



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:22 PM UTC

PDB ID : 5OQT / pdb_00005oqt
Title : Crystal structure of a bacterial cationic amino acid transporter (CAT) homologue
Authors : Jungnickel, K.E.J.; Newstead, S.
Deposited on : 2017-08-14
Resolution : 2.86 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

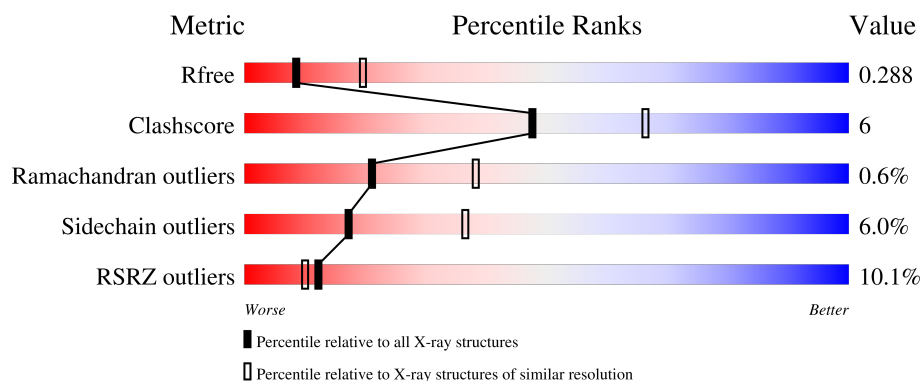
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	471	10% 80% 15% ...
2	C	31	3% 61% 19% 6% 13%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4127 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.

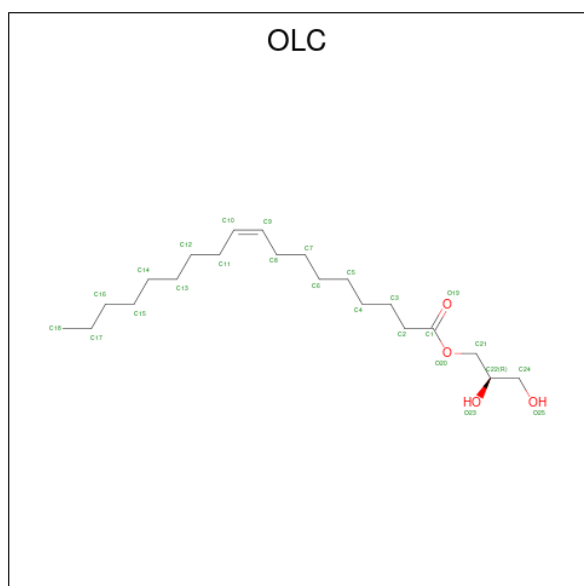
- Molecule 1 is a protein called Amino acid transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3478	2331	547	589	11			

- Molecule 2 is a protein called Uncharacterized protein YneM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	27	Total	C	N	O	S	0	0	0
			207	141	31	32	3			

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



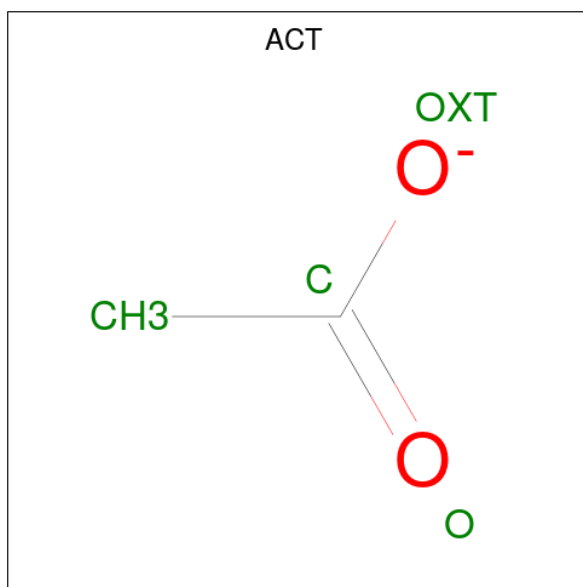
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	21	4		
3	A	1	Total	C	O	0	0
			25	21	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C 11 11	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	A	1	Total C O 25 21 4	0	0
3	C	1	Total C O 25 21 4	0	0

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).

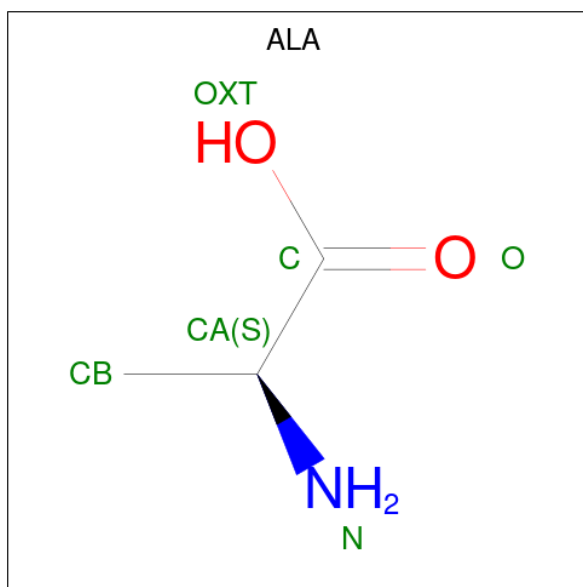


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

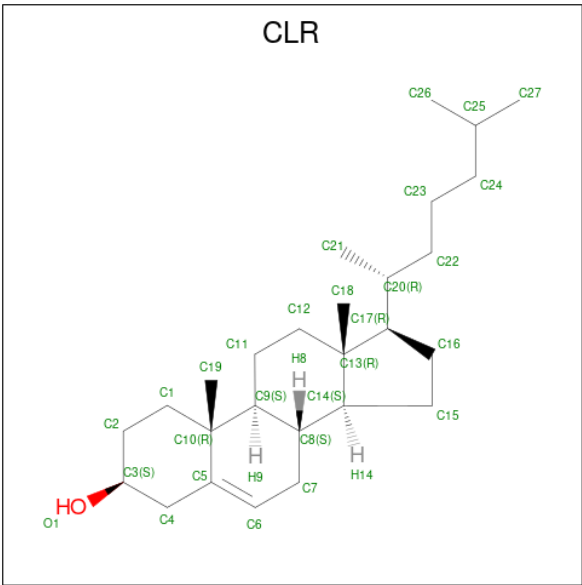
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is ALANINE (CCD ID: ALA) (formula: C₃H₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			28	27	1		

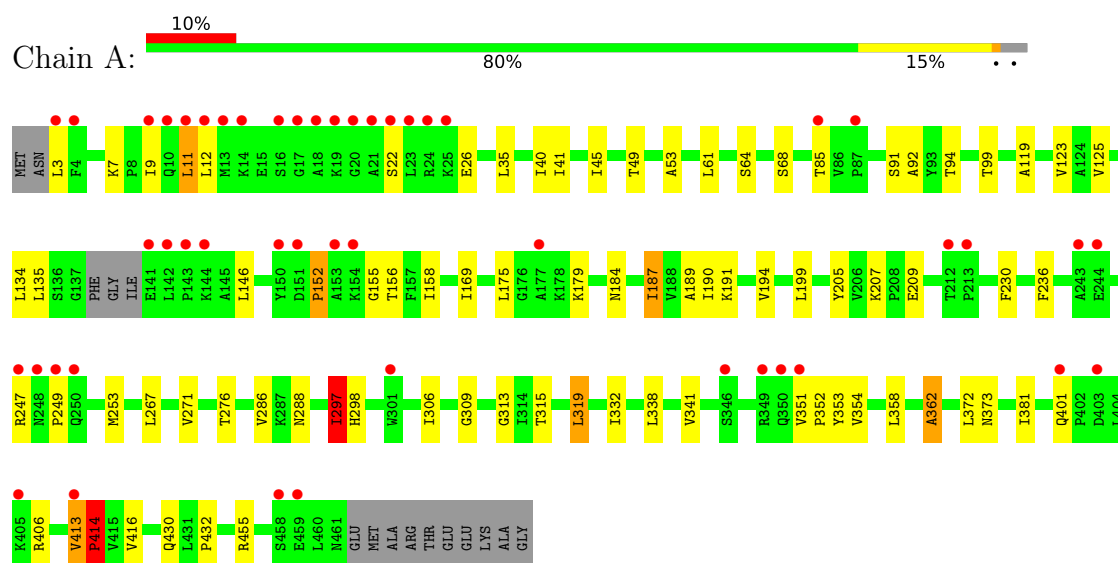
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	106	Total	O	0	0
			106	106		
8	C	2	Total	O	0	0
			2	2		

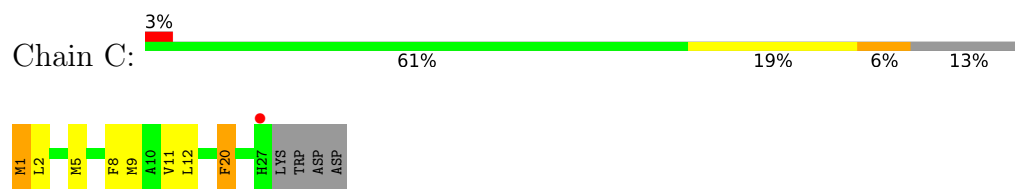
3 Residue-property plots [i](#)

