

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 250801ha_z3098046_0m

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: 250801ha_z3098046_0m

Bond precision:	C-C = 0.0059 Å	Wavelength=1.54178	
Cell:	a=12.5702 (3)	b=13.3715 (3)	c=21.2980 (4)
	alpha=84.105 (1)	beta=84.441 (1)	gamma=65.775 (1)
Temperature:	193 K		
	Calculated	Reported	
Volume	3241.41 (13)	3241.41 (12)	
Space group	P -1	P-1	
Hall group	-P 1	-P 1	
Moiety formula	C98 H110 Co8 O42 S8 [+ solvent]	C98 H110 Co8 O42 S8	
Sum formula	C98 H110 Co8 O42 S8 [+ solvent]	C98 H110 Co8 O42 S8	
Mr	2687.78	2687.77	
Dx, g cm ⁻³	1.377	1.377	
Z	1	1	
Mu (mm ⁻¹)	9.644	9.644	
F000	1378.0	1378.0	
F000'	1365.85		
h, k, lmax	15, 16, 25	15, 16, 25	
Nref	11895	11829	
Tmin, Tmax	0.438, 0.462	0.617, 0.753	
Tmin'	0.331		

Correction method= # Reported T Limits: Tmin=0.617 Tmax=0.753
AbsCorr = NONE

Data completeness= 0.994

Theta (max)= 68.390

PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H38	x,y,z = ..H39F	=	1_555	Check
						1.76 Ang.
			x,y,z =		1_555	Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Crystal Structure					! Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				405	Note
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed					! Info
PLAT910_ALERT_3_G	Missing FCF Reflection(s) Below Theta(Min) [Deg]=				3.63	Note
	0 0 1,					
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600				33	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity				3.4	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value				2.376	Note
	Predicted wR2: Based on SigI**2 5.84 or SHELX Weight 13.00					
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				4	Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 14 ALERT type 2 Indicator that the structure model may be wrong or deficient
 22 ALERT type 3 Indicator that the structure quality may be low
 6 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.

