

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) YS-PD-107-100K

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: YS-PD-107-100K

Bond precision:	C-C = 0.0130 A	Wavelength=0.71073
Cell:	a=20.4123 (4)	b=20.4123 (4) c=32.2304 (8)
	alpha=90	beta=90 gamma=120
Temperature:	153 K	
	Calculated	Reported
Volume	11630.0 (5)	11630.1 (5)
Space group	R -3	R -3 :H
Hall group	-R 3	-R 3
Moiety formula	C144 H114 Cl13 Dy7 N12 Ni6 O30, 2 (Cl)	C144 H114 Cl13 Dy7 N12 Ni6 O30, 2 (Cl)
Sum formula	C144 H114 Cl15 Dy7 N12 Ni6 O30	C144 H114 Cl15 Dy7 N12 Ni6 O30
Mr	4513.85	4513.98
Dx, g cm-3	1.934	1.934
Z	3	3
Mu (mm-1)	4.368	4.368
F000	6561.0	6561.0
F000'	6572.02	
h, k, lmax	24, 24, 38	23, 24, 38
Nref	4568	4561
Tmin, Tmax	0.334, 0.476	0.334, 0.476
Tmin'	0.309	

Correction method= # Reported T Limits: Tmin=0.334 Tmax=0.476

AbsCorr = MULTI-SCAN

Data completeness= 0.998

Theta(max)= 25.011

R(reflections)= 0.0489(4074)

wR2(reflections)=
0.1383(4561)

S = 1.105

Npar= 395

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	C	Ueq(max)/Ueq(min)	Range	4.2	Ratio
PLAT220_ALERT_2_C	NonSolvent	Resd 1	Cl	Ueq(max)/Ueq(min)	Range	4.8	Ratio
PLAT222_ALERT_3_C	NonSolvent	Resd 1	H	Uiso(max)/Uiso(min)	Range	4.9	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O3	--C13	.		6.6	s.u.
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Dy1	--O4_d	.		6.3	s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	Nil	--N1	.		0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	Cl2	--C22	.		0.16	Ang.
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of			C16	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of			O3	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including		Cl4			0.200	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including		Cl4'			0.199	Check
PLAT303_ALERT_2_C	Full Occupancy Atom	H13B	with # Connections			1.13	Check
PLAT336_ALERT_2_C	Long Bond Distance for C22	-Cl2			1.929	Ang.
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds			0.013	Ang.
PLAT420_ALERT_2_C	D-H Bond Without Acceptor	Cl3	--H13B	.		Please	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595				4	Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..					1	Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.53Ang	From Cl2'			1.55	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.11Ang	From Cl3'			1.53	eA-3



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite					16	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...					39	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms					3	Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical					?	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large				281.76	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records					2	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records					7	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records					1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records					5	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records					2	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used					0.0100	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used					0.0100	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used					0.0100	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par					0.0200	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	Cl2'	--C22	.		6.0	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of	Dy2	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	Cl2	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	Cl2'	Constrained at			0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	Cl1	Constrained at			0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	Cl1'	Constrained at			0.3333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	Cl3	Constrained at			0.1333	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	Cl3'	Constrained at			0.1	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	Cl12	Constrained at			0.3333	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of O5	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O5'	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H51	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl4	Constrained at	0.1667	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Cl4'	Constrained at	0.1667	Check
PLAT301_ALERT_3_G	Main Residue Disorder	(Resd 1)	19%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder	(Resd 3)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 2)	0.17	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in	(Resd 3)	0.17	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn	H13A ..H15A	1.98	Ang.
		2/3-x,1/3-y,1/3-z =	13_555	Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn	H13C ..H15A	2.09	Ang.
		2/3-x,1/3-y,1/3-z =	13_555	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C13 ..C15	2.96	Ang.
		2/3-x,1/3-y,1/3-z =	13_555	Check
PLAT480_ALERT_4_G	Long H...A H-Bond Reported	H13C ..CL2	2.90	Ang.
PLAT721_ALERT_1_G	Bond Calc	0.97000, Rep	0.96000	Dev...
	C15 -H15C	1_555 1_555		# 68 Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		322	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary			Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still		75%	Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		3	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		2	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		3.3	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged			Please Check
PLAT967_ALERT_5_G	Note: Two-Theta Cutoff Value in Embedded .res ..		50.0	Degree
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		2	Info

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

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

