



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:04 PM UTC

PDB ID : 7Q4H / pdb_00007q4h
Title : A thermostable lipase from Thermoanaerobacter thermohydrosulfuricus in complex with PMSF
Authors : Pinotsis, N.; Wilmanns, M.
Deposited on : 2021-10-30
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

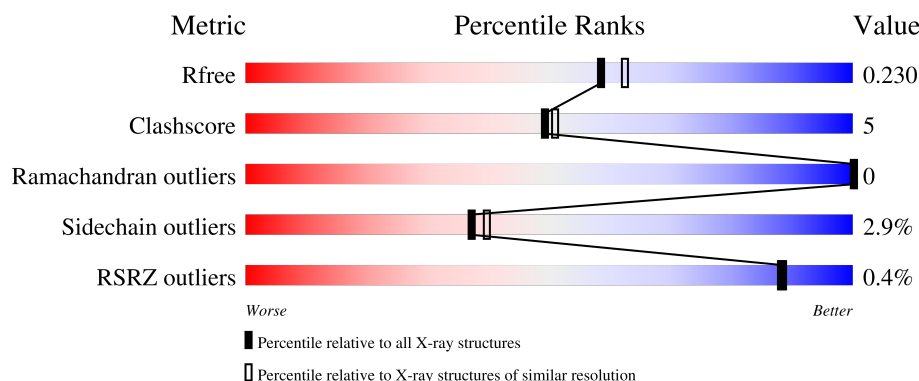
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	259	 89% 10% .
2	B	259	 83% 15% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	303	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4326 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hydrolase_4 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	1	0
			2048	1317	333	386	12			

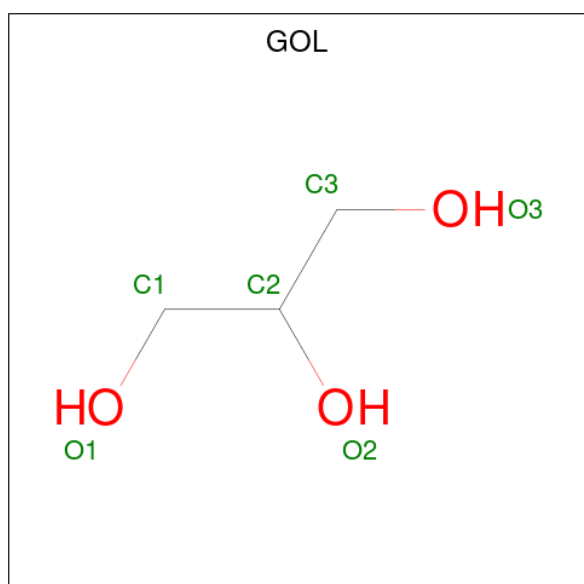
- Molecule 2 is a protein called Hydrolase_4 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	0	1	0
			2071	1332	335	392	12			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



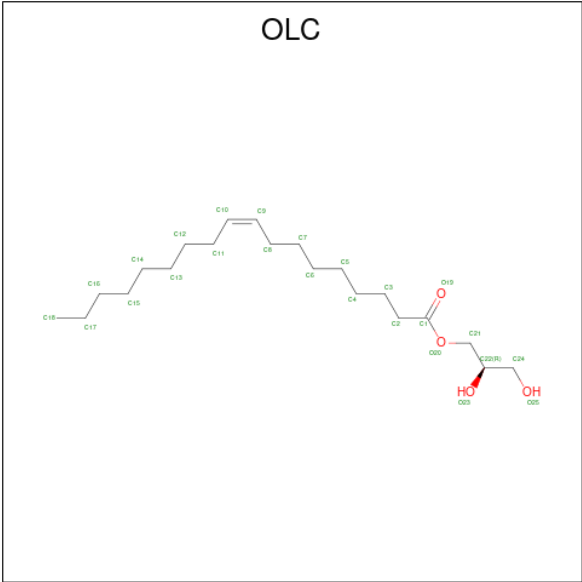
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			12	6	6		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			25	21	4		

