

## checkCIF (basic structural check) running

## checkCIF/PLATON (basic structural check)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found.  
Please wait while processing ....

[CIF dictionary](#)  
[Interpreting this report](#)

[Structure factor report](#)

### Datablock: I

Bond precision:	= 0.0000 A	Wavelength=0.71073
Cell:	a=18.12800      b=19.92500      c=11.54200	
	alpha=90      beta=95.9200      gamma=90	
Temperature:	0 K	
	Calculated	Reported
Volume	4146.741	4147
Space group	A a	A 1 a 1
Hall group	A -2ya	?
Moiety formula	As18 Fe18 O84, 18(O), 12(Ca)	?
Sum formula	As18 Ca12 Fe18 O102	Ca2 Fe3 As3 O17
Mr	4466.82	0.00
Dx,g cm-3	3.577	0.000
Z	2	0
Mu (mm-1)	11.073	0.000
F000	4236.0	0.0
F000'	4258.21	
h,k,lmax		
Nref		
Tmin,Tmax		
Tmin'		
Correction method=	Not given	
Data completeness=		Theta(max)=
R(reflections)=		wR2(reflections)=
S =	Npar=	

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 A

[SYMM001\\_ALERT\\_1\\_A](#) \_symmetry\_cell\_setting is missing  
The cell setting should be one of the following

- \* triclinic
- \* monoclinic
- \* orthorhombic
- \* tetragonal
- \* rhombohedral
- \* trigonal
- \* hexagonal
- \* cubic

The following tests will not be performed.  
SYMMS\_01, SYMMS\_02

[EXPT005\\_ALERT\\_1\\_A](#) \_exptl\_crystal\_description is missing  
Crystal habit description.  
The following tests will not be performed.  
CRYSR\_01

[DIFF003\\_ALERT\\_1\\_A](#) \_diffrn\_measurement\_device\_type is missing  
Diffractometer make and type. Replaces \_diffrn\_measurement\_type.

[ATOM007\\_ALERT\\_1\\_A](#) \_atom\_site\_aniso\_label is missing  
Unique label identifying the atom site.

<a href="#">GEOM001_ALERT_1_A</a>	_geom_bond_atom_site_label_1 is missing Label identifying the atom site 1.	
<a href="#">GEOM002_ALERT_1_A</a>	_geom_bond_atom_site_label_2 is missing Label identifying the atom site 2.	
<a href="#">GEOM003_ALERT_1_A</a>	_geom_bond_distance is missing Distance between atom sites 1 and 2.	
<a href="#">GEOM006_ALERT_1_A</a>	_geom_angle_atom_site_label_2 is missing Label identifying the atom site 2.	
<a href="#">GEOM007_ALERT_1_A</a>	_geom_angle_atom_site_label_3 is missing Label identifying the atom site 3.	
<a href="#">PLAT029_ALERT_3_A</a>	_diffn_measured_fraction_theta_full value Low .	0.000 Why?
<a href="#">PLAT043_ALERT_1_A</a>	Calculated and Reported Mol. Weight Differ by ..	4466.82 Check
<a href="#">PLAT129_ALERT_4_A</a>	Unusual Space Group Specified .....	A1a1 Check
<a href="#">PLAT183_ALERT_1_A</a>	Missing _cell_measurement_reflns_used Value ....	Please Do !
<a href="#">PLAT184_ALERT_1_A</a>	Missing _cell_measurement_theta_min Value .....	Please Do !
<a href="#">PLAT185_ALERT_1_A</a>	Missing _cell_measurement_theta_max Value .....	Please Do !
<a href="#">PLAT197_ALERT_1_A</a>	Missing _cell_measurement_temperature Datum ....	Please Add
<a href="#">PLAT198_ALERT_1_A</a>	Missing _diffn_ambient_temperature Datum ....	Please Add
	As1 As2 As3 As4 As5 As6	etc.
<a href="#">PLAT699_ALERT_1_A</a>	Missing _exptl_crystal_description Value .....	Please Do !
<a href="#">PLAT880_ALERT_1_A</a>	N0 datum for _diffn_reflns_number .....	Please Do !
<a href="#">PLAT881_ALERT_1_A</a>	No Datum for _diffn_reflns_av_R_equivalents ...	Please Do !

