



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:11 PM UTC

PDB ID : 6Z70 / pdb_00006z70
Title : Structure of the MATE family multidrug resistance transporter Aq_128 from Aquifex aeolicus in the outward-facing state
Authors : Zhao, J.; Safarian, S.; Thielmann, Y.; Xie, H.; Wang, J.; Michel, H.
Deposited on : 2020-05-29
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

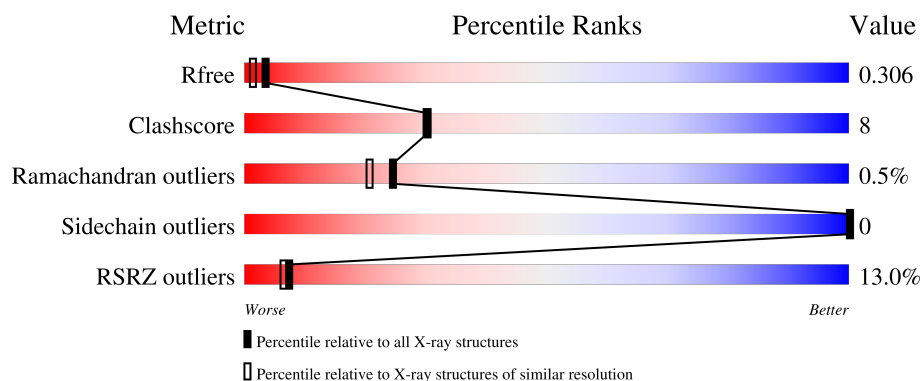
1 Overall quality at a glance

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	496	11% 74% 15% 10%
1	B	496	12% 79% 10% 10%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7154 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 Aq128.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3486	2348	544	579	15			
1	B	444	Total	C	N	O	S	0	0	0
			3487	2349	544	579	15			

There are 48 discrepancies between the modelled and reference sequences:

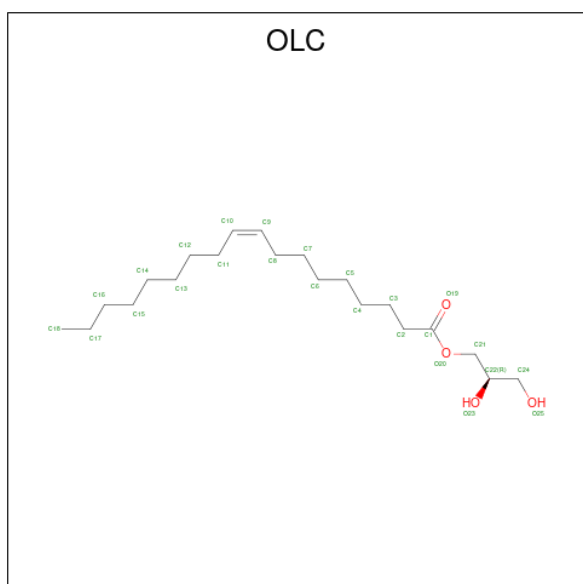
Chain	Residue	Modelled	Actual	Comment	Reference
A	473	ARG	-	expression tag	UNP O66528
A	474	ASN	-	expression tag	UNP O66528
A	475	SER	-	expression tag	UNP O66528
A	476	GLU	-	expression tag	UNP O66528
A	477	ASN	-	expression tag	UNP O66528
A	478	LEU	-	expression tag	UNP O66528
A	479	TYR	-	expression tag	UNP O66528
A	480	PHE	-	expression tag	UNP O66528
A	481	GLN	-	expression tag	UNP O66528
A	482	GLY	-	expression tag	UNP O66528
A	483	GLY	-	expression tag	UNP O66528
A	484	ARG	-	expression tag	UNP O66528
A	485	GLY	-	expression tag	UNP O66528
A	486	SER	-	expression tag	UNP O66528
A	487	HIS	-	expression tag	UNP O66528
A	488	HIS	-	expression tag	UNP O66528
A	489	HIS	-	expression tag	UNP O66528
A	490	HIS	-	expression tag	UNP O66528
A	491	HIS	-	expression tag	UNP O66528
A	492	HIS	-	expression tag	UNP O66528
A	493	HIS	-	expression tag	UNP O66528
A	494	HIS	-	expression tag	UNP O66528
A	495	HIS	-	expression tag	UNP O66528
A	496	HIS	-	expression tag	UNP O66528
B	473	ARG	-	expression tag	UNP O66528

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Chain	Residue	Modelled	Actual	Comment	Reference
B	474	ASN	-	expression tag	UNP O66528
B	475	SER	-	expression tag	UNP O66528
B	476	GLU	-	expression tag	UNP O66528
B	477	ASN	-	expression tag	UNP O66528
B	478	LEU	-	expression tag	UNP O66528
B	479	TYR	-	expression tag	UNP O66528
B	480	PHE	-	expression tag	UNP O66528
B	481	GLN	-	expression tag	UNP O66528
B	482	GLY	-	expression tag	UNP O66528
B	483	GLY	-	expression tag	UNP O66528
B	484	ARG	-	expression tag	UNP O66528
B	485	GLY	-	expression tag	UNP O66528
B	486	SER	-	expression tag	UNP O66528
B	487	HIS	-	expression tag	UNP O66528
B	488	HIS	-	expression tag	UNP O66528
B	489	HIS	-	expression tag	UNP O66528
B	490	HIS	-	expression tag	UNP O66528
B	491	HIS	-	expression tag	UNP O66528
B	492	HIS	-	expression tag	UNP O66528
B	493	HIS	-	expression tag	UNP O66528
B	494	HIS	-	expression tag	UNP O66528
B	495	HIS	-	expression tag	UNP O66528
B	496	HIS	-	expression tag	UNP O66528

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$) (labeled as "Ligand of Interest" by depositor).

