

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) IlyasSakh5\_0ma\_a

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: IlyasSakh5\_0ma\_a

---

Bond precision:	C-C = 0.0025 A	Wavelength=0.71073	
Cell:	a=18.3716(10)	b=11.4111(6)	c=13.2287(12)
	alpha=90	beta=132.282(2)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	2051.8(3)	2051.8(2)	
Space group	C 2/c	C 2/c	
Hall group	-C 2yc	-C 2yc	
Moiety formula	C12 H12 Br4 Co N4 O8	?	
Sum formula	C12 H12 Br4 Co N4 O8	C12 H12 Br4 Co N4 O8	
Mr	718.79	718.83	
Dx, g cm <sup>-3</sup>	2.327	2.327	
Z	4	4	
Mu (mm <sup>-1</sup> )	8.674	8.674	
F000	1372.0	1372.0	
F000'	1369.75		
h, k, lmax	31, 19, 22	30, 19, 22	
Nref	5369	4908	
Tmin, Tmax	0.787, 0.855	0.331, 0.747	
Tmin'	0.626		

Correction method= # Reported T Limits: Tmin=0.331 Tmax=0.747  
AbsCorr = MULTI-SCAN

Data completeness= 0.914      Theta(max)= 37.384

R(reflections)= 0.0324( 4079)	wR2(reflections)= 0.0790( 4908)
S = 1.019	Npar= 139

---

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 O11	has ADP max/min Ratio .....	3.2	prolat
PLAT213_ALERT_2_C	Atom O12	has ADP max/min Ratio .....	3.5	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range		3.4	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for O10 --N3		5.6	s.u.
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 ....		2.2	Note
PLAT431_ALERT_2_C	Short Inter HL..A Contact Br3 ..O12		3.15	Ang.
	-1/2+x,-1/2+y,-1+z =		3_444	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....		2.023	Check
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.58Ang From Br6		-1.83	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.65Ang From Br3		-1.59	eA-3

---



### Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		1	Info
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group C2/c		I2/a	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Co1 (II)		1.99	Info
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		456	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....		4.8	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please	Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		3	Info

---

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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
11 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  
2 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

