_555		# 2869 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	24.70 Deg.
C80 -C79 -C77	1_555 1_555 6_555		# 2870 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	6.00 Deg.
C65 -C80 -C61	1_555 1_555 6_555		# 2878 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	10.30 Deg.
C76 -C80 -C68	6_555 1_555 1_555		# 2891 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	29.50 Deg.
C77 -C80 -C61	6_555 1_555 6_555		# 2896 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	34.40 Deg.
C77 -C80 -C65	6_555 1_555 1_555		# 2897 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	40.30 Deg.
C79 -C80 -C78	1_555 1_555 6_555		# 2911 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	39.80 Deg.
C75 -C81 -C82	6_555 1_555 1_555		# 2918 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	39.80 Deg.
C75 -C81 -C82	1_555 1_555 6_555		# 2919 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	40.30 Deg.
C79 -C81 -C79	6_555 1_555 1_555		# 2922 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	39.40 Deg.
C74 -C82 -C69	6_555 1_555 1_555		# 2933 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	25.80 Deg.
U1 -N1 -U3	1_555 1_555 1_555		# 3276 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant	(Bond) Angle(s) in CIF ...	25.80 Deg.

U1	-N1	-U3	6_555	1_555	6_555		# 3279 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF ...	40.80 Deg.
U2	-N1	-U3	1_555	1_555	6_555		# 3280 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF ...	40.80 Deg.
U2	-N1	-U3	1_555	1_555	1_555		# 3281 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF ...	26.40 Deg.
U4	-N1	-U1	1_555	1_555	1_555		# 3283 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF ...	26.40 Deg.
U4	-N1	-U1	6_555	1_555	6_555		# 3284 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF ...	29.60 Deg.
U5	-N1	-U1	1_555	1_555	1_555		# 3294 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF ...	29.60 Deg.
U5	-N1	-U1	6_555	1_555	6_555		# 3296 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF ...	31.60 Deg.
U5	-N1	-U4	6_555	1_555	6_555		# 3305 Check
PLAT779_ALERT_4_G	Suspect	or	Irrelevant	(Bond)	Angle(s)	in CIF ...	31.60 Deg.
U5	-N1	-U4	1_555	1_555	1_555		# 3307 Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms						! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints						1383 Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).						3 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600					103 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.						12 Info
PLAT984_ALERT_1_G	The Ni-f' =	0.3120	Deviates from the B&C-Value				0.2982 Check
PLAT984_ALERT_1_G	The S-f' =	0.1246	Deviates from the B&C-Value				0.1576 Check
PLAT984_ALERT_1_G	The U-f' =	-6.3260	Deviates from the B&C-Value				-6.1890 Check
PLAT985_ALERT_1_G	The Ni-f" =	1.4720	Deviates from the B&C-Value				1.4582 Check
PLAT985_ALERT_1_G	The S-f" =	0.1234	Deviates from the B&C-Value				0.1682 Check
PLAT985_ALERT_1_G	The U-f" =	5.5940	Deviates from the B&C-Value				5.0831 Check

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

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 78 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
 538 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.

