

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 14aH3, 14aH7, 15aH72HCl, 15bH, 20aPb, 22aZn, 22bCd, 22bHg, 22bZn

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: 14aH3

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Bond precision:    C-C = 0.0034 Å                      Wavelength=0.71073

Cell:                      a=12.185 (3)              b=9.096 (2)              c=20.334 (3)  
                                    alpha=90                      beta=102.14 (3)              gamma=90

Temperature:              100 K

	Calculated	Reported
Volume	2203.3 (8)	2203.3 (8)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C23 H26 N4 O2, H2 O	C23 H26 N4 O2, H2 O
Sum formula	C23 H28 N4 O3	C23 H28 N4 O3
Mr	408.49	408.49
Dx, g cm <sup>-3</sup>	1.232	1.231
Z	4	4
Mu (mm <sup>-1</sup> )	0.083	0.083
F000	872.0	872.0
F000'	872.36	
h, k, lmax	20, 15, 34	18, 11, 33
Nref	11040	6315
Tmin, Tmax	0.972, 0.988	0.879, 1.000
Tmin'	0.952	

Correction method= # Reported T Limits: Tmin=0.879 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.572                      Theta (max)= 36.782

R(reflections)= 0.0762 ( 3272)

wR2(reflections)=  
0.2137 ( 6315)

S = 1.033

Npar= 275

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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.

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● **Alert level C**

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	19.879	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.626	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	4.662	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.284	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	5	Note

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● **Alert level G**

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	4	Report
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL/	2018	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	3613	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.5	Low
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	2	Units
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	4	Units
PLAT956_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Hmax Differ	2	Units
PLAT957_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Kmax Differ	4	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	2	Check

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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
5 **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

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

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## Datablock: 14aH7

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Bond precision: C-C = 0.0000 A

Wavelength=1.54184

Cell: a=8.520(2) b=17.383(3) c=15.051(3)

alpha=90 beta=90 gamma=90

Temperature: 100 K



PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	6	Report
PLAT012_ALERT_1_G	N.O.K. _shelx_res_checksum Found in CIF .....		Please Check
PLAT013_ALERT_1_G	N.O.K. _shelx_hkl_checksum Found in CIF .....		Please Check
PLAT169_ALERT_4_G	The CIF-Embedded .res File Contains AFIX 1 Recds	2	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of H1W Constrained at	0.886	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11W Constrained at	0.114	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )	100%	Note
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 2 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4 )	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 1 )	52.27	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 2 )	6.73	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 3 )	2.66	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 4 )	0.34	Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O9 .	93.7	Degree
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	9	Note
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C1A --C2A	1.82	Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	37.80	Deg.
	C10 -O9 -C100 1_555 1_555 7_565 ..... #	15	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	37.40	Deg.
	C100 -C10 -C100 7_565 1_555 1_555 ..... #	19	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	40.00	Deg.
	C10 -C10 -C100 7_565 1_555 1_555 ..... #	20	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...	40.00	Deg.
	C100 -C100 -C10 7_565 1_555 1_555 ..... #	23	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	102	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	5	Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Info

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

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## Datablock: 15aH72HCl

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Bond precision: C-C = 0.0057 A

Wavelength=1.54184

Cell: a=13.411(5) b=10.170(3) c=20.383(6)

alpha=90 beta=97.98(3) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2753.1(16)	2753.1(16)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C27 H40 N4 O3, 2(C1)	C27 H40 N4 O3, 2C1
Sum formula	C27 H40 Cl2 N4 O3	C27 H40 Cl2 N4 O3
Mr	539.53	539.53
Dx, g cm <sup>-3</sup>	1.302	1.302
Z	4	4
Mu (mm <sup>-1</sup> )	2.403	2.403
F000	1152.0	1152.0
F000'	1157.79	
h, k, lmax	16, 12, 24	16, 12, 24
Nref	4900	4896
Tmin, Tmax	0.771, 0.845	0.755, 0.841
Tmin'	0.714	

Correction method= # Reported T Limits: Tmin=0.755 Tmax=0.841  
AbsCorr = ANALYTICAL

Data completeness= 0.999                      Theta(max)= 66.994

R(reflections)= 0.0751( 3240)                      wR2(reflections)=  
0.2295( 4896)  
S = 1.087                      Npar= 489

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
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	2.29 Report
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	5.6 Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	5.6 Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for N27 --C4 .	5.3 s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference N25 --C26 .	0.18 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C19 --C20 .	0.20 Ang.
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00569 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	6.788 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.009 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.597	6 Report

### ● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	38 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	36 Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	10 Report





PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 63 Note  
 PLAT915\_ALERT\_3\_G No Flack x Check Done: Low Friedel Pair Coverage 59 %  
 PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 3.9 Low  
 PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 1 Info