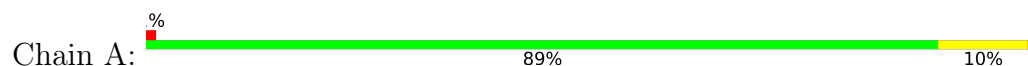
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	72	Total	O	0	0
			72	72		
7	B	64	Total	O	0	0
			64	64		

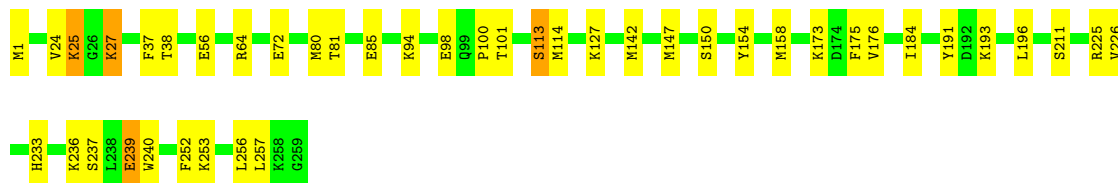
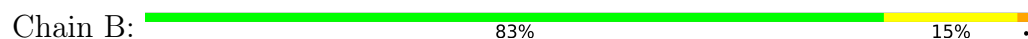
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Hydrolase_4 domain-containing protein



- Molecule 2: Hydrolase_4 domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	84.81Å 84.81Å 157.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.00 29.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.98-2.00) 98.1 (29.98-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.184 , 0.228 0.188 , 0.230	Depositor DCC
R_{free} test set	1219 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4326	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SEB, MLZ, OLC, SO4, GOL, MLY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/2014	0.74	0/2705
2	B	0.32	0/2015	0.70	0/2705
All	All	0.33	0/4029	0.72	0/5410