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: Amino acid transporter



- Molecule 2: Uncharacterized protein YneM



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.92Å 83.15Å 119.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.72 – 2.86 64.72 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.2 (64.72-2.86) 99.2 (64.72-2.86)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.215 , 0.271 0.229 , 0.288	Depositor DCC
R_{free} test set	901 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 70.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4127	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, CLR, CL, 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	0.87	1/3568 (0.0%)	1.45	18/4875 (0.4%)
2	C	0.76	0/212	1.62	3/284 (1.1%)
All	All	0.86	1/3780 (0.0%)	1.46	21/5159 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	GLN	CA-C	6.78	1.58	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	GLY	CA-C-N	7.22	132.06	121.31
1	A	155	GLY	C-N-CA	7.22	132.06	121.31
1	A	414	PRO	CA-C-N	6.30	129.02	120.77
1	A	414	PRO	C-N-CA	6.30	129.02	120.77
2	C	20	PHE	CA-CB-CG	6.22	120.02	113.80
1	A	416	VAL	N-CA-CB	5.46	114.71	110.45
1	A	22	SER	CA-C-N	5.30	128.38	120.90
1	A	22	SER	C-N-CA	5.30	128.38	120.90
1	A	68	SER	CA-C-N	5.19	125.71	120.00
1	A	68	SER	C-N-CA	5.19	125.71	120.00
1	A	297	ILE	CA-C-N	5.09	129.37	122.19
1	A	297	ILE	C-N-CA	5.09	129.37	122.19
1	A	362	ALA	CA-C-N	5.08	126.97	120.56
1	A	362	ALA	C-N-CA	5.08	126.97	120.56
1	A	247	ARG	N-CA-C	-5.08	101.47	109.25
2	C	12	LEU	CA-C-N	5.07	125.61	119.98
2	C	12	LEU	C-N-CA	5.07	125.61	119.98
1	A	230	PHE	CA-C-N	5.07	128.42	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	PHE	C-N-CA	5.07	128.42	120.82
1	A	276	THR	CA-C-N	5.05	125.55	120.00
1	A	276	THR	C-N-CA	5.05	125.55	120.00

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	3478	0	3631	39	0
2	C	207	0	211	8	0
3	A	271	0	434	13	0
3	C	25	0	40	1	0
4	A	4	0	3	0	0
5	A	1	0	0	0	0
6	A	5	0	4	0	0
7	C	28	0	46	1	0
8	A	106	0	0	0	0
8	C	2	0	0	0	0
All	All	4127	0	4369	47	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 6.

All (47) 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:A:413:VAL:HG13	1:A:414:PRO:HD3	1.60	0.82
1:A:207:LYS:HG3	3:A:501:OLC:H24	1.74	0.67
1:A:85:THR:CG2	1:A:406:ARG:HG2	2.29	0.62
3:A:503:OLC:H11	3:A:512:OLC:H2A	1.82	0.61
1:A:53:ALA:HB2	1:A:61:LEU:HD22	1.83	0.61
1:A:205:TYR:HB3	1:A:297:ILE:HG12	1.83	0.59
1:A:191:LYS:HG3	1:A:313:GLY:HA3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ILE:HD11	1:A:315:THR:HG23	1.87	0.56
1:A:184:ASN:HB2	3:A:509:OLC:H22	1.88	0.55
1:A:199:LEU:HB3	3:A:501:OLC:H14	1.90	0.54
1:A:85:THR:HG22	1:A:406:ARG:HG2	1.90	0.53
1:A:179:LYS:HB2	3:A:509:OLC:H24A	1.90	0.53
1:A:12:LEU:HD22	1:A:94:THR:HG23	1.90	0.53
1:A:286:VAL:HG12	1:A:288:ASN:H	1.74	0.53
2:C:2:LEU:H	2:C:5:MET:HE3	1.74	0.53
1:A:249:PRO:HB2	1:A:253:MET:HE2	1.91	0.52
1:A:267:LEU:O	1:A:271:VAL:HG23	2.11	0.51
1:A:189:ALA:CB	2:C:11:VAL:HG23	2.40	0.51
1:A:152:PRO:HD3	1:A:156:THR:O	2.12	0.50
1:A:189:ALA:HB1	2:C:11:VAL:HG23	1.94	0.48
2:C:1:MET:HG2	2:C:5:MET:HE2	1.96	0.47
3:A:501:OLC:H17A	3:A:512:OLC:H10	1.96	0.47
2:C:9:MET:HB3	3:C:102:OLC:H4	1.97	0.46
1:A:351:VAL:HB	1:A:352:PRO:HD2	1.97	0.46
2:C:20:PHE:CD1	7:C:101:CLR:H211	2.50	0.46
1:A:362:ALA:HB2	3:A:506:OLC:H6	1.98	0.45
1:A:7:LYS:HE3	1:A:11:LEU:HD12	1.98	0.45
1:A:205:TYR:CB	1:A:297:ILE:HG12	2.46	0.45
1:A:45:ILE:O	1:A:49:THR:CG2	2.65	0.45
1:A:194:VAL:HG11	1:A:309:GLY:HA3	1.99	0.44
3:A:503:OLC:H13	3:A:512:OLC:H4A	1.99	0.44
1:A:40:ILE:HD11	1:A:236:PHE:HB3	1.99	0.44
1:A:125:VAL:HG11	1:A:372:LEU:HB2	1.99	0.44
1:A:358:LEU:HB3	3:A:506:OLC:H4	1.99	0.44
1:A:319:LEU:HD13	3:A:509:OLC:H3	1.99	0.43
1:A:119:ALA:O	1:A:123:VAL:HG23	2.18	0.43
1:A:3:LEU:HG	1:A:455:ARG:HH22	1.83	0.43
1:A:189:ALA:HB3	2:C:11:VAL:CG2	2.49	0.42
1:A:41:ILE:HB	1:A:191:LYS:HD2	2.02	0.42
1:A:338:LEU:HD23	1:A:338:LEU:HA	1.97	0.42
1:A:187:ILE:HA	1:A:190:ILE:HD12	2.02	0.42
1:A:354:VAL:HG22	3:A:506:OLC:H24	2.01	0.42
1:A:332:ILE:HG22	1:A:338:LEU:HB2	2.02	0.41
3:A:504:OLC:H7A	3:A:509:OLC:H4A	2.02	0.41
1:A:189:ALA:HB2	2:C:8:PHE:CD1	2.55	0.41
1:A:432:PRO:HA	3:A:507:OLC:H4A	2.03	0.41
1:A:341:VAL:HG12	1:A:353:TYR:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	452/471 (96%)	424 (94%)	25 (6%)	3 (1%)	18	35
2	C	25/31 (81%)	24 (96%)	1 (4%)	0	100	100
All	All	477/502 (95%)	448 (94%)	26 (6%)	3 (1%)	21	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	PRO
1	A	92	ALA
1	A	414	PRO

5.3.2 Protein sidechains

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	362/373 (97%)	340 (94%)	22 (6%)	17	35
2	C	21/25 (84%)	20 (95%)	1 (5%)	23	46
All	All	383/398 (96%)	360 (94%)	23 (6%)	17	36

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	11	LEU
1	A	26	GLU

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Mol	Chain	Res	Type
1	A	35	LEU
1	A	64	SER
1	A	91	SER
1	A	99	THR
1	A	134	LEU
1	A	135	LEU
1	A	146	LEU
1	A	158	ILE
1	A	175	LEU
1	A	187	ILE
1	A	209	GLU
1	A	297	ILE
1	A	298	HIS
1	A	306	ILE
1	A	319	LEU
1	A	373	ASN
1	A	381	ILE
1	A	413	VAL
1	A	430	GLN
2	C	1	MET

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	132	GLN
1	A	350	GLN
1	A	373	ASN
1	A	430	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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
3	OLC	A	504	-	24,24,24	0.89	1 (4%)	25,25,25	0.98	2 (8%)
3	OLC	C	102	-	24,24,24	0.88	1 (4%)	25,25,25	0.89	2 (8%)
4	ACT	A	513	-	3,3,3	1.18	0	3,3,3	0.85	0
6	ALA	A	515	-	3,4,5	0.86	0	2,4,6	1.49	1 (50%)
3	OLC	A	502	-	24,24,24	0.94	2 (8%)	25,25,25	0.98	2 (8%)
3	OLC	A	507	-	24,24,24	0.87	1 (4%)	25,25,25	0.93	1 (4%)
3	OLC	A	511	-	24,24,24	0.77	0	25,25,25	0.68	0
3	OLC	A	501	-	24,24,24	0.95	2 (8%)	25,25,25	0.73	0
7	CLR	C	101	-	31,31,31	1.75	10 (32%)	48,48,48	1.60	7 (14%)
3	OLC	A	505	-	10,10,24	0.45	0	9,9,25	0.70	0
3	OLC	A	512	-	24,24,24	0.83	1 (4%)	25,25,25	0.74	0
3	OLC	A	509	-	24,24,24	0.80	0	25,25,25	0.72	0
3	OLC	A	508	-	9,9,24	0.51	0	8,8,25	0.58	0
3	OLC	A	510	-	24,24,24	0.82	1 (4%)	25,25,25	0.65	0
3	OLC	A	506	-	24,24,24	0.81	0	25,25,25	0.76	0
3	OLC	A	503	-	24,24,24	0.95	2 (8%)	25,25,25	0.94	2 (8%)

