

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lamnt_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: lamnt_0m

Bond precision: C-C = 0.0023 Å Wavelength=0.71073

Cell: a=36.5860 (9) b=13.7473 (3) c=19.4992 (5)
 alpha=90 beta=109.152 (1) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	9264.5 (4)	9264.5 (4)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C64 La4 N32 S32, 22 (C N0.50), 4 (C N0.50 Na), 2 (C1.50 N), 16 (Na)	C27.75 La N14 Na5 S8
Sum formula	C111 La4 N56 Na20 S32	C27.75 La N14 Na5 S8
Mr	4159.03	1039.76
Dx, g cm ⁻³	1.491	1.491
Z	2	8
Mu (mm ⁻¹)	1.367	1.367
F000	4036.0	4036.0
F000'	4043.42	
h, k, lmax	59, 22, 31	59, 22, 31
Nref	21134	21096
Tmin, Tmax	0.768, 0.872	0.672, 0.747
Tmin'	0.753	

Correction method= # Reported T Limits: Tmin=0.672 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta (max)= 35.474

R(reflections)= 0.0304(18448)

wR2(reflections)=
0.0777(21096)

S = 1.055

Npar= 619

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

PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: C64 La4 N32 S32, 22(C N0.50), 4(C N0.50 Na), 2(C1.50 N), 16(
Rep.: C27.75 La N14 Na5 S8

PLAT216_ALERT_3_C Disordered C8# (An/Solv) ADP max/min Ratio 5.2 Note

PLAT221_ALERT_2_C Solv./Anion Resd 2 C Ueq(max)/Ueq(min) Range 4.4 Ratio

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of S6 Check

PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C22 Check

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C019 Check

PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 17 Report

3	1	0,	4	0	0,	5	1	0,	-3	1	1,	1	1	1,	6	2	1,
-4	0	2,	-3	1	2,	-2	0	2,	-1	1	2,	0	0	2,	2	0	2,
-4	2	3,	-3	1	3,	-4	0	4,	-9	1	6,	-4	0	6,			

PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 3 Check

PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.84Ang From S6 -1.53 eA-3



Alert level G

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 19.95 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

C017	C0	C17	C25	C018	C26	C27	C28
N9	C18	N18	N19	C20	C21	Na4A	Na4B
N20	C23	C24	N01H	C01B	C01F	N21	C01G
Na1A	Na1B						

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 4) 67% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 5) 67% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 6) 100% 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) 50% Note

PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 10) 100% Note

PLAT432_ALERT_2_G Short Inter X...Y Contact N20 ..C18 . 2.99 Ang.

1-x,1-y,1-z = 5_666 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact C18 ..C23 . 3.07 Ang.

1-x,1-y,1-z = 5_666 Check

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 14 Note

La01	N00H	N00Q	N016	C017	C018	C019	C01A
C01B	C01C	C01F	C01G	N01H	C0		

PLAT773_ALERT_2_G Check long C-C Bond in CIF: C017 --C25 1.74 Ang.

PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 9 Check

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PLAT794_ALERT_5_G Tentative Bond Valency for La01      (III)      .      3.28 Info
PLAT822_ALERT_4_G CIF-embedded .res Contains Negative PART Numbers      7 Check
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).      2 Note
      1 1 0, 2 0 0,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600      18 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File      10 Note
      1 1 1, -2 0 2, -3 1 1, -4 0 6, -3 1 3, -4 0 4,
      5 1 0, 6 2 1, -9 1 6, -4 2 3,
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value .....      3.592 Note
      Predicted wR2: Based on SigI**2 2.16 or SHELX Weight 7.36

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
17 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

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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.

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

Datablock lamnt_0m - ellipsoid plot

