



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:29 pm BST

PDB ID : 6IS6
Title : Crystal structure of Thermoplasmatales archaeon heliorhodopsin
Authors : Shihoya, W.; Yamashita, K.; Nureki, O.
Deposited on : 2018-11-15
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

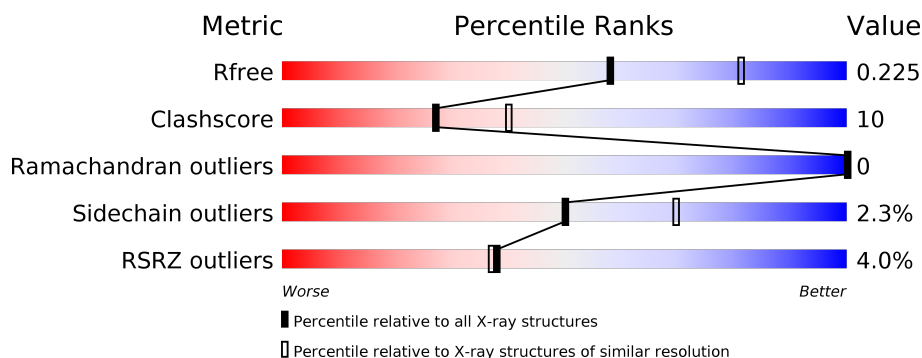
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	<div> <div>4%</div> <div>81%</div> <div>15%</div> <div>.</div> </div>

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
2	OLC	A	312	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2397 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.

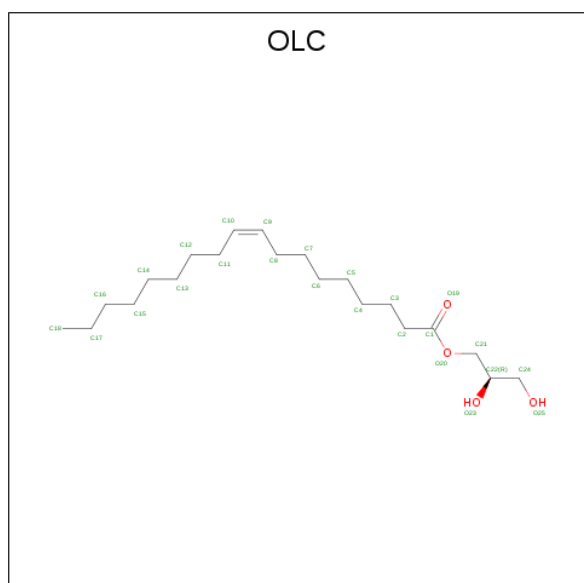
- Molecule 1 is a protein called heliorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	2014	1354	312	335	13	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

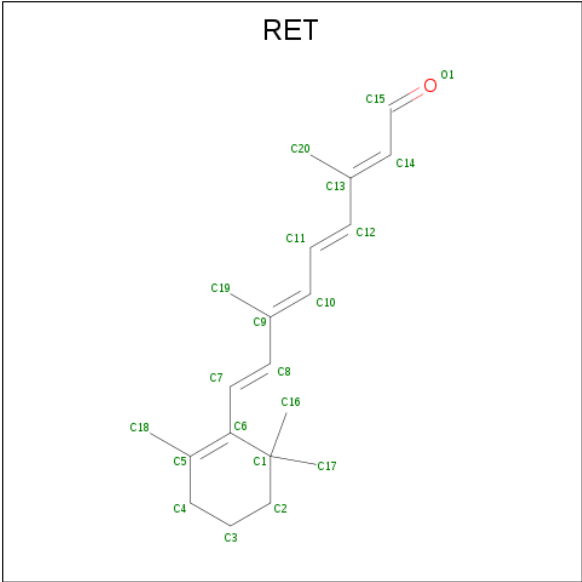
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP A0A151EDA9
A	-4	HIS	-	expression tag	UNP A0A151EDA9
A	-3	HIS	-	expression tag	UNP A0A151EDA9
A	-2	HIS	-	expression tag	UNP A0A151EDA9
A	-1	HIS	-	expression tag	UNP A0A151EDA9
A	0	HIS	-	expression tag	UNP A0A151EDA9
A	1	HIS	-	expression tag	UNP A0A151EDA9

- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			19	15	4		
2	A	1	Total	C	O	0	0
			17	13	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	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			21	17	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	A	1	Total	C	O	0	0
			25	21	4		
2	A	1	Total	C	O	0	0
			25	21	4		

- Molecule 3 is RETINAL (three-letter code: RET) (formula: C₂₀H₂₈O) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 20 20	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	31	Total O 31 31	0	0

- Molecule 1: heliorhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	51.98Å 109.35Å 107.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.77 – 2.40 48.77 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.77-2.40) 99.9 (48.77-2.40)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.189 , 0.225 0.189 , 0.225	Depositor DCC
R_{free} test set	641 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2397	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.39% 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: OLC, RET

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	0/2070	0.51	0/2822

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	2014	0	2067	32	0
2	A	332	0	516	31	0
3	A	20	0	27	4	0
4	A	31	0	0	0	0
All	All	2397	0	2610	50	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 10.

All (50) 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:248:GLY:HA2	2:A:309:OLC:H15A	1.67	0.75
1:A:203:PHE:HB3	2:A:303:OLC:H7	1.66	0.75
3:A:313:RET:H161	3:A:313:RET:H8	1.73	0.70
1:A:209:ASN:ND2	1:A:220:TRP:HE1	1.92	0.68
1:A:92:ARG:HD2	2:A:306:OLC:H14	1.75	0.67
1:A:191:PHE:HB3	2:A:309:OLC:H15	1.78	0.65
1:A:96:ASN:HD21	2:A:306:OLC:H12A	1.62	0.64
1:A:246:PHE:HA	1:A:250:LEU:HB2	1.85	0.59
1:A:169:ILE:HG23	2:A:308:OLC:H16A	1.84	0.58
2:A:304:OLC:H13	2:A:307:OLC:H24A	1.88	0.55
2:A:303:OLC:H11	2:A:311:OLC:H11A	1.87	0.55
1:A:120:ILE:O	1:A:124:THR:HG23	2.06	0.54
1:A:105:ARG:NH1	1:A:227:GLU:OE2	2.41	0.54
1:A:73:MET:HE3	1:A:73:MET:HA	1.91	0.53
1:A:150:GLU:HA	1:A:214:TYR:OH	2.10	0.52
1:A:172:PHE:CE1	2:A:303:OLC:H10	2.46	0.51
1:A:178:ILE:O	1:A:181:PRO:HD2	2.11	0.51
1:A:76:PHE:CG	2:A:301:OLC:H24	2.46	0.51
1:A:105:ARG:HG3	1:A:109:TYR:CZ	2.47	0.50
1:A:225:HIS:HD2	2:A:305:OLC:O23	1.95	0.49
2:A:304:OLC:H15A	2:A:307:OLC:H21	1.95	0.49
1:A:209:ASN:HD21	1:A:220:TRP:HE1	1.58	0.48
2:A:309:OLC:H7A	2:A:309:OLC:H4	1.73	0.47
3:A:313:RET:C8	3:A:313:RET:H161	2.44	0.47
2:A:303:OLC:H4A	2:A:303:OLC:H7A	1.38	0.46
1:A:248:GLY:HA2	2:A:309:OLC:C15	2.42	0.46
2:A:315:OLC:H8	2:A:315:OLC:H11A	1.52	0.46
2:A:309:OLC:H13A	2:A:309:OLC:H10	1.74	0.46
1:A:78:SER:HB2	1:A:238:LYS:HE2	1.98	0.45
1:A:30:VAL:O	1:A:34:SER:OG	2.30	0.45
1:A:69:PRO:HB2	2:A:301:OLC:H7A	1.99	0.45
2:A:305:OLC:H10	2:A:305:OLC:H14A	2.00	0.44
1:A:180:ILE:HB	1:A:181:PRO:HD3	1.99	0.44
3:A:313:RET:H7	3:A:313:RET:H181	1.78	0.43
1:A:65:ILE:HD11	2:A:307:OLC:H12A	2.00	0.43
1:A:34:SER:HB3	1:A:250:LEU:HB3	1.99	0.43
2:A:309:OLC:H13	2:A:309:OLC:H16	1.68	0.42
2:A:304:OLC:H21A	2:A:304:OLC:H2	1.85	0.42
1:A:80:THR:HG21	2:A:304:OLC:H5	2.01	0.42
2:A:305:OLC:H10	2:A:305:OLC:C14	2.49	0.41
1:A:77:ILE:HD13	1:A:111:ILE:HG22	2.01	0.41
1:A:175:TRP:CD1	2:A:303:OLC:H8	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:OLC:H3A	2:A:301:OLC:H7	2.02	0.41
1:A:195:ILE:O	1:A:199:ILE:HG12	2.21	0.41
2:A:303:OLC:H8A	2:A:303:OLC:H11A	1.70	0.41
3:A:313:RET:H11	3:A:313:RET:H191	1.90	0.41
1:A:96:ASN:ND2	2:A:306:OLC:H12A	2.33	0.41
1:A:73:MET:SD	2:A:304:OLC:H10	2.61	0.40
2:A:309:OLC:H8	2:A:309:OLC:H11	1.71	0.40
1:A:193:ILE:HD12	2:A:311:OLC:H2	2.03	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	248/259 (96%)	243 (98%)	5 (2%)	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	220/232 (95%)	215 (98%)	5 (2%)	50	70

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	53	ASN
1	A	58	VAL
1	A	157	GLN
1	A	186	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	143	ASN
1	A	204	ASN
1	A	209	ASN
1	A	225	HIS
1	A	244	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

