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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**

PLAT220_ALERT_2_B	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min)	Range	7.4	Ratio
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 **Alert level C**

PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min)	Range	7.1	Ratio
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of			Mol	Check
PLAT260_ALERT_2_C	Large Average	Ueq of Residue Including		C11		0.153	Check
PLAT260_ALERT_2_C	Large Average	Ueq of Residue Including		C11C		0.153	Check
PLAT303_ALERT_2_C	Full Occupancy	Atom H19B	with #	Connections		1.20	Check
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds	.....			0.0083	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	.....				2.450	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600				9	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.45A	From	Mol		2.12	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.30A	From	Mol		2.00	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.36A	From	Mol		1.96	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.33A	From	C11C		1.84	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.56A	From	C12C		-1.67	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.53A	From	C12C		-1.67	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.67A	From	C11C		-1.57	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.07A	From	C11B		-1.54	eA-3

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 **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite					9	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...					9	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension					2	Info
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ					Please	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large					25.51	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records					1	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records					2	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records					1	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C11B	--O3_b	.		15.5	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Mol	--S5	.		11.6	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Mol	--C22	.		6.7	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Mol	--C23	.		7.2	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Mol	--C24	.		7.0	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder	.....(Resd 1 )				1%	Note
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
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond	C14	-	C19	.	1.50	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	O4	..C27C			2.15	Ang.
			-x,1-y,-z =			5_565	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C25	..C27C			2.40	Ang.
			-x,1-y,-z =			5_565	Check
PLAT780_ALERT_1_G	Coordinates do not Form a Properly Connected Set					Please	Do !
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #					15	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	.....				64	Note
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).					4	Note

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=	0.600	63	Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...		6	Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity .....		4.9	Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		1	Info

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 26 ALERT type 2 Indicator that the structure model may be wrong or deficient  
 8 ALERT type 3 Indicator that the structure quality may be low  
 7 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 13/07/2021; check.def file version of 13/07/2021**

