
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

PLAT431_ALERT_2_A	Short Inter HL..A Contact	Br3	..Sel	.	3.05 Ang.
			x,y,z =		1_555 Check

Alert level B

PLAT434_ALERT_2_B	Short Inter HL..HL Contact	Br1	..Br3	.	3.24 Ang.
			x,y,-1+z =		1_554 Check
PLAT434_ALERT_2_B	Short Inter HL..HL Contact	Br2	..Br2	.	3.23 Ang.
			1-y,1-x,1-z =		8_666 Check
PLAT434_ALERT_2_B	Short Inter HL..HL Contact	Br3	..Br4	.	3.13 Ang.
			x,y,z =		1_555 Check
PLAT434_ALERT_2_B	Short Inter HL..HL Contact	Br3	..Br4	.	3.13 Ang.
			3/2-y,x,z =		3_655 Check
PLAT434_ALERT_2_B	Short Inter HL..HL Contact	Br3	..Br4	.	3.13 Ang.
			y,3/2-x,z =		4_565 Check
PLAT434_ALERT_2_B	Short Inter HL..HL Contact	Br3	..Br4	.	3.13 Ang.
			3/2-x,3/2-y,z =		2_665 Check

Alert level C

PLAT350_ALERT_3_C	Short C-H (X0.96,N1.08A)	C1	- H2	.	0.83 Ang.
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N1	--H1A	.	Please Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N1	--H1B	.	Please Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			3.791 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600			2 Report

Alert level G

PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.				1 Note
PLAT168_ALERT_4_G	The CIF-Embedded .res File Contains EXYZ Records				2 Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records				2 Report
PLAT300_ALERT_4_G	Atom Site Occupancy of N1	Constrained at			0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2	Constrained at			0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1A	Constrained at			0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1B	Constrained at			0.5 Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)			50% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 4)			0.12 Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...				0.00 Deg.
	H1A -C2 -H1B	1_555 1_555 1_555	#		9 Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary				Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600			1 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF				2 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File				2 Note
PLAT961_ALERT_5_G	Dataset Contains no Negative Intensities				Please Check
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged				Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				0 Info

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

6 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
17 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 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
10 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.

