

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: MnDy

Bond precision: C-C = 0.0052 Å

Wavelength=0.71073

Cell: a=13.2219(2) b=13.5495(3) c=14.1560(2)
 alpha=71.5364(15) beta=64.2521(15) gamma=81.4352(15)
Temperature: 106 K

	Calculated	Reported
Volume	2166.48(7)	2166.49(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C50 H90 Dy2 Mn2 O22, 2(C6 H16 N), 3(C2 N)	C50 H90 Dy2 Mn2 O22, 2(C6 H16 N), 3(C2 N)
Sum formula	C68 H122 Dy2 Mn2 N5 O22	C68 H122 Dy2 Mn2 N5 O22
Mr	1796.59	1796.58
Dx,g cm-3	1.377	1.377
Z	1	1
Mu (mm-1)	2.055	2.055
F000	923.0	923.0
F000'	923.66	
h,k,lmax	16,16,17	16,16,17
Nref	8855	8838
Tmin,Tmax	0.457,0.540	0.740,1.000
Tmin'	0.423	

Correction method= # Reported T Limits: Tmin=0.740 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998

Theta(max)= 26.372

R(reflections)= 0.0260(8482)

wR2(reflections)= 0.0704(8838)

S = 1.049

Npar= 572

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

PLAT213_ALERT_2_C	Atom C1	has ADP max/min Ratio	3.3	prolat
PLAT214_ALERT_2_C	Atom C32A	(Anion/Solvent) ADP max/min Ratio	4.5	prolat
PLAT220_ALERT_2_C	Large Non-Solvent	C Ueq(max)/Ueq(min) Range	4.0	Ratio
PLAT220_ALERT_2_C	Large Non-Solvent	O Ueq(max)/Ueq(min) Range	3.8	Ratio
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	03	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	09	Check
PLAT241_ALERT_2_C	High	Ueq as Compared to Neighbors for	C1	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	01	Check
PLAT242_ALERT_2_C	Low	Ueq as Compared to Neighbors for	C12	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	3.7	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.7	Note



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite		7	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms	...	18	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms		2	Report
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal		0.00150	Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records		1	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records		3	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records		1	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		1	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	O2A -- C1 ..	11.5	su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C2 -- C4B ..	5.7	su
PLAT230_ALERT_2_G	Hirshfeld Test Diff for	C2 -- C3A ..	6.0	su
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Dy1 -- O4 ..	8.3	su
PLAT300_ALERT_4_G	Atom Site Occupancy of	>O2 is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	<O2A is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	>C3B is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	>C4B is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	>C5B is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	<C3A is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	<C4A is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	<C5A is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	>O2_a is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	<O2A_a is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	>C3B_a is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	>C4B_a is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	>C5B_a is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	<C3A_a is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	<C4A_a is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	<C5A_a is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	>N1B is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	>C26B is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	>C27B is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	>C28B is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	>C29B is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	>C30B is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	>C31B is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	<N1A is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	<C26A is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	<C27A is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	<C28A is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of	<C29A is Constrained at	0.412	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of <C30A	is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C31A	is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >N2B	is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of >C32B	is Constrained at	0.588	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <N2A	is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of <C32A	is Constrained at	0.412	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *N3	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C34	is Constrained at	0.500	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of *C35	is Constrained at	0.500	Check
PLAT301_ALERT_3_G	Main Residue Disorder	Percentage =	11	Note
PLAT302_ALERT_4_G	Anion/Solvent Disorder	Percentage =	91	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (13.52) in Resd. #		2	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (9.48) in Resd. #		3	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms (1.50) in Resd. #		5	Check
PLAT309_ALERT_2_G	Single Bonded Oxygen (C-O > 1.3 Ang)		02	Check
PLAT309_ALERT_2_G	Single Bonded Oxygen (C-O > 1.3 Ang)		02A	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		19	Note
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .		1.15	Ratio
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		44	Note

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 19 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
 48 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*, 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.

