
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

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full	value Low	0.978	Why?
PLAT220_ALERT_2_C	NonSolvent	Resd 1 C Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	C5	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.458	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	113	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF	57	Note



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		14	Note
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records		9	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records		6	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used		0.0400	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	N3 --C11	9.1	s.u.
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	N3 --C11A	7.3	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of C9	Constrained at	0.58	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C10	Constrained at	0.58	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16	Constrained at	0.68	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17	Constrained at	0.68	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C9A	Constrained at	0.42	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C10A	Constrained at	0.42	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16A	Constrained at	0.32	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17A	Constrained at	0.32	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9A	Constrained at	0.58	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9B	Constrained at	0.58	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10A	Constrained at	0.58	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10B	Constrained at	0.58	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10C	Constrained at	0.58	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16A	Constrained at	0.68	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16B	Constrained at	0.68	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17A	Constrained at	0.68	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17B	Constrained at	0.68	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17C	Constrained at	0.68	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9AA	Constrained at	0.42	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9AB	Constrained at	0.42	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10D	Constrained at	0.42	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10E	Constrained at	0.42	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10F	Constrained at	0.42	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16C	Constrained at	0.32	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16D	Constrained at	0.32	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17D	Constrained at	0.32	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17E	Constrained at	0.32	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17F	Constrained at	0.32	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	17%	Note
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn	H19C ..H16D	2.07	Ang.
		x, y, z =	1_555	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn	H6C ..H12D	2.13	Ang.
		1/2-x, 1/2+y, 1/2-z =	2_555	Check

PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	2	Note
PLAT793_ALERT_4_G	Model has Chirality at P1 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at P2 (Centro SPGR)	R	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	27	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	4	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	1827	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.5	Low
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	4	Units
PLAT958_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Lmax Differ.	4	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	4	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 50 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 8 ALERT type 2 Indicator that the structure model may be wrong or deficient
 11 ALERT type 3 Indicator that the structure quality may be low
 34 ALERT type 4 Improvement, methodology, query or suggestion
 1 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 28/11/2022; check.def file version of 28/11/2022

Datablock msb_sr_419 - ellipsoid plot

