

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) vv3y

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: vv3y

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Bond precision:	C-C = 0.0066 Å	Wavelength=0.71073	
Cell:	a=14.240 (2)	b=14.240 (2)	c=21.691 (4)
	alpha=90	beta=90	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	4398.5 (15)	4398.4 (15)	
Space group	P -4 n 2	P -4 n 2	
Hall group	P -4 -2n	P -4 -2n	
Moiety formula	C20 H12 Na O12 Y	C20 H12 Na O12 Y	
Sum formula	C20 H12 Na O12 Y	C20 H12 Na O12 Y	
Mr	556.20	556.20	
Dx, g cm <sup>-3</sup>	1.680	1.680	
Z	8	8	
Mu (mm <sup>-1</sup> )	2.736	2.736	
F000	2224.0	2224.0	
F000'	2203.21		
h, k, lmax	17, 17, 27	17, 17, 27	
Nref	4498 [ 2444]	4496	
Tmin, Tmax	0.849, 0.921	0.371, 0.432	
Tmin'	0.761		

Correction method= # Reported T Limits: Tmin=0.371 Tmax=0.432  
AbsCorr = MULTI-SCAN

Data completeness= 1.84/1.00      Theta(max)= 26.372

R(reflections)= 0.0296 ( 4418)	wR2(reflections)= 0.0817 ( 4496)
S = 1.043	Npar= 308



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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 C

PLAT090_ALERT_3_C	Poor Data / Parameter Ratio (Zmax > 18) .....	7.94	Note
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.2	Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range	3.6	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for O9 --C14 .	5.7	s.u.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	03	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	09	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	012	Check
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.00662	Ang.
PLAT601_ALERT_2_C	Unit Cell Contains Solvent Accessible VOIDS of .	39	Ang**3

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### ● Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu not performed for this radiation type.		
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	3	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	3	Report
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O3 .	108.6	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O6 .	106.8	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O9 .	107.3	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O12 .	106.1	Degree
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.11	Ratio
PLAT774_ALERT_1_G	Check X-Y Bond in CIF: Y1 --Y1 ..	4.02	Ang.
PLAT774_ALERT_1_G	Check X-Y Bond in CIF: Y2 --Y2 ..	4.01	Ang.
PLAT794_ALERT_5_G	Tentative Bond Valency for Y1 (III) .	3.27	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Y2 (III) .	3.26	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	14	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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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  
18 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
13 ALERT type 2 Indicator that the structure model may be wrong or deficient  
3 ALERT type 3 Indicator that the structure quality may be low  
4 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.



