

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: jc_tp_h_108_1

Bond precision: C-C = 0.0083 A Wavelength=1.54178

Cell: a=17.1371(4) b=17.1371(4) c=29.0104(8)
alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	8519.8(5)	8519.8(5)
Space group	P 43 21 2	P 43 21 2
Hall group	P 4nw 2abw	P 4nw 2abw
Moiety formula	C103 H136 Cl7 N23 O30 S7 [+ solvent]	2(C51.5 H68 Cl3.5 N11.5 O15 S3.5)
Sum formula	C103 H136 Cl7 N23 O30 S7 [+ solvent]	C103 H136 Cl7 N23 O30 S7
Mr	2648.92	2648.91
Dx,g cm-3	1.033	1.033
Z	2	2
Mu (mm-1)	2.369	2.369
F000	2772.0	2772.0
F000'	2789.50	
h,k,lmax	21,21,36	21,19,36
Nref	8767[4979]	8717
Tmin,Tmax	0.685,0.735	0.786,1.000
Tmin'	0.436	

Correction method= # Reported T Limits: Tmin=0.786 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.75/0.99 Theta(max)= 74.807

R(reflections)= 0.0661(6970) wR2(reflections)= 0.2183(8717)

S = 1.069 Npar= 419

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

PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 2 Check

● Alert level C

PLAT234_ALERT_4_C	Large Hirshfeld Difference C12	--C13	.	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C43	--C44	.	0.22	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C44	--C45	.	0.19	Ang.
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C118		0.120	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds			0.00833	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		4	Report
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.			0	Info
PLAT987_ALERT_1_C	The Flack x is >> 0 - Do a BASF/TWIN Refinement				Please Check

● Alert level G

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_5_G	Number of Unrefined Donor-H Atoms			8	Report
PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero .			0.143	Note
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ				Please Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large			0.15	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 C148	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 S39	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 O40	Constrained at		0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O41	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 N34	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 C35	Constrained at		0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C36	Constrained at		0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C38	Constrained at		0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C42	Constrained at		0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C43	Constrained at		0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C44	Constrained at		0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C45	Constrained at		0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C46	Constrained at		0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C47	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 H33A	Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H33B	Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H35A	Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H35B	Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H36	Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H37	Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H38A	Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H38B	Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H38C	Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H43	Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H44	Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H46	Constrained at	0.875	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H47	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
PLAT300_ALERT_4_G	Atom Site Occupancy of H33C	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H33D	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H33E	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H37A	Constrained at	0.125	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H37B	Constrained at	0.125	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)		58%	Note
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C12 -C17		0.24	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C42 -C47		0.16	Ang.
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure		!	Info
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		96	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 !	
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		24	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...		3	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		3	Check

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
74 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.

