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) AB1609

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: AB1609

Bond precision: C–C = 0.0039 A Wavelength=0.71073

Cell: a=8.2840(6) b=10.2385(6) c=10.3631(8)
alpha=68.118(6) beta=71.449(7) gamma=87.541(6)

Temperature: 173 K

	Calculated	Reported
Volume	770.38(11)	770.38(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C17 H16 Br2 N2	C17 H16 Br2 N2
Sum formula	C17 H16 Br2 N2	C17 H16 Br2 N2
Mr	408.12	408.14
Dx,g cm-3	1.759	1.759
Z	2	2
Mu (mm-1)	5.256	5.255
F000	404.0	403.0
F000'	403.02	
h,k,lmax	10,13,13	9,13,13
Nref	3701	3026
Tmin,Tmax	0.153,0.359	0.274,0.472
Tmin'	0.116	

Correction method= # Reported T Limits: Tmin=0.274 Tmax=0.472
AbsCorr = ANALYTICAL

Data completeness= 0.818 Theta(max)= 27.930

R(reflections)= 0.0268(2410) wR2(reflections)= 0.0401(3026)

S = 0.967 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 H12A is N.P.D. or (nearly) 2D . Please Check
PLAT211_ALERT_2_A ADP of Atom H14 is N.P.D. or (nearly) 2D . Please Check

Alert level C

PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C6 - H6 . 1.12 Ang.
And 6 other PLAT351 Alerts
Less ...

PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C8 - H8A . 1.14 Ang.

PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C9 - H9A . 1.16 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C11 - H11A . 1.11 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C12 - H12B . 1.14 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C14 - H14 . 1.11 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C17 - H17 . 1.12 Ang.

PLAT353_ALERT_3_C Long N-H (N0.87,N1.01A) N19 - H19 . 1.04 Ang.

Alert level G

PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 14 Note
PLAT434_ALERT_2_G Short Inter HL..HL Contact Br5 ..Br15 . 3.59 Ang.
2+x,y,-1+z = 1_754 Check
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
0 2 0,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 1.5 Low
PLAT963_ALERT_2_G Both SHELXL WEIGHT Parameter Values Zero ..... Please Check
PLAT979_ALERT_1_G NoSpherA2 Scattering Factors Used ..... Please Note

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2 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
8 **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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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

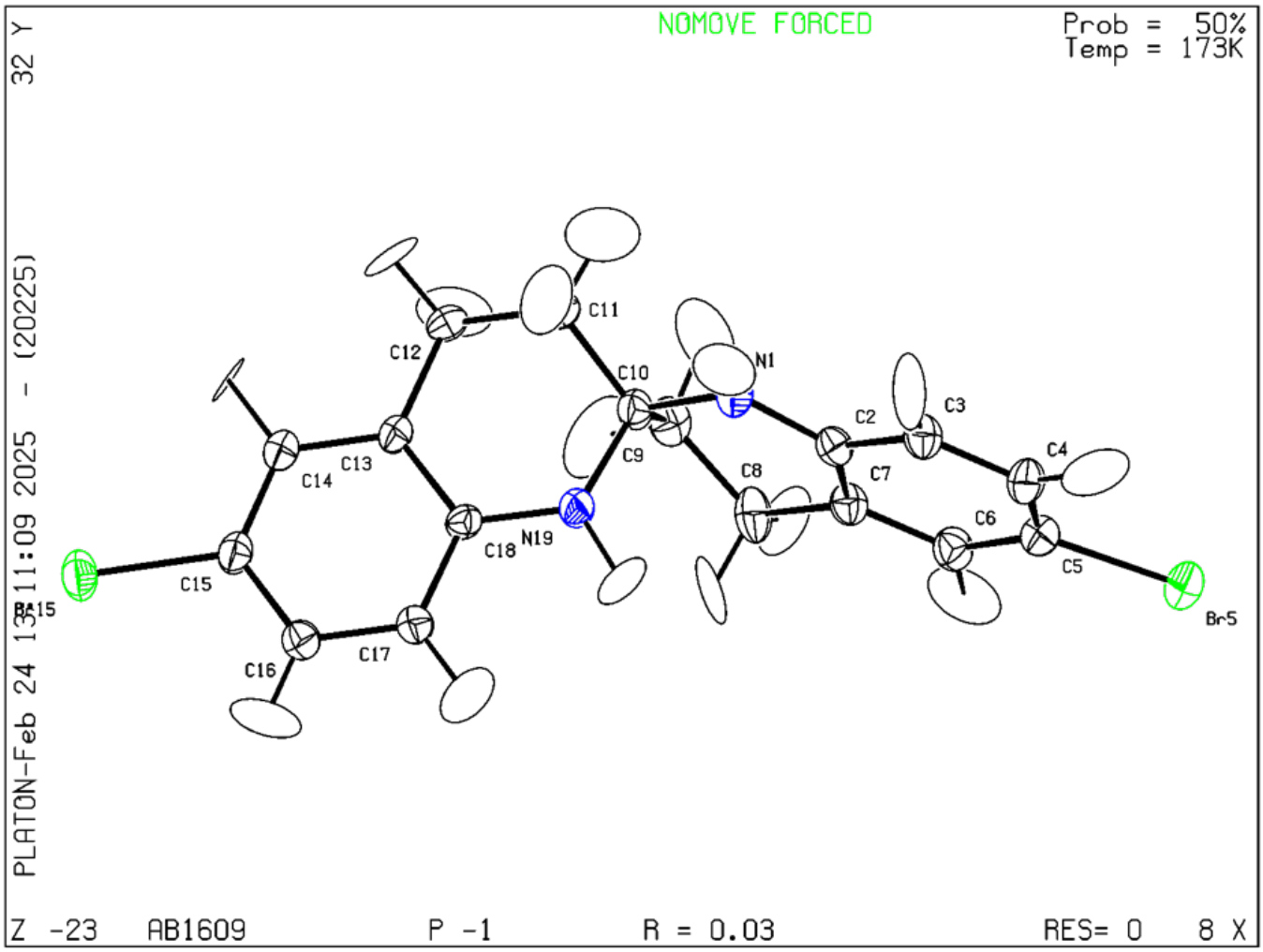
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 AB1609 - ellipsoid plot



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