Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2023 – 10:24 am BST

PDB ID	:	7ZN0
Title	:	Crystal structure of the light-driven inward proton pump xenorhodopsin BcXeR in the M 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	:	1.70 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:

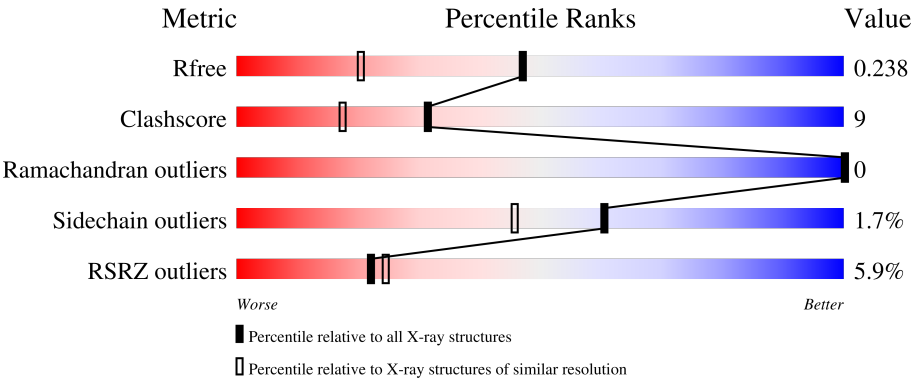
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	7% 83% 14%
1	B	229	3% 81% 15%
1	C	229	7% 84% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LFA	A	502	-	-	-	X
2	LFA	C	316	-	-	-	X

2 Entry composition (i)

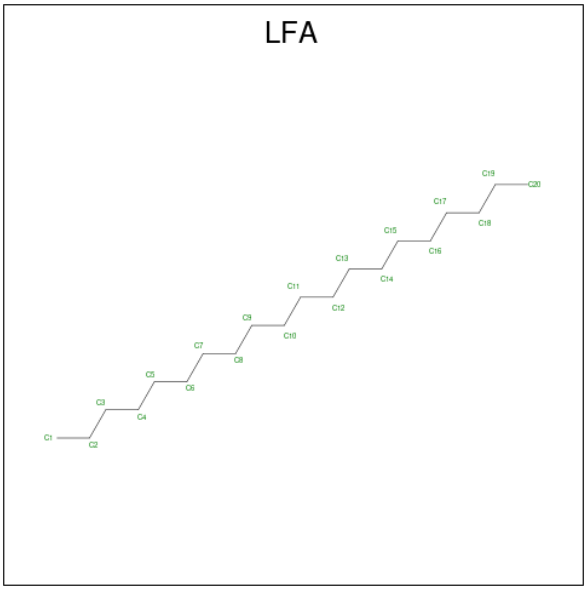
There are 6 unique types of molecules in this entry. The entry contains 6290 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	223	Total	C	N	O	S	0	7	0
			1819	1240	274	298	7			
1	B	220	Total	C	N	O	S	0	6	0
			1785	1215	271	292	7			
1	C	223	Total	C	N	O	S	0	6	0
			1807	1234	270	296	7			

- Molecule 2 is EICOSANE (three-letter code: 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
			7	7		
2	A	1	Total	C	0	0
			9	9		

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

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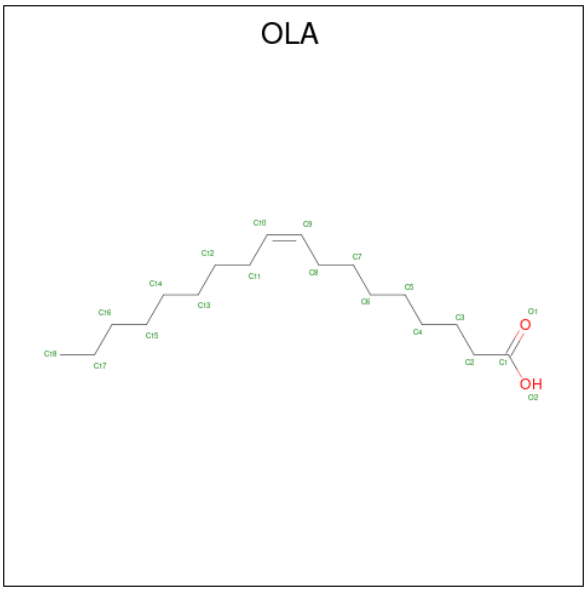
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 8 8	0	0
2	B	1	Total C 16 16	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C 13 13	0	0
2	C	1	Total C 17 17	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 11 11	0	0
2	C	1	Total C 4 4	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 4 4	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 16 16	0	0
2	C	1	Total C 12 12	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 11 11	0	0

- Molecule 3 is OLEIC ACID (three-letter code: 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 20 18 2	0	0
3	A	1	Total C O 15 13 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	A	1	Total C O 13 11 2	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C O 17 15 2	0	0
3	B	1	Total C O 16 14 2	0	0
3	B	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 16 14 2	0	0

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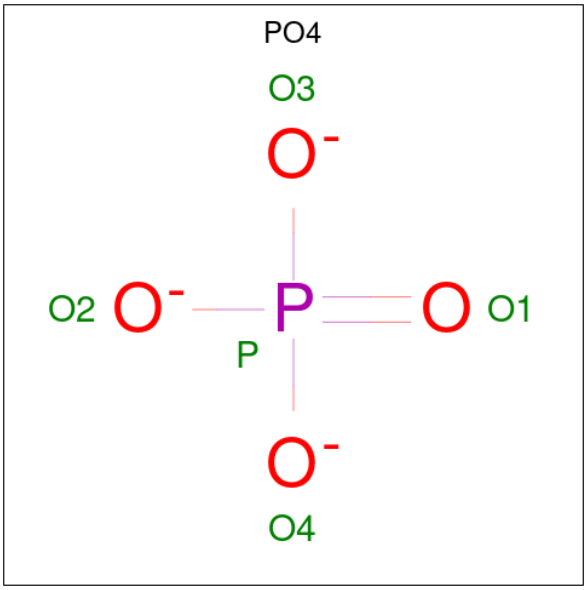
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 13 11 2	0	0
3	C	1	Total C O 15 13 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	81	Total O 82 82	0	3

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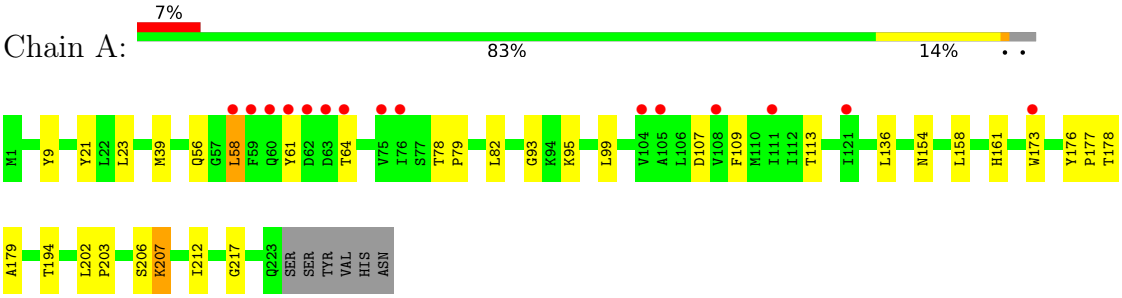
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	78	Total O 78 78	0	3
6	C	81	Total O 81 81	0	1

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.

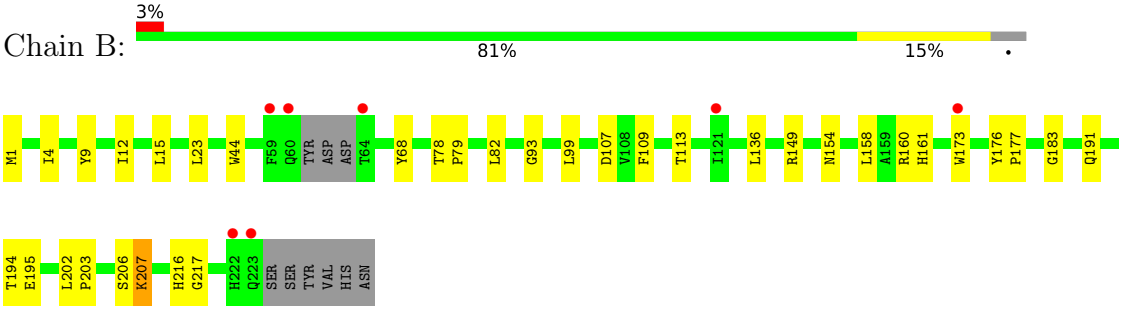
• Molecule 1: xenorhodopsin

Chain A:



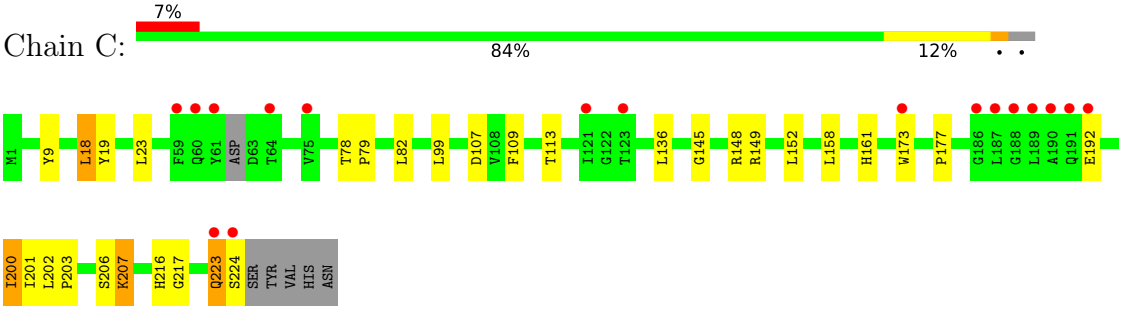
• Molecule 1: xenorhodopsin

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	68.50Å 109.50Å 119.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 49.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	70.0 (20.00-1.70) 70.0 (49.74-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.199 , 0.228 0.210 , 0.238	Depositor DCC
R_{free} test set	3360 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.8	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	0.95	EDS
Total number of atoms	6290	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.93% 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: FME, LFA, LYR, PO4, OLA, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.63	0/1827	0.61	0/2495
1	B	0.63	0/1791	0.61	0/2444
1	C	0.63	0/1814	0.62	0/2476
All	All	0.63	0/5432	0.61	0/7415

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1819	0	1894	41	0
1	B	1785	0	1865	34	0
1	C	1807	0	1886	28	0
2	A	109	0	197	6	0
2	B	159	0	292	11	0
2	C	120	0	225	6	0
3	A	89	0	125	11	0
3	B	90	0	125	5	0
3	C	60	0	80	5	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	5	0	0	0	0
5	A	1	0	0	0	0
6	A	82	0	0	0	0
6	B	78	0	0	2	0
6	C	81	0	0	1	0
All	All	6290	0	6689	115	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 9.

All (115) 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:148:ARG:O	1:C:152:LEU:HD23	1.74	0.87
2:A:519:LFA:H202	2:B:314:LFA:H132	1.62	0.82
1:A:58:LEU:HD22	1:A:58:LEU:C	2.07	0.74
2:B:321:LFA:C10	2:B:323:LFA:C8	2.68	0.72
1:B:207:LYR:H192	1:B:207:LYR:H9	1.70	0.71
1:A:202:LEU:HB2	1:A:203:PRO:HD3	1.73	0.71
3:B:304:OLA:H41	2:B:319:LFA:H21	1.74	0.70
1:A:61:TYR:O	1:A:64:THR:HG22	1.93	0.68
2:A:520:LFA:C19	2:C:311:LFA:H72	2.24	0.68
3:C:305:OLA:C3	2:C:309:LFA:H203	2.25	0.67
1:C:202:LEU:HB2	1:C:203:PRO:HD3	1.76	0.67
1:B:202:LEU:HB2	1:B:203:PRO:HD3	1.79	0.64
3:B:308:OLA:H121	1:C:109:PHE:HB2	1.80	0.64
1:A:161:HIS:CE1	1:A:217:GLY:HA3	2.32	0.64
1:B:161:HIS:CE1	1:B:217:GLY:HA3	2.33	0.63
3:C:305:OLA:H31	2:C:309:LFA:H203	1.80	0.63
1:B:183:GLY:HA3	1:B:195[A]:GLU:OE2	1.99	0.63
1:C:207:LYR:H183	1:C:207:LYR:H9	1.82	0.62
1:C:161:HIS:CE1	1:C:217:GLY:HA3	2.35	0.62
1:A:56:GLN:HB3	3:A:505:OLA:H52	1.82	0.62
1:A:93:GLY:HA3	1:A:154:ASN:HD21	1.63	0.62
1:A:82:LEU:HD21	1:A:173[A]:TRP:CZ2	2.35	0.62
1:A:207:LYR:H9	1:A:207:LYR:H183	1.81	0.61
1:A:56:GLN:HB3	3:A:505:OLA:C5	2.30	0.61
1:A:173[B]:TRP:CZ3	1:A:207:LYR:C4	2.85	0.59
1:C:99[B]:LEU:C	1:C:99[B]:LEU:HD23	2.23	0.59
1:B:82:LEU:HD21	1:B:173[A]:TRP:CZ2	2.38	0.58
1:A:95:LYS:HE2	3:A:507:OLA:O2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99[B]:LEU:O	1:A:99[B]:LEU:HD23	2.05	0.57
1:B:207:LYR:H192	1:B:207:LYR:C9	2.35	0.56
1:A:173[B]:TRP:CZ3	1:A:207:LYR:H43	2.41	0.55
1:A:99[B]:LEU:HD23	1:A:99[B]:LEU:C	2.27	0.55
3:A:506:OLA:H62	2:A:517:LFA:C5	2.37	0.54
1:C:99[B]:LEU:HD23	1:C:99[B]:LEU:O	2.07	0.54
1:A:58:LEU:HD22	1:A:58:LEU:O	2.07	0.54
1:C:207:LYR:H9	1:C:207:LYR:H192	1.90	0.54
1:C:78:THR:N	1:C:79:PRO:HD2	2.23	0.53
1:C:207:LYR:H192	1:C:207:LYR:C9	2.37	0.53
1:A:58:LEU:C	1:A:58:LEU:CD2	2.77	0.53
1:C:148:ARG:O	1:C:152:LEU:CD2	2.53	0.52
1:C:203:PRO:HA	1:C:206[A]:SER:OG	2.08	0.52
3:A:504:OLA:H9	2:C:301:LFA:H122	1.90	0.52
1:B:194:THR:HG21	3:B:305:OLA:H31	1.91	0.52
1:B:78:THR:N	1:B:79:PRO:HD2	2.24	0.52
1:A:78:THR:N	1:A:79:PRO:HD2	2.25	0.51
1:B:44:TRP:CE3	3:B:308:OLA:H152	2.46	0.51
1:A:212:ILE:HG21	3:A:508:OLA:H41	1.92	0.51
1:C:149:ARG:NH2	3:C:305:OLA:O1	2.44	0.51
1:A:212:ILE:HG22	3:A:508:OLA:H21	1.91	0.50
1:B:195[A]:GLU:HB2	2:B:321:LFA:H11	1.93	0.50
1:A:207:LYR:H192	1:A:207:LYR:C9	2.42	0.50
1:A:95:LYS:HE2	3:A:507:OLA:C1	2.42	0.50
1:B:82:LEU:HD12	1:B:107:ASP:HB2	1.94	0.49
2:A:519:LFA:C20	2:B:314:LFA:H132	2.38	0.49
1:A:203:PRO:HA	1:A:206[A]:SER:OG	2.13	0.49
1:C:145:GLY:HA3	3:C:305:OLA:H22	1.93	0.49
1:C:18[A]:LEU:HD12	2:C:312:LFA:H72	1.95	0.48
1:B:203:PRO:HA	1:B:206[A]:SER:OG	2.13	0.48
1:A:82:LEU:HD21	1:A:173[A]:TRP:CH2	2.49	0.47
1:A:82:LEU:CD2	1:A:173[A]:TRP:CZ2	2.97	0.47
1:C:19:TYR:OH	1:C:216:HIS:CE1	2.67	0.47
1:C:9:TYR:CE1	1:C:203:PRO:HB2	2.49	0.47
1:C:136[B]:LEU:C	1:C:136[B]:LEU:HD23	2.36	0.47
1:B:82:LEU:HD21	1:B:173[A]:TRP:CH2	2.50	0.46
1:B:207:LYR:H9	1:B:207:LYR:H183	1.98	0.46
1:C:82:LEU:HD12	1:C:107:ASP:HB2	1.98	0.46
1:C:173[A]:TRP:O	1:C:177:PRO:HD2	2.16	0.46
1:A:56:GLN:HB3	3:A:505:OLA:H51	1.97	0.46
1:B:9:TYR:CE1	1:B:203:PRO:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ILE:HG23	2:B:322:LFA:C12	2.45	0.45
1:A:107:ASP:OD1	1:A:173[B]:TRP:HZ2	2.00	0.45
3:C:305:OLA:H32	2:C:309:LFA:H203	1.97	0.45
1:A:207:LYR:H9	1:A:207:LYR:H192	1.98	0.45
1:C:9:TYR:HE1	1:C:203:PRO:HB2	1.81	0.45
1:A:82:LEU:HD12	1:A:107:ASP:HB2	1.97	0.45
1:A:178:THR:HG21	2:A:515:LFA:H12	1.98	0.45
1:A:207:LYR:H6	1:A:207:LYR:H41	1.82	0.45
1:B:158:LEU:C	1:B:158:LEU:HD13	2.38	0.45
1:B:93:GLY:HA3	1:B:154:ASN:HD21	1.81	0.44
3:B:305:OLA:H51	2:B:323:LFA:H151	1.99	0.44
1:A:158:LEU:C	1:A:158:LEU:HD13	2.38	0.44
1:A:176:TYR:N	1:A:177:PRO:HD2	2.33	0.44
1:A:21:TYR:HB2	1:A:39[B]:MET:CE	2.48	0.44
1:B:109:PHE:O	1:B:113:THR:HG23	2.17	0.44
1:A:194:THR:HG21	3:A:506:OLA:H22	1.99	0.44
1:C:19:TYR:HH	1:C:216:HIS:CE1	2.36	0.43
1:A:136[B]:LEU:C	1:A:136[B]:LEU:HD23	2.38	0.43
1:B:82:LEU:CD2	1:B:173[A]:TRP:CZ2	3.01	0.43
1:B:136[B]:LEU:C	1:B:136[B]:LEU:HD23	2.38	0.43
1:B:9:TYR:HE1	1:B:203:PRO:HB2	1.83	0.43
1:B:160:ARG:HG2	6:B:468:HOH:O	2.17	0.43
1:C:200:ILE:HG22	1:C:201:ILE:HG13	2.00	0.43
1:B:207:LYR:H6	1:B:207:LYR:H41	1.83	0.43
3:A:508:OLA:H81	3:A:508:OLA:H51	1.78	0.43
1:B:194:THR:OG1	2:B:323:LFA:H202	2.19	0.43
1:A:173[B]:TRP:CZ3	1:A:207:LYR:H41	2.53	0.43
1:C:158:LEU:C	1:C:158:LEU:HD13	2.39	0.43
1:A:109:PHE:O	1:A:113:THR:HG23	2.20	0.42
1:B:207:LYR:C	6:B:413[A]:HOH:O	2.68	0.42
1:C:109:PHE:O	1:C:113:THR:HG23	2.20	0.42
1:A:9:TYR:CE1	1:A:203:PRO:HB2	2.55	0.42
1:B:176:TYR:N	1:B:177:PRO:HD2	2.35	0.42
1:B:1:FME:O1	1:B:4:ILE:HG12	2.19	0.41
1:B:107:ASP:OD1	1:B:173[B]:TRP:HZ2	2.03	0.41
1:A:58:LEU:H	1:A:58:LEU:HD13	1.85	0.41
1:B:99[B]:LEU:HD23	1:B:99[B]:LEU:C	2.41	0.41
1:A:179:ALA:O	2:A:517:LFA:H13	2.19	0.41
1:C:223:GLN:O	1:C:224:SER:CB	2.69	0.41
1:A:58:LEU:HD13	1:A:58:LEU:N	2.36	0.41
1:B:216:HIS:CE1	2:B:322:LFA:H22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LYR:H6	1:C:207:LYR:H41	1.81	0.41
1:C:192:GLU:HG3	6:C:401:HOH:O	2.21	0.40
1:B:68:TYR:CD2	2:B:315:LFA:H61	2.56	0.40
1:B:15:LEU:HB3	2:B:322:LFA:H101	2.04	0.40
1:B:202:LEU:N	1:B:203:PRO:CD	2.85	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	227/229 (99%)	226 (100%)	1 (0%)	0	100	100
1	B	221/229 (96%)	220 (100%)	1 (0%)	0	100	100
1	C	224/229 (98%)	223 (100%)	1 (0%)	0	100	100
All	All	672/687 (98%)	669 (100%)	3 (0%)	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	184/189 (97%)	182 (99%)	2 (1%)	73	63
1	B	182/189 (96%)	179 (98%)	3 (2%)	62	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	183/189 (97%)	178 (97%)	5 (3%)	44 26
All	All	549/567 (97%)	539 (98%)	10 (2%)	60 43

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	58	LEU
1	B	23	LEU
1	B	149	ARG
1	B	191	GLN
1	C	18[A]	LEU
1	C	18[B]	LEU
1	C	23	LEU
1	C	200	ILE
1	C	223	GLN

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

Mol	Chain	Res	Type
1	A	154	ASN
1	A	191	GLN
1	B	60	GLN
1	B	154	ASN
1	B	191	GLN
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)

6 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	B	207	1	27,29,30	1.31	3 (11%)	30,37,39	1.26	4 (13%)
1	FME	B	1	1	8,9,10	0.38	0	7,9,11	0.72	0
1	FME	C	1	1	8,9,10	0.41	0	7,9,11	0.71	0
1	FME	A	1	1	8,9,10	0.39	0	7,9,11	0.69	0
1	LYR	C	207	1	27,29,30	1.28	3 (11%)	30,37,39	1.15	3 (10%)
1	LYR	A	207	1	27,29,30	1.32	3 (11%)	30,37,39	1.17	2 (6%)

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	B	207	1	-	2/22/40/42	0/1/1/1
1	FME	B	1	1	-	0/7/9/11	-
1	FME	C	1	1	-	1/7/9/11	-
1	FME	A	1	1	-	0/7/9/11	-
1	LYR	C	207	1	-	6/22/40/42	0/1/1/1
1	LYR	A	207	1	-	2/22/40/42	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	LYR	C7-C80	4.21	1.41	1.35
1	A	207	LYR	C7-C80	4.07	1.41	1.35
1	C	207	LYR	C7-C80	3.80	1.40	1.35
1	C	207	LYR	C9-C80	-2.98	1.39	1.45
1	A	207	LYR	C9-C80	-2.87	1.39	1.45
1	B	207	LYR	C9-C80	-2.62	1.40	1.45
1	A	207	LYR	C4-C3	-2.17	1.46	1.50
1	B	207	LYR	C4-C3	-2.10	1.46	1.50
1	C	207	LYR	C4-C3	-2.09	1.46	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	207	LYR	C8-C80-C7	-4.40	116.76	122.92
1	C	207	LYR	C8-C80-C7	-4.17	117.08	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	207	LYR	C8-C80-C7	-4.14	117.13	122.92
1	B	207	LYR	C9-C80-C7	2.81	123.25	118.94
1	C	207	LYR	C9-C80-C7	2.76	123.18	118.94
1	A	207	LYR	C9-C80-C7	2.66	123.02	118.94
1	B	207	LYR	C7-C6-C5	2.05	129.60	123.22
1	C	207	LYR	C7-C6-C5	2.03	129.54	123.22
1	B	207	LYR	C16-C17-C11	2.00	113.56	110.48

