
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

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	S2	--C13	.	7.9 s.u.
PLAT230_ALERT_2_B	Hirshfeld Test Diff for	O7	--C58	.	18.9 s.u.
PLAT234_ALERT_4_B	Large Hirshfeld Difference	O1	--C66	.	0.30 Ang.
PLAT234_ALERT_4_B	Large Hirshfeld Difference	O6	--C62	.	0.28 Ang.
PLAT342_ALERT_3_B	Low Bond Precision on	C-C Bonds		0.03034 Ang.

Alert level C

PLAT213_ALERT_2_C	Atom C15	has ADP max/min Ratio	3.2	prolat
PLAT213_ALERT_2_C	Atom C16	has ADP max/min Ratio	3.6	prolat
PLAT213_ALERT_2_C	Atom C63	has ADP max/min Ratio	3.4	prolat
PLAT220_ALERT_2_C	NonSolvent	Resd 1 C	Ueq(max)/Ueq(min) Range	4.8	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 2 C	Ueq(max)/Ueq(min) Range	3.9	Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference	O4	--C14	.	0.24 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C14	--C16	.	0.22 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C48	--C49	.	0.21 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C62	--C64	.	0.24 Ang.
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	S1	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	O4	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C66	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	S3	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	S4	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	O7	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C62	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Au1	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Au2	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Au3	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	Au4	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C58	Check
PLAT309_ALERT_2_C	Single Bonded Oxygen	(C-O > 1.3 Ang)	O3	Check
PLAT361_ALERT_2_C	Long	C(sp3)-C(sp3) Bond	C66 - C68	.	1.66 Ang.
PLAT361_ALERT_2_C	Long	C(sp3)-C(sp3) Bond	C58 - C60	.	1.68 Ang.
PLAT361_ALERT_2_C	Long	C(sp3)-C(sp3) Bond	C62 - C64	.	1.71 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		10.645	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.776	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		25	Report

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	11	Note
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	443.78	Why ?
PLAT112_ALERT_2_G	ADDSYM Detects New (Pseudo) Symm. Elem	sub	88 %Fit
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	5	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	7	Report
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O4	136.7	Degree
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	7	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed	!	Info
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	15 Note

PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	6	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.7	Low

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

1	ALERT type 1	CIF construction/syntax error, inconsistent or missing data
28	ALERT type 2	Indicator that the structure model may be wrong or deficient
6	ALERT type 3	Indicator that the structure quality may be low
10	ALERT type 4	Improvement, methodology, query or suggestion
0	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.

