



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:09 AM UTC

PDB ID : 7E4G / pdb_00007e4g
Title : Crystal structure of schizorhodopsin 4
Authors : Shihoya, W.; Nureki, O.
Deposited on : 2021-02-12
Resolution : 2.10 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

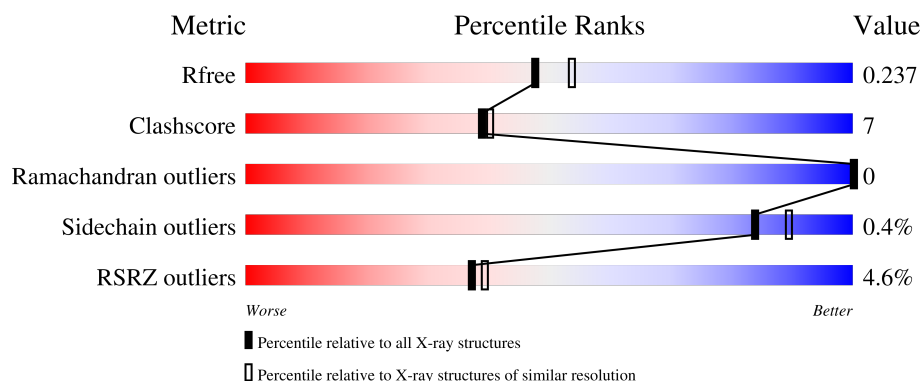
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	210	3% 87% 8% 5%
1	B	210	6% 82% 11% 7%
1	C	210	4% 81% 11% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5782 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 schizorhodopsin 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1624	1112	238	265	9			
1	B	196	Total	C	N	O	S	0	0	0
			1600	1098	234	259	9			
1	C	193	Total	C	N	O	S	0	0	0
			1575	1085	226	255	9			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

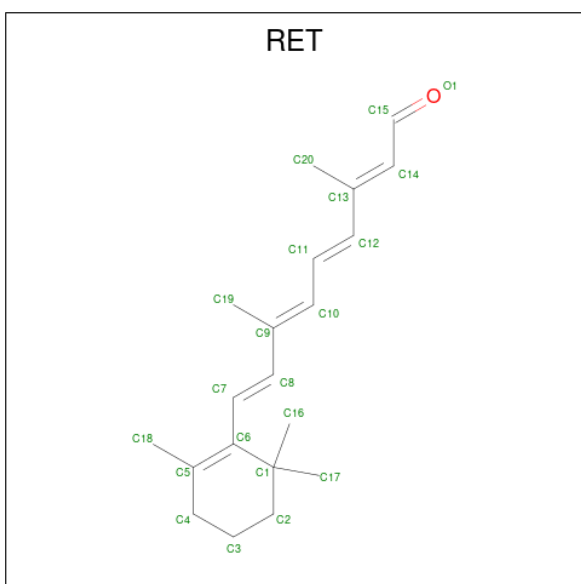
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	2	Total	Zn	0	0
			2	2		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



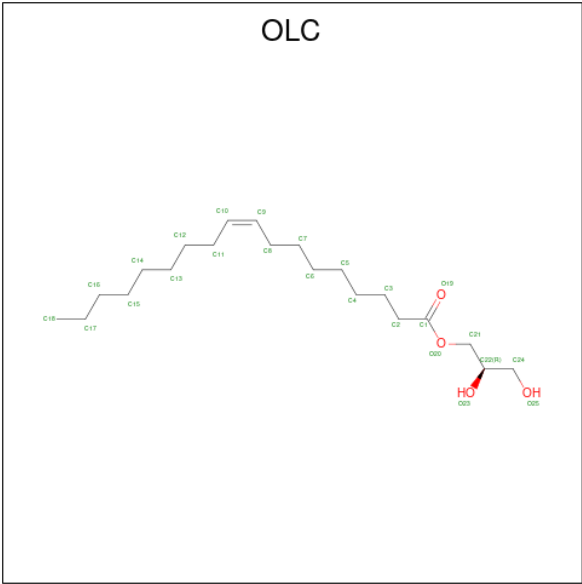
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is RETINAL (CCD ID: RET) (formula: $C_{20}H_{28}O$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 25 21 4	0	0
5	A	1	Total C O 25 21 4	0	0
5	A	1	Total C O 25 21 4	0	0
5	A	1	Total C O 25 21 4	0	0
5	A	1	Total C O 13 9 4	0	0
5	A	1	Total C O 14 10 4	0	0
5	A	1	Total C O 14 10 4	0	0
5	A	1	Total C O 25 21 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			23	19	4		
5	A	1	Total	C	O	0	0
			20	16	4		
5	B	1	Total	C	O	0	0
			22	18	4		
5	B	1	Total	C	O	0	0
			25	21	4		
5	B	1	Total	C	O	0	0
			25	21	4		
5	B	1	Total	C	O	0	0
			25	21	4		
5	B	1	Total	C	O	0	0
			25	21	4		
5	B	1	Total	C	O	0	0
			25	21	4		
5	B	1	Total	C	O	0	0
			25	21	4		
5	B	1	Total	C	O	0	0
			25	21	4		
5	B	1	Total	C	O	0	0
			25	21	4		
5	B	1	Total	C	O	0	0
			25	21	4		
5	B	1	Total	C	O	0	0
			22	18	4		
5	B	1	Total	C	O	0	0
			25	21	4		
5	C	1	Total	C	O	0	0
			25	21	4		
5	C	1	Total	C	O	0	0
			25	21	4		
5	C	1	Total	C	O	0	0
			25	21	4		
5	C	1	Total	C	O	0	0
			25	21	4		
5	C	1	Total	C	O	0	0
			25	21	4		
5	C	1	Total	C	O	0	0
			25	21	4		

Continued on next page...

Continued from previous page...

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

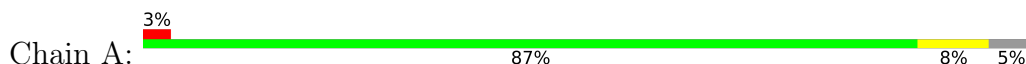
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	53	Total	O	0	0
			53	53		
6	B	46	Total	O	0	0
			46	46		
6	C	45	Total	O	0	0
			45	45		

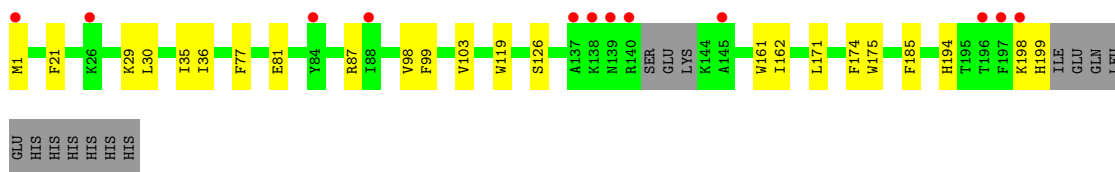
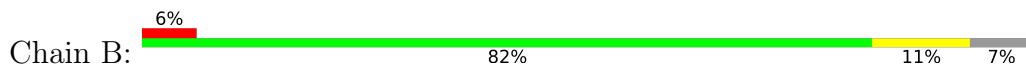
3 Residue-property plots [i](#)

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.

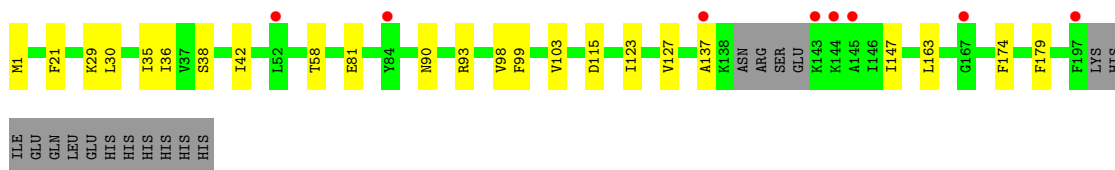
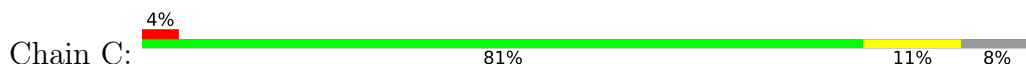
- Molecule 1: schizorhodopsin 4



- Molecule 1: schizorhodopsin 4



- Molecule 1: schizorhodopsin 4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.00Å 61.14Å 98.75Å 90.00° 99.35° 90.00°	Depositor
Resolution (Å)	49.56 – 2.10 49.56 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.56-2.10) 99.9 (49.56-2.10)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.202 , 0.237 0.201 , 0.237	Depositor DCC
R_{free} test set	1728 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5782	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.38% 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: OLC, ZN, RET, SO4

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	0.09	0/1671	0.22	0/2269
1	B	0.08	0/1646	0.22	0/2235
1	C	0.09	0/1620	0.25	1/2199 (0.0%)
All	All	0.09	0/4937	0.23	1/6703 (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	C	115	ASP	CB-CA-C	-5.41	109.88	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1624	0	1679	12	0
1	B	1600	0	1654	18	0
1	C	1575	0	1639	16	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
3	A	15	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	5	0	0	0	0
4	A	20	0	27	3	0
4	B	20	0	27	3	0
4	C	20	0	27	4	0
5	A	209	0	309	21	0
5	B	294	0	462	22	0
5	C	250	0	400	9	0
6	A	53	0	0	1	0
6	B	46	0	0	1	0
6	C	45	0	0	2	0
All	All	5782	0	6224	81	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 7.

All (81) 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:126:SER:HB3	5:B:315:OLC:H9	1.70	0.73
5:B:304:OLC:H13	5:B:306:OLC:H14A	1.72	0.72
4:B:303:RET:H8	4:B:303:RET:H171	1.80	0.64
1:A:79:MET:HE2	1:A:96:ILE:HG21	1.81	0.63
4:A:307:RET:H171	4:A:307:RET:H8	1.83	0.60
1:C:1:MET:HG3	1:C:174:PHE:HB2	1.83	0.60
1:A:76:SER:HB3	5:A:308:OLC:H6A	1.84	0.60
4:C:303:RET:H8	4:C:303:RET:H161	1.83	0.59
1:B:162:ILE:HG12	5:B:311:OLC:H10	1.84	0.58
1:B:175:TRP:CD1	5:B:309:OLC:H10	2.38	0.58
1:C:137:ALA:HA	1:C:147:ILE:HD13	1.86	0.57
1:A:21:PHE:HA	1:A:35:ILE:HD11	1.87	0.57
5:A:308:OLC:H12A	5:A:309:OLC:H13	1.88	0.55
1:C:90:ASN:ND2	6:C:403:HOH:O	2.39	0.54
5:B:304:OLC:H14	5:B:306:OLC:H10	1.88	0.54
5:A:313:OLC:H22	5:A:316:OLC:H12	1.90	0.54
1:B:30:LEU:HD22	1:B:81:GLU:HG3	1.90	0.53
1:B:29:LYS:NZ	6:B:401:HOH:O	2.43	0.52
1:B:77:PHE:CE2	5:B:304:OLC:H9	2.44	0.52
1:A:22:PHE:HE1	5:A:315:OLC:H12A	1.75	0.52
1:C:123:ILE:HG23	5:C:311:OLC:H11A	1.92	0.51
1:B:194:HIS:HD2	5:B:314:OLC:H24A	1.75	0.51
1:A:122:PHE:CE2	5:A:312:OLC:H2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:308:OLC:H2	5:A:309:OLC:H3	1.91	0.51
1:A:140:ARG:NH1	6:A:401:HOH:O	2.44	0.50
1:C:21:PHE:HA	1:C:35:ILE:HD11	1.94	0.50
5:B:309:OLC:H5	5:B:310:OLC:H7A	1.94	0.49
1:B:171:LEU:HA	5:B:309:OLC:H11A	1.94	0.48
1:C:179:PHE:HZ	5:C:306:OLC:H7A	1.77	0.48
5:A:311:OLC:H11	5:A:311:OLC:H8A	1.61	0.48
5:B:306:OLC:H13A	5:B:307:OLC:H16A	1.95	0.48
5:C:306:OLC:H14A	5:C:308:OLC:H16A	1.95	0.48
1:B:21:PHE:HA	1:B:35:ILE:HD11	1.96	0.47
1:A:36:ILE:HG23	1:C:98:VAL:HG11	1.96	0.47
1:A:53:PHE:HB3	1:A:65:TRP:CZ2	2.49	0.46
1:C:99:PHE:O	1:C:103:VAL:HG23	2.16	0.46
1:C:58:THR:O	5:C:307:OLC:H14A	2.16	0.46
5:C:312:OLC:H8	5:C:312:OLC:H11	1.61	0.46
1:B:98:VAL:HG11	1:C:36:ILE:HG23	1.97	0.46
5:A:311:OLC:H16A	5:B:305:OLC:H8A	1.98	0.46
5:A:315:OLC:H24	5:A:316:OLC:H10	1.96	0.46
1:B:198:LYS:HE3	1:B:199:HIS:CE1	2.50	0.46
1:A:127:VAL:HG21	5:B:308:OLC:H8A	1.97	0.45
4:B:303:RET:H171	4:B:303:RET:C8	2.47	0.45
4:C:303:RET:H181	4:C:303:RET:H7	1.73	0.45
5:A:311:OLC:H3A	5:A:311:OLC:H6	1.85	0.44
5:A:310:OLC:H8	5:A:310:OLC:H11	1.66	0.44
4:A:307:RET:H181	4:A:307:RET:H7	1.73	0.44
1:A:10:ILE:HG21	5:A:314:OLC:H2A	1.98	0.44
4:B:303:RET:H7	4:B:303:RET:H181	1.72	0.44
5:B:310:OLC:H11	5:B:310:OLC:H8	1.73	0.44
5:B:309:OLC:H4	5:B:310:OLC:H5A	1.99	0.43
5:A:313:OLC:H2A	1:C:127:VAL:HG21	1.99	0.43
5:C:311:OLC:H11A	5:C:311:OLC:H14A	1.85	0.43
1:C:163:LEU:HD13	5:C:308:OLC:H5	2.00	0.43
5:B:306:OLC:H8A	5:B:306:OLC:H5	1.78	0.43
5:A:309:OLC:H11	5:A:309:OLC:H8	1.83	0.43
1:B:99:PHE:O	1:B:103:VAL:HG23	2.18	0.43
5:A:308:OLC:H17A	5:A:308:OLC:H14	1.79	0.43
5:B:314:OLC:H8A	5:B:314:OLC:H5	1.78	0.43
5:A:309:OLC:H5A	5:B:306:OLC:H18	2.01	0.42
1:B:119:TRP:CE2	5:B:311:OLC:H5	2.54	0.42
1:A:119:TRP:CE2	5:A:312:OLC:H22	2.55	0.42
1:C:38:SER:O	1:C:42:ILE:HG13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:316:OLC:H8	5:A:316:OLC:H11	1.86	0.42
1:A:98:VAL:HG11	1:B:36:ILE:HG23	2.01	0.42
1:B:1:MET:HG3	1:B:174:PHE:CD1	2.55	0.42
5:A:309:OLC:H13A	5:A:309:OLC:H16A	1.89	0.41
1:B:161:TRP:HZ3	5:B:311:OLC:H9	1.85	0.41
1:B:119:TRP:NE1	5:B:311:OLC:H5	2.35	0.41
5:A:315:OLC:H8	5:A:315:OLC:H11	1.85	0.41
1:B:185:PHE:CD2	5:B:312:OLC:H14	2.56	0.41
5:C:304:OLC:H12A	5:C:304:OLC:H15A	1.80	0.41
5:C:313:OLC:H6A	5:C:313:OLC:H9	1.66	0.41
4:A:307:RET:H171	4:A:307:RET:C8	2.48	0.41
5:B:307:OLC:H3	1:C:93:ARG:NH1	2.36	0.41
1:C:30:LEU:HD22	1:C:81:GLU:HG3	2.03	0.41
4:C:303:RET:H11	4:C:303:RET:H191	1.95	0.41
4:C:303:RET:H161	4:C:303:RET:C8	2.49	0.40
1:C:29:LYS:NZ	6:C:405:HOH:O	2.54	0.40
5:A:308:OLC:H13	5:A:309:OLC:H15	2.03	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	197/210 (94%)	193 (98%)	4 (2%)	0	100	100
1	B	192/210 (91%)	191 (100%)	1 (0%)	0	100	100
1	C	189/210 (90%)	187 (99%)	2 (1%)	0	100	100
All	All	578/630 (92%)	571 (99%)	7 (1%)	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	177/189 (94%)	176 (99%)	1 (1%)	78	86
1	B	174/189 (92%)	173 (99%)	1 (1%)	78	86
1	C	172/189 (91%)	172 (100%)	0	100	100
All	All	523/567 (92%)	521 (100%)	2 (0%)	84	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	B	87	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	B	34	ASN
1	B	194	HIS
1	B	199	HIS
1	C	131	ASN