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	207	LYR	5	0
1	B	1	FME	1	0
1	C	207	LYR	4	0
1	A	207	LYR	7	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 63 ligands modelled in this entry, 1 is monoatomic - leaving 62 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	$\#\|Z\| > 2$
2	LFA	A	515	-	5,5,19	0.13	0	4,4,18	0.10	0
2	LFA	A	513	-	6,6,19	0.12	0	5,5,18	0.08	0
2	LFA	A	518	-	6,6,19	0.11	0	5,5,18	0.09	0
3	OLA	A	506	-	10,10,19	0.65	0	10,10,19	0.67	0
2	LFA	A	520	-	9,9,19	0.09	0	8,8,18	0.07	0
2	LFA	B	315	-	7,7,19	0.11	0	6,6,18	0.11	0
2	LFA	C	312	-	15,15,19	0.08	0	14,14,18	0.06	0
2	LFA	A	511	-	6,6,19	0.11	0	5,5,18	0.12	0
2	LFA	B	317	-	15,15,19	0.08	0	14,14,18	0.05	0
2	LFA	B	320	-	11,11,19	0.09	0	10,10,18	0.07	0
3	OLA	A	505	-	14,14,19	0.60	0	14,14,19	0.55	0
2	LFA	B	321	-	9,9,19	0.11	0	8,8,18	0.07	0
4	PO4	A	522	-	4,4,4	0.65	0	6,6,6	0.42	0
2	LFA	A	516	-	2,2,19	0.03	0	0,1,18	-	-
3	OLA	A	507	-	18,18,19	0.54	0	18,18,19	0.49	0
3	OLA	B	305	-	9,9,19	0.28	0	8,8,19	0.18	0
2	LFA	C	306	-	9,9,19	0.10	0	8,8,18	0.07	0
2	LFA	A	519	-	6,6,19	0.11	0	5,5,18	0.09	0
2	LFA	A	514	-	7,7,19	0.10	0	6,6,18	0.07	0
3	OLA	C	305	-	14,14,19	0.61	0	14,14,19	0.53	0
2	LFA	C	315	-	8,8,19	0.08	0	7,7,18	0.13	0
3	OLA	B	308	-	18,18,19	0.54	0	18,18,19	0.49	0
2	LFA	C	309	-	7,7,19	0.11	0	6,6,18	0.07	0
2	LFA	A	501	-	5,5,19	0.13	0	4,4,18	0.10	0
2	LFA	B	302	-	8,8,19	0.10	0	7,7,18	0.07	0
2	LFA	B	313	-	5,5,19	0.12	0	4,4,18	0.12	0
2	LFA	B	316	-	7,7,19	0.11	0	6,6,18	0.07	0
2	LFA	B	309	-	5,5,19	0.12	0	4,4,18	0.09	0
2	LFA	B	319	-	8,8,19	0.10	0	7,7,18	0.08	0
2	LFA	B	301	-	5,5,19	0.13	0	4,4,18	0.12	0
3	OLA	B	303	-	13,13,19	0.62	0	12,13,19	0.58	0
3	OLA	A	504	-	19,19,19	0.51	0	19,19,19	0.48	0
3	OLA	B	304	-	13,13,19	0.61	0	12,13,19	0.60	0
2	LFA	C	316	-	10,10,19	0.09	0	9,9,18	0.07	0
2	LFA	B	323	-	12,12,19	0.09	0	11,11,18	0.08	0
3	OLA	C	302	-	15,15,19	0.57	0	15,15,19	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LFA	B	314	-	14,14,19	0.08	0	13,13,18	0.06	0
2	LFA	A	509	-	8,8,19	0.11	0	7,7,18	0.09	0
2	LFA	C	314	-	9,9,19	0.09	0	8,8,18	0.07	0
2	LFA	A	512	-	11,11,19	0.09	0	10,10,18	0.06	0
2	LFA	C	301	-	16,16,19	0.08	0	15,15,18	0.06	0
2	LFA	C	307	-	10,10,19	0.09	0	9,9,18	0.09	0
4	PO4	C	317	-	4,4,4	0.67	0	6,6,6	0.44	0
2	LFA	B	312	-	4,4,19	0.14	0	3,3,18	0.22	0
2	LFA	C	313	-	11,11,19	0.11	0	10,10,18	0.05	0
2	LFA	B	311	-	4,4,19	0.13	0	3,3,18	0.23	0
2	LFA	B	318	-	11,11,19	0.09	0	10,10,18	0.06	0
2	LFA	C	310	-	3,3,19	0.24	0	2,2,18	0.44	0
2	LFA	A	502	-	6,6,19	0.11	0	5,5,18	0.13	0
2	LFA	A	510	-	8,8,19	0.11	0	7,7,18	0.08	0
3	OLA	A	503	-	10,10,19	0.69	0	10,10,19	0.63	0
2	LFA	A	521	-	5,5,19	0.11	0	4,4,18	0.11	0
2	LFA	B	310	-	6,6,19	0.11	0	5,5,18	0.08	0
3	OLA	B	306	-	16,16,19	0.57	0	16,16,19	0.51	0
2	LFA	C	308	-	3,3,19	0.23	0	2,2,18	0.44	0
2	LFA	B	322	-	11,11,19	0.09	0	10,10,18	0.06	0
3	OLA	B	307	-	15,15,19	0.60	0	15,15,19	0.51	0
3	OLA	A	508	-	12,12,19	0.64	0	12,12,19	0.61	0
3	OLA	C	304	-	12,12,19	0.64	0	12,12,19	0.62	0
2	LFA	A	517	-	4,4,19	0.15	0	3,3,18	0.22	0
3	OLA	C	303	-	15,15,19	0.59	0	15,15,19	0.53	0
2	LFA	C	311	-	7,7,19	0.11	0	6,6,18	0.08	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
2	LFA	A	515	-	-	2/3/3/17	-
2	LFA	A	513	-	-	1/4/4/17	-
2	LFA	A	518	-	-	0/4/4/17	-
3	OLA	A	506	-	-	3/8/8/17	-
2	LFA	A	520	-	-	0/7/7/17	-
2	LFA	B	315	-	-	1/5/5/17	-
2	LFA	C	312	-	-	4/13/13/17	-
2	LFA	A	511	-	-	0/4/4/17	-
2	LFA	B	317	-	-	3/13/13/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	B	320	-	-	1/9/9/17	-
3	OLA	A	505	-	-	7/12/12/17	-
2	LFA	B	321	-	-	3/7/7/17	-
3	OLA	A	507	-	-	7/16/16/17	-
3	OLA	B	305	-	-	2/7/7/17	-
2	LFA	C	306	-	-	3/7/7/17	-
2	LFA	A	519	-	-	2/4/4/17	-
2	LFA	A	514	-	-	0/5/5/17	-
3	OLA	C	305	-	-	6/12/12/17	-
2	LFA	C	315	-	-	1/6/6/17	-
3	OLA	B	308	-	-	10/16/16/17	-
2	LFA	C	309	-	-	0/5/5/17	-
2	LFA	A	501	-	-	2/3/3/17	-
2	LFA	B	302	-	-	1/6/6/17	-
2	LFA	B	313	-	-	2/3/3/17	-
2	LFA	B	316	-	-	1/5/5/17	-
2	LFA	B	309	-	-	2/3/3/17	-
2	LFA	B	319	-	-	0/6/6/17	-
2	LFA	B	301	-	-	0/3/3/17	-
3	OLA	B	303	-	-	4/11/11/17	-
3	OLA	A	504	-	-	11/17/17/17	-
3	OLA	B	304	-	-	4/11/11/17	-
2	LFA	C	316	-	-	2/8/8/17	-
2	LFA	B	323	-	-	0/10/10/17	-
3	OLA	C	302	-	-	8/13/13/17	-
2	LFA	B	314	-	-	6/12/12/17	-
2	LFA	A	509	-	-	1/6/6/17	-
2	LFA	C	314	-	-	5/7/7/17	-
2	LFA	A	512	-	-	7/9/9/17	-
2	LFA	C	301	-	-	11/14/14/17	-
2	LFA	C	307	-	-	2/8/8/17	-
2	LFA	B	312	-	-	1/2/2/17	-
2	LFA	C	313	-	-	3/9/9/17	-
2	LFA	B	311	-	-	0/2/2/17	-
2	LFA	B	318	-	-	3/9/9/17	-
2	LFA	C	310	-	-	0/1/1/17	-
2	LFA	A	502	-	-	0/4/4/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	A	510	-	-	4/6/6/17	-
3	OLA	A	503	-	-	5/8/8/17	-
2	LFA	A	521	-	-	2/3/3/17	-
2	LFA	B	310	-	-	1/4/4/17	-
3	OLA	B	306	-	-	5/14/14/17	-
2	LFA	C	308	-	-	0/1/1/17	-
2	LFA	B	322	-	-	1/9/9/17	-
3	OLA	B	307	-	-	3/13/13/17	-
3	OLA	A	508	-	-	3/10/10/17	-
3	OLA	C	304	-	-	7/10/10/17	-
2	LFA	A	517	-	-	2/2/2/17	-
3	OLA	C	303	-	-	11/13/13/17	-
2	LFA	C	311	-	-	3/5/5/17	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (179) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	508	OLA	C11-C10-C9-C8
3	B	307	OLA	C11-C10-C9-C8
3	C	302	OLA	C11-C10-C9-C8
3	A	508	OLA	C5-C6-C7-C8
3	B	306	OLA	C11-C10-C9-C8
3	A	504	OLA	C12-C13-C14-C15
2	C	312	LFA	C9-C10-C11-C12
2	B	310	LFA	C3-C4-C5-C6
2	B	314	LFA	C9-C10-C11-C12
2	C	313	LFA	C11-C10-C9-C8
3	C	304	OLA	C3-C4-C5-C6
3	B	303	OLA	C11-C10-C9-C8
2	B	321	LFA	C2-C3-C4-C5
2	C	301	LFA	C11-C12-C13-C14
3	A	507	OLA	C11-C12-C13-C14
3	B	308	OLA	C11-C12-C13-C14
2	B	314	LFA	C4-C5-C6-C7
2	C	314	LFA	C5-C6-C7-C8
3	C	303	OLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	C	314	LFA	C4-C5-C6-C7
3	C	304	OLA	C4-C5-C6-C7
3	C	302	OLA	C10-C11-C12-C13
2	A	510	LFA	C2-C3-C4-C5
2	A	510	LFA	C5-C6-C7-C8
2	A	512	LFA	C4-C5-C6-C7
2	C	301	LFA	C7-C8-C9-C10
2	C	301	LFA	C10-C11-C12-C13
2	C	312	LFA	C12-C13-C14-C15
3	A	508	OLA	C4-C5-C6-C7
2	C	314	LFA	C6-C7-C8-C9
2	A	512	LFA	C6-C7-C8-C9
2	A	512	LFA	C7-C8-C9-C10
2	C	301	LFA	C13-C14-C15-C16
2	C	316	LFA	C3-C4-C5-C6
3	B	303	OLA	C3-C4-C5-C6
3	C	303	OLA	C4-C5-C6-C7
3	C	303	OLA	C3-C4-C5-C6
2	B	313	LFA	C3-C4-C5-C6
2	B	320	LFA	C13-C14-C15-C16
2	C	301	LFA	C3-C4-C5-C6
2	C	313	LFA	C5-C6-C7-C8
2	B	321	LFA	C6-C7-C8-C9
3	A	503	OLA	C2-C3-C4-C5
3	A	504	OLA	C10-C11-C12-C13
3	C	304	OLA	C6-C7-C8-C9
3	C	305	OLA	C1-C2-C3-C4
2	B	314	LFA	C11-C10-C9-C8
3	A	504	OLA	C13-C14-C15-C16
2	C	313	LFA	C3-C4-C5-C6
2	C	314	LFA	C3-C4-C5-C6
3	B	308	OLA	C6-C7-C8-C9
3	B	306	OLA	C2-C3-C4-C5
2	C	301	LFA	C6-C7-C8-C9
3	B	304	OLA	C1-C2-C3-C4
2	B	314	LFA	C10-C11-C12-C13
3	B	306	OLA	C10-C11-C12-C13
3	C	303	OLA	C6-C7-C8-C9
2	C	301	LFA	C1-C2-C3-C4
2	A	517	LFA	C1-C2-C3-C4
2	A	519	LFA	C14-C15-C16-C17
2	A	512	LFA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	A	510	LFA	C1-C2-C3-C4
3	A	503	OLA	C6-C7-C8-C9
2	C	315	LFA	C2-C3-C4-C5
2	A	512	LFA	C9-C10-C11-C12
3	C	304	OLA	C5-C6-C7-C8
3	A	506	OLA	C4-C5-C6-C7
2	A	517	LFA	C2-C3-C4-C5
2	B	302	LFA	C6-C7-C8-C9
2	C	306	LFA	C3-C4-C5-C6
3	C	302	OLA	C4-C5-C6-C7
3	C	305	OLA	C11-C10-C9-C8
2	A	521	LFA	C14-C15-C16-C17
3	B	308	OLA	C5-C6-C7-C8
2	B	314	LFA	C11-C12-C13-C14
2	B	316	LFA	C13-C14-C15-C16
3	A	507	OLA	C3-C4-C5-C6
3	A	505	OLA	C11-C10-C9-C8
3	C	302	OLA	C5-C6-C7-C8
2	A	501	LFA	C15-C16-C17-C18
2	A	513	LFA	C3-C4-C5-C6
3	A	504	OLA	C15-C16-C17-C18
3	C	303	OLA	C11-C12-C13-C14
3	B	307	OLA	C5-C6-C7-C8
2	B	309	LFA	C2-C3-C4-C5
2	B	312	LFA	C17-C18-C19-C20
2	C	312	LFA	C10-C11-C12-C13
2	B	318	LFA	C4-C5-C6-C7
2	C	312	LFA	C3-C4-C5-C6
3	C	305	OLA	C2-C3-C4-C5
3	C	305	OLA	C3-C4-C5-C6
2	A	509	LFA	C5-C6-C7-C8
3	C	304	OLA	C11-C10-C9-C8
2	C	311	LFA	C1-C2-C3-C4
3	A	507	OLA	C12-C13-C14-C15
3	A	504	OLA	C6-C7-C8-C9
3	B	303	OLA	C5-C6-C7-C8
3	C	304	OLA	C2-C3-C4-C5
2	C	307	LFA	C7-C8-C9-C10
2	A	512	LFA	C5-C6-C7-C8
2	B	318	LFA	C9-C10-C11-C12
2	A	510	LFA	C6-C7-C8-C9
2	A	512	LFA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	C	306	LFA	C5-C6-C7-C8
2	C	311	LFA	C5-C6-C7-C8
2	A	515	LFA	C1-C2-C3-C4
2	C	306	LFA	C4-C5-C6-C7
2	C	314	LFA	C7-C8-C9-C10
2	C	301	LFA	C14-C15-C16-C17
3	A	507	OLA	C5-C6-C7-C8
2	C	307	LFA	C11-C10-C9-C8
3	A	505	OLA	C10-C11-C12-C13
3	B	308	OLA	C10-C11-C12-C13
3	B	308	OLA	C13-C14-C15-C16
2	C	311	LFA	C2-C3-C4-C5
3	A	504	OLA	C2-C3-C4-C5
3	B	308	OLA	C11-C10-C9-C8
2	A	519	LFA	C15-C16-C17-C18
2	B	322	LFA	C11-C10-C9-C8
3	C	303	OLA	C11-C10-C9-C8
2	B	309	LFA	C1-C2-C3-C4
3	A	504	OLA	C1-C2-C3-C4
3	B	305	OLA	C4-C5-C6-C7
3	B	304	OLA	C11-C10-C9-C8
2	B	313	LFA	C4-C5-C6-C7
3	B	304	OLA	C7-C8-C9-C10
3	A	507	OLA	C2-C3-C4-C5
3	A	507	OLA	C7-C8-C9-C10
3	A	506	OLA	O1-C1-C2-C3
2	A	521	LFA	C15-C16-C17-C18
3	C	303	OLA	C1-C2-C3-C4
2	C	301	LFA	C11-C10-C9-C8
3	B	307	OLA	C9-C10-C11-C12
3	A	504	OLA	C4-C5-C6-C7
3	C	303	OLA	C2-C3-C4-C5
2	A	515	LFA	C2-C3-C4-C5
3	A	505	OLA	O1-C1-C2-C3
3	B	308	OLA	C12-C13-C14-C15
2	B	314	LFA	C2-C3-C4-C5
3	C	303	OLA	C7-C8-C9-C10
3	C	305	OLA	C7-C8-C9-C10
3	A	506	OLA	O2-C1-C2-C3
2	C	316	LFA	C6-C7-C8-C9
3	B	305	OLA	C1-C2-C3-C4
2	C	301	LFA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	505	OLA	C2-C3-C4-C5
3	B	306	OLA	C7-C8-C9-C10
2	A	501	LFA	C17-C18-C19-C20
3	A	503	OLA	C1-C2-C3-C4
3	A	505	OLA	C9-C10-C11-C12
3	B	303	OLA	C7-C8-C9-C10
3	A	504	OLA	O2-C1-C2-C3
3	A	504	OLA	O1-C1-C2-C3
2	B	321	LFA	C3-C4-C5-C6
2	B	318	LFA	C3-C4-C5-C6
2	B	317	LFA	C6-C7-C8-C9
3	A	505	OLA	C7-C8-C9-C10
2	B	315	LFA	C5-C6-C7-C8
3	A	505	OLA	O2-C1-C2-C3
3	C	302	OLA	O1-C1-C2-C3
3	C	302	OLA	C1-C2-C3-C4
3	C	302	OLA	O2-C1-C2-C3
3	A	504	OLA	C3-C4-C5-C6
3	B	308	OLA	C9-C10-C11-C12
3	B	304	OLA	C3-C4-C5-C6
3	C	303	OLA	C9-C10-C11-C12
3	B	308	OLA	O2-C1-C2-C3
3	A	507	OLA	C14-C15-C16-C17
2	C	301	LFA	C5-C6-C7-C8
3	A	503	OLA	O2-C1-C2-C3
2	B	317	LFA	C12-C13-C14-C15
3	A	503	OLA	O1-C1-C2-C3
3	B	308	OLA	O1-C1-C2-C3
2	B	317	LFA	C4-C5-C6-C7
3	B	306	OLA	O2-C1-C2-C3
3	C	305	OLA	O1-C1-C2-C3
3	C	303	OLA	O2-C1-C2-C3
3	C	302	OLA	C11-C12-C13-C14
3	C	304	OLA	O2-C1-C2-C3

There are no ring outliers.

23 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	515	LFA	1	0
3	A	506	OLA	2	0
2	A	520	LFA	1	0

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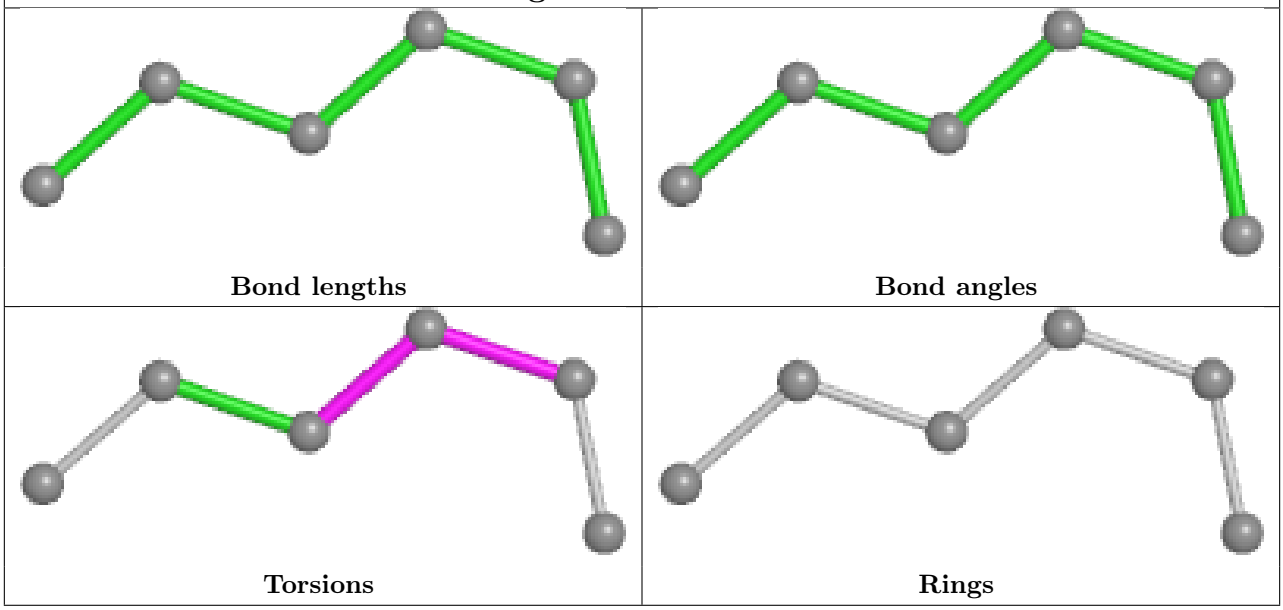
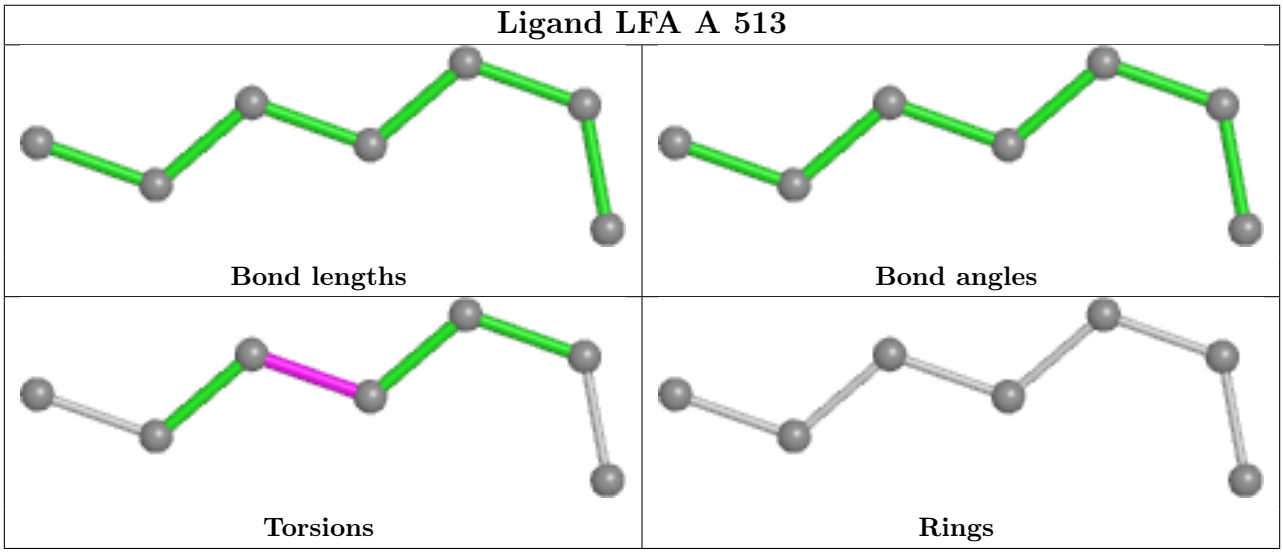
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	315	LFA	1	0
2	C	312	LFA	1	0
3	A	505	OLA	3	0
2	B	321	LFA	2	0
3	A	507	OLA	2	0
3	B	305	OLA	2	0
2	A	519	LFA	2	0
3	C	305	OLA	5	0
3	B	308	OLA	2	0
2	C	309	LFA	3	0
2	B	319	LFA	1	0
3	A	504	OLA	1	0
3	B	304	OLA	1	0
2	B	323	LFA	3	0
2	B	314	LFA	2	0
2	C	301	LFA	1	0
2	B	322	LFA	3	0
3	A	508	OLA	3	0
2	A	517	LFA	2	0
2	C	311	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.

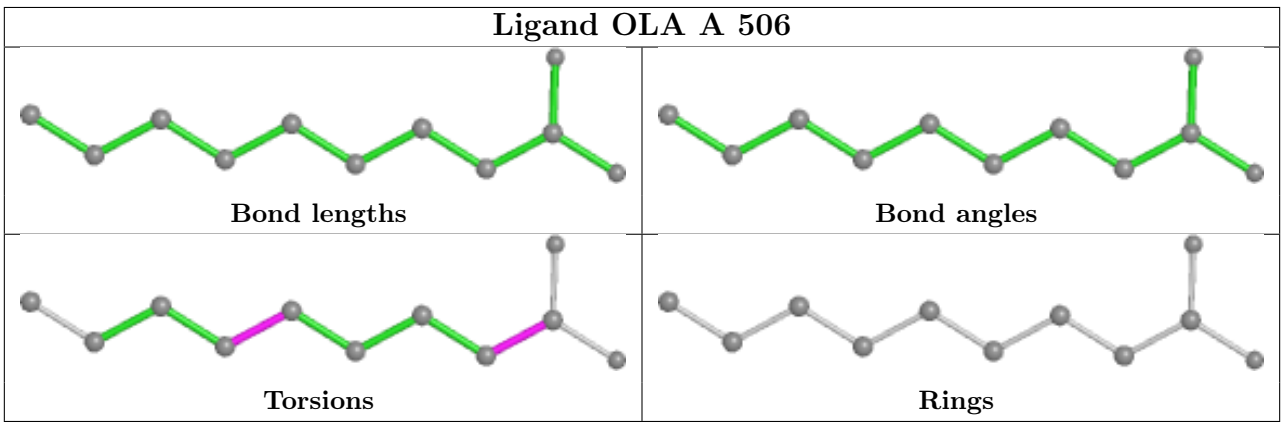
Ligand LFA A 515



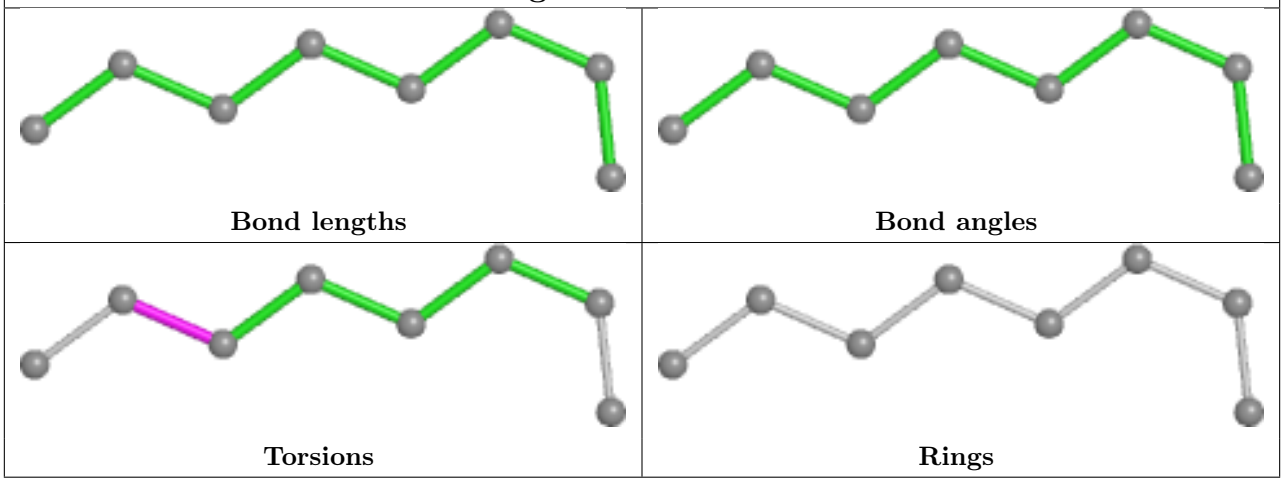
Ligand LFA A 513



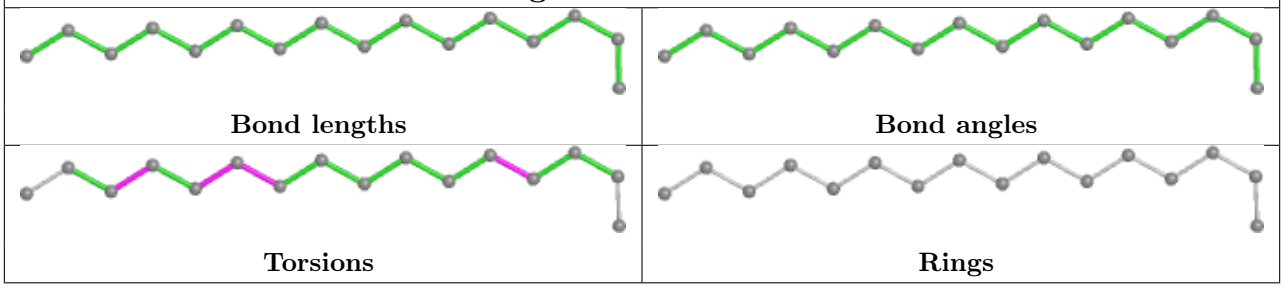
Ligand OLA A 506



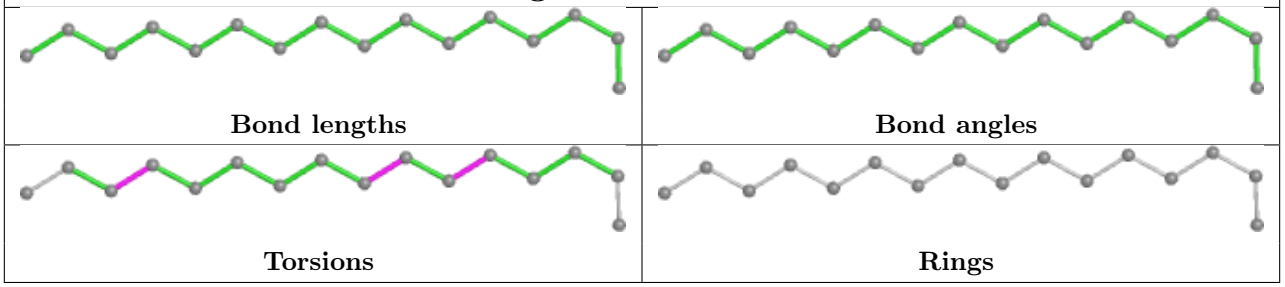
Ligand LFA B 315



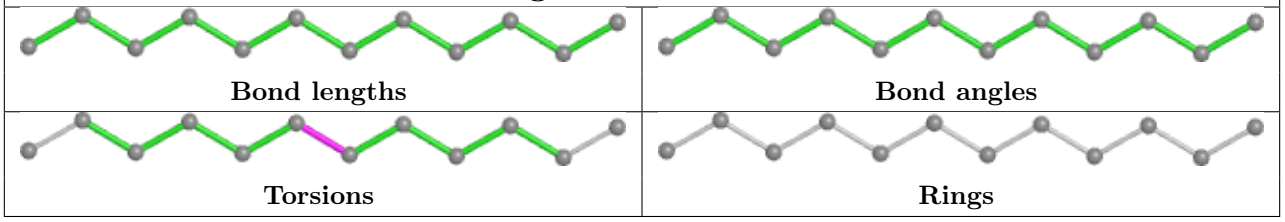
Ligand LFA C 312



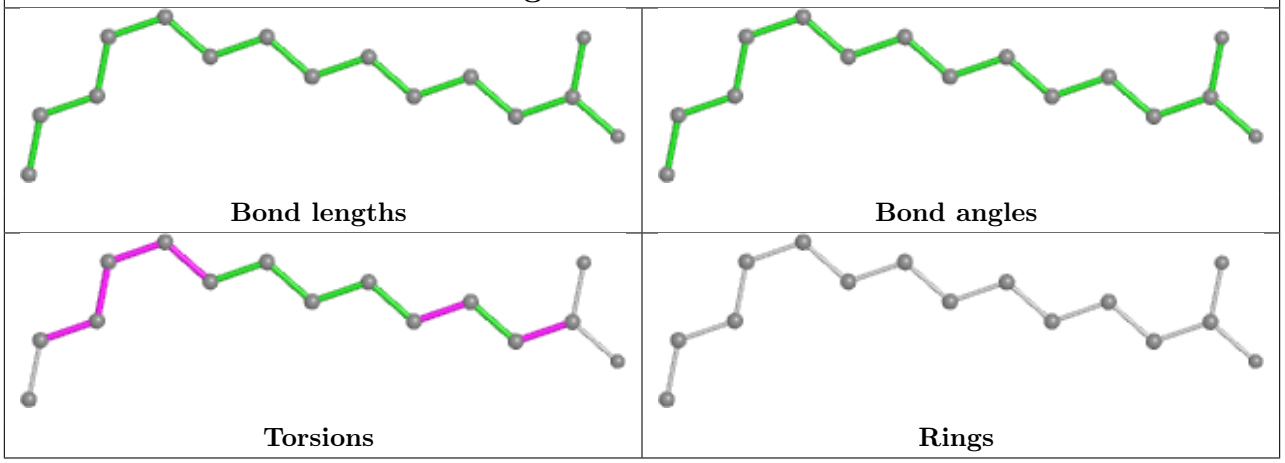
Ligand LFA B 317



Ligand LFA B 320



Ligand OLA A 505



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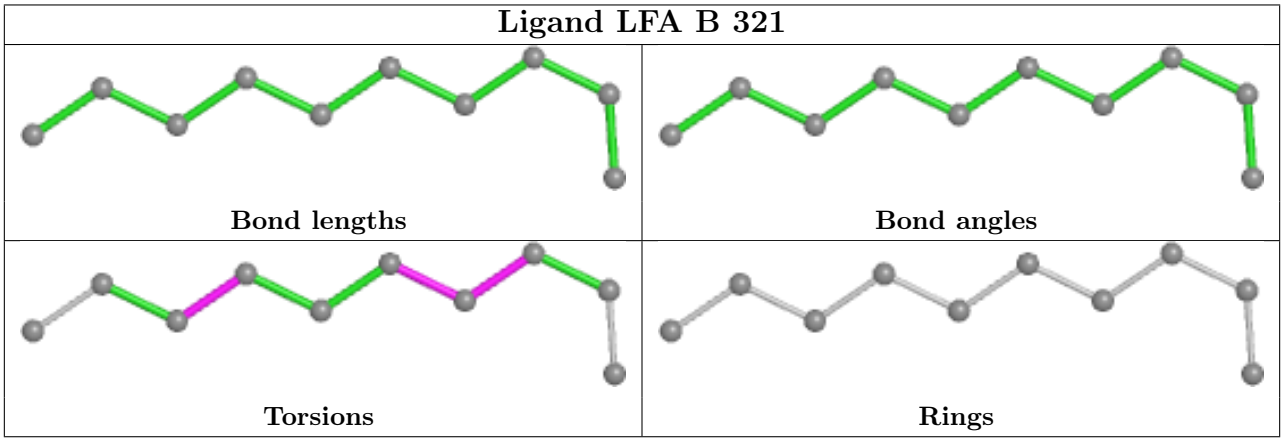

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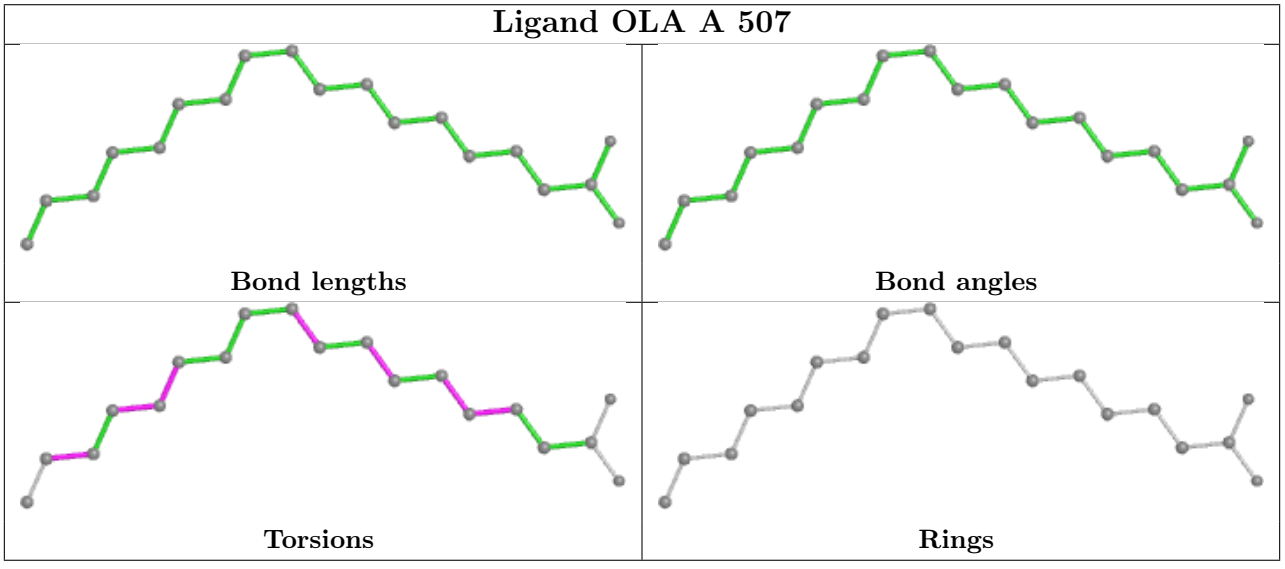

