



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:18 AM UTC

PDB ID : 7ZNC / pdb_00007znc
Title : Crystal structure of the light-driven inward proton pump xenorhodopsin BcXeR in the ground state at pH 7.6 in the absence 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

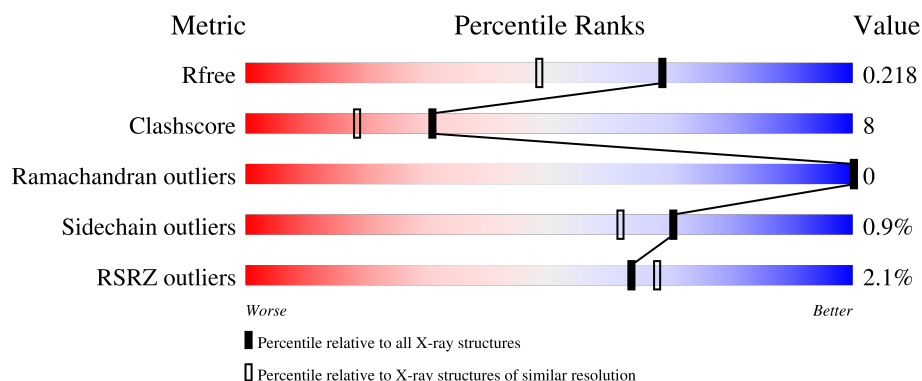
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

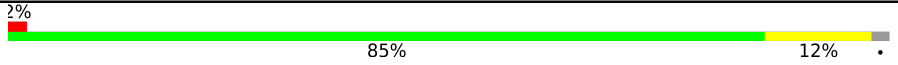
The reported resolution of this entry is 1.70 Å.

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	229	
1	B	229	
1	C	229	

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
1	FME	C	1	X	-	-	-

2 Entry composition [i](#)

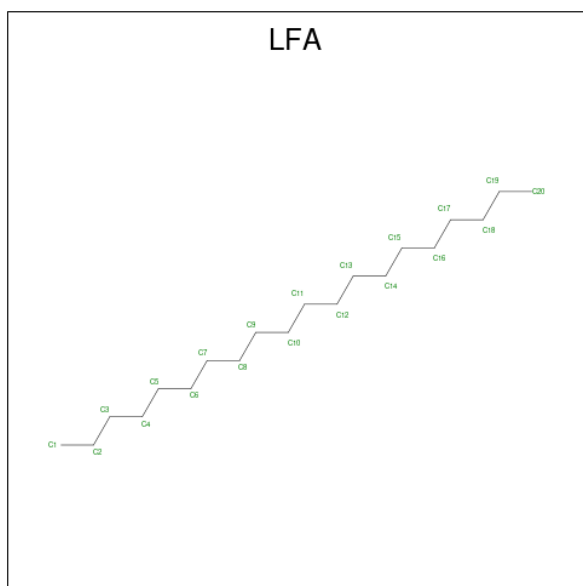
There are 6 unique types of molecules in this entry. The entry contains 6609 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	224	Total	C	N	O	S	0	6	0
			1824	1235	278	304	7			
1	B	222	Total	C	N	O	S	0	5	0
			1787	1217	268	295	7			
1	C	224	Total	C	N	O	S	0	6	0
			1811	1230	275	299	7			

- 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
			8	8		
2	A	1	Total	C	0	0
			9	9		

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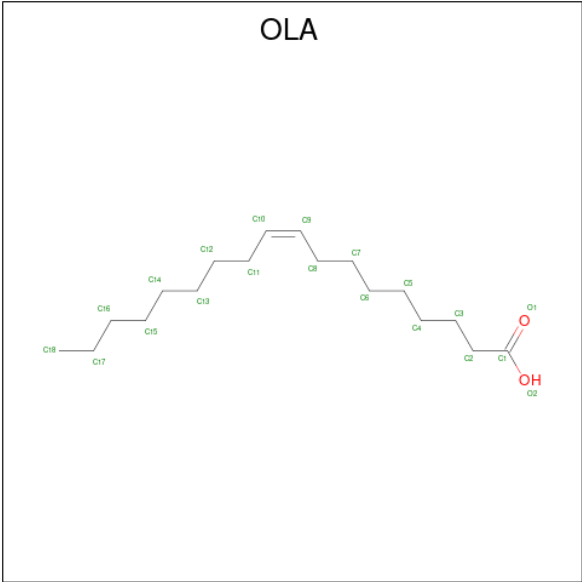
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 9 9	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 4 4	0	0
2	A	1	Total C 20 20	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 11 11	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 10 10	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 15 15	0	0
2	C	1	Total C 12 12	0	0
2	C	1	Total C 13 13	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 5 5	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 11 11	0	0
2	C	1	Total C 15 15	0	0
2	C	1	Total C 5 5	0	0
2	C	1	Total C 16 16	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 16 16	0	0

- Molecule 3 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



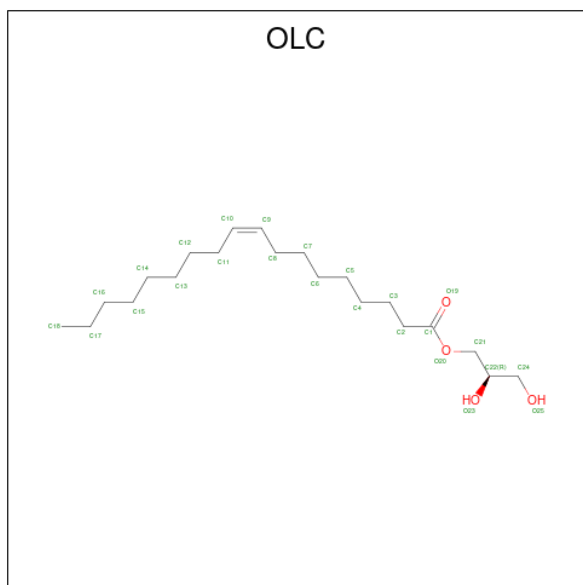
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	10	2		
3	A	1	Total	C	O	0	0
			14	12	2		
3	A	1	Total	C	O	0	0
			16	14	2		
3	A	1	Total	C	O	0	0
			20	18	2		
3	A	1	Total	C	O	0	0
			19	17	2		
3	A	1	Total	C	O	0	0
			20	18	2		
3	B	1	Total	C	O	0	0
			20	18	2		
3	B	1	Total	C	O	0	0
			16	14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

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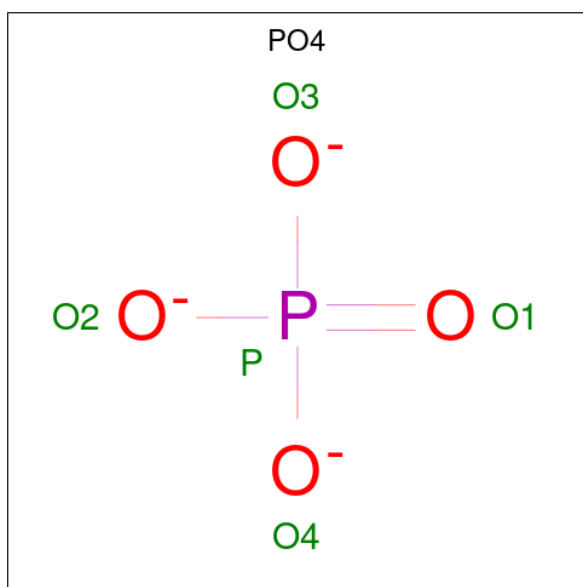
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			9	7	2		

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	15	2		
4	A	1	Total	C	O	0	0
			19	16	3		
4	A	1	Total	C	O	0	0
			19	15	4		
4	B	1	Total	C	O	0	0
			19	15	4		
4	B	1	Total	C	O	0	0
			20	18	2		
4	B	1	Total	C	O	0	0
			13	11	2		
4	C	1	Total	C	O	0	0
			17	13	4		
4	C	1	Total	C	O	0	0
			15	13	2		
4	C	1	Total	C	O	0	0
			19	15	4		

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



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

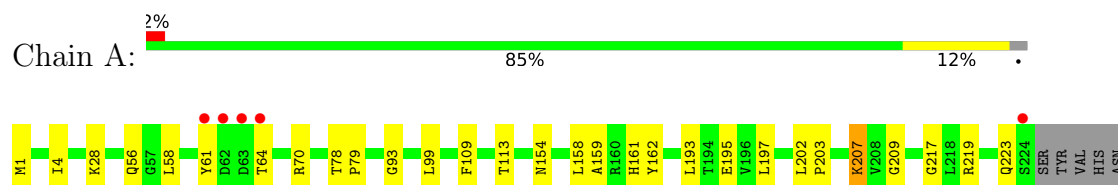
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	126	Total	O	0	4
			129	129		
6	B	113	Total	O	0	4
			116	116		
6	C	128	Total	O	0	4
			130	130		

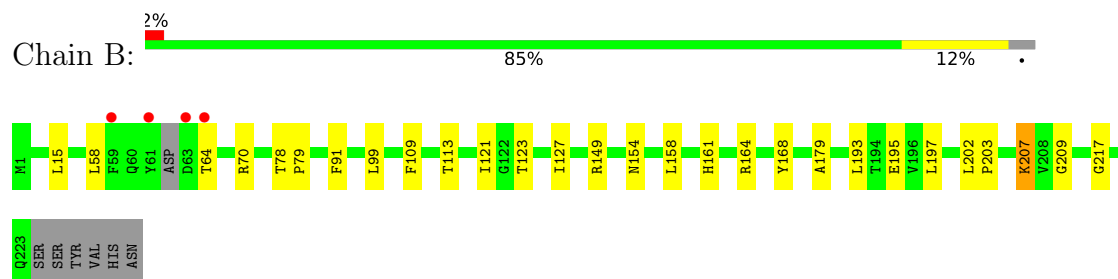
3 Residue-property plots [i](#)

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.

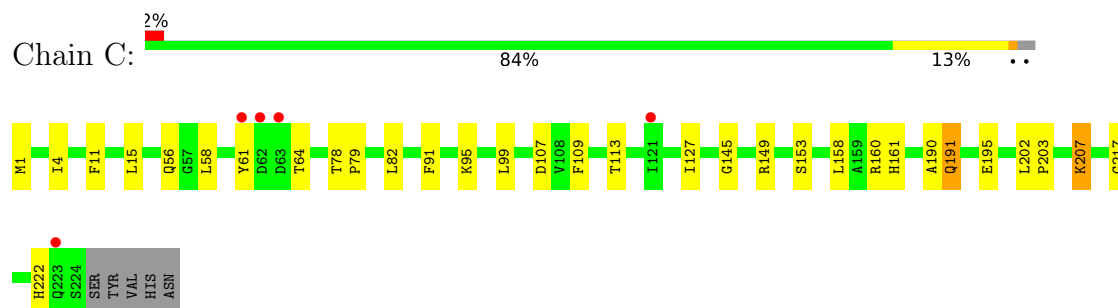
- Molecule 1: xenorhodopsin



- Molecule 1: xenorhodopsin



- Molecule 1: xenorhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.45Å 109.63Å 118.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	84.0 (20.00-1.70) 84.0 (20.00-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.184 , 0.208 0.198 , 0.218	Depositor DCC
R_{free} test set	4092 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6609	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, OLC, PO4, LYR, OLA, 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	0.94	0/1831	1.35	0/2498
1	B	0.95	0/1793	1.34	0/2448
1	C	0.95	0/1818	1.36	0/2482
All	All	0.95	0/5442	1.35	0/7428

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	1	FME	CA

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	1824	0	1902	27	0
1	B	1787	0	1863	33	0
1	C	1811	0	1893	41	0
2	A	97	0	184	1	0
2	B	173	0	319	13	0
2	C	146	0	265	3	0
3	A	101	0	149	3	0
3	B	103	0	141	4	0
3	C	29	0	43	0	0
4	A	55	0	71	5	0
4	B	52	0	74	4	0
4	C	51	0	65	10	0
5	C	5	0	0	0	0
6	A	129	0	0	7	1
6	B	116	0	0	3	0
6	C	130	0	0	10	1
All	All	6609	0	6969	110	1

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 8.

All (110) 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)
2:B:1002:LFA:C13	2:B:1019:LFA:C11	2.22	1.16
1:A:159:ALA:C	6:A:601:HOH:O	1.96	1.05
1:A:162:TYR:N	6:A:601:HOH:O	1.91	1.03
1:A:159:ALA:O	6:A:601:HOH:O	1.76	1.00
1:B:195[A]:GLU:HB2	2:B:1024:LFA:H11	1.59	0.84
1:C:127:ILE:HD13	4:C:913:OLC:H2	1.61	0.83
1:A:70:ARG:HD2	6:A:692[B]:HOH:O	1.79	0.82
1:C:149:ARG:HH22	4:C:908:OLC:H21A	1.45	0.81
1:C:127:ILE:CD1	4:C:913:OLC:H2	2.15	0.77
1:B:127[B]:ILE:HD13	2:B:1025:LFA:H112	1.67	0.76
1:B:70:ARG:HD2	6:B:1181[B]:HOH:O	1.86	0.76
1:B:202:LEU:HB2	1:B:203:PRO:HD3	1.75	0.68
1:B:127[B]:ILE:CD1	2:B:1025:LFA:H112	2.23	0.67
1:A:202:LEU:HB2	1:A:203:PRO:HD3	1.77	0.67
1:C:195[B]:GLU:OE1	6:C:1001:HOH:O	2.12	0.66
1:C:95:LYS:NZ	6:C:1002:HOH:O	2.22	0.66
1:C:160:ARG:HD3	6:C:1100:HOH:O	1.98	0.63
1:C:202:LEU:HB2	1:C:203:PRO:HD3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99[A]:LEU:C	1:C:99[A]:LEU:HD23	2.25	0.61
1:C:91:PHE:HD1	6:C:1010:HOH:O	1.83	0.61
1:C:207:LYR:H192	1:C:207:LYR:H9	1.82	0.61
1:B:207:LYR:H192	1:B:207:LYR:H9	1.83	0.61
1:A:99:LEU:HD23	1:A:99:LEU:C	2.26	0.60
1:A:28:LYS:HD2	1:A:219:ARG:NH1	2.17	0.60
1:B:99:LEU:C	1:B:99:LEU:HD23	2.27	0.59
1:A:56:GLN:HB3	4:A:507:OLC:H3	1.85	0.59
4:A:507:OLC:H6A	2:B:1001:LFA:H21	1.84	0.57
1:A:56:GLN:HB3	4:A:507:OLC:H5A	1.87	0.57
1:A:158:LEU:C	1:A:158:LEU:HD13	2.30	0.56
2:B:1002:LFA:C19	3:B:1009:OLA:C12	2.83	0.56
1:C:158:LEU:C	1:C:158:LEU:HD13	2.30	0.56
4:B:1017:OLC:H6A	4:C:913:OLC:H3A	1.88	0.56
3:A:503:OLA:O1	6:A:602:HOH:O	2.18	0.54
1:B:158:LEU:C	1:B:158:LEU:HD13	2.32	0.54
1:A:161:HIS:CE1	1:A:217:GLY:HA3	2.43	0.54
1:C:145:GLY:HA3	4:C:908:OLC:H21	1.91	0.52
1:C:191:GLN:HE21	1:C:191:GLN:HA	1.74	0.52
1:B:195[B]:GLU:HG3	2:B:1024:LFA:H11	1.92	0.52
1:A:207:LYR:H9	1:A:207:LYR:H183	1.91	0.51
1:C:153[B]:SER:HB2	6:C:1024[B]:HOH:O	2.10	0.51
1:C:58:LEU:C	1:C:58:LEU:HD12	2.35	0.51
2:A:510:LFA:H152	3:A:514:OLA:O2	2.11	0.51
1:B:164:ARG:NH1	4:B:1028:OLC:O20	2.35	0.50
1:B:58:LEU:C	1:B:58:LEU:HD12	2.36	0.50
1:C:191:GLN:HG2	6:C:1121:HOH:O	2.11	0.50
1:B:207:LYR:H192	1:B:207:LYR:C9	2.42	0.50
1:C:149:ARG:HH22	4:C:908:OLC:C21	2.19	0.49
1:C:207:LYR:H192	1:C:207:LYR:C9	2.43	0.49
1:A:1:FME:O	1:A:4:ILE:HG23	2.12	0.49
1:C:95:LYS:HD2	6:C:1036:HOH:O	2.12	0.49
1:B:161:HIS:CE1	1:B:217:GLY:HA3	2.48	0.49
1:C:1:FME:HCN	6:C:1082:HOH:O	2.12	0.48
1:A:193:LEU:O	1:A:197:LEU:HD23	2.14	0.48
1:B:195[B]:GLU:HB2	2:B:1024:LFA:H11	1.94	0.48
2:C:904:LFA:C6	2:C:906:LFA:C2	2.92	0.48
1:A:207:LYR:H9	1:A:207:LYR:H192	1.95	0.48
1:B:207:LYR:H9	1:B:207:LYR:H183	1.96	0.48
1:A:93:GLY:HA3	1:A:154:ASN:HD21	1.78	0.48
1:B:15[A]:LEU:HB3	3:B:1012:OLA:H10	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:THR:O	1:B:127[B]:ILE:HG12	2.13	0.47
1:B:168:TYR:HE1	4:B:1028:OLC:H3A	1.79	0.47
1:B:78:THR:N	1:B:79:PRO:HD2	2.29	0.47
1:B:127[B]:ILE:HD13	2:B:1025:LFA:C11	2.41	0.47
1:B:179:ALA:O	2:B:1024:LFA:H13	2.15	0.47
1:C:99[A]:LEU:HD23	1:C:99[A]:LEU:O	2.15	0.47
1:C:127:ILE:CD1	4:C:913:OLC:C2	2.90	0.47
1:C:1:FME:O1	1:C:4:ILE:HG12	2.15	0.47
1:C:149:ARG:NH2	4:C:908:OLC:H21A	2.23	0.47
1:C:127:ILE:HD11	4:C:913:OLC:C2	2.45	0.47
1:A:61:TYR:O	1:A:64:THR:HG22	2.14	0.46
1:C:207:LYR:H9	1:C:207:LYR:H183	1.98	0.46
1:C:161:HIS:CE1	1:C:217:GLY:HA3	2.50	0.46
1:C:58:LEU:HD12	1:C:58:LEU:O	2.15	0.46
4:A:507:OLC:C22	4:A:507:OLC:H2	2.45	0.46
1:A:207:LYR:H192	1:A:207:LYR:C9	2.46	0.45
1:B:91:PHE:HD1	6:B:1101:HOH:O	1.99	0.45
1:A:109:PHE:O	1:A:113:THR:HG23	2.16	0.45
1:A:99:LEU:HD23	1:A:99:LEU:O	2.16	0.45
1:C:78:THR:N	1:C:79:PRO:HD2	2.31	0.45
1:B:99:LEU:HD23	1:B:99:LEU:O	2.17	0.45
1:A:1:FME:HA	1:A:4:ILE:CG2	2.47	0.45
1:B:168:TYR:CD1	4:B:1028:OLC:H2	2.52	0.44
1:B:202:LEU:CB	1:B:203:PRO:HD3	2.45	0.44
1:C:56:GLN:HB3	4:C:912:OLC:H5A	1.99	0.44
1:C:109:PHE:O	1:C:113:THR:HG23	2.17	0.44
1:A:78:THR:N	1:A:79:PRO:HD2	2.32	0.44
1:B:195[B]:GLU:CB	2:B:1024:LFA:H11	2.46	0.44
1:B:109:PHE:O	1:B:113:THR:HG23	2.17	0.44
1:C:222:HIS:CE1	6:C:1009:HOH:O	2.71	0.43
1:A:1:FME:O	1:A:4:ILE:CG2	2.66	0.43
1:B:209:GLY:HA2	3:B:1013:OLA:H82	2.00	0.43
1:B:154:ASN:ND2	6:B:1107:HOH:O	2.51	0.43
1:B:193:LEU:O	1:B:197:LEU:HD23	2.18	0.43
1:C:191:GLN:HE21	1:C:191:GLN:CA	2.32	0.43
1:C:202:LEU:CB	1:C:203:PRO:HD3	2.47	0.43
1:C:11:PHE:CE1	1:C:15[B]:LEU:HD11	2.54	0.42
1:B:195[B]:GLU:CG	2:B:1024:LFA:H11	2.49	0.42
1:C:11:PHE:HB2	2:C:906:LFA:H32	2.01	0.42
1:A:58:LEU:HD23	1:A:58:LEU:N	2.35	0.42
1:A:209:GLY:HA2	4:A:519:OLC:H4	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:509:OLA:H32	2:B:1004:LFA:H82	2.02	0.42
1:A:162:TYR:HB3	6:A:601:HOH:O	2.20	0.42
1:C:195[A]:GLU:HG2	6:C:1064[A]:HOH:O	2.20	0.42
1:C:190:ALA:CB	2:C:920:LFA:H22	2.50	0.41
1:C:61:TYR:O	1:C:64:THR:HG22	2.20	0.41
1:C:207:LYR:HG2	1:C:207:LYR:H1	2.02	0.41
1:B:127[A]:ILE:CD1	3:B:1016:OLA:H51	2.51	0.41
1:B:197:LEU:HD13	1:B:197:LEU:HA	1.97	0.41
1:C:82:LEU:HD12	1:C:107:ASP:HB2	2.04	0.40
1:A:195[A]:GLU:OE2	6:A:603:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:689:HOH:O	6:C:1099:HOH:O[4_445]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/229 (99%)	226 (100%)	1 (0%)	0	100	100
1	B	222/229 (97%)	221 (100%)	1 (0%)	0	100	100
1	C	227/229 (99%)	226 (100%)	1 (0%)	0	100	100
All	All	676/687 (98%)	673 (100%)	3 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/189 (99%)	186 (100%)	1 (0%)	81	76
1	B	181/189 (96%)	178 (98%)	3 (2%)	53	38
1	C	185/189 (98%)	184 (100%)	1 (0%)	81	76
All	All	553/567 (98%)	548 (99%)	5 (1%)	70	62

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

Mol	Chain	Res	Type
1	A	223	GLN
1	B	64	THR
1	B	121	ILE
1	B	149	ARG
1	C	191	GLN

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

Mol	Chain	Res	Type
1	A	154	ASN
1	B	60	GLN
1	B	154	ASN
1	C	191	GLN
1	C	222	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.09	3 (11%)	30,37,39	1.26	3 (10%)
1	FME	A	1	1	8,9,10	0.41	0	8,9,11	0.65	0
1	LYR	A	207	1	27,29,30	1.02	2 (7%)	30,37,39	1.27	3 (10%)
1	LYR	C	207	1	27,29,30	1.04	2 (7%)	30,37,39	1.24	3 (10%)
1	FME	B	1	1	8,9,10	0.42	0	8,9,11	0.71	0
1	FME	C	1	1	8,9,10	0.44	0	8,9,11	0.66	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
1	LYR	B	207	1	-	2/22/40/42	0/1/1/1
1	FME	A	1	1	-	0/7/9/11	-
1	LYR	A	207	1	-	3/22/40/42	0/1/1/1
1	LYR	C	207	1	-	3/22/40/42	0/1/1/1
1	FME	B	1	1	-	1/7/9/11	-
1	FME	C	1	1	1/1/1/4	3/7/9/11	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	LYR	C5-C3	-2.61	1.40	1.46
1	B	207	LYR	C9-C80	-2.53	1.40	1.46
1	C	207	LYR	C9-C80	-2.45	1.40	1.46
1	C	207	LYR	C5-C3	-2.30	1.41	1.46
1	B	207	LYR	C5-C3	-2.28	1.41	1.46
1	A	207	LYR	C9-C80	-2.21	1.41	1.46
1	B	207	LYR	C4-C3	-2.01	1.46	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	LYR	C8-C80-C7	-3.64	116.92	122.82
1	C	207	LYR	C8-C80-C7	-3.56	117.04	122.82
1	B	207	LYR	C8-C80-C7	-3.48	117.18	122.82
1	A	207	LYR	C8-C80-C9	3.29	123.11	118.09
1	C	207	LYR	C8-C80-C9	3.27	123.09	118.09
1	B	207	LYR	C8-C80-C9	3.19	122.96	118.09
1	A	207	LYR	C5-C3-C2	-2.03	115.66	118.49
1	C	207	LYR	C5-C3-C2	-2.01	115.69	118.49
1	B	207	LYR	C17-C11-C10	2.01	121.10	115.65

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	1	FME	CA

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	1	FME	O1-CN-N-CA
1	C	1	FME	O-C-CA-CB
1	C	207	LYR	C1-C2-C3-C5
1	B	1	FME	CA-CB-CG-SD
1	B	207	LYR	C2-C1-NZ-CE
1	A	207	LYR	C1-C2-C3-C4
1	C	207	LYR	C1-C2-C3-C4
1	C	207	LYR	CD-CE-NZ-C1
1	A	207	LYR	CD-CE-NZ-C1
1	B	207	LYR	CD-CE-NZ-C1
1	C	1	FME	CB-CA-N-CN
1	A	207	LYR	C1-C2-C3-C5

There are no ring outliers.

