

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3HoCr

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: 3HoCr

---

Bond precision:	C-C = 0.0030 A	Wavelength=0.71073
Cell:	a=12.8518(7)	b=12.8157(7)      c=17.2114(10)
	alpha=90	beta=103.557(6)      gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	2755.8(3)	2755.8(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C17 H19 Cr Ho N13 O4, 3(H2 O)	C17 H19 Cr Ho N13 O4, 3(H2 O)
Sum formula	C17 H25 Cr Ho N13 O7	C17 H25 Cr Ho N13 O7
Mr	740.43	740.43
Dx, g cm <sup>-3</sup>	1.785	1.785
Z	4	4
Mu (mm <sup>-1</sup> )	3.306	3.306
F000	1460.0	1460.0
F000'	1460.88	
h, k, lmax	19, 19, 26	19, 19, 26
Nref	10273	9216
Tmin, Tmax	0.525, 0.891	0.569, 1.000
Tmin'	0.343	

Correction method= # Reported T Limits: Tmin=0.569 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.897      Theta(max)= 32.863

R(reflections)= 0.0233( 8479)	wR2(reflections)= 0.0575( 9216)
S = 1.008	Npar= 402

---

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

PLAT220_ALERT_2_C	NonSolvent	Resd 1	N	Ueq(max)/Ueq(min)	Range	3.4	Ratio
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N2	--H2B	.		Please	Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N3	--H3	.		Please	Check
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	N4	--H4	.		Please	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600				4	Report
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.77Ang	From O4	.		0.50	eA-3
PLAT975_ALERT_2_C	Check Calcd Resid. Dens.	0.90Ang	From O1	.		0.48	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density	on H3A	.			-0.31	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density	on H3C	.			-0.35	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density	on H4	.			-0.40	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density	on H11B	.			-0.35	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density	on H11C	.			-0.60	eA-3

---



### Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite					15	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension					1	Info
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records					1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Ho1	--N5	.		7.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Ho1	--N12	.		8.7	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Ho1	--N13	.		6.7	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C12	.		7.6	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C14	.		9.1	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C15	.		9.1	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C16	.		8.4	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C17	.		8.4	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C13_a	.		7.5	s.u.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported	H3	..N14	.		2.64	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported	H4	..N12	.		2.66	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported	H4	..N13	.		2.73	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported	H3B	..O7	.		2.61	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported	H6	..O7	.		2.63	Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported	H8	..O2	.		2.62	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	.....				10	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	.....				45	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600				1053	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File					14	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	.....				2.5	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged					Please	Check
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  
12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
25 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

24 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  
9 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.

---

**PLATON version of 19/02/2022; check.def file version of 19/02/2022**

