

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 109_autored

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: 109 authored

Bond precision:	C-C = 0.0026 Å	Wavelength=1.54184	
Cell:	a=15.0697 (6)	b=8.5154 (3)	c=19.8597 (7)
	alpha=90	beta=108.128 (4)	gamma=90
Temperature:	293 K		

	Calculated	Reported
Volume	2421.99 (16)	2421.99 (16)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C24 H28 O3 S [+ solvent]	C24 H28 O3 S
Sum formula	C24 H28 O3 S [+ solvent]	C24 H28 O3 S
Mr	396.52	396.52
Dx, g cm ⁻³	1.087	1.087
Z	4	4
Mu (mm ⁻¹)	1.331	1.331
F000	848.0	848.0
F000'	851.58	
h, k, l _{max}	18, 10, 25	18, 10, 24
Nref	5071	5047
Tmin, Tmax	0.709, 0.923	0.472, 1.000
Tmin'	0.590	

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Correction method= # Reported T Limits: Tmin=0.472 Tmax=1.000
AbsCorr = GAUSSIAN
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Data completeness= 0.995 Theta(max)= 76.233

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R(reflections)= 0.0469( 4329)      wR2(reflections)=
S = 1.045                          0.1414( 5047)
Npar= 366
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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.



Alert level C

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	S1	--O3	.	5.3 s.u.
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of		C7 Check
PLAT355_ALERT_3_C	Long	O-H (X0.82,N0.98A)	O2	- H2	1.02 Ang.



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	35	Note
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	19	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffn_ambient_temperature (K)	293	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	36%	Note
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	215	A**3
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	169	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	23	Note
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	4.845	Note
	Predicted wR2: Based on SigI**2 2.91 or SHELX Weight 13.53		
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	3	Check

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

- 2 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
3 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check
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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.