5 monomers are involved in 15 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

68 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	LFA	B	1022	-	9,9,19	0.08	0	8,8,18	0.07	0
2	LFA	C	915	-	10,10,19	0.09	0	9,9,18	0.07	0
2	LFA	B	1002	-	6,6,19	0.13	0	5,5,18	0.14	0
2	LFA	B	1018	-	5,5,19	0.13	0	4,4,18	0.09	0
2	LFA	B	1021	-	7,7,19	0.11	0	6,6,18	0.08	0
2	LFA	B	1005	-	8,8,19	0.08	0	7,7,18	0.12	0
3	OLA	A	508	-	15,15,19	0.58	0	15,15,19	0.55	0
3	OLA	A	514	-	19,19,19	0.55	0	19,19,19	0.48	0
2	LFA	C	902	-	12,12,19	0.10	0	11,11,18	0.07	0
2	LFA	C	904	-	5,5,19	0.11	0	4,4,18	0.10	0
4	OLC	B	1028	-	12,12,24	1.37	2 (16%)	12,12,25	1.42	2 (16%)
3	OLA	B	1006	-	19,19,19	0.51	0	19,19,19	0.49	0
3	OLA	B	1008	-	15,15,19	0.57	0	15,15,19	0.56	0
2	LFA	B	1007	-	9,9,19	0.10	0	8,8,18	0.07	0
2	LFA	A	517	-	3,3,19	0.20	0	2,2,18	0.46	0
3	OLA	A	509	-	19,19,19	0.53	0	19,19,19	0.49	0
2	LFA	B	1003	-	8,8,19	0.11	0	7,7,18	0.11	0
3	OLA	B	1013	-	13,13,19	0.64	0	13,13,19	0.56	0
4	OLC	A	511	-	18,18,24	0.29	0	18,18,25	0.20	0
4	OLC	B	1015	-	18,18,24	0.28	0	19,19,25	0.25	0
2	LFA	A	504	-	8,8,19	0.10	0	7,7,18	0.10	0
4	OLC	A	507	-	16,16,24	0.34	0	16,16,25	0.16	0
2	LFA	B	1020	-	5,5,19	0.11	0	4,4,18	0.10	0
2	LFA	B	1004	-	10,10,19	0.10	0	9,9,18	0.06	0
2	LFA	B	1010	-	7,7,19	0.10	0	6,6,18	0.12	0
2	LFA	B	1025	-	13,13,19	0.08	0	12,12,18	0.12	0
2	LFA	B	1026	-	9,9,19	0.09	0	8,8,18	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LFA	C	901	-	11,11,19	0.10	0	10,10,18	0.09	0
3	OLA	C	910	-	8,8,19	0.78	0	8,8,19	0.72	0
2	LFA	A	505	-	8,8,19	0.10	0	7,7,18	0.09	0
2	LFA	A	515	-	9,9,19	0.09	0	8,8,18	0.07	0
3	OLA	A	506	-	13,13,19	0.63	0	13,13,19	0.56	0
5	PO4	C	914	-	4,4,4	0.72	0	6,6,6	0.46	0
3	OLA	B	1009	-	13,13,19	0.61	0	13,13,19	0.58	0
2	LFA	B	1027	-	14,14,19	0.08	0	13,13,18	0.08	0
2	LFA	C	918	-	15,15,19	0.07	0	14,14,18	0.07	0
2	LFA	C	920	-	6,6,19	0.11	0	5,5,18	0.08	0
3	OLA	B	1014	-	13,13,19	0.62	0	13,13,19	0.58	0
4	OLC	B	1017	-	19,19,24	0.30	0	19,19,25	0.27	0
2	LFA	B	1024	-	9,9,19	0.12	0	8,8,18	0.08	0
2	LFA	B	1019	-	10,10,19	0.11	0	9,9,18	0.07	0
2	LFA	C	905	-	7,7,19	0.09	0	6,6,18	0.12	0
2	LFA	C	909	-	8,8,19	0.07	0	7,7,18	0.09	0
2	LFA	C	917	-	4,4,19	0.13	0	3,3,18	0.20	0
2	LFA	C	919	-	5,5,19	0.13	0	4,4,18	0.10	0
3	OLA	A	503	-	11,11,19	0.67	0	11,11,19	0.63	0
2	LFA	C	906	-	9,9,19	0.10	0	8,8,18	0.11	0
3	OLA	A	512	-	18,18,19	0.55	0	18,18,19	0.51	0
3	OLA	C	903	-	19,19,19	0.54	0	19,19,19	0.49	0
4	OLC	C	908	-	16,16,24	0.27	0	17,17,25	0.26	0
2	LFA	C	921	-	15,15,19	0.09	0	14,14,18	0.06	0
2	LFA	C	916	-	14,14,19	0.10	0	13,13,18	0.07	0
4	OLC	C	913	-	18,18,24	0.24	0	19,19,25	0.25	0
4	OLC	C	912	-	14,14,24	0.23	0	14,14,25	0.15	0
3	OLA	B	1016	-	10,10,19	0.71	0	10,10,19	0.63	0
2	LFA	A	513	-	11,11,19	0.16	0	10,10,18	0.08	0
2	LFA	B	1011	-	10,10,19	0.11	0	9,9,18	0.07	0
2	LFA	A	510	-	10,10,19	0.08	0	9,9,18	0.09	0
2	LFA	A	516	-	7,7,19	0.12	0	6,6,18	0.08	0
2	LFA	B	1001	-	6,6,19	0.11	0	5,5,18	0.10	0
2	LFA	C	911	-	6,6,19	0.13	0	5,5,18	0.11	0
2	LFA	A	502	-	7,7,19	0.09	0	6,6,18	0.09	0
2	LFA	C	907	-	4,4,19	0.14	0	3,3,18	0.19	0
2	LFA	B	1023	-	10,10,19	0.10	0	9,9,18	0.06	0
4	OLC	A	519	-	18,18,24	0.24	0	19,19,25	0.26	0
3	OLA	B	1012	-	13,13,19	0.63	0	13,13,19	0.56	0
2	LFA	A	501	-	5,5,19	0.14	0	4,4,18	0.12	0
2	LFA	A	518	-	19,19,19	0.09	0	18,18,18	0.05	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	B	1022	-	-	6/7/7/17	-
2	LFA	C	915	-	-	2/8/8/17	-
2	LFA	B	1002	-	-	3/4/4/17	-
2	LFA	B	1018	-	-	0/3/3/17	-
2	LFA	B	1021	-	-	3/5/5/17	-
2	LFA	B	1005	-	-	2/6/6/17	-
3	OLA	A	508	-	-	8/13/13/17	-
3	OLA	A	514	-	-	9/17/17/17	-
2	LFA	C	902	-	-	4/10/10/17	-
2	LFA	C	904	-	-	0/3/3/17	-
4	OLC	B	1028	-	-	4/10/10/24	-
3	OLA	B	1006	-	-	4/17/17/17	-
3	OLA	B	1008	-	-	4/13/13/17	-
2	LFA	B	1007	-	-	4/7/7/17	-
2	LFA	A	517	-	-	0/1/1/17	-
3	OLA	A	509	-	-	6/17/17/17	-
2	LFA	B	1003	-	-	1/6/6/17	-
3	OLA	B	1013	-	-	7/11/11/17	-
4	OLC	A	511	-	-	8/17/17/24	-
4	OLC	B	1015	-	-	11/18/18/24	-
2	LFA	A	504	-	-	1/6/6/17	-
4	OLC	A	507	-	-	8/15/15/24	-
2	LFA	B	1020	-	-	2/3/3/17	-
2	LFA	B	1004	-	-	5/8/8/17	-
2	LFA	B	1010	-	-	2/5/5/17	-
2	LFA	B	1025	-	-	2/11/11/17	-
2	LFA	B	1026	-	-	2/7/7/17	-
2	LFA	C	901	-	-	3/9/9/17	-
3	OLA	C	910	-	-	2/6/6/17	-
2	LFA	A	505	-	-	4/6/6/17	-
2	LFA	A	515	-	-	1/7/7/17	-
3	OLA	A	506	-	-	6/11/11/17	-
3	OLA	B	1009	-	-	5/11/11/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	B	1027	-	-	3/12/12/17	-
2	LFA	C	918	-	-	6/13/13/17	-
2	LFA	C	920	-	-	0/4/4/17	-
3	OLA	B	1014	-	-	8/11/11/17	-
4	OLC	B	1017	-	-	11/17/17/24	-
2	LFA	B	1024	-	-	3/7/7/17	-
2	LFA	B	1019	-	-	1/8/8/17	-
2	LFA	C	905	-	-	3/5/5/17	-
2	LFA	C	909	-	-	1/6/6/17	-
2	LFA	C	917	-	-	0/2/2/17	-
2	LFA	C	919	-	-	1/3/3/17	-
3	OLA	A	503	-	-	4/9/9/17	-
2	LFA	C	906	-	-	3/7/7/17	-
3	OLA	A	512	-	-	8/16/16/17	-
3	OLA	C	903	-	-	10/17/17/17	-
4	OLC	C	908	-	-	5/16/16/24	-
2	LFA	C	921	-	-	2/13/13/17	-
2	LFA	C	916	-	-	5/12/12/17	-
4	OLC	C	913	-	-	7/18/18/24	-
4	OLC	C	912	-	-	7/13/13/24	-
3	OLA	B	1016	-	-	7/8/8/17	-
2	LFA	A	513	-	-	4/9/9/17	-
2	LFA	B	1011	-	-	2/8/8/17	-
2	LFA	A	510	-	-	5/8/8/17	-
2	LFA	A	516	-	-	3/5/5/17	-
2	LFA	B	1001	-	-	2/4/4/17	-
2	LFA	C	911	-	-	2/4/4/17	-
2	LFA	A	502	-	-	3/5/5/17	-
2	LFA	C	907	-	-	1/2/2/17	-
2	LFA	B	1023	-	-	6/8/8/17	-
4	OLC	A	519	-	-	6/18/18/24	-
3	OLA	B	1012	-	-	7/11/11/17	-
2	LFA	A	501	-	-	1/3/3/17	-
2	LFA	A	518	-	-	6/17/17/17	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1028	OLC	O19-C1	3.53	1.33	1.22
4	B	1028	OLC	O20-C1	-3.07	1.20	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1028	OLC	O19-C1-C2	-3.49	112.02	123.09
4	B	1028	OLC	O20-C1-C2	3.37	124.66	114.00

There are no chirality outliers.

All (272) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1015	OLC	C21-C22-C24-O25
4	A	507	OLC	C2-C1-O20-C21
4	A	507	OLC	O19-C1-O20-C21
4	A	519	OLC	O19-C1-O20-C21
4	A	519	OLC	C2-C1-O20-C21
4	B	1015	OLC	C2-C1-O20-C21
4	B	1015	OLC	O19-C1-O20-C21
3	B	1014	OLA	C11-C10-C9-C8
2	C	918	LFA	C3-C4-C5-C6
4	B	1015	OLC	O20-C21-C22-C24
4	A	511	OLC	C1-C2-C3-C4
3	B	1012	OLA	C11-C10-C9-C8
3	A	506	OLA	C1-C2-C3-C4
3	A	509	OLA	C1-C2-C3-C4
3	C	903	OLA	C1-C2-C3-C4
3	B	1014	OLA	C1-C2-C3-C4
4	C	908	OLC	C2-C1-O20-C21
3	A	514	OLA	C14-C15-C16-C17
4	B	1015	OLC	O20-C21-C22-O23
3	A	512	OLA	C1-C2-C3-C4
4	B	1028	OLC	C1-C2-C3-C4
4	B	1015	OLC	C1-C2-C3-C4
4	C	908	OLC	O19-C1-O20-C21
4	A	519	OLC	C21-C22-C24-O25
4	C	913	OLC	C1-C2-C3-C4
4	A	511	OLC	C6-C7-C8-C9
4	A	511	OLC	O20-C21-C22-O23
4	C	912	OLC	C2-C1-O20-C21
2	A	513	LFA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	B	1022	LFA	C4-C5-C6-C7
2	B	1023	LFA	C5-C6-C7-C8
3	B	1008	OLA	C3-C4-C5-C6
4	A	507	OLC	C3-C4-C5-C6
4	B	1015	OLC	C2-C3-C4-C5
2	C	916	LFA	C5-C6-C7-C8
2	B	1022	LFA	C6-C7-C8-C9
2	B	1023	LFA	C6-C7-C8-C9
4	B	1015	OLC	C4-C5-C6-C7
4	B	1015	OLC	O23-C22-C24-O25
3	B	1009	OLA	C5-C6-C7-C8
4	B	1017	OLC	C1-C2-C3-C4
3	A	514	OLA	C13-C14-C15-C16
3	B	1008	OLA	C4-C5-C6-C7
2	C	901	LFA	C7-C8-C9-C10
3	B	1016	OLA	C2-C3-C4-C5
3	B	1006	OLA	C11-C12-C13-C14
2	B	1019	LFA	C5-C6-C7-C8
2	A	516	LFA	C4-C5-C6-C7
2	C	918	LFA	C5-C6-C7-C8
2	B	1023	LFA	C2-C3-C4-C5
2	C	905	LFA	C4-C5-C6-C7
3	B	1013	OLA	C11-C10-C9-C8
2	A	502	LFA	C2-C3-C4-C5
2	C	901	LFA	C11-C10-C9-C8
4	C	912	OLC	C5-C6-C7-C8
2	A	518	LFA	C13-C14-C15-C16
2	C	902	LFA	C7-C8-C9-C10
2	A	518	LFA	C14-C15-C16-C17
3	A	514	OLA	C3-C4-C5-C6
4	A	519	OLC	C9-C10-C11-C12
4	C	912	OLC	C9-C10-C11-C12
4	C	913	OLC	C9-C10-C11-C12
3	B	1016	OLA	C1-C2-C3-C4
3	A	514	OLA	C6-C7-C8-C9
3	B	1012	OLA	C6-C7-C8-C9
4	B	1017	OLC	C6-C7-C8-C9
3	A	506	OLA	C4-C5-C6-C7
3	B	1008	OLA	C5-C6-C7-C8
4	A	507	OLC	C1-C2-C3-C4
3	A	512	OLA	C6-C7-C8-C9
3	B	1009	OLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	B	1004	LFA	C6-C7-C8-C9
3	B	1012	OLA	C4-C5-C6-C7
4	B	1017	OLC	C7-C8-C9-C10
2	B	1023	LFA	C7-C8-C9-C10
2	C	902	LFA	C4-C5-C6-C7
2	B	1001	LFA	C3-C4-C5-C6
2	B	1004	LFA	C2-C3-C4-C5
2	C	921	LFA	C11-C10-C9-C8
3	B	1012	OLA	C1-C2-C3-C4
2	C	902	LFA	C10-C11-C12-C13
4	C	913	OLC	C5-C6-C7-C8
3	A	506	OLA	C6-C7-C8-C9
3	C	903	OLA	C6-C7-C8-C9
4	A	507	OLC	C6-C7-C8-C9
2	A	510	LFA	C12-C13-C14-C15
2	A	513	LFA	C11-C10-C9-C8
2	B	1004	LFA	C5-C6-C7-C8
3	A	512	OLA	C10-C11-C12-C13
2	A	516	LFA	C2-C3-C4-C5
2	A	510	LFA	C11-C12-C13-C14
4	C	912	OLC	C2-C3-C4-C5
3	A	509	OLA	C2-C3-C4-C5
3	B	1012	OLA	C3-C4-C5-C6
2	C	919	LFA	C2-C3-C4-C5
2	A	518	LFA	C9-C10-C11-C12
2	C	906	LFA	C4-C5-C6-C7
2	C	918	LFA	C9-C10-C11-C12
4	C	913	OLC	C2-C3-C4-C5
3	B	1014	OLA	C4-C5-C6-C7
3	A	508	OLA	C10-C11-C12-C13
3	B	1014	OLA	C6-C7-C8-C9
4	C	913	OLC	C6-C7-C8-C9
2	A	510	LFA	C14-C15-C16-C17
2	B	1021	LFA	C5-C6-C7-C8
3	A	506	OLA	C11-C10-C9-C8
3	B	1013	OLA	C5-C6-C7-C8
4	A	511	OLC	C2-C1-O20-C21
2	B	1023	LFA	C11-C10-C9-C8
2	B	1020	LFA	C2-C3-C4-C5
2	C	921	LFA	C7-C8-C9-C10
2	A	505	LFA	C12-C13-C14-C15
4	A	519	OLC	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	B	1005	LFA	C4-C5-C6-C7
2	B	1002	LFA	C13-C14-C15-C16
2	A	513	LFA	C7-C8-C9-C10
2	B	1007	LFA	C1-C2-C3-C4
2	B	1011	LFA	C7-C8-C9-C10
3	A	503	OLA	C2-C3-C4-C5
4	B	1017	OLC	C2-C3-C4-C5
2	C	901	LFA	C6-C7-C8-C9
2	C	906	LFA	C2-C3-C4-C5
2	B	1002	LFA	C16-C17-C18-C19
2	B	1007	LFA	C6-C7-C8-C9
2	B	1007	LFA	C7-C8-C9-C10
2	C	915	LFA	C10-C11-C12-C13
3	A	508	OLA	C11-C10-C9-C8
3	A	508	OLA	C4-C5-C6-C7
3	A	514	OLA	C5-C6-C7-C8
3	A	512	OLA	C7-C8-C9-C10
3	A	512	OLA	C5-C6-C7-C8
3	B	1012	OLA	C5-C6-C7-C8
2	B	1010	LFA	C5-C6-C7-C8
2	C	916	LFA	C11-C10-C9-C8
2	A	505	LFA	C13-C14-C15-C16
3	B	1006	OLA	C12-C13-C14-C15
2	C	907	LFA	C1-C2-C3-C4
2	B	1025	LFA	C4-C5-C6-C7
2	B	1023	LFA	C1-C2-C3-C4
2	A	505	LFA	C17-C18-C19-C20
2	B	1024	LFA	C6-C7-C8-C9
2	C	911	LFA	C1-C2-C3-C4
2	A	510	LFA	C13-C14-C15-C16
2	B	1026	LFA	C4-C5-C6-C7
2	A	505	LFA	C15-C16-C17-C18
3	C	903	OLA	C15-C16-C17-C18
4	C	912	OLC	O19-C1-O20-C21
4	A	511	OLC	O19-C1-O20-C21
2	B	1022	LFA	C3-C4-C5-C6
3	A	514	OLA	C4-C5-C6-C7
4	B	1017	OLC	C3-C4-C5-C6
4	B	1015	OLC	C5-C6-C7-C8
4	B	1017	OLC	C12-C13-C14-C15
2	A	502	LFA	C1-C2-C3-C4
2	C	918	LFA	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
2	B	1021	LFA	C4-C5-C6-C7
2	B	1011	LFA	C11-C10-C9-C8
2	A	513	LFA	C6-C7-C8-C9
2	C	902	LFA	C5-C6-C7-C8
2	A	510	LFA	C7-C8-C9-C10
4	B	1017	OLC	C5-C6-C7-C8
3	B	1013	OLA	C9-C10-C11-C12
2	B	1004	LFA	C4-C5-C6-C7
2	A	516	LFA	C5-C6-C7-C8
4	C	908	OLC	O20-C1-C2-C3
2	B	1022	LFA	C7-C8-C9-C10
3	A	514	OLA	C2-C3-C4-C5
2	A	515	LFA	C7-C8-C9-C10
3	A	503	OLA	C7-C8-C9-C10
3	C	903	OLA	C3-C4-C5-C6
2	C	918	LFA	C1-C2-C3-C4
2	B	1005	LFA	C2-C3-C4-C5
2	C	905	LFA	C5-C6-C7-C8
3	B	1009	OLA	C2-C3-C4-C5
3	C	910	OLA	C2-C3-C4-C5
2	C	918	LFA	C12-C13-C14-C15
2	B	1021	LFA	C1-C2-C3-C4
3	A	503	OLA	C4-C5-C6-C7
3	A	509	OLA	C6-C7-C8-C9
2	A	518	LFA	C16-C17-C18-C19
3	C	903	OLA	C7-C8-C9-C10
2	A	518	LFA	C10-C11-C12-C13
2	B	1004	LFA	C1-C2-C3-C4
2	C	906	LFA	C6-C7-C8-C9
3	B	1013	OLA	C2-C3-C4-C5
2	B	1002	LFA	C15-C16-C17-C18
3	A	512	OLA	C9-C10-C11-C12
2	B	1027	LFA	C9-C10-C11-C12
2	C	905	LFA	C6-C7-C8-C9
4	C	908	OLC	C2-C3-C4-C5
3	B	1013	OLA	C1-C2-C3-C4
4	A	519	OLC	O23-C22-C24-O25
2	B	1022	LFA	C2-C3-C4-C5
2	C	916	LFA	C9-C10-C11-C12
4	B	1017	OLC	C14-C15-C16-C17
3	B	1014	OLA	C3-C4-C5-C6
2	A	501	LFA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
2	A	518	LFA	C11-C10-C9-C8
3	B	1006	OLA	C15-C16-C17-C18
3	C	903	OLA	C11-C12-C13-C14
2	B	1020	LFA	C1-C2-C3-C4
3	A	514	OLA	C11-C12-C13-C14
3	B	1013	OLA	C6-C7-C8-C9
4	C	912	OLC	C6-C7-C8-C9
2	B	1024	LFA	C4-C5-C6-C7
3	B	1013	OLA	C7-C8-C9-C10
3	B	1016	OLA	C3-C4-C5-C6
2	B	1010	LFA	C2-C3-C4-C5
3	A	509	OLA	C7-C8-C9-C10
2	C	916	LFA	C4-C5-C6-C7
2	C	915	LFA	C14-C15-C16-C17
4	B	1015	OLC	C7-C8-C9-C10
3	A	506	OLA	C2-C3-C4-C5
4	B	1017	OLC	O19-C1-C2-C3
4	B	1028	OLC	C7-C8-C9-C10
2	C	916	LFA	C7-C8-C9-C10
3	A	508	OLA	C6-C7-C8-C9
3	A	512	OLA	O2-C1-C2-C3
3	C	903	OLA	O1-C1-C2-C3
3	A	514	OLA	C10-C11-C12-C13
3	B	1014	OLA	O1-C1-C2-C3
4	B	1017	OLC	O20-C1-C2-C3
3	B	1014	OLA	O2-C1-C2-C3
2	B	1001	LFA	C1-C2-C3-C4
3	B	1016	OLA	O2-C1-C2-C3
3	B	1016	OLA	C6-C7-C8-C9
2	C	909	LFA	C5-C6-C7-C8
2	B	1007	LFA	C4-C5-C6-C7
4	A	511	OLC	C5-C6-C7-C8
3	A	512	OLA	O1-C1-C2-C3
3	C	903	OLA	O2-C1-C2-C3
3	A	508	OLA	C5-C6-C7-C8
2	A	504	LFA	C1-C2-C3-C4
3	A	509	OLA	O2-C1-C2-C3
2	B	1027	LFA	C12-C13-C14-C15
4	C	912	OLC	C7-C8-C9-C10
3	A	503	OLA	C1-C2-C3-C4
3	A	508	OLA	C2-C3-C4-C5
3	B	1016	OLA	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	B	1025	LFA	C6-C7-C8-C9
2	A	502	LFA	C5-C6-C7-C8
2	C	911	LFA	C4-C5-C6-C7
3	B	1006	OLA	C7-C8-C9-C10
2	B	1024	LFA	C3-C4-C5-C6
2	B	1022	LFA	C5-C6-C7-C8
3	A	509	OLA	O1-C1-C2-C3
3	A	506	OLA	C7-C8-C9-C10
2	B	1026	LFA	C5-C6-C7-C8
3	C	903	OLA	C13-C14-C15-C16
4	A	507	OLC	C2-C3-C4-C5
4	C	913	OLC	O20-C21-C22-C24
3	B	1008	OLA	C7-C8-C9-C10
3	B	1012	OLA	C7-C8-C9-C10
4	A	507	OLC	C7-C8-C9-C10
2	B	1027	LFA	C3-C4-C5-C6
3	B	1009	OLA	O2-C1-C2-C3
4	A	507	OLC	C9-C10-C11-C12
4	A	511	OLC	C9-C10-C11-C12
2	B	1003	LFA	C6-C7-C8-C9
3	C	910	OLA	C3-C4-C5-C6
4	B	1017	OLC	C4-C5-C6-C7
4	C	908	OLC	O19-C1-C2-C3
3	B	1014	OLA	C5-C6-C7-C8
3	A	508	OLA	O2-C1-C2-C3
3	B	1009	OLA	O1-C1-C2-C3
4	C	913	OLC	O20-C21-C22-O23
3	B	1016	OLA	C5-C6-C7-C8
4	B	1028	OLC	O20-C1-C2-C3
4	A	511	OLC	O20-C1-C2-C3
3	C	903	OLA	C14-C15-C16-C17
4	B	1028	OLC	O19-C1-C2-C3
3	A	508	OLA	O1-C1-C2-C3

There are no ring outliers.

24 monomers are involved in 38 short contacts:

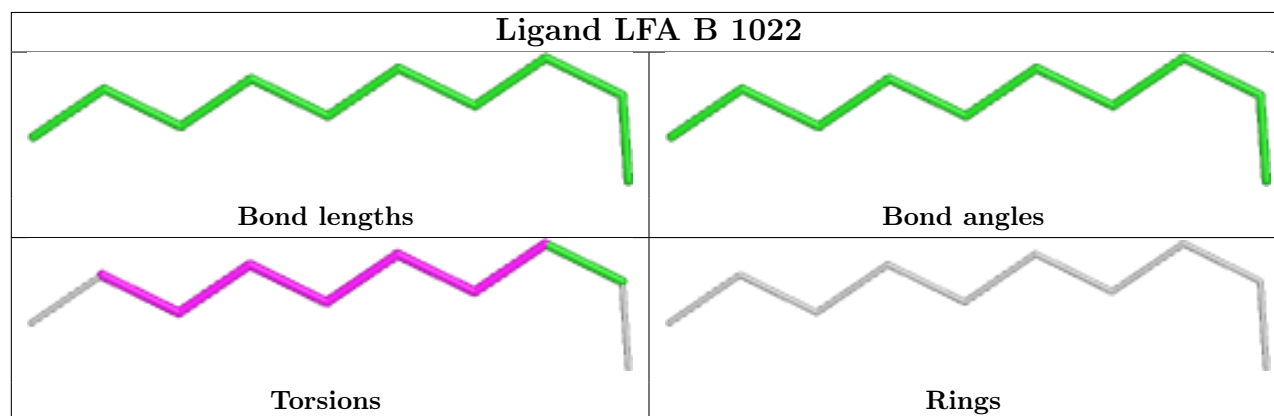
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	LFA	2	0
3	A	514	OLA	1	0
2	C	904	LFA	1	0
4	B	1028	OLC	3	0