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2048	0	2023	18	0
2	B	2071	0	2062	26	0
3	A	1	0	0	0	0
4	A	24	0	32	6	0
4	B	6	0	8	0	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
6	B	25	0	40	3	0
7	A	72	0	0	1	0
7	B	64	0	0	1	0
All	All	4326	0	4165	45	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:SER:HA	2:B:154:TYR:HB2	1.52	0.89
6:B:301:OLC:H16	6:B:301:OLC:H12A	1.72	0.71
2:B:94:LYS:NZ	2:B:98:GLU:OE2	2.22	0.66
1:A:45:HIS:H	4:A:303:GOL:C1	2.10	0.65
2:B:158:MET:HE2	2:B:173:LYS:HA	1.78	0.65
1:A:236:MLY:HH22	4:A:303:GOL:H32	1.78	0.63
1:A:45:HIS:H	4:A:303:GOL:H11	1.64	0.63
2:B:113:SEB:OD2	2:B:233:HIS:NE2	2.31	0.63
1:A:44:SER:HA	4:A:303:GOL:H12	1.81	0.63
1:A:90:ARG:NH2	7:A:405:HOH:O	2.38	0.57
2:B:196:LEU:HD11	2:B:226:VAL:HG23	1.87	0.56
2:B:127:LYS:O	2:B:193:LYS:NZ	2.38	0.56
2:B:80:MET:HE3	2:B:85:GLU:CD	2.31	0.56
2:B:147:MET:HE1	2:B:176:VAL:HG13	1.88	0.55
1:A:196:LEU:HD11	1:A:226:VAL:HG23	1.91	0.53
2:B:80:MET:HE1	2:B:175:PHE:HE2	1.74	0.53
1:A:253:MLZ:HG3	1:A:257:LEU:HD12	1.91	0.53
1:A:43:GLU:OE1	4:A:302[A]:GOL:H31	2.10	0.52
1:A:142:MET:HA	1:A:145:LEU:HD12	1.91	0.52
2:B:239[A]:GLU:HG2	2:B:240:TRP:N	2.23	0.51
2:B:237:SER:HG	2:B:240:TRP:CG	2.29	0.50
2:B:80:MET:HE2	2:B:81:THR:C	2.38	0.49
2:B:253:MLY:HG3	2:B:257:LEU:HD12	1.95	0.48
1:A:150:SER:HA	1:A:154:TYR:CD2	2.49	0.48
2:B:158:MET:HE1	2:B:176:VAL:CG2	2.44	0.48
2:B:113:SEB:HI1	6:B:301:OLC:H12A	1.94	0.48
2:B:27:MLZ:HD3	2:B:100:PRO:O	2.16	0.46
2:B:252:PHE:O	2:B:256:LEU:HB2	2.16	0.46
1:A:193:MLY:HD3	1:A:193:MLY:HH23	1.60	0.45
1:A:64:ARG:HH22	2:B:72:GLU:CD	2.25	0.44
1:A:146:ILE:HD13	1:A:175:PHE:HE1	1.84	0.43
6:B:301:OLC:H2	6:B:301:OLC:H21	1.74	0.43
1:A:134:VAL:HG22	1:A:196:LEU:HB3	2.00	0.43
1:A:64:ARG:NH2	2:B:72:GLU:OE2	2.52	0.43
2:B:211:SER:OG	2:B:225:ARG:NH1	2.50	0.42
4:A:303:GOL:H31	7:B:431:HOH:O	2.18	0.42
2:B:191:TYR:CZ	2:B:193:LYS:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:MET:HE1	2:B:176:VAL:HG23	2.02	0.42
2:B:25:MLZ:HD3	2:B:25:MLZ:HA	1.64	0.42
1:A:236:MLY:HH23	1:A:236:MLY:HD2	1.80	0.41
1:A:113:SEB:HA	1:A:137:ALA:O	2.21	0.41
1:A:143:PRO:HD3	1:A:184:ILE:HD12	2.03	0.41
2:B:37:PHE:O	2:B:38:THR:OG1	2.35	0.41
2:B:80:MET:HE2	2:B:81:THR:O	2.21	0.40
2:B:114:MET:SD	2:B:142:MET:HE2	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	252/259 (97%)	245 (97%)	7 (3%)	0	100	100
2	B	250/259 (96%)	243 (97%)	7 (3%)	0	100	100
All	All	502/518 (97%)	488 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/216 (97%)	204 (98%)	5 (2%)	43	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	212/214 (99%)	204 (96%)	8 (4%)	29	29
All	All	421/430 (98%)	408 (97%)	13 (3%)	37	37

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	106	ARG
1	A	146	ILE
1	A	152	LYS
1	A	224	THR
2	B	1	MET
2	B	24	VAL
2	B	56	GLU
2	B	64	ARG
2	B	101	THR
2	B	184	ILE
2	B	239[A]	GLU
2	B	239[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	99	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

