Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:25 PM UTC

PDB ID	:	7ZN3 / pdb_00007zn3
Title	:	Crystal structure of the light-driven inward proton pump xenorhodopsin BcXeR in the L state at pH 8.2 in the presence of sodium at 100K
Authors	:	Kovalev, K.; Tsybrov, F.; Alekseev, A.; Bourenkov, G.; Gordeliy, V.
Deposited on	:	2022-04-20
Resolution	:	1.60 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:

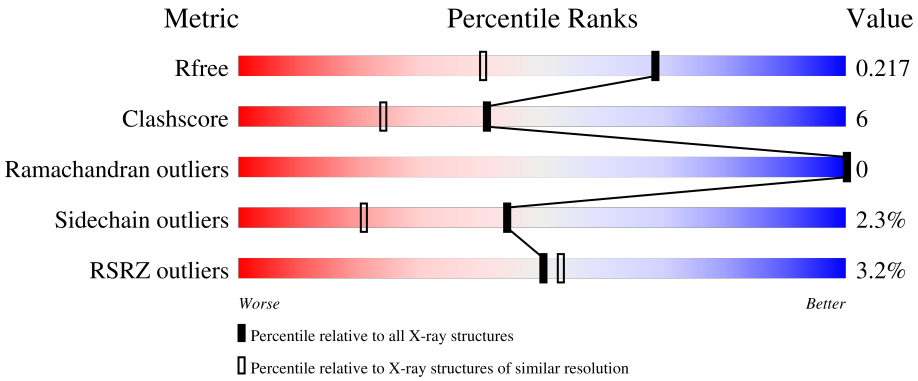
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 <=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	229	3% 87% 9%
1	B	229	2% 83% 11%
1	C	229	4% 85% 10%

2 Entry composition (i)

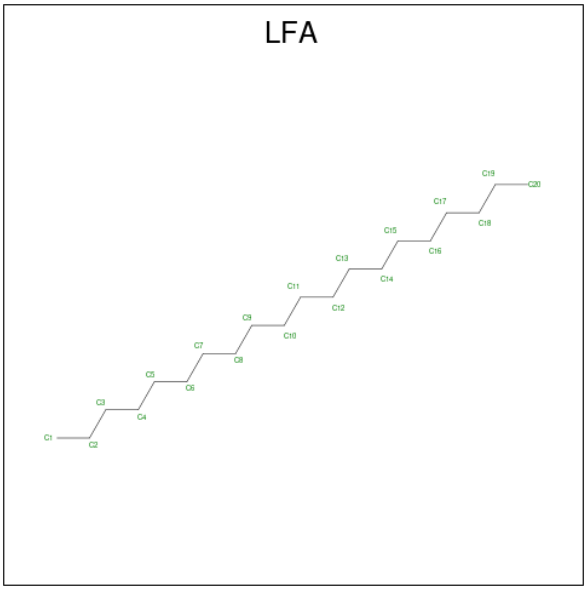
There are 6 unique types of molecules in this entry. The entry contains 6468 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 xenorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	12	0
			1872	1284	279	303	6			
1	B	219	Total	C	N	O	S	0	13	0
			1853	1270	278	299	6			
1	C	222	Total	C	N	O	S	0	14	0
			1885	1294	279	306	6			

- Molecule 2 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			6	6		
2	A	1	Total	C	0	0
			9	9		
2	A	1	Total	C	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 9 9	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 3 3	0	0
2	A	1	Total C 5 5	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 10 10	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 15 15	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 5 5	0	0
2	B	1	Total C 5 5	0	0

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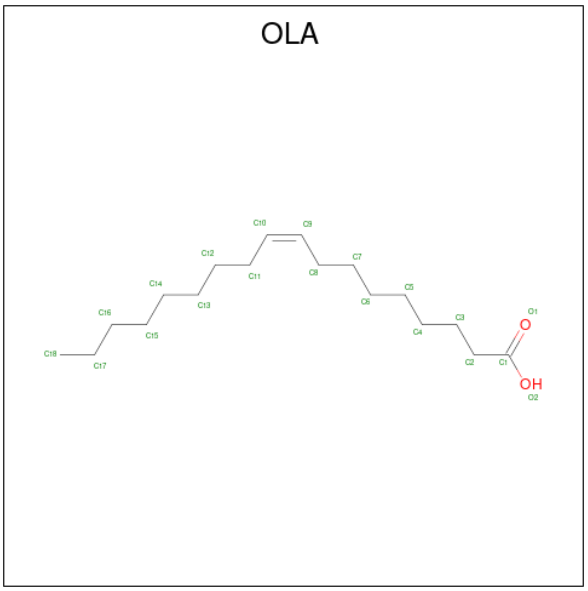
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 6 6	0	0
2	B	1	Total C 4 4	0	0
2	B	1	Total C 15 15	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 10 10	0	0
2	C	1	Total C 17 17	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 16 16	0	0
2	C	1	Total C 4 4	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 11 11	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 5 5	0	0
2	C	1	Total C 8 8	0	0

- Molecule 3 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



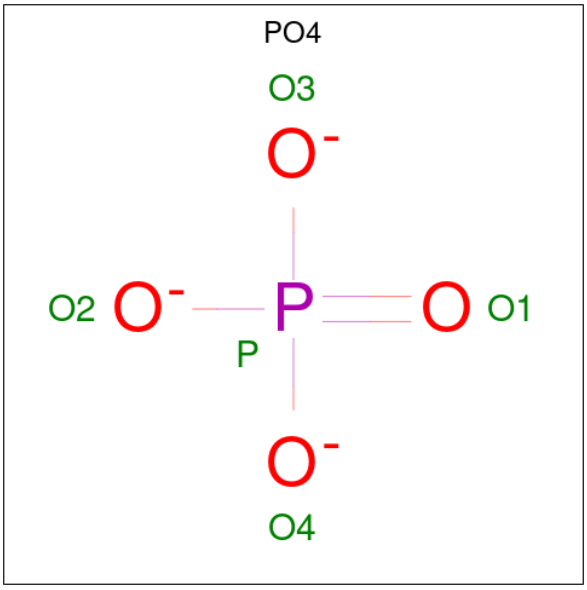
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 9 2	0	0
3	A	1	Total C O 40 36 4	0	1
3	A	1	Total C O 16 14 2	0	0
3	A	1	Total C O 11 9 2	0	0
3	A	1	Total C O 19 17 2	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C O 16 14 2	0	0
3	B	1	Total C O 12 10 2	0	0
3	B	1	Total C O 20 18 2	0	0
3	C	1	Total C O 16 14 2	0	0
3	C	1	Total C O 19 17 2	0	0
3	C	1	Total C O 16 14 2	0	0
3	C	1	Total C O 13 11 2	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest"

by depositor).

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

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 6 is water.

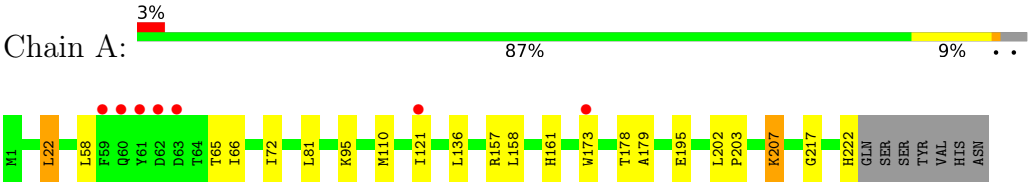
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	78	Total O 81 81	0	7
6	B	76	Total O 79 79	0	8
6	C	83	Total O 86 86	0	7

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.

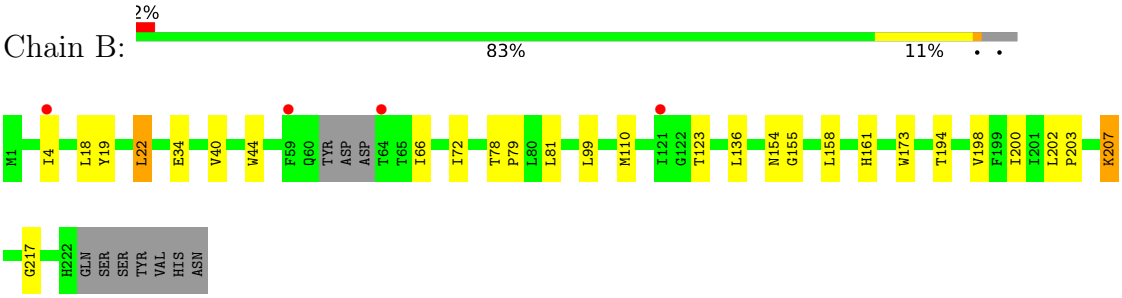
• Molecule 1: xenorhodopsin

Chain A:



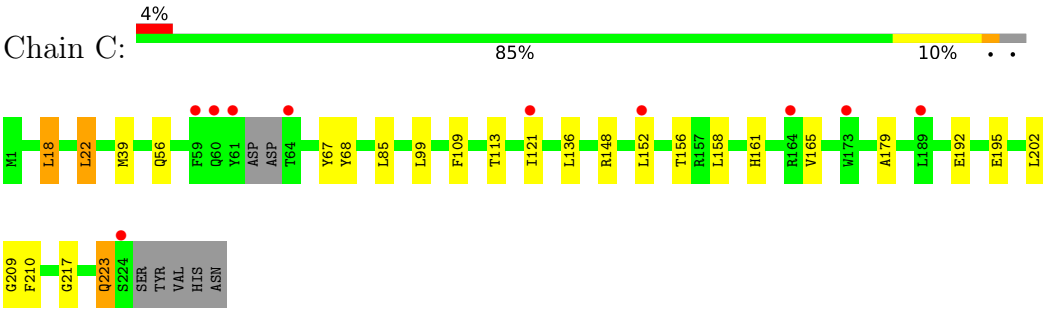
• Molecule 1: xenorhodopsin

Chain B:



• Molecule 1: xenorhodopsin

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.39Å 109.49Å 119.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 1.60 19.98 – 1.60	Depositor EDS
% Data completeness (in resolution range)	66.2 (19.98-1.60) 66.3 (19.98-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.203 , 0.216 0.205 , 0.217	Depositor DCC
R_{free} test set	3860 reflections (3.25%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6468	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, OLA, PO4, LYR, FME, LFA

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	1.04	0/1855	1.28	1/2532 (0.0%)
1	B	1.05	0/1835	1.24	3/2503 (0.1%)
1	C	1.03	0/1867	1.31	1/2548 (0.0%)
All	All	1.04	0/5557	1.28	5/7583 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	222	HIS	CA-C-O	-7.42	108.19	120.80
1	C	156	THR	CA-CB-OG1	-6.23	100.26	109.60
1	B	200	ILE	N-CA-C	-5.34	106.59	111.67
1	B	155	GLY	CA-C-O	-5.34	118.30	122.52
1	B	123	THR	CA-CB-OG1	-5.03	102.06	109.60

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	1872	0	1949	24	0
1	B	1853	0	1937	26	0
1	C	1885	0	1961	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	108	0	199	7	0
2	B	137	0	246	6	0
2	C	131	0	248	9	0
3	A	97	0	144	2	0
3	B	62	0	88	4	0
3	C	64	0	88	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	5	0	0	0	0
5	C	5	0	0	0	0
6	A	81	0	0	0	0
6	B	79	0	0	3	0
6	C	86	0	0	0	0
All	All	6468	0	6860	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (85) 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:C:56:GLN:HB3	3:C:305:OLA:H31	1.49	0.92
1:B:207[A]:LYR:H192	1:B:207[A]:LYR:H9	1.68	0.75
1:C:148:ARG:O	1:C:152:LEU:HD23	1.90	0.72
1:B:72:ILE:HD11	2:B:319:LFA:H71	1.73	0.68
1:C:165[A]:VAL:HG13	1:C:210[A]:PHE:CE1	2.28	0.68
1:B:202:LEU:HB2	1:B:203:PRO:HD3	1.77	0.67
1:A:207[C]:LYR:H183	1:A:207[C]:LYR:H9	1.76	0.67
1:B:40:VAL:HG13	3:C:303:OLA:H132	1.79	0.62
1:C:195[B]:GLU:HB2	2:C:313:LFA:H11	1.82	0.61
1:C:207[C]:LYR:H9	1:C:207[C]:LYR:H183	1.81	0.61
1:A:207[A]:LYR:H183	1:A:207[A]:LYR:H9	1.82	0.61
1:A:58:LEU:C	1:A:58:LEU:HD12	2.26	0.60
1:B:207[C]:LYR:H183	1:B:207[C]:LYR:H9	1.83	0.60
1:C:99[B]:LEU:C	1:C:99[B]:LEU:HD23	2.26	0.59
3:B:306:OLA:H72	2:C:317:LFA:H41	1.85	0.59
1:B:207[C]:LYR:H9	1:B:207[C]:LYR:H192	1.85	0.58
1:A:195[A]:GLU:HB2	2:A:518:LFA:H11	1.85	0.58
3:C:305:OLA:H52	2:C:316:LFA:H92	1.86	0.57
1:B:207[A]:LYR:H192	1:B:207[A]:LYR:C9	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:C	1:A:158:LEU:HD13	2.31	0.55
1:A:202:LEU:HB2	1:A:203:PRO:HD3	1.87	0.55
1:B:34:GLU:OE1	6:B:401:HOH:O	2.18	0.55
1:A:207[A]:LYR:H9	1:A:207[A]:LYR:H192	1.89	0.54
1:A:207[A]:LYR:C9	1:A:207[A]:LYR:H192	2.38	0.54
1:B:207[C]:LYR:H192	1:B:207[C]:LYR:C9	2.39	0.53
1:B:99[B]:LEU:HD23	1:B:99[B]:LEU:C	2.34	0.53
1:C:207[A]:LYR:H9	1:C:207[A]:LYR:H183	1.91	0.52
1:B:158:LEU:C	1:B:158:LEU:HD13	2.36	0.51
1:A:95:LYS:HE2	3:A:508:OLA:C1	2.41	0.51
1:C:18:LEU:O	1:C:22:LEU:HD22	2.10	0.51
3:B:306:OLA:H10	3:B:306:OLA:C14	2.41	0.50
1:C:136[C]:LEU:C	1:C:136[C]:LEU:HD23	2.37	0.50
1:C:202:LEU:HB2	1:C:203:PRO:HD3	1.93	0.50
1:A:207[C]:LYR:C9	1:A:207[C]:LYR:H192	2.42	0.50
1:A:178:THR:HG21	2:A:516:LFA:H12	1.93	0.49
1:C:158:LEU:C	1:C:158:LEU:HD13	2.37	0.49
1:A:179:ALA:O	2:A:518:LFA:H13	2.12	0.49
1:B:81[C]:LEU:HD23	1:B:173[C]:TRP:HZ3	1.76	0.48
1:A:195[B]:GLU:HB2	2:A:518:LFA:H11	1.95	0.48
1:C:68:TYR:CZ	2:C:319:LFA:H42	2.48	0.48
1:C:99[B]:LEU:HD23	1:C:99[B]:LEU:O	2.14	0.48
1:B:18:LEU:O	1:B:22:LEU:HD22	2.14	0.47
1:B:161:HIS:CE1	1:B:217:GLY:HA3	2.48	0.47
1:C:161:HIS:CE1	1:C:217:GLY:HA3	2.49	0.47
1:C:207[C]:LYR:H192	1:C:207[C]:LYR:C9	2.44	0.47
1:C:207[C]:LYR:H9	1:C:207[C]:LYR:H192	1.97	0.47
1:B:81[C]:LEU:HD13	6:B:403[C]:HOH:O	2.15	0.47
1:C:207[A]:LYR:H9	1:C:207[A]:LYR:H192	1.96	0.47
1:A:58:LEU:HD12	1:A:58:LEU:O	2.14	0.47
1:A:161:HIS:CE1	1:A:217:GLY:HA3	2.50	0.47
1:B:136[C]:LEU:HD22	2:B:301:LFA:C19	2.45	0.46
2:B:320:LFA:H81	2:B:320:LFA:H112	1.78	0.46
1:A:110:MET:HE1	1:A:173[C]:TRP:CZ2	2.51	0.45
1:B:19:TYR:CZ	2:B:304:LFA:H62	2.51	0.45
1:C:209[C]:GLY:HA2	2:C:307:LFA:H21	1.99	0.45
1:A:207[C]:LYR:H6	1:A:207[C]:LYR:H41	1.83	0.45
1:A:81[C]:LEU:HD23	1:A:173[C]:TRP:HZ3	1.82	0.45
2:A:512:LFA:C7	2:A:517:LFA:H11	2.48	0.44
1:A:136[C]:LEU:HD22	2:A:501:LFA:H201	2.00	0.44
1:A:207[C]:LYR:H9	1:A:207[C]:LYR:H192	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:HD12	1:A:22:LEU:HA	1.92	0.43
1:C:39[B]:MET:HE1	2:C:315:LFA:H81	2.00	0.43
1:C:209[C]:GLY:CA	2:C:307:LFA:H21	2.48	0.43
1:C:207[A]:LYR:H192	1:C:207[A]:LYR:C9	2.49	0.43
1:B:78:THR:N	1:B:79:PRO:HD2	2.34	0.42
1:B:194:THR:HG21	3:B:307:OLA:H21	2.01	0.42
1:C:39[B]:MET:CE	2:C:315:LFA:H81	2.49	0.42
1:B:207[C]:LYR:HA	6:B:403[C]:HOH:O	2.17	0.42
1:B:207[C]:LYR:H6	1:B:207[C]:LYR:H41	1.83	0.42
1:B:154:ASN:HD22	1:B:154:ASN:HA	1.74	0.42
1:C:223:GLN:HE21	1:C:223:GLN:HA	1.85	0.42
1:C:109:PHE:O	1:C:113:THR:HG23	2.20	0.41
1:C:207[C]:LYR:H81	1:C:207[C]:LYR:H10	1.84	0.41
1:C:179:ALA:O	2:C:313:LFA:H13	2.19	0.41
1:B:18:LEU:HD23	2:B:312:LFA:C1	2.50	0.41
1:B:110:MET:HE1	1:B:173[C]:TRP:CZ2	2.55	0.41
1:B:44:TRP:CE3	3:C:303:OLA:H152	2.56	0.41
1:C:67:TYR:OH	1:C:192:GLU:OE1	2.30	0.41
1:A:207[C]:LYR:H10	1:A:207[C]:LYR:H81	1.91	0.40
3:B:306:OLA:C14	3:B:306:OLA:C10	2.98	0.40
1:C:85:LEU:CD1	1:C:165[A]:VAL:HG12	2.51	0.40
1:A:72:ILE:HG13	2:A:520:LFA:H41	2.03	0.40
1:C:207[A]:LYR:H6	1:C:207[A]:LYR:H41	1.86	0.40
1:A:95:LYS:HE2	3:A:508:OLA:O2	2.21	0.40
1:B:198:VAL:HG22	2:B:311:LFA:H82	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	230/229 (100%)	227 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	226/229 (99%)	223 (99%)	3 (1%)	0	100	100
1	C	230/229 (100%)	228 (99%)	2 (1%)	0	100	100
All	All	686/687 (100%)	678 (99%)	8 (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	187/189 (99%)	182 (97%)	5 (3%)	39	16
1	B	187/189 (99%)	184 (98%)	3 (2%)	55	33
1	C	189/189 (100%)	185 (98%)	4 (2%)	47	23
All	All	563/567 (99%)	551 (98%)	12 (2%)	44	23

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	65	THR
1	A	66	ILE
1	A	121	ILE
1	A	157	ARG
1	B	4	ILE
1	B	22	LEU
1	B	66	ILE
1	C	18	LEU
1	C	22	LEU
1	C	121	ILE
1	C	223	GLN

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

Mol	Chain	Res	Type
1	A	154	ASN
1	B	154	ASN
1	B	222	HIS
1	C	223	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)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	LYR	A	207[C]	1	27,29,30	1.14	2 (7%)	30,37,39	1.14	3 (10%)
1	LYR	B	207[A]	1	27,29,30	1.14	2 (7%)	30,37,39	1.37	5 (16%)
1	FME	A	1	1	6,7,10	0.56	0	7,7,11	1.09	0
1	LYR	A	207[A]	1	27,29,30	1.14	2 (7%)	30,37,39	1.33	6 (20%)
1	LYR	B	207[C]	1	27,29,30	1.18	3 (11%)	30,37,39	1.15	3 (10%)
1	FME	C	1	1	6,7,10	0.59	0	7,7,11	1.25	0
1	FME	B	1	1	5,6,10	0.68	0	4,6,11	0.94	0
1	LYR	C	207[C]	1	27,29,30	1.13	2 (7%)	30,37,39	1.20	3 (10%)
1	LYR	C	207[A]	1	27,29,30	1.28	3 (11%)	30,37,39	1.35	5 (16%)

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
1	LYR	A	207[C]	1	-	5/22/40/42	0/1/1/1
1	LYR	B	207[A]	1	-	3/22/40/42	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	0/5/7/11	-
1	LYR	A	207[A]	1	-	4/22/40/42	0/1/1/1
1	LYR	B	207[C]	1	-	5/22/40/42	0/1/1/1
1	FME	C	1	1	-	1/5/7/11	-
1	FME	B	1	1	-	1/3/5/11	-
1	LYR	C	207[C]	1	-	5/22/40/42	0/1/1/1
1	LYR	C	207[A]	1	-	3/22/40/42	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	207[A]	LYR	C5-C3	-3.41	1.38	1.46
1	A	207[A]	LYR	C5-C3	-3.36	1.38	1.46
1	B	207[C]	LYR	C9-C80	-2.77	1.40	1.46
1	A	207[C]	LYR	C9-C80	-2.76	1.40	1.46
1	C	207[A]	LYR	C9-C80	-2.75	1.40	1.46
1	C	207[C]	LYR	C9-C80	-2.57	1.40	1.46
1	B	207[A]	LYR	C7-C80	2.44	1.41	1.35
1	C	207[C]	LYR	C7-C80	2.40	1.41	1.35
1	A	207[C]	LYR	C7-C80	2.35	1.41	1.35
1	B	207[C]	LYR	C7-C80	2.32	1.41	1.35
1	B	207[A]	LYR	C9-C80	-2.29	1.41	1.46
1	C	207[A]	LYR	C16-C15	-2.22	1.47	1.52
1	A	207[A]	LYR	C7-C80	2.11	1.40	1.35
1	B	207[C]	LYR	O-C	2.08	1.27	1.20

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	207[C]	LYR	C8-C80-C7	-3.62	116.95	122.82
1	A	207[C]	LYR	C8-C80-C7	-3.61	116.97	122.82
1	B	207[C]	LYR	C8-C80-C7	-3.52	117.11	122.82
1	C	207[A]	LYR	C6-C7-C80	3.20	131.76	127.28
1	B	207[A]	LYR	C5-C3-C2	-3.17	114.08	118.49
1	B	207[A]	LYR	C8-C80-C9	2.98	122.64	118.09
1	C	207[A]	LYR	C5-C3-C2	-2.93	114.42	118.49
1	C	207[C]	LYR	C9-C80-C7	2.91	123.58	119.01
1	A	207[A]	LYR	C8-C80-C7	-2.90	118.11	122.82
1	A	207[A]	LYR	C8-C80-C9	2.78	122.34	118.09
1	B	207[A]	LYR	C1-NZ-CE	-2.78	107.22	112.85
1	B	207[A]	LYR	C8-C80-C7	-2.70	118.44	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	207[A]	LYR	C4-C3-C2	2.65	128.33	123.73
1	A	207[A]	LYR	C6-C7-C80	2.59	130.91	127.28
1	C	207[A]	LYR	C8-C80-C7	-2.53	118.71	122.82
1	A	207[A]	LYR	C1-NZ-CE	-2.50	107.79	112.85
1	A	207[A]	LYR	C5-C3-C2	-2.45	115.08	118.49
1	A	207[C]	LYR	C9-C80-C7	2.38	122.75	119.01
1	A	207[C]	LYR	C7-C6-C5	2.37	130.08	123.20
1	B	207[A]	LYR	C4-C3-C2	2.29	127.71	123.73
1	B	207[C]	LYR	C7-C6-C5	2.21	129.62	123.20
1	C	207[C]	LYR	C7-C6-C5	2.18	129.51	123.20
1	B	207[C]	LYR	C9-C80-C7	2.18	122.43	119.01
1	C	207[A]	LYR	C1-NZ-CE	-2.12	108.56	112.85
1	A	207[A]	LYR	C16-C17-C11	2.02	113.37	110.44

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1	FME	O-C-CA-CB
1	C	1	FME	O-C-CA-CB
1	A	207[A]	LYR	C1-C2-C3-C4
1	A	207[A]	LYR	C1-C2-C3-C5
1	A	207[C]	LYR	C1-C2-C3-C4
1	A	207[C]	LYR	C1-C2-C3-C5
1	B	207[A]	LYR	C1-C2-C3-C4
1	B	207[A]	LYR	C1-C2-C3-C5
1	B	207[C]	LYR	C1-C2-C3-C4
1	B	207[C]	LYR	C1-C2-C3-C5
1	C	207[A]	LYR	C1-C2-C3-C4
1	C	207[A]	LYR	C1-C2-C3-C5
1	C	207[C]	LYR	C1-C2-C3-C4
1	C	207[C]	LYR	C1-C2-C3-C5
1	A	207[C]	LYR	C2-C1-NZ-CE
1	B	207[C]	LYR	C2-C1-NZ-CE
1	C	207[C]	LYR	C2-C1-NZ-CE
1	C	207[C]	LYR	CD-CE-NZ-C1
1	A	207[C]	LYR	CD-CE-NZ-C1
1	C	207[C]	LYR	CG-CD-CE-NZ
1	A	207[A]	LYR	CD-CE-NZ-C1
1	B	207[A]	LYR	CD-CE-NZ-C1
1	B	207[C]	LYR	CG-CD-CE-NZ
1	C	207[A]	LYR	CD-CE-NZ-C1

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Mol	Chain	Res	Type	Atoms
1	A	207[C]	LYR	CG-CD-CE-NZ
1	B	207[C]	LYR	CD-CE-NZ-C1
1	A	207[A]	LYR	CG-CD-CE-NZ

