



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 10:43 AM EDT

PDB ID : 7ZND / pdb_00007znd
Title : Crystal structure of the light-driven inward proton pump xenorhodopsin BcXeR in the M 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 : 1.99 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

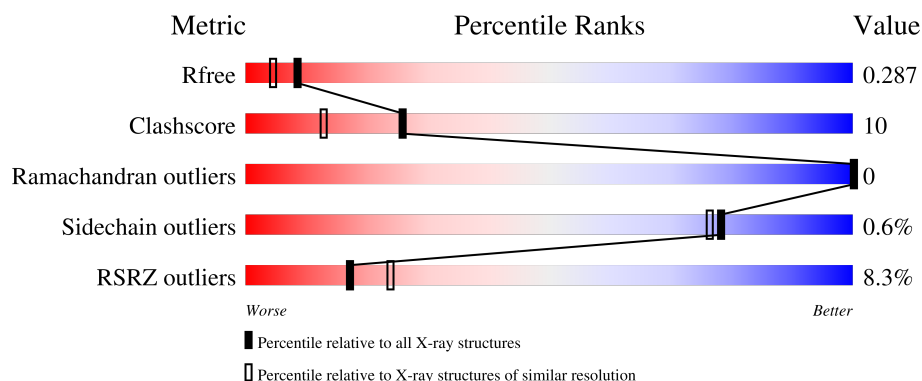
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	6% 80% 16% .
1	B	229	10% 79% 18% .
1	C	229	9% 83% 14% ..

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](#)

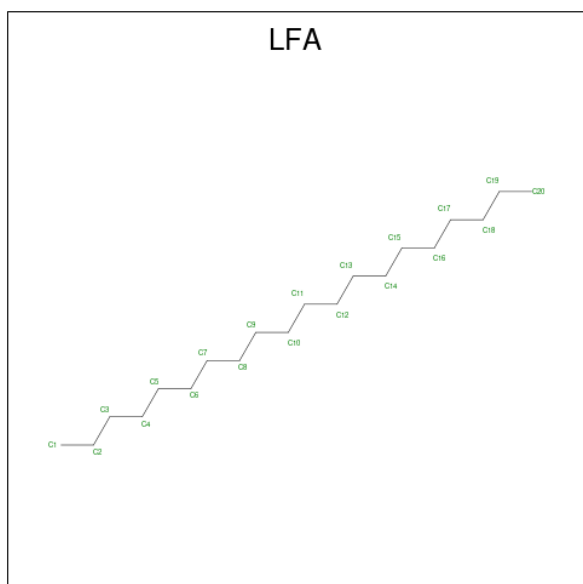
There are 6 unique types of molecules in this entry. The entry contains 6178 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called xenorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	1	0
			1760	1201	266	287	6			
1	B	222	Total	C	N	O	S	0	2	0
			1770	1209	266	289	6			
1	C	224	Total	C	N	O	S	0	0	0
			1766	1202	269	289	6			

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			6	6		
2	A	1	Total	C	0	0
			8	8		
2	A	1	Total	C	0	0
			9	9		

Continued on next page...

Continued from previous page...

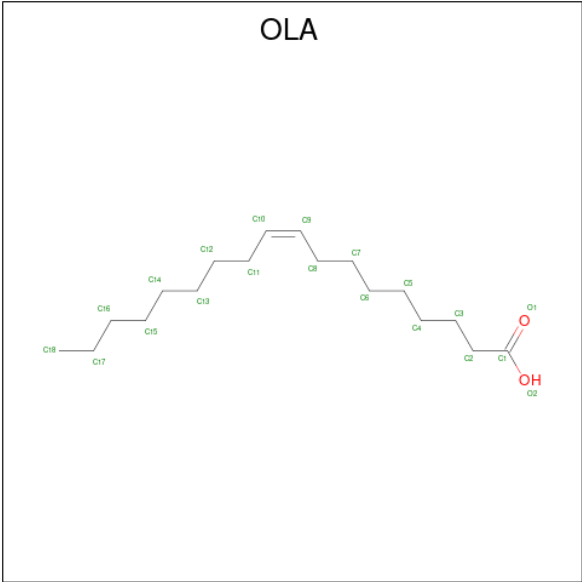
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 9 9	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 4 4	0	0
2	A	1	Total C 20 20	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 12 12	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 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).



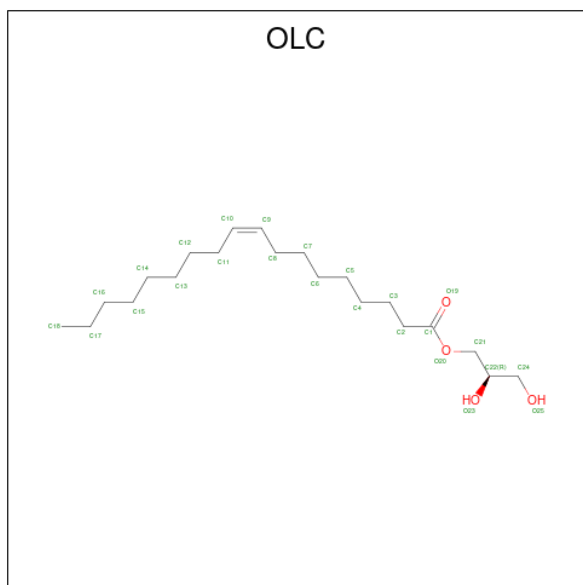
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	10	2		
3	A	1	Total	C	O	0	0
			14	12	2		
3	A	1	Total	C	O	0	0
			16	14	2		
3	A	1	Total	C	O	0	0
			20	18	2		
3	A	1	Total	C	O	0	0
			19	17	2		
3	A	1	Total	C	O	0	0
			20	18	2		
3	B	1	Total	C	O	0	0
			20	18	2		
3	B	1	Total	C	O	0	0
			16	14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

Continued on next page...

Continued from previous page...

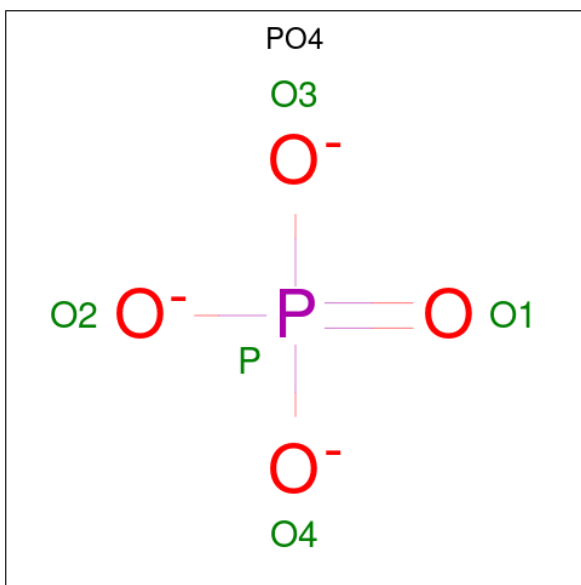
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			9	7	2		

- 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
			19	15	4		
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		

- 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		

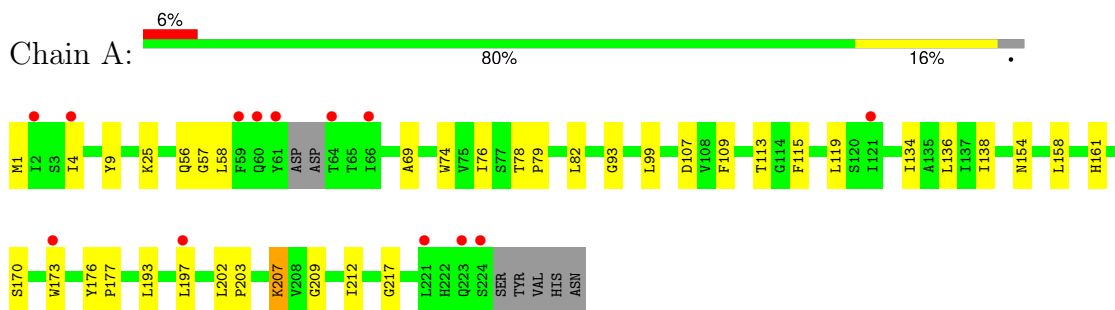
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	1
			28	28		
6	B	22	Total	O	0	1
			22	22		
6	C	25	Total	O	0	0
			25	25		

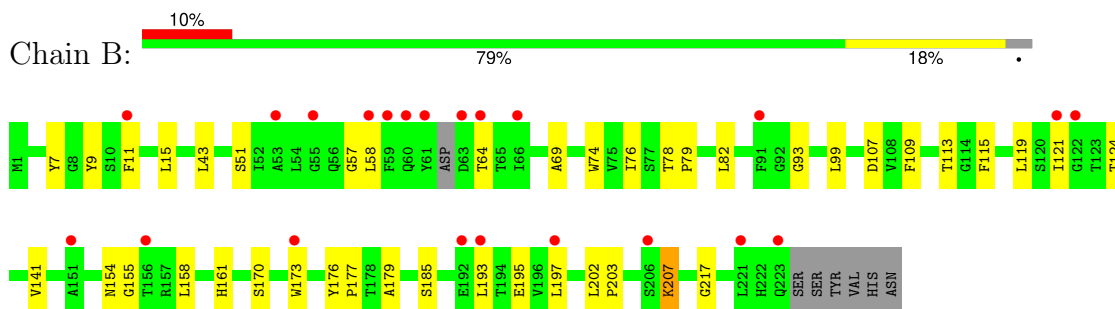
3 Residue-property plots [i](#)

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.

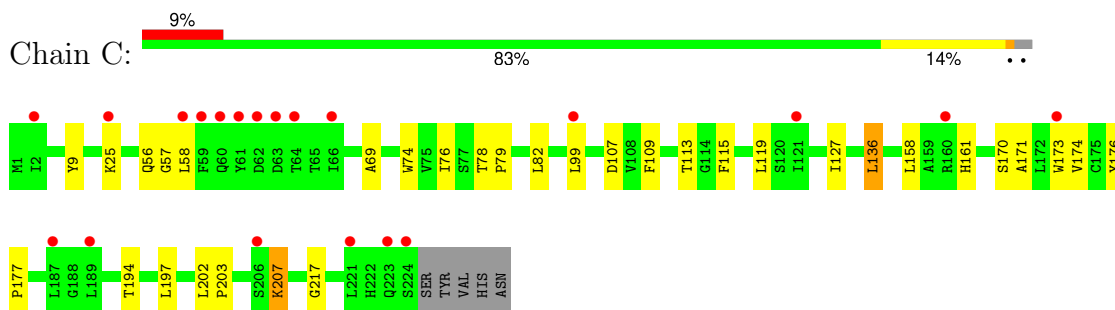
- Molecule 1: xenorhodopsin



- 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	69.09Å 109.36Å 119.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.99 20.00 – 1.99	Depositor EDS
% Data completeness (in resolution range)	66.9 (20.00-1.99) 67.0 (20.00-1.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.249 , 0.282 0.255 , 0.287	Depositor DCC
R_{free} test set	2076 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6178	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% 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, LYR, OLA, LFA, PO4, OLC

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	0.95	0/1767	1.53	0/2413
1	B	0.95	0/1778	1.54	1/2430 (0.0%)
1	C	0.96	0/1773	1.54	0/2422
All	All	0.95	0/5318	1.54	1/7265 (0.0%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	GLY	CA-C-O	-5.15	118.87	122.22

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	1760	0	1841	42	0
1	B	1770	0	1845	41	0
1	C	1766	0	1852	34	0
2	A	85	0	161	0	0
2	B	173	0	319	8	0
2	C	153	0	279	3	0
3	A	101	0	149	1	0
3	B	103	0	141	3	0
3	C	29	0	43	0	0
4	A	55	0	71	5	0
4	B	71	0	99	6	0
4	C	32	0	40	1	0
5	C	5	0	0	0	0
6	A	28	0	0	0	0
6	B	22	0	0	1	0
6	C	25	0	0	0	0
All	All	6178	0	6840	123	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:TYR:HE1	1:C:203:PRO:HB2	1.52	0.74
1:A:202:LEU:HB2	1:A:203:PRO:HD3	1.71	0.71
1:B:202:LEU:HB2	1:B:203:PRO:HD3	1.74	0.69
1:B:9:TYR:HE1	1:B:203:PRO:HB2	1.56	0.69
1:C:202:LEU:HB2	1:C:203:PRO:HD3	1.74	0.68
1:A:207:LYR:H192	1:A:207:LYR:H9	1.76	0.68
1:A:9:TYR:HE1	1:A:203:PRO:HB2	1.59	0.67
1:C:9:TYR:CE1	1:C:203:PRO:HB2	2.29	0.67
1:C:207:LYR:H192	1:C:207:LYR:H9	1.77	0.67
1:B:207:LYR:H192	1:B:207:LYR:H9	1.76	0.66
1:B:9:TYR:CE1	1:B:203:PRO:HB2	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLN:HB3	4:A:507:OLC:H5A	1.78	0.65
3:B:1016:OLA:H42	2:B:1023:LFA:H41	1.80	0.64
1:B:78:THR:N	1:B:79:PRO:HD2	2.14	0.63
4:B:1018:OLC:H2	1:C:127:ILE:HD13	1.81	0.62
1:A:9:TYR:CE1	1:A:203:PRO:HB2	2.34	0.62
1:A:78:THR:N	1:A:79:PRO:HD2	2.15	0.62
1:C:58:LEU:C	1:C:58:LEU:HD12	2.24	0.62
1:C:207:LYR:H9	1:C:207:LYR:H183	1.82	0.62
1:C:78:THR:N	1:C:79:PRO:HD2	2.15	0.61
1:B:58:LEU:C	1:B:58:LEU:HD12	2.26	0.61
1:A:207:LYR:H192	1:A:207:LYR:C9	2.31	0.60
1:A:207:LYR:H9	1:A:207:LYR:H183	1.84	0.60
1:C:207:LYR:H192	1:C:207:LYR:C9	2.32	0.59
1:A:161:HIS:CE1	1:A:217:GLY:HA3	2.37	0.59
1:A:25:LYS:HA	1:A:25:LYS:HE2	1.83	0.59
1:B:195:GLU:HG3	2:B:1025:LFA:H11	1.84	0.58
1:B:207:LYR:H192	1:B:207:LYR:C9	2.33	0.58
1:B:207:LYR:H9	1:B:207:LYR:H183	1.86	0.58
1:B:161:HIS:CE1	1:B:217:GLY:HA3	2.40	0.56
1:C:161:HIS:CE1	1:C:217:GLY:HA3	2.41	0.56
1:A:136:LEU:C	1:A:136:LEU:HD23	2.31	0.55
1:A:58:LEU:HD23	1:A:58:LEU:N	2.22	0.55
1:A:212:ILE:HG22	4:A:518:OLC:H21A	1.88	0.55
3:B:1016:OLA:C9	2:B:1026:LFA:C15	2.85	0.54
1:B:193:LEU:O	1:B:197:LEU:HD23	2.08	0.53
1:A:209:GLY:HA2	4:A:518:OLC:H4	1.91	0.53
2:B:1021:LFA:H21	2:B:1025:LFA:C9	2.39	0.53
1:A:93:GLY:HA3	1:A:154:ASN:HD21	1.74	0.53
1:C:25:LYS:HA	1:C:25:LYS:HE2	1.90	0.52
1:A:1:FME:O	1:A:4:ILE:CG2	2.57	0.52
1:B:93:GLY:HA3	1:B:154:ASN:HD21	1.75	0.52
4:B:1018:OLC:H2	1:C:127:ILE:CD1	2.40	0.52
1:B:7:TYR:CE1	4:B:1017:OLC:H2A	2.45	0.52
1:A:158:LEU:C	1:A:158:LEU:HD13	2.35	0.51
1:B:82:LEU:HD21	1:B:173[A]:TRP:CZ2	2.46	0.51
1:C:158:LEU:C	1:C:158:LEU:HD13	2.36	0.51
1:B:158:LEU:C	1:B:158:LEU:HD13	2.36	0.51
1:A:58:LEU:HD23	1:A:58:LEU:H	1.76	0.50
1:A:82:LEU:HD21	1:A:173[A]:TRP:CZ2	2.47	0.50
1:B:99:LEU:C	1:B:99:LEU:HD23	2.37	0.50
2:C:905:LFA:H82	2:C:906:LFA:H42	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:SER:OG	6:B:1101:HOH:O	2.19	0.49
1:A:99:LEU:HD23	1:A:99:LEU:C	2.36	0.49
1:B:82:LEU:HD12	1:B:107:ASP:HB2	1.93	0.49
1:C:99:LEU:C	1:C:99:LEU:HD23	2.37	0.49
1:A:193:LEU:O	1:A:197:LEU:HD23	2.13	0.48
1:C:194:THR:HA	2:C:916:LFA:H31	1.95	0.48
1:A:1:FME:O	1:A:4:ILE:HG22	2.14	0.48
1:A:176:TYR:N	1:A:177:PRO:HD2	2.28	0.48
1:B:176:TYR:N	1:B:177:PRO:HD2	2.29	0.48
1:A:74:TRP:CD1	1:A:207:LYR:H1	2.49	0.47
1:A:56:GLN:NE2	1:B:124:THR:HG21	2.29	0.47
1:A:82:LEU:HD21	1:A:173[A]:TRP:CH2	2.49	0.47
1:C:136:LEU:HD23	1:C:136:LEU:O	2.14	0.47
1:B:82:LEU:HD21	1:B:173[A]:TRP:CH2	2.49	0.47
1:C:197:LEU:CD1	2:C:916:LFA:H22	2.45	0.46
1:C:82:LEU:HD12	1:C:107:ASP:HB2	1.97	0.46
1:B:57:GLY:HA3	1:B:69:ALA:HB2	1.98	0.46
1:A:82:LEU:HD12	1:A:107:ASP:HB2	1.96	0.46
1:C:115:PHE:CZ	1:C:119:LEU:HD11	2.51	0.45
1:A:170:SER:HA	1:A:173[A]:TRP:CE3	2.51	0.45
2:B:1022:LFA:H51	4:B:1029:OLC:H6A	1.98	0.45
1:C:76:ILE:O	1:C:79:PRO:HG2	2.16	0.45
1:C:173:TRP:O	1:C:177:PRO:HD2	2.16	0.45
1:A:82:LEU:CD2	1:A:173[A]:TRP:CZ2	2.99	0.45
4:A:507:OLC:H6A	2:B:1001:LFA:H21	1.98	0.45
1:B:179:ALA:O	2:B:1025:LFA:H13	2.16	0.45
1:A:212:ILE:CG2	4:A:518:OLC:H21A	2.46	0.45
1:B:78:THR:N	1:B:79:PRO:CD	2.79	0.45
1:C:176:TYR:N	1:C:177:PRO:HD2	2.33	0.45
1:B:82:LEU:CD2	1:B:173[A]:TRP:CZ2	3.01	0.44
1:A:115:PHE:CZ	1:A:119:LEU:HD11	2.53	0.44
1:B:141:VAL:HA	3:B:1009:OLA:H51	1.99	0.44
1:C:58:LEU:HD12	1:C:58:LEU:O	2.17	0.44
1:A:57:GLY:HA3	1:A:69:ALA:HB2	2.00	0.44
1:A:76:ILE:O	1:A:79:PRO:HG2	2.17	0.44
1:C:82:LEU:HD21	1:C:173:TRP:CH2	2.53	0.44
1:B:109:PHE:O	1:B:113:THR:HG23	2.18	0.44
1:B:11:PHE:O	1:B:15:LEU:HD23	2.18	0.43
1:C:57:GLY:HA3	1:C:69:ALA:HB2	2.01	0.43
3:A:509:OLA:H32	2:B:1004:LFA:H82	1.99	0.43
1:C:56:GLN:HB3	4:C:913:OLC:C5	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LYR:H10	1:C:207:LYR:H81	1.89	0.43
1:A:109:PHE:O	1:A:113:THR:HG23	2.18	0.43
1:B:43:LEU:HA	4:B:1017:OLC:H18	1.99	0.43
1:B:173[B]:TRP:CZ3	1:B:207:LYR:H43	2.53	0.43
1:A:78:THR:N	1:A:79:PRO:CD	2.80	0.43
1:B:173[B]:TRP:CZ3	1:B:207:LYR:C4	3.02	0.43
1:C:78:THR:N	1:C:79:PRO:CD	2.80	0.43
1:B:207:LYR:H6	1:B:207:LYR:H41	1.81	0.42
1:B:115:PHE:CZ	1:B:119:LEU:HD11	2.55	0.42
1:B:76:ILE:O	1:B:79:PRO:HG2	2.18	0.42
1:B:170:SER:HA	1:B:173[A]:TRP:CE3	2.55	0.42
1:A:1:FME:O	1:A:4:ILE:HG23	2.20	0.42
1:C:109:PHE:O	1:C:113:THR:HG23	2.19	0.42
1:B:74:TRP:CD1	1:B:207:LYR:H1	2.54	0.42
1:C:203:PRO:O	1:C:207:LYR:N	2.52	0.42
1:A:207:LYR:H10	1:A:207:LYR:H81	1.87	0.41
1:A:107:ASP:OD1	1:A:173[B]:TRP:HZ2	2.03	0.41
1:B:203:PRO:O	1:B:207:LYR:N	2.53	0.41
1:C:74:TRP:CD1	1:C:207:LYR:H1	2.55	0.41
1:C:171:ALA:O	1:C:174:VAL:HG22	2.20	0.41
1:C:207:LYR:H41	1:C:207:LYR:H6	1.77	0.41
1:A:173[A]:TRP:O	1:A:177:PRO:HD2	2.21	0.41
1:B:51:SER:HB2	4:B:1015:OLC:H6	2.02	0.41
1:B:207:LYR:H10	1:B:207:LYR:H81	1.88	0.41
1:A:134:ILE:O	1:A:138:ILE:HG13	2.21	0.41
1:B:173[A]:TRP:O	1:B:177:PRO:HD2	2.20	0.41
1:C:170:SER:HA	1:C:173:TRP:CE3	2.56	0.41
1:A:203:PRO:O	1:A:207:LYR:N	2.53	0.41
1:A:207:LYR:H6	1:A:207:LYR:H41	1.80	0.41
1:B:207:LYR:C9	1:B:207:LYR:H183	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/229 (95%)	217 (100%)	1 (0%)	0	100	100
1	B	219/229 (96%)	219 (100%)	0	0	100	100
1	C	221/229 (96%)	220 (100%)	1 (0%)	0	100	100
All	All	658/687 (96%)	656 (100%)	2 (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	177/189 (94%)	177 (100%)	0	100	100
1	B	178/189 (94%)	176 (99%)	2 (1%)	65	61
1	C	179/189 (95%)	178 (99%)	1 (1%)	78	76
All	All	534/567 (94%)	531 (99%)	3 (1%)	78	76

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	64	THR
1	B	121	ILE
1	C	136	LEU

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	60	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	FME	A	1	1	8,9,10	0.44	0	8,9,11	0.61	0
1	LYR	A	207	1	27,29,30	1.16	3 (11%)	30,37,39	1.32	4 (13%)
1	FME	C	1	1	8,9,10	0.43	0	8,9,11	0.58	0
1	LYR	B	207	1	27,29,30	1.12	3 (11%)	30,37,39	1.32	4 (13%)
1	FME	B	1	1	8,9,10	0.43	0	8,9,11	0.66	0
1	LYR	C	207	1	27,29,30	1.14	2 (7%)	30,37,39	1.31	4 (13%)

