

# 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: a

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Bond precision:	C-C = 0.0064 Å	Wavelength=0.71073
Cell:	a=11.9767(3)	b=24.3621(7)      c=12.6637(3)
	alpha=90	beta=101.163(3)      gamma=90
Temperature:	173 K	
	Calculated	Reported
Volume	3625.08(17)	3625.07(16)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	?
	2(C20 H28 N12 Na O9), 2(C6	
Moiety formula	H5 N O3), 2(Br0.47 H2 O), ?	
	1.06(Br),	
Sum formula	C52 H86 Br2 N26 Na2 O35	C52 H86 Br2 N26 Na2 O35
Mr	1841.25	1841.25
Dx,g cm-3	1.687	1.687
Z	2	2
Mu (mm-1)	1.243	1.243
F000	1904.0	1904.0
F000'	1903.94	
h,k,lmax	14,28,15	14,28,15
Nref	6386	6374
Tmin,Tmax	0.577,0.689	0.577,0.689
Tmin'	0.566	

Correction method= MULTI-SCAN

Data completeness= 0.998      Theta(max)= 25.000

R(reflections)= 0.0767( 5365)      wR2(reflections)= 0.2226( 6374)

S = 1.070      Npar= 551

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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.

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### Alert level B

PLAT220\_ALERT\_2\_B Large Non-Solvent      0      Ueq(max)/Ueq(min) ...      4.4 Ratio

PLAT222_ALERT_3_B	Large Non-Solvent	H	Uiso(max)/Uiso(min)	..	7.3	Ratio
PLAT417_ALERT_2_B	Short Inter D-H..H-D	H9	..	H105	..	2.05 Ang.
PLAT417_ALERT_2_B	Short Inter D-H..H-D	H105	..	H102	..	1.84 Ang.
PLAT420_ALERT_2_B	D-H Without Acceptor	O3W	-	H103	...	?

### ● Alert level C

PLAT303_ALERT_2_C	Full Occupancy H-Atom	H102	with # Connections	1.47
PLAT341_ALERT_3_C	Low Bond Precision on	C-C Bonds	.....	0.0064 Ang
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H107	.. O4 ..	2.66 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H105	.. BR1' ..	2.97 Ang.
PLAT480_ALERT_4_C	Long H...A H-Bond Reported	H206	.. BR1' ..	3.12 Ang.
PLAT481_ALERT_4_C	Long D...A H-Bond Reported	O6W	.. BR1' ..	3.93 Ang.
PLAT774_ALERT_1_C	Suspect X-Y Bond in CIF:	NA1	-- NA1 ..	3.57 Ang.

### ● 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
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large.	0.12
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	14.77
PLAT128_ALERT_4_G	Alternate Setting of Space-group P21/c	P21/n
PLAT302_ALERT_4_G	Note: Anion/Solvent Disorder	23 Perc.
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	O9W'
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	O9W
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	17
PLAT793_ALERT_4_G	The Model has Chirality at C3 (Verify)	R
PLAT793_ALERT_4_G	The Model has Chirality at C4 (Verify)	R
PLAT793_ALERT_4_G	The Model has Chirality at C8 (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)	R
PLAT793_ALERT_4_G	The Model has Chirality at C20 (Verify)	S

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
9 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  
13 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.

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**PLATON version of 22/10/2012; check.def file version of 16/10/2012**

