

# checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: shelxl

---

Bond precision:    C-C = 0.0030 A                      Wavelength=0.71069

Cell:                a=10.895(4)                b=11.095(6)                c=16.340(3)  
                      alpha=88.789(1)        beta=82.016(2)        gamma=76.973(3)

Temperature:    150 K

	Calculated	Reported
Volume	1905.6(13)	1905.6(14)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	C32 H28 N20 Nd2 O30, 2(C8 H4 N5 O6), 14(H2 O)	?
Sum formula	C48 H64 N30 Nd2 O56	C48 H64 N30 Nd2 O56
Mr	2245.77	2245.77
Dx,g cm-3	1.957	1.957
Z	1	1
Mu (mm-1)	1.490	1.490
F000	1130.0	1130.0
F000'	1130.29	
h,k,lmax	14,14,21	14,14,21
Nref	8746	8692
Tmin,Tmax	0.494,0.640	0.722,0.788
Tmin'	0.470	

Correction method= # Reported T Limits: Tmin=0.722 Tmax=0.788  
AbsCorr = MULTI-SCAN

Data completeness= 0.994                      Theta(max)= 27.490

R(reflections)= 0.0196( 8246)                wR2(reflections)= 0.0651( 8692)

S = 1.126                      Npar= 738

---

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

PLAT352_ALERT_3_C	Short	N-H (X0.87,N1.01A)	N37	- H102	.	0.72 Ang.
PLAT352_ALERT_3_C	Short	N-H (X0.87,N1.01A)	N106	- H105	.	0.70 Ang.
PLAT354_ALERT_3_C	Short	O-H (X0.82,N0.98A)	O12	- H6	.	0.69 Ang.
PLAT354_ALERT_3_C	Short	O-H (X0.82,N0.98A)	O202	- H4	.	0.68 Ang.
PLAT354_ALERT_3_C	Short	O-H (X0.82,N0.98A)	O206	- H10	.	0.67 Ang.
PLAT354_ALERT_3_C	Short	O-H (X0.82,N0.98A)	O207	- H50	.	0.71 Ang.
PLAT355_ALERT_3_C	Long	O-H (X0.82,N0.98A)	O206	- H9	.	1.04 Ang.



#### Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details Found	in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	.....	1 Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Nd1 --07	5.1 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Nd1 --09	8.1 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Nd1 --N100	5.6 s.u.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O24 ..C62	2.83 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C58 ..C64	3.16 Ang.
PLAT794_ALERT_5_G	Tentative Bond Valency for Nd1	(II)	1.81 Info
PLAT899_ALERT_4_G	SHELXL97	is Deprecated and Succeeded by SHELXL	2018 Note

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
5 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  
1 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.

