

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) im_1_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: im_1_1

Bond precision:	C-C = 0.0065 A	Wavelength=0.71073
Cell:	a=12.5362 (4)	b=12.9887 (4) c=17.3319 (8)
	alpha=90	beta=98.597 (4) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	2790.43 (18)	2790.44 (18)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C16 H36 N, C3 H4 Br4 N3 O Re	C3 H4 Br4 N3 O Re, C16 H36 N
Sum formula	C19 H40 Br4 N4 O Re	C19 H40 Br4 N4 O Re
Mr	846.36	846.39
Dx, g cm ⁻³	2.015	2.015
Z	4	4
Mu (mm ⁻¹)	10.099	10.099
F000	1620.0	1620.0
F000'	1612.67	
h, k, lmax	16, 17, 23	16, 17, 22
Nref	6896	6336
Tmin, Tmax	0.488, 0.731	0.591, 0.774
Tmin'	0.437	

Correction method= # Reported T Limits: Tmin=0.591 Tmax=0.774
AbsCorr = GAUSSIAN

Data completeness= 0.919 Theta(max)= 28.238

R(reflections)= 0.0337 (4976)	wR2(reflections)= 0.0459 (6336)
S = 0.975	Npar= 266

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 C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.733 Check
PLAT977_ALERT_2_C	Check Negative Difference Density on H32A .	-0.39 eA-3



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1 Report
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	558 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.4 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
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- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
1 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

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checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hpz

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: hpz

Bond precision: C-C = 0.0071 Å Wavelength=0.71073

Cell: a=12.621 (2) b=12.784 (2) c=18.410 (4)
 alpha=90 beta=99.546 (5) gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	2929.3 (9)	2929.3 (10)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C16 H36 N, C3 H4 Br4 N3 O Re	C3 H4 Br4 N3 O Re, C16 H36 N
Sum formula	C19 H40 Br4 N4 O Re	C19 H40 Br4 N4 O Re
Mr	846.36	846.39
Dx, g cm ⁻³	1.919	1.919
Z	4	4
Mu (mm ⁻¹)	9.621	9.621
F000	1620.0	1620.0
F000'	1612.67	
h, k, lmax	16, 16, 23	16, 16, 23
Nref	6312	6293
Tmin, Tmax	0.157, 0.477	0.532, 0.745
Tmin'	0.049	

Correction method= # Reported T Limits: Tmin=0.532 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 26.872

R(reflections)= 0.0264 (4831)

wR2(reflections)=
0.0494 (6293)

S = 1.039

Npar= 264

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 C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.7 Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.6 Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C32 --C33	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C33 --C34	0.20 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C2 --C4	0.16 Ang.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Rel Check
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C33 - C34	1.35 Ang.
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	8 Note

Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1 Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293 Check
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	11 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 Info

