

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_20211124_ny_1_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: mo_20211124_ny_1_0m

Bond precision:	C-C = 0.0048 Å	Wavelength=0.71073
Cell:	a=14.3732(7) b=11.6437(5) c=27.9984(15)	
	alpha=90 beta=103.558(2) gamma=90	
Temperature:	191 K	
	Calculated	Reported
Volume	4555.2(4)	4555.2(4)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C57 H36, 0.5(C6 H14), C H2 C12	C H2 C12, C57 H36, C3 H7
Sum formula	C61 H45 C12	C61 H45 C12
Mr	848.87	848.87
Dx, g cm ⁻³	1.238	1.238
Z	4	4
Mu (mm ⁻¹)	0.183	0.183
F000	1780.0	1780.0
F000'	1781.79	
h,k,lmax	18,15,36	18,15,36
Nref	10493	10472
Tmin,Tmax	0.973,0.978	0.667,0.746
Tmin'	0.973	
Correction method= # Reported T Limits:	Tmin=0.667 Tmax=0.746	
AbsCorr = MULTI-SCAN		
Data completeness=	0.998	Theta(max)= 27.529
R(reflections)=	0.0817(6763)	wR2(reflections)=
		0.2367(10472)
S =	1.060	Npar= 570

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

DIFMX02_ALERT_1_C The maximum difference density is $> 0.1 \cdot Z_{\text{MAX}} \cdot 0.75$

The relevant atom site should be identified.

PLAT031_ALERT_4_C	Refined Extinction Parameter Within Range	3.000	Sigma
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	1.34	eA-3
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.9	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C1 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C2 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		C5 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		C60 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of		C58 Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including C11	0.120	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00476	Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C60 - C61	1.41	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	8.481	Check
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1	Check



Alert level G

PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ	Please	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	6.39	Why ?
PLAT793_ALERT_4_G	Model has Chirality at C7 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C20 (Centro SPGR)	S	Verify
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	17	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	8	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
14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected
- 2 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
4 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