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	FME	A	1	1	-	1/7/9/11	-
1	LYR	A	207	1	-	4/22/40/42	0/1/1/1
1	FME	C	1	1	1/1/1/4	3/7/9/11	-
1	LYR	B	207	1	-	2/22/40/42	0/1/1/1
1	FME	B	1	1	-	0/7/9/11	-
1	LYR	C	207	1	-	4/22/40/42	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	LYR	C7-C80	2.70	1.42	1.35
1	B	207	LYR	C7-C80	2.64	1.41	1.35
1	C	207	LYR	C7-C80	2.63	1.41	1.35
1	C	207	LYR	C9-C80	-2.55	1.40	1.46
1	A	207	LYR	C9-C80	-2.44	1.40	1.46
1	B	207	LYR	C9-C80	-2.22	1.41	1.46
1	A	207	LYR	C4-C3	-2.15	1.46	1.50
1	B	207	LYR	C4-C3	-2.00	1.46	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	LYR	C8-C80-C7	-3.68	116.85	122.82
1	A	207	LYR	C5-C3-C2	3.57	123.46	118.49
1	A	207	LYR	C8-C80-C7	-3.57	117.04	122.82
1	C	207	LYR	C5-C3-C2	3.49	123.35	118.49
1	C	207	LYR	C8-C80-C7	-3.48	117.18	122.82
1	B	207	LYR	C5-C3-C2	3.16	122.89	118.49
1	B	207	LYR	C9-C80-C7	2.98	123.70	119.01
1	A	207	LYR	C9-C80-C7	2.90	123.57	119.01
1	C	207	LYR	C9-C80-C7	2.56	123.04	119.01
1	C	207	LYR	C7-C6-C5	2.40	130.15	123.20
1	B	207	LYR	C7-C6-C5	2.27	129.79	123.20
1	A	207	LYR	C7-C6-C5	2.10	129.28	123.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	1	FME	CA

All (14) 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	O-C-CA-CB
1	C	207	LYR	CG-CD-CE-NZ
1	B	207	LYR	CD-CE-NZ-C1
1	B	207	LYR	CA-CB-CG-CD
1	A	207	LYR	CG-CD-CE-NZ
1	C	1	FME	CB-CA-N-CN

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

4 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	3	0
1	A	207	LYR	7	0
1	B	207	LYR	10	0
1	C	207	LYR	7	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

67 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	1002	-	6,6,19	0.09	0	5,5,18	0.13	0
2	LFA	B	1024	-	10,10,19	0.10	0	9,9,18	0.06	0
2	LFA	C	907	-	11,11,19	0.10	0	10,10,18	0.07	0
2	LFA	A	514	-	9,9,19	0.10	0	8,8,18	0.07	0
3	OLA	C	911	-	8,8,19	0.77	0	8,8,19	0.72	0
2	LFA	B	1025	-	9,9,19	0.11	0	8,8,18	0.07	0
2	LFA	C	912	-	6,6,19	0.11	0	5,5,18	0.09	0
3	OLA	B	1013	-	13,13,19	0.63	0	13,13,19	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OLC	A	507	-	16,16,24	0.34	0	16,16,25	0.17	0
4	OLC	C	909	-	16,16,24	0.26	0	17,17,25	0.25	0
5	PO4	C	914	-	4,4,4	0.71	0	6,6,6	0.47	0
2	LFA	C	918	-	5,5,19	0.11	0	4,4,18	0.11	0
2	LFA	B	1010	-	7,7,19	0.11	0	6,6,18	0.10	0
2	LFA	C	917	-	15,15,19	0.08	0	14,14,18	0.06	0
2	LFA	C	919	-	6,6,19	0.10	0	5,5,18	0.12	0
2	LFA	B	1005	-	8,8,19	0.08	0	7,7,18	0.09	0
2	LFA	B	1001	-	6,6,19	0.11	0	5,5,18	0.11	0
4	OLC	B	1017	-	19,19,24	0.29	0	19,19,25	0.25	0
2	LFA	A	505	-	8,8,19	0.09	0	7,7,18	0.09	0
4	OLC	B	1018	-	18,18,24	0.24	0	19,19,25	0.25	0
3	OLA	B	1012	-	13,13,19	0.63	0	13,13,19	0.57	0
2	LFA	B	1007	-	9,9,19	0.10	0	8,8,18	0.08	0
2	LFA	B	1020	-	10,10,19	0.10	0	9,9,18	0.07	0
3	OLA	A	503	-	11,11,19	0.68	0	11,11,19	0.60	0
3	OLA	B	1009	-	13,13,19	0.63	0	13,13,19	0.56	0
2	LFA	B	1021	-	5,5,19	0.11	0	4,4,18	0.10	0
4	OLC	A	511	-	18,18,24	0.28	0	18,18,25	0.20	0
2	LFA	B	1027	-	9,9,19	0.09	0	8,8,18	0.09	0
2	LFA	B	1019	-	5,5,19	0.11	0	4,4,18	0.09	0
2	LFA	C	908	-	4,4,19	0.14	0	3,3,18	0.22	0
3	OLA	B	1006	-	19,19,19	0.53	0	19,19,19	0.48	0
2	LFA	A	516	-	3,3,19	0.22	0	2,2,18	0.46	0
2	LFA	B	1022	-	7,7,19	0.11	0	6,6,18	0.09	0
4	OLC	B	1015	-	18,18,24	0.25	0	19,19,25	0.25	0
3	OLA	A	512	-	18,18,19	0.54	0	18,18,19	0.49	0
2	LFA	C	910	-	8,8,19	0.09	0	7,7,18	0.09	0
2	LFA	A	501	-	5,5,19	0.12	0	4,4,18	0.11	0
2	LFA	B	1023	-	9,9,19	0.10	0	8,8,18	0.07	0
2	LFA	C	915	-	10,10,19	0.08	0	9,9,18	0.07	0
2	LFA	B	1011	-	10,10,19	0.09	0	9,9,18	0.07	0
4	OLC	B	1029	-	12,12,24	1.35	2 (16%)	12,12,25	1.47	2 (16%)
3	OLA	B	1016	-	10,10,19	0.69	0	10,10,19	0.66	0
3	OLA	A	506	-	13,13,19	0.63	0	13,13,19	0.56	0
2	LFA	B	1026	-	13,13,19	0.08	0	12,12,18	0.08	0
2	LFA	C	902	-	12,12,19	0.08	0	11,11,18	0.07	0
3	OLA	A	509	-	19,19,19	0.53	0	19,19,19	0.47	0
2	LFA	A	504	-	8,8,19	0.11	0	7,7,18	0.10	0
3	OLA	B	1014	-	13,13,19	0.62	0	13,13,19	0.57	0
2	LFA	C	901	-	11,11,19	0.08	0	10,10,18	0.07	0
2	LFA	C	904	-	5,5,19	0.12	0	4,4,18	0.10	0
2	LFA	A	502	-	7,7,19	0.09	0	6,6,18	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LFA	B	1004	-	10,10,19	0.09	0	9,9,18	0.06	0
2	LFA	C	906	-	9,9,19	0.08	0	8,8,18	0.10	0
3	OLA	A	513	-	19,19,19	0.53	0	19,19,19	0.49	0
4	OLC	C	913	-	14,14,24	0.26	0	14,14,25	0.13	0
2	LFA	C	920	-	15,15,19	0.08	0	14,14,18	0.06	0
2	LFA	C	916	-	14,14,19	0.08	0	13,13,18	0.06	0
2	LFA	A	515	-	7,7,19	0.11	0	6,6,18	0.08	0
3	OLA	C	903	-	19,19,19	0.53	0	19,19,19	0.48	0
2	LFA	C	905	-	7,7,19	0.09	0	6,6,18	0.12	0
3	OLA	B	1008	-	15,15,19	0.59	0	15,15,19	0.54	0
2	LFA	A	517	-	19,19,19	0.09	0	18,18,18	0.04	0
3	OLA	A	508	-	15,15,19	0.60	0	15,15,19	0.54	0
4	OLC	A	518	-	18,18,24	0.23	0	19,19,25	0.24	0
2	LFA	B	1003	-	8,8,19	0.10	0	7,7,18	0.08	0
2	LFA	B	1028	-	14,14,19	0.09	0	13,13,18	0.07	0
2	LFA	A	510	-	10,10,19	0.08	0	9,9,18	0.07	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	1002	-	-	1/4/4/17	-
2	LFA	B	1024	-	-	7/8/8/17	-
2	LFA	C	907	-	-	4/9/9/17	-
2	LFA	A	514	-	-	1/7/7/17	-
3	OLA	C	911	-	-	2/6/6/17	-
2	LFA	B	1025	-	-	2/7/7/17	-
2	LFA	C	912	-	-	1/4/4/17	-
3	OLA	B	1013	-	-	1/11/11/17	-
4	OLC	A	507	-	-	10/15/15/24	-
4	OLC	C	909	-	-	2/16/16/24	-
2	LFA	C	918	-	-	0/3/3/17	-
2	LFA	B	1010	-	-	3/5/5/17	-
2	LFA	C	917	-	-	5/13/13/17	-
2	LFA	C	919	-	-	0/4/4/17	-
2	LFA	B	1005	-	-	4/6/6/17	-
2	LFA	B	1001	-	-	1/4/4/17	-
4	OLC	B	1017	-	-	6/17/17/24	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	A	505	-	-	2/6/6/17	-
4	OLC	B	1018	-	-	7/18/18/24	-
3	OLA	B	1012	-	-	6/11/11/17	-
2	LFA	B	1007	-	-	4/7/7/17	-
2	LFA	B	1020	-	-	0/8/8/17	-
3	OLA	A	503	-	-	5/9/9/17	-
3	OLA	B	1009	-	-	7/11/11/17	-
2	LFA	B	1021	-	-	2/3/3/17	-
4	OLC	A	511	-	-	3/17/17/24	-
2	LFA	B	1027	-	-	1/7/7/17	-
2	LFA	B	1019	-	-	0/3/3/17	-
2	LFA	C	908	-	-	1/2/2/17	-
3	OLA	B	1006	-	-	3/17/17/17	-
2	LFA	A	516	-	-	0/1/1/17	-
2	LFA	B	1022	-	-	0/5/5/17	-
4	OLC	B	1015	-	-	11/18/18/24	-
3	OLA	A	512	-	-	9/16/16/17	-
2	LFA	C	910	-	-	1/6/6/17	-
2	LFA	A	501	-	-	0/3/3/17	-
2	LFA	B	1023	-	-	0/7/7/17	-
2	LFA	C	915	-	-	2/8/8/17	-
2	LFA	B	1011	-	-	0/8/8/17	-
4	OLC	B	1029	-	-	2/10/10/24	-
3	OLA	B	1016	-	-	6/8/8/17	-
3	OLA	A	506	-	-	6/11/11/17	-
2	LFA	B	1026	-	-	1/11/11/17	-
2	LFA	C	902	-	-	4/10/10/17	-
3	OLA	A	509	-	-	4/17/17/17	-
2	LFA	A	504	-	-	1/6/6/17	-
3	OLA	B	1014	-	-	6/11/11/17	-
2	LFA	C	901	-	-	4/9/9/17	-
2	LFA	C	904	-	-	0/3/3/17	-
2	LFA	A	502	-	-	2/5/5/17	-
2	LFA	B	1004	-	-	3/8/8/17	-
2	LFA	C	906	-	-	1/7/7/17	-
3	OLA	A	513	-	-	6/17/17/17	-
4	OLC	C	913	-	-	8/13/13/24	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	C	920	-	-	6/13/13/17	-
2	LFA	C	916	-	-	6/12/12/17	-
2	LFA	A	515	-	-	1/5/5/17	-
3	OLA	C	903	-	-	7/17/17/17	-
2	LFA	C	905	-	-	1/5/5/17	-
3	OLA	B	1008	-	-	6/13/13/17	-
2	LFA	A	517	-	-	6/17/17/17	-
3	OLA	A	508	-	-	7/13/13/17	-
4	OLC	A	518	-	-	6/18/18/24	-
2	LFA	B	1003	-	-	1/6/6/17	-
2	LFA	B	1028	-	-	5/12/12/17	-
2	LFA	A	510	-	-	5/8/8/17	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1029	OLC	O19-C1	3.45	1.33	1.22
4	B	1029	OLC	O20-C1	-3.05	1.20	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1029	OLC	O19-C1-C2	-3.61	111.64	123.09
4	B	1029	OLC	O20-C1-C2	3.50	125.06	114.00

There are no chirality outliers.

All (225) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1015	OLC	O20-C21-C22-C24
4	B	1018	OLC	O20-C21-C22-C24
4	A	518	OLC	O19-C1-O20-C21
4	B	1015	OLC	C2-C1-O20-C21
4	A	518	OLC	C2-C1-O20-C21
3	B	1012	OLA	C11-C10-C9-C8
4	A	507	OLC	O19-C1-O20-C21
4	B	1015	OLC	O19-C1-O20-C21
4	A	507	OLC	C2-C1-O20-C21
3	A	509	OLA	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	1015	OLC	O23-C22-C24-O25
3	B	1012	OLA	C1-C2-C3-C4
3	A	506	OLA	C1-C2-C3-C4
4	A	507	OLC	C1-C2-C3-C4
3	A	512	OLA	C1-C2-C3-C4
4	B	1015	OLC	O20-C21-C22-O23
4	B	1029	OLC	C1-C2-C3-C4
3	B	1016	OLA	C1-C2-C3-C4
4	A	507	OLC	C10-C11-C12-C13
4	B	1018	OLC	O20-C21-C22-O23
4	B	1015	OLC	C21-C22-C24-O25
3	A	508	OLA	C4-C5-C6-C7
4	A	518	OLC	C1-C2-C3-C4
2	C	907	LFA	C4-C5-C6-C7
3	B	1006	OLA	C11-C12-C13-C14
2	C	901	LFA	C11-C10-C9-C8
2	C	916	LFA	C6-C7-C8-C9
3	A	506	OLA	C4-C5-C6-C7
4	B	1015	OLC	C1-C2-C3-C4
3	C	911	OLA	C3-C4-C5-C6
2	B	1010	LFA	C3-C4-C5-C6
3	A	513	OLA	C4-C5-C6-C7
4	B	1015	OLC	C4-C5-C6-C7
4	A	511	OLC	O20-C21-C22-O23
4	A	507	OLC	C3-C4-C5-C6
4	A	511	OLC	C1-C2-C3-C4
2	C	902	LFA	C5-C6-C7-C8
2	C	910	LFA	C5-C6-C7-C8
3	B	1008	OLA	C4-C5-C6-C7
2	A	517	LFA	C14-C15-C16-C17
3	A	512	OLA	C6-C7-C8-C9
3	B	1008	OLA	C3-C4-C5-C6
2	B	1025	LFA	C6-C7-C8-C9
4	B	1018	OLC	C2-C3-C4-C5
2	B	1024	LFA	C5-C6-C7-C8
2	B	1024	LFA	C6-C7-C8-C9
4	B	1017	OLC	C11-C12-C13-C14
3	C	911	OLA	C2-C3-C4-C5
4	B	1015	OLC	C2-C3-C4-C5
3	A	503	OLA	C1-C2-C3-C4
4	C	913	OLC	C9-C10-C11-C12
2	B	1001	LFA	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	506	OLA	C6-C7-C8-C9
3	A	508	OLA	C10-C11-C12-C13
3	A	512	OLA	C10-C11-C12-C13
3	B	1012	OLA	C6-C7-C8-C9
2	A	517	LFA	C10-C11-C12-C13
2	B	1024	LFA	C2-C3-C4-C5
2	B	1005	LFA	C4-C5-C6-C7
3	A	512	OLA	C5-C6-C7-C8
2	C	920	LFA	C7-C8-C9-C10
2	C	901	LFA	C7-C8-C9-C10
4	C	913	OLC	C2-C3-C4-C5
2	C	907	LFA	C11-C10-C9-C8
4	B	1017	OLC	C6-C7-C8-C9
3	A	509	OLA	C2-C3-C4-C5
3	B	1006	OLA	C12-C13-C14-C15
3	B	1009	OLA	C5-C6-C7-C8
3	A	512	OLA	C7-C8-C9-C10
2	A	505	LFA	C13-C14-C15-C16
3	B	1009	OLA	C2-C3-C4-C5
3	C	903	OLA	C13-C14-C15-C16
2	B	1004	LFA	C6-C7-C8-C9
3	B	1012	OLA	C5-C6-C7-C8
2	C	920	LFA	C11-C10-C9-C8
2	A	510	LFA	C11-C12-C13-C14
4	B	1015	OLC	C5-C6-C7-C8
2	A	517	LFA	C13-C14-C15-C16
3	A	506	OLA	C11-C10-C9-C8
3	A	508	OLA	C11-C10-C9-C8
3	A	506	OLA	C2-C3-C4-C5
3	B	1009	OLA	C6-C7-C8-C9
2	C	902	LFA	C10-C11-C12-C13
3	B	1014	OLA	C1-C2-C3-C4
3	B	1016	OLA	C2-C3-C4-C5
2	A	502	LFA	C2-C3-C4-C5
2	C	902	LFA	C4-C5-C6-C7
3	A	508	OLA	C6-C7-C8-C9
2	A	510	LFA	C12-C13-C14-C15
4	B	1018	OLC	C5-C6-C7-C8
3	B	1012	OLA	C3-C4-C5-C6
3	B	1008	OLA	C5-C6-C7-C8
2	B	1007	LFA	C1-C2-C3-C4
2	B	1010	LFA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	505	LFA	C12-C13-C14-C15
3	A	508	OLA	C11-C12-C13-C14
2	B	1007	LFA	C7-C8-C9-C10
2	C	901	LFA	C6-C7-C8-C9
2	B	1007	LFA	C6-C7-C8-C9
2	C	907	LFA	C2-C3-C4-C5
2	A	510	LFA	C14-C15-C16-C17
3	B	1016	OLA	C5-C6-C7-C8
3	C	903	OLA	C3-C4-C5-C6
2	A	517	LFA	C9-C10-C11-C12
2	B	1010	LFA	C2-C3-C4-C5
2	B	1028	LFA	C9-C10-C11-C12
2	B	1028	LFA	C3-C4-C5-C6
2	C	917	LFA	C2-C3-C4-C5
3	A	513	OLA	C3-C4-C5-C6
2	B	1003	LFA	C6-C7-C8-C9
4	B	1018	OLC	C1-C2-C3-C4
2	B	1004	LFA	C2-C3-C4-C5
3	A	503	OLA	C2-C3-C4-C5
4	A	507	OLC	C5-C6-C7-C8
2	B	1024	LFA	C7-C8-C9-C10
3	A	503	OLA	C7-C8-C9-C10
2	B	1028	LFA	C12-C13-C14-C15
2	C	915	LFA	C10-C11-C12-C13
4	C	913	OLC	C2-C1-O20-C21
3	B	1008	OLA	C11-C12-C13-C14
2	C	920	LFA	C3-C4-C5-C6
2	B	1005	LFA	C2-C3-C4-C5
4	B	1018	OLC	C9-C10-C11-C12
2	C	908	LFA	C1-C2-C3-C4
2	B	1028	LFA	C5-C6-C7-C8
2	C	902	LFA	C7-C8-C9-C10
4	C	913	OLC	C3-C4-C5-C6
3	A	513	OLA	C5-C6-C7-C8
2	B	1024	LFA	C1-C2-C3-C4
4	B	1017	OLC	C2-C3-C4-C5
2	A	502	LFA	C1-C2-C3-C4
3	A	508	OLA	C2-C3-C4-C5
2	B	1024	LFA	C11-C10-C9-C8
4	A	507	OLC	C6-C7-C8-C9
2	B	1027	LFA	C4-C5-C6-C7
2	B	1021	LFA	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1026	LFA	C9-C10-C11-C12
2	C	906	LFA	C11-C10-C9-C8
2	C	920	LFA	C6-C7-C8-C9
2	A	517	LFA	C16-C17-C18-C19
2	C	912	LFA	C3-C4-C5-C6
4	B	1017	OLC	C1-C2-C3-C4
2	C	917	LFA	C6-C7-C8-C9
2	C	915	LFA	C14-C15-C16-C17
2	A	514	LFA	C7-C8-C9-C10
2	C	916	LFA	C4-C5-C6-C7
2	C	916	LFA	C9-C10-C11-C12
2	B	1021	LFA	C1-C2-C3-C4
4	A	518	OLC	C2-C3-C4-C5
3	A	509	OLA	C7-C8-C9-C10
4	A	511	OLC	C9-C10-C11-C12
3	A	513	OLA	C14-C15-C16-C17
2	B	1025	LFA	C2-C3-C4-C5
3	B	1014	OLA	C2-C3-C4-C5
4	A	518	OLC	C9-C10-C11-C12
2	A	510	LFA	C10-C11-C12-C13
3	A	509	OLA	C6-C7-C8-C9
4	C	913	OLC	C6-C7-C8-C9
2	A	517	LFA	C17-C18-C19-C20
3	B	1012	OLA	C4-C5-C6-C7
2	B	1028	LFA	C7-C8-C9-C10
3	C	903	OLA	C11-C12-C13-C14
2	C	916	LFA	C11-C10-C9-C8
3	B	1016	OLA	C6-C7-C8-C9
4	B	1029	OLC	C7-C8-C9-C10
2	C	901	LFA	C10-C11-C12-C13
3	A	512	OLA	O1-C1-C2-C3
2	C	907	LFA	C7-C8-C9-C10
4	A	507	OLC	C9-C10-C11-C12
2	B	1024	LFA	C4-C5-C6-C7
4	C	913	OLC	C5-C6-C7-C8
3	A	506	OLA	C5-C6-C7-C8
3	A	513	OLA	O2-C1-C2-C3
2	C	920	LFA	C5-C6-C7-C8
4	B	1015	OLC	C7-C8-C9-C10
3	A	513	OLA	O1-C1-C2-C3
3	A	512	OLA	O2-C1-C2-C3
4	C	913	OLC	O19-C1-O20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1002	LFA	C13-C14-C15-C16
3	A	503	OLA	C4-C5-C6-C7
3	A	512	OLA	C4-C5-C6-C7
2	C	905	LFA	C2-C3-C4-C5
3	B	1009	OLA	O2-C1-C2-C3
2	C	916	LFA	C12-C13-C14-C15
3	A	503	OLA	C6-C7-C8-C9
3	B	1014	OLA	O2-C1-C2-C3
3	B	1009	OLA	C1-C2-C3-C4
3	B	1009	OLA	C7-C8-C9-C10
3	B	1013	OLA	C7-C8-C9-C10
3	C	903	OLA	C7-C8-C9-C10
4	A	507	OLC	C7-C8-C9-C10
4	C	909	OLC	C4-C5-C6-C7
4	B	1018	OLC	C6-C7-C8-C9
3	B	1016	OLA	O2-C1-C2-C3
3	A	512	OLA	C9-C10-C11-C12
3	B	1006	OLA	C7-C8-C9-C10
3	B	1008	OLA	C7-C8-C9-C10
2	A	510	LFA	C13-C14-C15-C16
2	C	917	LFA	C13-C14-C15-C16
2	B	1005	LFA	C3-C4-C5-C6
4	C	913	OLC	C7-C8-C9-C10
3	B	1009	OLA	O1-C1-C2-C3
3	B	1014	OLA	O1-C1-C2-C3
3	B	1016	OLA	O1-C1-C2-C3
3	C	903	OLA	C2-C3-C4-C5
2	B	1007	LFA	C2-C3-C4-C5
2	B	1004	LFA	C5-C6-C7-C8
3	B	1014	OLA	C7-C8-C9-C10
4	C	909	OLC	O20-C1-C2-C3
4	A	507	OLC	C2-C3-C4-C5
3	C	903	OLA	O1-C1-C2-C3
2	C	917	LFA	C12-C13-C14-C15
4	B	1017	OLC	O19-C1-C2-C3
4	B	1017	OLC	O20-C1-C2-C3
3	B	1014	OLA	C9-C10-C11-C12
2	C	916	LFA	C11-C12-C13-C14
2	C	920	LFA	C10-C11-C12-C13
3	C	903	OLA	O2-C1-C2-C3
3	A	508	OLA	O2-C1-C2-C3
2	A	515	LFA	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1008	OLA	C11-C10-C9-C8
2	A	504	LFA	C1-C2-C3-C4
2	B	1005	LFA	C7-C8-C9-C10
2	C	917	LFA	C5-C6-C7-C8
4	A	518	OLC	O20-C1-C2-C3