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

Of 45 ligands modelled in this entry, 6 are monoatomic - leaving 39 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
5	OLC	A	311	-	24,24,24	0.92	1 (4%)	25,25,25	0.89	1 (4%)
5	OLC	B	306	-	24,24,24	0.93	1 (4%)	25,25,25	0.88	1 (4%)
5	OLC	B	311	-	24,24,24	0.92	1 (4%)	25,25,25	0.76	1 (4%)
5	OLC	B	308	-	24,24,24	0.92	1 (4%)	25,25,25	0.94	1 (4%)
5	OLC	A	316	-	22,22,24	0.96	1 (4%)	23,23,25	0.86	1 (4%)
5	OLC	A	309	-	24,24,24	0.91	1 (4%)	25,25,25	0.83	1 (4%)
5	OLC	C	307	-	24,24,24	0.91	1 (4%)	25,25,25	0.87	1 (4%)
3	SO4	A	306	-	4,4,4	0.23	0	6,6,6	0.08	0
5	OLC	A	310	-	24,24,24	0.91	1 (4%)	25,25,25	0.89	1 (4%)
5	OLC	B	312	-	24,24,24	0.94	1 (4%)	25,25,25	0.98	2 (8%)
4	RET	A	307	1	20,20,21	2.55	5 (25%)	27,27,28	1.36	5 (18%)
5	OLC	C	305	-	24,24,24	0.93	1 (4%)	25,25,25	0.89	1 (4%)
5	OLC	B	310	-	24,24,24	0.93	1 (4%)	25,25,25	0.96	2 (8%)
5	OLC	C	309	-	24,24,24	0.93	1 (4%)	25,25,25	0.86	1 (4%)
5	OLC	B	305	-	24,24,24	0.91	1 (4%)	25,25,25	0.74	0
4	RET	B	303	1	20,20,21	2.50	5 (25%)	27,27,28	1.36	6 (22%)
5	OLC	A	315	-	24,24,24	0.93	1 (4%)	25,25,25	0.92	2 (8%)
5	OLC	C	306	-	24,24,24	0.91	1 (4%)	25,25,25	0.82	1 (4%)
5	OLC	A	317	-	19,19,24	1.03	1 (5%)	20,20,25	0.94	1 (5%)
5	OLC	B	307	-	24,24,24	0.91	1 (4%)	25,25,25	0.76	0
5	OLC	C	304	-	24,24,24	0.93	1 (4%)	25,25,25	0.82	1 (4%)
5	OLC	C	311	-	24,24,24	0.93	1 (4%)	25,25,25	0.93	1 (4%)
5	OLC	B	304	-	21,21,24	0.99	1 (4%)	22,22,25	0.91	1 (4%)
5	OLC	B	314	-	21,21,24	0.99	1 (4%)	22,22,25	0.99	2 (9%)
5	OLC	B	309	-	24,24,24	0.93	1 (4%)	25,25,25	0.99	2 (8%)
5	OLC	A	314	-	13,13,24	1.24	1 (7%)	14,14,25	1.10	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	305	-	4,4,4	0.23	0	6,6,6	0.08	0
5	OLC	A	313	-	13,13,24	1.22	1 (7%)	14,14,25	0.92	1 (7%)
5	OLC	C	312	-	24,24,24	0.92	1 (4%)	25,25,25	0.89	1 (4%)
5	OLC	C	310	-	24,24,24	0.93	1 (4%)	25,25,25	0.91	2 (8%)
4	RET	C	303	1	20,20,21	2.49	5 (25%)	27,27,28	1.38	5 (18%)
3	SO4	A	304	2	4,4,4	0.23	0	6,6,6	0.09	0
5	OLC	C	313	-	24,24,24	0.92	1 (4%)	25,25,25	0.85	1 (4%)
3	SO4	C	302	-	4,4,4	0.24	0	6,6,6	0.09	0
5	OLC	C	308	-	24,24,24	0.93	1 (4%)	25,25,25	0.94	1 (4%)
5	OLC	A	312	-	12,12,24	1.28	1 (8%)	13,13,25	1.17	2 (15%)
5	OLC	B	315	-	24,24,24	0.92	1 (4%)	25,25,25	0.81	1 (4%)
5	OLC	B	313	-	24,24,24	0.92	1 (4%)	25,25,25	0.90	2 (8%)
5	OLC	A	308	-	24,24,24	0.90	1 (4%)	25,25,25	0.99	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
5	OLC	A	311	-	-	6/24/24/24	-
5	OLC	B	306	-	-	6/24/24/24	-
5	OLC	B	311	-	-	8/24/24/24	-
5	OLC	B	308	-	-	4/24/24/24	-
5	OLC	A	316	-	-	6/22/22/24	-
5	OLC	A	309	-	-	5/24/24/24	-
5	OLC	C	307	-	-	4/24/24/24	-
5	OLC	A	310	-	-	0/24/24/24	-
5	OLC	B	312	-	-	3/24/24/24	-
4	RET	A	307	1	-	0/13/30/31	0/1/1/1
5	OLC	C	305	-	-	1/24/24/24	-
5	OLC	B	310	-	-	5/24/24/24	-
5	OLC	C	309	-	-	7/24/24/24	-
5	OLC	B	305	-	-	5/24/24/24	-
4	RET	B	303	1	-	0/13/30/31	0/1/1/1
5	OLC	A	315	-	-	8/24/24/24	-
5	OLC	C	306	-	-	7/24/24/24	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLC	A	317	-	-	6/19/19/24	-
5	OLC	B	307	-	-	7/24/24/24	-
5	OLC	C	304	-	-	12/24/24/24	-
5	OLC	C	311	-	-	12/24/24/24	-
5	OLC	B	304	-	-	6/21/21/24	-
5	OLC	B	314	-	-	8/21/21/24	-
5	OLC	B	309	-	-	9/24/24/24	-
5	OLC	A	314	-	-	2/13/13/24	-
5	OLC	A	313	-	-	5/13/13/24	-
5	OLC	C	312	-	-	7/24/24/24	-
5	OLC	C	310	-	-	1/24/24/24	-
4	RET	C	303	1	-	0/13/30/31	0/1/1/1
5	OLC	C	313	-	-	16/24/24/24	-
5	OLC	C	308	-	-	7/24/24/24	-
5	OLC	A	312	-	-	5/12/12/24	-
5	OLC	B	315	-	-	10/24/24/24	-
5	OLC	B	313	-	-	10/24/24/24	-
5	OLC	A	308	-	-	5/24/24/24	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	307	RET	C14-C13	9.65	1.40	1.33
4	B	303	RET	C14-C13	9.33	1.40	1.33
4	C	303	RET	C14-C13	9.26	1.40	1.33
5	B	312	OLC	O20-C1	4.34	1.46	1.33
5	C	308	OLC	O20-C1	4.33	1.46	1.33
5	A	315	OLC	O20-C1	4.33	1.46	1.33
5	B	310	OLC	O20-C1	4.32	1.45	1.33
5	B	314	OLC	O20-C1	4.32	1.45	1.33
5	C	310	OLC	O20-C1	4.32	1.45	1.33
5	B	306	OLC	O20-C1	4.31	1.45	1.33
5	C	305	OLC	O20-C1	4.31	1.45	1.33
5	C	311	OLC	O20-C1	4.31	1.45	1.33
5	A	317	OLC	O20-C1	4.30	1.45	1.33
5	B	304	OLC	O20-C1	4.30	1.45	1.33
5	B	309	OLC	O20-C1	4.30	1.45	1.33
5	C	309	OLC	O20-C1	4.29	1.45	1.33
5	C	304	OLC	O20-C1	4.28	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	314	OLC	O20-C1	4.28	1.45	1.33
5	C	313	OLC	O20-C1	4.26	1.45	1.33
5	B	308	OLC	O20-C1	4.26	1.45	1.33
5	C	312	OLC	O20-C1	4.26	1.45	1.33
5	A	312	OLC	O20-C1	4.25	1.45	1.33
5	B	313	OLC	O20-C1	4.25	1.45	1.33
5	A	311	OLC	O20-C1	4.25	1.45	1.33
5	A	309	OLC	O20-C1	4.24	1.45	1.33
5	A	310	OLC	O20-C1	4.24	1.45	1.33
5	B	315	OLC	O20-C1	4.23	1.45	1.33
5	A	316	OLC	O20-C1	4.23	1.45	1.33
5	C	307	OLC	O20-C1	4.23	1.45	1.33
5	B	311	OLC	O20-C1	4.23	1.45	1.33
5	C	306	OLC	O20-C1	4.21	1.45	1.33
5	A	313	OLC	O20-C1	4.21	1.45	1.33
5	B	307	OLC	O20-C1	4.21	1.45	1.33
5	A	308	OLC	O20-C1	4.20	1.45	1.33
5	B	305	OLC	O20-C1	4.18	1.45	1.33
4	B	303	RET	C8-C9	-2.80	1.40	1.46
4	C	303	RET	C8-C9	-2.77	1.40	1.46
4	C	303	RET	C15-C14	-2.75	1.39	1.49
4	A	307	RET	C8-C9	-2.74	1.40	1.46
4	B	303	RET	C15-C14	-2.74	1.39	1.49
4	A	307	RET	C15-C14	-2.69	1.39	1.49
4	B	303	RET	C10-C9	2.28	1.41	1.35
4	A	307	RET	C10-C9	2.28	1.41	1.35
4	C	303	RET	C10-C9	2.26	1.41	1.35
4	C	303	RET	C12-C13	-2.21	1.41	1.46
4	B	303	RET	C12-C13	-2.21	1.41	1.46
4	A	307	RET	C12-C13	-2.15	1.41	1.46

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	303	RET	C19-C9-C10	-3.37	117.36	122.82
5	B	310	OLC	O20-C1-C2	3.27	121.81	111.83
5	B	309	OLC	O20-C1-C2	3.25	121.76	111.83
4	A	307	RET	C19-C9-C10	-3.25	117.55	122.82
5	B	312	OLC	O20-C1-C2	3.19	121.57	111.83
4	B	303	RET	C19-C9-C10	-3.17	117.67	122.82
5	A	312	OLC	O20-C1-C2	3.13	121.39	111.83
5	C	308	OLC	O20-C1-C2	3.03	121.06	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	311	OLC	O20-C1-C2	3.02	121.04	111.83
5	A	308	OLC	O20-C1-C2	3.02	121.03	111.83
5	B	314	OLC	O20-C1-C2	3.02	121.03	111.83
5	A	315	OLC	O20-C1-C2	3.00	120.97	111.83
5	B	308	OLC	O20-C1-C2	2.95	120.84	111.83
5	B	313	OLC	O20-C1-C2	2.88	120.63	111.83
5	B	304	OLC	O20-C1-C2	2.86	120.57	111.83
5	C	310	OLC	O20-C1-C2	2.85	120.53	111.83
5	A	314	OLC	O20-C1-C2	2.85	120.51	111.83
5	C	313	OLC	O20-C1-C2	2.73	120.15	111.83
5	C	305	OLC	O20-C1-C2	2.72	120.13	111.83
5	B	306	OLC	O20-C1-C2	2.72	120.12	111.83
5	A	310	OLC	O20-C1-C2	2.71	120.09	111.83
5	C	312	OLC	O20-C1-C2	2.68	120.01	111.83
5	A	311	OLC	O20-C1-C2	2.67	119.97	111.83
4	C	303	RET	C2-C1-C6	2.66	114.30	110.44
5	C	309	OLC	O20-C1-C2	2.65	119.92	111.83
5	C	307	OLC	O20-C1-C2	2.63	119.86	111.83
5	C	304	OLC	O20-C1-C2	2.63	119.85	111.83
5	A	316	OLC	O20-C1-C2	2.60	119.76	111.83
5	A	317	OLC	O20-C1-C2	2.50	119.45	111.83
5	A	309	OLC	O20-C1-C2	2.47	119.38	111.83
4	A	307	RET	C2-C1-C6	2.46	114.01	110.44
4	B	303	RET	C2-C1-C6	2.38	113.90	110.44
4	B	303	RET	C19-C9-C8	2.38	121.72	118.09
4	B	303	RET	C1-C6-C7	2.37	122.08	115.65
5	B	315	OLC	O20-C1-C2	2.36	119.02	111.83
4	C	303	RET	C1-C6-C7	2.34	122.01	115.65
4	A	307	RET	C1-C6-C7	2.34	122.00	115.65
5	C	306	OLC	O20-C1-C2	2.31	118.89	111.83
4	A	307	RET	C19-C9-C8	2.29	121.58	118.09
4	C	303	RET	C19-C9-C8	2.27	121.55	118.09
5	A	313	OLC	O20-C1-C2	2.26	118.73	111.83
5	B	309	OLC	O20-C1-O19	-2.21	118.11	123.63
5	B	310	OLC	O20-C1-O19	-2.18	118.17	123.63
4	C	303	RET	C1-C6-C5	-2.13	119.73	122.64
5	B	311	OLC	O20-C1-C2	2.12	118.30	111.83
5	A	312	OLC	O20-C1-O19	-2.09	118.40	123.63
5	B	312	OLC	O20-C1-O19	-2.09	118.41	123.63
5	B	314	OLC	O20-C1-O19	-2.09	118.41	123.63
4	B	303	RET	C1-C6-C5	-2.07	119.81	122.64
4	A	307	RET	C1-C6-C5	-2.06	119.82	122.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	303	RET	C11-C10-C9	2.03	130.13	127.28
5	C	310	OLC	O20-C1-O19	-2.03	118.54	123.63
5	B	313	OLC	O20-C1-O19	-2.02	118.59	123.63
5	A	315	OLC	O20-C1-O19	-2.02	118.59	123.63

There are no chirality outliers.

All (203) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	317	OLC	C10-C11-C12-C13
5	A	317	OLC	O20-C21-C22-O23
5	B	314	OLC	O20-C21-C22-O23
5	C	306	OLC	O20-C21-C22-C24
5	C	307	OLC	O20-C21-C22-C24
5	C	309	OLC	O20-C21-C22-C24
5	C	313	OLC	O20-C21-C22-C24
5	A	311	OLC	C2-C1-O20-C21
5	B	304	OLC	C2-C1-O20-C21
5	B	307	OLC	C2-C1-O20-C21
5	B	307	OLC	O19-C1-O20-C21
5	B	305	OLC	C2-C1-O20-C21
5	B	309	OLC	O20-C21-C22-O23
5	C	307	OLC	O20-C21-C22-O23
5	C	313	OLC	O20-C21-C22-O23
5	B	305	OLC	O19-C1-O20-C21
5	A	311	OLC	O19-C1-O20-C21
5	B	304	OLC	O19-C1-O20-C21
5	A	313	OLC	C2-C1-O20-C21
5	B	309	OLC	C2-C1-O20-C21
5	B	311	OLC	C2-C1-O20-C21
5	C	306	OLC	C2-C1-O20-C21
5	B	315	OLC	C11-C12-C13-C14
5	B	314	OLC	O20-C21-C22-C24
5	B	309	OLC	O19-C1-O20-C21
5	A	308	OLC	O20-C21-C22-O23
5	B	311	OLC	O19-C1-O20-C21
5	B	313	OLC	C2-C1-O20-C21
5	C	306	OLC	O19-C1-O20-C21
5	A	313	OLC	O19-C1-O20-C21
5	A	312	OLC	O20-C21-C22-O23
5	C	309	OLC	O20-C21-C22-O23
5	C	308	OLC	C2-C1-O20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	313	OLC	C6-C7-C8-C9
5	A	308	OLC	O20-C21-C22-C24
5	A	312	OLC	O20-C21-C22-C24
5	B	313	OLC	O19-C1-O20-C21
5	C	306	OLC	O20-C21-C22-O23
5	B	307	OLC	C21-C22-C24-O25
5	A	308	OLC	C2-C1-O20-C21
5	C	312	OLC	C1-C2-C3-C4
5	C	312	OLC	C4-C5-C6-C7
5	B	311	OLC	C5-C6-C7-C8
5	A	314	OLC	C2-C1-O20-C21
5	A	315	OLC	C4-C5-C6-C7
5	B	308	OLC	C11-C12-C13-C14
5	A	315	OLC	C3-C4-C5-C6
5	B	304	OLC	C3-C4-C5-C6
5	C	313	OLC	C5-C6-C7-C8
5	B	309	OLC	C2-C3-C4-C5
5	A	317	OLC	C1-C2-C3-C4
5	C	313	OLC	C11-C12-C13-C14
5	C	313	OLC	C4-C5-C6-C7
5	C	308	OLC	O19-C1-O20-C21
5	B	313	OLC	C6-C7-C8-C9
5	B	311	OLC	C14-C15-C16-C17
5	C	306	OLC	C11-C12-C13-C14
5	A	308	OLC	O19-C1-O20-C21
5	B	306	OLC	C4-C5-C6-C7
5	C	311	OLC	C13-C14-C15-C16
5	B	306	OLC	C13-C14-C15-C16
5	B	313	OLC	C4-C5-C6-C7
5	B	313	OLC	C11-C12-C13-C14
5	A	314	OLC	O19-C1-O20-C21
5	B	306	OLC	C12-C13-C14-C15
5	C	312	OLC	C3-C4-C5-C6
5	A	316	OLC	C1-C2-C3-C4
5	B	310	OLC	C1-C2-C3-C4
5	C	304	OLC	C10-C11-C12-C13
5	C	306	OLC	C1-C2-C3-C4
5	A	316	OLC	C3-C4-C5-C6
5	B	315	OLC	C13-C14-C15-C16
5	C	309	OLC	C5-C6-C7-C8
5	B	306	OLC	C10-C11-C12-C13
5	B	313	OLC	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	313	OLC	C10-C11-C12-C13
5	B	315	OLC	O20-C21-C22-O23
5	A	317	OLC	O20-C21-C22-C24
5	B	304	OLC	C6-C7-C8-C9
5	B	312	OLC	C11-C12-C13-C14
5	A	309	OLC	C2-C1-O20-C21
5	C	313	OLC	C2-C1-O20-C21
5	C	311	OLC	C12-C13-C14-C15
5	C	307	OLC	C11-C12-C13-C14
5	C	313	OLC	C14-C15-C16-C17
5	C	311	OLC	C2-C1-O20-C21
5	A	309	OLC	C10-C11-C12-C13
5	B	315	OLC	C6-C7-C8-C9
5	B	305	OLC	C5-C6-C7-C8
5	B	304	OLC	C4-C5-C6-C7
5	B	310	OLC	C15-C16-C17-C18
5	C	304	OLC	C15-C16-C17-C18
5	B	315	OLC	C2-C1-O20-C21
5	C	312	OLC	C2-C1-O20-C21
5	C	312	OLC	C12-C13-C14-C15
5	A	312	OLC	C1-C2-C3-C4
5	A	315	OLC	C2-C1-O20-C21
5	A	309	OLC	O19-C1-O20-C21
5	C	304	OLC	C6-C7-C8-C9
5	B	309	OLC	C1-C2-C3-C4
5	B	304	OLC	C2-C3-C4-C5
5	C	311	OLC	C6-C7-C8-C9
5	C	313	OLC	O19-C1-O20-C21
5	C	311	OLC	O20-C21-C22-C24
5	C	311	OLC	O20-C21-C22-O23
5	C	308	OLC	C11-C12-C13-C14
5	B	310	OLC	C3-C4-C5-C6
5	B	306	OLC	C11-C12-C13-C14
5	A	315	OLC	O23-C22-C24-O25
5	C	304	OLC	C2-C1-O20-C21
5	C	304	OLC	C5-C6-C7-C8
5	B	315	OLC	O19-C1-O20-C21
5	C	311	OLC	O19-C1-O20-C21
5	A	308	OLC	C4-C5-C6-C7
5	C	305	OLC	C10-C11-C12-C13
5	C	312	OLC	O19-C1-O20-C21
5	A	313	OLC	O20-C21-C22-O23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	314	OLC	C2-C1-O20-C21
5	B	313	OLC	C12-C13-C14-C15
5	C	304	OLC	O19-C1-O20-C21
5	C	304	OLC	C14-C15-C16-C17
5	C	304	OLC	C12-C13-C14-C15
5	A	317	OLC	C4-C5-C6-C7
5	B	313	OLC	C2-C3-C4-C5
5	A	315	OLC	O19-C1-O20-C21
5	C	312	OLC	C14-C15-C16-C17
5	C	313	OLC	C2-C3-C4-C5
5	B	314	OLC	O19-C1-O20-C21
5	C	309	OLC	C15-C16-C17-C18
5	B	309	OLC	C11-C12-C13-C14
5	C	310	OLC	C2-C3-C4-C5
5	B	315	OLC	C14-C15-C16-C17
5	C	308	OLC	C10-C11-C12-C13
5	B	308	OLC	C3-C4-C5-C6
5	A	311	OLC	C4-C5-C6-C7
5	B	315	OLC	C1-C2-C3-C4
5	C	309	OLC	C1-C2-C3-C4
5	B	309	OLC	C14-C15-C16-C17
5	B	311	OLC	C13-C14-C15-C16
5	A	316	OLC	O20-C21-C22-O23
5	B	309	OLC	C7-C8-C9-C10
5	A	316	OLC	C4-C5-C6-C7
5	B	309	OLC	O20-C21-C22-C24
5	A	312	OLC	C2-C1-O20-C21
5	B	310	OLC	C2-C3-C4-C5
5	B	314	OLC	C7-C8-C9-C10
5	C	304	OLC	C7-C8-C9-C10
5	C	308	OLC	C9-C10-C11-C12
5	C	304	OLC	O20-C21-C22-O23
5	C	311	OLC	C14-C15-C16-C17
5	A	312	OLC	O19-C1-O20-C21
5	C	313	OLC	C1-C2-C3-C4
5	C	304	OLC	C9-C10-C11-C12
5	B	307	OLC	C13-C14-C15-C16
5	B	315	OLC	C5-C6-C7-C8
5	A	316	OLC	C2-C3-C4-C5
5	B	306	OLC	C5-C6-C7-C8
5	B	311	OLC	O20-C1-C2-C3
5	B	315	OLC	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	311	OLC	C14-C15-C16-C17
5	C	309	OLC	C12-C13-C14-C15
5	B	307	OLC	O23-C22-C24-O25
5	C	311	OLC	C2-C3-C4-C5
5	A	317	OLC	C9-C10-C11-C12
5	B	308	OLC	C5-C6-C7-C8
5	A	311	OLC	O20-C21-C22-C24
5	A	313	OLC	O20-C21-C22-C24
5	B	314	OLC	C9-C10-C11-C12
5	C	309	OLC	C7-C8-C9-C10
5	A	311	OLC	O20-C21-C22-O23
5	C	313	OLC	C7-C8-C9-C10
5	B	308	OLC	C2-C3-C4-C5
5	B	311	OLC	C9-C10-C11-C12
5	B	311	OLC	C2-C3-C4-C5
5	A	316	OLC	C7-C8-C9-C10
5	B	307	OLC	C7-C8-C9-C10
5	C	311	OLC	C9-C10-C11-C12
5	B	313	OLC	O20-C1-C2-C3
5	C	313	OLC	C15-C16-C17-C18
5	A	315	OLC	C2-C3-C4-C5
5	A	309	OLC	O20-C21-C22-C24
5	C	304	OLC	O20-C21-C22-C24
5	C	306	OLC	C2-C3-C4-C5
5	A	315	OLC	O20-C1-C2-C3
5	C	308	OLC	O20-C1-C2-C3
5	B	307	OLC	O20-C1-C2-C3
5	B	312	OLC	C12-C13-C14-C15
5	B	314	OLC	O23-C22-C24-O25
5	C	313	OLC	O20-C1-C2-C3
5	C	311	OLC	C11-C12-C13-C14
5	B	310	OLC	C12-C13-C14-C15
5	C	311	OLC	C4-C5-C6-C7
5	B	314	OLC	C4-C5-C6-C7
5	A	313	OLC	C4-C5-C6-C7
5	C	307	OLC	C12-C13-C14-C15
5	B	305	OLC	C4-C5-C6-C7
5	A	309	OLC	C9-C10-C11-C12
5	C	308	OLC	O19-C1-C2-C3
5	B	313	OLC	O19-C1-C2-C3
5	B	305	OLC	O20-C21-C22-O23
5	A	315	OLC	O19-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	312	OLC	C2-C1-O20-C21
5	C	313	OLC	O19-C1-C2-C3

