



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:19 AM UTC

PDB ID : 7ZNA / pdb_00007zna
Title : Crystal structure of the light-driven inward proton pump xenorhodopsin BcXeR in the ground state at pH 5.2 in the presence of sodium at 100K
Authors : Kovalev, K.; Tsybrov, F.; Alekseev, A.; Bourenkov, G.; Gordeliy, V.
Deposited on : 2022-04-20
Resolution : 1.80 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

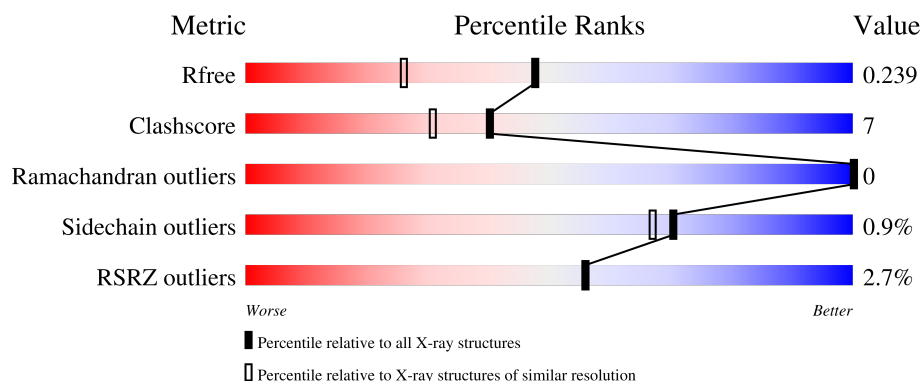
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

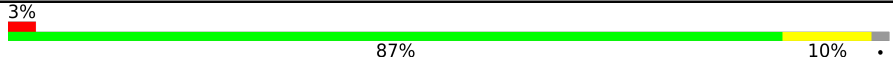
The reported resolution of this entry is 1.80 Å.

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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	

2 Entry composition [i](#)

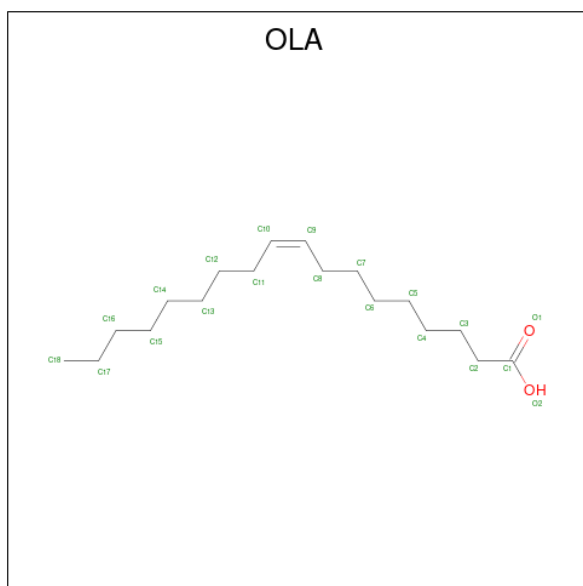
There are 7 unique types of molecules in this entry. The entry contains 6386 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	5	0
			1808	1225	275	301	7			
1	B	221	Total	C	N	O	S	0	5	0
			1780	1210	269	294	7			
1	C	222	Total	C	N	O	S	0	4	0
			1776	1210	264	295	7			

- Molecule 2 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	18	2		
2	A	1	Total	C	O	0	0
			14	12	2		
2	A	1	Total	C		0	0
			8	8			

Continued on next page...

Continued from previous page...

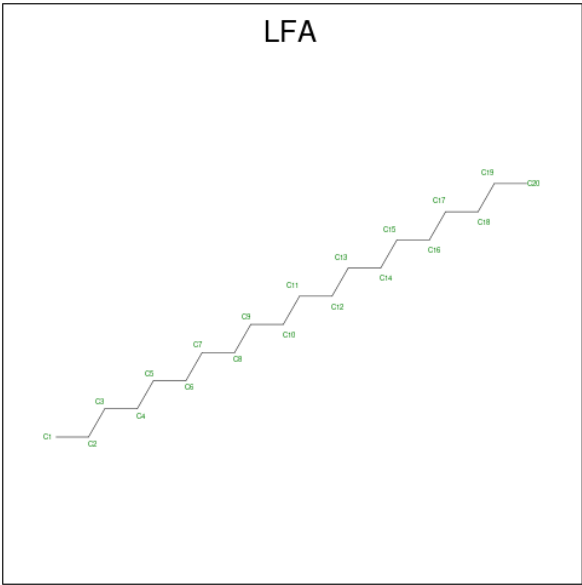
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	12	2		
2	B	1	Total	C	O	0	0
			13	11	2		
2	B	1	Total	C	O	0	0
			16	14	2		
2	B	1	Total	C	O	0	0
			12	10	2		
2	B	1	Total	C	O	0	0
			19	17	2		
2	B	1	Total	C	O	0	0
			16	14	2		
2	B	1	Total	C	O	0	0
			19	17	2		
2	B	1	Total	C	O	0	0
			14	12	2		
2	C	1	Total	C	O	0	0
			16	14	2		
2	C	1	Total	C	O	0	0
			19	17	2		
2	C	1	Total	C	O	0	0
			16	14	2		
2	C	1	Total	C	O	0	0
			15	13	2		
2	C	1	Total	C	O	0	0
			20	18	2		

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



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

- Molecule 4 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			9	9		
4	A	1	Total	C	0	0
			9	9		
4	A	1	Total	C	0	0
			12	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 8 8	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 3 3	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 4 4	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 13 13	0	0
4	A	1	Total C 13 13	0	0
4	A	1	Total C 17 17	0	0
4	A	1	Total C 11 11	0	0
4	A	1	Total C 8 8	0	0
4	A	1	Total C 8 8	0	0
4	A	1	Total C 6 6	0	0
4	A	1	Total C 4 4	0	0
4	B	1	Total C 7 7	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C 6 6	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C 7 7	0	0
4	B	1	Total C 5 5	0	0

Continued on next page...

Continued from previous page...

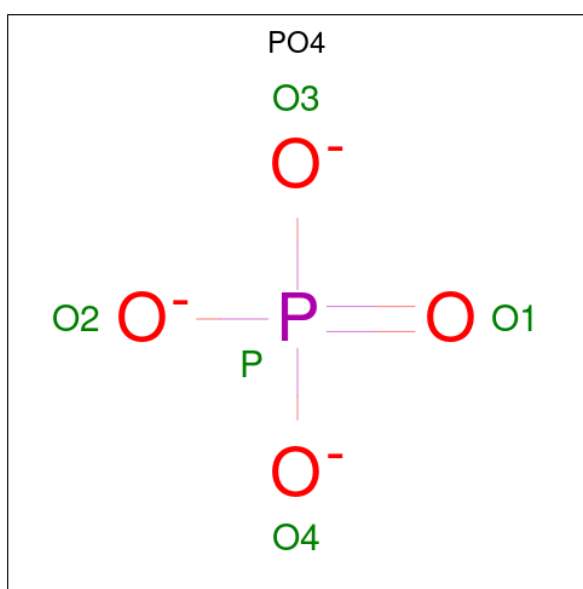
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C 15 15	0	0
4	B	1	Total C 8 8	0	0
4	B	1	Total C 11 11	0	0
4	B	1	Total C 10 10	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C 14 14	0	0
4	B	1	Total C 4 4	0	0
4	B	1	Total C 11 11	0	0
4	B	1	Total C 9 9	0	0
4	C	1	Total C 9 9	0	0
4	C	1	Total C 12 12	0	0
4	C	1	Total C 8 8	0	0
4	C	1	Total C 9 9	0	0
4	C	1	Total C 6 6	0	0
4	C	1	Total C 8 8	0	0
4	C	1	Total C 8 8	0	0
4	C	1	Total C 12 12	0	0
4	C	1	Total C 10 10	0	0
4	C	1	Total C 8 8	0	0
4	C	1	Total C 7 7	0	0
4	C	1	Total C 15 15	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C 12 12	0	0
4	C	1	Total C 9 9	0	0
4	C	1	Total C 9 9	0	0
4	C	1	Total C 7 7	0	0

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



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

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

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

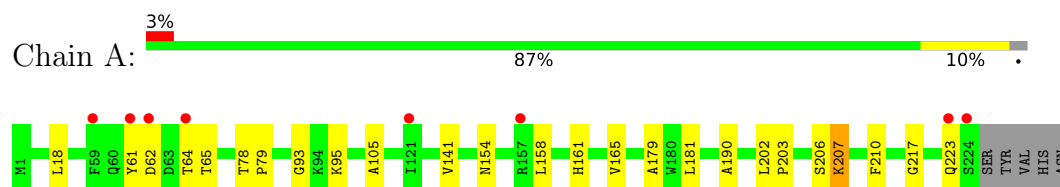
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	95	Total 96	O 96	0	2
7	B	82	Total 83	O 83	0	2
7	C	109	Total 110	O 110	0	2

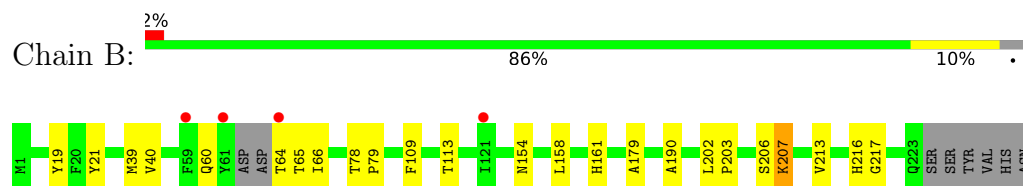
3 Residue-property plots [i](#)

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.

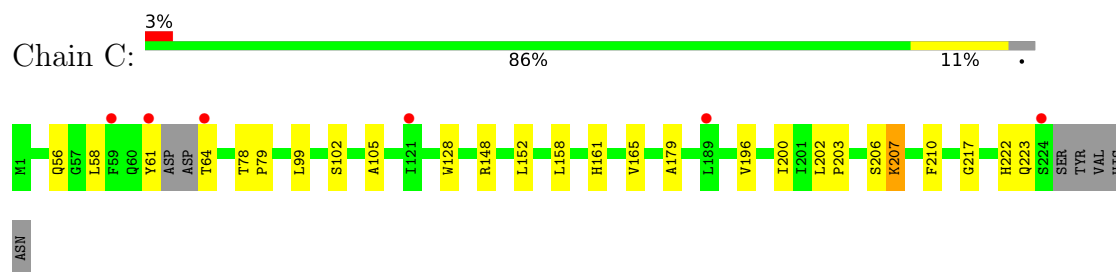
- Molecule 1: xenorhodopsin



- 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	68.57Å 109.59Å 119.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	77.5 (20.00-1.80) 77.5 (20.00-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.197 , 0.230 0.207 , 0.239	Depositor DCC
R_{free} test set	3196 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.9	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	6386	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LFA, NA, OLA, PO4, OLC, LYR, FME

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	0/1816	1.38	0/2480
1	B	0.94	0/1786	1.38	0/2438
1	C	0.94	0/1782	1.36	0/2434
All	All	0.94	0/5384	1.37	0/7352

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1808	0	1872	25	0
1	B	1780	0	1858	25	0
1	C	1776	0	1845	26	0
2	A	56	0	81	2	0
2	B	109	0	149	10	0
2	C	86	0	125	3	0
3	A	25	0	40	7	0
4	A	161	0	304	6	0
4	B	134	0	238	5	0
4	C	149	0	273	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	5	0	0	0	0
5	C	5	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	96	0	0	0	0
7	B	83	0	0	2	0
7	C	110	0	0	2	0
All	All	6386	0	6785	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:ARG:O	1:C:152:LEU:HD23	1.81	0.79
1:C:222:HIS:HE1	7:C:801:HOH:O	1.66	0.78
1:B:64:THR:OG1	7:B:401:HOH:O	2.01	0.76
1:B:190:ALA:CB	4:B:318:LFA:H192	2.16	0.74
1:A:190:ALA:CB	4:A:1020:LFA:H72	2.20	0.71
1:A:95:LYS:HE2	3:A:1004:OLC:H21	1.73	0.70
3:A:1004:OLC:H21A	2:B:306:OLA:H32	1.72	0.70
1:A:179:ALA:O	4:A:1020:LFA:C8	2.40	0.69
1:C:99[B]:LEU:C	1:C:99[B]:LEU:HD23	2.17	0.69
1:C:222:HIS:CE1	7:C:801:HOH:O	2.45	0.67
1:B:207:LYR:H192	1:B:207:LYR:H9	1.77	0.65
1:C:99[B]:LEU:O	1:C:102[B]:SER:OG	2.14	0.63
1:B:190:ALA:HB1	4:B:318:LFA:H192	1.80	0.62
1:C:61:TYR:O	1:C:64:THR:HG22	2.00	0.62
4:C:711:LFA:C8	4:C:721:LFA:C7	2.77	0.61
1:A:161:HIS:CE1	1:A:217:GLY:HA3	2.35	0.61
3:A:1004:OLC:H24A	2:B:306:OLA:H31	1.82	0.61
1:A:165:VAL:HG13	1:A:210:PHE:CE1	2.36	0.61
1:A:190:ALA:HB3	4:A:1020:LFA:H72	1.82	0.61
1:A:207:LYR:H192	1:A:207:LYR:H9	1.83	0.61
3:A:1004:OLC:H24A	2:B:306:OLA:C3	2.31	0.60
1:B:161:HIS:CE1	1:B:217:GLY:HA3	2.38	0.59
1:A:95:LYS:HE2	3:A:1004:OLC:C21	2.32	0.58
1:C:99[B]:LEU:HD23	1:C:99[B]:LEU:O	2.05	0.57
1:C:207:LYR:H183	1:C:207:LYR:H9	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:VAL:HG13	2:C:703:OLA:H132	1.87	0.56
1:A:95:LYS:HE2	3:A:1004:OLC:C22	2.35	0.56
1:C:161:HIS:CE1	1:C:217:GLY:HA3	2.40	0.56
1:C:207:LYR:H9	1:C:207:LYR:H192	1.87	0.56
1:C:179:ALA:HB1	4:C:712:LFA:H13	1.89	0.54
2:B:304:OLA:H10	2:B:304:OLA:C14	2.38	0.53
1:A:95:LYS:HE2	3:A:1004:OLC:H22	1.91	0.53
1:A:207:LYR:H192	1:A:207:LYR:C9	2.40	0.52
1:C:196:VAL:O	1:C:200:ILE:HG12	2.10	0.51
1:A:61:TYR:O	1:A:64:THR:HG22	2.11	0.51
1:B:202:LEU:HB2	1:B:203:PRO:HD3	1.93	0.51
1:C:58:LEU:HD23	1:C:58:LEU:N	2.26	0.51
1:B:207:LYR:H192	1:B:207:LYR:C9	2.40	0.50
1:B:213:VAL:HG22	2:B:307:OLA:H42	1.94	0.50
1:C:165:VAL:HG13	1:C:210:PHE:CE1	2.47	0.50
1:A:78:THR:N	1:A:79:PRO:HD2	2.26	0.50
1:A:202:LEU:HB2	1:A:203:PRO:HD3	1.93	0.49
1:C:78:THR:N	1:C:79:PRO:HD2	2.28	0.49
1:A:207:LYR:H9	1:A:207:LYR:H183	1.95	0.49
1:C:207:LYR:H192	1:C:207:LYR:C9	2.42	0.49
1:A:181:LEU:HD23	4:A:1018:LFA:H81	1.95	0.48
1:B:190:ALA:HB3	4:B:318:LFA:H192	1.94	0.48
1:B:78:THR:N	1:B:79:PRO:HD2	2.28	0.48
2:B:304:OLA:C14	1:C:128:TRP:CZ3	2.96	0.48
1:A:105:ALA:HB2	2:A:1001:OLA:H131	1.95	0.47
1:B:39[B]:MET:HE1	2:B:309:OLA:H111	1.96	0.47
1:B:179:ALA:O	4:B:318:LFA:H202	2.13	0.47
1:A:158:LEU:C	1:A:158:LEU:HD13	2.39	0.47
1:C:105:ALA:HB1	2:C:703:OLA:H142	1.97	0.47
2:B:304:OLA:C14	2:B:304:OLA:C10	2.93	0.46
1:C:207:LYR:HG2	1:C:207:LYR:H1	1.98	0.46
1:A:93:GLY:HA3	1:A:154:ASN:HD21	1.79	0.46
2:B:307:OLA:H52	4:B:320:LFA:C16	2.47	0.45
1:C:158:LEU:C	1:C:158:LEU:HD13	2.41	0.45
1:B:19:TYR:OH	1:B:216:HIS:NE2	2.45	0.45
1:B:158:LEU:C	1:B:158:LEU:HD13	2.42	0.45
1:C:58:LEU:HD23	1:C:58:LEU:H	1.82	0.45
4:A:1018:LFA:H102	4:A:1018:LFA:H72	1.71	0.45
1:C:202:LEU:HB2	1:C:203:PRO:HD3	1.99	0.44
1:B:60:GLN:NE2	1:B:65:THR:OG1	2.50	0.44
4:A:1023:LFA:H201	4:C:717:LFA:H121	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:LYR:HG2	1:B:207:LYR:H1	2.01	0.42
1:C:206:SER:HB3	1:C:207:LYR:H42	2.00	0.42
1:C:56:GLN:HB3	2:C:705:OLA:H31	2.01	0.42
1:B:21:TYR:HB2	1:B:39[B]:MET:HE3	2.01	0.42
1:B:207:LYR:H9	1:B:207:LYR:H183	2.02	0.42
1:A:206:SER:HB3	1:A:207:LYR:H42	2.02	0.42
1:B:39[B]:MET:CE	2:B:309:OLA:C12	2.97	0.42
1:B:154:ASN:ND2	7:B:410:HOH:O	2.53	0.42
1:B:203:PRO:HA	1:B:206:SER:HB2	2.01	0.42
1:B:206:SER:HB3	1:B:207:LYR:H42	2.02	0.42
1:C:203:PRO:HA	1:C:206:SER:HB2	2.02	0.42
1:A:62:ASP:C	1:A:64:THR:H	2.28	0.41
1:A:207:LYR:H1	1:A:207:LYR:HG2	2.02	0.41
1:B:202:LEU:N	1:B:203:PRO:HD2	2.36	0.41
1:C:202:LEU:HD23	1:C:202:LEU:HA	1.94	0.41
1:A:203:PRO:HA	1:A:206:SER:HB2	2.02	0.40
1:B:109:PHE:O	1:B:113:THR:HG23	2.22	0.40
1:A:141:VAL:HA	2:A:1005:OLA:H51	2.03	0.40
1:A:202:LEU:N	1:A:203:PRO:HD2	2.37	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	226/229 (99%)	222 (98%)	4 (2%)	0	100	100
1	B	221/229 (96%)	220 (100%)	1 (0%)	0	100	100
1	C	221/229 (96%)	220 (100%)	1 (0%)	0	100	100
All	All	668/687 (97%)	662 (99%)	6 (1%)	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	184/189 (97%)	181 (98%)	3 (2%)	55	47
1	B	182/189 (96%)	181 (100%)	1 (0%)	81	80
1	C	180/189 (95%)	179 (99%)	1 (1%)	78	77
All	All	546/567 (96%)	541 (99%)	5 (1%)	70	67

