

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) jr272

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: jr272

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Bond precision:    C-C = 0.0034 Å                      Wavelength=1.54184

Cell:                      a=17.10349(6)              b=17.98863(8)              c=28.79512(12)  
                            alpha=90                      beta=90                      gamma=90  
Temperature:              150 K

	Calculated	Reported
Volume	8859.35(6)	8859.35(6)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C38 H26 Cr N6, 0.174(C F3 O3 S), 2.826(F6 P), 2(C2 H3 N)	C38 H26 Cr N6, 2.826(F6 P), 0.174(C F3 O3 S), 2(C2 H3 N)
Sum formula	C42.17 H32 Cr F17.48 N8 O0.52 P2.83 S0.17	C42.17 H32 Cr F17.48 N8 O0.52 P2.83 S0.17
Mr	1136.38	1136.37
Dx,g cm-3	1.704	1.704
Z	8	8
Mu (mm-1)	4.261	4.261
F000	4573.6	4574.0
F000'	4597.27	
h,k,lmax	21,22,35	21,22,35
Nref	9053	8997
Tmin,Tmax	0.332,0.447	0.180,1.000
Tmin'	0.223	

Correction method= # Reported T Limits: Tmin=0.180 Tmax=1.000  
AbsCorr = GAUSSIAN

Data completeness= 0.994                      Theta(max)= 74.427

R(reflections)= 0.0452( 8817)              wR2(reflections)= 0.1206( 8997)

S = 1.040                      Npar= 712

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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 C

PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density ....	2.13 Report
PLAT244_ALERT_4_C	Low Solvent Ueq as Compared to Neighbors of	C40 Check
PLAT244_ALERT_4_C	Low Solvent Ueq as Compared to Neighbors of	C43 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance .....	2.024 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	4 Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.82A From P1	1.79 eA-3

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### ● Alert level G

CELLZ01\_ALERT\_1\_G Difference between formula and atom\_site contents detected.

CELLZ01\_ALERT\_1\_G ALERT: check formula stoichiometry or atom site occupancies.

From the CIF: \_cell\_formula\_units\_Z 8

From the CIF: \_chemical\_formula\_sum C42.17 H32 Cr F17.48 N8 O0.52 P2.8

TEST: Compare cell contents of formula and atom\_site data

atom	Z*formula	cif sites	diff
C	337.36	337.39	-0.03
H	256.00	256.00	0.00
Cr	8.00	8.00	0.00
F	139.84	139.82	0.02
N	64.00	64.00	0.00
O	4.16	4.18	-0.02
P	22.64	22.61	0.03
S	1.36	1.39	-0.03

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	15 Note
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	12.01 Why ?
PLAT142_ALERT_4_G	s.u. on b - Axis Small or Missing .....	0.00008 Ang.
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing .....	0.00012 Ang.
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2 Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3 Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2 Report
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) P2 --F10	5.1 s.u.
PLAT244_ALERT_4_G	Low Solvent Ueq as Compared to Neighbors of	P1 Check
PLAT244_ALERT_4_G	Low Solvent Ueq as Compared to Neighbors of	P2 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5 )	100% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 2 )	1.39 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 5 )	5.78 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F12 ..C23	2.97 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F18 ..C30	2.73 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F20 ..C22	2.39 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F20 ..C23	2.85 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F21 ..C21	2.70 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact F21 ..C22	2.84 Ang.
	x,y,z =	1_555 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C22 ..C41	3.02 Ang.

	x,y,z =	1_555	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F7 ..F21	2.77	Ang.
	1/2+x,y,3/2-z =	6_657	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Cr1 (III)	3.15	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	137	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	52	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2	Info

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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  
 30 **ALERT level G** = General information/check it is not something unexpected

4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 13 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  
 16 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.

