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-177D

> 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-177D

Bond precision: C-C = 0.0094 A   Wavelength=1.54184

Cell: a=11.9616(9)   b=13.3224(8)   c=20.6454(7)
             alpha=97.484(4)   beta=96.376(5)   gamma=110.942(7)

Temperature: 100 K

	Calculated	Reported
Volume	3002.0(3)	3002.0(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C28 H16 F2 N6 O8 Zn, 2(C16 H36 N)	C28 H16 F2 N6 O8 Zn, 2(C16 H36 N)
Sum formula	C60 H88 F2 N8 O8 Zn	C60 H88 F2 N8 O8 Zn
Mr	1152.77	1152.75
Dx,g cm-3	1.275	1.275
Z	2	2
Mu (mm-1)	1.103	1.103
F000	1232.0	1232.0
F000'	1232.42	
h,k,lmax	14,15,24	14,15,24
Nref	10584	17129
Tmin,Tmax		0.040,0.135
Tmin'		

Correction method= # Reported T Limits: Tmin=0.040 Tmax=0.135 AbsCorr =
SPHERE

Data completeness= 1.618   Theta(max)= 66.497

R(reflections)= 0.0793(13018)   wR2(reflections)= 0.2463(17129)

S = 1.080   Npar= 743

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
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....   2.88 Report
PLAT260_ALERT_2_C Large Average Ueq of Residue Including   N7   0.108 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ....   0.00945 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond C1   - C2   .   1.53 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond C15   - C16   .   1.54 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......   6.452 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.595   73 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .   10 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .   25.01 Check

⬤Alert level G
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   5 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX 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 2)   12% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3)   6% Note
PLAT410_ALERT_2_G Short Intra H...H Contact H33B   ..H38C   .   2.02 Ang.
                            x,y,z =   1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H37B   ..H39D   .   1.99 Ang.
                            x,y,z =   1_555 Check
PLAT410_ALERT_2_G Short Intra H...H Contact H41B   ..H38B   .   1.93 Ang.
                            x,y,z =   1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn   H25   ..H52A   .   1.92 Ang.
                            1+x,y,z =   1_655 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #   2 Note
            C16 H36 N
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. #   3 Note
            C16 H36 N
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1   (II)   .   1.92 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   592 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..   ! Info
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   49% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).   1 Note
PLAT931_ALERT_5_G CIFcalcFCF Twin Law   [2 5 1] Est.d BASF   0.83 Check
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...   26 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ....   1.6 Low
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ....   Please Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged   Please Check
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by   5 Check

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

 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
 9 ALERT type 3 Indicator that the structure quality may be low
 7 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.
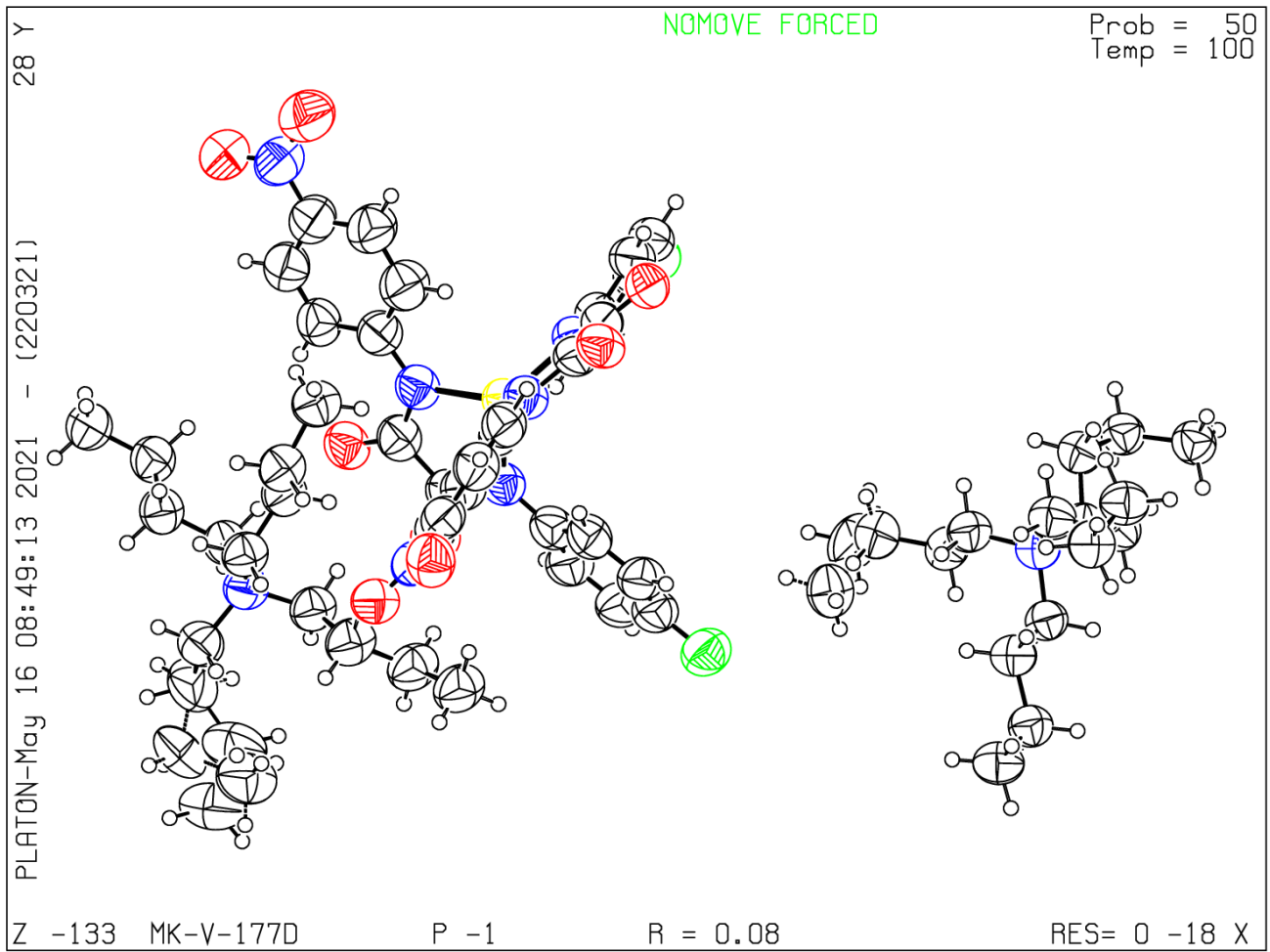
Publication of your CIF in IUCr journals

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-177D - ellipsoid plot

NOMOVE FORCED
Prob = 50
Temp = 100

28 Y

PLATON-May 16 08:49:13 2021 - (220321)

Z -133   MK-V-177D   P -1   R = 0.08   RES= 0 -18 X