

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) jr281

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: jr281

Bond precision: C-C = 0.0042 Å Wavelength=1.54184

Cell: a=13.1076(5) b=13.8460(5) c=14.7792(5)
 alpha=100.865(3) beta=90.278(3) gamma=108.118(3)
Temperature: 150 K

	Calculated	Reported
Volume	2497.76(17)	2497.76(16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C47 H32 Cr N6 O, 3(C F3 O3 S), C2 H3 N	C47 H32 Cr N6 O, 3(C F3 O3 S), C2 H3 N
Sum formula	C52 H35 Cr F9 N7 O10 S3	C52 H35 Cr F9 N7 O10 S3
Mr	1237.05	1237.05
Dx, g cm ⁻³	1.645	1.645
Z	2	2
Mu (mm ⁻¹)	3.975	3.975
F000	1258.0	1258.0
F000'	1264.13	
h,k,lmax	16,16,18	15,16,18
Nref	9562	9338
Tmin,Tmax	0.294,0.521	0.324,1.000
Tmin'	0.109	

Correction method= # Reported T Limits: Tmin=0.324 Tmax=1.000
AbsCorr = GAUSSIAN

Data completeness= 0.977 Theta(max)= 70.573

R(reflections)= 0.0500(8986) wR2(reflections)= 0.1283(9338)

S = 1.041 Npar= 742

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

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.38	Report
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	1.85	eA-3
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	S3	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	23	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.10A From S2	1.87	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.89A From O8	0.47	eA-3



Alert level G

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.003	Degree
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) S1 --C49 .	5.1	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) S2 --O4 .	5.8	s.u.
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	C49	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	C51	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	C50	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C5 ..C5	3.18	Ang.
	1-x,2-y,-z =	2_675	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Cr1 (III) .	3.07	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	198	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.0	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	3	Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 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
7 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