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

Mol	Chain	Res	Type
1	A	18	LEU
1	A	65	THR
1	A	223	GLN
1	B	66	ILE
1	C	223	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	222	HIS
1	A	223	GLN
1	B	60	GLN
1	B	154	ASN
1	B	222	HIS
1	C	222	HIS
1	C	223	GLN

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	C	1	1	8,9,10	0.43	0	8,9,11	0.63	0
1	FME	B	1	1	8,9,10	0.43	0	8,9,11	0.67	0
1	LYR	A	207	1	27,29,30	1.09	3 (11%)	30,37,39	1.24	3 (10%)
1	LYR	B	207	1	27,29,30	1.05	3 (11%)	30,37,39	1.33	3 (10%)
1	FME	A	1	1	8,9,10	0.43	0	8,9,11	0.63	0
1	LYR	C	207	1	27,29,30	1.01	2 (7%)	30,37,39	1.28	3 (10%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	207	LYR	C9-C80	-2.66	1.40	1.46
1	A	207	LYR	C9-C80	-2.54	1.40	1.46
1	B	207	LYR	C9-C80	-2.32	1.41	1.46
1	B	207	LYR	C5-C3	-2.24	1.41	1.46
1	A	207	LYR	C5-C3	-2.17	1.41	1.46
1	A	207	LYR	C16-C15	-2.15	1.47	1.52
1	C	207	LYR	C5-C3	-2.09	1.41	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	LYR	C4-C3	-2.04	1.46	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	LYR	C8-C80-C7	-3.72	116.79	122.82
1	C	207	LYR	C8-C80-C7	-3.49	117.17	122.82
1	A	207	LYR	C8-C80-C7	-3.39	117.32	122.82
1	C	207	LYR	C5-C3-C2	-3.17	114.08	118.49
1	B	207	LYR	C8-C80-C9	2.87	122.47	118.09
1	C	207	LYR	C8-C80-C9	2.87	122.47	118.09
1	A	207	LYR	C5-C3-C2	-2.81	114.58	118.49
1	A	207	LYR	C8-C80-C9	2.63	122.11	118.09
1	B	207	LYR	C5-C3-C2	-2.50	115.01	118.49

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 15 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 71 ligands modelled in this entry, 3 are monoatomic - leaving 68 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	OLA	B	303	-	12,12,19	0.68	0	12,12,19	0.59	0
5	PO4	C	722	-	4,4,4	0.72	0	6,6,6	0.47	0
4	LFA	C	719	-	8,8,19	0.10	0	7,7,18	0.10	0
4	LFA	B	322	-	8,8,19	0.14	0	7,7,18	0.15	0
2	OLA	B	309	-	13,13,19	0.67	0	13,13,19	0.50	0
4	LFA	B	314	-	14,14,19	0.14	0	13,13,18	0.09	0
4	LFA	C	720	-	8,8,19	0.12	0	7,7,18	0.10	0
4	LFA	A	1010	-	5,5,19	0.16	0	4,4,18	0.15	0
4	LFA	C	715	-	7,7,19	0.13	0	6,6,18	0.11	0
2	OLA	A	1003	-	7,7,19	0.17	0	6,6,19	0.11	0
4	LFA	A	1018	-	16,16,19	0.10	0	15,15,18	0.13	0
4	LFA	A	1020	-	7,7,19	0.14	0	6,6,18	0.15	0
5	PO4	A	1024	-	4,4,4	0.67	0	6,6,6	0.48	0
4	LFA	C	709	-	8,8,19	0.14	0	7,7,18	0.10	0
4	LFA	C	712	-	7,7,19	0.16	0	6,6,18	0.17	0
4	LFA	B	315	-	7,7,19	0.08	0	6,6,18	0.16	0
4	LFA	A	1008	-	11,11,19	0.10	0	10,10,18	0.05	0
2	OLA	C	702	-	15,15,19	0.55	0	15,15,19	0.58	0
4	LFA	A	1015	-	9,9,19	0.09	0	8,8,18	0.08	0
4	LFA	A	1007	-	8,8,19	0.09	0	7,7,18	0.14	0
4	LFA	C	710	-	5,5,19	0.12	0	4,4,18	0.14	0
4	LFA	A	1013	-	3,3,19	0.16	0	2,2,18	0.55	0
4	LFA	A	1022	-	5,5,19	0.14	0	4,4,18	0.13	0
4	LFA	C	714	-	9,9,19	0.13	0	8,8,18	0.11	0
4	LFA	B	310	-	5,5,19	0.13	0	4,4,18	0.13	0
2	OLA	A	1001	-	19,19,19	0.49	0	19,19,19	0.55	0
4	LFA	B	311	-	8,8,19	0.12	0	7,7,18	0.15	0
4	LFA	B	321	-	10,10,19	0.13	0	9,9,18	0.08	0
4	LFA	A	1014	-	9,9,19	0.11	0	8,8,18	0.09	0
2	OLA	A	1002	-	13,13,19	0.60	0	13,13,19	0.59	0
2	OLA	A	1005	-	13,13,19	0.68	0	13,13,19	0.53	0
4	LFA	B	319	-	13,13,19	0.10	0	12,12,18	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LFA	C	717	-	14,14,19	0.09	0	13,13,18	0.07	0
2	OLA	B	305	-	11,11,19	0.67	0	11,11,19	0.69	0
2	OLA	C	705	-	14,14,19	0.59	0	14,14,19	0.57	0
4	LFA	B	313	-	4,4,19	0.15	0	3,3,18	0.22	0
2	OLA	B	307	-	15,15,19	0.59	0	15,15,19	0.53	0
2	OLA	C	706	-	19,19,19	0.49	0	19,19,19	0.54	0
4	LFA	A	1016	-	12,12,19	0.08	0	11,11,18	0.07	0
4	LFA	C	713	-	11,11,19	0.09	0	10,10,18	0.07	0
4	LFA	B	312	-	6,6,19	0.10	0	5,5,18	0.14	0
2	OLA	C	703	-	18,18,19	0.56	0	18,18,19	0.51	0
4	LFA	A	1023	-	3,3,19	0.21	0	2,2,18	0.45	0
2	OLA	B	304	-	15,15,19	0.58	0	15,15,19	0.56	0
2	OLA	B	308	-	18,18,19	0.54	0	18,18,19	0.58	0
4	LFA	C	707	-	11,11,19	0.09	0	10,10,18	0.09	0
4	LFA	A	1021	-	7,7,19	0.13	0	6,6,18	0.10	0
4	LFA	B	301	-	6,6,19	0.14	0	5,5,18	0.12	0
4	LFA	A	1019	-	10,10,19	0.12	0	9,9,18	0.09	0
4	LFA	B	318	-	8,8,19	0.19	0	7,7,18	0.14	0
4	LFA	B	316	-	10,10,19	0.09	0	9,9,18	0.10	0
4	LFA	B	320	-	3,3,19	0.26	0	2,2,18	0.42	0
3	OLC	A	1004	-	24,24,24	0.26	0	25,25,25	0.27	0
4	LFA	C	718	-	11,11,19	0.09	0	10,10,18	0.07	0
4	LFA	A	1012	-	9,9,19	0.14	0	8,8,18	0.09	0
2	OLA	C	704	-	15,15,19	0.60	0	15,15,19	0.57	0
4	LFA	C	708	-	7,7,19	0.10	0	6,6,18	0.09	0
4	LFA	C	721	-	6,6,19	0.15	0	5,5,18	0.14	0
4	LFA	B	302	-	8,8,19	0.10	0	7,7,18	0.15	0
4	LFA	A	1017	-	12,12,19	0.13	0	11,11,18	0.09	0
4	LFA	B	317	-	9,9,19	0.07	0	8,8,18	0.10	0
4	LFA	C	701	-	8,8,19	0.13	0	7,7,18	0.14	0
4	LFA	A	1006	-	8,8,19	0.11	0	7,7,18	0.10	0
4	LFA	C	711	-	7,7,19	0.13	0	6,6,18	0.10	0
4	LFA	C	716	-	6,6,19	0.12	0	5,5,18	0.12	0
4	LFA	A	1011	-	2,2,19	0.08	0	1,1,18	0.17	0
2	OLA	B	306	-	18,18,19	0.54	0	18,18,19	0.58	0
4	LFA	A	1009	-	7,7,19	0.12	0	6,6,18	0.21	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	OLA	B	303	-	-	2/10/10/17	-
4	LFA	C	719	-	-	2/6/6/17	-
4	LFA	B	322	-	-	1/6/6/17	-
2	OLA	B	309	-	-	7/11/11/17	-
4	LFA	B	314	-	-	3/12/12/17	-
4	LFA	C	720	-	-	1/6/6/17	-
4	LFA	A	1010	-	-	2/3/3/17	-
4	LFA	C	715	-	-	1/5/5/17	-
2	OLA	A	1003	-	-	2/5/5/17	-
4	LFA	A	1018	-	-	5/14/14/17	-
4	LFA	A	1020	-	-	3/5/5/17	-
4	LFA	C	709	-	-	3/6/6/17	-
4	LFA	C	712	-	-	2/5/5/17	-
4	LFA	B	315	-	-	2/5/5/17	-
4	LFA	A	1008	-	-	6/9/9/17	-
2	OLA	C	702	-	-	6/13/13/17	-
4	LFA	A	1015	-	-	4/7/7/17	-
4	LFA	A	1007	-	-	0/6/6/17	-
4	LFA	C	710	-	-	2/3/3/17	-
4	LFA	A	1013	-	-	1/1/1/17	-
4	LFA	A	1022	-	-	2/3/3/17	-
4	LFA	C	714	-	-	0/7/7/17	-
4	LFA	B	310	-	-	0/3/3/17	-
2	OLA	A	1001	-	-	8/17/17/17	-
4	LFA	B	311	-	-	2/6/6/17	-
4	LFA	B	321	-	-	6/8/8/17	-
4	LFA	A	1014	-	-	1/7/7/17	-
2	OLA	A	1002	-	-	2/11/11/17	-
2	OLA	A	1005	-	-	6/11/11/17	-
4	LFA	B	319	-	-	3/11/11/17	-
4	LFA	C	717	-	-	7/12/12/17	-
2	OLA	B	305	-	-	4/9/9/17	-
2	OLA	C	705	-	-	7/12/12/17	-
4	LFA	B	313	-	-	0/2/2/17	-
2	OLA	B	307	-	-	4/13/13/17	-
2	OLA	C	706	-	-	4/17/17/17	-
4	LFA	A	1016	-	-	4/10/10/17	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LFA	C	713	-	-	5/9/9/17	-
4	LFA	B	312	-	-	1/4/4/17	-
2	OLA	C	703	-	-	10/16/16/17	-
4	LFA	A	1023	-	-	0/1/1/17	-
2	OLA	B	304	-	-	7/13/13/17	-
2	OLA	B	308	-	-	6/16/16/17	-
4	LFA	C	707	-	-	2/9/9/17	-
4	LFA	A	1021	-	-	2/5/5/17	-
4	LFA	B	301	-	-	2/4/4/17	-
4	LFA	A	1019	-	-	1/8/8/17	-
4	LFA	B	318	-	-	1/6/6/17	-
4	LFA	B	316	-	-	4/8/8/17	-
4	LFA	B	320	-	-	0/1/1/17	-
3	OLC	A	1004	-	-	13/24/24/24	-
4	LFA	C	718	-	-	4/9/9/17	-
4	LFA	A	1012	-	-	1/7/7/17	-
2	OLA	C	704	-	-	8/13/13/17	-
4	LFA	C	708	-	-	0/5/5/17	-
4	LFA	C	721	-	-	1/4/4/17	-
4	LFA	B	302	-	-	2/6/6/17	-
4	LFA	A	1017	-	-	6/10/10/17	-
4	LFA	B	317	-	-	3/7/7/17	-
4	LFA	C	701	-	-	3/6/6/17	-
4	LFA	A	1006	-	-	3/6/6/17	-
4	LFA	C	711	-	-	4/5/5/17	-
4	LFA	C	716	-	-	0/4/4/17	-
2	OLA	B	306	-	-	3/16/16/17	-
4	LFA	A	1009	-	-	1/5/5/17	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (208) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1004	OLC	O20-C21-C22-O23
4	A	1013	LFA	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	702	OLA	C11-C10-C9-C8
2	C	705	OLA	C11-C10-C9-C8
2	B	307	OLA	C11-C10-C9-C8
2	B	304	OLA	C1-C2-C3-C4
2	B	305	OLA	C5-C6-C7-C8
4	A	1018	LFA	C7-C8-C9-C10
2	B	304	OLA	C11-C10-C9-C8
2	B	308	OLA	C1-C2-C3-C4
3	A	1004	OLC	C1-C2-C3-C4
3	A	1004	OLC	O20-C21-C22-C24
2	C	703	OLA	C1-C2-C3-C4
3	A	1004	OLC	C21-C22-C24-O25
2	A	1005	OLA	C1-C2-C3-C4
4	A	1015	LFA	C14-C15-C16-C17
2	C	704	OLA	C11-C10-C9-C8
2	A	1003	OLA	C3-C4-C5-C6
4	C	711	LFA	C2-C3-C4-C5
4	A	1018	LFA	C11-C10-C9-C8
2	C	705	OLA	C3-C4-C5-C6
4	C	718	LFA	C12-C13-C14-C15
2	A	1005	OLA	C2-C3-C4-C5
4	C	717	LFA	C5-C6-C7-C8
4	C	717	LFA	C11-C12-C13-C14
2	C	704	OLA	C5-C6-C7-C8
2	C	705	OLA	C5-C6-C7-C8
4	A	1021	LFA	C3-C4-C5-C6
4	A	1014	LFA	C15-C16-C17-C18
4	B	319	LFA	C5-C6-C7-C8
2	A	1001	OLA	C1-C2-C3-C4
4	A	1017	LFA	C5-C6-C7-C8
4	B	318	LFA	C14-C15-C16-C17
4	A	1016	LFA	C13-C14-C15-C16
2	C	703	OLA	C11-C12-C13-C14
2	C	704	OLA	C3-C4-C5-C6
4	A	1020	LFA	C2-C3-C4-C5
2	A	1002	OLA	C9-C10-C11-C12
2	C	706	OLA	C11-C12-C13-C14
4	A	1018	LFA	C4-C5-C6-C7
2	B	304	OLA	C11-C12-C13-C14
4	C	717	LFA	C6-C7-C8-C9
4	B	316	LFA	C14-C15-C16-C17
3	A	1004	OLC	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1001	OLA	C9-C10-C11-C12
2	C	704	OLA	C4-C5-C6-C7
4	A	1016	LFA	C12-C13-C14-C15
2	B	307	OLA	C2-C3-C4-C5
4	B	316	LFA	C16-C17-C18-C19
4	C	713	LFA	C13-C14-C15-C16
2	C	706	OLA	C12-C13-C14-C15
2	A	1005	OLA	C6-C7-C8-C9
2	C	703	OLA	C13-C14-C15-C16
4	C	713	LFA	C9-C10-C11-C12
2	C	706	OLA	C6-C7-C8-C9
4	A	1020	LFA	C3-C4-C5-C6
4	B	312	LFA	C3-C4-C5-C6
2	A	1002	OLA	C2-C3-C4-C5
4	A	1008	LFA	C4-C5-C6-C7
3	A	1004	OLC	C6-C7-C8-C9
2	A	1005	OLA	C11-C10-C9-C8
4	A	1006	LFA	C4-C5-C6-C7
4	A	1016	LFA	C11-C10-C9-C8
4	A	1020	LFA	C5-C6-C7-C8
2	C	703	OLA	C5-C6-C7-C8
4	A	1010	LFA	C2-C3-C4-C5
2	C	703	OLA	C2-C3-C4-C5
3	A	1004	OLC	C4-C5-C6-C7
4	C	713	LFA	C15-C16-C17-C18
4	B	321	LFA	C11-C10-C9-C8
2	B	303	OLA	C2-C3-C4-C5
4	C	711	LFA	C1-C2-C3-C4
2	A	1001	OLA	C2-C3-C4-C5
4	A	1006	LFA	C6-C7-C8-C9
4	A	1019	LFA	C11-C10-C9-C8
4	C	718	LFA	C10-C11-C12-C13
4	A	1008	LFA	C9-C10-C11-C12
4	B	321	LFA	C5-C6-C7-C8
2	A	1001	OLA	C11-C12-C13-C14
4	A	1008	LFA	C5-C6-C7-C8
4	A	1015	LFA	C12-C13-C14-C15
4	B	317	LFA	C12-C13-C14-C15
4	C	701	LFA	C2-C3-C4-C5
4	A	1022	LFA	C15-C16-C17-C18
4	B	311	LFA	C11-C10-C9-C8
4	B	321	LFA	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	314	LFA	C4-C5-C6-C7
2	B	303	OLA	C11-C10-C9-C8
4	A	1008	LFA	C1-C2-C3-C4
2	C	703	OLA	C3-C4-C5-C6
4	A	1017	LFA	C1-C2-C3-C4
4	A	1017	LFA	C3-C4-C5-C6
4	B	316	LFA	C15-C16-C17-C18
4	B	322	LFA	C7-C8-C9-C10
4	C	712	LFA	C4-C5-C6-C7
4	C	713	LFA	C14-C15-C16-C17
3	A	1004	OLC	C13-C14-C15-C16
4	C	715	LFA	C13-C14-C15-C16
3	A	1004	OLC	C11-C12-C13-C14
4	A	1010	LFA	C1-C2-C3-C4
4	C	701	LFA	C5-C6-C7-C8
3	A	1004	OLC	C2-C3-C4-C5
2	C	703	OLA	C6-C7-C8-C9
2	C	704	OLA	C6-C7-C8-C9
4	C	710	LFA	C4-C5-C6-C7
4	A	1017	LFA	C4-C5-C6-C7
4	A	1016	LFA	C15-C16-C17-C18
4	A	1008	LFA	C7-C8-C9-C10
4	A	1008	LFA	C6-C7-C8-C9
2	B	304	OLA	C3-C4-C5-C6
4	A	1012	LFA	C5-C6-C7-C8
4	C	717	LFA	C10-C11-C12-C13
2	C	702	OLA	C11-C12-C13-C14
4	C	719	LFA	C17-C18-C19-C20
4	C	707	LFA	C9-C10-C11-C12
2	B	309	OLA	C5-C6-C7-C8
2	B	305	OLA	C4-C5-C6-C7
4	B	301	LFA	C13-C14-C15-C16
2	B	305	OLA	C7-C8-C9-C10
4	B	321	LFA	C2-C3-C4-C5
4	B	316	LFA	C17-C18-C19-C20
2	C	702	OLA	C3-C4-C5-C6
2	A	1003	OLA	C4-C5-C6-C7
2	C	704	OLA	C11-C12-C13-C14
4	B	319	LFA	C11-C10-C9-C8
2	B	309	OLA	C9-C10-C11-C12
4	C	712	LFA	C2-C3-C4-C5
4	C	717	LFA	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1018	LFA	C11-C12-C13-C14
4	B	321	LFA	C6-C7-C8-C9
2	A	1001	OLA	C7-C8-C9-C10
2	C	704	OLA	C1-C2-C3-C4
4	C	721	LFA	C4-C5-C6-C7
2	B	308	OLA	C4-C5-C6-C7
2	B	306	OLA	C11-C10-C9-C8
4	A	1015	LFA	C13-C14-C15-C16
4	C	710	LFA	C3-C4-C5-C6
2	C	703	OLA	C7-C8-C9-C10
2	B	306	OLA	C13-C14-C15-C16
4	C	709	LFA	C5-C6-C7-C8
4	C	717	LFA	C1-C2-C3-C4
4	B	302	LFA	C1-C2-C3-C4
4	A	1021	LFA	C1-C2-C3-C4
2	A	1001	OLA	O1-C1-C2-C3
2	B	307	OLA	C7-C8-C9-C10
2	B	304	OLA	C7-C8-C9-C10
2	B	308	OLA	C14-C15-C16-C17
3	A	1004	OLC	C14-C15-C16-C17
2	C	705	OLA	O1-C1-C2-C3
4	C	709	LFA	C3-C4-C5-C6
2	A	1001	OLA	O2-C1-C2-C3
2	B	308	OLA	O2-C1-C2-C3
2	B	308	OLA	O1-C1-C2-C3
4	C	718	LFA	C15-C16-C17-C18
2	C	705	OLA	O2-C1-C2-C3
4	B	302	LFA	C3-C4-C5-C6
4	C	717	LFA	C3-C4-C5-C6
2	B	304	OLA	O1-C1-C2-C3
4	C	718	LFA	C11-C12-C13-C14
4	B	315	LFA	C1-C2-C3-C4
2	A	1001	OLA	C11-C10-C9-C8
4	A	1022	LFA	C17-C18-C19-C20
4	C	709	LFA	C6-C7-C8-C9
2	C	702	OLA	C4-C5-C6-C7
2	B	305	OLA	C2-C3-C4-C5
4	C	713	LFA	C17-C18-C19-C20
4	A	1017	LFA	C11-C10-C9-C8
2	B	308	OLA	C7-C8-C9-C10
4	B	317	LFA	C11-C12-C13-C14
4	A	1017	LFA	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