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-
-

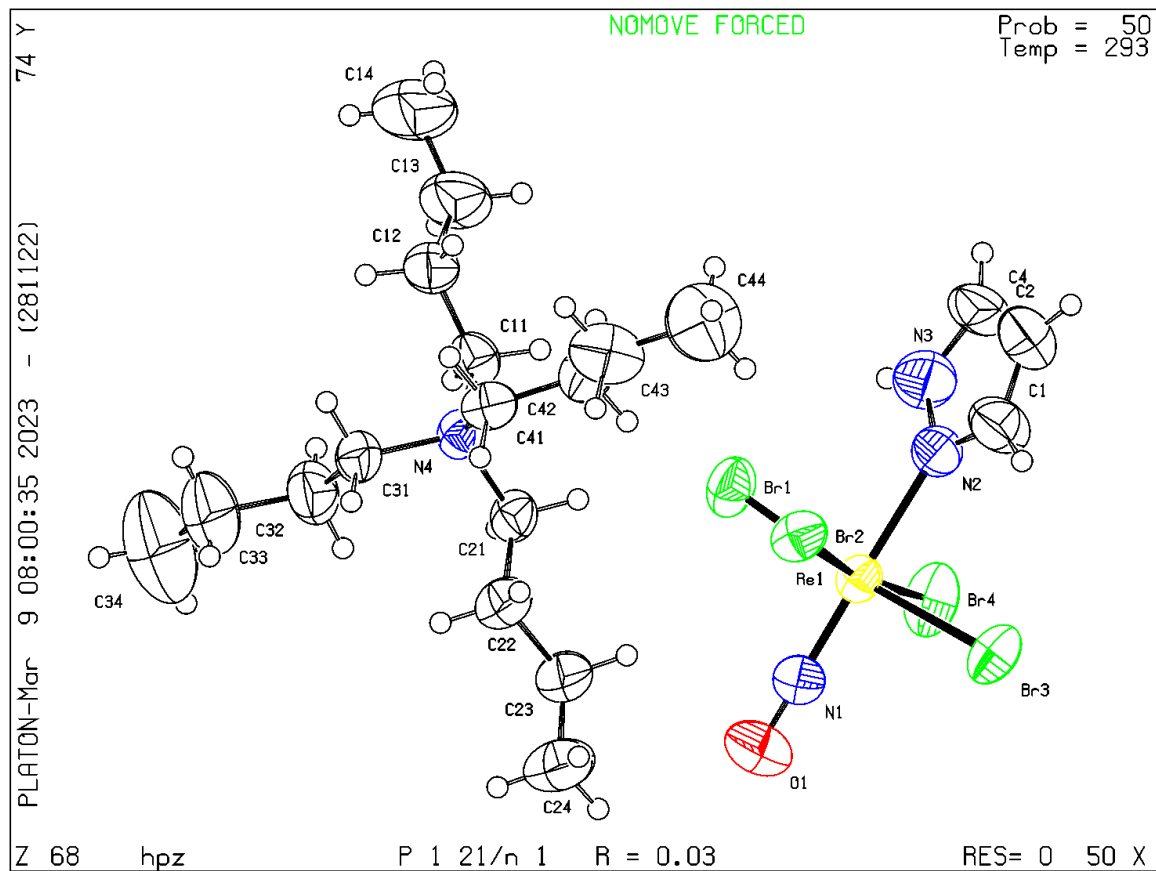
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checkCIF/PLATON report

Structure factors have been supplied for datablock(s) tri_1_2

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Datablock: tri_1_2

Bond precision:	C-C = 0.0063 Å	Wavelength=0.71073
Cell:	a=12.5889(2)	b=12.8366(2) c=17.3631(5)
	alpha=90	beta=98.6314(19) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	2774.08(10)	2774.06(10)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C16 H36 N, C2 H3 Br4 N4 O Re	C2 H3 Br4 N4 O Re, C16 H36 N
Sum formula	C18 H39 Br4 N5 O Re	C18 H39 Br4 N5 O Re
Mr	847.35	847.38
Dx, g cm ⁻³	2.029	2.029
Z	4	4
Mu (mm ⁻¹)	10.160	10.160
F000	1620.0	1620.0
F000'	1612.66	
h, k, lmax	16, 17, 23	15, 16, 21
Nref	6901	6188
Tmin, Tmax	0.171, 0.444	0.143, 0.473
Tmin'	0.050	

Correction method= # Reported T Limits: Tmin=0.143 Tmax=0.473
AbsCorr = GAUSSIAN

Data completeness= 0.897 Theta(max)= 28.310

R(reflections)= 0.0299(5178)	wR2(reflections)= 0.0587(6188)
S = 1.046	Npar= 252

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 C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.21Ang From C1	1.55 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H3	-0.52 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H13B	-0.31 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H23A	-0.33 eA-3



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1 Report
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	1 Note
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1 Report
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	594 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	1 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.8 Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	2 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.	1 Info

