

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1DyCr

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: 1DyCr

Bond precision: C-C = 0.0020 Å Wavelength=0.71073

Cell: a=12.84505(12) b=12.79181(10) c=17.18315(16)
 alpha=90 beta=103.3953(9) gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	2746.58(4)	2746.58(4)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C17 H19 Cr Dy N13 O4, 3(H2 O)	C17 H19 Dy Cr N13 O4, 3(H2 O)
Sum formula	C17 H25 Cr Dy N13 O7	C17 H25 Cr Dy N13 O7
Mr	738.00	738.00
Dx, g cm ⁻³	1.785	1.785
Z	4	4
Mu (mm ⁻¹)	3.156	3.156
F000	1456.0	1456.0
F000'	1457.00	
h, k, lmax	19, 19, 26	19, 18, 25
Nref	10287	9358
Tmin, Tmax	0.750, 0.857	0.728, 1.000
Tmin'	0.326	

Correction method= # Reported T Limits: Tmin=0.728 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.910

Theta(max)= 32.923

R(reflections)= 0.0159(8567)

wR2(reflections)=
0.0373(9358)

S = 1.006

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

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
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		2.576	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		7	Report
PLAT977_ALERT_2_C	Check Negative Difference Density on H3A			-0.39	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H11A			-0.31	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H11C			-0.35	eA-3



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite			12	Note
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension			1	Info
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ				Please Check
PLAT142_ALERT_4_G	s.u. on b - Axis Small or Missing		0.00010	Ang.
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing		0.00016	Ang.
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records			1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Dy1	--O1	.	5.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Dy1	--O2	.	6.8 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Dy1	--N5	.	7.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Dy1	--N6	.	6.4 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Dy1	--N12	.	9.6 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Dy1	--N13	.	10.8 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C12	.	11.4 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C14	.	11.7 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C15	.	11.2 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C16	.	12.0 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C17	.	11.8 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Cr1	--C13_a	.	11.2 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	.	2.71 Ang.
PLAT480_ALERT_4_G	Long H...A H-Bond Reported	H4	..N13	.	2.75 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	.	2.61 Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		10	Note
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		28	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).			1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		862	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		1	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File			7	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		3.8	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.			7	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
22 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
11 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

