

```
R(reflections)= 0.1288( 3708)      wR2(reflections)=
S = 1.824                        0.3838( 3986)
Npar= 203
```

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

PLAT029_ALERT_3_A	_diffn_measured_fraction_theta_full	value Low	0.937	Why?
PLAT934_ALERT_3_A	Number of (Iobs-Icalc)/Sigma(W)	> 10 Outliers	11	Check
PLAT971_ALERT_2_A	Check Calcd Resid. Dens.	1.08Ang From I1	8.11	eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens.	1.06Ang From I1	7.57	eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens.	1.12Ang From I3	7.24	eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens.	1.13Ang From I4	6.90	eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens.	1.04Ang From I3	6.52	eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens.	1.11Ang From I2	6.47	eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens.	1.17Ang From I4	6.39	eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens.	1.05Ang From I2	6.36	eA-3
PLAT971_ALERT_2_A	Check Calcd Resid. Dens.	2.50Ang From C5	4.10	eA-3

Alert level B

SHFSU01_ALERT_2_B	The absolute value of parameter shift to su ratio > 0.10			
	Absolute value of the parameter shift to su ratio given			0.199
Additional refinement cycles may be required.				
PLAT080_ALERT_2_B	Maximum Shift/Error		0.20	Why ?
PLAT084_ALERT_3_B	High wR2 Value (i.e. > 0.25)		0.38	Report
PLAT097_ALERT_2_B	Large Reported Max. (Positive) Residual Density		7.14	eA-3
PLAT972_ALERT_2_B	Check Calcd Resid. Dens.	0.74Ang From I1	-3.41	eA-3
PLAT972_ALERT_2_B	Check Calcd Resid. Dens.	0.67Ang From I4	-3.21	eA-3
PLAT972_ALERT_2_B	Check Calcd Resid. Dens.	0.74Ang From I4	-3.04	eA-3
PLAT972_ALERT_2_B	Check Calcd Resid. Dens.	0.66Ang From I4	-2.97	eA-3
PLAT972_ALERT_2_B	Check Calcd Resid. Dens.	0.75Ang From I3	-2.92	eA-3
PLAT972_ALERT_2_B	Check Calcd Resid. Dens.	0.73Ang From I2	-2.68	eA-3
PLAT972_ALERT_2_B	Check Calcd Resid. Dens.	0.70Ang From I3	-2.51	eA-3
PLAT972_ALERT_2_B	Check Calcd Resid. Dens.	1.30Ang From I2	-2.51	eA-3

Alert level C

DIFMX02_ALERT_1_C	The maximum difference density is > 0.1*ZMAX*0.75			
The relevant atom site should be identified.				
PLAT082_ALERT_2_C	High R1 Value		0.13	Report
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density		2.26	Report
PLAT234_ALERT_4_C	Large Hirshfeld Difference C8	--C9	0.16	Ang.
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds		0.02	Ang.
PLAT412_ALERT_2_C	Short Intra XH3 .. XHn	H2 ..H7A	1.87	Ang.
		x,y,z =	1_555	Check
PLAT413_ALERT_2_C	Short Inter XH3 .. XHn	H7B ..H13C	2.14	Ang.
		1-x,1-y,1-z =	2_666	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		13.100	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600	238	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	1.42Ang From N3	1.74	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	2.14Ang From C13	1.55	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.72Ang From I1	-2.39	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.96Ang From I1	-2.38	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.88Ang From C8	-2.21	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.93Ang From I4	-2.14	eA-3

PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.66Ang From I3	-2.09 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.05Ang From I1	-2.06 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.17Ang From I4	-2.05 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.70Ang From I4	-2.00 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.84Ang From N3	-1.97 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.64Ang From I1	-1.96 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.92Ang From I1	-1.88 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.75Ang From N3	-1.81 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.97Ang From C5	-1.76 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.91Ang From C5	-1.67 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.32Ang From C5	-1.67 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.61Ang From I3	-1.64 eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	1.34Ang From C7	-1.62 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H4	.	-1.12 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H8	.	-1.33 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H11	.	-0.55 eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H12	.	-0.64 eA-3

● Alert level G

PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.20 Report
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	458 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.2 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 Info

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- 11 **ALERT level A** = Most likely a serious problem - resolve or explain
 - 12 **ALERT level B** = A potentially serious problem, consider carefully
 - 32 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 - 5 **ALERT level G** = General information/check it is not something unexpected
-
- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 49 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
 - 2 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.