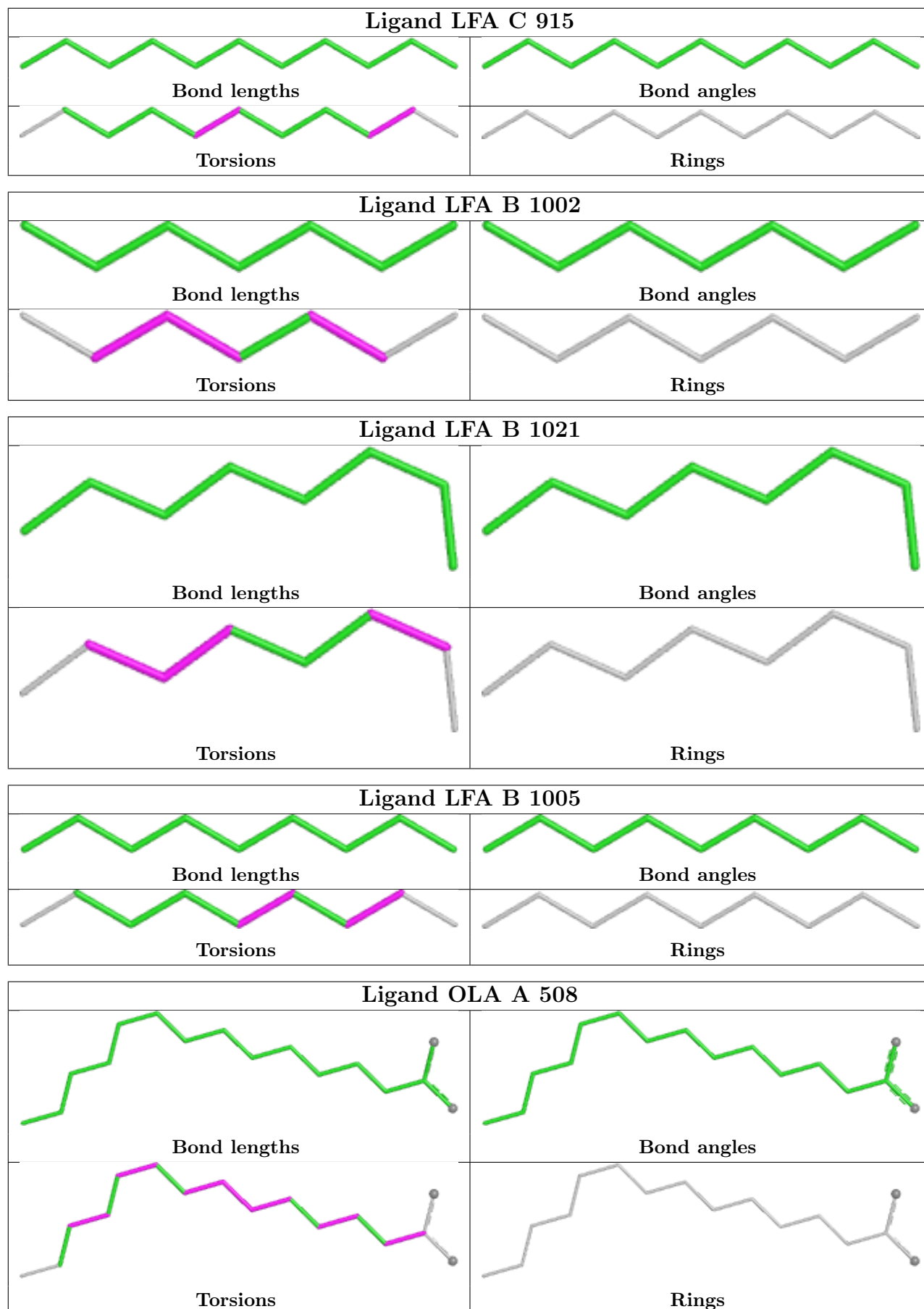
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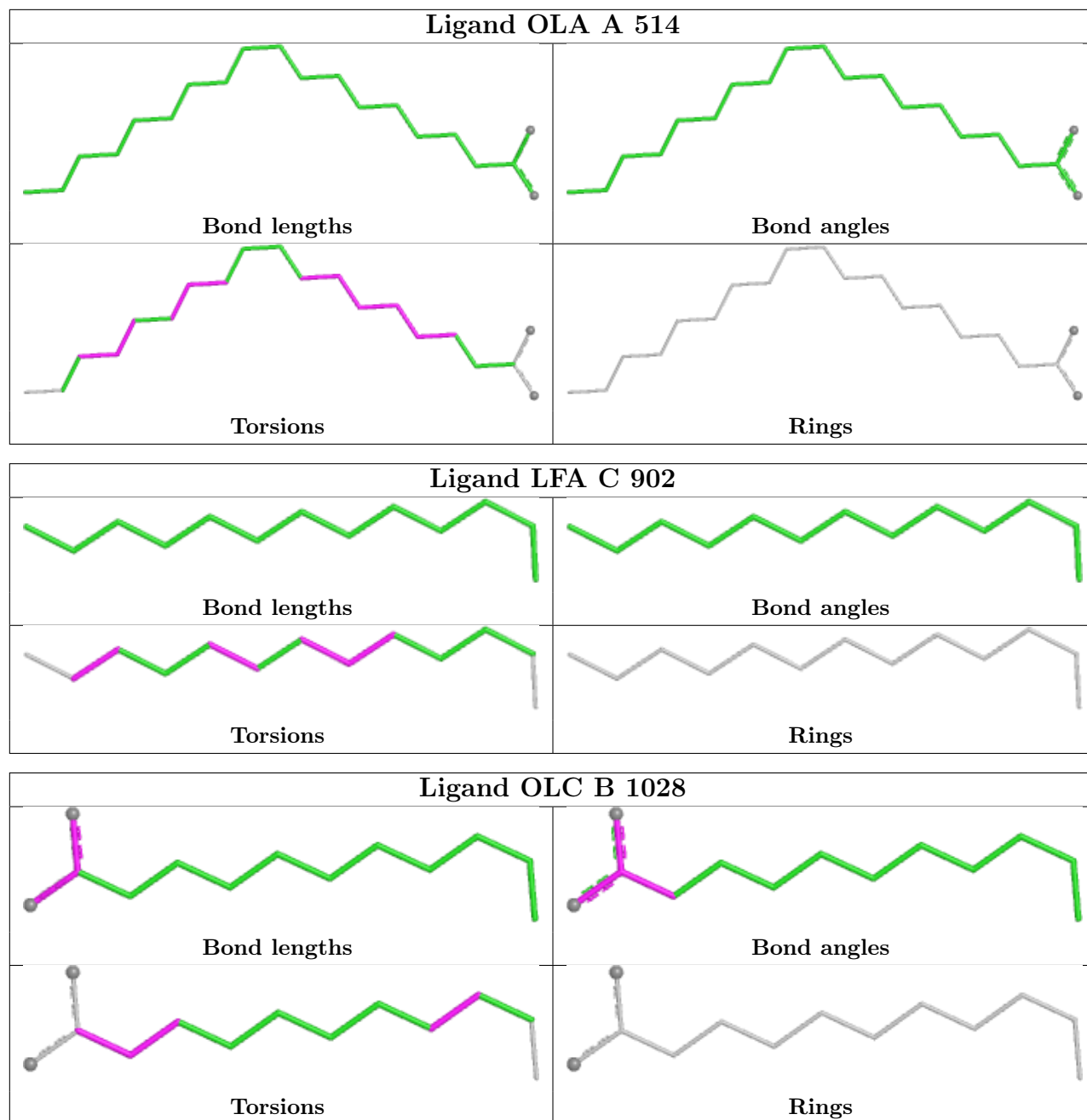
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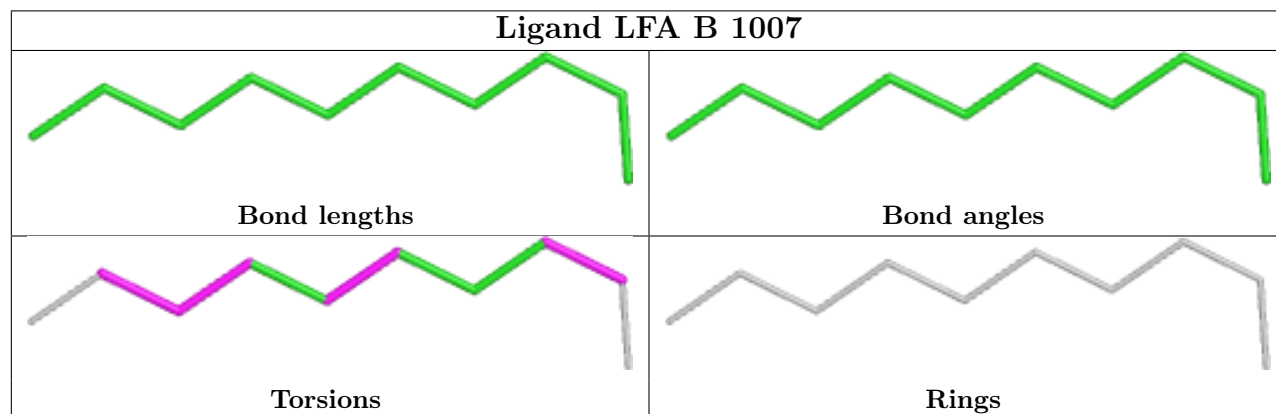
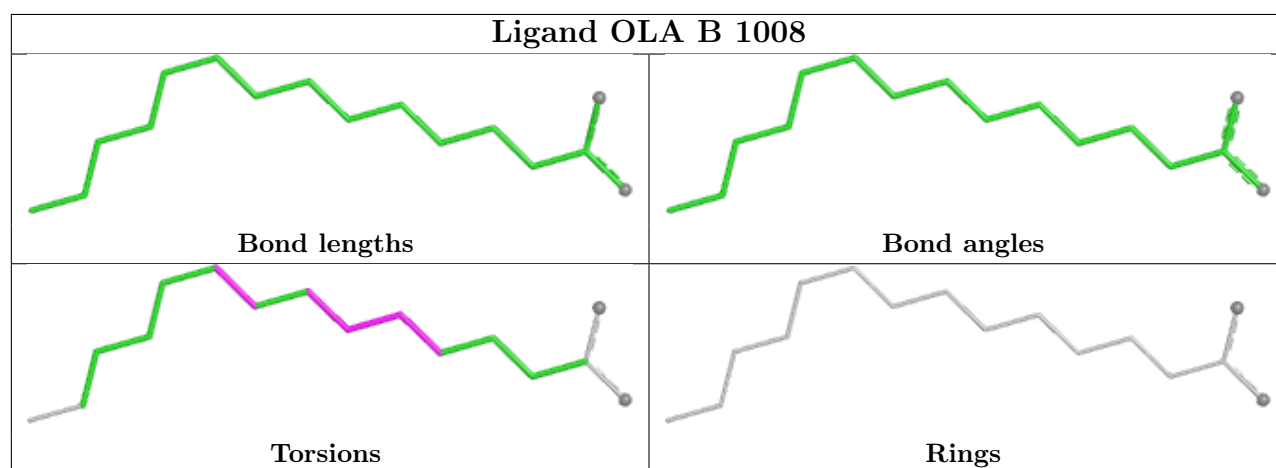
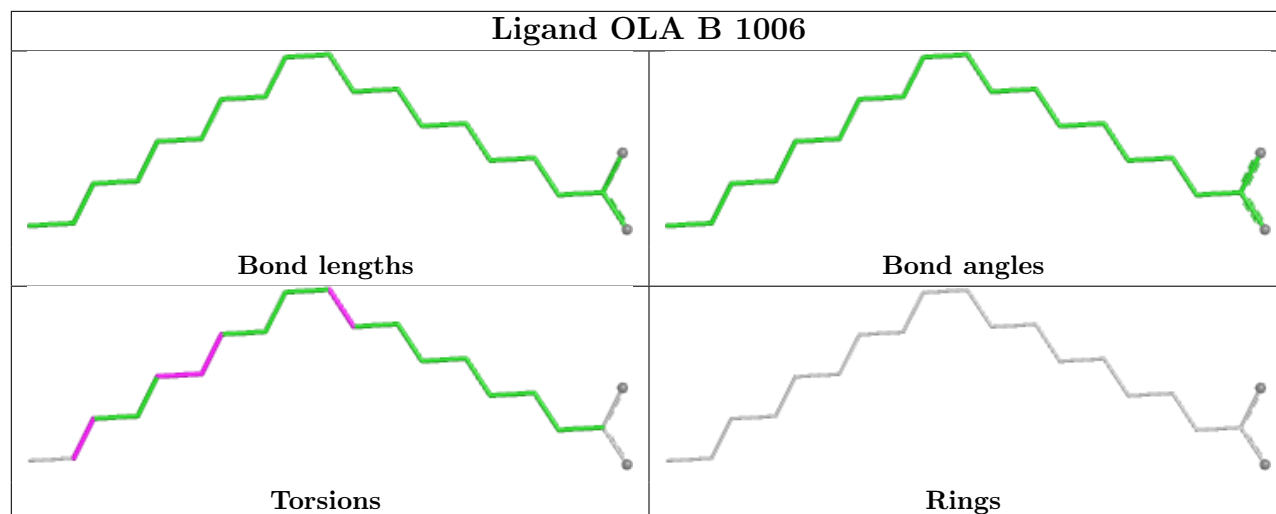
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	509	OLA	1	0
3	B	1013	OLA	1	0
4	A	507	OLC	4	0
2	B	1004	LFA	1	0
2	B	1025	LFA	3	0
3	B	1009	OLA	1	0
2	C	920	LFA	1	0
4	B	1017	OLC	1	0
2	B	1024	LFA	6	0
2	B	1019	LFA	1	0
3	A	503	OLA	1	0
2	C	906	LFA	2	0
4	C	908	OLC	4	0
4	C	913	OLC	5	0
4	C	912	OLC	1	0
3	B	1016	OLA	1	0
2	A	510	LFA	1	0
2	B	1001	LFA	1	0
4	A	519	OLC	1	0
3	B	1012	OLA	1	0

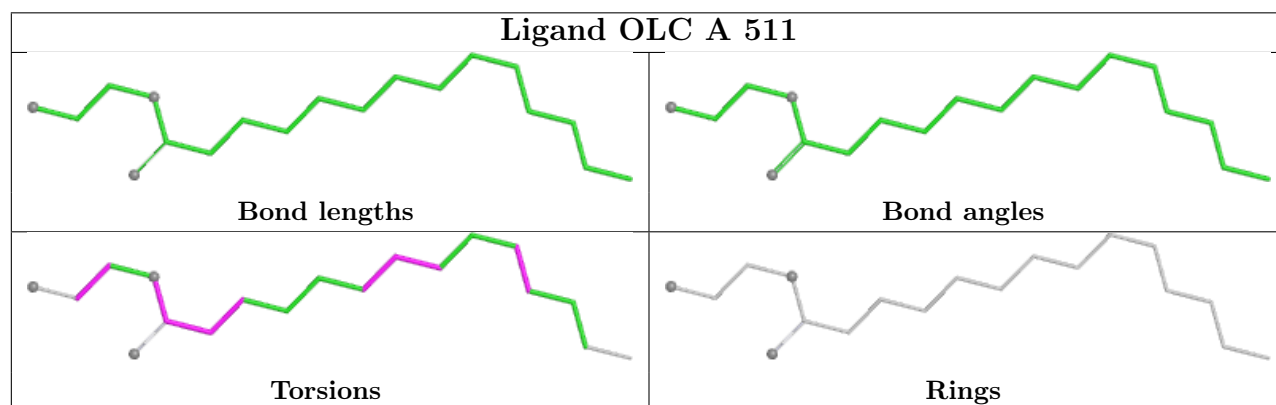
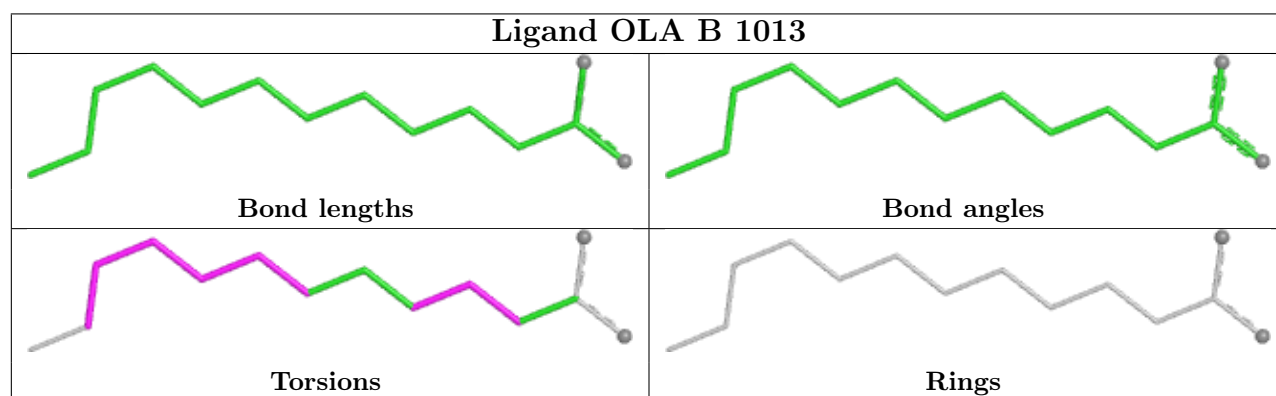
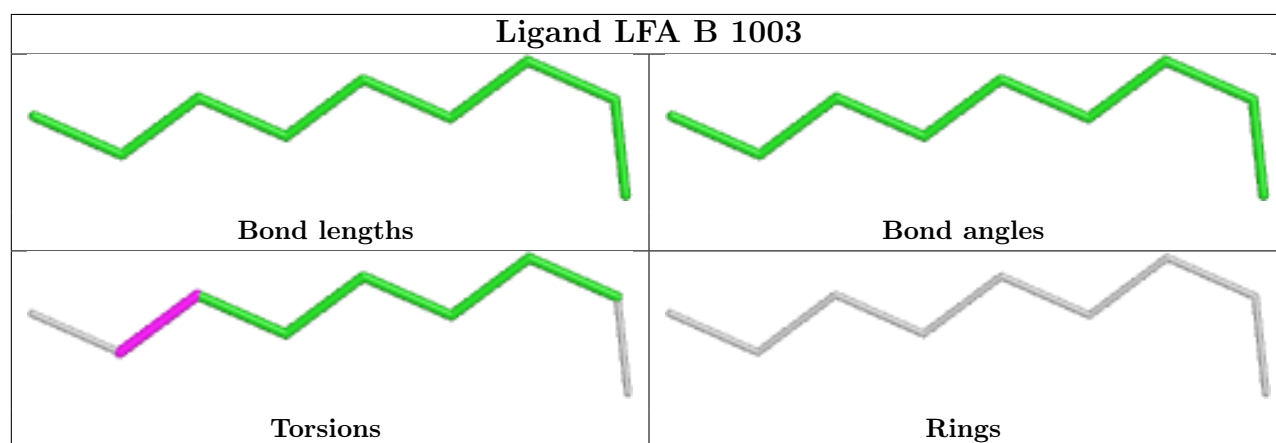
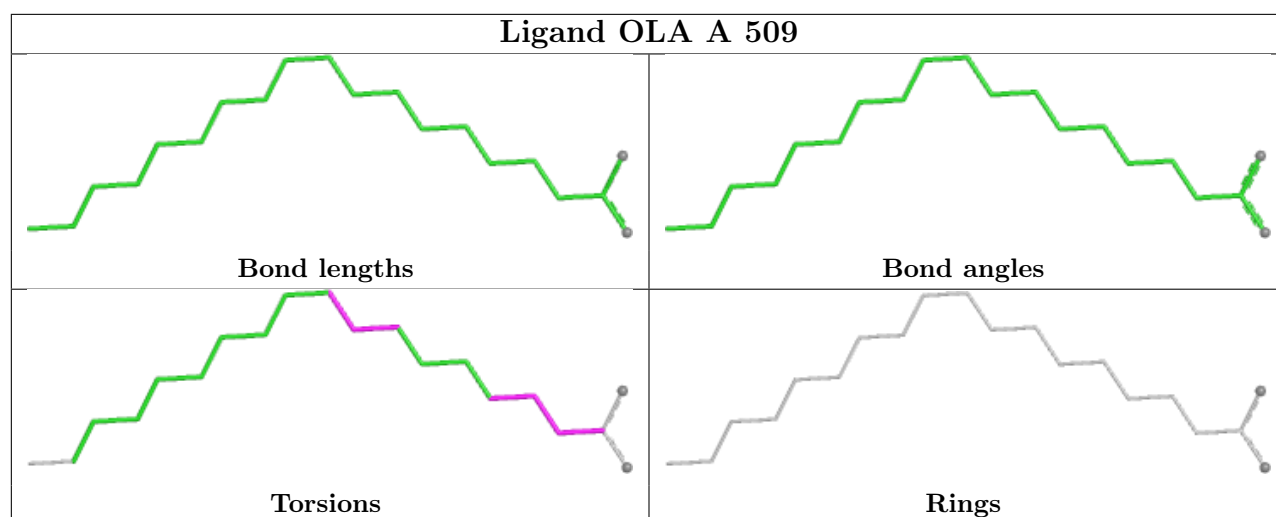
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

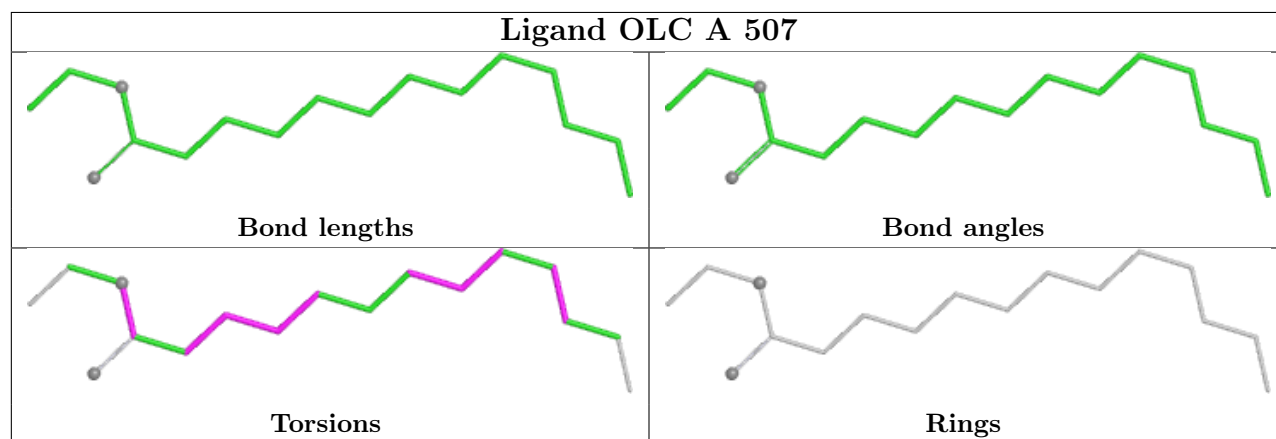
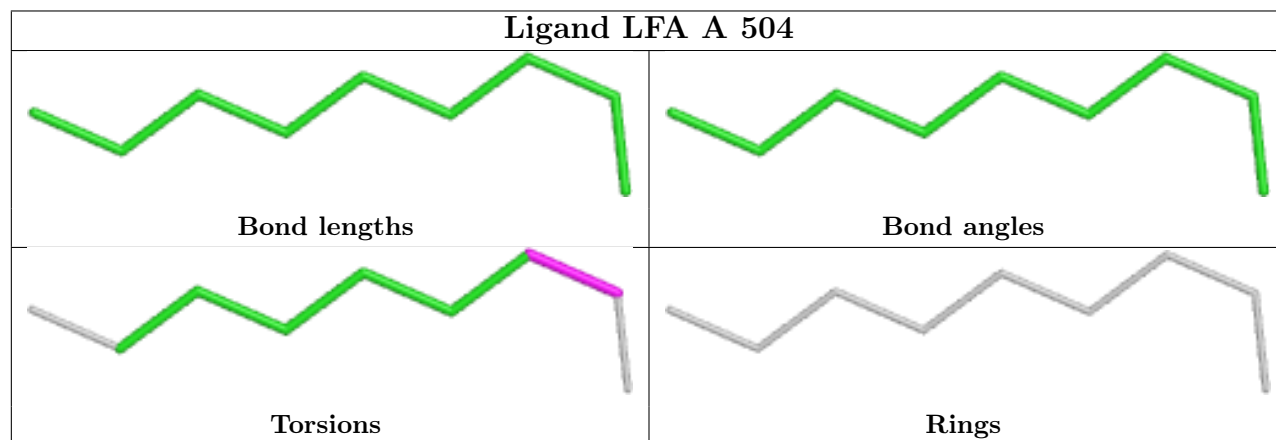
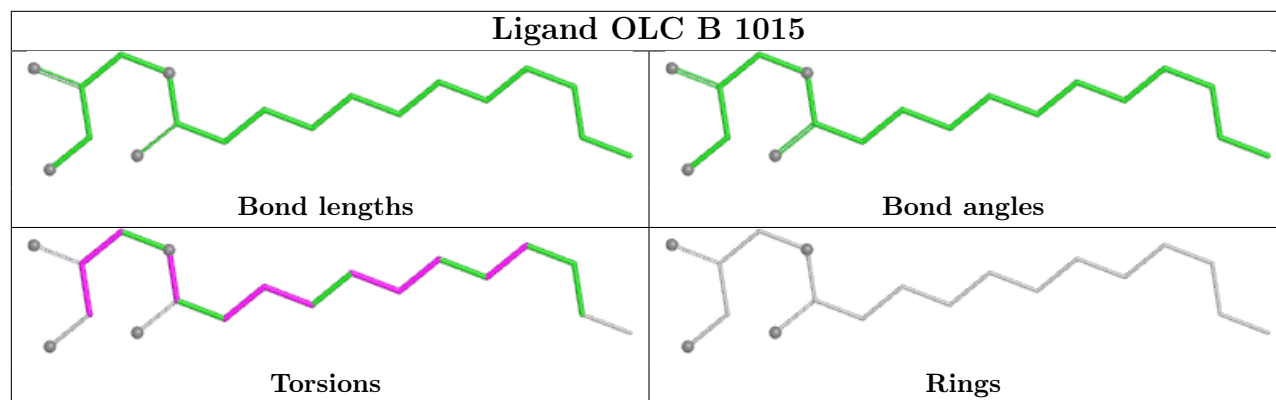


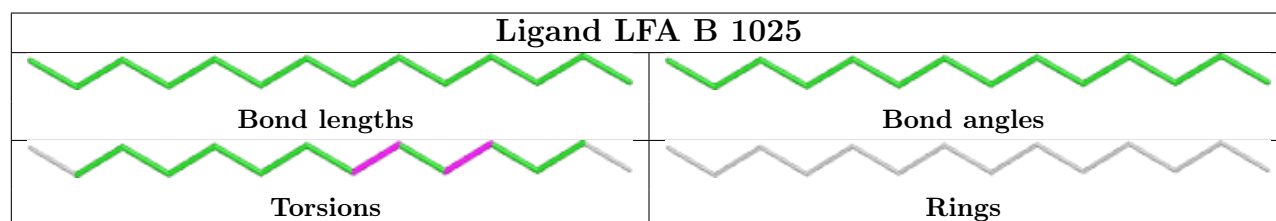
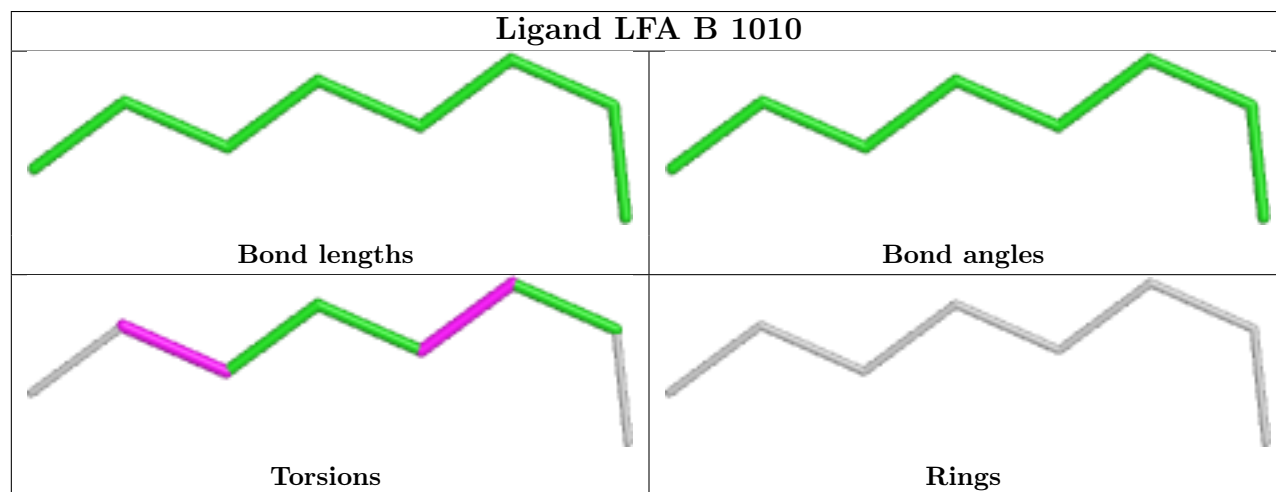
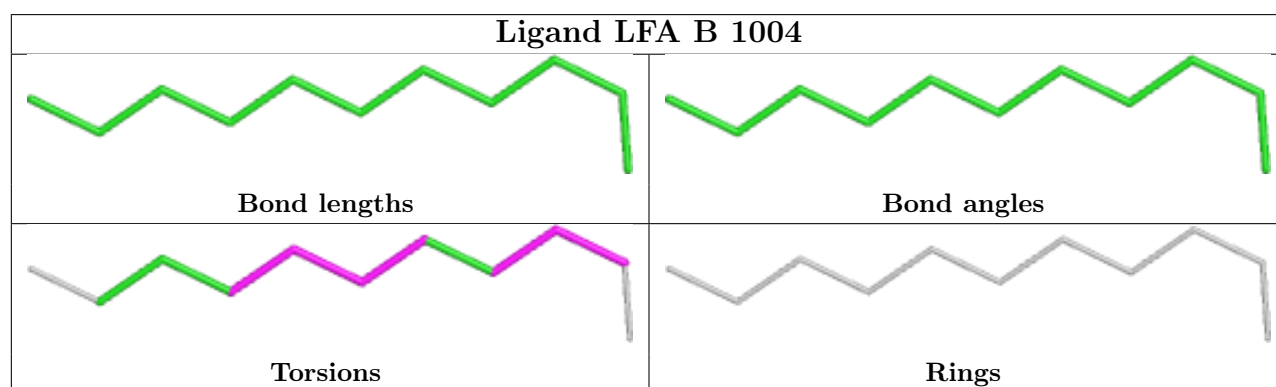
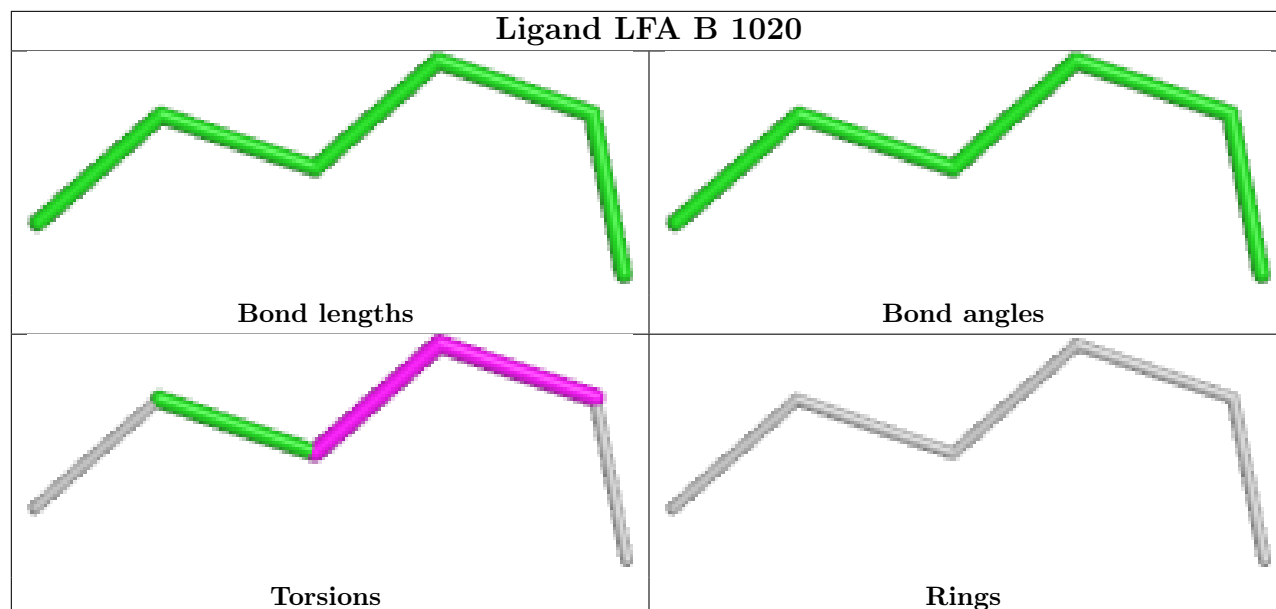