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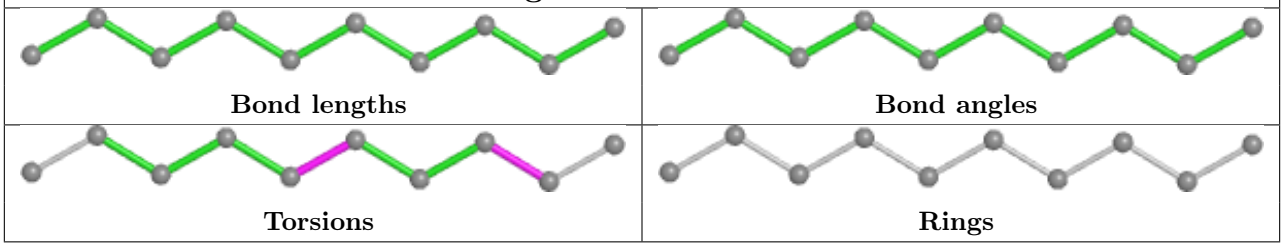
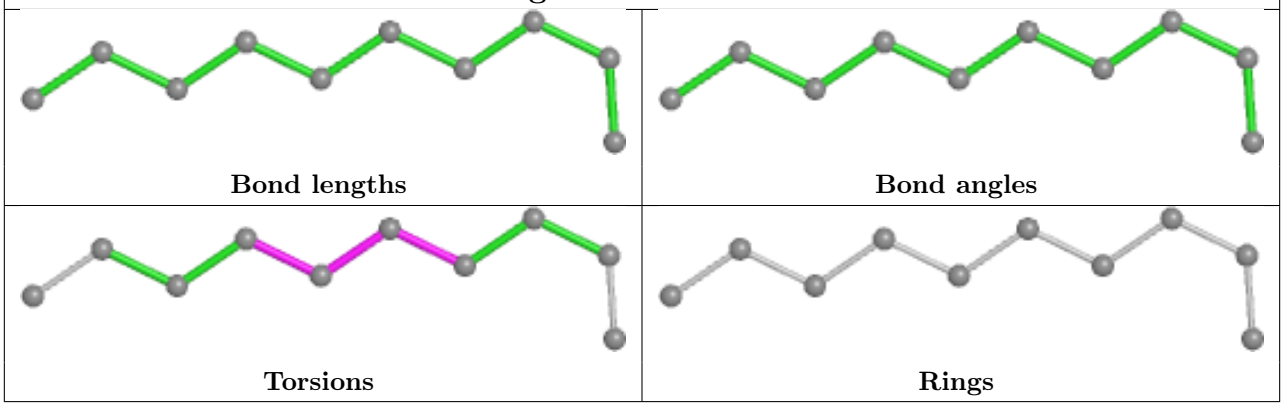


Ligand LFA C 306



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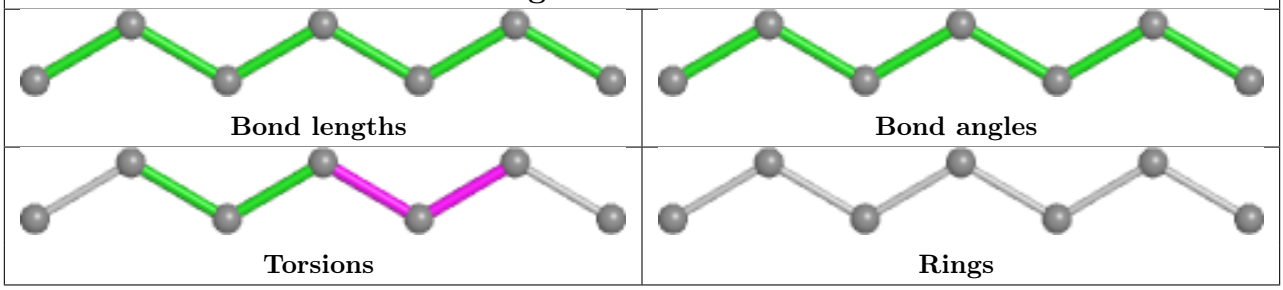
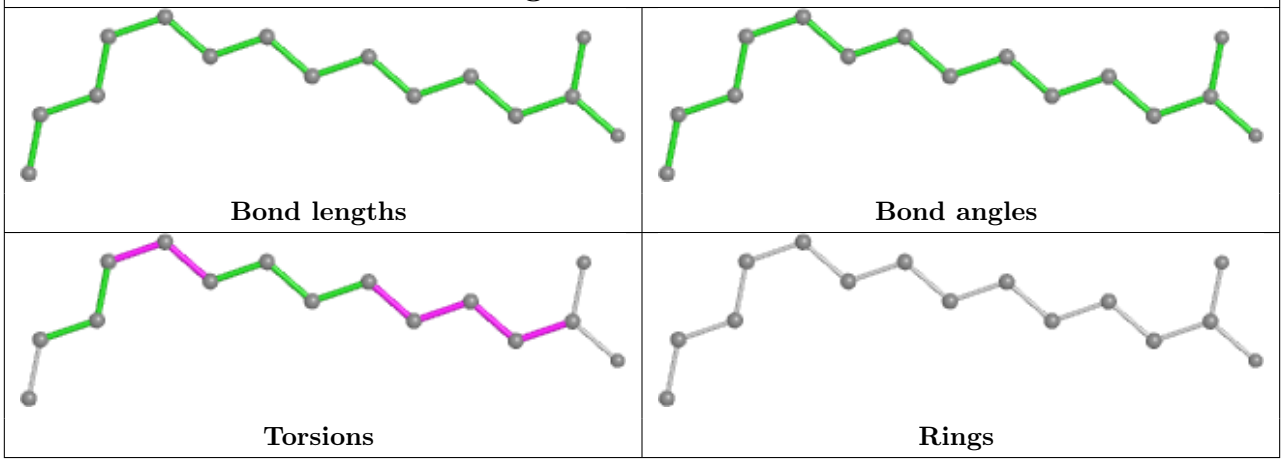
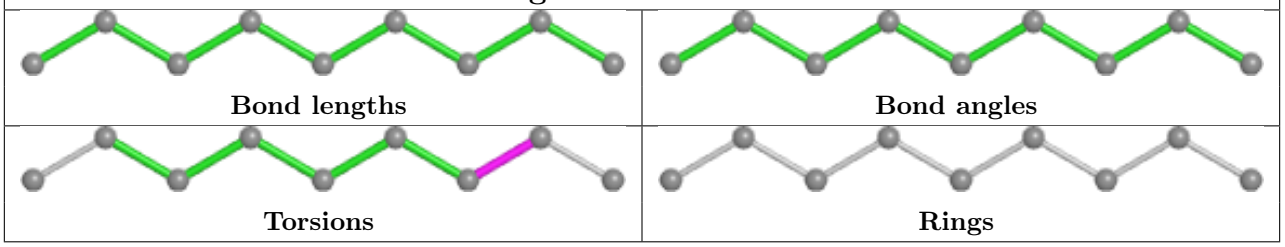


Ligand OLA C 305



Ligand LFA C 315



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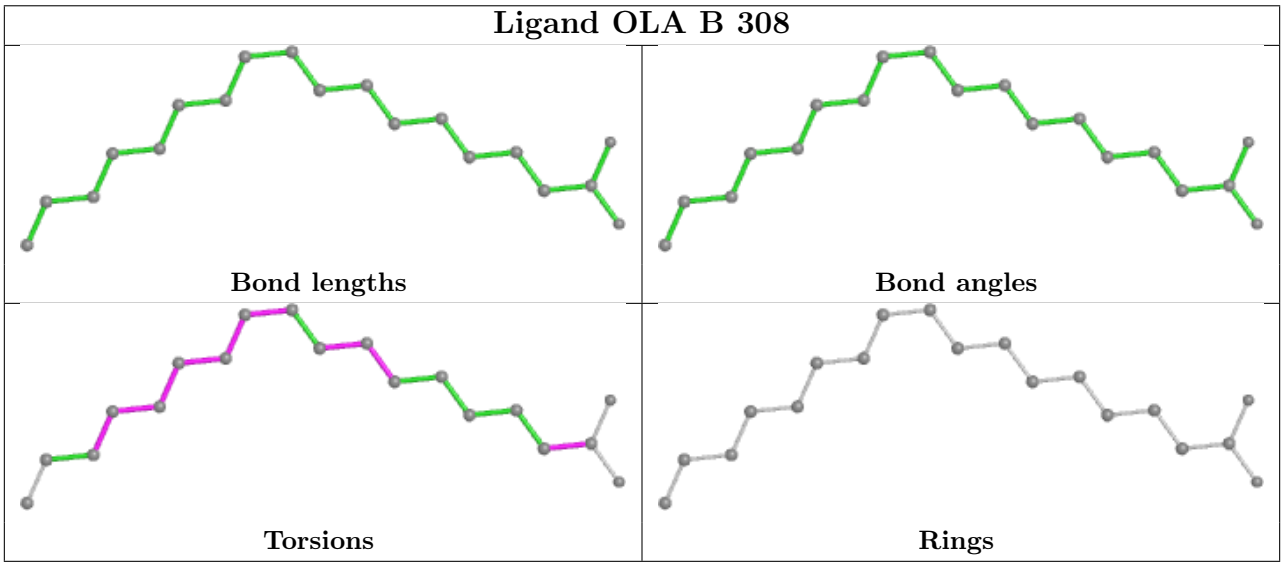
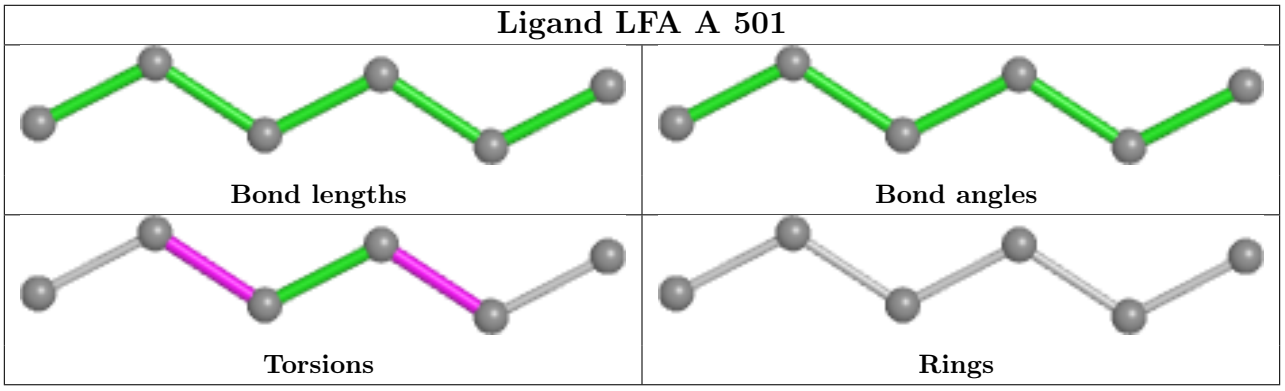


Ligand LFA A 501



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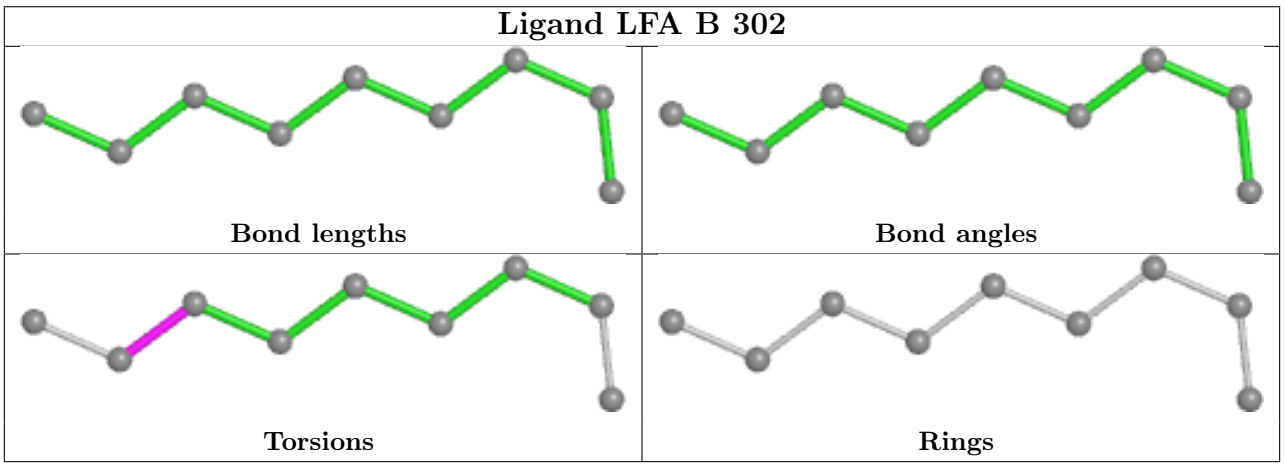
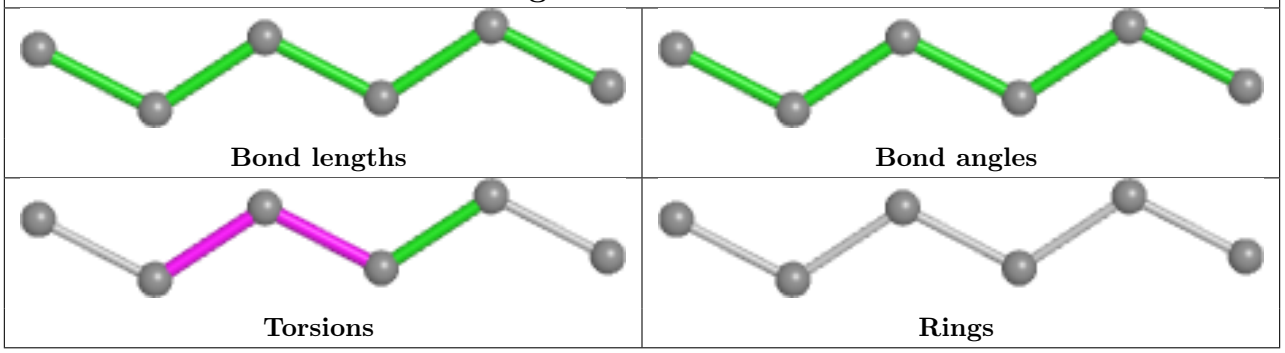


Ligand LFA B 313



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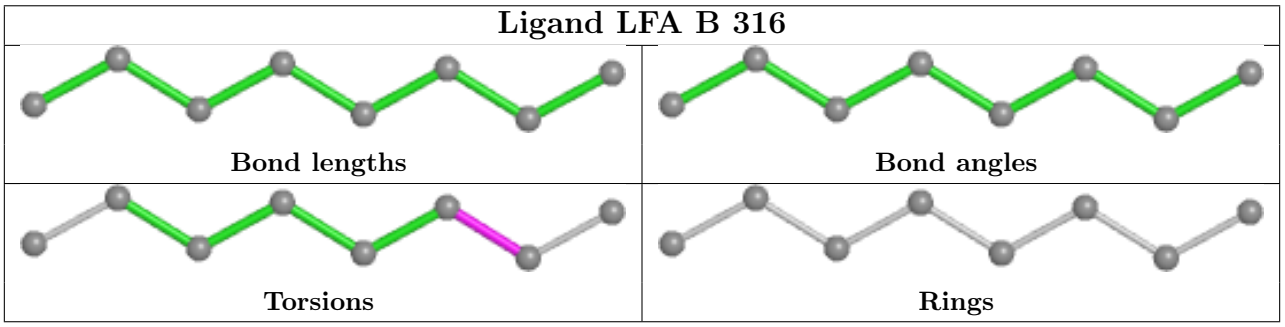

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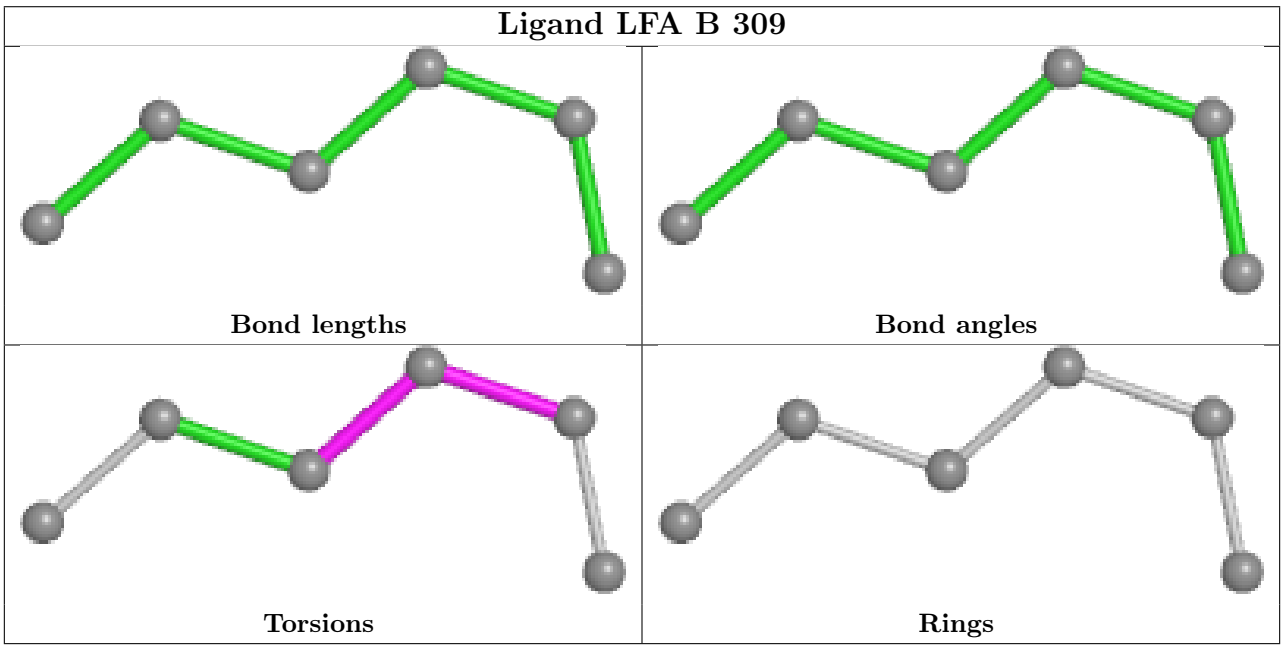

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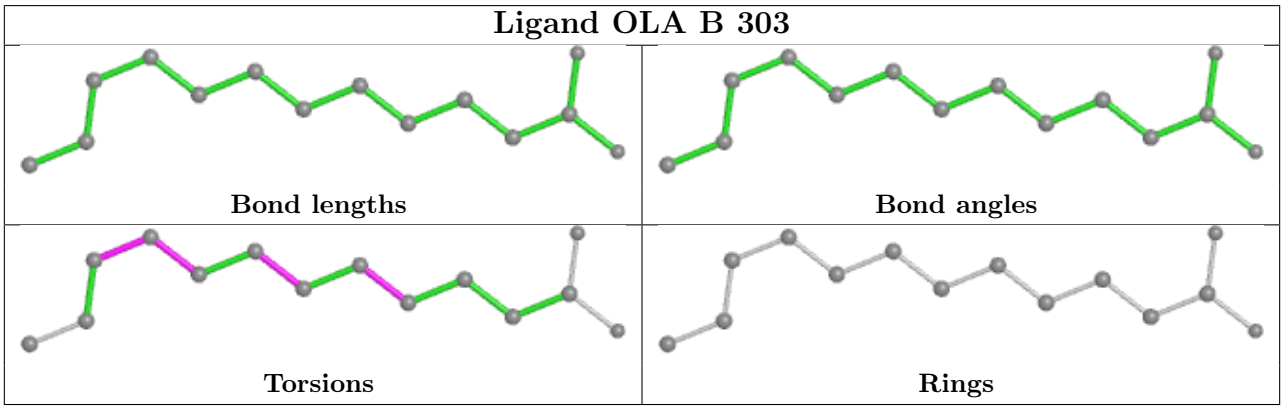

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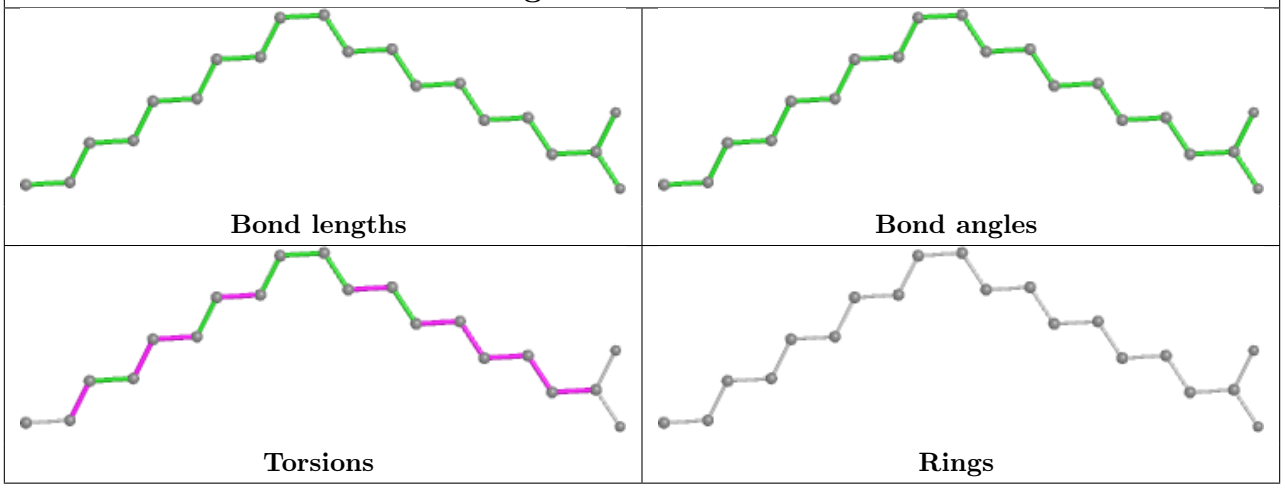

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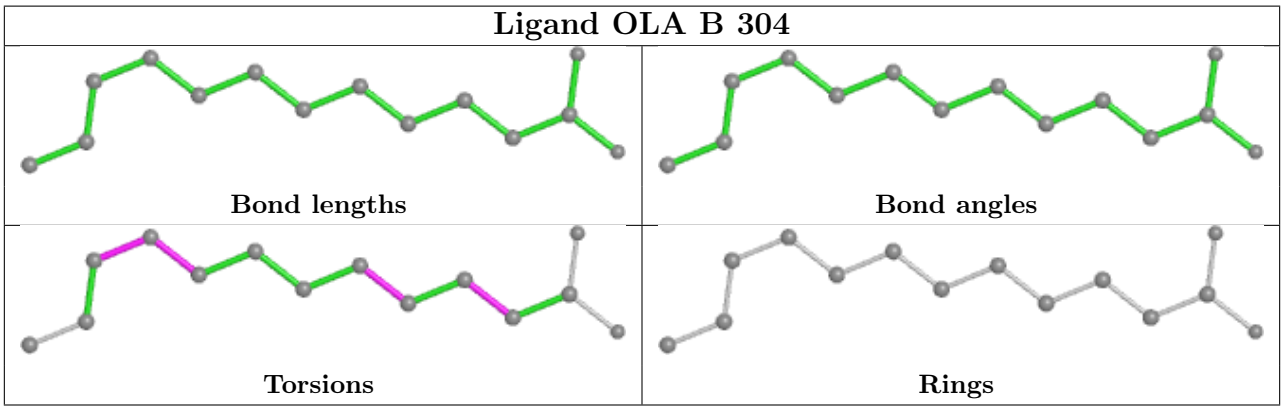

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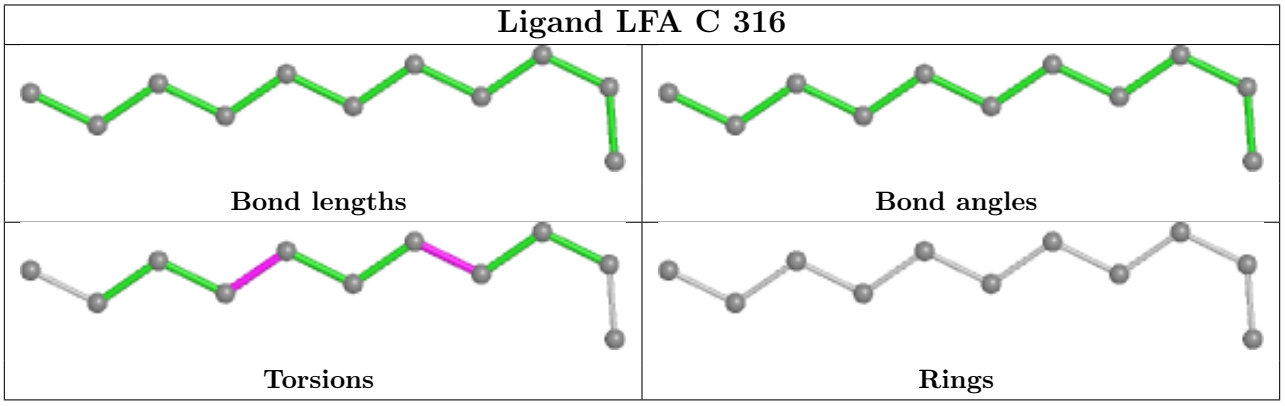

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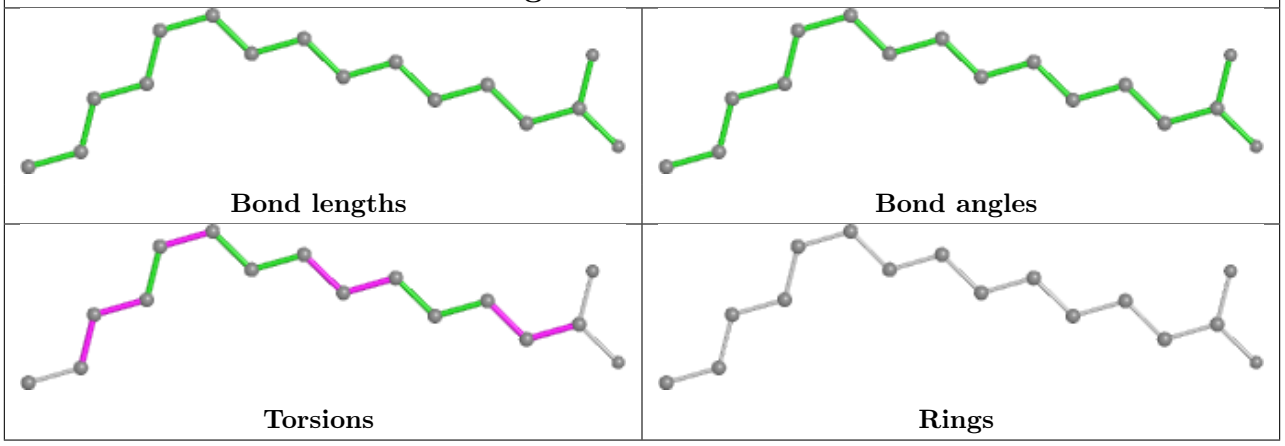

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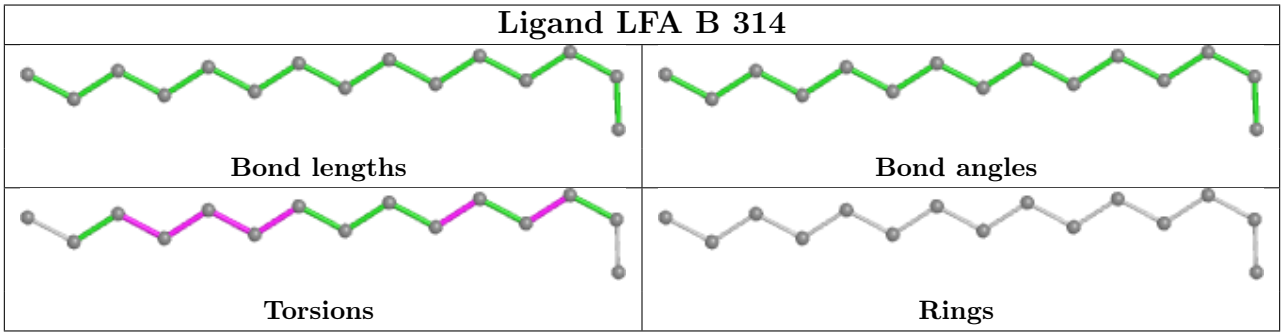
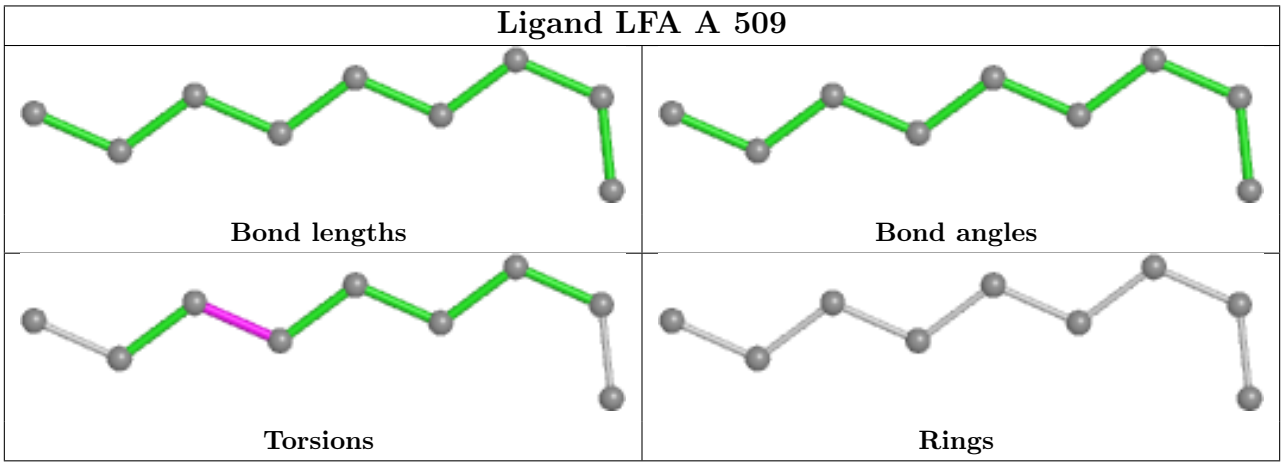
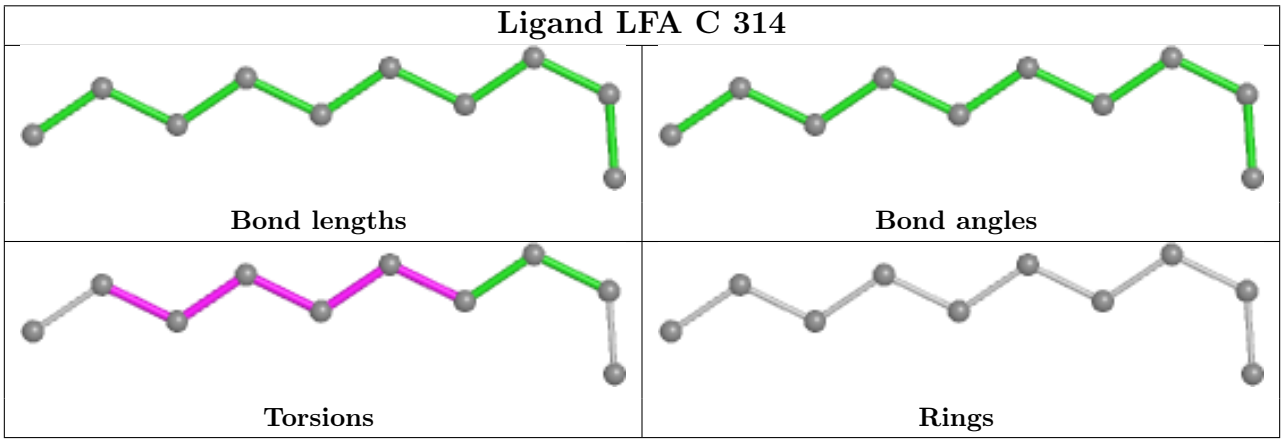