### Alert level B

<a href="#">PLAT306_ALERT_2_B</a>	Isolated Oxygen Atom (H-atoms Missing ?) .....	043 Check
<b>And 8 other PLAT306 Alerts</b>		
<a href="#">PLAT306_ALERT_2_B</a>	Isolated Oxygen Atom (H-atoms Missing ?) .....	044 Check
<a href="#">PLAT306_ALERT_2_B</a>	Isolated Oxygen Atom (H-atoms Missing ?) .....	045 Check
<a href="#">PLAT306_ALERT_2_B</a>	Isolated Oxygen Atom (H-atoms Missing ?) .....	046 Check
<a href="#">PLAT306_ALERT_2_B</a>	Isolated Oxygen Atom (H-atoms Missing ?) .....	047 Check
<a href="#">PLAT306_ALERT_2_B</a>	Isolated Oxygen Atom (H-atoms Missing ?) .....	048 Check
<a href="#">PLAT306_ALERT_2_B</a>	Isolated Oxygen Atom (H-atoms Missing ?) .....	049 Check
<a href="#">PLAT306_ALERT_2_B</a>	Isolated Oxygen Atom (H-atoms Missing ?) .....	050 Check
<a href="#">PLAT306_ALERT_2_B</a>	Isolated Oxygen Atom (H-atoms Missing ?) .....	051 Check

### Alert level C

<a href="#">PLAT034_ALERT_1_C</a>	No Flack Parameter Given. Z > Si, NonCentro ....	Please Do !
<a href="#">PLAT141_ALERT_4_C</a>	s.u. on a - Axis Small or Missing .....	0.00000 Ang.
<a href="#">PLAT142_ALERT_4_C</a>	s.u. on b - Axis Small or Missing .....	0.00000 Ang.
<a href="#">PLAT143_ALERT_4_C</a>	s.u. on c - Axis Small or Missing .....	0.00000 Ang.
<a href="#">PLAT145_ALERT_4_C</a>	s.u. on beta Small or Missing .....	0.0000 Degree
<a href="#">PLAT151_ALERT_1_C</a>	No s.u. (esd) Given on Volume .....	Please Do !
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	CA1 Check
<b>And 74 other PLAT161 Alerts</b>		

<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	CA2 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	CA3 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	CA4 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	CA5 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	CA6 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	FE1 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	FE2 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	FE3 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	FE4 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	FE5 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	FE6 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	FE7 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	FE8 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	FE9 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	AS1 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	AS2 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	AS3 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	AS4 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	AS5 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	AS6 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	AS7 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	AS8 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	AS9 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	01 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	02 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	03 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	04 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	05 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	06 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	07 Check
<a href="#">PLAT161_ALERT_4_C</a>	Missing or Zero s.u. (esd) on x-coordinate for .	08 Check







<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	09	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	010	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	011	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	012	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	013	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	014	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	015	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	016	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	017	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	018	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	019	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	020	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	021	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	022	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	023	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	024	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	025	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	026	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	027	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	028	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	029	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	030	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	031	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	032	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	033	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	034	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	035	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	036	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	037	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	038	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	039	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	040	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	041	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	042	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	043	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	044	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	045	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	046	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	047	Check			
<a href="#">PLAT163_ALERT_4_C</a>	Missing or Zero s.u. (esd) on z-coordinate for .	048	Check			
<a href="#">PLAT202_ALERT_3_C</a>	Isotropic non-H Atoms in Anion/Solvent .....	15	Check			
043	044	045	046	047	048	etc.

