

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) khriz011

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: khriz011

Bond precision: C-C = 0.0059 Å Wavelength=0.71073

Cell: a=11.4754(3) b=13.0017(4) c=16.9515(5)
 alpha=90.9576(10) beta=103.9529(10) gamma=90.4510(11)
Temperature: 105 K

	Calculated	Reported
Volume	2454.01(12)	2454.01(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C52 H35 Br2 Mn2 N5 O3), 3(C4 H8 O)	C52 H35 Br2 Mn2 N5 O3, 1.5(C4 H8 O)
Sum formula	C116 H94 Br4 Mn4 N10 O9	C58 H47 Br2 Mn2 N5 O4.50
Mr	2311.38	1155.70
Dx, g cm ⁻³	1.564	1.564
Z	1	2
Mu (mm ⁻¹)	2.199	2.199
F000	1172.0	1172.0
F000'	1172.58	
h,k,lmax	13,15,20	13,15,20
Nref	8994	8993
Tmin,Tmax	0.969,0.985	0.847,0.928
Tmin'	0.806	

Correction method= # Reported T Limits: Tmin=0.847 Tmax=0.928
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.349

R(reflections)= 0.0430(6802)	wR2(reflections)= 0.1180(8993)
S = 1.057	Npar= 713

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

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including O5'	0.124 Check

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	15	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	15	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500	Check
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	6	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records	3	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	2	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	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	0.0050	Report
PLAT189_ALERT_3_G	A Non-default SAME Restraint Value for First Par	0.0100	Report
PLAT189_ALERT_3_G	A Non-default SAME Restraint Value for First Par	0.0100	Report
PLAT189_ALERT_3_G	A Non-default SAME Restraint Value for First Par	0.0100	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of O5' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C51' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C52' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C53' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C54' Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H51A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H51B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H52B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H53A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H53B Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H54A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H54B Constrained at	0.5	Check
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
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 2)	9.85	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 3)	6.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 4)	3.15	Check
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O5'	103.4	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O4'	107.2	Degree
PLAT411_ALERT_2_G	Short Inter H...H Contact H24 ..H44D	2.10	Ang.
	2-x,2-y,1-z =	2_776	Check
PLAT411_ALERT_2_G	Short Inter H...H Contact H33B ..H41D	1.95	Ang.
	-1+x,y,z =	1_455	Check
PLAT411_ALERT_2_G	Short Inter H...H Contact H52A ..H108	2.10	Ang.
	-x,-y,-z =	2_555	Check
PLAT411_ALERT_2_G	Short Inter H...H Contact H54A ..H108	1.98	Ang.
	x,y,z =	1_555	Check
PLAT411_ALERT_2_G	Short Inter H...H Contact H54A ..H110	1.97	Ang.
	x,y,z =	1_555	Check
PLAT411_ALERT_2_G	Short Inter H...H Contact H54B ..H55	1.74	Ang.
	x,-1+y,z =	1_545	Check

PLAT411_ALERT_2_G Short Inter H...H Contact	H54B	..H110	.	1.93 Ang.
		x,y,z =		1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C54'	..C110	.	3.17 Ang.
		x,y,z =		1_555 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group	#			13 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.	#			2 Note
	C4 H8 O			
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.	#			4 Note
	C4 H8 O			
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1	(II)	.		2.16 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mn2	(II)	.		2.14 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters				10 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints				324 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary	.			Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).				3 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File				1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.				6 Info

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 15 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
 27 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.