14 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLY	B	3	2	9,10,11	0.83	0	6,11,13	0.82	0
2	MLZ	B	27	2	8,9,10	0.64	0	4,9,11	1.45	1 (25%)
1	MLZ	A	253	1	8,9,10	0.64	0	4,9,11	1.49	1 (25%)
2	MLY	B	253	2	9,10,11	0.58	0	6,11,13	0.90	0
1	MLY	A	193	1	9,10,11	0.62	0	6,11,13	0.57	0
1	MLZ	A	12	1	8,9,10	0.60	0	4,9,11	1.41	1 (25%)
2	SEB	B	113	2	15,16,17	2.14	5 (33%)	16,21,23	1.74	3 (18%)
2	MLZ	B	25	2	8,9,10	0.62	0	4,9,11	1.48	1 (25%)
2	MLY	B	131	2	9,10,11	0.61	0	6,11,13	0.74	0
1	MLY	A	236	1	9,10,11	0.61	0	6,11,13	0.94	0
1	SEB	A	113	1	15,16,17	2.01	4 (26%)	16,21,23	1.56	2 (12%)
2	MLZ	B	236	2	8,9,10	0.60	0	4,9,11	1.51	1 (25%)
2	MLY	B	194	2	9,10,11	0.59	0	6,11,13	0.76	0
1	MLZ	A	189	1	8,9,10	0.61	0	4,9,11	1.53	1 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLY	B	3	2	-	3/8/9/11	-
2	MLZ	B	27	2	-	4/7/8/10	-
1	MLZ	A	253	1	-	3/7/8/10	-
2	MLY	B	253	2	-	3/8/9/11	-
1	MLY	A	193	1	-	2/8/9/11	-
1	MLZ	A	12	1	-	1/7/8/10	-
2	SEB	B	113	2	-	3/10/13/15	0/1/1/1
2	MLZ	B	25	2	-	4/7/8/10	-
2	MLY	B	131	2	-	6/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-
1	SEB	A	113	1	-	0/10/13/15	0/1/1/1
2	MLZ	B	236	2	-	2/7/8/10	-
2	MLY	B	194	2	-	2/8/9/11	-
1	MLZ	A	189	1	-	3/7/8/10	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	113	SEB	CE-SD	5.48	1.84	1.78
1	A	113	SEB	CE-SD	4.76	1.83	1.78
2	B	113	SEB	OG-SD	-4.50	1.42	1.56
1	A	113	SEB	OG-SD	-4.25	1.43	1.56
1	A	113	SEB	OD1-SD	2.83	1.51	1.44
2	B	113	SEB	OD1-SD	2.54	1.50	1.44
1	A	113	SEB	OD2-SD	2.44	1.50	1.44
2	B	113	SEB	OD2-SD	2.19	1.49	1.44
2	B	113	SEB	CE-CZ	2.12	1.55	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	113	SEB	OG-CB-CA	4.44	113.07	107.63
1	A	113	SEB	OG-SD-CE	4.43	116.40	104.18
2	B	113	SEB	OG-SD-CE	4.23	115.83	104.18
1	A	113	SEB	CB-OG-SD	3.42	126.66	119.30
2	B	25	MLZ	CM-NZ-CE	2.88	120.02	112.01
1	A	189	MLZ	CM-NZ-CE	2.87	120.00	112.01
2	B	236	MLZ	CM-NZ-CE	2.80	119.83	112.01
1	A	253	MLZ	CM-NZ-CE	2.79	119.77	112.01
2	B	27	MLZ	CM-NZ-CE	2.69	119.51	112.01
2	B	113	SEB	CB-OG-SD	-2.66	113.58	119.30
1	A	12	MLZ	CM-NZ-CE	2.62	119.31	112.01

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	189	MLZ	C-CA-CB-CG
1	A	236	MLY	N-CA-CB-CG
1	A	236	MLY	C-CA-CB-CG
1	A	253	MLZ	N-CA-CB-CG
1	A	253	MLZ	C-CA-CB-CG
2	B	25	MLZ	CD-CE-NZ-CM
2	B	27	MLZ	N-CA-CB-CG
2	B	27	MLZ	C-CA-CB-CG
2	B	113	SEB	SD-CE-CZ-CH2
2	B	113	SEB	SD-CE-CZ-CH1
2	B	131	MLY	N-CA-CB-CG
2	B	131	MLY	C-CA-CB-CG
2	B	253	MLY	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	B	253	MLY	C-CA-CB-CG
2	B	131	MLY	CD-CE-NZ-CH2
1	A	193	MLY	CG-CD-CE-NZ
2	B	131	MLY	CG-CD-CE-NZ
2	B	131	MLY	CD-CE-NZ-CH1
2	B	25	MLZ	CG-CD-CE-NZ
2	B	25	MLZ	CA-CB-CG-CD
2	B	194	MLY	CG-CD-CE-NZ
2	B	3	MLY	CG-CD-CE-NZ
2	B	27	MLZ	CA-CB-CG-CD
1	A	193	MLY	CD-CE-NZ-CH2
2	B	27	MLZ	CE-CD-CG-CB
1	A	189	MLZ	CE-CD-CG-CB
1	A	236	MLY	CE-CD-CG-CB
2	B	253	MLY	CE-CD-CG-CB
1	A	253	MLZ	CE-CD-CG-CB
2	B	25	MLZ	CE-CD-CG-CB
2	B	3	MLY	CE-CD-CG-CB
2	B	131	MLY	CA-CB-CG-CD
2	B	113	SEB	CB-OG-SD-OD1
1	A	189	MLZ	CG-CD-CE-NZ
2	B	3	MLY	CD-CE-NZ-CH1
2	B	236	MLZ	N-CA-CB-CG
2	B	236	MLZ	CE-CD-CG-CB
2	B	194	MLY	CD-CE-NZ-CH2
1	A	12	MLZ	N-CA-CB-CG

