

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) MK-V-177C

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.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

[Structure factor report](#)

Datablock: MK-V-177C

Bond precision:	C-C = 0.0036 Å	Wavelength=1.54184
Cell:	a=11.6176(2) b=16.2017(3) c=18.5816(3)	
	alpha=76.716(1) beta=75.622(1) gamma=70.836(2)	
Temperature:	100 K	
	Calculated	Reported
Volume	3157.93(10)	3157.93(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C30 H22 N6 O8 Zn, 2(C16 H36 N), H2 O	C30 H22 N6 O8 Zn, 2(C16 H36 N), H2 O
Sum formula	C62 H96 N8 O9 Zn	C62 H96 N8 O9 Zn
Mr	1162.86	1162.83
Dx, g cm ⁻³	1.223	1.223
Z	2	2
Mu (mm ⁻¹)	1.016	1.016
F000	1252.0	1252.0
F000'	1252.30	
h, k, lmax	14, 20, 23	14, 20, 23
Nref	13102	12645
Tmin, Tmax	0.941, 0.950	0.825, 1.000
Tmin'	0.903	
Correction method=	# Reported T Limits: Tmin=0.825 Tmax=1.000 AbsCorr =	
	MULTI-SCAN	
Data completeness=	0.965 Theta(max)= 75.423	
R(reflections)=	0.0501(11218) wR2(reflections)= 0.1355(12645)	
S =	1.032 Npar= 935	

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

[PLAT369_ALERT_2_C](#) Long C(sp2)-C(sp2) Bond C1 - C2 . 1.55 Ang.
[PLAT369_ALERT_2_C](#) Long C(sp2)-C(sp2) Bond C16 - C17 . 1.55 Ang.
[PLAT601_ALERT_2_C](#) Unit Cell Contains Solvent Accessible VOIDS of . 95 Ang**3
[PLAT911_ALERT_3_C](#) Missing FCF Refl Between Thmin & STh/L= 0.600 26 Report

● Alert level G

[PLAT002_ALERT_2_G](#) Number of Distance or Angle Restraints on AtSite 58 Note
[PLAT003_ALERT_2_G](#) Number of Uiso or Uij Restrained non-H Atoms ... 32 Report
[PLAT171_ALERT_4_G](#) The CIF-Embedded .res File Contains EADP Records 2 Report
[PLAT172_ALERT_4_G](#) The CIF-Embedded .res File Contains DFIX Records 10 Report
[PLAT173_ALERT_4_G](#) The CIF-Embedded .res File Contains DANG Records 7 Report
[PLAT174_ALERT_4_G](#) The CIF-Embedded .res File Contains FLAT Records 2 Report
[PLAT178_ALERT_4_G](#) The CIF-Embedded .res File Contains SIMU Records 4 Report

PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 3 Report
 PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
 PLAT230_ALERT_2_G Hirshfeld Test Diff for O3 --N3 . 5.5 s.u.
And 4 other PLAT230 Alerts
 Less ...

PLAT230_ALERT_2_G Hirshfeld Test Diff for O8 --N6 . 5.5 s.u.
 PLAT230_ALERT_2_G Hirshfeld Test Diff for C6 --C15' . 7.7 s.u.
 PLAT230_ALERT_2_G Hirshfeld Test Diff for C12 --C15 . 5.5 s.u.
 PLAT230_ALERT_2_G Hirshfeld Test Diff for N7 --C35 . 5.9 s.u.

PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 18% Note
 PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 94% Note
 PLAT413_ALERT_2_G Short Inter XH3 .. XHn H22 ..H42E . 2.14 Ang.
 x,y,z = 1_555 Check
 PLAT413_ALERT_2_G Short Inter XH3 .. XHn H49A ..H30E . 2.06 Ang.
 1-x,1-y,1-z = 2_666 Check
 PLAT432_ALERT_2_G Short Inter X...Y Contact O8' ..C6 2.80 Ang.
 -1+x,y,z = 1_455 Check
 PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 4 Note
 H2 O

PLAT794_ALERT_5_G Tentative Bond Valency for Zn1 (II) . 1.90 Info
 PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ! Info
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 1008 Note
 PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
 PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 430 Note
 PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 17 Note
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.7 Low
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info
 PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 3 Check