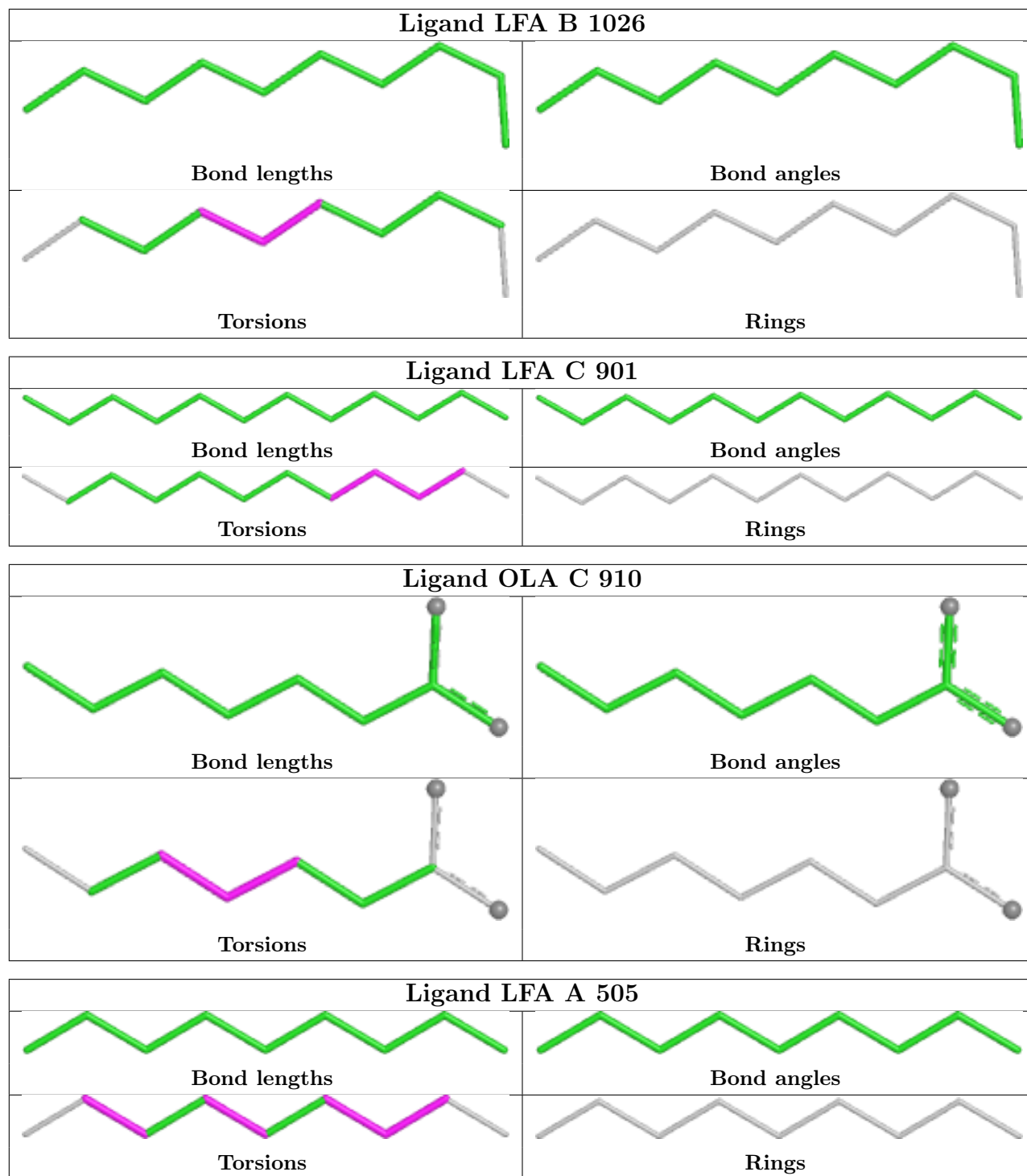


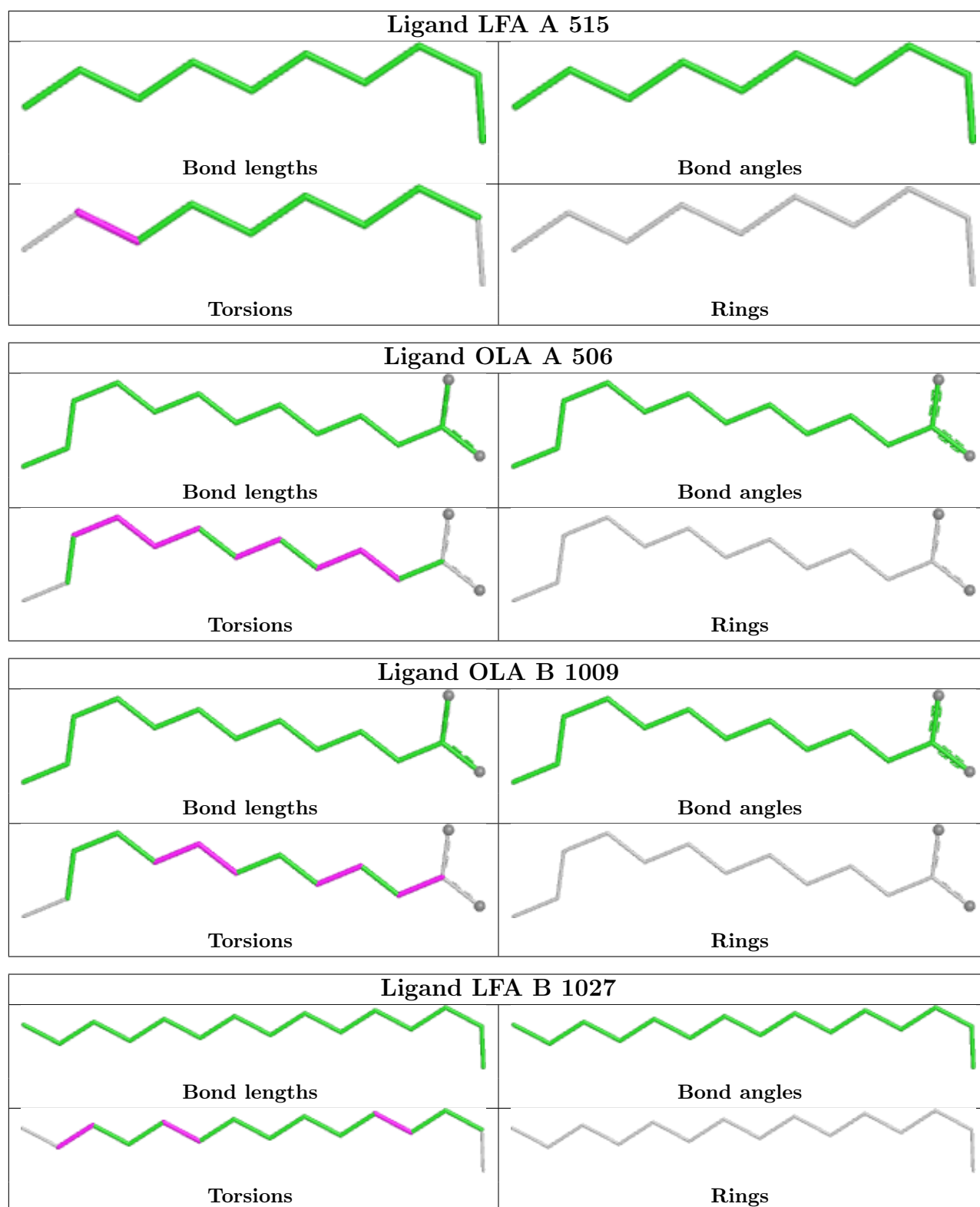


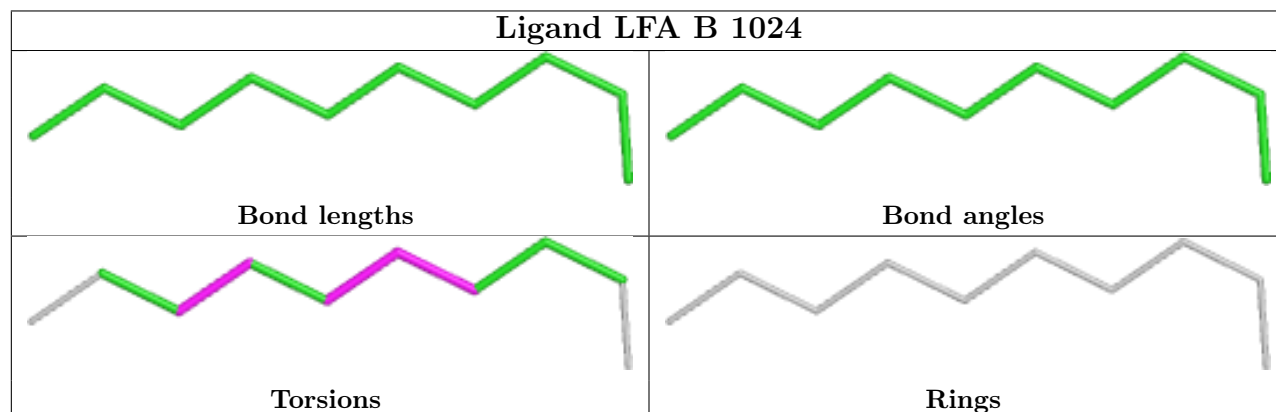
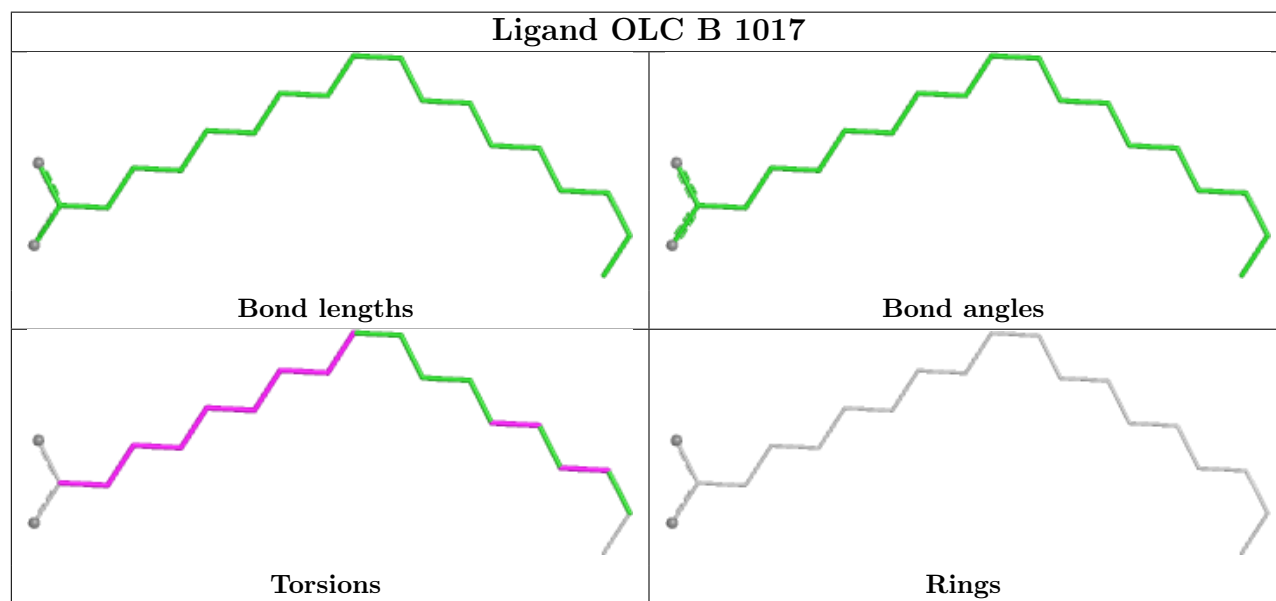
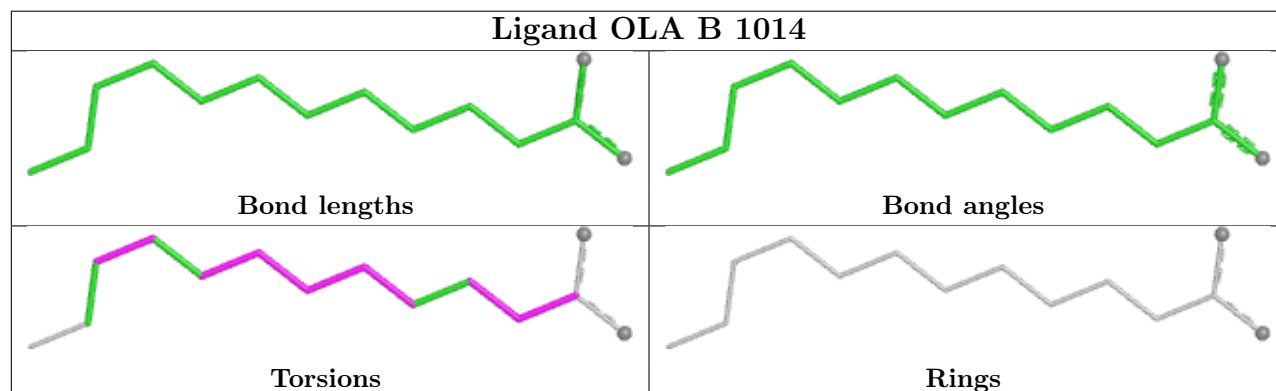
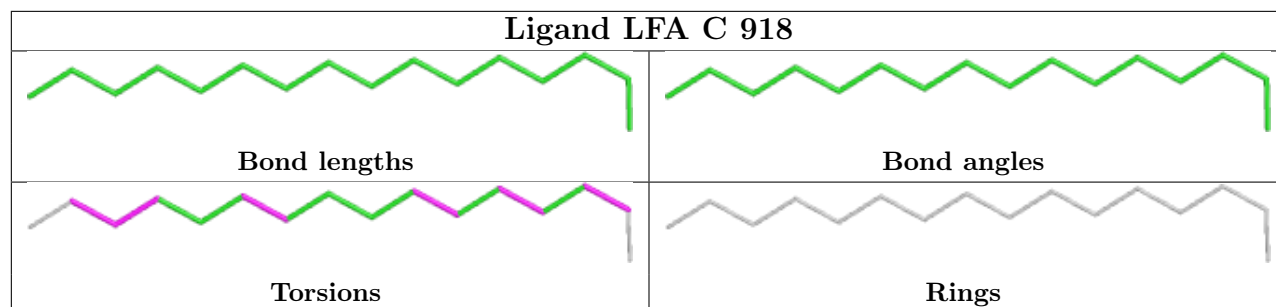


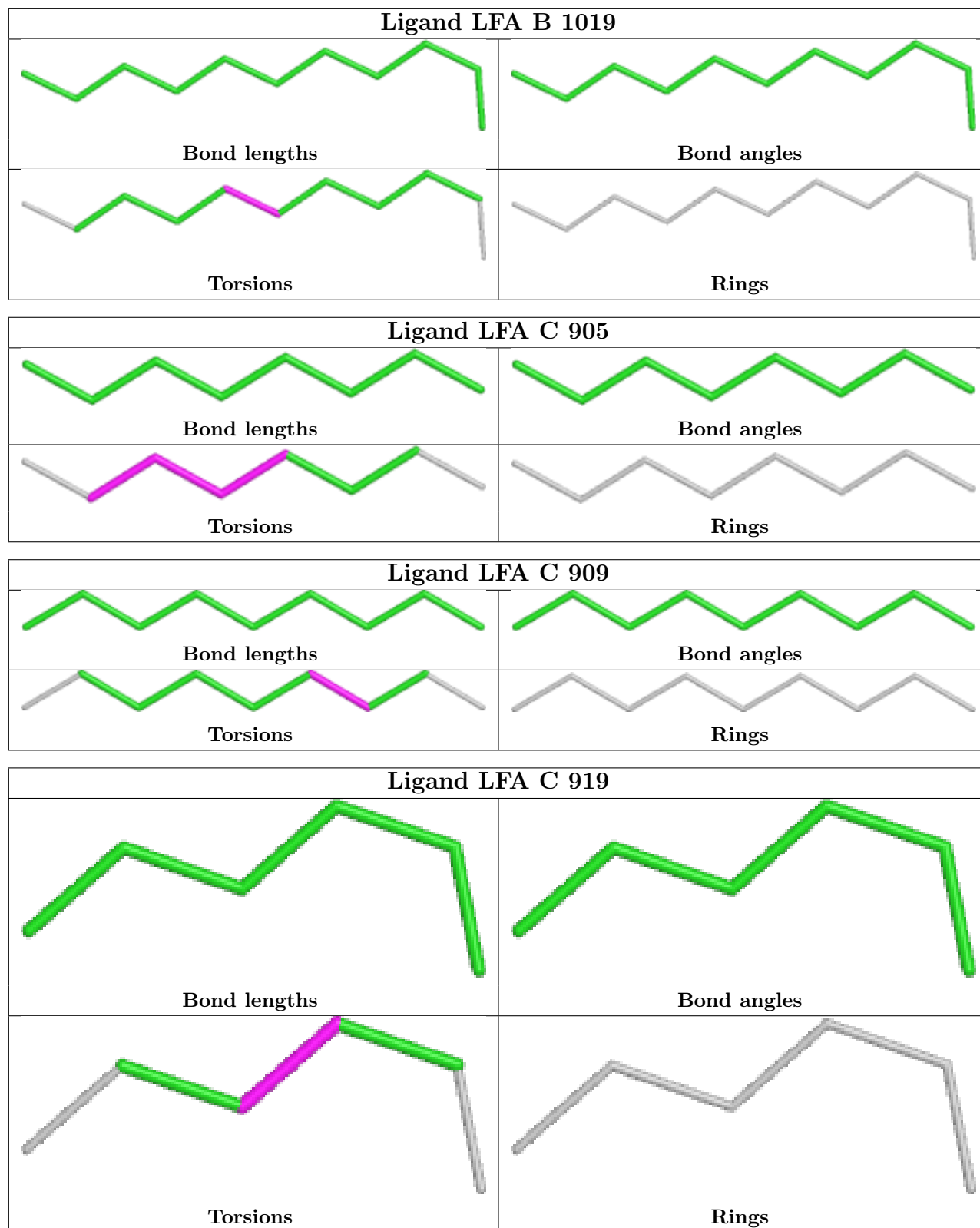


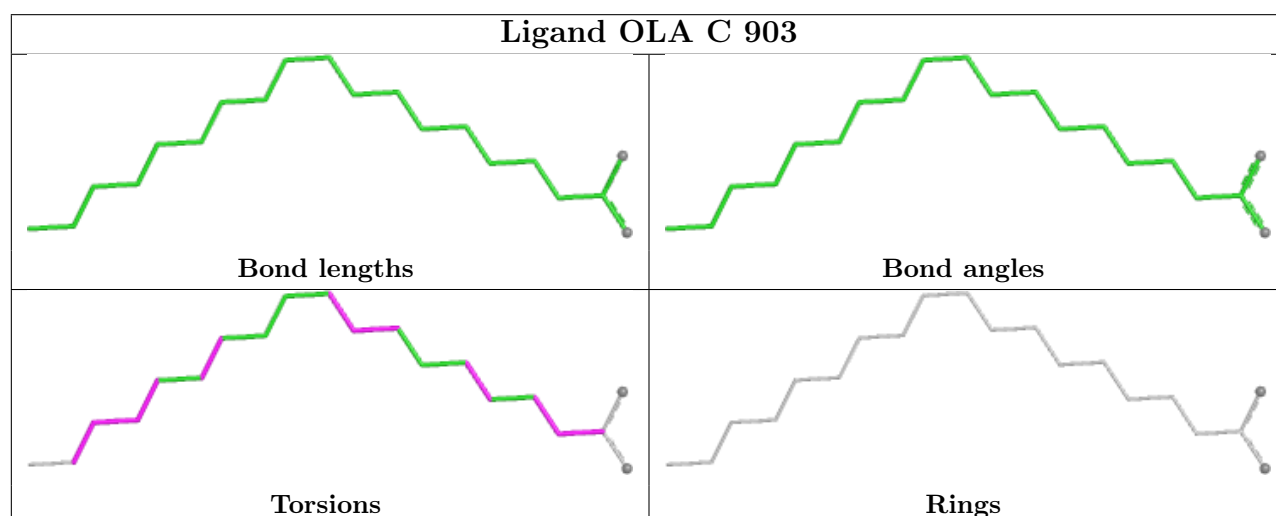
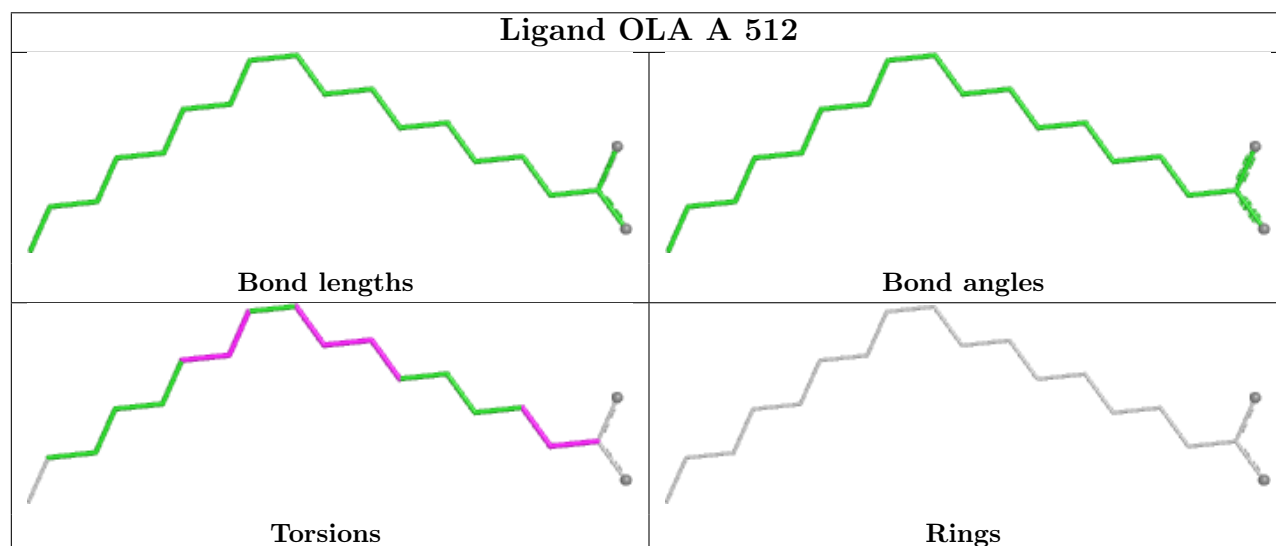
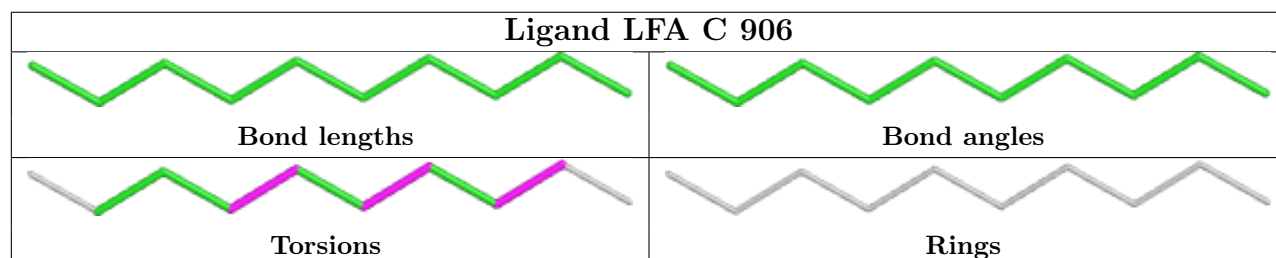
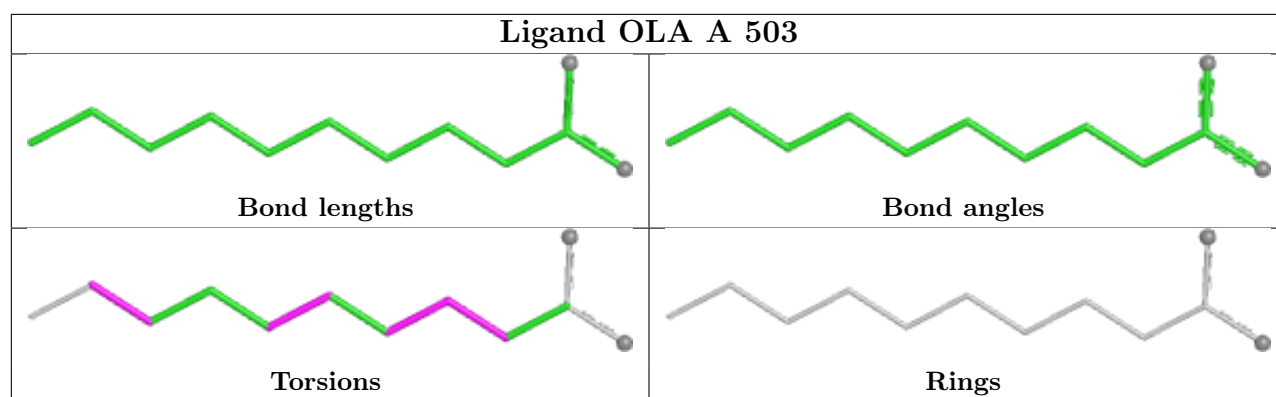


