

```
R(reflections)= 0.0328( 1738)      wR2(reflections)=
S = 1.074                          0.0906( 2057)
Npar= 200
```

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 G

PLAT242_ALERT_2_G	Low	'MainMol' Ueq as Compared to Neighbors of	C12	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F1A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F1B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F2A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F2B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F3	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of F4	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	19%	Note
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond	C11 - C12	1.51	Ang.
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd)	.	1.36	Ratio
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		15.00	Deg.
	C13 -C12 -C13	2_556 1_555 1_555	# 34	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		42.00	Deg.
	F3 -C13 -F3	2_556 1_555 1_555	# 40	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		32.00	Deg.
	C13 -C13 -F4	2_556 1_555 2_556	# 53	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		19.70	Deg.
	C13 -F3 -C13	2_556 1_555 1_555	# 61	Check
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		9.80	Deg.
	C13 -F4 -C13	1_555 1_555 2_556	# 67	Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary	.		Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still		63%	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		10	Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
13 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.

