

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ndmnt\_new\_0m

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: ndmnt\_new\_0m

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Bond precision:	C-C = 0.0039 Å	Wavelength=0.71073
Cell:	a=36.2857 (17) alpha=90	b=13.7022 (6) beta=108.918 (2) c=19.4470 (9) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	9146.7 (7)	9146.6 (7)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C64 N32 Nd4 S32, 24 (C N0.50), 4 (C N0.50), 14.667 (Na0.50), 4 (Na0	C27.5 N14 Na5 Nd S8, 0.5 (C)
Sum formula	C112 N56 Na20 Nd4 S32	C28.11 N14.03 Na5 Nd S8
Mr	4192.36	1049.86
Dx, g cm <sup>-3</sup>	1.522	1.525
Z	2	8
Mu (mm <sup>-1</sup> )	1.586	1.586
F000	4072.0	4079.0
F000'	4080.17	
h, k, lmax	66, 24, 35	66, 24, 35
Nref	28876	28829
Tmin, Tmax	0.724, 0.753	0.489, 0.748
Tmin'	0.710	

Correction method= # Reported T Limits: Tmin=0.489 Tmax=0.748  
AbsCorr = MULTI-SCAN

Data completeness= 0.998

Theta (max)= 40.309

R(reflections)= 0.0398( 23501)

wR2(reflections)=  
0.1035( 28829)

S = 1.036

Npar= 579

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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.

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#### Alert level B

PLAT972\_ALERT\_2\_B Check Calcd Resid. Dens. 0.69Ang From Nd01 -2.53 eA-3

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#### Alert level C

PLAT041\_ALERT\_1\_C Calc. and Reported SumFormula Strings Differ Please Check  
Calc: C28 N14 Na5 Nd S8  
Rep.: C28.11 N14.03 Na5 Nd S8

PLAT042\_ALERT\_1\_C Calc. and Reported MoietyFormula Strings Differ Please Check  
Calc: C64 N32 Nd4 S32, 24(C N0.50), 4(C N0.50), 14.667(Na0.50), 4(  
Rep.: C27.5 N14 Na5 Nd S8, 0.5(C)

PLAT043\_ALERT\_1\_C Calculated and Reported Mol. Weight Differ by .. 7.08 Check

PLAT068\_ALERT\_1\_C Reported F000 Differs from Calcd (or Missing)... Please Check

PLAT214\_ALERT\_2\_C Atom C010 (Anion/Solvent) ADP max/min Ratio 4.5 prolat

PLAT243\_ALERT\_4\_C High 'Solvent' Ueq as Compared to Neighbors of C01B Check

PLAT244\_ALERT\_4\_C Low 'Solvent' Ueq as Compared to Neighbors of C018 Check

PLAT244\_ALERT\_4\_C Low 'Solvent' Ueq as Compared to Neighbors of C017 Check

PLAT244\_ALERT\_4\_C Low 'Solvent' Ueq as Compared to Neighbors of C019 Check

PLAT244\_ALERT\_4\_C Low 'Solvent' Ueq as Compared to Neighbors of C01L Check

PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including N00P 0.131 Check

PLAT260\_ALERT\_2\_C Large Average Ueq of Residue Including N01H 0.127 Check

PLAT910\_ALERT\_3\_C Missing # of FCF Reflection(s) Below Theta(Min). 7 Note  
1 1 0, 2 0 0, -3 1 1, -1 1 1, 1 1 1, -2 0 2,  
0 0 2,

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 5 Report  
4 0 0, 5 1 0, -11 3 1, -1 1 2, -26 0 10,

PLAT934\_ALERT\_3\_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check  
-4 0 6,

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.63Ang From Nd01 2.17 eA-3

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.61Ang From Nd01 2.07 eA-3

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.61Ang From Nd01 2.07 eA-3

PLAT971\_ALERT\_2\_C Check Calcd Resid. Dens. 0.65Ang From Nd01 1.64 eA-3

PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 0.61Ang From Nd01 -2.11 eA-3

PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 0.65Ang From Nd01 -2.01 eA-3

PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 0.59Ang From Nd01 -1.85 eA-3

PLAT972\_ALERT\_2\_C Check Calcd Resid. Dens. 0.72Ang From S5 -1.71 eA-3

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#### Alert level G

FORMU01\_ALERT\_1\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and \_chemical\_formula\_moiety. This is  
usually due to the moiety formula being in the wrong format.  
Atom count from \_chemical\_formula\_sum: C28.11 N14.03 Na5 Nd1 S8  
Atom count from \_chemical\_formula\_moiety:C28 N14 Na5 Nd1 S8

FORMU01\_ALERT\_2\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and the formula from the \_atom\_site\* data.

Atom count from \_chemical\_formula\_sum: C28.11 N14.03 Na5 Nd1 S8  
 Atom count from the \_atom\_site data: C28 N14 Na5 Nd1 S8  
 CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.  
 CELLZ01\_ALERT\_1\_G ALERT: Large difference may be due to a  
 symmetry error - see SYMMG tests  
 From the CIF: \_cell\_formula\_units\_Z 8  
 From the CIF: \_chemical\_formula\_sum C28.11 N14.03 Na5 Nd S8  
 TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	224.88	224.00	0.88
N	112.24	112.00	0.24
Na	40.00	40.00	0.00
Nd	8.00	8.00	0.00
S	64.00	64.00	0.00

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2	Info
PLAT040_ALERT_1_G	No H-atoms in this Carbon Containing Compound ..	Please	Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	15.78	Why ?
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group C2/c	I2/a	Note
PLAT299_ALERT_4_G	Atom Site Occupancy Constrained at .....	0.5	Check
	N10 N25 C01D C22 N11 C19 N9 C17		
	C21 N12 C28 C30 Na4A Na4B		
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2A Constrained at	0.6667	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Na2B Constrained at	0.3333	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	67%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	67%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 8)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 9)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 11)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 13)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 14)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 16)	100%	Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact N9 ..C19 .	2.98	Ang.
	x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C17 ..C19 .	3.06	Ang.
	x,y,z =	1_555	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	14	Note
	Nd01 N00P N00S N016 C017 C018 C019 C01B		
	C01D C01E C01F N01H C01L C01O		
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	7	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Nd01 (III) .	3.31	Info
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers	4	Check
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	35	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	5	Note
	1 1 1, -3 1 1, -2 0 2, -1 1 2, 5 1 0,		
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....	1.716	Note
	Predicted wR2: Based on SigI**2 6.04 or SHELX Weight 9.99		

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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  
 23 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 29 **ALERT level G** = General information/check it is not something unexpected

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

17 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
21 ALERT type 4 Improvement, methodology, query or suggestion  
3 ALERT type 5 Informative message, check

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## Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT972_ndmnt_new_0m
;
PROBLEM: Check Calcd Resid. Dens. 0.69Ang From Nd01 -2.53 eA-3
RESPONSE: ...
;
# end Validation Reply Form
```

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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.

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**PLATON version of 15/07/2024; check.def file version of 15/07/2024**