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	27	MLZ	1	0
1	A	253	MLZ	1	0
2	B	253	MLY	1	0
1	A	193	MLY	1	0
2	B	113	SEB	2	0
2	B	25	MLZ	1	0
1	A	236	MLY	2	0
1	A	113	SEB	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	A	303	-	5,5,5	0.39	0	5,5,5	0.62	0
5	SO4	B	303	-	4,4,4	0.23	0	6,6,6	0.12	0
4	GOL	A	302[A]	-	5,5,5	0.38	0	5,5,5	0.21	0
4	GOL	A	304	-	5,5,5	0.36	0	5,5,5	0.36	0
5	SO4	A	305	-	4,4,4	0.24	0	6,6,6	0.05	0
5	SO4	A	306	-	4,4,4	0.25	0	6,6,6	0.11	0
6	OLC	B	301	-	24,24,24	0.89	1 (4%)	25,25,25	0.93	1 (4%)
4	GOL	B	302	-	5,5,5	0.36	0	5,5,5	0.52	0
4	GOL	A	302[B]	-	5,5,5	0.35	0	5,5,5	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	303	-	-	2/4/4/4	-
4	GOL	A	302[A]	-	-	3/4/4/4	-
4	GOL	A	304	-	-	3/4/4/4	-
6	OLC	B	301	-	-	4/24/24/24	-
4	GOL	B	302	-	-	0/4/4/4	-
4	GOL	A	302[B]	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	301	OLC	C11-C10	-2.25	1.37	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	301	OLC	O20-C1-C2	2.82	120.44	111.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	GOL	O1-C1-C2-C3
4	A	304	GOL	C1-C2-C3-O3
6	B	301	OLC	C2-C1-O20-C21
6	B	301	OLC	O19-C1-O20-C21
4	A	303	GOL	O1-C1-C2-O2
4	A	304	GOL	O2-C2-C3-O3
4	A	304	GOL	O1-C1-C2-O2
4	A	302[A]	GOL	O1-C1-C2-O2
4	A	302[A]	GOL	O1-C1-C2-C3
4	A	302[A]	GOL	C1-C2-C3-O3
6	B	301	OLC	C7-C8-C9-C10
6	B	301	OLC	C9-C10-C11-C12

