

## checkCIF (basic structural check) running

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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)

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Structure factors have been supplied for datablock(s) nha59\_sq

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: nha59\_sq

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Bond precision:	C-C = 0.0103 A	Wavelength=0.71073	
Cell:	a=19.1169(2)	b=16.8263(2)	c=23.7598(3)
	alpha=90	beta=96.560(1)	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	7592.70(15)	7592.70(15)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C68 H103 Li2 N5 O2 U [+ solvent]	C68 H103 Li2 N5 O2 U [+ solvent]	
Sum formula	C68 H103 Li2 N5 O2 U [+ solvent]	C68 H103 Li2 N5 O2 U	
Mr	1274.47	1274.46	
Dx, g cm <sup>-3</sup>	1.115	1.115	
Z	4	4	
Mu (mm <sup>-1</sup> )	2.177	2.177	
F000	2640.0	2640.0	
F000'	2602.21		
h,k,lmax	24,21,30	26,23,32	
Nref	17424	17390	
Tmin,Tmax	0.366,0.520	0.034,0.520	
Tmin'	0.338		
Correction method=	# Reported T Limits: Tmin=0.034 Tmax=0.520 AbsCorr =		
	MULTI-SCAN		
Data completeness=	0.998	Theta(max)= 27.485	
R(reflections)=	0.0496( 12434)	wR2(reflections)= 0.1209( 17390)	
S =	1.110	Npar= 729	

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 B

[PLAT971\\_ALERT\\_2\\_B](#) Check Calcd Resid. Dens. 0.95Ang From U1 3.15 eA-3

**Author Response: All large Q peaks nearby uranium. Data collected on vintage instrument (produced 1997) with limited data processing and absorption correction options.**

**And 3 other PLAT971 Alerts**

More ...

**Alert level C**

PLAT220\_ALERT\_2\_C NonSolvent Resid 1 C Ueq(max)/Ueq(min) Range 3.7 Ratio  
 PLAT230\_ALERT\_2\_C Hirshfeld Test Diff for N1 --C10 . 6.0 s.u.  
 PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of C2 Check

**And 2 other PLAT241 Alerts**

More ...

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of C16 Check

**And 2 other PLAT242 Alerts**

More ...

PLAT342\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.0103 Ang.  
 PLAT420\_ALERT\_2\_C D-H Bond Without Acceptor N4 --H4N . Please Check  
 PLAT905\_ALERT\_3\_C Negative K value in the Analysis of Variance ... -1.025 Report  
 PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 22 Report  
 0 2 0, 1 1 0, 2 0 0, 2 2 0, -20 3 1, -1 1 1,  
 -1 14 1, 0 1 1, 1 1 1, 1 14 1, 20 3 1, -21 2 2,  
 -1 0 2, 0 0 2, 0 1 2, 1 0 2, 2 0 2, -3 14 3,  
 -1 1 3, 0 2 3, 0 13 4, 1 11 20,  
 PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 1.15Ang From U1 -1.90 eA-3  
 PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 0.76Ang From N1 -1.55 eA-3  
 PLAT973\_ALERT\_2\_C Check Calcd Positive Resid. Density on U1 1.11 eA-3  
 PLAT975\_ALERT\_2\_C Check Calcd Resid. Dens. 0.90Ang From N5 . 0.69 eA-3  
 PLAT976\_ALERT\_2\_C Check Calcd Resid. Dens. 1.01Ang From N5 . -0.60 eA-3  
 PLAT992\_ALERT\_5\_C Repd & Actual \_reflns\_number\_gt Values Differ by 15 Check

**Alert level G**

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 4 Note  
 PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 24.75 Why ?  
 PLAT172\_ALERT\_4\_G The CIF-Embedded .res File Contains DFIX Records 1 Report  
 PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) U1 --N1 . 7.5 s.u.  
 PLAT232\_ALERT\_2\_G Hirshfeld Test Diff (M-X) U1 --N5 . 8.7 s.u.  
 PLAT303\_ALERT\_2\_G Full Occupancy Atom H5N with # Connections 2.00 Check  
 PLAT606\_ALERT\_4\_G Solvent Accessible VOID(S) in Crystal Structure ! Info  
 PLAT779\_ALERT\_4\_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 43.80 Deg.  
 N5 -C50 -LI1 1\_555 1\_555 1\_555 ..... # 238 Check  
 PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 5 Note  
 PLAT869\_ALERT\_4\_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info  
 PLAT912\_ALERT\_4\_G Missing # of FCF Reflections Above STh/L= 0.600 11 Note  
 PLAT913\_ALERT\_3\_G Missing # of Very Strong Reflections in FCF .... 2 Note  
 1 1 0, 0 0 2,  
 PLAT933\_ALERT\_2\_G Number of HKL-OMIT Records in Embedded .res File 13 Note  
 -1 14 1, 0 13 4, -3 14 3, -1 1 3, 0 1 2, 2 2 0,  
 0 1 1, 1 1 0, -1 1 1, 0 2 0, 0 2 3, 2 0 2,  
 1 14 1,  
 PLAT941\_ALERT\_3\_G Average HKL Measurement Multiplicity ..... 1.0 Low  
 PLAT950\_ALERT\_5\_G Calculated (ThMax) and CIF-Reported Hmax Differ -2 Units  
 PLAT951\_ALERT\_5\_G Calculated (ThMax) and CIF-Reported Kmax Differ -2 Units  
 PLAT952\_ALERT\_5\_G Calculated (ThMax) and CIF-Reported Lmax Differ. -2 Units  
 PLAT953\_ALERT\_1\_G Reported (CIF) and Actual (FCF) Hmax Differ by . 2 Units  
 PLAT954\_ALERT\_1\_G Reported (CIF) and Actual (FCF) Kmax Differ by . 2 Units  
 PLAT955\_ALERT\_1\_G Reported (CIF) and Actual (FCF) Lmax Differ by . 2 Units  
 PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 2.872 Note  
 Predicted wR2: Based on SigI\*\*2 4.21 or SHELX Weight 10.90  
 PLAT978\_ALERT\_2\_G Number C-C Bonds with Positive Residual Density. 0 Info