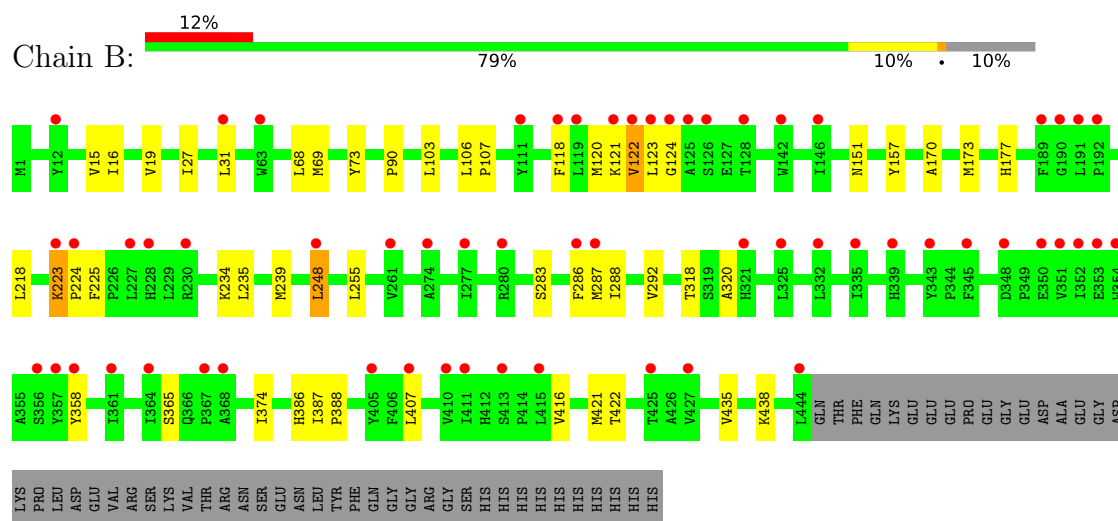


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			25	21	4		
2	B	1	Total	C	O	0	0
			25	21	4		
2	B	1	Total	C	O	0	0
			25	21	4		
2	B	1	Total	C	O	0	0
			25	21	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	3	Total	O	0	0
			3	3		

- Molecule 1: Aq128



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.10Å 116.10Å 137.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.00 19.99 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.99-2.00) 99.0 (19.99-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.01Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.266 , 0.284 0.266 , 0.306	Depositor DCC
R_{free} test set	752 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtrriage
Anisotropy	0.526	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.41$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7154	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6430e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: OLC

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	0.39	0/3585	0.52	0/4875
1	B	0.37	0/3586	0.51	1/4876 (0.0%)
All	All	0.38	0/7171	0.52	1/9751 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	LEU	CA-CB-CG	-5.74	96.22	116.30

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	3486	0	3643	68	0
1	B	3487	0	3648	53	0
2	A	100	0	160	24	0
2	B	75	0	120	14	0
3	A	3	0	0	1	0
3	B	3	0	0	1	0
All	All	7154	0	7571	123	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 8.