15 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	303	-	24,24,24	0.92	1 (4%)	25,25,25	0.93	2 (8%)
2	OLC	A	308	-	24,24,24	0.90	1 (4%)	25,25,25	0.91	1 (4%)
2	OLC	A	310	-	24,24,24	0.92	1 (4%)	25,25,25	0.90	1 (4%)
2	OLC	A	311	-	24,24,24	0.96	1 (4%)	25,25,25	0.89	2 (8%)
2	OLC	A	306	-	24,24,24	0.98	1 (4%)	25,25,25	0.83	1 (4%)
2	OLC	A	315	-	24,24,24	0.96	1 (4%)	25,25,25	0.91	2 (8%)
2	OLC	A	305	-	24,24,24	0.93	1 (4%)	25,25,25	0.89	1 (4%)
2	OLC	A	302	-	16,16,24	1.20	1 (6%)	17,17,25	1.10	1 (5%)
2	OLC	A	301	-	18,18,24	1.13	1 (5%)	18,19,25	0.86	1 (5%)
2	OLC	A	314	-	24,24,24	0.95	1 (4%)	25,25,25	0.79	1 (4%)
3	RET	A	313	1	20,20,21	2.54	4 (20%)	27,27,28	1.39	3 (11%)
2	OLC	A	304	-	24,24,24	0.98	1 (4%)	25,25,25	0.92	1 (4%)
2	OLC	A	312	-	24,24,24	0.97	1 (4%)	25,25,25	0.88	1 (4%)
2	OLC	A	309	-	24,24,24	0.90	1 (4%)	25,25,25	1.01	2 (8%)
2	OLC	A	307	-	20,20,24	0.99	1 (5%)	21,21,25	1.16	2 (9%)

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	303	-	-	9/24/24/24	-
2	OLC	A	308	-	-	8/24/24/24	-
2	OLC	A	310	-	-	12/24/24/24	-
2	OLC	A	311	-	-	7/24/24/24	-
2	OLC	A	306	-	-	14/24/24/24	-
2	OLC	A	315	-	-	6/24/24/24	-
2	OLC	A	305	-	-	8/24/24/24	-
2	OLC	A	302	-	-	4/16/16/24	-
2	OLC	A	301	-	-	9/18/18/24	-
2	OLC	A	314	-	-	10/24/24/24	-
3	RET	A	313	1	-	0/13/30/31	0/1/1/1
2	OLC	A	304	-	-	11/24/24/24	-
2	OLC	A	312	-	-	13/24/24/24	-
2	OLC	A	309	-	-	9/24/24/24	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	307	-	-	11/20/20/24	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	313	RET	C14-C13	9.21	1.40	1.33
2	A	304	OLC	O20-C1	4.58	1.46	1.33
2	A	302	OLC	O20-C1	4.55	1.46	1.33
2	A	301	OLC	O20-C1	4.53	1.46	1.33
2	A	312	OLC	O20-C1	4.50	1.46	1.33
2	A	306	OLC	O20-C1	4.49	1.46	1.33
2	A	315	OLC	O20-C1	4.41	1.46	1.33
2	A	314	OLC	O20-C1	4.40	1.46	1.33
2	A	311	OLC	O20-C1	4.39	1.46	1.33
2	A	305	OLC	O20-C1	4.31	1.45	1.33
2	A	310	OLC	O20-C1	4.30	1.45	1.33
2	A	303	OLC	O20-C1	4.30	1.45	1.33
3	A	313	RET	C10-C9	4.28	1.41	1.35
2	A	307	OLC	O20-C1	4.21	1.45	1.33
2	A	308	OLC	O20-C1	4.09	1.45	1.33
2	A	309	OLC	O20-C1	4.08	1.45	1.33
3	A	313	RET	C8-C9	-2.62	1.40	1.45
3	A	313	RET	C12-C13	-2.12	1.41	1.45

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	313	RET	C19-C9-C10	-4.02	117.29	122.92
2	A	302	OLC	O20-C1-C2	3.23	122.04	111.91
2	A	309	OLC	O20-C1-C2	2.95	121.15	111.91
2	A	307	OLC	O20-C1-C2	2.91	121.04	111.91
2	A	304	OLC	O20-C1-C2	2.82	120.75	111.91
2	A	310	OLC	O20-C1-C2	2.75	120.55	111.91
3	A	313	RET	C2-C1-C6	2.75	114.72	110.48
2	A	311	OLC	O20-C1-C2	2.75	120.53	111.91
2	A	315	OLC	O20-C1-C2	2.71	120.41	111.91
2	A	306	OLC	O20-C1-C2	2.62	120.11	111.91
2	A	312	OLC	O20-C1-C2	2.59	120.03	111.91
2	A	308	OLC	O20-C1-C2	2.56	119.94	111.91
3	A	313	RET	C8-C9-C10	2.44	122.69	118.94
2	A	303	OLC	O20-C1-C2	2.35	119.27	111.91
2	A	301	OLC	O20-C1-C2	2.33	119.22	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	303	OLC	C4-C3-C2	-2.29	104.97	113.19
2	A	309	OLC	O20-C1-O19	-2.27	117.85	123.59
2	A	311	OLC	O20-C1-O19	-2.24	117.93	123.59
2	A	305	OLC	O20-C1-C2	2.19	118.78	111.91
2	A	315	OLC	O20-C1-O19	-2.16	118.14	123.59
2	A	314	OLC	O20-C1-C2	2.07	118.41	111.91
2	A	307	OLC	C3-C2-C1	-2.05	106.18	113.62

There are no chirality outliers.

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	303	OLC	C21-C22-C24-O25
2	A	310	OLC	C21-C22-C24-O25
2	A	310	OLC	O23-C22-C24-O25
2	A	306	OLC	O20-C21-C22-C24
2	A	306	OLC	C2-C1-O20-C21
2	A	306	OLC	O19-C1-O20-C21
2	A	315	OLC	O20-C21-C22-C24
2	A	314	OLC	O20-C21-C22-C24
2	A	314	OLC	O20-C21-C22-O23
2	A	304	OLC	O20-C21-C22-O23
2	A	304	OLC	C2-C1-O20-C21
2	A	304	OLC	O19-C1-O20-C21
2	A	301	OLC	O19-C1-O20-C21
2	A	301	OLC	C2-C1-O20-C21
2	A	307	OLC	O20-C21-C22-O23
2	A	312	OLC	C12-C13-C14-C15
2	A	307	OLC	C2-C1-O20-C21
2	A	303	OLC	C4-C5-C6-C7
2	A	315	OLC	O20-C21-C22-O23
2	A	301	OLC	C1-C2-C3-C4
2	A	314	OLC	C2-C1-O20-C21
2	A	310	OLC	C1-C2-C3-C4
2	A	309	OLC	C1-C2-C3-C4
2	A	302	OLC	C1-C2-C3-C4
2	A	307	OLC	O19-C1-O20-C21
2	A	306	OLC	O20-C21-C22-O23
2	A	314	OLC	O19-C1-O20-C21
2	A	309	OLC	C13-C14-C15-C16
2	A	309	OLC	C4-C5-C6-C7
2	A	312	OLC	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	312	OLC	C2-C3-C4-C5
2	A	311	OLC	C12-C13-C14-C15
2	A	306	OLC	C14-C15-C16-C17
2	A	305	OLC	C12-C13-C14-C15
2	A	304	OLC	C3-C4-C5-C6
2	A	306	OLC	C11-C12-C13-C14
2	A	312	OLC	C3-C4-C5-C6
2	A	308	OLC	C11-C12-C13-C14
2	A	315	OLC	C21-C22-C24-O25
2	A	312	OLC	C21-C22-C24-O25
2	A	306	OLC	C3-C4-C5-C6
2	A	314	OLC	C11-C12-C13-C14
2	A	309	OLC	C5-C6-C7-C8
2	A	311	OLC	C10-C11-C12-C13
2	A	301	OLC	C6-C7-C8-C9
2	A	307	OLC	C4-C5-C6-C7
2	A	304	OLC	C2-C3-C4-C5
2	A	314	OLC	C4-C5-C6-C7
2	A	306	OLC	C4-C5-C6-C7
2	A	303	OLC	O23-C22-C24-O25
2	A	312	OLC	O23-C22-C24-O25
2	A	314	OLC	C13-C14-C15-C16
2	A	302	OLC	C2-C3-C4-C5
2	A	308	OLC	C12-C13-C14-C15
2	A	307	OLC	C5-C6-C7-C8
2	A	310	OLC	C13-C14-C15-C16
2	A	303	OLC	C5-C6-C7-C8
2	A	310	OLC	C6-C7-C8-C9
2	A	311	OLC	C6-C7-C8-C9
2	A	304	OLC	C6-C7-C8-C9
2	A	305	OLC	C1-C2-C3-C4
2	A	307	OLC	O20-C21-C22-C24
2	A	312	OLC	C4-C5-C6-C7
2	A	312	OLC	C13-C14-C15-C16
2	A	301	OLC	C4-C5-C6-C7
2	A	307	OLC	C2-C3-C4-C5
2	A	305	OLC	C13-C14-C15-C16
2	A	314	OLC	C1-C2-C3-C4
2	A	314	OLC	C3-C4-C5-C6
2	A	309	OLC	C14-C15-C16-C17
2	A	314	OLC	C15-C16-C17-C18
2	A	315	OLC	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	306	OLC	C15-C16-C17-C18
2	A	306	OLC	C13-C14-C15-C16
2	A	303	OLC	C15-C16-C17-C18
2	A	312	OLC	C11-C12-C13-C14
2	A	311	OLC	C2-C1-O20-C21
2	A	305	OLC	C15-C16-C17-C18
2	A	309	OLC	C11-C12-C13-C14
2	A	309	OLC	C10-C11-C12-C13
2	A	305	OLC	C11-C12-C13-C14
2	A	310	OLC	C4-C5-C6-C7
2	A	310	OLC	C2-C1-O20-C21
2	A	311	OLC	O19-C1-O20-C21
2	A	301	OLC	O23-C22-C24-O25
2	A	308	OLC	C2-C3-C4-C5
2	A	306	OLC	C10-C11-C12-C13
2	A	310	OLC	O20-C21-C22-C24
2	A	304	OLC	O20-C21-C22-C24
2	A	312	OLC	C14-C15-C16-C17
2	A	310	OLC	O19-C1-O20-C21
2	A	311	OLC	C11-C12-C13-C14
2	A	315	OLC	O23-C22-C24-O25
2	A	305	OLC	C4-C5-C6-C7
2	A	312	OLC	C7-C8-C9-C10
2	A	312	OLC	C2-C1-O20-C21
2	A	302	OLC	C5-C6-C7-C8
2	A	307	OLC	O23-C22-C24-O25
2	A	308	OLC	C2-C1-O20-C21
2	A	312	OLC	O19-C1-O20-C21
2	A	304	OLC	C10-C11-C12-C13
2	A	308	OLC	C5-C6-C7-C8
2	A	306	OLC	C9-C10-C11-C12
2	A	306	OLC	C12-C13-C14-C15
2	A	307	OLC	C3-C4-C5-C6
2	A	304	OLC	C9-C10-C11-C12
2	A	308	OLC	O19-C1-O20-C21
2	A	305	OLC	C9-C10-C11-C12
2	A	301	OLC	C3-C4-C5-C6
2	A	304	OLC	O20-C1-C2-C3
2	A	305	OLC	C2-C3-C4-C5
2	A	309	OLC	C2-C3-C4-C5
2	A	310	OLC	C9-C10-C11-C12
2	A	301	OLC	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	315	OLC	C15-C16-C17-C18
2	A	311	OLC	C7-C8-C9-C10
2	A	310	OLC	O20-C21-C22-O23
2	A	307	OLC	C9-C10-C11-C12
2	A	308	OLC	C3-C4-C5-C6
2	A	303	OLC	O20-C1-C2-C3
2	A	308	OLC	C9-C10-C11-C12
2	A	301	OLC	C21-C22-C24-O25
2	A	307	OLC	C21-C22-C24-O25
2	A	310	OLC	C12-C13-C14-C15
2	A	304	OLC	O19-C1-C2-C3
2	A	306	OLC	O20-C1-C2-C3
2	A	303	OLC	O19-C1-C2-C3
2	A	303	OLC	C2-C3-C4-C5
2	A	303	OLC	C7-C8-C9-C10
2	A	309	OLC	O20-C1-C2-C3
2	A	302	OLC	C3-C4-C5-C6

