

Structure factors have been supplied for datablock(s) t_a

No syntax errors found. CIF dictionary Interpreting this report

Bond precision:	C-C = 0.0055 Å	Wavelength=1.54178		
Cell:	a=50.275 (3)	b=50.275 (3)	c=10.5646 (6)	
	alpha=90	beta=90	gamma=120	
Temperature:	233 K			

	Calculated	Reported
Volume	23125(3)	23125(3)
Space group	R -3	R -3
Hall group	-R 3	-R 3
Moiety formula	C56 H34, C H Cl3 [+ solvent]	C56 H34, C H Cl3
Sum formula	C57 H35 Cl3 [+ solvent]	C57 H35 Cl3
Mr	826.20	826.20
Dx, g cm-3	1.068	1.068
Z	18	18
Mu (mm-1)	1.858	1.858
F000	7704.0	7704.0
F000'	7741.54	
h, k, lmax	60, 60, 12	60, 60, 12
Nref	9361	9342
Tmin, Tmax	0.956, 0.964	0.525, 0.753
Tmin'	0.830	

Data completeness= 0.998 Theta (max)= 67.910

R(reflections)= 0.0823(5148)	wR2(reflections)= 0.2767(9342)
S = 0.984	Npar= 542

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

PLAT260_ALERT_2_B Large Average Ueq of Residue Including C11 0.695 Check

 Alert level C

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.136

PLAT020_ALERT_3_C	The Value of Rint is Greater Than 0.12	0.136	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.28	Report
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C53 --C54 .	5.5	s.u.
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C57	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C11	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C13	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00554	Ang.
PLAT767_ALERT_4_C	INS Embedded LIST 6 Instruction Should be LIST 4		Please Check
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...	-1.195	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	4	Check
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1	Check

 Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	4	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	4	Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.18	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	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT344_ALERT_2_G	Unusual sp3 Angle Range in Solvent/Ion for	C57	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C29 ..C57 .	3.12	Ang.
	1/3+x-y,-1/3+x,5/3-z =	18_546	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C30 ..C57 .	2.94	Ang.
	1/3+x-y,-1/3+x,5/3-z =	18_546	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C31 ..C57 .	3.04	Ang.
	1/3+x-y,-1/3+x,5/3-z =	18_546	Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	42	Note
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed	!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	18	Note
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

1 **ALERT level B** = A potentially serious problem, consider carefully

12 **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

0 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
9 ALERT type 3 Indicator that the structure quality may be low
11 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.

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