
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

CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.

yellowish

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.

PLAT213_ALERT_2_C	Atom O13	has ADP max/min Ratio	3.8	prolat
PLAT220_ALERT_2_C	NonSolvent	Resd 1 O	Ueq(max)/Ueq(min) Range	6.0	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1 H	Uiso(max)/Uiso(min) Range	9.4	Ratio
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Tb01	Check
PLAT245_ALERT_2_C	U(iso) H1A	Smaller than U(eq) O20	by	0.018	Ang**2
PLAT245_ALERT_2_C	U(iso) H1B	Smaller than U(eq) O20	by	0.018	Ang**2
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.84Ang From O20	.	1.18	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.97Ang From O20	.	0.64	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	1.07Ang From O13	.	0.42	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.44Ang From O13	.	-0.53	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens.	0.67Ang From O13	.	-0.53	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density	on H1B	.	-0.33	eA-3



Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	5	Report
PLAT128_ALERT_4_G	Alternate Setting for Input Space Group	C2/c	I2/a	Note
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Tb01 --O2	13.4	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of O19	Constrained at	0.7	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O18	Constrained at	0.3	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19A	Constrained at	0.7	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18A	Constrained at	0.3	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	2%	Note
PLAT303_ALERT_2_G	Full Occupancy Atom H100	with # Connections	2.00	Check
PLAT416_ALERT_2_G	Short Intra D-H..H-D	H1 ..H1C	0.98	Ang.
		x,y,z =	1_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O5 ..C2	2.96	Ang.
		3/2-x,1/2-y,1-z =	7_656	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O9 ..C29	2.96	Ang.
		3/2-x,-1/2+y,3/2-z =	4_646	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure		179	A**3
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	1	Note
PLAT767_ALERT_4_G	INS Embedded LIST 6 Instruction Should be LIST 4			Please Check
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE	Suppressed	!	Info
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).		2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	18	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.8	Low
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities		Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		8	Info

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

0 **ALERT level B** = A potentially serious problem, consider carefully

14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
24 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
17 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
12 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

