checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx_a_pl

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: shelx_a_pl

```
Bond precision:  C-C = 0.0124 A          Wavelength=1.54186

Cell:            a=9.8240(3)    b=9.2835(3)         c=21.7931(6)
                 alpha=90       beta=100.383(2)     gamma=90
Temperature:     93 K
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	Calculated	Reported
Volume	1955.01(10)	1955.01(10)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C38 H42 Cl4 N4 Na2 O10	C38 H38 Cl4 N4 Na2 O8, 2(H2O)
Sum formula	C38 H42 Cl4 N4 Na2 O10	C38 H42 Cl4 N4 Na2 O10
Mr	902.54	902.53
Dx,g cm-3	1.533	1.533
Z	2	2
Mu (mm-1)	3.521	3.521
F000	936.0	936.0
F000’	941.94	
h,k,lmax	11,11,26	11,11,26
Nref	7139[3808]	6778
Tmin,Tmax	0.557,0.872	0.656,0.875
Tmin’	0.483	

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Correction method= # Reported T Limits: Tmin=0.656 Tmax=0.875
AbsCorr = MULTI-SCAN

Data completeness= 1.78/0.95      Theta(max)= 68.229

R(reflections)= 0.0743( 4942)     wR2(reflections)= 0.1893( 6778)

S = 1.023                 Npar= 555
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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.

Alert level B

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PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds ...............    0.01239 Ang.
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Alert level C

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RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
            Rint given   0.136
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .........      0.136 Report
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) ........       6.85 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.14 Report
PLAT915_ALERT_3_C No Flack x Check Done: Low Friedel Pair Coverage         89 %
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.03A   From N2              0.53 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          8 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          4 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          6 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT111_ALERT_2_G ADDSYM Detects New (Pseudo) Centre of Symmetry .         89 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New  Space Group      P21/c Check
PLAT169_ALERT_4_G The CIF-Embedded .res File Contains AFIX 1 Recds          2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of H32A       Constrained at     0.6529 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32B       Constrained at     0.3471 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         3% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          2 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        151 Check
              O4   -C28  -NA1     1.555   1.555   2.745             42.00 Deg.
PLAT780_ALERT_1_G Coordinates do not Form a Properly Connected Set     Please Do !
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON           4 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         37 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          7 Note
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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
   7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  22 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 ALERT type 2 Indicator that the structure model may be wrong or deficient
   8 ALERT type 3 Indicator that the structure quality may be low
   9 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
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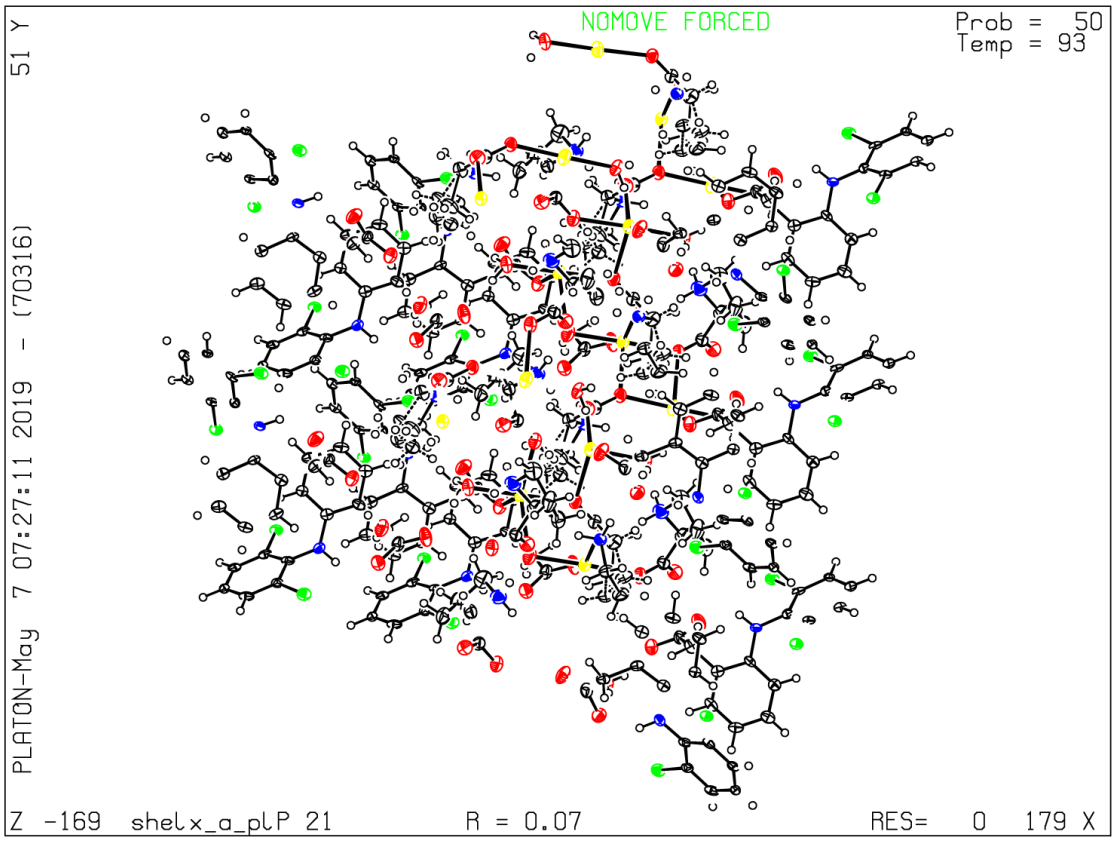
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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 03/05/2019; check.def file version of 29/04/2019

Datablock shelx_a_pl - ellipsoid plot