checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...
No extractable fcf data in found in CIF

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) AB1607

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: AB1607

Bond precision: C-C = 0.0022 A Wavelength=0.71073

Cell: a=18.6804(6) b=18.6804(6) c=7.6330(4)
alpha=90 beta=90 gamma=90

Temperature: 173 K

	Calculated	Reported
Volume	2663.6(2)	2663.59(17)
Space group	I -4	I -4
Hall group	I -4	I -4
Moiety formula	C17 H18 N2	C17 H18 N2
Sum formula	C17 H18 N2	C17 H18 N2
Mr	250.33	250.35
Dx,g cm-3	1.248	1.249
Z	8	8
Mu (mm-1)	0.074	0.074
F000	1072.0	1072.6
F000'	1072.34	
h,k,lmax	24,24,10	24,24,10
Nref	3232[1739]	2775
Tmin,Tmax	0.963,0.986	0.974,0.990
Tmin'	0.962	

Correction method= # Reported T Limits: Tmin=0.974 Tmax=0.990
AbsCorr = ANALYTICAL

Data completeness= 1.60/0.86 Theta(max)= 28.030

R(reflections)= 0.0337(2305) wR2(reflections)= 0.0547(2775)

S = 1.029 Npar= 334

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

PLAT089_ALERT_3_B Poor Data / Parameter Ratio (Zmax < 18) ..... 5.21 Note

Alert level C

STRVA01_ALERT_4_C Flack parameter is too small
From the CIF: _refine_ls_abs_structure_Flack -1.000
From the CIF: _refine_ls_abs_structure_Flack_su 1.500
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C9 - H9A . 1.14 Ang.
And 2 other PLAT351 Alerts
More ...

PLAT353_ALERT_3_C Long N-H (N0.87,N1.01A) N1 - H1 . 1.03 Ang.
PLAT353_ALERT_3_C Long N-H (N0.87,N1.01A) N19 - H19 . 1.02 Ang.
PLAT420_ALERT_2_C D-H Bond Without Acceptor N1 --H1 . Please Check
PLAT420_ALERT_2_C D-H Bond Without Acceptor N19 --H19 . Please Check

Alert level G

PLAT032_ALERT_4_G Std. Uncertainty on Flack Parameter Value High . 1.500 Report
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 3 Units
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.9 Low
PLAT979_ALERT_1_G NoSpherA2 Scattering Factors Used ..... Please Note

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
0 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

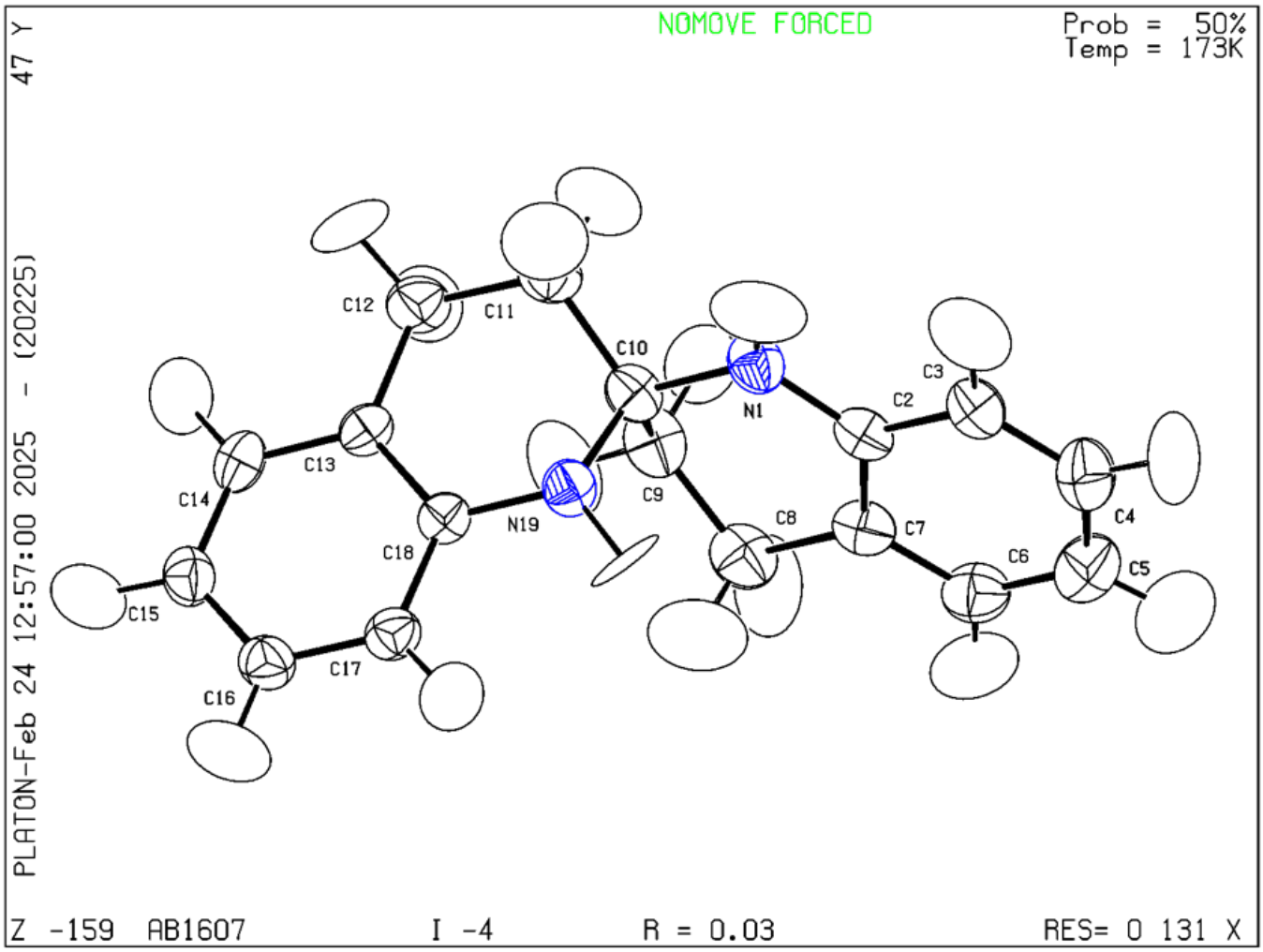
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 02/02/2025; check.def file version of 02/02/2025

Datablock AB1607 - ellipsoid plot



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Test a new CIF entry