checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SGGAR1

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: SGGAR1

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Bond precision:   C-C = 0.0191 A          Wavelength=0.71073

Cell:             a=15.603(2)    b=17.630(2)          c=15.3019(19)
                  alpha=90       beta=118.175(4)      gamma=90
Temperature:      150 K
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	Calculated	Reported
Volume	3710.5(8)	3710.5(8)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C26 H34 B6 Co2 O5 S5 W [+ solvent]	C26 H34 B6 Co2 O5 S5 W
Sum formula	C26 H34 B6 Co2 O5 S5 W [+ solvent]	C26 H34 B6 Co2 O5 S5 W
Mr	953.39	953.40
Dx,g cm-3	1.707	1.707
Z	4	4
Mu (mm-1)	4.291	4.291
F000	1872.0	1872.0
F000'	1874.44	
h,k,lmax	20,22,19	20,22,19
Nref	8530	8479
Tmin,Tmax	0.441,0.651	0.454,0.651
Tmin'	0.408	

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Correction method= # Reported T Limits: Tmin=0.454 Tmax=0.651
AbsCorr = MULTI-SCAN

Data completeness= 0.994           Theta(max)= 27.522
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R(reflections)= 0.0735(7089)

wR2(reflections)= 0.1947(8479)

S = 1.124 Npar= 417

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

PLAT342_ALERT_3_C	Low Bond Precision on C–C Bonds	0.0191	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	4.322	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.102	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	22	Report
PLAT977_ALERT_2_C	Check Negative Difference Density on H3 .	−0.33	eA−3
PLAT977_ALERT_2_C	Check Negative Difference Density on H5 .	−0.33	eA−3
PLAT977_ALERT_2_C	Check Negative Difference Density on H6 .	−0.35	eA−3
PLAT977_ALERT_2_C	Check Negative Difference Density on H13C .	−0.56	eA−3
PLAT977_ALERT_2_C	Check Negative Difference Density on H14A .	−0.48	eA−3
PLAT977_ALERT_2_C	Check Negative Difference Density on H25B .	−1.00	eA−3

Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	153.46	Why ?
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	121	A**3
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	28	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	10	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.6	Low
PLAT978_ALERT_2_G	Number C–C Bonds with Positive Residual Density.	0	Info

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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
8 **ALERT level G** = General information/check it is not something unexpected

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

PLATON version of 20/01/2022; check.def file version of 19/01/2022

Datablock SGGAR1 - ellipsoid plot