

## 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) sh1718a

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: sh1718a

Bond precision:	C-C = 0.0039 Å	Wavelength=0.71073
Cell:	a=9.6243(3)      b=9.8590(2)      c=12.5952(3)	
	alpha=68.645(2)      beta=72.467(2)      gamma=75.230(2)	
Temperature: 293 K		
	Calculated	Reported
Volume	1047.06(5)	1047.06(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C20 H24 N6 O4	C20 H24 N6 O4
Sum formula	C20 H24 N6 O4	C20 H24 N6 O4
Mr	412.45	412.45
Dx, g cm-3	1.308	1.308
Z	2	2
Mu (mm-1)	0.094	0.094
F000	436.0	436.0
F000'	436.19	
h,k,lmax	11,11,14	11,11,14
Nref	3683	3684
Tmin,Tmax	0.983,0.988	0.917,1.000
Tmin'	0.983	
Correction method=	# Reported T Limits: Tmin=0.917 Tmax=1.000	
AbsCorr =	MULTI-SCAN	
Data completeness=	1.000	Theta(max)= 24.999
R(reflections)=	0.0465( 2287)	wR2(reflections)= 0.1359( 3684)
S =	1.002	Npar= 296

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

PLAT220\_ALERT\_2\_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C11 --C12A . 0.17 Ang.  
PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C11 --C12B . 0.18 Ang.  
PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C13 Check  
PLAT331\_ALERT\_2\_C Small Aver Phenyl C-C Dist C16 --C21 . 1.37 Ang.  
PLAT905\_ALERT\_3\_C Negative K value in the Analysis of Variance ... -3.318 Report

### Alert level G

PLAT154\_ALERT\_1\_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.002 Degree

## And 2 other PLAT793 Alerts

PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
 PLAT965\_ALERT\_2\_G The SHELXL WEIGHT Optimisation has not Converged Please Check  
 PLAT967\_ALERT\_5\_G Note: Two-Theta Cutoff Value in Embedded .res .. 50.0 Degree  
 PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 0 Info

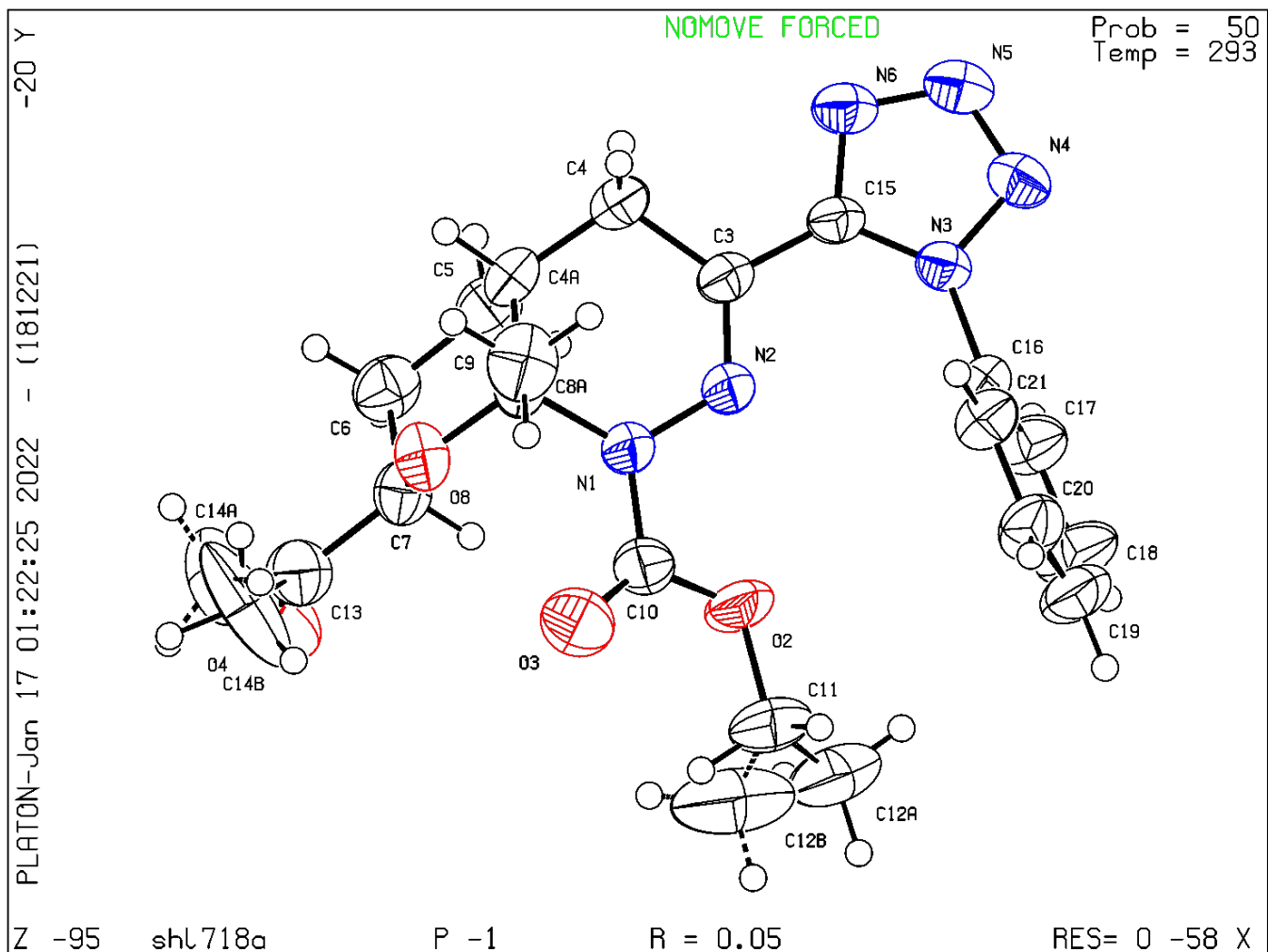
5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
8 ALERT type 2 Indicator that the structure model may be wrong or deficient  
2 ALERT type 3 Indicator that the structure quality may be low  
7 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative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

## Publication of your CIF in IUCr journals

### Publication of your CIF in other journals

**PLATON version of 18/12/2021; check.def file version of 18/12/2021**

## Datablock sh1718a - ellipsoid plot



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