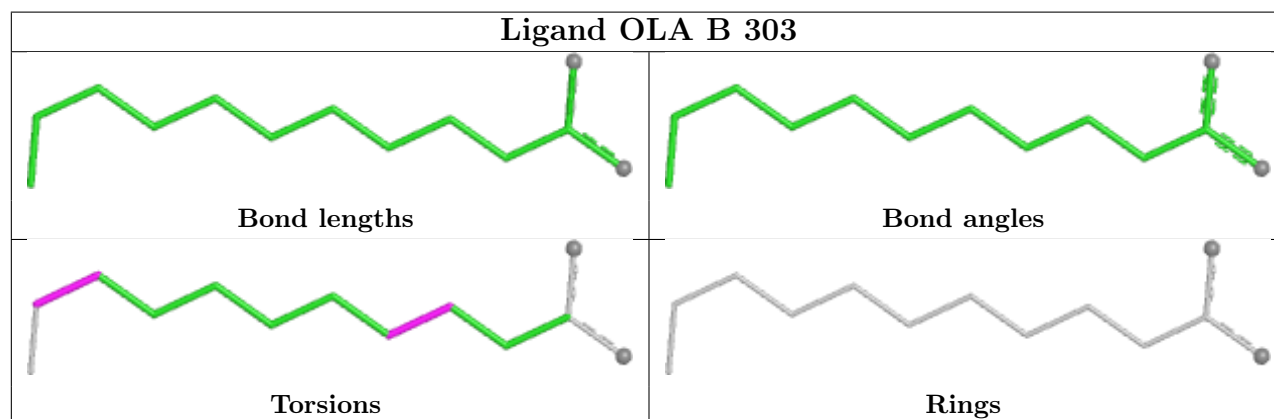
Mol	Chain	Res	Type	Atoms
2	A	1005	OLA	C7-C8-C9-C10
4	A	1006	LFA	C5-C6-C7-C8
2	B	309	OLA	C7-C8-C9-C10
2	C	705	OLA	C9-C10-C11-C12
4	C	711	LFA	C3-C4-C5-C6
3	A	1004	OLC	O23-C22-C24-O25
4	B	317	LFA	C14-C15-C16-C17
3	A	1004	OLC	C9-C10-C11-C12
2	C	702	OLA	O2-C1-C2-C3
2	B	307	OLA	C10-C11-C12-C13
2	B	309	OLA	C4-C5-C6-C7
4	B	314	LFA	C10-C11-C12-C13
2	B	304	OLA	O2-C1-C2-C3
2	C	702	OLA	O1-C1-C2-C3
4	A	1009	LFA	C4-C5-C6-C7
2	C	704	OLA	C7-C8-C9-C10
4	A	1018	LFA	C5-C6-C7-C8
4	B	314	LFA	C11-C12-C13-C14
4	B	301	LFA	C16-C17-C18-C19
4	C	707	LFA	C12-C13-C14-C15
2	B	309	OLA	C2-C3-C4-C5
4	C	720	LFA	C5-C6-C7-C8
4	B	319	LFA	C7-C8-C9-C10
2	C	703	OLA	C4-C5-C6-C7
4	B	315	LFA	C4-C5-C6-C7
2	B	309	OLA	O1-C1-C2-C3
2	B	309	OLA	O2-C1-C2-C3
2	A	1005	OLA	C3-C4-C5-C6
4	B	311	LFA	C6-C7-C8-C9
4	C	711	LFA	C5-C6-C7-C8
2	C	705	OLA	C6-C7-C8-C9
2	B	306	OLA	C14-C15-C16-C17
4	C	701	LFA	C7-C8-C9-C10
2	C	706	OLA	C1-C2-C3-C4
4	B	321	LFA	C4-C5-C6-C7
4	A	1015	LFA	C15-C16-C17-C18
4	C	719	LFA	C12-C13-C14-C15
2	C	703	OLA	C11-C10-C9-C8

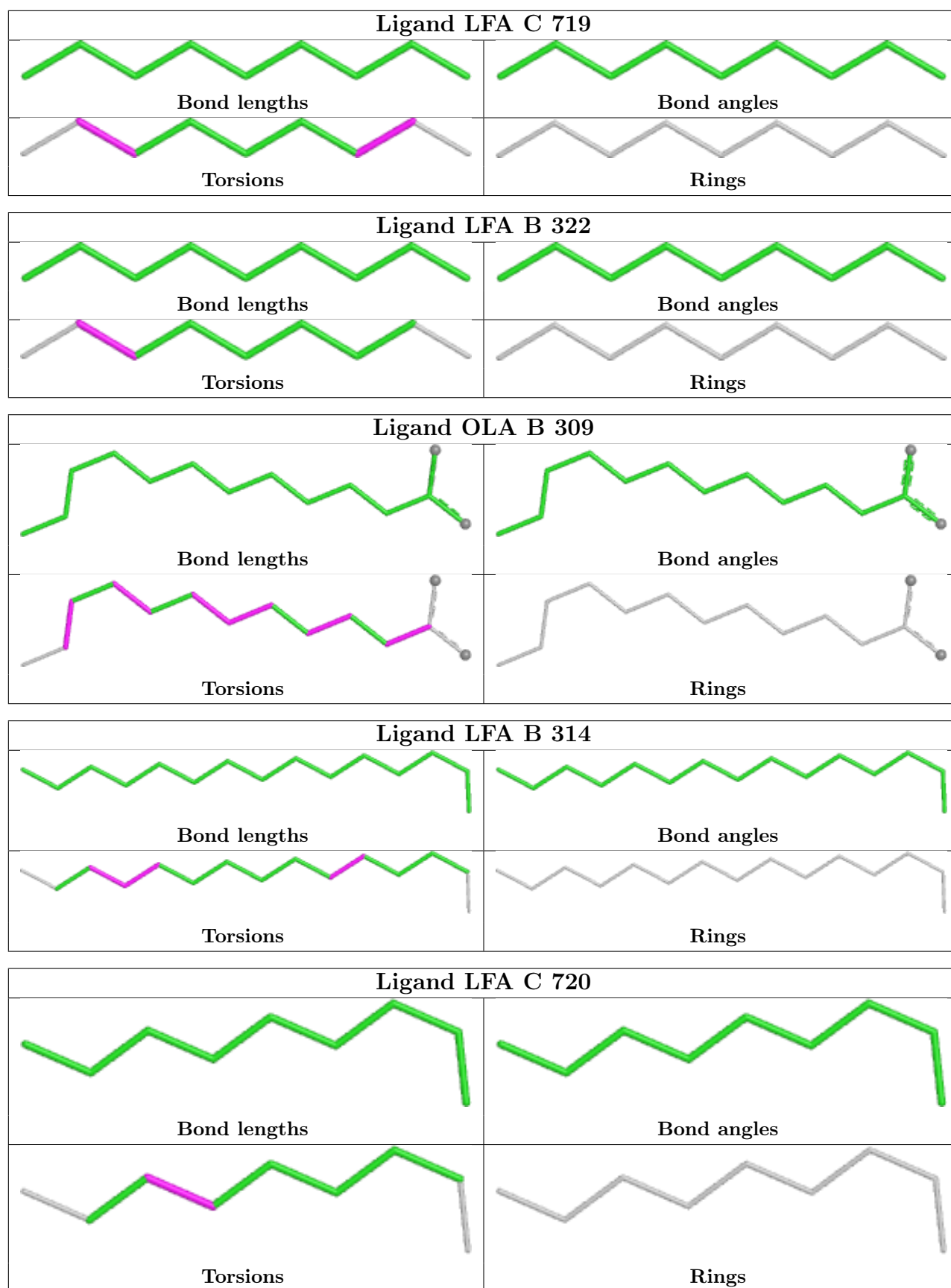
There are no ring outliers.