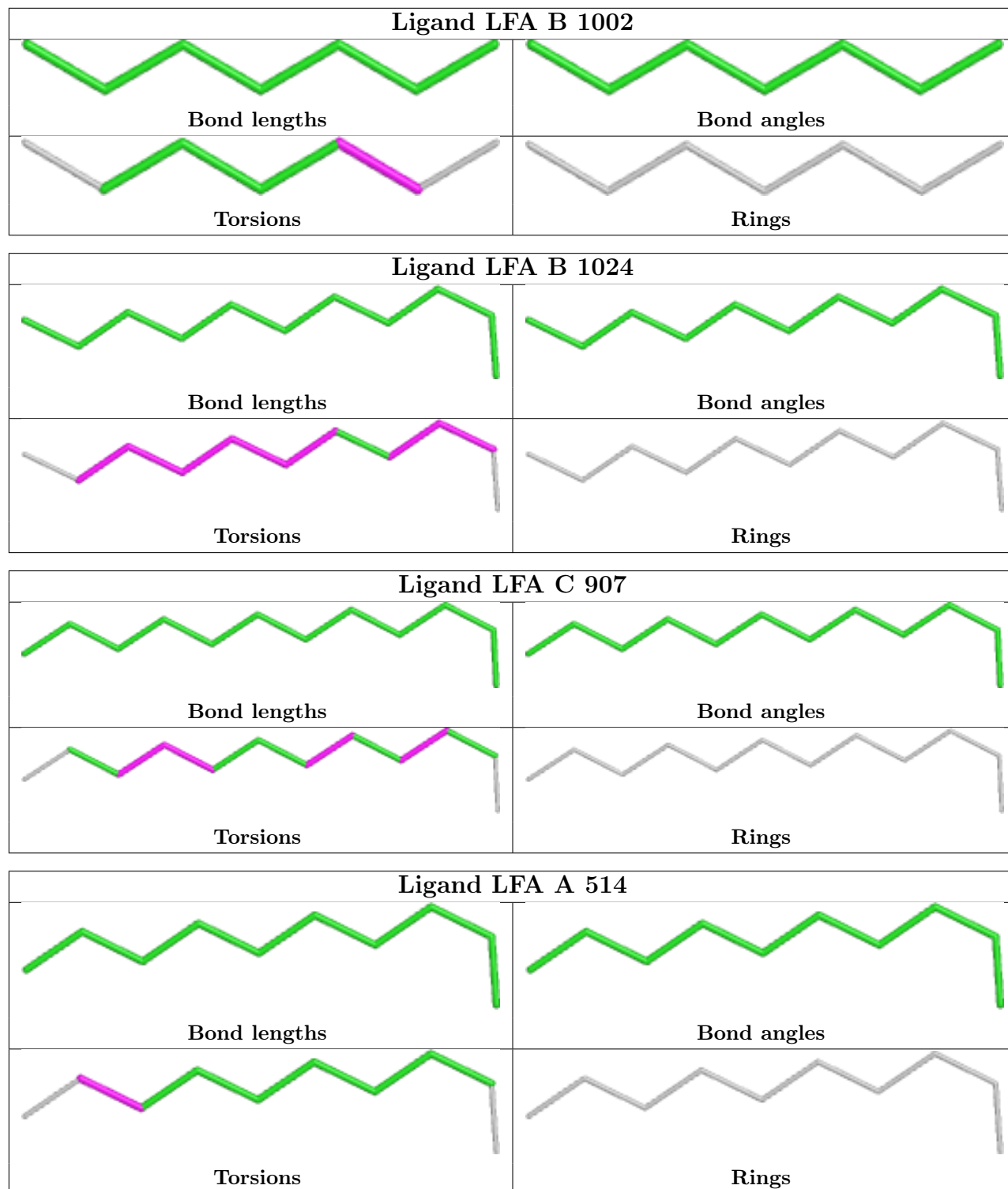
There are no ring outliers.

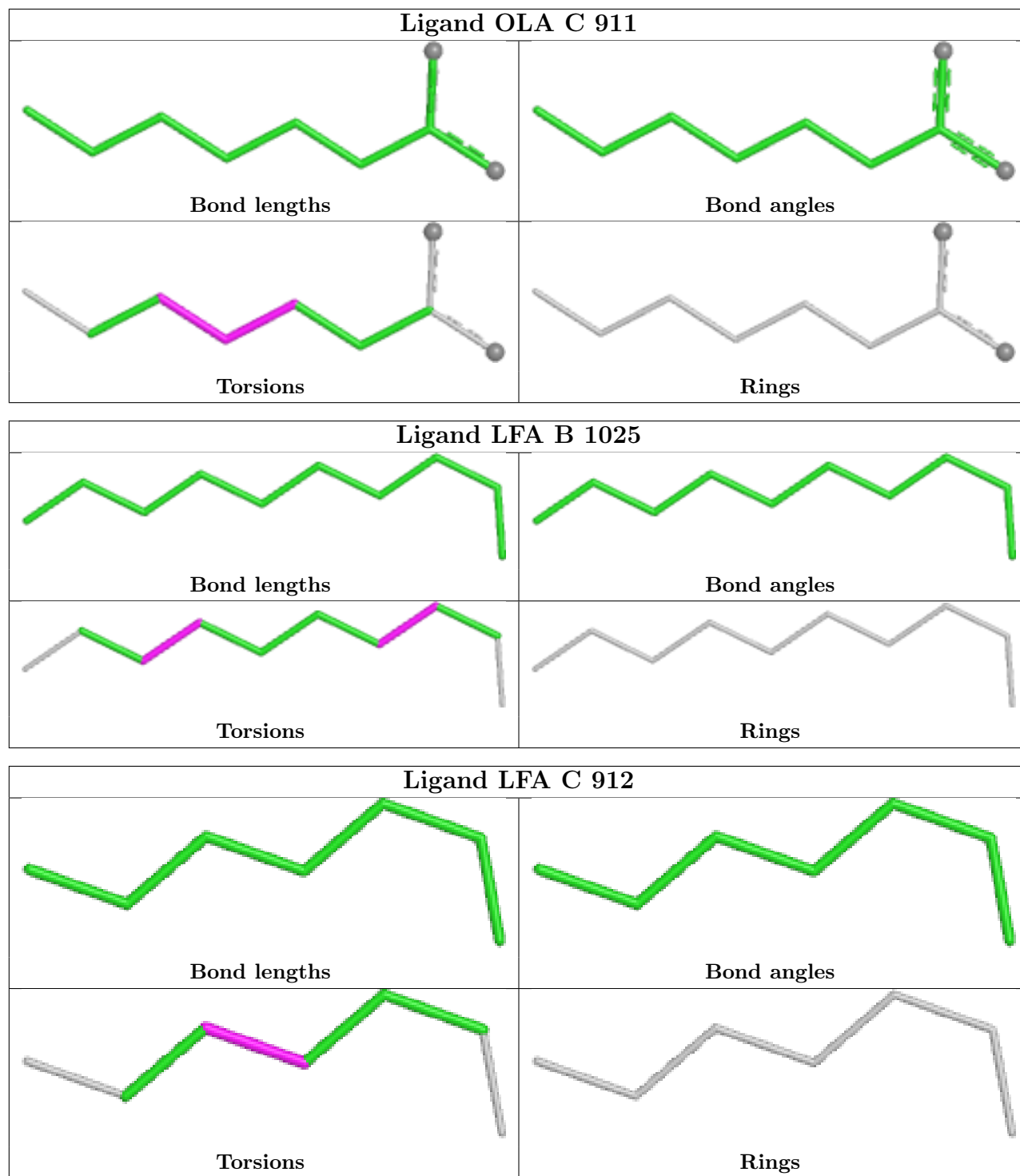
20 monomers are involved in 22 short contacts:

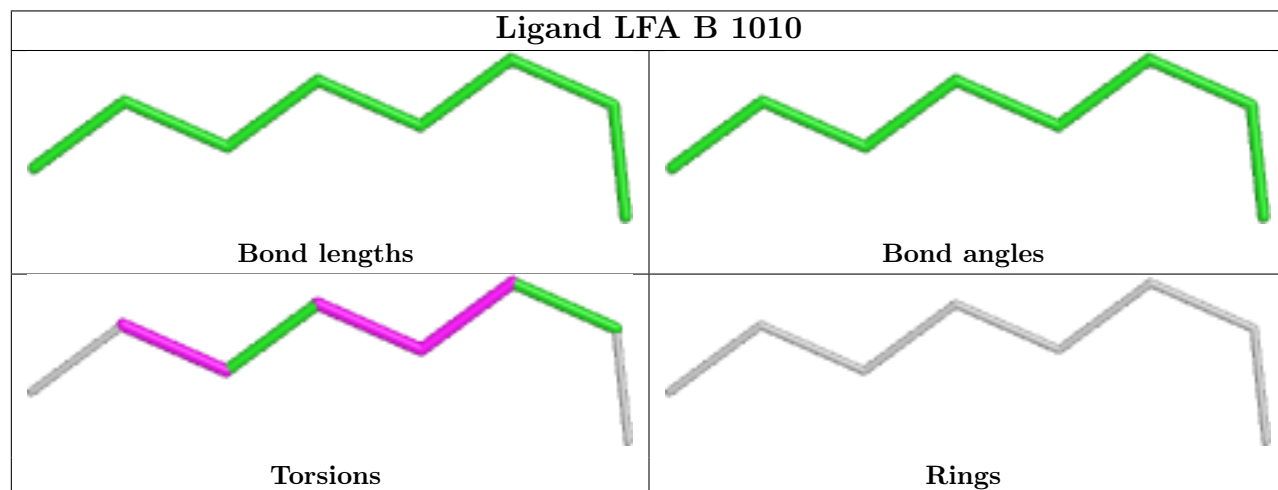
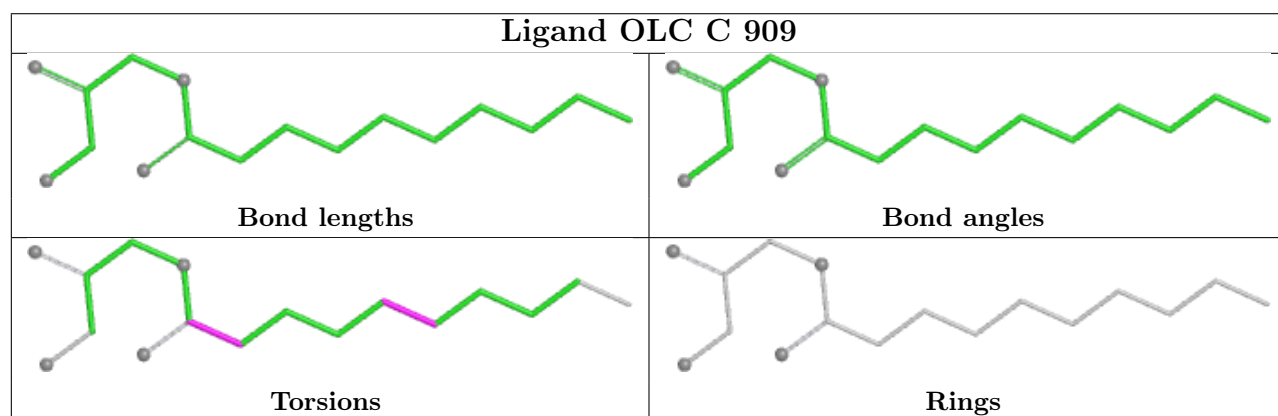
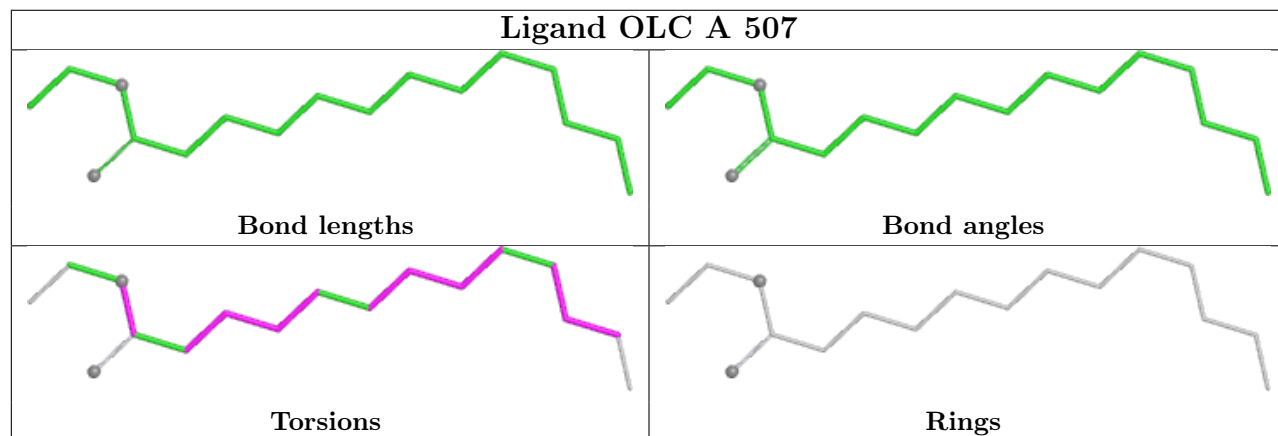
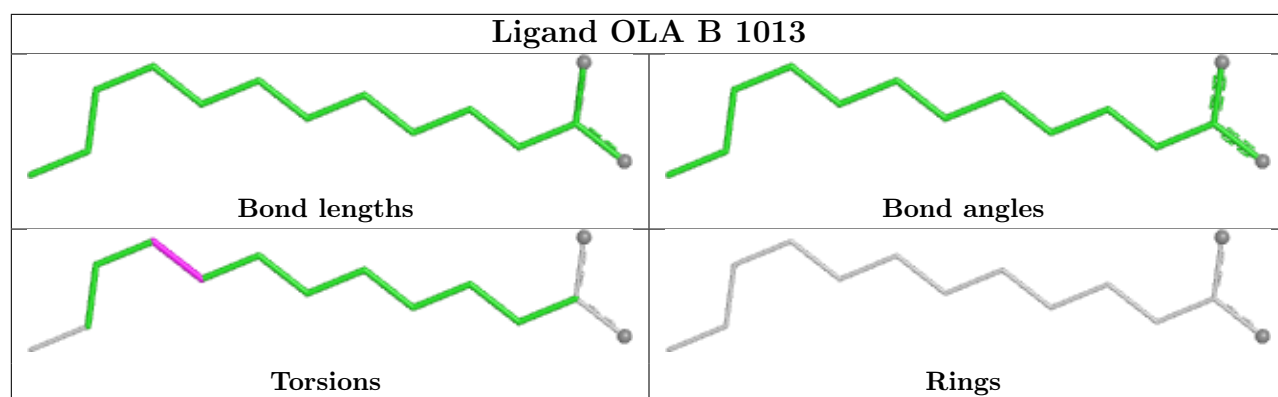
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1025	LFA	3	0
4	A	507	OLC	2	0
2	B	1001	LFA	1	0
4	B	1017	OLC	2	0
4	B	1018	OLC	2	0
3	B	1009	OLA	1	0
2	B	1021	LFA	1	0
2	B	1022	LFA	1	0
4	B	1015	OLC	1	0
2	B	1023	LFA	1	0
4	B	1029	OLC	1	0
3	B	1016	OLA	2	0
2	B	1026	LFA	1	0
3	A	509	OLA	1	0
2	B	1004	LFA	1	0
2	C	906	LFA	1	0
4	C	913	OLC	1	0
2	C	916	LFA	2	0
2	C	905	LFA	1	0
4	A	518	OLC	3	0

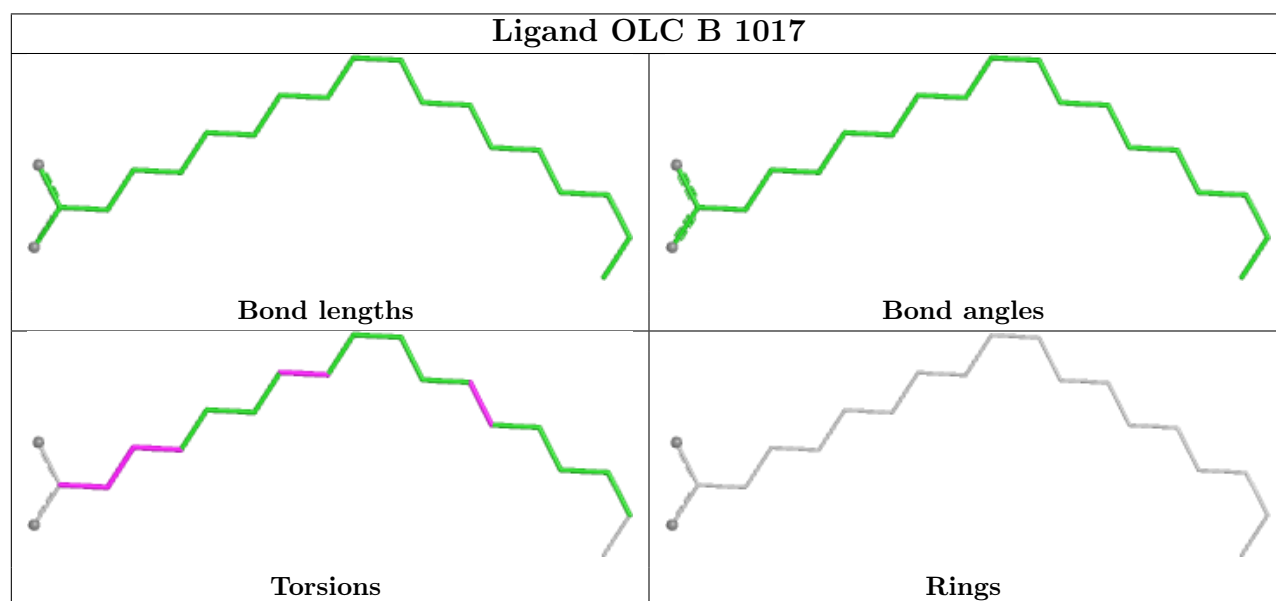
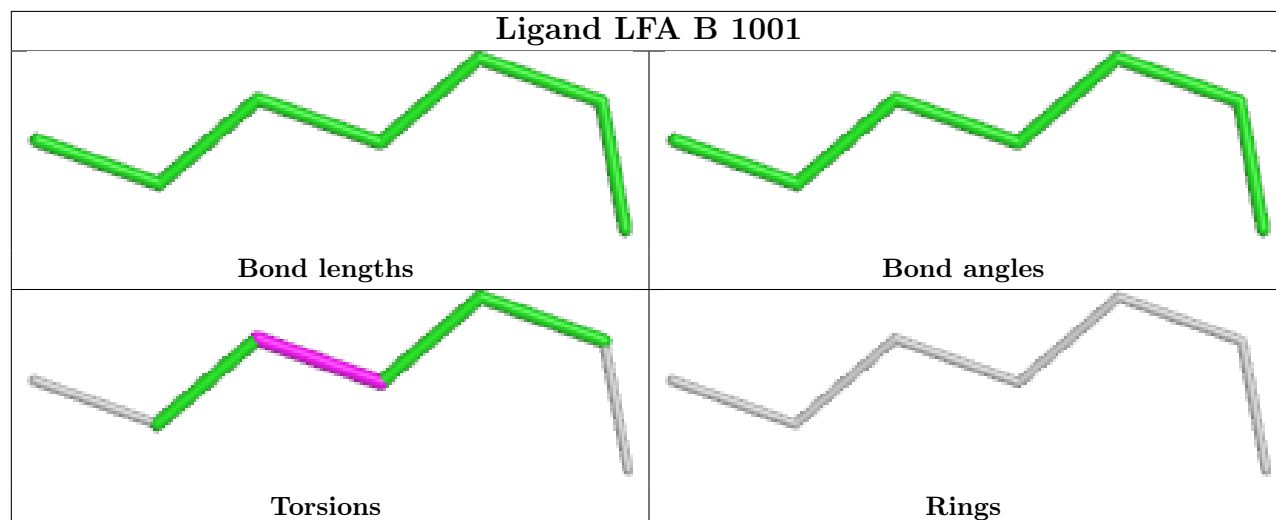
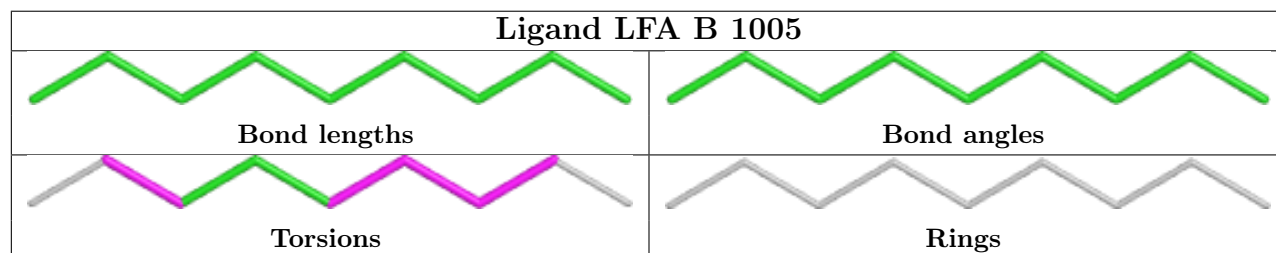
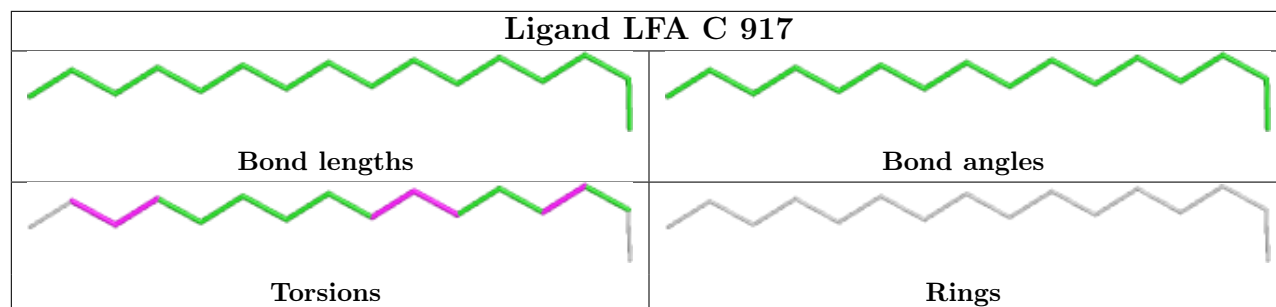
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

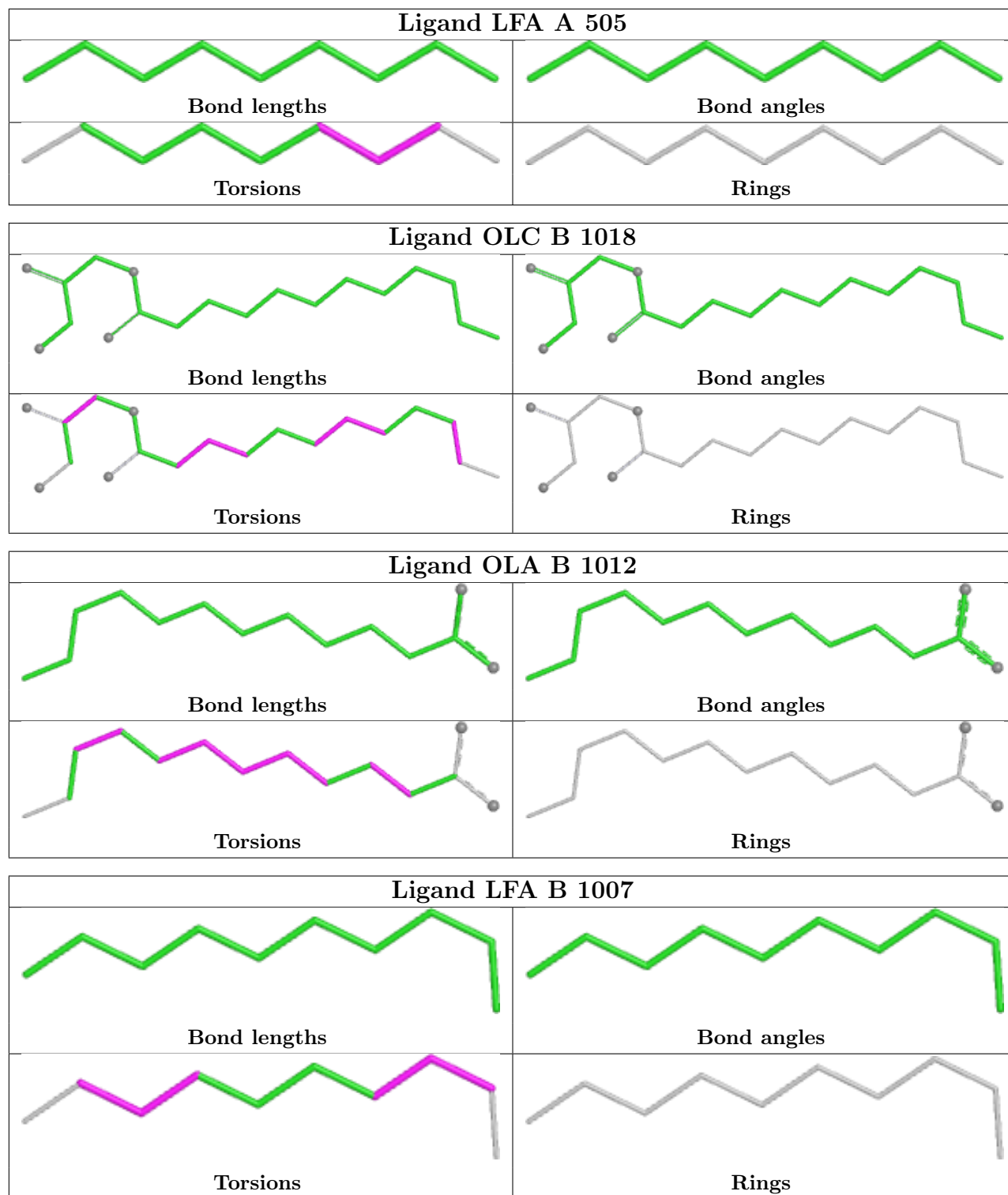
equivalents in the CSD to analyse the geometry.

