

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) MAB6

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: MAB6

Bond precision: O- B = 0.0059 A Wavelength=0.71075

Cell: a=9.7545 (3) b=15.4363 (4) c=17.0325 (5)
 alpha=90 beta=101.851 (3) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2509.98 (13)	2509.98 (13)
Space group	C c	C 1 c 1
Hall group	C -2yc	C -2yc
Moiety formula	C22 H46 N2, 2 (B5 H4 O10), 4 (B H3 O3)	C22 H46 N2, 2 (B5 H4 O10), 4 (B H3 O3)
Sum formula	C22 H66 B14 N2 O32	C22 H66 B14 N2 O32
Mr	1022.11	1022.10
Dx, g cm ⁻³	1.352	1.352
Z	2	2
Mu (mm ⁻¹)	0.117	0.117
F000	1076.0	1076.0
F000'	1076.74	
h, k, lmax	12, 20, 22	12, 20, 22
Nref	5768 [2889]	9481
Tmin, Tmax	0.990, 0.997	0.370, 1.000
Tmin'	0.981	

Correction method= # Reported T Limits: Tmin=0.370 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 3.28/1.64 Theta(max) = 27.518

R(reflections)= 0.0532 (8213)

wR2(reflections)=
0.1483 (9481)

S = 1.052

Npar= 437

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**

STRVA01_ALERT_4_C	Flack parameter is too small		
	From the CIF: <code>_refine_ls_abs_structure_Flack</code>	-2.200	
	From the CIF: <code>_refine_ls_abs_structure_Flack_su</code>	0.700	
PLAT089_ALERT_3_C	Poor Data / Parameter Ratio (Zmax < 18)	6.57	Note
PLAT215_ALERT_3_C	Disordered C20 has ADP max/min Ratio	3.2	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1)	2.2	Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 2)	2.9	Note
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.023	Check
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc) .	1	Check

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	28	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	47	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	10	Report
	H7 H8 H9 H10 H11 H12 H13 H21 H22 H23		
PLAT032_ALERT_4_G	Std. Uncertainty on Flack Parameter Value High .	0.700	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	9	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0600	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0300	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0600	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0300	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0300	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0600	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0600	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0600	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of N1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N2 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C5 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C6 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C7 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C8 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C9 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C10 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C11 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C12 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18 Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19 Constrained at	0.5	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of C20	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H11B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H15B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18C	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H20A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H20B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22C	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder (Resd 1)		100%	Note
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		70	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		!	Info
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers		1	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		617	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..		!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		19	Note
PLAT916_ALERT_2_G	Hooft y and Flack x Parameter Values Differ by .		2.70	Check

PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 3.3 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 10.35 Note
Predicted wR2: Based on SigI**2 1.43 or SHELX Weight 14.42

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
15 ALERT type 3 Indicator that the structure quality may be low
80 ALERT type 4 Improvement, methodology, query or suggestion
3 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.

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