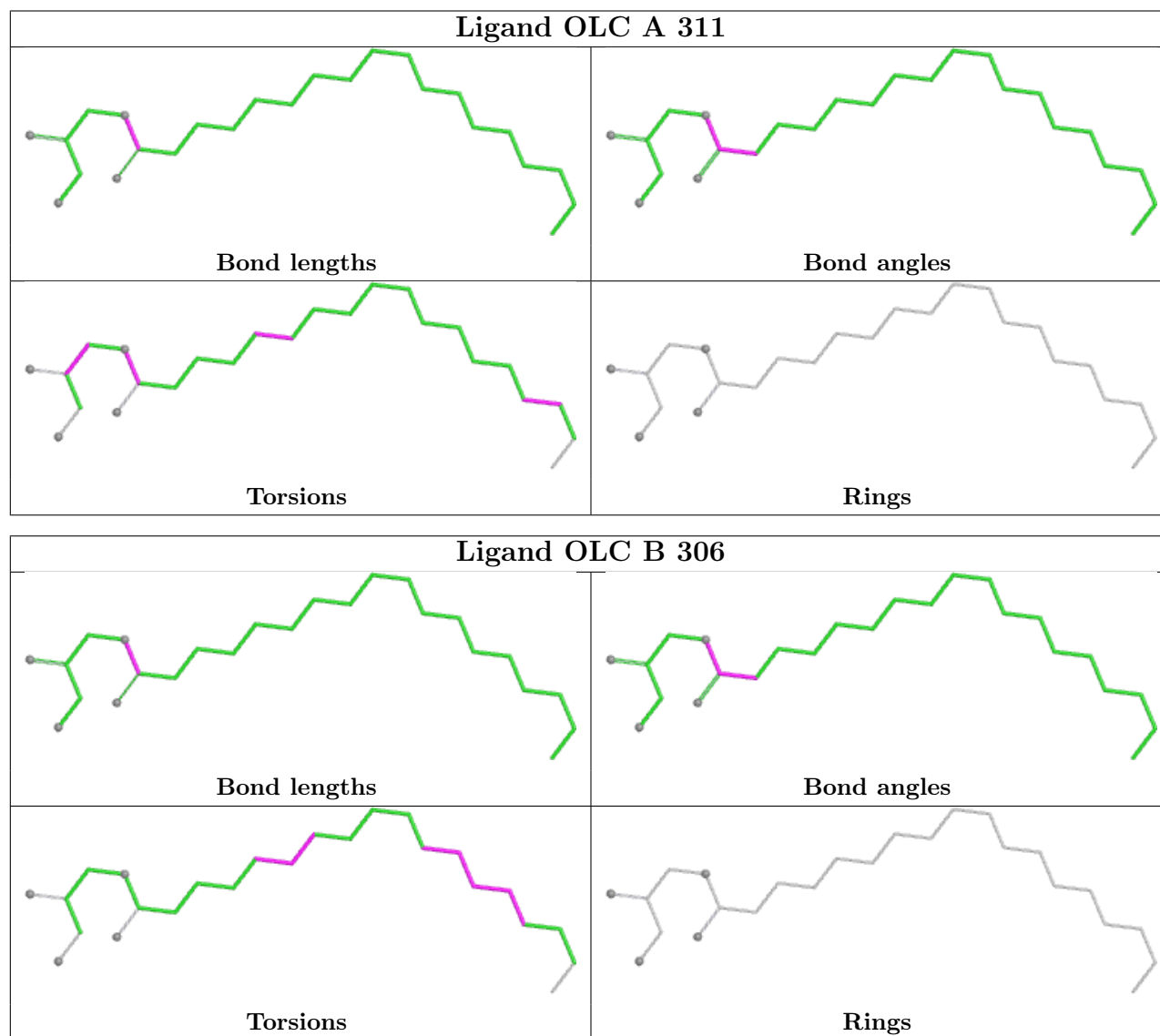
There are no ring outliers.

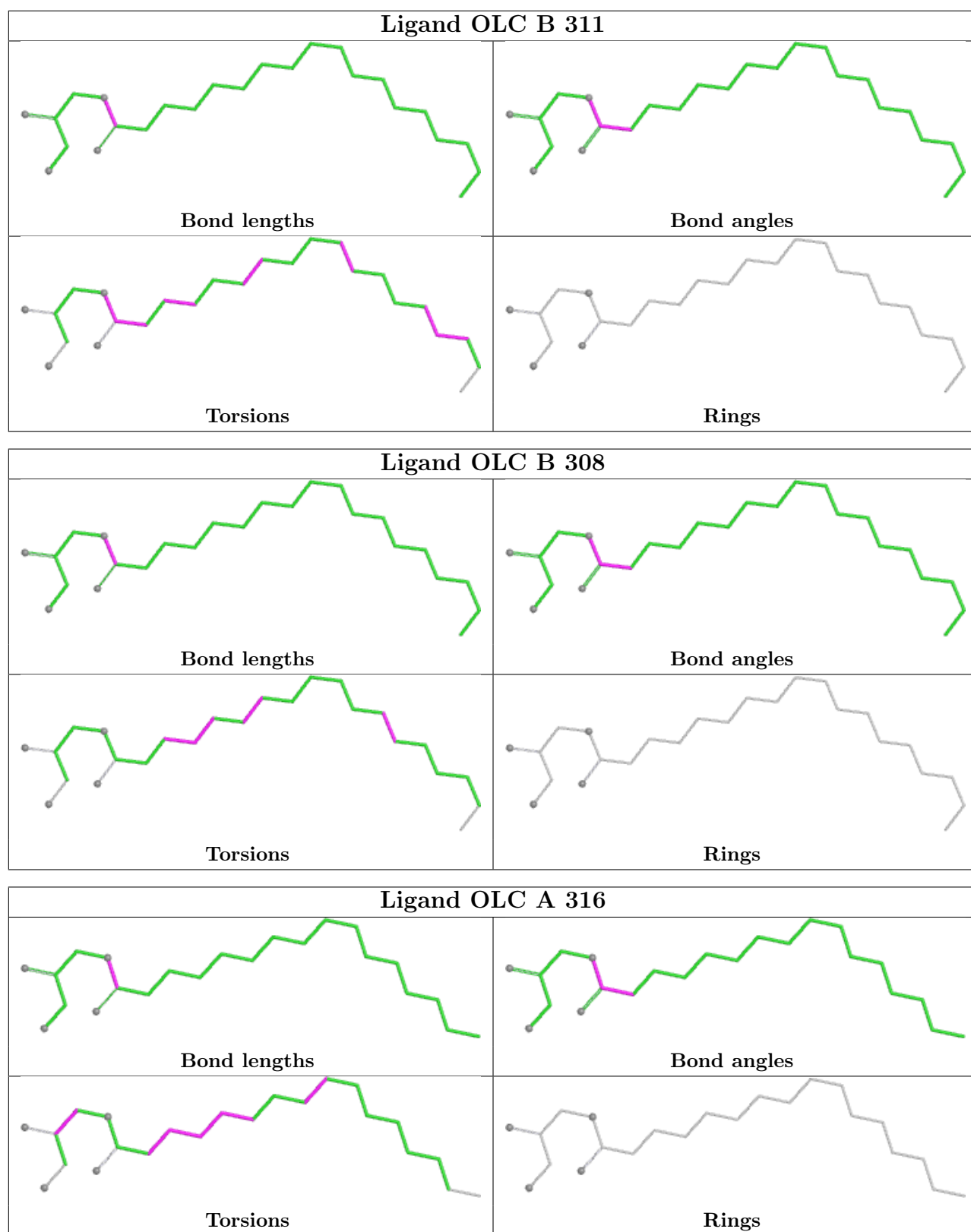
30 monomers are involved in 60 short contacts:

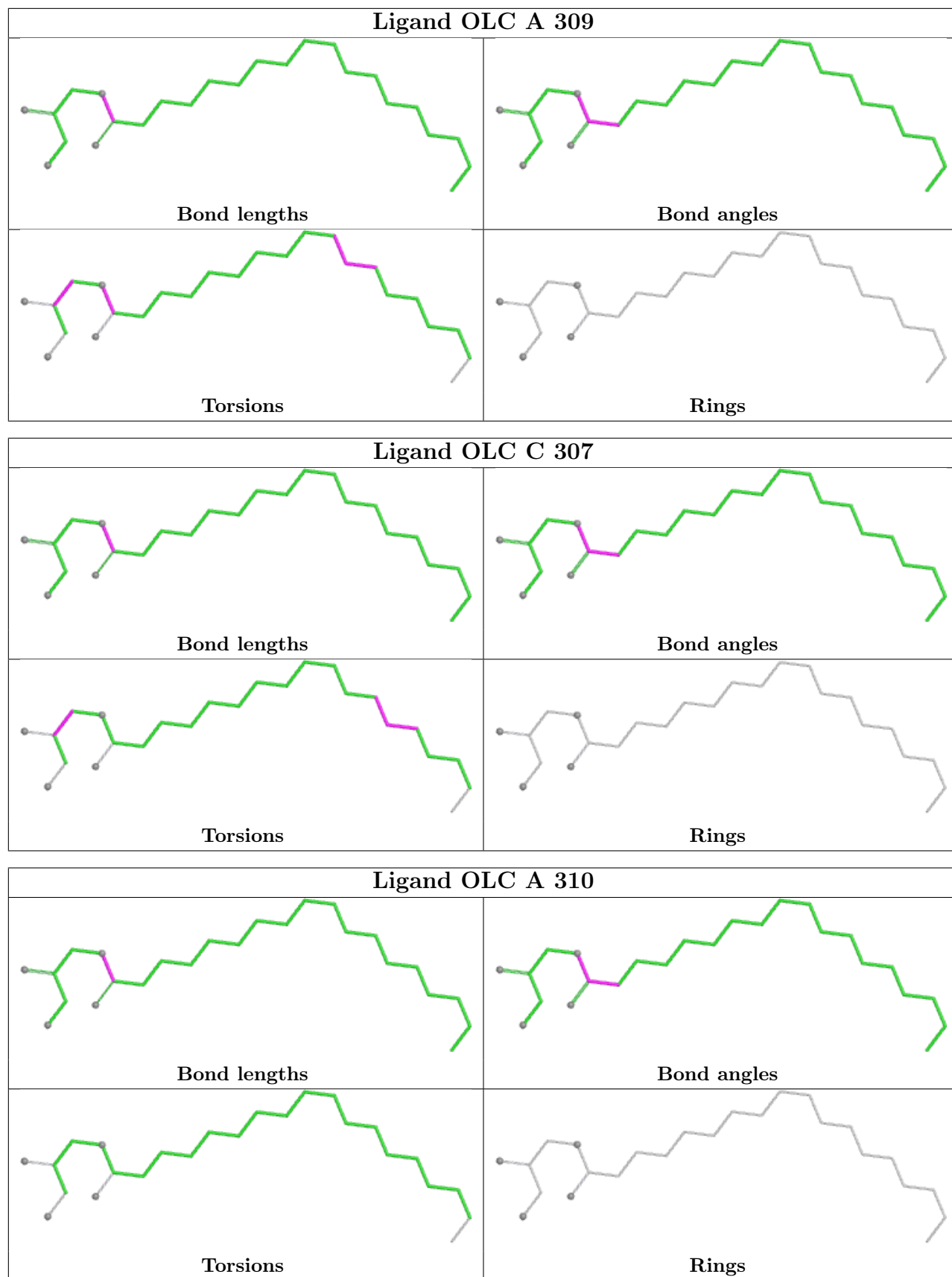
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	311	OLC	3	0
5	B	306	OLC	5	0
5	B	311	OLC	4	0
5	B	308	OLC	1	0
5	A	316	OLC	3	0
5	A	309	OLC	6	0
5	C	307	OLC	1	0
5	A	310	OLC	1	0
5	B	312	OLC	1	0
4	A	307	RET	3	0
5	B	310	OLC	3	0
5	B	305	OLC	1	0
4	B	303	RET	3	0
5	A	315	OLC	3	0
5	C	306	OLC	2	0
5	B	307	OLC	2	0
5	C	304	OLC	1	0
5	C	311	OLC	2	0
5	B	304	OLC	3	0
5	B	314	OLC	2	0
5	B	309	OLC	4	0
5	A	314	OLC	1	0
5	A	313	OLC	2	0
5	C	312	OLC	1	0
4	C	303	RET	4	0
5	C	313	OLC	1	0
5	C	308	OLC	2	0
5	A	312	OLC	2	0
5	B	315	OLC	1	0
5	A	308	OLC	5	0