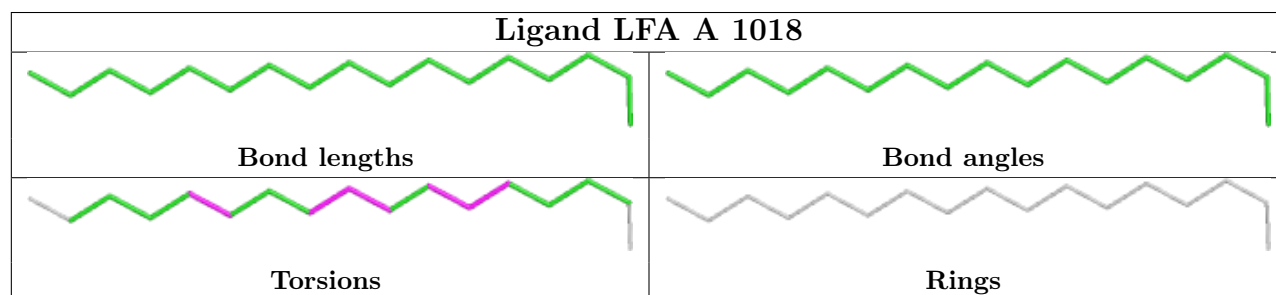
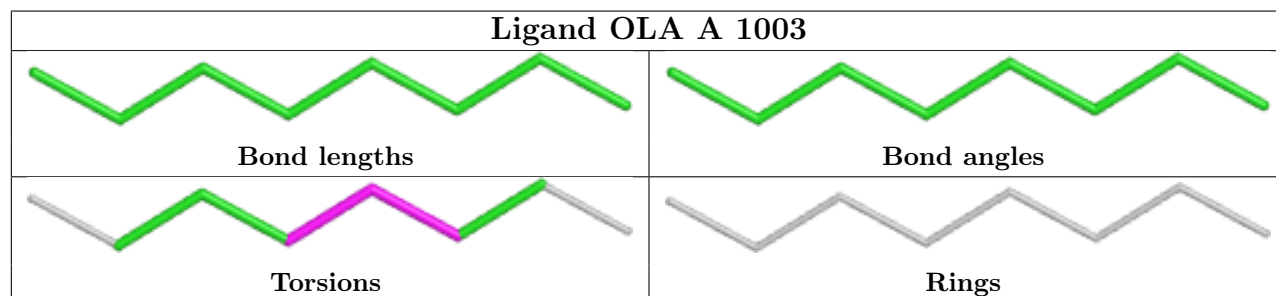
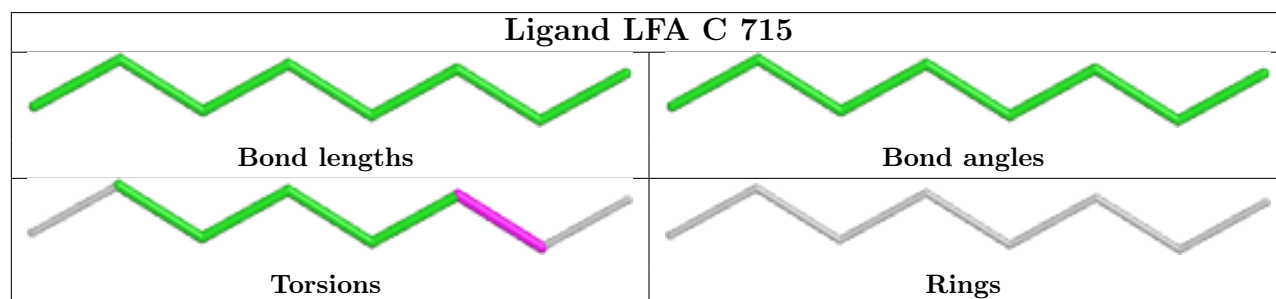
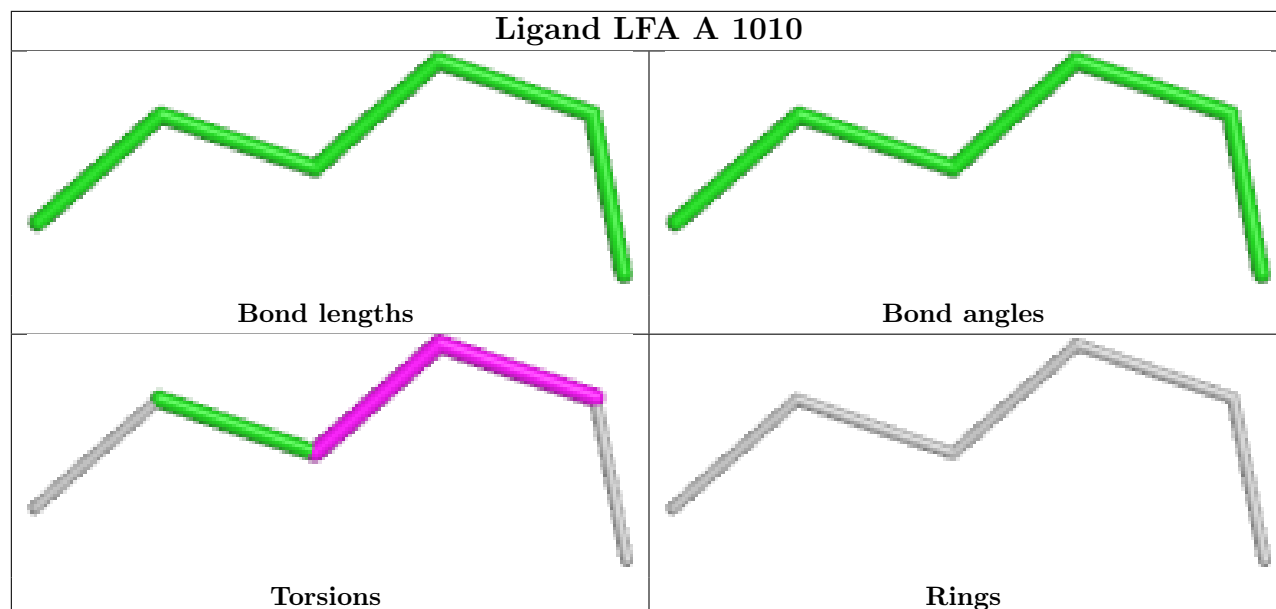
18 monomers are involved in 31 short contacts:

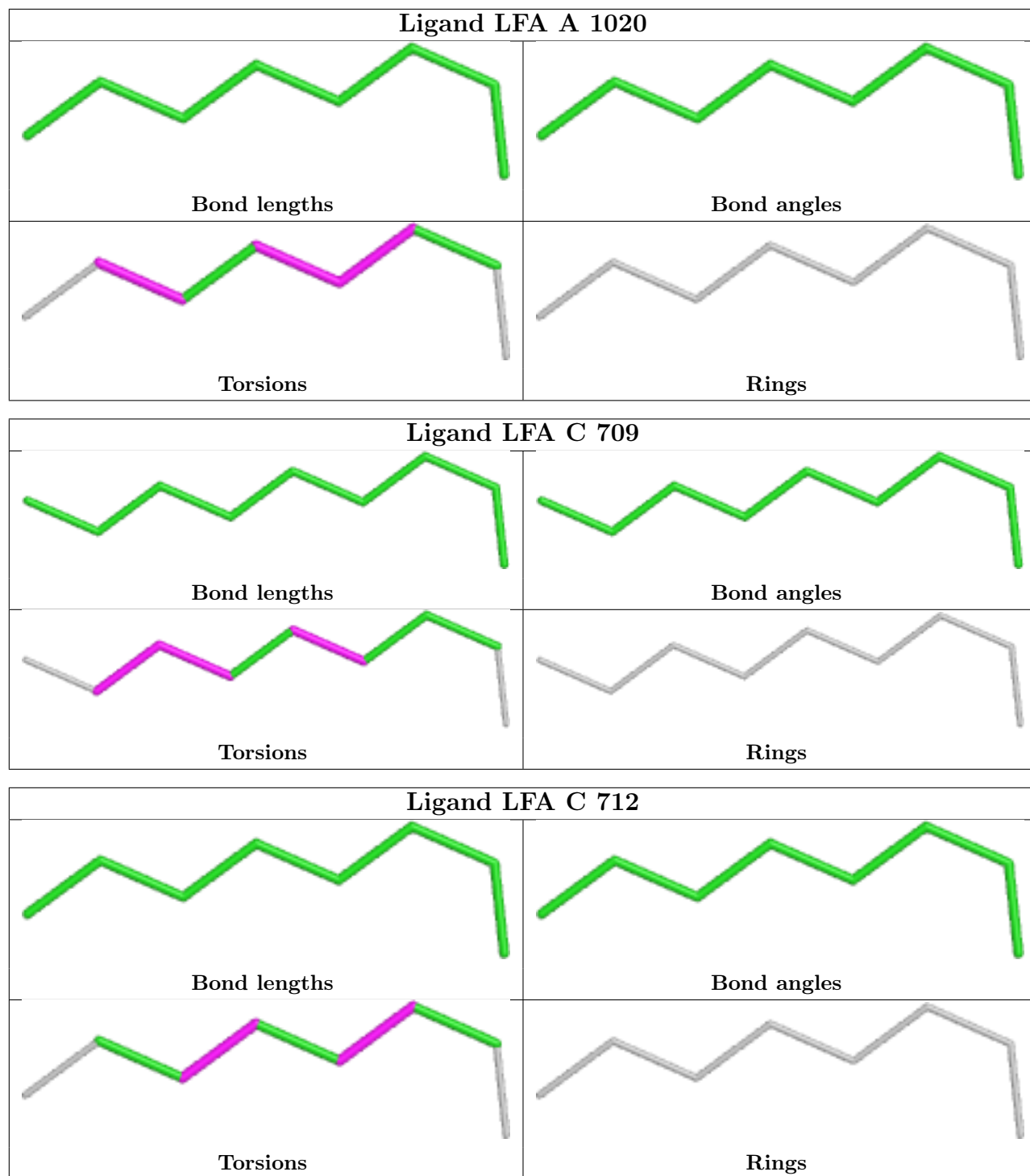
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	309	OLA	2	0
4	A	1018	LFA	2	0
4	A	1020	LFA	3	0
4	C	712	LFA	1	0
2	A	1001	OLA	1	0
2	A	1005	OLA	1	0
4	C	717	LFA	1	0
2	C	705	OLA	1	0
2	B	307	OLA	2	0
2	C	703	OLA	2	0
4	A	1023	LFA	1	0
2	B	304	OLA	3	0
4	B	318	LFA	4	0
4	B	320	LFA	1	0
3	A	1004	OLC	7	0
4	C	721	LFA	1	0
4	C	711	LFA	1	0
2	B	306	OLA	3	0

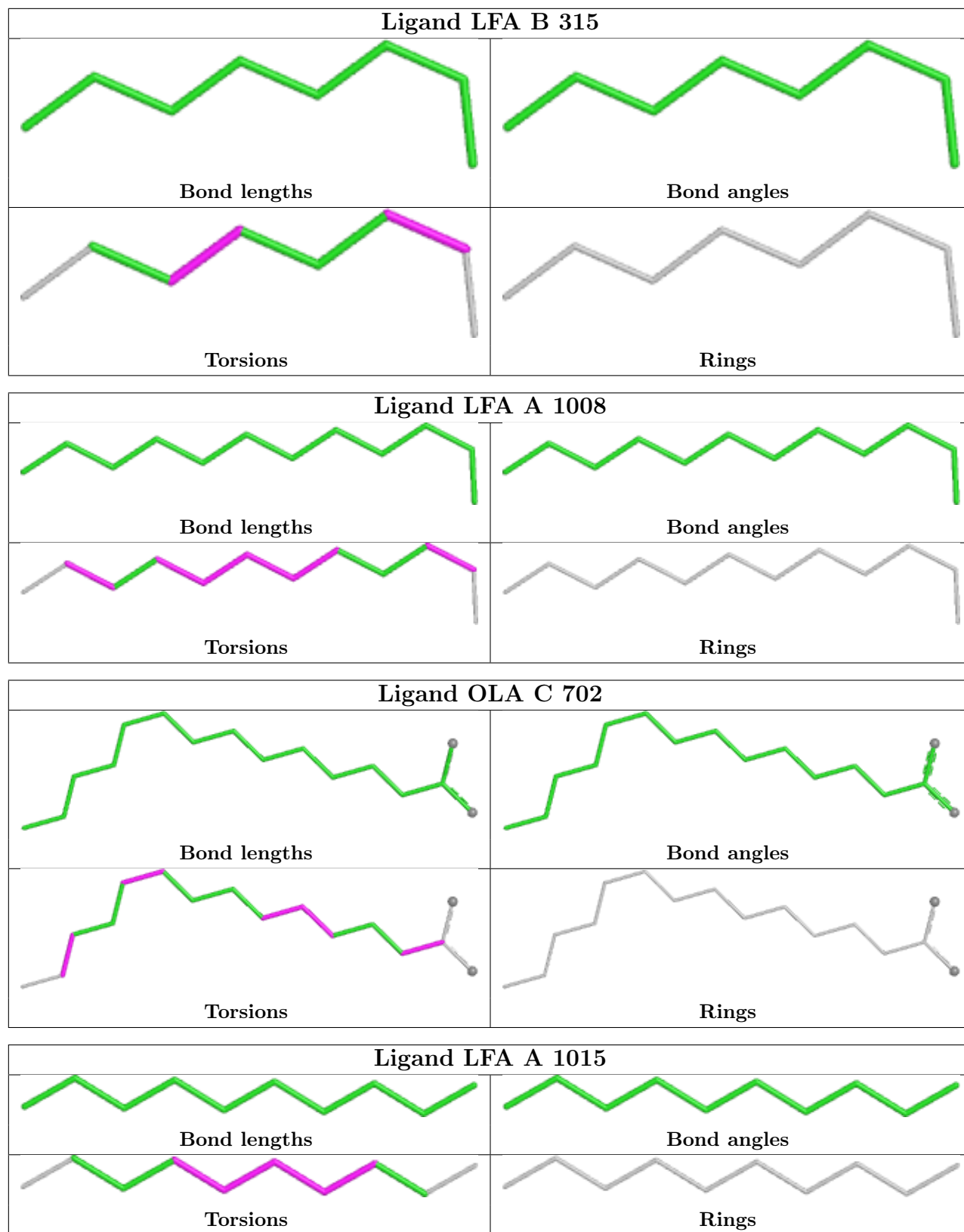
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