### Alert level G

<a href="#">PLAT004_ALERT_5_G</a>	Polymeric Structure Found with Maximum Dimension	2	Info
<a href="#">PLAT005_ALERT_5_G</a>	No Embedded Refinement Details Found in the CIF	Please	Do !
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 01 as	02	
<b>And 39 other PLAT017 Alerts</b>			
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 03 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 04 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 05 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 06 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 07 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 08 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 09 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 010 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 011 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 012 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 013 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 014 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 015 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 016 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 017 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 018 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 019 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 030 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 031 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 032 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 033 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 034 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 035 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 036 as	02	
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 037 as	02	

<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 038	as	02
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 039	as	02
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 040	as	02
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 041	as	02
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 042	as	02
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 043	as	02
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 044	as	02
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 045	as	02
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 046	as	02
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 047	as	02
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 048	as	02
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 049	as	02
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 050	as	02
<a href="#">PLAT017_ALERT_1_G</a>	Check Scattering Type Consistency of 051	as	02
<a href="#">PLAT045_ALERT_1_G</a>	Calculated and Reported Z Differ by a Factor ...	0.00	Check
<a href="#">PLAT104_ALERT_1_G</a>	The Reported Crystal System is Inconsistent with	Aa	Check
<a href="#">PLAT120_ALERT_1_G</a>	Reported Ala1 Inconsistent with Explicit	Aa	Check
<a href="#">PLAT128_ALERT_4_G</a>	Alternate Setting for Input Space Group	Aa	Cc Note
<a href="#">PLAT720_ALERT_4_G</a>	Number of Unusual/Non-Standard Labels .....	40	Note
<a href="#">PLAT794_ALERT_5_G</a>	Tentative Bond Valency for Fe1 (III)	.	2.85 Info
<b>And 8 other PLAT794 Alerts</b>			
<a href="#">PLAT794_ALERT_5_G</a>	Tentative Bond Valency for Fe2 (III)	.	2.87 Info
<a href="#">PLAT794_ALERT_5_G</a>	Tentative Bond Valency for Fe3 (III)	.	2.88 Info
<a href="#">PLAT794_ALERT_5_G</a>	Tentative Bond Valency for Fe4 (III)	.	2.90 Info
<a href="#">PLAT794_ALERT_5_G</a>	Tentative Bond Valency for Fe5 (III)	.	2.84 Info
<a href="#">PLAT794_ALERT_5_G</a>	Tentative Bond Valency for Fe6 (III)	.	2.82 Info
<a href="#">PLAT794_ALERT_5_G</a>	Tentative Bond Valency for Fe7 (III)	.	2.84 Info
<a href="#">PLAT794_ALERT_5_G</a>	Tentative Bond Valency for Fe8 (III)	.	2.92 Info
<a href="#">PLAT794_ALERT_5_G</a>	Tentative Bond Valency for Fe9 (III)	.	2.91 Info
<a href="#">PLAT808_ALERT_5_G</a>	No Parseable SHELXL Style Weighting Scheme Found		Please Check
<a href="#">PLAT882_ALERT_1_G</a>	No Datum for _diffrn_reflms_av_unetI/netI .....		Please Do !
<a href="#">PLAT883_ALERT_1_G</a>	No Info/Value for _atom_sites_solution_primary .		Please Do !
<a href="#">PLAT980_ALERT_1_G</a>	No Anomalous Scattering Factors Found in CIF ...		Please Check

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- 20 **ALERT level A** = Most likely a serious problem - resolve or explain  
9 **ALERT level B** = A potentially serious problem, consider carefully  
232 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
60 **ALERT level G** = General information/check it is not something unexpected
- 66 **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  
2 **ALERT type 3** Indicator that the structure quality may be low  
232 **ALERT type 4** Improvement, methodology, query or suggestion  
12 **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