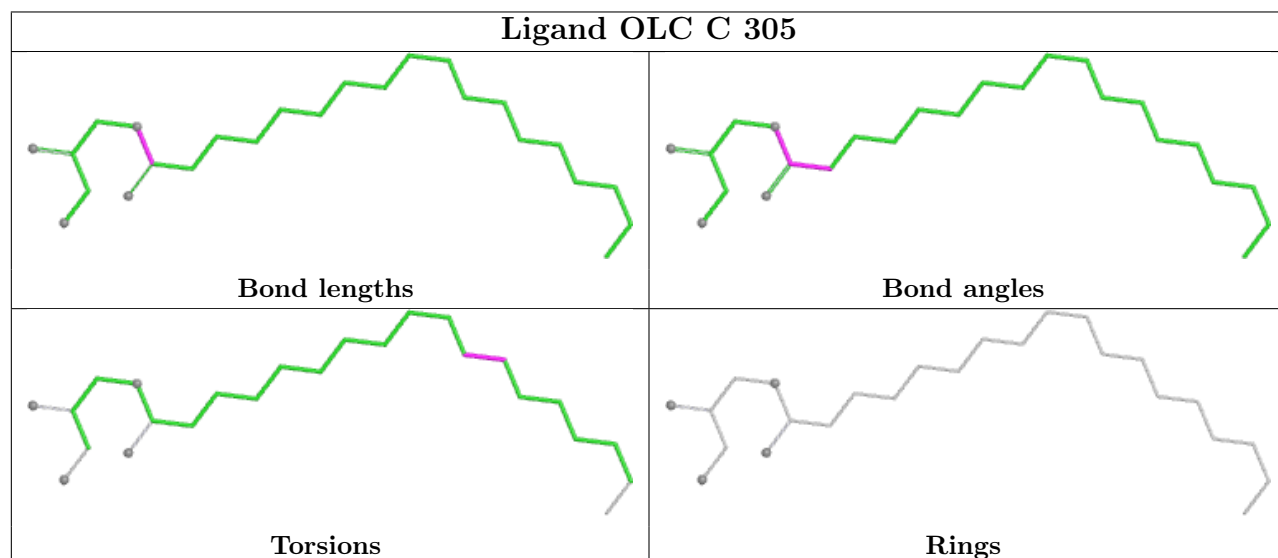
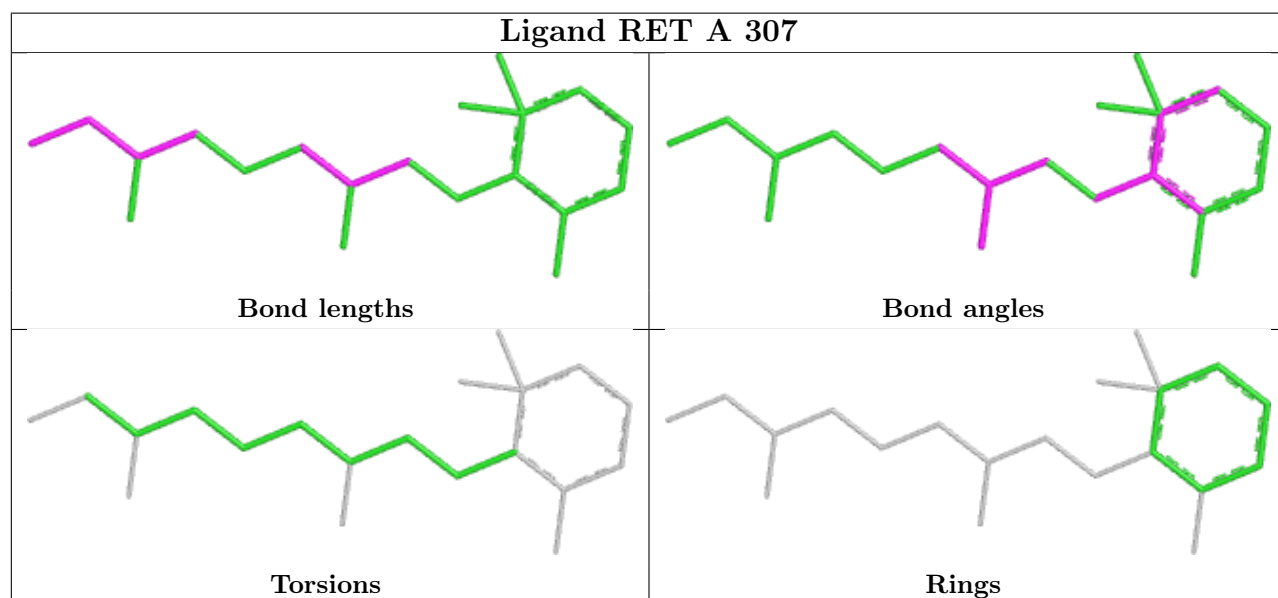
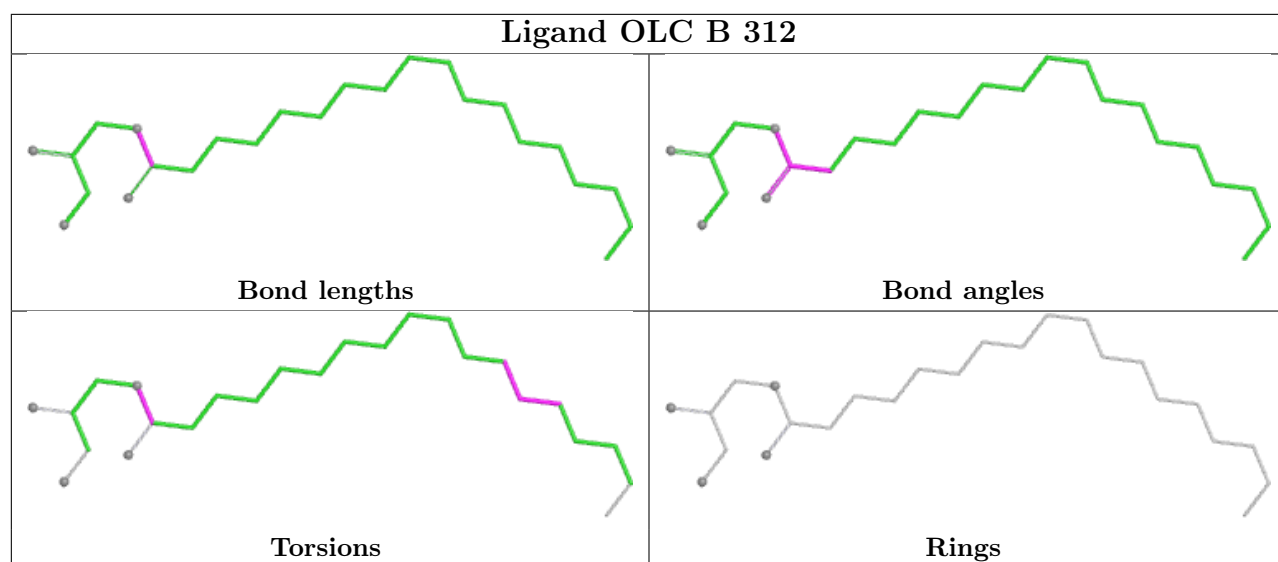
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

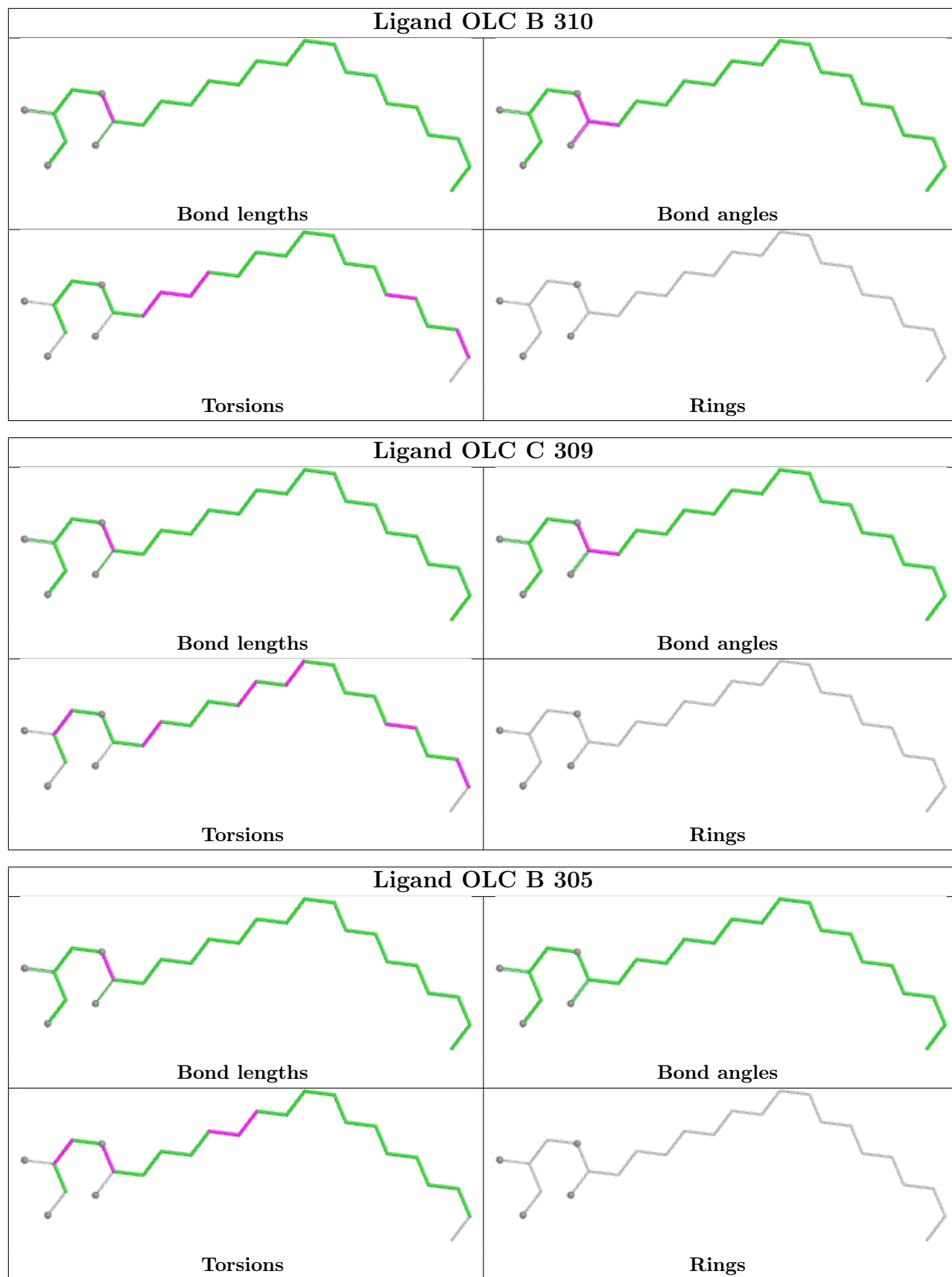
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

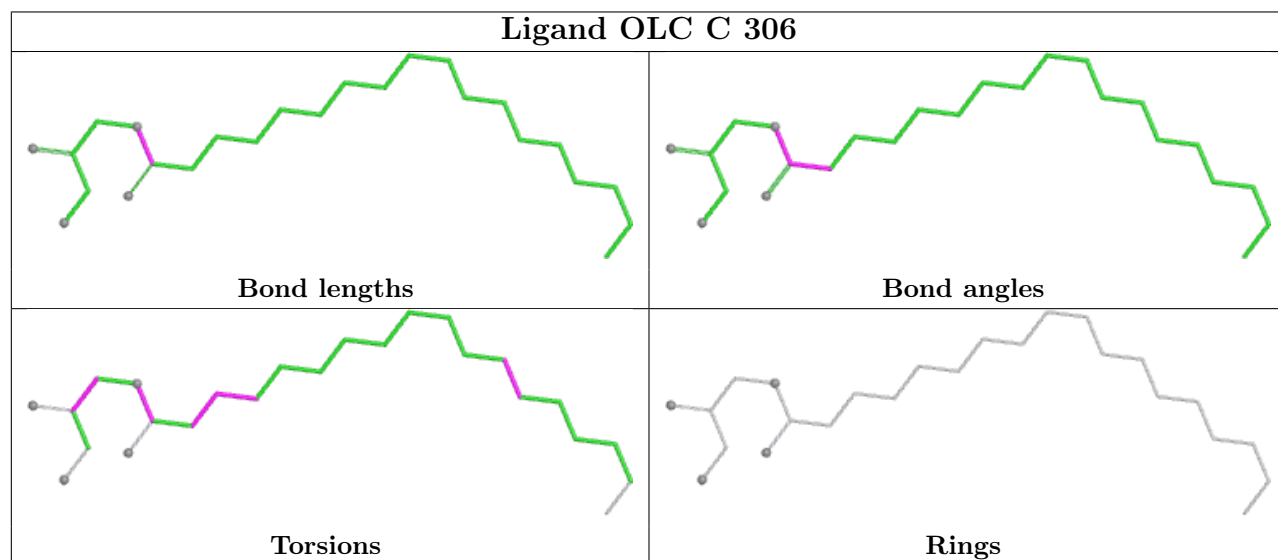
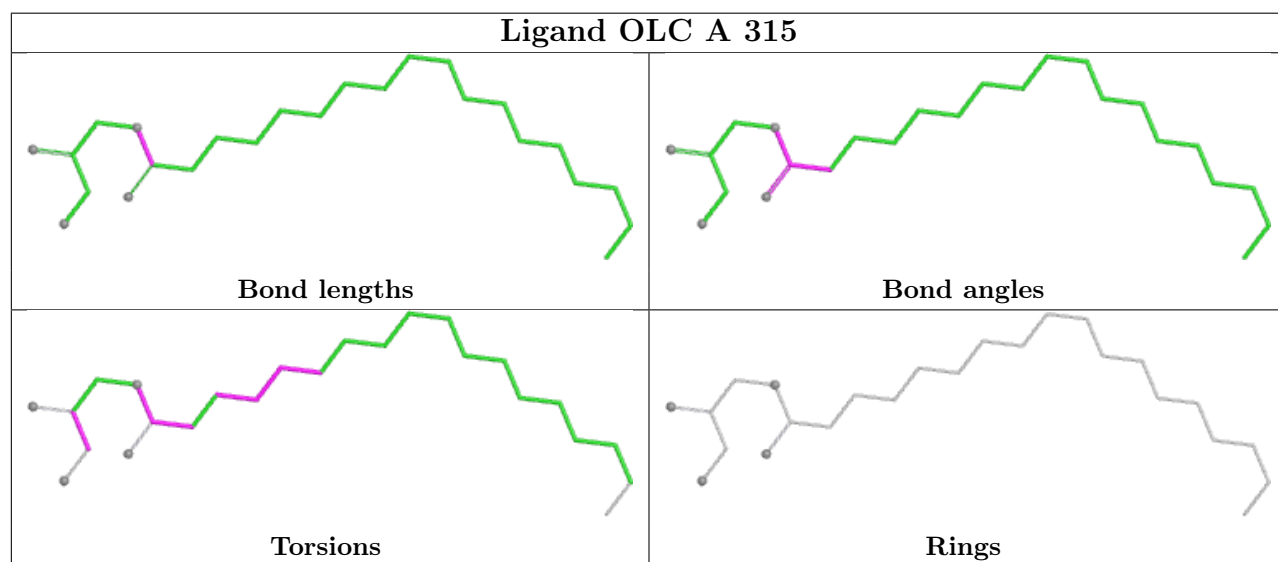
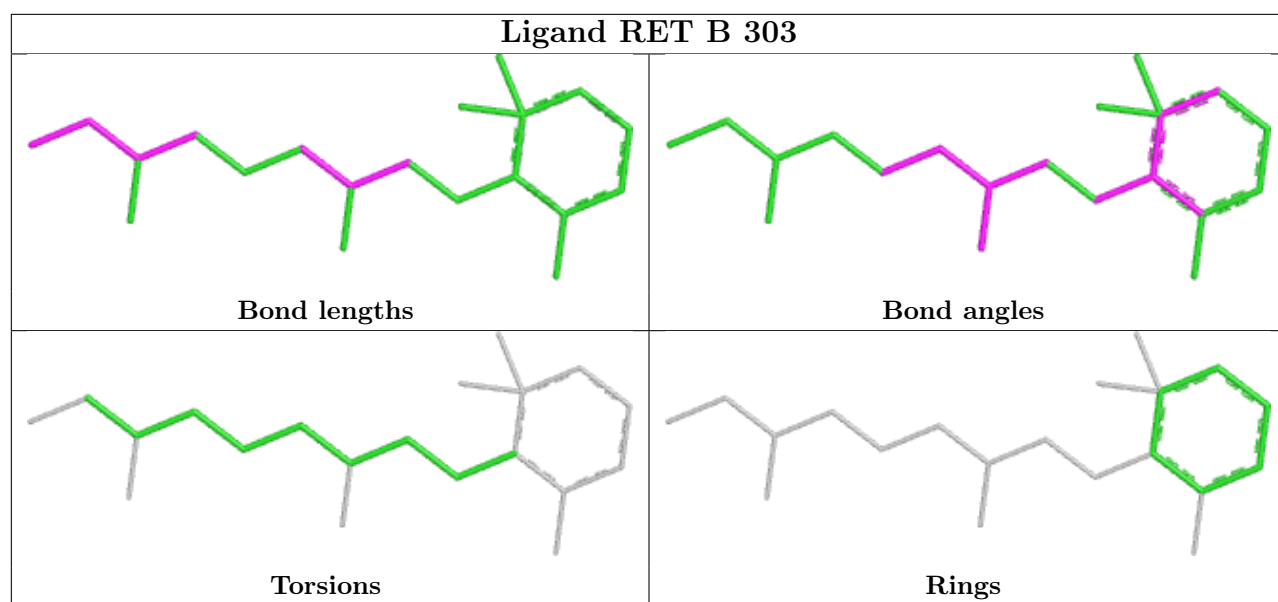


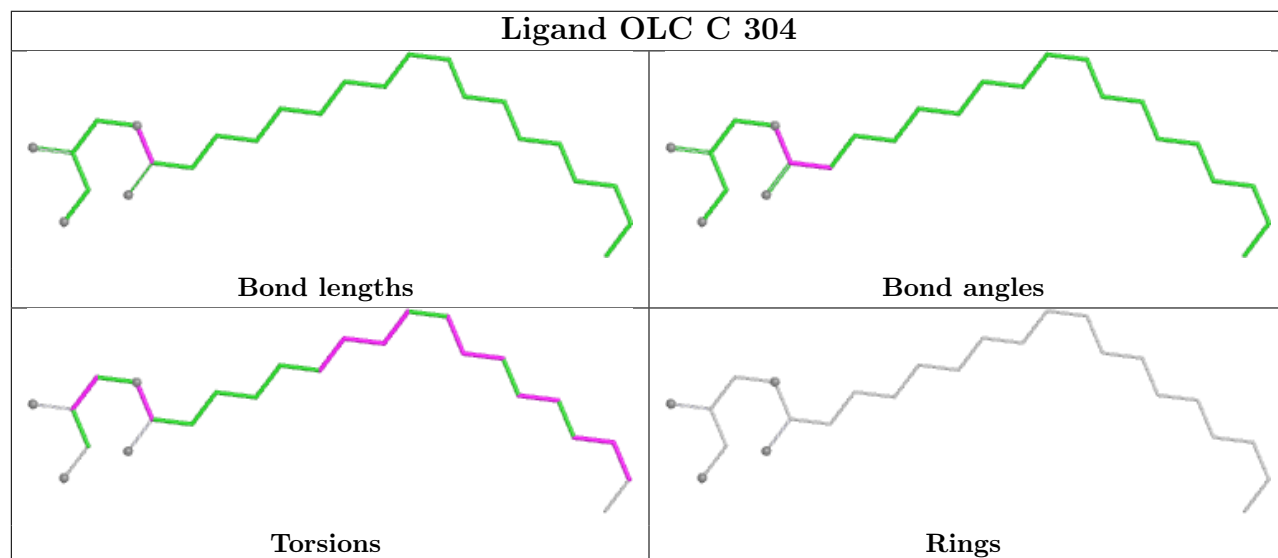
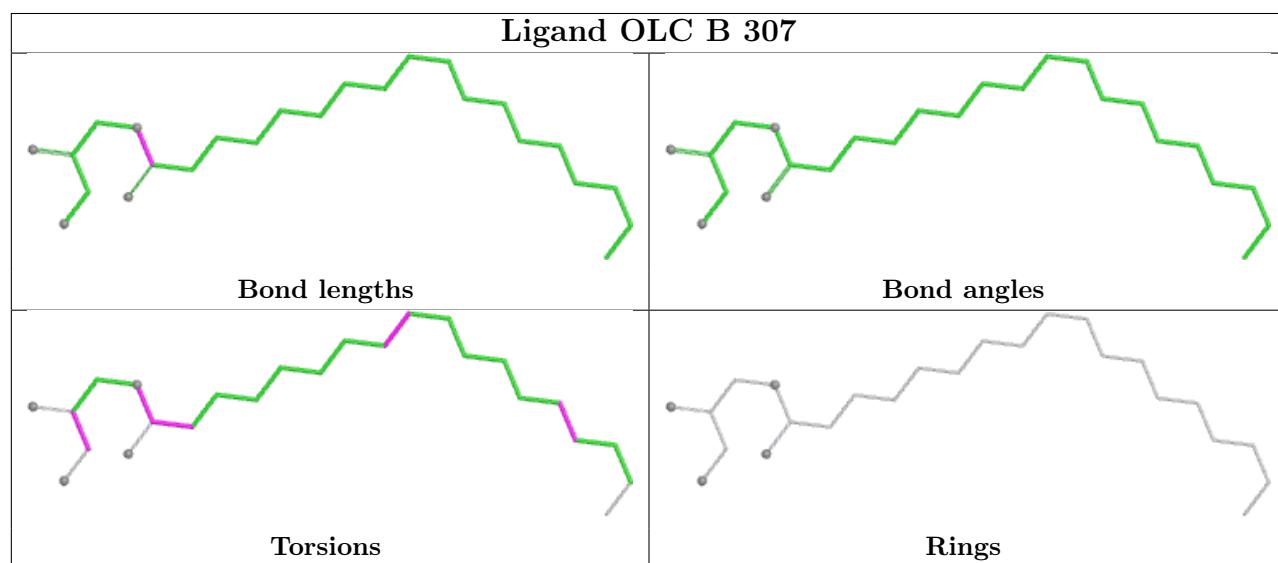
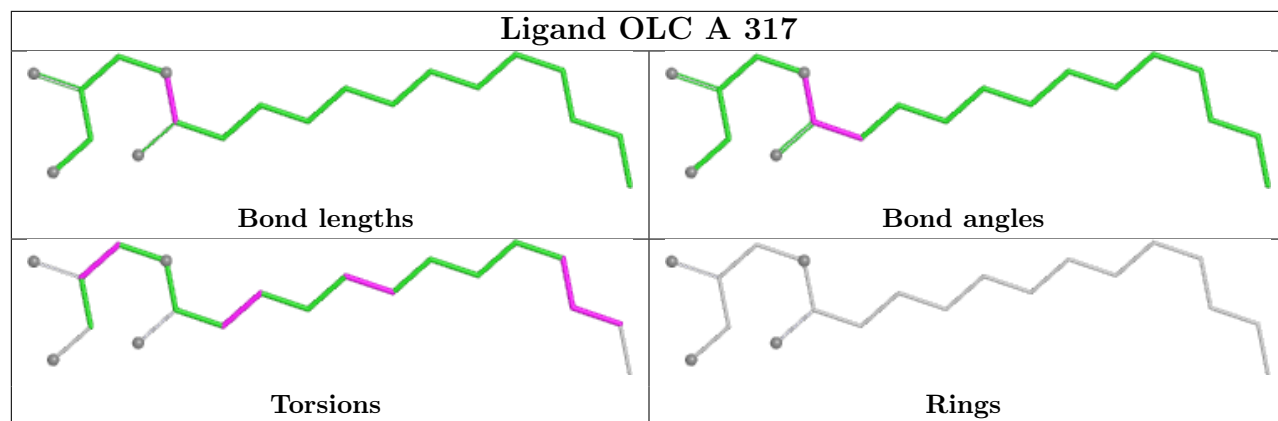


