
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	O2SA	--H2SA	.	Please Check
PLAT971_ALERT_2_B	Check Calcd Resid. Dens.	0.89A	From Er1		2.98 eA-3



Alert level C

PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor				2.1 Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600			87 Report
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.79A	From Er1		-1.81 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.72A	From Er1		-1.79 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.58A	From Er1		-1.72 eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on		Er1		1.07 eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.46A	From O3SA		1.21 eA-3



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite				15 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...				15 Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms				5 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large				6.93 Why ?
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)				0.002 Degree
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records				1 Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records				3 Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records				2 Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records				2 Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Er1	--Cl1	.	5.8 s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of O1SA		Constrained at		0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1SA		Constrained at		0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2SA		Constrained at		0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1S1		Constrained at		0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1S2		Constrained at		0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2S1		Constrained at		0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2S2		Constrained at		0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2S3		Constrained at		0.8 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2SA		Constrained at		0.6 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3SA		Constrained at		0.6 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4SA		Constrained at		0.6 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2SA		Constrained at		0.6 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3S1		Constrained at		0.6 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3S2		Constrained at		0.6 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4S1		Constrained at		0.6 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4S2		Constrained at		0.6 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4S3		Constrained at		0.6 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1SB		Constrained at		0.2 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1SB		Constrained at		0.2 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2SB		Constrained at		0.2 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1SB		Constrained at		0.2 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1S3		Constrained at		0.2 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1S4		Constrained at		0.2 Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H2S4	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2S5	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2S6	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2SB	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3SB	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4SB	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2SB	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3S3	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3S4	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4S4	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4S5	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4S6	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O3SA	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C5SA	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C6SA	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3SA	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5S1	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5S2	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6S1	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6S2	Constrained at	0.2	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6S3	Constrained at	0.2	Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)		100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 6)		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)		7.20	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 3)		5.40	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 4)		1.80	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 5)		1.80	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 6)		1.80	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H20 ..H4S5 .		2.09	Ang.
		x,y,z =	1_555	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H25C ..H2S5 .		2.12	Ang.
		-1+x,y,z =	1_455	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact O3 ..C4SB		2.61	Ang.
		1+x,1+y,z =	1_665	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C1 ..C4SB		2.91	Ang.
		1+x,1+y,z =	1_665	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		45	Note
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		9	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		170	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		1704	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		21	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		2.1	Low
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.		1	Info

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

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

19 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
62 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.

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