

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) syn-23123

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: syn-23123

Bond precision: C-C = 0.0132 Å Wavelength=1.54184

Cell: a=12.38796(9) b=14.12473(10) c=13.3245(1)
 alpha=90 beta=100.3448(7) gamma=90

Temperature: 93 K

	Calculated	Reported
Volume	2293.58(3)	2293.58(3)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C21 H18 Br F6 I N2 O2	C21 H18 Br F6 I N2 O2
Sum formula	C21 H18 Br F6 I N2 O2	C21 H18 Br F6 I N2 O2
Mr	651.17	651.18
Dx, g cm ⁻³	1.886	1.886
Z	4	4
Mu (mm ⁻¹)	13.663	13.663
F000	1264.0	1264.0
F000'	1264.22	
h,k,lmax	15,18,17	15,17,16
Nref	9956[5185]	9705
Tmin,Tmax	0.530,0.872	0.265,1.000
Tmin'	0.481	

Correction method= # Reported T Limits: Tmin=0.265 Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 1.87/0.97 Theta(max)= 79.806

R(reflections)= 0.0349(9470) wR2(reflections)= 0.0916(9705)

S = 1.083 Npar= 602

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 C

[PLAT094_ALERT_2_C](#) Ratio of Maximum / Minimum Residual Density 2.12 Report
[PLAT342_ALERT_3_C](#) Low Bond Precision on C-C Bonds 0.01315 Ang.
[PLAT971_ALERT_2_C](#) Check Calcd Resid. Dens. 0.39Ang From Br1_2 2.07 eA-3
[PLAT971_ALERT_2_C](#) Check Calcd Resid. Dens. 0.78Ang From Br1_2 1.61 eA-3

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.184 Note
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 9.37 Why ?
PLAT111_ALERT_2_G ADDSYM Detects New (Pseudo) Centre of Symmetry . 100 %Fit

Author Response: See the reply to PLAT113

PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem c 100 %Fit

Author Response: See the reply to PLAT113

PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New Space Group P21/c Check
Check Model Parameter Symmetry for Reflection Data Support

Author Response: The solution in P2(1)/c was explored. However, the pseudosymmetry of the c-glide requires the I and Br to occupy the same space. These distributions were freely refined and converged near 50/50. However, the refinement metrics of P2(1)/c are much worse than P2(1), implying the polar space group is correct. The I and Br atoms are not related by crystallographic symmetry.

PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing 0.00010 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing 0.00010 Ang.
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C21_1 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C13_2 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact I1_2 ..F4_2 . 3.24 Ang.
x,-1+y,z = 1_545 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 102 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 52 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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

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

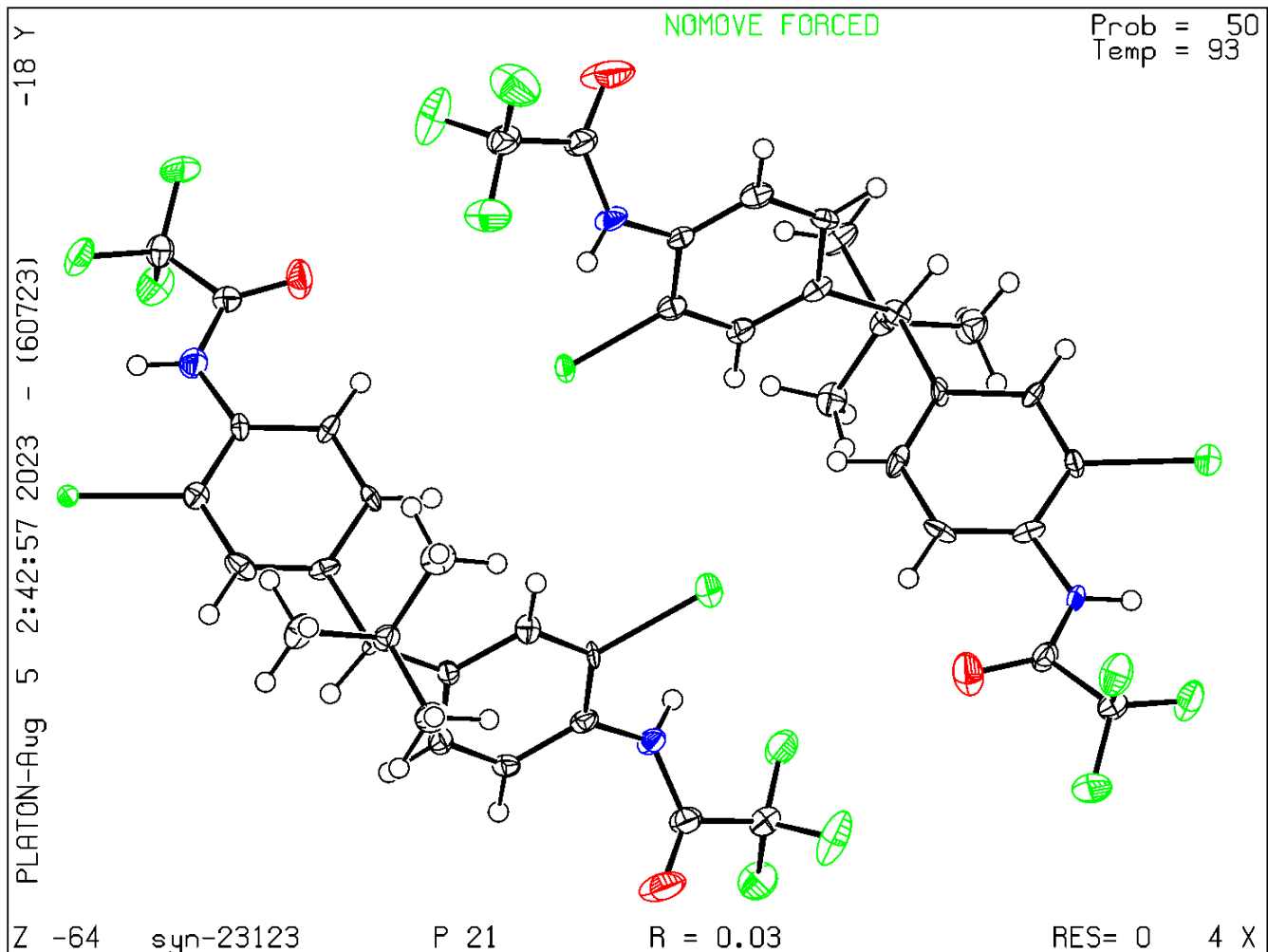
Publication of your CIF in IUCr journals

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 06/07/2023; check.def file version of 30/06/2023

Datablock syn-23123 - ellipsoid plot

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