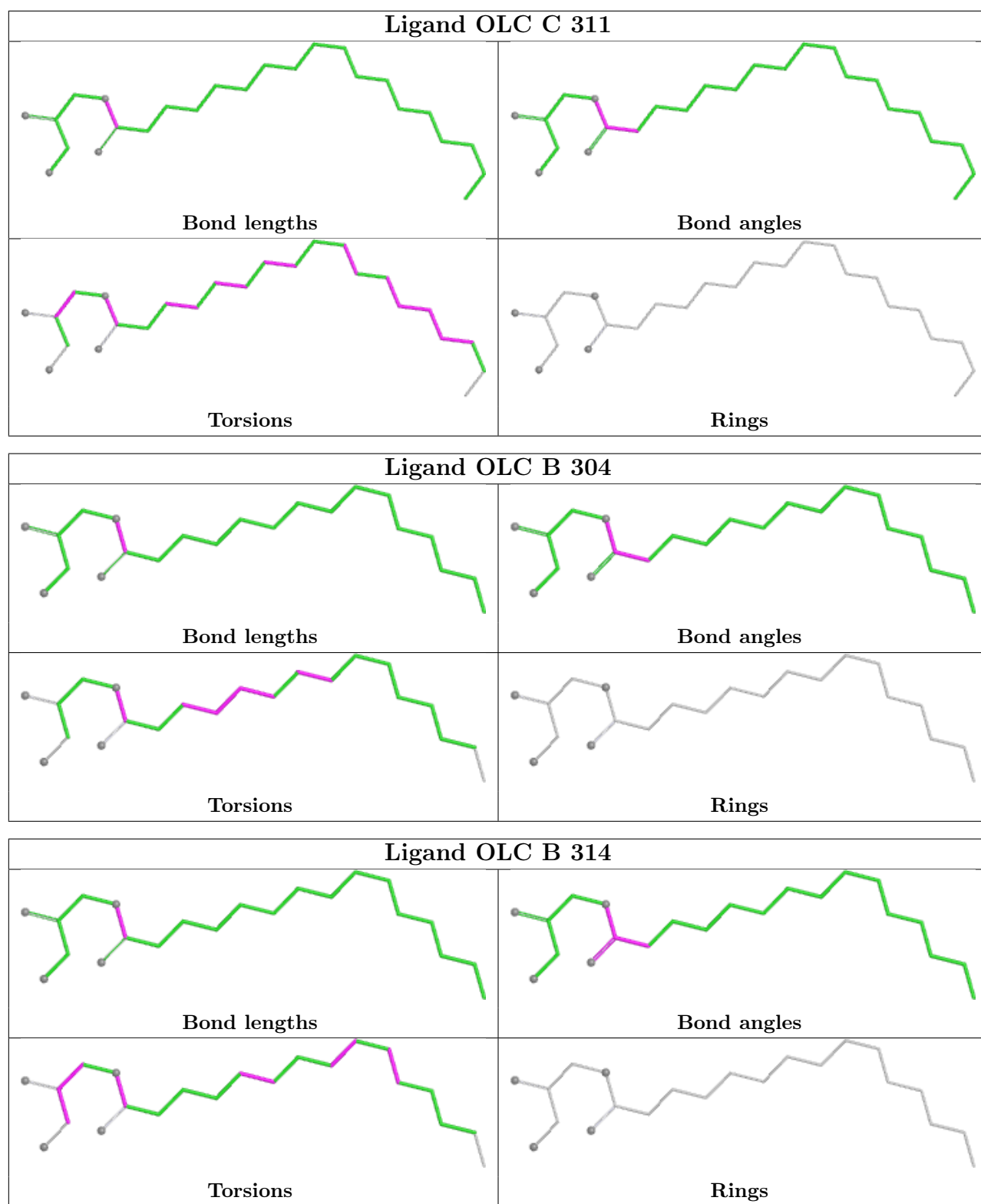


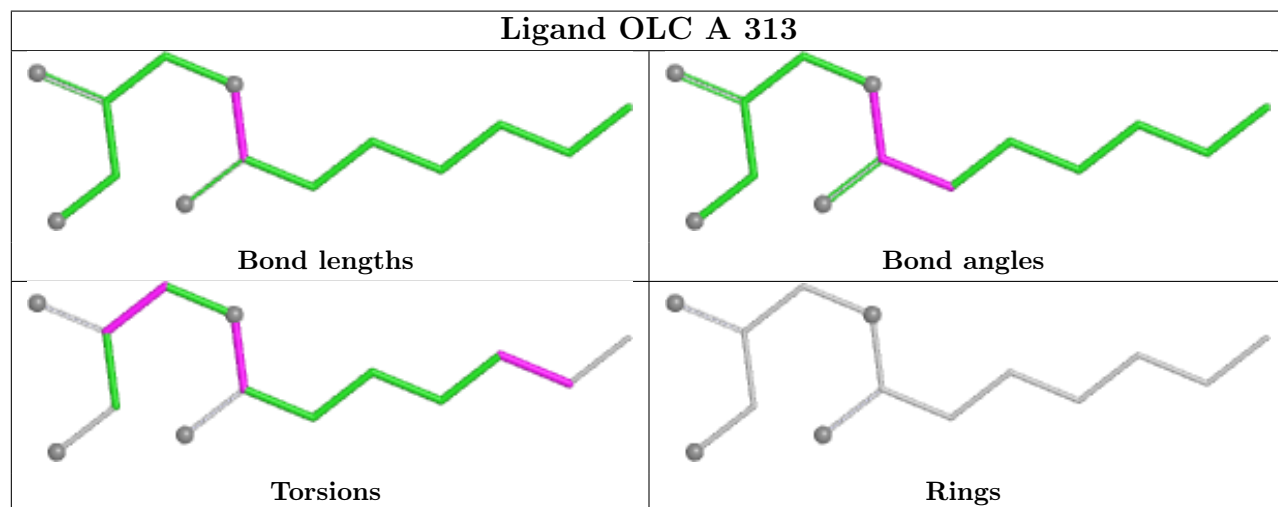
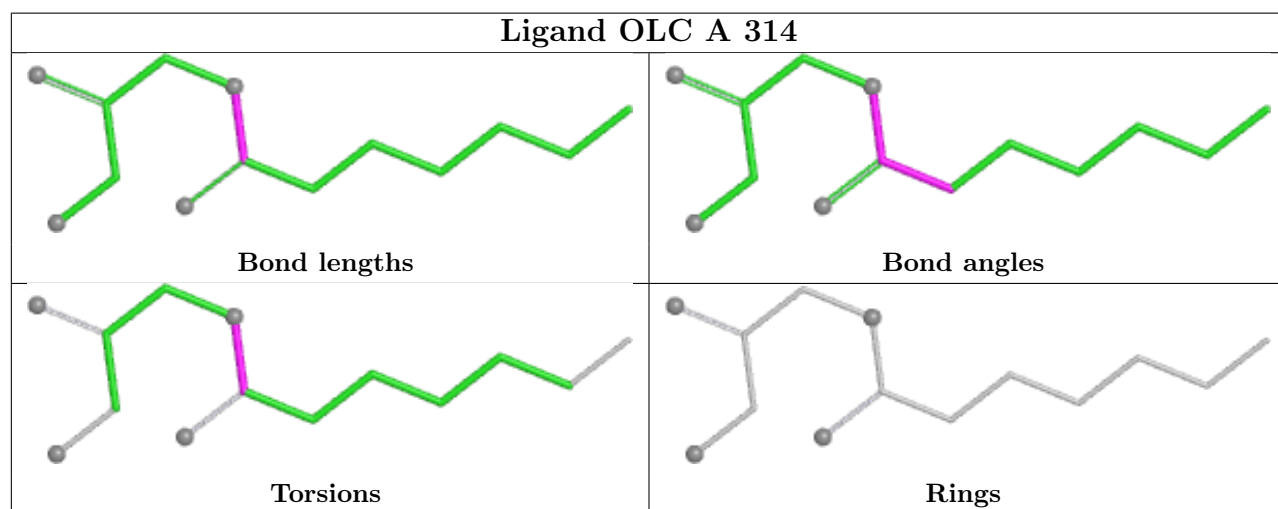
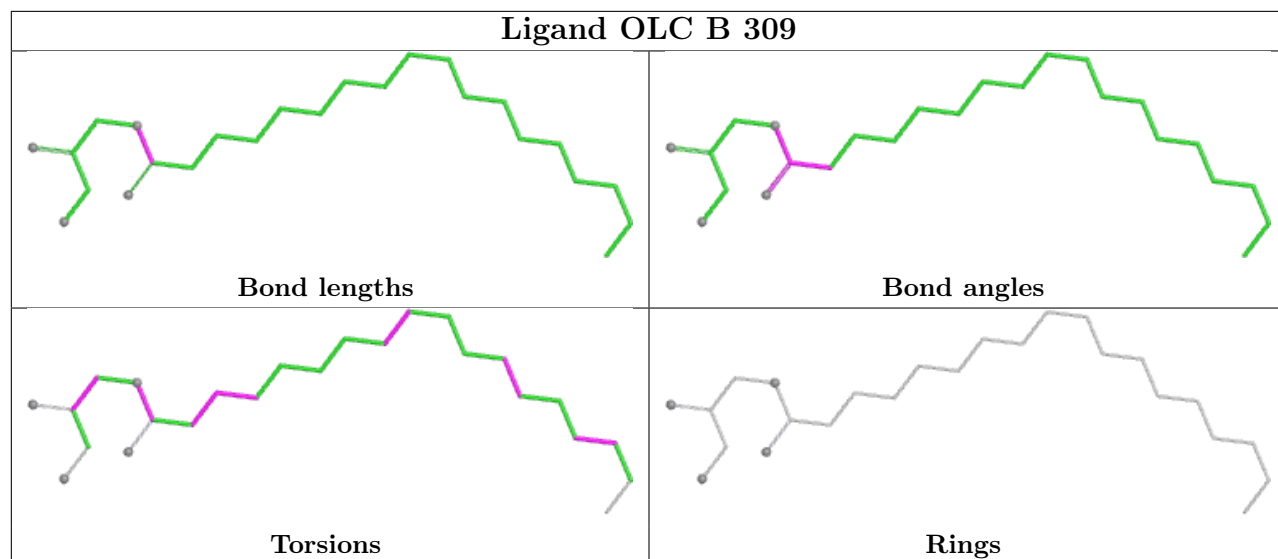


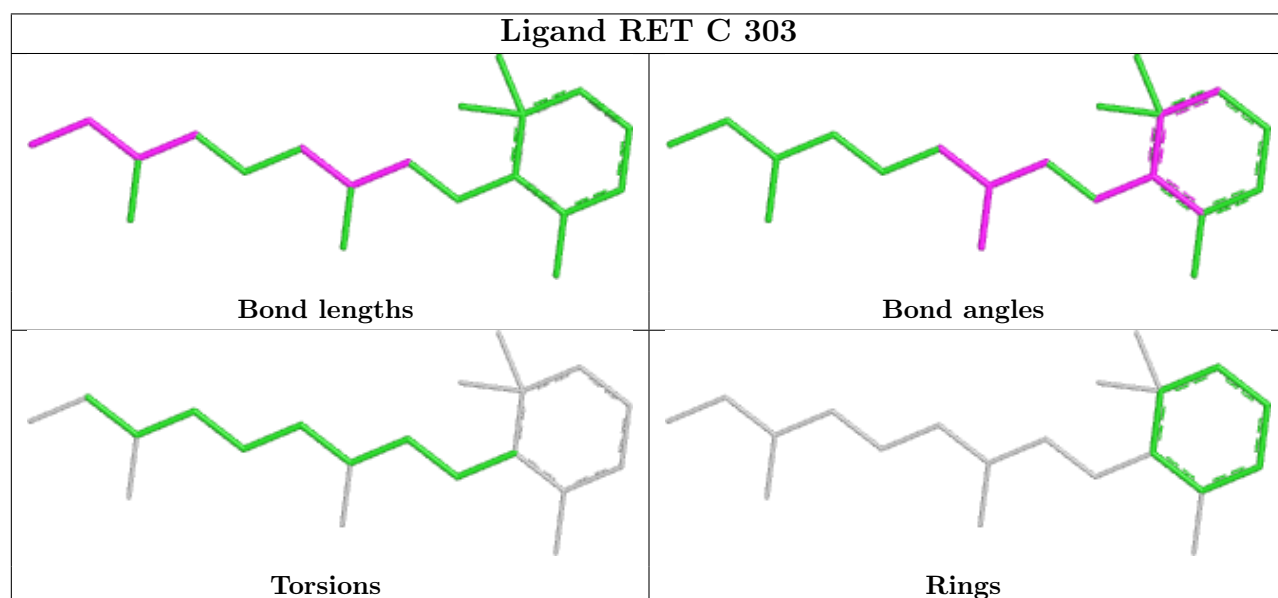
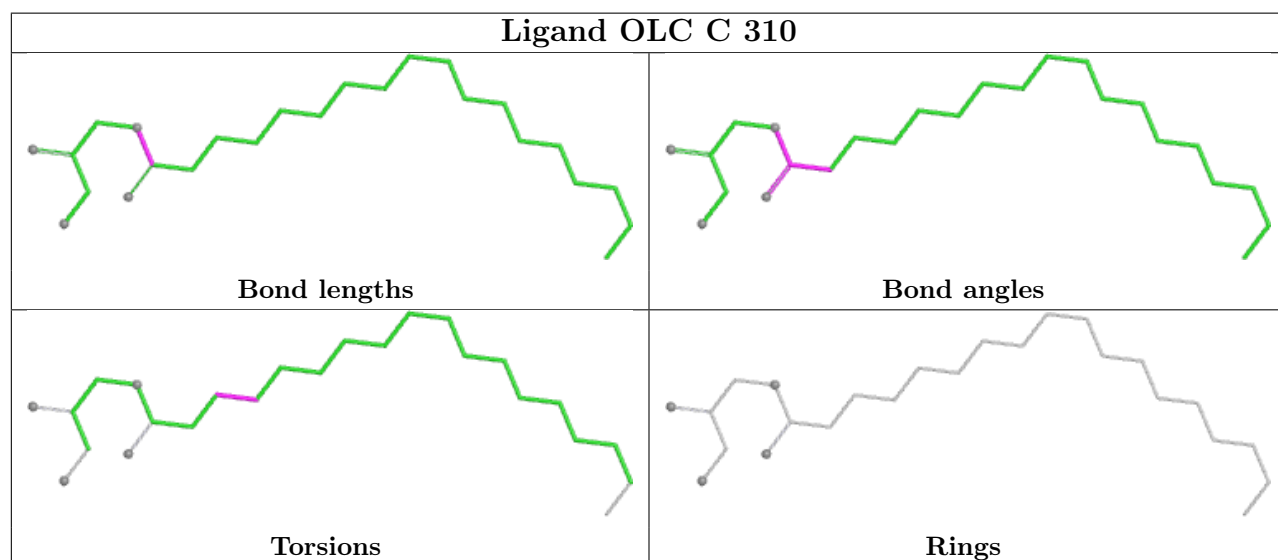
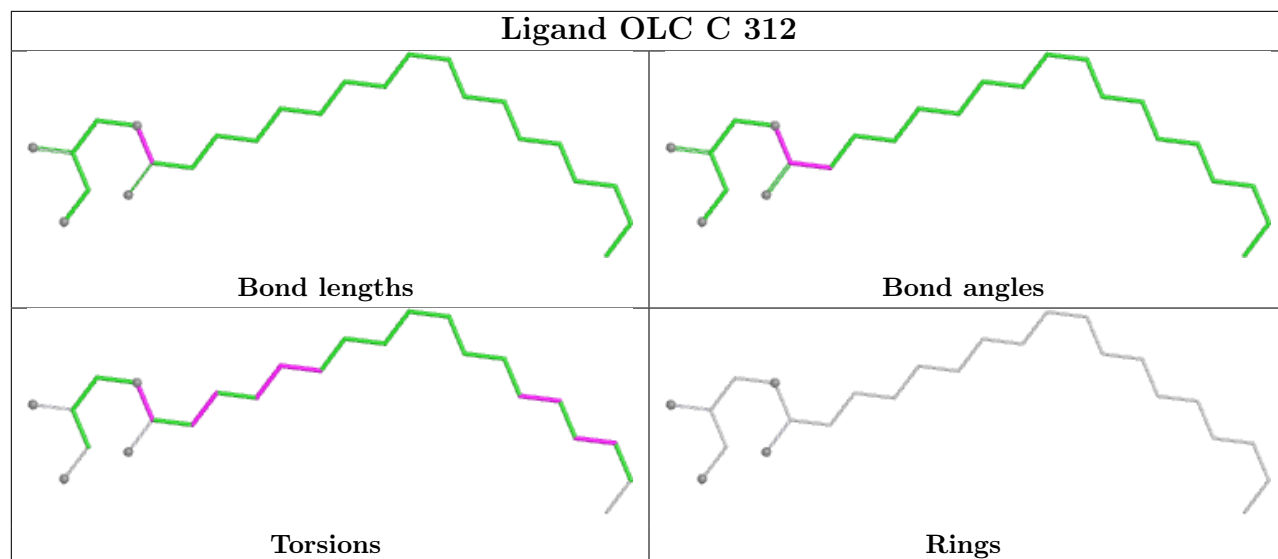