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

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

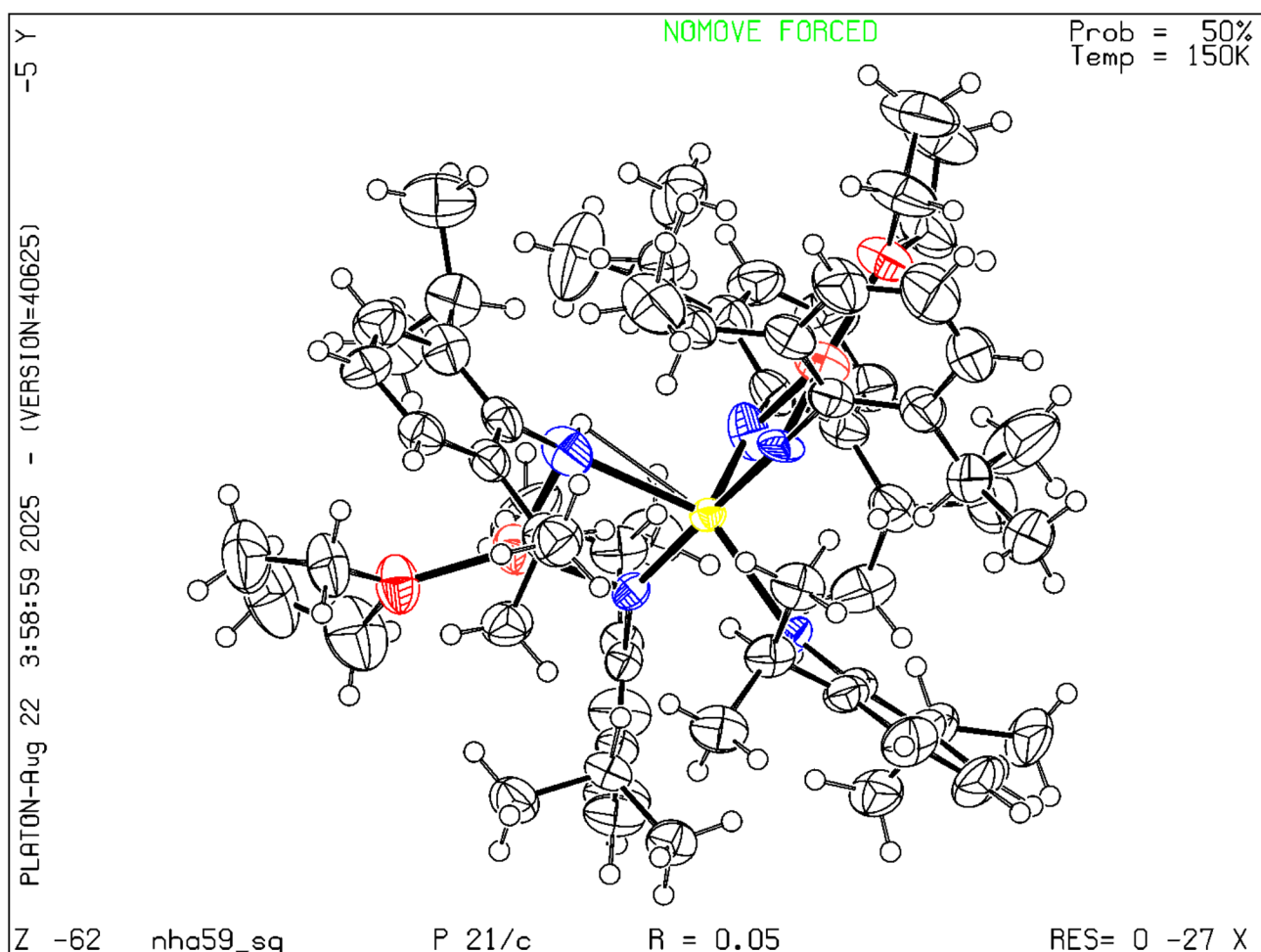
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 04/06/2025; check.def file version of 30/05/2025

## Datablock nha59\_sq - ellipsoid plot



[Test a new CIF entry](#)