## 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) AB1709

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: AB1709

Bond precision: C–C = 0.0072 A Wavelength=0.71073

Cell: a=12.6560(8) b=8.9013(6) c=16.6514(11)
alpha=90 beta=97.910(6) gamma=90

Temperature: 173 K

| | Calculated | Reported |
|---|---|---|
| Volume | 1858.0(2) | 1858.0(2) |
| Space group | P 21/c | P 1 21/c 1 |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C19 H16 Br4 N2 | C19 H16 Br4 N2 |
| Sum formula | C19 H16 Br4 N2 | C19 H16 Br4 N2 |
| Mr | 591.94 | 591.97 |
| Dx,g cm-3 | 2.116 | 2.116 |
| Z | 4 | 4 |
| Mu (mm-1) | 8.669 | 8.668 |
| F000 | 1136.0 | 1133.3 |
| F000' | 1132.13 | |
| h,k,lmax | 16,11,22 | 16,11,21 |
| Nref | 4604 | 3719 |
| Tmin,Tmax | 0.059,0.540 | 0.105,0.537 |
| Tmin' | 0.013 | |

Correction method= # Reported T Limits: Tmin=0.105 Tmax=0.537
AbsCorr = ANALYTICAL

Data completeness= 0.808 Theta(max)= 28.290

R(reflections)= 0.0410( 2465) wR2(reflections)= 0.0477( 3719)

S = 1.002 Npar= 371

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

PLAT203_ALERT_2_A Negative Isotropic ADP for H11 ..... -0.006 Report
PLAT211_ALERT_2_A ADP of Atom H1 is N.P.D. or (nearly) 2D . Please Check
**And 10 other PLAT211 Alerts**
Less ...

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 H9 is N.P.D. or (nearly) 2D . Please Check

PLAT211_ALERT_2_A ADP of Atom H11 is N.P.D. or (nearly) 2D . Please Check
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
PLAT211_ALERT_2_A ADP of Atom H19 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

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## Alert level B

PLAT351_ALERT_3_B Long C-H (X0.96,N1.08A) C11 - H11 . 1.20 Ang.

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## Alert level C

SHFSU01_ALERT_2_C The absolute value of parameter shift to su ratio > 0.05
Absolute value of the parameter shift to su ratio given 0.090
Additional refinement cycles may be required.
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT080_ALERT_2_C Maximum Shift/Error ..... 0.09 Why ?
PLAT245_ALERT_2_C U(iso) H11 Smaller than U(eq) C11 by 0.027 Ang**2
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00724 Ang.
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) C9 - H9 . 1.11 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 . 1.15 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C14 - H14 . 1.14 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C20 - H20B . 1.16 Ang.
PLAT351_ALERT_3_C Long C-H (X0.96,N1.08A) C21 - H21A . 1.11 Ang.

PLAT353_ALERT_3_C Long N-H (N0.87,N1.01A) N1 - H1 . 1.06 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact H4 ..H21A . 2.08 Ang.
1-x,1/2+y,1/2-z = 2_655 Check
PLAT411_ALERT_2_C Short Inter H...H Contact H11 ..H21A . 2.08 Ang.
1-x,1-y,1-z = 3_666 Check

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## 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 Br17 ..Br17 . 3.47 Ang.
-x,2-y,1-z = 3_576 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) R 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 1 Note
0 0 2,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 1.7 Low
PLAT979_ALERT_1_G NoSpherA2 Scattering Factors Used ..... Please Note

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
19 ALERT type 2 Indicator that the structure model may be wrong or deficient
11 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

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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.

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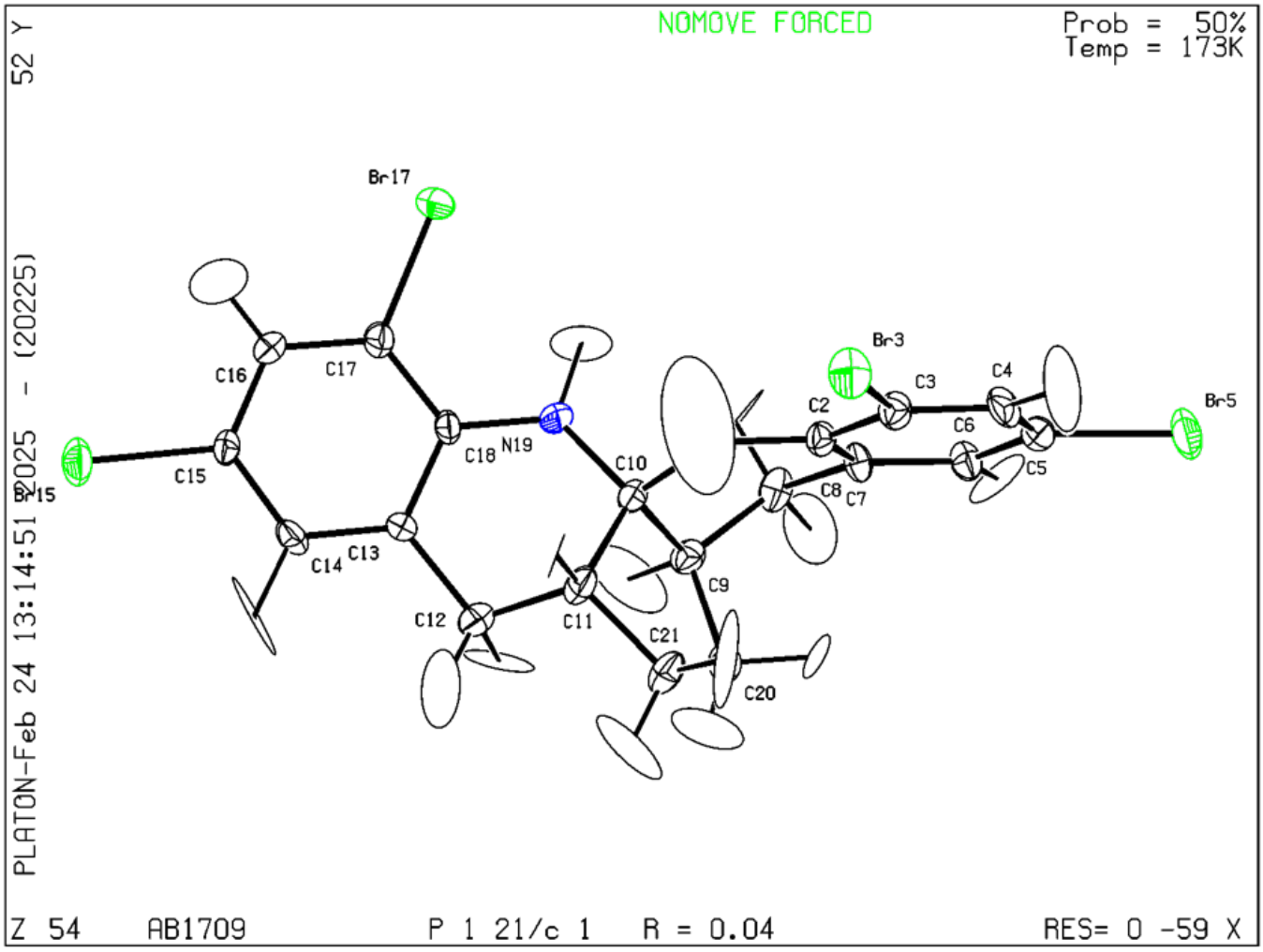
**PLATON version of 02/02/2025; check.def file version of 02/02/2025**

# **Datablock AB1709** - ellipsoid plot

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