

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) dwat21_0m_a_sq

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: dwat21_0m_a_sq

Bond precision: C-C = 0.0079 A

Wavelength=0.71073

Cell: a=6.9398(10) b=16.126(2) c=18.517(3)
 alpha=79.340(4) beta=80.010(4) gamma=89.242(4)
Temperature: 100 K

	Calculated	Reported
Volume	2005.2(5)	2005.2(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C8 H3 I N2 O4, C8 H6 N2 O [+ solvent]	C8 H3 I N2 O4, C8 H6 N2 O
Sum formula	C16 H9 I N4 O5 [+ solvent]	C16 H9 I N4 O5
Mr	464.17	464.17
Dx, g cm ⁻³	1.538	1.538
Z	4	4
Mu (mm ⁻¹)	1.628	1.628
F000	904.0	904.0
F000'	902.51	
h,k,lmax	8,20,23	8,20,23
Nref	8285	8062
Tmin,Tmax	0.683,0.823	0.519,0.745
Tmin'	0.608	

Correction method= # Reported T Limits: Tmin=0.519 Tmax=0.745

AbsCorr = MULTI-SCAN

Data completeness= 0.973

Theta(max)= 26.452

R(reflections)= 0.0484(6152)

wR2(reflections)= 0.1220(8062)

S = 1.043

Npar= 469

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**

PLAT213_ALERT_2_C	Atom O4	has ADP max/min Ratio	3.6	prolat
PLAT213_ALERT_2_C	Atom O5	has ADP max/min Ratio	3.9	prolat
PLAT234_ALERT_4_C	Large Hirshfeld Difference C18	--C19 .	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C19	--C20 .	0.16	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C18	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		N2	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		N3	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		2.6	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		2.8	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	78	Report
PLAT977_ALERT_2_C	Check Negative Difference Density on H19		-0.61	eA-3
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.		0	Info

● **Alert level G**

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.004	Degree
PLAT371_ALERT_2_G	Long C(sp2)-C(sp1) Bond C2	- C3 .	1.43	Ang.
PLAT371_ALERT_2_G	Long C(sp2)-C(sp1) Bond C10	- C11 .	1.43	Ang.
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O9		105.6	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O10		106.5	Degree
PLAT431_ALERT_2_G	Short Inter HL..A Contact I1	..N7 .	2.83	Ang.
		1-x,1-y,-z =	2_665	Check
PLAT431_ALERT_2_G	Short Inter HL..A Contact I2	..N5 .	2.79	Ang.
		1-x,1-y,-z =	2_665	Check
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure		!	Info
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed		!	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	143	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		2	Note
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by		2	Check

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
16 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
5 ALERT type 4 Improvement, methodology, query or suggestion
1 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* 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.

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