

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) li_780_3

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](#)

Please wait while processing [Interpreting this report](#)

Structure factor report

Datablock: li_780_3

Bond precision:	C-C = 0.0056 Å	Wavelength=0.71073
Cell:	a=29.359(2) b=9.2406(6) c=17.5828(15)	
	alpha=90 beta=91.338(3) gamma=90	
Temperature: 296 K		

	Calculated	Reported
Volume	4768.8(6)	4768.9(6)
Space group	C 2	C 2
Hall group	C 2y	C 2y
Moiety formula	C26 H42 N2	C26 H42 N2
Sum formula	C26 H42 N2	C26 H42 N2
Mr	382.62	382.61
Dx, g cm ⁻³	1.066	1.066
Z	8	8
Mu (mm ⁻¹)	0.061	0.061
F000	1696.0	1696.0
F000'	1696.51	
h,k,lmax	37,11,22	37,11,22
Nref	10511[5588]	10461
Tmin,Tmax	0.961,0.995	0.874,0.938
Tmin'	0.961	

Correction method= # Reported T Limits: Tmin=0.874 Tmax=0.938 AbsCorr =
MULTI-SCAN

Data completeness= 1.87/1.00 Theta(max)= 27.078

R(reflections)= 0.0601(6791) wR2(reflections)= 0.1942(10461)

S = 1.018 Npar= 513

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

STRVA01_ALERT_2_C

Chirality of atom sites is inverted?

From the CIF: _refine_ls_abs_structure_Flack 1.700

From the CIF: _refine_ls_abs_structure_Flack_su 1.000

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C7 Check

And 3 other PLAT241 Alerts

[More ...](#)

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C6 Check

And 3 other PLAT242 Alerts

[More ...](#)

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds 0.00559 Ång.

PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -1.469 Report

PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? . 1.70 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 6 Report
 0 2 0, 2 0 0, 4 0 0, -2 0 1, -1 1 1, 2 0 1,

Alert level G

PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 1.000 Report
 PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size .. 0.65 mm
 PLAT111_ALERT_2_G ADDSYM Detects New (Pseudo) Centre of Symmetry . 82 %Fit
 PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space Group C2/c Check
 Check Model Parameter Symmetry for Reflection Data Support
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 19 Note
 PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF 1 Note
 0 2 0,
 PLAT916_ALERT_2_G Hooft y and Flack x Parameter Values Differ by . 0.70 Check
 PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 5 Note
 2 0 0, -1 -1 1, -2 0 1, 1 -1 1, 2 0 1,
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.62 Note
 Predicted wR2: Based on SigI*2 7.42 or SHELX Weight 19.57
 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
 13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 10 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 15 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
 3 ALERT type 4 Improvement, methodology, query or suggestion
 1 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

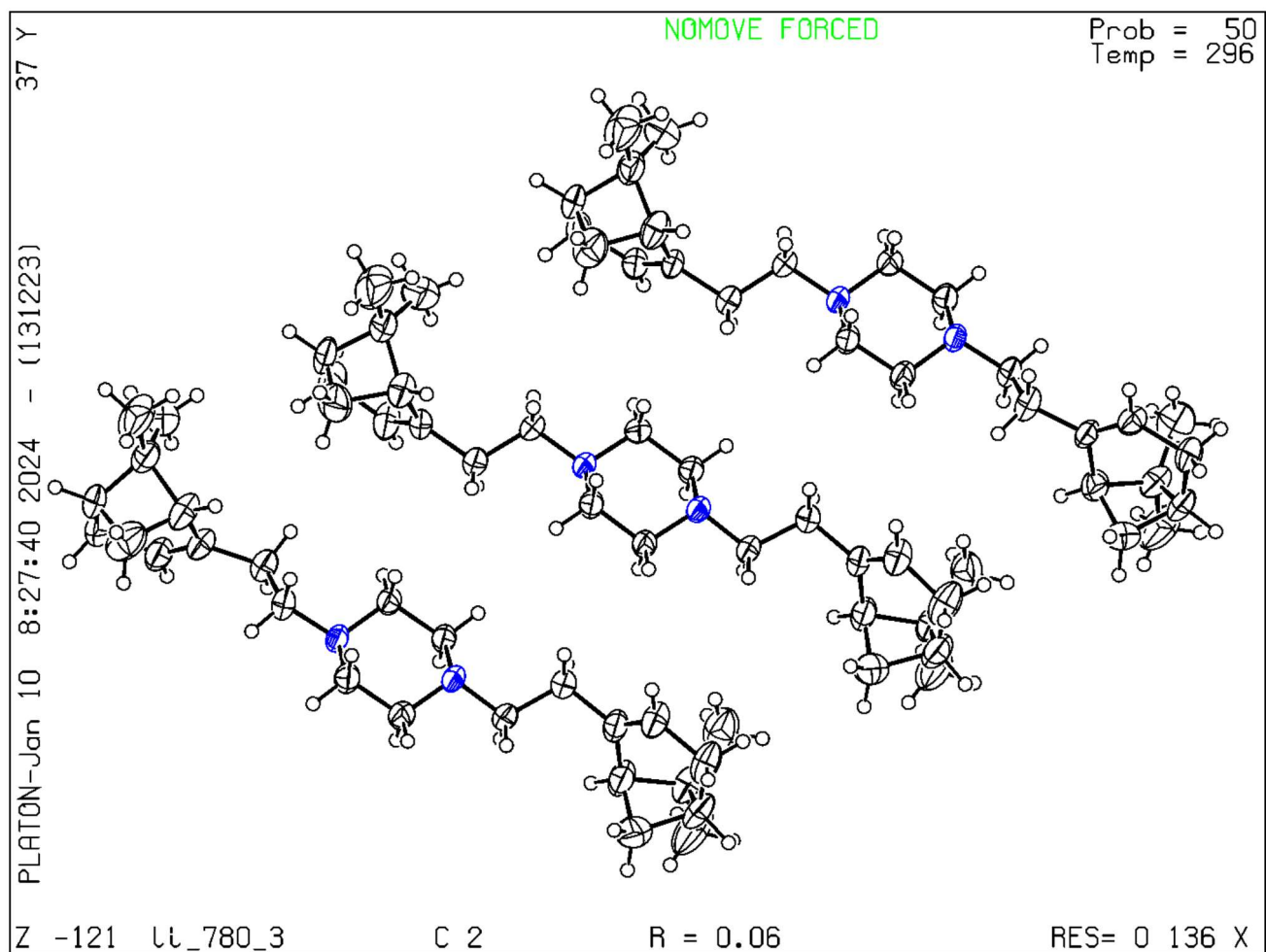
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 13/12/2023; check.def file version of 13/12/2023

Datablock li_780_3 - ellipsoid plot



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