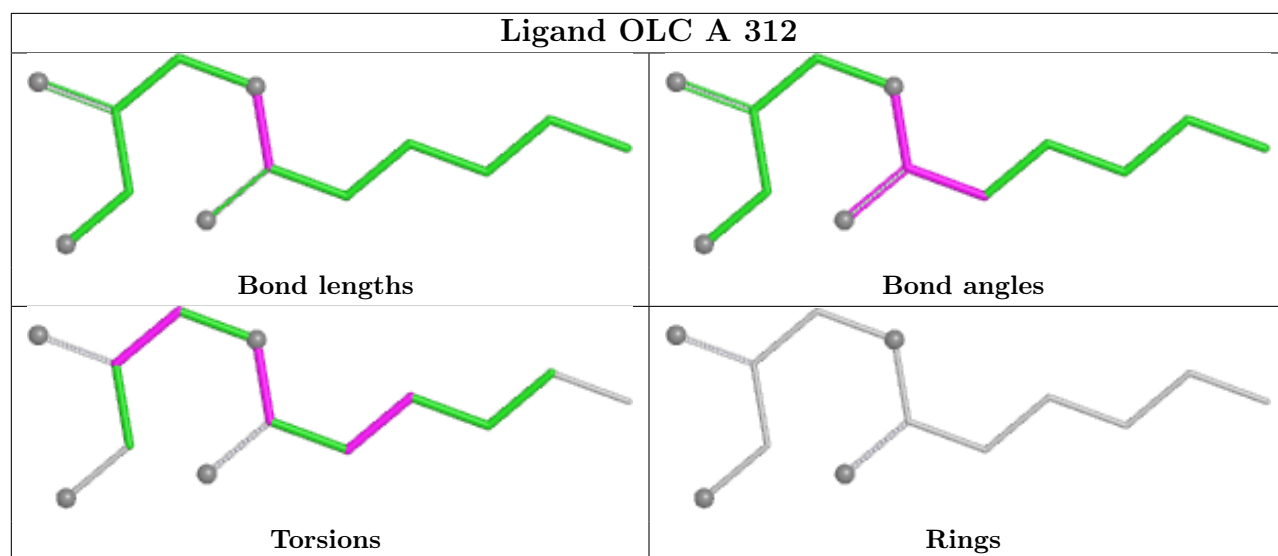
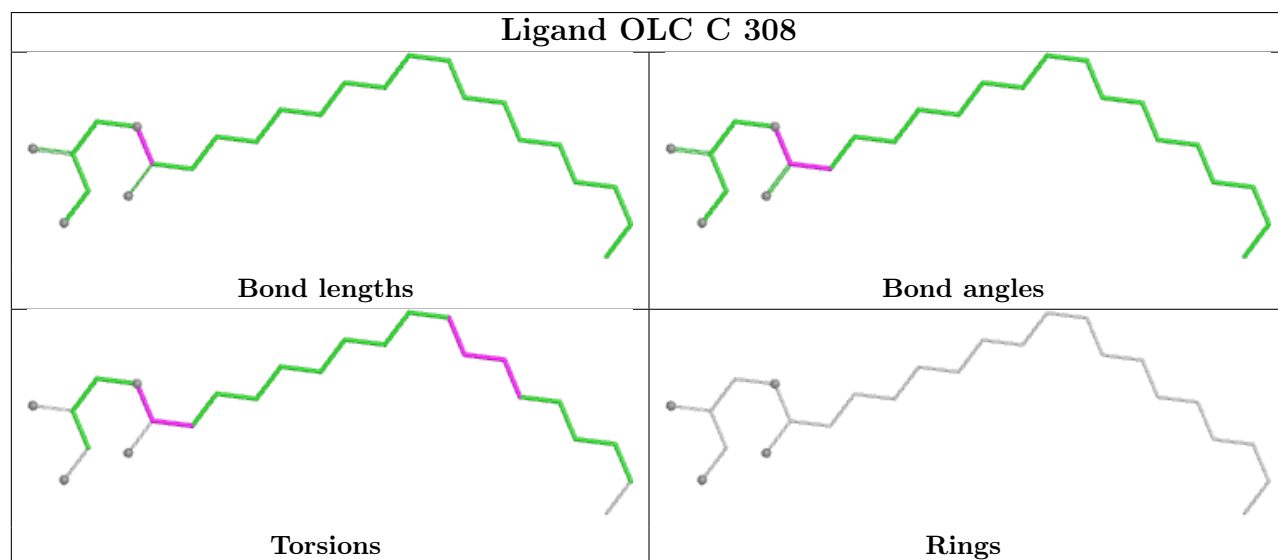
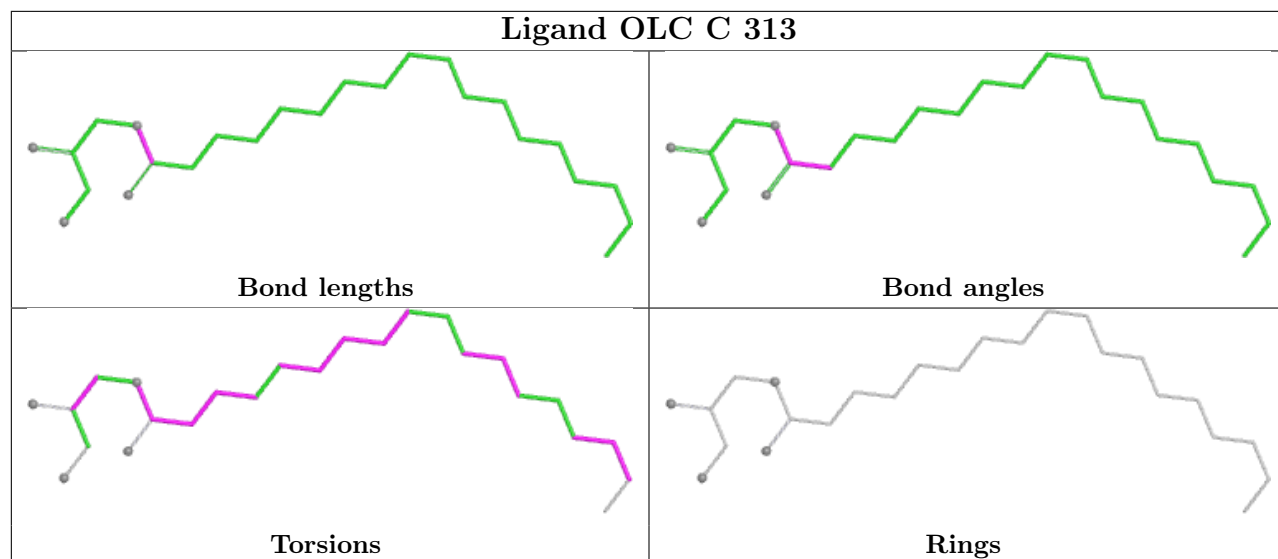


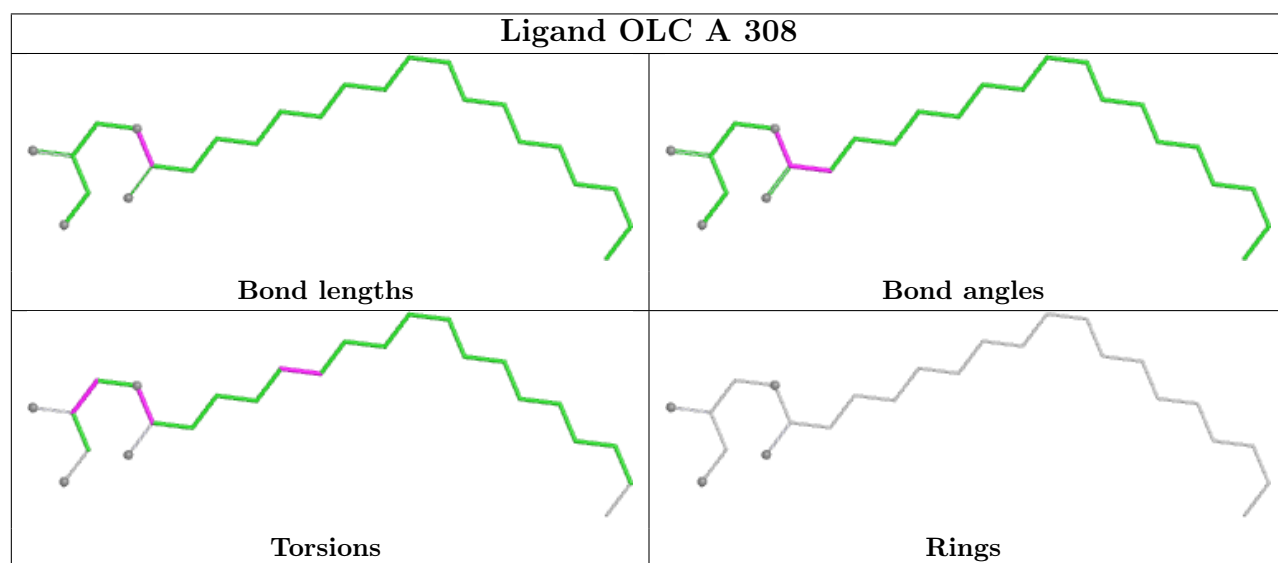
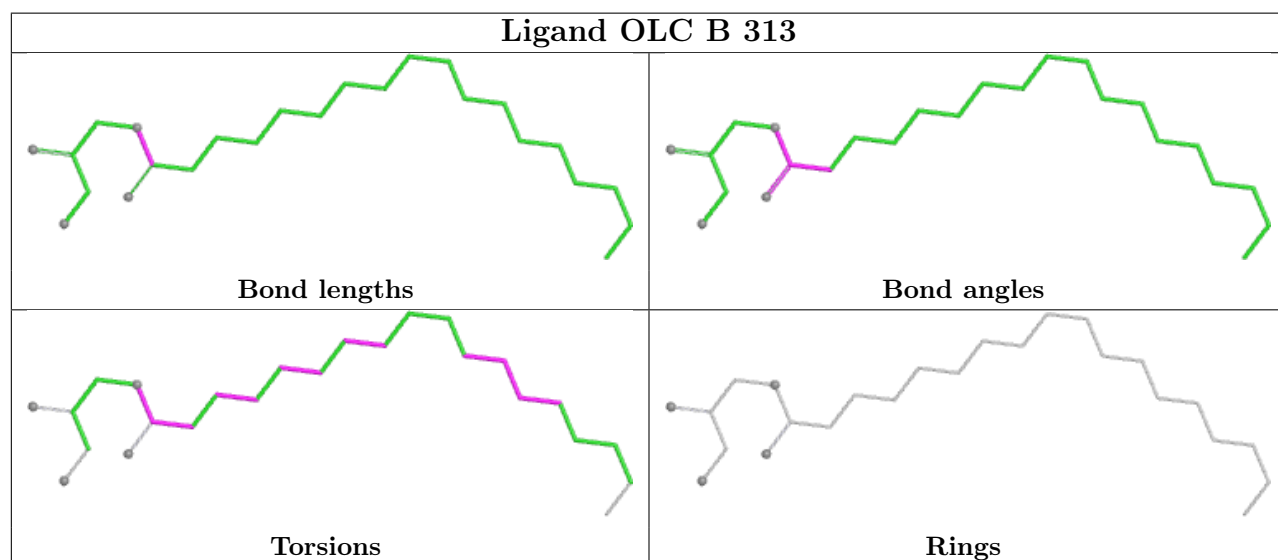
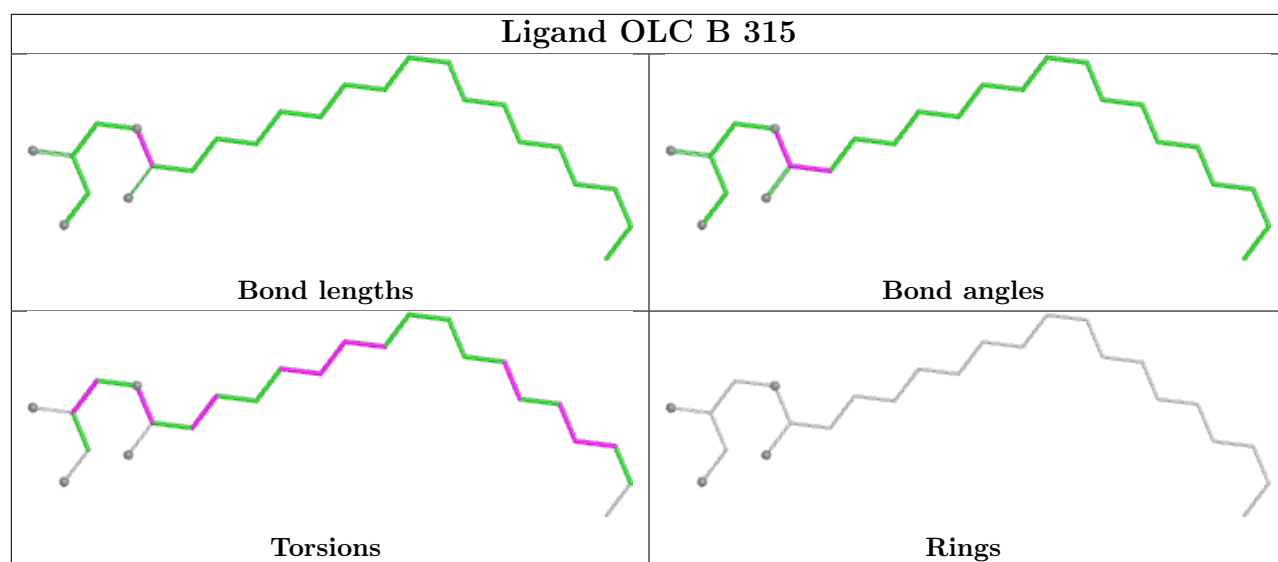












5.7 Other polymers [i](#)

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	199/210 (94%)	0.47	7 (3%) 47 49	18, 27, 53, 96	0
1	B	196/210 (93%)	0.55	12 (6%) 27 29	19, 29, 55, 102	0
1	C	193/210 (91%)	0.54	8 (4%) 41 43	19, 29, 56, 121	0
All	All	588/630 (93%)	0.52	27 (4%) 37 39	18, 28, 55, 121	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	ASN	3.9
1	B	140	ARG	3.6
1	B	1	MET	3.4
1	C	197	PHE	3.4
1	A	142	GLU	3.2
1	C	145	ALA	3.0
1	A	199	HIS	2.9
1	C	143	LYS	2.8
1	C	137	ALA	2.8
1	A	52	LEU	2.7
1	A	26	LYS	2.7
1	C	52	LEU	2.6
1	B	198	LYS	2.6
1	B	84	TYR	2.6
1	A	197	PHE	2.5
1	A	138	LYS	2.3
1	B	197	PHE	2.3
1	B	145	ALA	2.3
1	C	144	LYS	2.3
1	C	167	GLY	2.2
1	B	196	THR	2.2
1	B	137	ALA	2.1
1	A	25	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	138	LYS	2.1
1	B	88	ILE	2.0
1	B	26	LYS	2.0
1	C	84	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
5	OLC	B	313	25/25	0.55	0.20	38,63,85,87	0
5	OLC	A	315	25/25	0.63	0.20	51,66,74,79	0
5	OLC	B	314	22/25	0.64	0.20	52,66,75,78	0
5	OLC	C	309	25/25	0.65	0.20	51,66,75,77	0
5	OLC	C	313	25/25	0.65	0.19	64,73,82,84	0
5	OLC	C	311	25/25	0.67	0.21	50,64,82,85	0
5	OLC	A	311	25/25	0.67	0.19	51,66,78,81	0
5	OLC	A	317	20/25	0.68	0.18	51,60,68,72	0
5	OLC	C	307	25/25	0.69	0.21	43,54,59,62	0
5	OLC	B	310	25/25	0.69	0.19	47,57,67,71	0
5	OLC	A	312	13/25	0.70	0.20	38,45,53,54	0
5	OLC	A	310	25/25	0.71	0.17	36,66,97,99	0
5	OLC	B	315	25/25	0.71	0.17	44,48,57,62	0
5	OLC	A	314	14/25	0.72	0.16	53,60,72,77	0
5	OLC	B	305	25/25	0.72	0.20	48,70,78,80	0
5	OLC	B	308	25/25	0.72	0.17	48,62,69,71	0
5	OLC	B	309	25/25	0.72	0.18	39,50,68,70	0
5	OLC	B	306	25/25	0.73	0.21	61,67,76,83	0
5	OLC	C	312	25/25	0.73	0.18	45,56,66,75	0

Continued on next page...