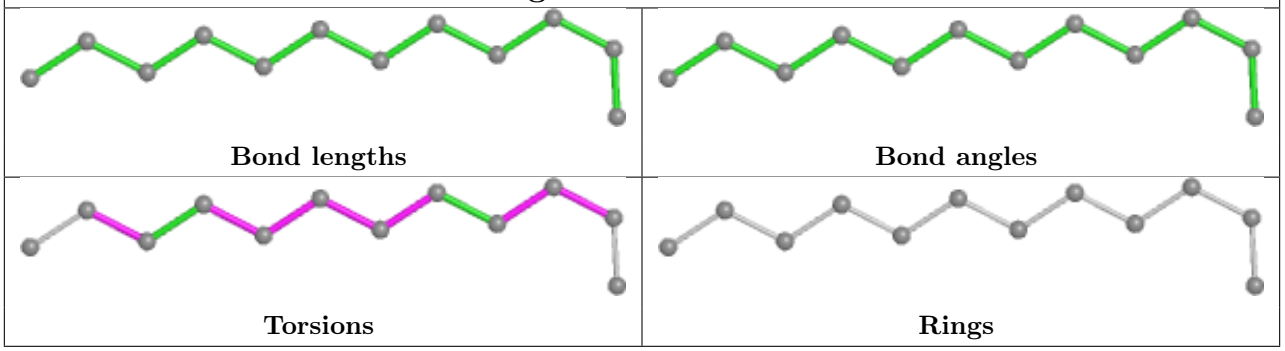
Ligand LFA A 509



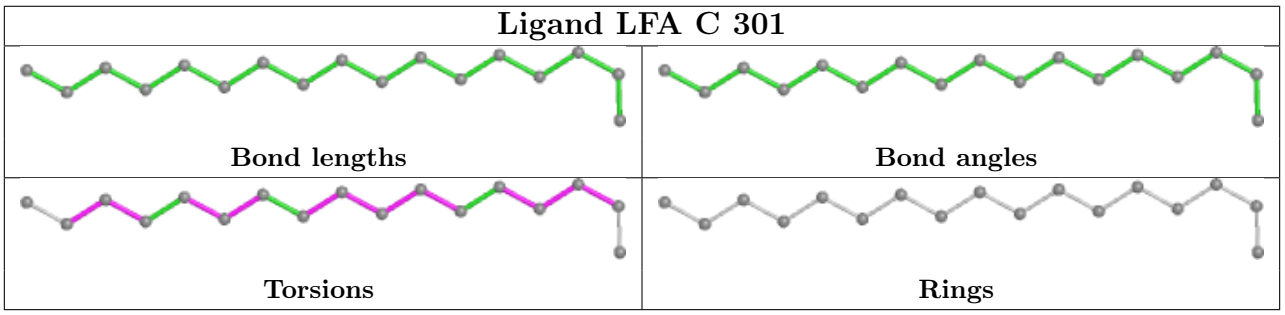
Ligand LFA C 314



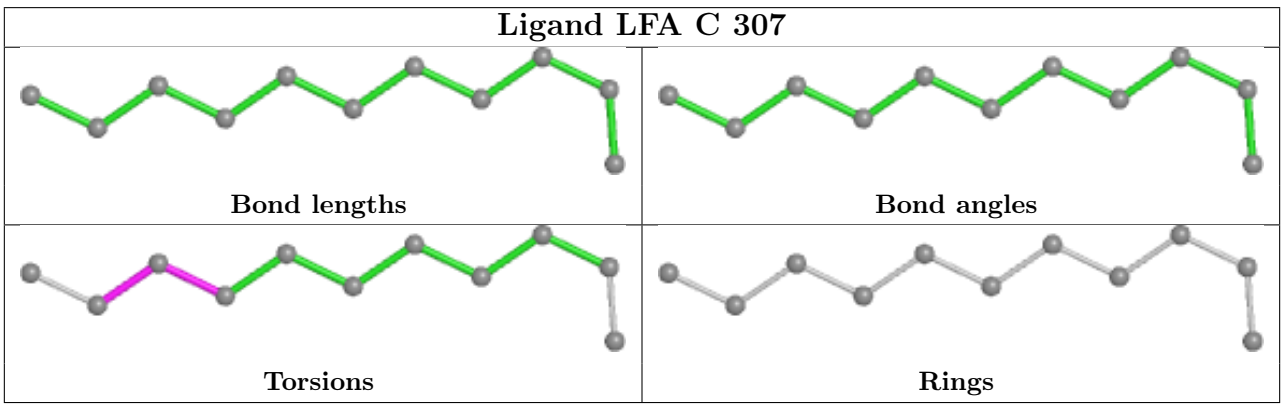
Ligand LFA A 512



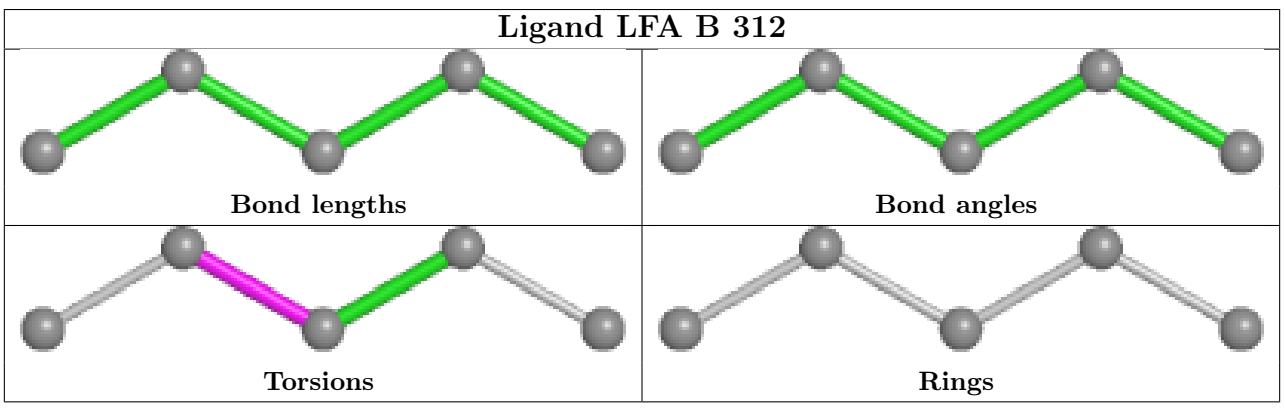
Ligand LFA C 301



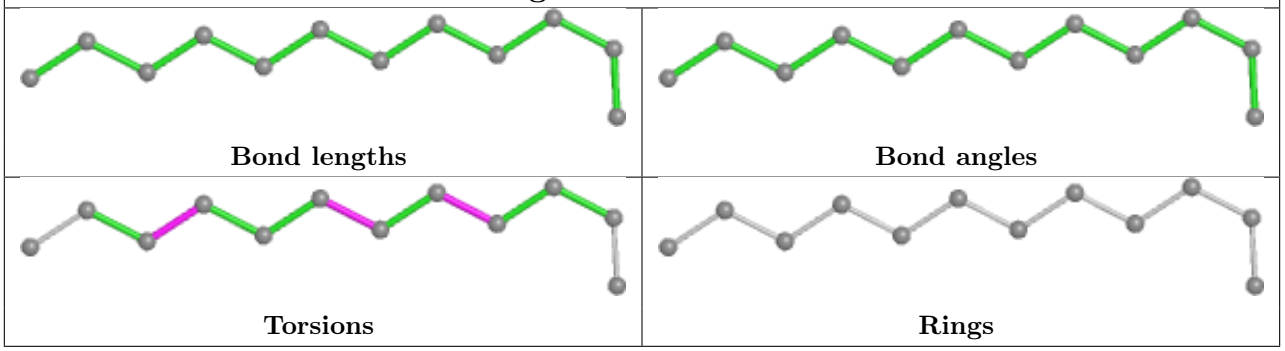
Ligand LFA C 307



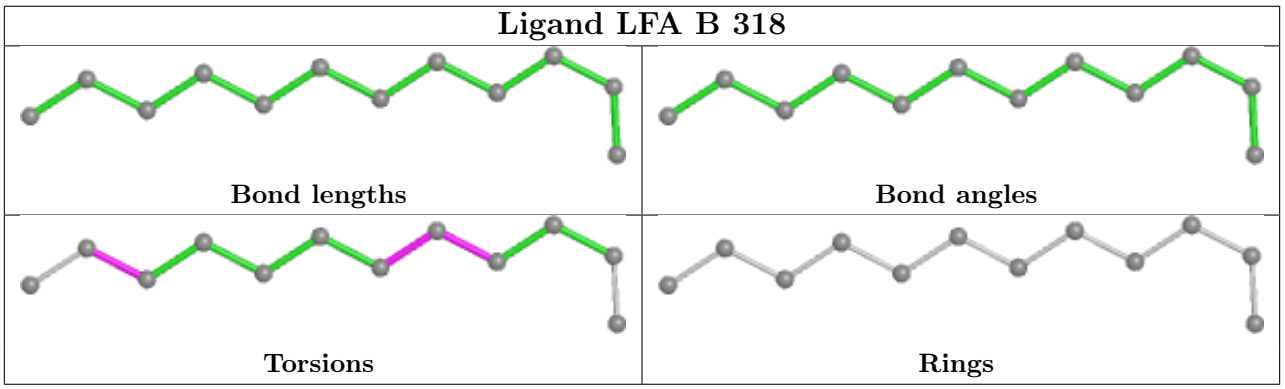
Ligand LFA B 312



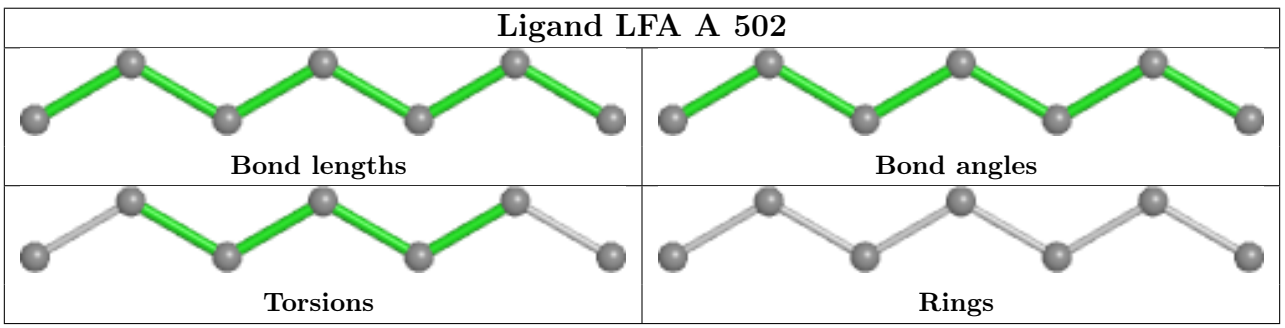
Ligand LFA C 313



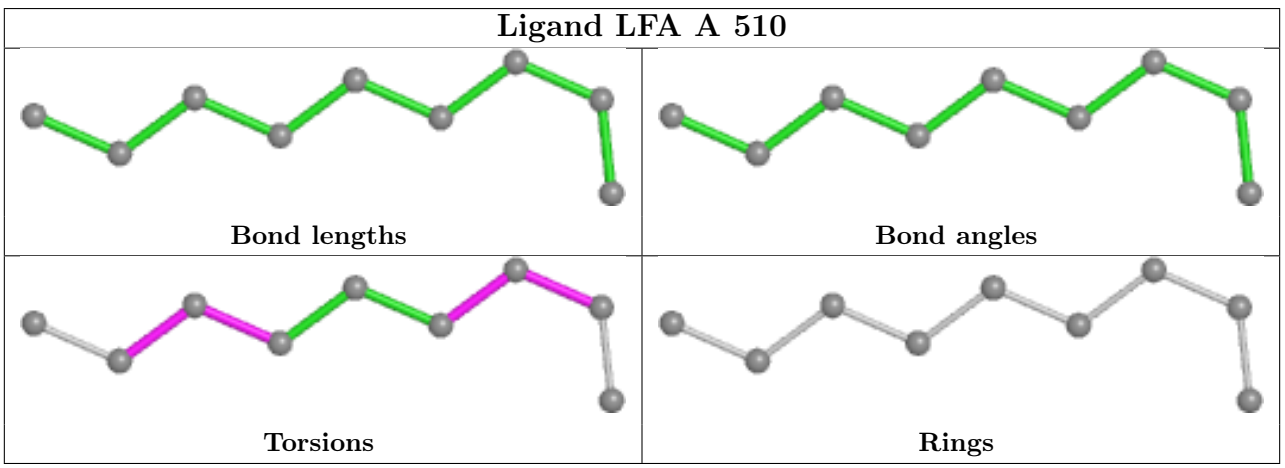
Ligand LFA B 318



Ligand LFA A 502

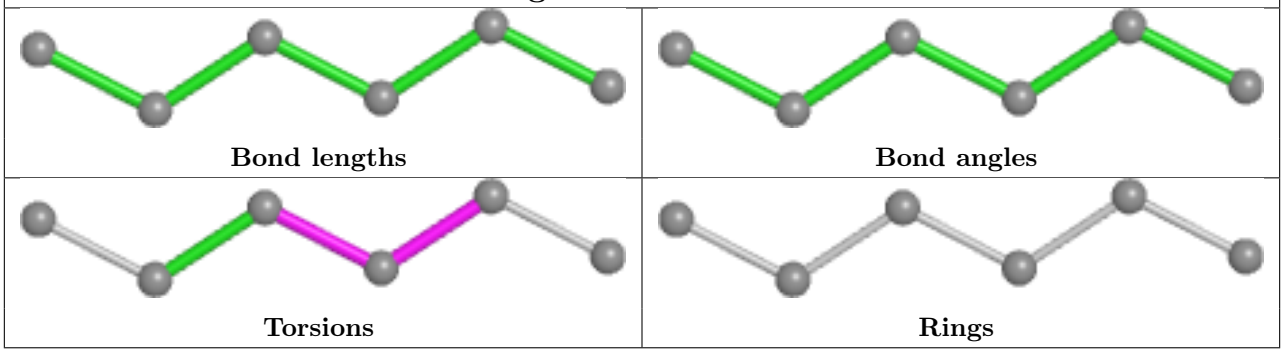


Ligand LFA A 510

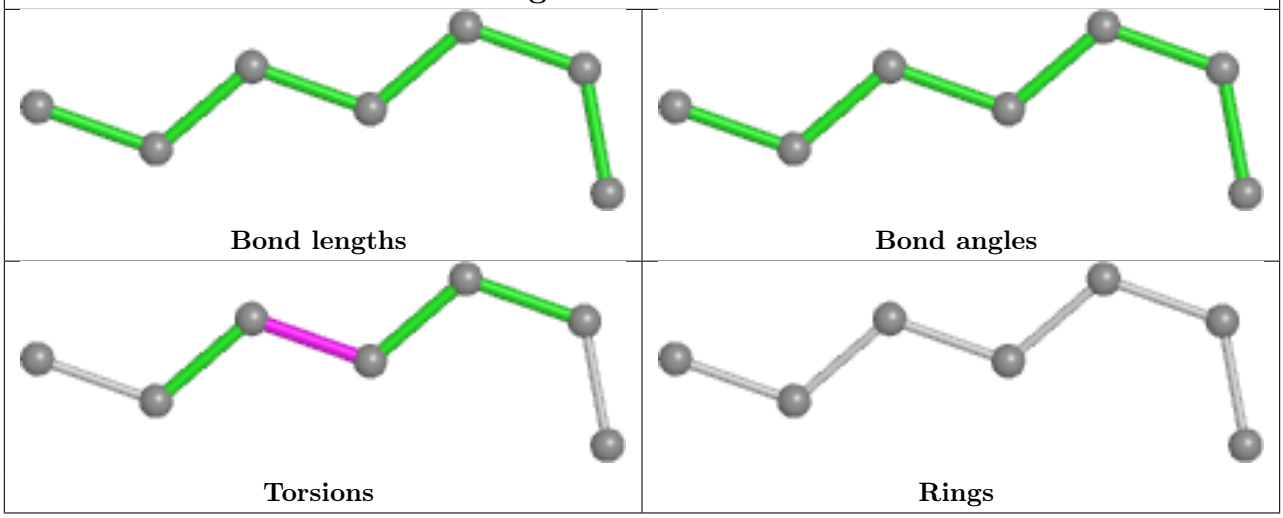


Ligand OLA A 503

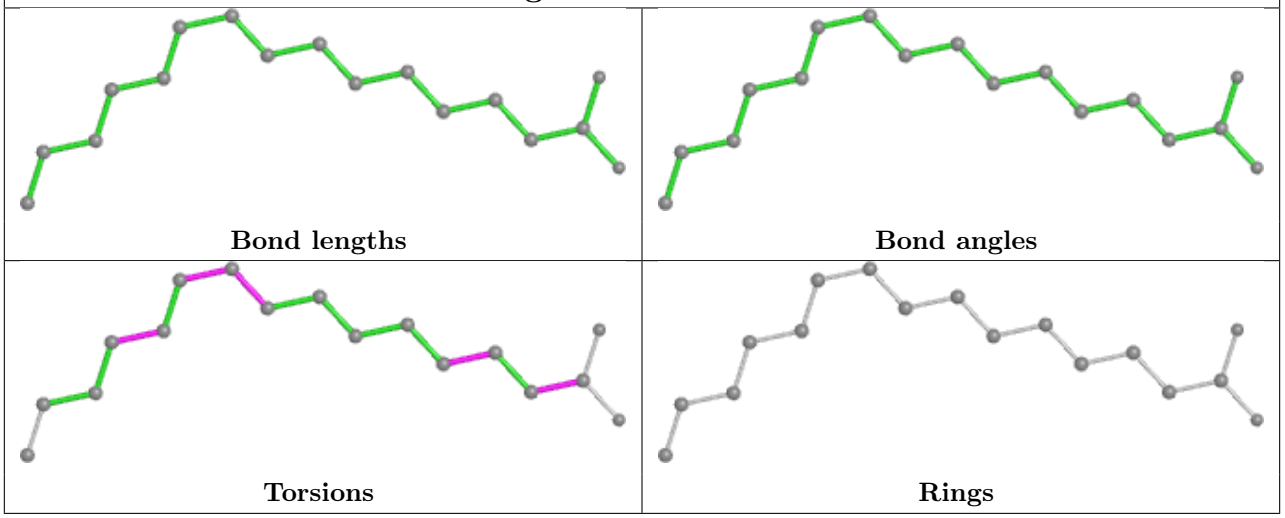
Ligand LFA A 521



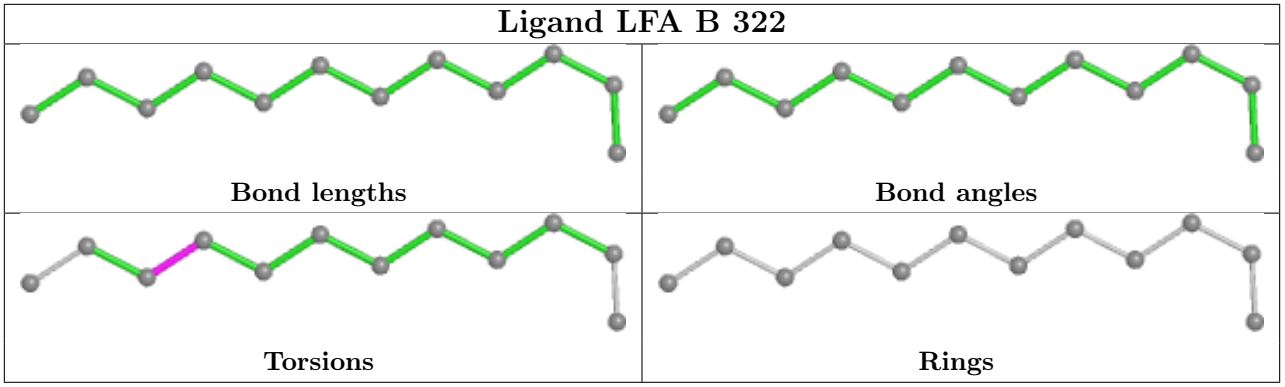
Ligand LFA B 310



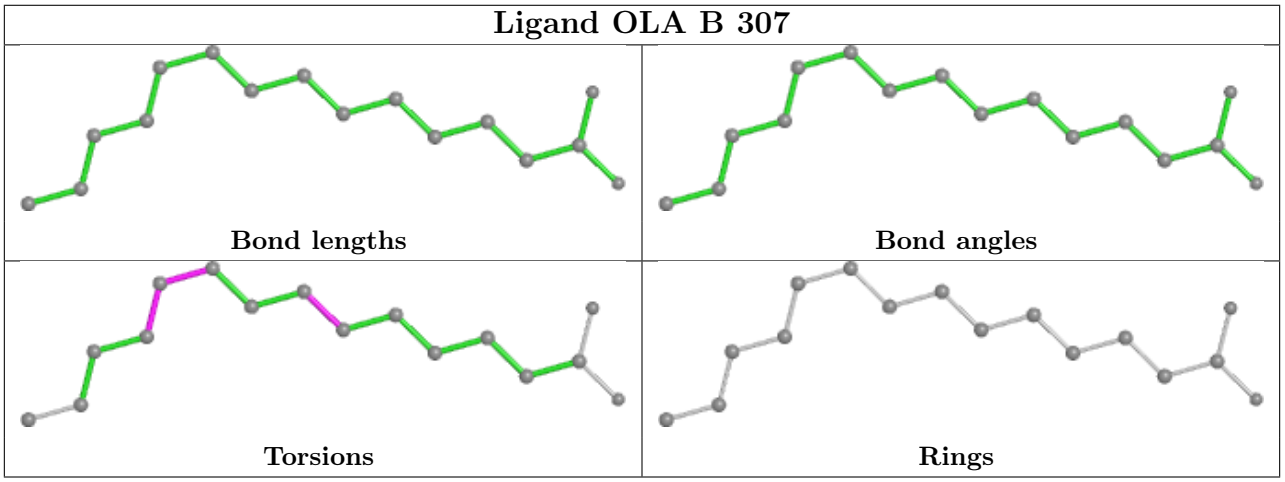
Ligand OLA B 306



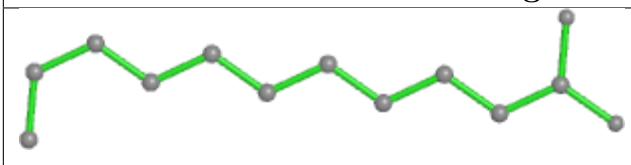
Ligand LFA B 322



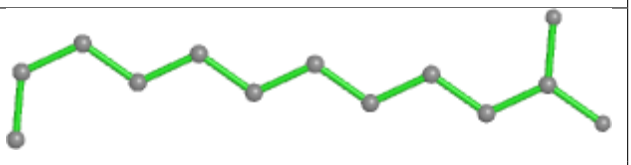
Ligand OLA B 307



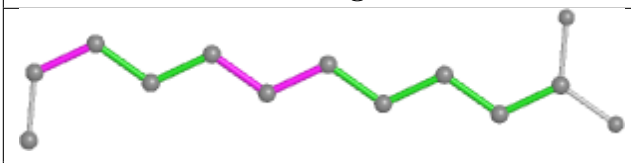
Ligand OLA A 508



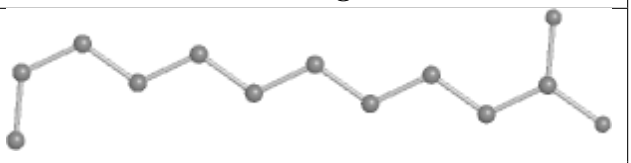
Bond lengths



Bond angles

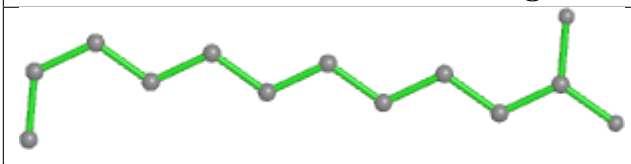


Torsions

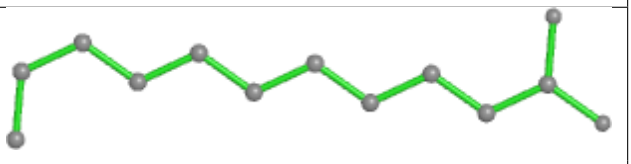


Rings

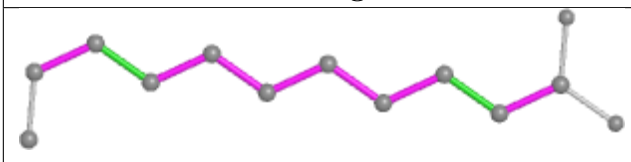
Ligand OLA C 304



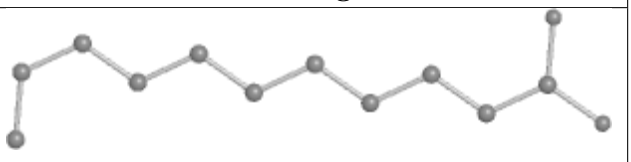
Bond lengths



Bond angles

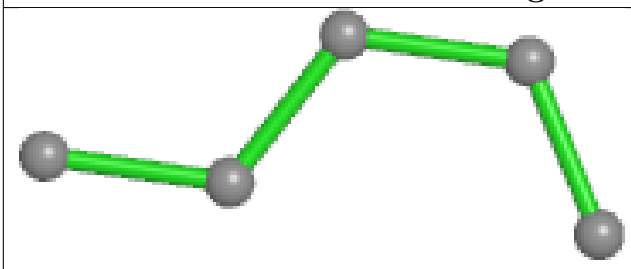


Torsions

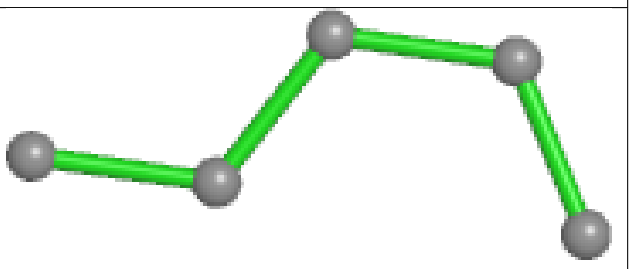


Rings

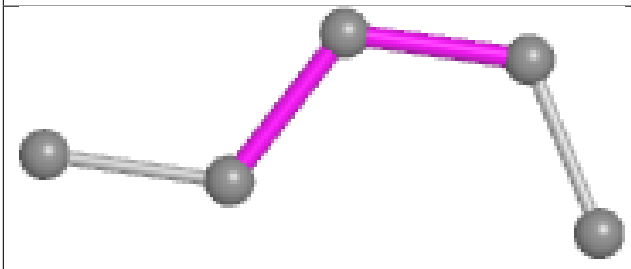
Ligand LFA A 517



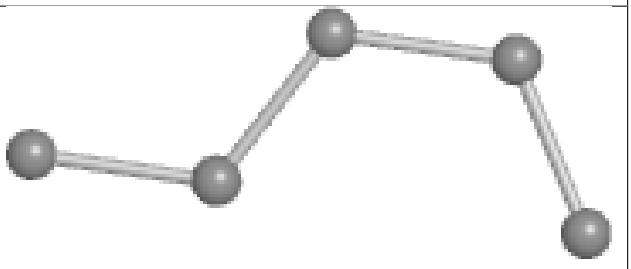
Bond lengths



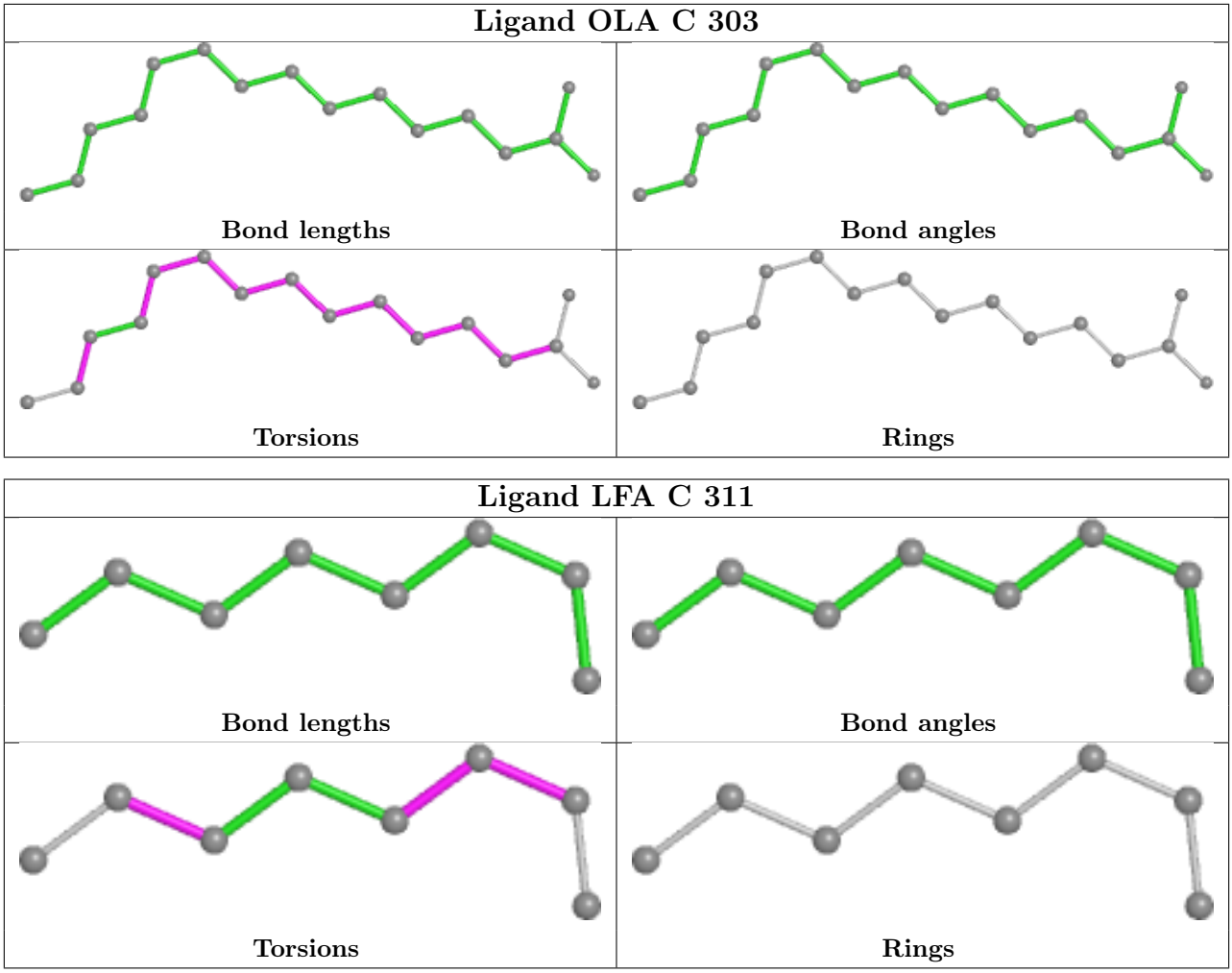
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	221/229 (96%)	0.22	15 (6%)	17	19	22, 29, 49, 86	0
1	B	218/229 (95%)	0.13	7 (3%)	47	52	22, 31, 49, 81	0
1	C	221/229 (96%)	0.23	17 (7%)	13	15	23, 32, 52, 94	0
All	All	660/687 (96%)	0.19	39 (5%)	22	24	22, 31, 51, 94	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	TYR	8.4
1	C	61	TYR	7.4
1	A	121	ILE	5.7
1	C	189	LEU	5.7
1	B	60	GLN	5.3
1	A	62	ASP	5.2
1	A	64	THR	4.9
1	B	59	PHE	4.6
1	A	59	PHE	4.6
1	B	223	GLN	4.5
1	C	64	THR	4.2
1	C	187	LEU	4.0
1	B	64	THR	4.0
1	A	63	ASP	3.5
1	C	60	GLN	3.4
1	A	108	VAL	3.3
1	C	188	GLY	3.2
1	C	173[A]	TRP	3.1
1	A	75	VAL	3.0
1	C	192	GLU	3.0
1	A	60	GLN	3.0
1	A	105	ALA	2.9
1	B	121	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	191	GLN	2.8
1	C	121	ILE	2.8
1	C	186	GLY	2.7
1	C	123	THR	2.6
1	C	223	GLN	2.6
1	A	58	LEU	2.6
1	A	173[A]	TRP	2.6
1	C	224	SER	2.6
1	B	222	HIS	2.4
1	B	173[A]	TRP	2.4
1	A	104	VAL	2.4
1	C	59	PHE	2.3
1	C	190	ALA	2.2
1	A	111	ILE	2.2
1	A	76	ILE	2.1
1	C	75	VAL	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, 95^{th} 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	A	1	10/11	0.88	0.21	41,51,93,108	0
1	LYR	C	207	29/30	0.89	0.11	26,32,38,42	0
1	FME	C	1	10/11	0.90	0.23	43,50,86,100	0
1	LYR	A	207	29/30	0.91	0.12	21,29,41,44	0
1	LYR	B	207	29/30	0.92	0.11	23,28,36,42	0
1	FME	B	1	10/11	0.93	0.16	42,54,92,92	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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
3	OLA	B	307	16/20	0.50	0.30	46,52,61,66	0
2	LFA	A	513	7/20	0.52	0.27	49,54,57,59	0
2	LFA	C	307	11/20	0.54	0.21	67,75,85,86	0
2	LFA	B	313	6/20	0.57	0.16	54,66,68,72	0
3	OLA	A	504	20/20	0.59	0.30	41,54,66,68	0
2	LFA	C	312	16/20	0.60	0.23	52,63,74,75	0
3	OLA	C	302	16/20	0.60	0.24	41,48,59,61	0
3	OLA	B	306	17/20	0.62	0.28	45,52,64,67	0
2	LFA	C	310	4/20	0.65	0.27	52,57,59,59	0
2	LFA	B	309	6/20	0.65	0.21	54,55,56,56	0
3	OLA	A	506	11/20	0.66	0.18	47,59,69,74	0
3	OLA	C	304	13/20	0.66	0.21	42,55,73,77	0
