

checkCIF/PLATON report

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

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: ComplexA

Bond precision: C-C = 0.0078 Å Wavelength=1.54184

Cell: a=13.5359(5) b=13.9046(4) c=19.5358(7)
 alpha=101.369(3) beta=92.861(3) gamma=114.983(3)
Temperature: 137 K

	Calculated	Reported
Volume	3230.5(2)	3230.6(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C61 H52 Fe Ni O2 P4 S2, 2(B F4), 2(C H2 Cl2)	?
Sum formula	C63 H56 B2 Cl4 F8 Fe Ni O2 P4 S2	C63 H56 B2 Cl4 F8 Fe Ni O2 P4 S2
Mr	1463.04	1463.05
Dx, g cm ⁻³	1.504	1.504
Z	2	2
Mu (mm ⁻¹)	5.792	5.792
F000	1492.0	1492.0
F000'	1493.99	
h, k, lmax	16, 17, 24	16, 16, 23
Nref	13126	11539
Tmin, Tmax	0.482, 0.499	0.586, 1.000
Tmin'	0.365	

Correction method= # Reported T Limits: Tmin=0.586 Tmax=1.000

AbsCorr = MULTII-SCAN

Data completeness= 0.879

Theta(max)= 74.066

R(reflections)= 0.0622(9672)

wR2(reflections)=
0.1706(11539)

S = 1.028

Npar= 807

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

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	2.15 eA-3
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.4 Ratio
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	B1 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	B2 Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00782 Ang.
PLAT430_ALERT_2_C	Short Inter D...A Contact 01 ..01 .	2.88 Ang.
	1-x,-y,1-z =	2_656 Check



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	16 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	15 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	9.33 Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.003 Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	7 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2 Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2 Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	2 Report
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) F1 --B1 .	11.7 s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) F2 --B1 .	26.0 s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) F4 --B1 .	10.2 s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) F1' --B1 .	24.2 s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) F2' --B1 .	13.0 s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) F3' --B1 .	14.2 s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) F4' --B1 .	5.7 s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) F5 --B2 .	8.5 s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) F6 --B2 .	11.0 s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) F7 --B2 .	7.7 s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) F5' --B2 .	14.2 s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) F6' --B2 .	6.2 s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) F7' --B2 .	9.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fe1 --C1 .	6.5 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fe1 --C2 .	7.5 s.u.
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	80% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	60% Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact F4 ..C12 .	2.83 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F3' ..C46 .	2.72 Ang.
	x,y,z =	1_555 Check
PLAT767_ALERT_4_G	INS Embedded LIST 6 Instruction Should be LIST 4	Please Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	134 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	11 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.0 Low

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

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

Datablock: Complex1

Bond precision:	C-C = 0.0049 A	Wavelength=1.54184
Cell:	a=12.16469(13)	b=23.5596(3) c=20.6266(2)
	alpha=90	beta=90.0624(9) gamma=90
Temperature:	152 K	
	Calculated	Reported
Volume	5911.48(11)	5911.48(11)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C61 H52 Fe N Ni O P4 S2, B F4, C H2 Cl2, H2 O	?
Sum formula	C62 H56 B Cl2 F4 Fe N Ni O2 P4 S2	C62 H56 B Cl2 F4 Fe N Ni O2 P4 S2
Mr	1307.33	1307.34
Dx, g cm ⁻³	1.469	1.469
Z	4	4
Mu (mm ⁻¹)	5.354	5.354
F000	2688.0	2688.0
F000'	2687.85	
h, k, lmax	14, 28, 24	14, 28, 24
Nref	10577	10570
Tmin, Tmax	0.446, 0.526	0.364, 1.000
Tmin'	0.404	

Correction method= # Reported T Limits: Tmin=0.364 Tmax=1.000
 AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 67.076

R(reflections)= 0.0425(8969)

wR2(reflections)=
0.1099(10570)

S = 1.019

Npar= 729

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

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of		C3	Check



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite				3	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...				1	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large				5.89	Why ?
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing				0.00020	Ang.
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records				2	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records				1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Nil	--S1	.	5.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fel	--C1	.	5.9	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fel	--C2	.	6.2	s.u.
PLAT244_ALERT_4_G	Low	'Solvent'	Ueq as Compared to Neighbors of		B1	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				9	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File				6	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity				3.8	Low

