

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_70415aa

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: mo_70415aa

Bond precision:	C-C = 0.0092 Å	Wavelength=0.71073
Cell:	a=30.6731(19) b=12.4071(8) c=25.1314(16)	
	alpha=90 beta=104.710(1) gamma=90	
Temperature:	173 K	
	Calculated	Reported
Volume	9250.6(10)	9250.6(10)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	4(C34 H44 B20 N4 Pd2 S2), C Cl3	?
Sum formula	C137 H176 B80 Cl3 N16 Pd8 S8	C34.25 H44.25 B20 Cl0.75 N4 Pd2 S2
Mr	4125.77	1031.69
Dx, g cm ⁻³	1.481	1.482
Z	2	8
Mu (mm ⁻¹)	0.945	0.945
F000	4114.0	4116.0
F000'	4101.64	
h,k,lmax	39,16,32	39,16,32
Nref	21336	21148
Tmin,Tmax	0.873,0.910	0.669,0.746
Tmin'	0.812	

Correction method= # Reported T Limits: Tmin=0.669 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 27.538

R(reflections)= 0.0504(13739) wR2(reflections)= 0.1483(21148)

S = 1.055 Npar= 1165

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

PLAT327_ALERT_2_B	Possible Missing H on sp3? Carbon	*C69	Check
PLAT934_ALERT_3_B	Number of (Iobs-Icalc)/SigmaW > 10 Outliers	10	Check

Alert level C

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT220_ALERT_2_C	Non-Solvent Resd 1	C Ueq(max)/Ueq(min) Range	3.3 Ratio
PLAT220_ALERT_2_C	Non-Solvent Resd 2	C Ueq(max)/Ueq(min) Range	4.1 Ratio
PLAT222_ALERT_3_C	Non-Solvent Resd 2	H Uiso(max)/Uiso(min) Range	6.6 Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference C30	-- C31 ..	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference B17	-- B18 ..	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C57	-- C58 ..	0.19 Ang.
PLAT245_ALERT_2_C	U(iso) H45	Smaller than U(eq) C45 by ...	0.016 AngSq
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds		0.00923 Ang.
PLAT351_ALERT_3_C	Long C-H (X0.96,N1.08A) C11	- H11A ..	1.12 Ang.
PLAT411_ALERT_2_C	Short Inter H...H Contact H5A	.. H33 .	2.12 Ang.
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance		4.024 Check
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L=	0.600	98 Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .		2 Check
PLAT977_ALERT_2_C	Check the Negative Difference Density on	H5	-0.47 eA-3
PLAT977_ALERT_2_C	Check the Negative Difference Density on	H13	-0.36 eA-3
PLAT977_ALERT_2_C	Check the Negative Difference Density on	H20A	-0.39 eA-3
PLAT977_ALERT_2_C	Check the Negative Difference Density on	H23A	-0.34 eA-3
PLAT977_ALERT_2_C	Check the Negative Difference Density on	H33	-0.31 eA-3
PLAT977_ALERT_2_C	Check the Negative Difference Density on	H67	-0.43 eA-3

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
 _chemical_formula_sum and the formula from the _atom_site* data.
 Atom count from _chemical_formula_sum: C34.25 H44.25 B20 Cl0.75 N4 Pd
 Atom count from the _atom_site data: C34.25 H44 B20 Cl0.75 N4 Pd2 S

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
 From the CIF: _cell_formula_units_Z 8
 From the CIF: _chemical_formula_sum C34.25 H44.25 B20 Cl0.75 N4 Pd2
 TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	274.00	274.00	0.00
H	354.00	352.00	2.00
B	160.00	160.00	0.00
Cl	6.00	6.00	0.00
N	32.00	32.00	0.00
Pd	16.00	16.00	0.00
S	16.00	16.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	10	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	5	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.25	Check
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	3	Note
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) Pd4	-- S4 ..	6.5 s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl1	is Constrained at	0.5 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of Cl2	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl3	is Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C69	is Constrained at	0.5	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)..		100	% Note
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for	C1	Check
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for	C2	Check
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for	C10	Check
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for	C11	Check
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for	C35	Check
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for	C36	Check
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for	C44	Check
PLAT343_ALERT_2_G	Unusual sp?	Angle Range in Main Residue for	C45	Check
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond C1 - C2 ..	1.66	Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond C1 - C3 ..	1.51	Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond C10 - C11 ..	1.65	Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond C10 - C12 ..	1.50	Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond C35 - C36 ..	1.65	Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond C35 - C37 ..	1.52	Ang.
PLAT367_ALERT_2_G	Long?	C(sp?)-C(sp?) Bond C44 - C45 ..	1.66	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl1 .. C69 ..	1.95	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl2 .. C69 ..	1.41	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	Cl3 .. C69 ..	2.58	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C69 .. C69 ..	1.70	Ang.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		963	Check
	CL2 -C69 -CL1	3.565 1.555 1.555	36.10	Deg.
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF #		968	Check
	CL2 -C69 -CL1	1.555 1.555 3.565	32.20	Deg.
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		35	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min)		2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		89	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		3	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		2	Note

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 36 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
 14 ALERT type 4 Improvement, methodology, query or suggestion
 0 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.

