

checkCIF (basic structural check) running

Checking for embedded fcf data in CIF ...

Found embedded fcf data in CIF. Extracting fcf data from uploaded CIF, please wait . . .

checkCIF/PLATON (basic structural check)

Structure factors have been supplied for datablock(s) hcl

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](#)

Please wait while processing [Interpreting this report](#)

[Structure factor report](#)

Datablock: hcl

Bond precision:	O- C = 0.0017 Å	Wavelength=0.71073
Cell:	a=10.0234(3) b=11.5131(3) c=16.2989(5)	
	alpha=90 beta=104.205(3) gamma=90	
Temperature: 293 K		
	Calculated	Reported
Volume	1823.39(9)	1823.39(9)
Space group	P 2/c	P 1 2/c 1
Hall group	-P 2yc	-P 2yc
Moiety formula	2(A12 Ca4 H20 O16), C O3, 2(Cl), 2(H2 O)	A12 Ca4 H20 O16, Cl, H2 O, C0.5 O1.5
Sum formula	C H44 Al4 Ca8 Cl2 O37	C0.50 H22 Al2 Ca4 Cl O18.50
Mr	1147.82	573.91
Dx, g cm-3	2.091	2.091
Z	2	4
Mu (mm-1)	1.517	1.517
F000	1184.0	1184.0
F000'	1189.44	
h,k,lmax	15,17,25	15,17,25
Nref	7290	6296
Tmin,Tmax	0.488,0.886	0.734,1.000
Tmin'	0.464	
Correction method= # Reported T Limits: Tmin=0.734 Tmax=1.000 AbsCorr =		
MULTI-SCAN		
Data completeness= 0.864	Theta(max)= 33.730	
R(reflections)= 0.0351(4548)	wR2(reflections)= 0.1070(6296)	
S = 1.049	Npar= 324	

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 B

[PLAT420_ALERT_2_B](#) D-H Bond Without Acceptor O5 --H5 . Please Check

●Alert level C

[PLAT041_ALERT_1_C](#) Calc. and Reported SumFormula Strings Differ Please Check
Calc: C H44 Al4 Ca8 Cl2 O37
Rep.: C0.50 H22 Al2 Ca4 Cl O18.50

[PLAT042_ALERT_1_C](#) Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: 2(A12 Ca4 H20 O16), C O3, 2(Cl), 2(H2 O)
Rep.: A12 Ca4 H20 O16, Cl, H2 O, C0.5 O1.5

[PLAT222_ALERT_3_C](#) NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 6.6 Ratio
[PLAT244_ALERT_4_C](#) Low 'Solvent' Ueq as Compared to Neighbors of C Check

PLAT355_ALERT_3_C Long O-H (X0.82,N0.98A) O12 - H12 . 1.03 Ang.
 PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 3.443 Check
 PLAT910_ALERT_3_C Missing FCF Reflection(s) Below Theta(Min)[Deg]= 3.13 Note
 1 0 0, 0 1 0, 1 1 0, -1 1 1, 0 1 1, -1 0 2,
 0 0 2,
 PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
 1 1 1, 1 0 2,

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 38 Note
 PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
 PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 4 Report
 H17A H17B H18A H18B
 PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check
 PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 9 Report
 PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
 PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
 PLAT299_ALERT_4_G Atom Site Occupancy Constrained at 0.5 Check
 H17A H17B H18A H18B
 PLAT417_ALERT_2_G Short Inter D-H..H-D H13B ..H17B . 1.60 Ang.
 x,-y,1/2+z = 4_556 Check
 PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.45 Ratio
 PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 30.60 Deg.
 H17A -O17 -H17A 1_555 1_555 2_655 # 487 Check
 PLAT794_ALERT_5_G Tentative Bond Valency for Al1 (III) . 2.72 Info
 PLAT794_ALERT_5_G Tentative Bond Valency for Al2 (III) . 2.73 Info
 PLAT860_ALERT_3_G Number of Least-Squares Restraints 24 Note
 PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !
 PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 986 Note
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 4.4 Low
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 2.614 Note
 Predicted wR2: Based on SigI**2 4.09 or SHELX Weight 10.20

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **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

6 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
 7 ALERT type 3 Indicator that the structure quality may be low
 6 ALERT type 4 Improvement, methodology, query or suggestion
 5 ALERT type 5 Informative message, check