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2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected
- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 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
5 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
-

Datablock: Complex2

Bond precision: C-C = 0.0136 A

Wavelength=1.54184

Cell:	a=13.6077(9)	b=13.8784(10)	c=20.6526(15)
	alpha=70.414(7)	beta=87.819(6)	gamma=74.103(6)
Temperature:	152 K		

	Calculated	Reported
Volume	3527.9(5)	3527.9(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C61 H52 Fe N Ni O P4 S3, B F4 [+ solvent]	?
Sum formula	C61 H52 B F4 Fe N Ni O P4 S3 [+ solvent]	C61 H52 B F4 Fe N Ni O P4 S3
Mr	1236.45	1236.46
Dx, g cm ⁻³	1.164	1.164
Z	2	2
Mu (mm ⁻¹)	4.037	4.037
F000	1272.0	1272.0
F000'	1270.98	
h,k,lmax	16,16,24	16,16,24
Nref	12601	12095
Tmin,Tmax	0.573,0.592	0.584,1.000
Tmin'	0.520	

Correction method= # Reported T Limits: Tmin=0.584 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.960 Theta(max)= 67.072

R(reflections)= 0.0790(6503) wR2(reflections)=
0.2390(12095)
S = 0.880 Npar= 695

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

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full	value Low	.	0.960	Why?
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	P2	--C14	.	6.7 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	P4	--C49	.	5.5 s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C39	--C40	.	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C40	--C41	.	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C53	--C54	.	0.17 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C56	--C61	.	0.16 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of			C37	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of			C40	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of			C44	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of			C36	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of			C39	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of			C42	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including		F1	0.126	Check

PLAT331_ALERT_2_C	Small Aver Phenyl C-C Dist C36	--C41	.	1.36 Ang.
PLAT331_ALERT_2_C	Small Aver Phenyl C-C Dist C42	--C47	.	1.37 Ang.
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds			0.0136 Ang.



Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	15	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	4	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	4	Report
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	B1	Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	64	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	495	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.9	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check

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 - 17 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 - 10 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: Complex4

Bond precision:	C-C = 0.0089 A	Wavelength=1.54184
Cell:	a=10.4504 (3)	b=17.3852 (6) c=17.3954 (6)
	alpha=85.080 (3)	beta=81.056 (3) gamma=75.973 (3)
Temperature:	100 K	

	Calculated	Reported
Volume	3025.10(18)	3025.10(18)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C57 H54 Fe N Ni O P4 S2, B F4, 2(C3 H6 O)	?
Sum formula	C63 H66 B F4 Fe N Ni O3 P4 S2	C63 H66 B F4 Fe N Ni O3 P4 S2
Mr	1274.52	1274.53
Dx, g cm ⁻³	1.399	1.399
Z	2	2
Mu (mm ⁻¹)	4.433	4.433
F000	1324.0	1324.0
F000'	1322.56	
h,k,lmax	12,20,20	12,20,20
Nref	10812	10804
Tmin,Tmax	0.517,0.587	0.426,1.000
Tmin'	0.469	

Correction method= # Reported T Limits: Tmin=0.426 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta(max)= 67.077

R(reflections)= 0.0705(8495) wR2(reflections)=
0.1968(10804)
S = 1.039 Npar= 726

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

PLAT213_ALERT_2_C Atom C23	has ADP max/min Ratio	3.2 prolat
PLAT220_ALERT_2_C NonSolvent Resd 1 C	Ueq(max)/Ueq(min) Range	3.5 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for N1	--C43	7.0 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of		C23 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of		C61 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of		C58 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds		0.00887 Ang.

