

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) jr286\_2

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: jr286\_2

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Bond precision:	C-C = 0.0049 A	Wavelength=1.54184
Cell:	a=21.14124(15)	b=22.83951(17)      c=20.55852(15)
	alpha=90	beta=90.3997(7)      gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	9926.55(13)	9926.55(12)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C40 H32 Cr N8, 3(F6 P), 2(C2 H3 N)	C40 H32 Cr N8, 3(F6 P), 2(C2 H3 N)
Sum formula	C44 H38 Cr F18 N10 P3	C44 H38 Cr F18 N10 P3
Mr	1193.75	1193.75
Dx,g cm-3	1.598	1.598
Z	8	8
Mu (mm-1)	3.837	3.837
F000	4824.0	4824.0
F000'	4848.40	
h,k,lmax	26,28,25	25,27,24
Nref	20103	18950
Tmin,Tmax	0.204,0.868	0.119,1.000
Tmin'	0.069	

Correction method= # Reported T Limits: Tmin=0.119 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.943      Theta(max)= 73.785

R(reflections)= 0.0542( 15427)      wR2(reflections)= 0.1579( 18950)

S = 1.065      Npar= 1377

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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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<b>Alert level C</b>				
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C38 Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	C2S Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	C5S Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	C8S Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	C11S Check
PLAT250_ALERT_2_C	Large	U3/U1 Ratio for Average U(i,j) Tensor	....	2.2 Note
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	N3S	0.124 Check
PLAT260_ALERT_2_C	Large	Average Ueq of Residue Including	N10S	0.124 Check
PLAT911_ALERT_3_C	Missing	FCF Refl Between Thmin & STh/L=	0.600	54 Report

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<b>Alert level G</b>				
PLAT063_ALERT_4_G	Crystal Size Possibly too Large for Beam Size	..	0.64 mm	
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large	7.40	Why ?
PLAT142_ALERT_4_G	s.u. on b - Axis Small or Missing	.....	0.00017	Ang.
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing	.....	0.00015	Ang.
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
PLAT244_ALERT_4_G	Low	'Solvent'	Ueq as Compared to Neighbors of	P3 Check
PLAT244_ALERT_4_G	Low	'Solvent'	Ueq as Compared to Neighbors of	P4 Check
PLAT244_ALERT_4_G	Low	'Solvent'	Ueq as Compared to Neighbors of	P5 Check
PLAT244_ALERT_4_G	Low	'Solvent'	Ueq as Compared to Neighbors of	P6 Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C21 ..C21B	3.07	Ang.
		1-x,1-y,1-z =	3_666	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	.....	9	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Cr1	(III)	3.18	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Cr1B	(III)	3.14	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	984	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	.....	4.6	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		0	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  
 9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 17 **ALERT level G** = General information/check it is not something unexpected

0 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  
 2 ALERT type 3 Indicator that the structure quality may be low  
 15 ALERT type 4 Improvement, methodology, query or suggestion  
 2 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.