All (123) 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)
1:B:157:TYR:OH	1:B:223:LYS:NZ	1.73	1.22
1:A:223:LYS:HG3	1:A:224:PRO:HD2	1.18	1.16
1:B:223:LYS:HG3	1:B:224:PRO:HD2	1.31	1.06
1:A:107:PRO:HG2	2:A:501:OLC:H13	1.54	0.86
1:A:37:ASN:HD21	2:A:504:OLC:H24A	1.40	0.86
1:A:223:LYS:HG3	1:A:224:PRO:CD	2.09	0.79
1:B:365:SER:HB3	1:B:422:THR:HG23	1.68	0.76
1:A:157:TYR:HE1	1:A:223:LYS:HE3	1.50	0.76
1:B:218:LEU:HA	1:B:223:LYS:HB2	1.69	0.74
1:A:122:VAL:HG22	1:B:122:VAL:HB	1.72	0.72
1:A:365:SER:HB3	1:A:422:THR:HG23	1.72	0.71
1:B:157:TYR:CZ	1:B:224:PRO:HD3	2.24	0.71
1:A:218:LEU:HA	1:A:223:LYS:HB2	1.71	0.70
1:B:157:TYR:CE2	1:B:223:LYS:NZ	2.60	0.68
1:A:157:TYR:CZ	1:A:224:PRO:HD3	2.27	0.68
1:A:223:LYS:CG	1:A:224:PRO:HD2	2.11	0.67
1:B:320:ALA:HA	1:B:374:ILE:HD12	1.76	0.67
1:A:41:MET:HE2	2:A:504:OLC:H24	1.76	0.67
1:A:320:ALA:HA	1:A:374:ILE:HD12	1.77	0.67
1:B:69:MET:HE1	2:B:503:OLC:H13	1.77	0.67
1:A:157:TYR:CE1	1:A:223:LYS:HE3	2.31	0.66
1:A:157:TYR:HE1	1:A:223:LYS:CE	2.08	0.65
1:A:234:LYS:HE2	2:B:502:OLC:H21A	1.79	0.64
1:A:157:TYR:CE1	1:A:223:LYS:CE	2.80	0.64
1:B:107:PRO:HG2	2:B:501:OLC:H12A	1.80	0.62
2:A:502:OLC:H14	2:B:501:OLC:H13	1.80	0.62
1:A:12:TYR:OH	1:A:321:HIS:ND1	2.25	0.61
1:A:248:LEU:HD21	1:B:248:LEU:HG	1.84	0.60
1:A:414:PRO:O	1:A:417:PRO:HD2	2.02	0.59
1:B:120:MET:O	1:B:122:VAL:N	2.35	0.59
1:A:37:ASN:HD21	2:A:504:OLC:C24	2.15	0.58
1:A:121:LYS:HD3	1:B:122:VAL:HA	1.85	0.58
1:A:37:ASN:ND2	2:A:504:OLC:H24A	2.14	0.57
1:A:182:TYR:CE1	1:A:188:LYS:HE2	2.39	0.57
2:A:502:OLC:H22	1:B:234:LYS:NZ	2.18	0.57
1:A:234:LYS:CE	2:B:502:OLC:H21A	2.35	0.57
1:A:66:TYR:CE2	2:A:503:OLC:H14	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:LEU:HB2	2:B:501:OLC:H18	1.87	0.56
1:A:63:TRP:HE1	2:A:504:OLC:H18B	1.70	0.56
1:A:394:SER:HB3	2:A:502:OLC:H12A	1.88	0.55
1:A:290:PHE:CE1	2:A:503:OLC:H5	2.41	0.55
1:A:224:PRO:HB2	1:A:225:PHE:CE1	2.43	0.54
2:A:502:OLC:H22	1:B:234:LYS:HZ2	1.72	0.54
1:A:393:ILE:HG21	2:B:501:OLC:H11A	1.90	0.53
1:A:290:PHE:HE1	2:A:503:OLC:H5	1.73	0.53
1:B:157:TYR:CE1	1:B:224:PRO:HD3	2.43	0.53
1:A:157:TYR:CE2	1:A:224:PRO:HD3	2.44	0.53
1:B:16:ILE:HD11	1:B:318:THR:HG22	1.91	0.52
1:A:248:LEU:CD2	1:B:248:LEU:HG	2.39	0.52
1:A:36:GLU:HG2	1:A:178:ILE:HD11	1.92	0.51
2:A:502:OLC:H14	2:B:501:OLC:C13	2.41	0.51
1:B:223:LYS:CG	1:B:224:PRO:HD2	2.22	0.51
1:A:360:GLN:O	1:A:364:ILE:HD12	2.11	0.51
1:B:435:VAL:HG13	2:B:502:OLC:H3A	1.93	0.50
1:A:90:PRO:HG2	1:A:225:PHE:CE2	2.46	0.50
1:B:122:VAL:C	1:B:124:GLY:H	2.19	0.49
1:A:214:TYR:HD2	1:A:223:LYS:HE2	1.76	0.49
1:B:283:SER:HA	1:B:286:PHE:HB2	1.93	0.49
1:B:177:HIS:HE1	3:B:602:HOH:O	1.95	0.49
1:A:93:ILE:HD13	1:A:235:LEU:HD13	1.93	0.49
1:B:73:TYR:HB2	1:B:151:ASN:HD21	1.77	0.49
1:A:288:ILE:O	1:A:292:VAL:HG23	2.12	0.48
2:B:503:OLC:H16	2:B:503:OLC:H13A	1.69	0.48
2:A:504:OLC:H21	2:A:504:OLC:H3A	1.95	0.48
1:A:63:TRP:NE1	2:A:504:OLC:H18B	2.29	0.48
1:A:416:VAL:HB	1:A:417:PRO:HD3	1.94	0.47
1:A:16:ILE:HD11	1:A:318:THR:HG22	1.96	0.47
1:A:177:HIS:HE1	3:A:603:HOH:O	1.99	0.46
1:B:358:TYR:OH	1:B:421:MET:HE1	2.15	0.46
1:A:66:TYR:CG	1:A:69:MET:HE2	2.50	0.46
2:A:503:OLC:H12A	2:A:503:OLC:H15	1.67	0.46
1:B:122:VAL:HG13	1:B:123:LEU:HD22	1.98	0.46
1:A:235:LEU:HB3	1:A:239:MET:HE3	1.97	0.46
1:A:283:SER:HA	1:A:286:PHE:HB2	1.96	0.46
2:B:503:OLC:H7A	2:B:503:OLC:H2A	1.98	0.46
1:B:224:PRO:HB2	1:B:225:PHE:CE1	2.51	0.45
1:B:170:ALA:HA	1:B:173:MET:HE2	1.98	0.45
1:B:234:LYS:O	1:B:234:LYS:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:TRP:HB3	2:B:501:OLC:H18B	1.99	0.45
1:A:127:GLU:HG2	1:A:130:ARG:NH2	2.32	0.45
1:B:235:LEU:HB3	1:B:239:MET:HE3	1.97	0.45
1:B:288:ILE:O	1:B:292:VAL:HG23	2.17	0.45
1:B:387:ILE:HB	1:B:388:PRO:HD3	1.99	0.44
2:A:503:OLC:H10	2:A:503:OLC:H7	1.67	0.44
1:B:90:PRO:HG2	1:B:225:PHE:CE2	2.53	0.44
1:A:277:ILE:HD13	1:A:280:ARG:HD3	2.00	0.44
1:B:248:LEU:HD22	1:B:248:LEU:N	2.33	0.44
1:B:407:LEU:HD12	1:B:416:VAL:CG1	2.47	0.44
1:B:122:VAL:C	1:B:124:GLY:N	2.76	0.43
1:B:283:SER:O	1:B:287:MET:HG2	2.18	0.43
1:A:185:ILE:HD11	1:A:199:ALA:HB2	2.01	0.43
1:A:349:PRO:HA	1:A:352:ILE:HD12	2.00	0.43
1:A:440:VAL:O	1:A:444:LEU:HG	2.18	0.43
1:B:218:LEU:HB2	1:B:223:LYS:HD3	1.99	0.43
1:B:365:SER:CB	1:B:422:THR:HG23	2.45	0.43
1:A:396:PHE:CE2	1:A:400:ARG:HD2	2.54	0.43
1:A:283:SER:O	1:A:287:MET:HG2	2.19	0.43
1:B:68:LEU:HD21	2:B:501:OLC:H10	2.00	0.43
1:A:248:LEU:HA	1:A:248:LEU:HD13	1.78	0.42
1:A:248:LEU:HD11	1:B:248:LEU:HD11	2.01	0.42
1:A:257:PHE:CZ	2:A:504:OLC:H12A	2.54	0.42
1:A:39:ILE:O	1:A:43:LEU:HG	2.19	0.42
2:A:504:OLC:H13A	2:A:504:OLC:H10	1.67	0.42
1:B:122:VAL:HG13	1:B:123:LEU:N	2.35	0.42
1:B:438:LYS:HD3	1:B:438:LYS:HA	1.82	0.42
1:A:224:PRO:HB2	1:A:225:PHE:CD1	2.54	0.42
1:A:59:LEU:HB3	2:A:504:OLC:H21A	2.01	0.41
1:A:180:THR:HG21	1:A:205:ILE:HD12	2.02	0.41
1:A:241:ARG:HD3	1:B:386:HIS:CE1	2.54	0.41
1:B:15:VAL:O	1:B:19:VAL:HG23	2.21	0.41
1:B:248:LEU:HD13	1:B:248:LEU:HA	1.56	0.41
1:B:68:LEU:HD11	2:B:501:OLC:C9	2.50	0.41
1:A:85:GLY:HA3	1:A:302:GLN:O	2.20	0.41
2:A:502:OLC:H11	1:B:103:LEU:HD12	2.02	0.41
1:A:71:LEU:C	1:A:71:LEU:HD23	2.46	0.41
2:A:501:OLC:H2	1:B:255:LEU:HB3	2.03	0.41
2:A:504:OLC:C10	2:A:504:OLC:H6A	2.47	0.41
1:A:173:MET:HG3	1:A:206:SER:HB2	2.02	0.40
1:A:122:VAL:HG11	1:B:118:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASN:O	1:A:154:TYR:HB3	2.22	0.40
1:A:327:MET:SD	1:A:370:ALA:HB2	2.61	0.40
1:B:27:ILE:O	1:B:31:LEU:HG	2.22	0.40
1:B:157:TYR:CZ	1:B:223:LYS:NZ	2.56	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	442/496 (89%)	432 (98%)	9 (2%)	1 (0%)	43	42
1	B	442/496 (89%)	429 (97%)	10 (2%)	3 (1%)	18	14
All	All	884/992 (89%)	861 (97%)	19 (2%)	4 (0%)	24	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	LYS
1	B	121	LYS
1	B	122	VAL
1	B	223	LYS

