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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.

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#### Alert level B

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	O1	--C11	.	10.1 s.u.
PLAT340_ALERT_3_B	Low Bond Precision on	C-C Bonds	.....		0.01067 Ang.

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#### Alert level C

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	48%	Check
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25) .....	0.26	Report
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C1	--C2 .
PLAT234_ALERT_4_C	Large Hirshfeld Difference S1A	--C6	. 0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C6	--C7	. 0.16 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	O1	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	O2	Check
PLAT245_ALERT_2_C	U(iso) H3	Smaller than U(eq) O3	by 0.027 Ang**2
PLAT355_ALERT_3_C	Long O-H (X0.82,N0.98A) O3	- H3	. 1.03 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.268	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).	5	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	9 Report

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#### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	5	Note
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF .....	Please	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.11	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	5	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of S1	Constrained at	0.75 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of S1A	Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C7	Constrained at	0.75 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C7A	Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7	Constrained at	0.75 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8A	Constrained at	0.75 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9A	Constrained at	0.75 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7A	Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8B	Constrained at	0.25 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9B	Constrained at	0.25 Check
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1 )	13% Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	5	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	1 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3	Note
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	2	Units
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0	Info

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

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

12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

21 **ALERT level G** = General information/check it is not something unexpected

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

9 ALERT type 2 Indicator that the structure model may be wrong or deficient  
9 ALERT type 3 Indicator that the structure quality may be low  
15 ALERT type 4 Improvement, methodology, query or suggestion  
1 ALERT type 5 Informative message, check

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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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**PLATON version of 06/07/2023; check.def file version of 30/06/2023**