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	207[C]	LYR	5	0
1	B	207[A]	LYR	2	0
1	A	207[A]	LYR	3	0
1	B	207[C]	LYR	5	0
1	C	207[C]	LYR	4	0
1	C	207[A]	LYR	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 63 ligands modelled in this entry, 3 are monoatomic - leaving 60 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OLA	B	306	-	15,15,19	0.70	0	15,15,19	0.65	0
2	LFA	A	512	-	6,6,19	0.29	0	5,5,18	0.33	0
2	LFA	A	511	-	8,8,19	0.14	0	7,7,18	0.19	0
2	LFA	C	309	-	3,3,19	0.13	0	2,2,18	0.47	0
2	LFA	B	321	-	9,9,19	0.14	0	8,8,18	0.08	0
3	OLA	A	505[A]	-	19,19,19	0.55	0	19,19,19	0.54	0
2	LFA	B	314	-	4,4,19	0.25	0	3,3,18	0.43	0
2	LFA	C	308	-	15,15,19	0.20	0	14,14,18	0.19	0
3	OLA	B	307	-	11,11,19	0.76	0	11,11,19	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LFA	B	301	-	6,6,19	0.27	0	5,5,18	0.41	0
2	LFA	A	501	-	5,5,19	0.14	0	4,4,18	0.11	0
2	LFA	B	304	-	6,6,19	0.09	0	5,5,18	0.27	0
2	LFA	C	318	-	4,4,19	0.11	0	3,3,18	0.21	0
2	LFA	A	517	-	2,2,19	0.08	0	1,1,18	0.08	0
2	LFA	A	519	-	9,9,19	0.21	0	8,8,18	0.17	0
3	OLA	C	305	-	12,12,19	0.64	0	12,12,19	0.65	0
2	LFA	B	310	-	5,5,19	0.13	0	4,4,18	0.10	0
2	LFA	A	520	-	9,9,19	0.13	0	8,8,18	0.05	0
2	LFA	B	317	-	3,3,19	0.30	0	2,2,18	0.44	0
3	OLA	A	504	-	10,10,19	0.84	0	10,10,19	0.53	0
3	OLA	A	506	-	15,15,19	0.63	0	15,15,19	0.53	0
2	LFA	C	315	-	8,8,19	0.13	0	7,7,18	0.07	0
3	OLA	A	505[B]	-	19,19,19	0.51	0	19,19,19	0.52	0
2	LFA	B	320	-	13,13,19	0.14	0	12,12,18	0.07	0
2	LFA	A	510	-	8,8,19	0.11	0	7,7,18	0.09	0
2	LFA	C	317	-	8,8,19	0.14	0	7,7,18	0.10	0
2	LFA	C	307	-	9,9,19	0.19	0	8,8,18	0.11	0
3	OLA	B	308	-	19,19,19	0.54	0	19,19,19	0.49	0
2	LFA	C	311	-	8,8,19	0.13	0	7,7,18	0.10	0
2	LFA	C	319	-	7,7,19	0.12	0	6,6,18	0.08	0
5	PO4	C	320	-	4,4,4	0.70	0	6,6,6	0.48	0
2	LFA	A	513	-	11,11,19	0.16	0	10,10,18	0.12	0
2	LFA	B	312	-	8,8,19	0.22	0	7,7,18	0.28	0
3	OLA	B	305	-	13,13,19	0.77	0	13,13,19	0.53	0
5	PO4	A	521	-	4,4,4	0.75	0	6,6,6	0.46	0
2	LFA	C	314	-	8,8,19	0.12	0	7,7,18	0.11	0
2	LFA	C	301	-	16,16,19	0.19	0	15,15,18	0.24	0
3	OLA	C	302	-	15,15,19	0.73	1 (6%)	15,15,19	0.63	0
2	LFA	C	313	-	7,7,19	0.18	0	6,6,18	0.24	0
2	LFA	B	313	-	6,6,19	0.22	0	5,5,18	0.28	0
2	LFA	A	515	-	7,7,19	0.17	0	6,6,18	0.22	0
2	LFA	B	315	-	4,4,19	0.14	0	3,3,18	0.30	0
2	LFA	B	303	-	8,8,19	0.18	0	7,7,18	0.26	0
2	LFA	C	310	-	7,7,19	0.12	0	6,6,18	0.20	0
2	LFA	B	316	-	5,5,19	0.17	0	4,4,18	0.20	0
2	LFA	A	516	-	5,5,19	0.22	0	4,4,18	0.13	0
2	LFA	B	302	-	14,14,19	0.28	0	13,13,18	0.19	0
3	OLA	C	304	-	15,15,19	0.64	0	15,15,19	0.45	0
3	OLA	A	507	-	10,10,19	0.66	0	10,10,19	0.87	0
2	LFA	A	518	-	4,4,19	0.27	0	3,3,18	0.13	0
2	LFA	A	502	-	8,8,19	0.12	0	7,7,18	0.16	0
2	LFA	A	503	-	6,6,19	0.22	0	5,5,18	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LFA	C	316	-	10,10,19	0.12	0	9,9,18	0.08	0
3	OLA	A	508	-	18,18,19	0.57	0	18,18,19	0.54	0
2	LFA	C	312	-	7,7,19	0.16	0	6,6,18	0.11	0
2	LFA	A	514	-	6,6,19	0.15	0	5,5,18	0.11	0
3	OLA	C	303	-	18,18,19	0.63	0	18,18,19	0.55	0
2	LFA	B	311	-	8,8,19	0.11	0	7,7,18	0.15	0
2	LFA	B	318	-	14,14,19	0.24	0	13,13,18	0.12	0
2	LFA	B	319	-	8,8,19	0.12	0	7,7,18	0.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLA	B	306	-	-	6/13/13/17	-
2	LFA	A	512	-	-	1/4/4/17	-
2	LFA	A	511	-	-	1/6/6/17	-
2	LFA	C	309	-	-	0/1/1/17	-
2	LFA	B	321	-	-	4/7/7/17	-
3	OLA	A	505[A]	-	-	9/17/17/17	-
2	LFA	B	314	-	-	1/2/2/17	-
2	LFA	C	308	-	-	4/13/13/17	-
3	OLA	B	307	-	-	2/9/9/17	-
2	LFA	B	301	-	-	2/4/4/17	-
2	LFA	A	501	-	-	2/3/3/17	-
2	LFA	B	304	-	-	1/4/4/17	-
2	LFA	C	318	-	-	1/2/2/17	-
3	OLA	C	305	-	-	8/10/10/17	-
2	LFA	A	519	-	-	2/7/7/17	-
2	LFA	B	310	-	-	2/3/3/17	-
2	LFA	A	520	-	-	4/7/7/17	-
2	LFA	B	317	-	-	0/1/1/17	-
3	OLA	A	504	-	-	3/8/8/17	-
3	OLA	A	506	-	-	9/13/13/17	-
2	LFA	C	315	-	-	4/6/6/17	-
3	OLA	A	505[B]	-	-	11/17/17/17	-
2	LFA	B	320	-	-	7/11/11/17	-
2	LFA	A	510	-	-	2/6/6/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	C	317	-	-	4/6/6/17	-
2	LFA	C	307	-	-	2/7/7/17	-
3	OLA	B	308	-	-	11/17/17/17	-
2	LFA	C	311	-	-	5/6/6/17	-
2	LFA	C	319	-	-	3/5/5/17	-
2	LFA	A	513	-	-	5/9/9/17	-
2	LFA	B	312	-	-	1/6/6/17	-
3	OLA	B	305	-	-	5/11/11/17	-
2	LFA	C	314	-	-	5/6/6/17	-
2	LFA	C	301	-	-	6/14/14/17	-
3	OLA	C	302	-	-	8/13/13/17	-
2	LFA	C	313	-	-	2/5/5/17	-
2	LFA	B	313	-	-	2/4/4/17	-
2	LFA	A	515	-	-	4/5/5/17	-
2	LFA	B	315	-	-	0/2/2/17	-
2	LFA	B	303	-	-	1/6/6/17	-
2	LFA	C	310	-	-	1/5/5/17	-
2	LFA	B	316	-	-	2/3/3/17	-
2	LFA	A	516	-	-	2/3/3/17	-
2	LFA	B	302	-	-	4/12/12/17	-
3	OLA	C	304	-	-	8/13/13/17	-
3	OLA	A	507	-	-	6/8/8/17	-
2	LFA	A	518	-	-	2/2/2/17	-
2	LFA	A	502	-	-	3/6/6/17	-
2	LFA	A	503	-	-	2/4/4/17	-
2	LFA	C	316	-	-	3/8/8/17	-
3	OLA	A	508	-	-	3/16/16/17	-
2	LFA	C	312	-	-	3/5/5/17	-
2	LFA	A	514	-	-	2/4/4/17	-
3	OLA	C	303	-	-	10/16/16/17	-
2	LFA	B	311	-	-	1/6/6/17	-
2	LFA	B	318	-	-	7/12/12/17	-
2	LFA	B	319	-	-	5/6/6/17	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	OLA	O1-C1	2.46	1.30	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (214) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	305	OLA	C11-C10-C9-C8
3	B	306	OLA	C11-C10-C9-C8
3	B	308	OLA	C11-C10-C9-C8
3	C	302	OLA	C11-C10-C9-C8
3	B	306	OLA	C1-C2-C3-C4
3	A	505[A]	OLA	C11-C10-C9-C8
3	C	303	OLA	C1-C2-C3-C4
3	C	303	OLA	C11-C10-C9-C8
3	B	307	OLA	C1-C2-C3-C4
3	B	305	OLA	C11-C10-C9-C8
2	C	312	LFA	C2-C3-C4-C5
3	A	505[B]	OLA	C11-C10-C9-C8
2	A	520	LFA	C2-C3-C4-C5
2	B	318	LFA	C4-C5-C6-C7
2	B	318	LFA	C11-C10-C9-C8
3	A	506	OLA	C5-C6-C7-C8
2	B	321	LFA	C16-C17-C18-C19
3	B	305	OLA	C2-C3-C4-C5
3	C	304	OLA	C5-C6-C7-C8
3	B	305	OLA	C3-C4-C5-C6
2	A	519	LFA	C3-C4-C5-C6
2	B	319	LFA	C2-C3-C4-C5
3	A	507	OLA	C4-C5-C6-C7
2	B	320	LFA	C6-C7-C8-C9
2	C	307	LFA	C3-C4-C5-C6
3	C	305	OLA	C1-C2-C3-C4
2	A	510	LFA	C4-C5-C6-C7
2	B	302	LFA	C6-C7-C8-C9
3	A	504	OLA	C2-C3-C4-C5
3	A	505[B]	OLA	C4-C5-C6-C7
3	A	506	OLA	C4-C5-C6-C7
2	B	319	LFA	C4-C5-C6-C7
2	A	502	LFA	C5-C6-C7-C8
2	C	314	LFA	C4-C5-C6-C7
3	A	507	OLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	C	319	LFA	C2-C3-C4-C5
3	A	505[B]	OLA	C5-C6-C7-C8
2	B	312	LFA	C1-C2-C3-C4
2	C	308	LFA	C9-C10-C11-C12
3	A	505[A]	OLA	C4-C5-C6-C7
3	C	303	OLA	C11-C12-C13-C14
3	C	304	OLA	C3-C4-C5-C6
2	C	314	LFA	C2-C3-C4-C5
2	C	317	LFA	C2-C3-C4-C5
3	C	304	OLA	C4-C5-C6-C7
2	B	319	LFA	C5-C6-C7-C8
3	C	302	OLA	C10-C11-C12-C13
3	A	507	OLA	C3-C4-C5-C6
3	B	306	OLA	C11-C12-C13-C14
2	C	301	LFA	C11-C10-C9-C8
2	B	318	LFA	C2-C3-C4-C5
2	C	313	LFA	C4-C5-C6-C7
2	B	313	LFA	C3-C4-C5-C6
3	A	508	OLA	C11-C12-C13-C14
3	C	305	OLA	C3-C4-C5-C6
3	C	304	OLA	C11-C10-C9-C8
3	C	303	OLA	C4-C5-C6-C7
3	C	303	OLA	C12-C13-C14-C15
2	A	514	LFA	C2-C3-C4-C5
3	A	505[A]	OLA	C10-C11-C12-C13
3	A	506	OLA	C6-C7-C8-C9
3	C	304	OLA	C6-C7-C8-C9
2	A	515	LFA	C1-C2-C3-C4
3	C	302	OLA	C4-C5-C6-C7
2	C	301	LFA	C6-C7-C8-C9
2	B	318	LFA	C7-C8-C9-C10
3	B	305	OLA	C5-C6-C7-C8
3	A	505[B]	OLA	C15-C16-C17-C18
2	A	519	LFA	C2-C3-C4-C5
3	C	303	OLA	C6-C7-C8-C9
3	C	303	OLA	C13-C14-C15-C16
2	C	317	LFA	C5-C6-C7-C8
2	B	310	LFA	C2-C3-C4-C5
2	C	314	LFA	C3-C4-C5-C6
3	B	307	OLA	C4-C5-C6-C7
2	A	520	LFA	C3-C4-C5-C6
2	A	513	LFA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	C	316	LFA	C2-C3-C4-C5
2	B	316	LFA	C3-C4-C5-C6
2	C	315	LFA	C3-C4-C5-C6
2	C	307	LFA	C4-C5-C6-C7
2	A	512	LFA	C3-C4-C5-C6
2	C	308	LFA	C11-C12-C13-C14
2	A	518	LFA	C1-C2-C3-C4
2	B	320	LFA	C9-C10-C11-C12
2	B	302	LFA	C3-C4-C5-C6
3	A	505[A]	OLA	C5-C6-C7-C8
2	A	520	LFA	C5-C6-C7-C8
2	B	316	LFA	C4-C5-C6-C7
2	B	320	LFA	C2-C3-C4-C5
3	C	304	OLA	C11-C12-C13-C14
2	A	510	LFA	C6-C7-C8-C9
2	C	311	LFA	C6-C7-C8-C9
2	C	315	LFA	C1-C2-C3-C4
3	A	505[B]	OLA	C3-C4-C5-C6
2	A	520	LFA	C7-C8-C9-C10
2	C	312	LFA	C1-C2-C3-C4
2	C	312	LFA	C3-C4-C5-C6
2	A	513	LFA	C9-C10-C11-C12
2	B	319	LFA	C6-C7-C8-C9
2	A	501	LFA	C15-C16-C17-C18
2	A	501	LFA	C16-C17-C18-C19
3	A	506	OLA	C2-C3-C4-C5
3	B	308	OLA	C1-C2-C3-C4
3	A	508	OLA	C11-C10-C9-C8
2	B	320	LFA	C5-C6-C7-C8
3	C	303	OLA	C2-C3-C4-C5
2	A	518	LFA	C2-C3-C4-C5
2	B	318	LFA	C10-C11-C12-C13
3	A	504	OLA	C6-C7-C8-C9
2	B	310	LFA	C1-C2-C3-C4
2	B	311	LFA	C11-C10-C9-C8
2	B	320	LFA	C11-C12-C13-C14
2	C	319	LFA	C1-C2-C3-C4
3	A	505[A]	OLA	C3-C4-C5-C6
2	C	319	LFA	C5-C6-C7-C8
2	B	321	LFA	C15-C16-C17-C18
3	A	505[B]	OLA	C14-C15-C16-C17
2	C	316	LFA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	B	318	LFA	C1-C2-C3-C4
2	C	301	LFA	C4-C5-C6-C7
3	C	303	OLA	C5-C6-C7-C8
2	C	317	LFA	C6-C7-C8-C9
2	A	513	LFA	C6-C7-C8-C9
2	B	320	LFA	C4-C5-C6-C7
2	C	317	LFA	C1-C2-C3-C4
2	C	311	LFA	C3-C4-C5-C6
3	C	303	OLA	C3-C4-C5-C6
2	C	308	LFA	C7-C8-C9-C10
2	A	516	LFA	C2-C3-C4-C5
2	B	301	LFA	C14-C15-C16-C17
3	B	308	OLA	C3-C4-C5-C6
2	A	503	LFA	C16-C17-C18-C19
2	C	301	LFA	C10-C11-C12-C13
3	A	505[B]	OLA	C10-C11-C12-C13
2	A	513	LFA	C1-C2-C3-C4
2	A	502	LFA	C2-C3-C4-C5
3	B	308	OLA	C13-C14-C15-C16
2	C	314	LFA	C1-C2-C3-C4
3	B	306	OLA	C3-C4-C5-C6
3	C	305	OLA	C2-C3-C4-C5
2	C	310	LFA	C17-C18-C19-C20
3	C	302	OLA	C3-C4-C5-C6
2	B	304	LFA	C3-C4-C5-C6
2	A	516	LFA	C1-C2-C3-C4
3	A	505[A]	OLA	C15-C16-C17-C18
2	B	303	LFA	C6-C7-C8-C9
2	B	313	LFA	C4-C5-C6-C7
2	C	311	LFA	C2-C3-C4-C5
2	A	515	LFA	C3-C4-C5-C6
3	B	308	OLA	C10-C11-C12-C13
3	A	508	OLA	C13-C14-C15-C16
3	B	308	OLA	C15-C16-C17-C18
2	B	319	LFA	C1-C2-C3-C4
2	C	301	LFA	C5-C6-C7-C8
2	B	320	LFA	C11-C10-C9-C8
3	B	305	OLA	C7-C8-C9-C10
2	A	502	LFA	C7-C8-C9-C10
3	C	305	OLA	C4-C5-C6-C7
3	B	308	OLA	C7-C8-C9-C10
2	B	301	LFA	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
3	A	505[B]	OLA	C6-C7-C8-C9
3	A	506	OLA	C1-C2-C3-C4
2	C	318	LFA	C17-C18-C19-C20
3	A	504	OLA	C1-C2-C3-C4
3	C	305	OLA	C5-C6-C7-C8
2	A	514	LFA	C4-C5-C6-C7
3	C	302	OLA	C11-C12-C13-C14
3	C	302	OLA	O2-C1-C2-C3
3	C	305	OLA	O2-C1-C2-C3
3	A	505[B]	OLA	O2-C1-C2-C3
2	C	308	LFA	C1-C2-C3-C4
3	B	306	OLA	O1-C1-C2-C3
2	B	321	LFA	C11-C12-C13-C14
3	A	505[A]	OLA	O2-C1-C2-C3
2	C	315	LFA	C4-C5-C6-C7
2	C	311	LFA	C5-C6-C7-C8
3	A	505[B]	OLA	O1-C1-C2-C3
3	C	305	OLA	O1-C1-C2-C3
3	A	507	OLA	O1-C1-C2-C3
3	B	306	OLA	O2-C1-C2-C3
2	A	513	LFA	C3-C4-C5-C6
2	A	511	LFA	C1-C2-C3-C4
2	B	314	LFA	C16-C17-C18-C19
3	C	302	OLA	O1-C1-C2-C3
3	A	507	OLA	C6-C7-C8-C9
2	B	318	LFA	C9-C10-C11-C12
3	A	507	OLA	O2-C1-C2-C3
2	B	321	LFA	C14-C15-C16-C17
3	A	505[A]	OLA	O1-C1-C2-C3
3	A	506	OLA	C9-C10-C11-C12
2	B	302	LFA	C4-C5-C6-C7
3	A	505[A]	OLA	C7-C8-C9-C10
3	B	308	OLA	C5-C6-C7-C8
2	C	301	LFA	C3-C4-C5-C6
2	A	515	LFA	C4-C5-C6-C7
3	A	505[B]	OLA	C7-C8-C9-C10
3	C	304	OLA	C7-C8-C9-C10
3	A	506	OLA	O1-C1-C2-C3
2	A	503	LFA	C17-C18-C19-C20
3	C	302	OLA	C2-C3-C4-C5
2	A	515	LFA	C5-C6-C7-C8
2	C	313	LFA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	C	316	LFA	C7-C8-C9-C10
3	B	308	OLA	C12-C13-C14-C15
2	B	302	LFA	C5-C6-C7-C8
3	C	304	OLA	C2-C3-C4-C5
3	B	308	OLA	C11-C12-C13-C14
3	A	506	OLA	O2-C1-C2-C3
2	C	315	LFA	C5-C6-C7-C8
2	C	314	LFA	C6-C7-C8-C9
2	C	311	LFA	C1-C2-C3-C4
3	A	506	OLA	C7-C8-C9-C10
3	B	308	OLA	O2-C1-C2-C3

There are no ring outliers.

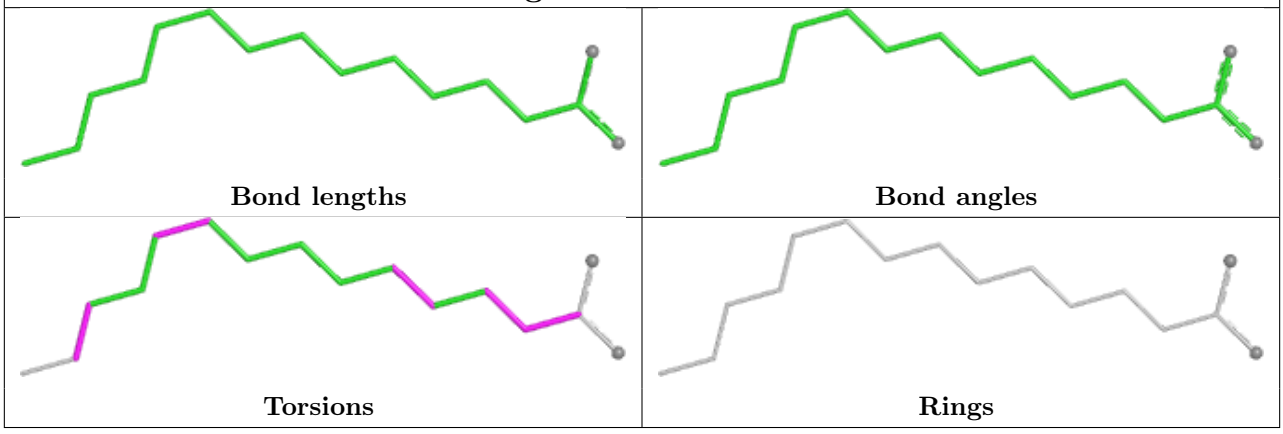
23 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	306	OLA	3	0
2	A	512	LFA	1	0
3	B	307	OLA	1	0
2	B	301	LFA	1	0
2	A	501	LFA	1	0
2	B	304	LFA	1	0
2	A	517	LFA	1	0
3	C	305	OLA	2	0
2	A	520	LFA	1	0
2	C	315	LFA	2	0
2	B	320	LFA	1	0
2	C	317	LFA	1	0
2	C	307	LFA	2	0
2	C	319	LFA	1	0
2	B	312	LFA	1	0
2	C	313	LFA	2	0
2	A	516	LFA	1	0
2	A	518	LFA	3	0
2	C	316	LFA	1	0
3	A	508	OLA	2	0
3	C	303	OLA	2	0
2	B	311	LFA	1	0
2	B	319	LFA	1	0

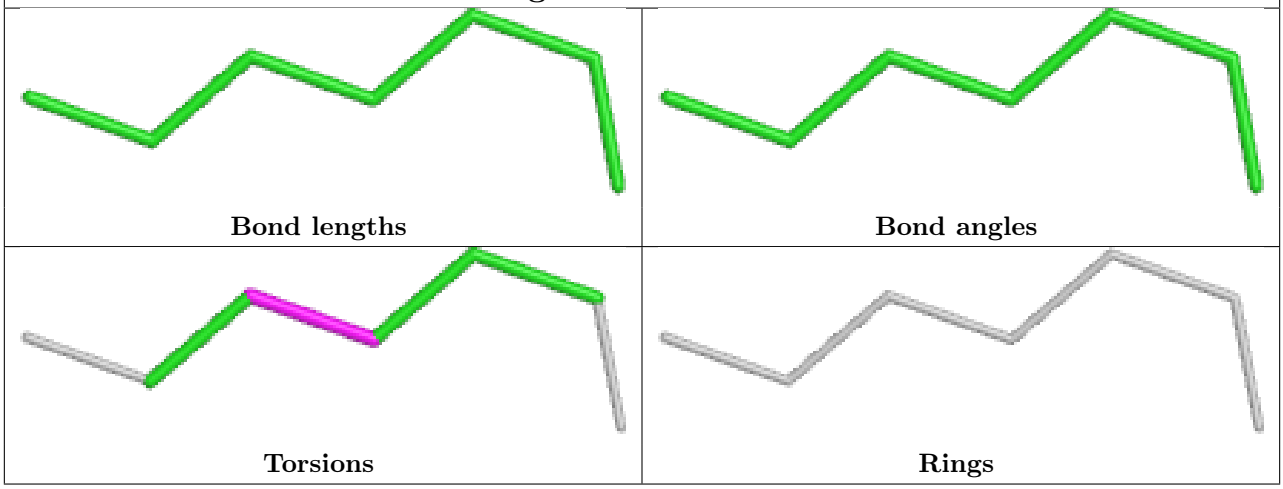
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

