

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_1456

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_1456

Bond precision: C-C = 0.0035 Å Wavelength=1.54184

Cell: a=10.2479(3) b=12.4899(4) c=21.9716(7)
alpha=74.823(3) beta=79.678(3) gamma=73.455(3)

Temperature: 293 K

	Calculated	Reported
Volume	2585.11(15)	2585.11(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H60 N2 O2 [+ solvent]	C44 H60 N2 O2
Sum formula	C44 H60 N2 O2 [+ solvent]	C44 H60 N2 O2
Mr	648.94	648.94
Dx, g cm ⁻³	0.834	0.834
Z	2	2
Mu (mm ⁻¹)	0.383	0.383
F000	708.0	708.0
F000'	709.81	
h, k, lmax	12, 14, 26	12, 14, 26
Nref	9234	8913
Tmin, Tmax	0.887, 0.933	0.489, 1.000
Tmin'	0.865	

Correction method= # Reported T Limits: Tmin=0.489 Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 0.965

Theta(max)= 67.079

R(reflections)= 0.0755(6011)

wR2(reflections)= 0.2531(8913)

S = 1.058

Npar= 489

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

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.965 Why?

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.5 Ratio

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C23 Check

● **Alert level G**

More ...

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_1456 - ellipsoid plot



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