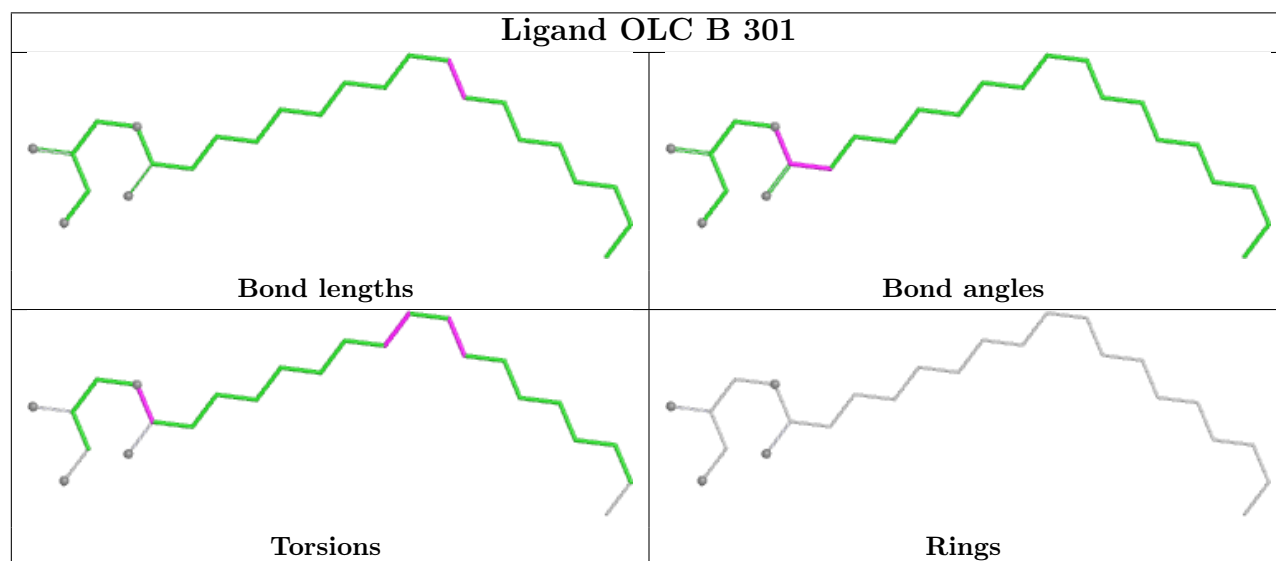
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	GOL	5	0
4	A	302[A]	GOL	1	0
6	B	301	OLC	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	253/259 (97%)	-0.23	2 (0%) 82 82	24, 42, 85, 138	1 (0%)
2	B	251/259 (96%)	-0.16	0 100 100	19, 46, 79, 104	1 (0%)
All	All	504/518 (97%)	-0.20	2 (0%) 88 88	19, 44, 80, 138	2 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	TYR	2.5
1	A	259	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MLZ	B	27	10/11	0.77	0.13	70,73,78,79	0
2	MLZ	B	25	10/11	0.78	0.16	60,78,82,85	0
2	MLY	B	131	11/12	0.84	0.14	55,60,89,90	0
1	MLY	A	236	11/12	0.85	0.14	36,42,66,70	0
1	MLZ	A	189	10/11	0.85	0.12	46,59,74,74	0
2	SEB	B	113	16/17	0.88	0.15	34,64,81,90	0
1	MLY	A	193	11/12	0.91	0.12	50,54,66,67	0
1	MLZ	A	253	10/11	0.92	0.08	46,53,59,61	0
2	MLY	B	253	11/12	0.92	0.09	49,55,62,64	0
2	MLY	B	194	11/12	0.93	0.08	50,61,72,73	0
1	SEB	A	113	16/17	0.93	0.11	30,60,67,73	0
2	MLZ	B	236	10/11	0.95	0.09	26,36,58,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MLZ	A	12	10/11	0.95	0.07	31,39,48,55	0
2	MLY	B	3	11/12	0.96	0.07	30,35,48,51	0

