

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ata_519c_0m

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: ata_519c_0m

Bond precision: C-C = 0.0140 Å Wavelength=0.71073

Cell: a=18.9040(7) b=18.9040(7) c=12.3051(9)
 alpha=90 beta=90 gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	4397.4(5)	4397.4(7)
Space group	P 4/n	P 4/n
Hall group	-P 4a	-P 4a
Moiety formula	C48 H52 Mn4 N4 O20 Tb, C16 H36 N, 5(C H2 Cl2)	C48 H52 Mn4 N4 O20 Tb, 5(C H2 Cl2), C16 H36 N
Sum formula	C69 H98 Cl10 Mn4 N5 O20 Tb	C69 H98 Cl10 Mn4 N5 O20 Tb
Mr	2050.71	2050.70
Dx, g cm ⁻³	1.549	1.549
Z	2	2
Mu (mm ⁻¹)	1.722	1.722
F000	2084.0	2084.0
F000'	2090.02	
h,k,lmax	23,23,15	23,23,15
Nref	4331	4332
Tmin,Tmax	0.440,0.842	0.588,0.746
Tmin'	0.406	

Correction method= # Reported T Limits: Tmin=0.588 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.994

R(reflections)= 0.0473(3891) wR2(reflections)= 0.1306(4332)

S = 1.283 Npar= 453

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

PLAT088_ALERT_3_C	Poor Data / Parameter Ratio	9.56	Note
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	5.1	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range	6.0	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C14	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C17	Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.014	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.407	Check
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/SigmaW > 10 Outliers	1	Check
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 1.26A From C18	-1.56	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H18B	-0.46	eA-3

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	17	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	26	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	22.74	Why ?
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	-2	Units
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	2	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	6	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C15 Constrained at	0.6	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16 Constrained at	0.6	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15B Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16B Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14A Constrained at	0.6	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14B Constrained at	0.6	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15A Constrained at	0.6	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15B Constrained at	0.6	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16A Constrained at	0.6	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16B Constrained at	0.6	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16C Constrained at	0.6	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14C Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14D Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15C Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15D Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16D Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16E Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16F Constrained at	0.4	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18 Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18A Constrained at	0.25	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18B Constrained at	0.25	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	99%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	47%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 4	1.25	Check
PLAT722_ALERT_1_G	Angle Calc 118.00, Rep 119.40 Dev...	1.40	Degree
	C1B -C2B -H2B 1.555 1.555 1.555 # 140		Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	5	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	196	Note

0	ALERT level A	= Most likely a serious problem - resolve or explain
0	ALERT level B	= A potentially serious problem, consider carefully
10	ALERT level C	= Check. Ensure it is not caused by an omission or oversight
42	ALERT level G	= General information/check it is not something unexpected
3	ALERT type 1	CIF construction/syntax error, inconsistent or missing data
8	ALERT type 2	Indicator that the structure model may be wrong or deficient
7	ALERT type 3	Indicator that the structure quality may be low
33	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.