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
3	OLC	A	504	-	-	8/24/24/24	-
3	OLC	C	102	-	-	7/24/24/24	-
6	ALA	A	515	-	-	0/1/2/4	-
3	OLC	A	502	-	-	9/24/24/24	-
3	OLC	A	507	-	-	8/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLC	A	511	-	-	8/24/24/24	-
3	OLC	A	501	-	-	9/24/24/24	-
7	CLR	C	101	-	-	9/10/68/68	0/4/4/4
3	OLC	A	505	-	-	2/8/8/24	-
3	OLC	A	512	-	-	6/24/24/24	-
3	OLC	A	509	-	-	5/24/24/24	-
3	OLC	A	508	-	-	2/7/7/24	-
3	OLC	A	510	-	-	9/24/24/24	-
3	OLC	A	506	-	-	5/24/24/24	-
3	OLC	A	503	-	-	10/24/24/24	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	101	CLR	C10-C9	3.49	1.61	1.56
7	C	101	CLR	C13-C17	3.42	1.61	1.55
7	C	101	CLR	C8-C9	3.02	1.59	1.53
3	A	503	OLC	O20-C1	2.97	1.42	1.33
7	C	101	CLR	C13-C14	2.70	1.59	1.55
7	C	101	CLR	C18-C13	2.68	1.58	1.54
3	A	502	OLC	O20-C1	2.57	1.40	1.33
3	A	504	OLC	O20-C1	2.51	1.40	1.33
7	C	101	CLR	C12-C13	2.46	1.58	1.54
3	A	501	OLC	O20-C1	2.46	1.40	1.33
7	C	101	CLR	C2-C3	2.43	1.57	1.51
3	C	102	OLC	O20-C1	2.39	1.40	1.33
3	A	507	OLC	O20-C1	2.33	1.40	1.33
7	C	101	CLR	C11-C9	2.33	1.57	1.53
7	C	101	CLR	C4-C3	2.30	1.56	1.52
3	A	512	OLC	O20-C1	2.29	1.40	1.33
7	C	101	CLR	C1-C10	2.28	1.58	1.54
3	A	510	OLC	O20-C1	2.20	1.39	1.33
3	A	501	OLC	C21-C22	2.16	1.58	1.51
3	A	503	OLC	C21-C22	2.10	1.58	1.51
3	A	502	OLC	C21-C22	2.09	1.58	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	101	CLR	C17-C13-C14	-5.84	93.39	100.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	101	CLR	C21-C20-C22	-4.35	103.60	110.34
7	C	101	CLR	C13-C17-C20	2.98	124.10	119.50
3	A	502	OLC	O20-C1-O19	-2.96	116.23	123.63
3	A	504	OLC	O20-C1-O19	-2.89	116.40	123.63
3	A	507	OLC	O20-C1-O19	-2.60	117.12	123.63
7	C	101	CLR	C18-C13-C14	2.56	116.33	111.68
3	C	102	OLC	O20-C1-O19	-2.47	117.45	123.63
3	A	503	OLC	O20-C1-O19	-2.41	117.59	123.63
3	A	504	OLC	C21-O20-C1	2.35	125.72	117.12
3	A	503	OLC	C21-O20-C1	2.34	125.66	117.12
3	A	502	OLC	C21-O20-C1	2.34	125.66	117.12
3	C	102	OLC	C21-O20-C1	2.33	125.64	117.12
6	A	515	ALA	O-C-CA	-2.10	117.50	124.23
7	C	101	CLR	C16-C17-C13	-2.06	101.42	103.84
7	C	101	CLR	C1-C2-C3	2.05	113.19	110.48
7	C	101	CLR	C2-C3-C4	2.03	113.15	110.29

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	OLC	O23-C22-C24-O25
3	A	502	OLC	O20-C21-C22-O23
3	A	502	OLC	C2-C1-O20-C21
3	A	502	OLC	O19-C1-O20-C21
3	A	503	OLC	C2-C1-O20-C21
3	A	503	OLC	O19-C1-O20-C21
3	A	504	OLC	C2-C1-O20-C21
3	A	504	OLC	O19-C1-O20-C21
3	A	507	OLC	C2-C1-O20-C21
3	A	507	OLC	O19-C1-O20-C21
3	C	102	OLC	C2-C1-O20-C21
3	C	102	OLC	O19-C1-O20-C21
7	C	101	CLR	C13-C17-C20-C21
7	C	101	CLR	C16-C17-C20-C22
7	C	101	CLR	C13-C17-C20-C22
3	A	501	OLC	O20-C21-C22-O23
7	C	101	CLR	C16-C17-C20-C21
3	A	501	OLC	O20-C21-C22-C24
7	C	101	CLR	C17-C20-C22-C23
7	C	101	CLR	C21-C20-C22-C23
3	A	501	OLC	C21-C22-C24-O25

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Mol	Chain	Res	Type	Atoms
3	A	503	OLC	C21-C22-C24-O25
3	A	510	OLC	C21-C22-C24-O25
3	A	511	OLC	C21-C22-C24-O25
3	A	504	OLC	C13-C14-C15-C16
3	A	509	OLC	C11-C12-C13-C14
3	A	510	OLC	C2-C3-C4-C5
3	A	503	OLC	C4-C5-C6-C7
3	A	510	OLC	C14-C15-C16-C17
3	A	512	OLC	C3-C4-C5-C6
3	A	501	OLC	C11-C12-C13-C14
3	A	501	OLC	C4-C5-C6-C7
3	A	512	OLC	C4-C5-C6-C7
3	A	507	OLC	C1-C2-C3-C4
3	A	511	OLC	C6-C7-C8-C9
3	A	512	OLC	C10-C11-C12-C13
3	C	102	OLC	C10-C11-C12-C13
3	A	512	OLC	C14-C15-C16-C17
3	A	503	OLC	C14-C15-C16-C17
3	A	511	OLC	C3-C4-C5-C6
3	A	501	OLC	C12-C13-C14-C15
3	A	511	OLC	C11-C12-C13-C14
3	A	504	OLC	C4-C5-C6-C7
3	A	510	OLC	C11-C12-C13-C14
3	A	504	OLC	C6-C7-C8-C9
3	A	508	OLC	C15-C16-C17-C18
3	A	502	OLC	C2-C3-C4-C5
3	C	102	OLC	C11-C12-C13-C14
3	A	502	OLC	C14-C15-C16-C17
3	A	506	OLC	C15-C16-C17-C18
3	A	509	OLC	C5-C6-C7-C8
3	A	504	OLC	C11-C12-C13-C14
3	A	503	OLC	C15-C16-C17-C18
3	A	502	OLC	O20-C21-C22-C24
3	A	512	OLC	C15-C16-C17-C18
3	A	503	OLC	C2-C3-C4-C5
3	A	503	OLC	C3-C4-C5-C6
3	A	510	OLC	C13-C14-C15-C16
3	A	505	OLC	C9-C10-C11-C12
3	A	511	OLC	C15-C16-C17-C18
7	C	101	CLR	C23-C24-C25-C27
3	A	503	OLC	C6-C7-C8-C9
7	C	101	CLR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
3	A	511	OLC	C4-C5-C6-C7
3	A	504	OLC	C10-C11-C12-C13
3	C	102	OLC	C15-C16-C17-C18
3	A	508	OLC	C9-C10-C11-C12
3	A	504	OLC	C9-C10-C11-C12
3	A	511	OLC	O20-C21-C22-O23
3	A	506	OLC	C7-C8-C9-C10
3	A	506	OLC	C6-C7-C8-C9
3	A	502	OLC	O23-C22-C24-O25
3	A	511	OLC	O23-C22-C24-O25
3	A	512	OLC	C7-C8-C9-C10
3	A	505	OLC	C7-C8-C9-C10
3	A	510	OLC	C3-C4-C5-C6
3	A	502	OLC	C9-C10-C11-C12
3	A	509	OLC	C13-C14-C15-C16
3	A	510	OLC	C9-C10-C11-C12
3	A	503	OLC	C13-C14-C15-C16
3	A	507	OLC	C14-C15-C16-C17
3	A	506	OLC	C2-C3-C4-C5
3	A	502	OLC	C21-C22-C24-O25
3	A	501	OLC	C1-C2-C3-C4
3	A	509	OLC	C14-C15-C16-C17
3	A	507	OLC	O20-C1-C2-C3
3	C	102	OLC	C13-C14-C15-C16
3	A	510	OLC	O20-C1-C2-C3
3	A	507	OLC	C7-C8-C9-C10
3	A	501	OLC	C9-C10-C11-C12
3	A	510	OLC	O19-C1-C2-C3
3	A	507	OLC	O20-C21-C22-O23
3	A	509	OLC	O23-C22-C24-O25
3	A	507	OLC	O19-C1-C2-C3
7	C	101	CLR	C22-C23-C24-C25
3	A	506	OLC	C4-C5-C6-C7
3	C	102	OLC	C14-C15-C16-C17

There are no ring outliers.