6.3 Carbohydrates [i](#)

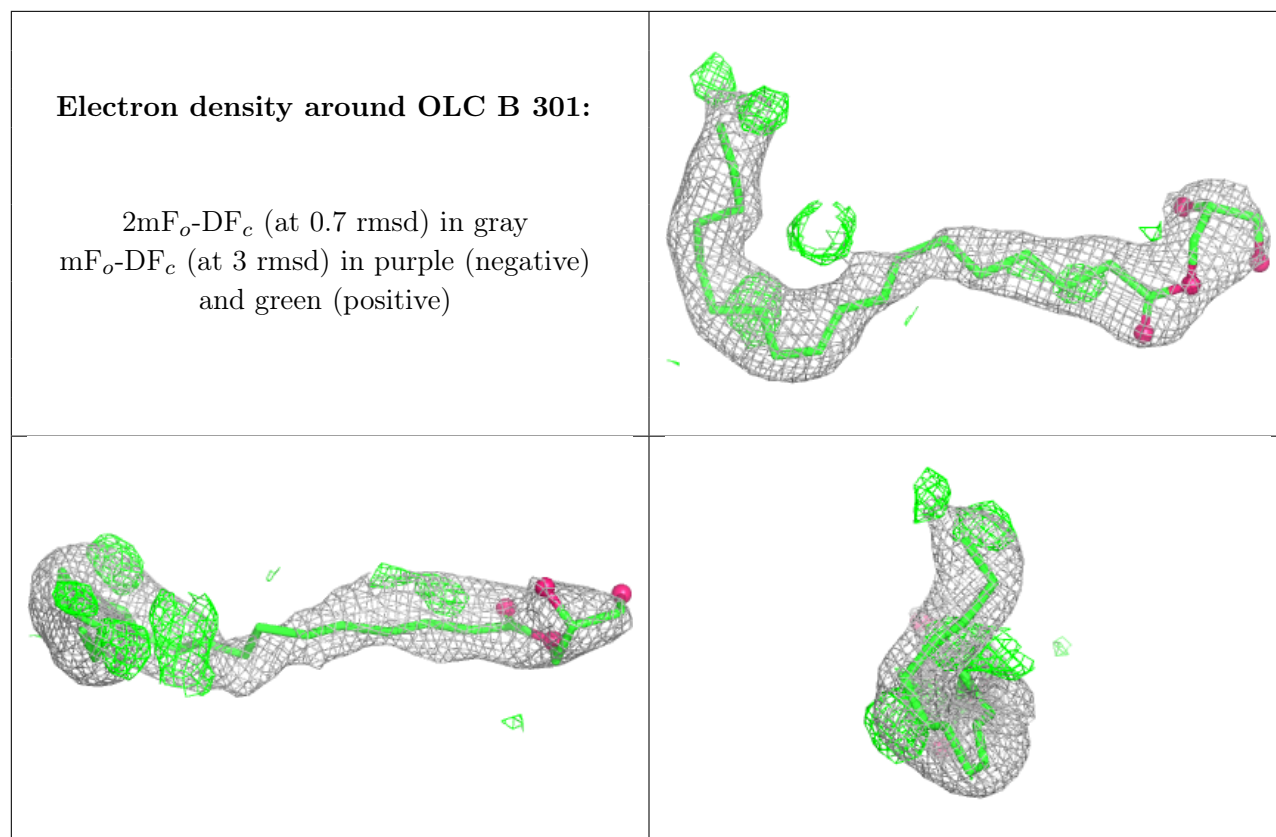
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	304	6/6	0.63	0.17	74,79,81,82	0
4	GOL	A	302[B]	6/6	0.70	0.17	28,54,55,61	6
4	GOL	A	302[A]	6/6	0.70	0.17	45,54,56,61	6
5	SO4	A	306	5/5	0.74	0.10	92,95,96,98	0
6	OLC	B	301	25/25	0.76	0.17	50,68,92,93	0
4	GOL	A	303	6/6	0.81	0.13	46,52,59,69	0
5	SO4	A	305	5/5	0.84	0.07	85,86,87,89	5
4	GOL	B	302	6/6	0.85	0.15	43,52,58,63	0
5	SO4	B	303	5/5	0.95	0.07	46,48,68,69	5
3	CL	A	301	1/1	1.00	0.02	32,32,32,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.