

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) exp_1455

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: exp_1455

Bond precision:	C-C = 0.0047 Å	Wavelength=1.54184
Cell:	a=9.5096(3)	b=12.0422(4)
	alpha=90	beta=90
		gamma=90
Temperature: 293 K		
	Calculated	Reported
Volume	3927.2(2)	3927.2(2)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C42 H54 N2 O2	C42 H54 N2 O2
Sum formula	C42 H54 N2 O2	C42 H54 N2 O2
Mr	618.87	618.87
Dx, g cm ⁻³	1.047	1.047
Z	4	4
Mu (mm ⁻¹)	0.485	0.485
F000	1344.0	1344.0
F000'	1347.49	
h, k, lmax	11, 14, 40	11, 14, 40
Nref	3514	3439
Tmin, Tmax	0.860, 0.916	0.535, 1.000
Tmin'	0.816	
Correction method= # Reported T Limits: Tmin=0.535 Tmax=1.000 AbsCorr = MULTI-SCAN		
Data completeness= 0.979	Theta(max)= 67.078	
R(reflections)= 0.0986(2680)	wR2(reflections)= 0.2865(3439)	
S = 1.065	Npar= 284	

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

PLAT420_ALERT_2_B D-H Without Acceptor	O1	--H1A	.	Please Check
PLAT420_ALERT_2_B D-H Without Acceptor	O2	--H15'	.	Please Check

●Alert level C

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low . 0.979 Why?
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) 0.29 Report
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of N1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C7 Check

And 3 other PLAT242 Alerts

More ...

PLAT260_ALERT_2_C Large Average Ueq of Residue Including O1 0.102 Check
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00469 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor N1 --H1 . Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 22.488 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.622 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.597 74 Report

●Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 14 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 14 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 3 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.15 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 12 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 12 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 13 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O1 Constrained at 0.5 Check

And 51 other PLAT300 Alerts

More ...

PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 30% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H3 ..H17C . 2.05 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H3 ..H17D . 1.97 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H3 ..H21C . 2.06 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H3 ..H21D . 2.07 Ang.
x,y,z = 1_555 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints 96 Note
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 52% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 74 Note
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

2 **ALERT level B** = A potentially serious problem, consider carefully

13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

18 ALERT type 2 Indicator that the structure model may be wrong or deficient

10 ALERT type 3 Indicator that the structure quality may be low

56 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 18/09/2020; check.def file version of 20/08/2020

Datablock exp_1455 - ellipsoid plot



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