9 monomers are involved in 15 short contacts:

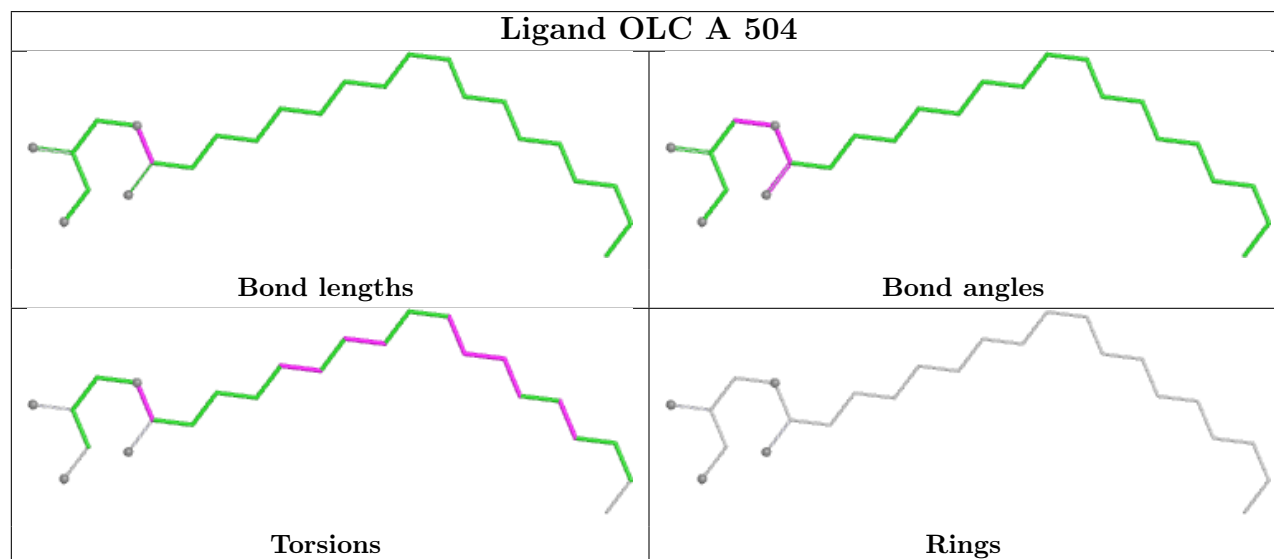
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	OLC	1	0
3	C	102	OLC	1	0
3	A	507	OLC	1	0

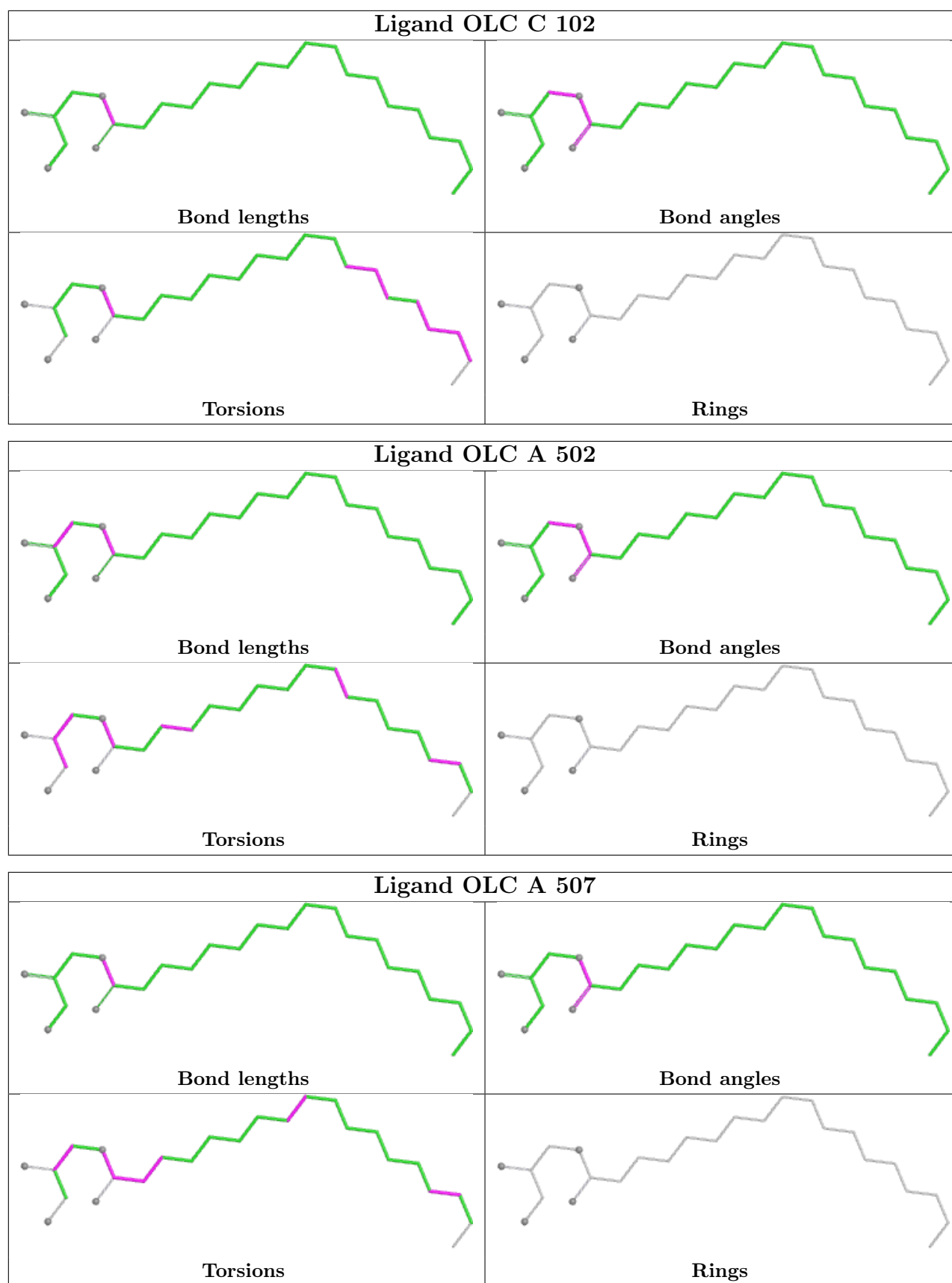
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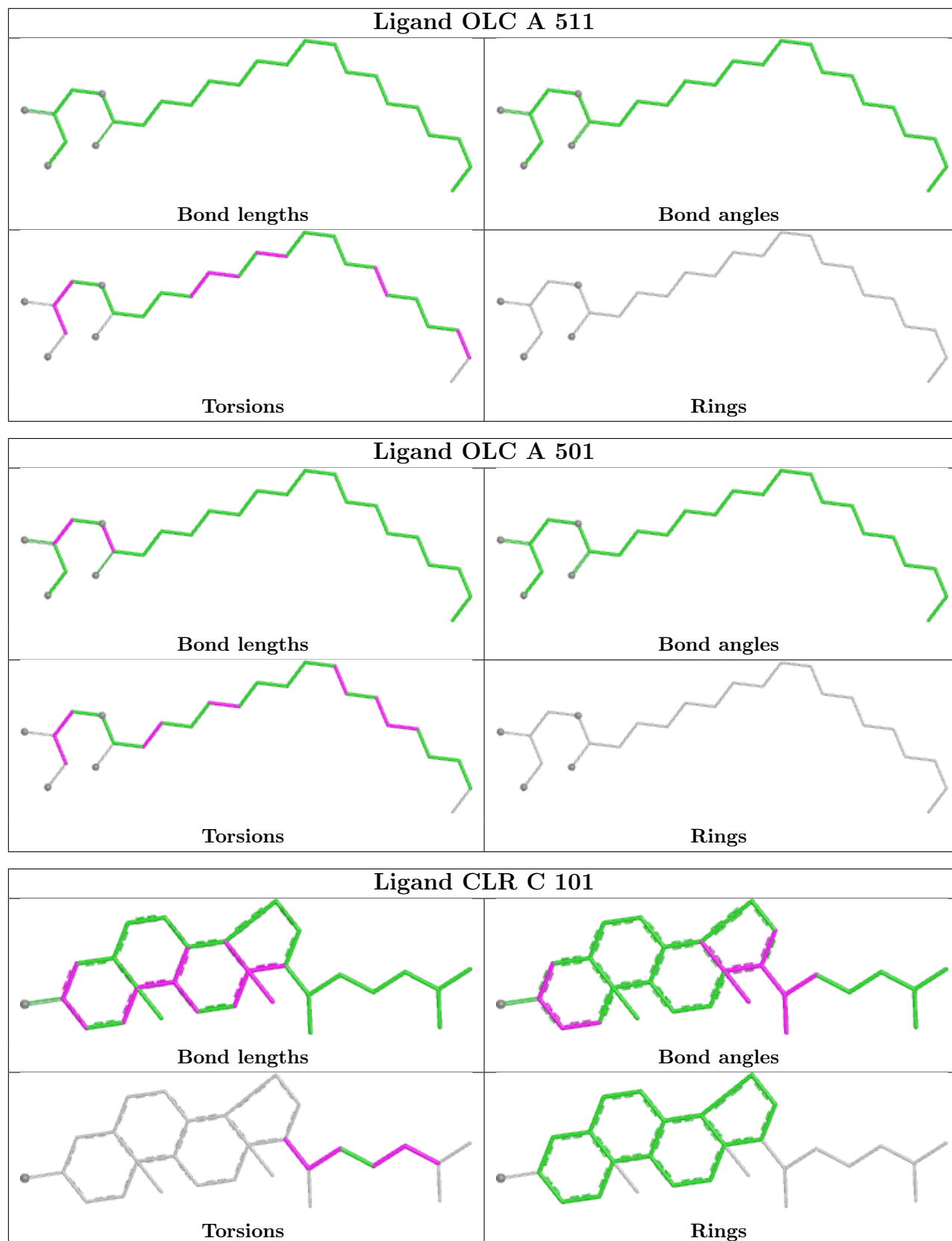
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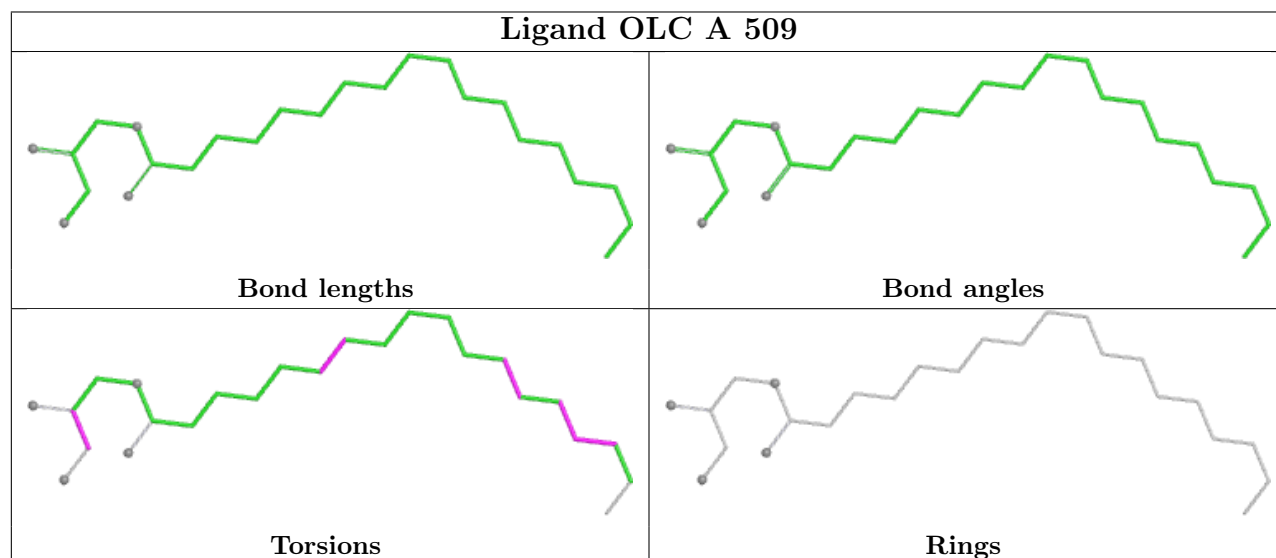
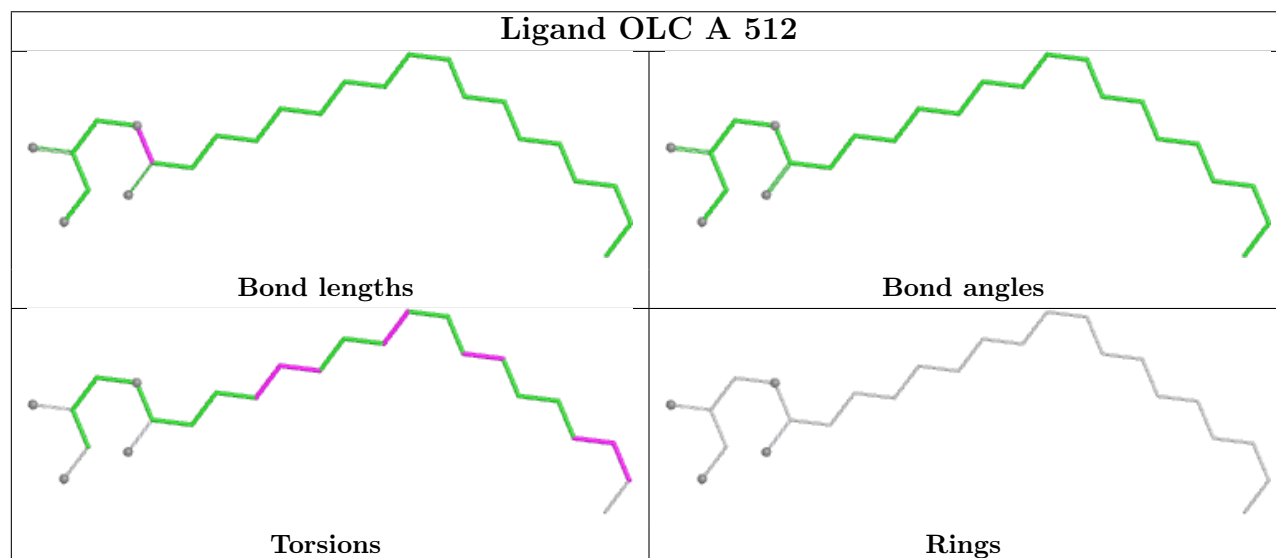
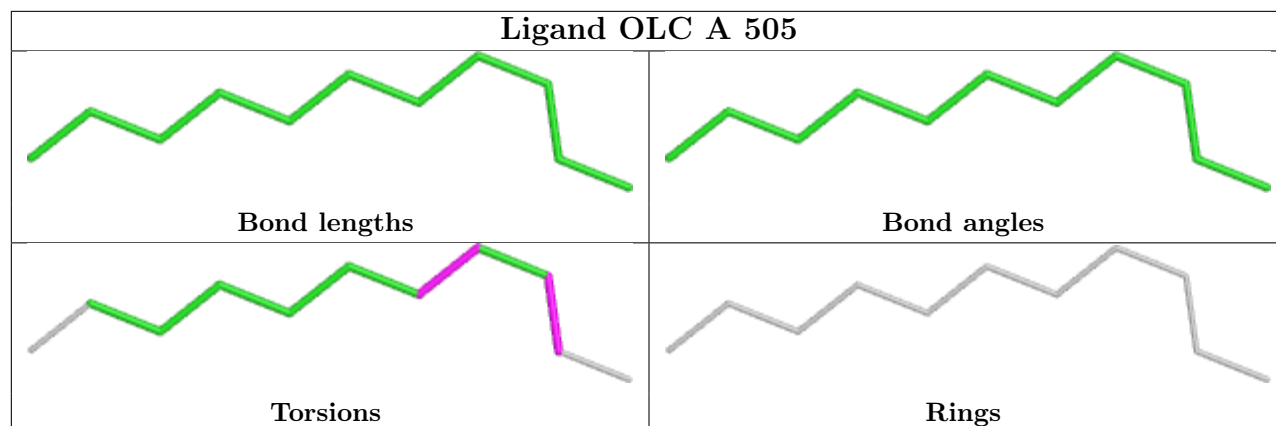
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	OLC	3	0
7	C	101	CLR	1	0
3	A	512	OLC	3	0
3	A	509	OLC	4	0
3	A	506	OLC	3	0
3	A	503	OLC	2	0