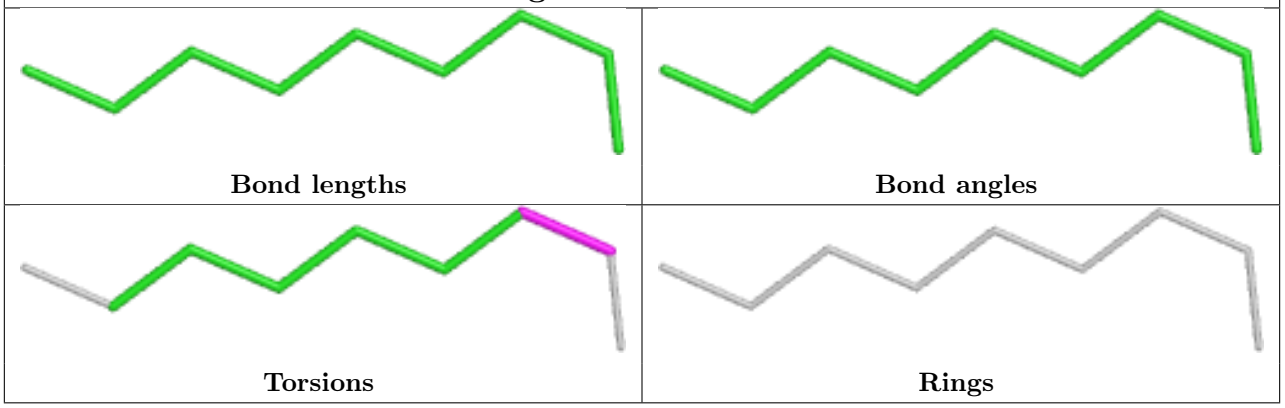
Ligand OLA B 306



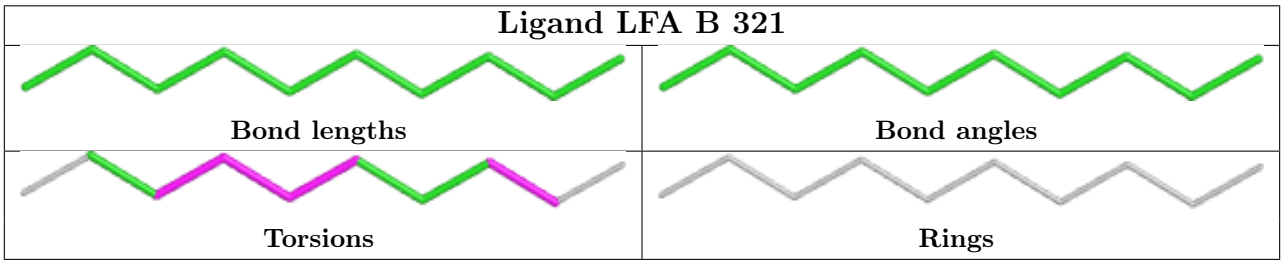
Ligand LFA A 512



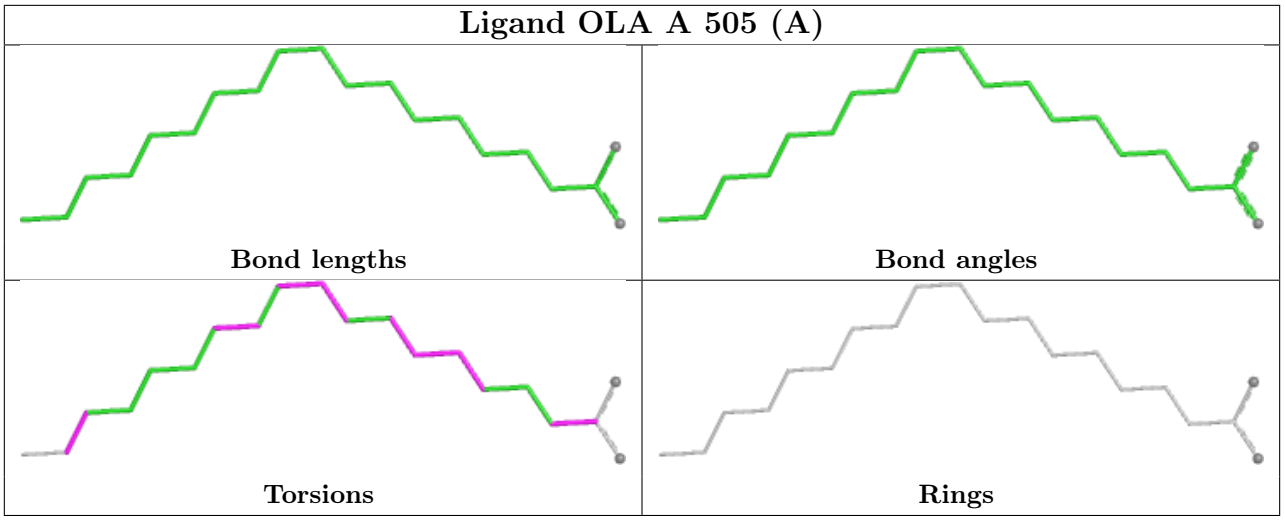
Ligand LFA A 511



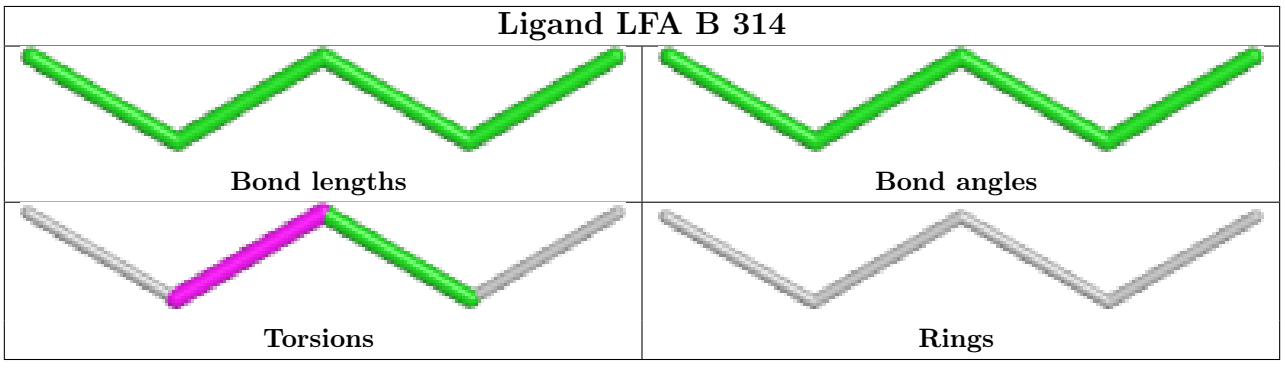
Ligand LFA B 321



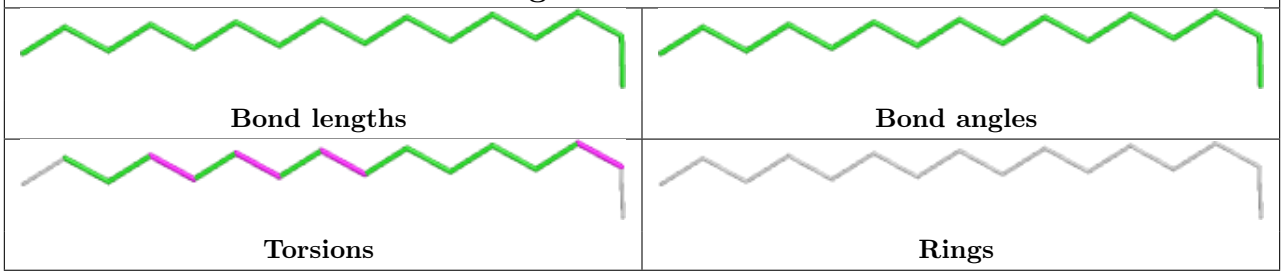
Ligand OLA A 505 (A)



Ligand LFA B 314



Ligand LFA C 308



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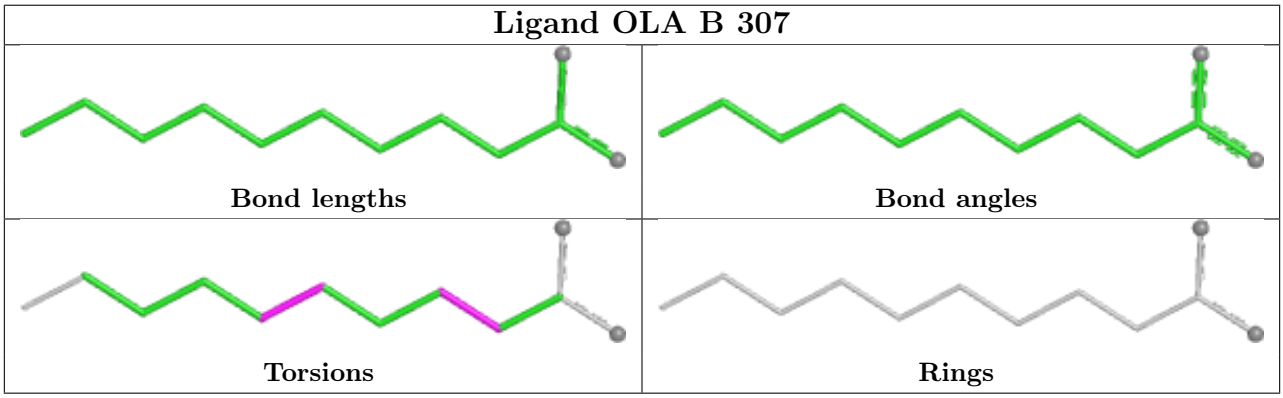
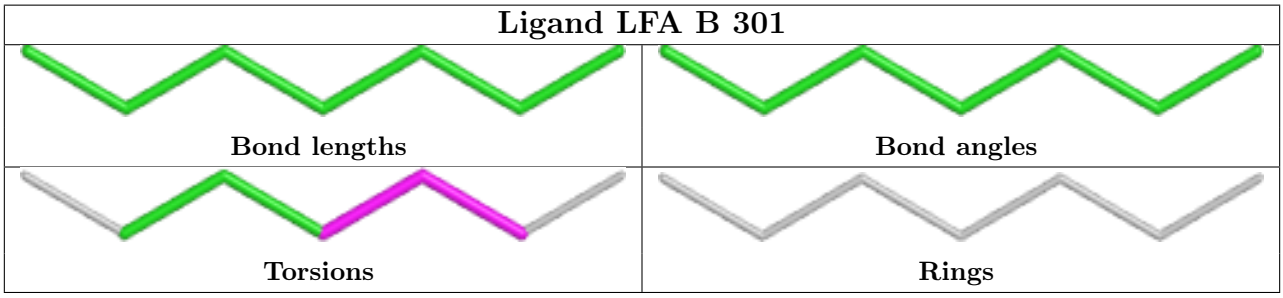
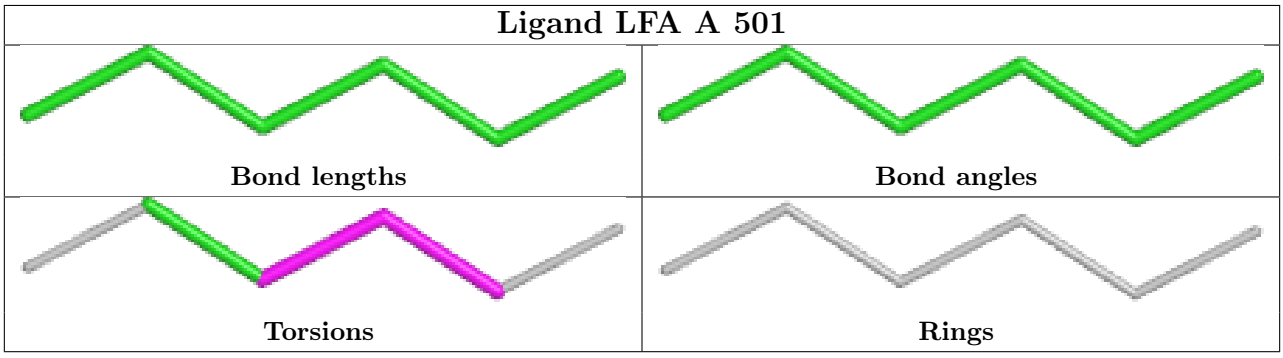


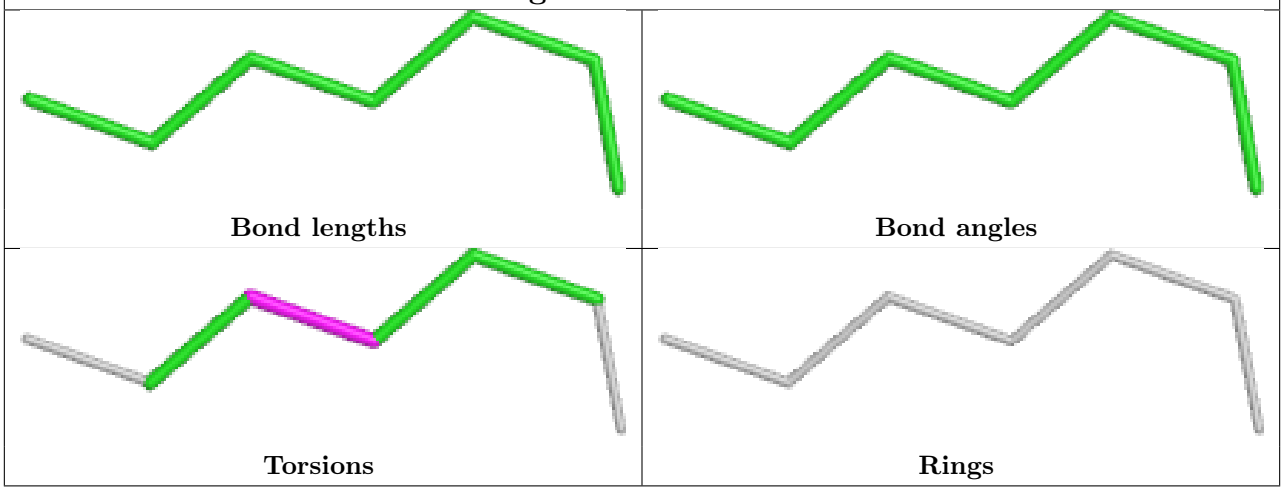
Ligand LFA B 301



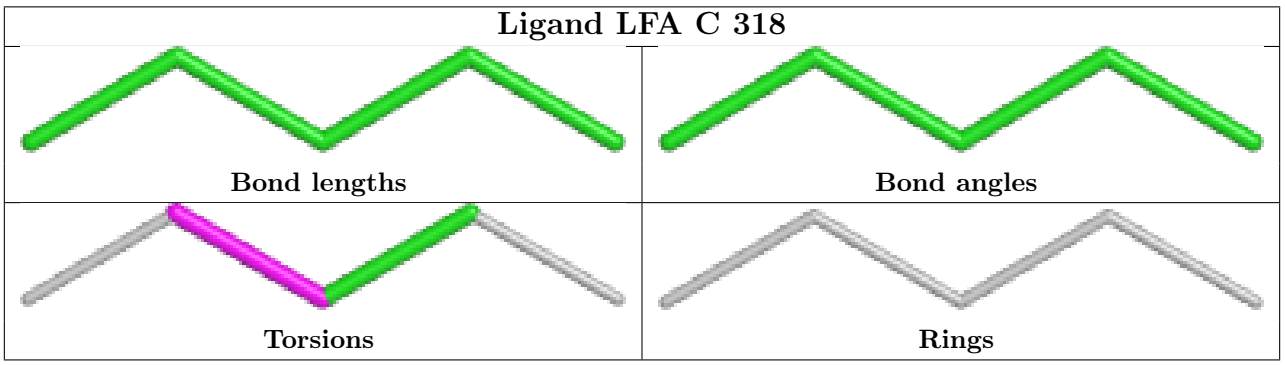
Ligand LFA A 501



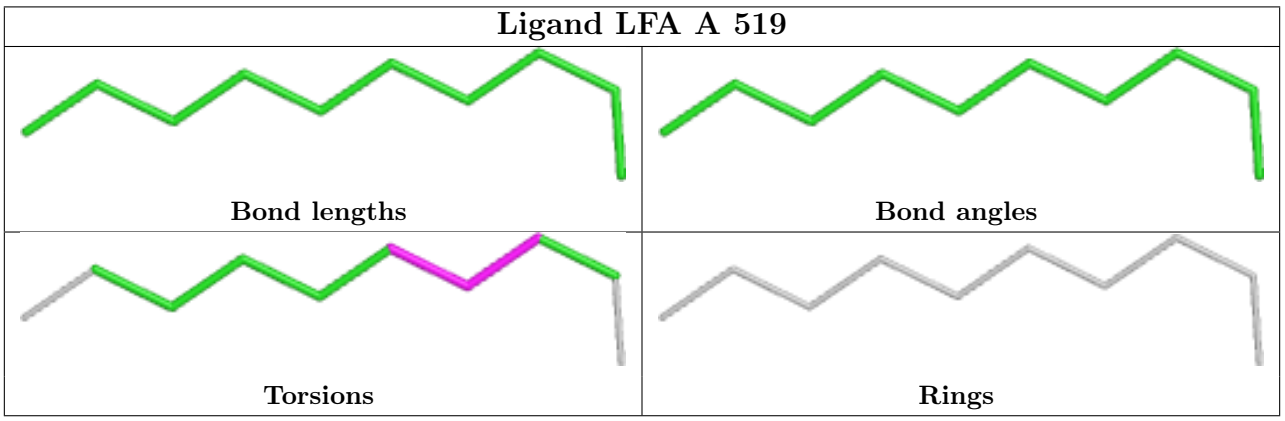
Ligand LFA B 304



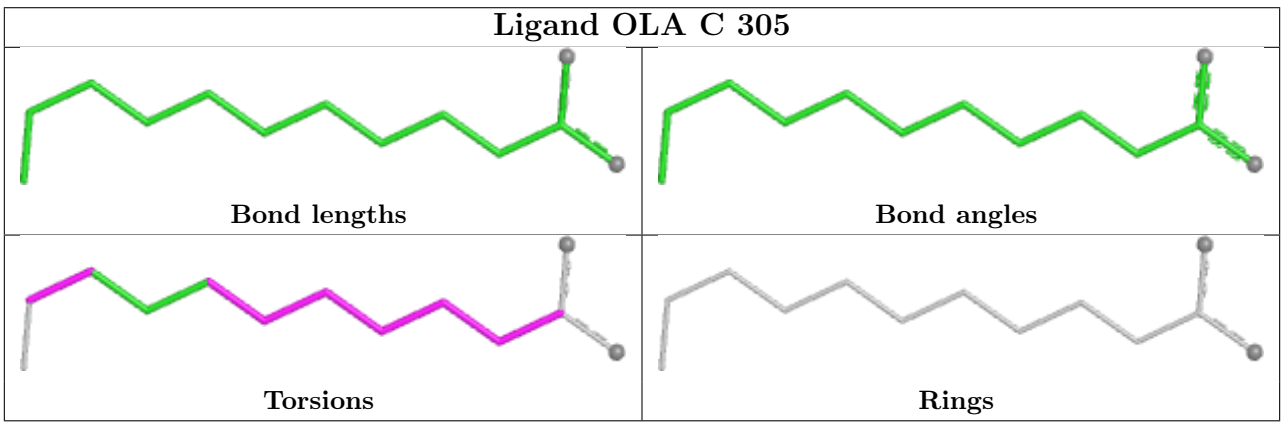
Ligand LFA C 318



Ligand LFA A 519



Ligand OLA C 305



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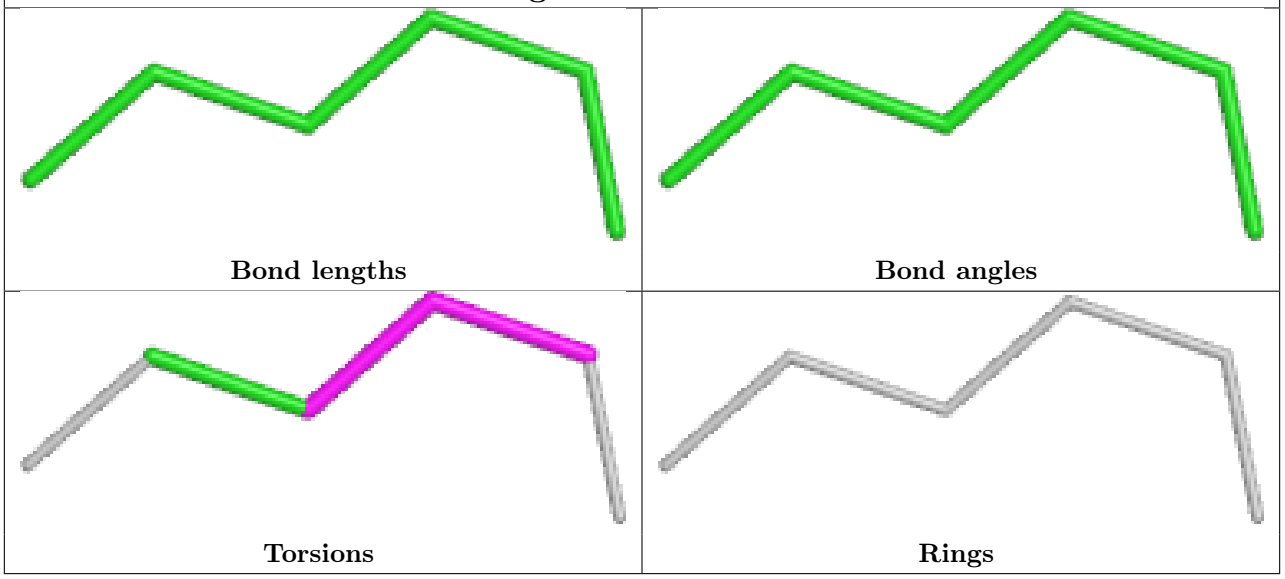
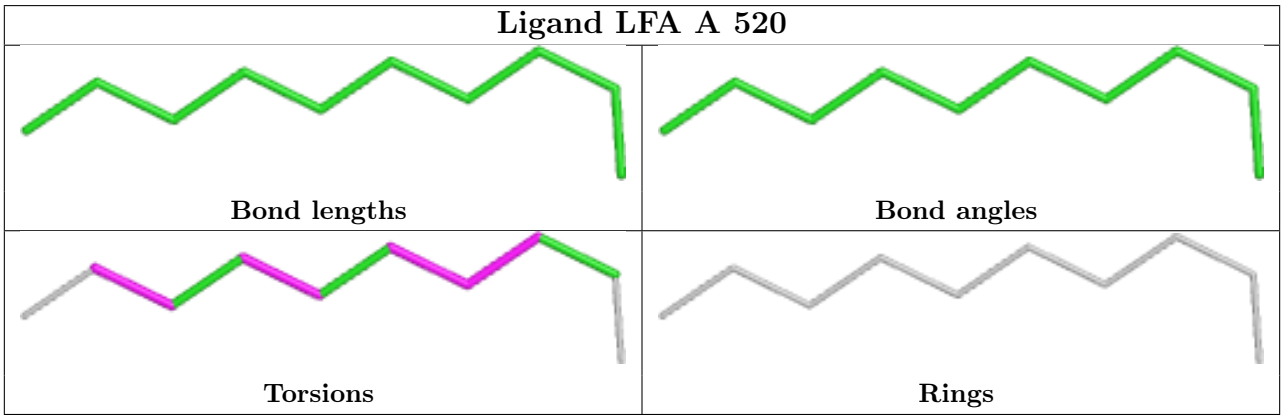
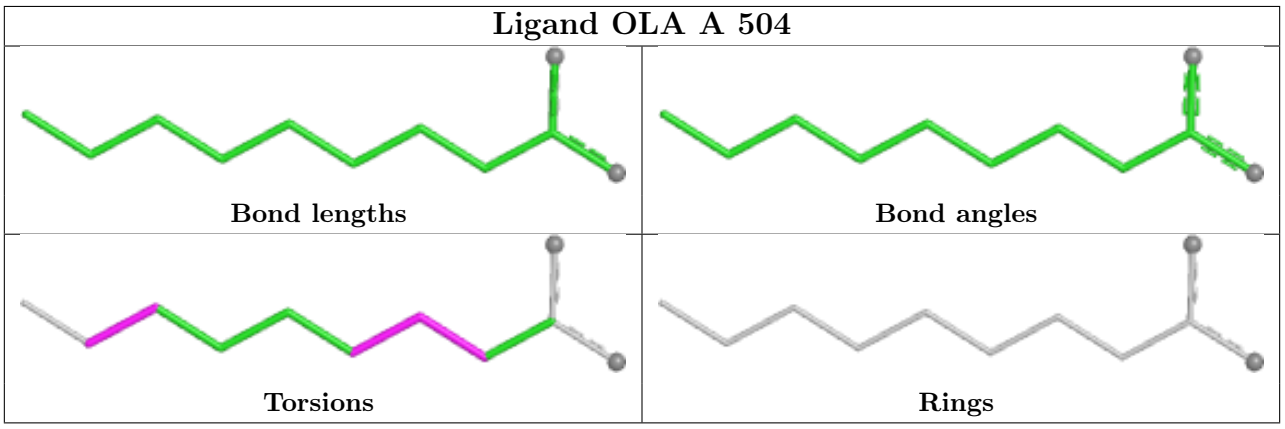


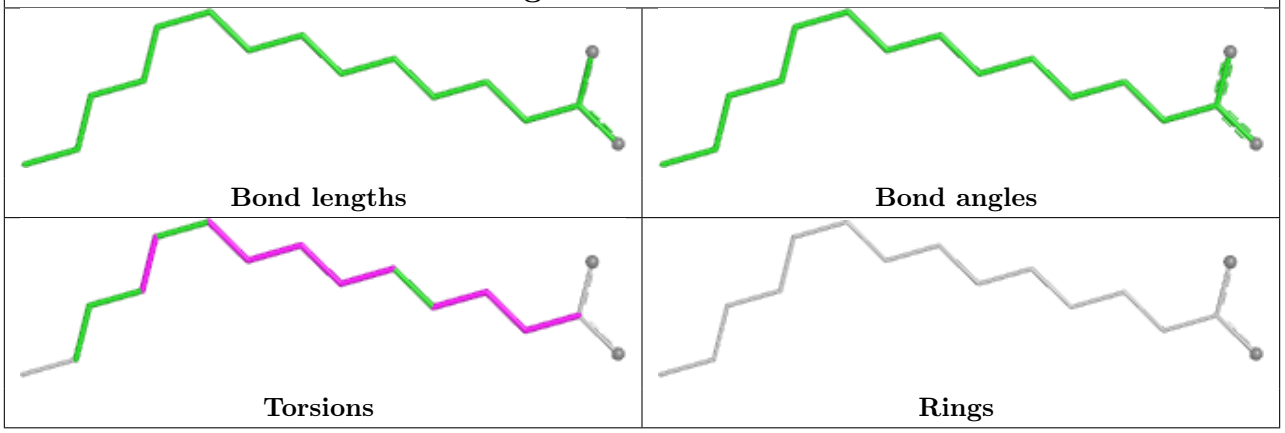
Ligand LFA A 520



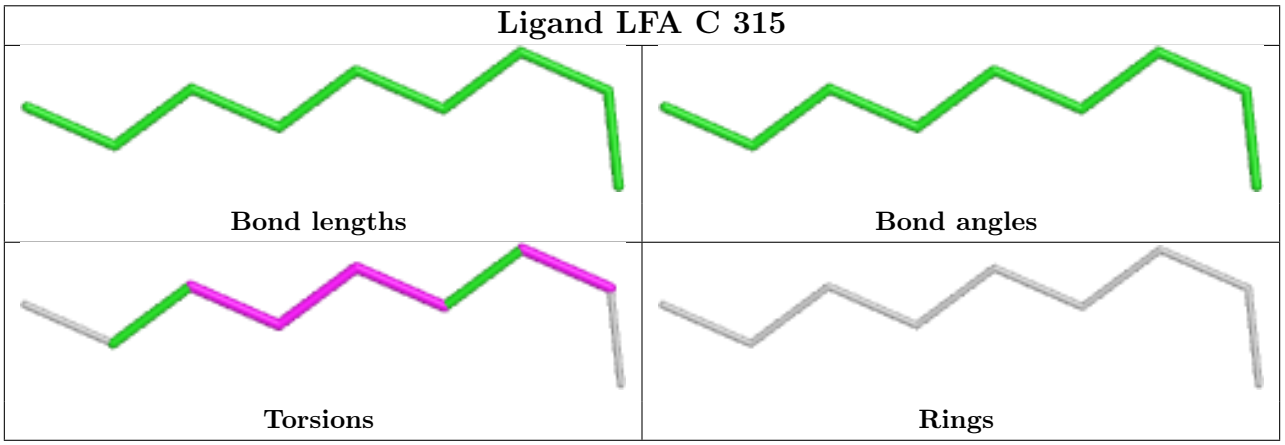
Ligand OLA A 504



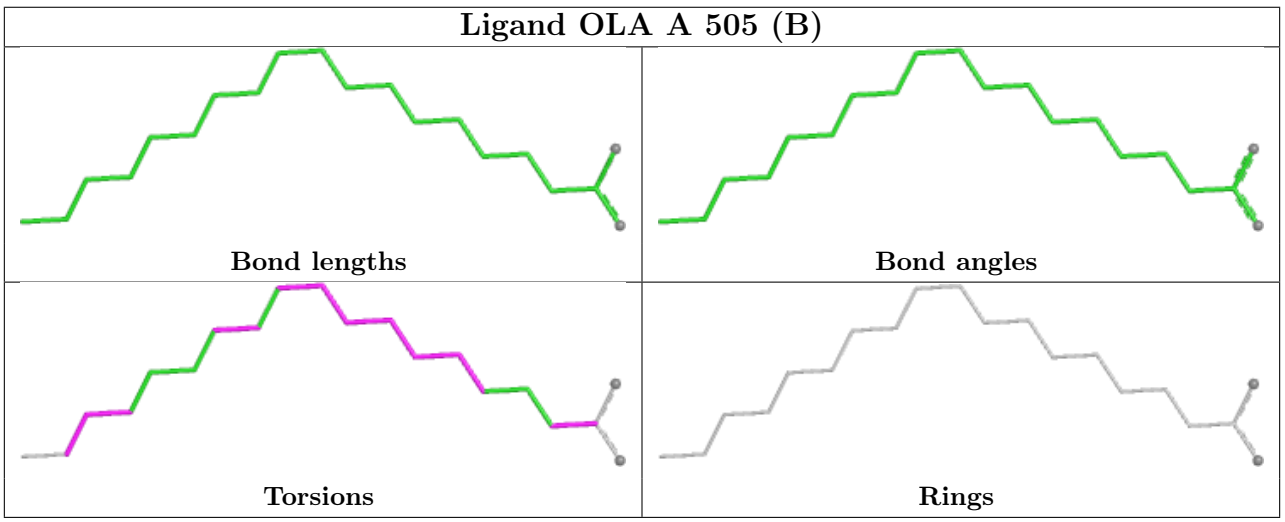
Ligand OLA A 506



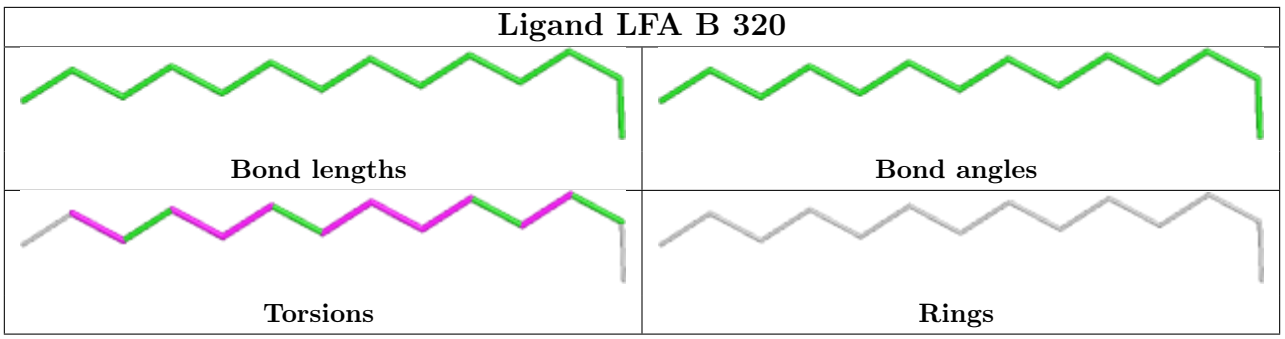
Ligand LFA C 315



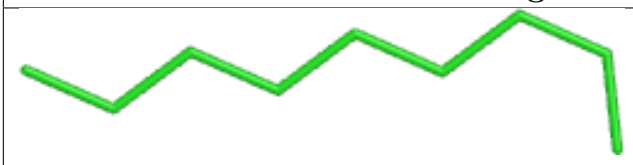
Ligand OLA A 505 (B)