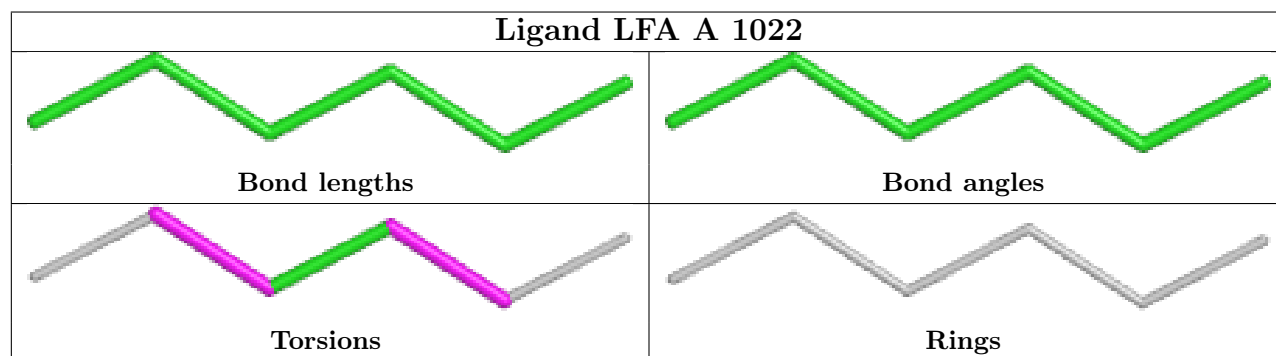
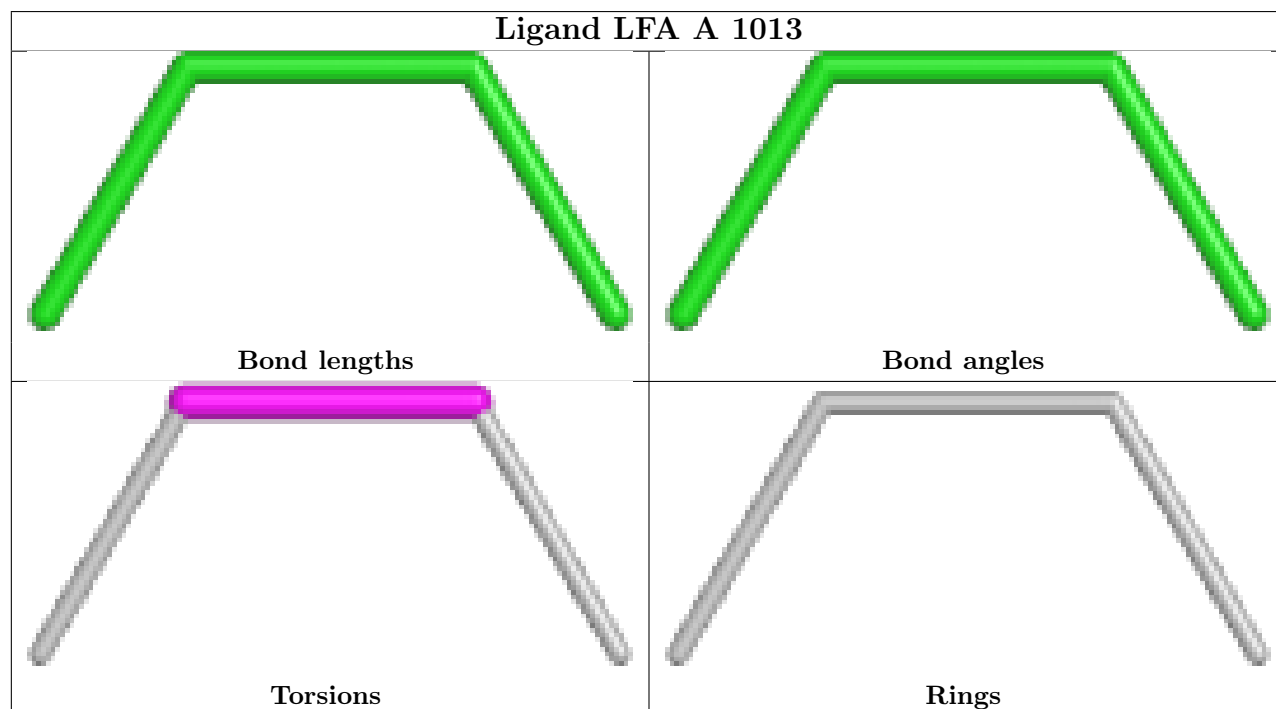
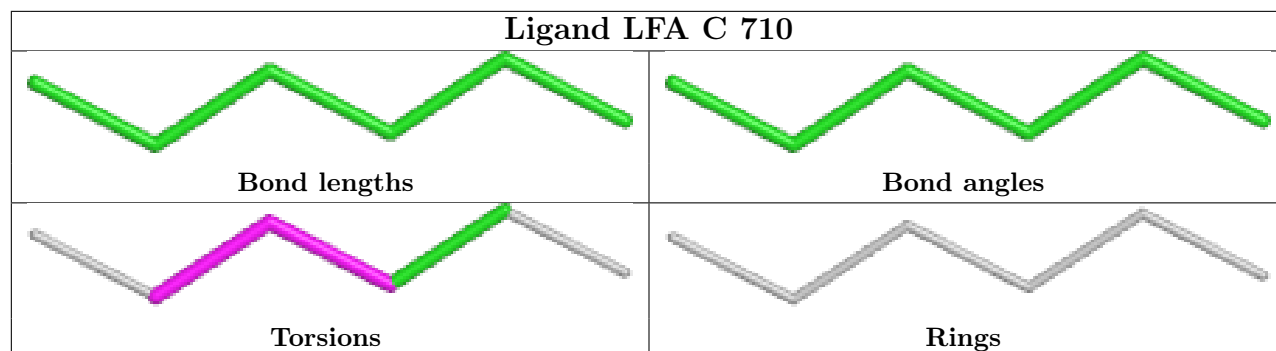


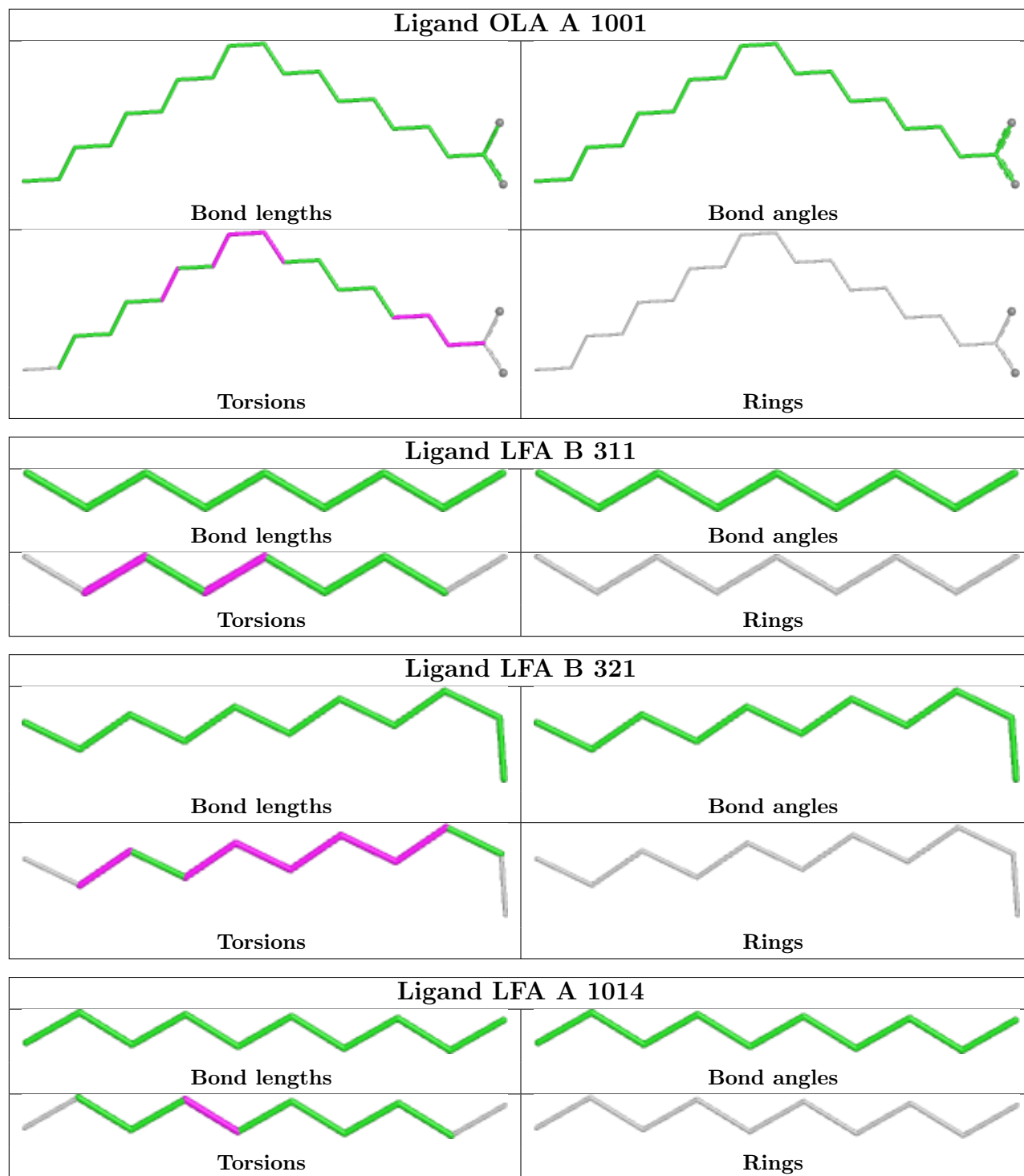


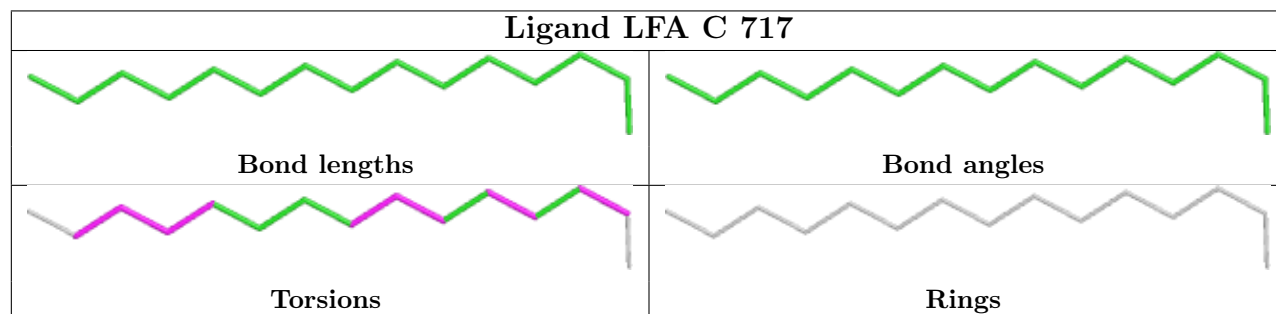
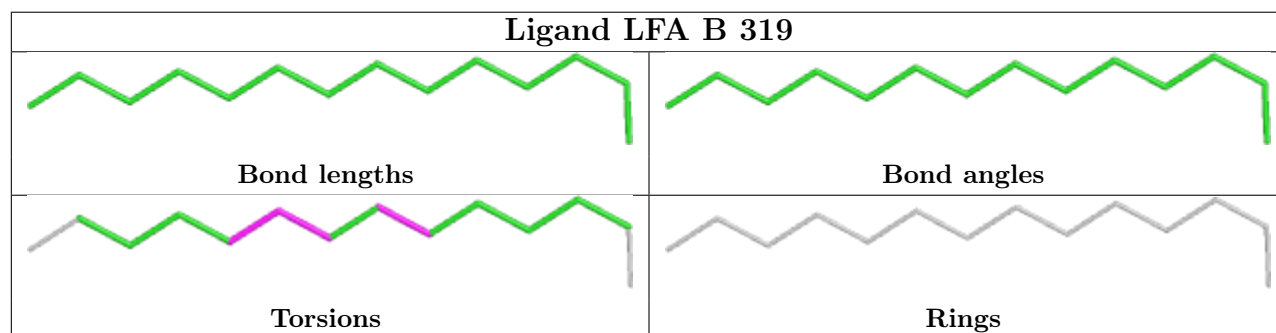
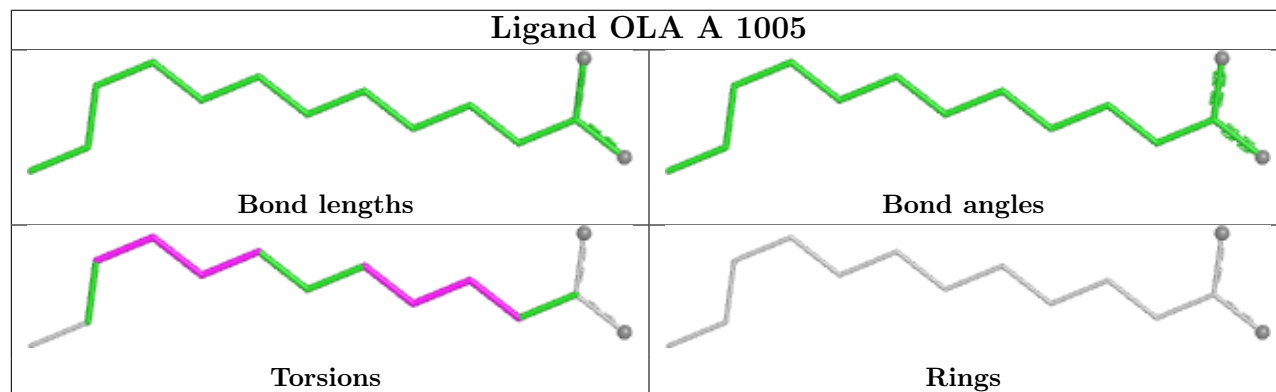
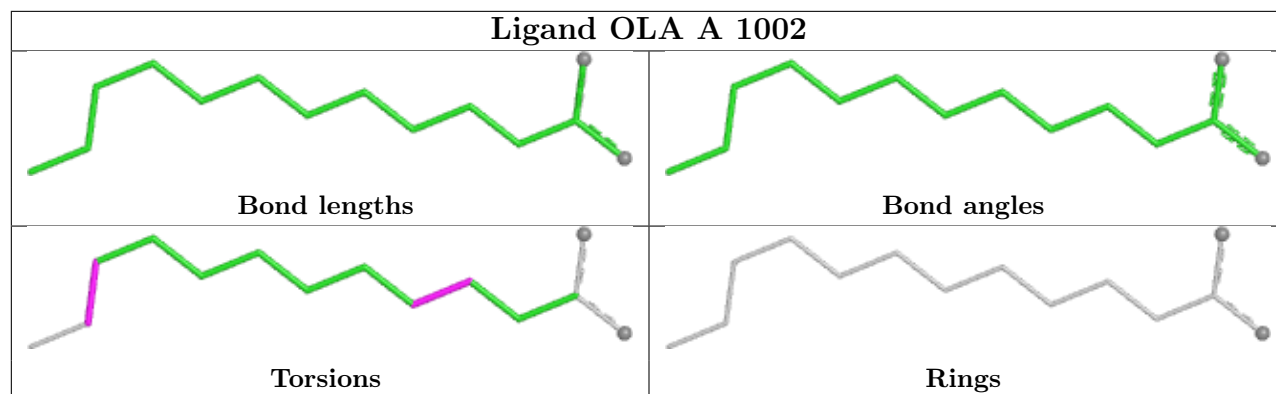


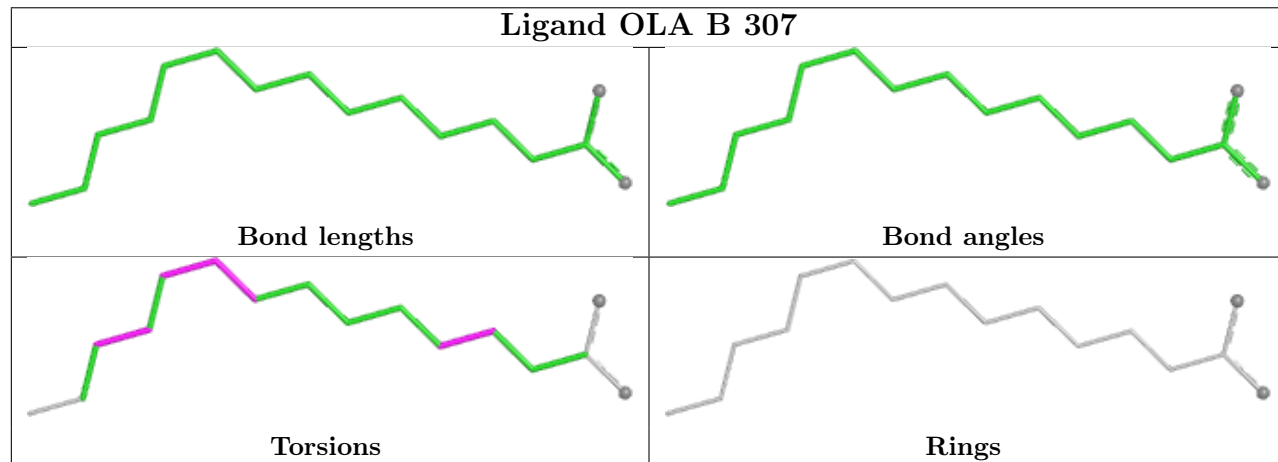
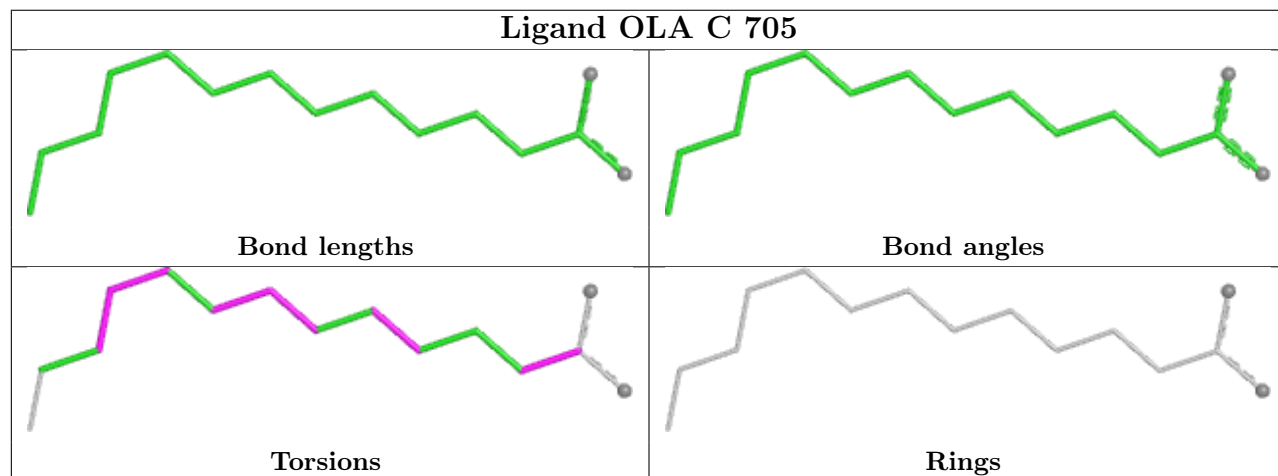
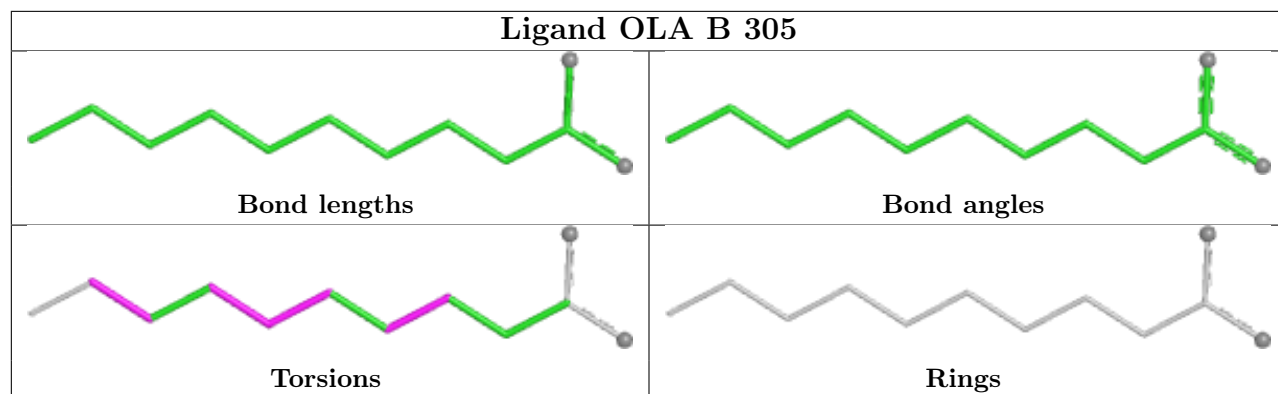