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
 30 **ALERT level G** = General information/check it is not something unexpected

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

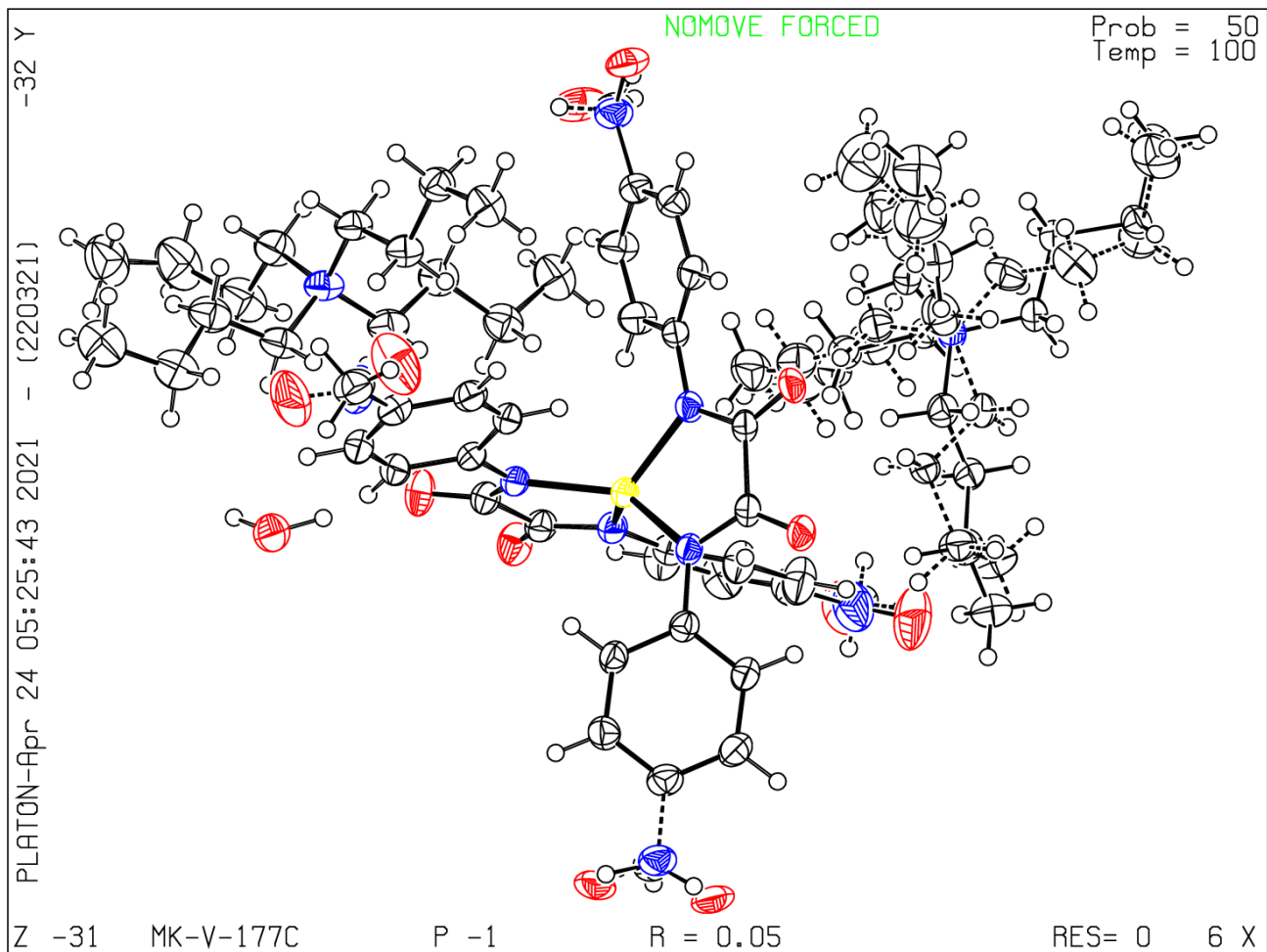
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 22/03/2021; check.def file version of 19/03/2021

Datablock MK-V-177C - ellipsoid plot



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