

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB8

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 Interpreting this report

Datablock: MAB8

Bond precision: O- B = 0.0031 A Wavelength=0.71075

Cell: a=9.1508(4) b=9.8599(4) c=13.5971(4)
 alpha=88.525(3) beta=70.627(3) gamma=65.245(4)
Temperature: 100 K

	Calculated	Reported
Volume	1041.79(8)	1041.79(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C4 H20 B6 N2 Ni O14, 5(H2 O)	C4 H20 B6 N2 Ni O14, 5(H2 O)
Sum formula	C4 H30 B6 N2 Ni O19	C4 H30 B6 N2 Ni O19
Mr	533.85	533.87
Dx,g cm-3	1.702	1.702
Z	2	2
Mu (mm-1)	1.023	1.023
F000	556.0	556.0
F000'	557.06	
h,k,lmax	11,12,17	11,12,17
Nref	4777	4713
Tmin,Tmax	0.958,0.985	0.703,1.000
Tmin'	0.884	

Correction method= # Reported T Limits: Tmin=0.703 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.987 Theta(max)= 27.483

R(reflections)= 0.0403(3882) wR2(reflections)= 0.1048(4713)

S = 1.064 Npar= 376

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

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.

bluish

PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range	4.3	Ratio
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)	01	Check
PLAT480_ALERT_4_C	Long H...A H-Bond Reported H35B ..N1B .	2.67	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.176	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	47	Report
PLAT977_ALERT_2_C	Check Negative Difference Density on H1BD	-0.35	eA-3

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	24	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	21	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	4	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	6	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	26%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 6)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 7)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	2.12	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	0.88	Check
PLAT417_ALERT_2_G	Short Inter D-H..H-D H32B ..H35B .	2.10	Ang.
	-1+x,1+y,z =	1_465	Check
PLAT417_ALERT_2_G	Short Inter D-H..H-D H33A ..H35B .	2.13	Ang.
	x,y,z =	1_555	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	12	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2	Note
	H2 O		
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	3	Note
	H2 O		
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	5	Note
	H2 O		
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	375	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	14	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.3	Low

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

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

1 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data

6 **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

15 **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 13/07/2021; check.def file version of 13/07/2021