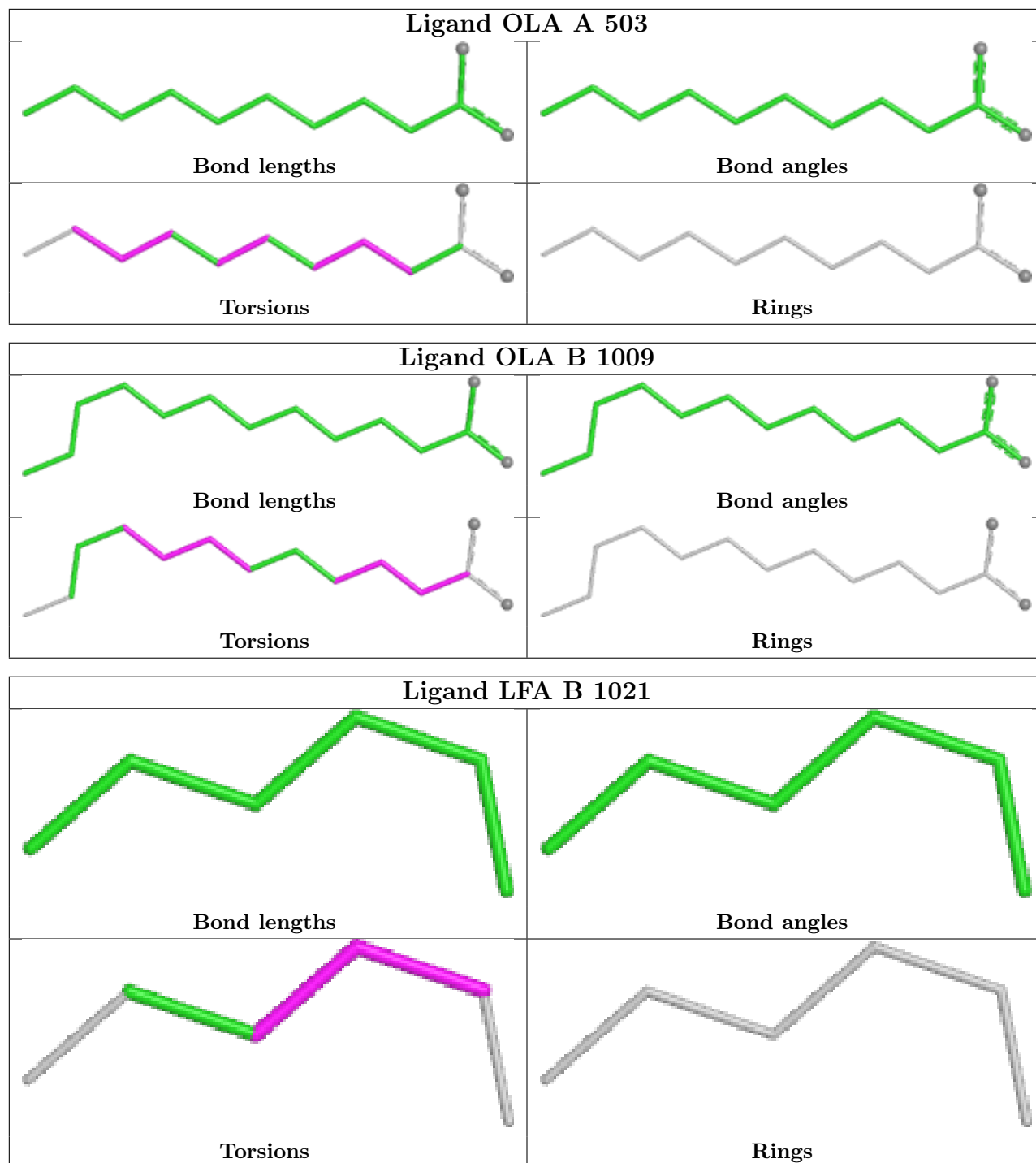


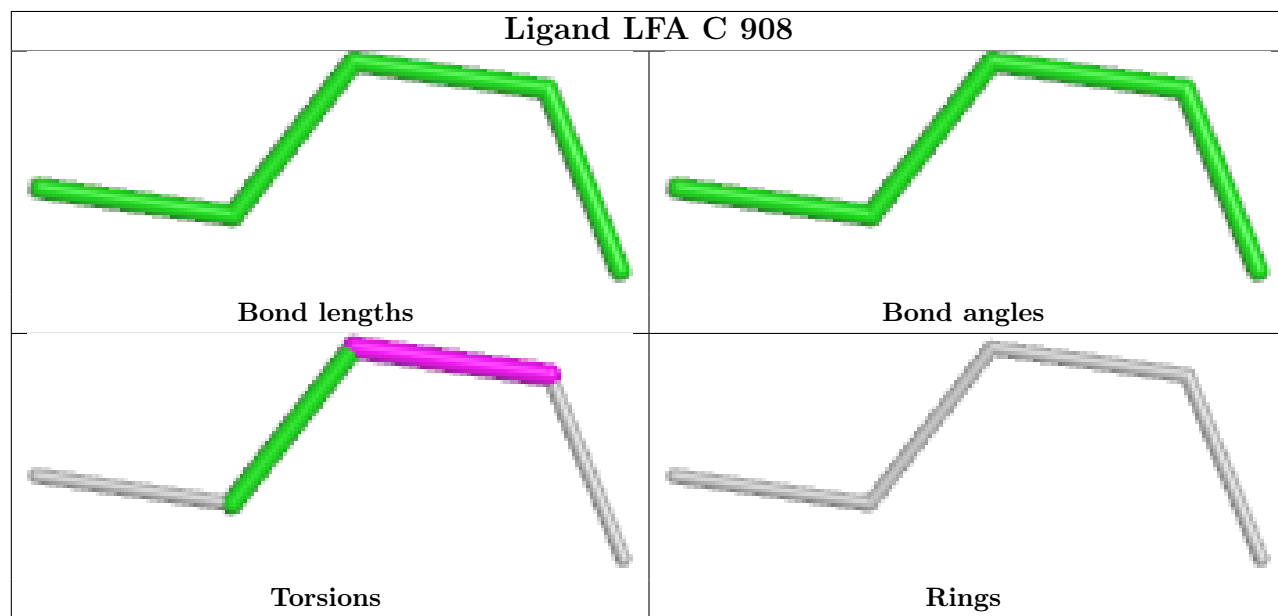
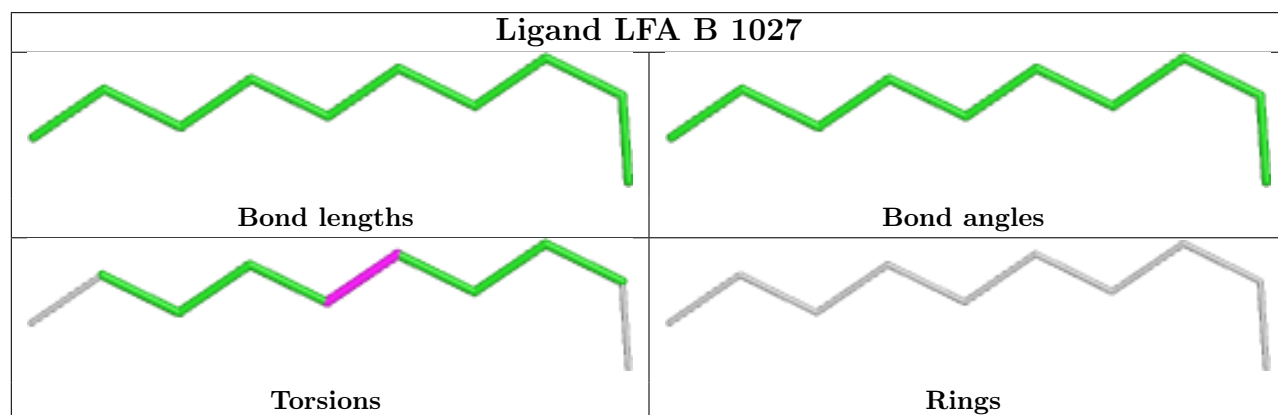
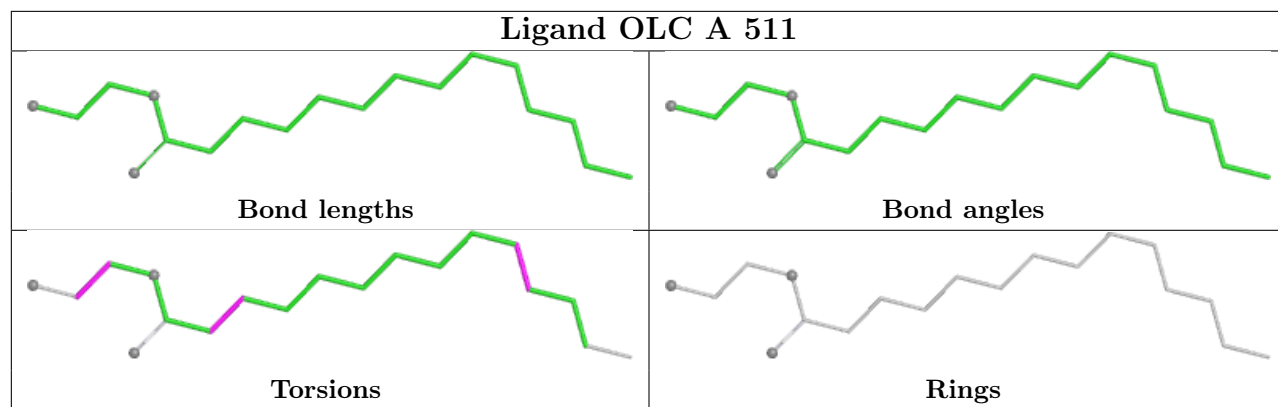


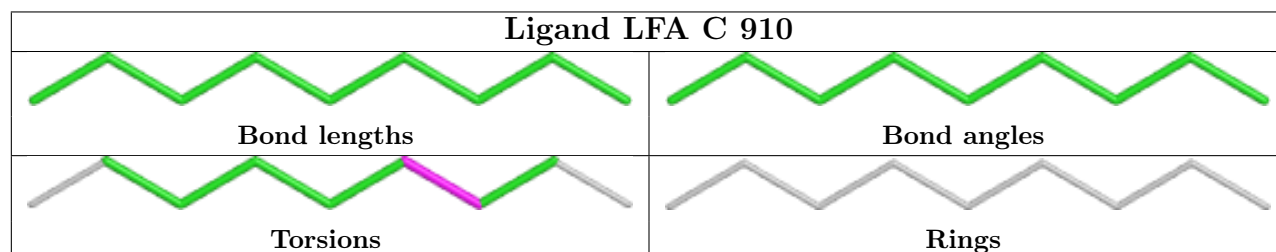
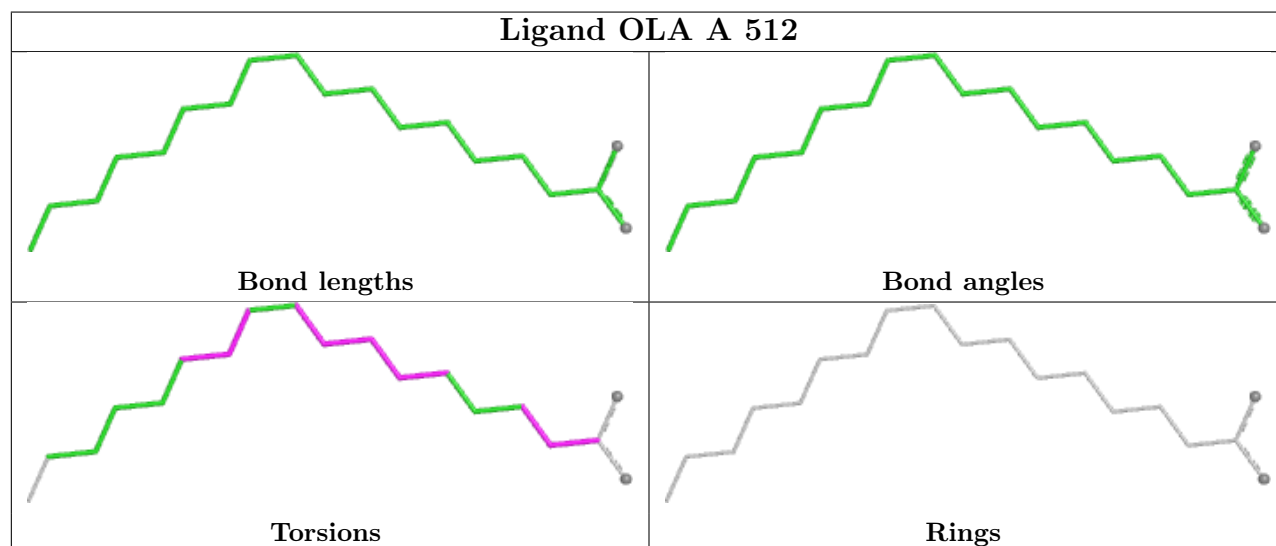
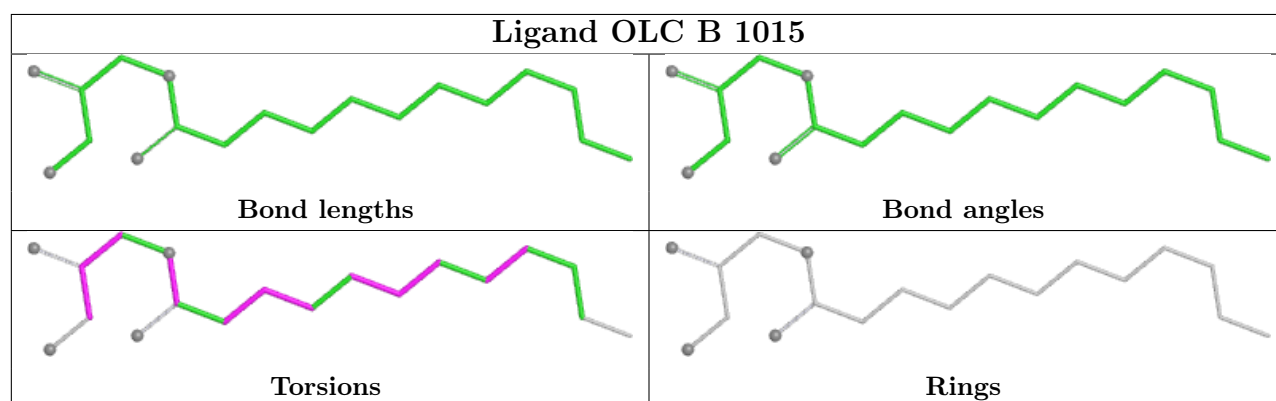
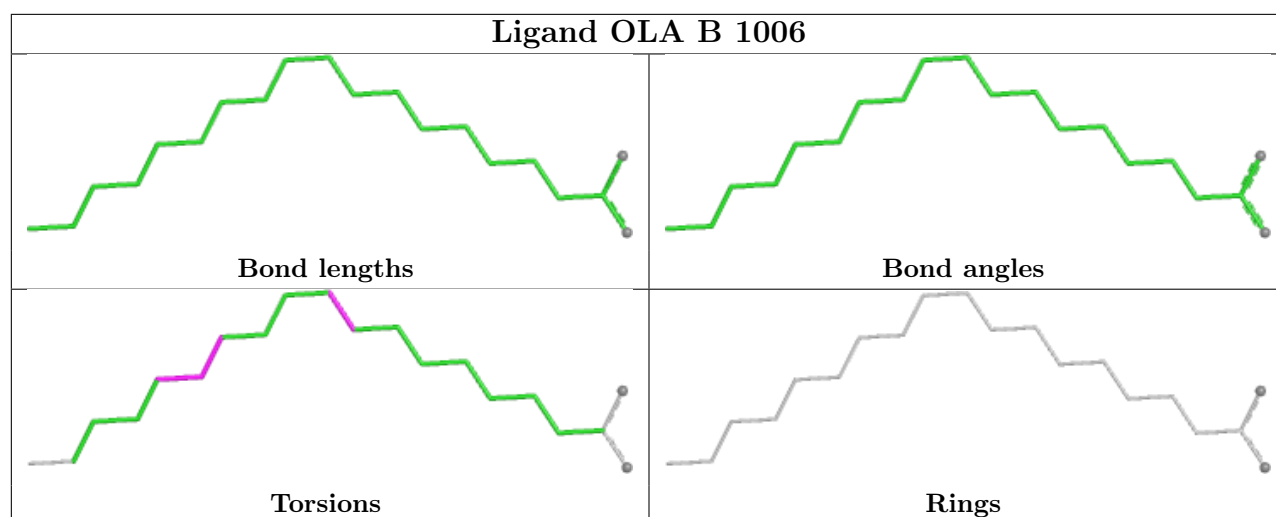


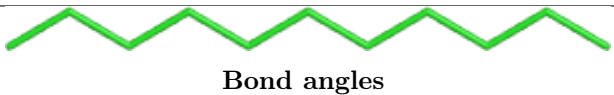


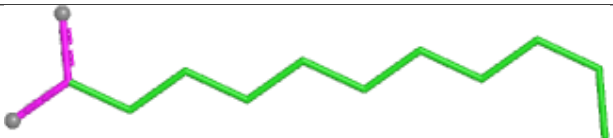
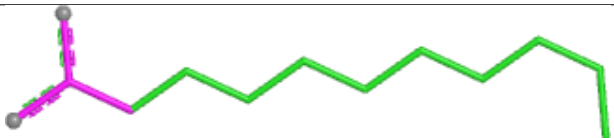
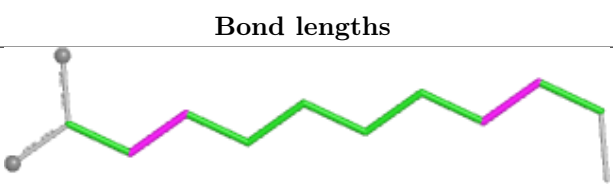
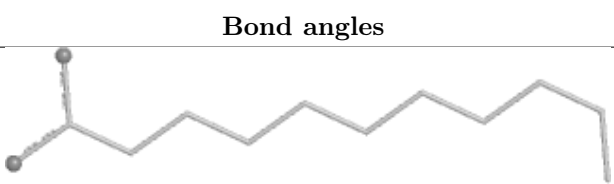


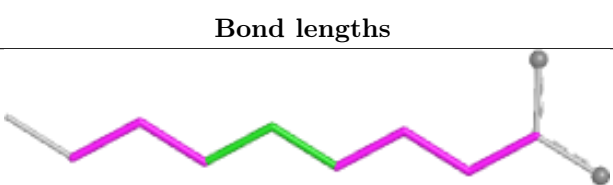
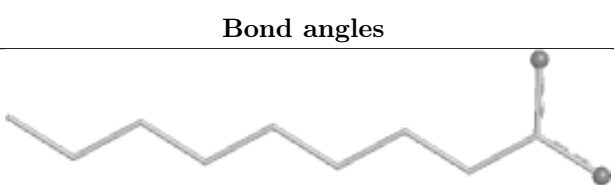


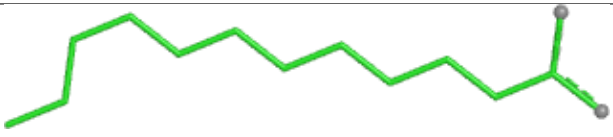
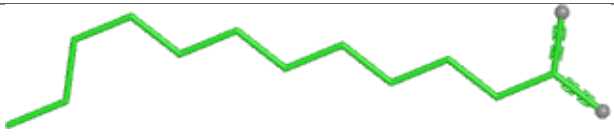
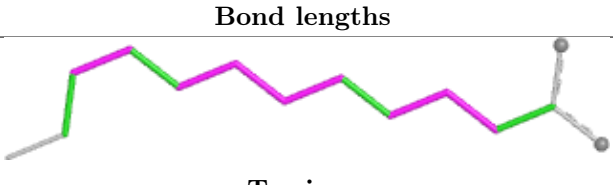
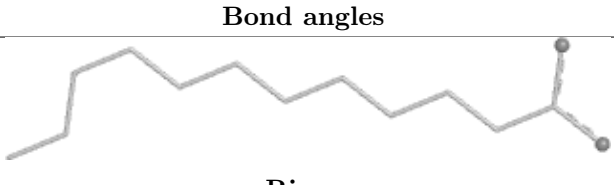