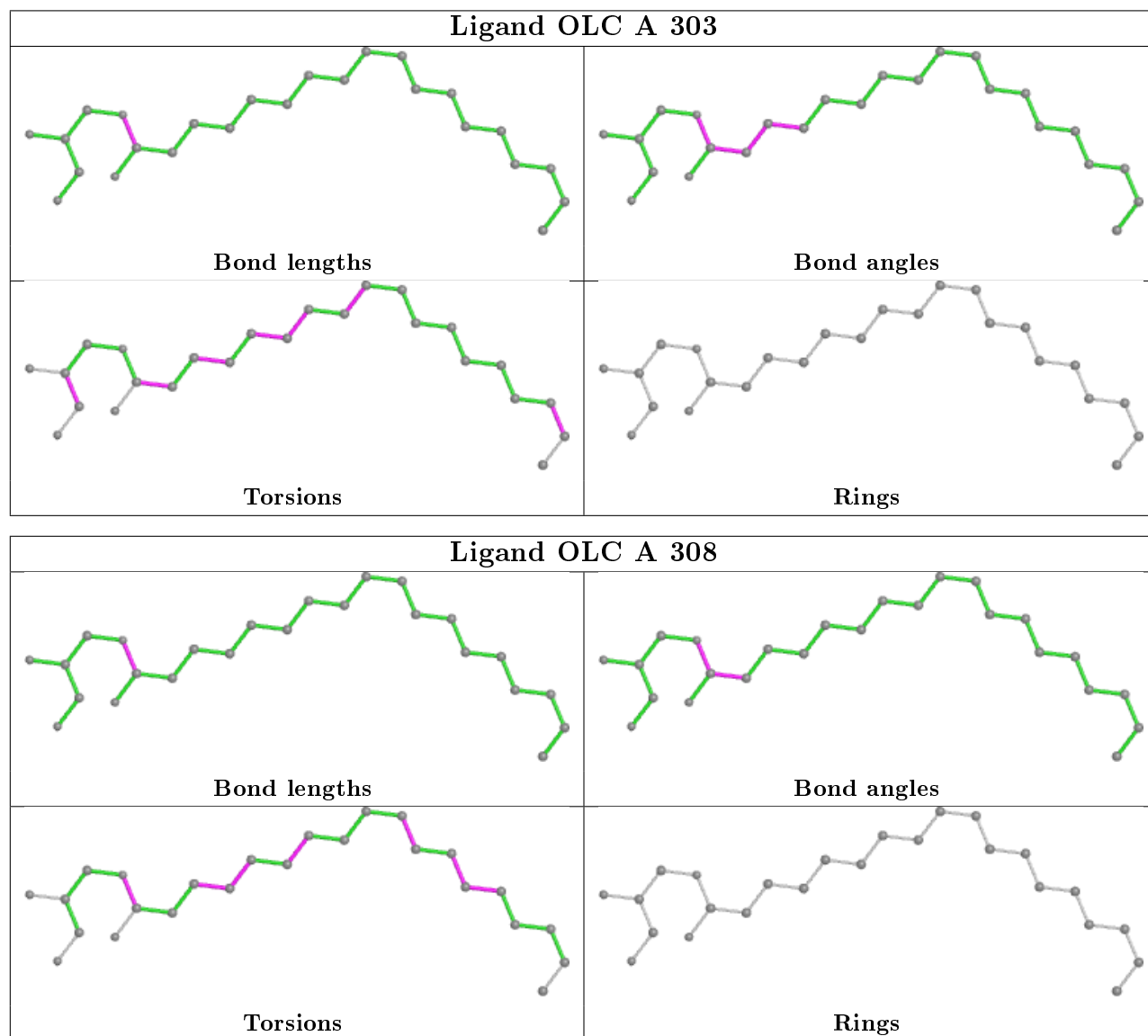
There are no ring outliers.

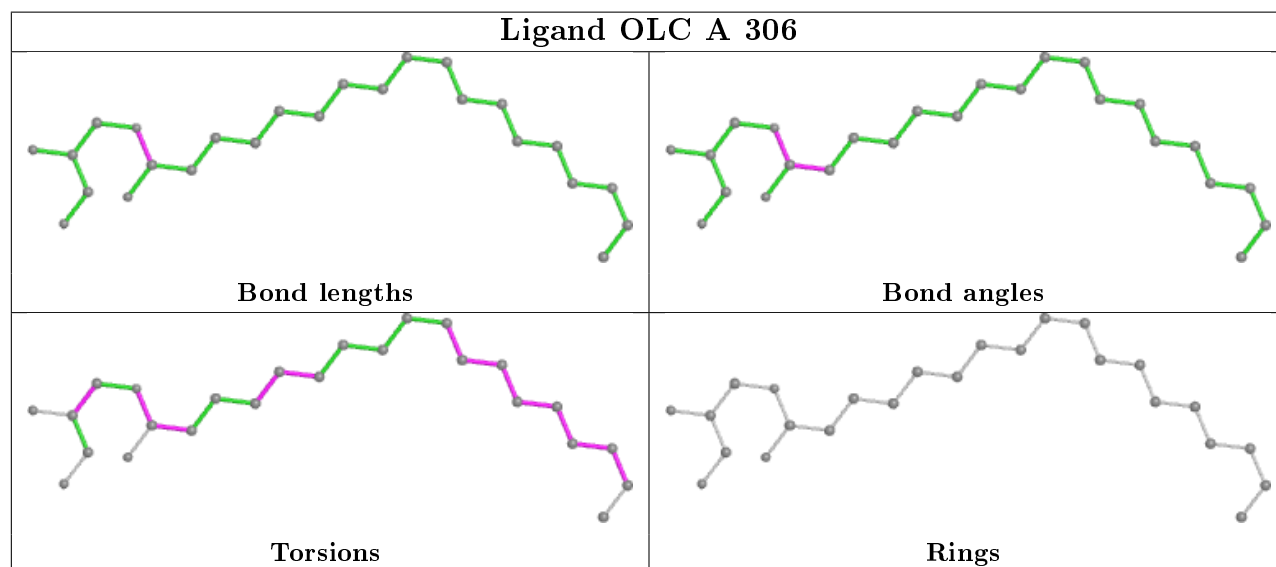
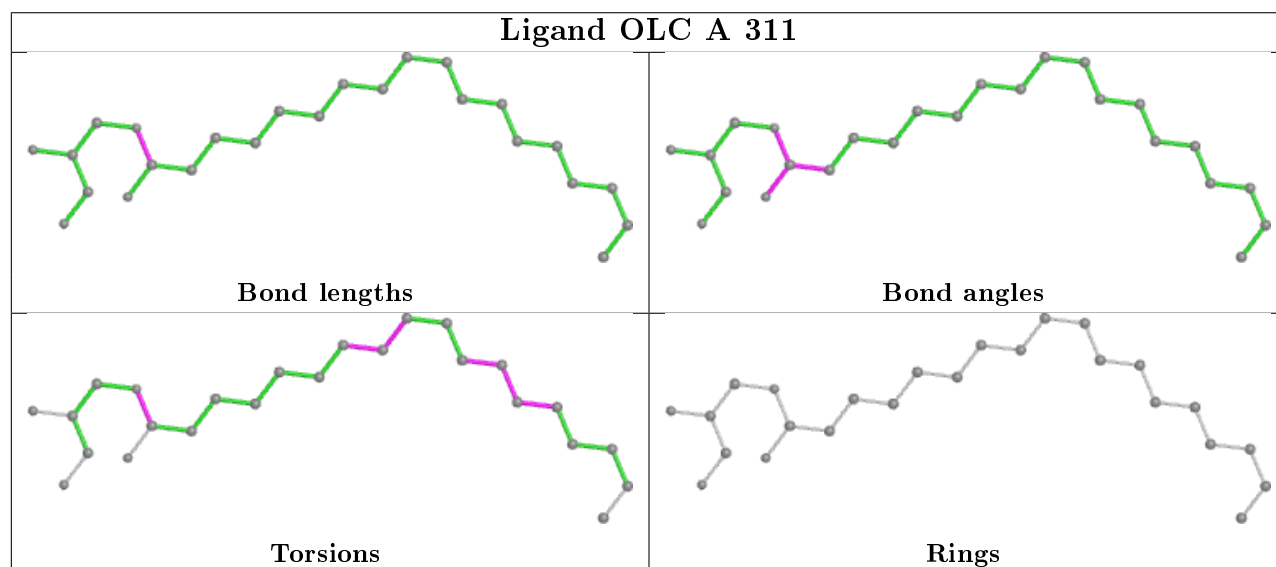
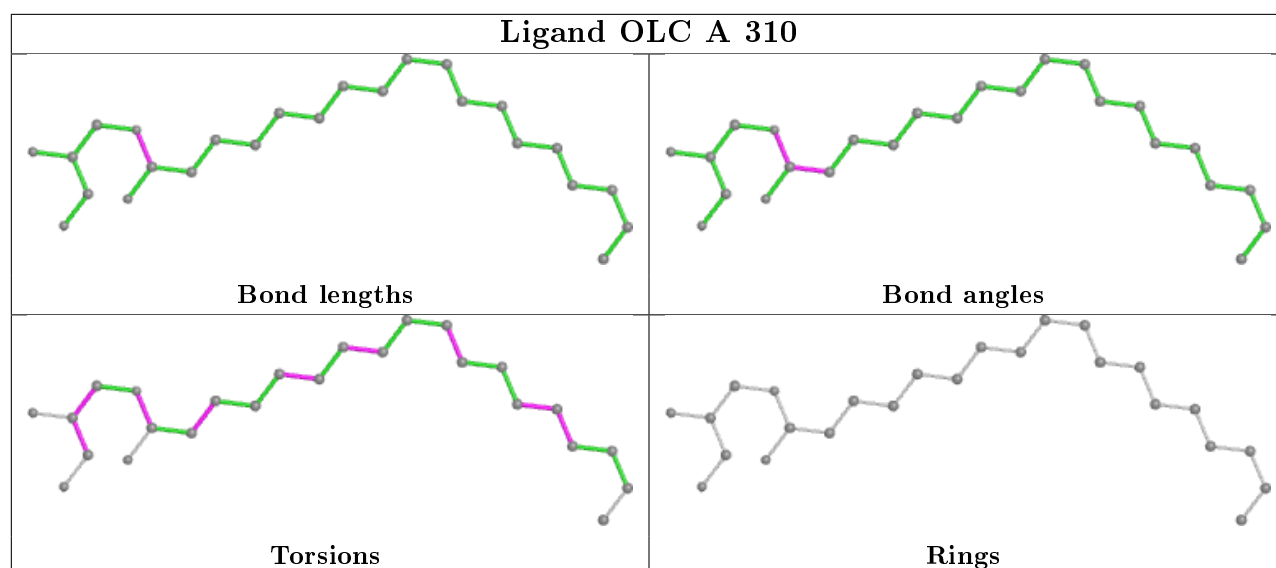
11 monomers are involved in 35 short contacts:

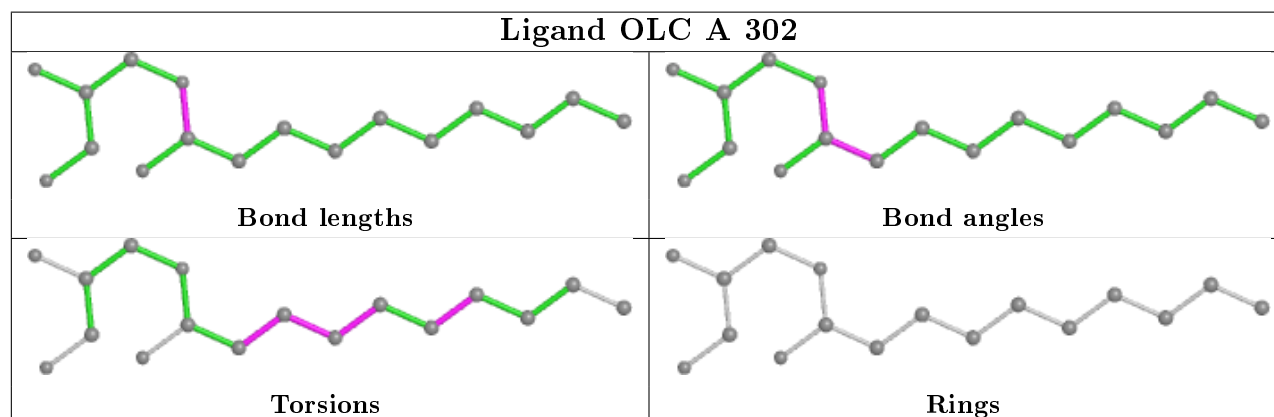
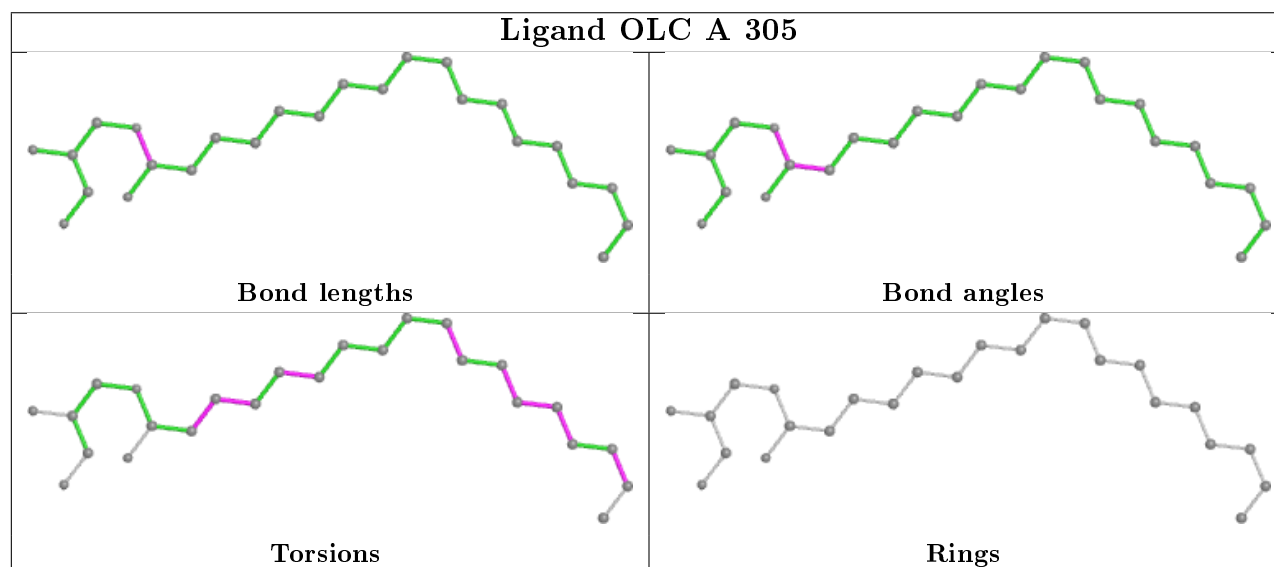
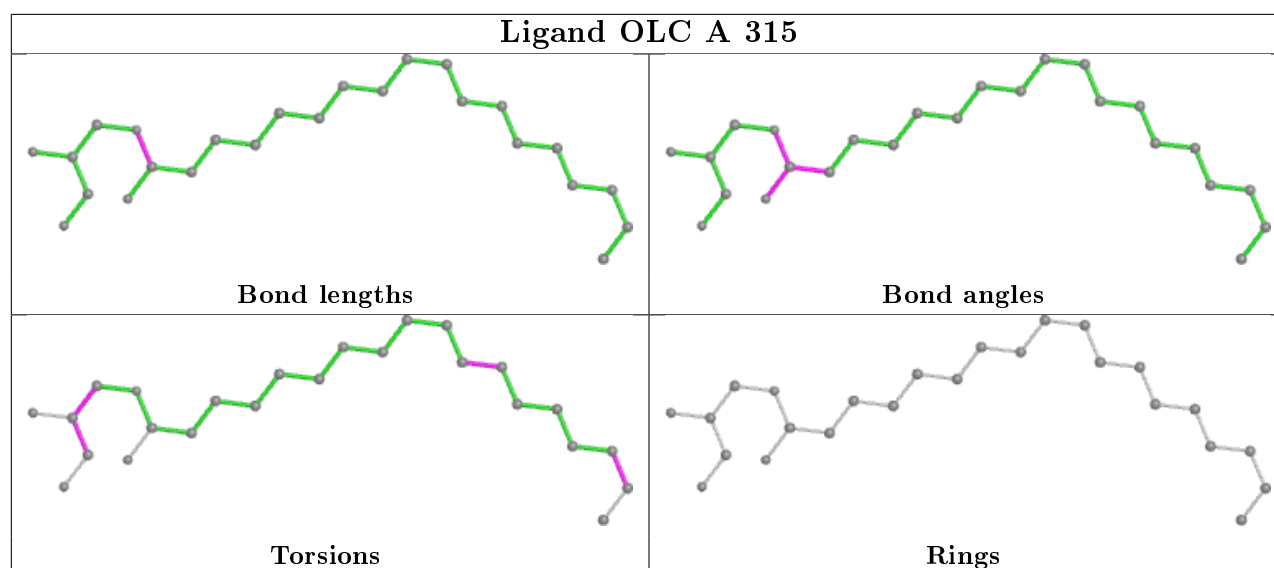
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	303	OLC	6	0
2	A	308	OLC	1	0
2	A	311	OLC	2	0
2	A	306	OLC	3	0
2	A	315	OLC	1	0
2	A	305	OLC	3	0
2	A	301	OLC	3	0
3	A	313	RET	4	0
2	A	304	OLC	5	0
2	A	309	OLC	7	0
2	A	307	OLC	3	0

