

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) EJC_05_177_Et2OPent_0m

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: EJC_05_177_Et2OPent_0m

Bond precision:	C-C = 0.0035 A	Wavelength=0.71073
Cell:	a=23.0613(9) b=21.5918(8) c=31.8077(12)	
	alpha=90 beta=90 gamma=90	
Temperature:	150 K	
	Calculated	Reported
Volume	15838.2(10)	15838.2(10)
Space group	I b c a	I b c a
Hall group	-I 2b 2c	-I 2b 2c
Moiety formula	C76 H125 K4 N5 O4 U	?
Sum formula	C76 H125 K4 N5 O4 U	C76 H125 K4 N5 O4 U
Mr	1567.24	1567.23
Dx, g cm ⁻³	1.314	1.315
Z	8	8
Mu (mm ⁻¹)	2.307	2.307
F000	6528.0	6528.0
F000'	6459.14	
h,k,lmax	32,29,44	32,29,44
Nref	11106	11097
Tmin,Tmax	0.637,0.630	0.503,0.570
Tmin'	0.624	
Correction method=	# Reported T Limits: Tmin=0.503 Tmax=0.570 AbsCorr =	
MULTI-SCAN		
Data completeness=	0.999 Theta(max)= 29.573	
R(reflections)=	0.0248(8978) wR2(reflections)= 0.0572(
		11097)
S =	1.076 Npar= 422	

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 5.3 Ratio

[PLAT222_ALERT_3_C](#) NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.4 Ratio

[PLAT230_ALERT_2_C](#) Hirshfeld Test Diff for N1 --C1 . 5.9 s.u.

[PLAT905_ALERT_3_C](#) Negative K value in the Analysis of Variance ... -1.518 Report

[PLAT910_ALERT_3_C](#) Missing FCF Reflection(s) Below Theta(Min)[Deg]= 2.56 Note

0 2 0, 2 0 0, 1 2 1, 2 1 1, 0 0 2, 0 2 2,

1 1 2, 2 0 2,

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 2.21Ang From C26 2.10 eA-3

PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.82Ang From N3 0.52 eA-3

Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 54.01 Why ?

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) U1 --N2 . 6.9 s.u.

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) U1 --N3 . 8.5 s.u.

PLAT303_ALERT_2_G Full Occupancy Atom H16A with # Connections 2.00 Check

And 3 other PLAT303 Alerts

More ...

PLAT343_ALERT_2_G Unusual Angle Range in Main Residue for C8 Check

PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.26 Ratio

PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 40.60 Deg.

K1 -C17 -H17B 1_555 1_555 1_555 # 257 Check

And 3 other PLAT779 Alerts

More ...

PLAT793_ALERT_4_G Model has Chirality at C15 (Centro SpGr) R Verify

And 3 other PLAT793 Alerts

More ...

PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 2 Note

0 4 0, 2 0 2,

PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 3.931 Note

Predicted wR2: Based on SigI**2 1.46 or SHELX Weight 5.32

PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 6 Info

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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 14 ALERT type 2 Indicator that the structure model may be wrong or deficient
 3 ALERT type 3 Indicator that the structure quality may be low
 9 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

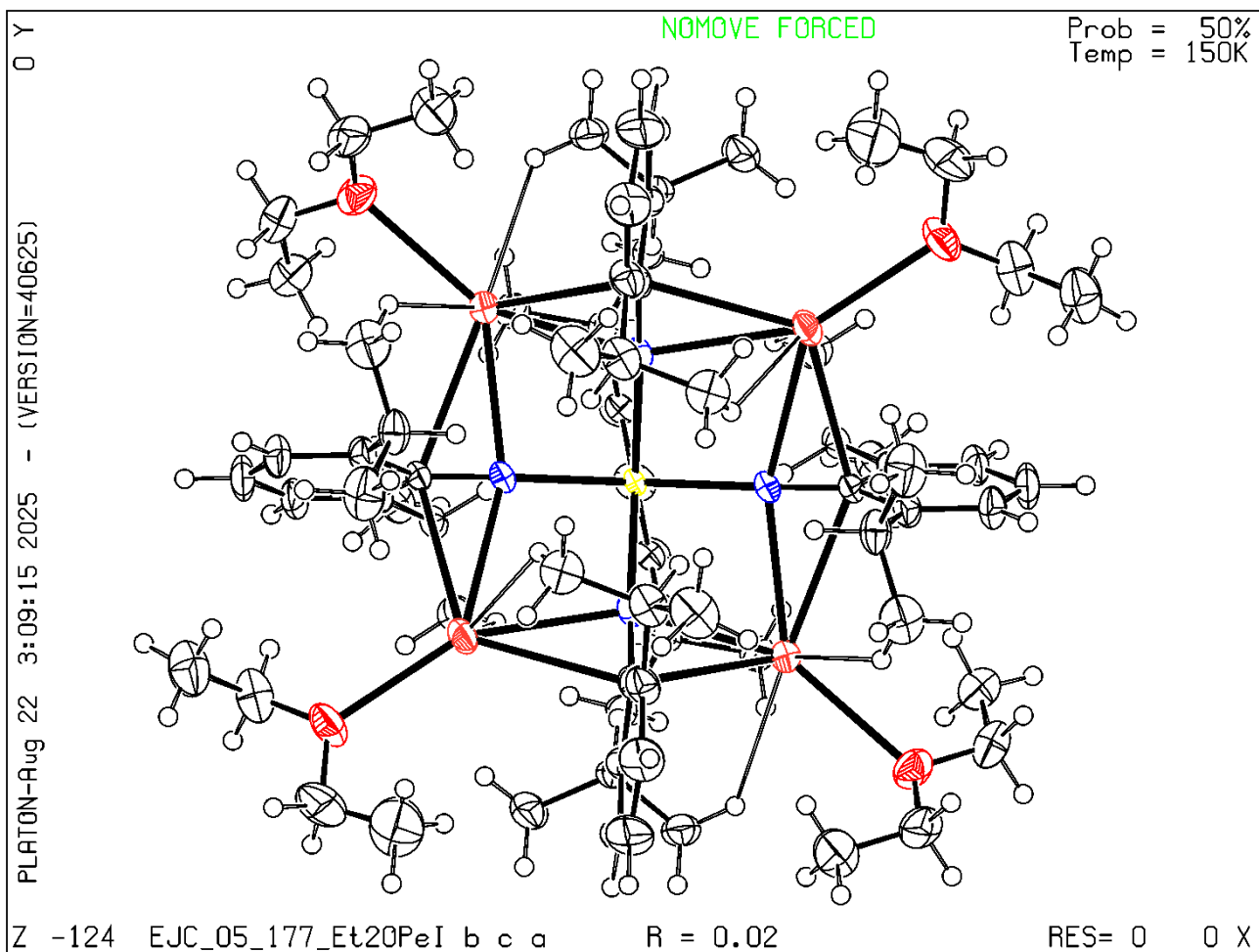
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

Datablock EJC_05_177_Et2OPent_0m - ellipsoid plot



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