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: ww

Bond precision: C-C = 0.0060 A Wavelength=0.71073

Cell: a=12.464(3) b=13.531(3) c=8.8035(18)
alpha=90 beta=95.06(3) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1478.9(6)	1478.9(6)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C28 H26 Ba Cl2 N6 O2	?
Sum formula	C28 H26 Ba Cl2 N6 O2	C28 H26 Ba Cl2 Mg0 N6 Na0 Nd0 O2
Mr	686.78	686.78
Dx,g cm-3	1.542	1.542
Z	2	2
Mu (mm-1)	1.559	1.559
F000	684.0	684.0
F000’	684.13	
h,k,lmax	16,17,11	16,17,11
Nref	3384	3353
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.991 Theta(max)= 27.479

R(reflections)= 0.0455(2936) wR2(reflections)= 0.1109(3353)

S = 1.098 Npar= 178

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

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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.38 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range       3.5 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C11    --  C12     ..       0.18 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C9 Check
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Alert level G

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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    2
           From the CIF: _chemical_formula_sum  C28 H26 Ba Cl2 Mg0 N6 Na0 Nd0 O2
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         56.00     56.00    0.00
           H         52.00     52.00    0.00
           Ba         2.00      2.00    0.00
           Cl         4.00      4.00    0.00
           Mg         2.00      0.00    2.00
           N         12.00     12.00    0.00
           Na         2.00      0.00    2.00
           Nd         2.00      0.00    2.00
           O          4.00      4.00    0.00
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms .............          1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)      293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)      293 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
5 **ALERT level G** = General information/check it is not something unexpected

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
1 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 27/03/2017; check.def file version of 24/03/2017

Datablock ww - ellipsoid plot