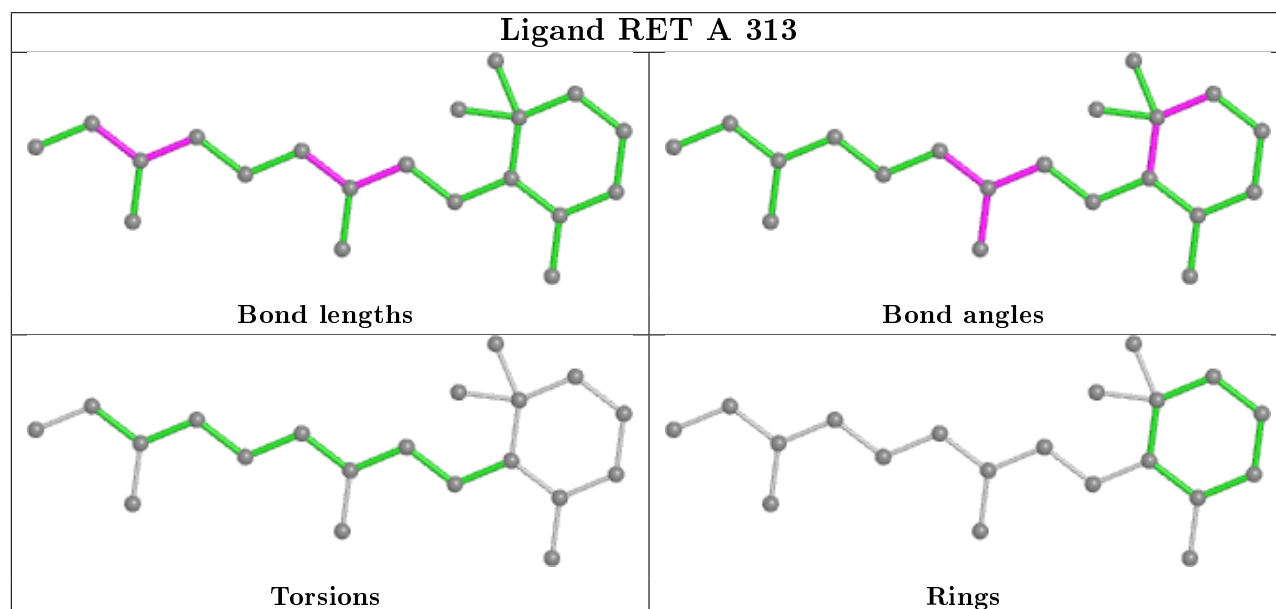
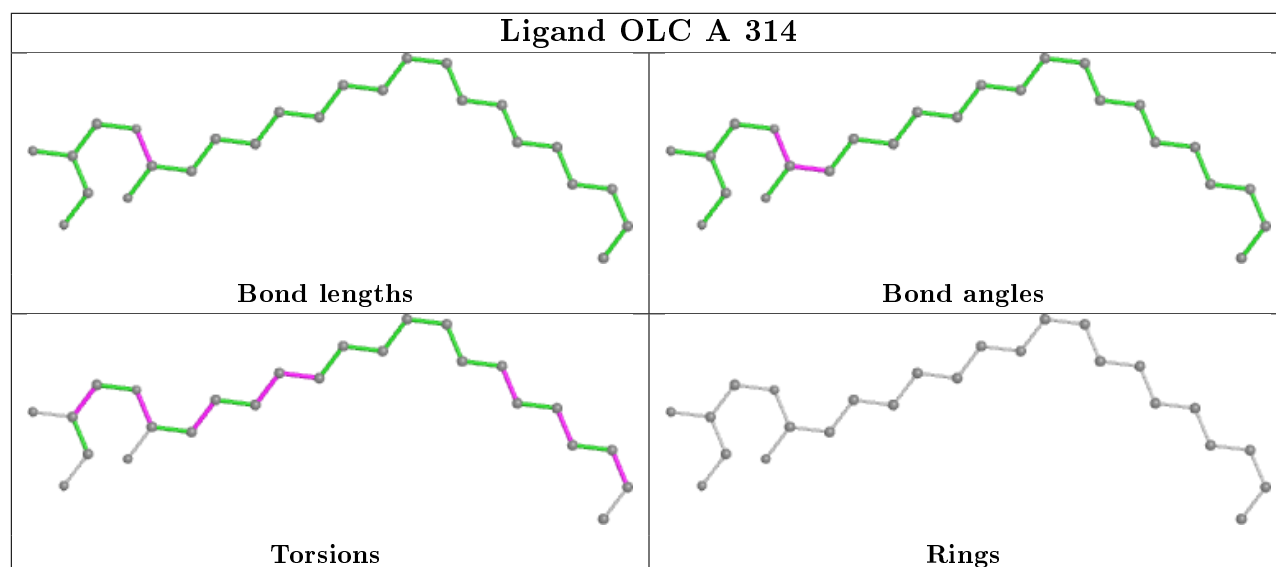
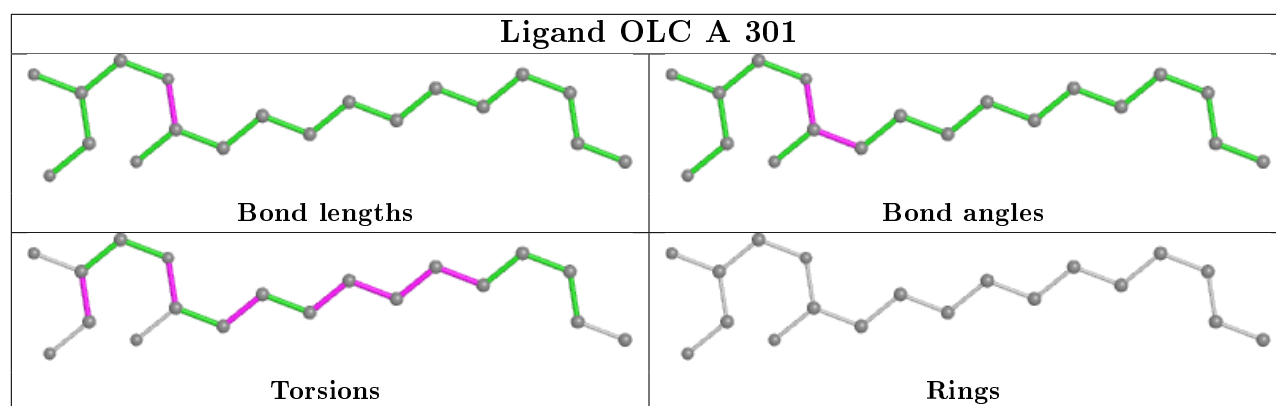
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

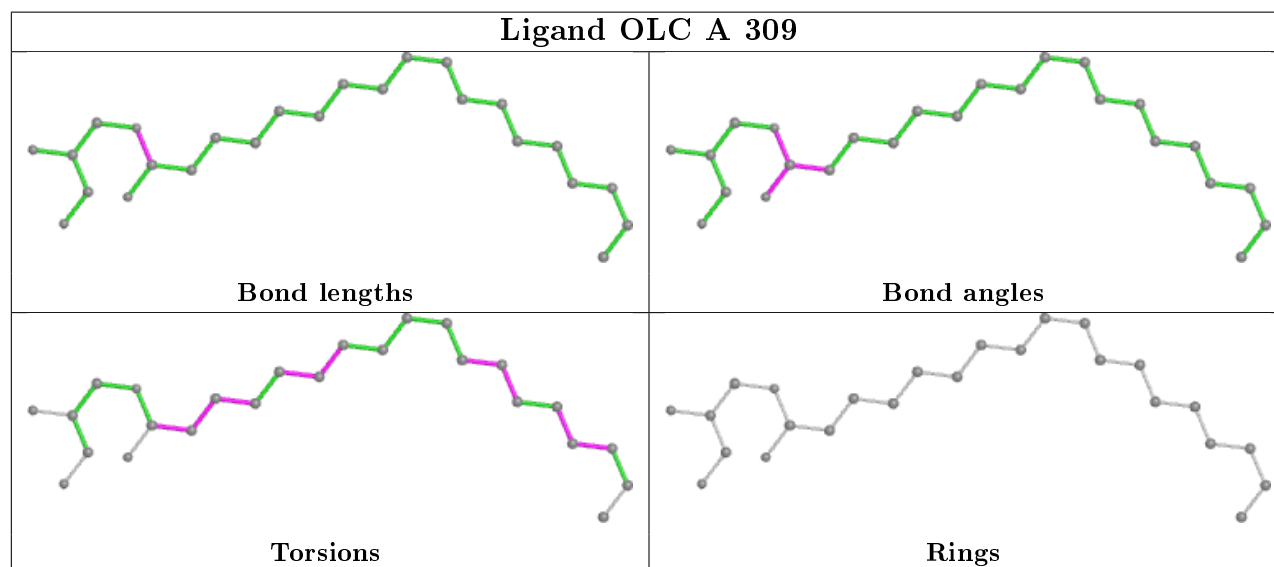
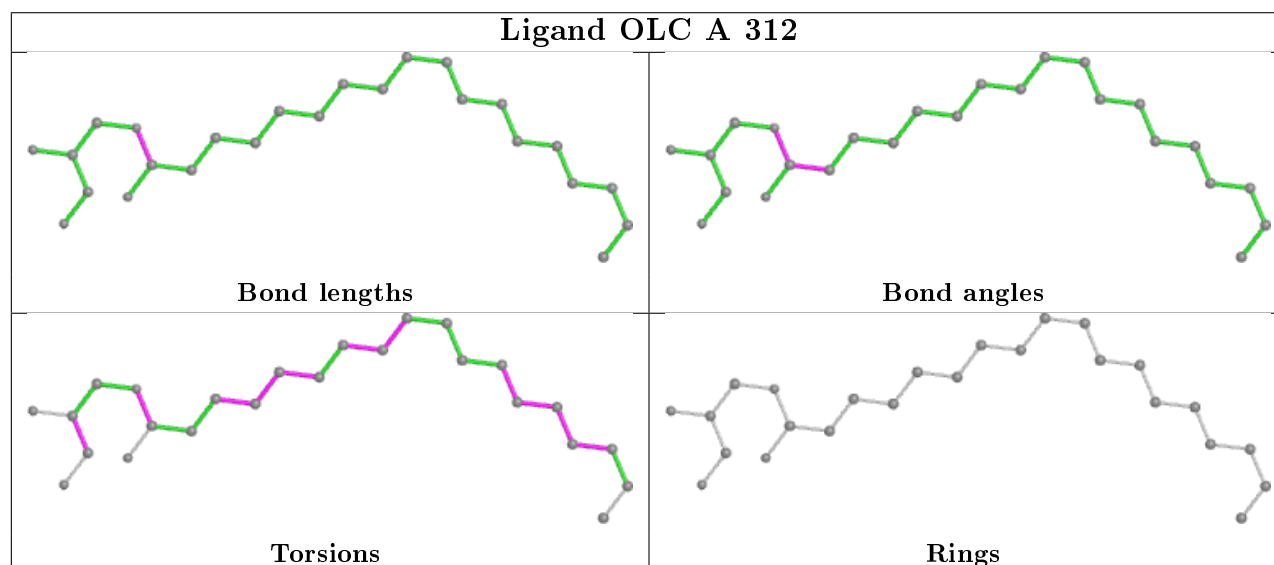
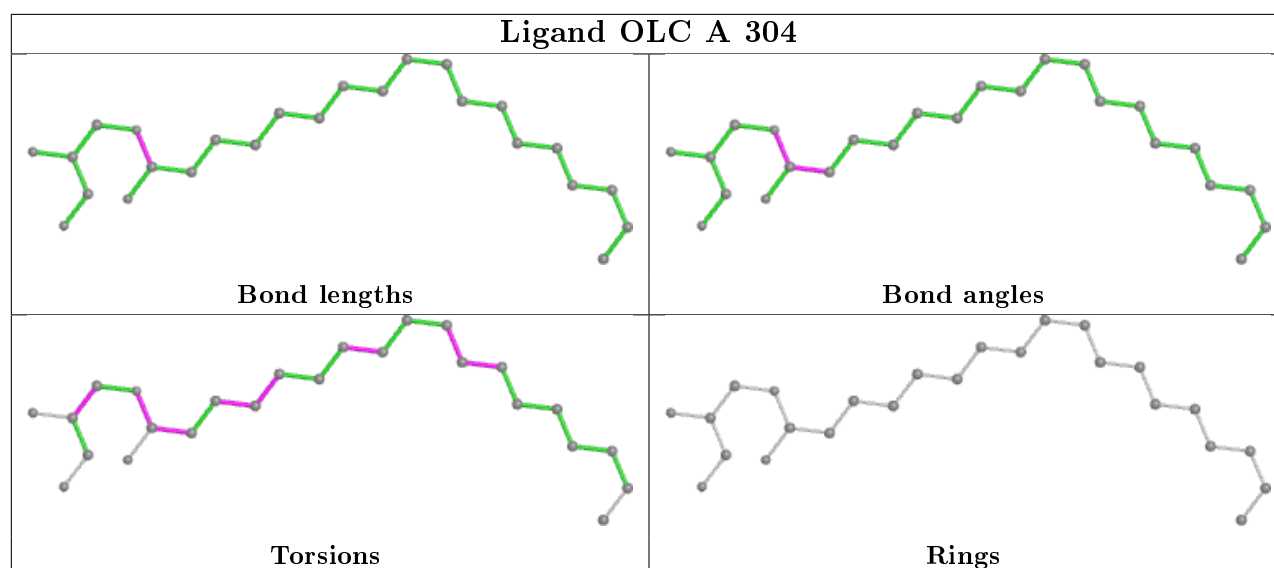
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