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-
-

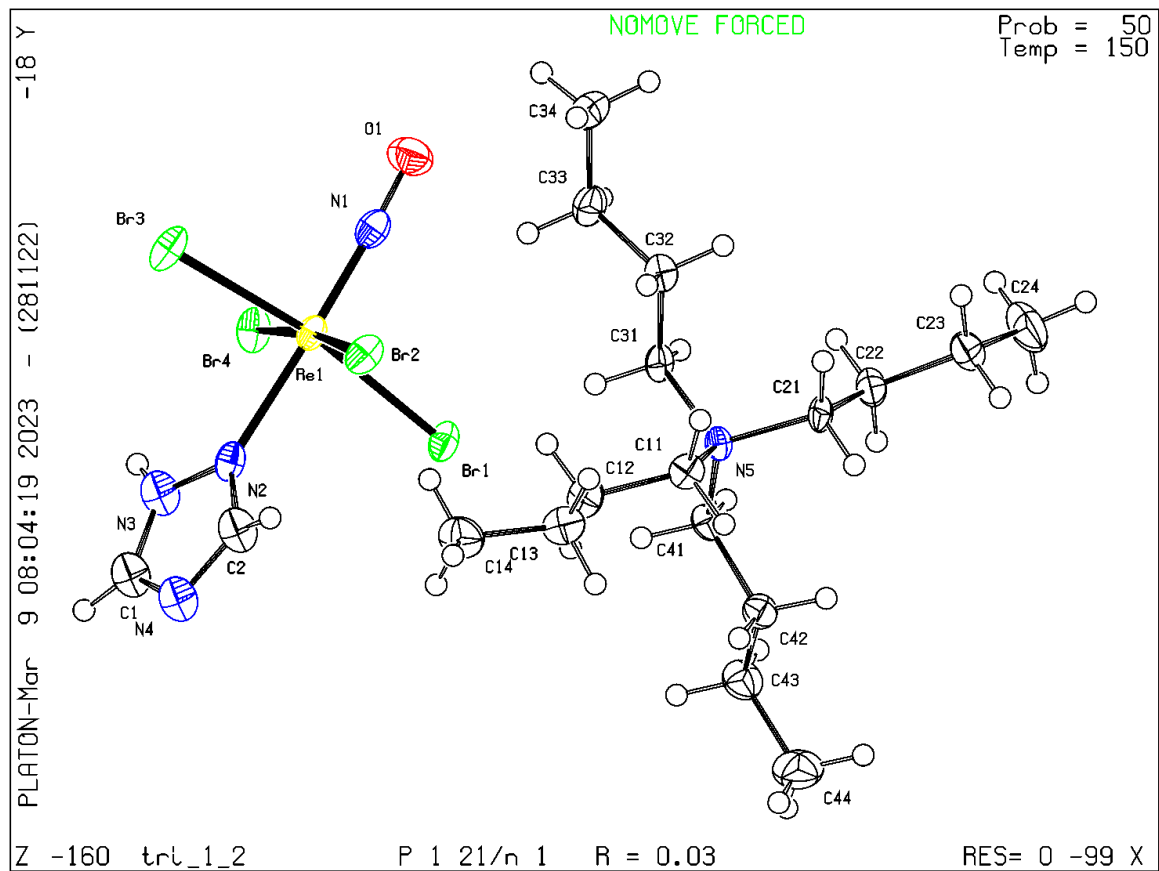
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Alert level A

PLAT410_ALERT_2_A	Short	Intra H...H Contact	H51A	..H71A	.	1.67 Ang.
				x,y,z =		1_555 Check
PLAT410_ALERT_2_A	Short	Intra H...H Contact	H51B	..H81B	.	1.58 Ang.
				x,y,z =		1_555 Check
PLAT410_ALERT_2_A	Short	Intra H...H Contact	H52A	..H53A	.	1.79 Ang.
				x,y,z =		1_555 Check
PLAT410_ALERT_2_A	Short	Intra H...H Contact	H61A	..H81A	.	1.63 Ang.
				x,y,z =		1_555 Check
PLAT410_ALERT_2_A	Short	Intra H...H Contact	H61B	..H71B	.	1.62 Ang.
				x,y,z =		1_555 Check

