



## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 260117ha\_z1493210\_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: 260117ha\_z1493210\_0m

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Bond precision:	C-C = 0.0117 Å	Wavelength=1.54178	
Cell:	a=16.2763 (3)	b=16.2763 (3)	c=31.0684 (11)
	alpha=90	beta=90	gamma=90
Temperature:	193 K		
	Calculated	Reported	
Volume	8230.6 (4)	8230.6 (4)	
Space group	I 4/m	I4/m	
Hall group	-I 4	-I 4	
Moiety formula	C120 H120 Co8 O42 S8, 4 (C2 H8 N) [+ solvent]	0.5 (C120 H120 Co8 O42 S8), 2 (C2 H8 N)	
Sum formula	C128 H152 Co8 N4 O42 S8 [+ solvent]	C64 H76 Co4 N2 O21 S4	
Mr	3146.46	1573.22	
Dx, g cm <sup>-3</sup>	1.270	1.270	
Z	2	4	
Mu (mm <sup>-1</sup> )	7.679	7.679	
F000	3256.0	3256.0	
F000'	3232.81		
h, k, lmax	19, 19, 37	19, 17, 37	
Nref	3871	3836	
Tmin, Tmax	0.424, 0.541	0.616, 0.753	
Tmin'	0.320		



PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records		1	Report
PLAT175_ALERT_4_G	The CIF-Embedded .res File Contains SAME Records		1	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		3	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR 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		0.0100	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used		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 SecondPar		0.0200	Report
PLAT299_ALERT_4_G	Atom Site Occupancy Constrained at .....		0.5	Check
	O4 O5 O6 O7 C11 C12 C13 C14			
	C15 C16 C17 C18 C19 C20 H12A H12B			
	H13 H16 H17 H18 H19 H20 N1 C21			
	C22 H1A H1B H21A H21B H21C H22A H22B			
	H22C			
PLAT301_ALERT_3_G	Main Residue Disorder .....	(Resd 1)	49%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)		100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in .....	(Resd 2)	5.50	Check
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H3 ..H8C .		2.04	Ang.
	x, y, z =		1_555	Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure		576	A**3
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....		6	Note
	H8AA H8AB H8AC H9AA H9AB H9AC			
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #		33	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 .....		270	Note
PLAT868_ALERT_4_G	ALERTS Due to the Use of _smtbx_masks Suppressed		!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		4	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....		3	Note
	0 1 1, 0 3 3, 0 0 8,			
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....		4.7	Low
PLAT951_ALERT_5_G	Calculated (ThMax) and CIF-Reported Kmax Differ		2	Units
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value .....		7.079	Note
	Predicted wR2: Based on SigI**2 4.87 or SHELX Weight 30.20			
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		2	Info

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
16 ALERT type 2 Indicator that the structure model may be wrong or deficient  
13 ALERT type 3 Indicator that the structure quality may be low  
16 ALERT type 4 Improvement, methodology, query or suggestion  
4 ALERT type 5 Informative message, check

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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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

**PLATON version of 26/09/2025; check.def file version of 20/09/2025**

Datablock 260117ha\_z1493210\_0m - ellipsoid plot

