



checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: sm_184_auto

Bond precision: C-C = 0.0042 Å

Wavelength=1.54184

Cell: a=9.2711 (2) b=26.2949 (4) c=26.3344 (4)
 alpha=61.892 (2) beta=80.279 (1) gamma=85.507 (2)
Temperature: 100 K

	Calculated	Reported
Volume	5581.4 (2)	5581.41 (19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C174 H114 O24, 8 (C4 H8 O2) [+ solvent]	C87 H57 O12, 4 (C4 H8 O2)
Sum formula	C206 H178 O40 [+ solvent]	C103 H89 O20
Mr	3293.49	1646.74
Dx, g cm ⁻³	0.980	0.980
Z	1	2
Mu (mm ⁻¹)	0.552	0.552
F000	1734.0	1734.0
F000'	1739.50	
h, k, lmax	11, 33, 33	11, 33, 33
Nref	24309	23600
Tmin, Tmax	0.980, 0.989	0.786, 1.000
Tmin'	0.978	

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

Data completeness= 0.971

Theta(max)= 79.707

R(reflections)= 0.0865(18159)

wR2(reflections)=
0.2976(23600)

S = 1.072

Npar= 1207

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

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)	0.30	Report
PLAT097_ALERT_2_C	Large Reported Max. (Positive) Residual Density	0.65	eA-3
PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT220_ALERT_2_C	NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range	3.2	Ratio
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	02B	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	02S	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 3)	2.1	Note
PLAT329_ALERT_4_C	Carbon Atom Hybridisation Unclear for	C5	Check
PLAT329_ALERT_4_C	Carbon Atom Hybridisation Unclear for	C6	Check
PLAT340_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00422	Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C15S - C16S .	1.41	Ang.
PLAT410_ALERT_2_C	Short Intra H...H Contact H4A ..H6C .	1.99	Ang.
	1-x,1-y,1-z =	2_666	Check
PLAT410_ALERT_2_C	Short Intra H...H Contact H4B ..H6A .	1.93	Ang.
	x,y,z =	1_555	Check



Alert level G

PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H-Atoms	5	Report
PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF		Please Check
PLAT041_ALERT_1_G	Calc. and Reported SumFormula Strings Differ		Please Check
	Calc: C206 H178 O40		
	Rep.: C103 H89 O20		
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ		Please Check
	Calc: C174 H114 O24, 8(C4 H8 O2)		
	Rep.: C87 H57 O12, 4(C4 H8 O2)		
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.500	Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.19	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	5	Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for O4C --C29C .	8.0	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) O7S2 --C16S .	7.0	s.u.
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) O8S --C13S .	7.7	s.u.
PLAT299_ALERT_4_G	Atom Site Occupancy Constrained at	0.5	Check
	C1 C2 C3 C4 C17C C18C C19C C20C		
	C21C C22C H1 H2 H3 H17C H18C H20C		
	H21C H22C O8S2 O7S2 O7S O8S H13A H13B		
	H13C H13D H14J H14K H14L H14M H15J H15K		
	H15L H15M H16A H16B H16C H16D		
PLAT300_ALERT_4_G	Atom Site Occupancy of O3C Constrained at	0.88	Check

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PLAT300_ALERT_4_G Atom Site Occupancy of O4B          Constrained at      0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O4C          Constrained at      0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O4B2        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O4C2        Constrained at      0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O3C2        Constrained at     0.12 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5          Constrained at      0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6          Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5          Constrained at      0.6 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H29B        Constrained at     0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H29C        Constrained at     0.75 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6          Constrained at      0.4 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H29A        Constrained at     0.25 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H29D        Constrained at     0.25 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd   1)      9% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd   2)     33% Note
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C1A      -C2A      .      1.43 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C1A      -C1C_a     .      1.44 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C1B      -C2B      .      1.43 Ang.
PLAT333_ALERT_2_G Large Aver C6-Ring C-C Dist C1C      -C1A_a     .      1.44 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C16C    -C21C     .      0.22 Ang.
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O8S2 .      104.1 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O7S2 .      107.8 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O7S .      105.4 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O8S .      106.8 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O1S .      108.8 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O2S .      109.3 Degree
PLAT412_ALERT_2_G Short Intra XH3 .. XHn      H2      ..H15D .      2.10 Ang.
                                     x,y,z =      1_555 Check
PLAT606_ALERT_4_G Solvent Accessible VOID(S) in Crystal Structure      ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....      23 Note
      H9SA      H9SB      H7SA      H7SB      H6SA      H6SB      H1SA      H1SB
      H5SA      H5SB      H8SA      H8SB      H2SA      H2SB      H4SA      H4SB
      H3SA      H3SB      O8S2      O7S2      O4B2      O4C2      O3C2
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....      30 Note
PLAT868_ALERT_4_G ALERTS Due to the Use of _smtbx_masks Suppressed      ! Info
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File      27 Note
      3  9  6,  3 -4  5,  1  3  5,  2  8  6,  8  1  1,  7  2  2,
      3  7  1, -5  5  9,  8  2  2,  1  2  4,  0 -4  1,  0  4  4,
     -1  0  3,  1 -1  2,  2  3  3, -2  2  1,  1  0  3,  2  1  0,
      1 -2  1,  0 -2  5,  0 -2  1, -1  5  1,  2  6 11, -1 -2  1,
      1  7  4, -1 10  1,  2  3  4,

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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
14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
45 ALERT level G = General information/check it is not something unexpected

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

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Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_DIFMX02_sm_184_auto
;
PROBLEM: The maximum difference density is > 0.1*ZMAX*0.75
RESPONSE: ...
;
_vrf_PLAT084_sm_184_auto
;
PROBLEM: High wR2 Value (i.e. > 0.25) ..... 0.30 Report
RESPONSE: ...
;
_vrf_PLAT097_sm_184_auto
;
PROBLEM: Large Reported Max. (Positive) Residual Density 0.65 eA-3
RESPONSE: ...
;
_vrf_PLAT220_sm_184_auto
;
PROBLEM: NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.5 Ratio
RESPONSE: ...
;
_vrf_PLAT242_sm_184_auto
;
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of 02B Check
RESPONSE: ...
;
_vrf_PLAT244_sm_184_auto
;
PROBLEM: Low 'Solvent' Ueq as Compared to Neighbors of 02S Check
RESPONSE: ...
;
_vrf_PLAT250_sm_184_auto
;
PROBLEM: Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 3) 2.1 Note
RESPONSE: ...
;
_vrf_PLAT329_sm_184_auto
;
PROBLEM: Carbon Atom Hybridisation Unclear for ..... C5 Check
RESPONSE: ...
;
_vrf_PLAT340_sm_184_auto
;
PROBLEM: Low Bond Precision on C-C Bonds ..... 0.00422 Ang.
RESPONSE: ...
;
_vrf_PLAT360_sm_184_auto
;
PROBLEM: Short C(sp3)-C(sp3) Bond C15S - C16S . 1.41 Ang.
RESPONSE: ...
;
_vrf_PLAT410_sm_184_auto
;
```

PROBLEM: Short Intra H...H Contact H4A ..H6C . 1.99 Ang.
RESPONSE: ...
;
end Validation Reply Form

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

duplicate check

No duplication found