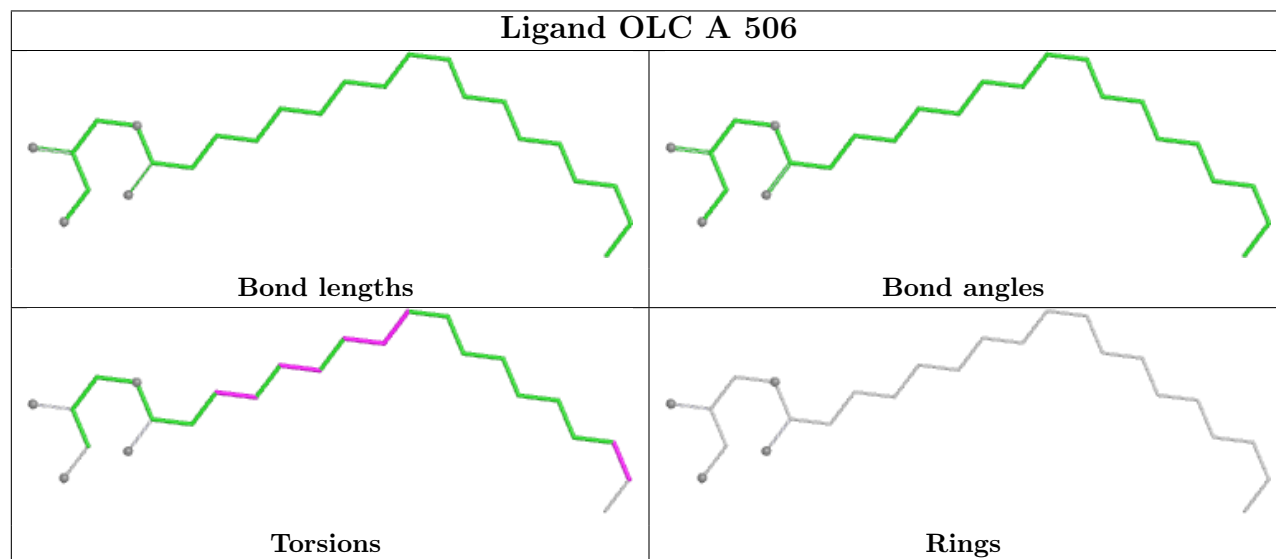
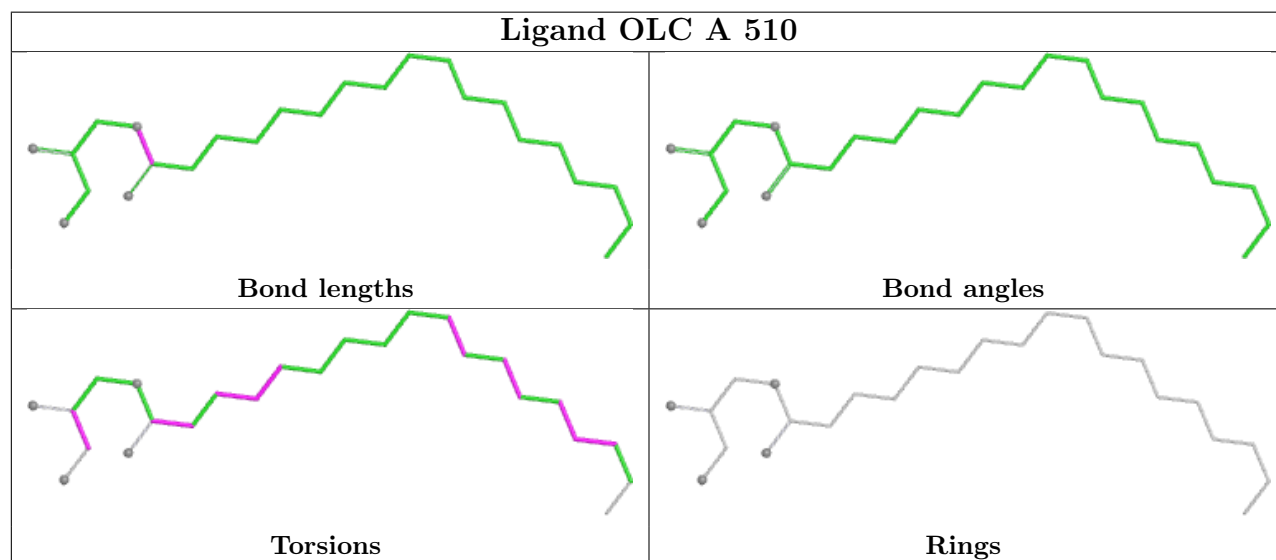
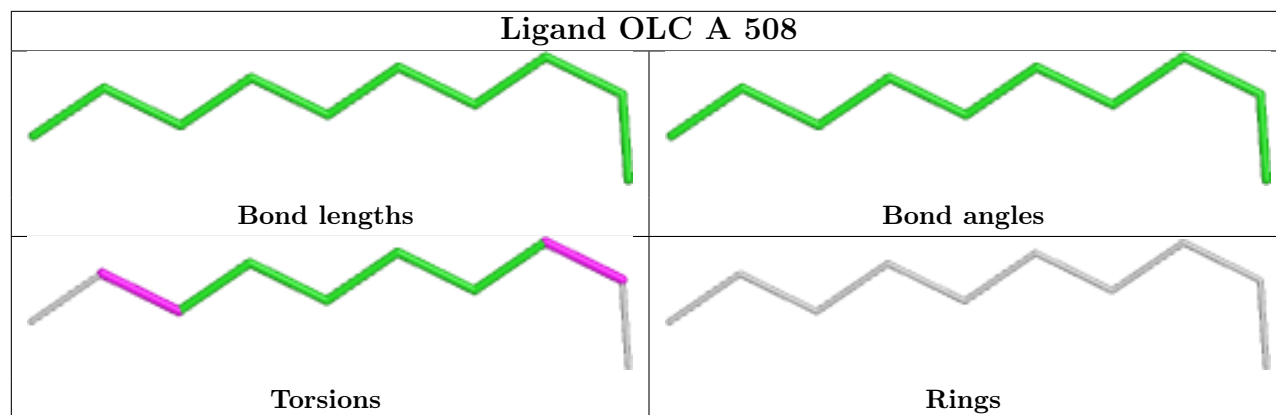
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