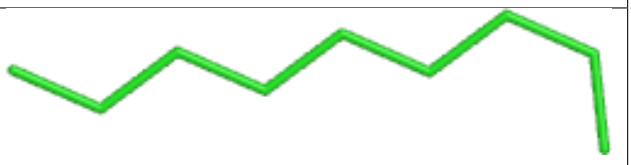
Ligand LFA B 320



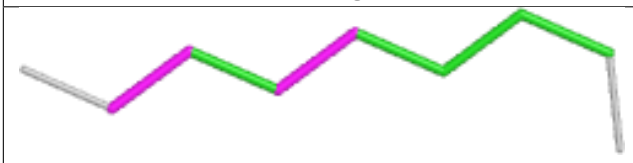
Ligand LFA A 510



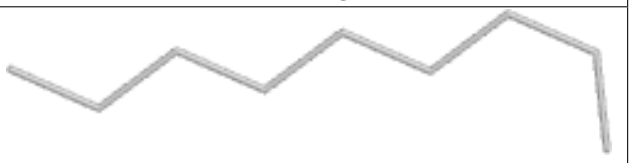
Bond lengths



Bond angles



Torsions

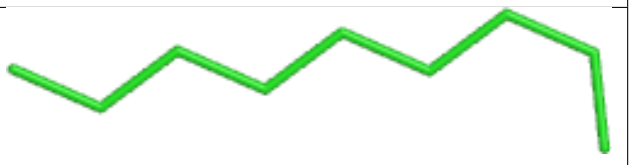


Rings

Ligand LFA C 317



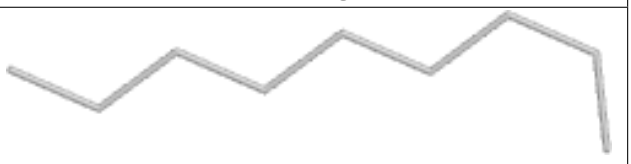
Bond lengths



Bond angles

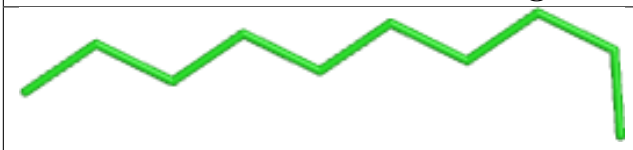


Torsions

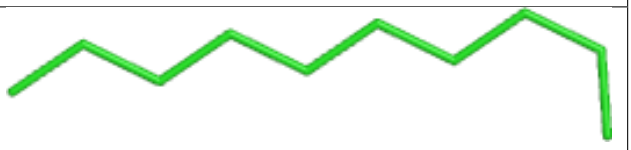


Rings

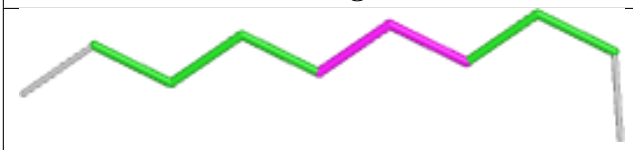
Ligand LFA C 307



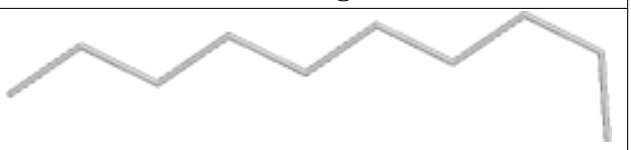
Bond lengths



Bond angles

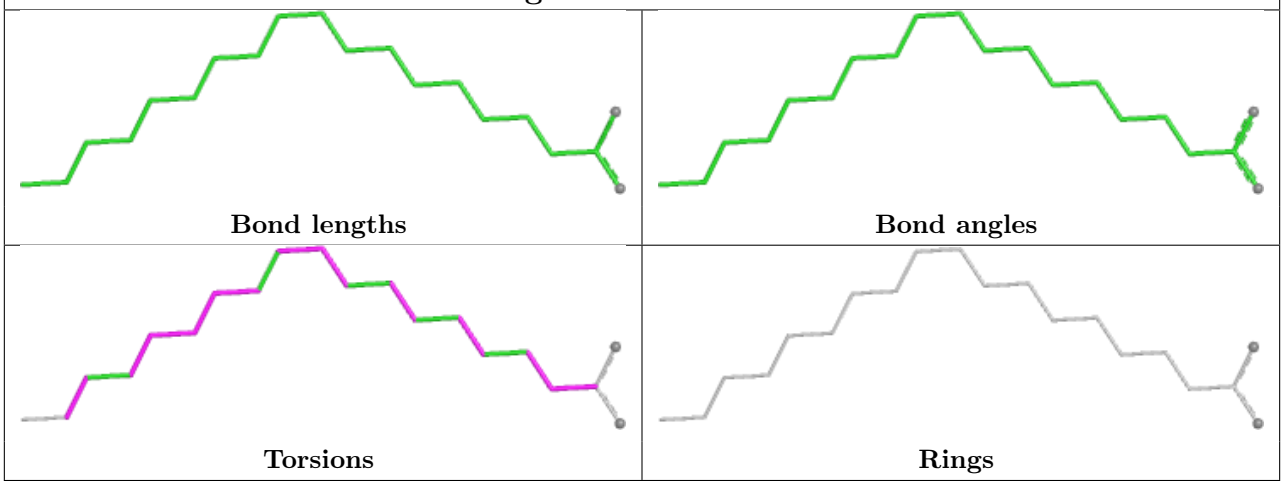


Torsions

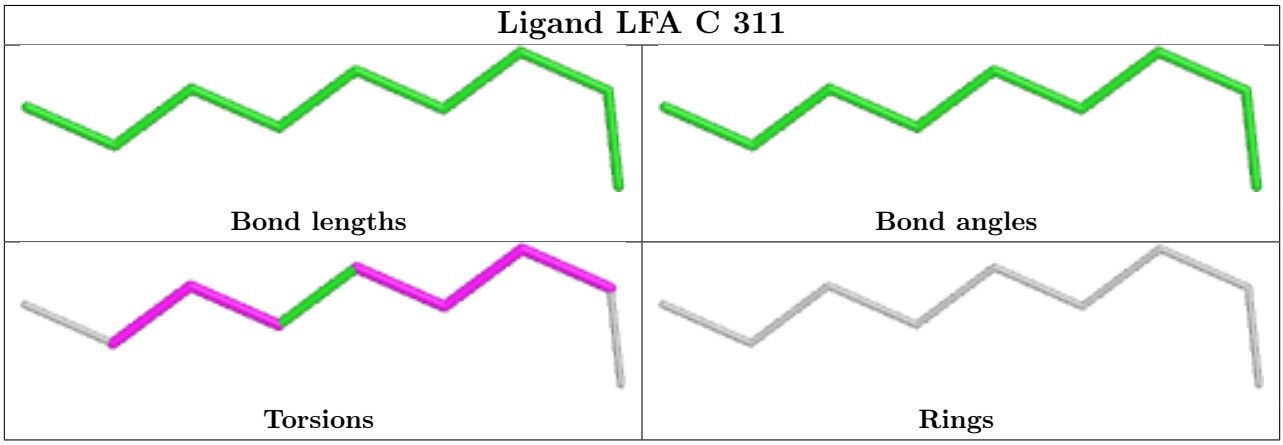


Rings

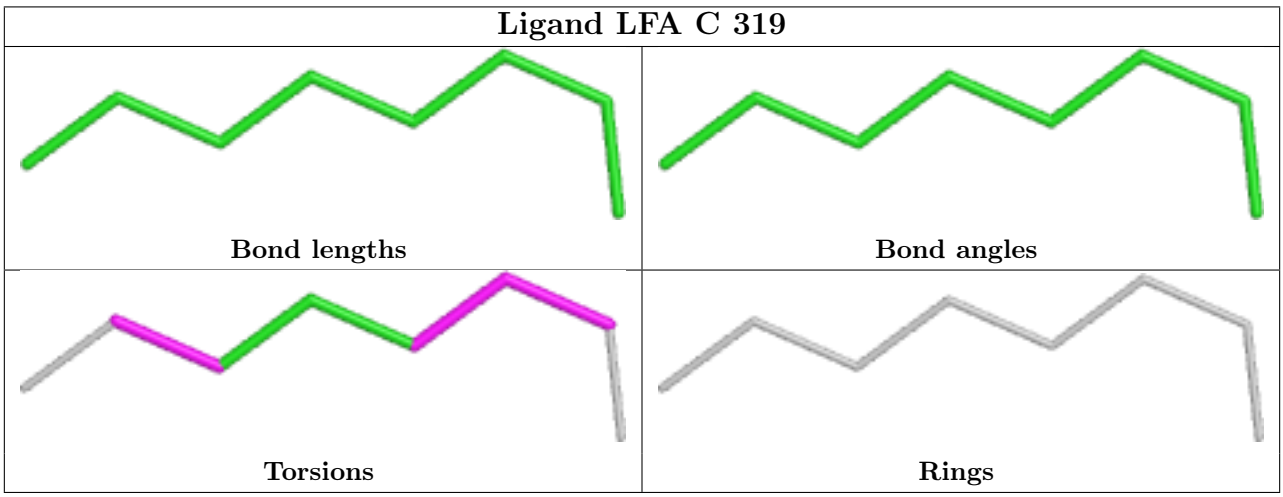
Ligand OLA B 308



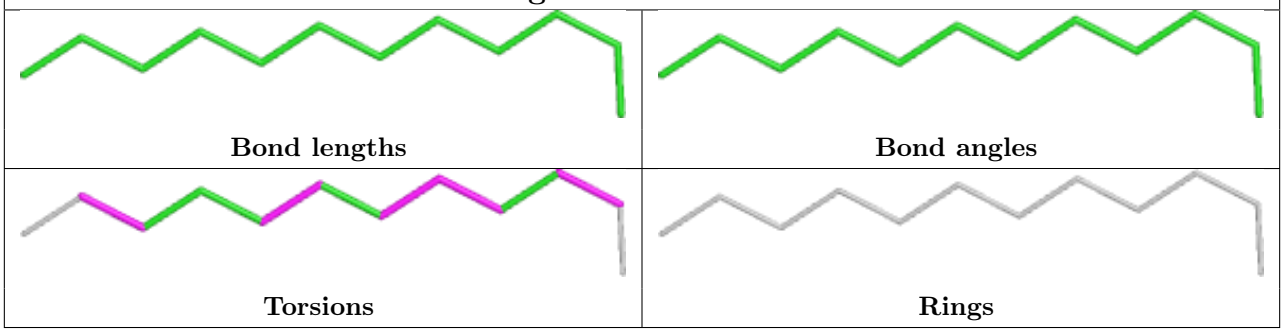
Ligand LFA C 311



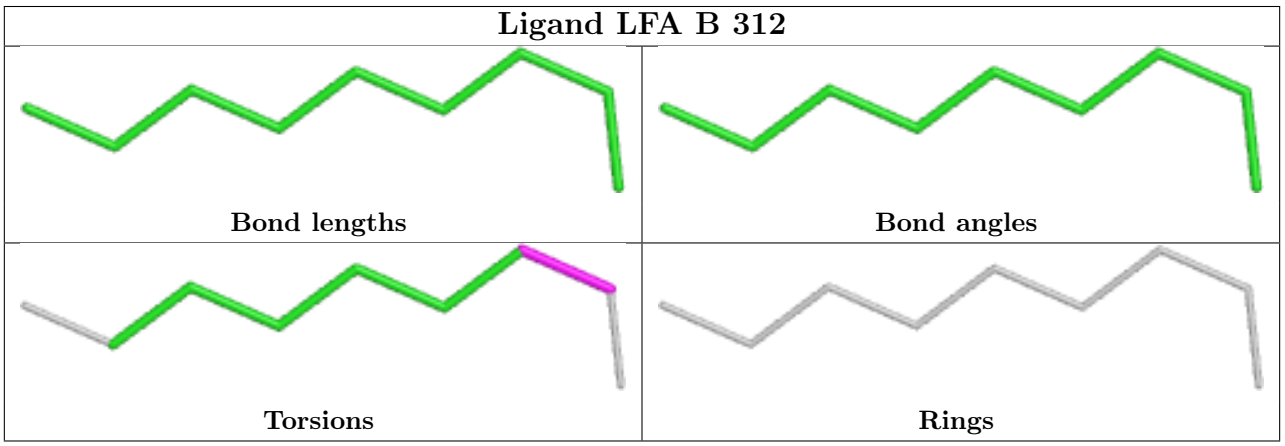
Ligand LFA C 319



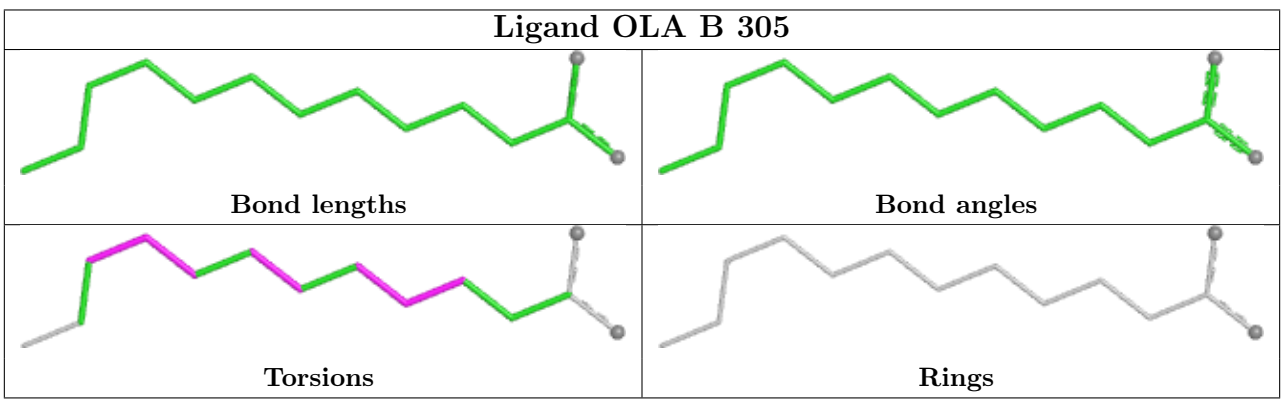
Ligand LFA A 513



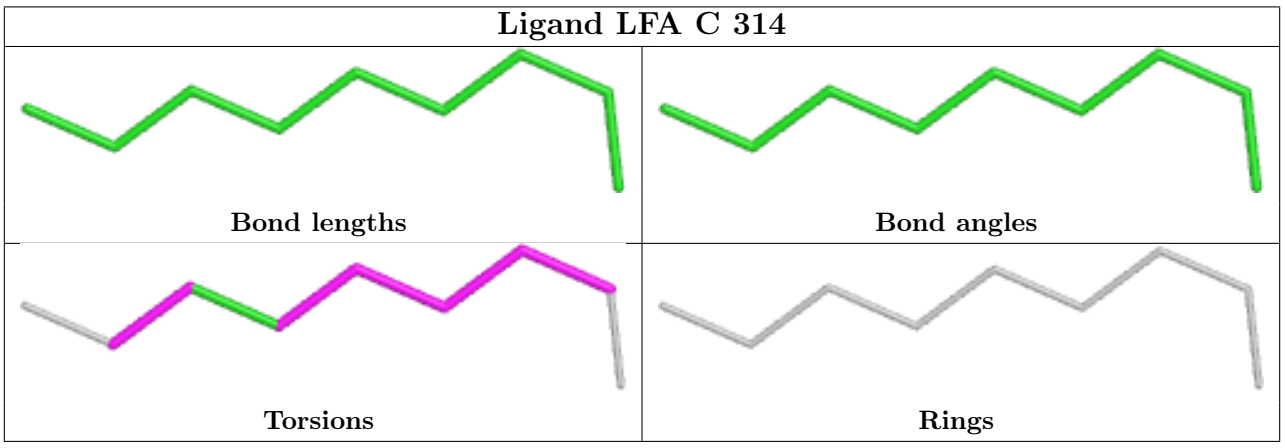
Ligand LFA B 312



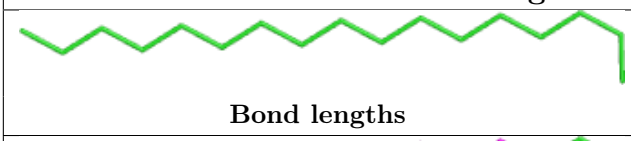
Ligand OLA B 305



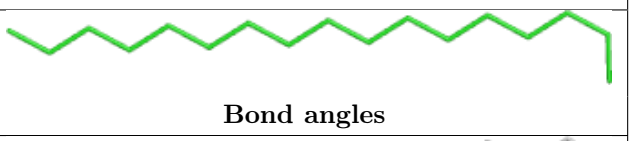
Ligand LFA C 314



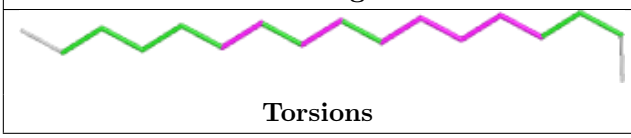
Ligand LFA C 301



Bond lengths



Bond angles

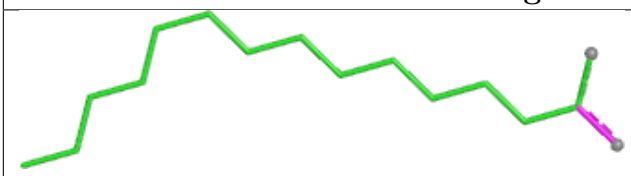


Torsions

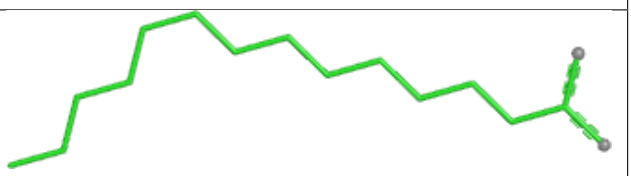


Rings

Ligand OLA C 302



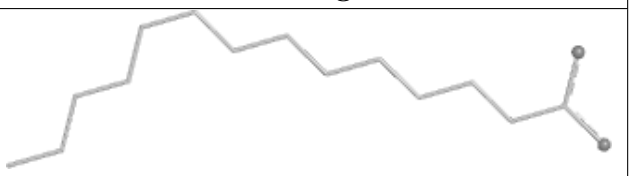
Bond lengths



Bond angles

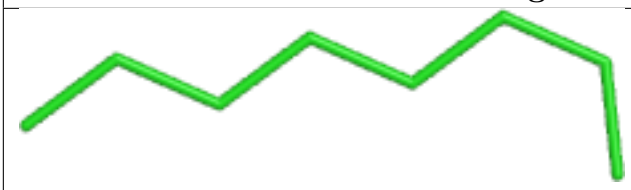


Torsions



Rings

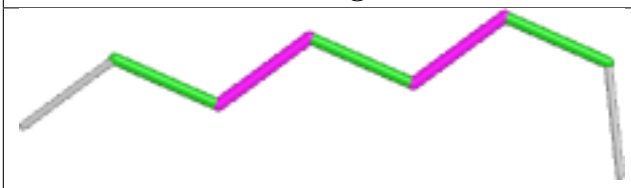
Ligand LFA C 313



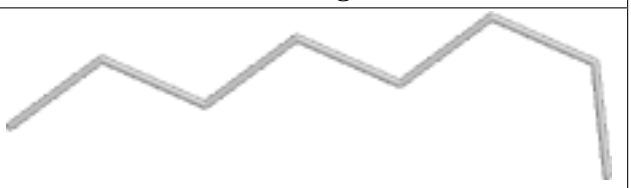
Bond lengths



Bond angles

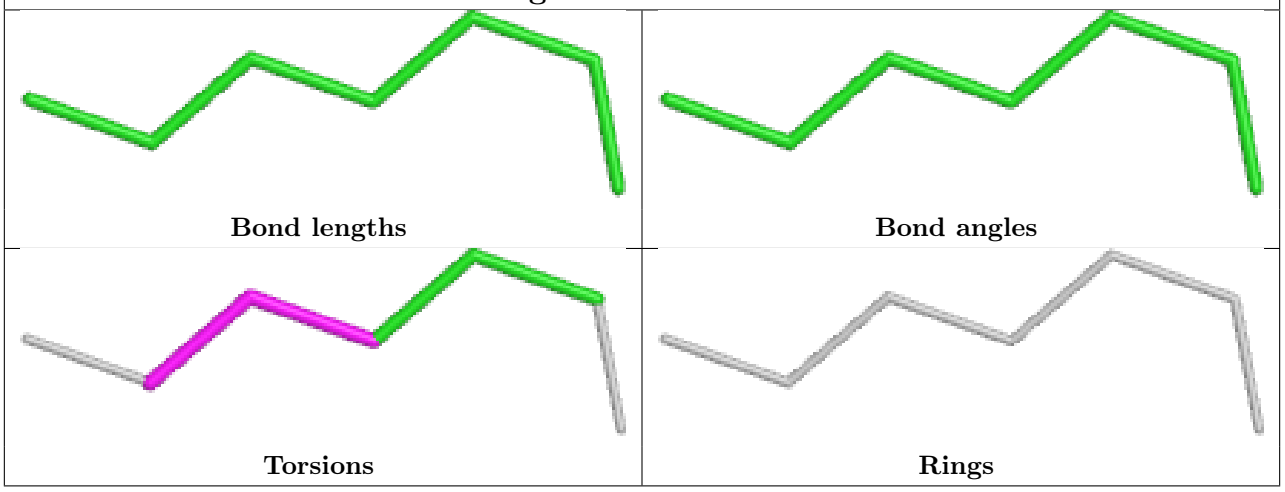


Torsions

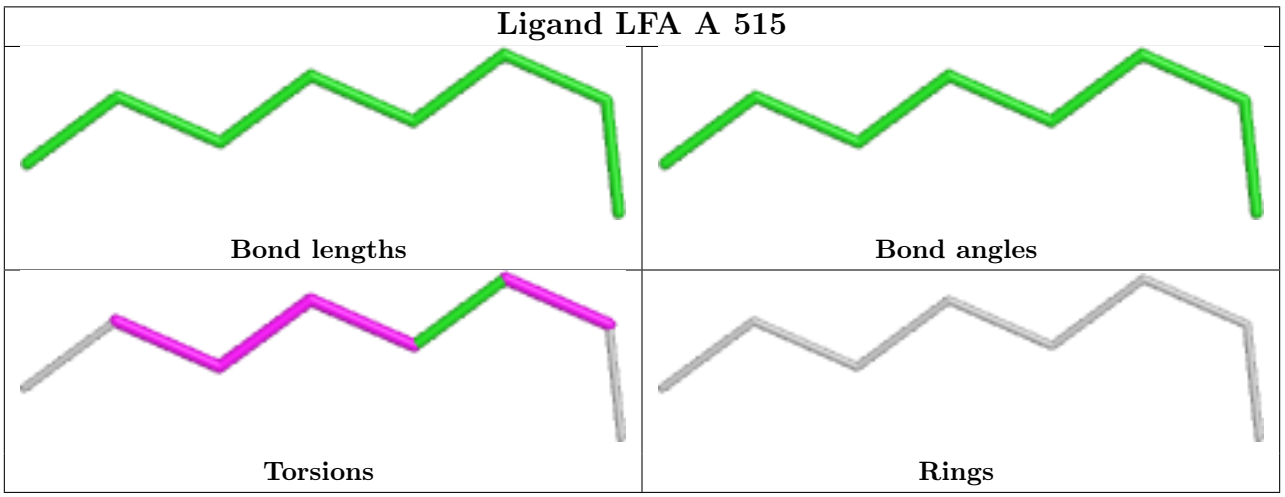


Rings

Ligand LFA B 313



Ligand LFA A 515



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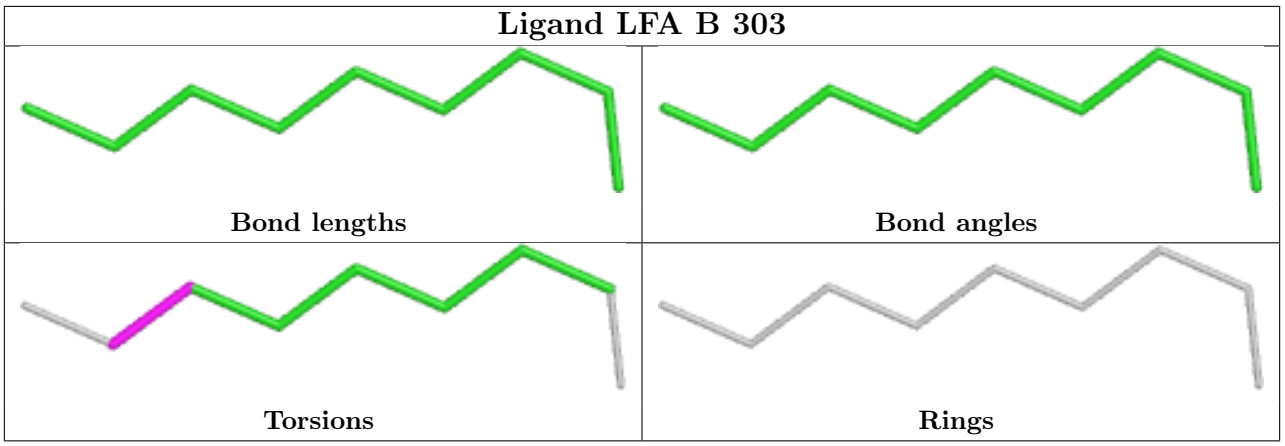
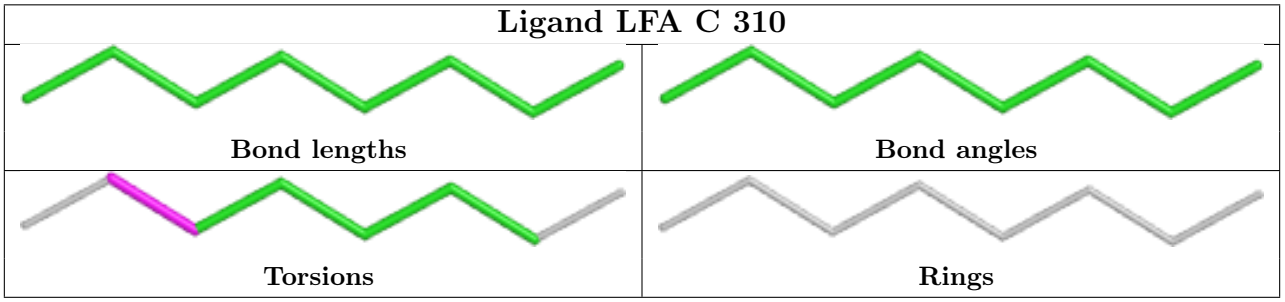