Alert level B

PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of		C62	Check
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of		C71	Check
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of		C81	Check
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of		N2	Check
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of		C53	Check
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of		C63	Check
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of		C73	Check
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of		C83	Check
PLAT342_ALERT_3_B	Low	Bond Precision on C-C Bonds		0.02183	Ang.
PLAT360_ALERT_2_B	Short	C(sp3)-C(sp3) Bond	C51 - C52	.	1.33	Ang.
PLAT360_ALERT_2_B	Short	C(sp3)-C(sp3) Bond	C52 - C53	.	1.33	Ang.
PLAT360_ALERT_2_B	Short	C(sp3)-C(sp3) Bond	C71 - C72	.	1.33	Ang.
PLAT360_ALERT_2_B	Short	C(sp3)-C(sp3) Bond	C81 - C82	.	1.32	Ang.
PLAT360_ALERT_2_B	Short	C(sp3)-C(sp3) Bond	C82 - C83	.	1.33	Ang.
PLAT362_ALERT_2_B	Short	C(sp3)-C(sp2) Bond	C62 - C63	.	1.27	Ang.
PLAT410_ALERT_2_B	Short	Intra H...H Contact	H82A	..H83B	.	1.80 Ang.
				x,y,z =		1_555 Check

Alert level C

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings	Differ		Please	Check
PLAT220_ALERT_2_C	NonSolvent Resd 2 C	Ueq(max)/Ueq(min) Range		4.4	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 2 H	Uiso(max)/Uiso(min) Range		5.5	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C62 --C63	.	0.24	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C63 --C64	.	0.20	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	N15 --N16	.	0.17	Ang.
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C51	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C52	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C61	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C72	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C82	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N15	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	N25	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C43	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Re1	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Re2	Check

PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	N22	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	0.159	Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	0.102	Check
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond C61 - C62	1.34	Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond C72 - C73	1.40	Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond C73 - C74	1.38	Ang.
PLAT360_ALERT_2_C	Short	C(sp3)-C(sp3) Bond C83 - C84	1.41	Ang.
PLAT410_ALERT_2_C	Short	Intra H...H Contact H61A ..H62B	1.97	Ang.
		x,y,z =	1_555	Check
PLAT410_ALERT_2_C	Short	Intra H...H Contact H81B ..H82B	1.93	Ang.
		x,y,z =	1_555	Check
PLAT790_ALERT_4_C	Centre of Gravity not Within Unit Cell: Resd. #		1	Note
	C16 H35 N			
PLAT906_ALERT_3_C	Large	K Value in the Analysis of Variance	9.321	Check
PLAT906_ALERT_3_C	Large	K Value in the Analysis of Variance	2.461	Check
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L=	0.600	65 Report
PLAT973_ALERT_2_C	Check	Calcd Positive Resid. Density on	1.04	eA-3
PLAT973_ALERT_2_C	Check	Calcd Positive Resid. Density on	1.02	eA-3
PLAT977_ALERT_2_C	Check	Negative Difference Density on H23B	-0.31	eA-3
PLAT977_ALERT_2_C	Check	Negative Difference Density on H44B	-0.34	eA-3
PLAT977_ALERT_2_C	Check	Negative Difference Density on H72A	-0.37	eA-3
PLAT977_ALERT_2_C	Check	Negative Difference Density on H74A	-0.34	eA-3

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	12	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	12	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	7.35	Why ?
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	6	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	5	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature	293	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for	C51	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for	C52	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for	C61	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for	C62	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for	C71	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for	C72	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for	C81	Check
PLAT343_ALERT_2_G	Unusual sp3 Angle Range in Main Residue for	C82	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Br13 ..Br23	3.57	Ang.
	x,3/2-y,1/2+z =	4_576	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	135	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	1750 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	24	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.0	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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PLATON version of 28/11/2022; check.def file version of 28/11/2022