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...		2 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large		6.25 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)		0.003 Degree
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records		1 Report

PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe1	--S1	.	5.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fe1	--C1	.	6.0 s.u.
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of				B1 Check
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for			C27 Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond	C27	- C28	.	1.53 Ang.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints			12 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity			1.9 Low

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 7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 11 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: Complex5

Bond precision:	C-C = 0.0067 A	Wavelength=1.54184
Cell:	a=26.3215 (7)	b=26.3215 (7) c=19.6548 (5)
	alpha=90	beta=90 gamma=120
Temperature:	293 K	
	Calculated	Reported
Volume	11792.9 (7)	11792.9 (7)
Space group	P -3	P -3
Hall group	-P 3	-P 3
Moiety formula	C62 H58 Fe N Ni O P4 S3, 0.5(C6 H14), B F4 [+ solvent]	?
Sum formula	C65 H65 B F4 Fe N Ni O P4 S3 [+ solvent]	C65 H65 B F4 Fe N Ni O P4 S3
Mr	1297.59	1297.61
Dx, g cm-3	1.096	1.096
Z	6	6
Mu (mm-1)	3.642	3.642
F000	4038.0	4038.0
F000'	4035.34	
h, k, lmax	32, 32, 24	31, 31, 24
Nref	15964	15472
Tmin, Tmax	0.489, 0.501	0.496, 1.000
Tmin'	0.443	

Correction method= # Reported T Limits: Tmin=0.496 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.969

Theta(max)= 74.028

R(reflections)= 0.0689(12139)

wR2(reflections)=
0.1981(15472)

S = 0.903

Npar= 787

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.18	Report
PLAT214_ALERT_2_C	Atom B3 (Anion/Solvent) ADP max/min Ratio	4.8	prolat
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including C63	0.132	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including F5	0.121	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00667	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact H4 ..H31A .	1.98	Ang.
	x,y,z =	1_555	Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor S3 --H3 .		Please Check



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	11	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	10	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Nil --S1 .	5.6	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fe1 --S2 .	5.2	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fe1 --C1 .	6.7	s.u.
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	B2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C63 Constrained at	0.5	Check
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 H63A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H63B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H63C Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H64A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H64B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H65A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H65B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H66A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H66B Constrained at	0.5	Check

PLAT300_ALERT_4_G Atom Site Occupancy of H67A	Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H67B	Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H68A	Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H68B	Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H68C	Constrained at	0.5	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5	Constrained at	0.3333	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F6	Constrained at	0.3333	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F7	Constrained at	0.3333	Check
PLAT300_ALERT_4_G Atom Site Occupancy of F8	Constrained at	0.3333	Check
PLAT300_ALERT_4_G Atom Site Occupancy of B3	Constrained at	0.3333	Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2)		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 5)		1.67	Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Structure		!	Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints		122	Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed		!	Info
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File		29	Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity		1.9	Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged			Please Check

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 0 **ALERT level B** = A potentially serious problem, consider carefully
 7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 46 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: ComplexD

Bond precision: C-C = 0.0063 A

Wavelength=0.71073

Cell: a=16.1180(9) b=24.5373(12) c=22.9864(14)
 alpha=90 beta=108.562(2) gamma=90

Temperature: 113 K

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	
DENSD01_ALERT_1_C	The ratio of the submitted crystal density and that calculated from the formula is outside the range 0.99 <> 1.01 Crystal density given = 1.412 Calculated crystal density = 1.363	
PLAT046_ALERT_1_C	Reported Z, MW and D(calc) are Inconsistent	1.363 Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C72 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C71 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C74 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including C11	0.103 Check

PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Cl3	0.169	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Cl5	0.118	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Cl7	0.157	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds		0.00626	Ang.



Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large	30.25	Why ?
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fe1	--C1	5.9	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fe1	--C2	6.1	s.u.
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		B1	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of		B2	Check
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H10	..S1	2.96	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H33	..O1	2.61	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H72B	..O1	2.64	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H73B	..CL2	2.96	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H74B	..F4	2.61	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H10	..S1	2.96	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H33	..O1	2.61	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H72B	..O1	2.64	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H73B	..CL2	2.96	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H74B	..F4	2.61	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H10	..S1	2.96	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H14	..F2	2.64	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H33	..O1	2.61	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H72B	..O1	2.64	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H73B	..CL2	2.96	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported H74B	..F4	2.61	Ang.
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure		!	Info
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE	Suppressed	!	Info
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		4.9	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged			Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..		50.0	Degree

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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.











