

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

Bond precision: As- O = 0.0046 Å Wavelength=0.71073

Cell: a=8.8418 (9) b=23.031 (2) c=13.5270 (14)
 alpha=90 beta=90 gamma=90

Temperature: 300 K

	Calculated	Reported
Volume	2754.6 (5)	2754.6 (5)
Space group	C m c a	C m c a
Hall group	-C 2bc 2	-C 2bc 2
Moiety formula	As ₈ Mn ₈ O ₄₀ , 8 (Ca _{0.50} O), 8 (O _{0.50}), 8 (O _{0.50}), 4 (O)	?
Sum formula	As ₈ Ca ₄ Mn ₈ O ₆₀	As ₂ Ca Mn ₂ O ₁₅
Mr	2159.20	539.80
Dx, g cm ⁻³	2.603	2.603
Z	2	8
Mu (mm ⁻¹)	7.045	7.045
F ₀₀₀	2048.0	2048.0
F ₀₀₀ '	2057.33	
h, k, lmax	11, 28, 16	11, 28, 16
Nref	1508	1507
Tmin, Tmax	0.662, 0.809	0.837, 0.915
Tmin'	0.489	

Correction method= # Reported T Limits: Tmin=0.837 Tmax=0.915
AbsCorr = MULTI-SCAN

Data completeness= 0.999 Theta (max)= 26.368

R(reflections)= 0.0385 (1195)

wR2(reflections)=
0.1047 (1507)

S = 1.068

Npar= 129

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 O6	has ADP max/min Ratio	3.1	prolat
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	04	Check
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	As1	Check
PLAT975_ALERT_2_C	Check	Calcd Resid. Dens. 1.04Ang From O9	0.53	eA-3
PLAT975_ALERT_2_C	Check	Calcd Resid. Dens. 0.72Ang From O12B	0.51	eA-3
PLAT975_ALERT_2_C	Check	Calcd Resid. Dens. 0.73Ang From O5	0.50	eA-3
PLAT975_ALERT_2_C	Check	Calcd Resid. Dens. 0.89Ang From O5	0.50	eA-3
PLAT975_ALERT_2_C	Check	Calcd Resid. Dens. 0.82Ang From O5	0.48	eA-3
PLAT975_ALERT_2_C	Check	Calcd Resid. Dens. 0.77Ang From O10	0.44	eA-3
PLAT975_ALERT_2_C	Check	Calcd Resid. Dens. 0.81Ang From O1	0.42	eA-3
PLAT975_ALERT_2_C	Check	Calcd Resid. Dens. 0.65Ang From O4	0.41	eA-3
PLAT975_ALERT_2_C	Check	Calcd Resid. Dens. 0.42Ang From O11	0.40	eA-3
PLAT976_ALERT_2_C	Check	Calcd Resid. Dens. 1.05Ang From O2	-0.44	eA-3
PLAT976_ALERT_2_C	Check	Calcd Resid. Dens. 1.03Ang From O5	-0.44	eA-3
PLAT976_ALERT_2_C	Check	Calcd Resid. Dens. 0.97Ang From O3	-0.42	eA-3



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.250	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	34.60	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of O7A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O7B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O8 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Ca2 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O12A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O12B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O9 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O10 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O11 Constrained at	0.5	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
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100%	Note
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	09	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	010	Check
PLAT311_ALERT_2_G	Isolated Disordered Oxygen Atom (No H's ?)	011	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT899_ALERT_4_G	SHELXL2018 is Deprecated and Succeeded by SHELXL	2019/3	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min). 0 2 0,	1	Note
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please	Check
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value Predicted wr2: Based on SigI**2 4.90 or SHELX Weight 10.25	2.14	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully
15 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
27 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
20 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
15 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* 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.

Datablock shelx - ellipsoid plot