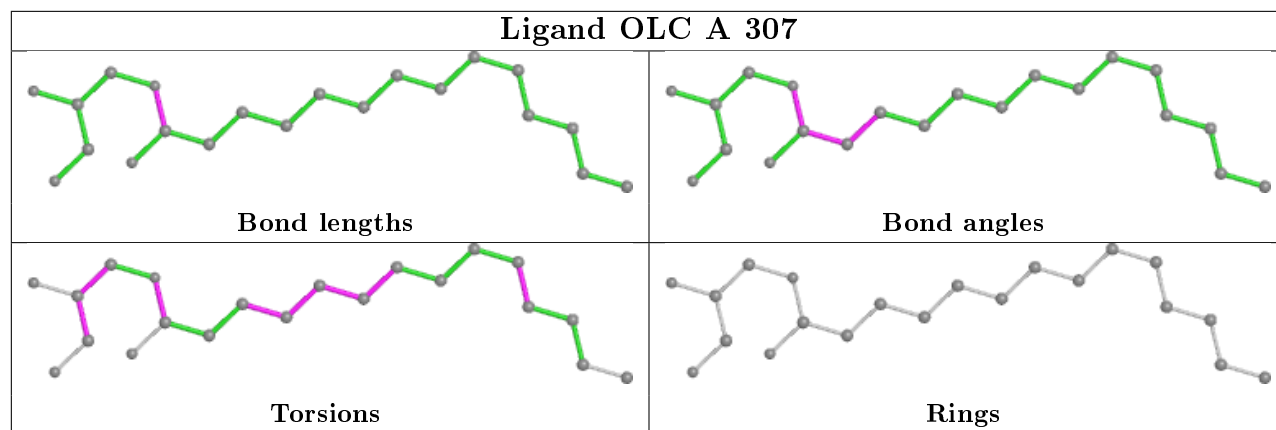












5.7 Other polymers [i](#)

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	250/259 (96%)	-0.20	10 (4%)	38 37	23, 32, 66, 97	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLU	6.3
1	A	51	ILE	3.7
1	A	50	GLU	3.5
1	A	4	ASN	3.4
1	A	54	SER	3.4
1	A	49	ASN	2.8
1	A	7	ILE	2.5
1	A	48	TYR	2.4
1	A	55	ILE	2.3
1	A	44	ASN	2.1

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](#)

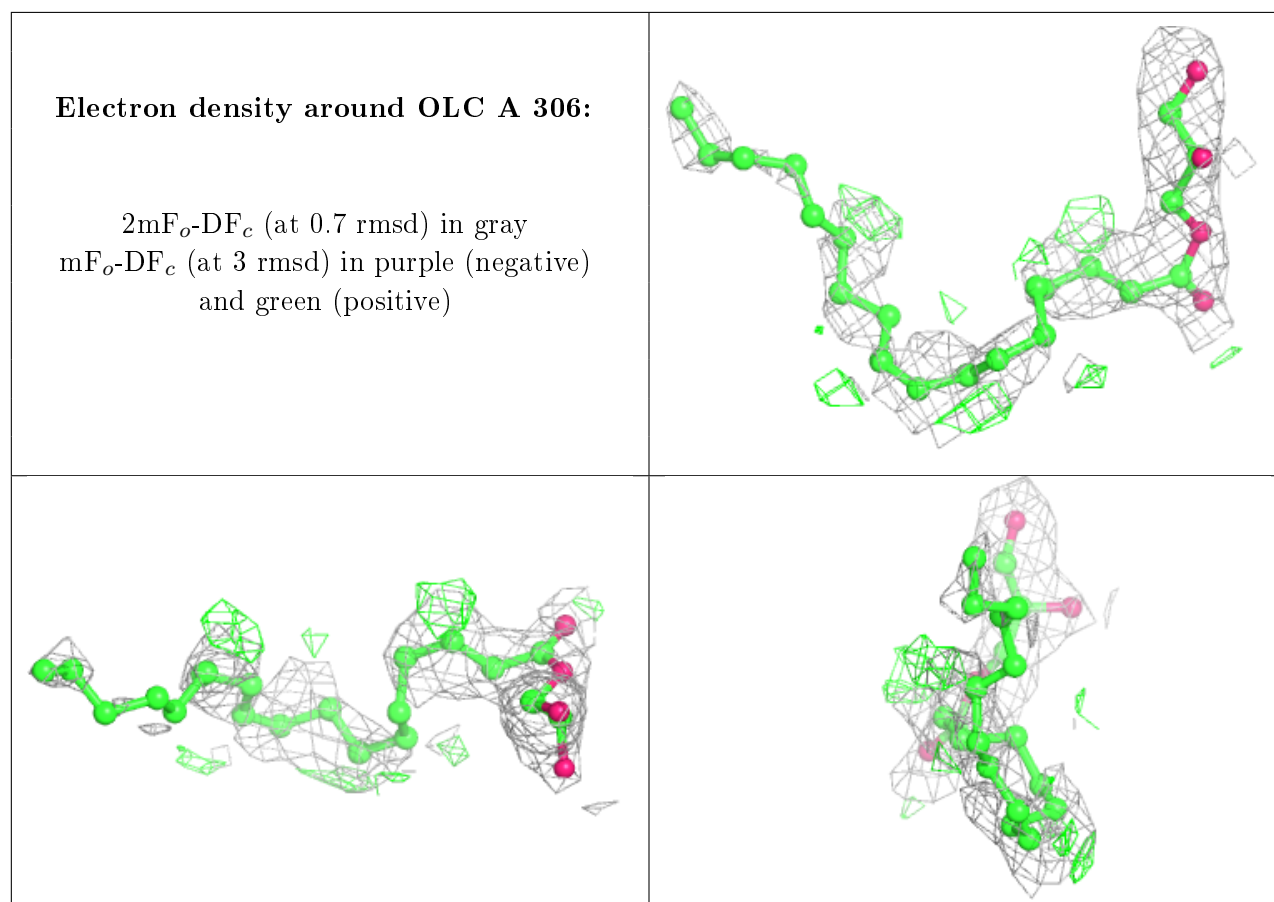
There are no carbohydrates in this entry.

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.

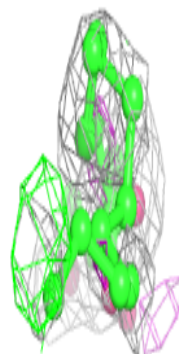
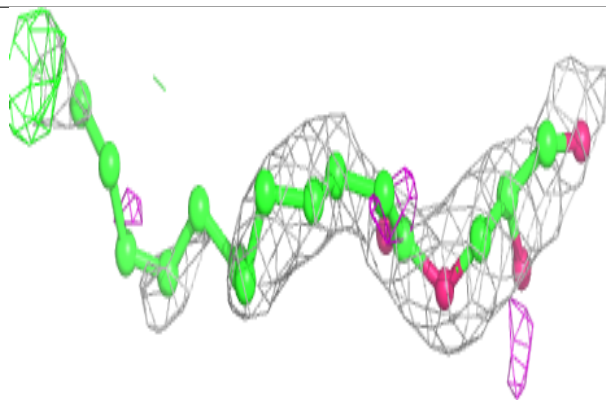
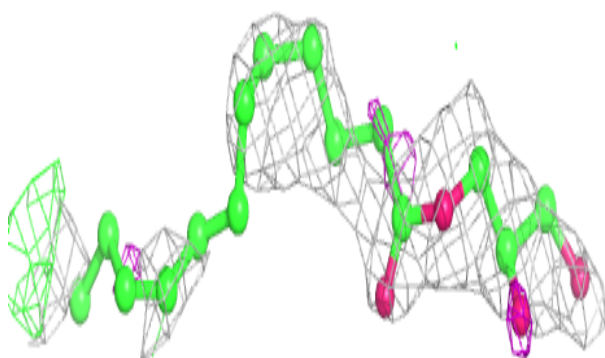
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OLC	A	306	25/25	0.72	0.28	41,56,62,65	0
2	OLC	A	301	19/25	0.76	0.37	45,54,61,63	0
2	OLC	A	310	25/25	0.77	0.33	52,60,64,74	0
2	OLC	A	314	25/25	0.77	0.26	47,59,71,73	0
2	OLC	A	305	25/25	0.78	0.25	35,43,51,60	0
2	OLC	A	315	25/25	0.79	0.22	48,64,67,69	0
2	OLC	A	312	25/25	0.80	0.48	47,60,79,81	0
2	OLC	A	304	25/25	0.82	0.25	41,52,67,72	0
2	OLC	A	308	25/25	0.83	0.28	43,51,57,59	0
2	OLC	A	303	25/25	0.84	0.25	36,46,56,63	0
2	OLC	A	302	17/25	0.84	0.24	50,56,66,68	0
2	OLC	A	311	25/25	0.85	0.27	45,57,64,65	0
2	OLC	A	309	25/25	0.85	0.26	33,43,49,52	0
2	OLC	A	307	21/25	0.85	0.23	34,51,72,80	0
3	RET	A	313	20/21	0.95	0.14	22,26,32,34	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.