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	376/424 (89%)	376 (100%)	0	100	100
1	B	376/424 (89%)	376 (100%)	0	100	100
All	All	752/848 (89%)	752 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	177	HIS
1	B	37	ASN
1	B	177	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands 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	OLC	A	503	-	24,24,24	0.81	1 (4%)	25,25,25	1.16	1 (4%)
2	OLC	B	501	-	24,24,24	0.72	0	25,25,25	1.19	2 (8%)
2	OLC	B	503	-	24,24,24	0.88	1 (4%)	25,25,25	1.23	1 (4%)
2	OLC	A	501	-	24,24,24	0.72	2 (8%)	25,25,25	1.15	1 (4%)
2	OLC	A	502	-	24,24,24	0.79	1 (4%)	25,25,25	1.05	1 (4%)
2	OLC	B	502	-	24,24,24	0.84	1 (4%)	25,25,25	1.09	1 (4%)
2	OLC	A	504	-	24,24,24	0.85	2 (8%)	25,25,25	1.02	1 (4%)

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	OLC	A	503	-	-	17/24/24/24	-
2	OLC	B	501	-	-	12/24/24/24	-
2	OLC	B	503	-	-	13/24/24/24	-
2	OLC	A	501	-	-	13/24/24/24	-
2	OLC	A	502	-	-	12/24/24/24	-
2	OLC	B	502	-	-	12/24/24/24	-
2	OLC	A	504	-	-	12/24/24/24	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	OLC	O20-C1	2.86	1.41	1.33
2	B	503	OLC	O20-C1	2.74	1.41	1.33
2	A	504	OLC	O20-C1	2.73	1.41	1.33
2	A	503	OLC	O20-C1	2.72	1.41	1.33
2	A	502	OLC	O20-C1	2.48	1.40	1.33
2	A	501	OLC	O20-C1	2.11	1.39	1.33
2	A	501	OLC	O20-C21	-2.07	1.40	1.45
2	A	504	OLC	O20-C21	-2.04	1.40	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	503	OLC	O20-C1-C2	3.92	123.78	111.83
2	A	503	OLC	O20-C1-C2	3.43	122.28	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	504	OLC	O20-C1-C2	3.20	121.58	111.83
2	A	501	OLC	O20-C1-C2	3.06	121.15	111.83
2	B	501	OLC	O20-C1-C2	3.05	121.14	111.83
2	B	502	OLC	O20-C1-C2	2.95	120.82	111.83
2	A	502	OLC	O20-C1-C2	2.81	120.39	111.83
2	B	501	OLC	O20-C1-O19	-2.18	118.18	123.63

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	OLC	C21-C22-C24-O25
2	A	502	OLC	C21-C22-C24-O25
2	A	503	OLC	O20-C21-C22-C24
2	A	503	OLC	O20-C21-C22-O23
2	A	504	OLC	C21-C22-C24-O25
2	B	501	OLC	O20-C21-C22-C24
2	B	501	OLC	O20-C21-C22-O23
2	B	503	OLC	C21-C22-C24-O25
2	A	504	OLC	O19-C1-O20-C21
2	A	504	OLC	C2-C1-O20-C21
2	A	504	OLC	C13-C14-C15-C16
2	A	502	OLC	O20-C21-C22-C24
2	B	503	OLC	O20-C21-C22-C24
2	A	502	OLC	O20-C21-C22-O23
2	A	502	OLC	O23-C22-C24-O25
2	A	501	OLC	C1-C2-C3-C4
2	B	503	OLC	C1-C2-C3-C4
2	B	502	OLC	C12-C13-C14-C15
2	B	503	OLC	O20-C21-C22-O23
2	A	503	OLC	C2-C1-O20-C21
2	A	503	OLC	C12-C13-C14-C15
2	B	502	OLC	C21-C22-C24-O25
2	A	503	OLC	O19-C1-O20-C21
2	A	503	OLC	C13-C14-C15-C16
2	B	502	OLC	C5-C6-C7-C8
2	A	503	OLC	C5-C6-C7-C8
2	A	504	OLC	O23-C22-C24-O25
2	B	503	OLC	O23-C22-C24-O25
2	A	502	OLC	C12-C13-C14-C15
2	B	502	OLC	C1-C2-C3-C4
2	B	501	OLC	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	A	502	OLC	C4-C5-C6-C7
2	A	502	OLC	C5-C6-C7-C8
2	B	501	OLC	C3-C4-C5-C6
2	A	501	OLC	C12-C13-C14-C15
2	A	504	OLC	C5-C6-C7-C8
2	A	504	OLC	C4-C5-C6-C7
2	B	501	OLC	C11-C12-C13-C14
2	A	503	OLC	C14-C15-C16-C17
2	B	501	OLC	C14-C15-C16-C17
2	B	501	OLC	C2-C3-C4-C5
2	A	503	OLC	C10-C11-C12-C13
2	A	501	OLC	C13-C14-C15-C16
2	A	501	OLC	C2-C3-C4-C5
2	A	501	OLC	C11-C12-C13-C14
2	B	501	OLC	C5-C6-C7-C8
2	B	501	OLC	C10-C11-C12-C13
2	B	503	OLC	C6-C7-C8-C9
2	A	502	OLC	C15-C16-C17-C18
2	B	501	OLC	C15-C16-C17-C18
2	A	504	OLC	C1-C2-C3-C4
2	A	501	OLC	O23-C22-C24-O25
2	B	502	OLC	O23-C22-C24-O25
2	A	501	OLC	C7-C8-C9-C10
2	A	503	OLC	C7-C8-C9-C10
2	B	503	OLC	C3-C4-C5-C6
2	A	503	OLC	C9-C10-C11-C12
2	B	502	OLC	C2-C3-C4-C5
2	B	502	OLC	C6-C7-C8-C9
2	B	502	OLC	C3-C4-C5-C6
2	A	504	OLC	C15-C16-C17-C18
2	A	503	OLC	C15-C16-C17-C18
2	A	502	OLC	C6-C7-C8-C9
2	B	503	OLC	C5-C6-C7-C8
2	B	501	OLC	C12-C13-C14-C15
2	A	502	OLC	C2-C1-O20-C21
2	A	502	OLC	O19-C1-O20-C21
2	A	504	OLC	C9-C10-C11-C12
2	B	502	OLC	C15-C16-C17-C18
2	A	501	OLC	C6-C7-C8-C9
2	A	503	OLC	C3-C4-C5-C6
2	A	501	OLC	O20-C1-C2-C3
2	A	504	OLC	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
2	A	503	OLC	C6-C7-C8-C9
2	A	501	OLC	C10-C11-C12-C13
2	A	501	OLC	C9-C10-C11-C12
2	A	504	OLC	C22-C21-O20-C1
2	A	501	OLC	C3-C4-C5-C6
2	B	503	OLC	C7-C8-C9-C10
2	B	503	OLC	C2-C3-C4-C5
2	B	501	OLC	C7-C8-C9-C10
2	B	502	OLC	O20-C21-C22-C24
2	A	502	OLC	C7-C8-C9-C10
2	B	502	OLC	C7-C8-C9-C10
2	A	503	OLC	O20-C1-C2-C3
2	B	503	OLC	O20-C1-C2-C3
2	B	502	OLC	C14-C15-C16-C17
2	A	503	OLC	O19-C1-C2-C3
2	A	503	OLC	C4-C5-C6-C7
2	B	503	OLC	O19-C1-C2-C3
2	B	503	OLC	C13-C14-C15-C16

