

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

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Bond precision:	Si- O = 0.0100 A	Wavelength=0.71073	
Cell:	a=4.7640 (3)	b=7.6938 (4)	c=9.9735 (7)
	alpha=90	beta=90.294 (6)	gamma=90
Temperature:	846 K		
	Calculated	Reported	
Volume	365.56 (4)	365.56 (4)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	Bi0.40 Mn0.47 O20 Si4.48 Y3.60, 3.52 (Be)	?	
Sum formula	Be3.52 Bi0.40 Mn0.47 O20 Si4.48 Y3.60	Be3.52 H4 Bi0.40 Ca0 Mn0.48 O20 Si4.48 Y3.60	
Mr	907.14	911.63	
Dx, g cm <sup>-3</sup>	4.121	4.141	
Z	1	1	
Mu (mm <sup>-1</sup> )	19.826	19.834	
F000	422.2	426.0	
F000'	411.47		
h, k, lmax	6, 10, 13	6, 10, 13	
Nref	979	874	
Tmin, Tmax	0.679, 0.673		
Tmin'	0.666		

Correction method= Not given

Data completeness= 0.893

Theta (max)= 29.066

R(reflections)= 0.0642 ( 706)

wR2(reflections)=  
0.1507 ( 874)

S = 1.267

Npar= 76

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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**

PLAT041_ALERT_1_C	Calc. and Reported SumFormula	Strings Differ	Please Check
PLAT043_ALERT_1_C	Calculated and Reported Mol. Weight	Differ by ..	4.49 Check
PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..		Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....		6.867 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....		2.117 Check
PLAT925_ALERT_1_C	The Reported and Calculated Rho(max) Differ by .		1.19 eA-3

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● **Alert level G**

FORMU01\_ALERT\_2\_G There is a discrepancy between the atom counts in the  
\_chemical\_formula\_sum and the formula from the \_atom\_site\* data.  
Atom count from \_chemical\_formula\_sum: H4 Be3.52 Bi0.4 Mn0.48 O20 Si4.4  
Atom count from the \_atom\_site data: Be3.52 Bi0.4 Mn0.4716 O20 Si4.48

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.

CELLZ01\_ALERT\_1\_G ALERT: Large difference may be due to a  
symmetry error - see SYMMG tests

From the CIF: \_cell\_formula\_units\_Z 1

From the CIF: \_chemical\_formula\_sum Be3.52 H4 Bi0.40 Ca0 Mn0.48 O20 Si

TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
Be	3.52	3.52	0.00
H	4.00	0.00	4.00
Bi	0.40	0.40	0.00
Ca	1.00	0.00	1.00
Mn	0.48	0.47	0.01
O	20.00	20.00	0.00
Si	4.48	4.48	0.00
Y	3.60	3.60	0.00

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension		3 Info
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large		11.94 Why ?
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records		2 Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		2 Report
PLAT300_ALERT_4_G	Atom Site Occupancy of Bi1	Constrained at	0.1 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Y1	Constrained at	0.9 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mn1	Constrained at	0.2358 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Si2	Constrained at	0.12 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Be2	Constrained at	0.88 Check
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1 )	18% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )		100% 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		105 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....		4.1 Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check

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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

8 **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

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

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**PLATON version of 28/11/2022; check.def file version of 28/11/2022**