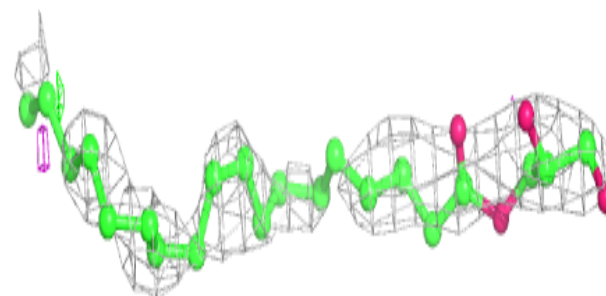
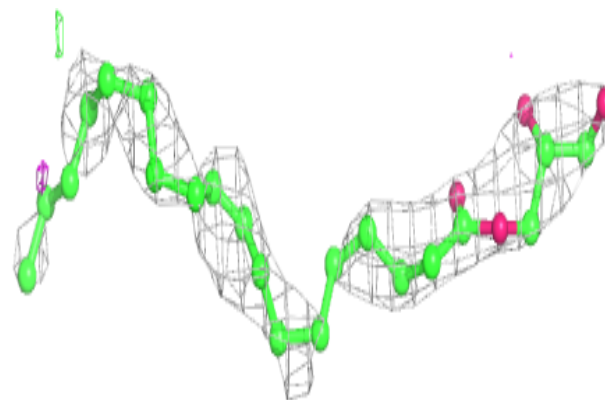


Electron density around OLC A 301:

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

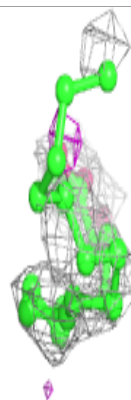
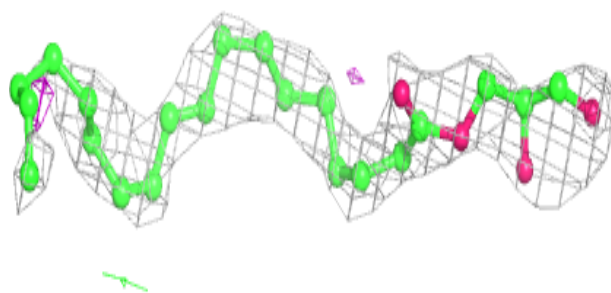
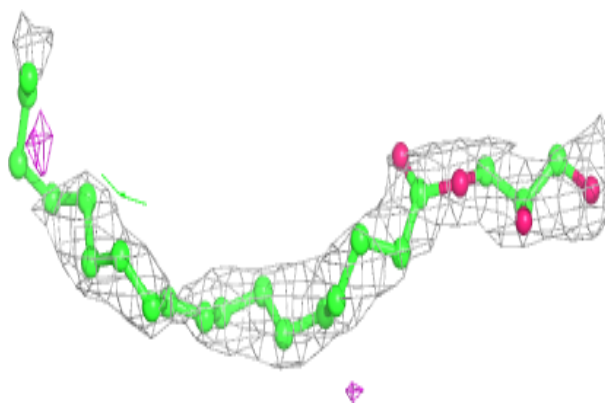
**Electron density around OLC A 310:**

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

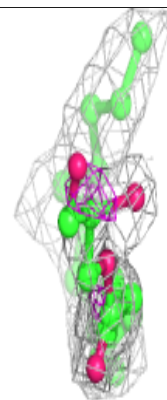
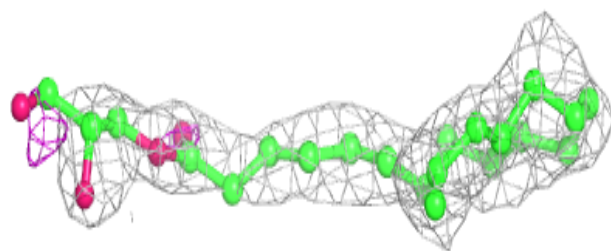
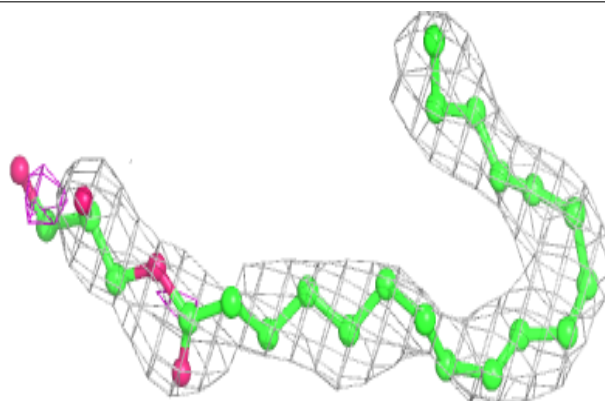


Electron density around OLC A 314:

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

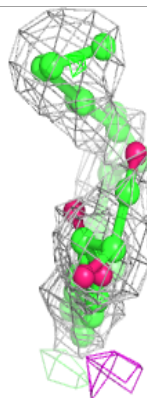
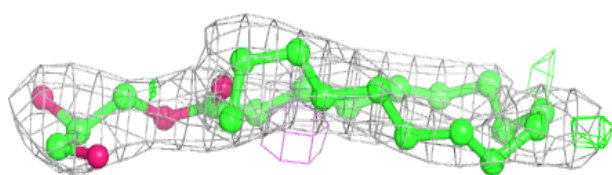
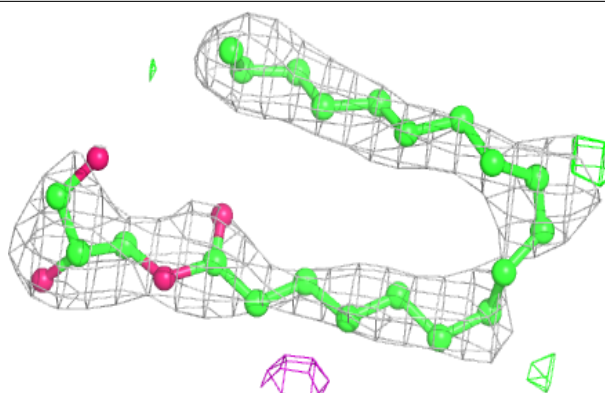
**Electron density around OLC A 305:**

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

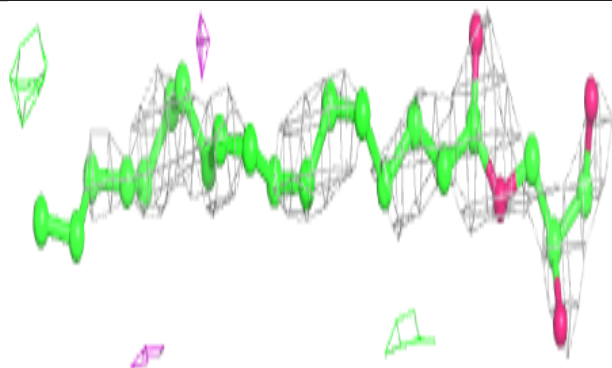
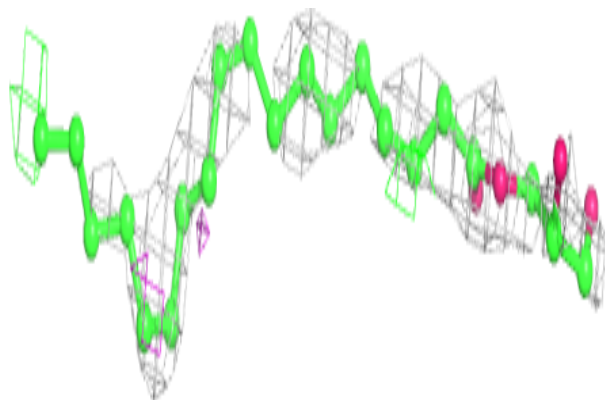


Electron density around OLC A 315:

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

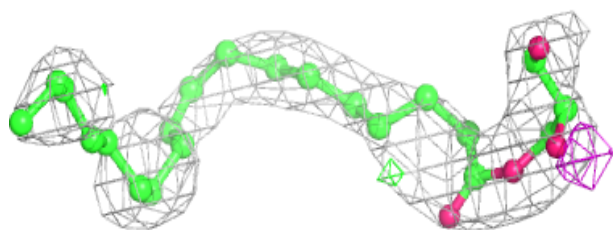
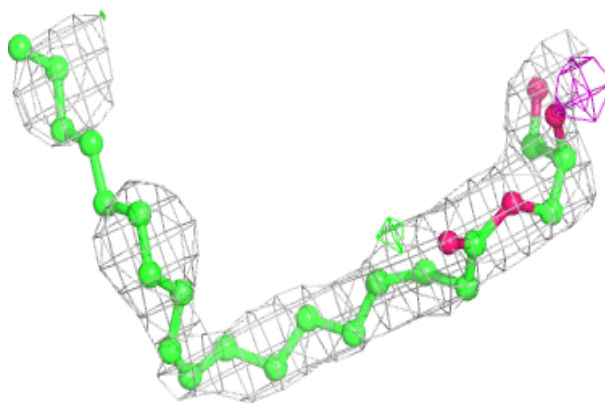
**Electron density around OLC A 312:**