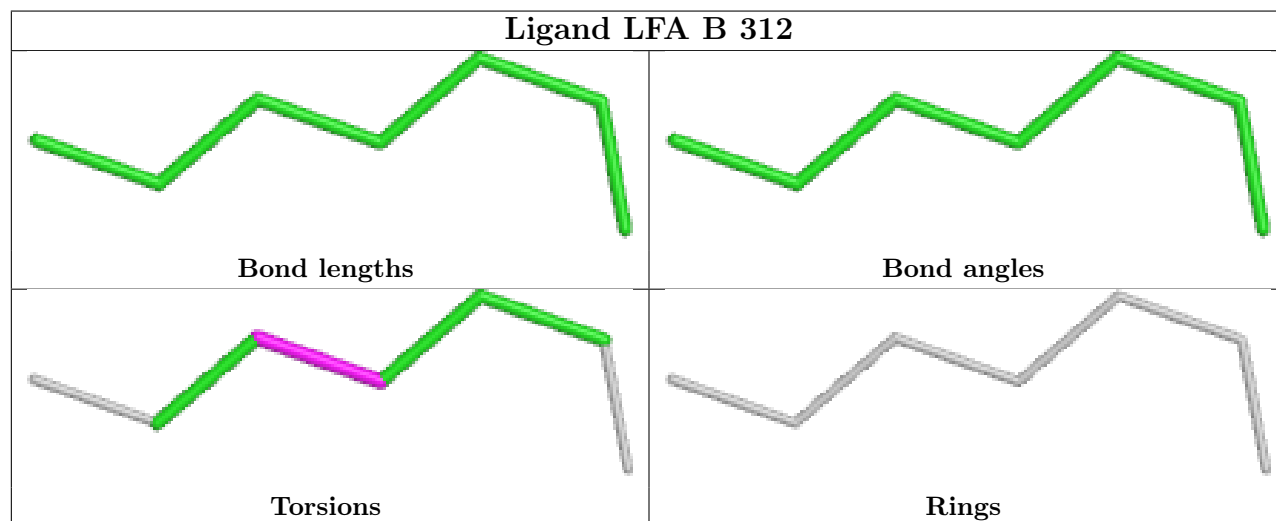
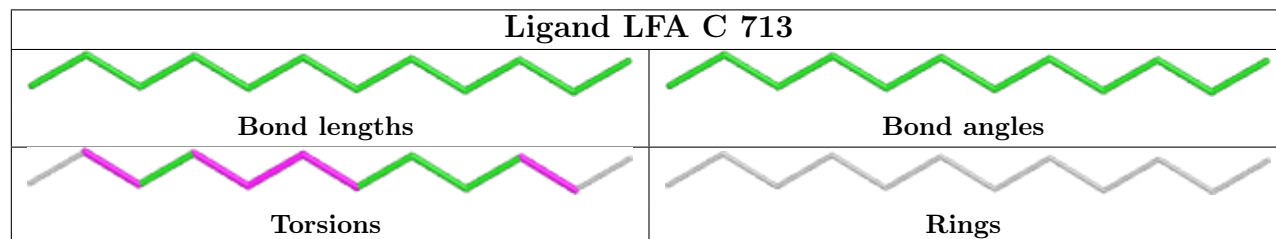
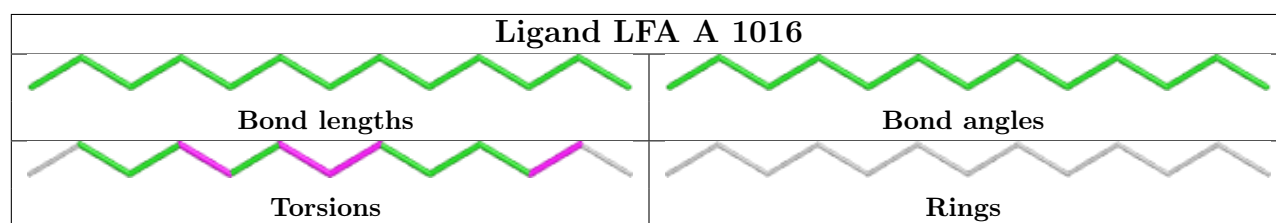
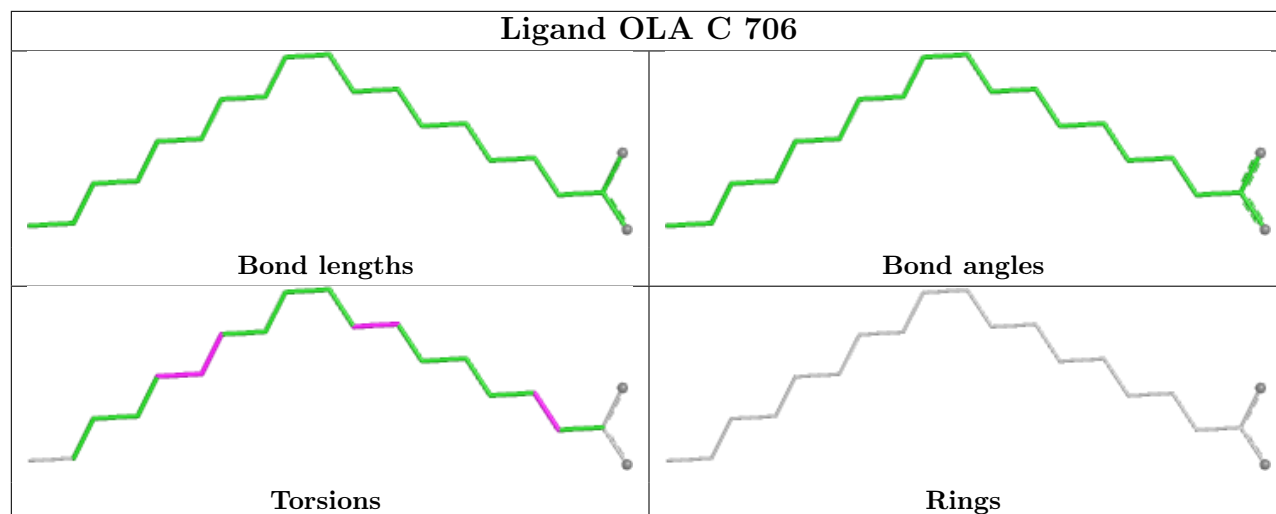


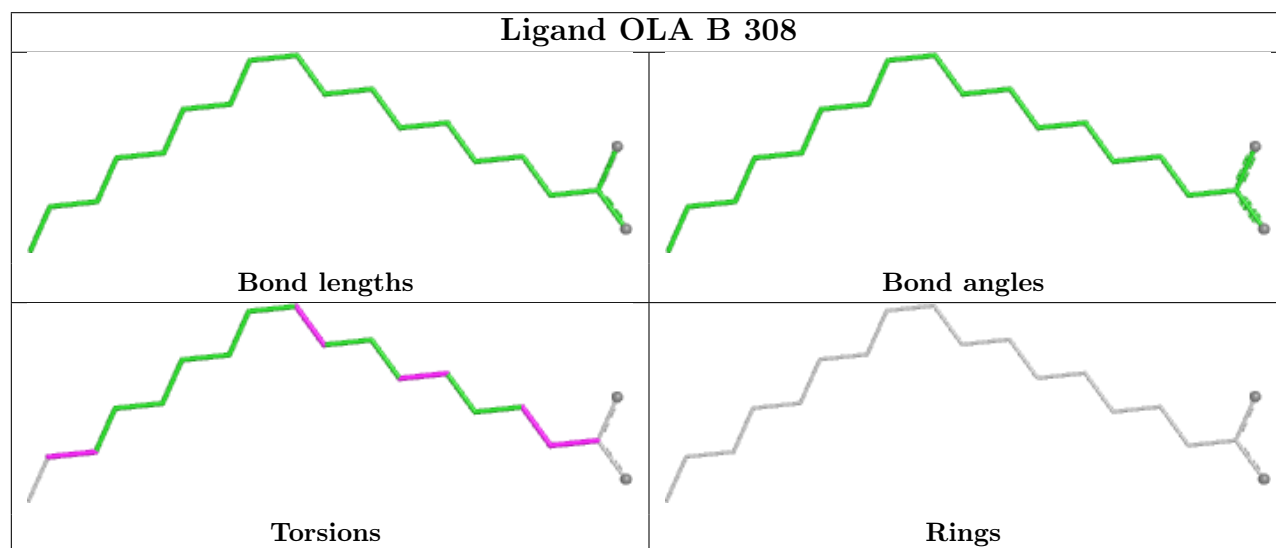
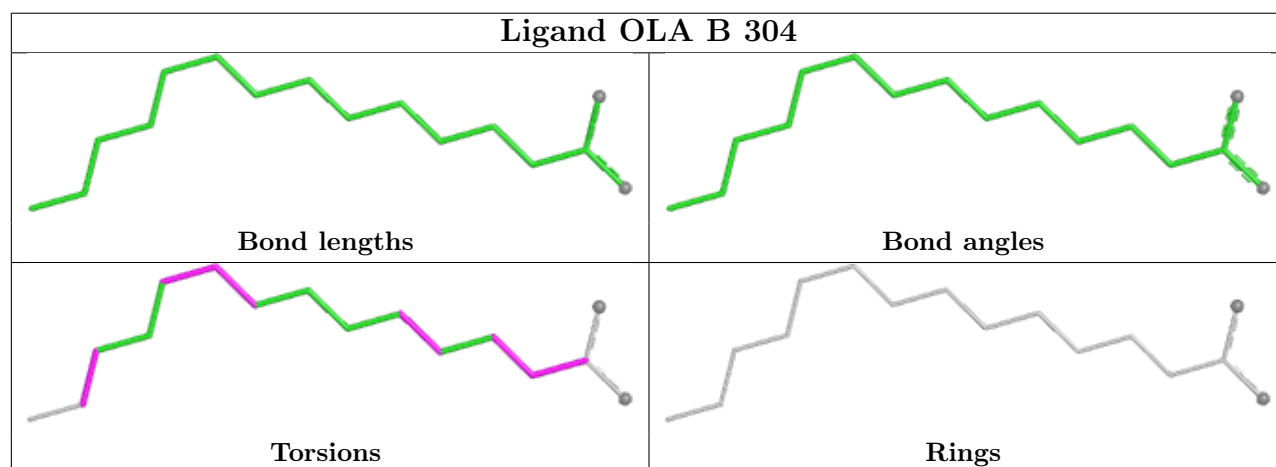
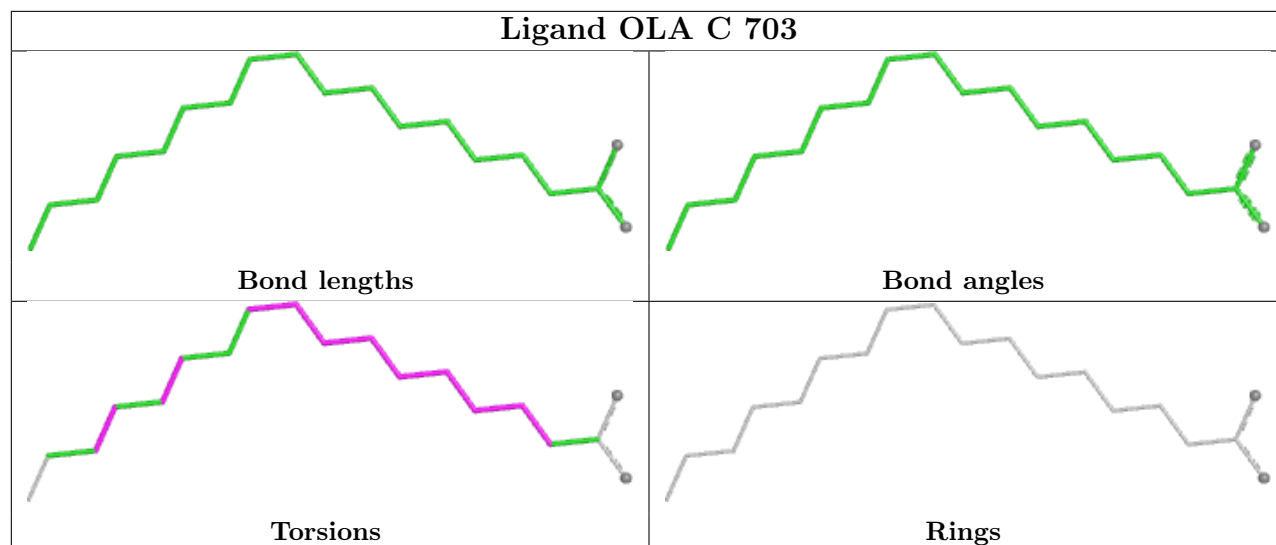


