

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a_a

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: a_a

Bond precision: C-C = 0.0121 Å Wavelength=1.54178

Cell: a=10.9914 (9) b=13.2868 (11) c=14.8616 (13)
 alpha=66.908 (4) beta=80.808 (5) gamma=89.602 (5)
Temperature: 223 K

	Calculated	Reported
Volume	1967.2 (3)	1967.1 (3)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	2 (C56 H34), C S2	0.5 (C S2), C56 H34
Sum formula	C113 H68 S2	C56.5 H34 S
Mr	1489.79	744.97
Dx, g cm ⁻³	1.258	1.258
Z	1	2
Mu (mm ⁻¹)	1.024	1.024
F000	778.0	780.9
F000'	780.62	
h, k, lmax	13, 16, 18	13, 16, 17
Nref	14682 [7341]	12602
Tmin, Tmax	0.815, 0.950	0.435, 0.753
Tmin'	0.815	

Correction method= # Reported T Limits: Tmin=0.435 Tmax=0.753
AbsCorr = NONE

Data completeness= 1.72/0.86 Theta (max)= 69.260

R(reflections)= 0.1089 (7723)	wR2(reflections)=
S = 1.119	0.3409 (12602)
Npar= 1037	

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

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01208 Ang.



Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.134

PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12	0.134	Report
PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ		Please Check
PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ		Please Check
PLAT057_ALERT_3_C	Correction for Absorption Required RT(exp) ...	1.17	Do !
PLAT082_ALERT_2_C	High R1 Value	0.11	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.34	Report
PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18)	6.92	Note
PLAT234_ALERT_4_C	Large Hirshfeld Difference C11 --C12 .	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C36 --C37 .	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C52 --C53 .	0.17	Ang.
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C113	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.2	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.2	Note
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including S1	0.131	Check
PLAT601_ALERT_2_C	Unit Cell Contains Solvent Accessible VOIDS of .	63	Ang**3
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4		Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.609	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	75	Report
PLAT915_ALERT_3_C	No Flack x Check Done: Low Friedel Pair Coverage	74	%
PLAT921_ALERT_1_C	R1 in the CIF and FCF Differ by	0.0011	Check
PLAT987_ALERT_1_C	The Flack x is >> 0 - Do a BASF/TWIN Refinement		Please Check



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	12	Note
PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero .	0.140	Note
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.20	Report
PLAT073_ALERT_1_G	H-atoms ref, but _hydrogen_treatment Reported as		constr Check
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2	Report
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	4	Note
PLAT769_ALERT_4_G	CIF Embedded explicitly supplied scattering data		Please Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	15	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	90	Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	8	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info
PLAT982_ALERT_1_G	The C-f' = 0.0192 Deviates from IT-value =	0.0181	Check
PLAT982_ALERT_1_G	The S-f' = 0.3354 Deviates from IT-value =	0.3331	Check
PLAT983_ALERT_1_G	The S-f'' = 0.5513 Deviates from IT-Value =	0.5567	Check
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	9	Check

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

10 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
11 ALERT type 3 Indicator that the structure quality may be low
10 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.

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