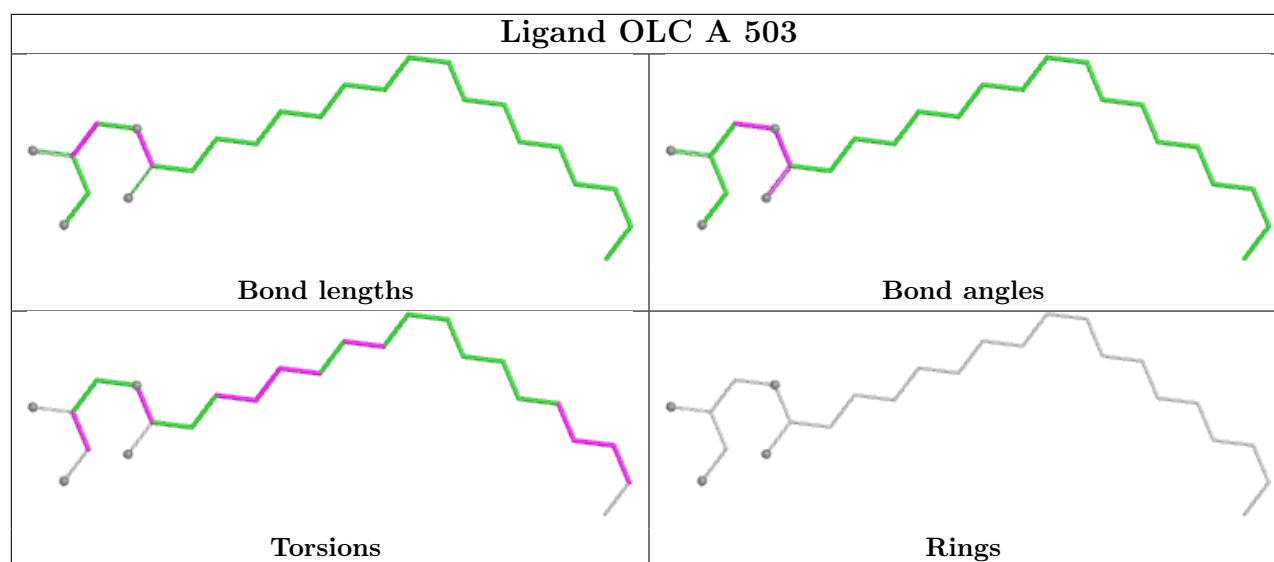












5.7 Other polymers [i](#)

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	456/471 (96%)	0.50	48 (10%) 11 9	49, 72, 117, 135	0
2	C	27/31 (87%)	0.53	1 (3%) 45 35	59, 69, 106, 134	0
All	All	483/502 (96%)	0.50	49 (10%) 12 10	49, 72, 117, 135	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	SER	8.3
1	A	21	ALA	7.5
1	A	17	GLY	6.3
1	A	10	GLN	5.7
1	A	247	ARG	5.7
1	A	23	LEU	5.6
1	A	20	GLY	5.3
1	A	18	ALA	4.9
1	A	14	LYS	4.7
1	A	244	GLU	4.6
1	A	87	PRO	4.5
1	A	403	ASP	4.3
1	A	25	LYS	4.2
1	A	413	VAL	4.0
1	A	142	LEU	3.7
1	A	212	THR	3.6
1	A	141	GLU	3.3
1	A	243	ALA	3.2
1	A	150	TYR	3.1
1	A	346	SER	3.0
2	C	27	HIS	3.0
1	A	13	MET	2.9
1	A	3	LEU	2.7
1	A	401	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	24	ARG	2.5
1	A	16	SER	2.5
1	A	143	PRO	2.5
1	A	248	ASN	2.4
1	A	12	LEU	2.4
1	A	4	PHE	2.4
1	A	19	LYS	2.4
1	A	144	LYS	2.4
1	A	350	GLN	2.4
1	A	85	THR	2.4
1	A	9	ILE	2.4
1	A	459	GLU	2.3
1	A	250	GLN	2.3
1	A	213	PRO	2.3
1	A	349	ARG	2.3
1	A	301	TRP	2.3
1	A	249	PRO	2.3
1	A	153	ALA	2.3
1	A	458	SER	2.2
1	A	177	ALA	2.2
1	A	351	VAL	2.2
1	A	154	LYS	2.2
1	A	405	LYS	2.1
1	A	11	LEU	2.0
1	A	151	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

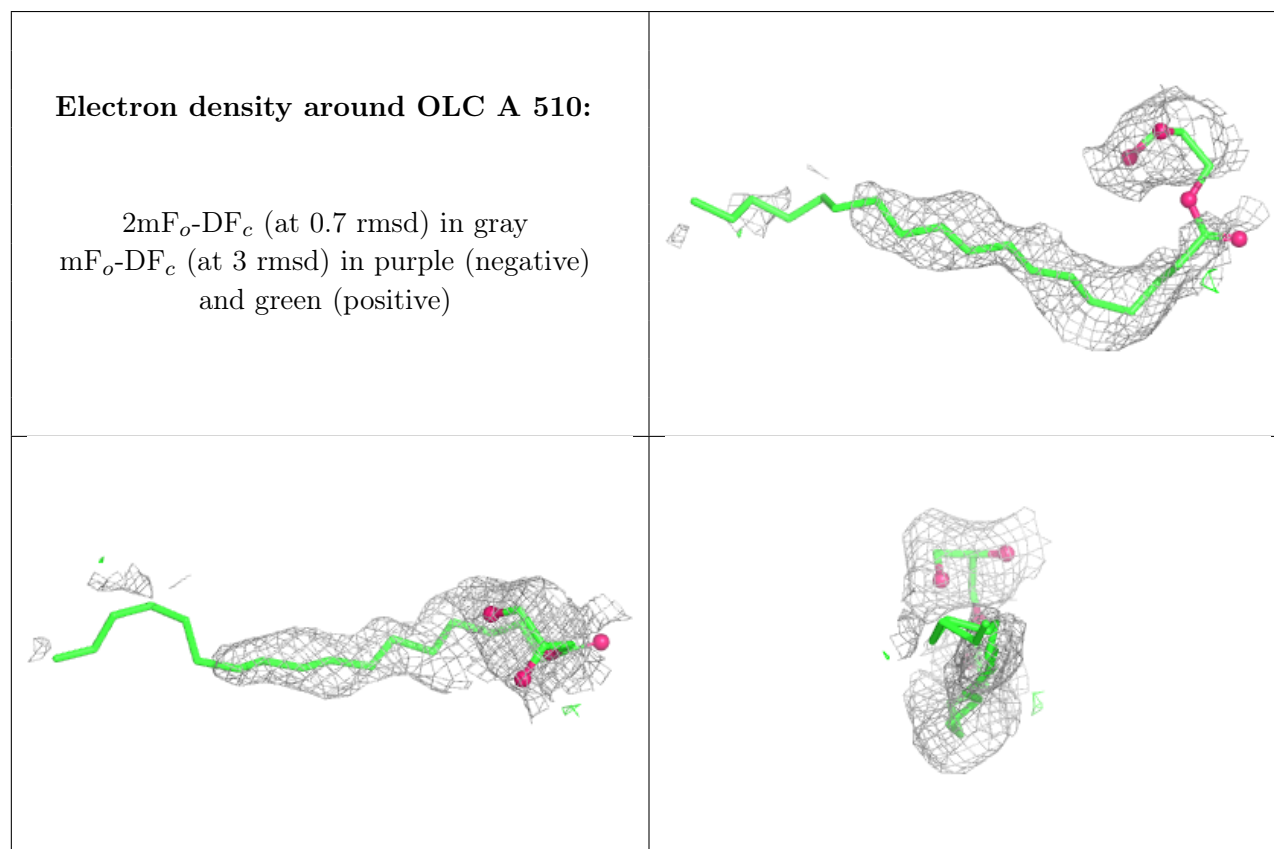
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