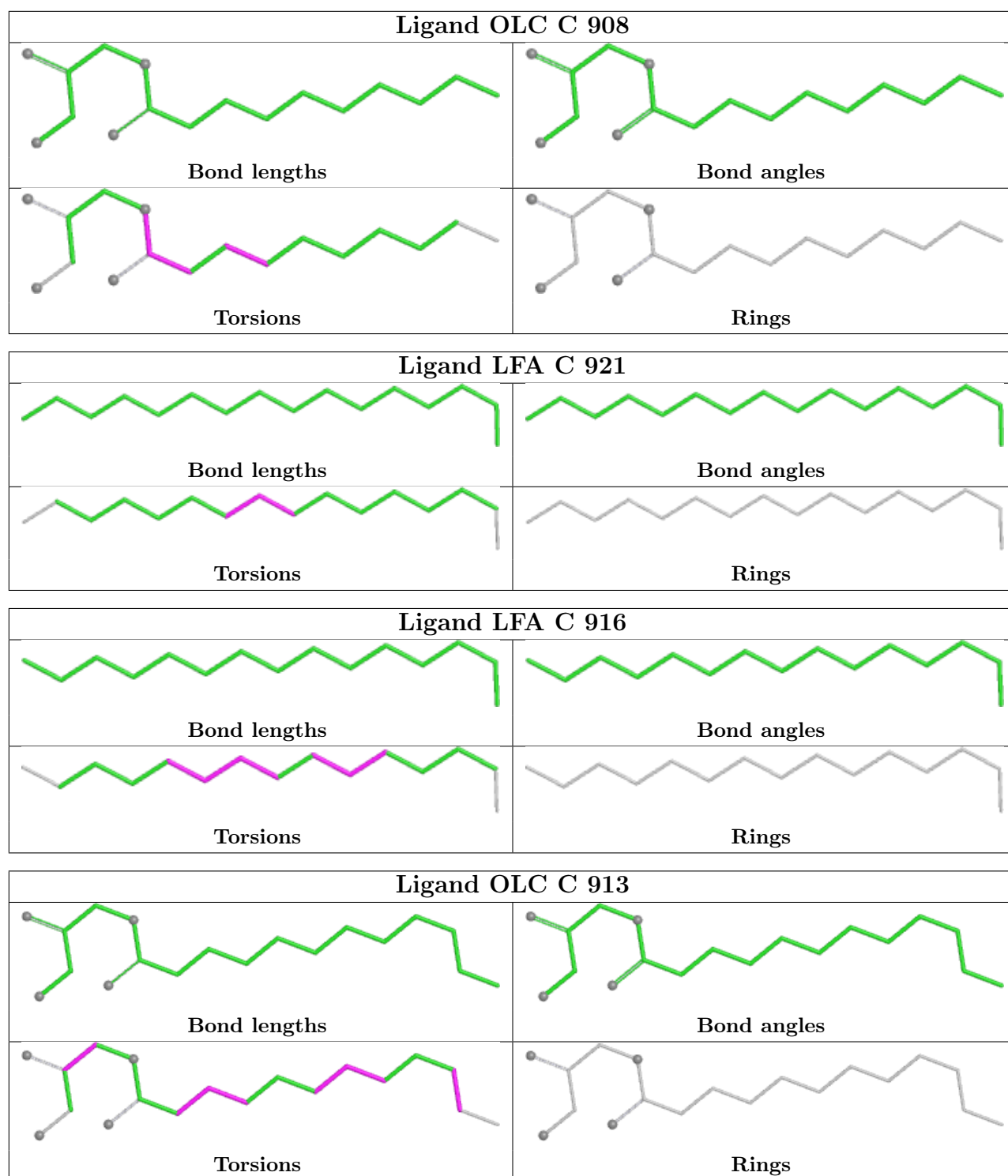


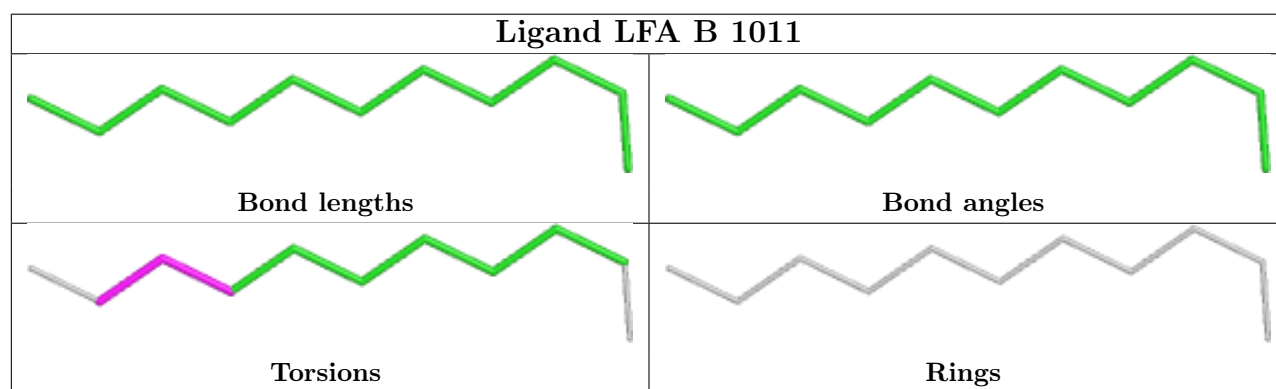
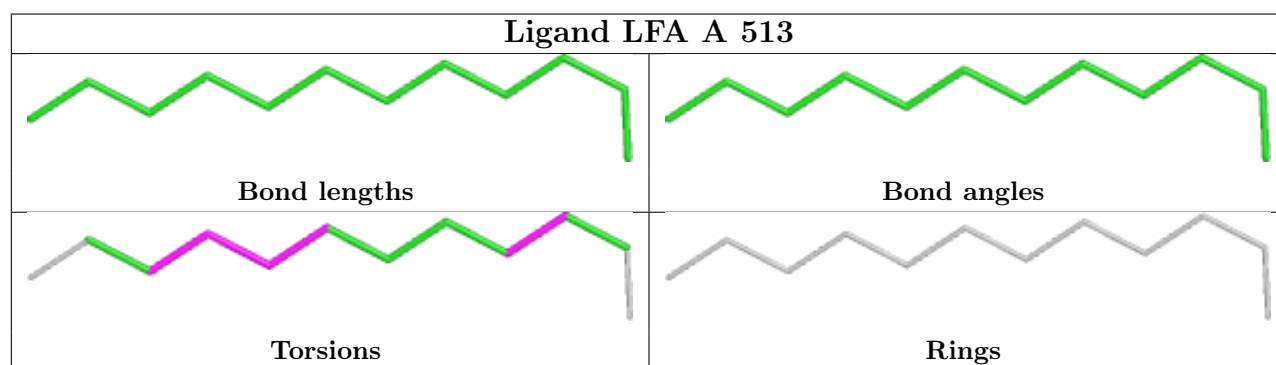
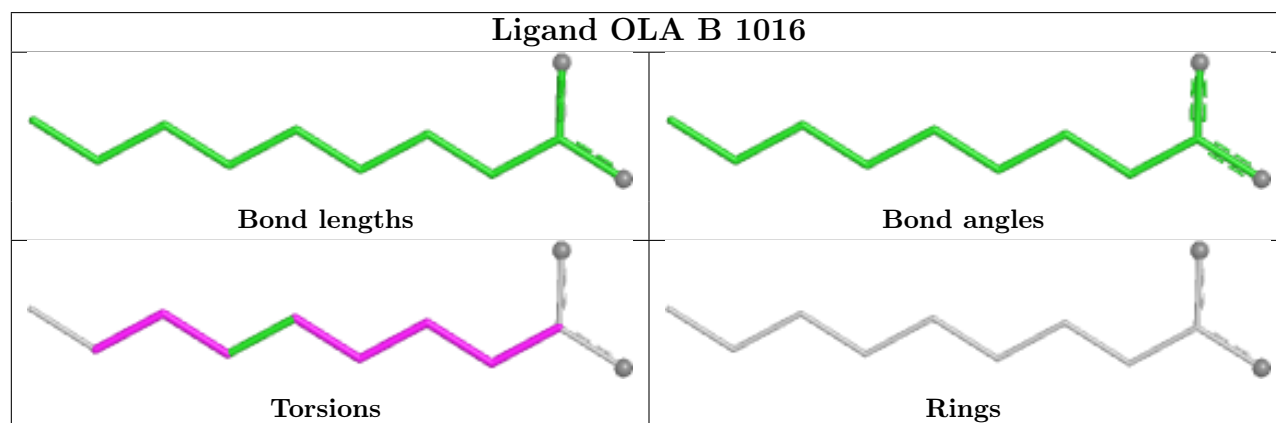
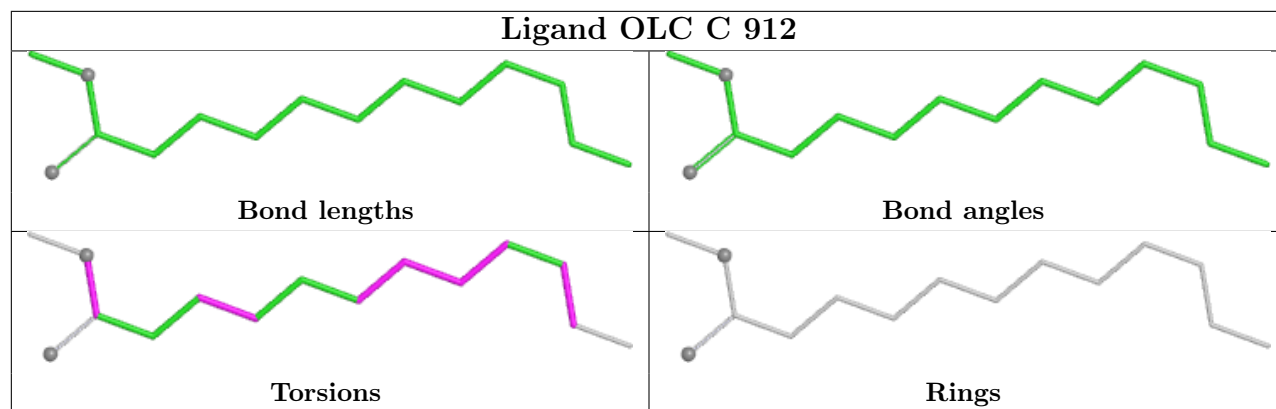


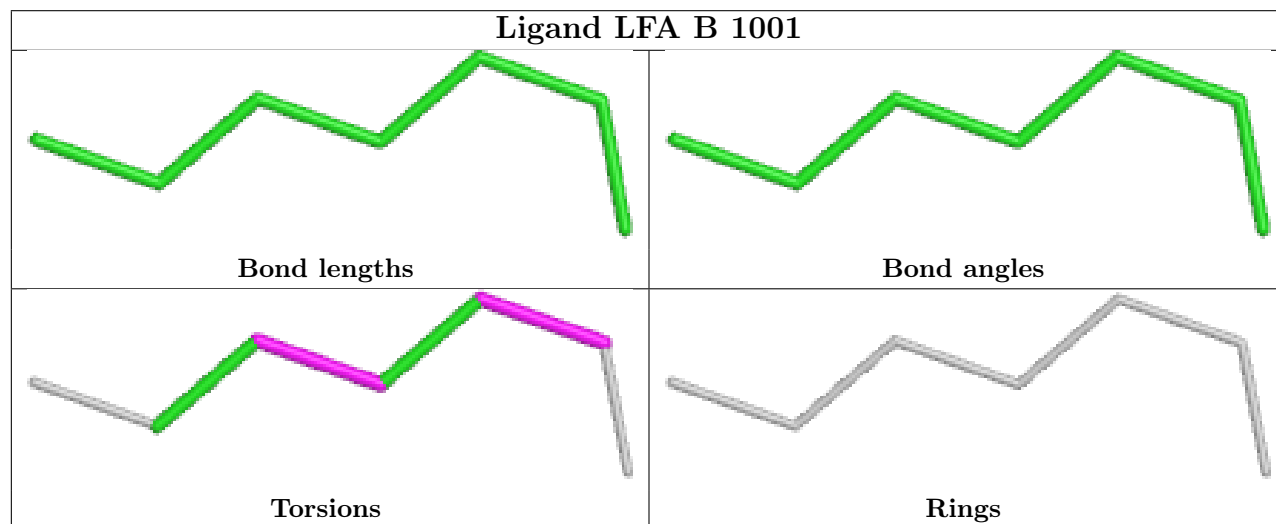
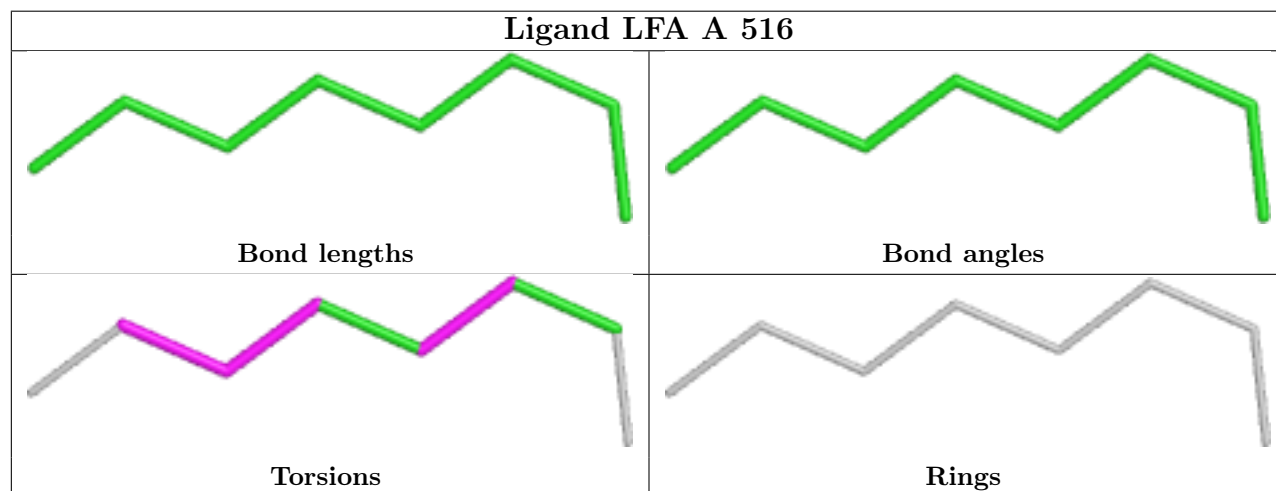
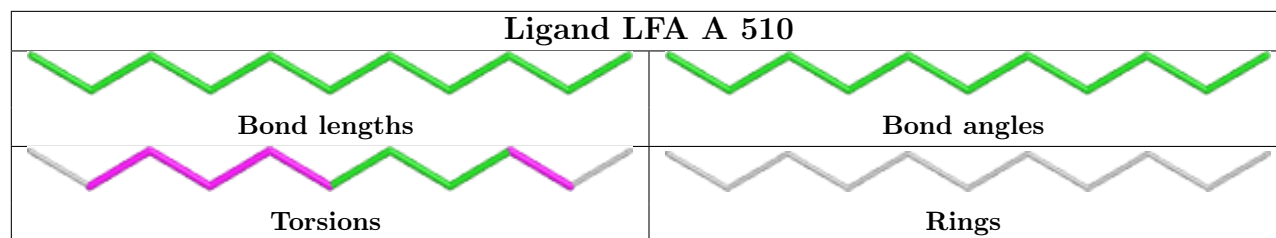


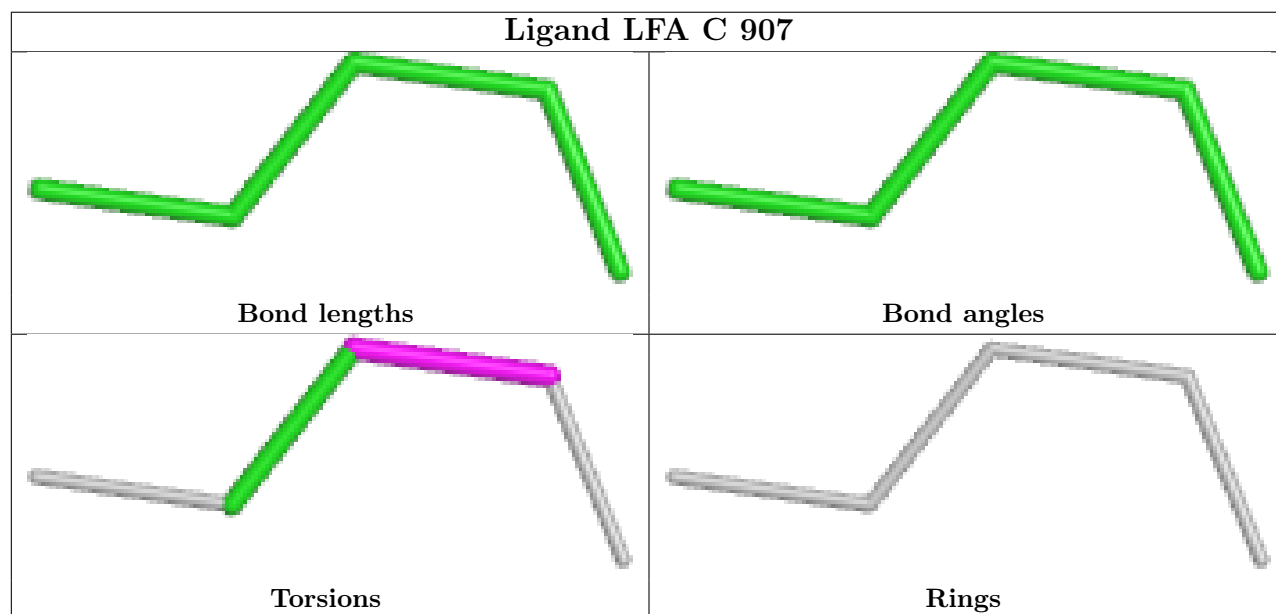
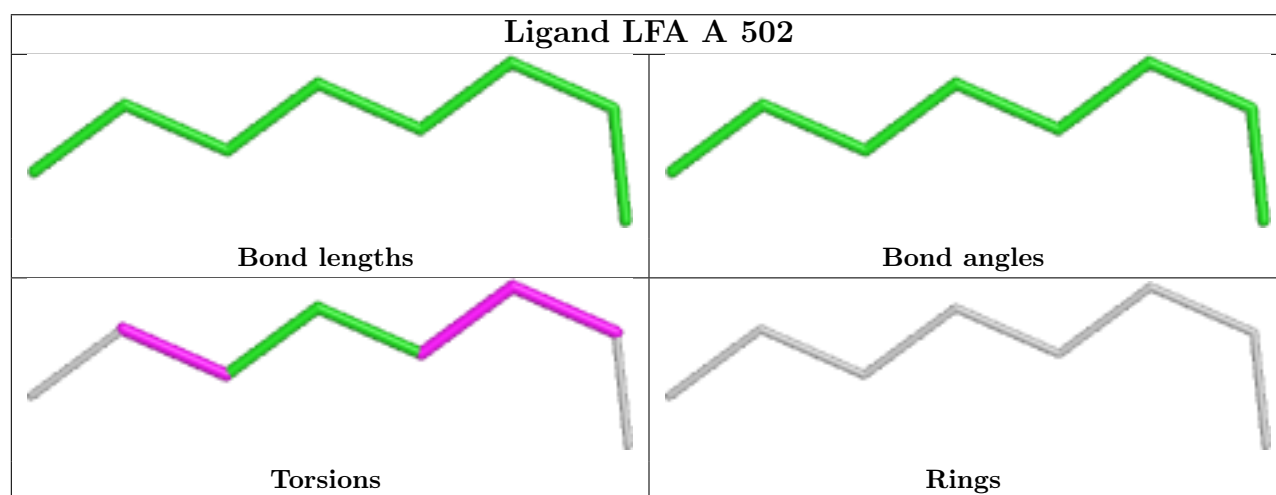
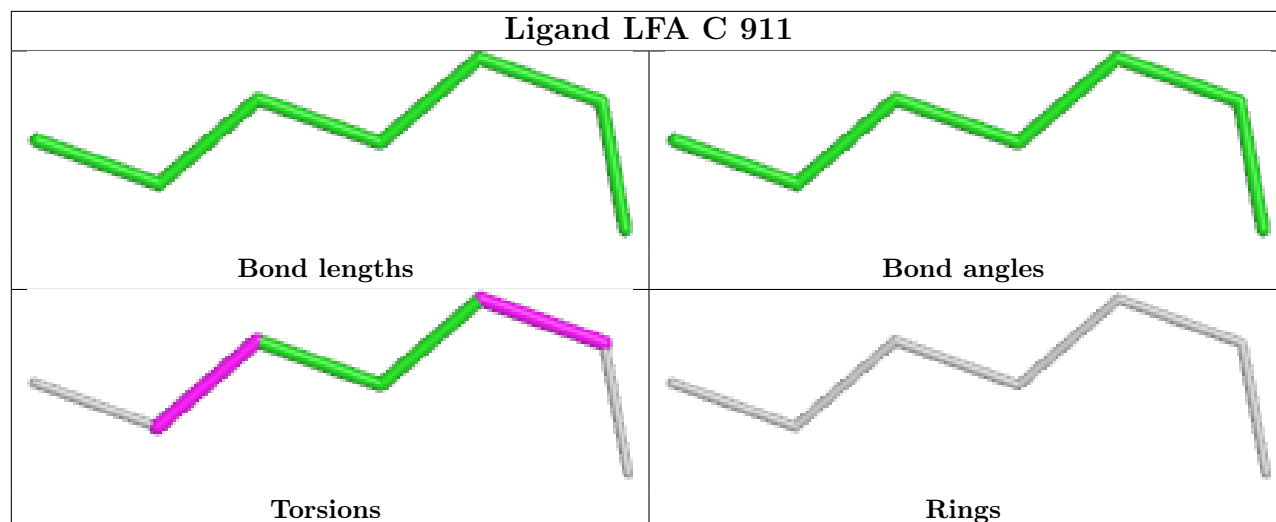


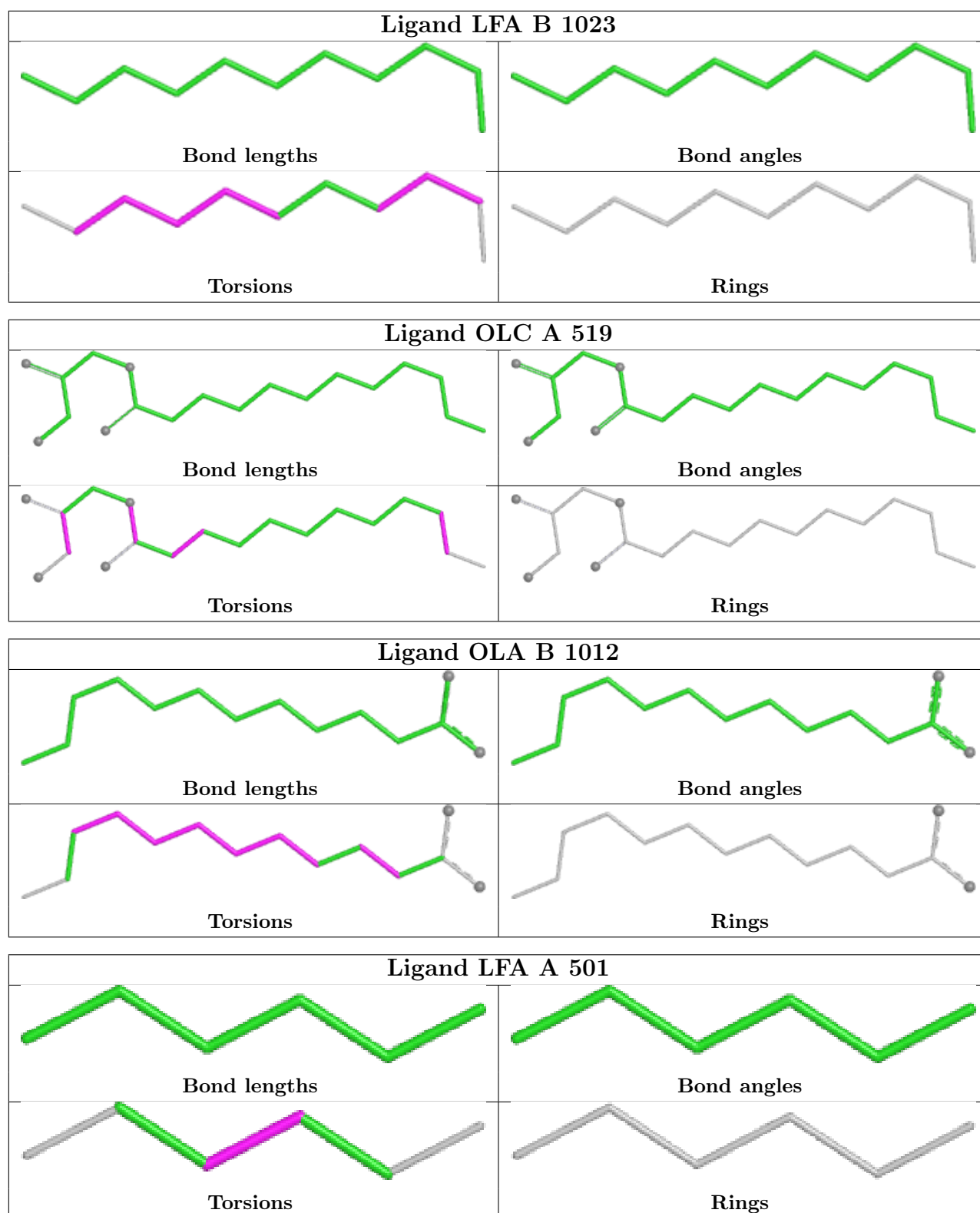


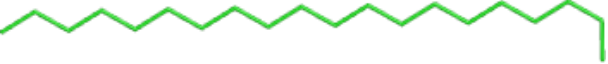
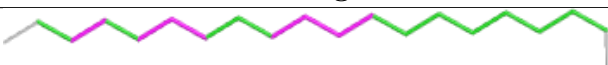
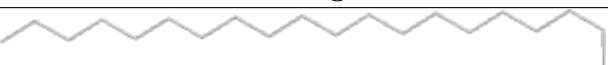