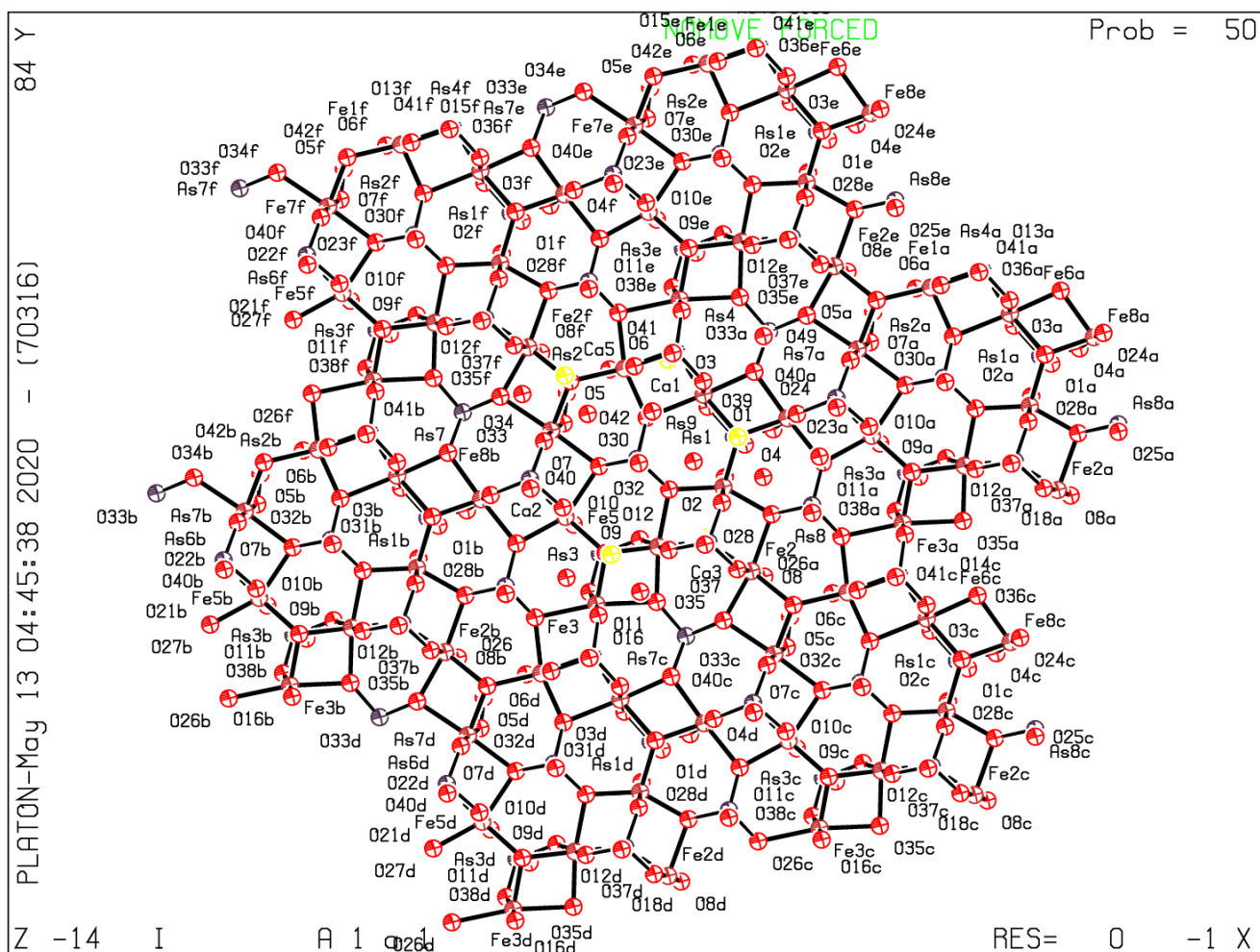
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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.

PLATON version of 22/04/2020; check.def file version of 09/03/2020

## Datablock I - ellipsoid plot



[Download CIF editor \(pubCIF\) from the IUCr](#)  
[Download CIF editor \(enCIFer\) from the CCDC](#)  
[Test a new CIF entry.](#)