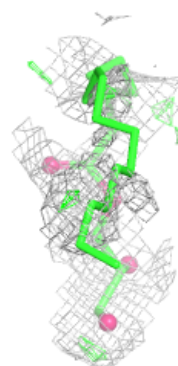
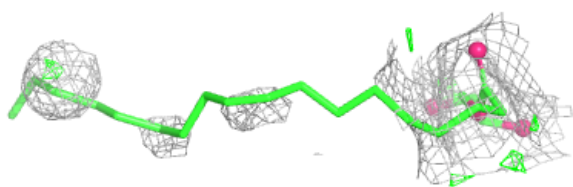
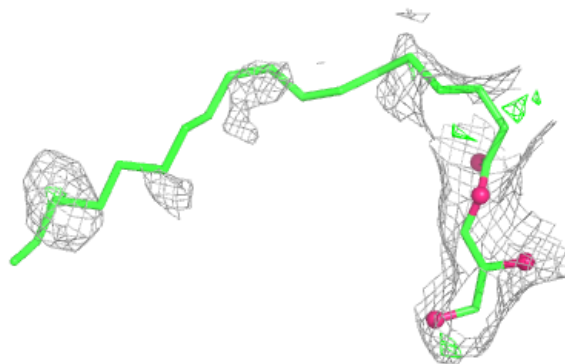
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	A	513	4/4	0.48	0.28	139,139,139,140	0
3	OLC	A	510	25/25	0.63	0.23	119,123,140,141	0
3	OLC	A	511	25/25	0.65	0.21	143,148,151,151	0
3	OLC	A	508	10/25	0.70	0.29	80,81,83,84	0
3	OLC	A	504	25/25	0.72	0.22	106,121,135,135	0
3	OLC	A	507	25/25	0.73	0.19	111,124,131,131	0
3	OLC	C	102	25/25	0.75	0.19	71,84,119,122	0
3	OLC	A	509	25/25	0.75	0.22	130,132,145,146	0
3	OLC	A	503	25/25	0.77	0.19	66,86,113,114	0
3	OLC	A	512	25/25	0.77	0.21	99,103,116,116	0
3	OLC	A	502	25/25	0.78	0.20	91,97,102,103	0
6	ALA	A	515	5/6	0.78	0.13	32,35,49,57	0
3	OLC	A	501	25/25	0.81	0.18	73,86,105,106	0
3	OLC	A	505	11/25	0.82	0.18	71,72,75,75	0
3	OLC	A	506	25/25	0.83	0.19	93,95,99,99	0
5	CL	A	514	1/1	0.89	0.21	79,79,79,79	0
7	CLR	C	101	28/28	0.89	0.15	71,83,90,91	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.

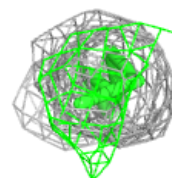
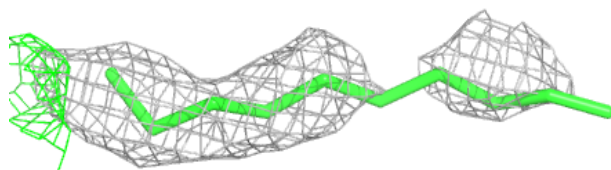
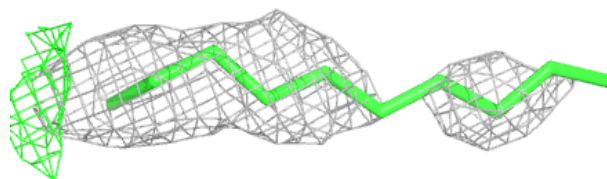


Electron density around OLC A 511:

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

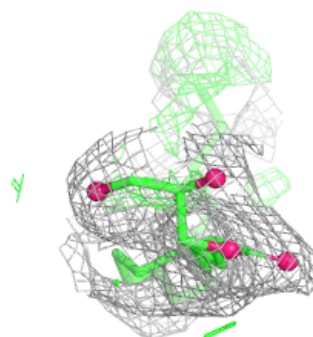
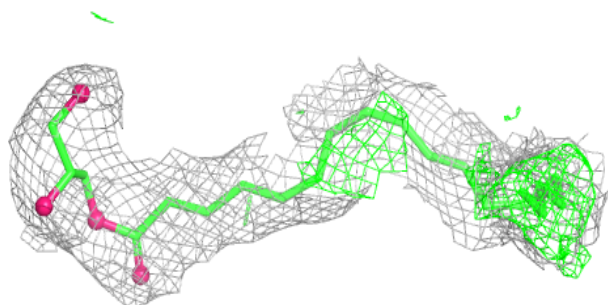
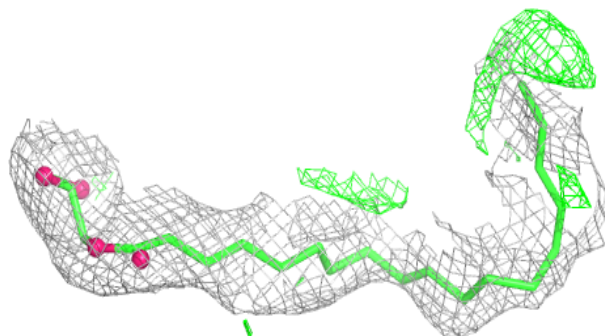
**Electron density around OLC A 508:**

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

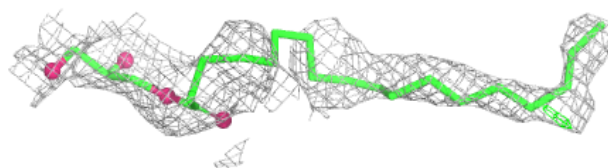
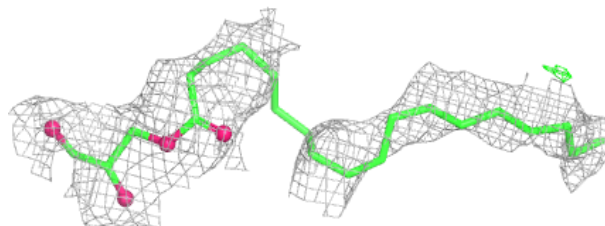


Electron density around OLC A 504:

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

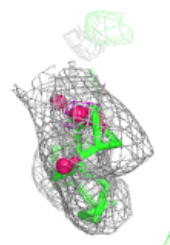
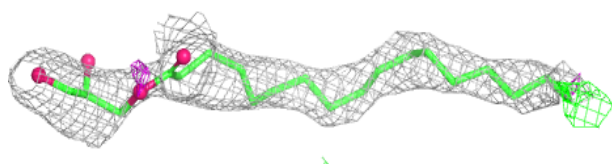
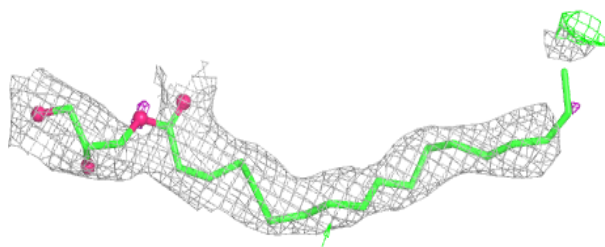
**Electron density around OLC A 507:**

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

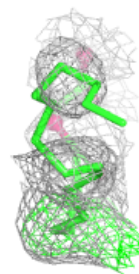
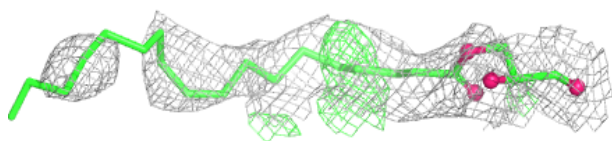
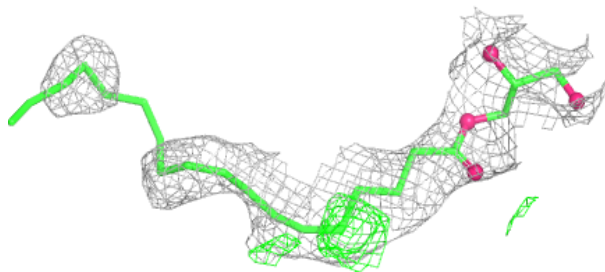


Electron density around OLC C 102:

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

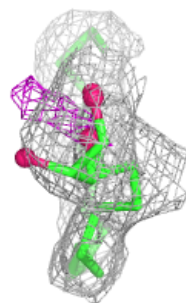
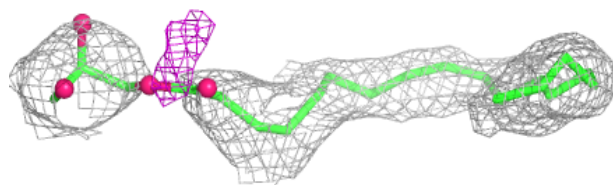
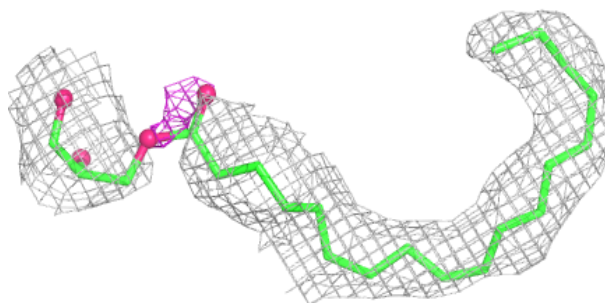
**Electron density around OLC A 509:**