3	OLA	C	305	15/20	0.66	0.23	52,64,74,75	0
3	OLA	B	308	19/20	0.67	0.26	46,57,76,88	0
2	LFA	B	323	13/20	0.68	0.19	56,65,73,73	0
2	LFA	A	518	7/20	0.68	0.36	42,52,57,57	0
2	LFA	B	315	8/20	0.68	0.22	47,52,57,57	0
2	LFA	B	317	16/20	0.69	0.18	53,64,74,76	0
2	LFA	A	520	10/20	0.71	0.13	62,70,75,76	0
3	OLA	A	507	19/20	0.71	0.32	38,54,69,69	0
3	OLA	B	305	10/20	0.71	0.19	34,59,67,73	0
2	LFA	A	509	9/20	0.73	0.24	60,66,74,74	0
3	OLA	A	503	11/20	0.73	0.15	42,51,59,65	0
2	LFA	C	306	10/20	0.73	0.19	56,59,66,69	0
3	OLA	B	303	14/20	0.74	0.17	44,55,65,71	0
2	LFA	C	316	11/20	0.74	0.43	60,64,70,74	0
3	OLA	C	303	16/20	0.75	0.18	52,62,73,82	0
3	OLA	B	304	14/20	0.75	0.15	44,52,64,64	0
3	OLA	A	505	15/20	0.75	0.14	43,54,90,96	0
2	LFA	A	517	5/20	0.76	0.20	46,49,54,62	0
2	LFA	C	315	9/20	0.77	0.24	48,63,67,71	0
2	LFA	B	316	8/20	0.78	0.22	56,57,60,61	0
2	LFA	A	502	7/20	0.78	0.44	44,51,55,56	0
2	LFA	B	310	7/20	0.78	0.14	53,56,61,62	0
2	LFA	C	314	10/20	0.80	0.34	52,57,66,66	0
2	LFA	A	512	12/20	0.80	0.14	40,52,61,62	0
2	LFA	A	519	7/20	0.80	0.14	53,54,60,61	0
2	LFA	A	510	9/20	0.81	0.18	48,52,59,60	0
3	OLA	A	508	13/20	0.81	0.15	47,64,75,80	0
2	LFA	A	511	7/20	0.83	0.10	46,48,51,53	0
2	LFA	A	514	8/20	0.83	0.13	54,59,64,69	0

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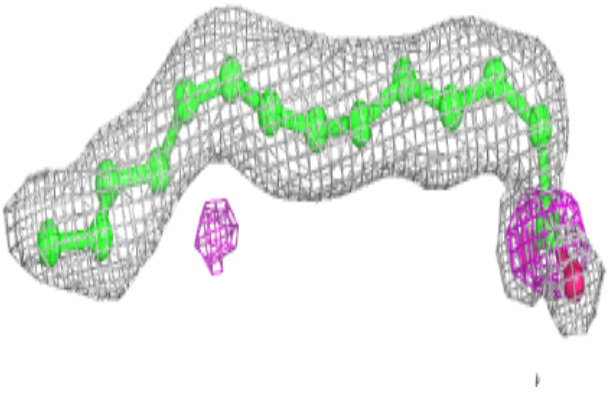
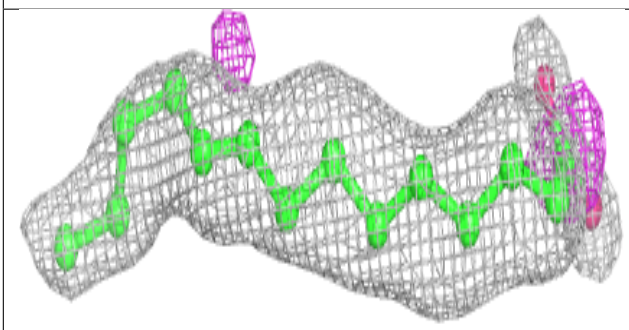
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LFA	C	308	4/20	0.84	0.15	51,54,54,58	0
2	LFA	C	313	12/20	0.84	0.22	43,49,52,52	0
2	LFA	B	318	12/20	0.84	0.14	46,57,63,65	0
2	LFA	C	301	17/20	0.85	0.34	43,49,57,60	0
2	LFA	B	302	9/20	0.86	0.33	51,54,57,60	0
2	LFA	B	319	9/20	0.86	0.22	57,58,63,67	0
2	LFA	B	320	12/20	0.86	0.11	55,61,64,66	0
2	LFA	A	516	3/20	0.86	0.28	62,62,62,62	0
2	LFA	B	314	15/20	0.86	0.18	42,52,70,75	0
2	LFA	B	322	12/20	0.87	0.11	48,52,66,68	0
2	LFA	C	309	8/20	0.87	0.10	55,61,64,64	0
2	LFA	C	311	8/20	0.88	0.14	57,59,63,64	0
2	LFA	B	321	10/20	0.88	0.16	46,57,66,66	0
2	LFA	A	515	6/20	0.89	0.26	45,54,55,58	0
2	LFA	B	312	5/20	0.90	0.32	57,58,61,62	0
2	LFA	A	501	6/20	0.90	0.19	49,49,53,55	0
2	LFA	B	311	5/20	0.91	0.10	49,50,51,58	0
2	LFA	A	521	6/20	0.92	0.13	48,53,59,61	0
2	LFA	B	301	6/20	0.93	0.18	42,44,49,53	0
4	PO4	C	317	5/5	0.94	0.21	73,73,78,79	5
4	PO4	A	522	5/5	0.96	0.24	108,109,111,113	5
5	NA	A	523[B]	1/1	0.98	0.05	16,16,16,16	1

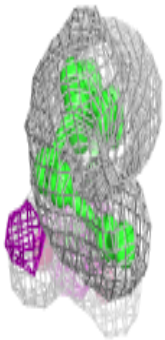
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA 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)

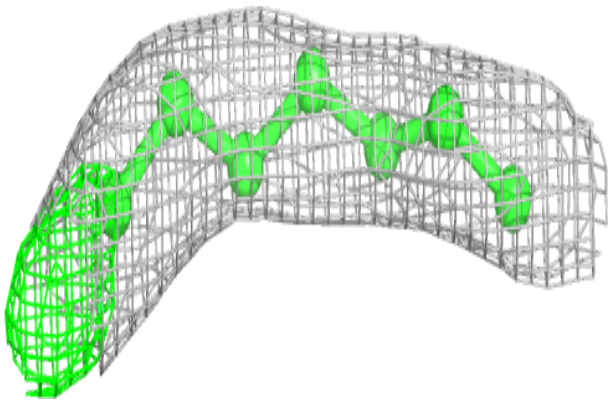


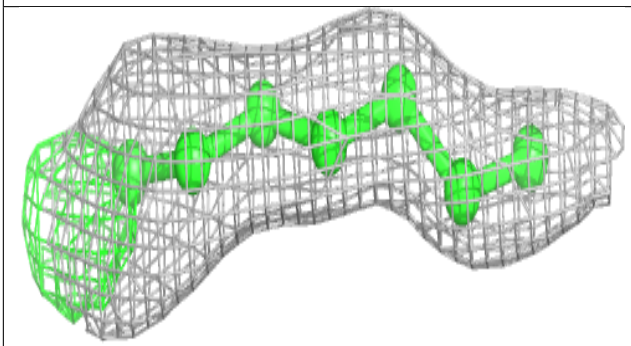


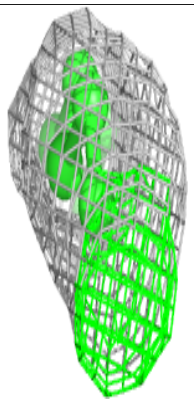


Electron density around LFA A 513:

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

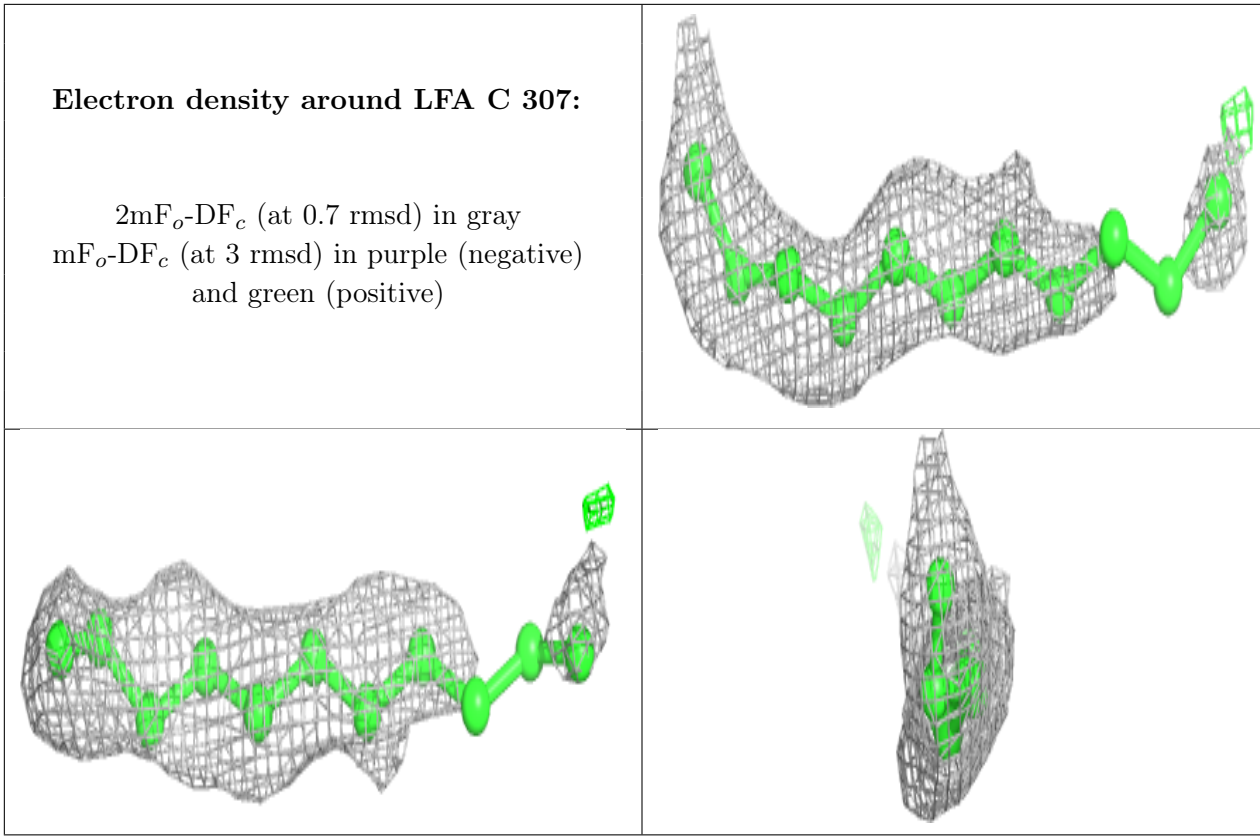






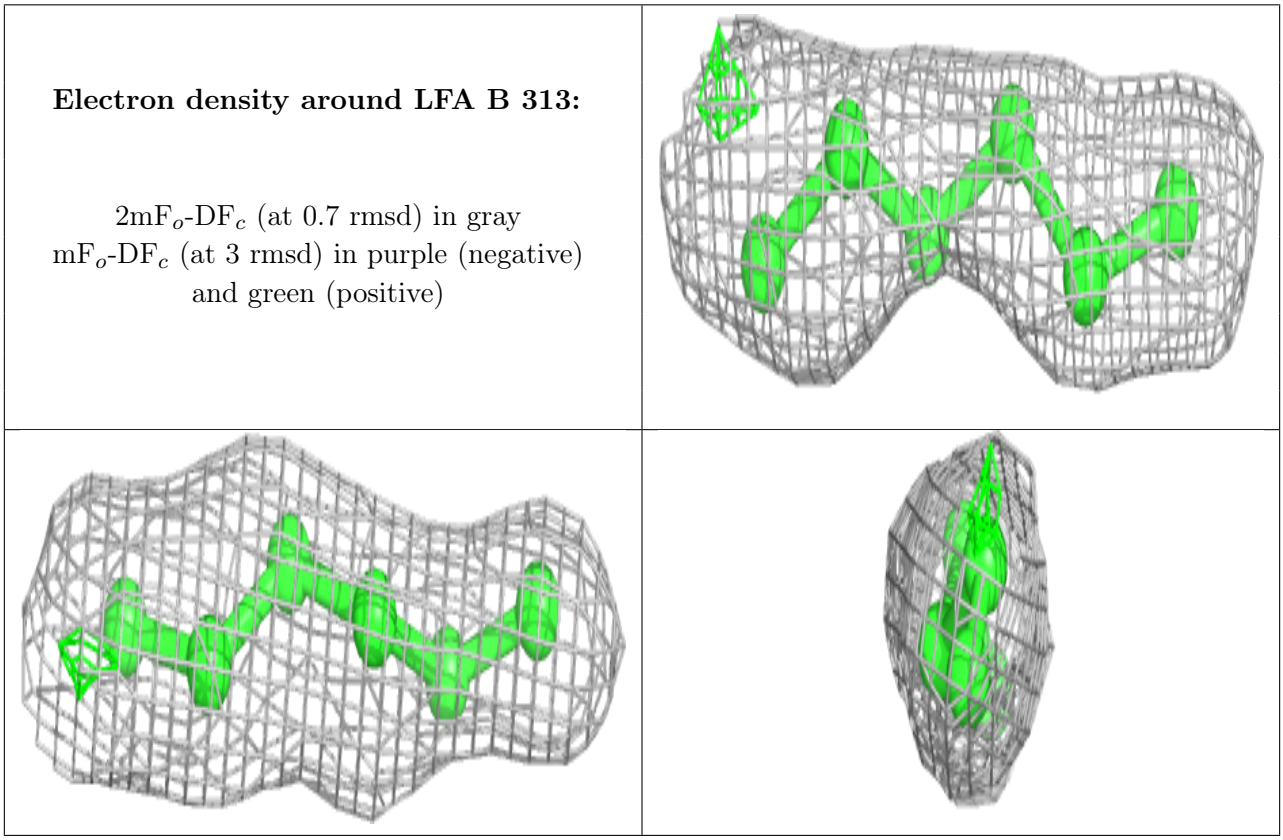
Electron density around LFA C 307:

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



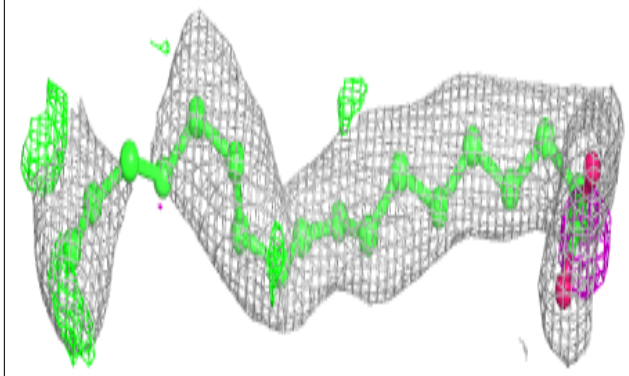
Electron density around LFA B 313:

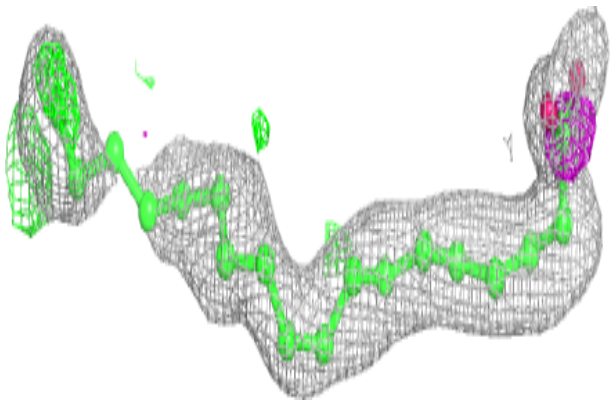
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

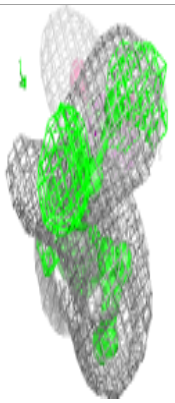


Electron density around OLA A 504:

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

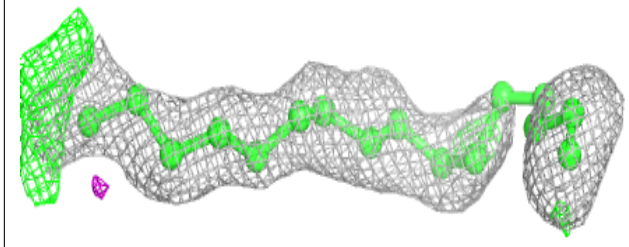


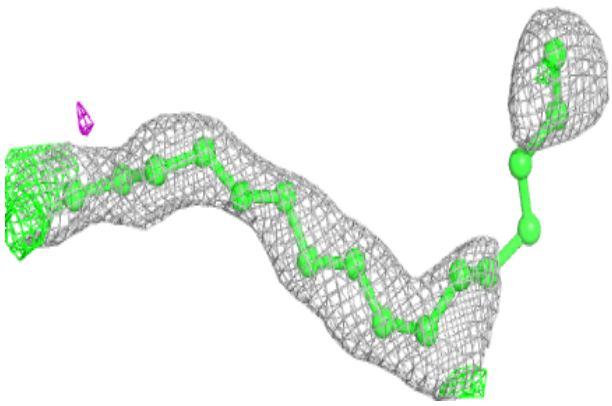


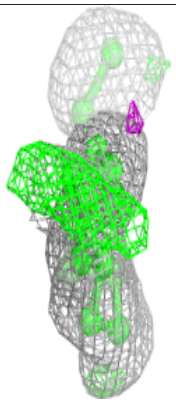


Electron density around LFA C 312:

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

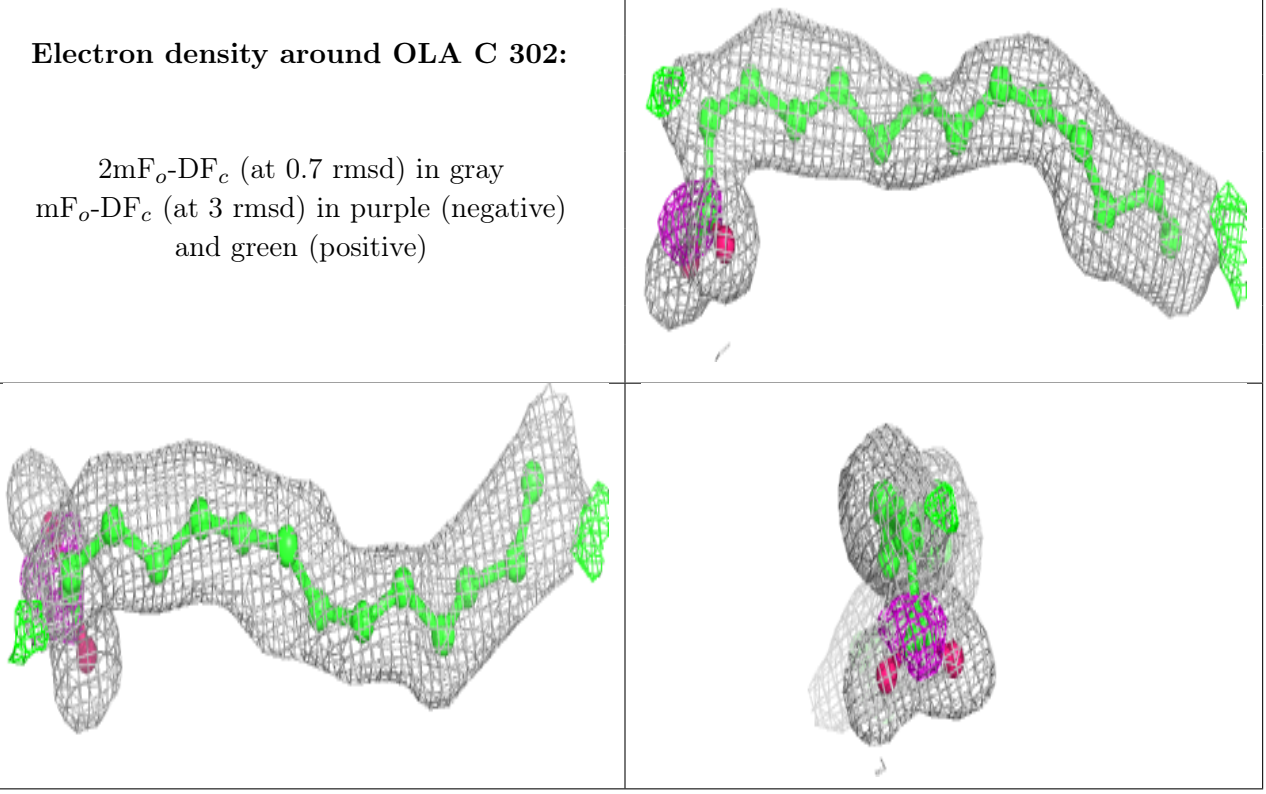






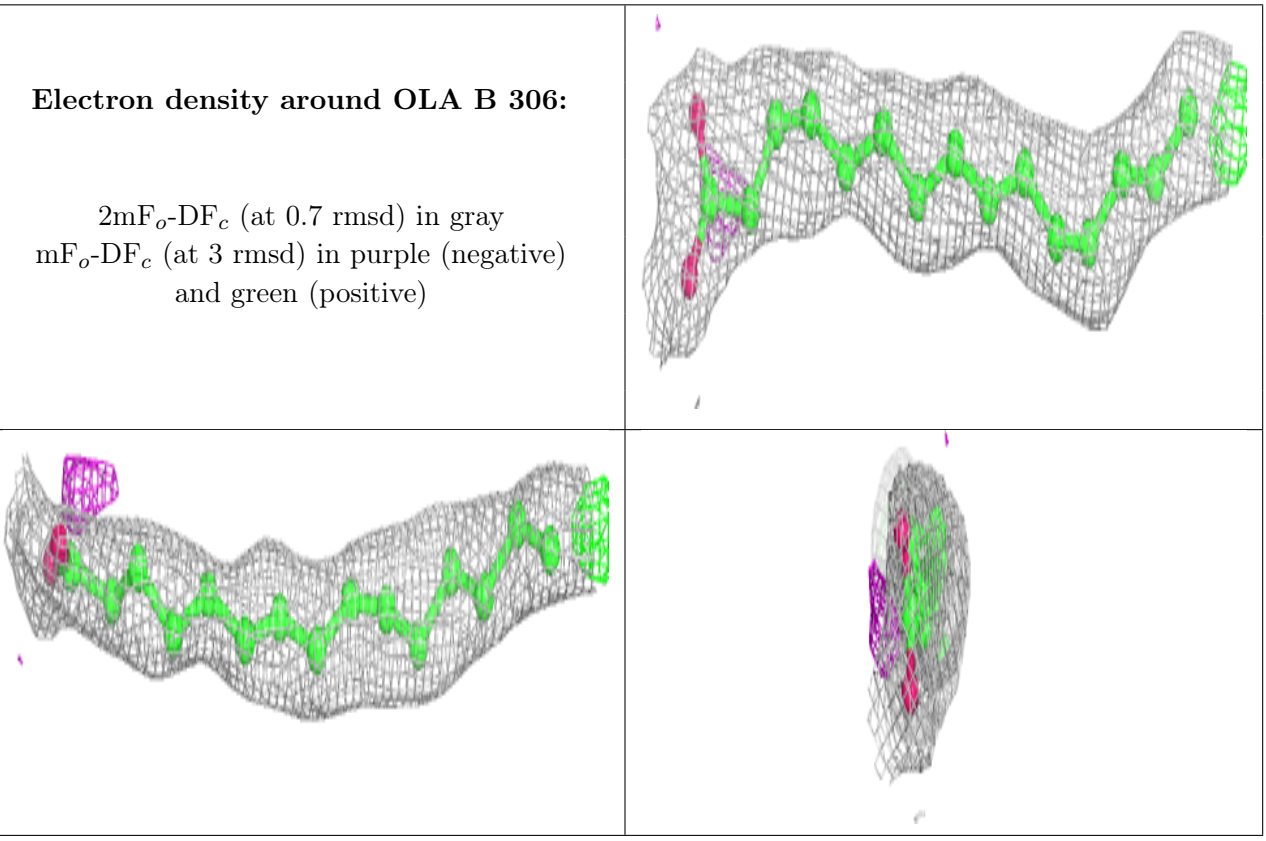
Electron density around OLA C 302:

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



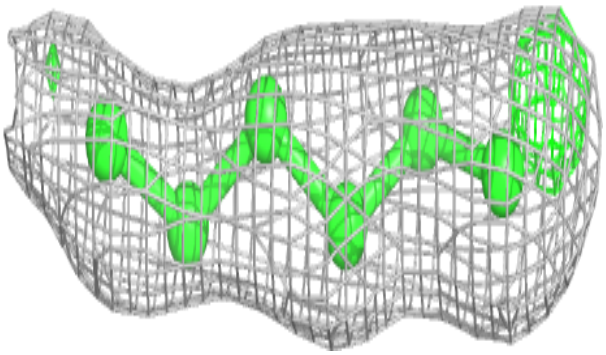
Electron density around OLA B 306:

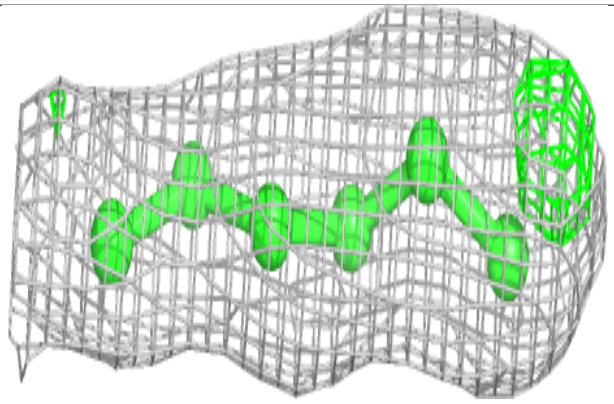
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

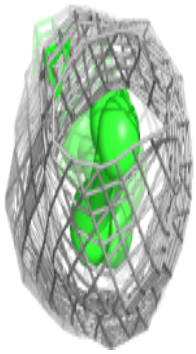


Electron density around LFA B 309:

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

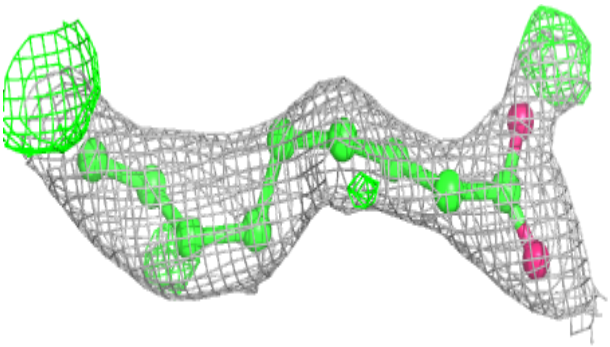


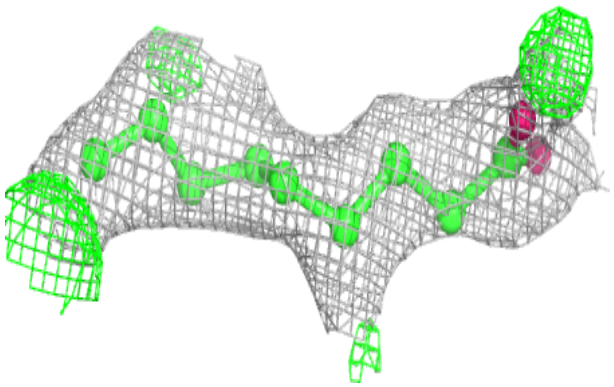


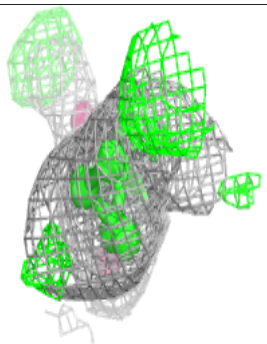


Electron density around OLA A 506:

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

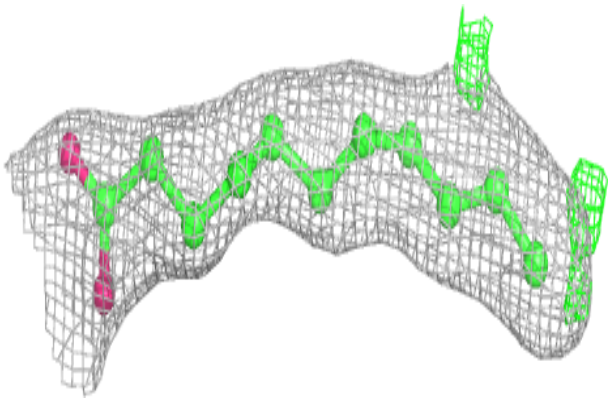


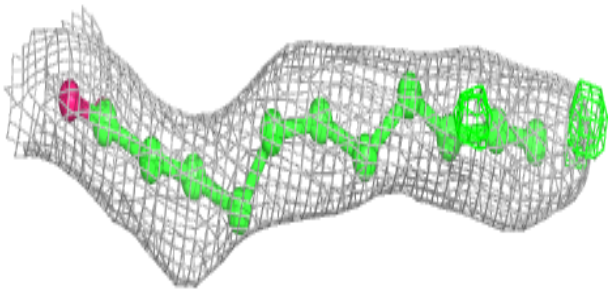


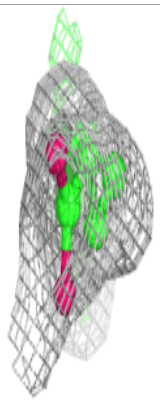


Electron density around OLA C 304:

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

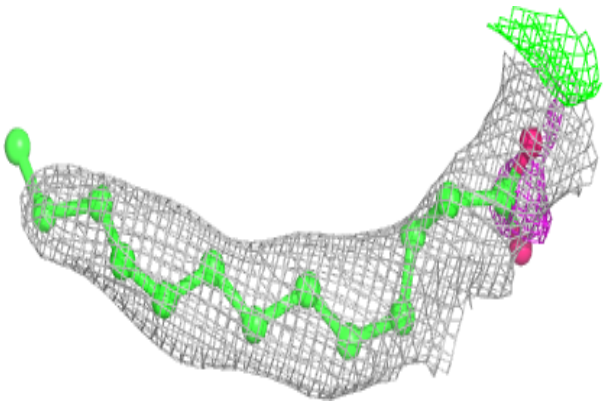


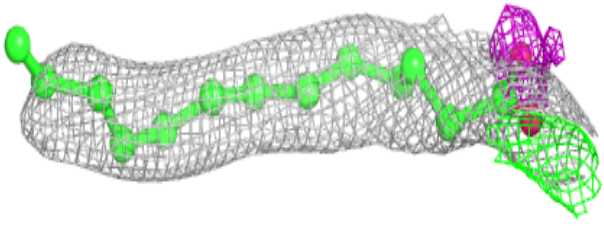


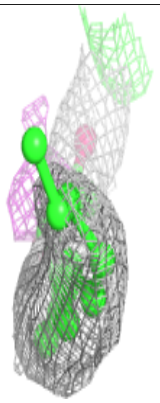


Electron density around OLA C 305:

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

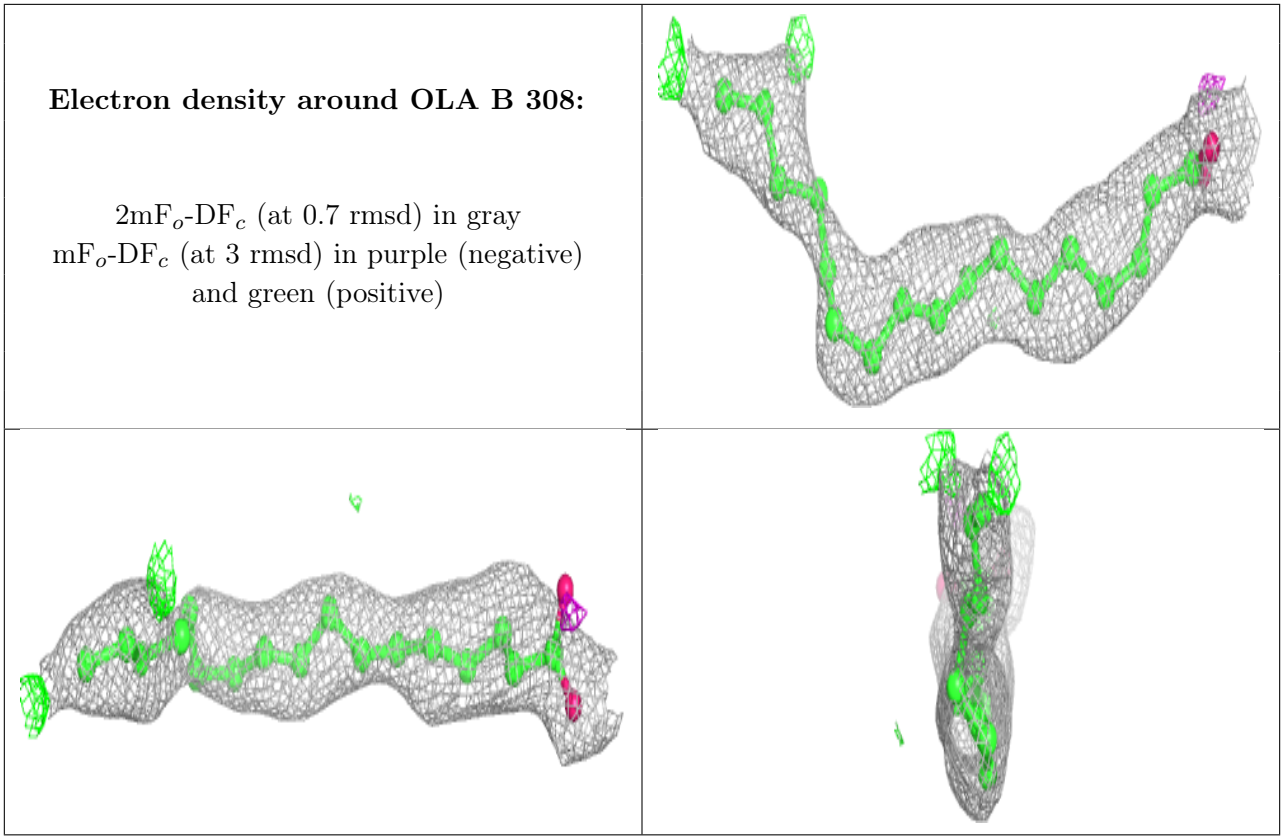






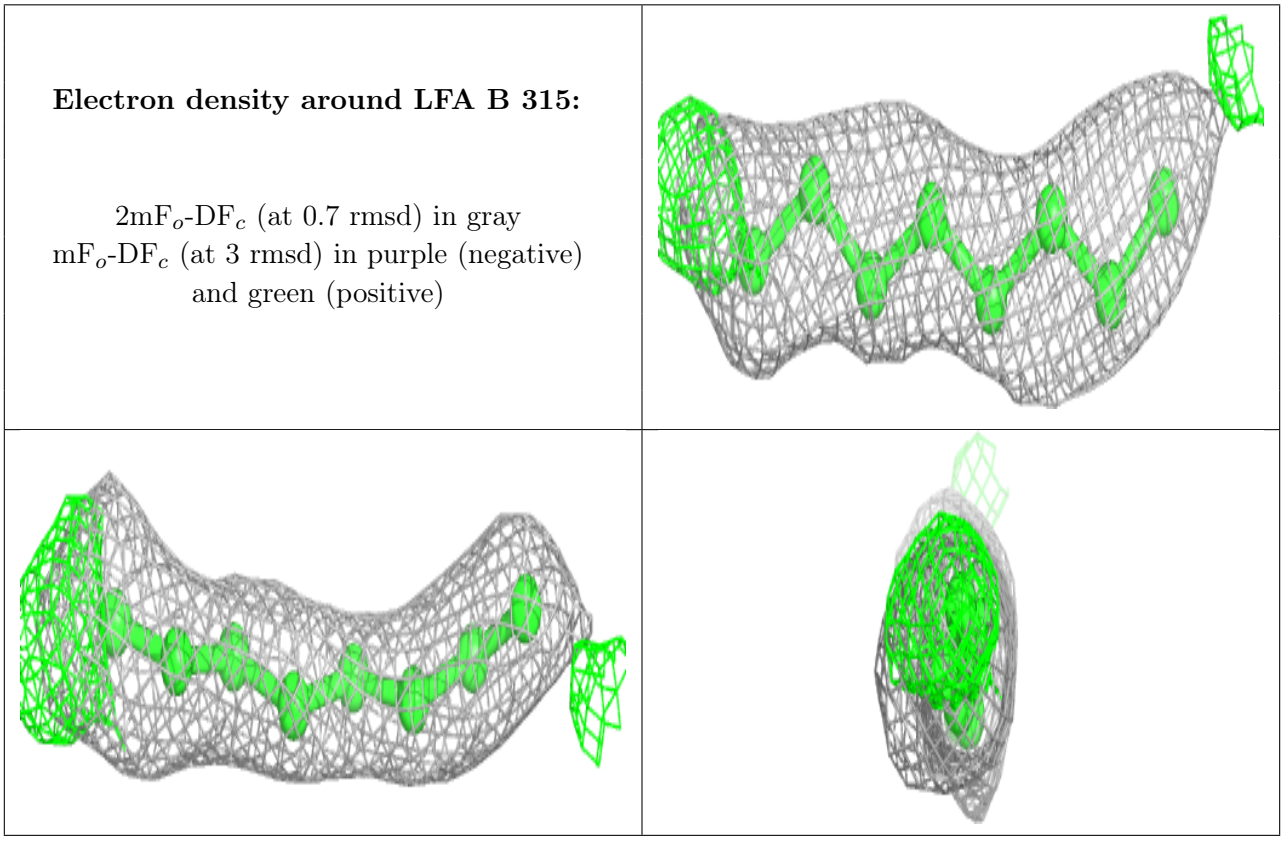
Electron density around OLA B 308:

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



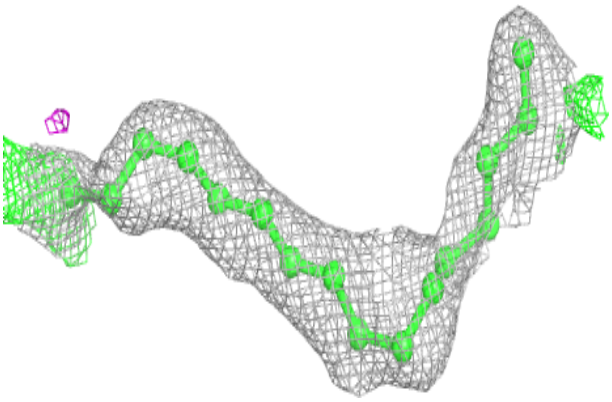
Electron density around LFA B 315:

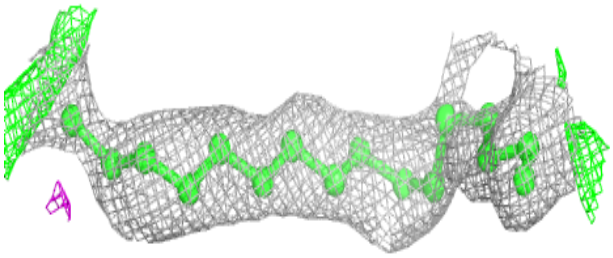
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

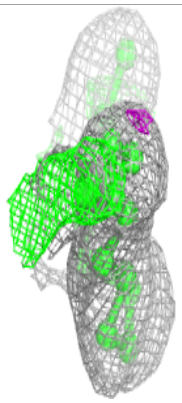


Electron density around LFA B 317:

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

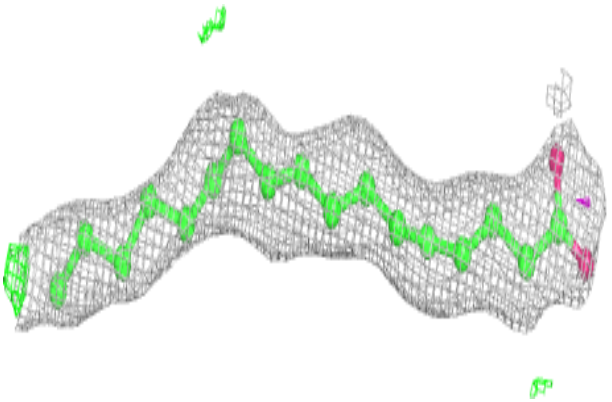


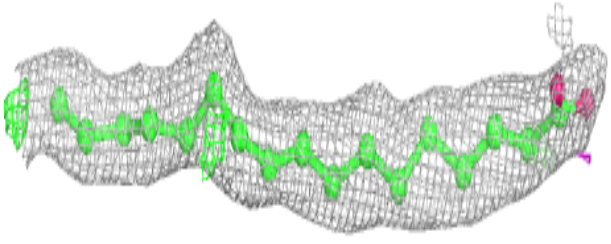


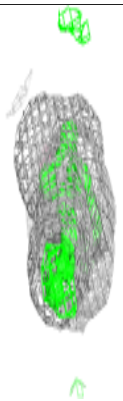


Electron density around OLA A 507:

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

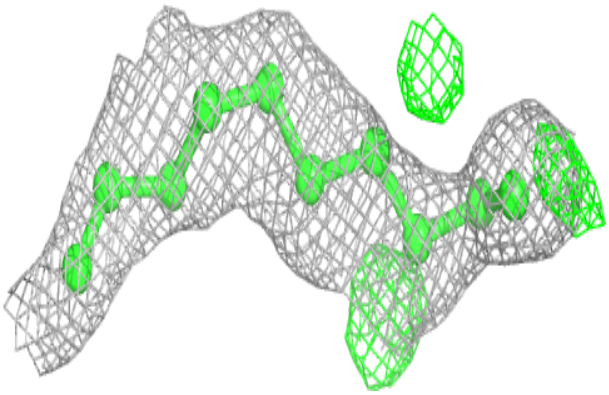


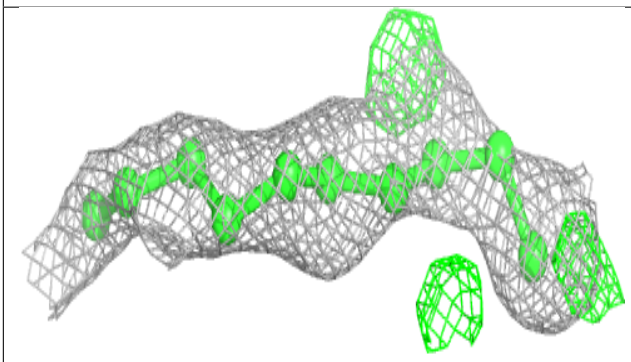


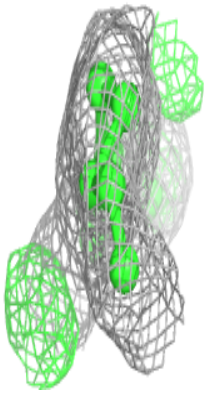


Electron density around OLA B 305:

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

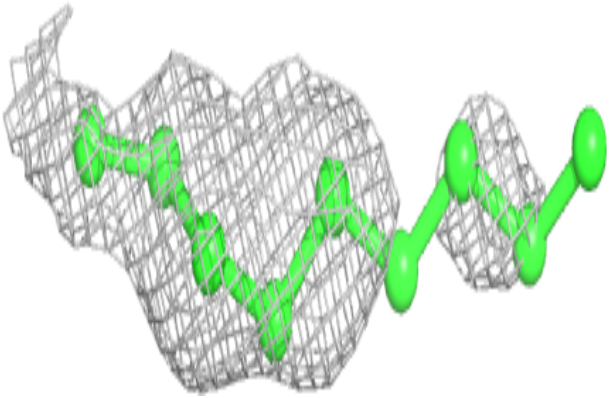


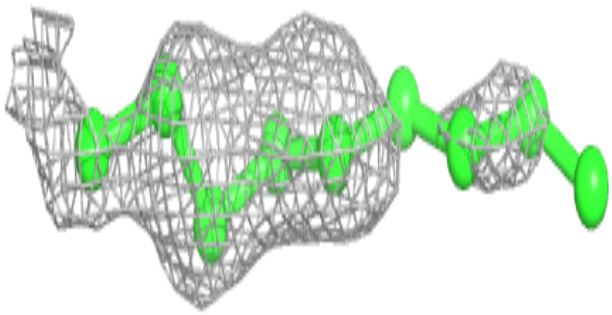


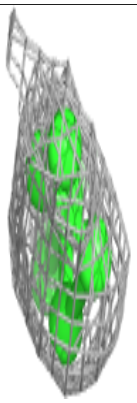


Electron density around LFA A 509:

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

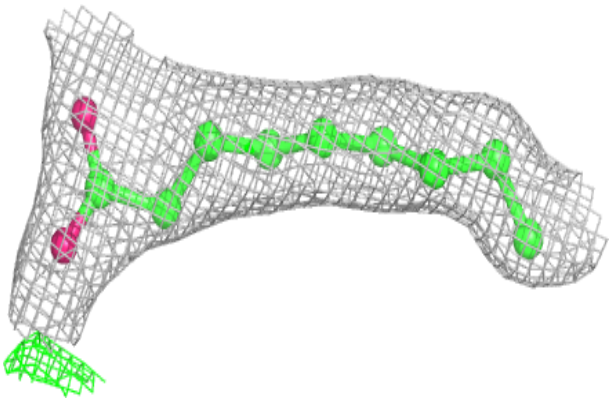


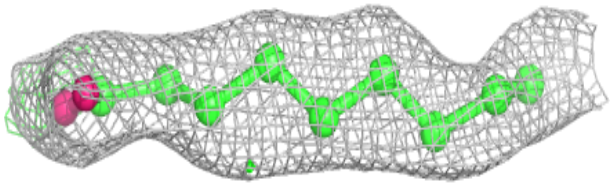


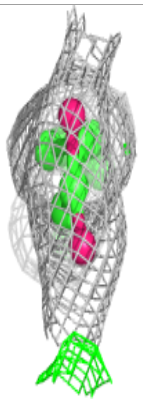


Electron density around OLA A 503:

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

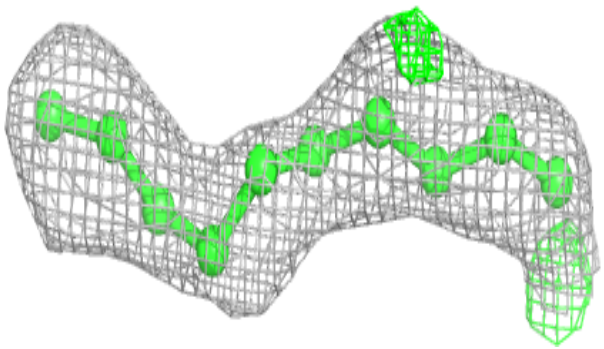


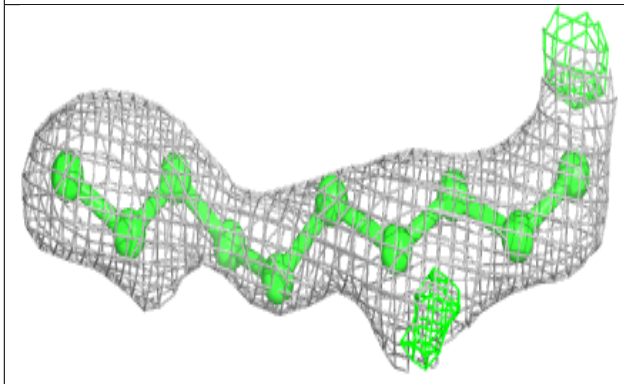


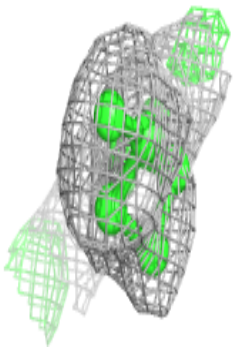


Electron density around LFA C 306:

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

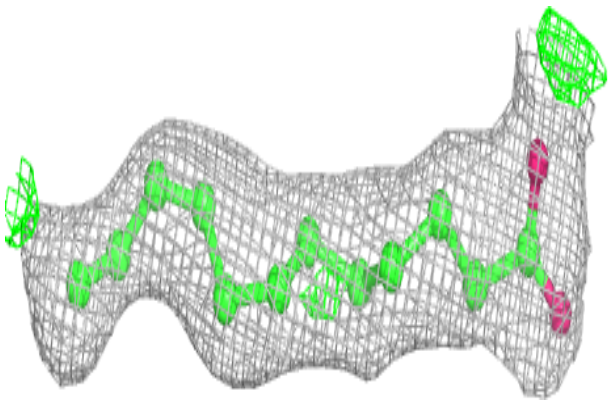


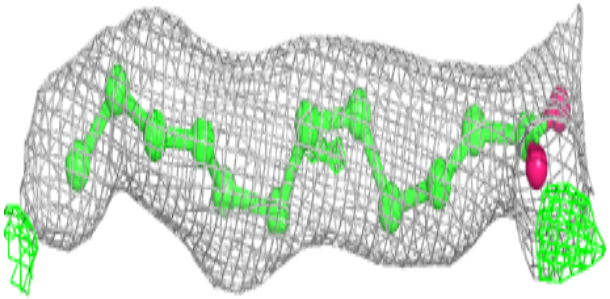


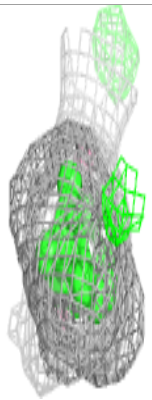


Electron density around OLA B 303:

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

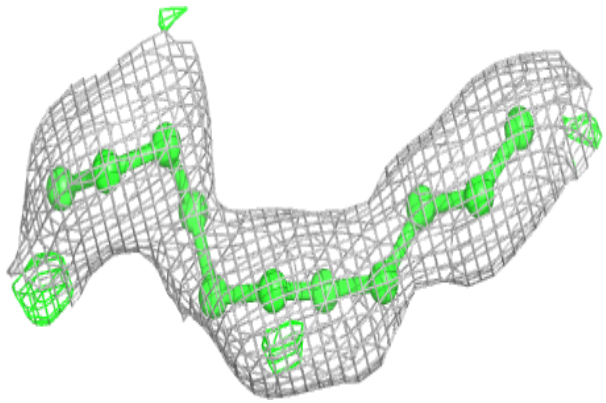


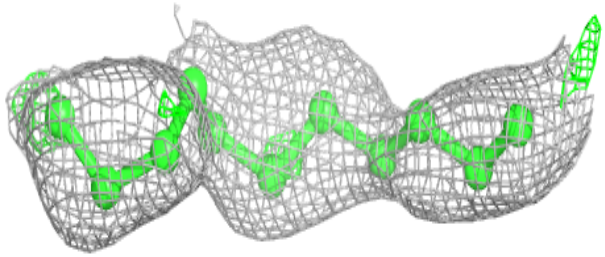


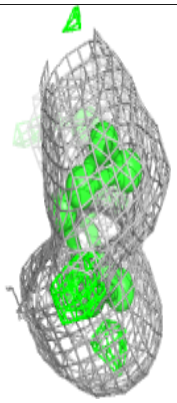


Electron density around LFA C 316:

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

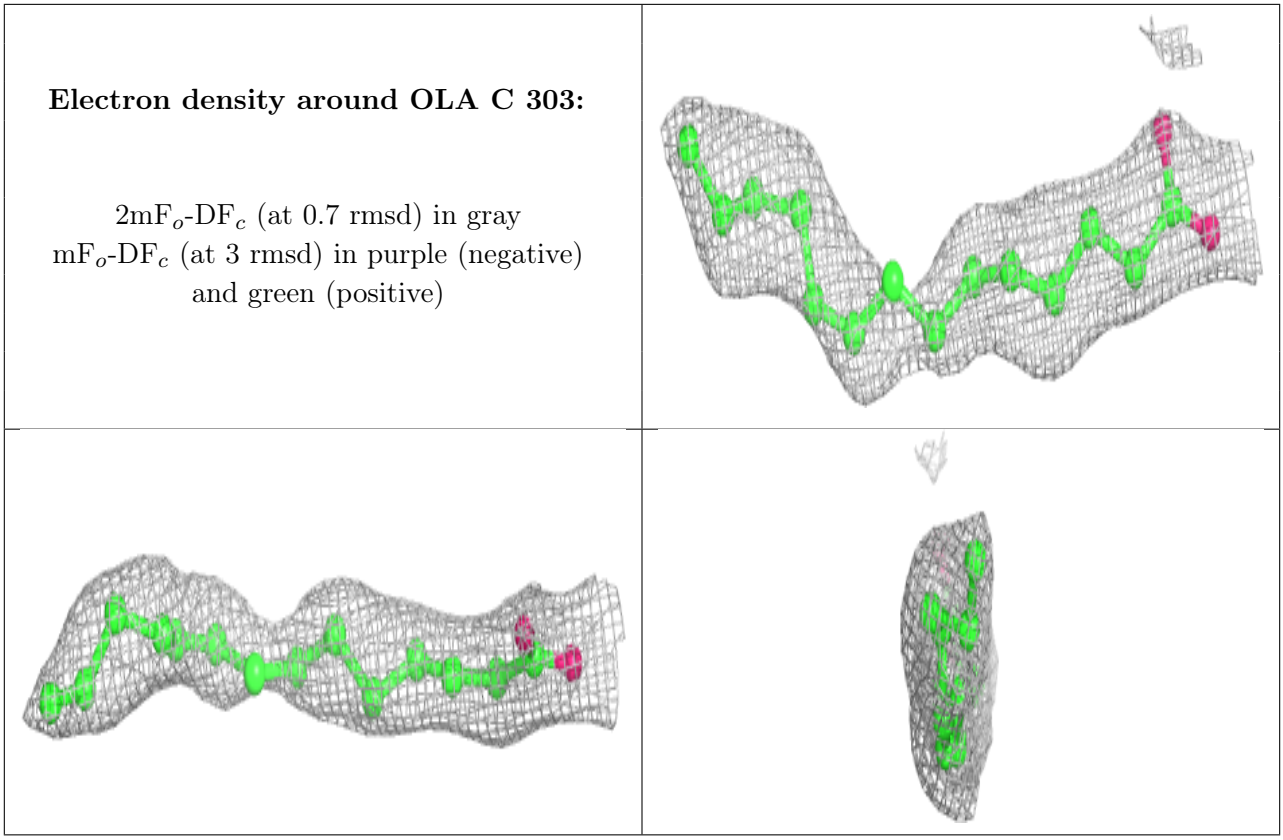






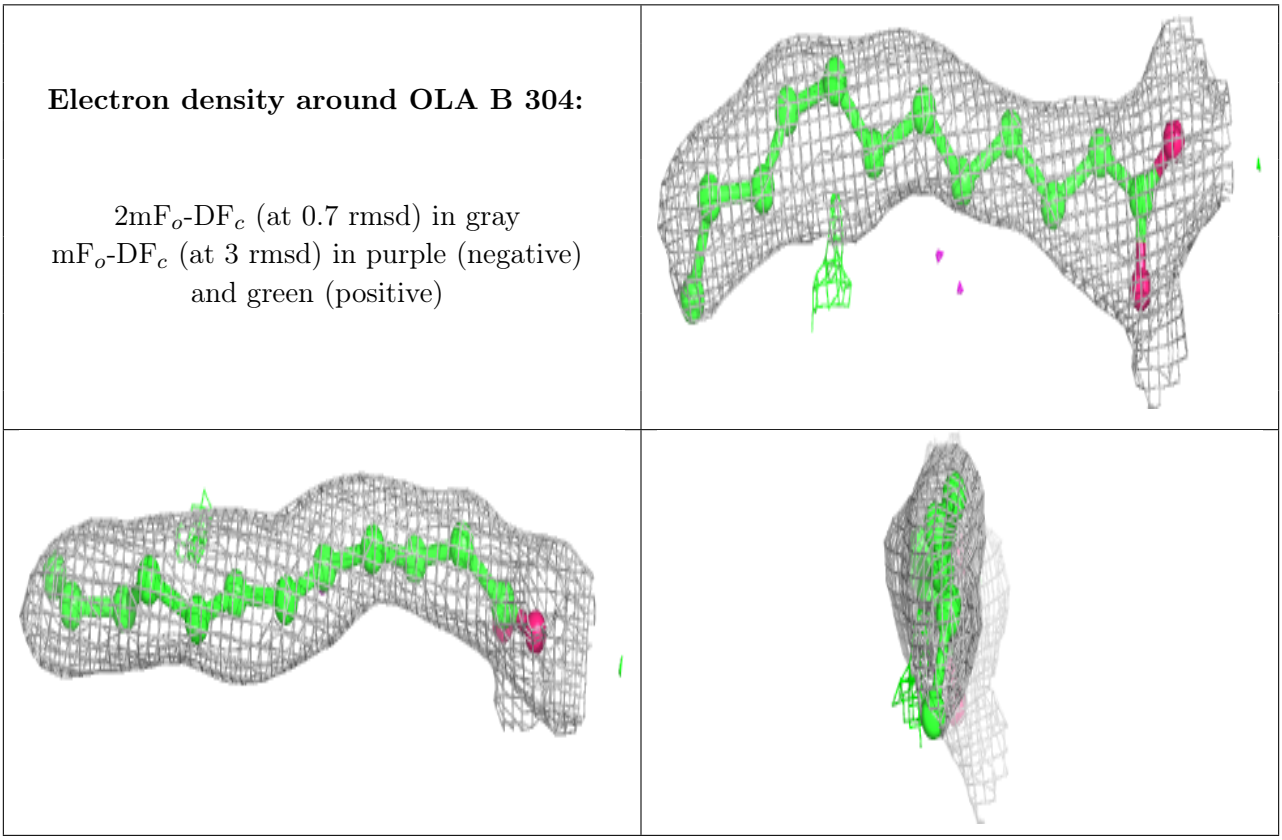
Electron density around OLA C 303:

