

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4c\_benzo\_mes\_I3

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: 4c\_benzo\_mes\_I3

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Bond precision:      C-C = 0.0049 Å

Wavelength=0.71073

Cell:                      a=10.7490(12)              b=13.7879(14)              c=16.0621(16)  
                             alpha=78.407(3)              beta=75.739(3)              gamma=89.266(4)  
Temperature:              150 K

	Calculated	Reported
Volume	2258.4(4)	2258.4(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C47 H51 N O), C4 H10 O, 2(I3)	2(C47 H51 N O), C4 H10 O, 2(I3)
Sum formula	C98 H112 I6 N2 O3	C98 H112 I6 N2 O3
Mr	2127.30	2127.29
Dx, g cm <sup>-3</sup>	1.564	1.564
Z	1	1
Mu (mm <sup>-1</sup> )	2.113	2.113
F000	1056.0	1056.0
F000'	1053.49	
h,k,lmax	13,16,19	13,16,19
Nref	8576	8547
Tmin,Tmax	0.608,0.760	0.673,0.760
Tmin'	0.548	

Correction method= # Reported T Limits: Tmin=0.673 Tmax=0.760  
AbsCorr = MULTI-SCAN

Data completeness= 0.997

Theta(max)= 25.681

R(reflections)= 0.0304( 7586)

wR2(reflections)=  
0.0803( 8547)

S = 1.041

Npar= 500

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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

PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including O2 0.116 Check  
PLAT410\_ALERT\_2\_C Short Intra H...H Contact H25B ..H33 . 1.98 Ang.  
x,y,z = 1\_555 Check  
PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 26 Report  
3 8 0, 0 -1 1, -1 0 1, 1 0 1, 3 9 1, -7 4 2,  
0 1 3, 2 -8 4, 4 -7 4, -2 3 4, 1 5 4, -5 6 4,  
5 7 5, -5 2 6, 6 -4 7, -4 3 7, 4 7 7, 4 -4 8,  
1 1 8, 2 -5 9, 0 1 10, 1 1 10, 0 2 11, 1 2 11,  
1 3 12, -5 4 15,  
PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.06Ang From C50 2.45 eA-3  
PLAT977\_ALERT\_2\_C Check Negative Difference Density on H48A . -0.36 eA-3  
PLAT977\_ALERT\_2\_C Check Negative Difference Density on H48B . -0.32 eA-3  
PLAT977\_ALERT\_2\_C Check Negative Difference Density on H49B . -0.35 eA-3  
PLAT977\_ALERT\_2\_C Check Negative Difference Density on H51C . -0.47 eA-3

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### Alert level G

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 5 Note  
PLAT003\_ALERT\_2\_G Number of Uiso or U(i,j) Restrained non-H-Atoms 5 Report  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 7.52 Why ?  
PLAT171\_ALERT\_4\_G The CIF-Embedded .res File Contains EADP Records 1 Report  
PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 4 Report  
PLAT186\_ALERT\_4\_G The CIF-Embedded .res File Contains ISOR Records 1 Report  
PLAT299\_ALERT\_4\_G Atom Site Occupancy Constrained at ..... 0.5 Check  
O2 C48 C49 C50 C51 H48A H48B H48C  
H49A H49B H50A H50B H51A H51B H51C  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... (Resd 2) 7.50 Check  
PLAT413\_ALERT\_2\_G Short Inter XH3 .. XHn H12 ..H51B . 1.99 Ang.  
x,-1+y,1+z = 1\_546 Check  
PLAT413\_ALERT\_2\_G Short Inter XH3 .. XHn H16 ..H48C . 2.12 Ang.  
x,-1+y,z = 1\_545 Check  
PLAT789\_ALERT\_4\_G Atoms with Negative \_atom\_site\_disorder\_group # 15 Check  
PLAT793\_ALERT\_4\_G Model has Chirality at C5 (Centro SpGr) S Verify  
PLAT822\_ALERT\_4\_G CIF-embedded .res Contains Negative PART Numbers 1 Check  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 38 Note  
PLAT910\_ALERT\_3\_G Missing FCF Reflection(s) Below Theta(Min) [Deg]= 1.96 Note  
0 1 0, 0 0 1, 0 1 1,  
PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 1 Note  
-2 3 4,  
PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 3.6 Low  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 3.078 Note  
Predicted wR2: Based on SigI\*\*2 2.61 or SHELX Weight 7.71  
PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 12 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  
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
20 **ALERT level G** = General information/check it is not something unexpected

0 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  
4 ALERT type 3 Indicator that the structure quality may be low  
9 ALERT type 4 Improvement, methodology, query or suggestion  
1 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.

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**PLATON version of 04/06/2025; check.def file version of 30/05/2025**

