

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) d8v20176

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.

Please wait while processing

[CIF dictionary](#)

[Interpreting this report](#)

[Structure factor report](#)

Datablock: d8v20176

Bond precision: C-C = 0.0112 Å Wavelength=0.71073

Cell: a=19.776(2) b=18.2753(15) c=16.4263(15)
alpha=90 beta=90.339(3) gamma=90

Temperature: 192 K

	Calculated	Reported
Volume	5936.6(9)	5936.7(9)
Space group	P c	P c
Hall group	P -2yc	P -2yc
Moiety formula	C36 H32 B2 O2 [+ solvent]	?
Sum formula	C36 H32 B2 O2 [+ solvent]	C36 H32 B2 O2
Mr	518.24	518.23
Dx, g cm ⁻³	1.160	1.160
Z	8	8
Mu (mm ⁻¹)	0.069	0.069
F000	2192.0	2192.0
F000'	2192.87	
h, k, lmax	23, 21, 19	23, 21, 19
Nref	20911[10466]	19509
Tmin, Tmax	0.988, 0.993	0.524, 0.746
Tmin'	0.988	

Correction method= # Reported T Limits: Tmin=0.524 Tmax=0.746 AbsCorr = MULTI-SCAN

Data completeness= 1.86/0.93 Theta(max)= 24.999

R(reflections)= 0.0755(12937) wR2(reflections)= 0.2132(19509)

S = 1.001 Npar= 1467

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 B

PLAT340_ALERT_3_B Low Bond Precision on C-C Bonds 0.01117 Ång.

PLAT990_ALERT_1_B Deprecated .res/.hkl Input Style SQUEEZE Job ... ! Note

●Alert level C

STRVA01_ALERT_4_C Flack parameter is too small
From the CIF: `_refine_ls_abs_structure_Flack` -0.400
From the CIF: `_refine_ls_abs_structure_Flack_su` 1.000
PLAT018_ALERT_1_C `_diffn_measured_fraction_theta_max` .NE. *_full ! Check
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) 7.12 Note
PLAT234_ALERT_4_C Large Hirshfeld Difference C5 --C6 . 0.16 Ang.

And 6 other PLAT234 Alerts

More ...

PLAT334_ALERT_2_C Small Aver. Benzene C-C Dist C1 -C6 1.37 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.393 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 7 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 8 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 5 Note

●Alert level G

PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 1.000 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.12 Report
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp²)-Methyl Moiety C35B Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure ! Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT883_ALERT_1_G No Info/Value for `_atom_sites_solution_primary` . Please Do !
PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.30 Check
PLAT931_ALERT_5_G CIFcalcFCF Twin Law [1 0 0] Est.d BASF 0.10 Check
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 8 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities Please Check
PLAT992_ALERT_5_G Repd & Actual `_reflns_number_gt` Values Differ by 4 Check

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

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 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
13 ALERT type 4 Improvement, methodology, query or suggestion
3 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 22/04/2020; check.def file version of 09/03/2020

Datablock d8v20176 - ellipsoid plot



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