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



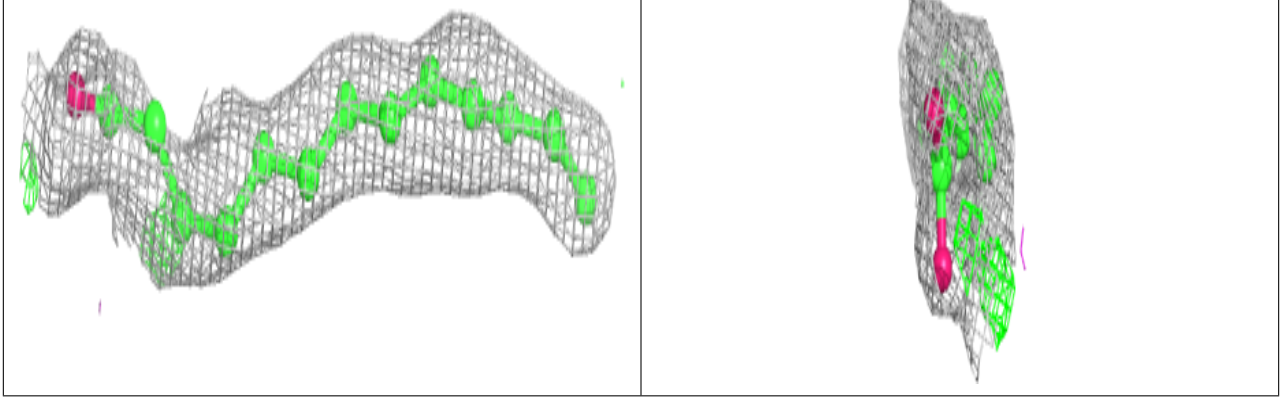
Electron density around OLA B 304:

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



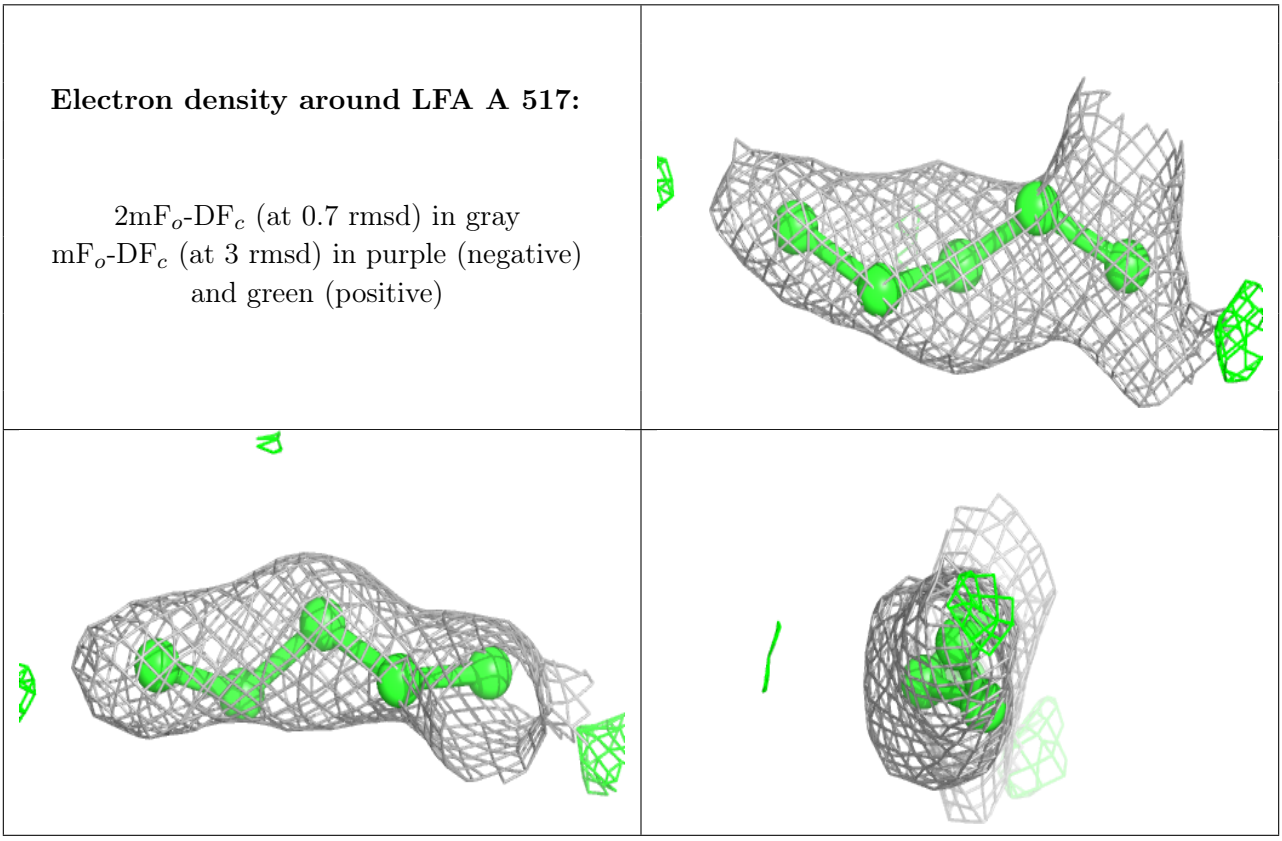
Electron density around OLA A 505:

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



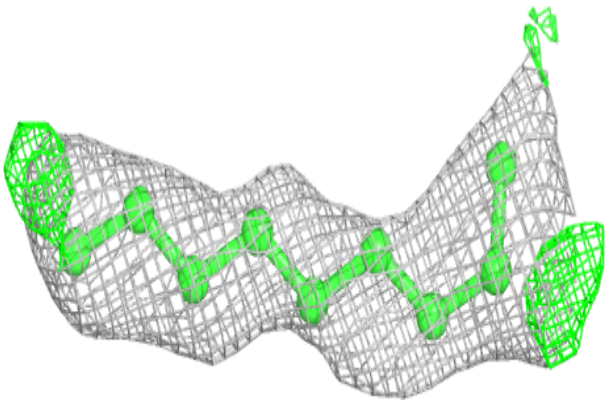
Electron density around LFA A 517:

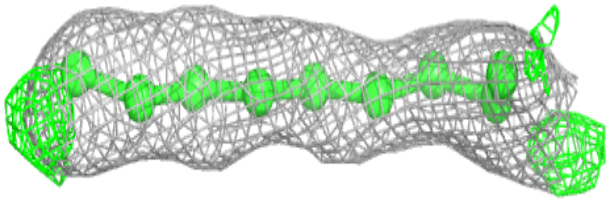
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

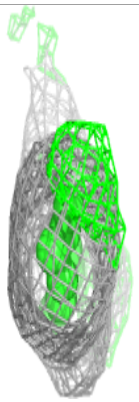


Electron density around LFA C 315:

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

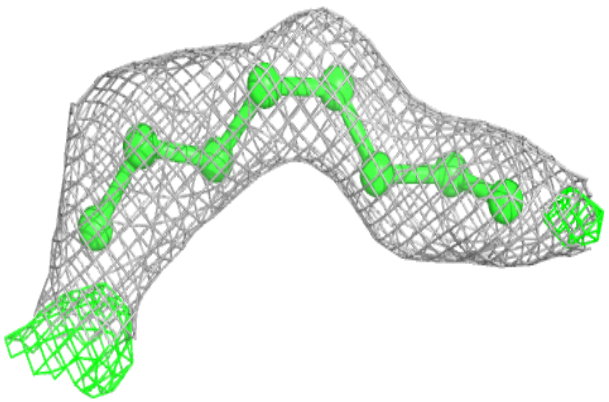


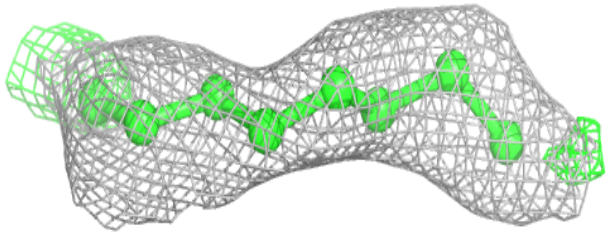


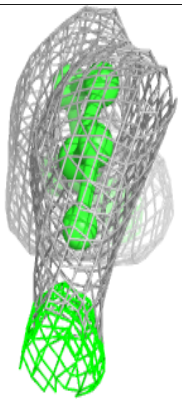


Electron density around LFA B 316:

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

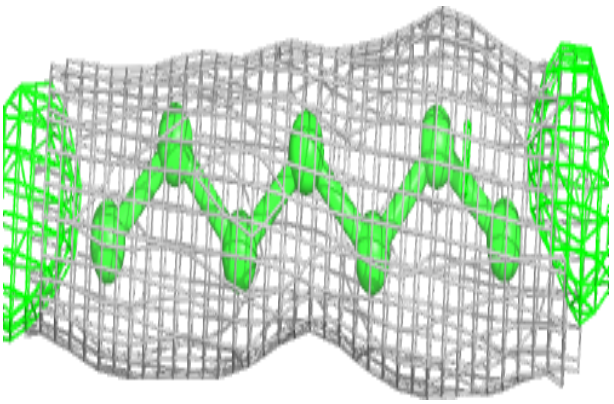


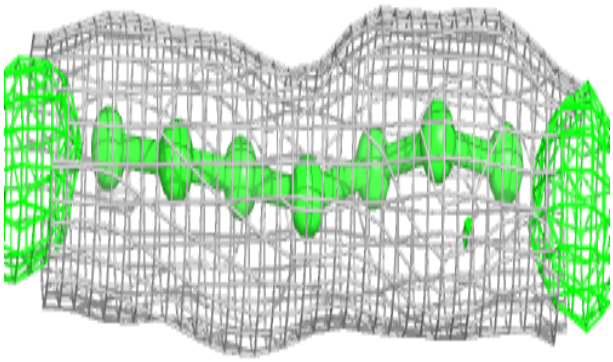


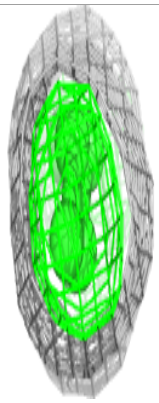


Electron density around LFA A 502:

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

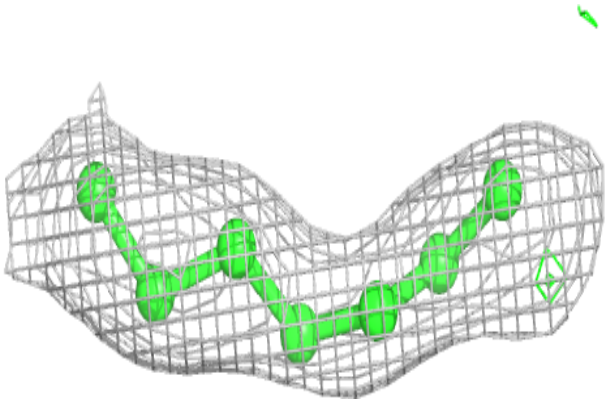


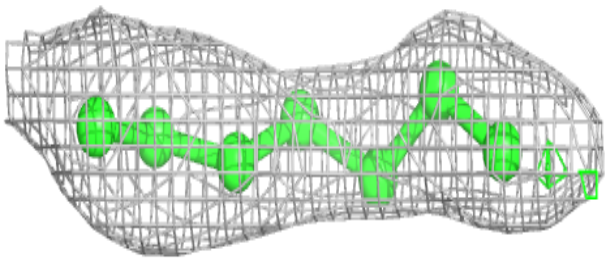


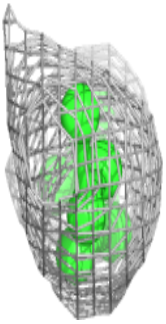


Electron density around LFA B 310:

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

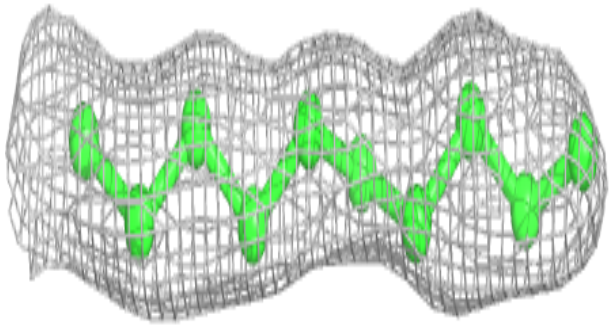


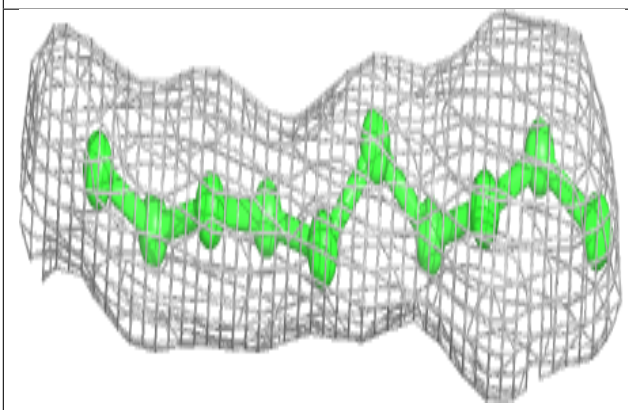


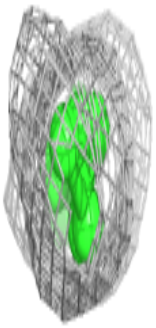


Electron density around LFA C 314:

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

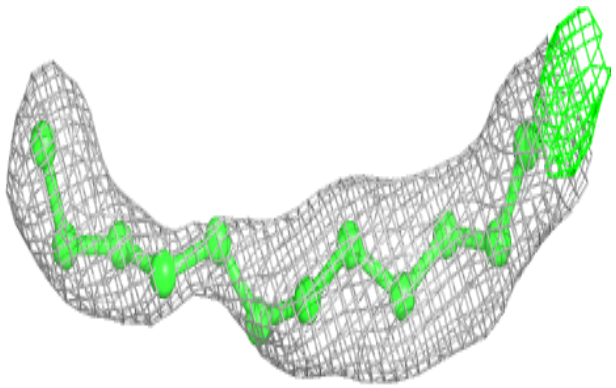


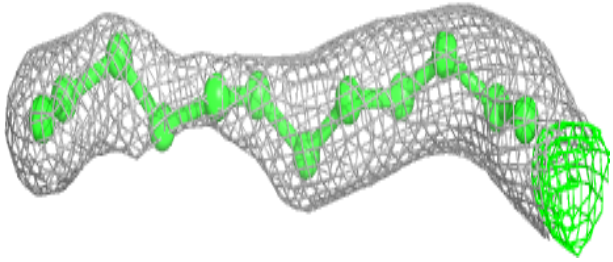


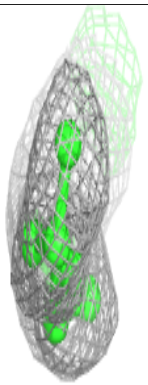


Electron density around LFA A 512:

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

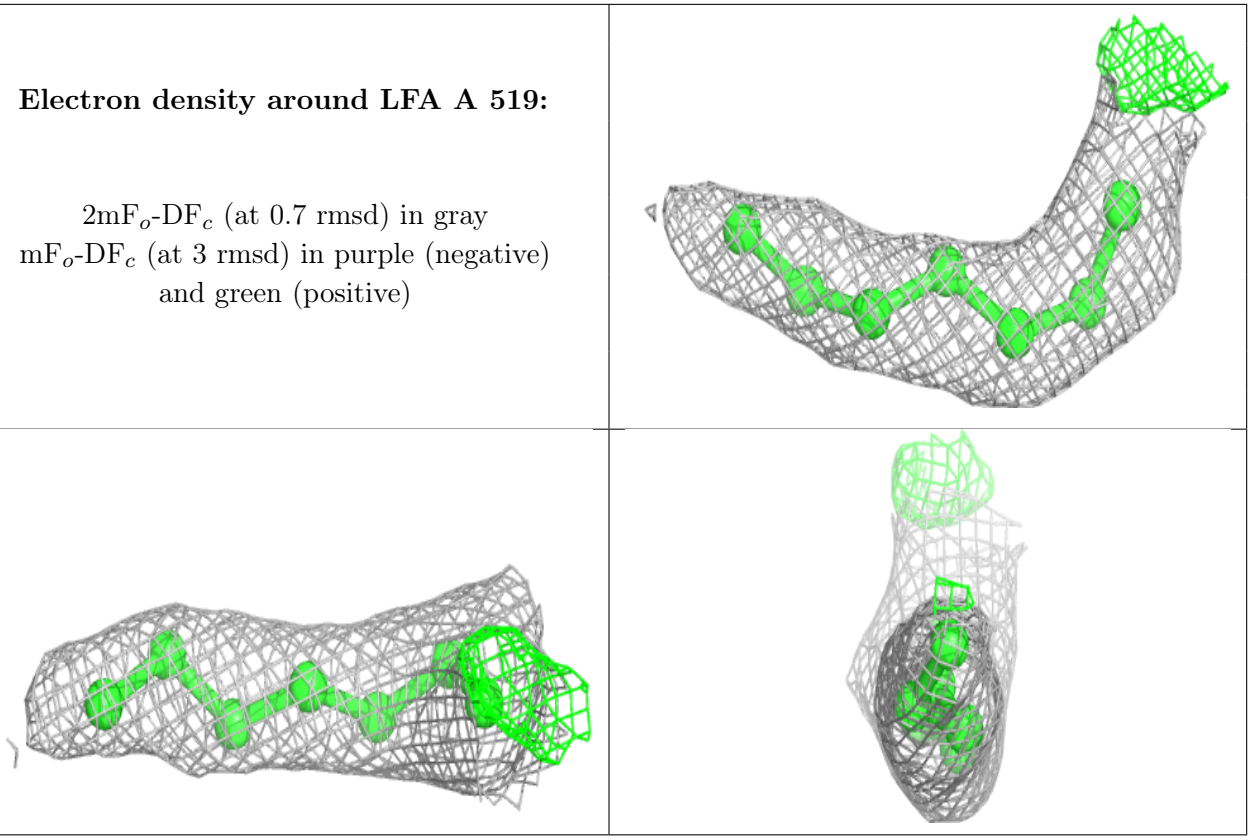






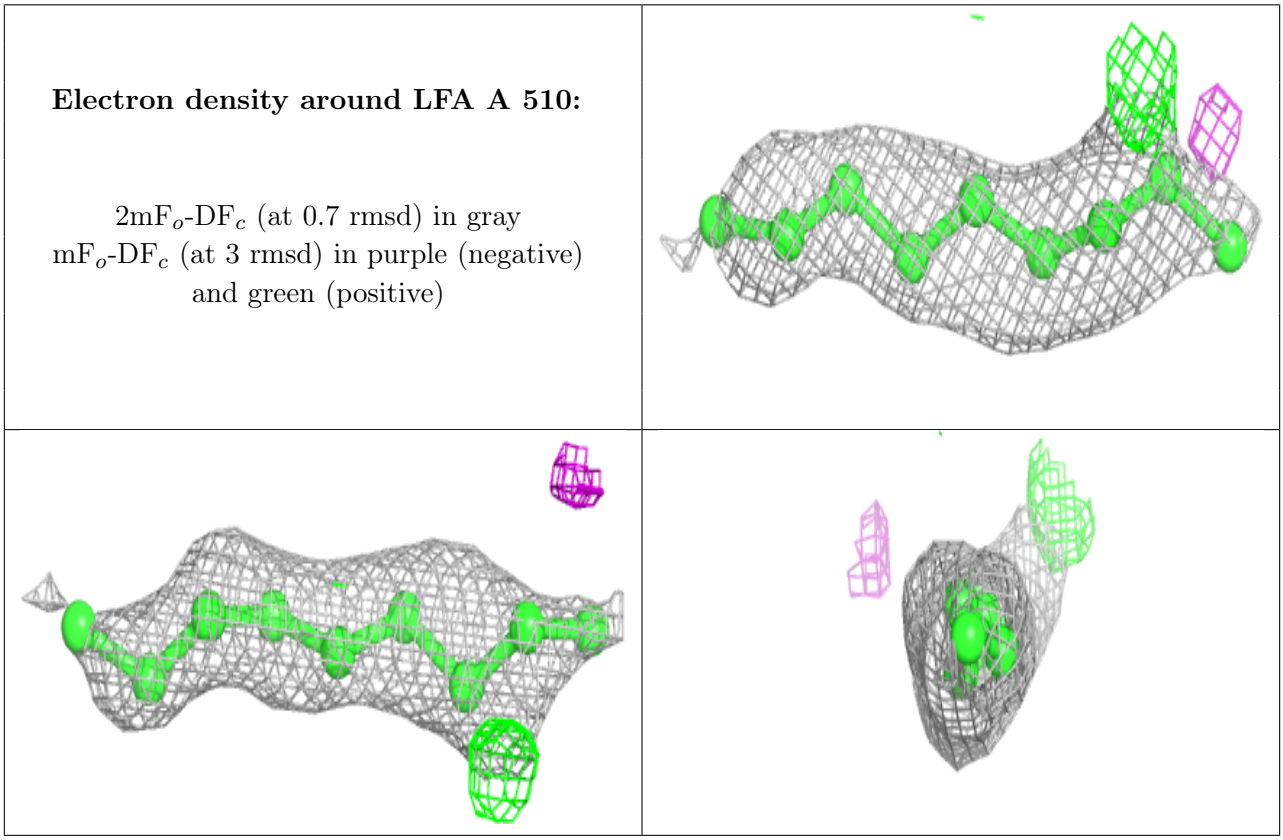
Electron density around LFA A 519:

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



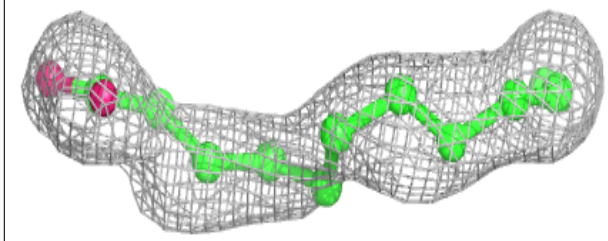
Electron density around LFA A 510:

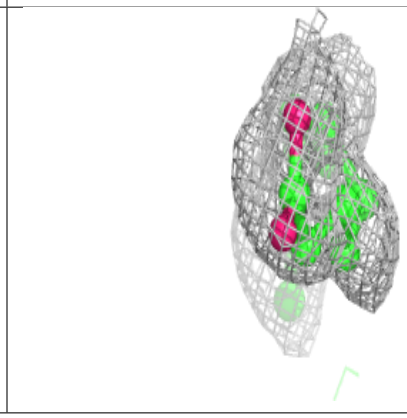
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around OLA A 508:

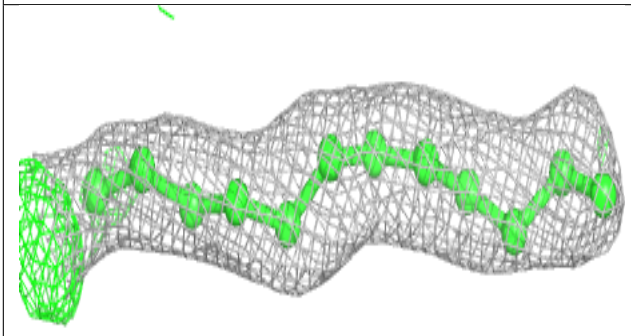
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

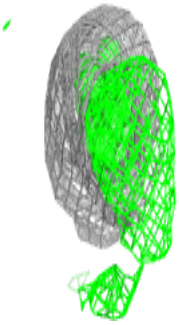




Electron density around LFA C 313:

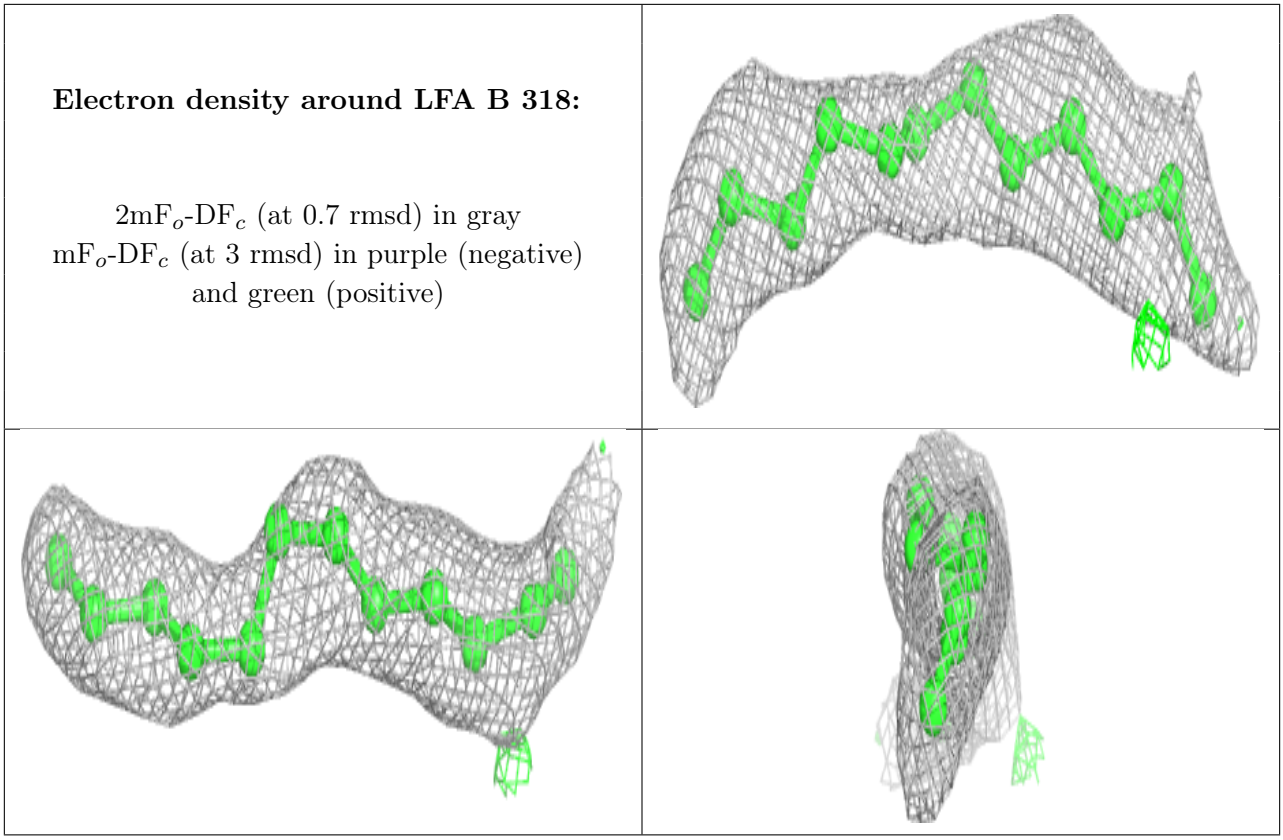
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