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

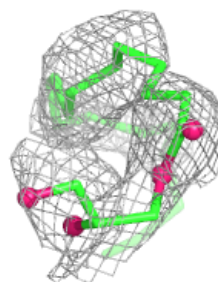
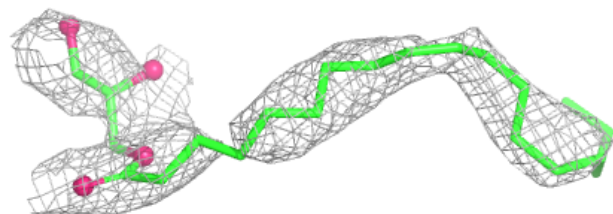
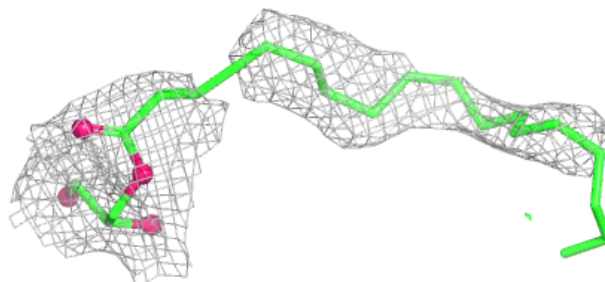


Electron density around OLC A 503:

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

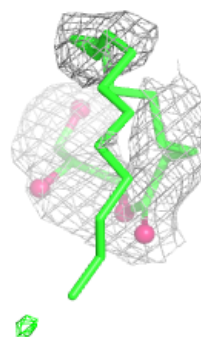
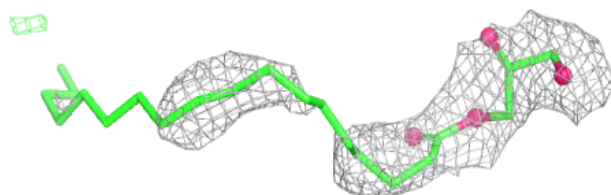
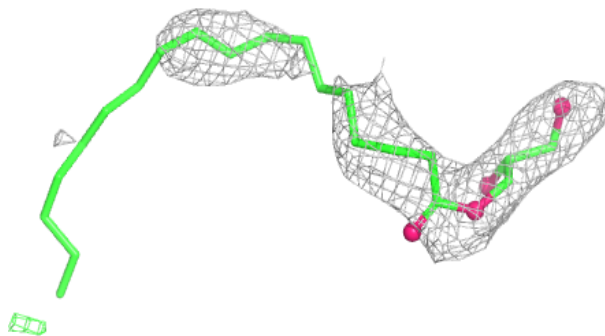
**Electron density around OLC A 512:**

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

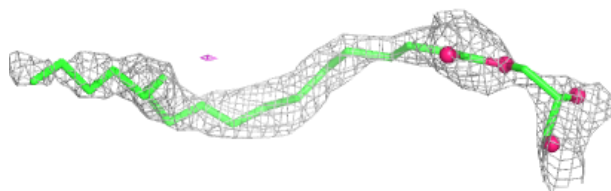
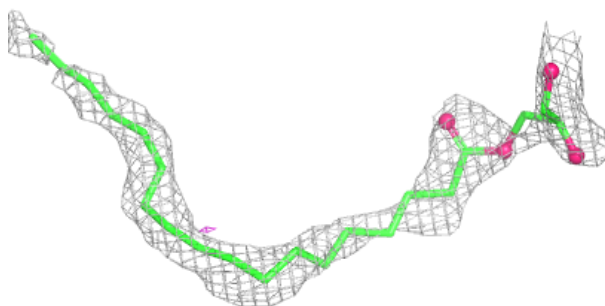


Electron density around OLC A 502:

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

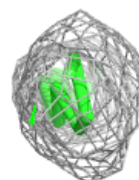
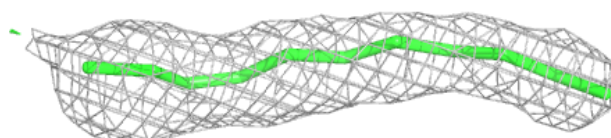
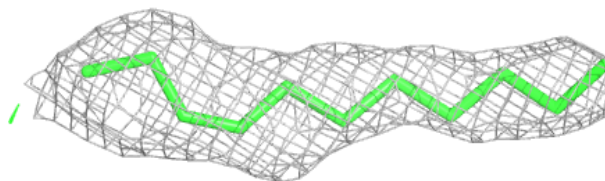
**Electron density around OLC A 501:**

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

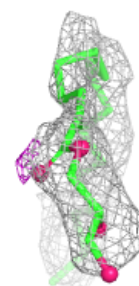
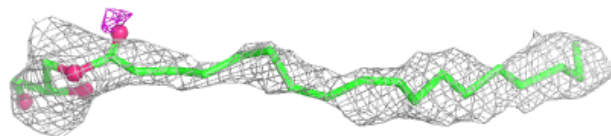
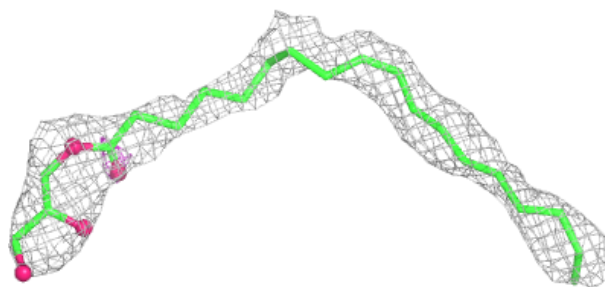


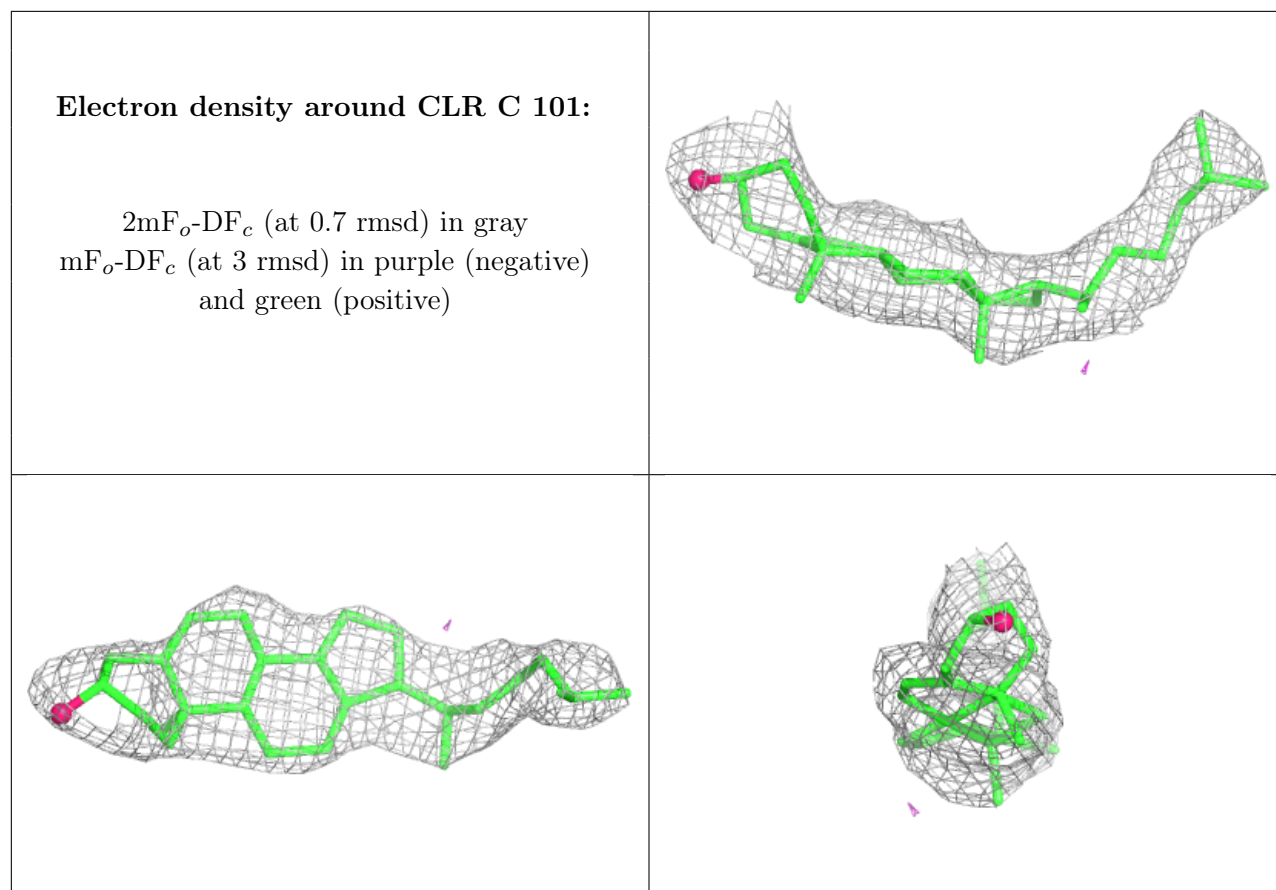
Electron density around OLC A 505:

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

**Electron density around OLC A 506:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.