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: chinleite-Nd

Bond precision: S- O = 0.0070 A Wavelength=0.71075

Cell: a=6.9540(7) b=6.9540(7) c=12.8590(9)
alpha=90 beta=90 gamma=120
Temperature: 293 K

	Calculated	Reported
Volume	538.53(11)	538.52(11)
Space group	P 32 2 1	P 32 2 1
Hall group	P 32 2"	P 32 2"
Moiety formula	Nd2.11 O27 S6, 1.17(O), 1.728(Ca), 2.16(Na)	?
Sum formula	Ca1.73 Na2.16 Nd2.11 O28.17 S6	Ca0.58 Na0.72 Nd0.70 O9.39 S2
Mr	1066.63	355.48
Dx,g cm-3	3.289	3.288
Z	1	3
Mu (mm-1)	6.204	6.202
F000	506.4	506.0
F000'	507.49	
h,k,lmax	9,9,16	8,9,16
Nref	820[506]	814
Tmin,Tmax	0.557,0.780	0.506,1.000
Tmin'	0.367	

Correction method= # Reported T Limits: Tmin=0.506 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.61/0.99 Theta(max)= 27.444

R(reflections)= 0.0259(791)

wR2(reflections)= 0.0585(814)

S = 1.194 Npar= 69

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

PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18)	7.33 Note
PLAT220_ALERT_2_C	NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range	3.4 Ratio
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including O6	0.111 Check

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Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.333 Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem c/2	83 %Fit
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records	2 Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2 Report
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	3 Note
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293 Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1)	11% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100% Note
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	O6 Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	4 Note

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

5 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
2 ALERT type 3 Indicator that the structure quality may be low
8 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 09/05/2022; check.def file version of 21/03/2022

Datablock chinleite-Nd - ellipsoid plot