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) AB1608b

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: AB1608b

Bond precision: C–C = 0.0072 A Wavelength=1.54184

Cell: a=8.7964(3) b=12.5727(4) c=15.8234(5)
alpha=90 beta=100.818(3) gamma=90

Temperature: 173 K

	Calculated	Reported
Volume	1718.88(10)	1718.88(10)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C17 H14 Br4 N2	C17 H14 Br4 N2
Sum formula	C17 H14 Br4 N2	C17 H14 Br4 N2
Mr	565.90	565.93
Dx,g cm-3	2.187	2.187
Z	4	4
Mu (mm-1)	11.422	11.422
F000	1080.0	1071.2
F000'	1070.66	
h,k,lmax	10,15,19	10,15,19
Nref	3460	3310
Tmin,Tmax	0.318,0.423	0.257,0.533
Tmin'	0.054	

Correction method= # Reported T Limits: Tmin=0.257 Tmax=0.533
AbsCorr = ANALYTICAL

Data completeness= 0.957 Theta(max)= 73.810

R(reflections)= 0.0338(2760) wR2(reflections)= 0.0777(3310)

S = 1.101 Npar= 335

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 A

PLAT211_ALERT_2_A ADP of Atom H1 is N.P.D. or (nearly) 2D . Please Check
And 9 other PLAT211 Alerts
Less ...

PLAT211_ALERT_2_A ADP of Atom H4 is N.P.D. or (nearly) 2D . Please Check
PLAT211_ALERT_2_A ADP of Atom H6 is N.P.D. or (nearly) 2D . Please Check
PLAT211_ALERT_2_A ADP of Atom H8A is N.P.D. or (nearly) 2D . Please Check
PLAT211_ALERT_2_A ADP of Atom H8B is N.P.D. or (nearly) 2D . Please Check
PLAT211_ALERT_2_A ADP of Atom H9B is N.P.D. or (nearly) 2D . Please Check

PLAT211_ALERT_2_A ADP of Atom H11A is N.P.D. or (nearly) 2D . Please Check
PLAT211_ALERT_2_A ADP of Atom H11B is N.P.D. or (nearly) 2D . Please Check
PLAT211_ALERT_2_A ADP of Atom H16 is N.P.D. or (nearly) 2D . Please Check
PLAT211_ALERT_2_A ADP of Atom H19 is N.P.D. or (nearly) 2D . Please Check

PLAT351_ALERT_3_A Long C-H (X0.96,N1.08A) C8 - H8B . 1.31 Ang.
PLAT770_ALERT_2_A Suspect C-H Bond in CIF: C8 --H8B . 1.31 Ang.

Alert level B

PLAT351_ALERT_3_B Long C-H (X0.96,N1.08A) C8 - H8A . 1.18 Ang.
PLAT351_ALERT_3_B Long C-H (X0.96,N1.08A) C11 - H11A . 1.21 Ang.
PLAT353_ALERT_3_B Long N-H (N0.87,N1.01A) N1 - H1 . 1.09 Ang.

Alert level C

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 7.7 Ratio
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00722 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C4 - H4 . 1.11 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C9 - H9B . 1.12 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X H1 ..H12A . 1.99 Ang.
x,y,z = 1_555 Check

Alert level G

PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 12 Note
PLAT434_ALERT_2_G Short Inter HL..HL Contact Br3 ..Br5 . 3.43 Ang.
-1+x,y,z = 1_455 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact Br15 ..Br17 . 3.55 Ang.
-1+x,y,z = 1_455 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 1.7 Low
PLAT979_ALERT_1_G NoSpherA2 Scattering Factors Used ..... Please Note

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 ALERT type 2 Indicator that the structure model may be wrong or deficient
9 ALERT type 3 Indicator that the structure quality may be low
2 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