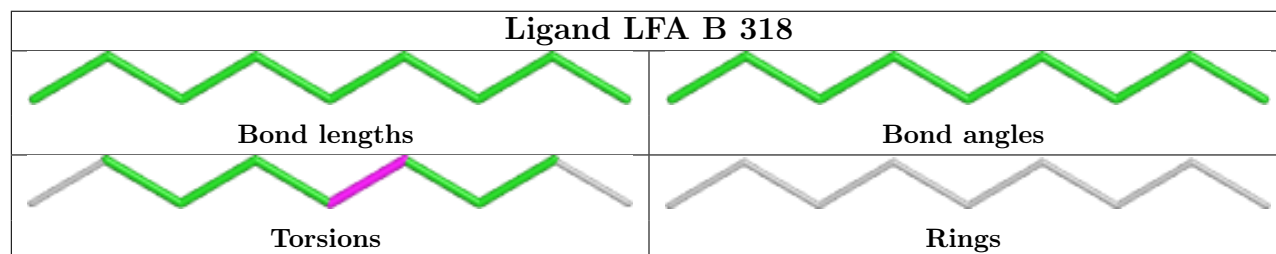
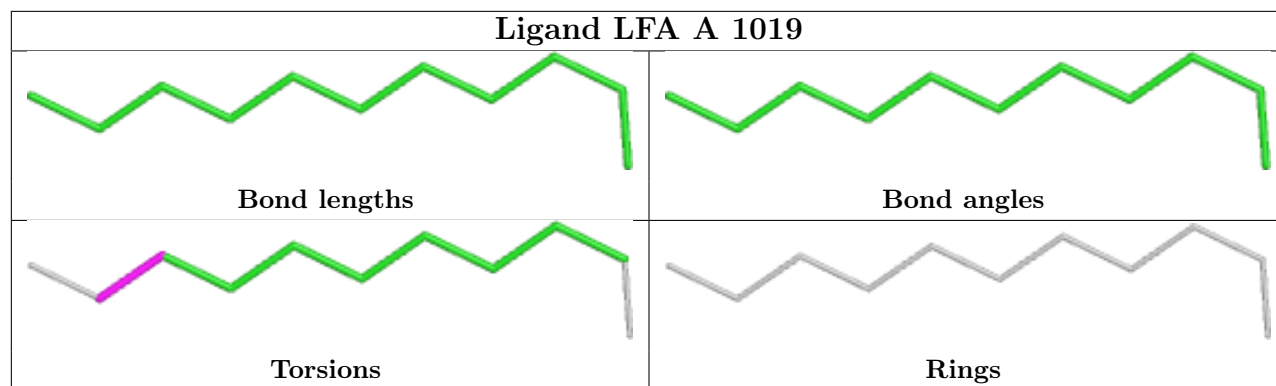
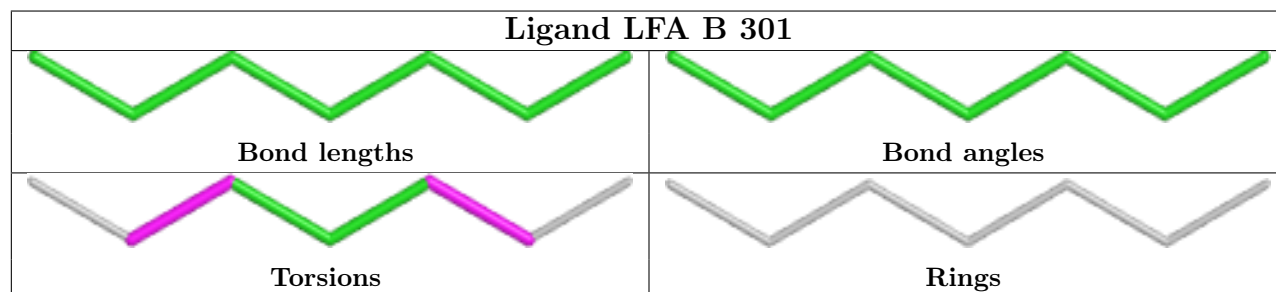
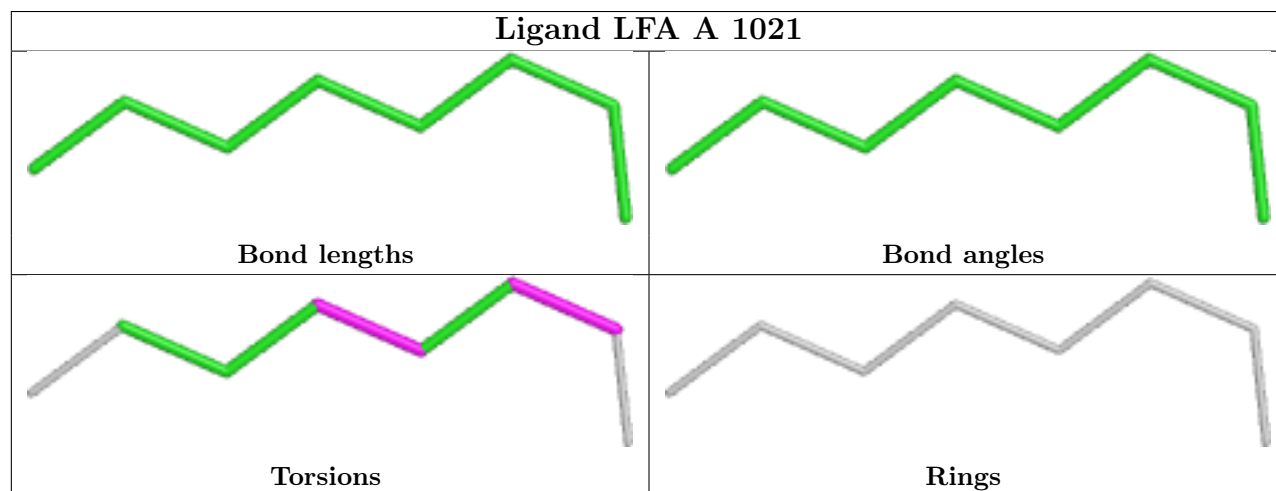
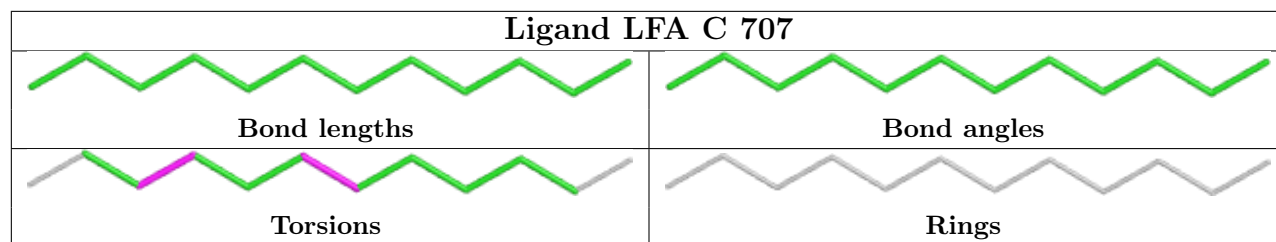


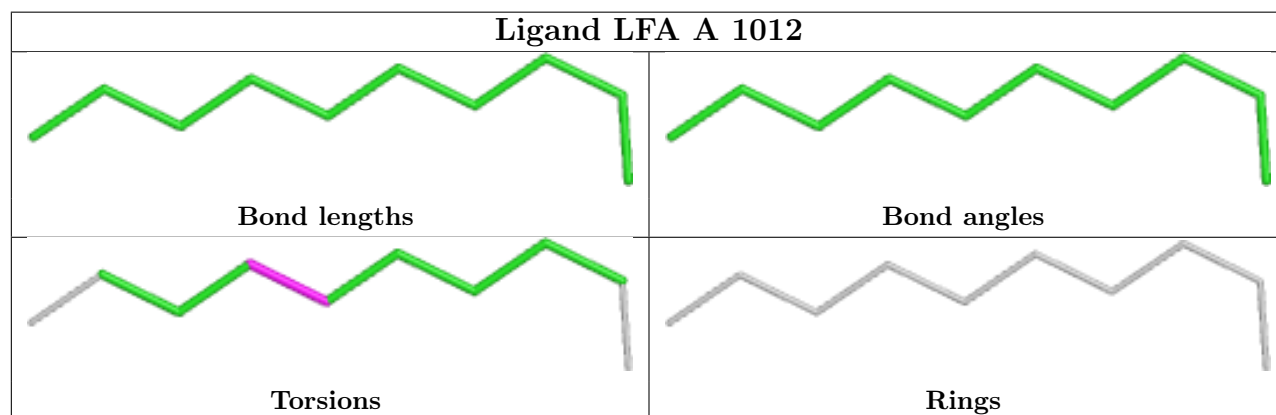
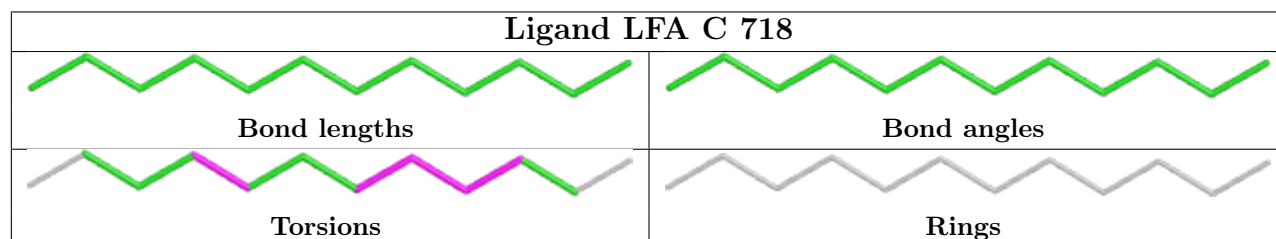
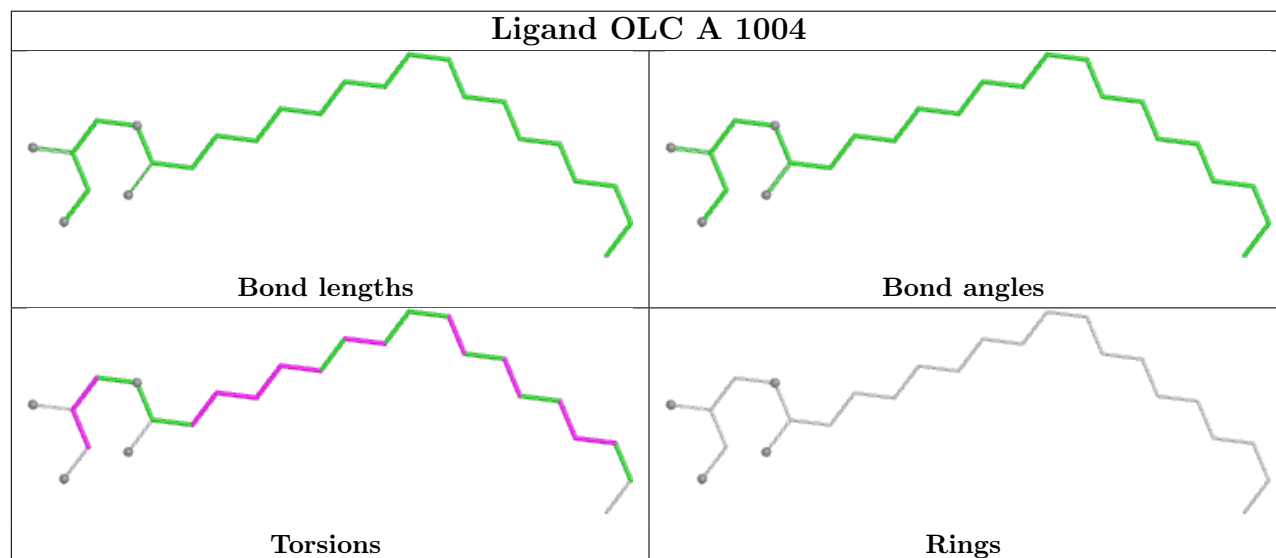
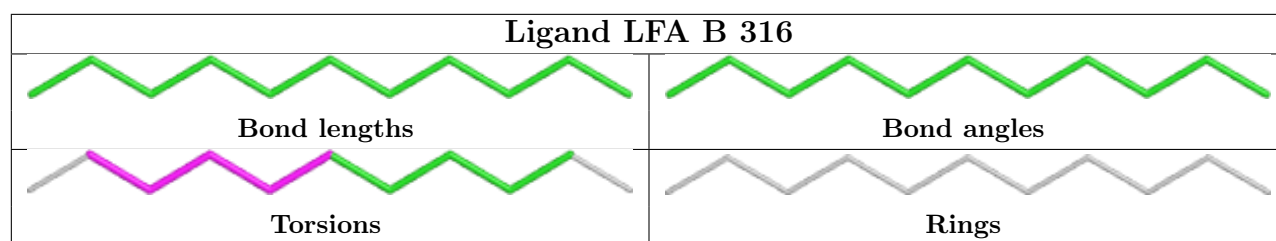


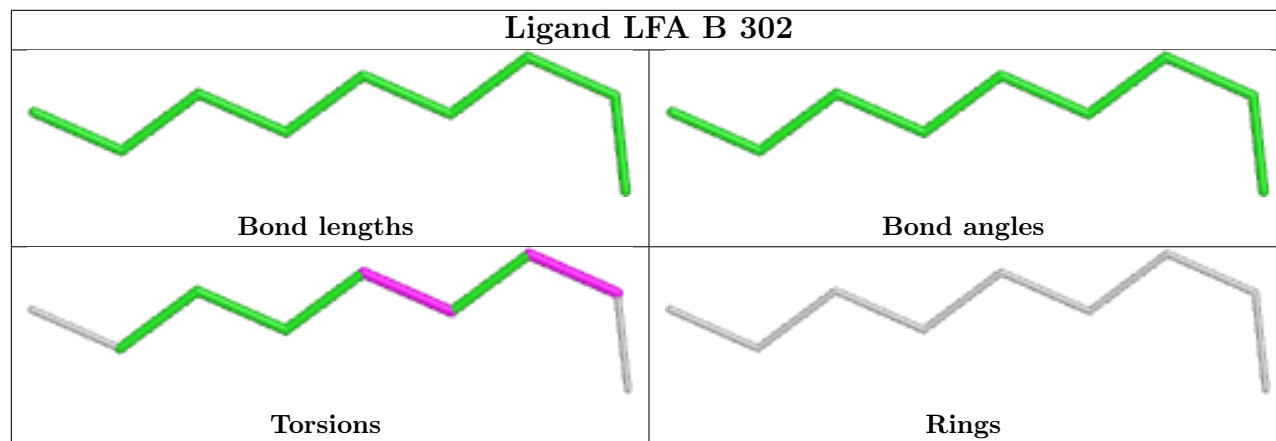
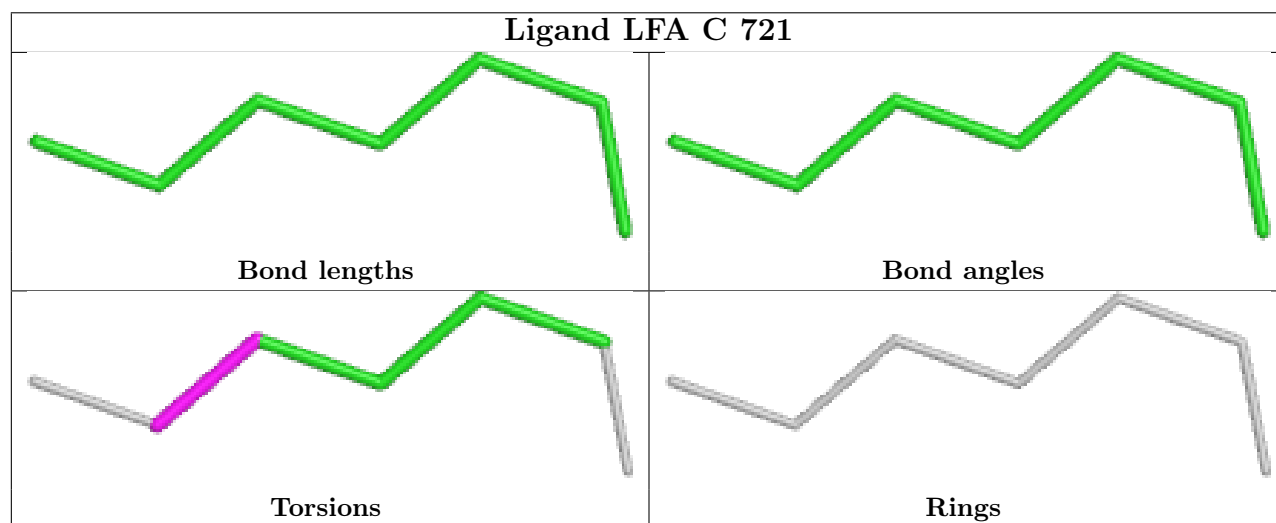
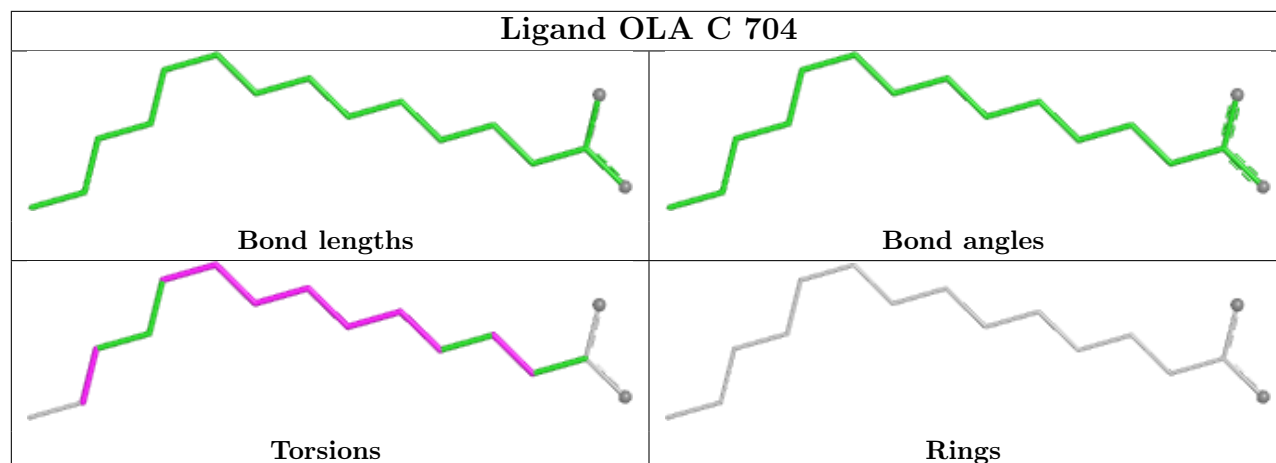


