

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) mh182_auto

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: mh182_auto

Bond precision:	C-C = 0.0037 Å		Wavelength=1.54184
Cell:	a=18.6072(1)	b=15.7408(1)	c=28.3753(2)
	alpha=90	beta=106.953(1)	gamma=90
Temperature: 100 K			
	Calculated	Reported	
Volume	7949.75(10)	7949.74(10)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C80 H77 Ga N4 O, C20 H18 O [+ solvent]	C80 H77 Ga N4 O, C20 H18 O	
Sum formula	C100 H95 Ga N4 O2 [+ solvent]	C100 H95 Ga N4 O2	
Mr	1454.52	1454.51	
Dx, g cm-3	1.215	1.215	
Z	4	4	
Mu (mm-1)	0.883	0.883	
F000	3080.0	3080.0	
F000'	3082.48		
h,k,lmax	22,19,34	22,19,34	
Nref	15349	15009	
Tmin,Tmax		0.849,1.000	
Tmin'			
Correction method= # Reported T Limits: Tmin=0.849 Tmax=1.000 AbsCorr = MULTI-SCAN			
Data completeness= 0.978	Theta(max)= 70.921		
R(reflections)= 0.0496(12926)	wR2(reflections)= 0.1421(15009)		
S = 1.043	Npar= 1006		

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

PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density 4.02 Report

●Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...	Please Check
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	2.61 eA-3
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	4.4 Ratio
PLAT221_ALERT_2_C	Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range	6.3 Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.9 Ratio
PLAT223_ALERT_4_C	Solv./Anion Resd 2 H Ueq(max)/Ueq(min) Range	6.8 Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C97 Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2)	2.2 Note

PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C97 - C99 . 1.41 Ang.
 PLAT361_ALERT_2_C Long C(sp3)-C(sp3) Bond C97 - C98 . 1.65 Ang.
 PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.86Ang From C29 2.47 eA-3

Alert level G

PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 108 Report
 PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 8.22 Why ?
 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 0.00020 Ang.
 PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
 PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
 PLAT299_ALERT_4_G Atom Site Occupancy Constrained at 0.5 Check
 C50A C50B H50A H50B H50C H50D H50E H50F
 PLAT300_ALERT_4_G Atom Site Occupancy of C49A Constrained at 0.6 Check

And 7 other PLAT300 Alerts

More ...

PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 2% Note
 PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C44 - C47 . 1.53 Ang.
 PLAT367_ALERT_2_G Long? C(sp?)-C(sp?) Bond C47 - C48 . 1.53 Ang.
 PLAT412_ALERT_2_G Short Intra XH3 .. XHn H43 ..H49A . 2.13 Ang.
 x,y,z = 1_555 Check
 PLAT412_ALERT_2_G Short Intra XH3 .. XHn H45 ..H50D . 2.06 Ang.
 x,y,z = 1_555 Check
 PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 65 A**3
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 750 Note
 PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed ! Info
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 339 Note
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 5.167 Note
 Predicted wR2: Based on SigI**2 2.75 or SHELX Weight 13.61
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

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

- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 16 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
 17 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

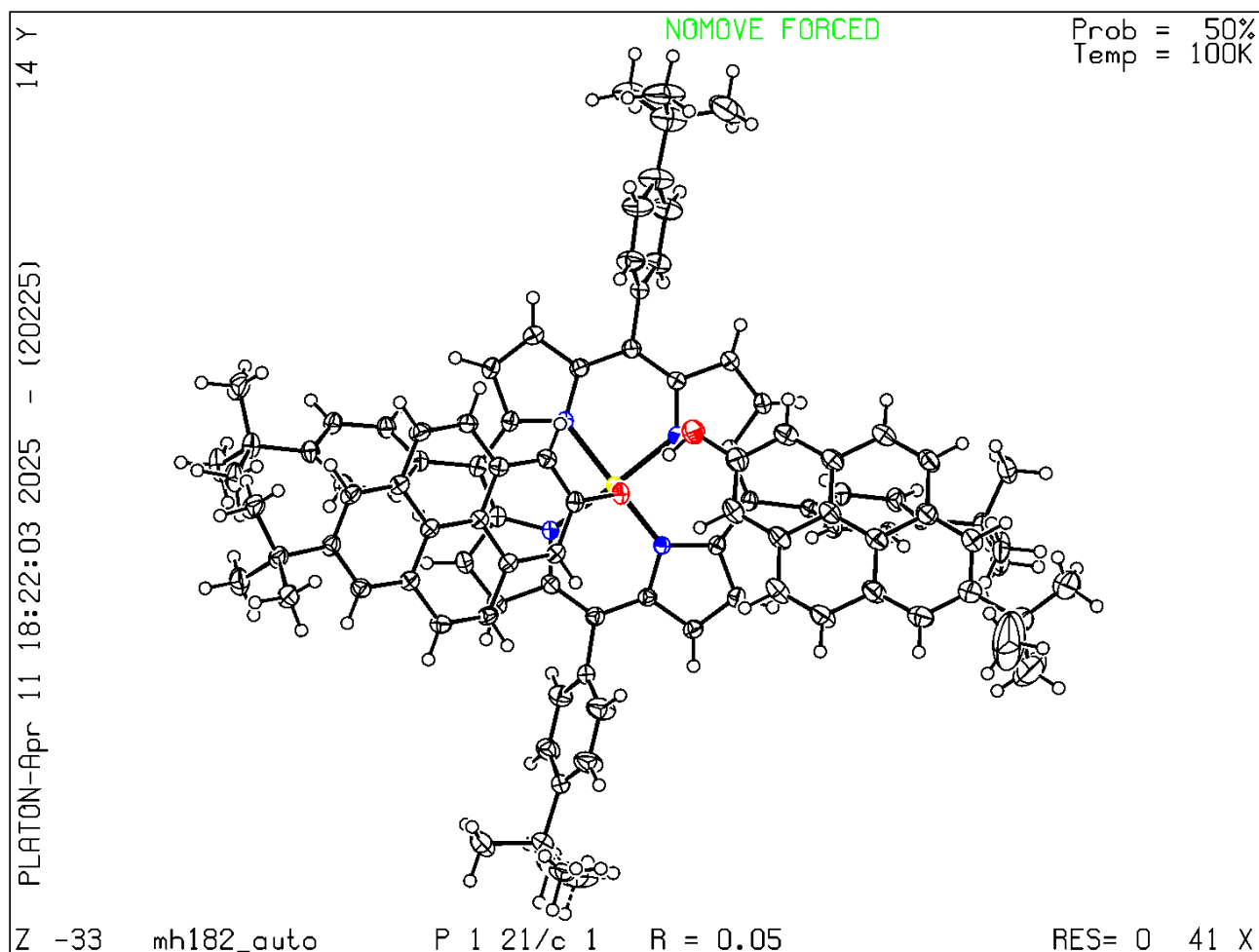
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 02/02/2025; check.def file version of 02/02/2025

Datablock mh182_auto - ellipsoid plot



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