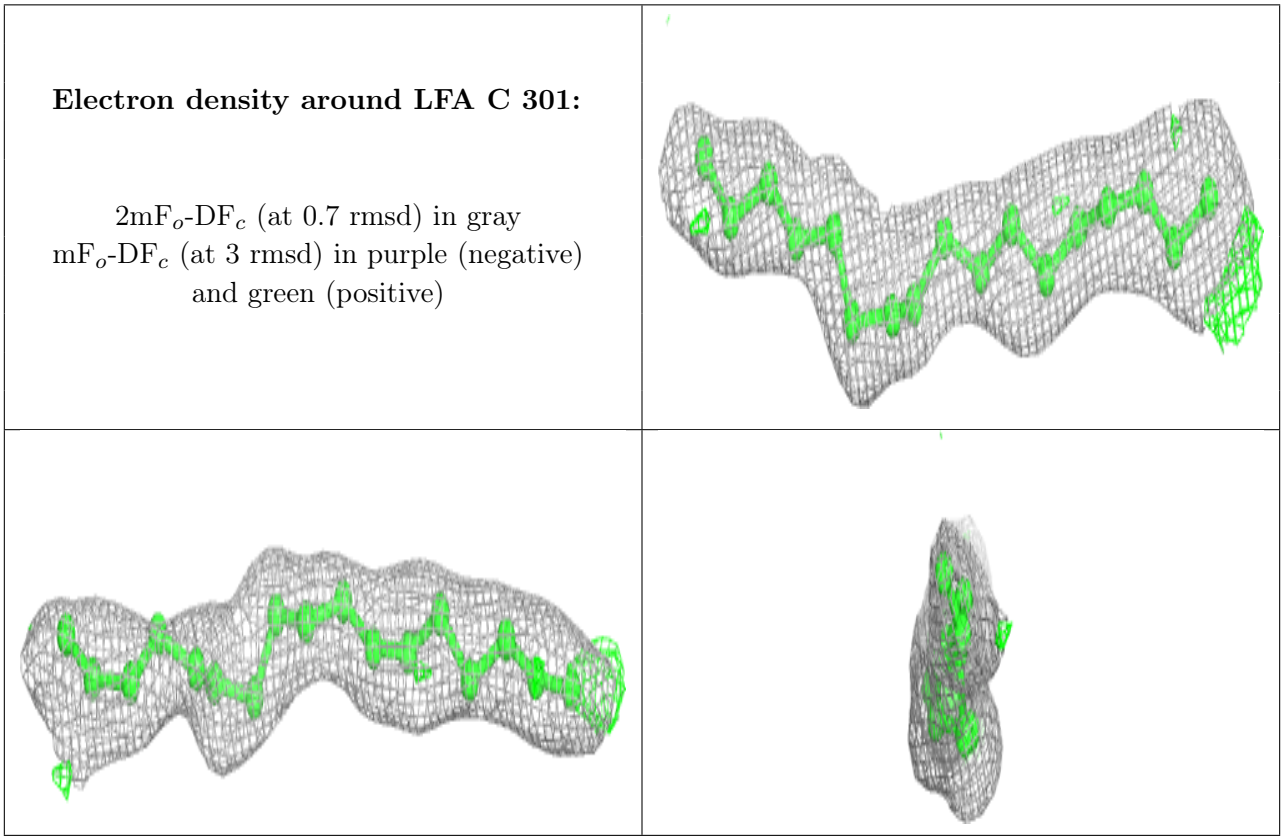
Electron density around LFA B 318:

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



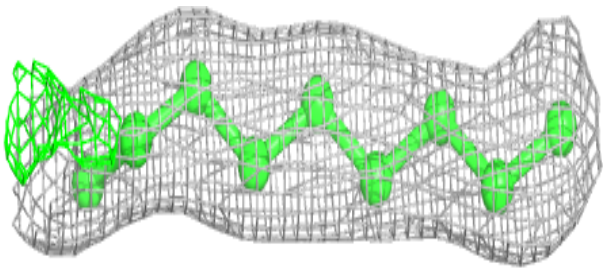
Electron density around LFA C 301:

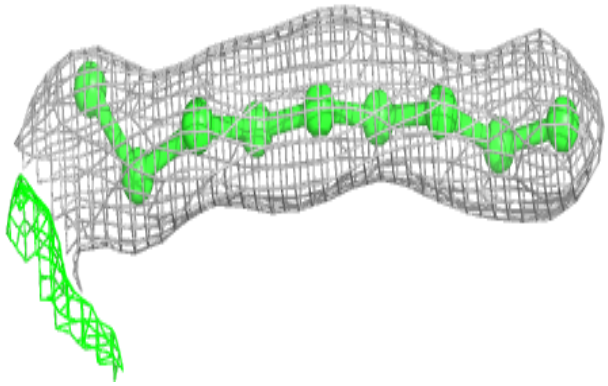
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

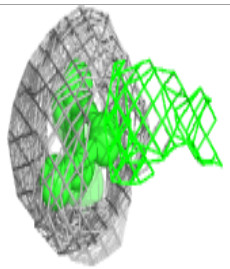


Electron density around LFA B 302:

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

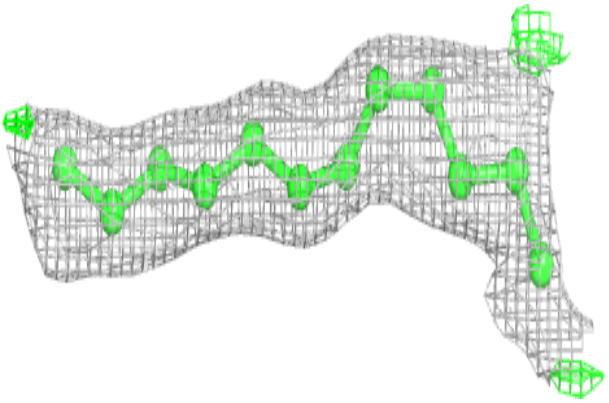


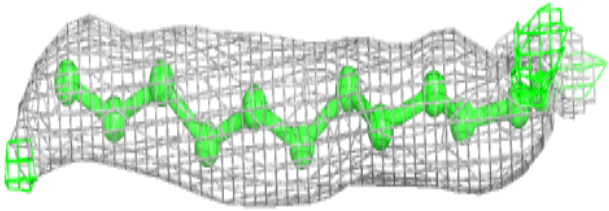


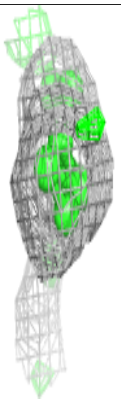


Electron density around LFA B 320:

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

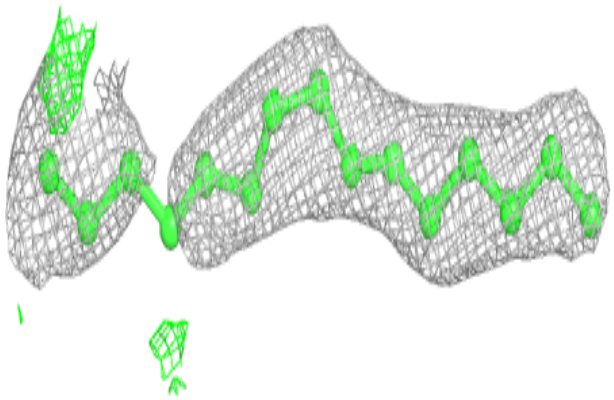


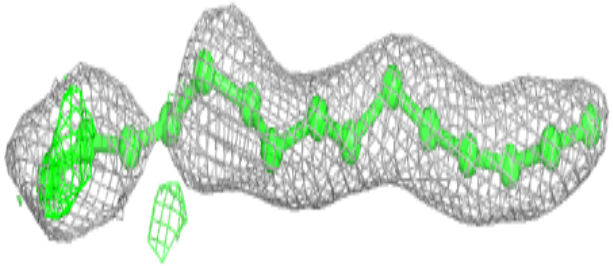


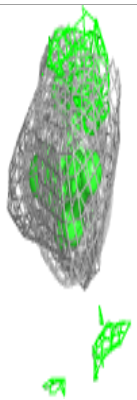


Electron density around LFA B 314:

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

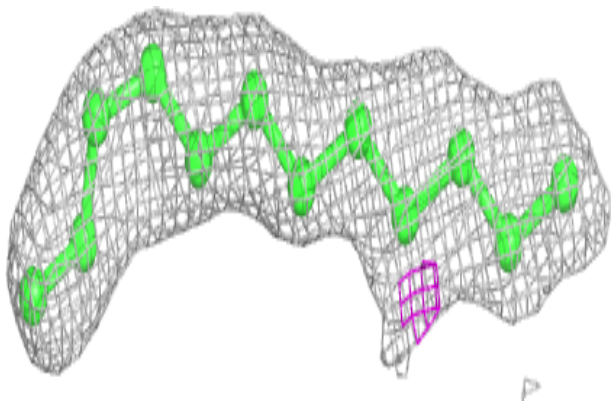


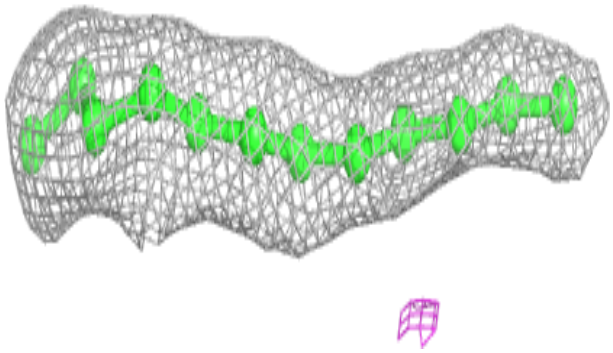


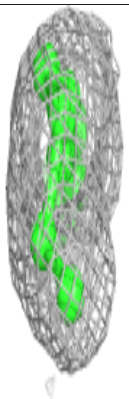


Electron density around LFA B 322:

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

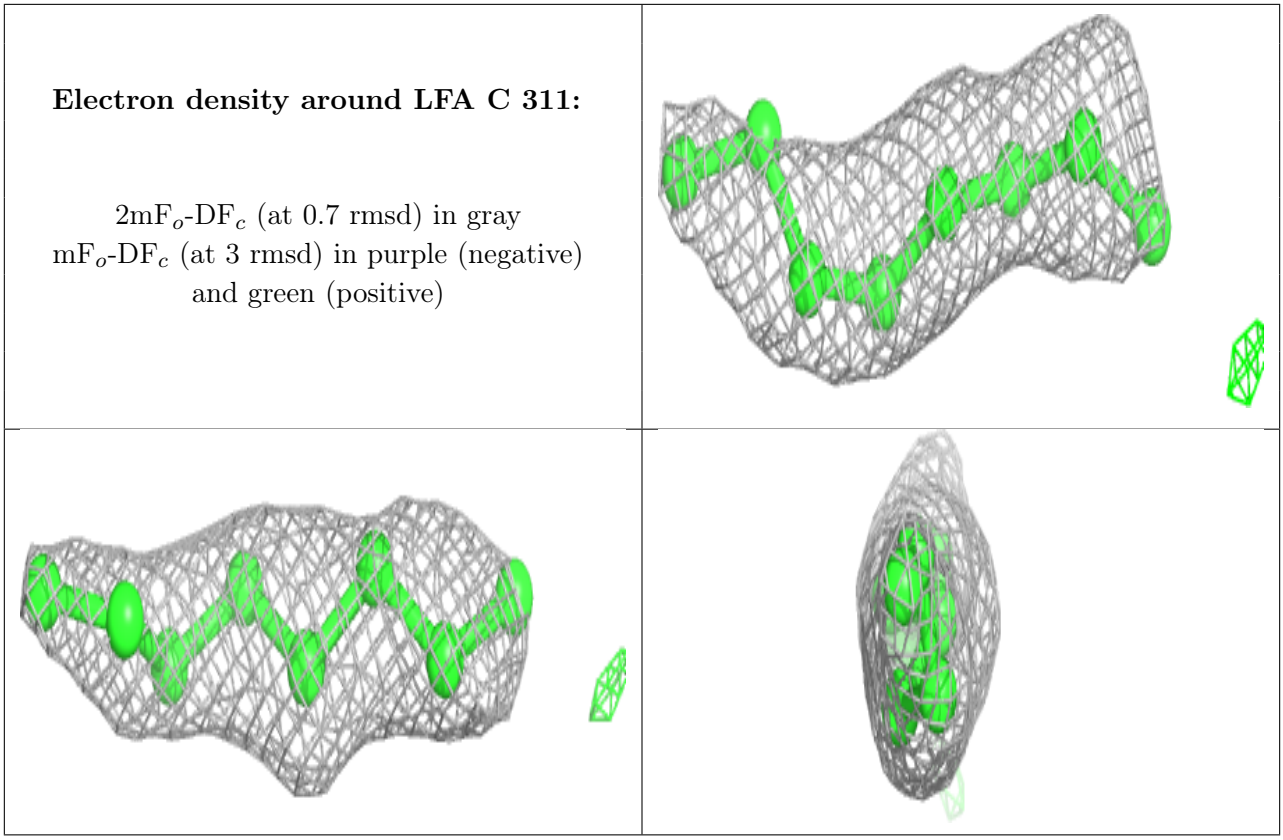






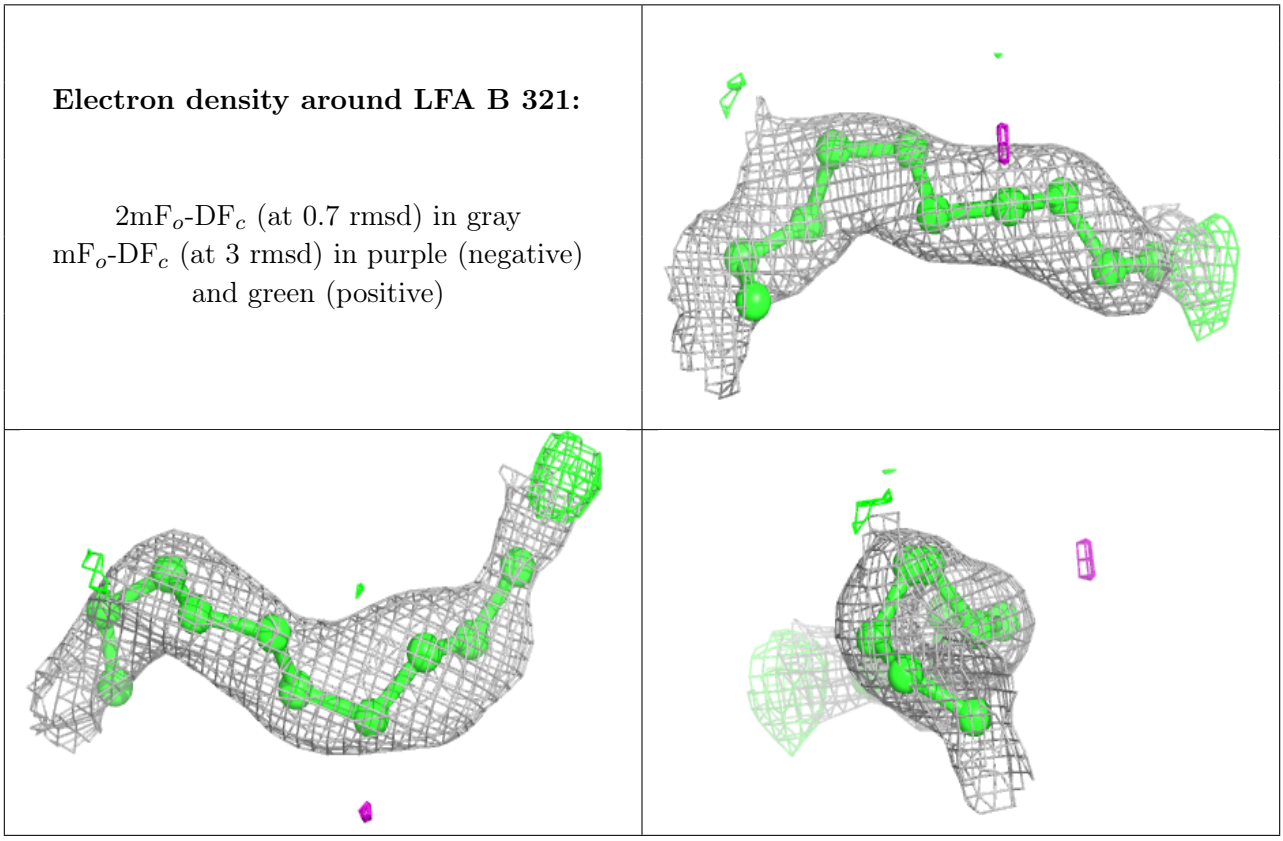
Electron density around LFA C 311:

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



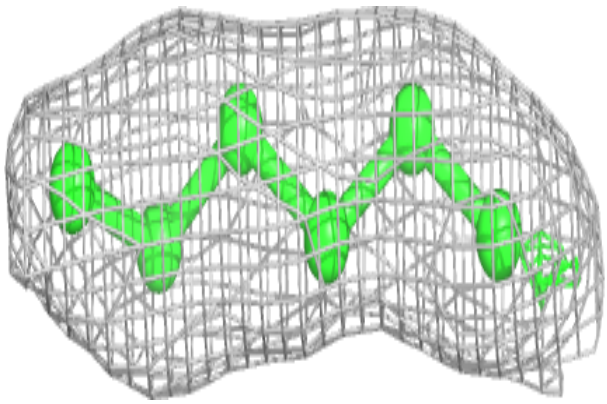
Electron density around LFA B 321:

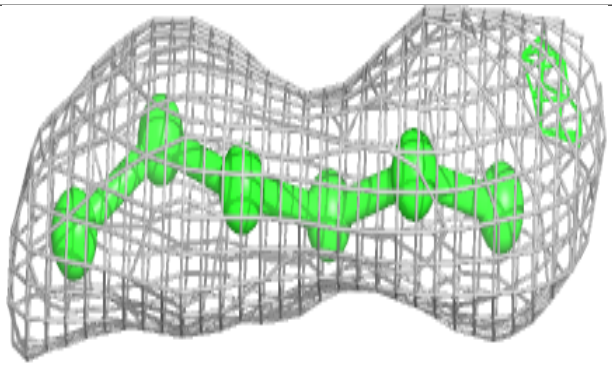
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

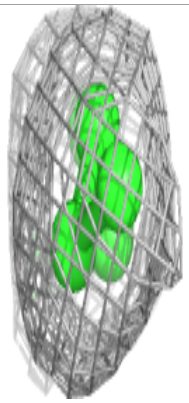


Electron density around LFA A 515:

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

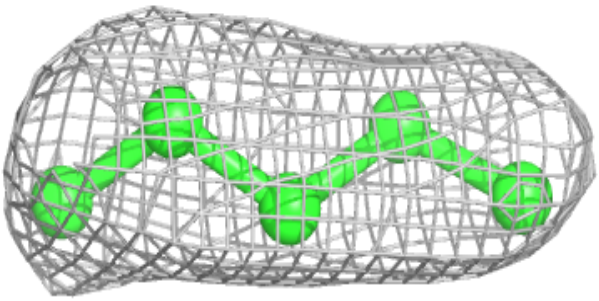


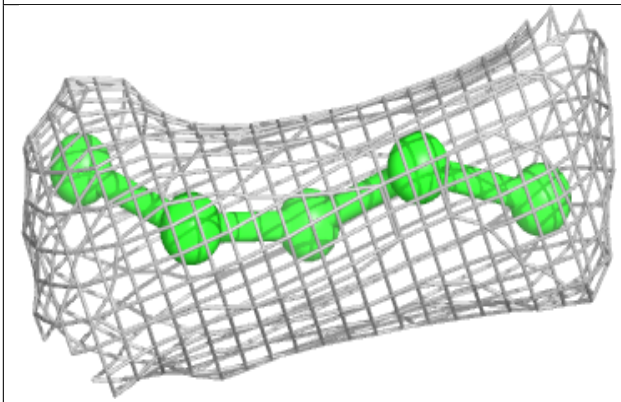


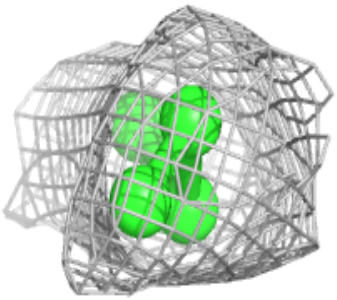


Electron density around LFA B 312:

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

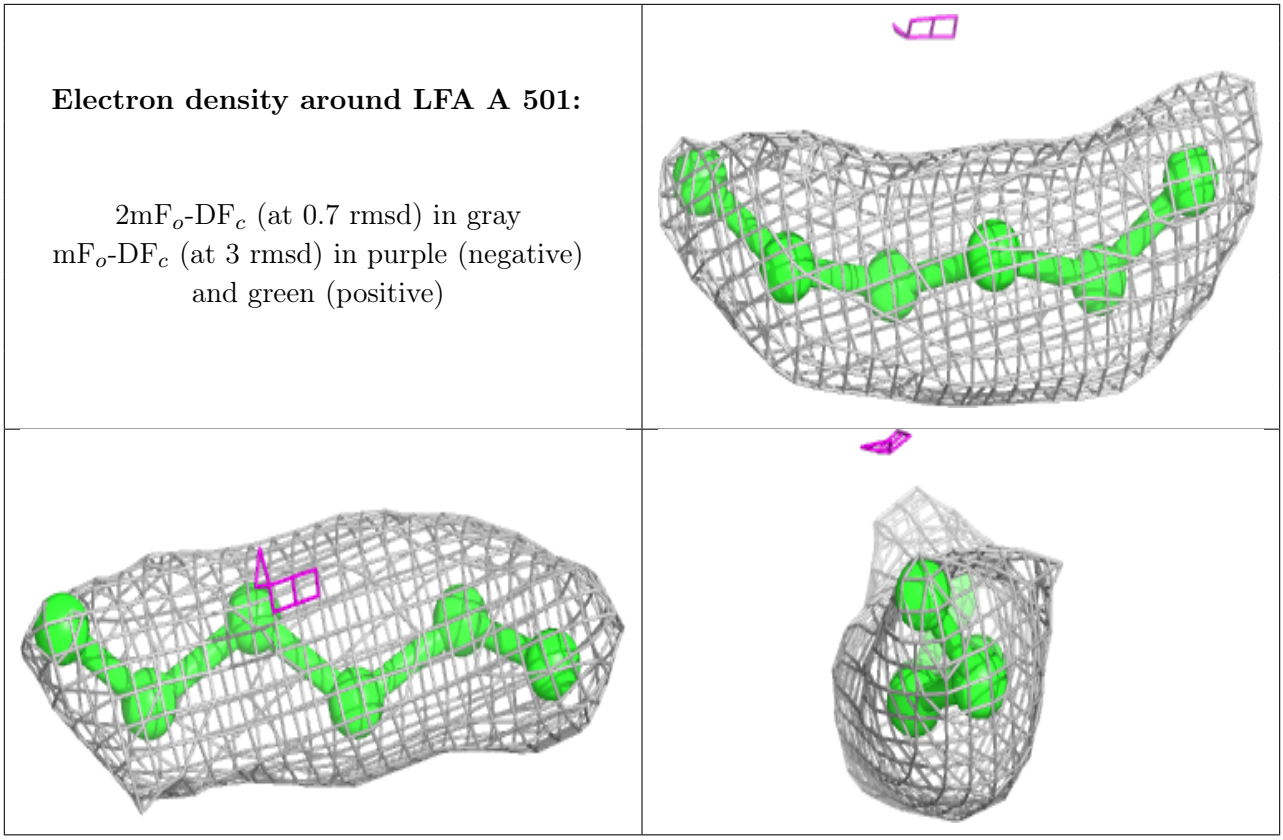






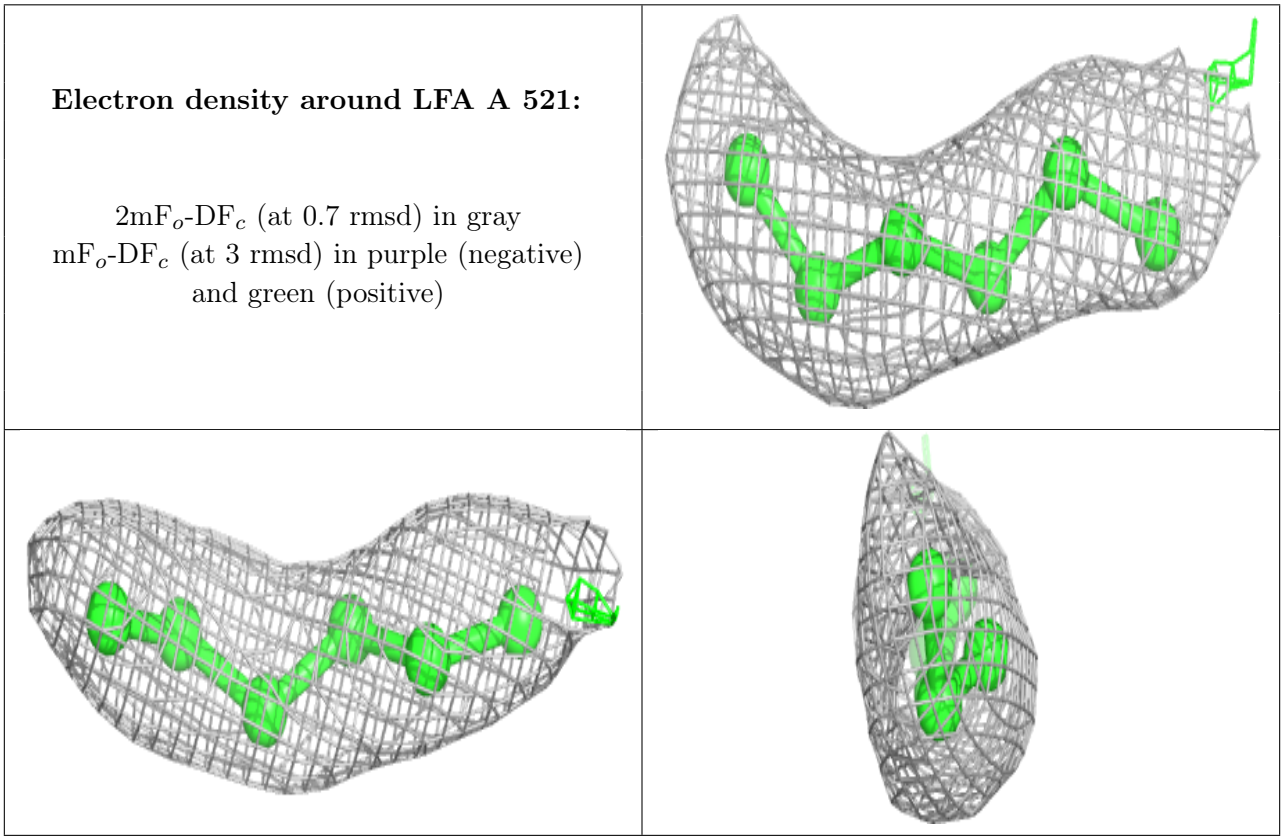
Electron density around LFA A 501:

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



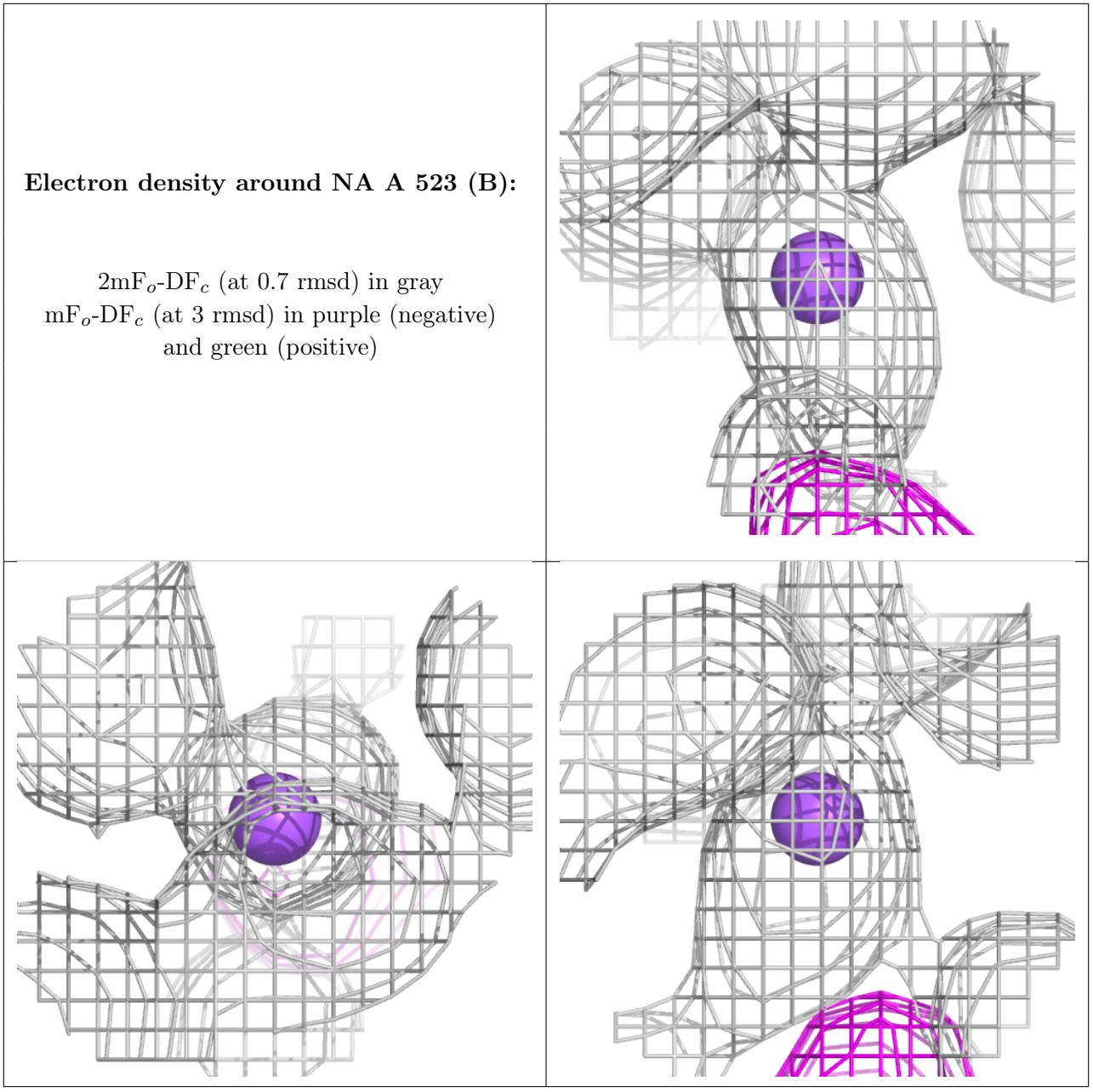
Electron density around LFA A 521:

$2mF_o$-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 523 (B):

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



6.5 Other polymers

There are no such residues in this entry.