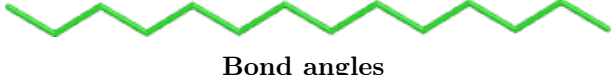


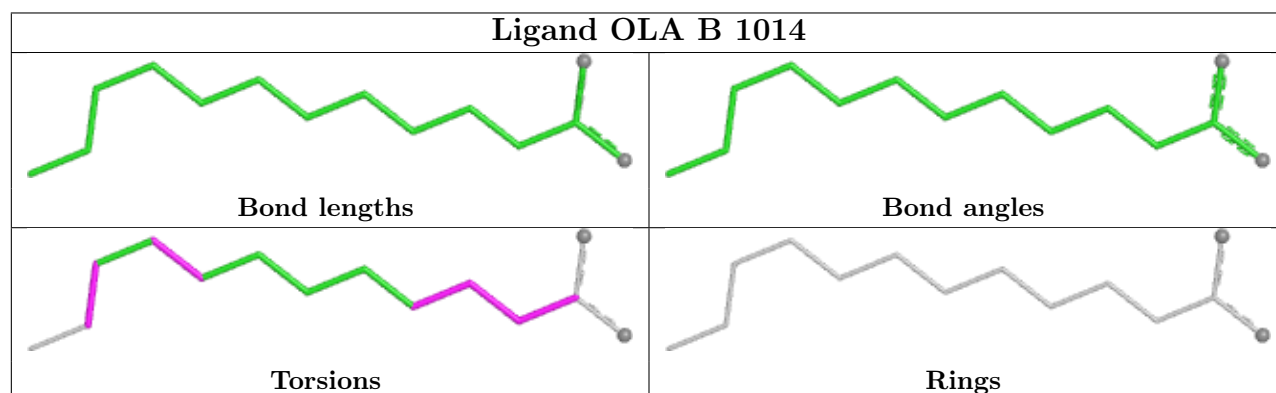
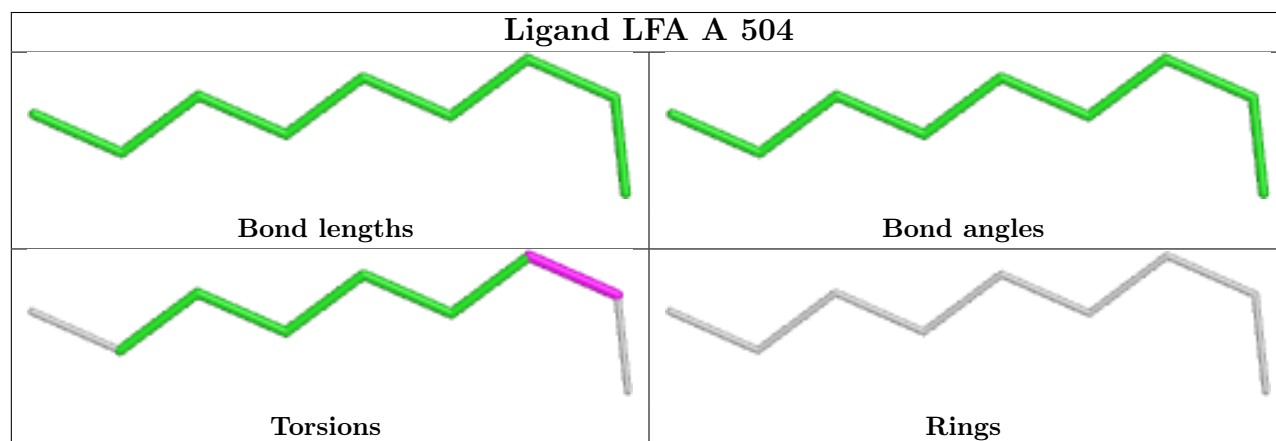
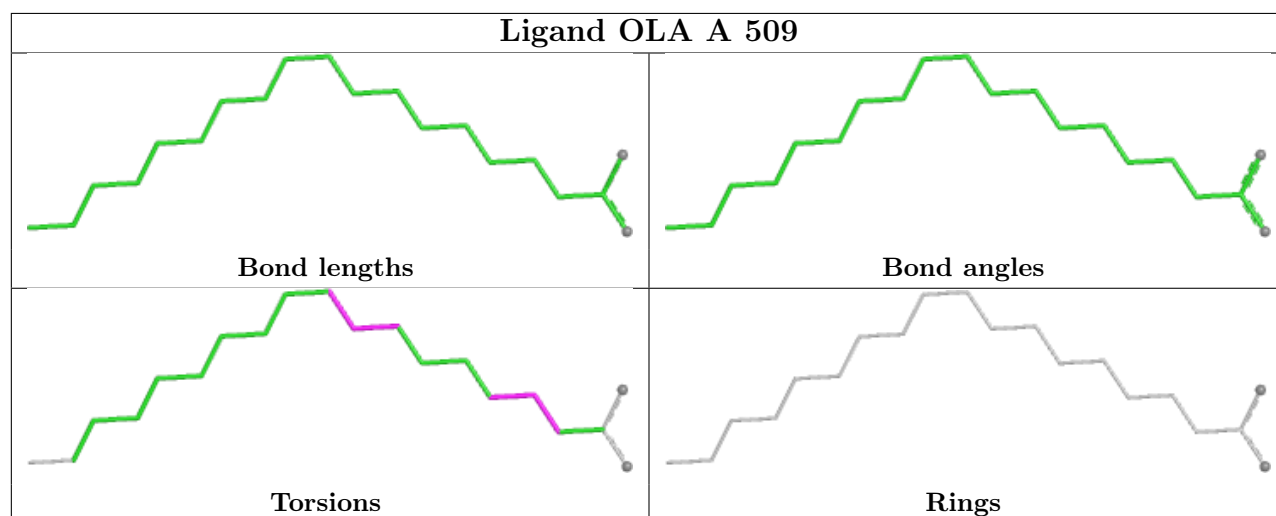
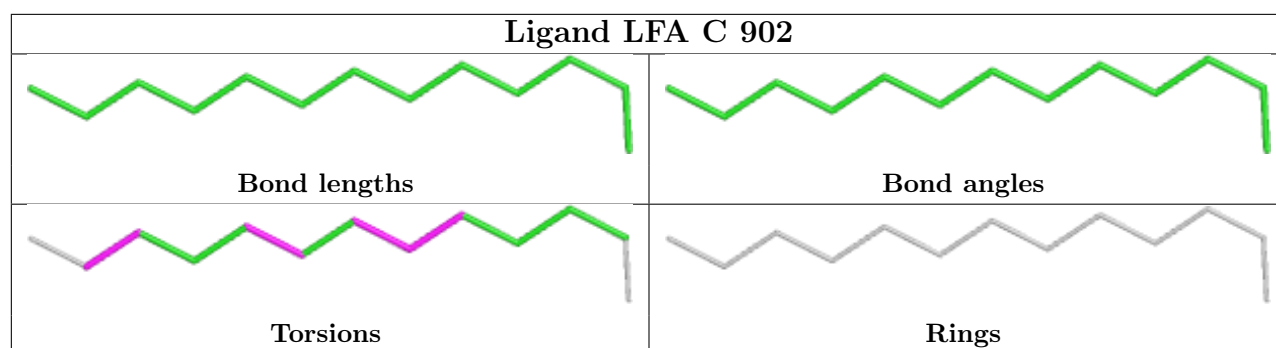
Ligand LFA C 915			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

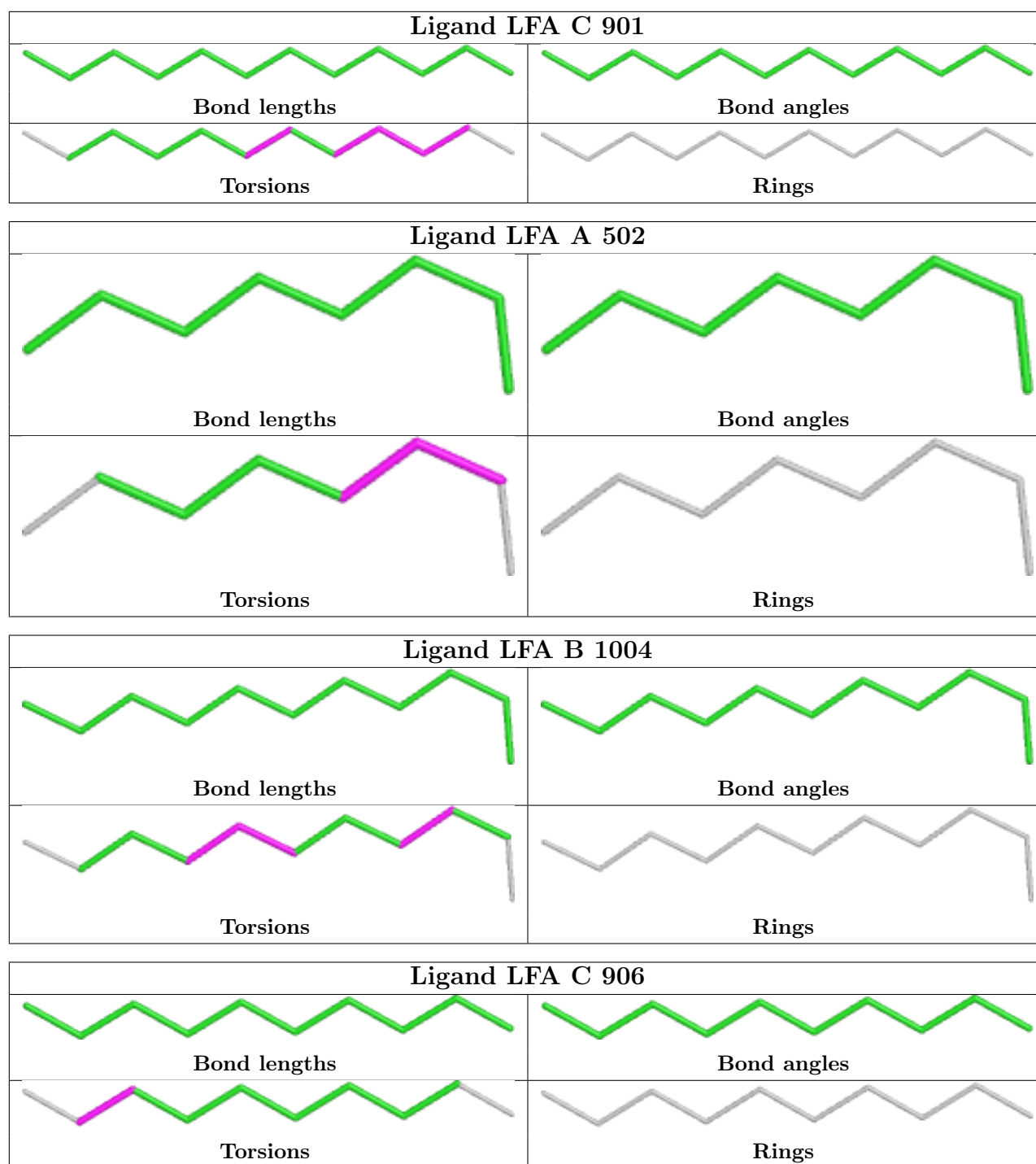
Ligand OLC B 1029			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

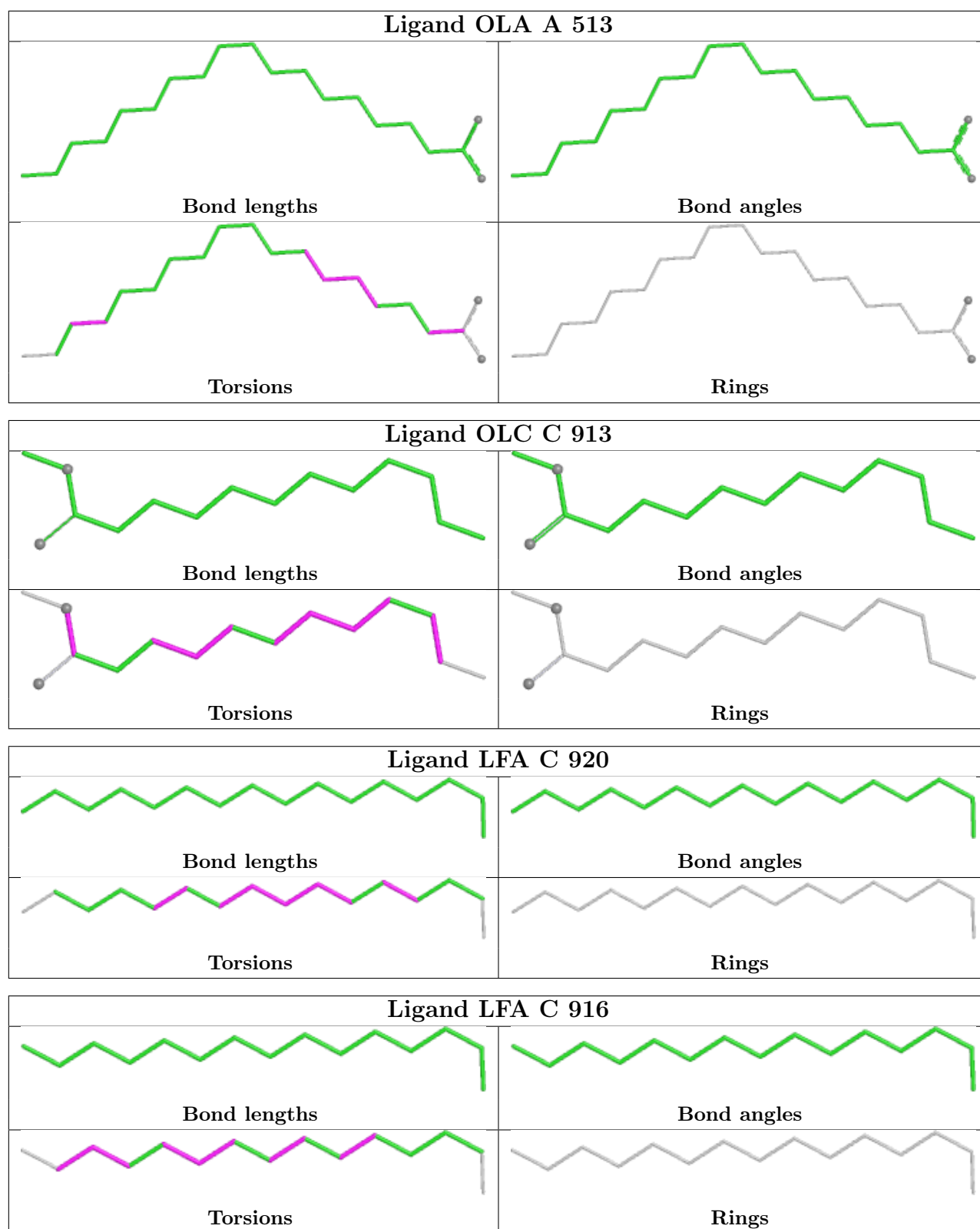
Ligand OLA B 1016			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

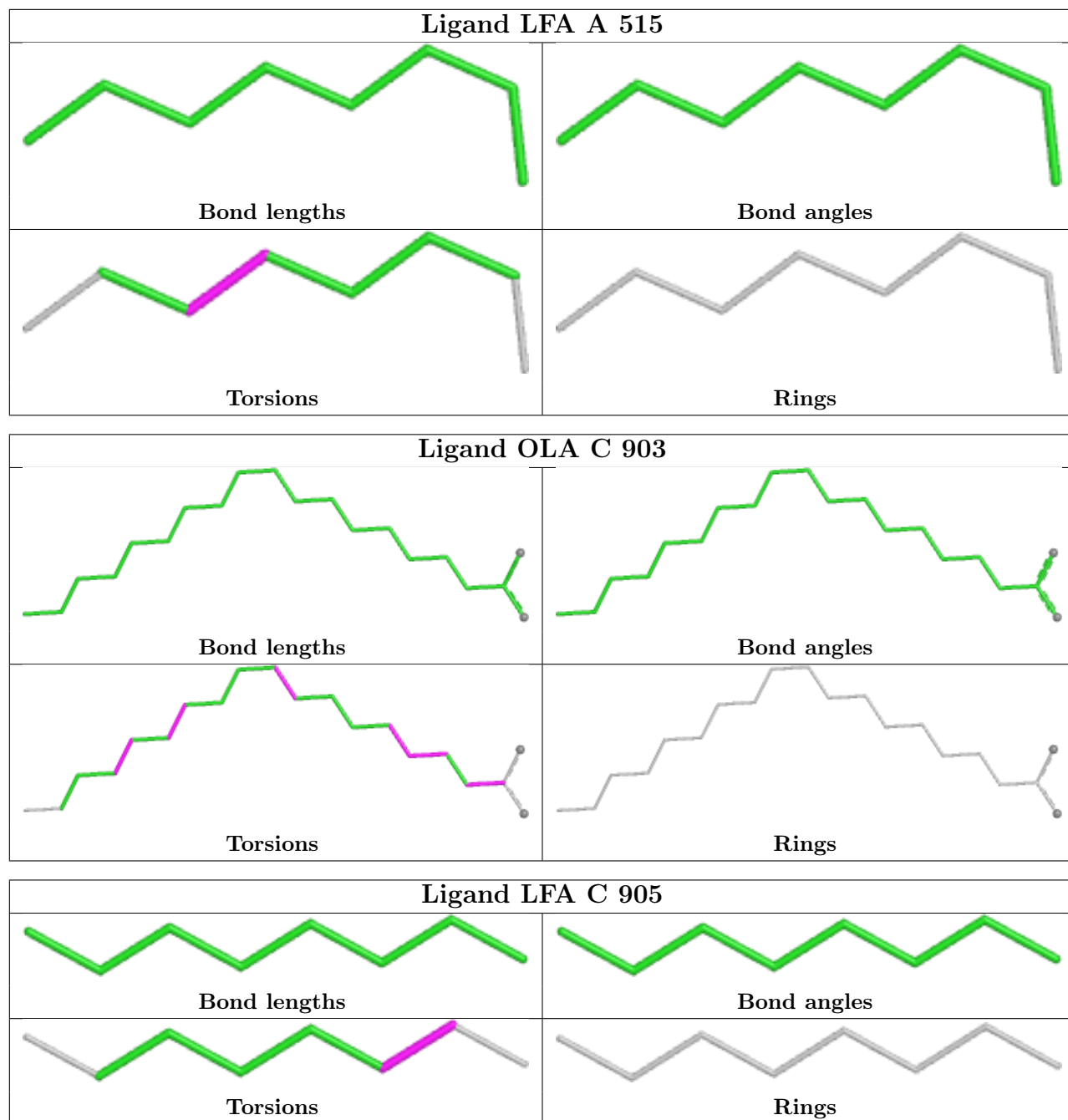
Ligand OLA A 506			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

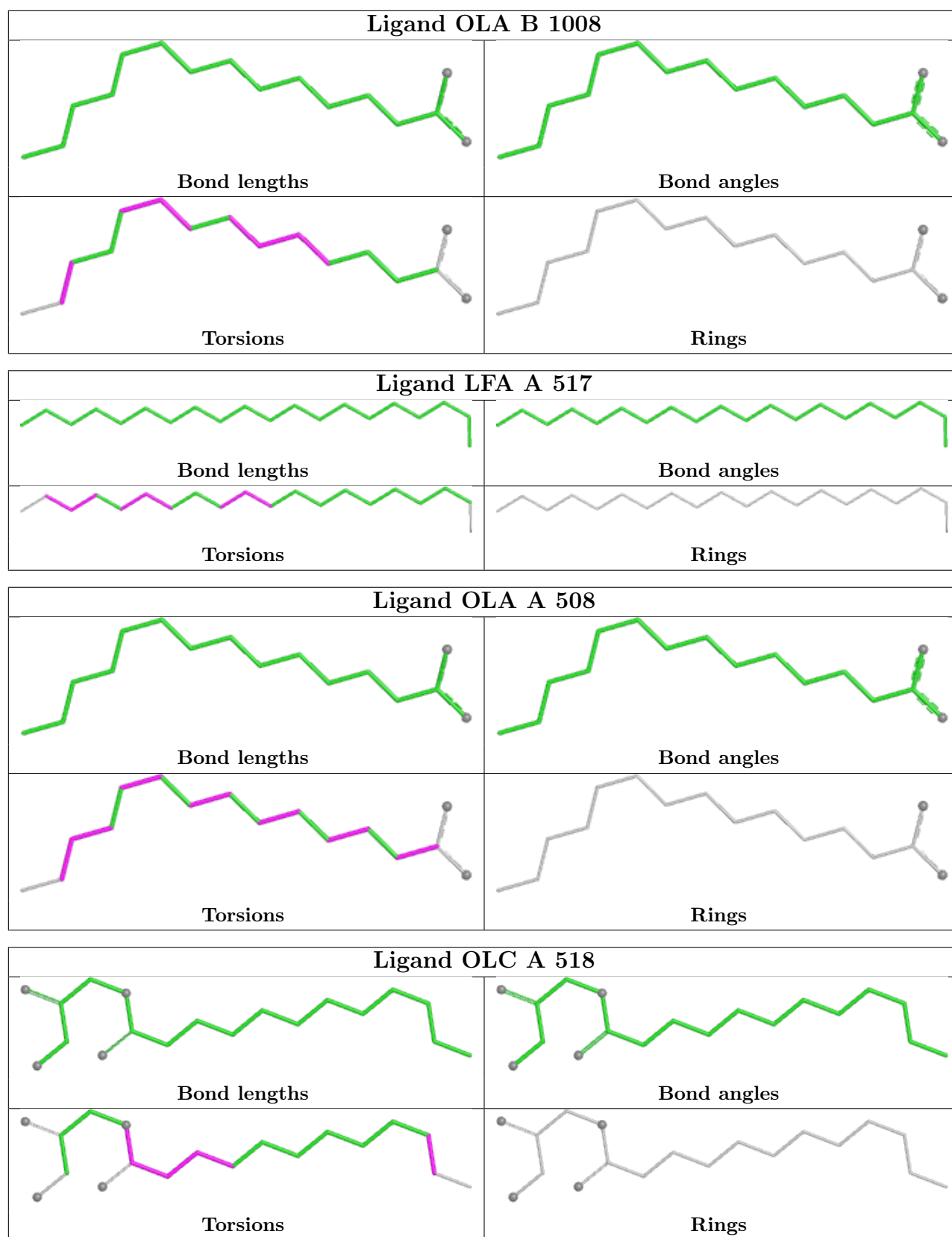
Ligand LFA B 1026			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