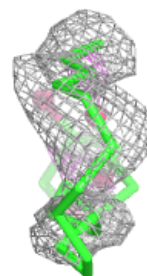
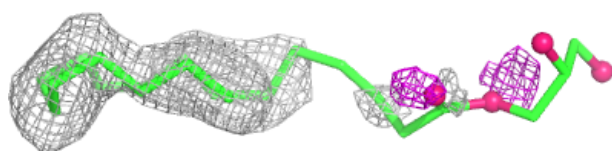
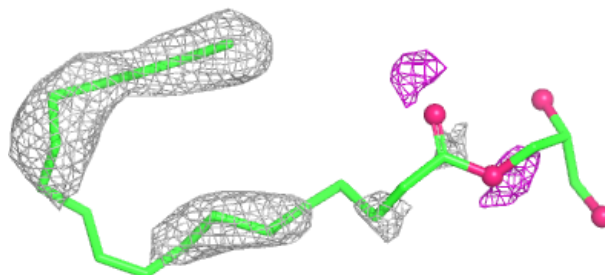
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	OLC	C	310	25/25	0.73	0.16	37,48,62,64	0
5	OLC	A	316	23/25	0.74	0.16	41,67,75,75	0
3	SO4	C	302	5/5	0.74	0.12	61,67,74,80	0
5	OLC	B	304	22/25	0.74	0.19	39,54,73,75	0
5	OLC	C	304	25/25	0.74	0.19	56,63,78,80	0
5	OLC	A	313	14/25	0.74	0.17	50,59,71,73	0
5	OLC	B	311	25/25	0.75	0.18	35,48,74,77	0
5	OLC	B	312	25/25	0.76	0.17	39,50,71,76	0
5	OLC	C	308	25/25	0.77	0.16	48,59,69,73	0
5	OLC	C	306	25/25	0.77	0.17	47,56,65,68	0
5	OLC	B	307	25/25	0.78	0.18	43,54,75,78	0
2	ZN	A	301	1/1	0.79	0.10	101,101,101,101	0
5	OLC	A	308	25/25	0.81	0.18	50,58,70,72	0
5	OLC	C	305	25/25	0.81	0.16	31,56,72,74	0
3	SO4	A	304	5/5	0.83	0.12	71,71,73,73	0
2	ZN	B	301	1/1	0.84	0.13	149,149,149,149	1
5	OLC	A	309	25/25	0.84	0.17	61,67,75,77	0
2	ZN	A	303	1/1	0.85	0.15	90,90,90,90	0
2	ZN	B	302	1/1	0.86	0.09	109,109,109,109	0
4	RET	A	307	20/21	0.86	0.10	18,24,30,32	0
4	RET	B	303	20/21	0.89	0.09	17,24,31,33	0
2	ZN	C	301	1/1	0.89	0.09	106,106,106,106	0
2	ZN	A	302	1/1	0.89	0.08	109,109,109,109	1
4	RET	C	303	20/21	0.91	0.08	17,22,28,29	0
3	SO4	A	305	5/5	0.92	0.14	52,56,57,68	0
3	SO4	A	306	5/5	0.92	0.13	42,45,46,46	5

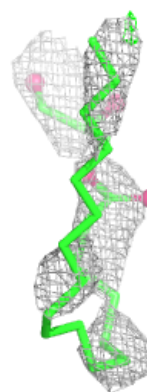
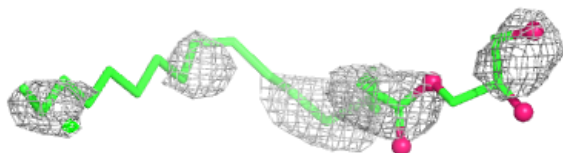
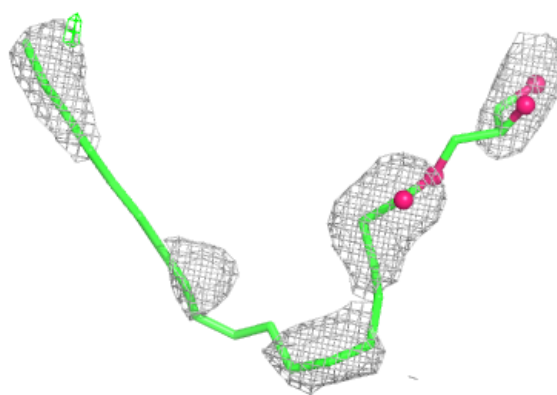
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC B 313:

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

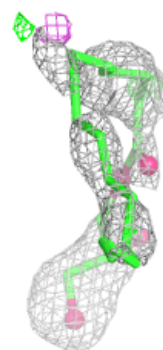
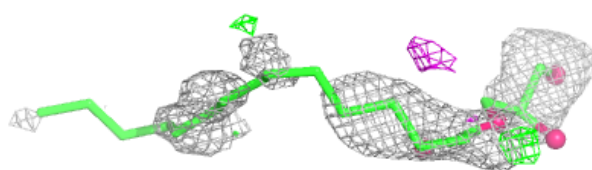
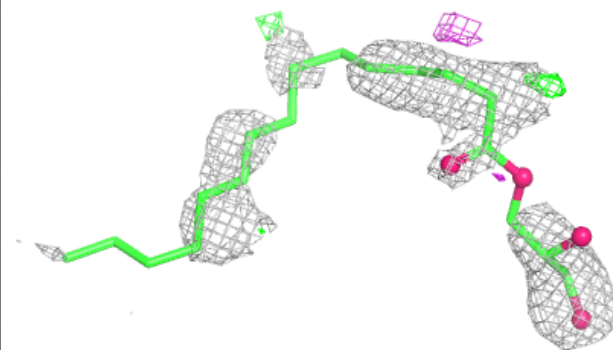
**Electron density around OLC A 315:**

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

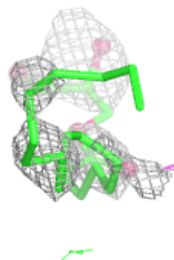
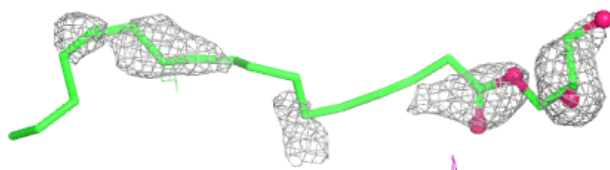
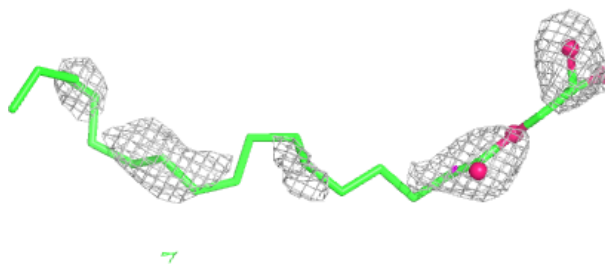


Electron density around OLC B 314:

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

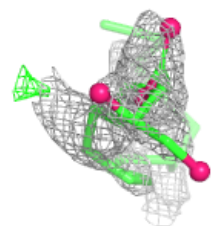
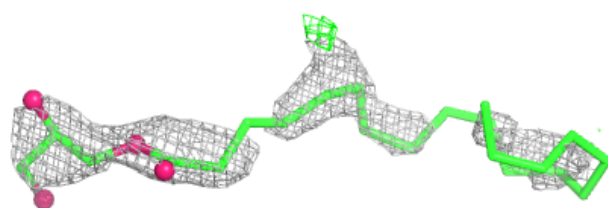
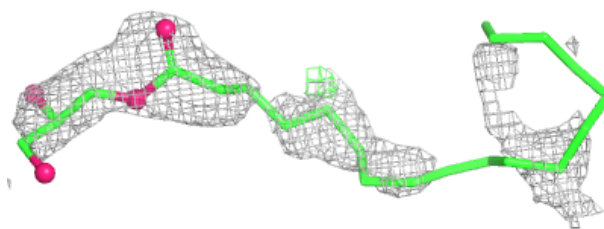
**Electron density around OLC C 309:**

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

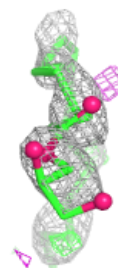
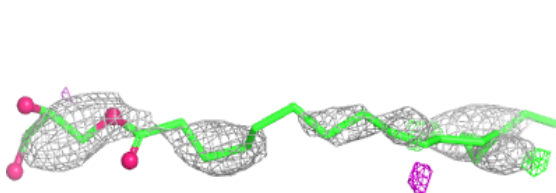
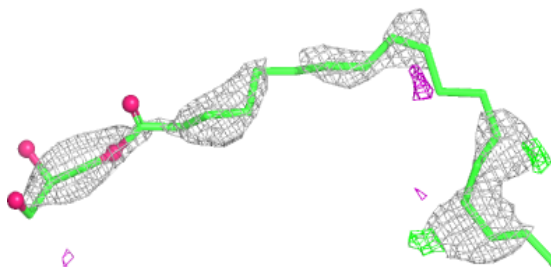


Electron density around OLC C 313:

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

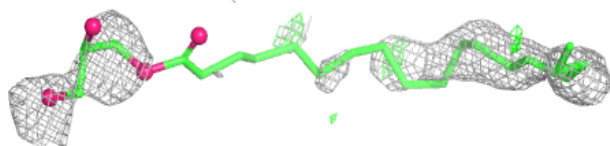
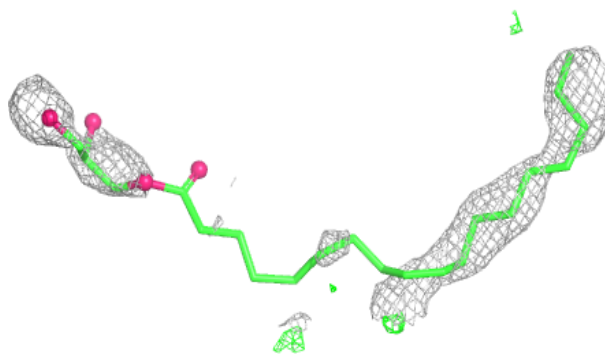
**Electron density around OLC C 311:**

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

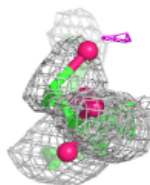
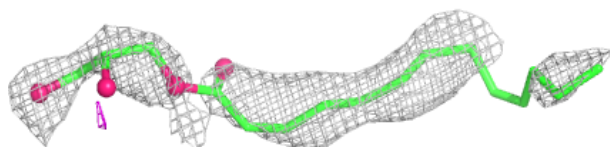
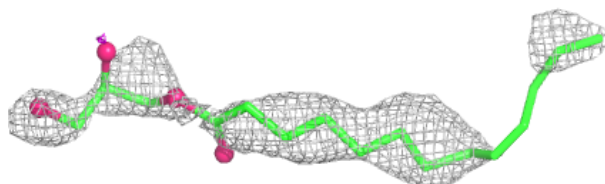


Electron density around OLC A 311:

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

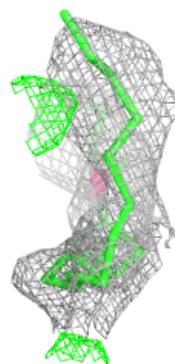
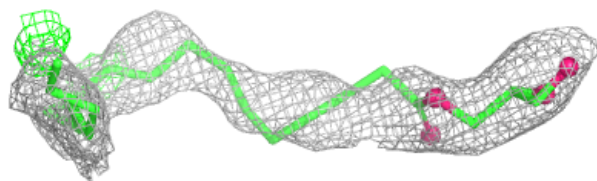
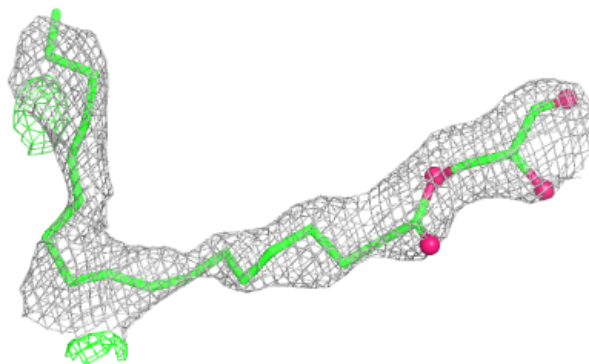
**Electron density around OLC A 317:**

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

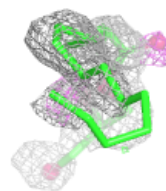
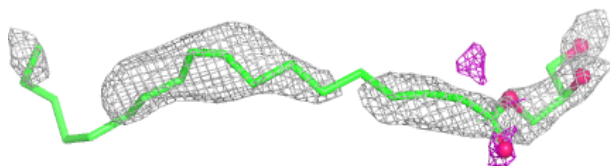
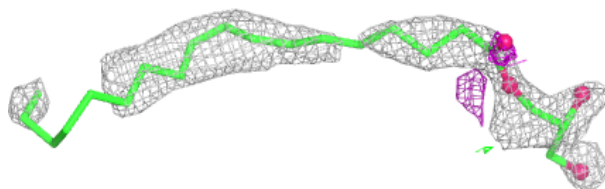


Electron density around OLC C 307:

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

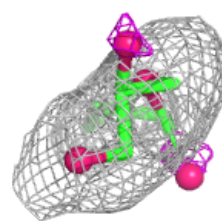
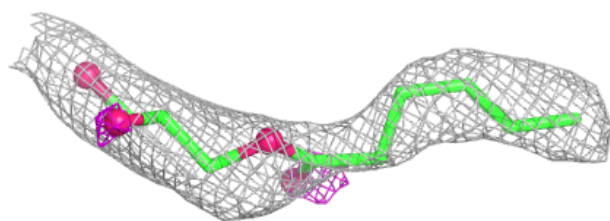
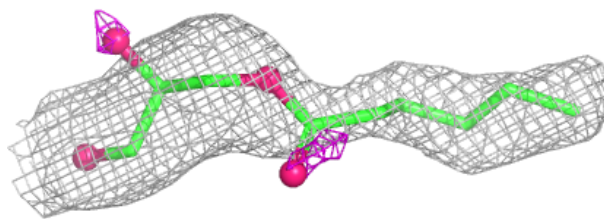
**Electron density around OLC B 310:**

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

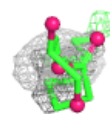
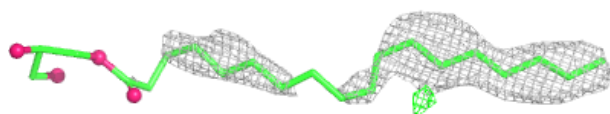
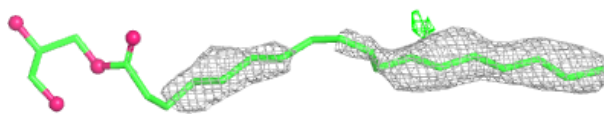


Electron density around OLC A 312:

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

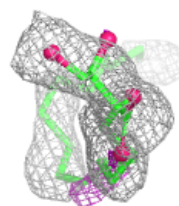
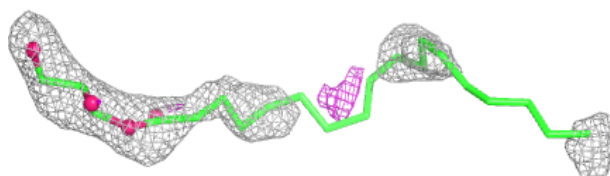
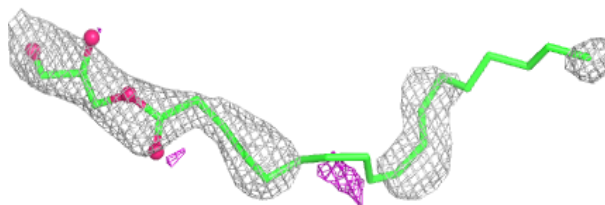
**Electron density around OLC A 310:**

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

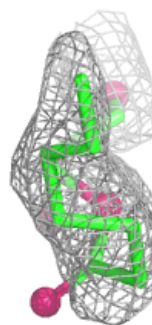
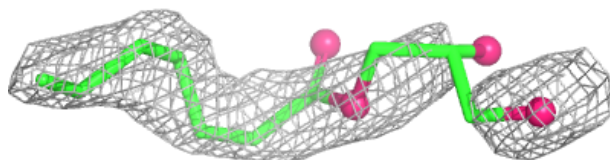
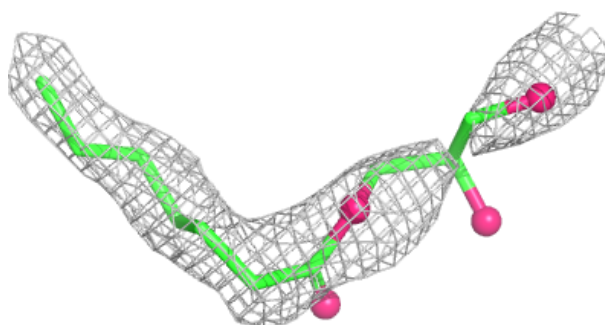


Electron density around OLC B 315:

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

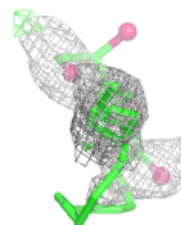
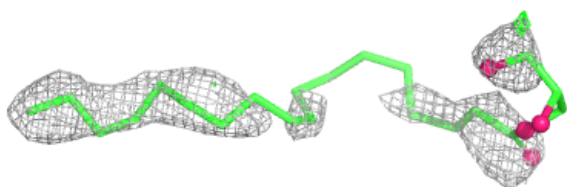
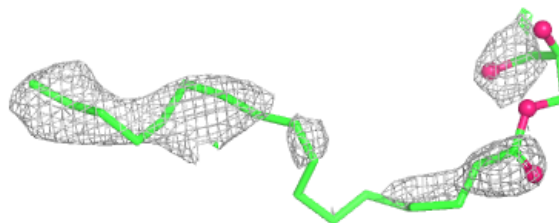
**Electron density around OLC A 314:**

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

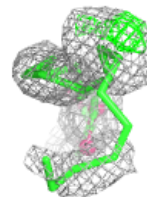
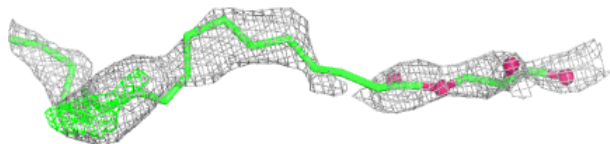
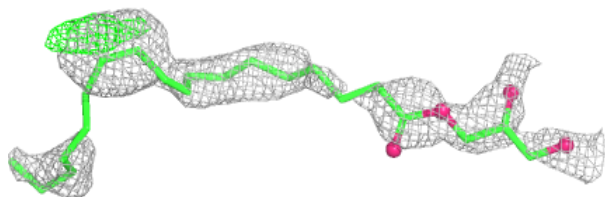


Electron density around OLC B 305:

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

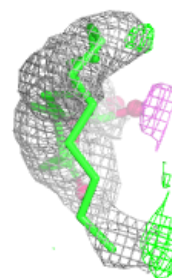
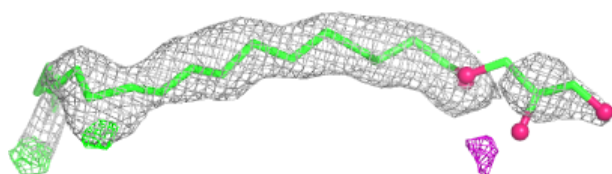
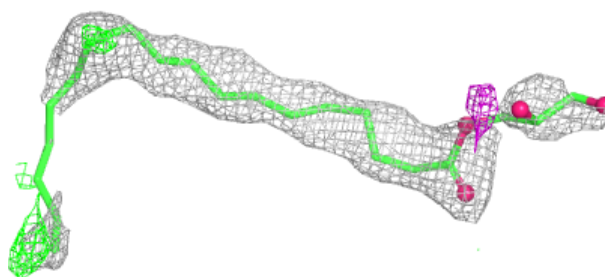
**Electron density around OLC B 308:**

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

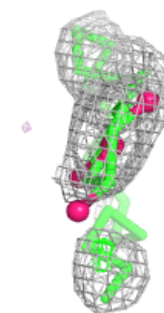
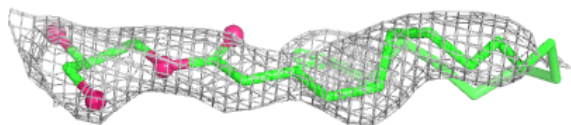
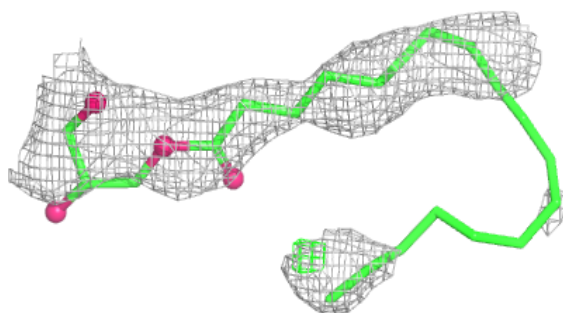