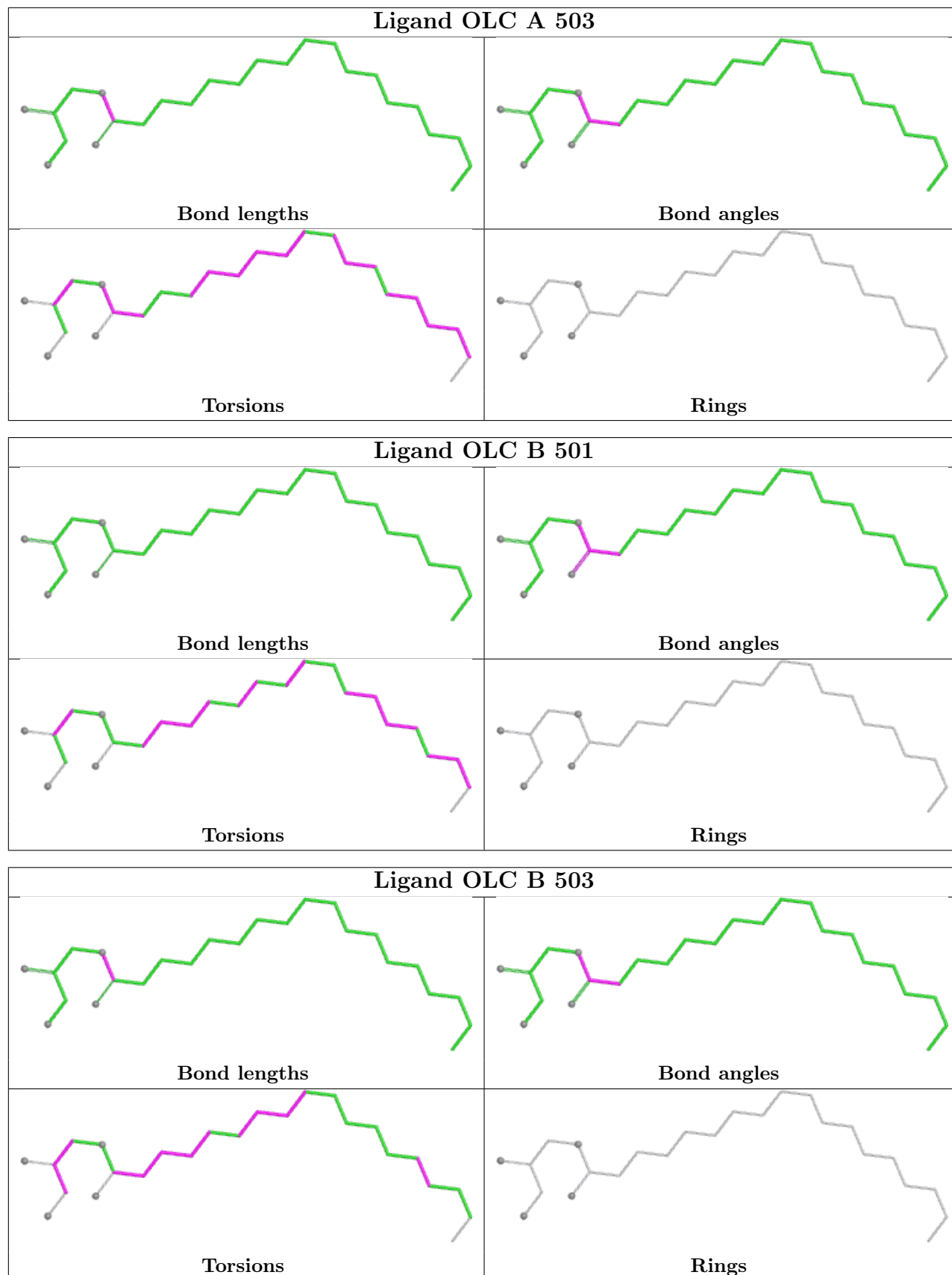
There are no ring outliers.

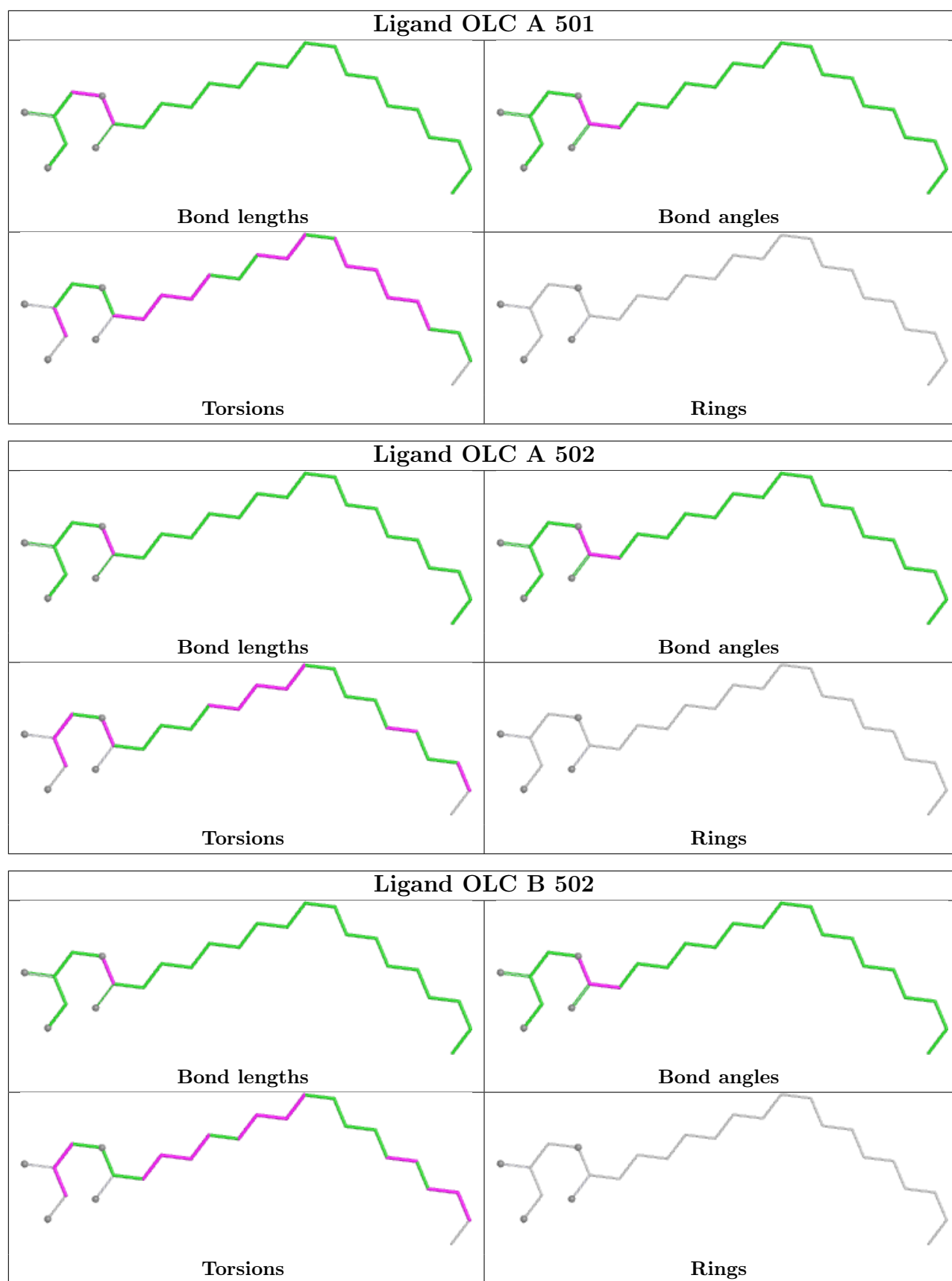
7 monomers are involved in 36 short contacts:

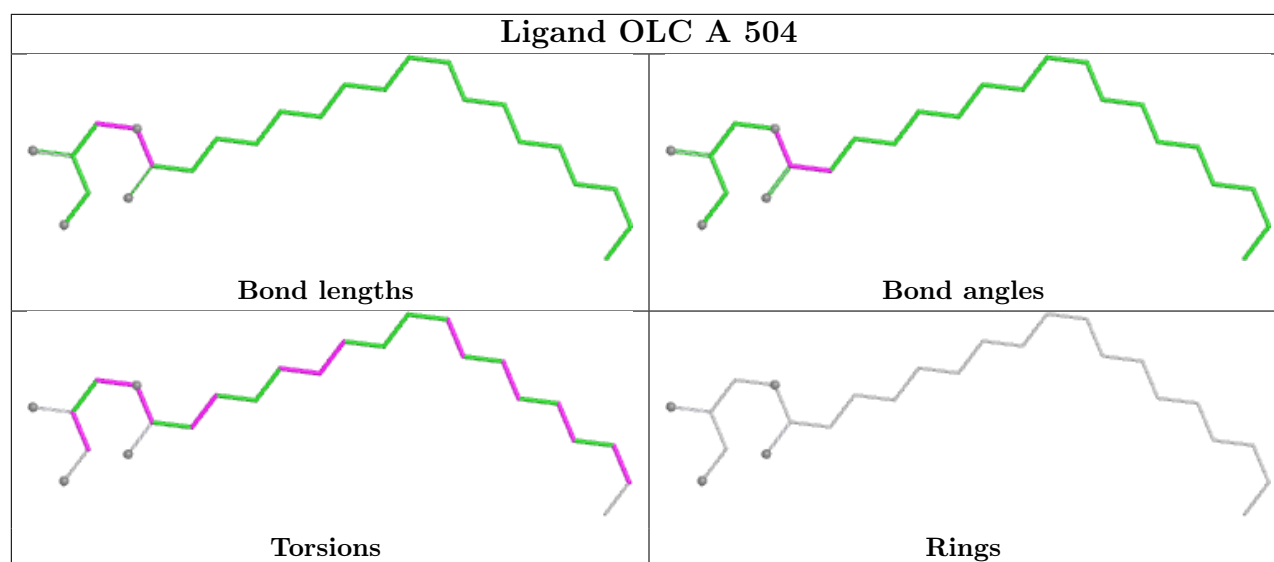
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	OLC	5	0
2	B	501	OLC	8	0
2	B	503	OLC	3	0
2	A	501	OLC	2	0
2	A	502	OLC	6	0
2	B	502	OLC	3	0
2	A	504	OLC	11	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	444/496 (89%)	1.10	55 (12%) 8 7	27, 39, 60, 70	0
1	B	444/496 (89%)	0.84	60 (13%) 7 6	26, 38, 58, 73	0
All	All	888/992 (89%)	0.97	115 (12%) 7 6	26, 39, 60, 73	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	PHE	7.7
1	B	357	TYR	7.6
1	B	124	GLY	6.7
1	B	224	PRO	6.6
1	B	122	VAL	6.6
1	A	122	VAL	6.5
1	B	286	PHE	6.4
1	B	125	ALA	6.2
1	A	124	GLY	5.1
1	A	357	TYR	5.1
1	B	223	LYS	5.1
1	B	118	PHE	4.9
1	A	189	PHE	4.6
1	A	111	TYR	4.5
1	B	123	LEU	4.5
1	B	111	TYR	4.4
1	A	224	PRO	4.4
1	B	248	LEU	4.3
1	B	415	LEU	4.2
1	B	121	LYS	4.2
1	A	192	PRO	4.1
1	B	190	GLY	4.1
1	A	118	PHE	3.9
1	B	189	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	223	LYS	3.9
1	A	1	MET	3.8
1	B	274	ALA	3.5
1	A	281	ILE	3.5
1	B	126	SER	3.5
1	A	287	MET	3.5
1	A	190	GLY	3.4
1	B	364	ILE	3.4
1	B	356	SER	3.3
1	B	228	HIS	3.2
1	B	191	LEU	3.2
1	A	369	MET	3.2
1	B	321	HIS	3.2
1	A	123	LEU	3.1
1	A	280	ARG	3.1
1	B	12	TYR	3.0
1	B	192	PRO	3.0
1	A	12	TYR	3.0
1	B	410	VAL	2.9
1	A	350	GLU	2.9
1	A	290	PHE	2.9
1	B	352	ILE	2.9
1	A	31	LEU	2.8
1	B	280	ARG	2.8
1	B	339	HIS	2.8
1	B	361	ILE	2.8
1	B	354	TRP	2.8
1	B	332	LEU	2.7
1	A	410	VAL	2.7
1	A	333	ILE	2.7
1	B	353	GLU	2.7
1	A	345	PHE	2.7
1	A	277	ILE	2.7
1	A	128	THR	2.6
1	B	358	TYR	2.6
1	B	261	VAL	2.6
1	B	351	VAL	2.6
1	B	227	LEU	2.6
1	B	413	SER	2.6
1	B	277	ILE	2.6
1	A	229	LEU	2.6
1	A	444	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	212	PHE	2.5
1	B	368	ALA	2.5
1	A	283	SER	2.5
1	A	284	ILE	2.5
1	B	128	THR	2.5
1	A	53	ALA	2.5
1	B	350	GLU	2.5
1	A	242	LEU	2.5
1	A	187	GLY	2.5
1	B	425	THR	2.4
1	B	230	ARG	2.4
1	B	335	ILE	2.4
1	B	119	LEU	2.4
1	B	63	TRP	2.4
1	A	182	TYR	2.3
1	B	348	ASP	2.3
1	A	47	ILE	2.3
1	B	142	TRP	2.3
1	B	31	LEU	2.3
1	A	322	PHE	2.3
1	B	345	PHE	2.3
1	A	74	SER	2.3
1	A	142	TRP	2.3
1	B	146	ILE	2.3
1	B	411	ILE	2.3
1	B	343	TYR	2.3
1	B	405	TYR	2.3
1	A	225	PHE	2.2
1	A	185	ILE	2.2
1	A	317	ASN	2.2
1	A	125	ALA	2.2
1	A	282	GLU	2.2
1	A	33	TYR	2.2
1	A	332	LEU	2.2
1	B	427	VAL	2.1
1	A	230	ARG	2.1
1	A	265	ALA	2.1
1	A	121	LYS	2.1
1	B	444	LEU	2.1
1	B	287	MET	2.1
1	A	45	SER	2.1
1	A	248	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	329	LEU	2.1
1	B	325	LEU	2.1
1	A	269	ASP	2.1
1	B	407	LEU	2.0
1	B	367	PRO	2.0
1	A	434	THR	2.0
1	A	371	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