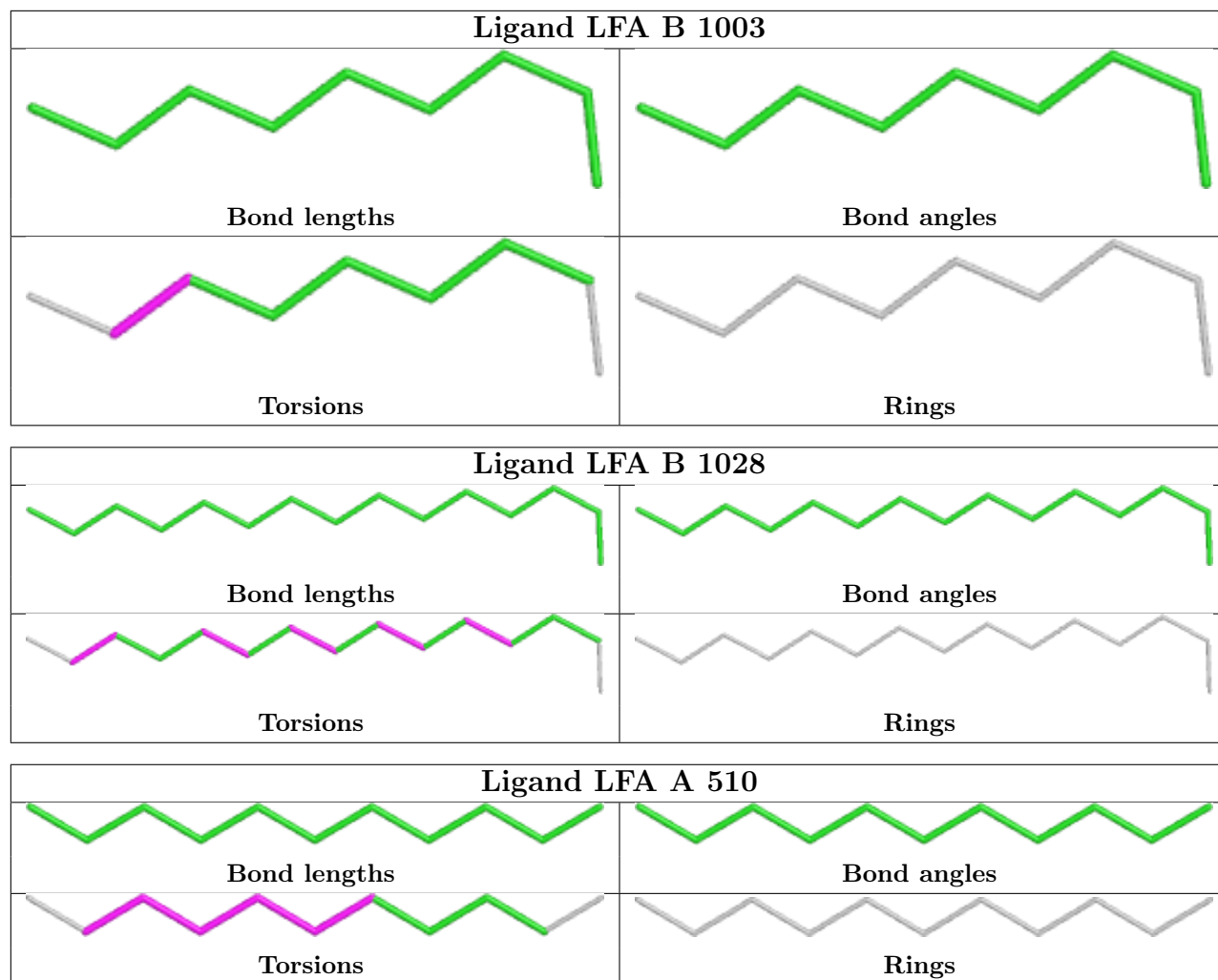












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	220/229 (96%)	0.82	13 (5%)	28	37	16, 28, 51, 74	1 (0%)
1	B	220/229 (96%)	0.87	22 (10%)	12	18	11, 30, 48, 86	2 (0%)
1	C	222/229 (96%)	0.90	20 (9%)	15	21	21, 30, 51, 114	0
All	All	662/687 (96%)	0.86	55 (8%)	17	24	11, 29, 50, 114	3 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	62	ASP	7.2
1	A	61	TYR	5.5
1	B	61	TYR	4.9
1	C	61	TYR	4.8
1	B	64	THR	4.5
1	B	59	PHE	4.3
1	A	64	THR	4.2
1	B	63	ASP	4.1
1	C	173	TRP	3.9
1	C	2	ILE	3.8
1	C	59	PHE	3.7
1	C	223	GLN	3.6
1	A	59	PHE	3.5
1	B	173[A]	TRP	3.5
1	A	66	ILE	3.5
1	C	60	GLN	3.5
1	C	66	ILE	3.3
1	B	66	ILE	3.2
1	C	63	ASP	3.2
1	A	223	GLN	3.0
1	A	173[A]	TRP	3.0
1	C	189	LEU	3.0
1	C	58	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	58	LEU	2.9
1	A	121	ILE	2.8
1	B	122	GLY	2.8
1	A	4	ILE	2.8
1	C	121	ILE	2.7
1	B	121	ILE	2.6
1	C	187	LEU	2.6
1	A	224	SER	2.6
1	A	221	LEU	2.5
1	A	60	GLN	2.5
1	B	197	LEU	2.4
1	A	197	LEU	2.4
1	B	206	SER	2.4
1	B	223	GLN	2.3
1	C	64	THR	2.3
1	B	11	PHE	2.2
1	C	224	SER	2.2
1	C	99	LEU	2.2
1	B	156	THR	2.2
1	C	221	LEU	2.2
1	B	55	GLY	2.1
1	C	25	LYS	2.1
1	B	91	PHE	2.1
1	C	160	ARG	2.1
1	B	192	GLU	2.1
1	B	193	LEU	2.1
1	B	151	ALA	2.1
1	A	2	ILE	2.0
1	B	221	LEU	2.0
1	B	53	ALA	2.0
1	C	206	SER	2.0
1	B	60	GLN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	FME	C	1	10/11	0.68	0.19	40,54,83,99	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	FME	A	1	10/11	0.72	0.16	45,59,77,90	0
1	FME	B	1	10/11	0.78	0.15	40,58,73,79	0
1	LYR	C	207	29/30	0.84	0.13	21,26,36,43	0
1	LYR	A	207	29/30	0.85	0.12	23,28,38,43	0
1	LYR	B	207	29/30	0.88	0.11	20,24,36,39	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
5	PO4	C	914	5/5	0.39	0.15	97,98,107,112	0
2	LFA	C	910	9/20	0.46	0.21	47,57,66,68	0
2	LFA	B	1027	10/20	0.52	0.19	56,61,67,68	0
4	OLC	A	518	19/25	0.57	0.28	58,84,101,102	0
2	LFA	B	1004	11/20	0.57	0.21	44,48,50,51	0
4	OLC	B	1029	13/25	0.60	0.18	62,79,87,91	0
2	LFA	C	904	6/20	0.61	0.23	45,52,55,56	0
2	LFA	A	517	20/20	0.62	0.27	65,74,86,87	0
2	LFA	A	516	4/20	0.63	0.17	47,47,56,59	0
2	LFA	C	905	8/20	0.63	0.19	52,53,55,55	0
4	OLC	C	909	17/25	0.64	0.23	50,67,84,86	0
2	LFA	B	1019	6/20	0.64	0.20	49,60,62,66	0
3	OLA	A	508	16/20	0.65	0.20	59,77,82,84	0
2	LFA	C	901	12/20	0.66	0.16	40,47,54,57	0
2	LFA	B	1023	10/20	0.66	0.18	65,72,73,75	0
2	LFA	A	515	8/20	0.66	0.17	47,58,64,65	0
2	LFA	B	1024	11/20	0.67	0.17	49,61,77,78	0
3	OLA	C	911	9/20	0.67	0.21	55,72,76,78	0
2	LFA	C	919	7/20	0.67	0.17	56,59,64,65	0
2	LFA	C	912	7/20	0.68	0.25	40,48,62,63	0
2	LFA	C	915	11/20	0.68	0.16	43,47,50,50	0
2	LFA	C	917	16/20	0.68	0.25	56,60,63,67	0
4	OLC	A	511	19/25	0.68	0.20	50,62,72,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LFA	A	510	11/20	0.69	0.14	43,48,58,59	0
3	OLA	A	513	20/20	0.70	0.21	50,62,84,91	0
3	OLA	B	1016	11/20	0.70	0.20	59,63,85,92	0
2	LFA	B	1001	7/20	0.71	0.16	43,43,51,52	0
2	LFA	C	902	13/20	0.71	0.23	63,70,78,80	0
2	LFA	B	1005	9/20	0.71	0.17	41,46,57,58	0
4	OLC	B	1018	19/25	0.72	0.20	57,76,91,99	0
2	LFA	B	1003	9/20	0.72	0.13	39,45,47,50	0
2	LFA	B	1020	11/20	0.73	0.17	56,63,74,76	0
2	LFA	B	1025	10/20	0.73	0.20	51,56,64,65	0
3	OLA	B	1008	16/20	0.73	0.15	38,42,53,54	0
3	OLA	B	1009	14/20	0.73	0.16	44,52,60,68	0
2	LFA	A	514	10/20	0.74	0.18	35,37,53,58	0
2	LFA	C	916	15/20	0.74	0.19	60,62,70,71	0
2	LFA	B	1028	15/20	0.74	0.23	47,59,78,79	0
4	OLC	B	1017	20/25	0.74	0.18	45,81,93,93	0
3	OLA	A	512	19/20	0.75	0.21	49,58,74,75	0
2	LFA	A	501	6/20	0.75	0.15	40,43,44,45	0
4	OLC	C	913	15/25	0.75	0.17	44,55,69,73	0
3	OLA	B	1013	14/20	0.75	0.16	52,62,73,75	0
3	OLA	B	1012	14/20	0.76	0.17	47,53,71,73	0
3	OLA	C	903	20/20	0.76	0.15	36,46,83,88	0
2	LFA	A	502	8/20	0.76	0.17	48,54,57,58	0
4	OLC	A	507	17/25	0.76	0.19	37,54,71,75	0
2	LFA	C	920	16/20	0.77	0.17	44,48,64,64	0
3	OLA	A	506	14/20	0.77	0.16	50,59,70,77	0
2	LFA	C	907	12/20	0.77	0.17	43,45,56,57	0
2	LFA	C	908	5/20	0.77	0.18	45,47,50,52	0
2	LFA	B	1022	8/20	0.77	0.16	51,54,57,61	0
2	LFA	C	918	6/20	0.77	0.22	63,63,64,65	0
2	LFA	B	1021	6/20	0.77	0.18	56,59,65,66	0
2	LFA	B	1026	14/20	0.78	0.17	57,71,76,76	0
3	OLA	A	509	20/20	0.78	0.15	41,49,65,67	0
4	OLC	B	1015	19/25	0.78	0.18	42,61,83,83	0
2	LFA	A	505	9/20	0.79	0.23	56,59,61,62	0
3	OLA	B	1014	14/20	0.79	0.17	49,58,73,75	0
3	OLA	A	503	12/20	0.79	0.12	47,54,63,63	0
2	LFA	B	1007	10/20	0.80	0.16	40,51,58,59	0
2	LFA	B	1010	8/20	0.80	0.17	53,55,57,58	0
2	LFA	B	1011	11/20	0.80	0.14	40,46,60,61	0
2	LFA	C	906	10/20	0.81	0.16	54,57,57,61	0
2	LFA	A	504	9/20	0.82	0.14	42,46,55,56	0

Continued on next page...

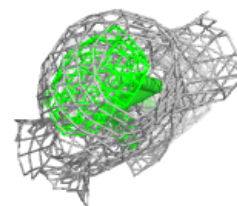
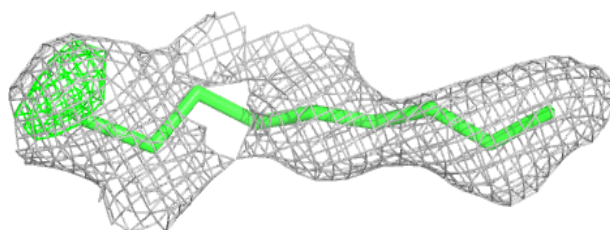
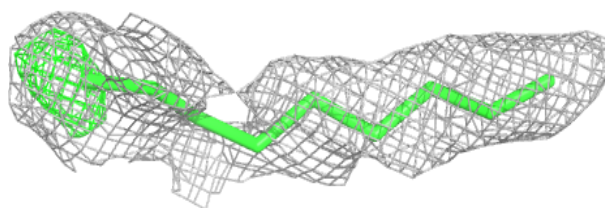
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OLA	B	1006	20/20	0.83	0.15	37,51,81,82	0
2	LFA	B	1002	7/20	0.86	0.13	39,40,43,52	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.

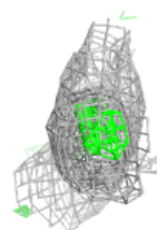
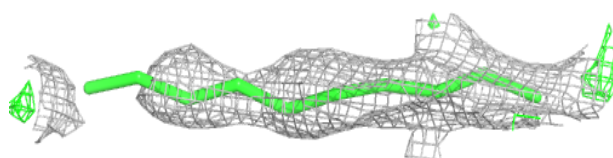
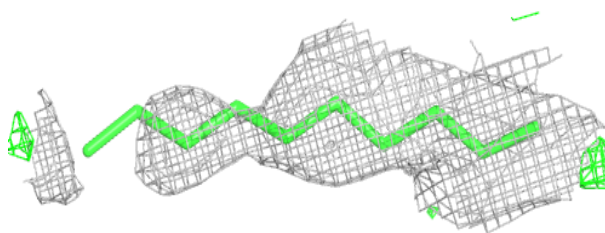
Electron density around LFA C 910:

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

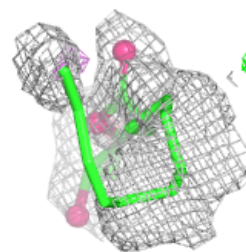
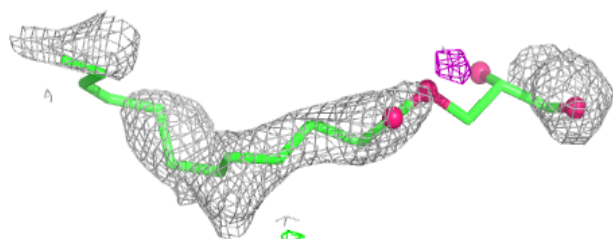
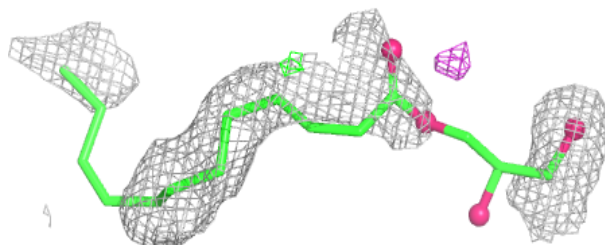


Electron density around LFA B 1027:

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

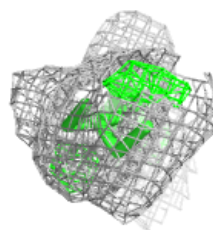
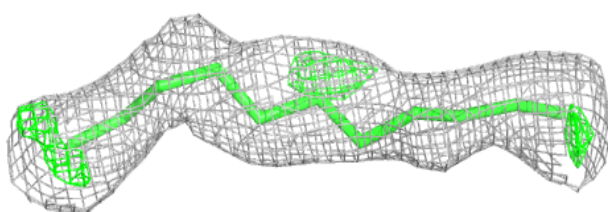
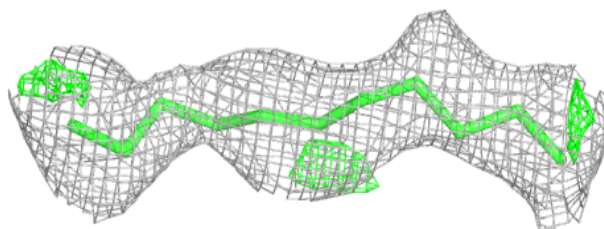
**Electron density around OLC A 518:**

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

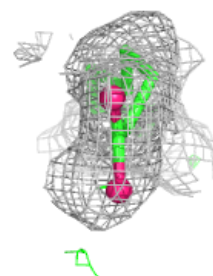
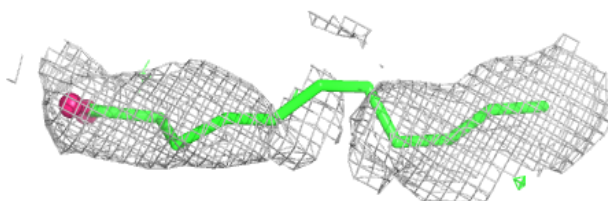
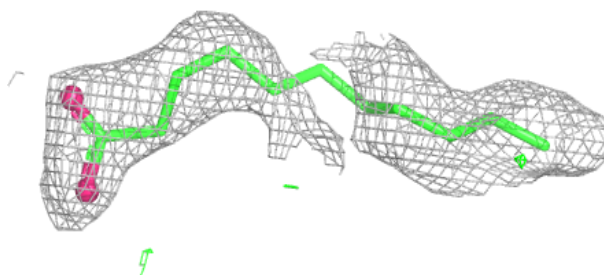


Electron density around LFA B 1004:

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

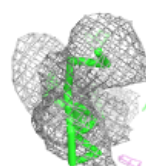
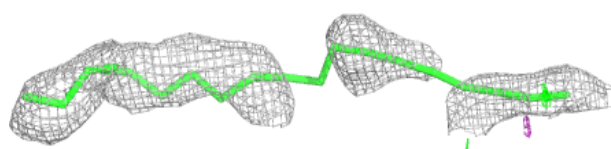
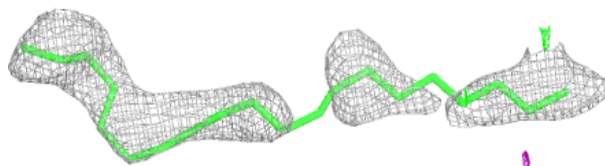
**Electron density around OLC B 1029:**

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

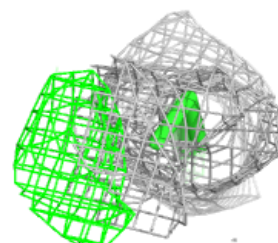
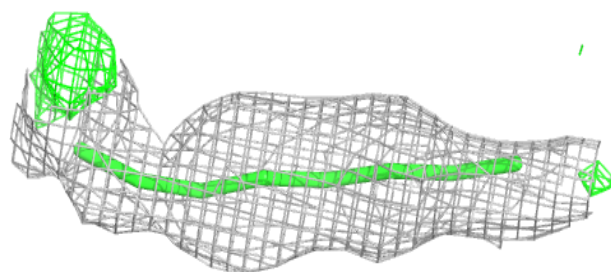
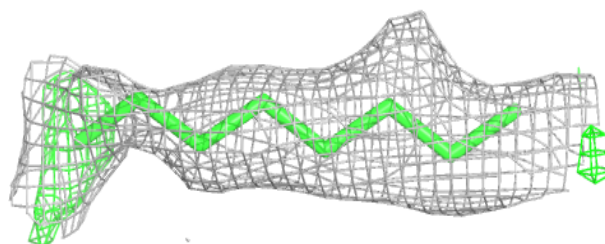


Electron density around LFA A 517:

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

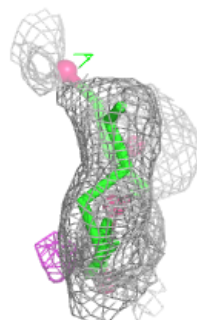
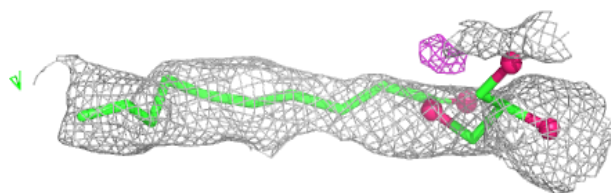
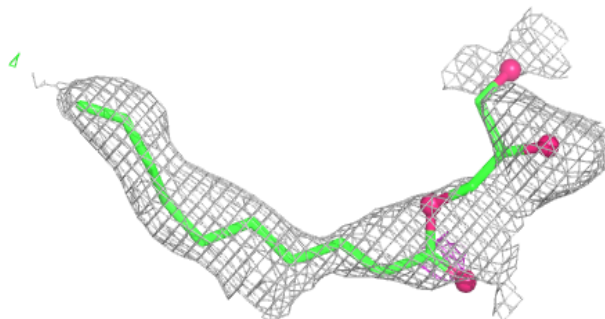
**Electron density around LFA C 905:**

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

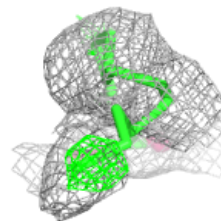
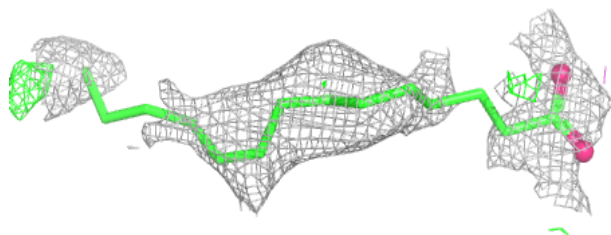
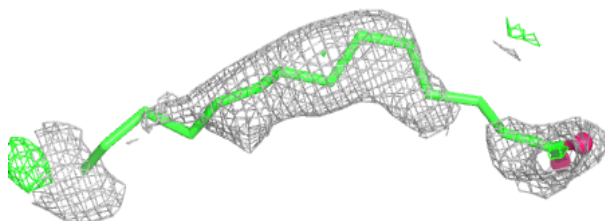


Electron density around OLC C 909:

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

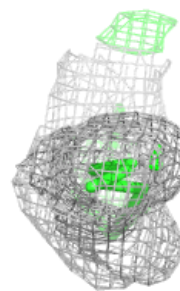
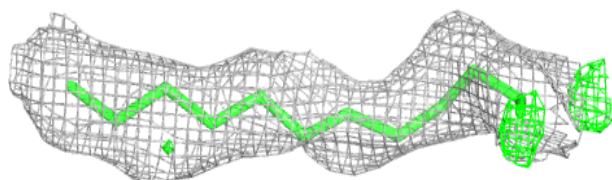
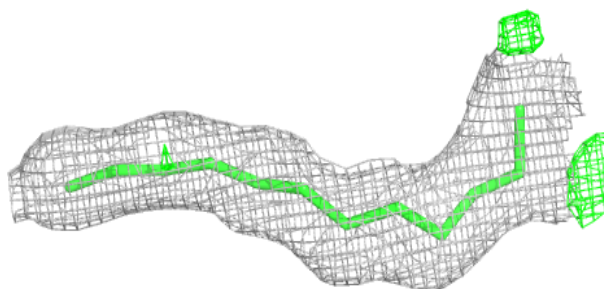
**Electron density around OLA A 508:**

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

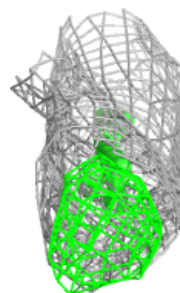
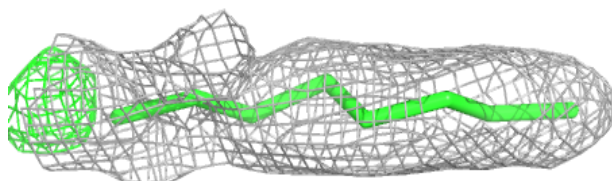
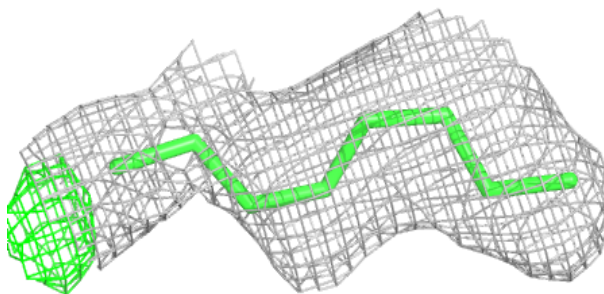


Electron density around LFA C 901:

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

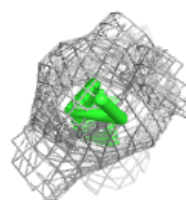
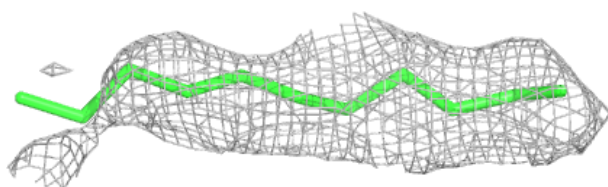
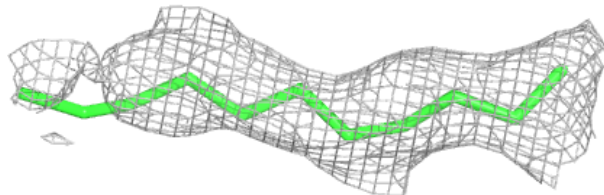
**Electron density around LFA A 515:**

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

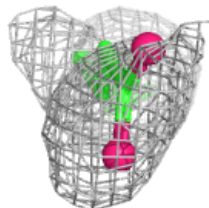
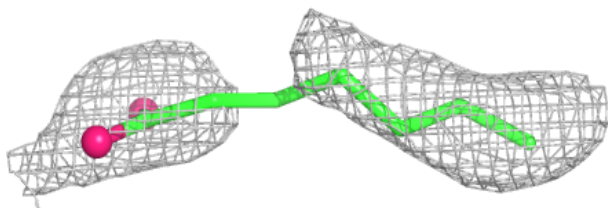
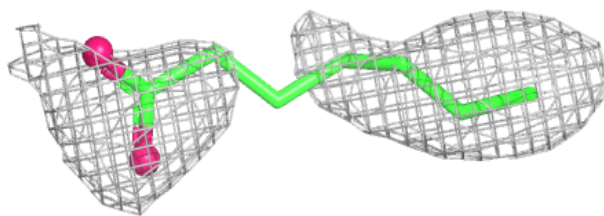


Electron density around LFA B 1024:

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

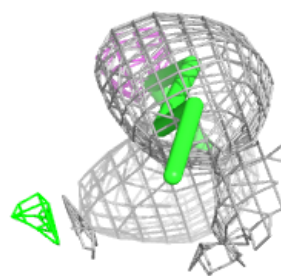
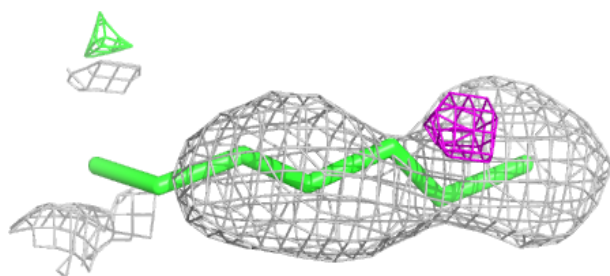
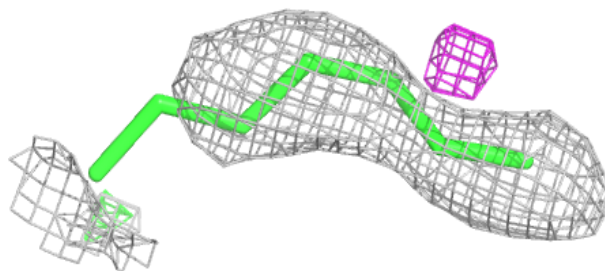
**Electron density around OLA C 911:**

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

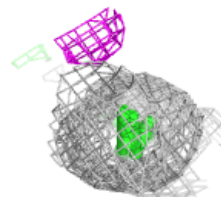
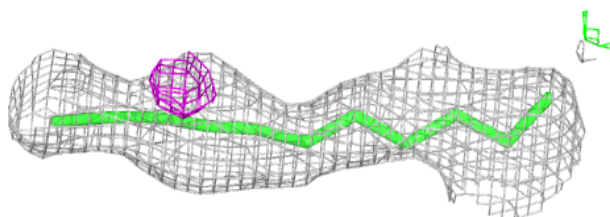
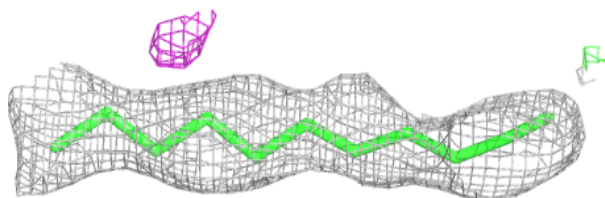


Electron density around LFA C 912:

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

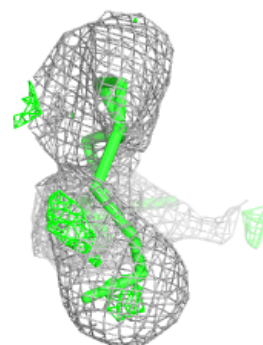
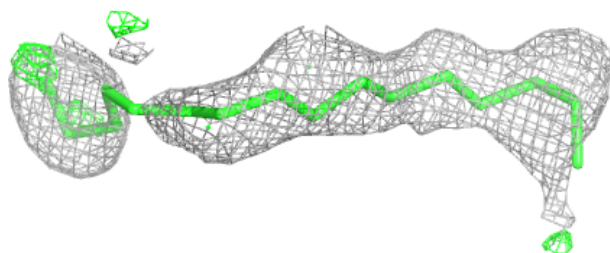
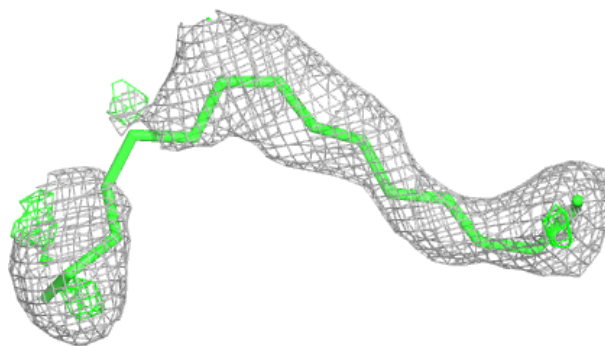
**Electron density around LFA C 915:**

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

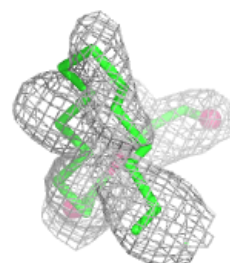
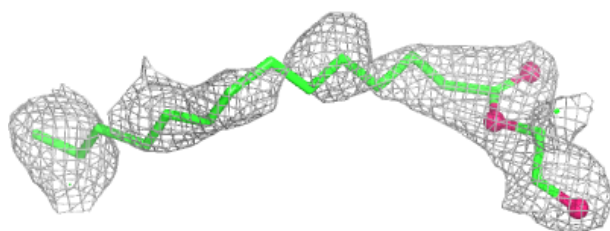
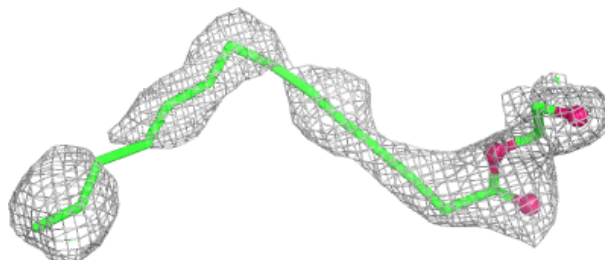


Electron density around LFA C 917:

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

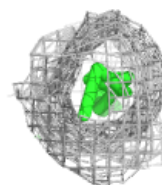
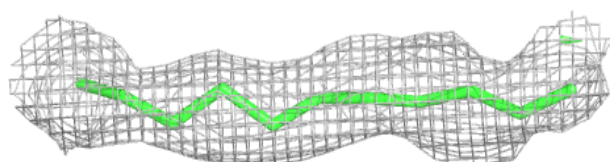
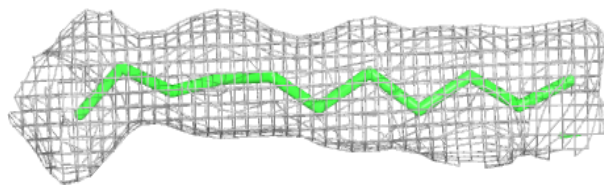
**Electron density around OLC A 511:**

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

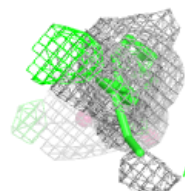
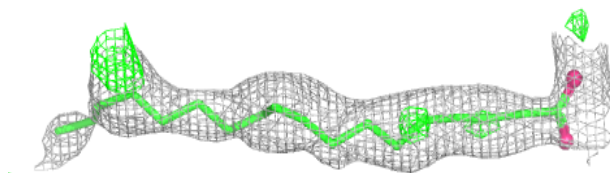
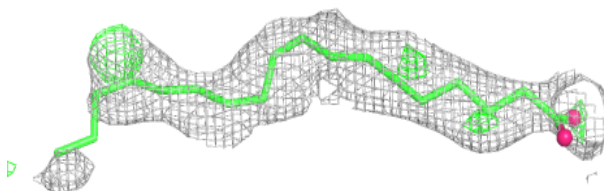


Electron density around LFA A 510:

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

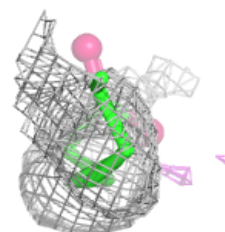
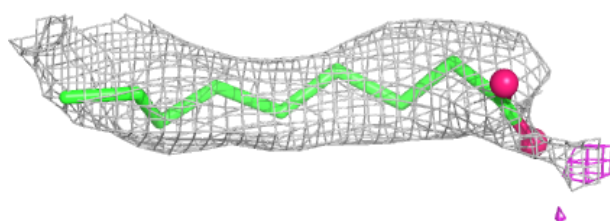
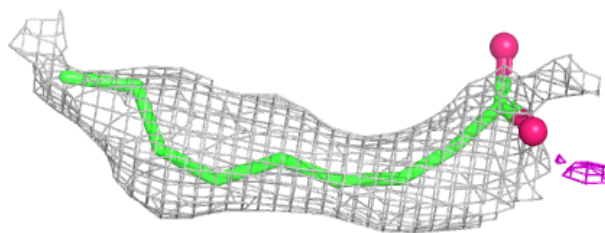
**Electron density around OLA A 513:**

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

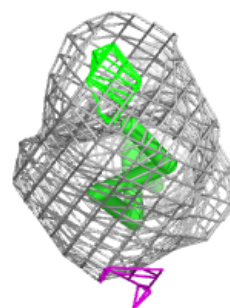
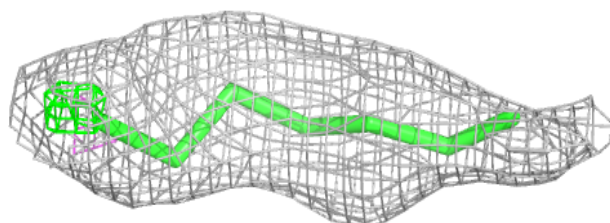
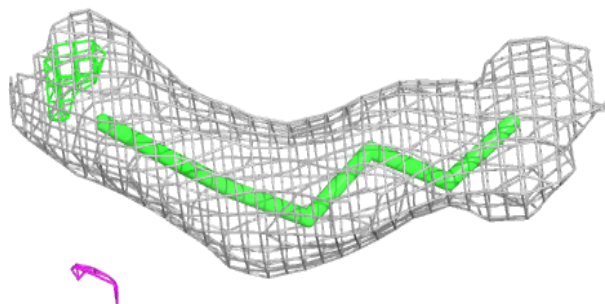


Electron density around OLA B 1016:

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

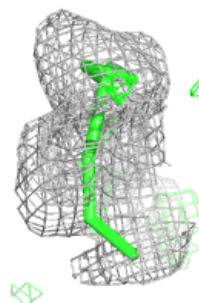
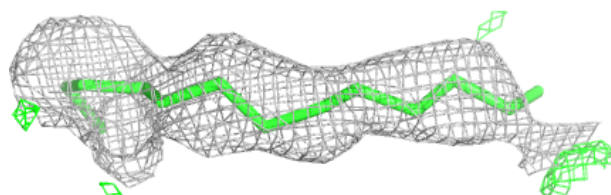
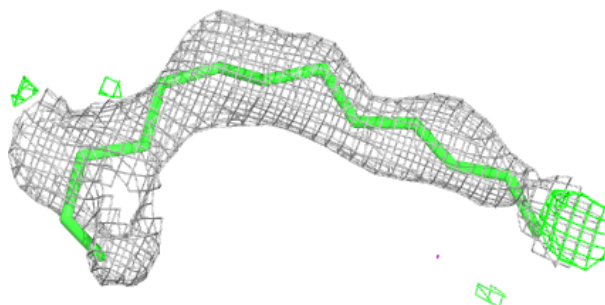
**Electron density around LFA B 1001:**

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

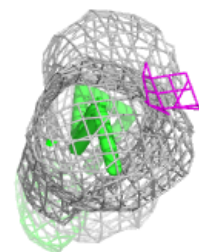
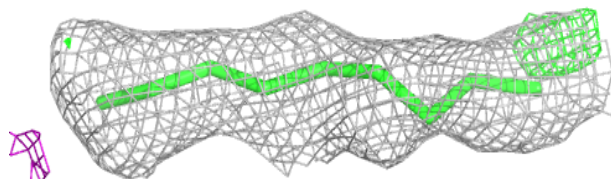
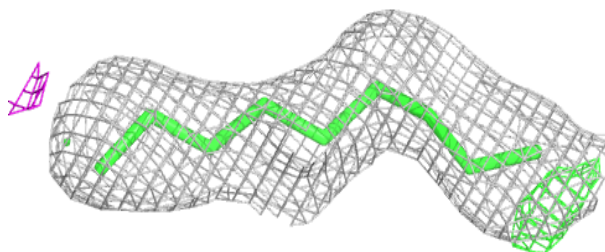


Electron density around LFA C 902:

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

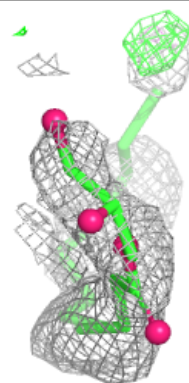
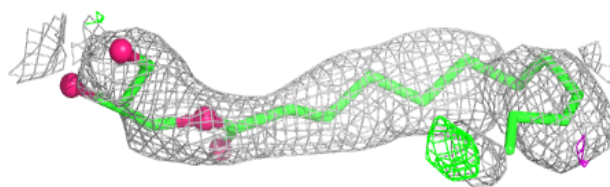
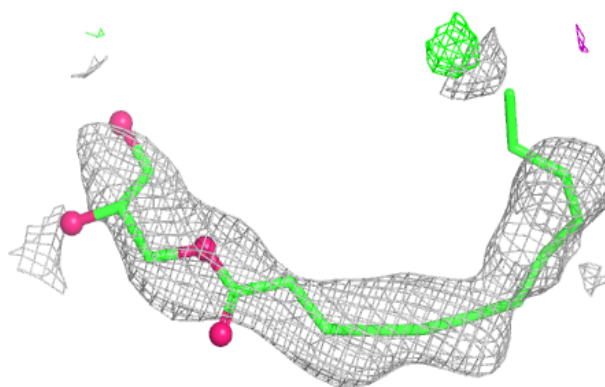
**Electron density around LFA B 1005:**

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

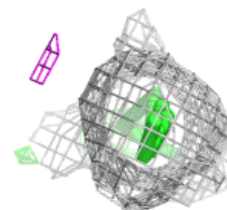
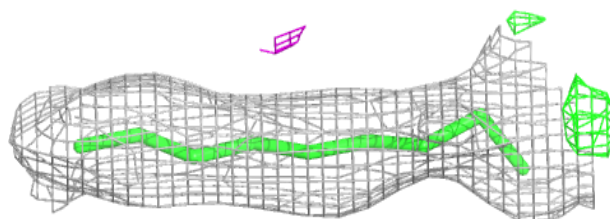
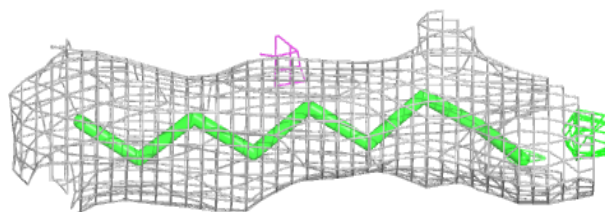


Electron density around OLC B 1018:

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

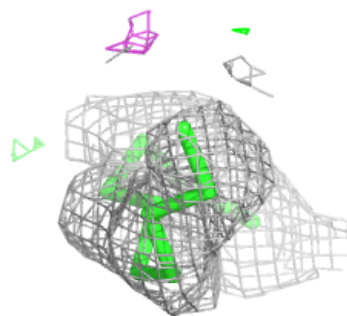
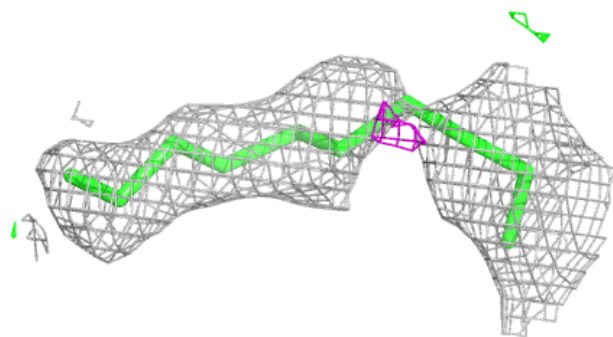
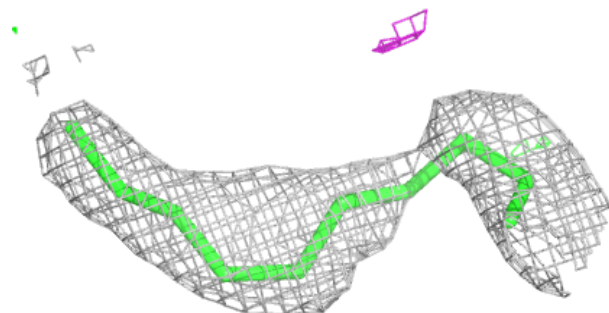
**Electron density around LFA B 1003:**

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

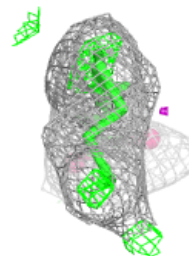
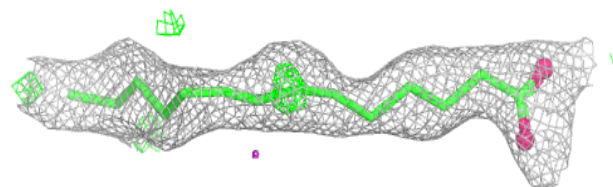
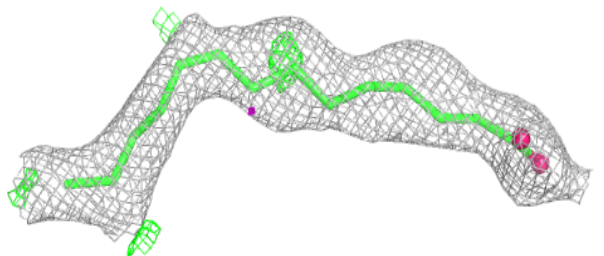


Electron density around LFA B 1025:

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

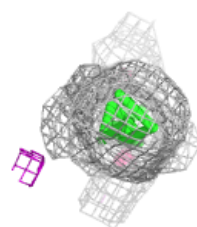
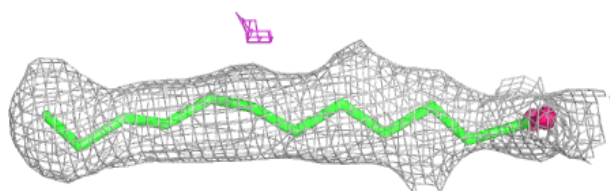
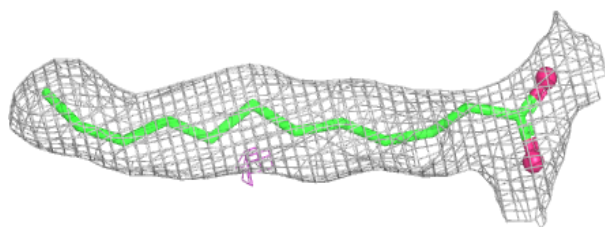
**Electron density around OLA B 1008:**

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

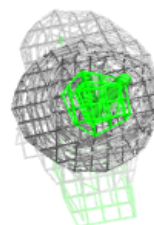
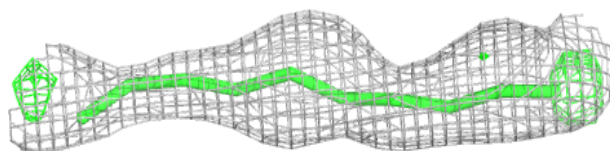
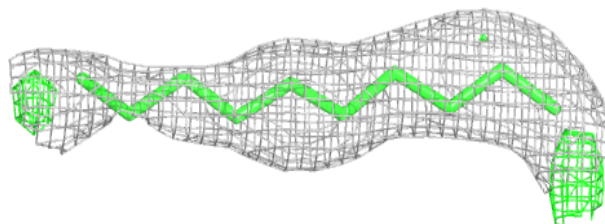


Electron density around OLA B 1009:

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

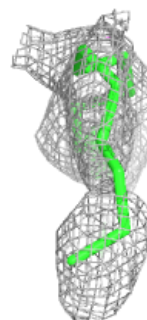
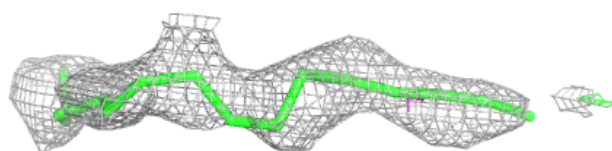
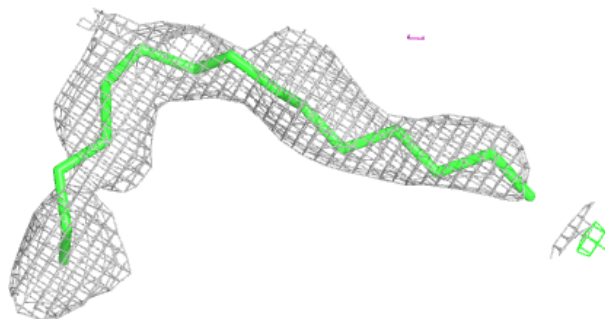
**Electron density around LFA A 514:**

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

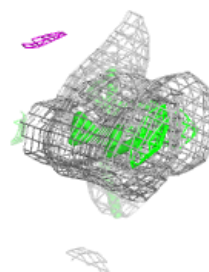
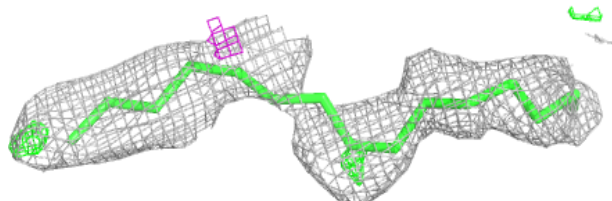
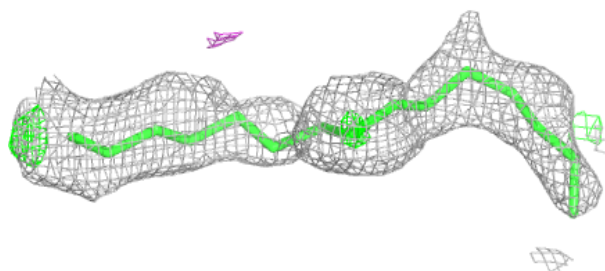


Electron density around LFA C 916:

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

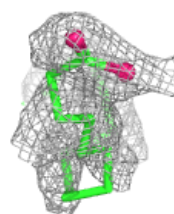
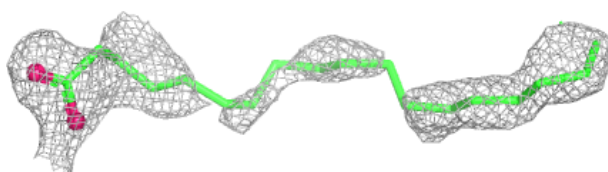
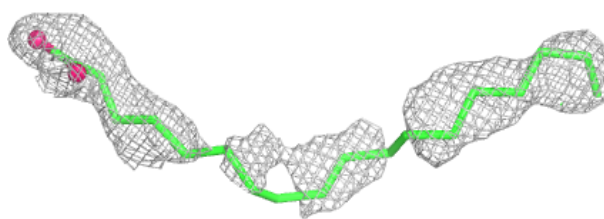
**Electron density around LFA B 1028:**

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

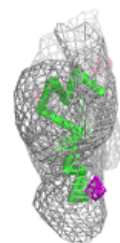
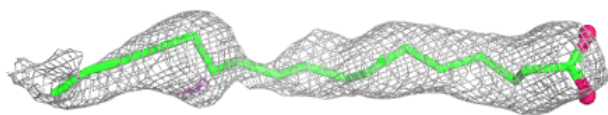
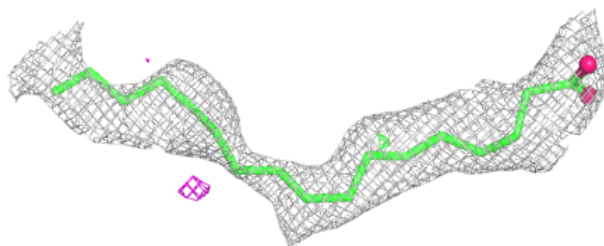


Electron density around OLC B 1017:

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

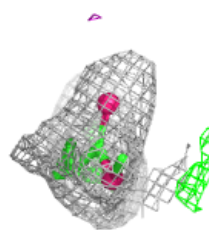
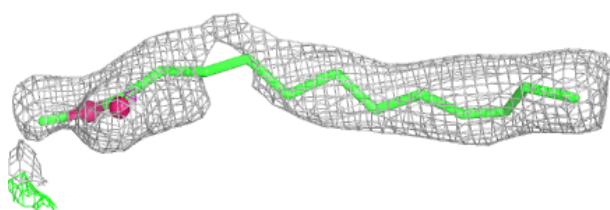
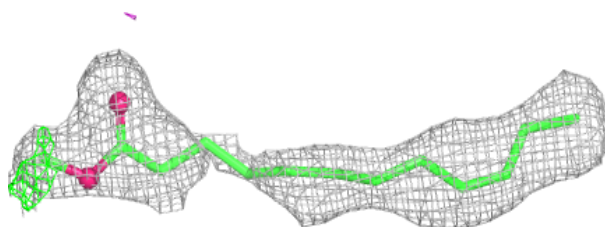
**Electron density around OLA A 512:**

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

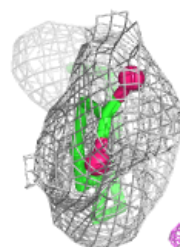
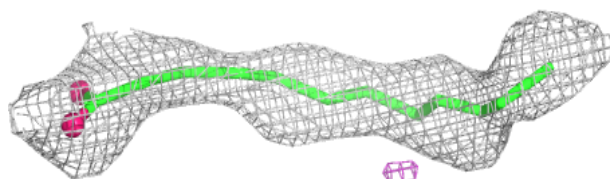
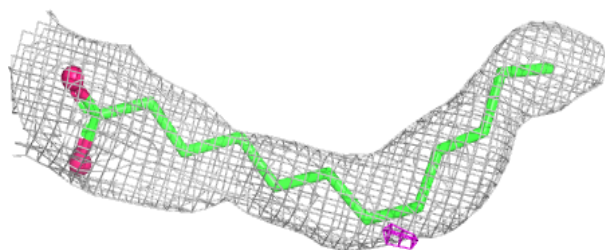


Electron density around OLC C 913:

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

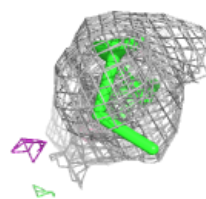
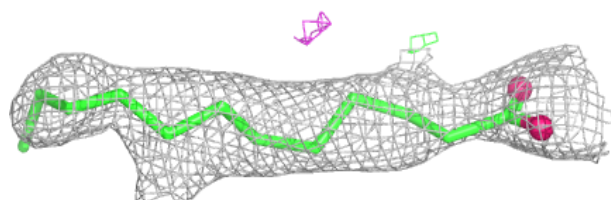
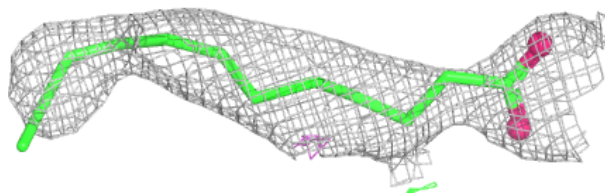
**Electron density around OLA B 1013:**

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

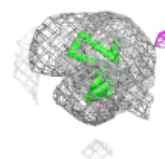
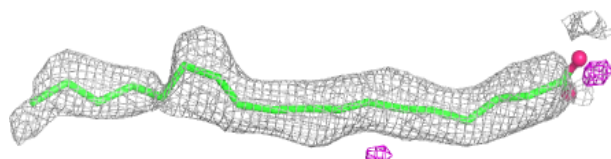
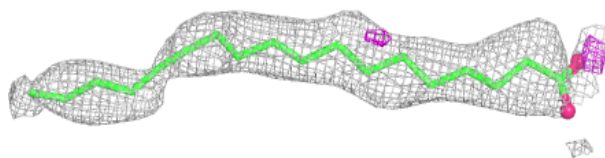


Electron density around OLA B 1012:

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

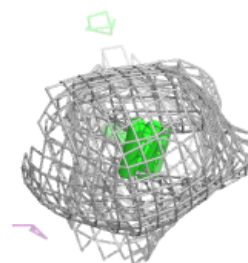
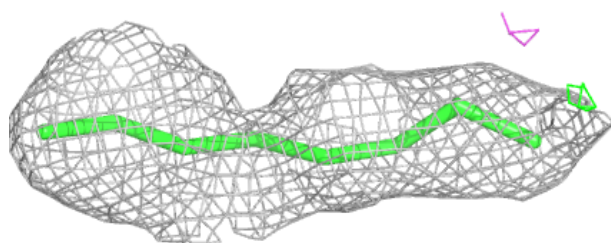
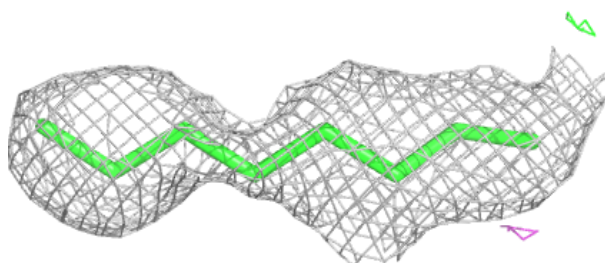
**Electron density around OLA C 903:**

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

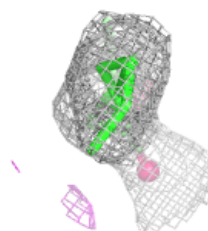
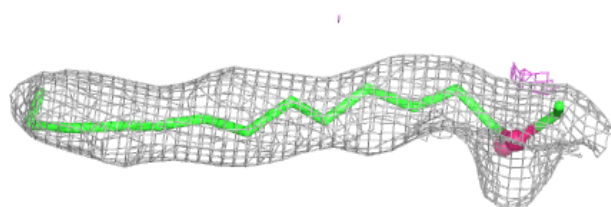
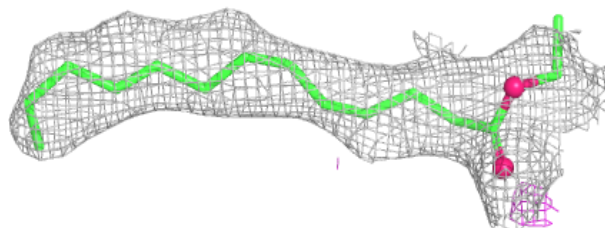


Electron density around LFA A 502:

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

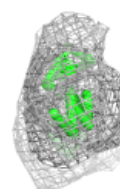
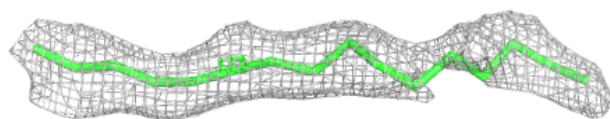
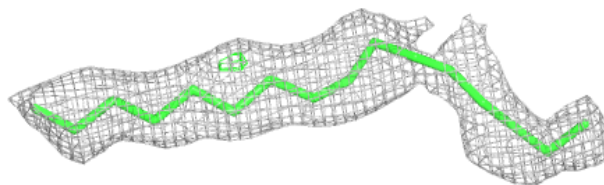
**Electron density around OLC A 507:**

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

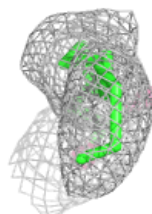
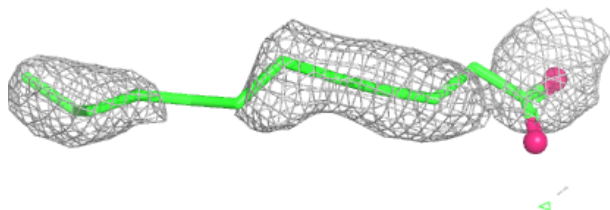
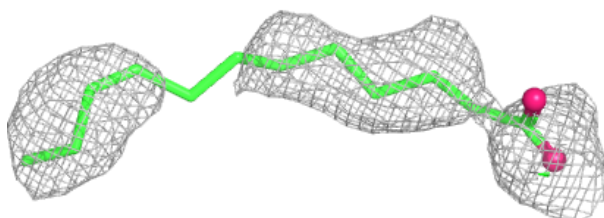


Electron density around LFA C 920:

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

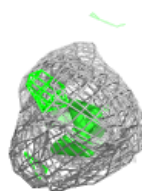
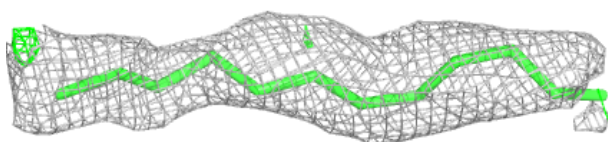
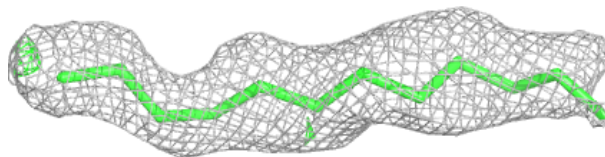
**Electron density around OLA A 506:**

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

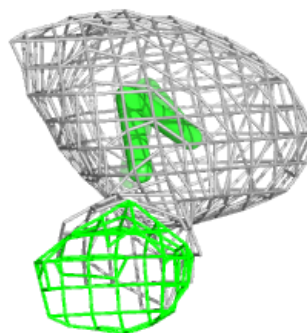
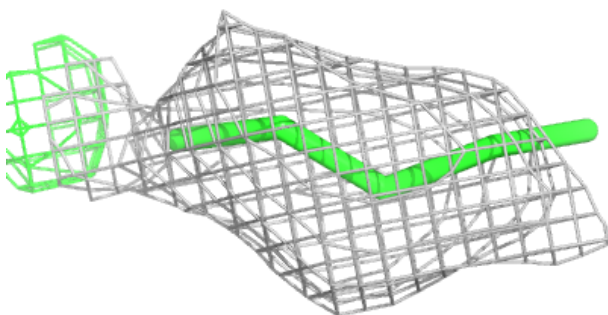
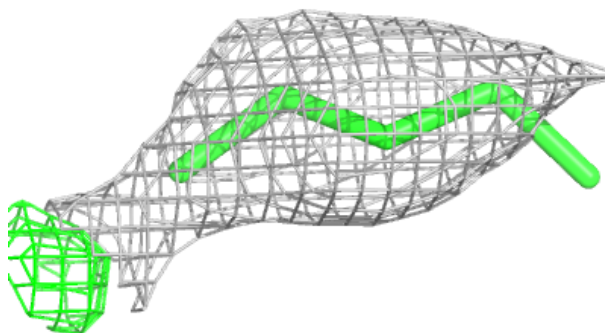


Electron density around LFA C 907:

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

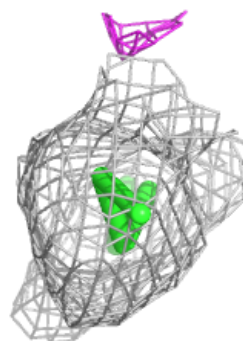
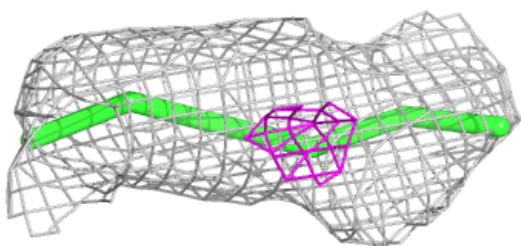
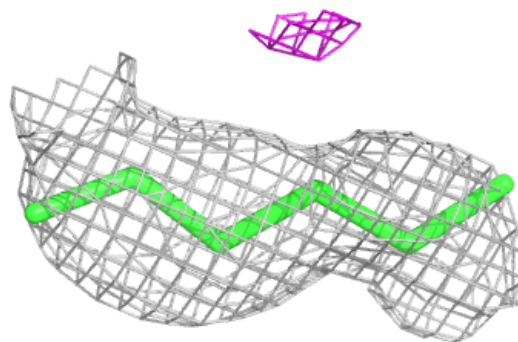
**Electron density around LFA C 908:**

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

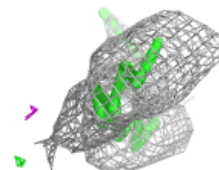
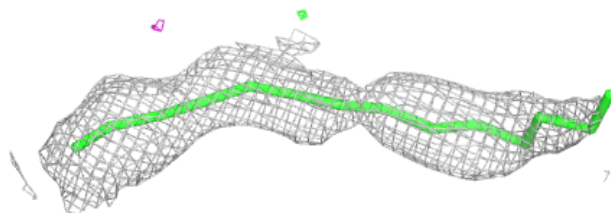
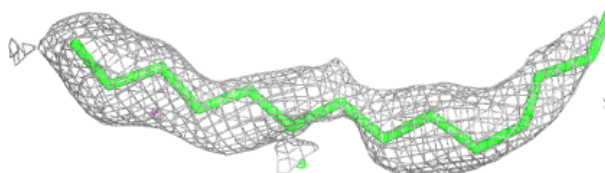


Electron density around LFA B 1021:

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

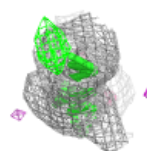
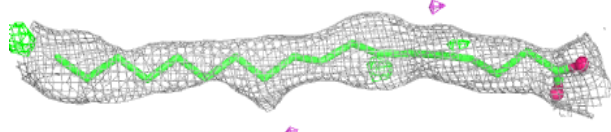
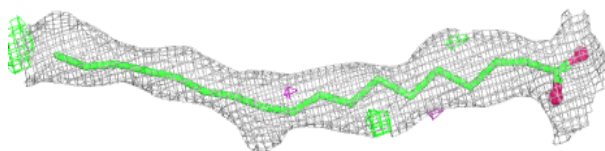
**Electron density around LFA B 1026:**

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

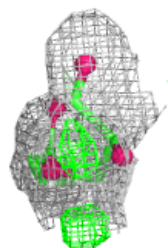
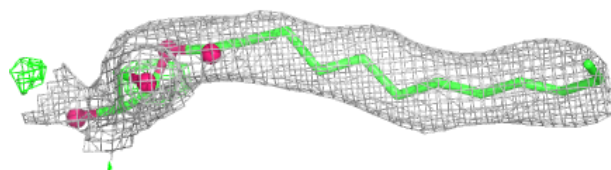
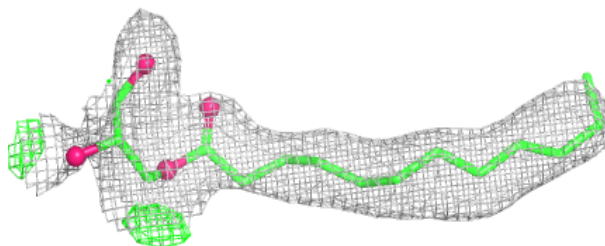


Electron density around OLA A 509:

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

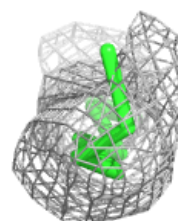
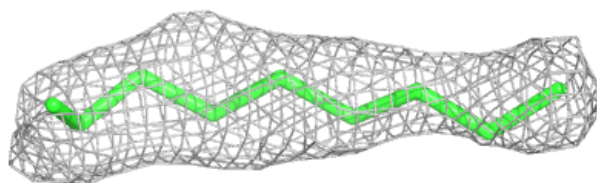
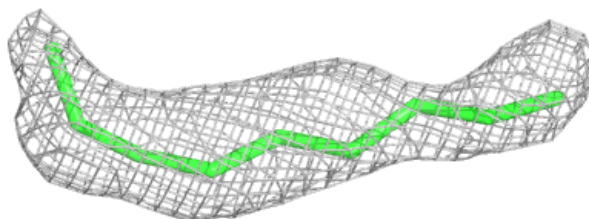
**Electron density around OLC B 1015:**

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

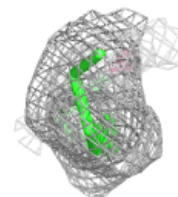
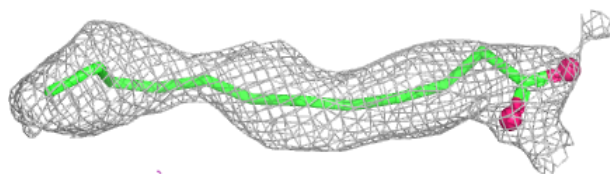
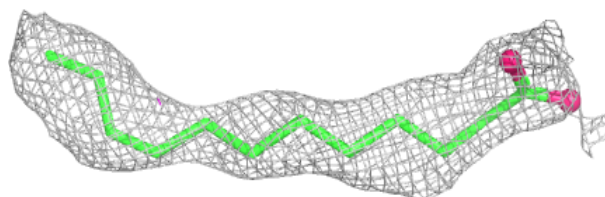


Electron density around LFA A 505:

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

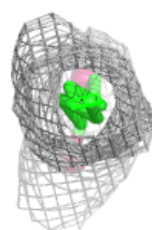
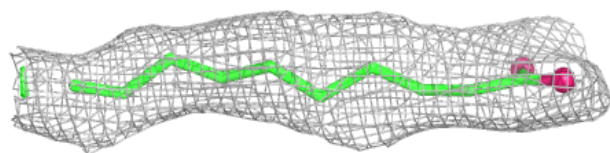
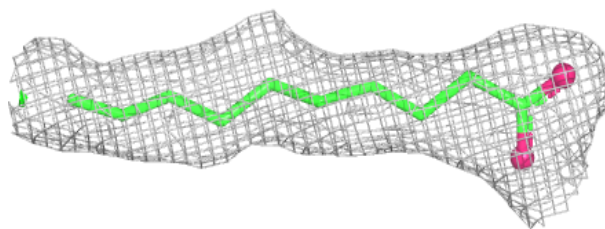
**Electron density around OLA B 1014:**

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

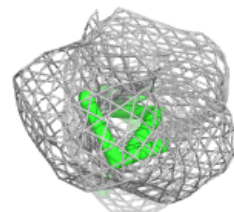
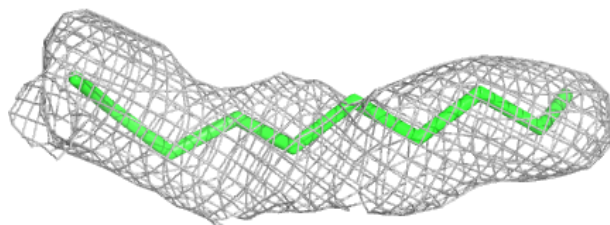
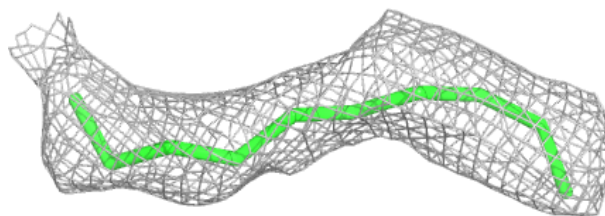


Electron density around OLA A 503:

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

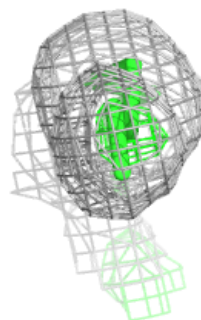
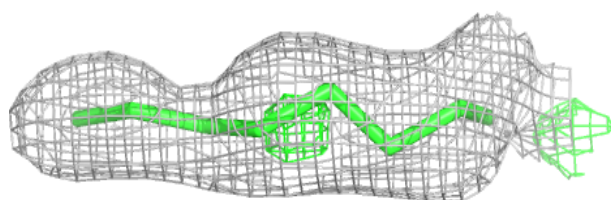
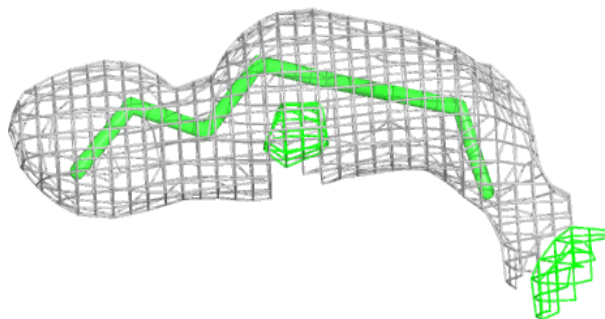
**Electron density around LFA B 1007:**

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

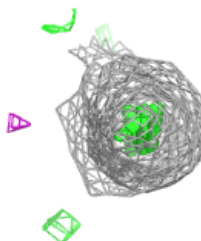
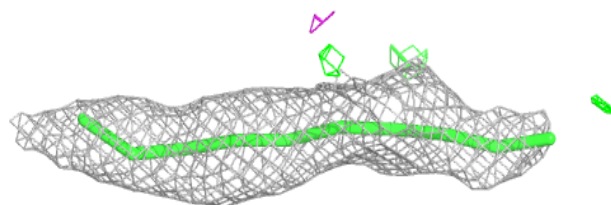
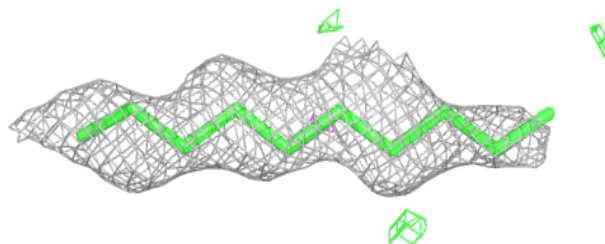


Electron density around LFA B 1010:

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

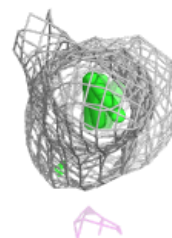
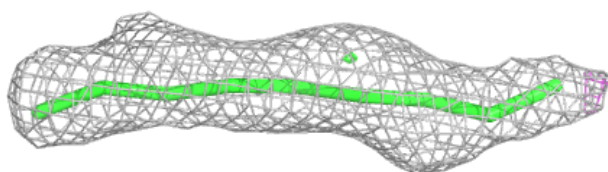
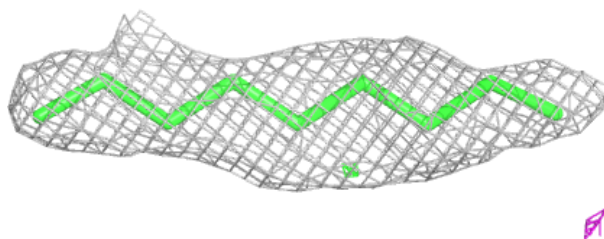
**Electron density around LFA C 906:**

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

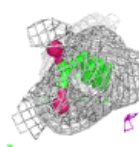
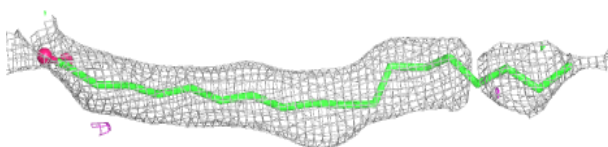
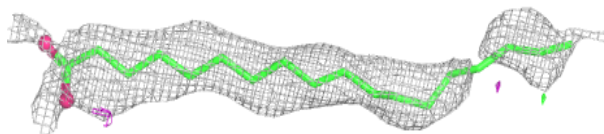


Electron density around LFA A 504:

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

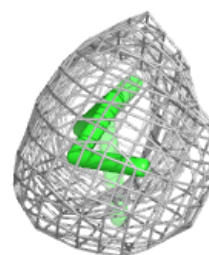
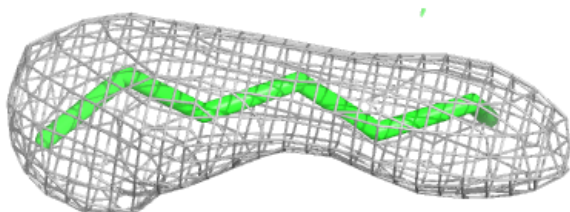
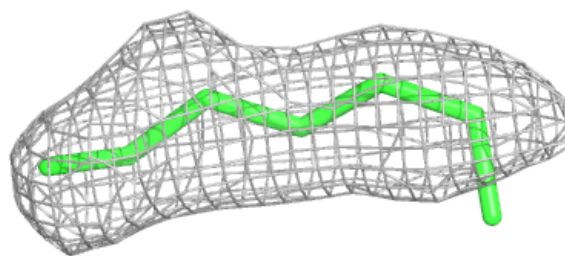
**Electron density around OLA B 1006:**

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.