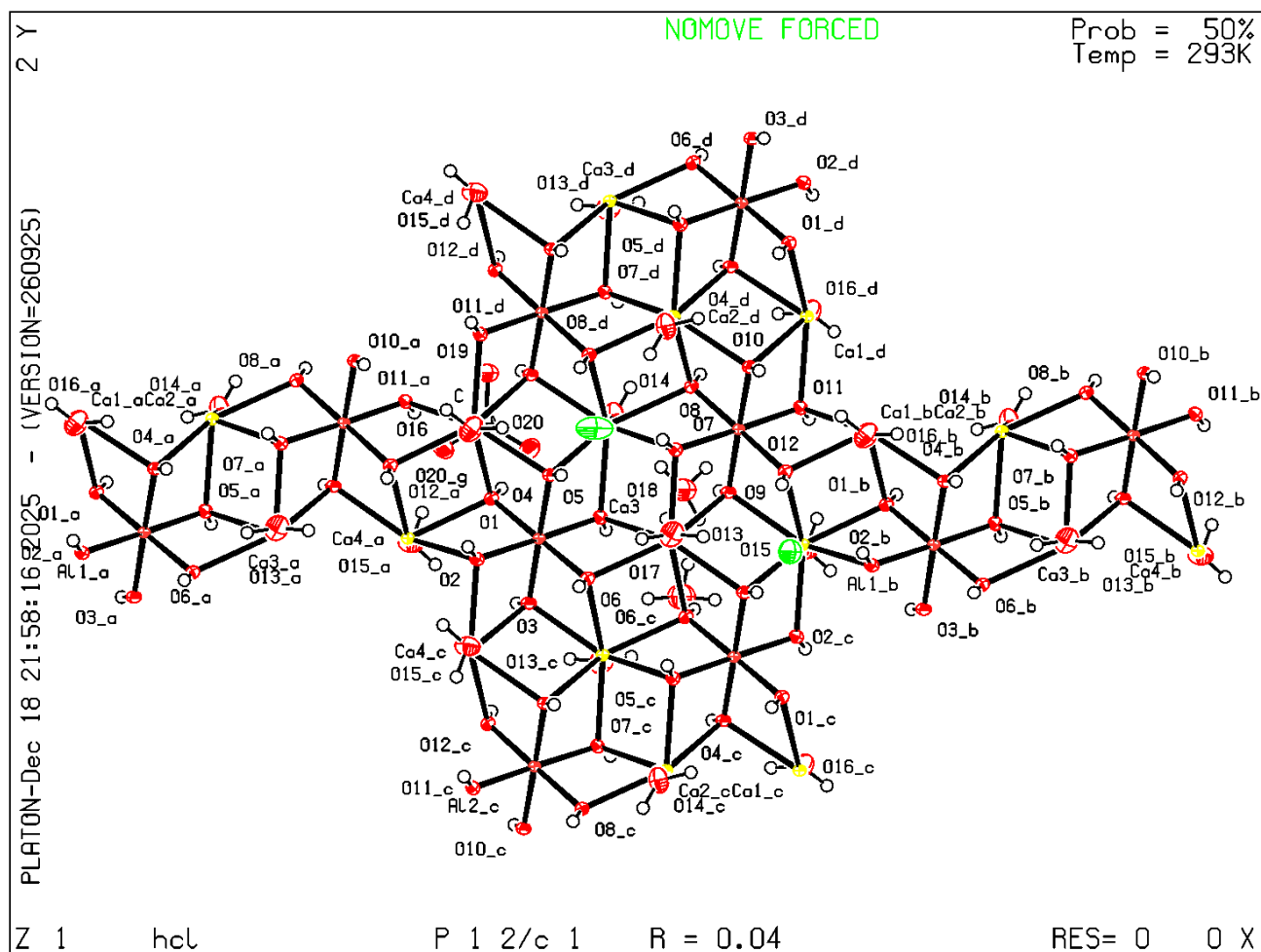
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

PLATON version of 26/09/2025; check.def file version of 20/09/2025

duplicate check

No duplication found

Datablock hcl - ellipsoid plot



Download CIF editor (pubCIF) from the IUCr
 Download CIF editor (enCIFer) from the CCDC
 Test a new CIF entry