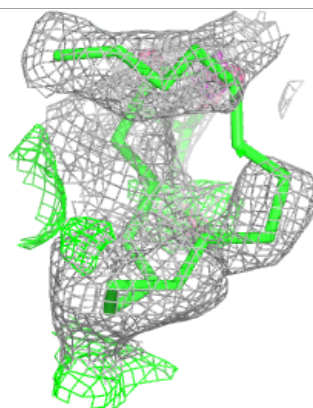
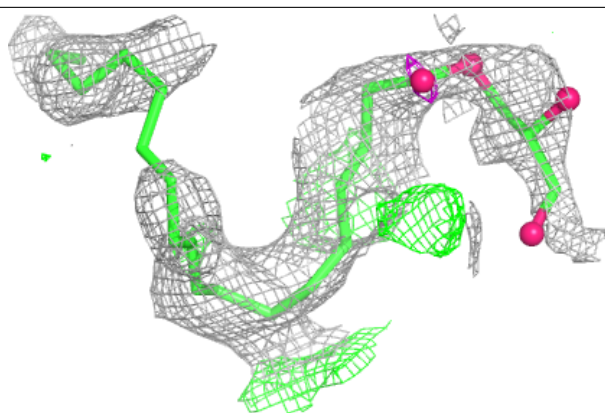
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OLC	A	504	25/25	0.41	0.23	51,64,70,75	0
2	OLC	B	501	25/25	0.66	0.20	35,48,65,68	0
2	OLC	B	502	25/25	0.68	0.19	35,45,68,72	0
2	OLC	B	503	25/25	0.70	0.19	44,54,63,64	0
2	OLC	A	503	25/25	0.72	0.19	46,53,59,63	0
2	OLC	A	501	25/25	0.75	0.17	30,50,65,72	0
2	OLC	A	502	25/25	0.79	0.16	31,43,67,70	0

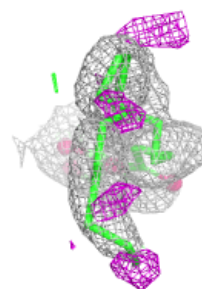
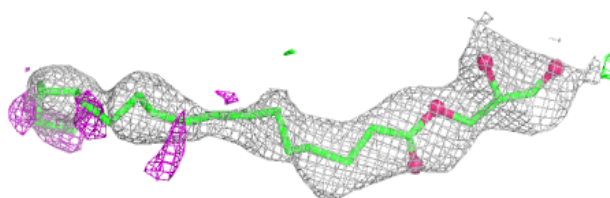
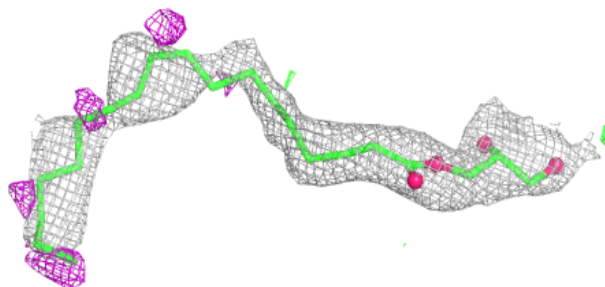
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

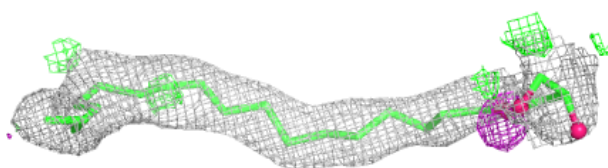
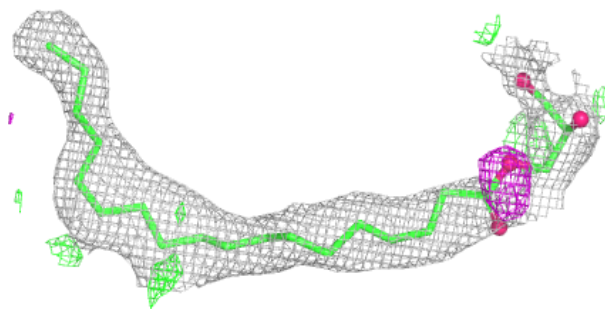
**Electron density around OLC B 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



