

checkCIF/PLATON report (basic structural check)

No syntax errors found.
Please wait while processing

CIF dictionary
Interpreting this report

Datablock: L618

Bond precision:	C-C = 0.0080 A	Wavelength=0.71073
Cell:	a=13.9237(6) b=14.5196(7) c=25.1289(10)	
	alpha=82.856(3) beta=79.710(3) gamma=65.545(3)	
Temperature: 150 K		
	Calculated	Reported
Volume	4542.9(4)	4542.9(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C62 H124 Dy2 Fe4 N10 O22, 2(C2 H3 N), C2 N	C62 H124 Dy2 Fe4 N10 O22, 3(C2 H3 N)
Sum formula	C68 H130 Dy2 Fe4 N13 O22	C68 H133 Dy2 Fe4 N13 O22
Mr	2030.26	2033.27
Dx, g cm-3	1.484	1.486
Z	2	2
Mu (mm-1)	2.315	2.315
F000	2082.0	2088.0
F000'	2084.74	
h,k,lmax	18,19,33	18,19,33
Nref	21843	21679
Tmin,Tmax	0.481,0.615	0.472,0.610
Tmin'	0.472	
Correction method=	MULTI-SCAN	
Data completeness=	0.992	Theta(max)= 27.950
R(reflections)=	0.0449(17985)	wR2(reflections)= 0.1201(21679)
S =	1.018	Npar= 979

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 B

Crystal system given = triclinic

PLAT201_ALERT_2_B	Isotropic non-H Atoms in Main Residue(s)	1
PLAT220_ALERT_2_B	Large Non-Solvent C Ueq(max)/Ueq(min) ...	4.5 Ratio
PLAT413_ALERT_2_B	Short Inter XH3 .. XHn H57D .. H74A ..	2.07 Ang.

●Alert level C

PLAT041_ALERT_1_C	Calc. and Reported SumFormula Strings Differ	? Check
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...	? Check
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	3
PLAT213_ALERT_2_C	Atom C47 has ADP max/min Ratio	3.4 prola
PLAT222_ALERT_3_C	Large Non-Solvent H Uiso(max)/Uiso(min) ..	6.1 Ratio
PLAT242_ALERT_2_C	Check Low Ueq as Compared to Neighbors for	C34

And 5 other PLAT242 Alerts

More ...

PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C71
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C73

●Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the _chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum: C68 H133 Dy2 Fe4 N13 O22
Atom count from the _atom_site data: C68 H130 Dy2 Fe4 N13 O22
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum C68 H133 Dy2 Fe4 N13 O22
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	136.00	136.00	0.00
H	266.00	260.00	6.00
Dy	4.00	4.00	0.00
Fe	8.00	8.00	0.00
N	26.00	26.00	0.00
O	44.00	44.00	0.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	23
PLAT005_ALERT_5_G	No _iucr_refine_instructions_details in the CIF	? Do !
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	? Check
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal	0.00300 Deg.
PLAT301_ALERT_3_G	Note: Main Residue Disorder	3 %
PLAT302_ALERT_4_G	Note: Anion/Solvent Disorder	33 %
PLAT793_ALERT_4_G	The Model has Chirality at N1 (Verify)	R

And 3 other PLAT793 Alerts

More ...

PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	50
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
 3 **ALERT level B** = A potentially serious problem, consider carefully
 13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 14 **ALERT level G** = General information/check it is not something unexpected

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 12 ALERT type 2 Indicator that the structure model may be wrong or deficient
 4 ALERT type 3 Indicator that the structure quality may be low
 7 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

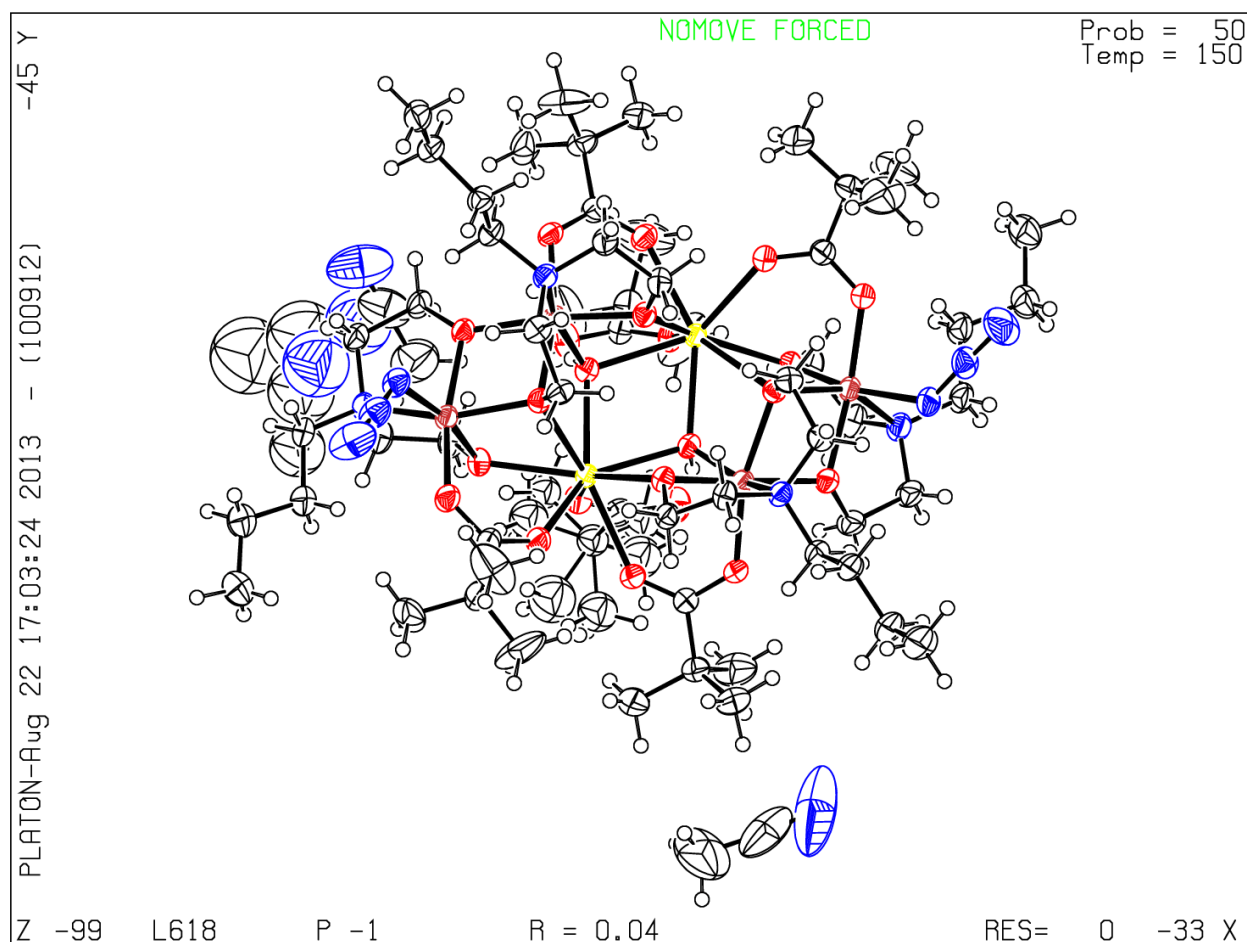
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, 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 01/06/2013; check.def file version of 24/05/2013

Datablock L618 - ellipsoid plot



[Test a new CIF entry](#)