

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Ellinaite

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: Ellinaite

Bond precision: Cr- O = 0.0050 A Wavelength=0.71073

Cell: a=8.868(9) b=2.885(3) c=10.355(11)
 alpha=90 beta=90 gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	264.9(5)	264.9(5)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	?
Moiety formula	Cr4 O8, 2(Ca)	?
Sum formula	Ca2 Cr4 O8	Ca Cr2 O4
Mr	416.16	208.08
Dx,g cm-3	5.218	5.217
Z	2	4
Mu (mm-1)	9.936	9.935
F000	400.0	400.0
F000'	403.63	
h,k,lmax	11,3,13	11,3,13
Nref	351	348
Tmin,Tmax	0.788,0.820	0.273,1.000
Tmin'	0.742	

Correction method= # Reported T Limits: Tmin=0.273 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 26.983

R(reflections)= 0.0588(312) wR2(reflections)= 0.1572(348)

S = 1.105 Npar= 43

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

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -1.834
Test value = -1.800

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	8.09	Note
PLAT098_ALERT_2_C	Large Reported Min. (Negative) Residual Density	-1.83	eA-3
PLAT148_ALERT_3_C	s.u. on the a - Axis is (Too) Large ...	0.009	Ang.
PLAT148_ALERT_3_C	s.u. on the b - Axis is (Too) Large ...	0.0030	Ang.
PLAT148_ALERT_3_C	s.u. on the c - Axis is (Too) Large ...	0.011	Ang.
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor ...	2.3	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	3	Report
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on Cr1	1.13	eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on Ca1	1.06	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.70A From O1	0.72	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 1.03A From O3	-0.88	eA-3

● Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.12	Report
PLAT794_ALERT_5_G	Tentative Bond Valency for Cr1 (IV)	4.12	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cr2 (IV)	3.97	Info
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	3	Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected
- 2 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
9 **ALERT type 2** Indicator that the structure model may be wrong or deficient
5 **ALERT type 3** Indicator that the structure quality may be low
0 **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.