Ligand LFA A 518	
 Bond lengths	 Bond angles
 Torsions	 Rings

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	222/229 (96%)	0.02	5 (2%) 61 65	9, 22, 44, 86	6 (2%)
1	B	220/229 (96%)	0.06	4 (1%) 67 72	9, 24, 43, 78	5 (2%)
1	C	222/229 (96%)	0.04	5 (2%) 61 65	8, 23, 44, 86	6 (2%)
All	All	664/687 (96%)	0.04	14 (2%) 63 68	8, 23, 44, 86	17 (2%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	62	ASP	3.8
1	B	61	TYR	3.7
1	C	61	TYR	3.6
1	B	63	ASP	3.3
1	A	61	TYR	3.2
1	C	63	ASP	3.2
1	B	64	THR	2.9
1	A	62	ASP	2.8
1	B	59	PHE	2.7
1	A	224	SER	2.6
1	A	63	ASP	2.3
1	C	121	ILE	2.2
1	C	223	GLN	2.1
1	A	64	THR	2.1

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($\text{\AA}^2$)	Q<0.9
1	FME	C	1	10/11	0.80	0.15	34,48,76,85	0
1	FME	A	1	10/11	0.88	0.11	33,43,65,68	0
1	FME	B	1	10/11	0.89	0.10	32,44,74,84	0
1	LYR	C	207	29/30	0.91	0.08	18,21,25,33	0
1	LYR	B	207	29/30	0.92	0.08	17,19,27,28	0
1	LYR	A	207	29/30	0.92	0.08	16,19,27,30	0

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($\text{\AA}^2$)	Q<0.9
2	LFA	B	1021	8/20	0.66	0.14	58,60,60,61	0
5	PO4	C	914	5/5	0.66	0.12	72,79,83,98	0
4	OLC	A	519	19/25	0.70	0.20	54,67,77,86	0
4	OLC	B	1028	13/25	0.71	0.18	52,79,89,92	0
4	OLC	C	908	17/25	0.71	0.18	43,58,72,75	0
2	LFA	B	1026	10/20	0.71	0.15	56,59,65,68	0
2	LFA	C	917	5/20	0.72	0.18	56,60,62,66	0
3	OLA	C	910	9/20	0.72	0.18	58,61,68,70	0
2	LFA	B	1027	15/20	0.73	0.19	42,53,66,68	0
4	OLC	C	913	19/25	0.74	0.15	50,66,82,96	0
2	LFA	C	909	9/20	0.75	0.15	34,49,57,58	0
2	LFA	A	518	20/20	0.76	0.17	51,60,67,68	0
3	OLA	B	1013	14/20	0.76	0.16	59,64,68,71	0
3	OLA	B	1016	11/20	0.76	0.14	52,59,65,65	0
2	LFA	B	1022	10/20	0.77	0.13	55,57,60,61	0
2	LFA	B	1025	14/20	0.77	0.17	48,62,66,66	0
2	LFA	A	517	4/20	0.78	0.12	51,52,53,54	0
2	LFA	B	1024	10/20	0.79	0.16	41,50,57,63	0
2	LFA	C	918	16/20	0.79	0.18	46,50,58,59	0
4	OLC	C	912	15/25	0.79	0.15	44,48,62,68	0
4	OLC	A	511	19/25	0.79	0.15	44,52,67,67	0
2	LFA	C	916	15/20	0.79	0.16	52,61,68,70	0
2	LFA	C	920	7/20	0.80	0.14	41,51,58,59	0

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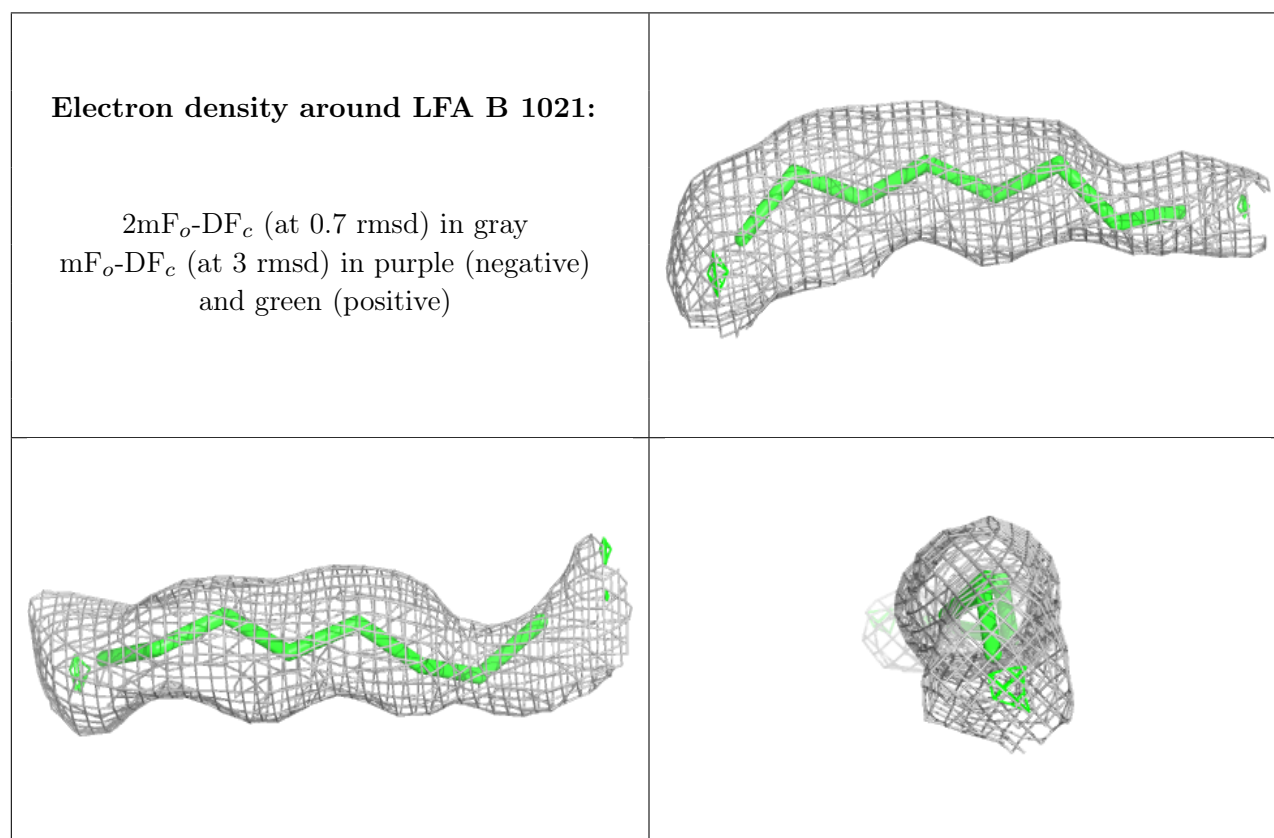
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OLA	A	503	12/20	0.80	0.14	39,55,68,71	0
2	LFA	B	1023	11/20	0.80	0.11	47,56,61,63	0
2	LFA	A	515	10/20	0.81	0.11	40,46,52,53	0
3	OLA	A	512	19/20	0.81	0.16	38,53,61,64	0
2	LFA	A	516	8/20	0.81	0.14	51,56,59,61	0
2	LFA	C	921	16/20	0.81	0.14	43,51,60,62	0
2	LFA	C	919	6/20	0.82	0.16	51,55,57,58	0
2	LFA	B	1018	6/20	0.82	0.12	45,50,54,57	0
2	LFA	B	1010	8/20	0.82	0.14	45,48,55,56	0
2	LFA	C	902	13/20	0.82	0.12	52,56,63,65	0
2	LFA	C	905	8/20	0.82	0.13	45,47,52,53	0
3	OLA	A	506	14/20	0.83	0.13	44,56,68,76	0
2	LFA	B	1011	11/20	0.83	0.14	40,45,57,57	0
3	OLA	B	1008	16/20	0.83	0.14	34,46,56,57	0
3	OLA	B	1012	14/20	0.83	0.13	48,50,65,67	0
2	LFA	B	1004	11/20	0.83	0.14	39,46,51,54	0
2	LFA	B	1019	11/20	0.83	0.12	48,53,60,62	0
2	LFA	A	505	9/20	0.83	0.15	43,49,56,56	0
2	LFA	B	1007	10/20	0.84	0.15	36,48,53,54	0
2	LFA	C	915	11/20	0.84	0.10	46,51,55,56	0
3	OLA	B	1014	14/20	0.84	0.14	48,56,73,96	0
2	LFA	B	1001	7/20	0.85	0.12	43,46,49,49	0
2	LFA	C	901	12/20	0.85	0.11	36,45,54,54	0
4	OLC	A	507	17/25	0.85	0.14	37,47,70,74	0
3	OLA	A	508	16/20	0.85	0.12	37,52,67,74	0
2	LFA	B	1020	6/20	0.85	0.12	45,48,53,58	0
4	OLC	B	1015	19/25	0.85	0.17	37,54,80,86	0
4	OLC	B	1017	20/25	0.85	0.12	40,57,82,87	0
3	OLA	A	514	20/20	0.85	0.13	37,48,63,65	0
2	LFA	C	904	6/20	0.85	0.12	40,45,50,54	0
2	LFA	A	504	9/20	0.85	0.12	46,47,51,52	0
2	LFA	A	502	8/20	0.85	0.12	37,44,49,49	0
2	LFA	C	911	7/20	0.85	0.15	35,42,54,59	0
3	OLA	B	1009	14/20	0.86	0.14	34,48,62,64	0
2	LFA	B	1005	9/20	0.86	0.12	36,47,56,56	0
2	LFA	B	1002	7/20	0.86	0.12	41,46,50,53	0
3	OLA	A	509	20/20	0.86	0.12	33,47,62,65	0
3	OLA	C	903	20/20	0.87	0.13	35,41,77,77	0
2	LFA	A	513	12/20	0.87	0.13	28,44,49,54	0
2	LFA	B	1003	9/20	0.87	0.09	41,47,50,53	0
2	LFA	A	510	11/20	0.87	0.09	40,46,53,55	0
2	LFA	C	907	5/20	0.88	0.10	40,41,42,45	0

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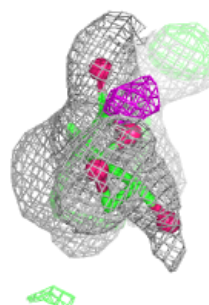
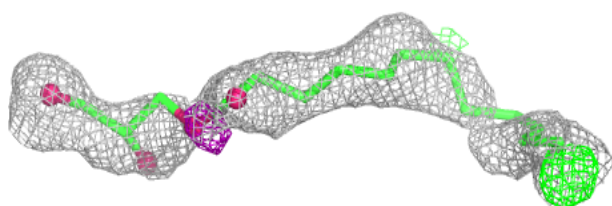
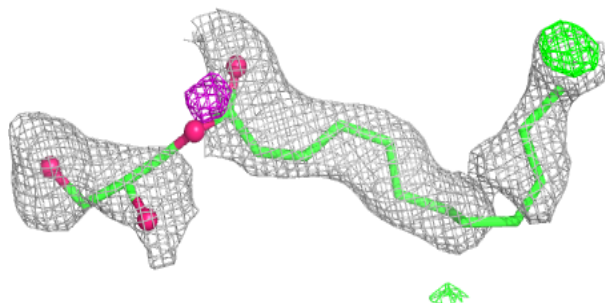
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LFA	A	501	6/20	0.89	0.11	37,38,44,44	0
2	LFA	C	906	10/20	0.89	0.10	43,47,51,55	0
3	OLA	B	1006	20/20	0.90	0.10	33,43,61,71	0

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

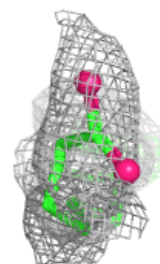
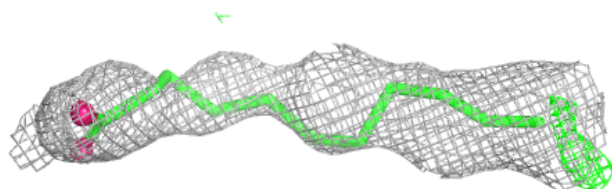
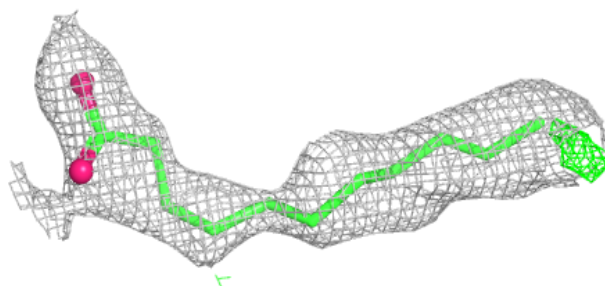


Electron density around OLC A 519:

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

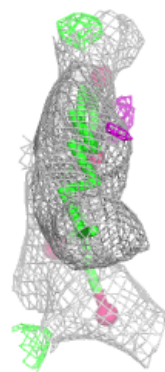
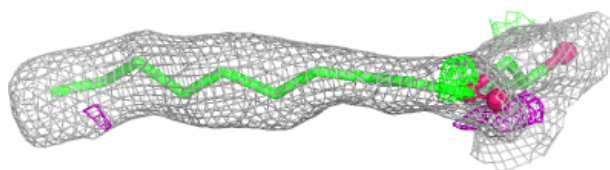
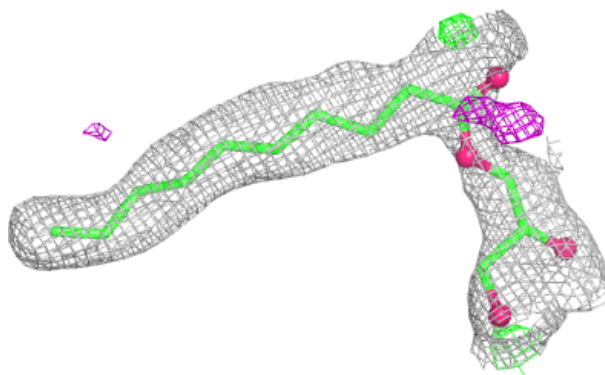
**Electron density around OLC B 1028:**

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

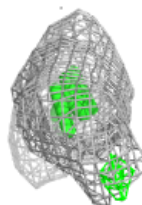
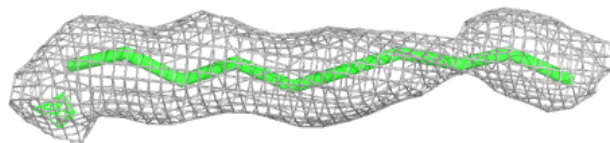
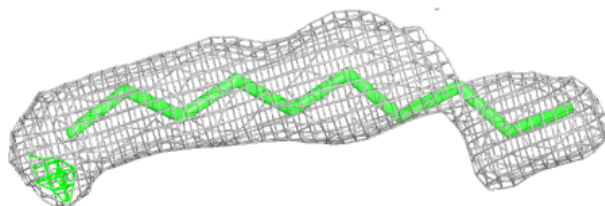


Electron density around OLC C 908:

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

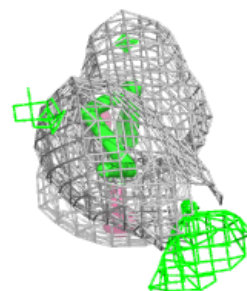
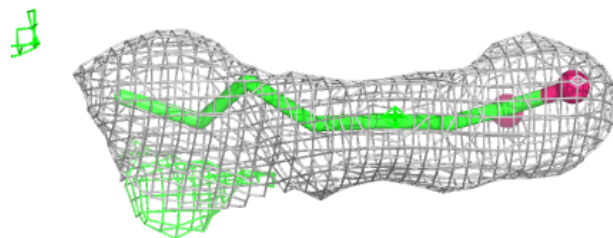
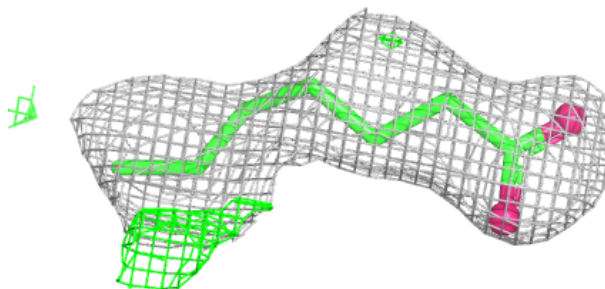
**Electron density around LFA B 1026:**

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

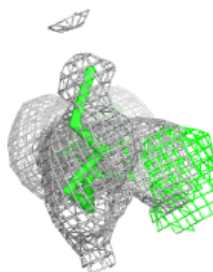
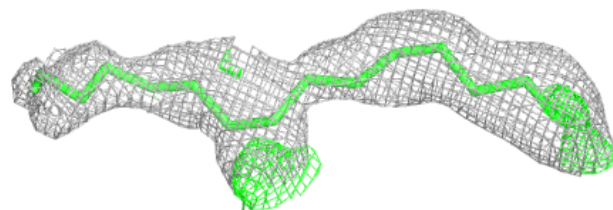
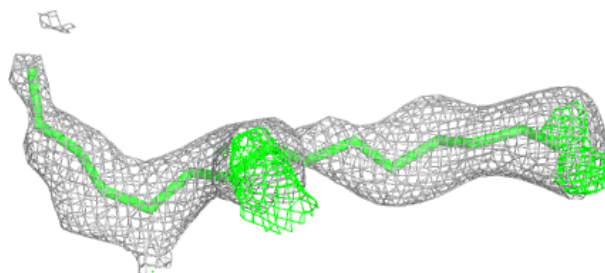


Electron density around OLA C 910:

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

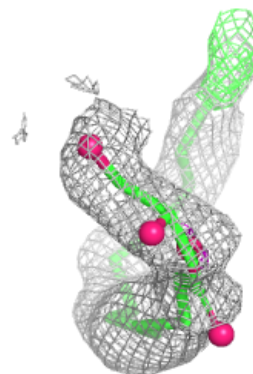
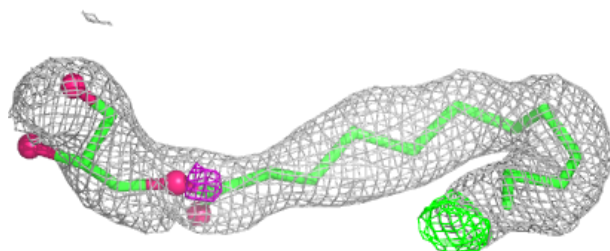
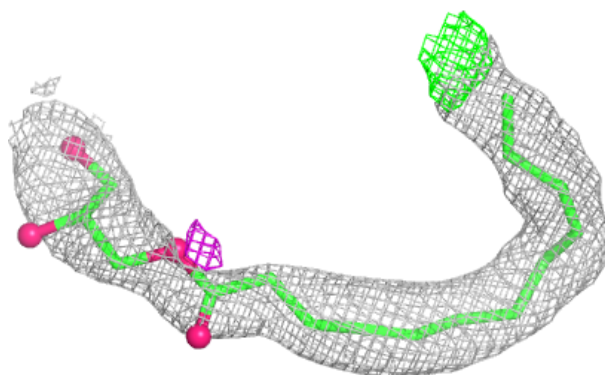
**Electron density around LFA B 1027:**

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

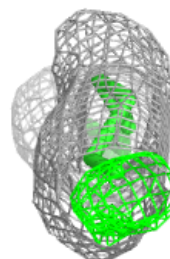
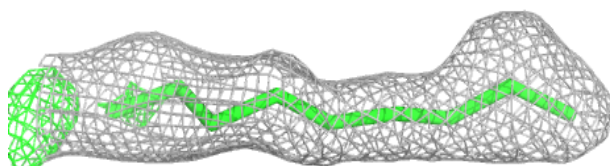
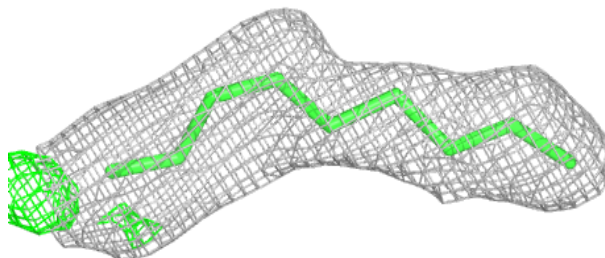


Electron density around OLC C 913:

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

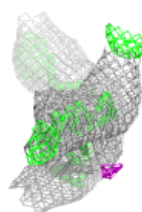
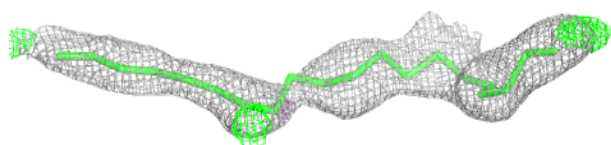
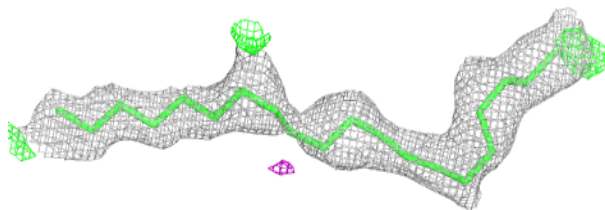
**Electron density around LFA C 909:**

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

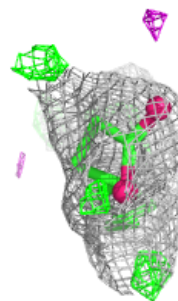
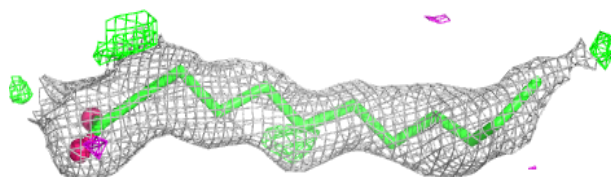
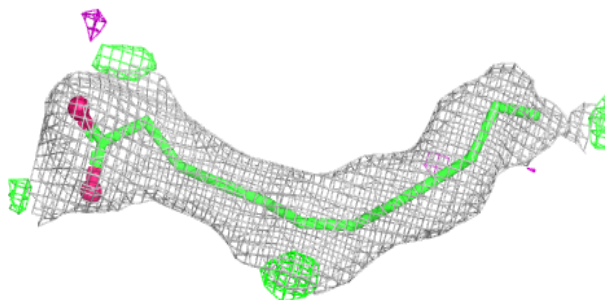


Electron density around LFA A 518:

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

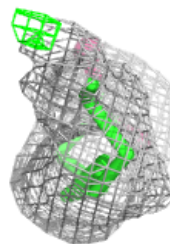
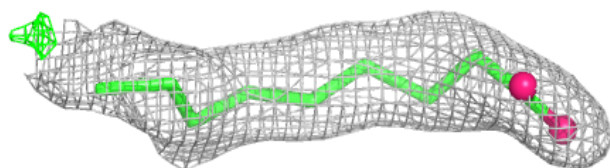
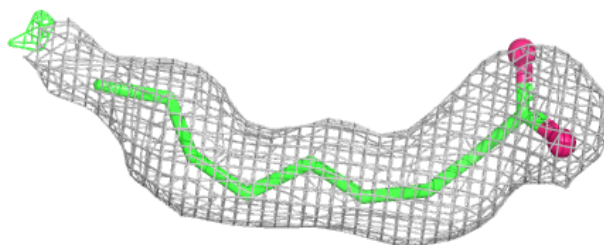
**Electron density around OLA B 1013:**

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

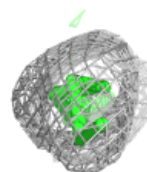
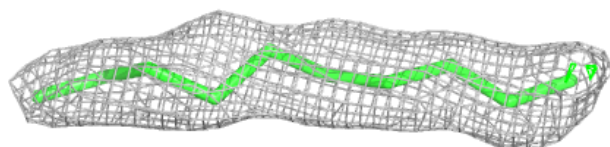
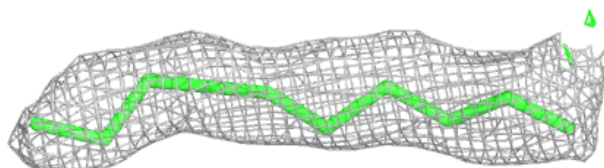


Electron density around OLA B 1016:

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

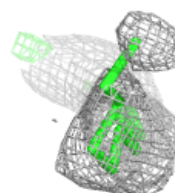
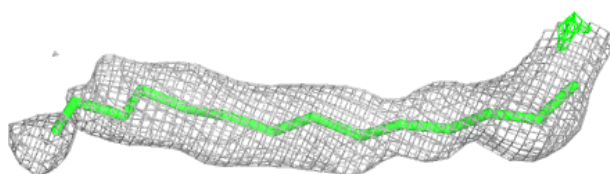
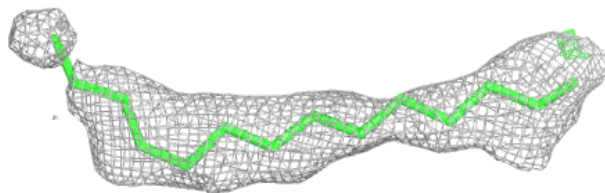
**Electron density around LFA B 1022:**

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

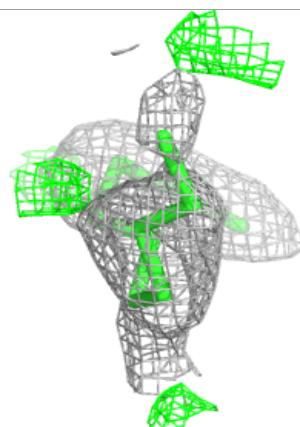
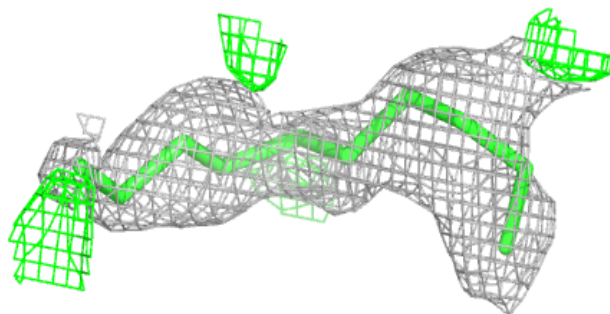
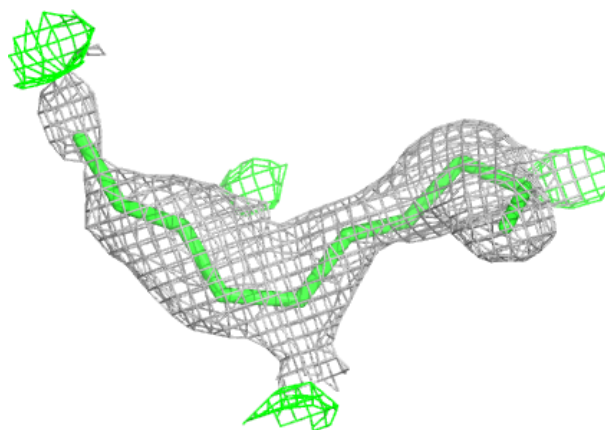