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

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Bond precision: C-C = 0.0134 A Wavelength=1.54184

Cell: a=19.442(2) b=13.794(2) c=19.055(2)  
 alpha=90 beta=113.33(3) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	4692.4(14)	4692.4(14)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C25 H26 N4 O4 Pb	C25 H26 N4 O4 Pb
Sum formula	C25 H26 N4 O4 Pb	C25 H26 N4 O4 Pb
Mr	653.70	653.69
Dx, g cm <sup>-3</sup>	1.851	1.851
Z	8	8
Mu (mm <sup>-1</sup> )	14.316	14.316
F000	2544.0	2544.0
F000'	2517.83	
h, k, lmax	24, 17, 23	24, 17, 23
Nref	9447	17047
Tmin, Tmax	0.291, 0.651	0.275, 1.000
Tmin'	0.066	

Correction method= # Reported T Limits: Tmin=0.275 Tmax=1.000  
 AbsCorr = MULTI-SCAN



Data completeness= 1.804

Theta(max)= 73.420

R(reflections)= 0.0509( 14374)

wR2(reflections)=  
0.1457( 17047)

S = 1.073

Npar= 614

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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.

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● **Alert level C**

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of	02 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .....	0.01338 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. #	1 Note
C25 H26 N4 O4 Pb	
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance .....	5.184 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600	21 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .	17 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .	24.31 Check

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● **Alert level G**

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	41.28 Why ?
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....	C31A Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....	4 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #	2 Note
C25 H26 N4 O4 Pb	
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) .	2.22 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2 (II) .	2.12 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..	! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	294 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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1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 ALERT type 2 Indicator that the structure model may be wrong or deficient  
6 ALERT type 3 Indicator that the structure quality may be low  
6 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check

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## Datablock: 22aZn

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Bond precision: C-C = 0.0021 A

Wavelength=1.54184

Cell: a=8.507(2) b=17.186(3) c=17.472(3)  
 alpha=100.29(2) beta=96.09(2) gamma=102.48(3)  
 Temperature: 100 K

	Calculated	Reported
Volume	2426.0(9)	2426.0(9)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C54 H62 N8 O6 Zn	C54 H62 N8 O6 Zn
Sum formula	C54 H62 N8 O6 Zn	C54 H62 N8 O6 Zn
Mr	984.51	984.48
Dx, g cm <sup>-3</sup>	1.348	1.348
Z	2	2
Mu (mm <sup>-1</sup> )	1.187	1.187
F000	1040.0	1040.0
F000'	1039.73	
h, k, lmax	10, 21, 21	10, 21, 21
Nref	10117	9909
Tmin, Tmax	0.843, 0.965	0.888, 1.000
Tmin'	0.770	

Correction method= # Reported T Limits: Tmin=0.888 Tmax=1.000  
 AbsCorr = MULTI-SCAN

Data completeness= 0.979 Theta(max)= 75.835

R(reflections)= 0.0338( 8945) wR2(reflections)=  
 0.0912( 9909)  
 S = 1.081 Npar= 650

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	3.2 Ratio
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600	7 Report



#### Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...	4 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records	1 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for O21 --C22 .	6.9 s.u.
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1 )	4% Note
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O21A .	108.1 Degree
PLAT410_ALERT_2_G Short Intra H...H Contact H16B ..H19D .	1.86 Ang.



	Calculated	Reported
Volume	5841.4(19)	5841.3(19)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C54 H52 F10 N8 O6 Zn [+ solvent]	C54 H52 F10 N8 O6 Zn [+ solvent]
Sum formula	C54 H52 F10 N8 O6 Zn [+ solvent]	C54 H52 F10 N8 O6 Zn [+ solvent]
Mr	1164.43	1164.40
Dx, g cm <sup>-3</sup>	1.324	1.324
Z	4	4
Mu (mm <sup>-1</sup> )	1.326	1.326
F000	2400.0	2400.0
F000'	2402.35	
h, k, lmax	16, 19, 35	16, 19, 35
Nref	12199	12000
Tmin, Tmax	0.867, 0.961	0.576, 1.000
Tmin'	0.864	

Correction method= # Reported T Limits: Tmin=0.576 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.984                      Theta(max)= 76.077

R(reflections)= 0.0617( 7895)                      wR2(reflections)=  
0.1912( 12000)  
S = 1.058                      Npar= 713

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

PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for C19 --C20 . 5.2 s.u.  
PLAT790\_ALERT\_4\_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note  
C54 H52 F10 N8 O6 Zn  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 5 Report  
PLAT934\_ALERT\_3\_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check

