

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: tp_7_mix

Bond precision: C-C = 0.0093 A Wavelength=1.54178

Cell: a=21.1606(12) b=21.1606(12) c=17.5048(11)
alpha=90 beta=90 gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	7838.1(10)	7838.1(10)
Space group	I 41/a	I 41/a
Hall group	-I 4ad	-I 4ad
Moiety formula	C103 H136 Cl7 N23 O30 S7 [+ solvent]	C103 H136 Cl7 N23 O30 S7
Sum formula	C103 H136 Cl7 N23 O30 S7 [+ solvent]	C103 H136 Cl7 N23 O30 S7
Mr	2648.92	2648.91
Dx,g cm-3	1.122	1.122
Z	2	2
Mu (mm-1)	2.575	2.575
F000	2772.0	2772.0
F000'	2789.50	
h,k,lmax	22,22,18	22,20,18
Nref	2422	2411
Tmin,Tmax	0.485,0.525	0.580,1.000
Tmin'	0.440	

Correction method= # Reported T Limits: Tmin=0.580 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 54.506

R(reflections)= 0.0891(1640) wR2(reflections)= 0.3173(2411)

S = 1.119 Npar= 210

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 A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5281

Author Response: Crystals did not diffract past ~ 0.95A

Alert level C

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.32	Report
PLAT234_ALERT_4_C	Large Hirshfeld Difference O21 --C22	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C6 --C8	0.19	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C22 --C23	0.16	Ang.
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including C118	0.172	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00933	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.933	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.126	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.528	11	Report
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0	Info

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	8	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1	Info
PLAT007_ALERT_2_G	Number of Unrefined Donor-H Atoms	4	Report
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.18	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of C118 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of S9 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O10 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O11 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N4 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C5 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C6 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C8 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C12 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C14 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C15 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C16 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C17 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3AA Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3AB Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5A Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H5B Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H6 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7A Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8A Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8B Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H8C Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H14 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H16 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H17 Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3BC Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3BD Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3BE Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7BA Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H7BB Constrained at	0.125	Check
PLAT301_ALERT_3_G	Main Residue Disorder (Resd 1)	58%	Note
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	222	A**3

PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	7	Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	102	Note
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed	!	Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ	2	Units
PLAT992_ALERT_5_G	Repd & Actual _reflns_number_gt Values Differ by	2	Check

1 **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
51 **ALERT level G** = General information/check it is not something unexpected

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