Electron density around LFA B 1025:

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

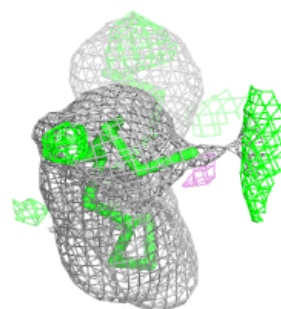
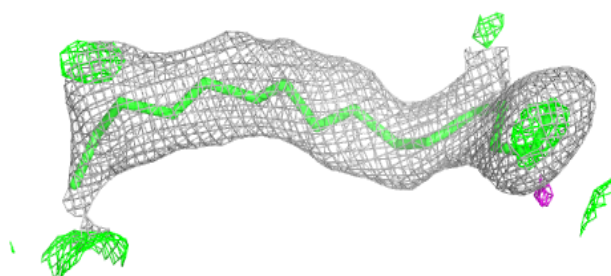
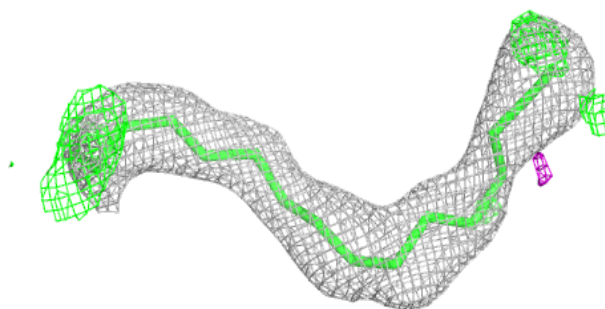
**Electron density around LFA B 1024:**

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

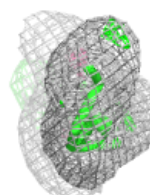
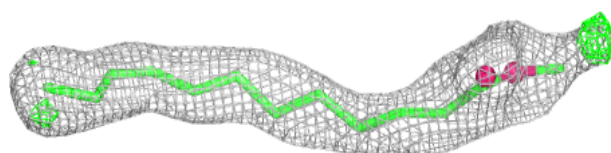
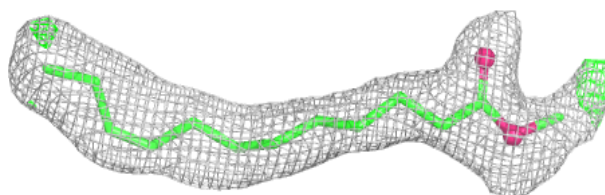


Electron density around LFA C 918:

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

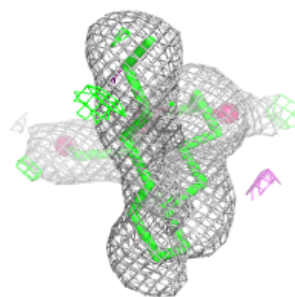
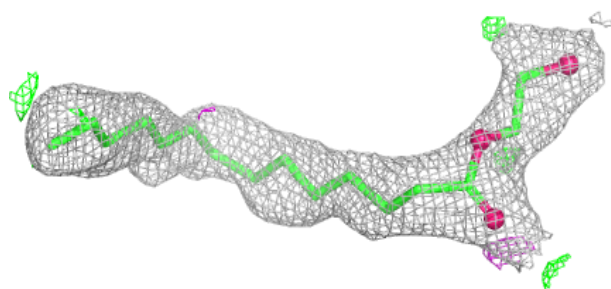
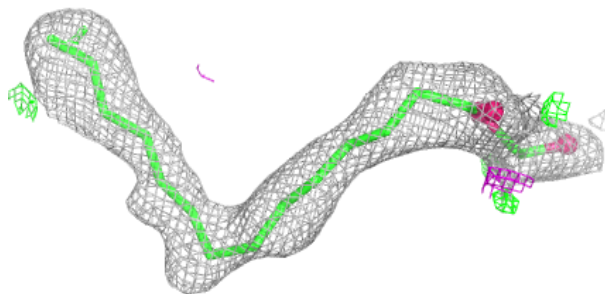
**Electron density around OLC C 912:**

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

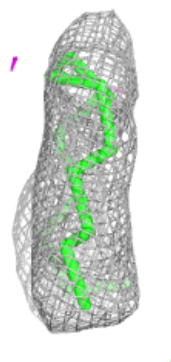
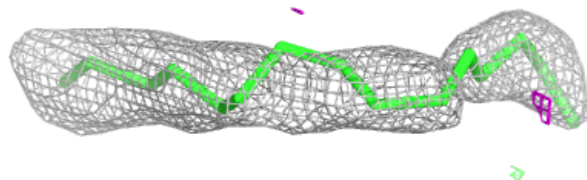
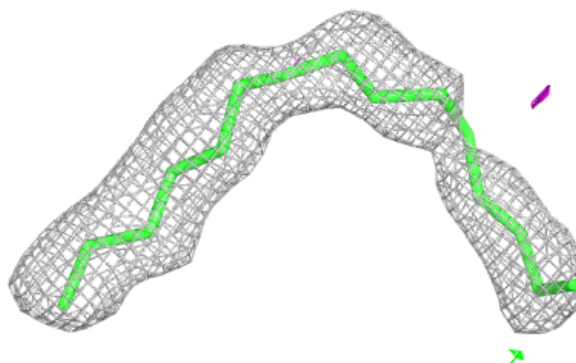


Electron density around OLC A 511:

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

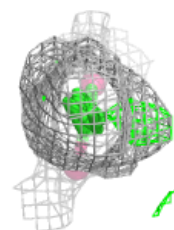
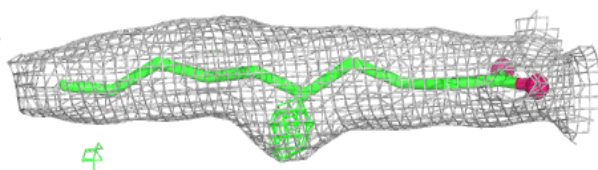
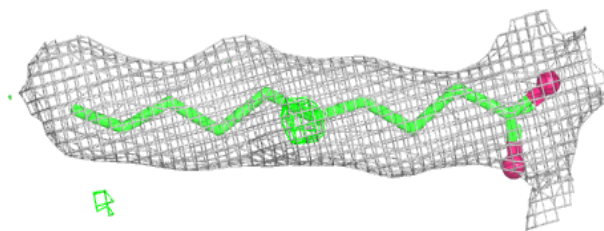
**Electron density around LFA C 916:**

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

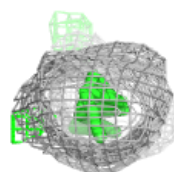
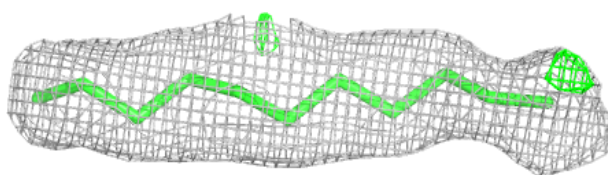
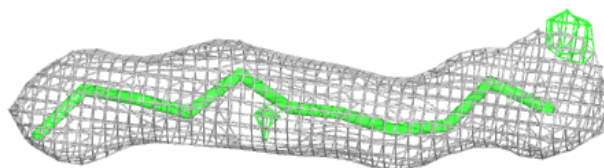


Electron density around OLA A 503:

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

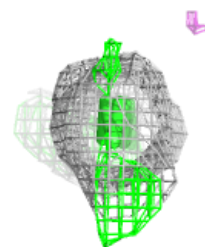
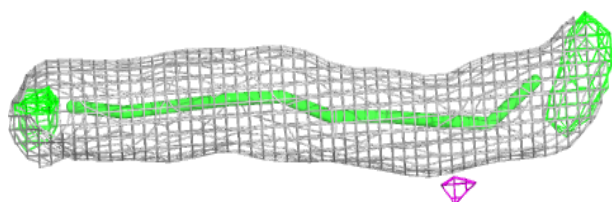
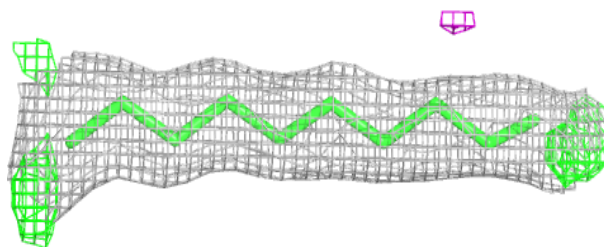
**Electron density around LFA B 1023:**

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

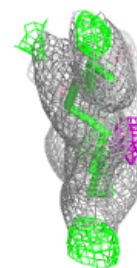
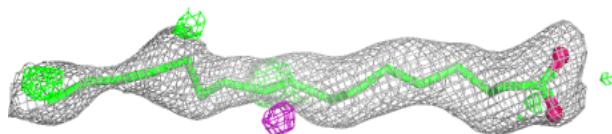
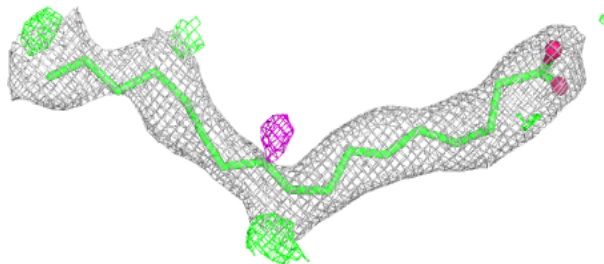


Electron density around LFA A 515:

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

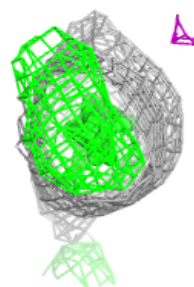
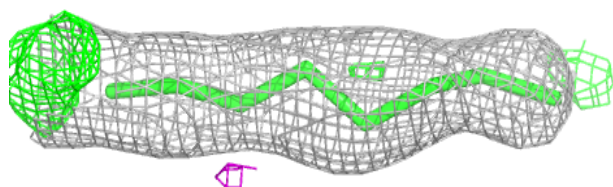
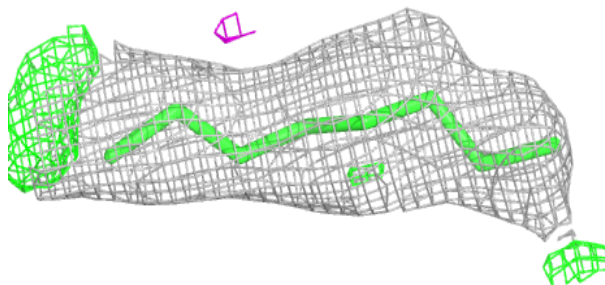
**Electron density around OLA A 512:**

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

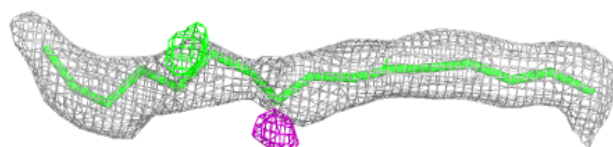
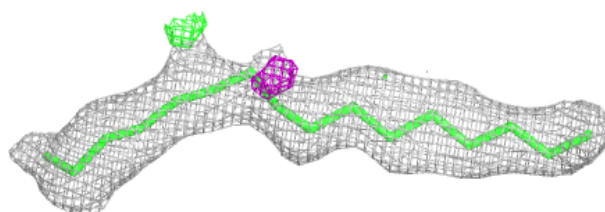


Electron density around LFA A 516:

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

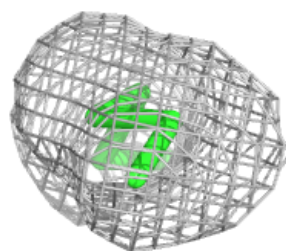
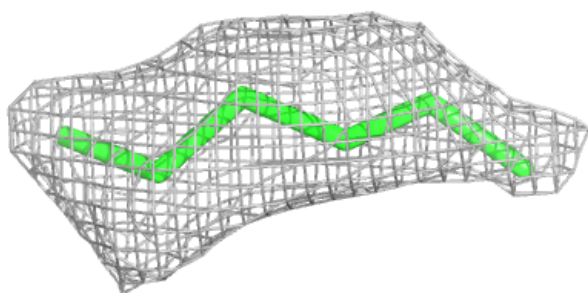
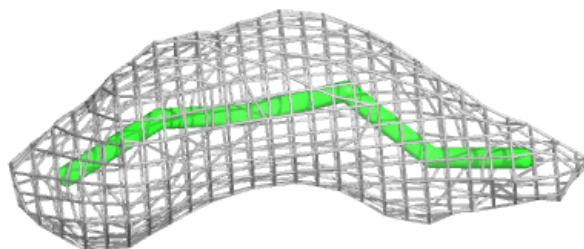
**Electron density around LFA C 921:**

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

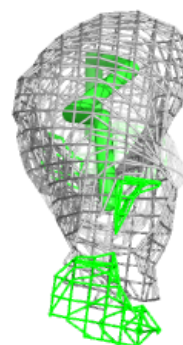
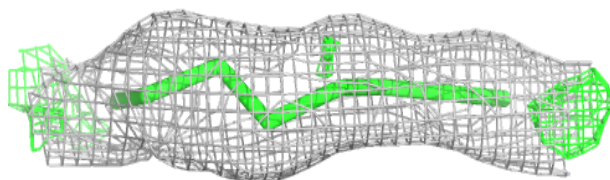
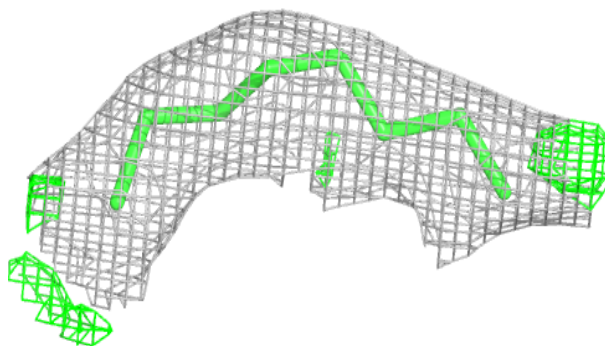


Electron density around LFA C 919:

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

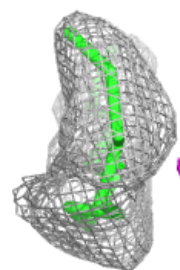
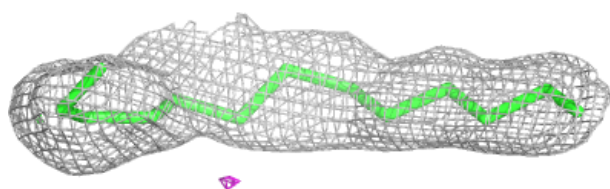
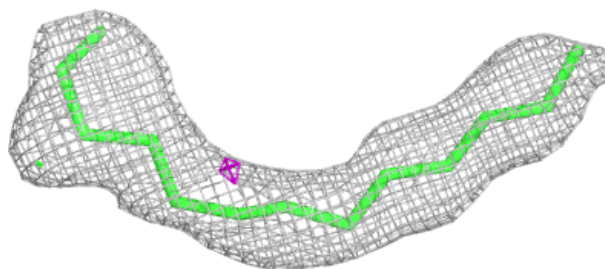
**Electron density around LFA B 1010:**

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

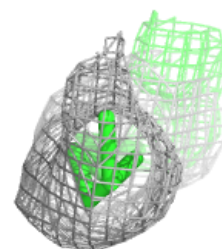
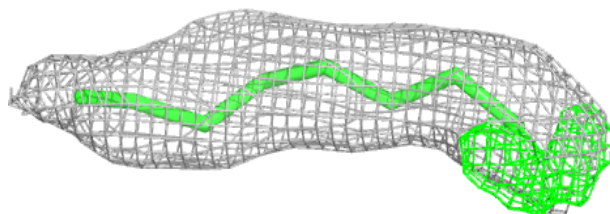
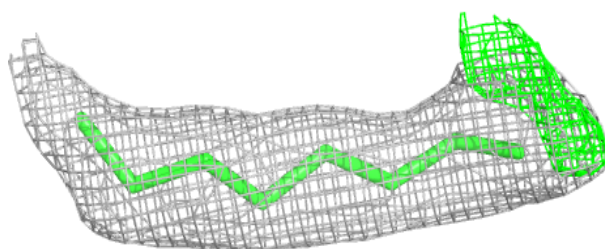


Electron density around LFA C 902:

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

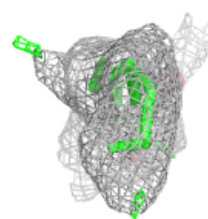
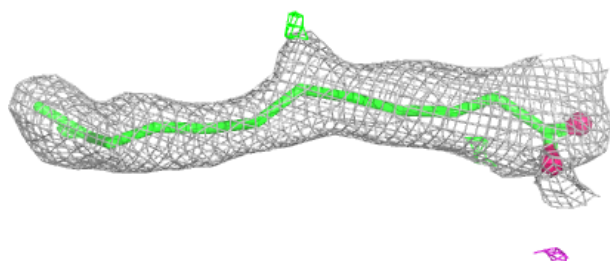
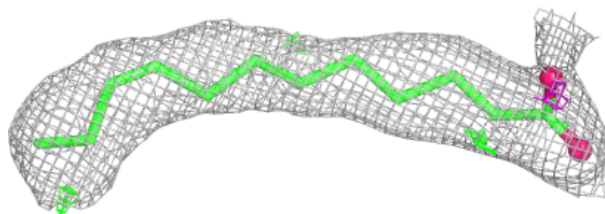
**Electron density around LFA C 905:**

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

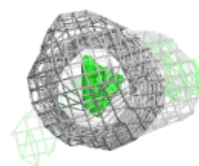
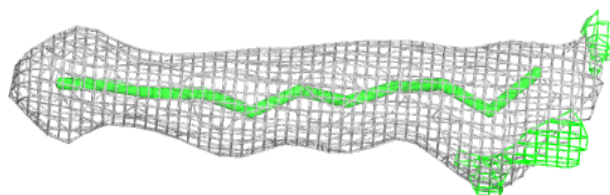
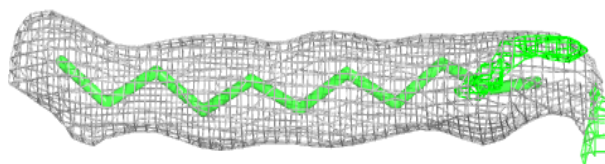


Electron density around OLA A 506:

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

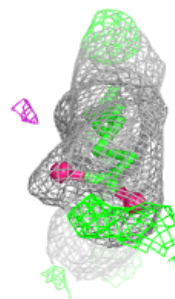
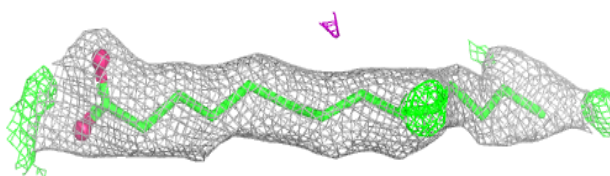
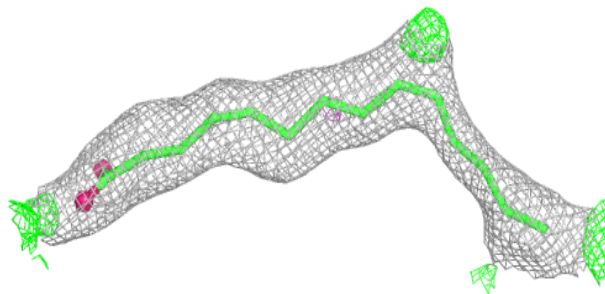
**Electron density around LFA B 1011:**

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

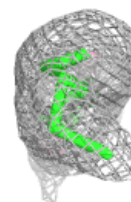
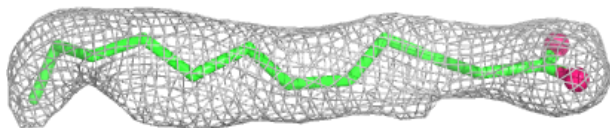
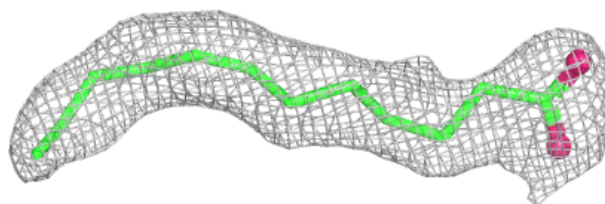


Electron density around OLA B 1008:

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

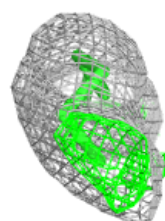
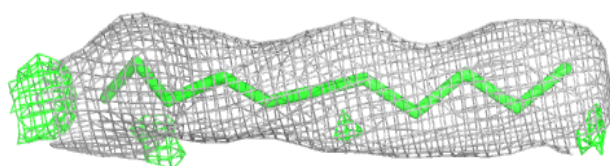
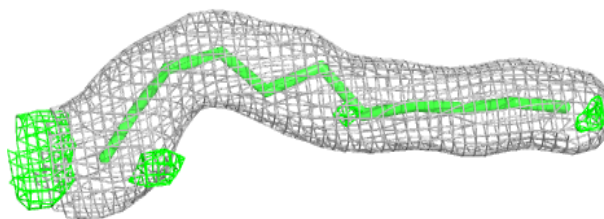
**Electron density around OLA B 1012:**

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

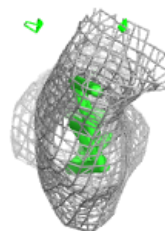
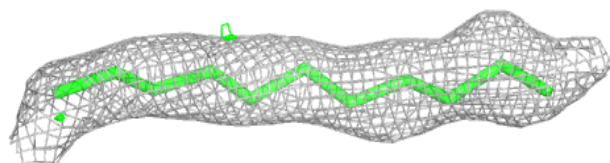
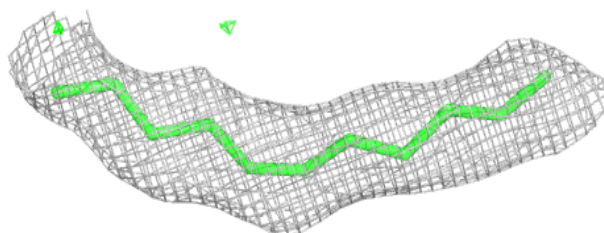


Electron density around LFA B 1004:

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

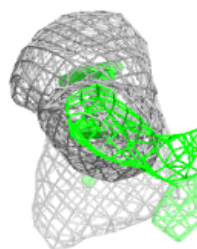
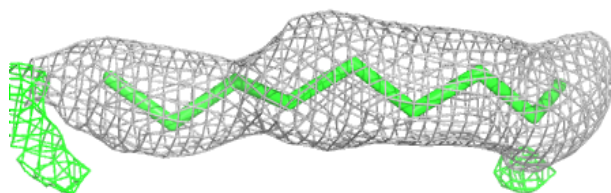
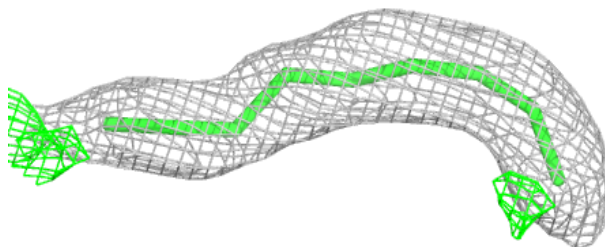
**Electron density around LFA B 1019:**

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

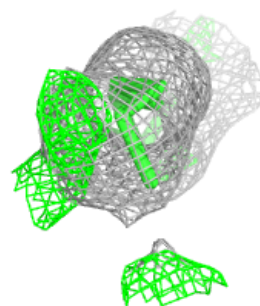
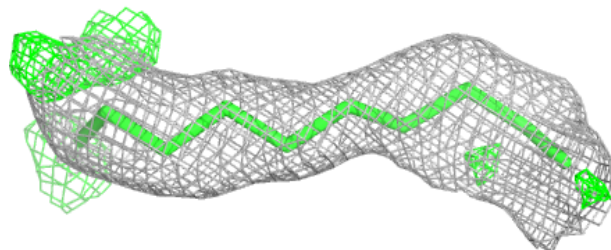
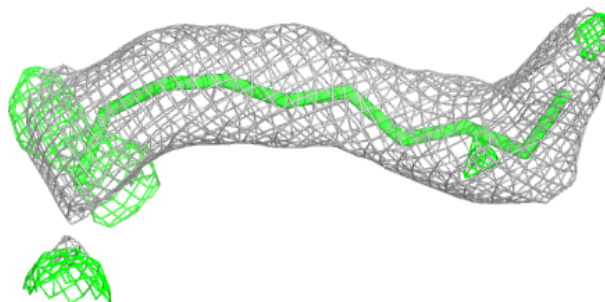


Electron density around LFA A 505:

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

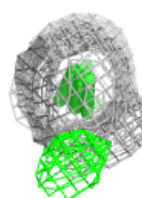
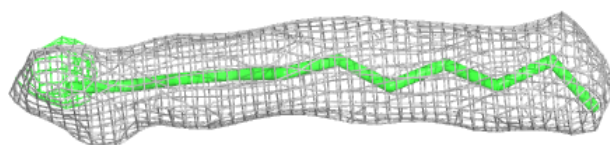
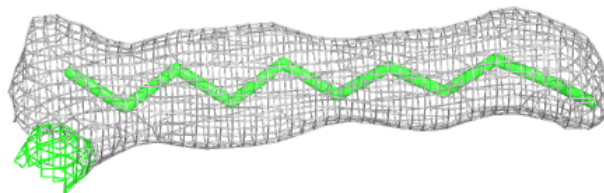
**Electron density around LFA B 1007:**

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

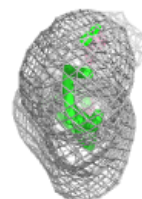
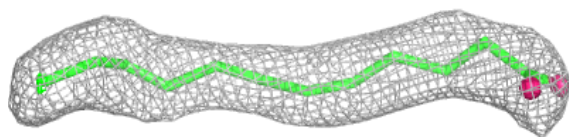
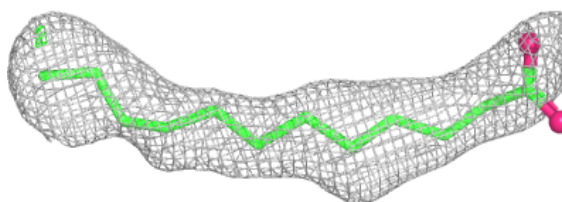


Electron density around LFA C 915:

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

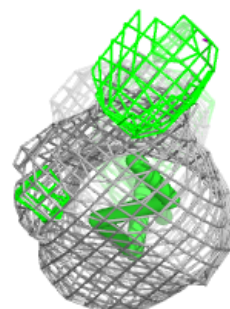
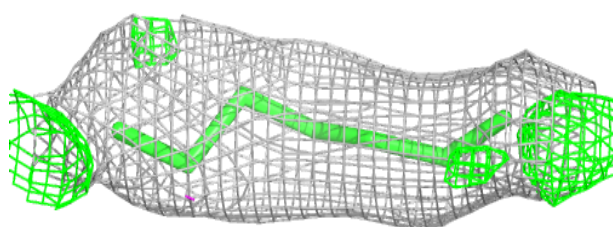
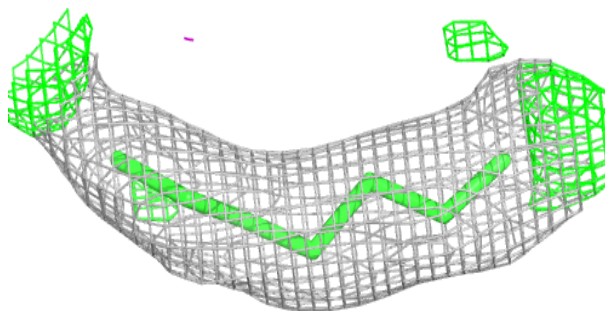
**Electron density around OLA B 1014:**