#### Alert level G

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
CELLZ01\_ALERT\_1\_G ALERT: Large difference may be due to a  
symmetry error - see SYMMG tests  
From the CIF: \_cell\_formula\_units\_Z 4  
From the CIF: \_chemical\_formula\_sum C54 H52 F10 N8 O6 Zn [+ solvent]  
TEST: Compare cell contents of formula and atom\_site data











PLAT300_ALERT_4_G	Atom Site Occupancy of H22C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H23D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H24D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H26B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H40D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H42A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H42B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H42C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H42D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H45A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H45B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H45C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H45D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H46A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H46B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H46C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H46D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H48D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O70	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O70A	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )		33%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3 )		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 2 )		0.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 3 )		0.50	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O70	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?) .....		O70A	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C38 - C39 .		1.58	Ang.
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O18A .		136.4	Degree
PLAT410_ALERT_2_G	Short Intra H...H Contact H48A ..H49B .		2.13	Ang.
		x,y,z =	1_555	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H48B ..H49B .		2.07	Ang.
		x,y,z =	1_555	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H48C ..H49A .		2.05	Ang.
		x,y,z =	1_555	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H48C ..H49B .		2.05	Ang.
		x,y,z =	1_555	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H48D ..H49B .		2.07	Ang.
		x,y,z =	1_555	Check

PLAT411_ALERT_2_G	Short Inter H...H Contact	H8A	..H24B	.	1.75 Ang.
			x,-1+y,z =		1_545 Check
PLAT411_ALERT_2_G	Short Inter H...H Contact	H8A	..H24D	.	2.11 Ang.
			x,-1+y,z =		1_545 Check
PLAT431_ALERT_2_G	Short Inter HL..A Contact	F60	..O18A	.	2.58 Ang.
			2-x,-1/2+y,3/2-z =		2_746 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O18A	..C60	.	2.68 Ang.
			2-x,1/2+y,3/2-z =		2_756 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	F61	..C60	.	2.79 Ang.
			2-x,1-y,1-z =		3_766 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C19A	..C60	.	3.20 Ang.
			2-x,1/2+y,3/2-z =		2_756 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C60	..C61	.	3.16 Ang.
			2-x,1-y,1-z =		3_766 Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....				! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....				1032 Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .				Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600				297 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....				3.8 Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged				Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				4 Info

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

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## Datablock: 22bCd

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Bond precision: C-C = 0.0176 A                      Wavelength=1.54184

Cell:                      a=23.482(3)              b=8.277(2)              c=28.339(3)  
                             alpha=90                      beta=106.77(2)              gamma=90

Temperature:              100 K



PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C34	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C66	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Cd1	0.124 Check
PLAT334_ALERT_2_C	Small <C-C> Benzene Dist. C63 -C68 .		1.37 Ang.
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds .....		0.01763 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....		2.938 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600		53 Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..		1 Check
PLAT977_ALERT_2_C	Check Negative Difference Density on H42B .		-0.34 eA-3

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**Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		70	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...		78	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records		1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records		19	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records		5	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records		1	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for N51 --C50 .		7.5	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C5 --C6 .		7.0	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C5 --C57 .		6.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cd1 --N53A .		5.0	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder ..... (Resd 1 )		49%	Note
PLAT410_ALERT_2_G	Short Intra H...H Contact H14A ..H16C .		1.99	Ang.
		x, y, z =	1_555	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H23A ..H22D .		1.98	Ang.
		x, y, z =	1_555	Check
PLAT410_ALERT_2_G	Short Intra H...H Contact H36A ..H38B .		2.02	Ang.
		x, y, z =	1_555	Check
PLAT411_ALERT_2_G	Short Inter H...H Contact H34A ..H50D .		1.79	Ang.
		x, -1+y, z =	1_545	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F66 ..C43A .		2.96	Ang.
		2-x, -1/2+y, 1/2-z =	2_745	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F68 ..C46 .		2.93	Ang.
		2-x, 1/2+y, 1/2-z =	2_755	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O15 ..C42A .		2.96	Ang.
		x, 1/2-y, -1/2+z =	4_565	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O44A ..C66 .		2.99	Ang.
		2-x, 1/2+y, 1/2-z =	2_755	Check
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C50 --C52		1.98	Ang.
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C4A --C5A		2.03	Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		33.60	Deg.
	N51 -C50 -C52 1_555 1_555 1_555 .....	#	98	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		42.80	Deg.
	N51 -C52 -C50 1_555 1_555 1_555 .....	#	128	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ....			! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....		1743	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .			Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta (Min).		1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		426	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....		3.4	Low
PLAT955_ALERT_1_G	Reported (CIF) and Actual (FCF) Lmax Differ by .		1	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		4	Info

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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.

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**PLATON version of 18/05/2022; check.def file version of 17/05/2022**



















