checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: complex1

```
Bond precision:  C-C = 0.0026 A          Wavelength=0.71073

Cell:            a=11.958(2)    b=24.461(5)          c=15.593(6)
                 alpha=90       beta=127.316(19)     gamma=90
Temperature:     173 K
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	Calculated	Reported
Volume	3627.4(19)	3627.4(17)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	?
Moiety formula	2(C20 H28 N12 Na O9), 2(C6 H5 N O3), 2(Cl), 10(H2 O), O	?
Sum formula	C52 H86 Cl2 N26 Na2 O35	C52 H86 Cl2 N26 Na2 O35
Mr	1752.35	1752.35
Dx,g cm-3	1.604	1.604
Z	2	2
Mu (mm-1)	0.214	0.214
F000	1832.0	1832.0
F000’	1833.70	
h,k,lmax	14,29,18	14,29,18
Nref	6390	6366
Tmin,Tmax	0.918,0.938	0.918,0.938
Tmin’	0.918	

```
Correction method= MULTI-SCAN

Data completeness= 0.996          Theta(max)= 25.000

R(reflections)= 0.0362( 5897)     wR2(reflections)= 0.0970( 6366)

S = 1.063                 Npar= 543
```

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

PLAT417_ALERT_2_B Short Inter D-H..H-D H2O2 .. H2O6 .. 2.07 Ang.

PLAT420_ALERT_2_B D-H Without Acceptor O4W - H2O4 ... ?

Alert level C

CELLV02_ALERT_1_C The supplied cell volume s.u. differs from that
calculated from the cell parameter s.u.'s by > 2
Calculated cell volume su = 19.25
Cell volume su given = 17.00
PLAT220_ALERT_2_C Large Non-Solvent O Ueq(max)/Ueq(min) ... 3.4 Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) .. 5.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for O2 -- C11 .. 5.3 su
PLAT314_ALERT_2_C Check Small Angle for H2O: Metal-O4W -H2O4 89.92 Deg.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1
C20 H28 N12 Na O9

Alert level G

PLAT004_ALERT_5_G Info: Polymeric Structure Found with Dimension . 1
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms 17
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ... 2 Units
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ..... 8 Perc.
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) ..... O7W'
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) O7W
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 17
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2
C6 H5 N O3
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 3
Cl
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 4
H2 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 5
H2 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 6
H2 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 7
H2 O
PLAT793_ALERT_4_G The Model has Chirality at C4 (Verify) .... S
PLAT793_ALERT_4_G The Model has Chirality at C5 (Verify) .... R
PLAT793_ALERT_4_G The Model has Chirality at C9 (Verify) .... S
PLAT793_ALERT_4_G The Model has Chirality at C10 (Verify) .... R
PLAT793_ALERT_4_G The Model has Chirality at C19 (Verify) .... S
PLAT793_ALERT_4_G The Model has Chirality at C20 (Verify) .... R

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
20 **ALERT level G** = General information/check it is not something unexpected

2 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
1 ALERT type 3 Indicator that the structure quality may be low
15 ALERT type 4 Improvement, methodology, query or suggestion
3 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*, 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 04/07/2012; check.def file version of 28/06/2012

Datablock complex1 - ellipsoid plot