checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20220615_double4helicene

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.

Datablock: 20220615_double4helicene

Bond precision:	C-C = 0.0031 A	Wavelength=0.71073	
Cell:	a=16.2348(3)	b=11.5347(2)	c=22.0250(4)
	alpha=90	beta=105.712(2)	gamma=90
Temperature:	93 K		
	Calculated	Reported	
Volume	3970.37(13)	3970.37(13)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C54 H50 O2	C54 H50 O2	
Sum formula	C54 H50 O2	C54 H50 O2	
Mr	730.94	730.94	
Dx,g cm-3	1.223	1.223	
Z	4	4	
Mu (mm-1)	0.072	0.072	
F000	1560.0	1560.0	
F000'	1560.61		
h,k,lmax	21,15,29	21,15,29	
Nref	9588	9576	
Tmin, Tmax	0.987,0.994	0.812,1.0	00
Tmin'	0.984		
Correction methodals AbsCorr = MULTI-	_	imits: Tmin=0.812 Tm	ax=1.000
Data completenes	ss= 0.999	Theta $(max) = 27.99$	7
R(reflections) =	0.0730(6828)		wR2(reflections) = 0.2191(9576)
S = 1.045	Npar= !	511	0.2101 (00.0)
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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.

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Alert level C
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DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75 The relevant atom site should be identified.

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.62 Report PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 0.66 eA-3 PLAT230_ALERT_2_C Hirshfeld Test Diff for C41 --C42 5.5 s.u. PLAT410_ALERT_2_C Short Intra H...H Contact H1 ..H27 1.93 Ang. x, y, z =1_555 Check PLAT410_ALERT_2_C Short Intra H...H Contact H12 ..H16 1.97 Ang. 1_555 Check x, y, z =PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 8.974 Check PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report

Alert level G

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.12 Report PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C37 Check 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 8 Note PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note 3.4 Low PLAT941_ALERT_3_G Average HKL Measurement Multiplicity PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res .. 56.0 Degree 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
- 0 ALERT level B = A potentially serious problem, consider carefully
- 8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
- 9 ALERT level G = General information/check it is not something unexpected
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
- 8 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
- 2 ALERT type 4 Improvement, methodology, query or suggestion
- 2 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 28/11/2022; check.def file version of 28/11/2022