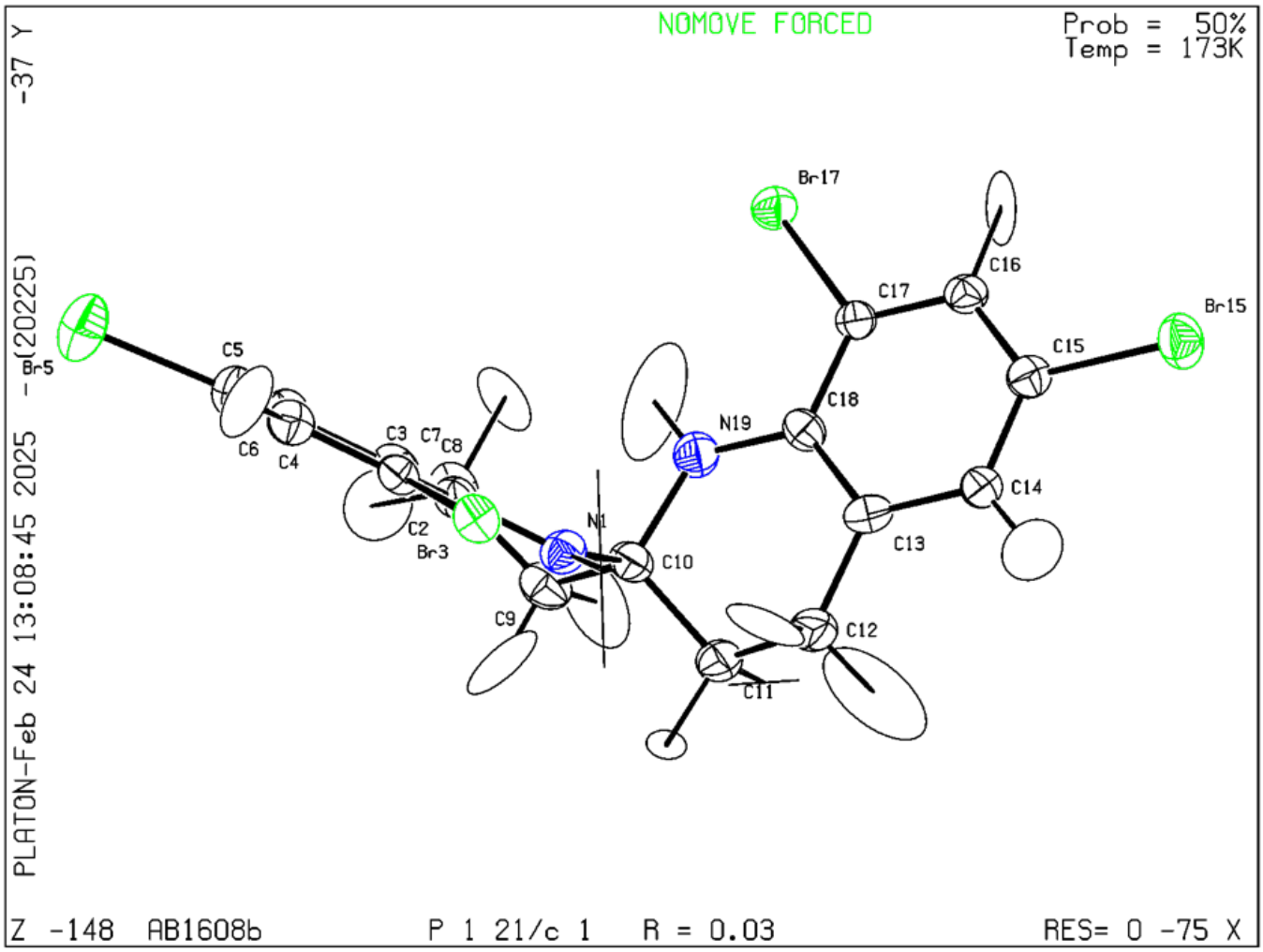
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 AB1608b - ellipsoid plot



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