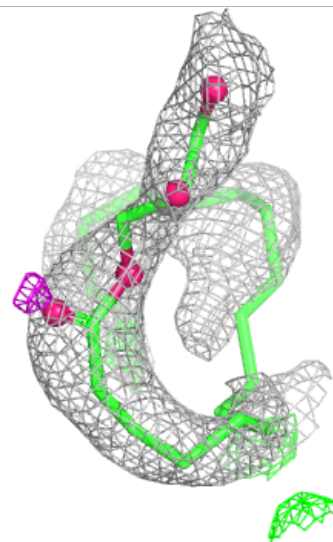
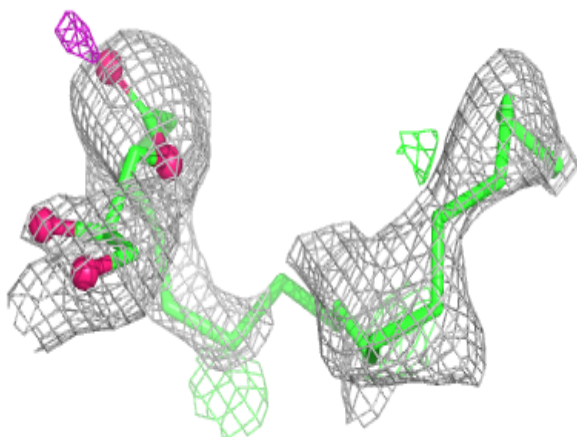
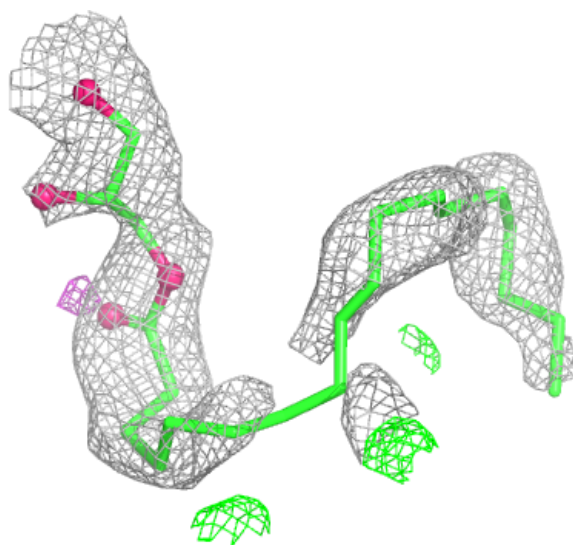
Electron density around OLC B 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



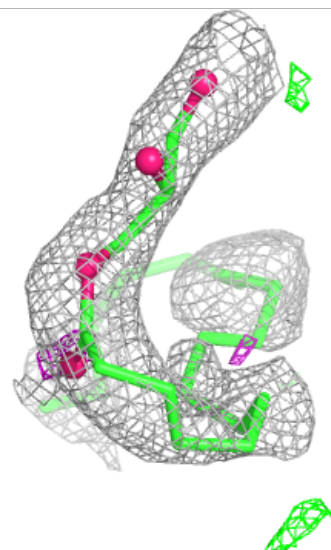
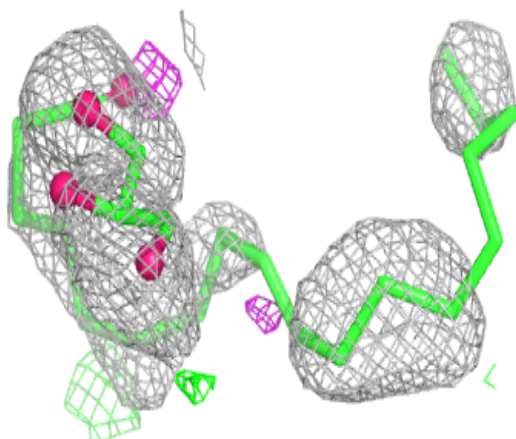
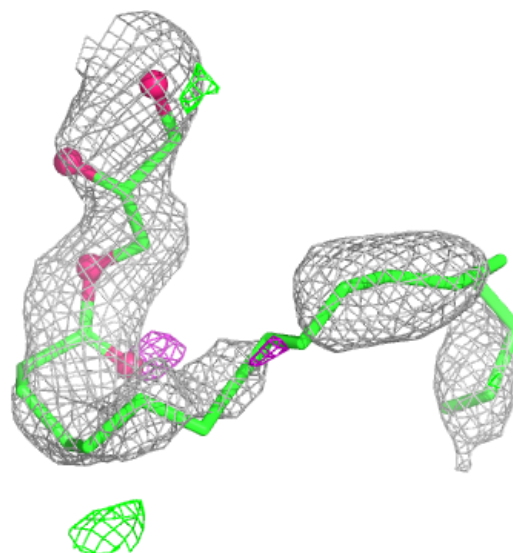
Electron density around OLC B 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



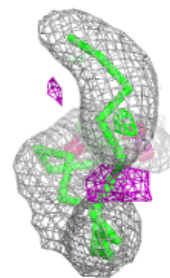
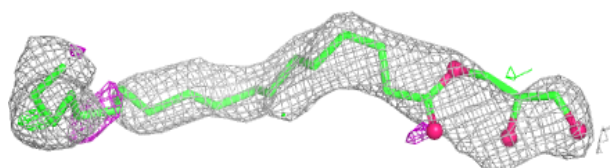
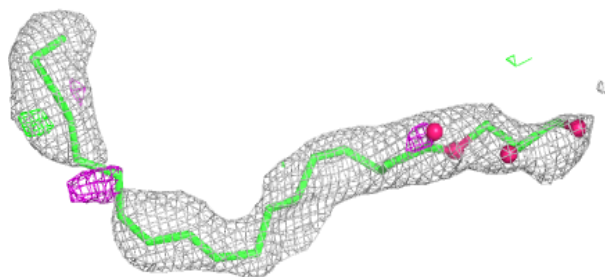
Electron density around OLC A 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

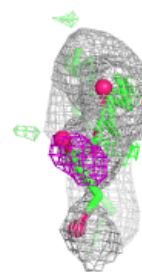
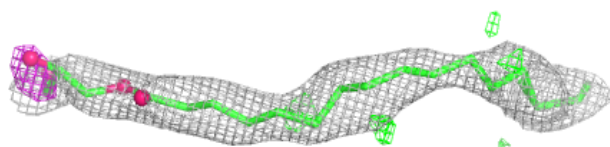
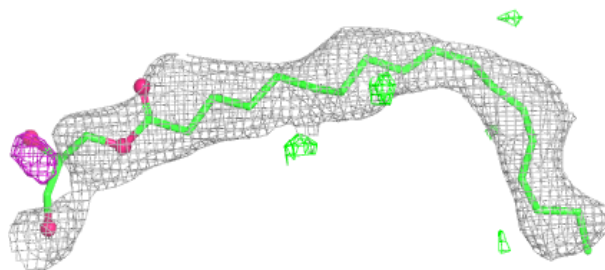


Electron density around OLC A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around OLC A 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.