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

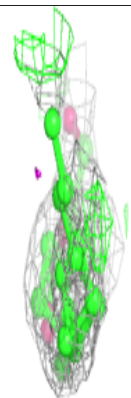
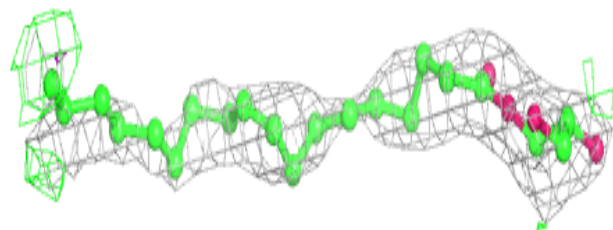
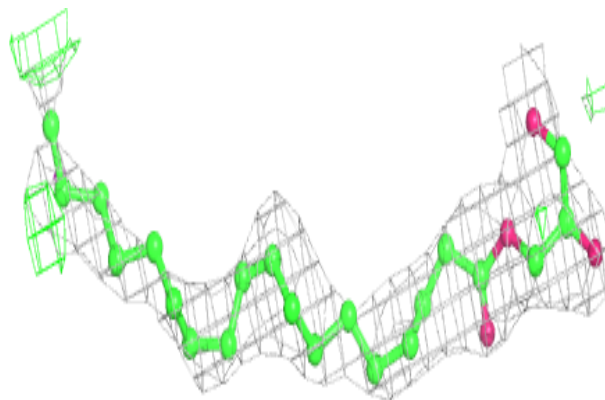


Electron density around OLC A 304:

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

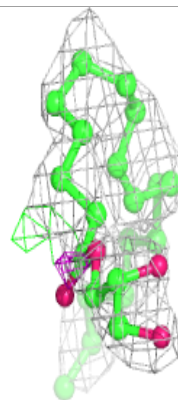
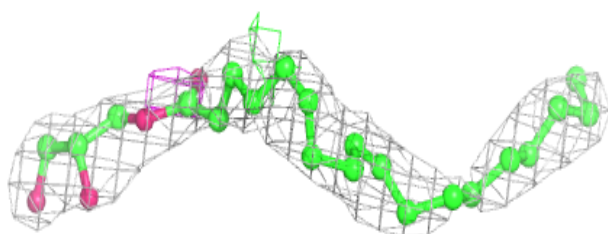
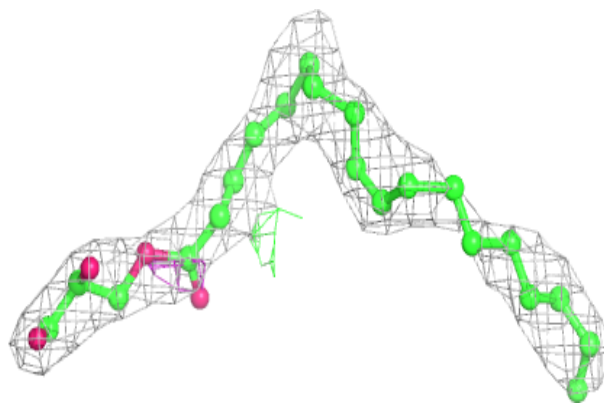
**Electron density around OLC A 308:**

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

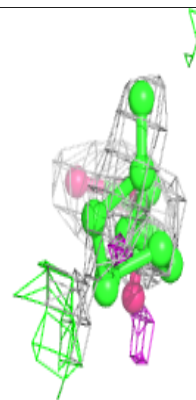
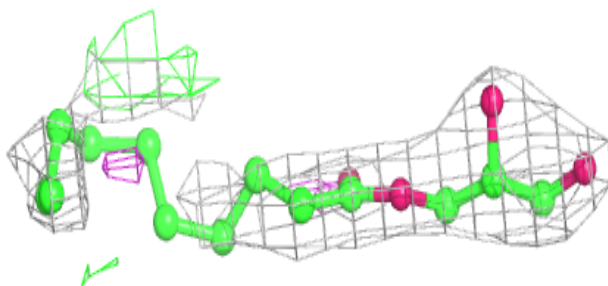
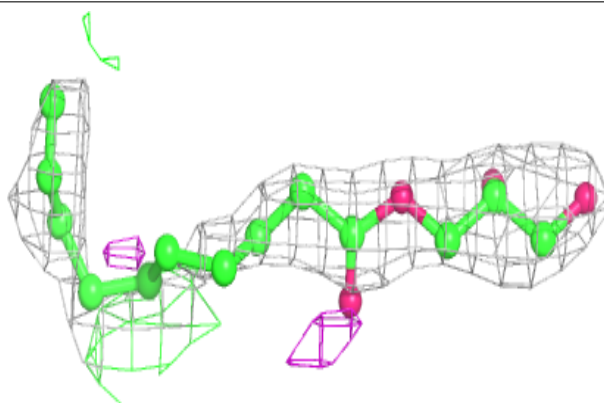


Electron density around OLC A 303:

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

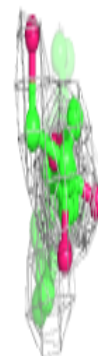
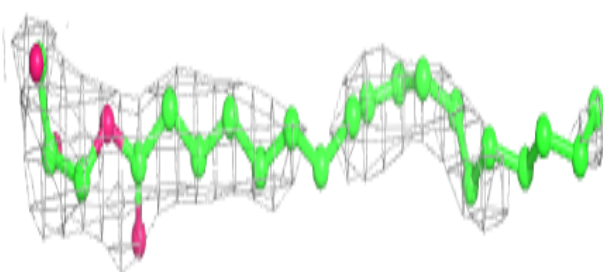
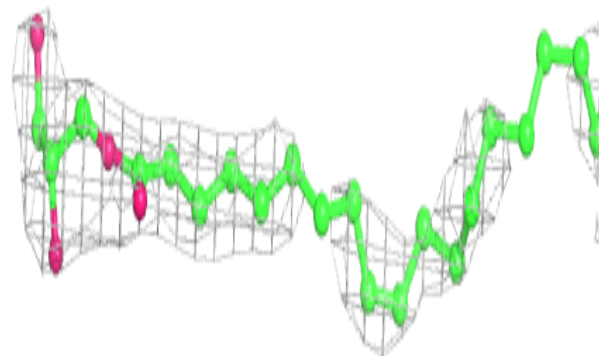
**Electron density around OLC A 302:**

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

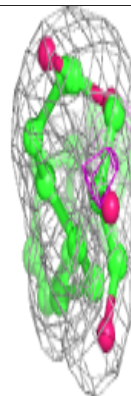
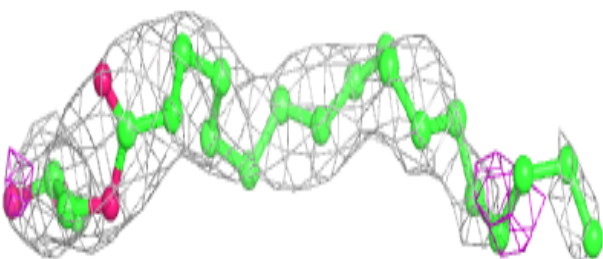
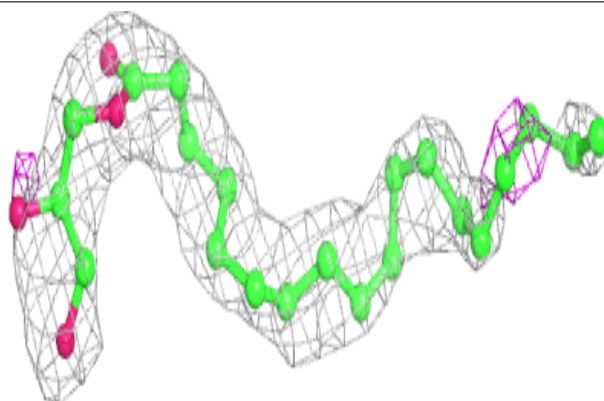


Electron density around OLC A 311:

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

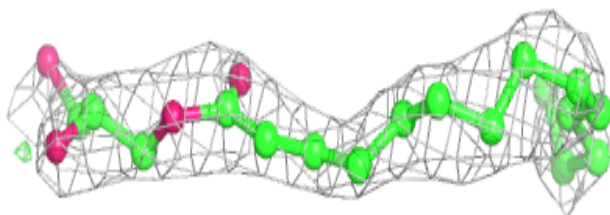
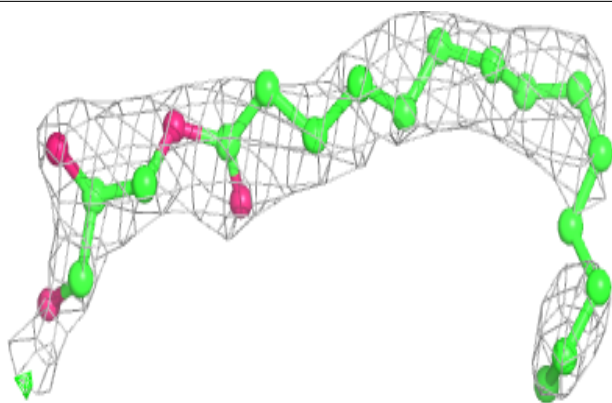
**Electron density around OLC A 309:**

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

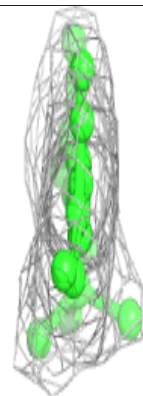
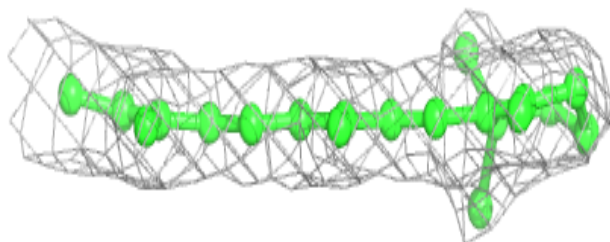
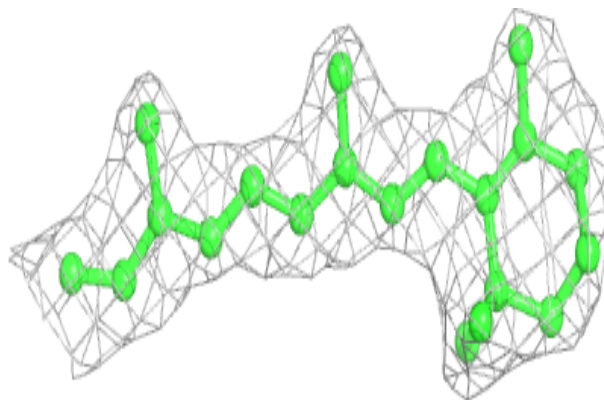


Electron density around OLC A 307:

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

**Electron density around RET A 313:**

$2mF_o-DF_c$ (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.