Ligand LFA C 310



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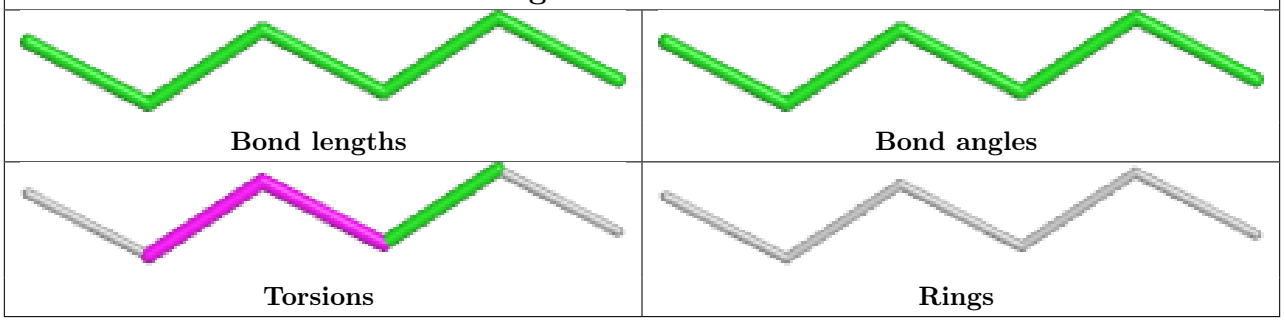
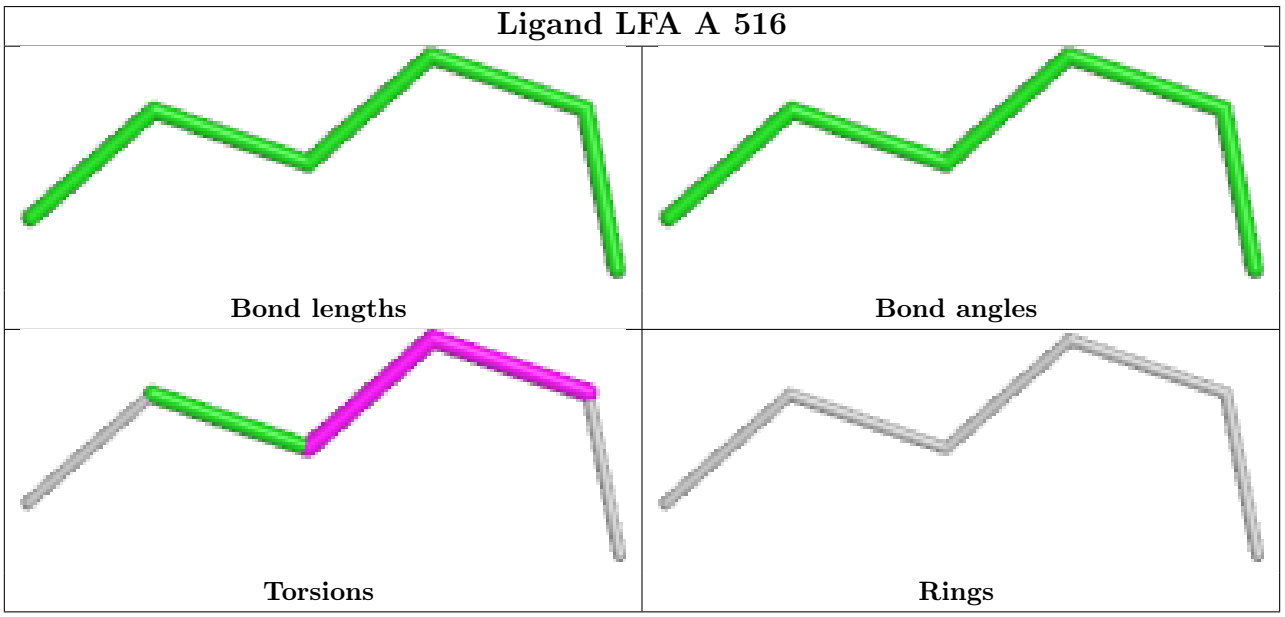


Ligand LFA A 516



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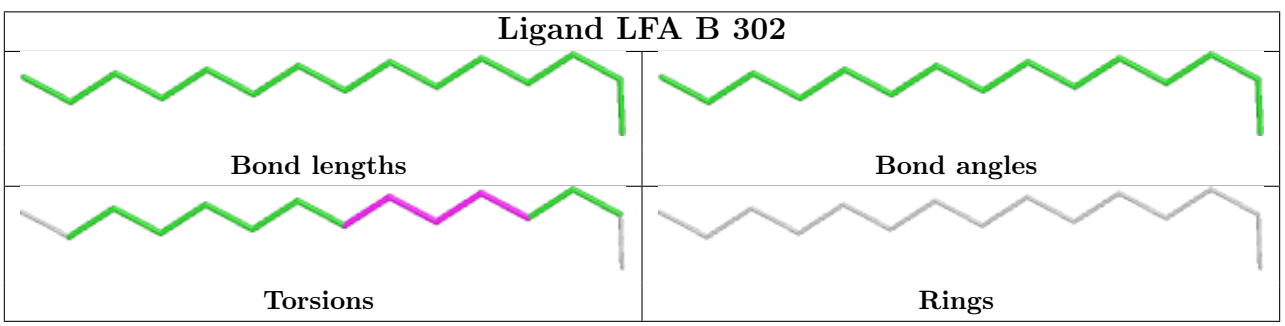
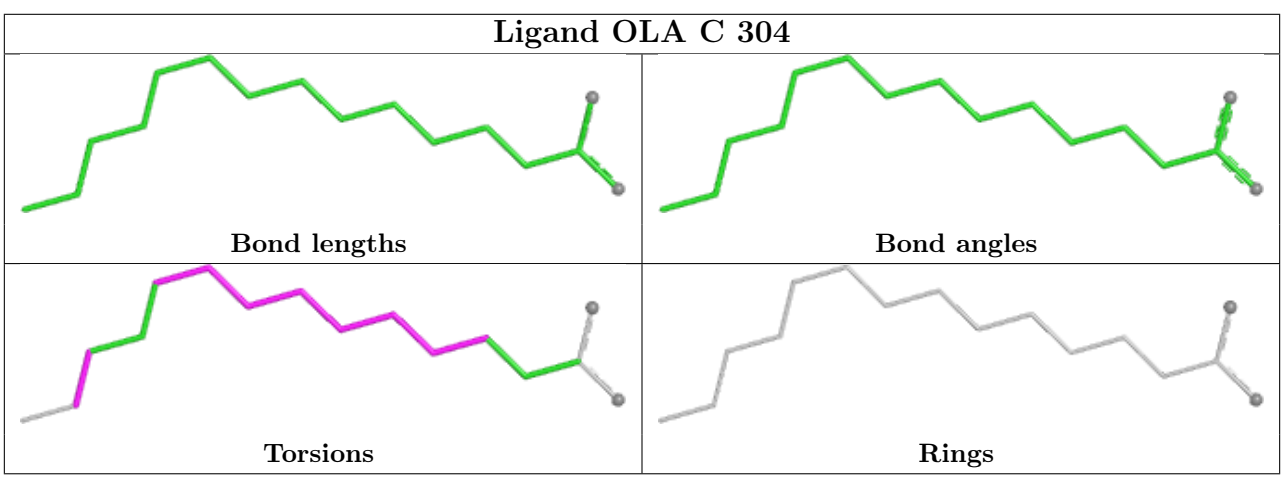
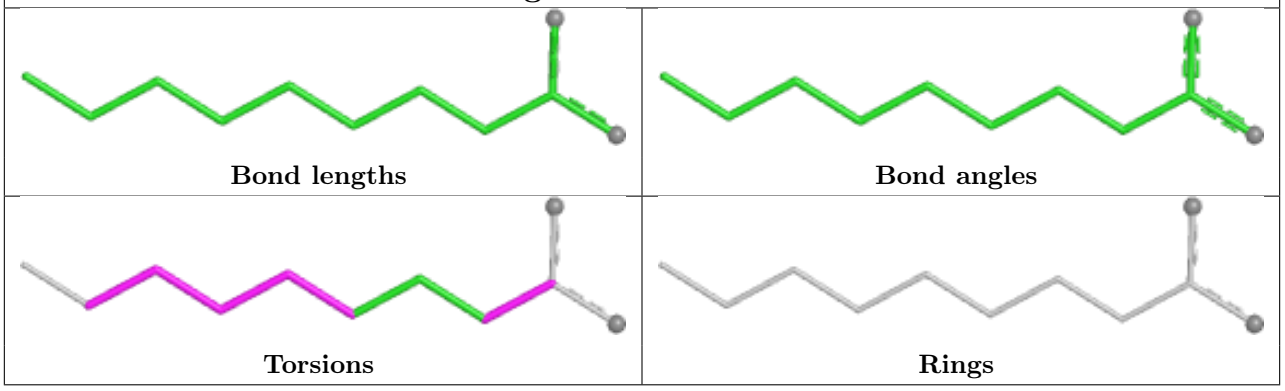


Ligand OLA C 304



Ligand OLA A 507



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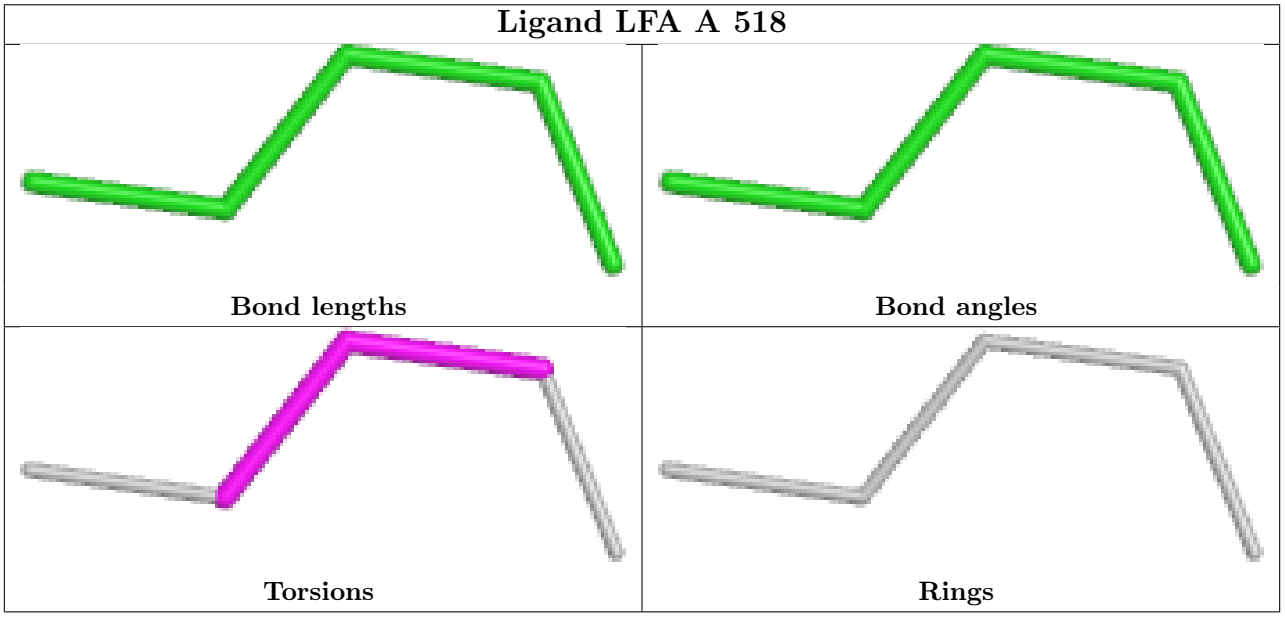

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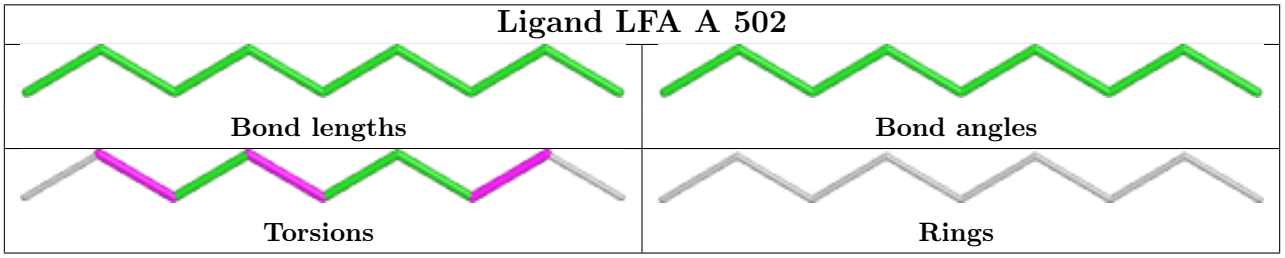

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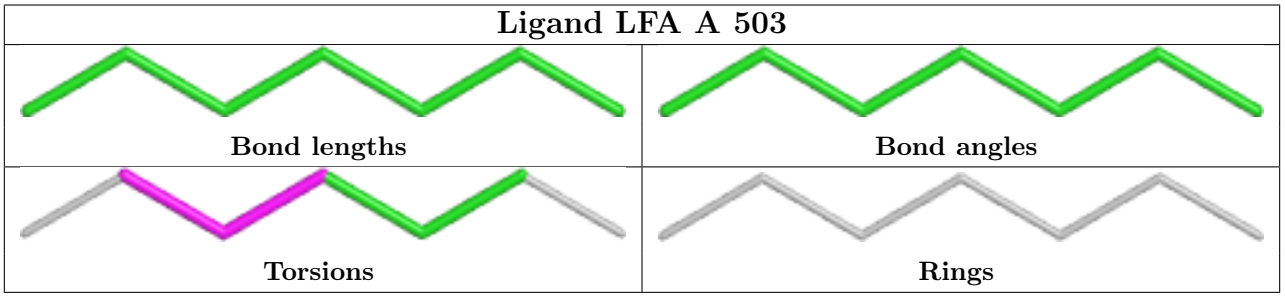
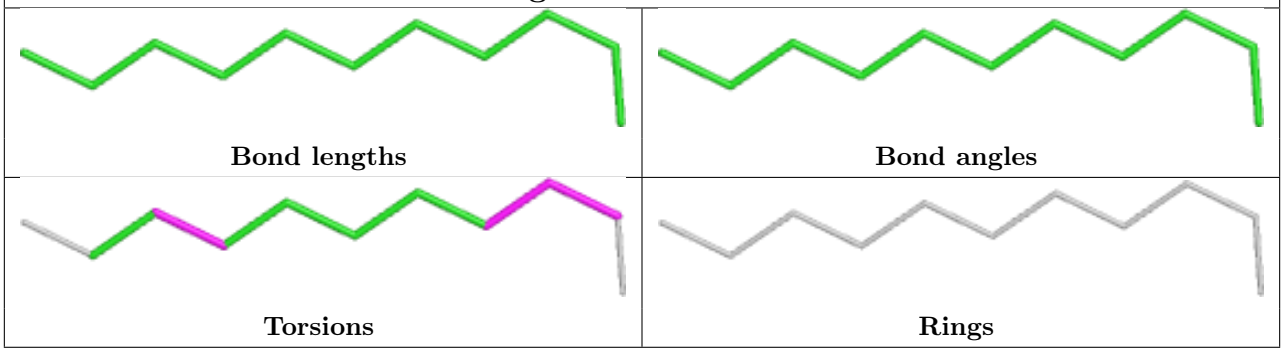


Ligand LFA C 316



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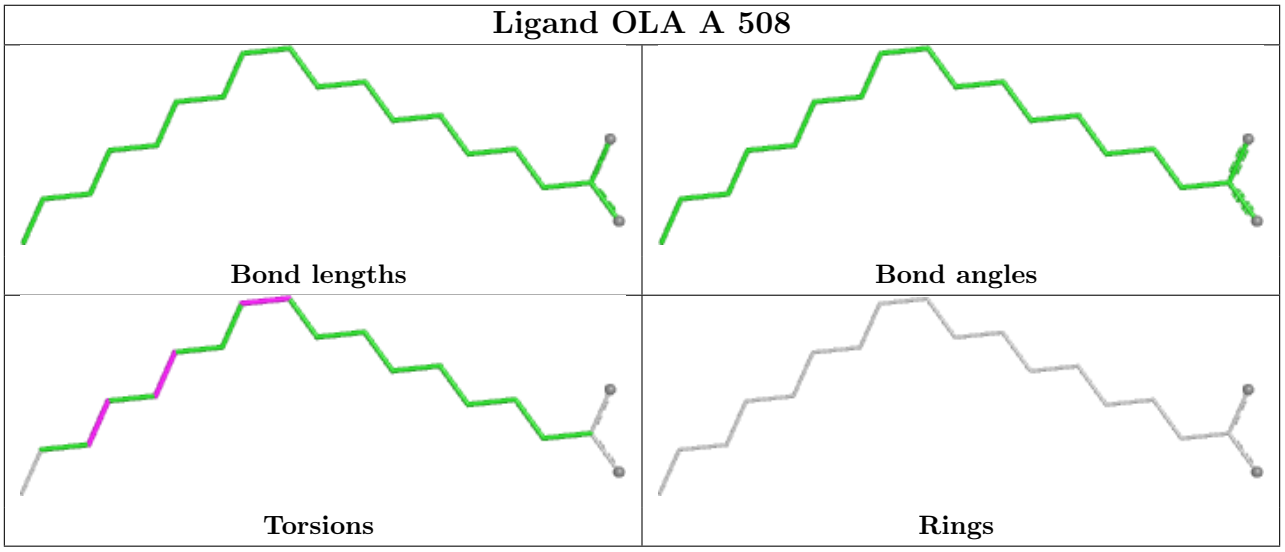
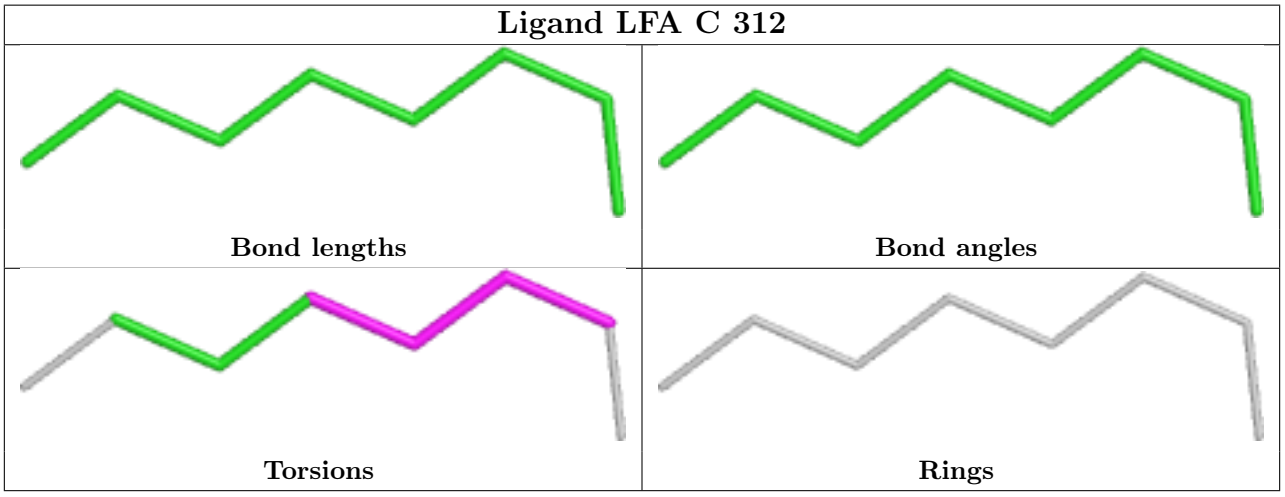
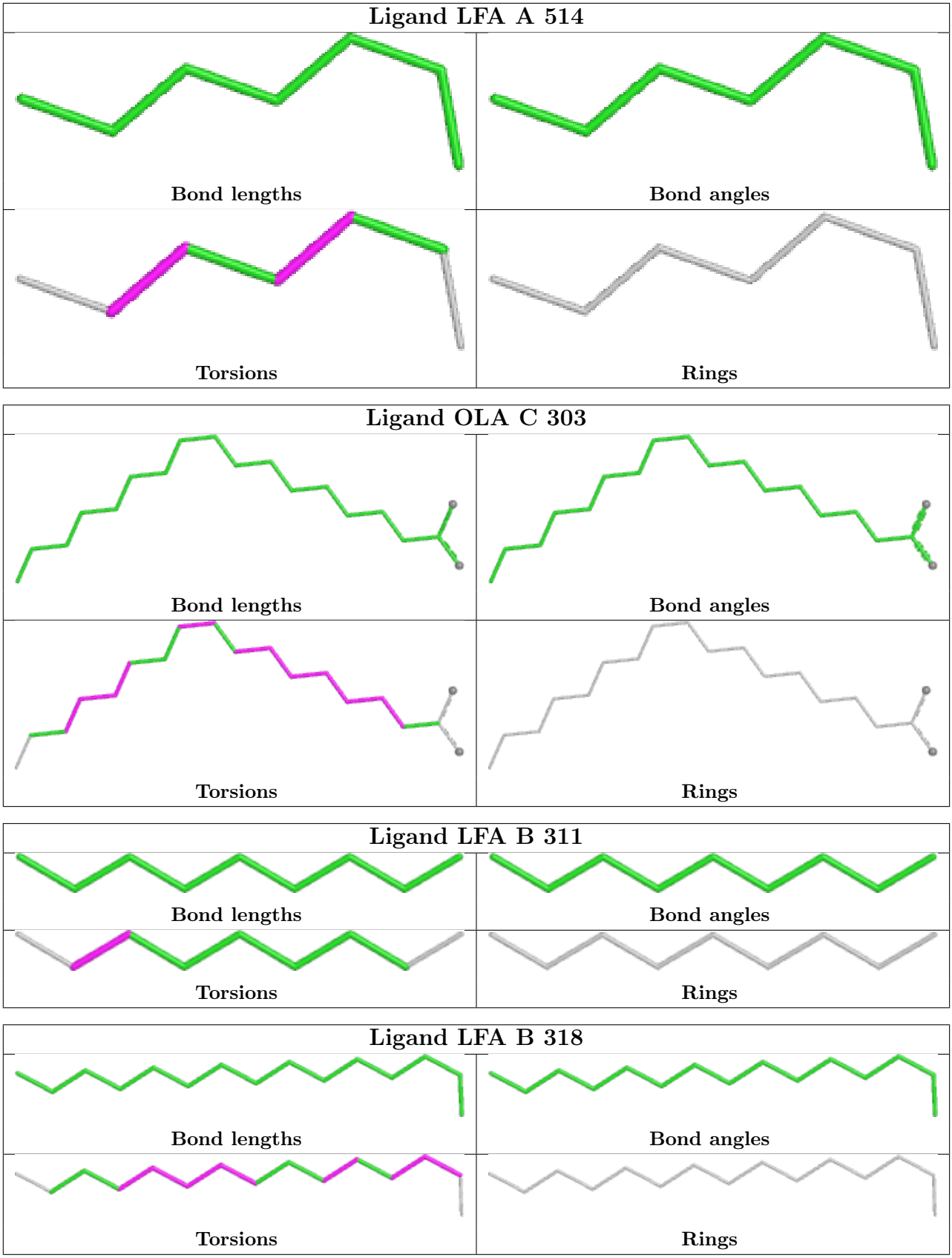
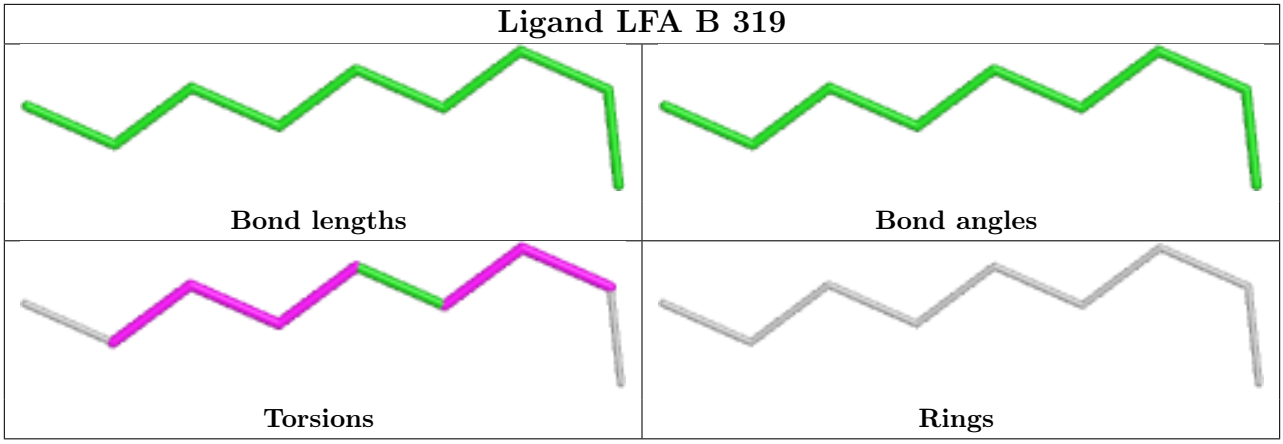