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

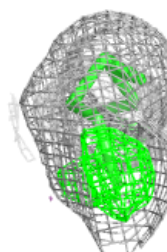
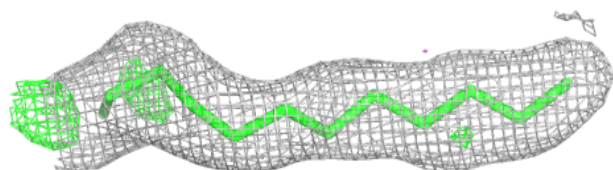
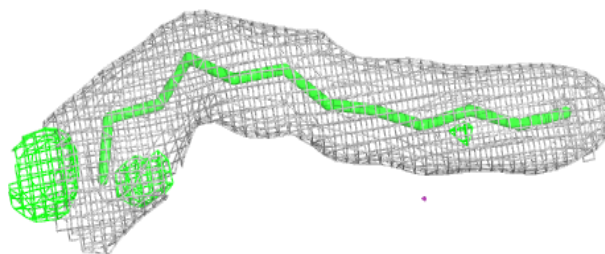


Electron density around LFA B 1001:

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

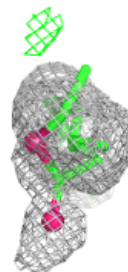
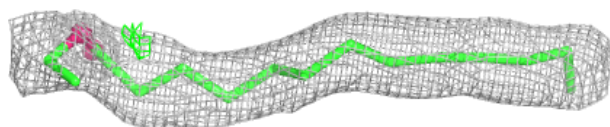
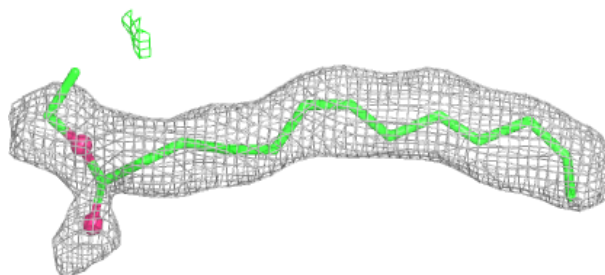
**Electron density around LFA C 901:**

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

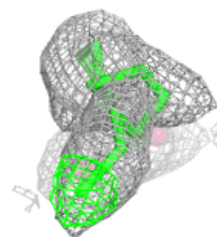
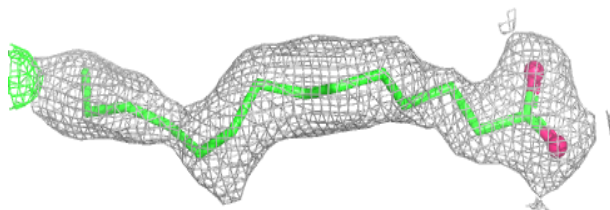
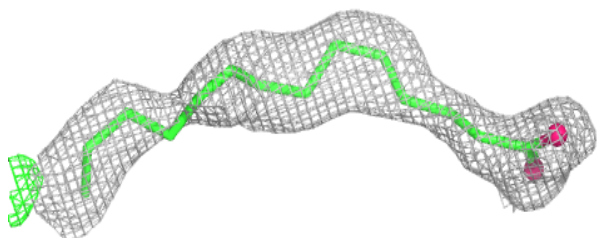


Electron density around OLC A 507:

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

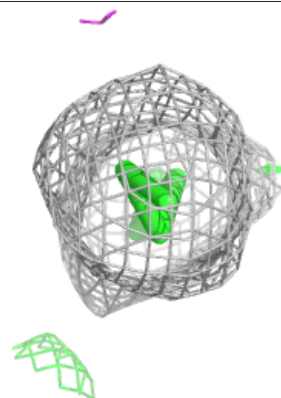
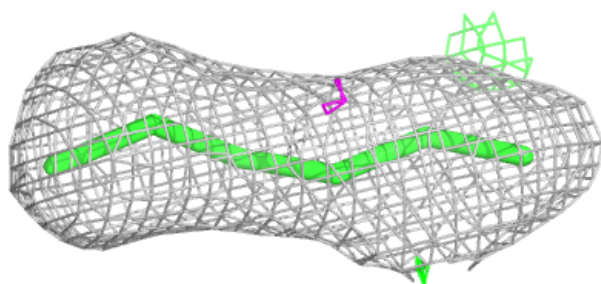
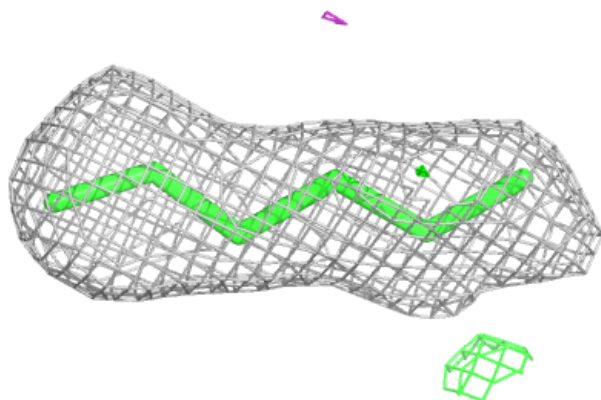
**Electron density around OLA A 508:**

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

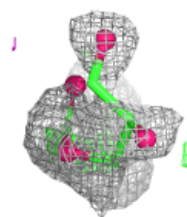
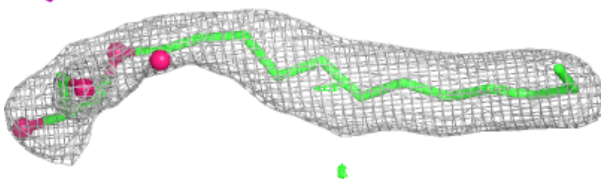
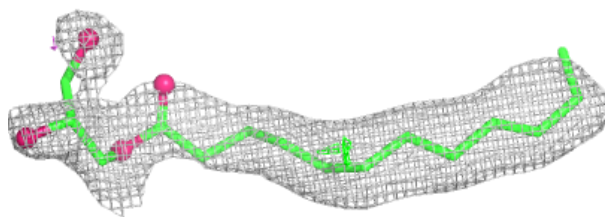


Electron density around LFA B 1020:

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

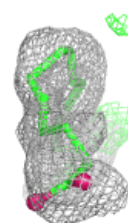
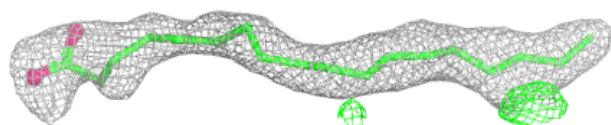
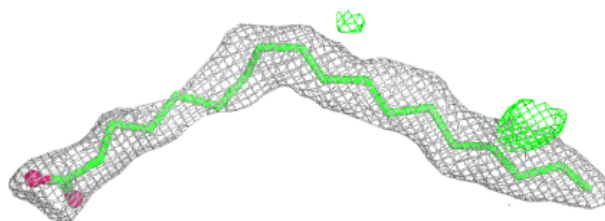
**Electron density around OLC B 1015:**

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

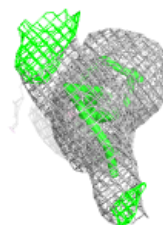
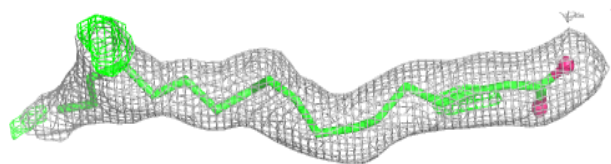
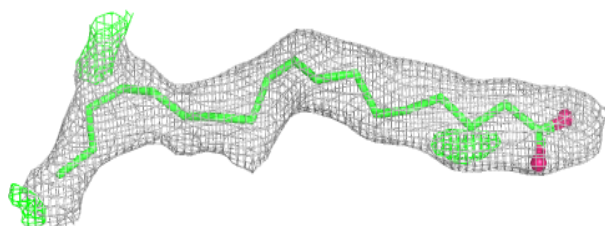


Electron density around OLC B 1017:

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

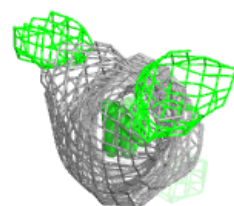
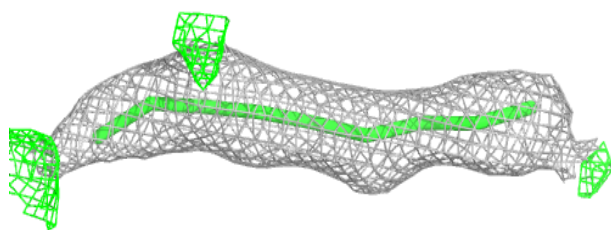
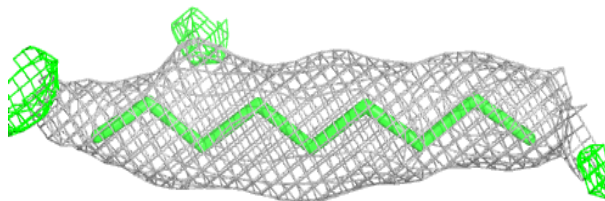
**Electron density around OLA A 514:**

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

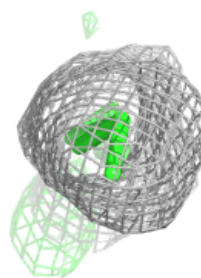
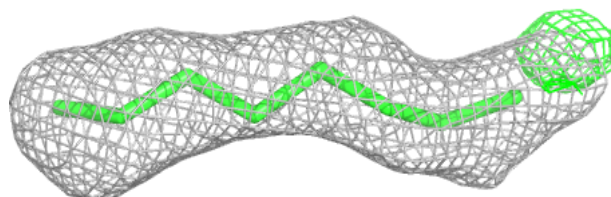
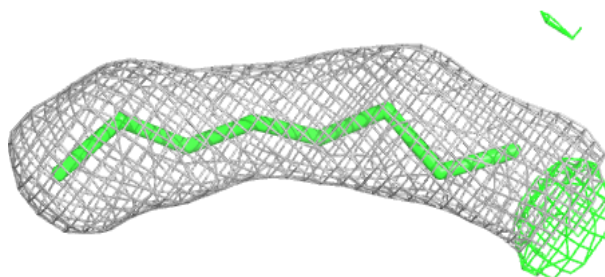


Electron density around LFA A 504:

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

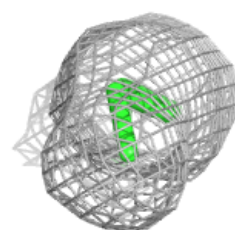
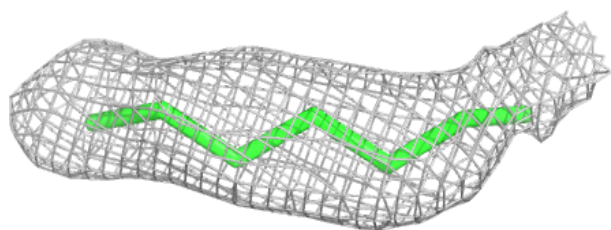
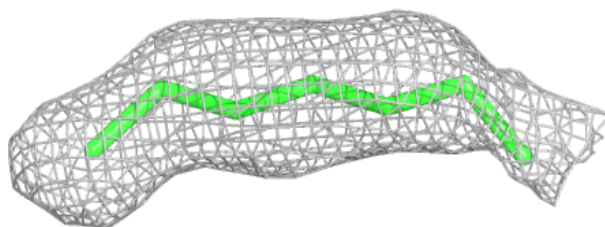
**Electron density around LFA A 502:**

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

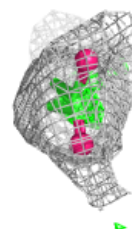
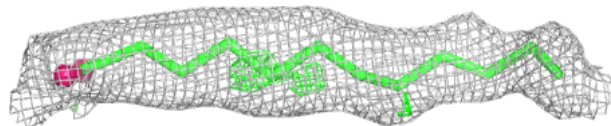
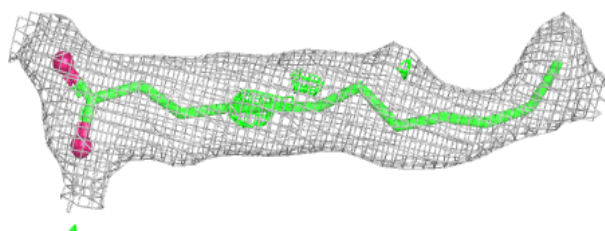


Electron density around LFA C 911:

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

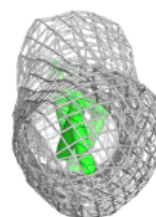
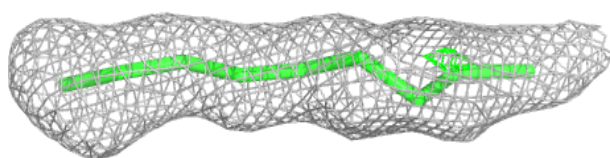
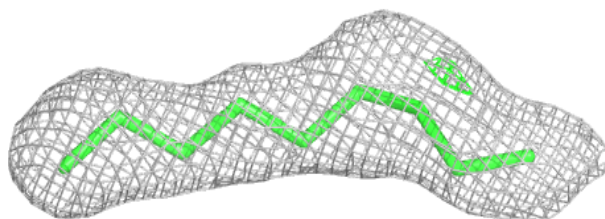
**Electron density around OLA B 1009:**

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

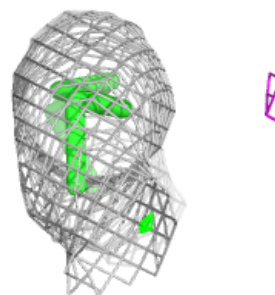
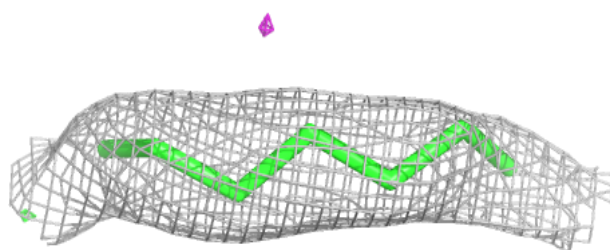
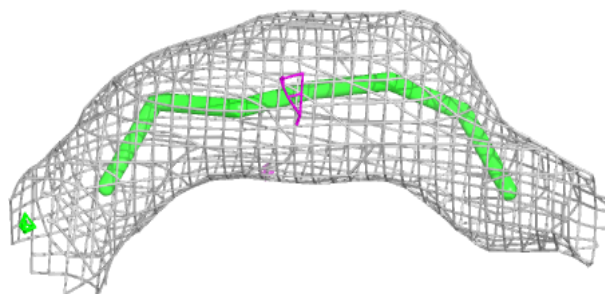


Electron density around LFA B 1005:

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

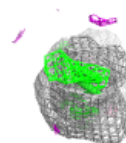
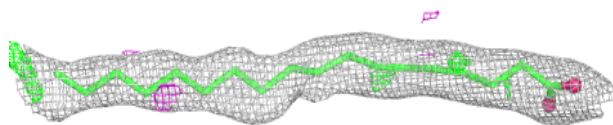
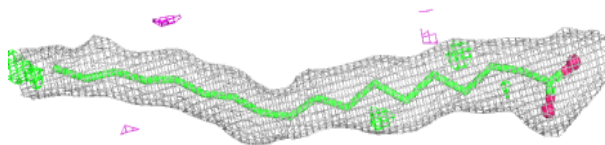
**Electron density around LFA B 1002:**

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

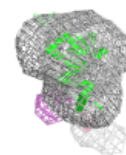
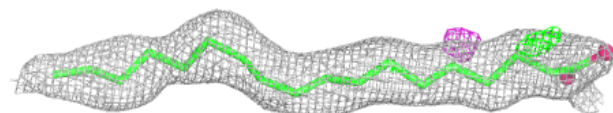
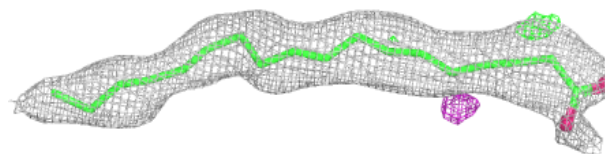


Electron density around OLA A 509:

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

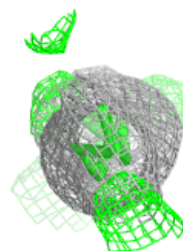
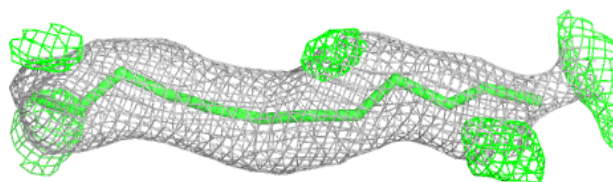
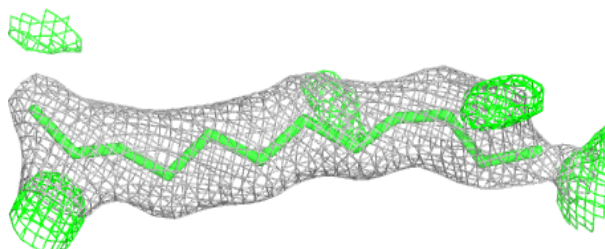
**Electron density around OLA C 903:**

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

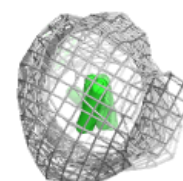
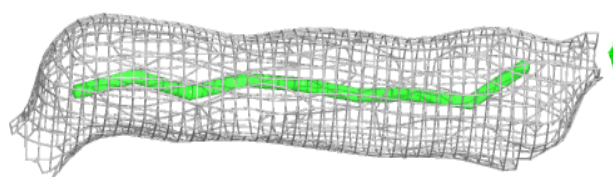
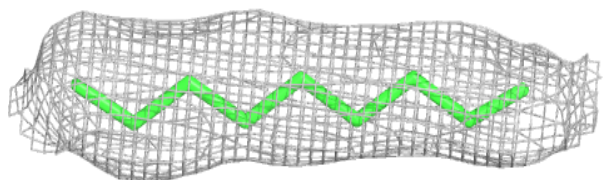


Electron density around LFA A 513:

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

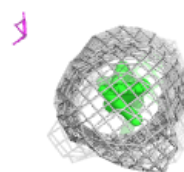
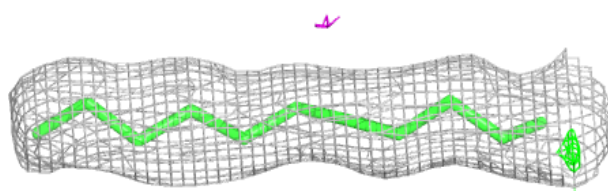
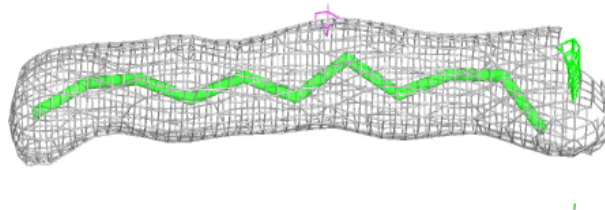
**Electron density around LFA B 1003:**

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

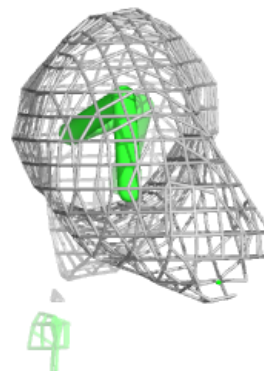
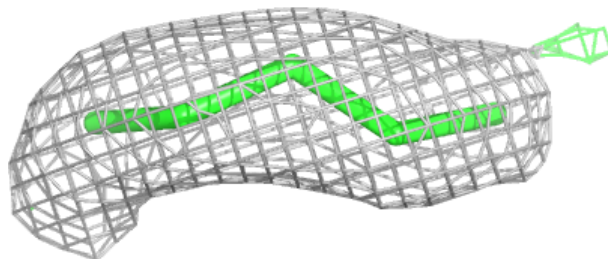
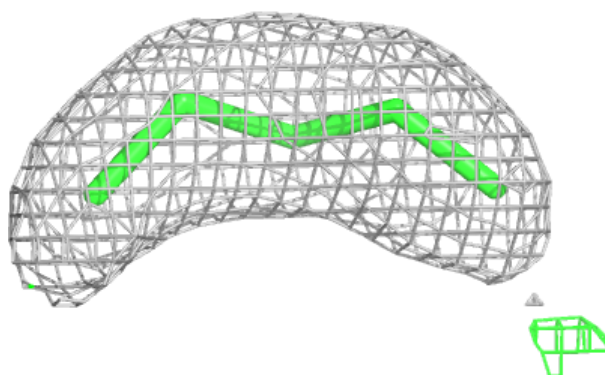


Electron density around LFA A 510:

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

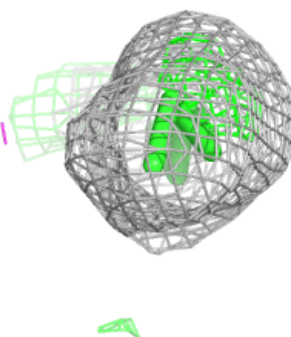
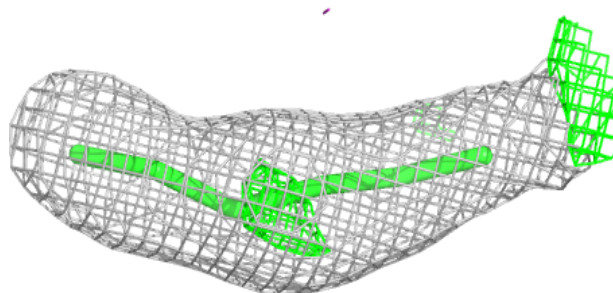
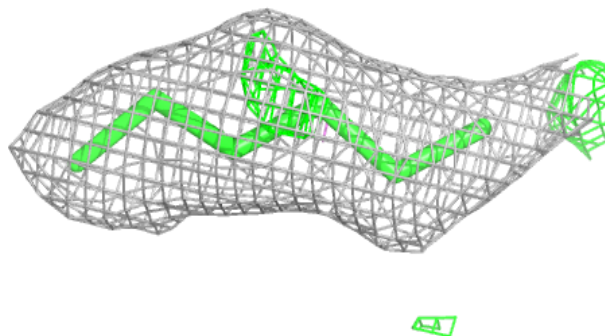
**Electron density around LFA C 907:**

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

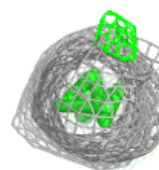
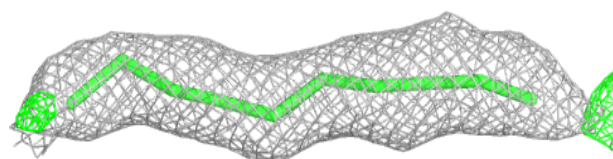
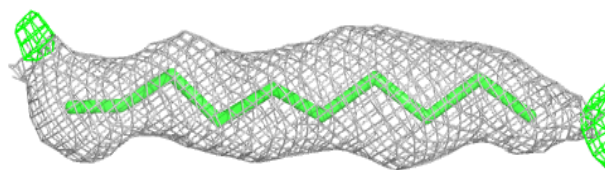


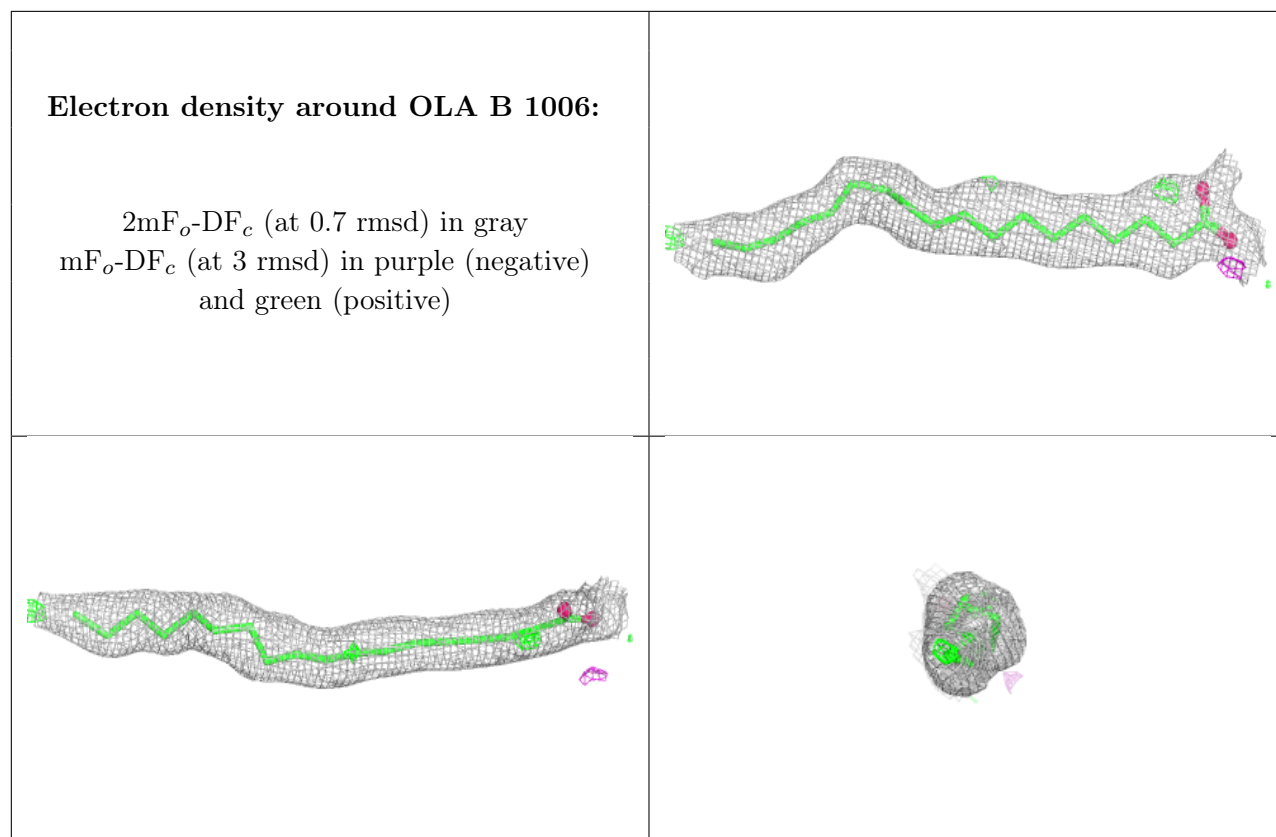
Electron density around LFA A 501:

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

**Electron density around LFA C 906:**

$2mF_o-DF_c$ (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.