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-177E

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: MK-V-177E

Bond precision: C-C = 0.0085 A Wavelength=1.54184

Cell: a=12.7359(1) b=23.1116(2) c=23.7682(2)
alpha=64.310(1) beta=76.402(1) gamma=81.357(1)

Temperature: 100 K

	Calculated	Reported
Volume	6118.49(10)	6118.49(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C28 H18 N6 O8 Zn, 2(C16 H36 N)	C28 H18 N6 O8 Zn, 2(C16 H36 N)
Sum formula	C60 H90 N8 O8 Zn	C60 H90 N8 O8 Zn
Mr	1116.79	1116.76
Dx,g cm-3	1.212	1.212
Z	4	4
Mu (mm-1)	1.017	1.017
F000	2400.0	2400.0
F000'	2400.27	
h,k,lmax	15,27,28	15,27,28
Nref	21580	21513
Tmin,Tmax	0.854,0.901	0.504,0.858
Tmin'	0.842	

Correction method= # Reported T Limits: Tmin=0.504 Tmax=0.858 AbsCorr = GAUSSIAN

Data completeness= 0.997 Theta(max)= 66.496

R(reflections)= 0.0906(18221) wR2(reflections)= 0.2587(21513)

S = 1.031 Npar= 1481

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. 1.00A From Zn2 2.57 eA-3

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.26 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.31 Report
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 2.38 eA-3
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C19 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C47 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C118 Check

And 3 other PLAT242 Alerts
Less ...

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C121 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C66 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C98 Check

PLAT260_ALERT_2_C Large Average Ueq of Residue Including N16 0.105 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00846 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C1 - C2 . 1.55 Ang.
And 3 other PLAT369 Alerts
Less ...

PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C15 - C16 . 1.53 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C29 - C30 . 1.55 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C43 - C44 . 1.53 Ang.

PLAT601_ALERT_2_C Unit Cell Contains Solvent Accessible VOIDS of . 57 Ang**3
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 6.643 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.595 65 Report
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.08A From O7 0.66 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 1.09A From O14 0.54 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 22 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 8 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 8.88 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 4 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 2 Report
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
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 47% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 12% Note
PLAT410_ALERT_2_G Short Intra H...H Contact H11J ..H11U . 2.07 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H11L ..H11S . 2.09 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H11U ..H13B . 2.08 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H12J ..H12A . 1.80 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H12K ..H12B . 2.11 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H76B ..H81B . 2.06 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H76B ..H81D . 2.14 Ang.
x,y,z = 1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H84A ..H81C . 2.09 Ang.
x,y,z = 1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H80A ..H83C . 1.97 Ang.
x,y,z = 1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H33 ..H83D . 2.14 Ang.
-x,1-y,1-z = 2_566 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H11V ..H11G . 1.87 Ang.
1-x,-y,1-z = 2_656 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn H12G ..H83B . 1.99 Ang.
-x,1-y,1-z = 2_566 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C118 ..C11A 3.20 Ang.
1-x,-y,1-z = 2_656 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 6 Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 5 Note
C16 H36 N
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1 (II) . 1.87 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn2 (II) . 1.90 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 1264 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 68% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 3 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 49 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ..... Please Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

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

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

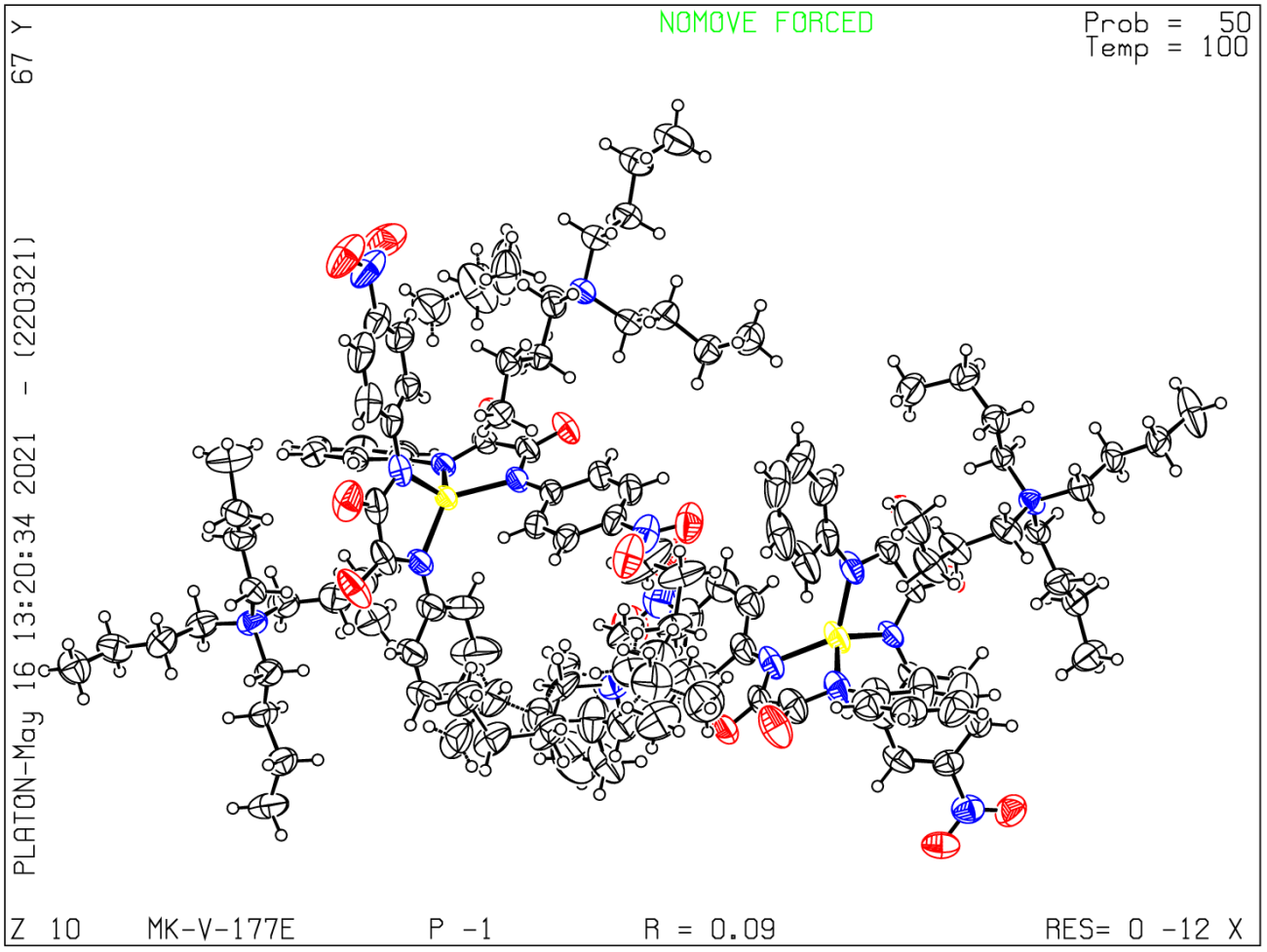
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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-177E - ellipsoid plot



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