Ligand LFA C 312




Ligand LFA A 514
Bond lengths
Bond angles
Torsions
Rings
Ligand OLA C 303
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA B 311
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA B 318
Bond lengths
Bond angles
Torsions
Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	220/229 (96%)	0.07	7 (3%)	50	53	11, 27, 44, 90	11 (5%)
1	B	217/229 (94%)	0.09	4 (1%)	67	71	11, 28, 45, 74	12 (5%)
1	C	220/229 (96%)	0.31	10 (4%)	38	40	11, 28, 45, 70	13 (5%)
All	All	657/687 (95%)	0.16	21 (3%)	50	53	11, 28, 45, 90	36 (5%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	TYR	4.4
1	C	64	THR	4.0
1	C	224	SER	3.9
1	A	62	ASP	3.9
1	A	59	PHE	3.8
1	C	61	TYR	3.7
1	C	59	PHE	3.6
1	A	63	ASP	3.6
1	C	121	ILE	3.3
1	B	59	PHE	3.3
1	A	121	ILE	2.9
1	B	64	THR	2.6
1	A	173[A]	TRP	2.5
1	C	152	LEU	2.4
1	C	189	LEU	2.4
1	A	60	GLN	2.4
1	B	121	ILE	2.4
1	C	173[A]	TRP	2.3
1	C	60	GLN	2.3
1	B	4	ILE	2.1
1	C	164	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	FME	B	1	7/11	0.85	0.10	36,41,51,51	0
1	FME	A	1	8/11	0.88	0.10	36,43,46,49	0
1	FME	C	1	8/11	0.88	0.10	36,41,48,49	0
1	LYR	B	207[A]	29/30	0.88	0.10	24,27,31,33	29
1	LYR	B	207[C]	29/30	0.88	0.10	24,27,30,32	29
1	LYR	C	207[A]	29/30	0.89	0.09	23,27,30,31	29
1	LYR	C	207[C]	29/30	0.89	0.09	23,27,30,30	29
1	LYR	A	207[A]	29/30	0.90	0.09	24,27,30,32	29
1	LYR	A	207[C]	29/30	0.90	0.09	24,27,30,32	29

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	PO4	C	320	5/5	0.65	0.14	63,65,72,73	5
5	PO4	A	521	5/5	0.67	0.13	63,64,71,72	5
3	OLA	A	507	11/20	0.72	0.18	36,46,56,57	0
3	OLA	A	505[A]	20/20	0.72	0.12	33,41,45,46	20
3	OLA	A	505[B]	20/20	0.72	0.12	35,41,45,47	20
2	LFA	B	310	6/20	0.73	0.13	42,44,48,48	0
2	LFA	C	315	9/20	0.75	0.15	40,43,49,49	0
3	OLA	B	307	12/20	0.76	0.17	40,49,57,68	0
2	LFA	C	308	16/20	0.76	0.16	43,53,64,66	0
2	LFA	C	313	8/20	0.76	0.15	37,45,58,60	0
2	LFA	A	520	10/20	0.77	0.12	34,52,56,57	0
2	LFA	B	316	6/20	0.78	0.12	51,59,59,62	0
2	LFA	C	319	8/20	0.78	0.12	42,51,56,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LFA	A	510	9/20	0.79	0.15	52,58,62,64	0
2	LFA	C	310	8/20	0.79	0.17	49,55,56,58	0
3	OLA	C	305	13/20	0.79	0.13	36,48,61,63	0
2	LFA	C	311	9/20	0.79	0.15	40,44,51,53	0
2	LFA	B	317	4/20	0.79	0.17	32,37,37,42	0
2	LFA	A	515	8/20	0.80	0.13	46,52,56,59	0
2	LFA	C	314	9/20	0.80	0.13	43,48,52,52	0
3	OLA	C	304	16/20	0.80	0.15	41,51,62,73	0
2	LFA	C	316	11/20	0.81	0.11	42,48,52,54	0
2	LFA	A	517	3/20	0.81	0.21	44,44,45,55	0
2	LFA	B	319	9/20	0.81	0.13	35,46,50,54	0
3	OLA	C	303	19/20	0.81	0.16	32,46,58,71	0
2	LFA	C	307	10/20	0.82	0.15	42,48,53,54	0
2	LFA	A	519	10/20	0.82	0.13	39,42,46,49	0
2	LFA	B	320	14/20	0.82	0.12	41,47,51,53	0
2	LFA	B	321	10/20	0.82	0.12	41,49,54,56	0
2	LFA	C	317	9/20	0.82	0.13	46,49,56,56	0
3	OLA	A	504	11/20	0.83	0.12	33,43,51,51	0
2	LFA	B	312	9/20	0.83	0.12	34,43,49,51	0
3	OLA	C	302	16/20	0.83	0.11	33,41,54,58	0
2	LFA	B	301	7/20	0.83	0.16	36,39,46,55	0
2	LFA	C	301	17/20	0.84	0.11	27,40,46,47	0
3	OLA	A	508	19/20	0.84	0.14	37,46,61,73	0
3	OLA	B	305	14/20	0.84	0.12	38,47,60,66	0
2	LFA	B	315	5/20	0.84	0.11	42,44,47,48	0
2	LFA	A	518	5/20	0.84	0.12	35,36,41,52	0
2	LFA	C	318	5/20	0.84	0.09	33,47,51,52	0
2	LFA	A	516	6/20	0.84	0.11	40,46,50,51	0
2	LFA	B	311	9/20	0.84	0.12	43,44,54,55	0
2	LFA	A	511	9/20	0.84	0.12	36,40,44,51	0
2	LFA	B	314	5/20	0.84	0.14	34,36,38,45	0
2	LFA	A	512	7/20	0.85	0.11	40,42,47,50	0
2	LFA	A	513	12/20	0.86	0.12	33,46,53,57	0
2	LFA	C	309	4/20	0.86	0.12	39,40,40,41	0
3	OLA	A	506	16/20	0.86	0.12	39,49,82,86	0
3	OLA	B	308	20/20	0.86	0.10	38,46,60,62	0
2	LFA	B	302	15/20	0.86	0.11	35,38,44,48	0
2	LFA	A	501	6/20	0.87	0.10	35,38,43,47	0
2	LFA	A	514	7/20	0.87	0.11	39,46,50,56	0
2	LFA	B	304	7/20	0.87	0.13	36,38,44,50	0
3	OLA	B	306	16/20	0.87	0.14	37,44,64,65	0
2	LFA	A	503	7/20	0.88	0.09	36,39,42,46	0

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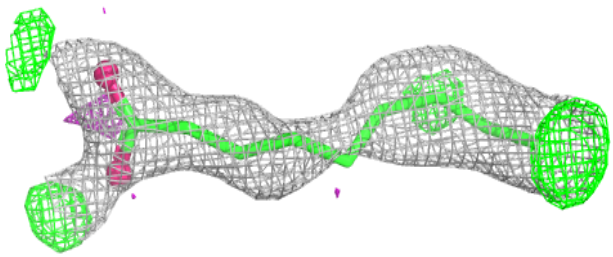
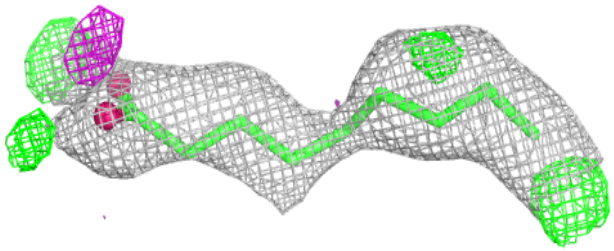
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LFA	C	312	8/20	0.89	0.10	36,41,44,45	0
2	LFA	B	303	9/20	0.89	0.11	37,44,52,54	0
2	LFA	A	502	9/20	0.90	0.09	29,32,42,43	0
2	LFA	B	313	7/20	0.90	0.10	45,46,54,58	0
2	LFA	B	318	15/20	0.90	0.12	31,41,57,57	0
4	NA	C	306	1/1	0.99	0.04	24,24,24,24	0
4	NA	A	509	1/1	0.99	0.02	24,24,24,24	0
4	NA	B	309	1/1	0.99	0.09	25,25,25,25	0

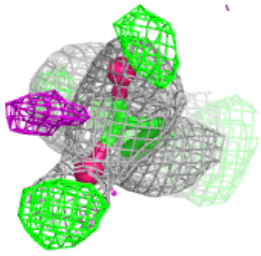
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 507:

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

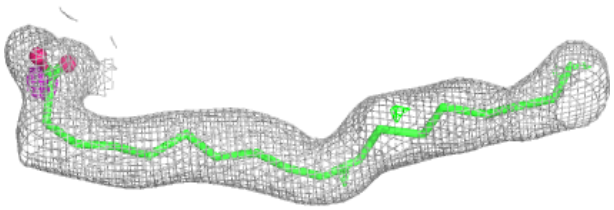


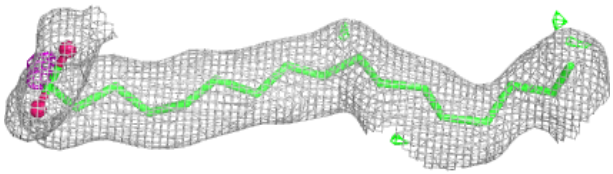


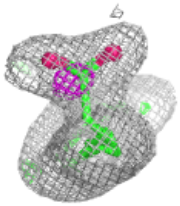


Electron density around OLA A 505 (A):

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

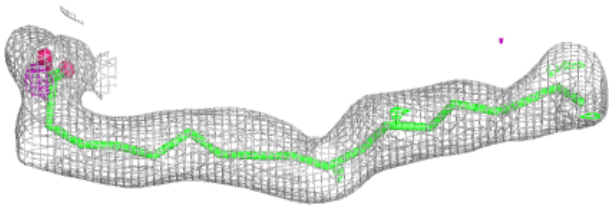


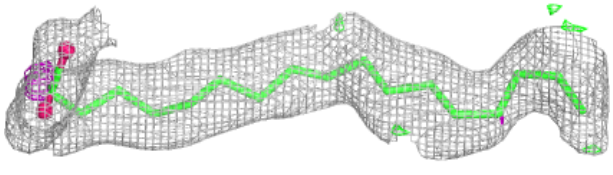


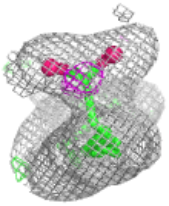


Electron density around OLA A 505 (B):

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

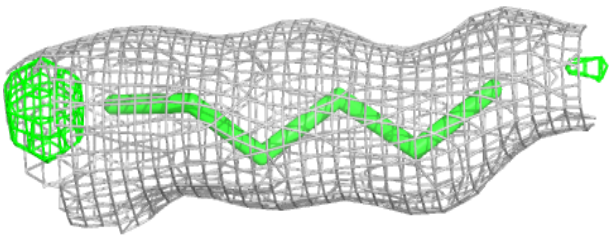


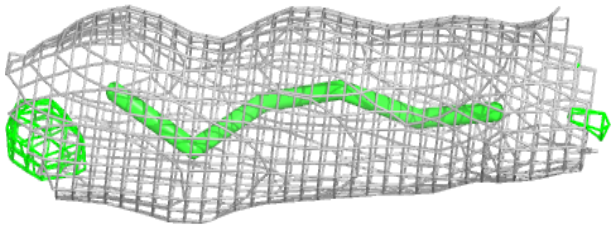


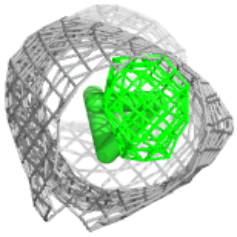


Electron density around LFA B 310:

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

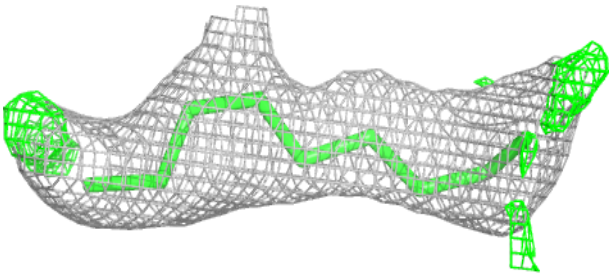


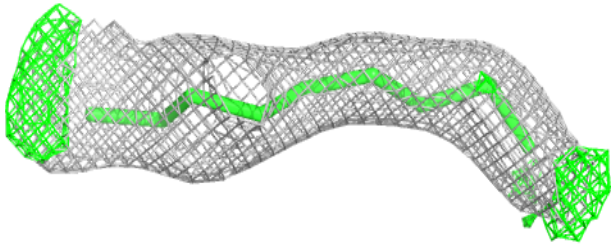


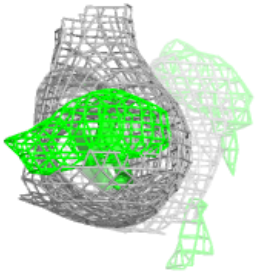


Electron density around LFA C 315:

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

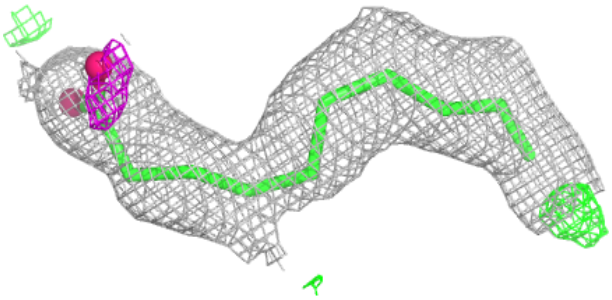


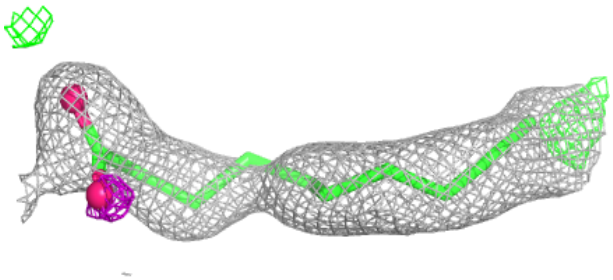


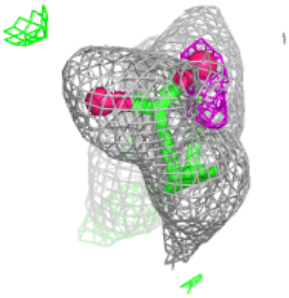


Electron density around OLA B 307:

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

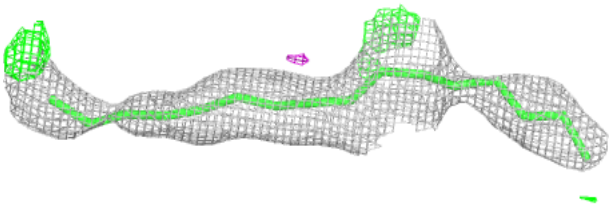


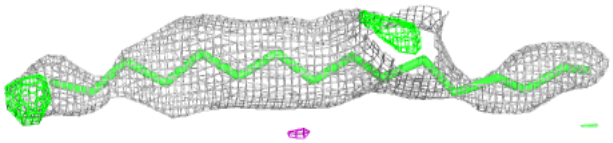


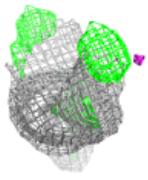


Electron density around LFA C 308:

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

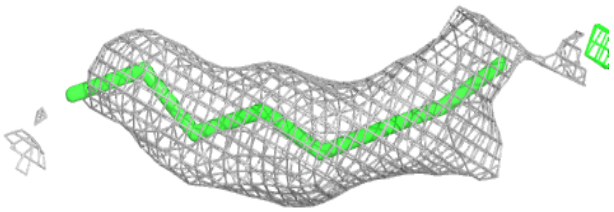


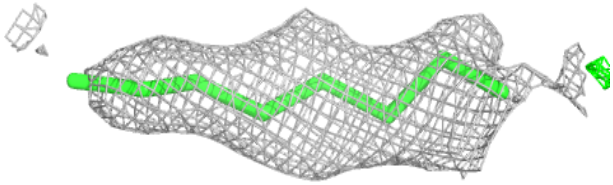


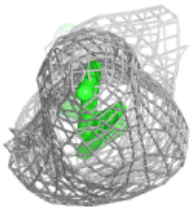


Electron density around LFA C 313:

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

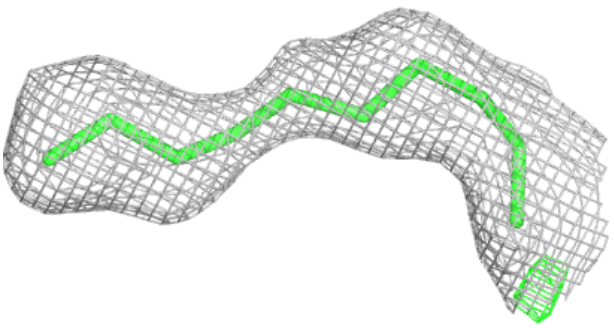


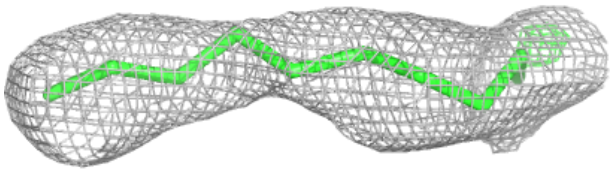


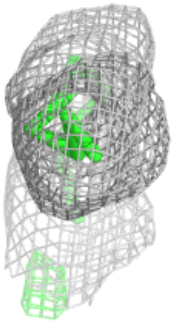


Electron density around LFA A 520:

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

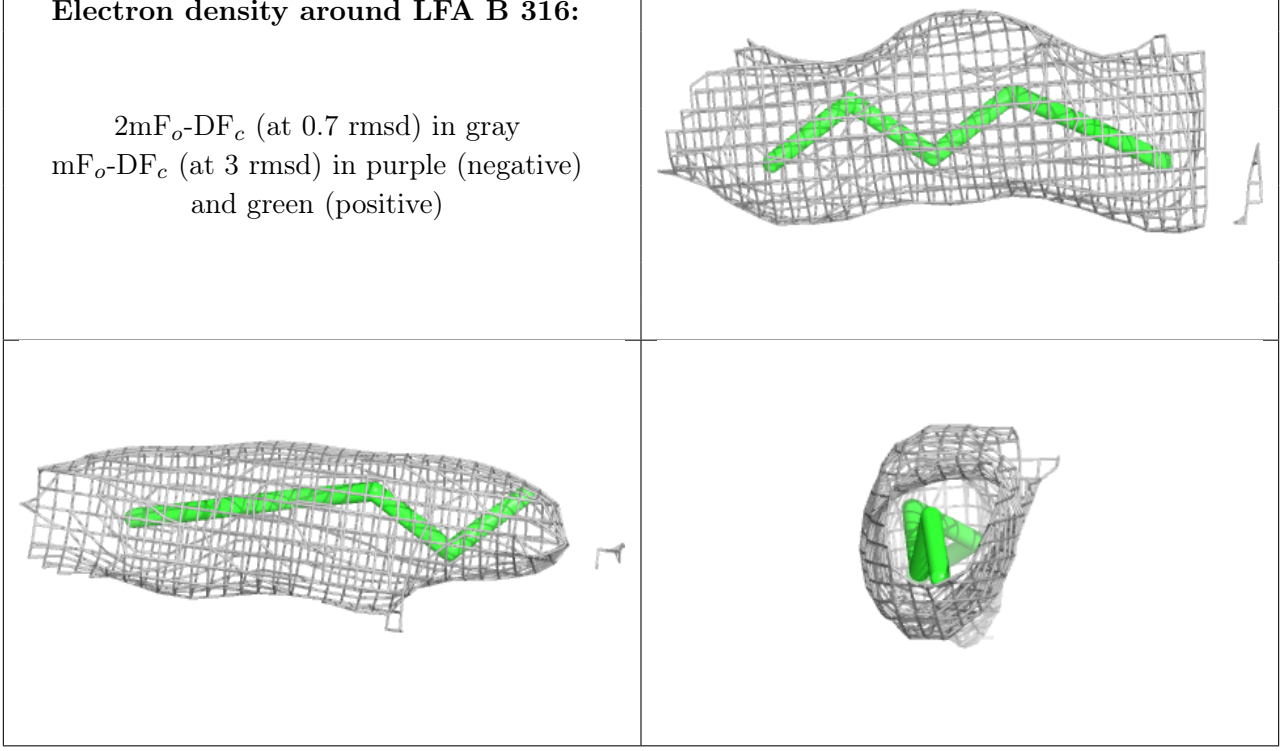






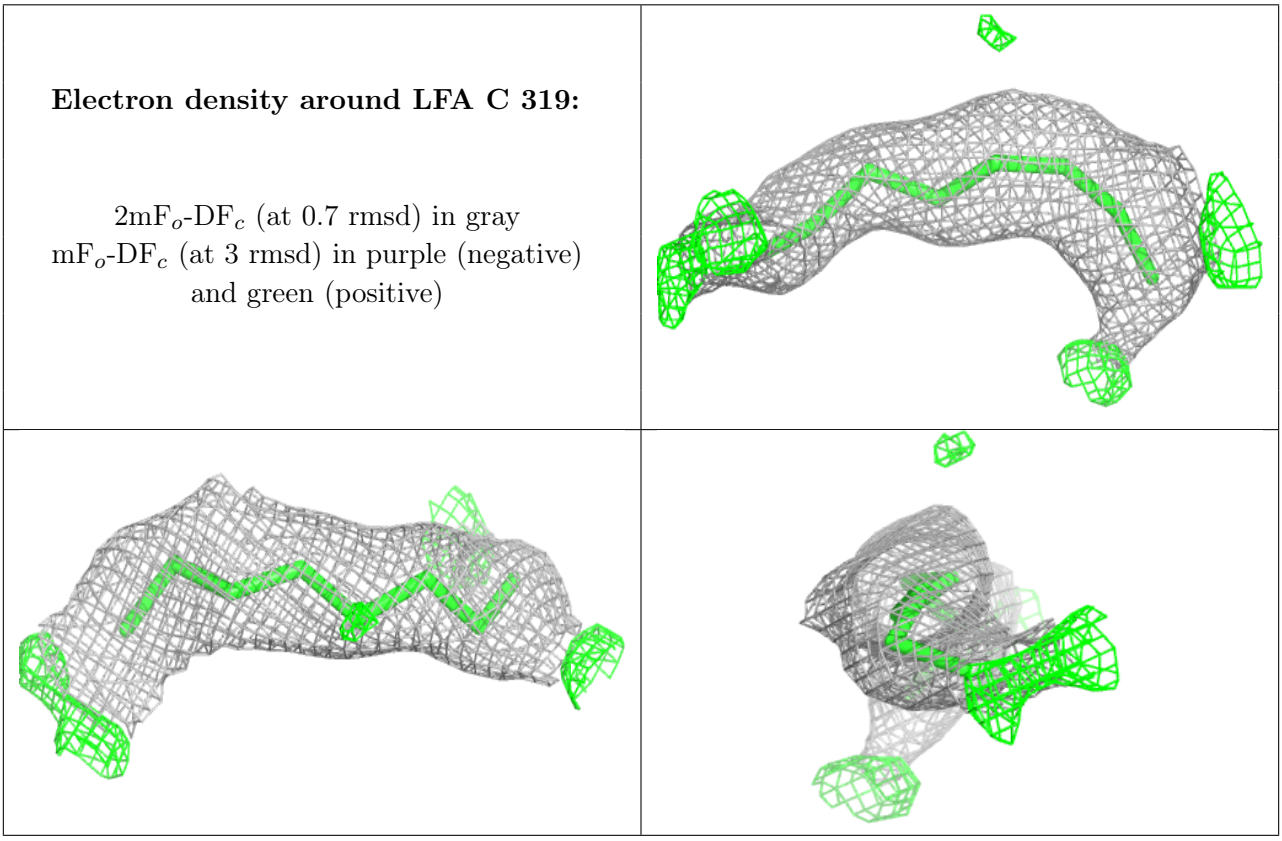
Electron density around LFA B 316:

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



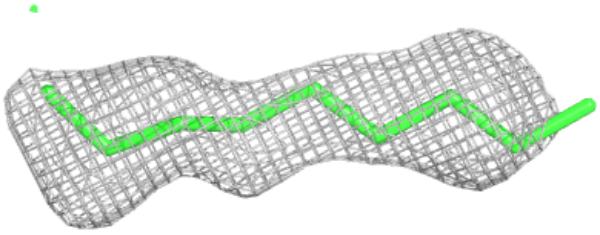
Electron density around LFA C 319:

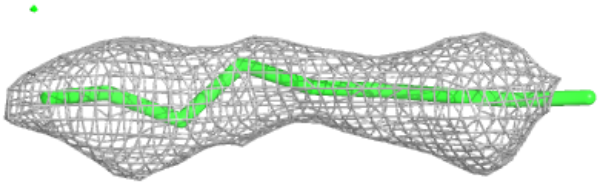
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

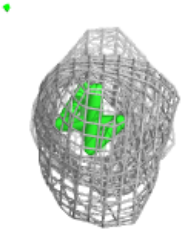


Electron density around LFA A 510:

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

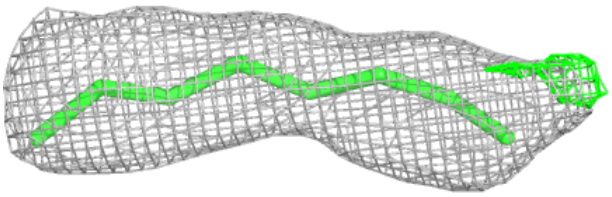


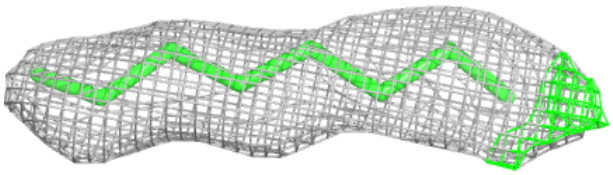


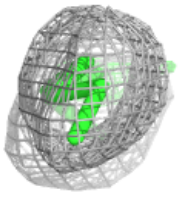


Electron density around LFA C 310:

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

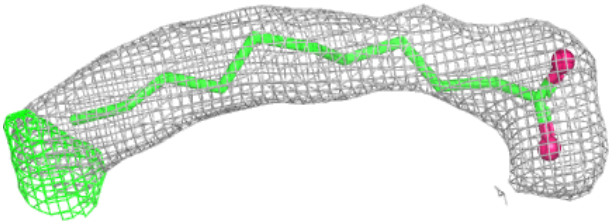


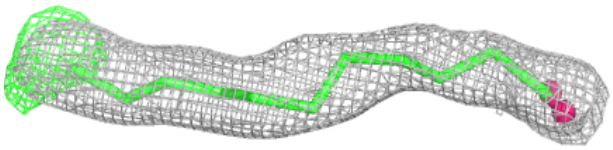


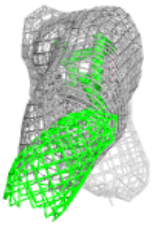


Electron density around OLA C 305:

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

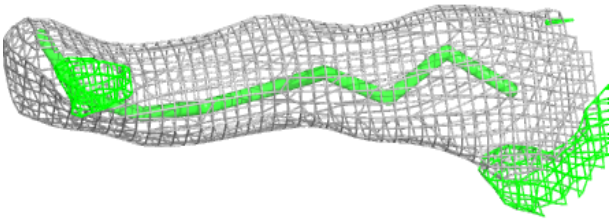


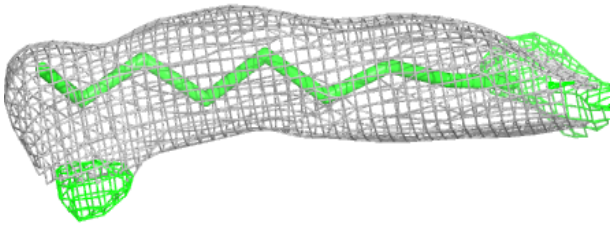


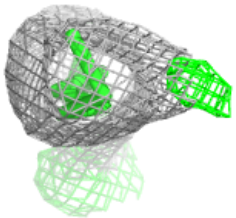


Electron density around LFA C 311:

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

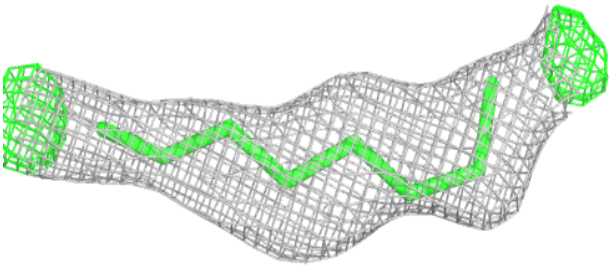


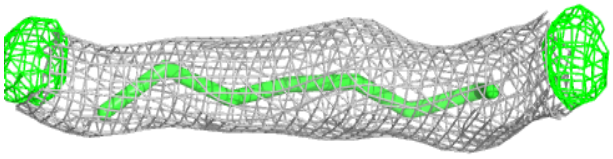


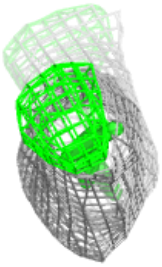


Electron density around LFA A 515:

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

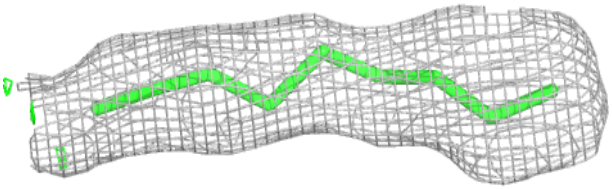


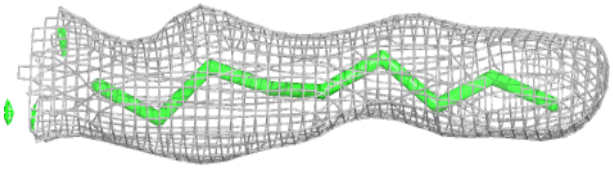


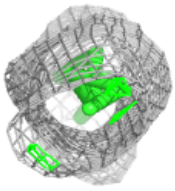


Electron density around LFA C 314:

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

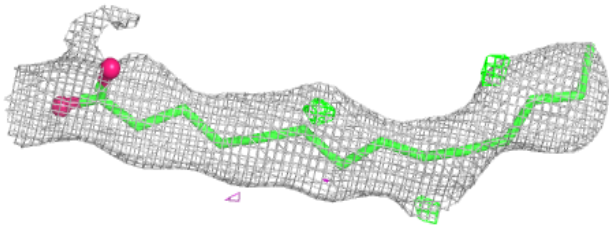


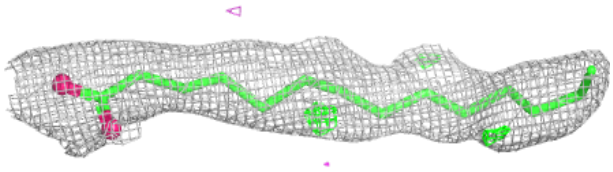


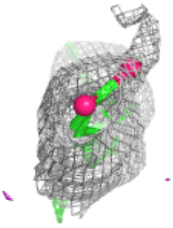


Electron density around OLA C 304:

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

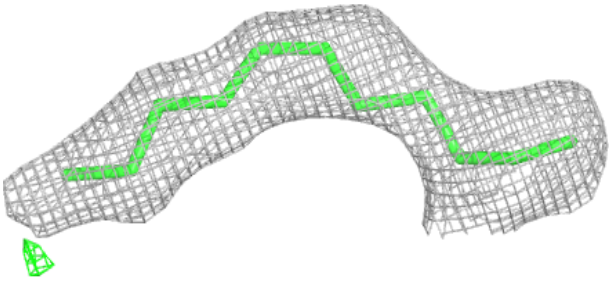


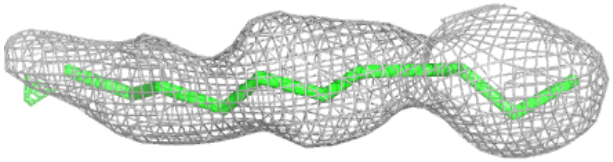


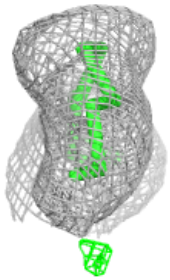


Electron density around LFA C 316:

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

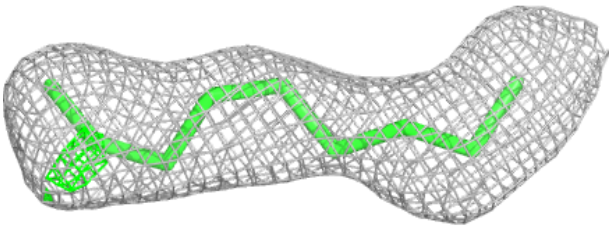


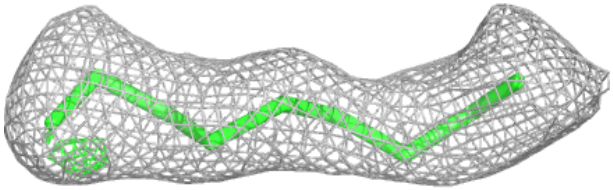


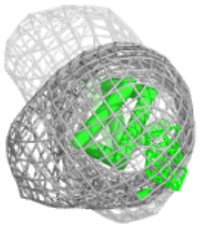


Electron density around LFA B 319:

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

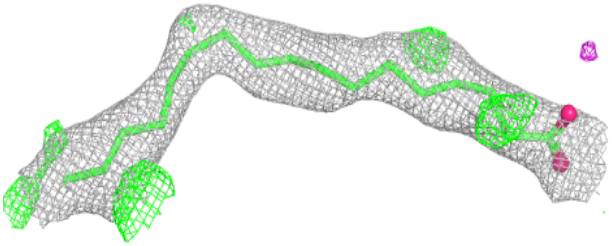


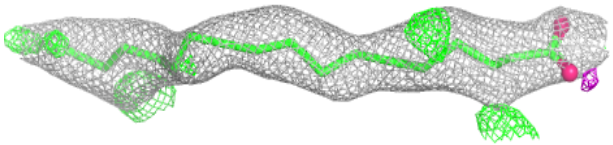


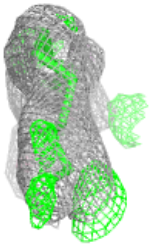


Electron density around OLA C 303:

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

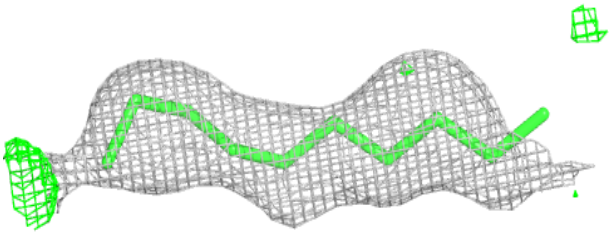


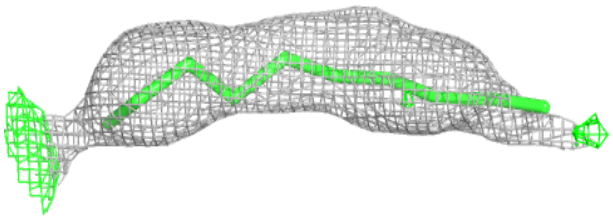


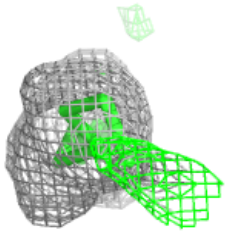


Electron density around LFA C 307:

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

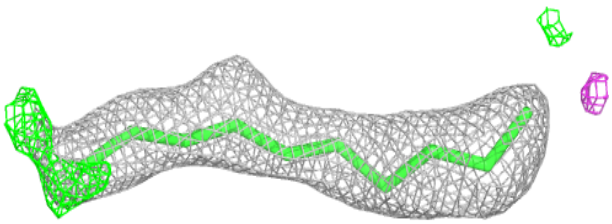


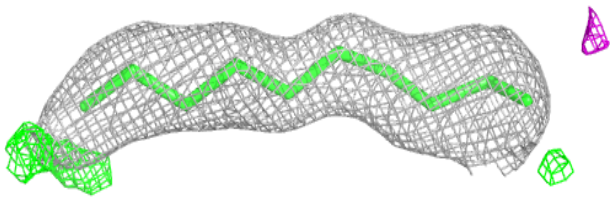


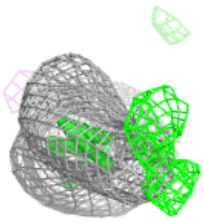


Electron density around LFA A 519:

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

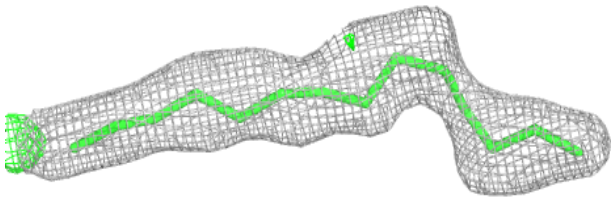


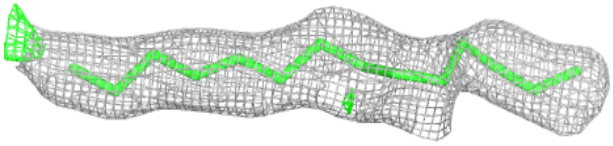


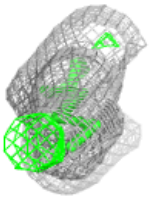


Electron density around LFA B 320:

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

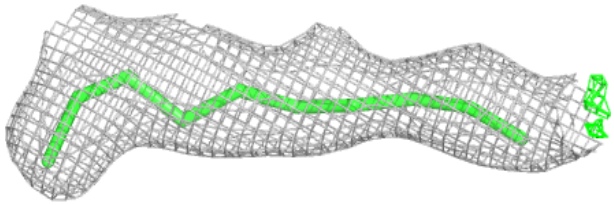


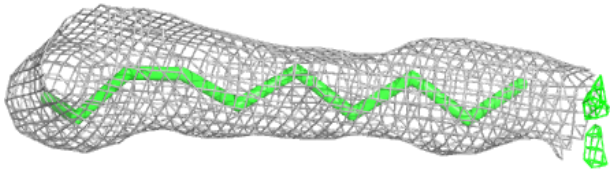


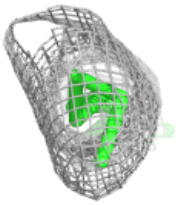


Electron density around LFA B 321:

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

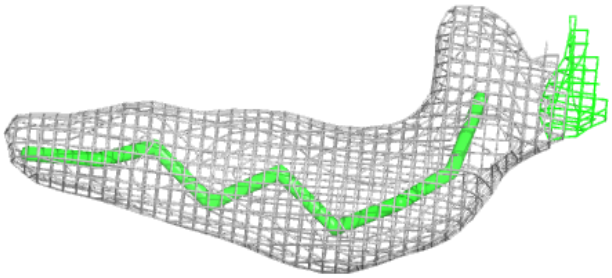


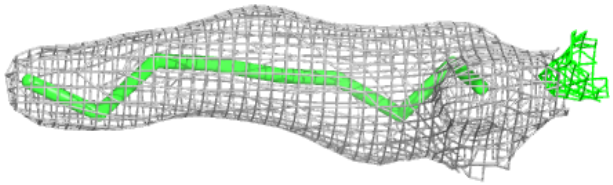


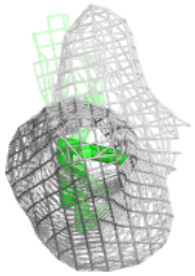


Electron density around LFA C 317:

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

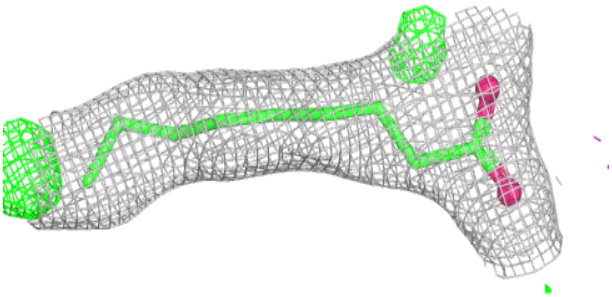


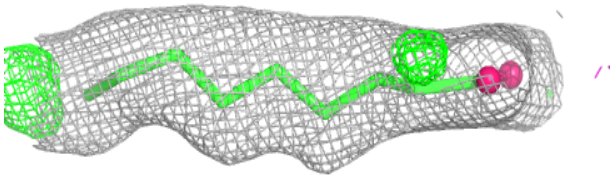


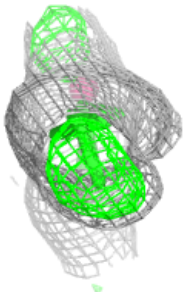


Electron density around OLA A 504:

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

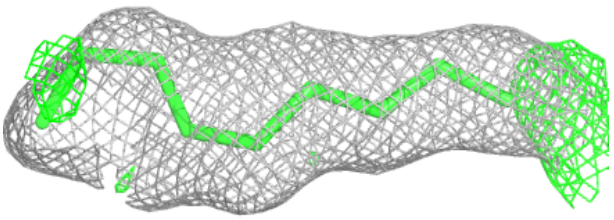


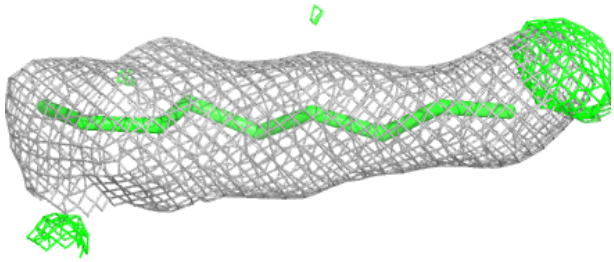


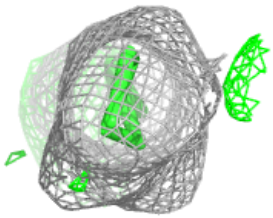


Electron density around LFA B 312:

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

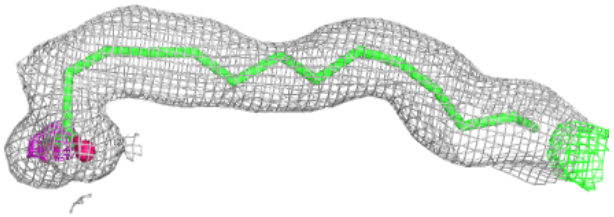


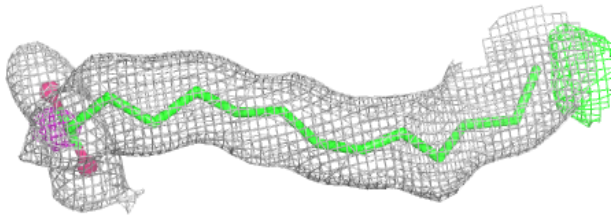


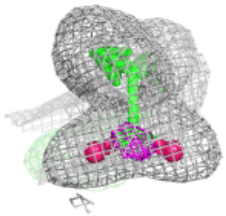


Electron density around OLA C 302:

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

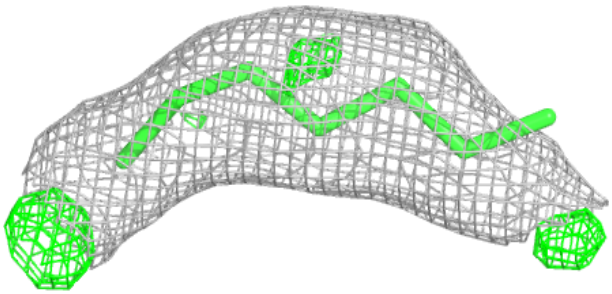


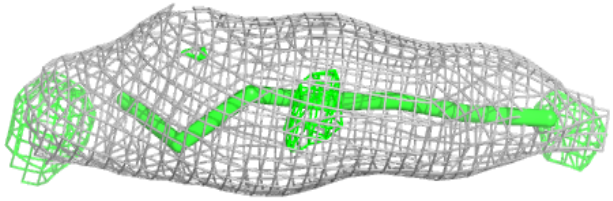


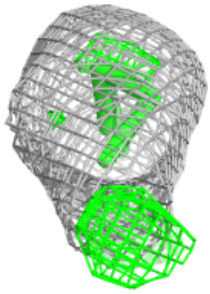


Electron density around LFA B 301:

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

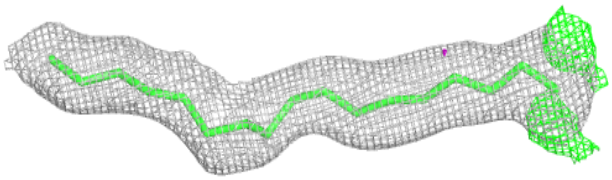


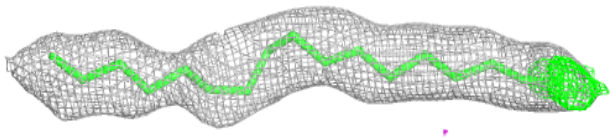


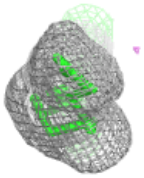


Electron density around LFA C 301:

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

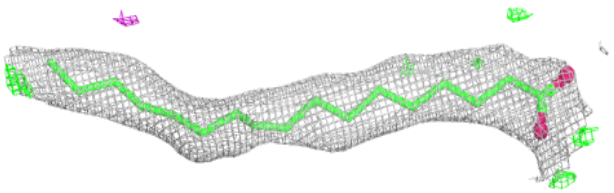


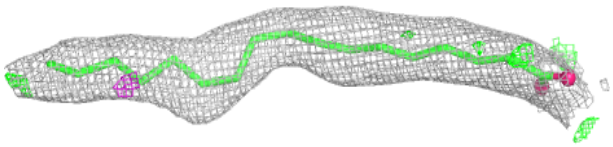


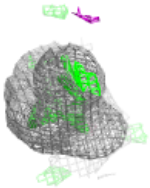


Electron density around OLA A 508:

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

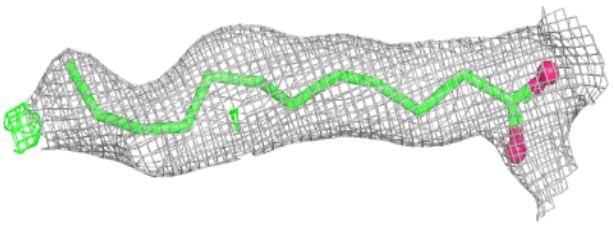


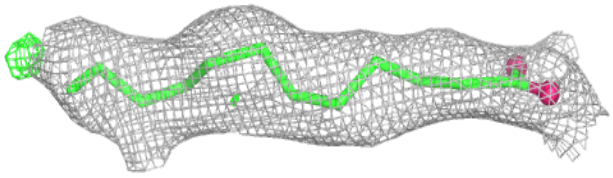


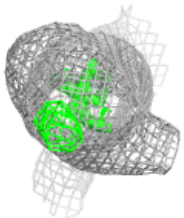


Electron density around OLA B 305:

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

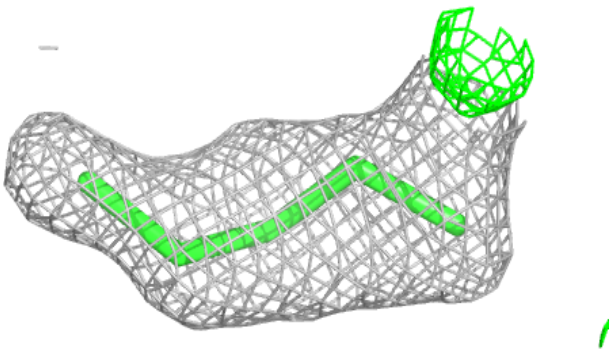


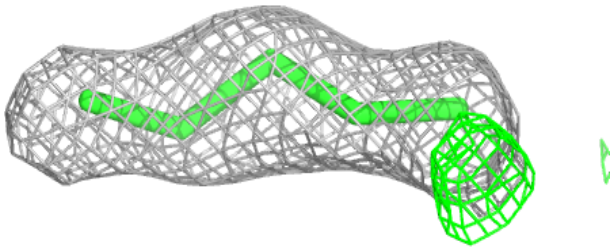


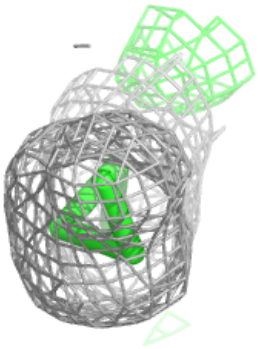


Electron density around LFA A 518:

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

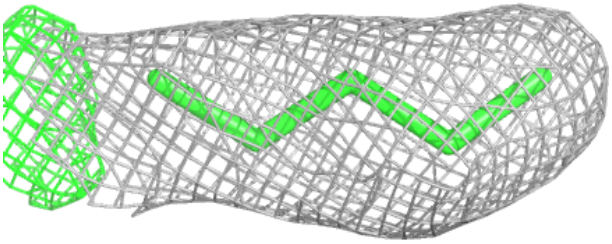


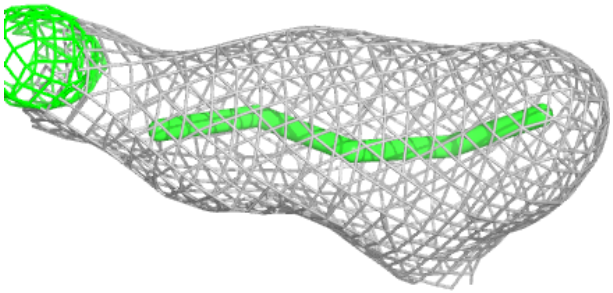


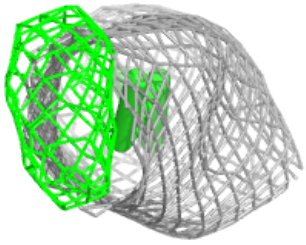


Electron density around LFA C 318:

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

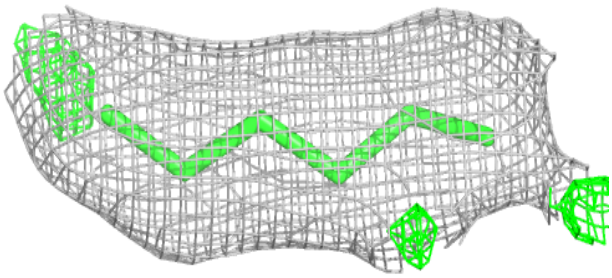


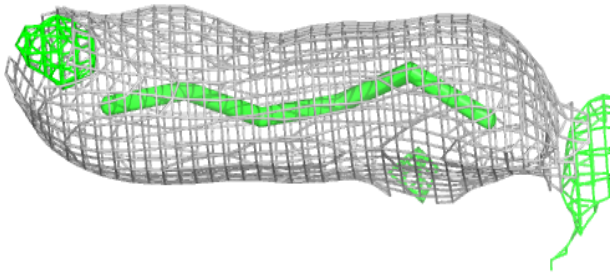


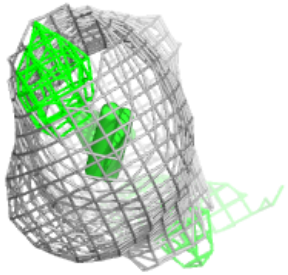


Electron density around LFA A 516:

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

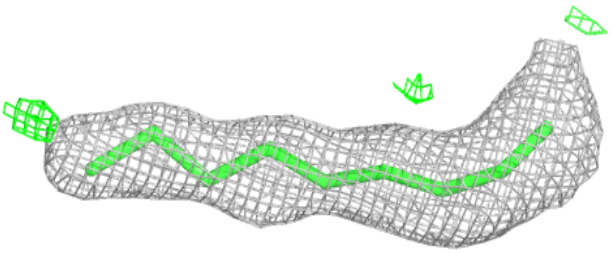


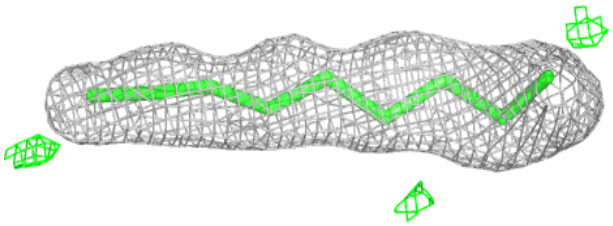


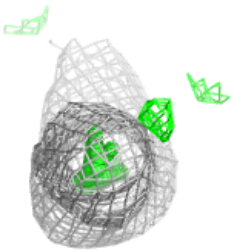


Electron density around LFA B 311:

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

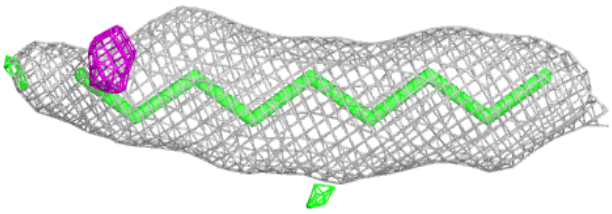


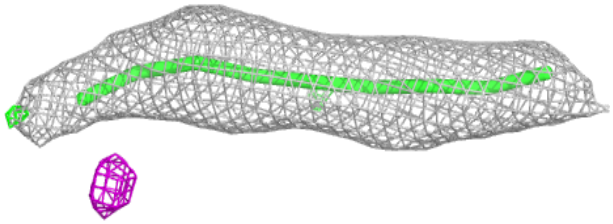


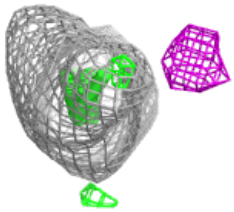


Electron density around LFA A 511:

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

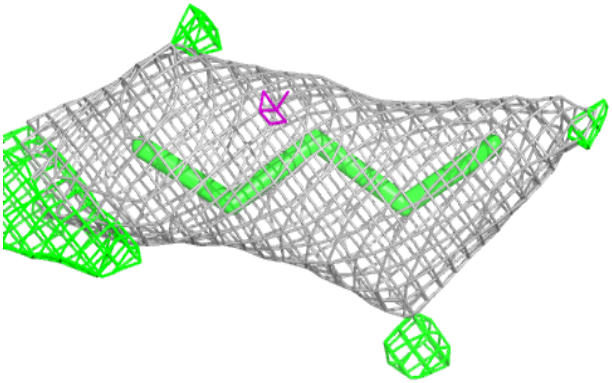


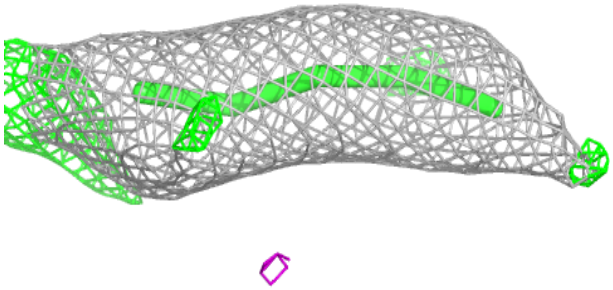


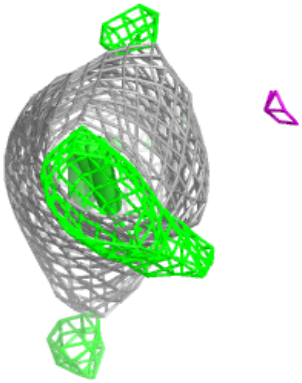


Electron density around LFA B 314:

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

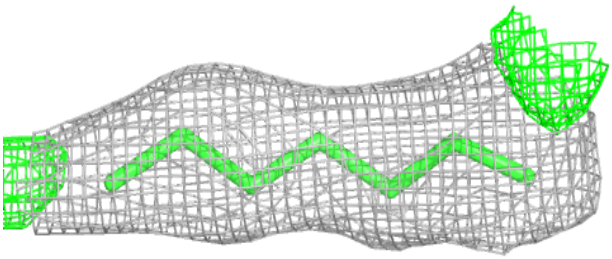


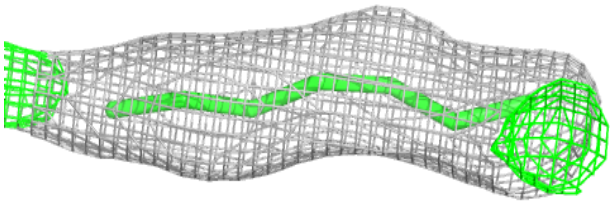


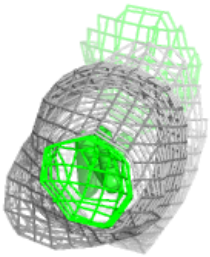


Electron density around LFA A 512:

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

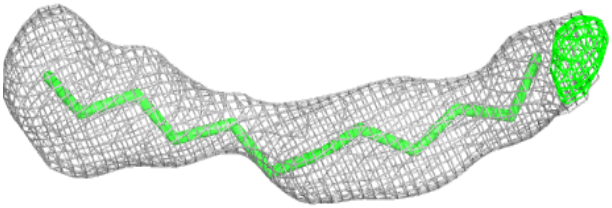


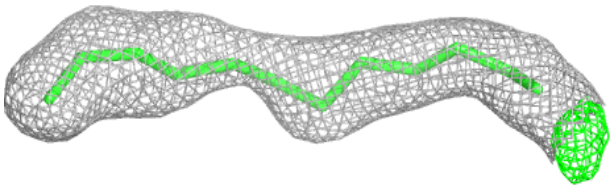


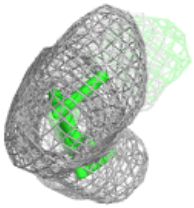


Electron density around LFA A 513:

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

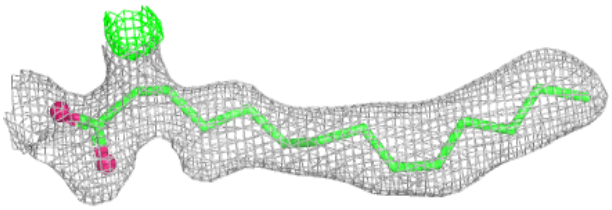


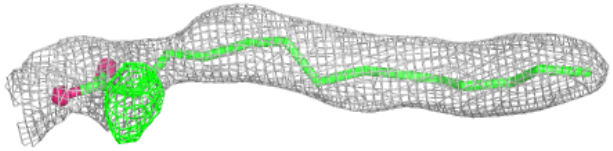


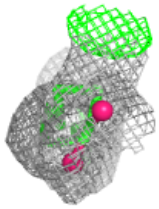


Electron density around OLA A 506:

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

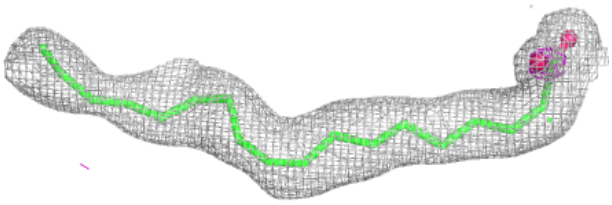


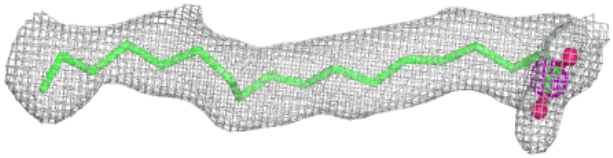




Electron density around OLA B 308:

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

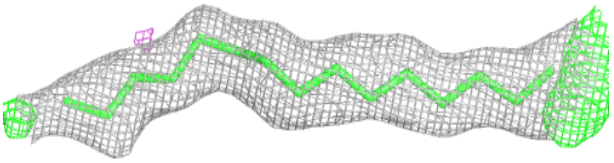


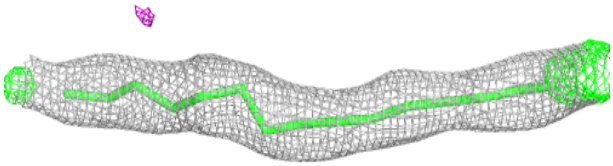


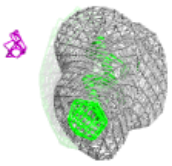


Electron density around LFA B 302:

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

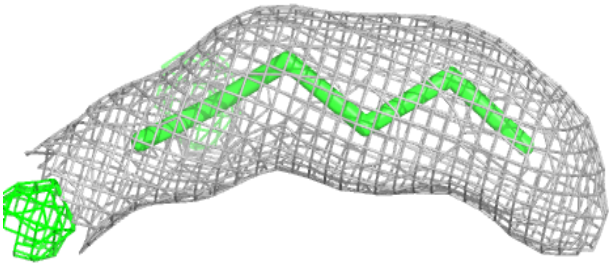


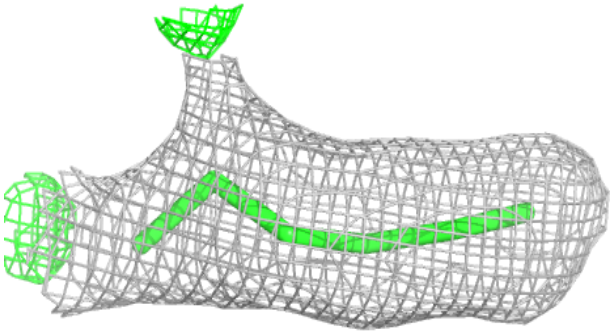


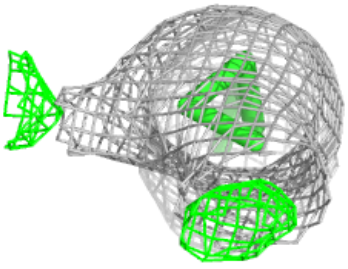


Electron density around LFA A 501:

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

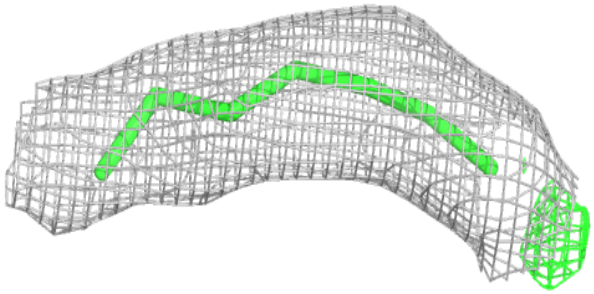


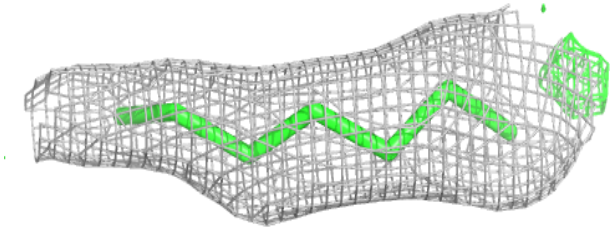


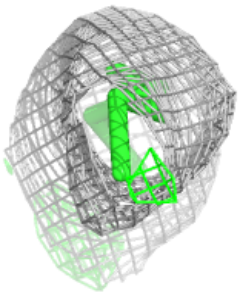


Electron density around LFA A 514:

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

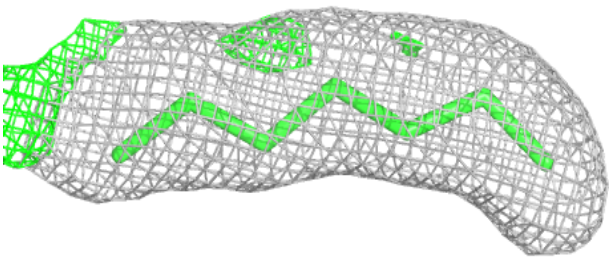


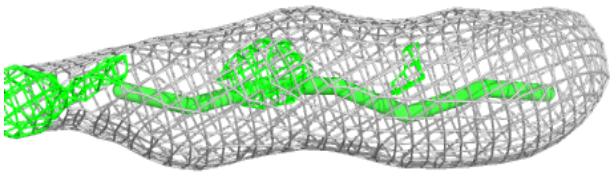


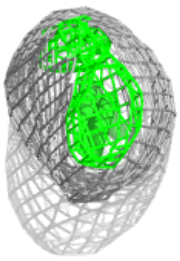


Electron density around LFA B 304:

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



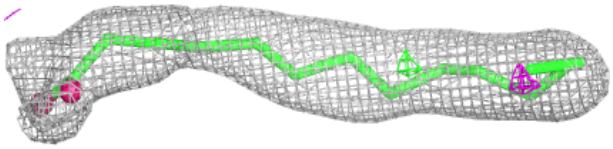


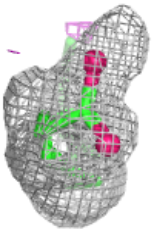


Electron density around OLA B 306:

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

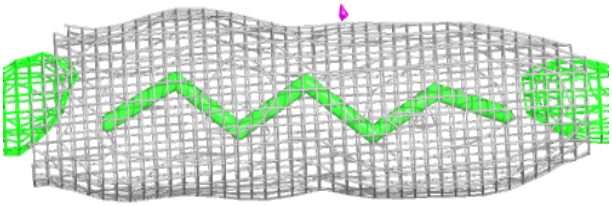


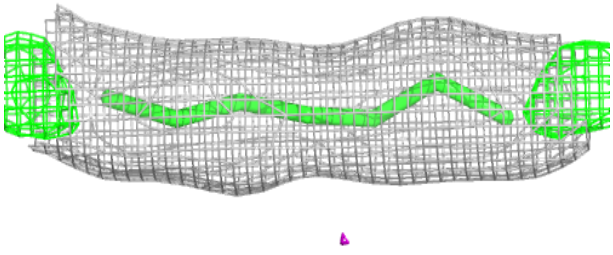


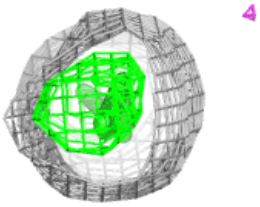


Electron density around LFA A 503:

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

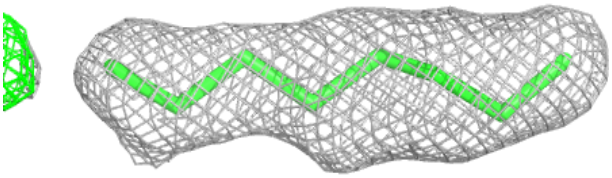


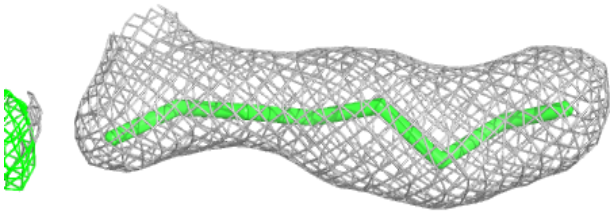


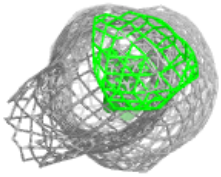


Electron density around LFA C 312:

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

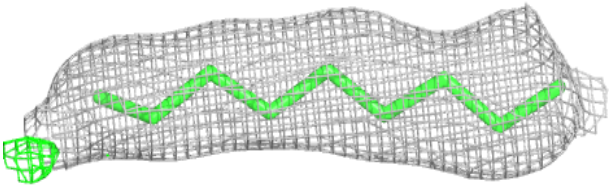


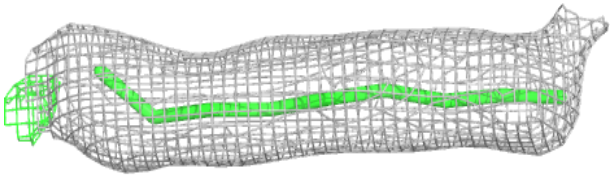


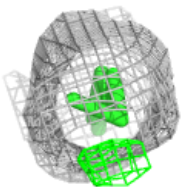


Electron density around LFA B 303:

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

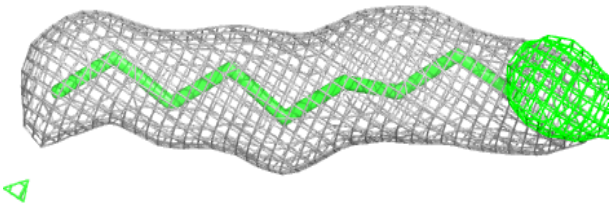


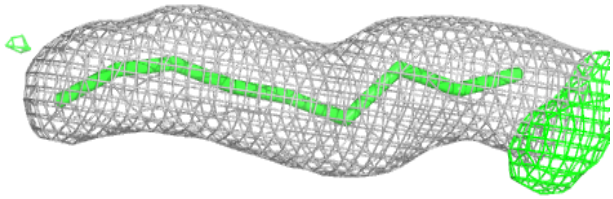


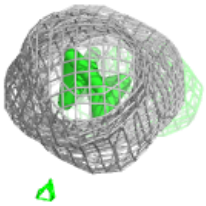


Electron density around LFA A 502:

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

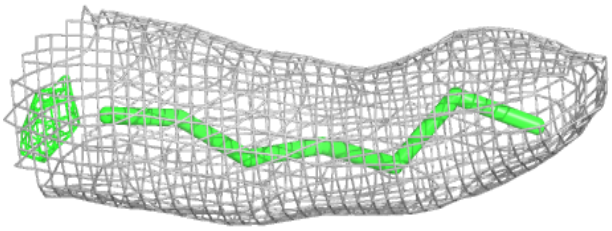


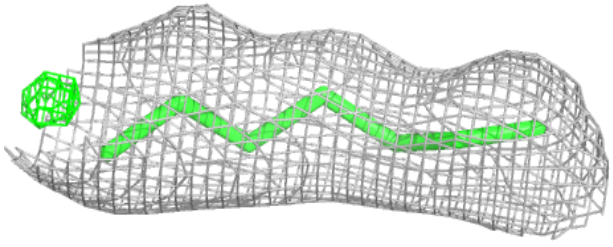


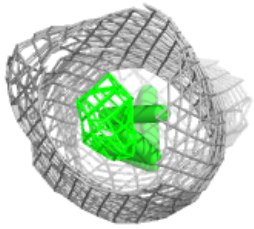


Electron density around LFA B 313:

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

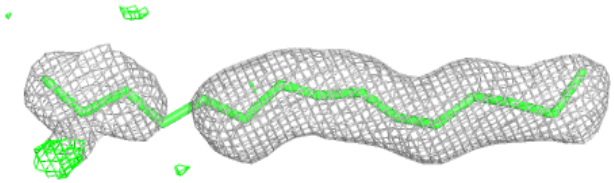


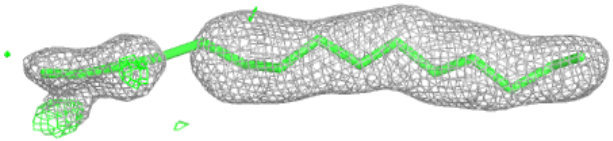


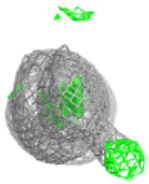


Electron density around LFA B 318:

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

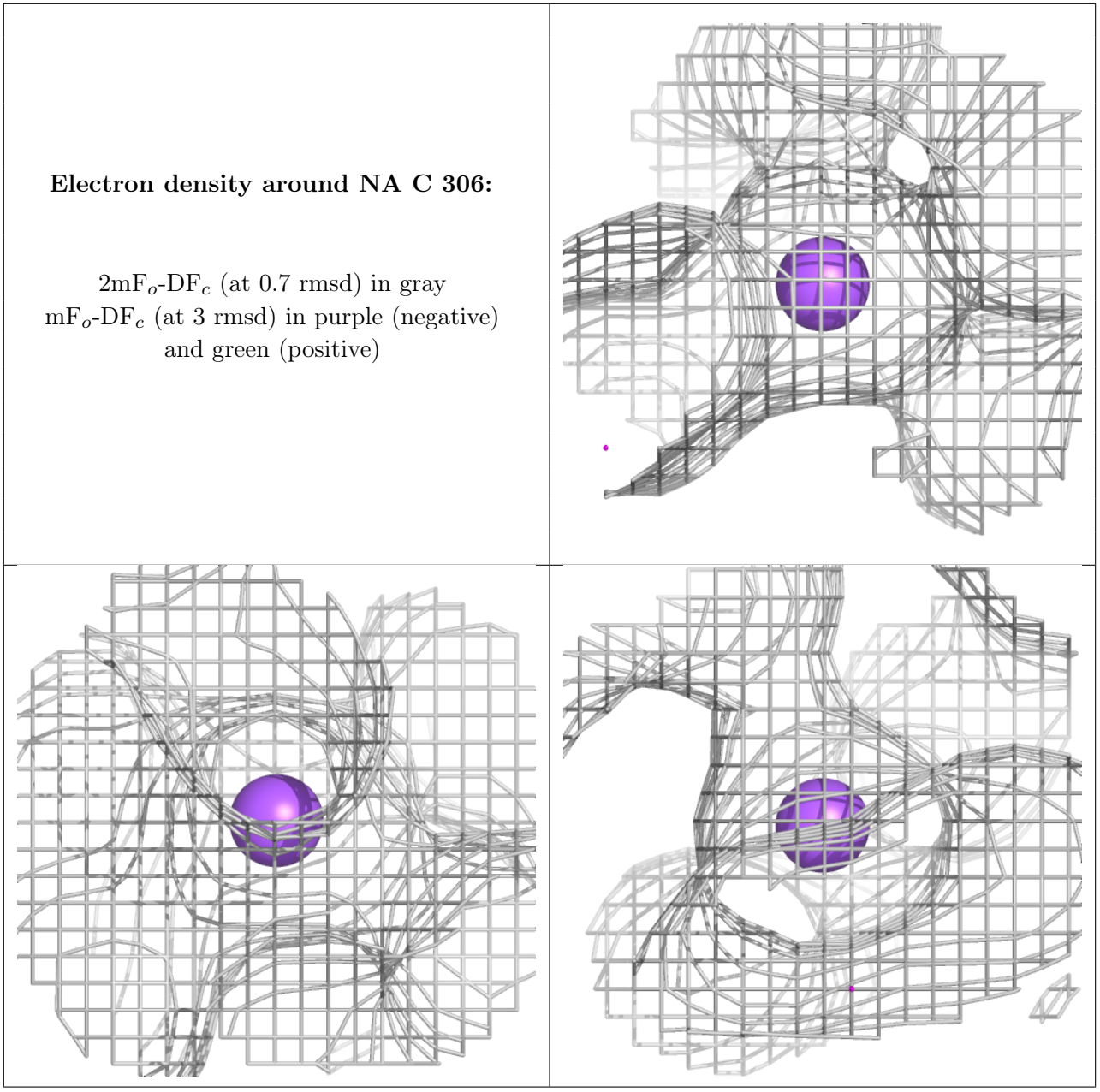






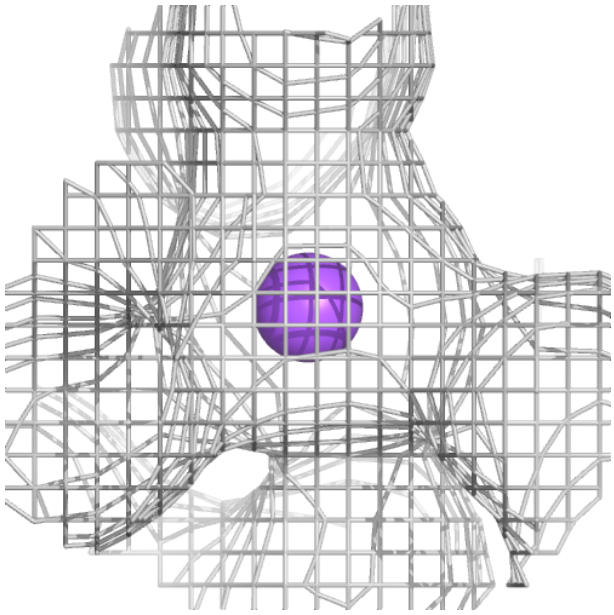
Electron density around NA C 306:

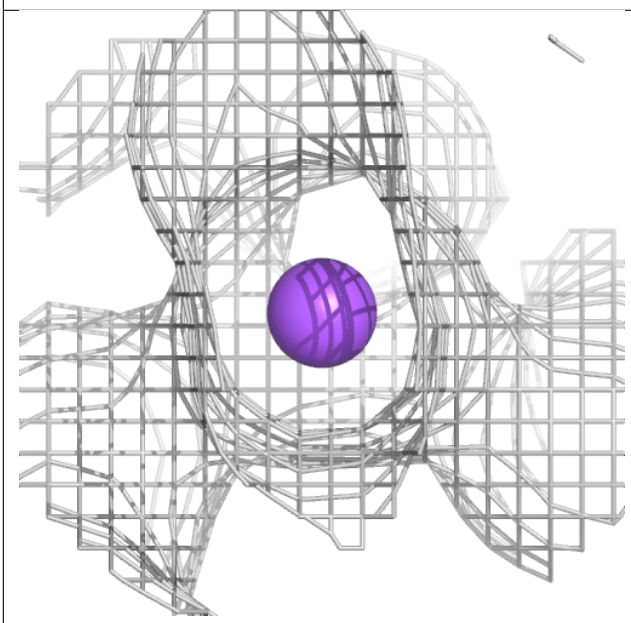
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

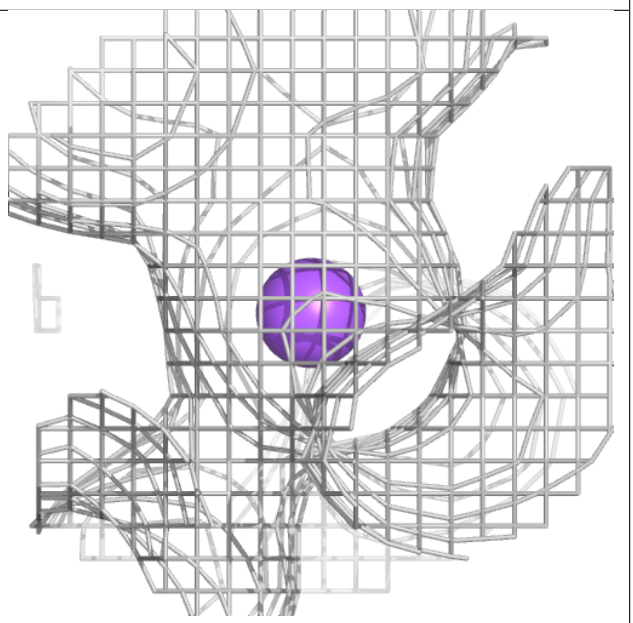


Electron density around NA A 509:

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

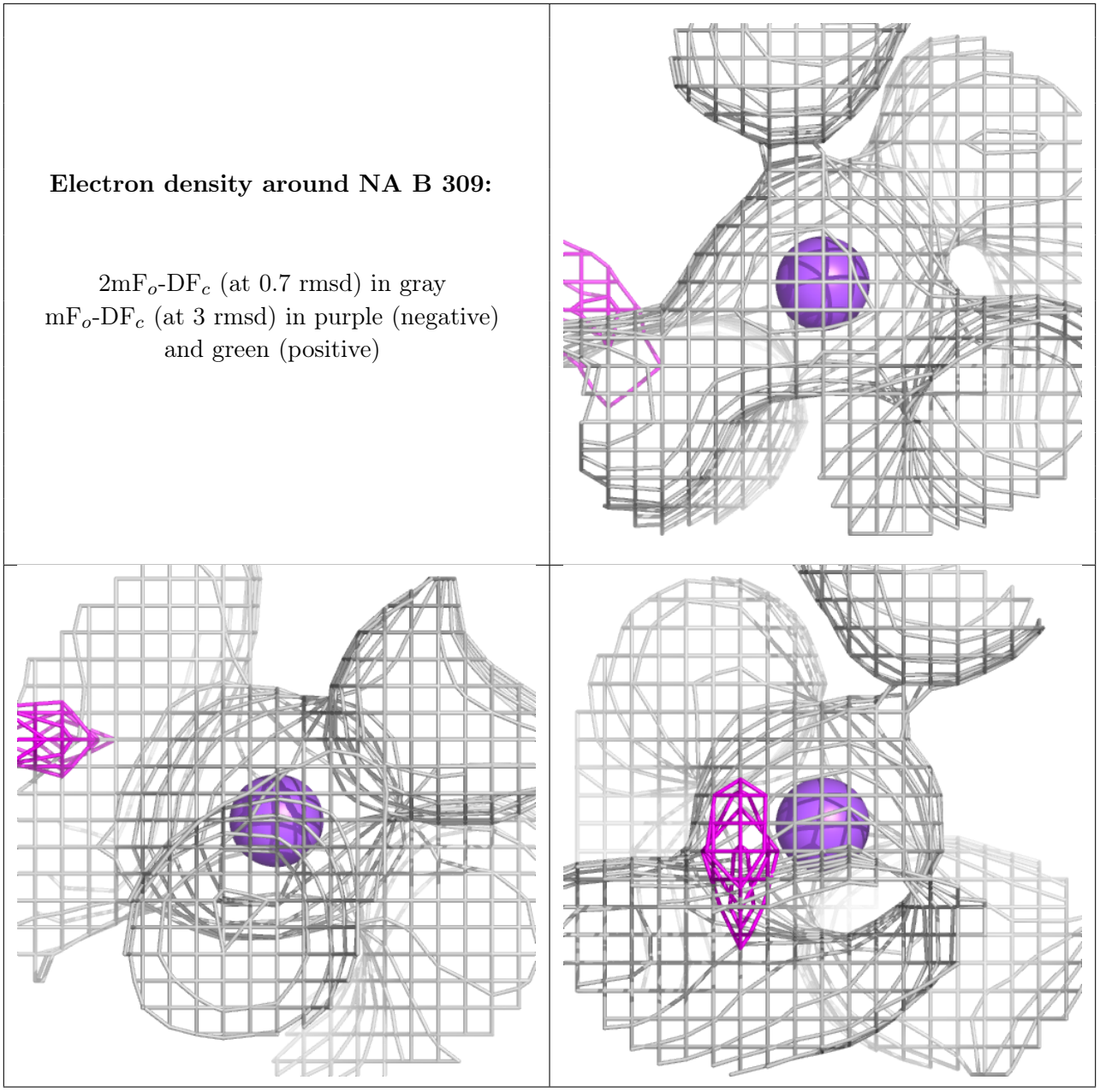






Electron density around NA B 309:

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



6.5 Other polymers (i)

There are no such residues in this entry.