Electron density around OLC B 309:

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

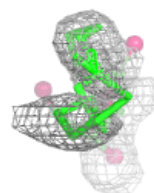
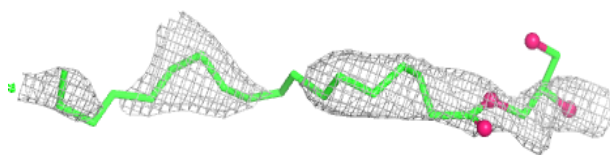
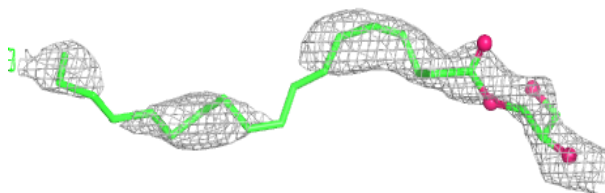
**Electron density around OLC B 306:**

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

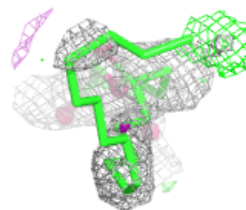
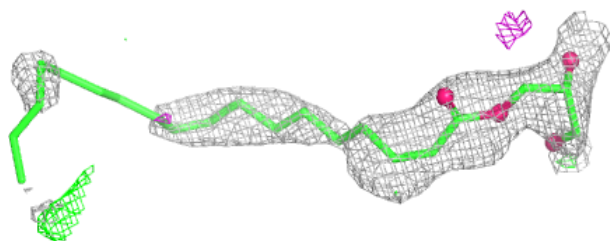
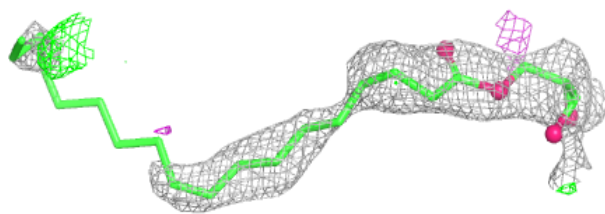


Electron density around OLC C 312:

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

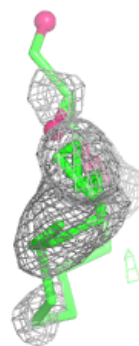
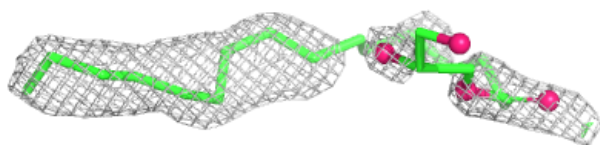
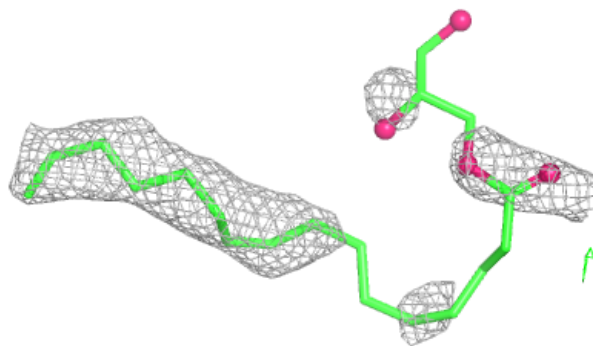
**Electron density around OLC C 310:**

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

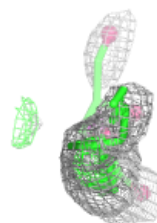
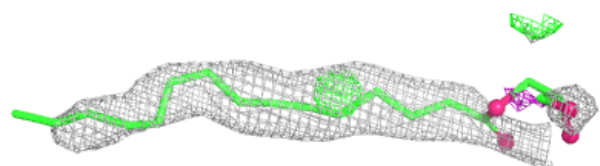
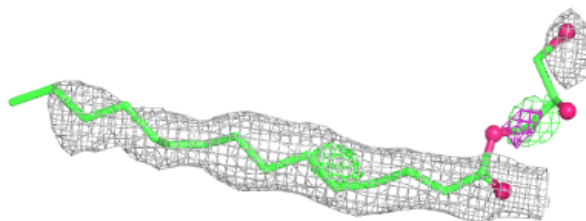


Electron density around OLC A 316:

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

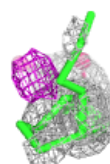
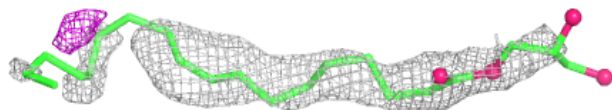
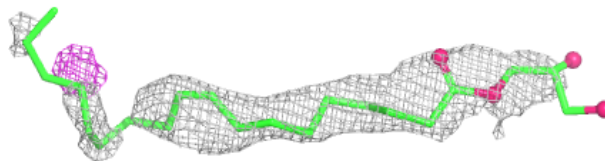
**Electron density around OLC B 304:**

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

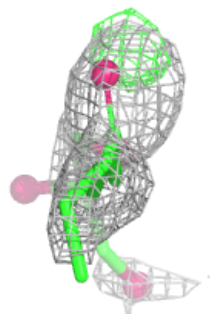
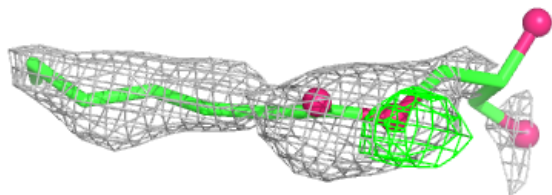
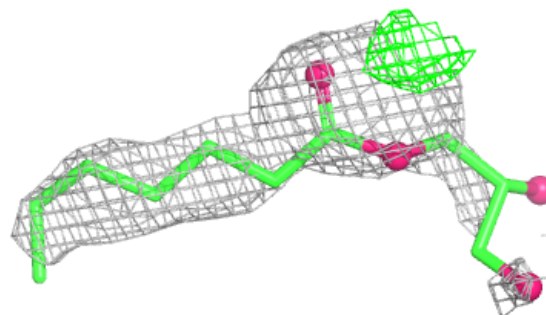


Electron density around OLC C 304:

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

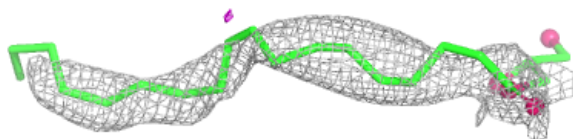
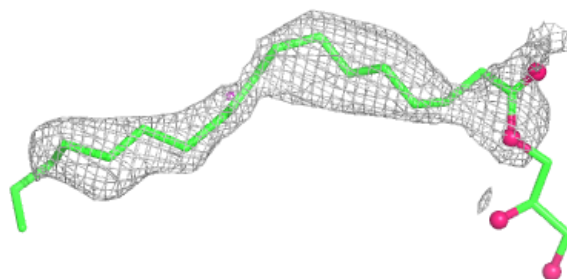
**Electron density around OLC A 313:**

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

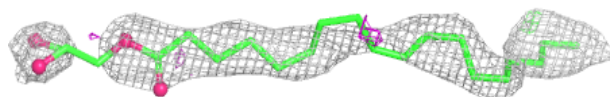
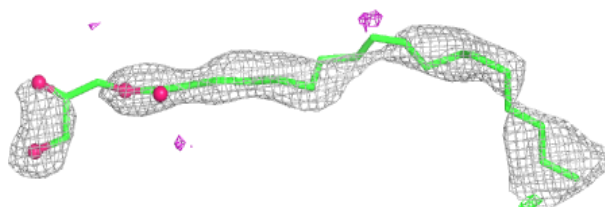


Electron density around OLC B 311:

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

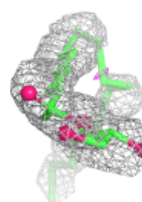
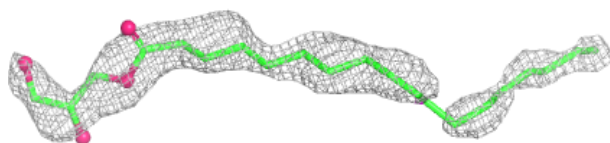
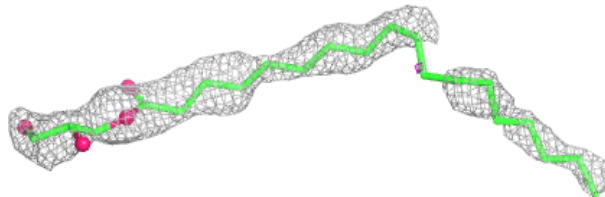
**Electron density around OLC B 312:**

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

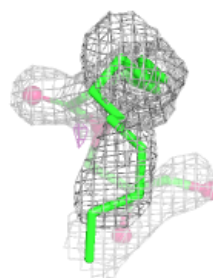
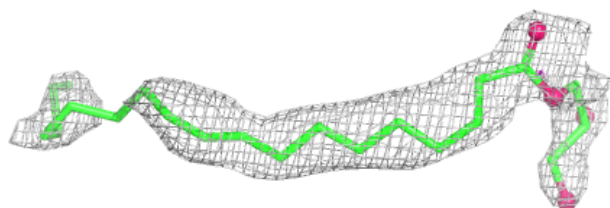
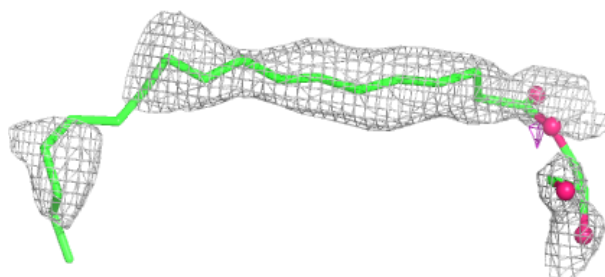


Electron density around OLC C 308:

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

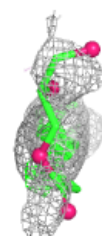
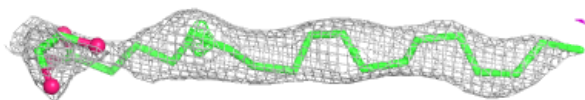
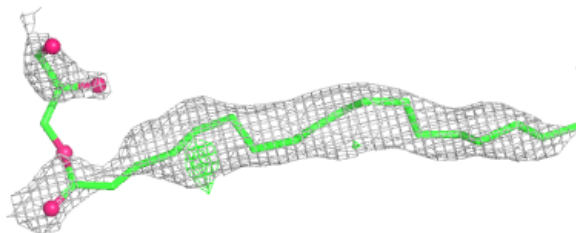
**Electron density around OLC C 306:**

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

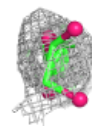
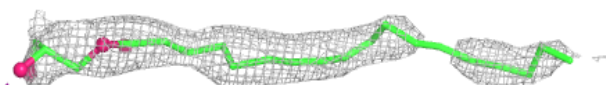
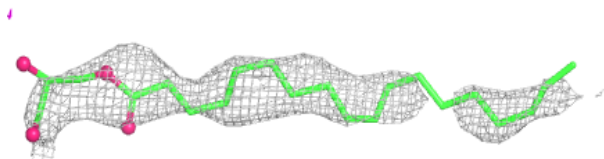


Electron density around OLC B 307:

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

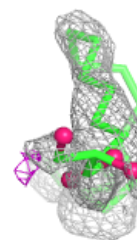
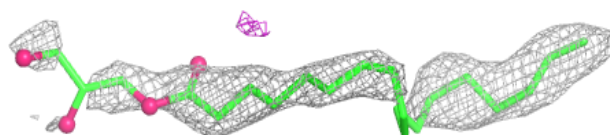
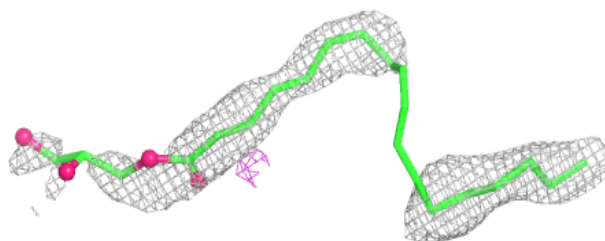
**Electron density around OLC A 308:**

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

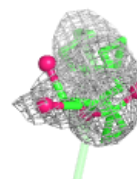
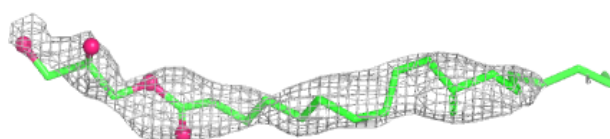
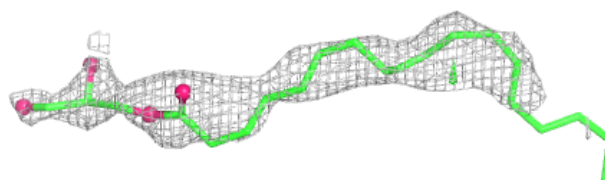


Electron density around OLC C 305:

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

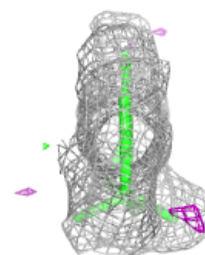
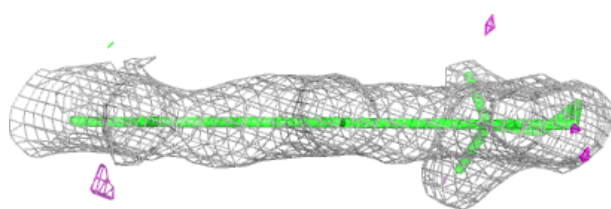
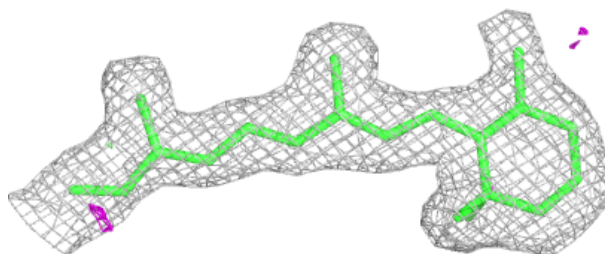
**Electron density around OLC A 309:**

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

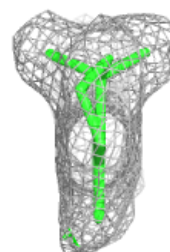
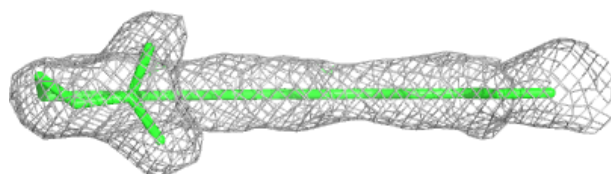
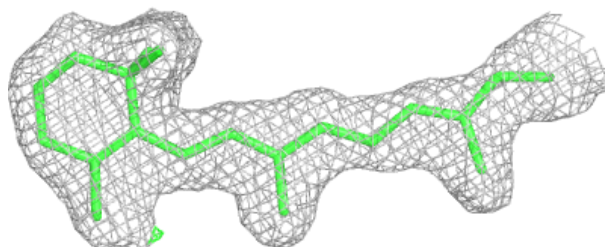


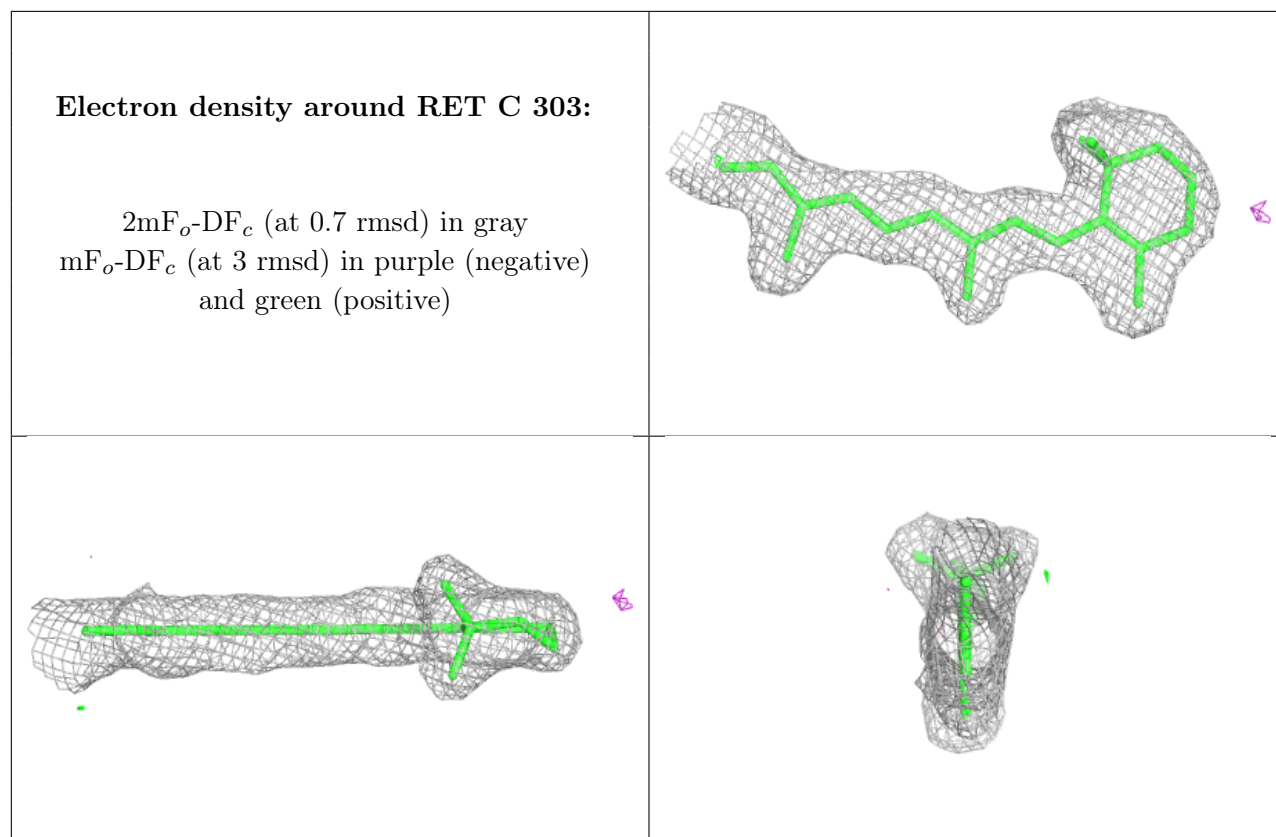
Electron density around RET A 307:

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

**Electron density around RET B 303:**

$2mF_o-DF_c$ (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.