

```
R(reflections)= 0.0449( 2144)      wR2(reflections)=
S = 1.071                          0.1339( 3120)
Npar= 183
```

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 C

PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	01	Check
PLAT241_ALERT_2_C	High	'MainMol' Ueq as Compared to Neighbors of	C11	Check
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...		-0.695	Report



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	5%	Note

Author Response: In the final cycles of refinement, one peak which was significantly larger (ca. 2 eA*3) was refined as a minor component of disorder from Mo1. This may be attributed to whole molecule disorder where only the minor component related to the Mo atom can be identified as the contribution is so small. This refinement works well and prevent the presence of an A-alert.

PLAT303_ALERT_2_G	Full Occupancy Atom H11A	with # Connections	1.03	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond	C11 - C12	1.53	Ang.
PLAT398_ALERT_2_G	Deviating C-O-C	Angle From 120 for O2	106.7	Degree
PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle(s) in CIF ...		25.40	Deg.
	MO1A -C11 -H11A	1_555 1_555 1_555	# 63	Check
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		2	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

start Validation Reply Form

_vrf_PLAT241_k1044

;

PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of 01 Check

RESPONSE: ...

;

_vrf_PLAT905_k1044

;

PROBLEM: Negative K value in the Analysis of Variance ... -0.695 Report

RESPONSE: ...

;

end Validation Reply Form

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.

PLATON version of 18/12/2021; check.def file version of 18/12/2021

