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) AB1710

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: AB1710

Bond precision: C–C = 0.0050 A Wavelength=0.71073

Cell: a=8.6429(5) b=9.5129(5) c=12.9337(6)
alpha=80.017(4) beta=72.909(5) gamma=77.318(5)

Temperature: 173 K

	Calculated	Reported
Volume	984.86(9)	984.87(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C20 H18 Br4 N2	C20 H18 Br4 N2
Sum formula	C20 H18 Br4 N2	C20 H18 Br4 N2
Mr	605.96	605.99
Dx,g cm-3	2.043	2.043
Z	2	2
Mu (mm-1)	8.180	8.179
F000	584.0	581.8
F000'	582.06	
h,k,lmax	11,12,17	11,12,17
Nref	4830	3873
Tmin,Tmax	0.073,0.116	0.151,0.272
Tmin'	0.031	

Correction method= # Reported T Limits: Tmin=0.151 Tmax=0.272
AbsCorr = ANALYTICAL

Data completeness= 0.802 Theta(max)= 28.150

R(reflections)= 0.0314(3033) wR2(reflections)= 0.0495(3873)

S = 1.040 Npar= 398

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 13 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 H9 is N.P.D. or (nearly) 2D . Please Check
PLAT211_ALERT_2_A ADP of Atom H12B 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
PLAT211_ALERT_2_A ADP of Atom H19 is N.P.D. or (nearly) 2D . Please Check
PLAT211_ALERT_2_A ADP of Atom H20A is N.P.D. or (nearly) 2D . Please Check
PLAT211_ALERT_2_A ADP of Atom H20B is N.P.D. or (nearly) 2D . Please Check
PLAT211_ALERT_2_A ADP of Atom H21A is N.P.D. or (nearly) 2D . Please Check
PLAT211_ALERT_2_A ADP of Atom H21B is N.P.D. or (nearly) 2D . Please Check
PLAT211_ALERT_2_A ADP of Atom H22A is N.P.D. or (nearly) 2D . Please Check
PLAT211_ALERT_2_A ADP of Atom H22B is N.P.D. or (nearly) 2D . Please Check

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Alert level B

PLAT351_ALERT_3_B Long C-H (X0.96,N1.08A) C22 - H22A . 1.18 Ang.

Alert level C

PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 5.3 Ratio
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C6 - H6 . 1.11 Ang.
And 8 other PLAT351 Alerts
Less ...

PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C8 - H8A . 1.12 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C9 - H9 . 1.14 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C12 - H12A . 1.13 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 . 1.15 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C20 - H20A . 1.14 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C20 - H20B . 1.12 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C21 - H21A . 1.14 Ang.

PLAT353_ALERT_3_C Long N-H (N0.87,N1.01A) N19 - H19 . 1.02 Ang.

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. 16 Note
PLAT434_ALERT_2_G Short Inter HL..HL Contact Br15 ..Br17 . 3.56 Ang.
1+x,y,z = 1_655 Check
PLAT793_ALERT_4_G Model has Chirality at C9 (Centro SpGr) R Verify
PLAT793_ALERT_4_G Model has Chirality at C11 (Centro SpGr) S Verify
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 2 Note
0 1 1, 1 0 0,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 1.5 Low
PLAT979_ALERT_1_G NoSpherA2 Scattering Factors Used ..... Please Note

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
16 ALERT type 2 Indicator that the structure model may be wrong or deficient
13 ALERT type 3 Indicator that the structure quality may be low
4 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

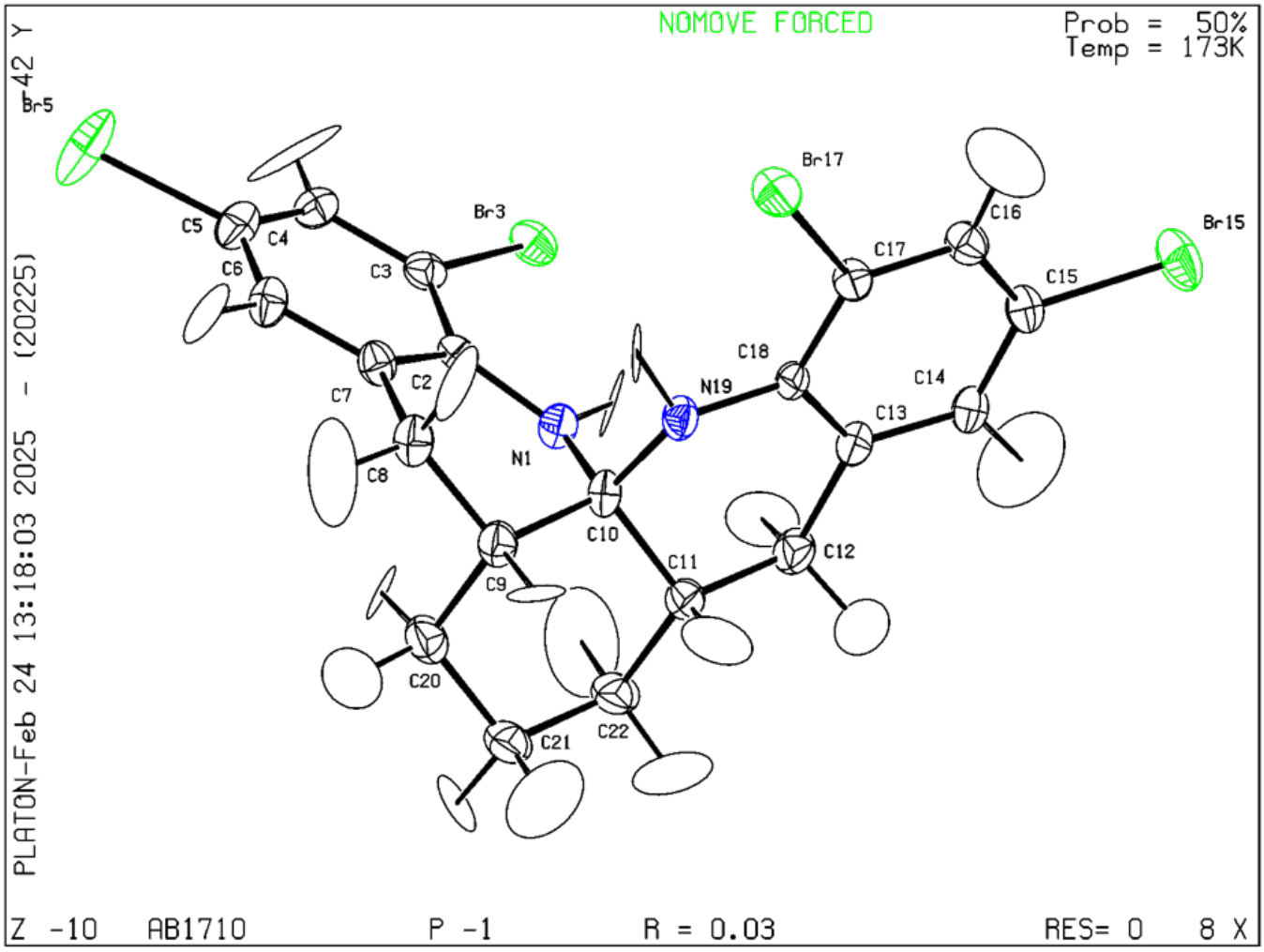
submission.

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 AB1710 - ellipsoid plot



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