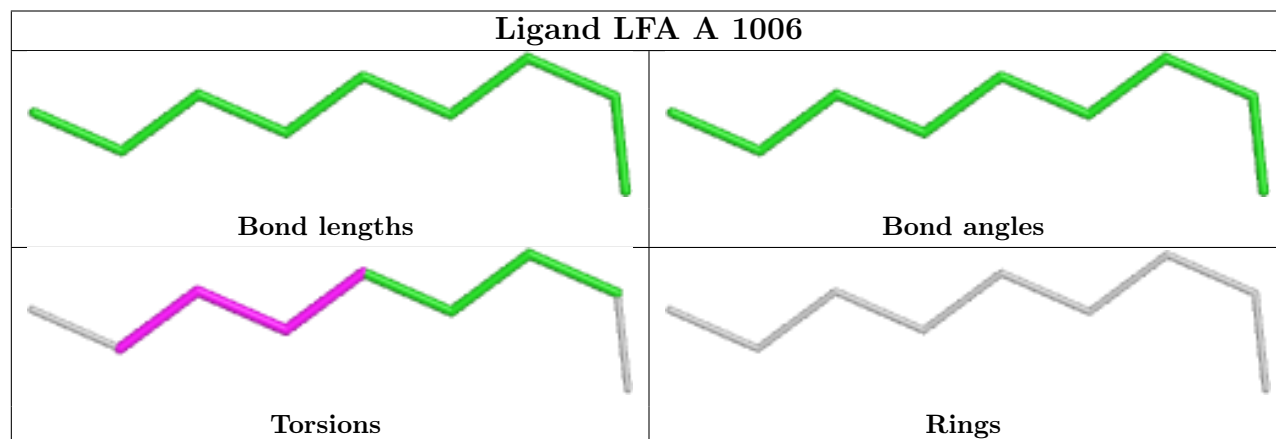
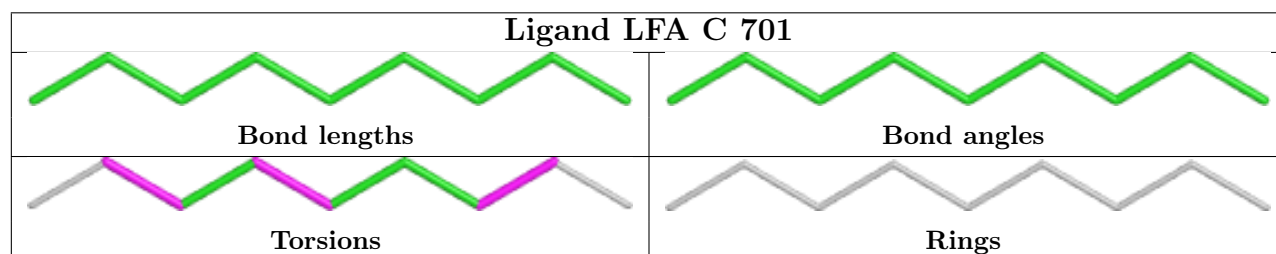
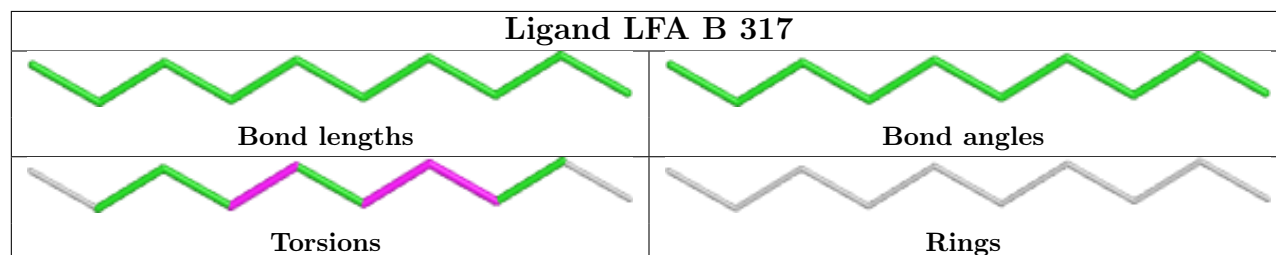
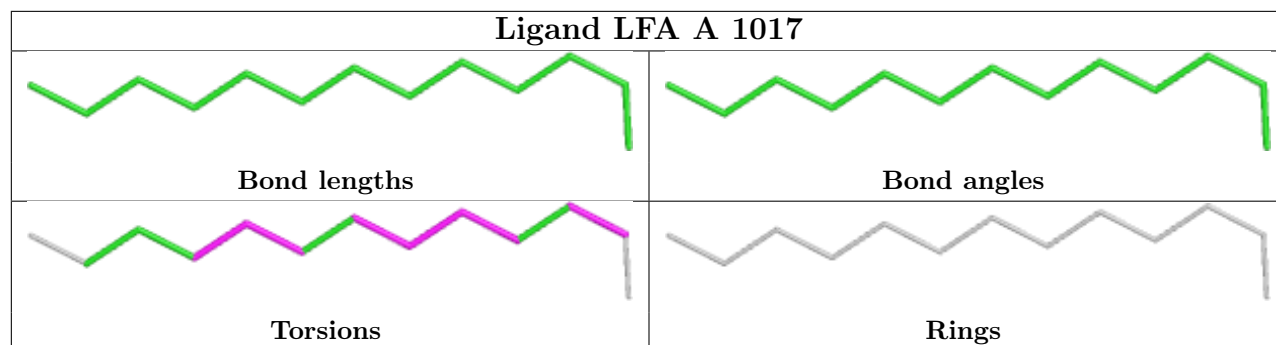


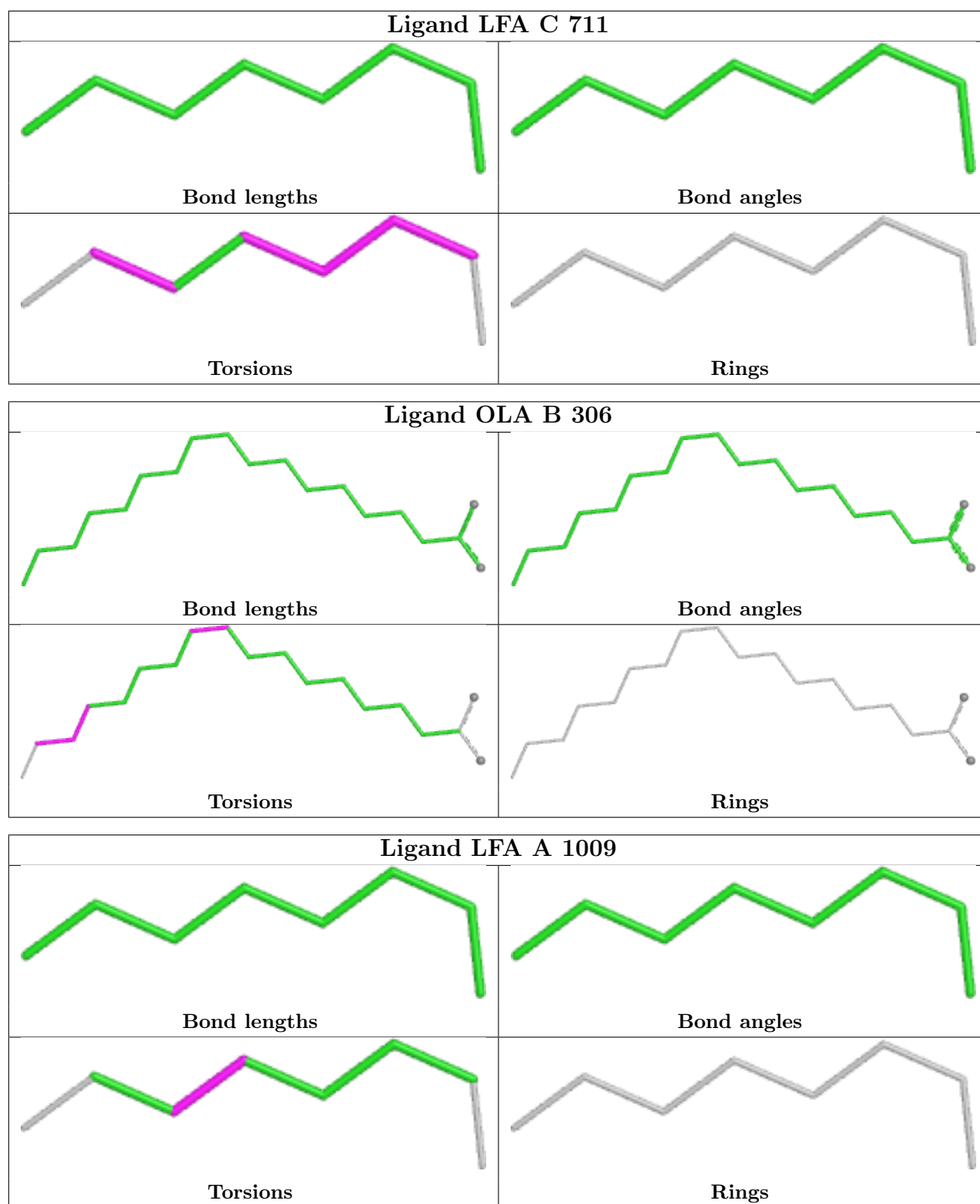












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	222/229 (96%)	-0.02	8 (3%)	46 46	11, 27, 48, 101	5 (2%)
1	B	219/229 (95%)	-0.04	4 (1%)	67 68	11, 28, 47, 83	5 (2%)
1	C	220/229 (96%)	0.03	6 (2%)	56 56	11, 29, 48, 93	4 (1%)
All	All	661/687 (96%)	-0.01	18 (2%)	56 56	11, 28, 48, 101	14 (2%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	PHE	3.8
1	A	224	SER	3.7
1	C	61	TYR	3.6
1	A	62	ASP	3.6
1	C	64	THR	3.2
1	C	224	SER	3.2
1	A	61	TYR	3.1
1	B	61	TYR	3.0
1	B	121	ILE	3.0
1	C	121	ILE	3.0
1	B	64	THR	2.8
1	A	121	ILE	2.6
1	B	59	PHE	2.6
1	C	59	PHE	2.6
1	C	189	LEU	2.5
1	A	64	THR	2.5
1	A	223	GLN	2.4
1	A	157	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	FME	B	1	10/11	0.77	0.15	39,56,82,90	0
1	FME	A	1	10/11	0.83	0.14	35,50,80,86	0
1	FME	C	1	10/11	0.87	0.12	43,50,96,100	0
1	LYR	C	207	29/30	0.91	0.09	22,25,31,43	0
1	LYR	B	207	29/30	0.92	0.09	20,24,30,38	0
1	LYR	A	207	29/30	0.92	0.08	21,25,30,41	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(Å ²)	Q<0.9
4	LFA	C	719	9/20	0.47	0.19	66,78,85,89	0
2	OLA	B	305	12/20	0.58	0.24	48,56,74,77	0
4	LFA	B	320	4/20	0.62	0.25	44,49,56,59	0
2	OLA	A	1003	8/20	0.65	0.19	52,57,66,69	0
4	LFA	A	1020	8/20	0.66	0.22	34,49,55,56	0
4	LFA	C	710	6/20	0.68	0.12	60,71,76,77	0
2	OLA	B	309	14/20	0.68	0.17	46,58,67,73	0
4	LFA	C	717	15/20	0.69	0.22	53,70,89,95	0
4	LFA	B	310	6/20	0.71	0.16	60,64,69,70	0
4	LFA	A	1014	10/20	0.71	0.20	55,63,73,74	0
4	LFA	B	321	11/20	0.71	0.20	49,61,67,69	0
4	LFA	A	1012	10/20	0.72	0.19	50,56,68,70	0
2	OLA	C	702	16/20	0.72	0.14	37,49,52,59	0
4	LFA	B	322	9/20	0.72	0.20	52,62,67,71	0
4	LFA	C	720	9/20	0.72	0.18	60,62,66,68	0
2	OLA	B	307	16/20	0.73	0.19	69,80,91,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	LFA	C	709	9/20	0.73	0.19	52,57,62,62	0
4	LFA	B	316	11/20	0.74	0.17	50,57,83,87	0
4	LFA	A	1006	9/20	0.74	0.14	60,63,72,77	0
4	LFA	B	311	9/20	0.74	0.19	54,69,74,76	0
2	OLA	A	1001	20/20	0.75	0.15	35,48,61,61	0
2	OLA	B	306	19/20	0.75	0.17	44,51,70,72	0
4	LFA	A	1021	8/20	0.77	0.14	57,60,64,66	0
4	LFA	A	1010	6/20	0.78	0.15	44,52,57,59	0
2	OLA	C	704	16/20	0.78	0.16	48,59,67,76	0
4	LFA	C	707	12/20	0.79	0.18	62,73,76,79	0
4	LFA	A	1009	8/20	0.79	0.13	50,55,60,64	0
4	LFA	A	1015	10/20	0.79	0.15	48,62,67,68	0
4	LFA	C	721	7/20	0.79	0.15	56,60,64,65	0
4	LFA	C	712	8/20	0.80	0.15	37,45,71,72	0
4	LFA	C	713	12/20	0.80	0.15	48,70,74,76	0
4	LFA	A	1022	6/20	0.80	0.17	48,50,55,56	0
4	LFA	C	718	12/20	0.80	0.16	57,65,74,75	0
4	LFA	C	708	8/20	0.80	0.14	59,61,65,66	0
4	LFA	A	1013	4/20	0.80	0.20	49,54,54,62	0
4	LFA	B	318	9/20	0.80	0.18	44,49,57,60	0
4	LFA	A	1011	3/20	0.81	0.29	56,56,58,63	0
4	LFA	A	1016	13/20	0.81	0.17	54,63,71,74	0
4	LFA	B	301	7/20	0.81	0.12	41,42,49,51	0
3	OLC	A	1004	25/25	0.81	0.13	35,50,65,69	0
4	LFA	C	715	8/20	0.81	0.15	50,54,58,59	0
4	LFA	B	312	7/20	0.82	0.12	47,49,50,50	0
4	LFA	B	313	5/20	0.82	0.14	51,52,54,54	0
2	OLA	B	303	13/20	0.82	0.13	40,48,67,70	0
4	LFA	A	1019	11/20	0.82	0.11	45,52,67,71	0
4	LFA	B	319	14/20	0.82	0.14	51,56,61,62	0
4	LFA	A	1008	12/20	0.83	0.14	44,51,61,61	0
4	LFA	B	315	8/20	0.83	0.12	38,45,53,57	0
4	LFA	C	714	10/20	0.83	0.11	49,51,54,55	0
2	OLA	A	1005	14/20	0.84	0.12	39,55,61,74	0
2	OLA	C	703	19/20	0.85	0.17	42,50,78,92	0
4	LFA	A	1017	13/20	0.86	0.14	50,51,62,64	0
4	LFA	A	1018	17/20	0.86	0.12	36,51,67,70	0
4	LFA	A	1023	4/20	0.86	0.13	64,67,67,68	0
4	LFA	B	314	15/20	0.86	0.16	40,49,70,72	0
4	LFA	A	1007	9/20	0.86	0.12	43,46,49,51	0
2	OLA	C	705	15/20	0.86	0.13	45,51,71,78	0
2	OLA	C	706	20/20	0.87	0.10	40,49,60,63	0

Continued on next page...

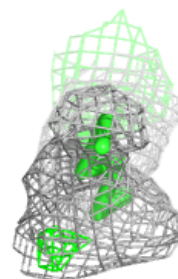
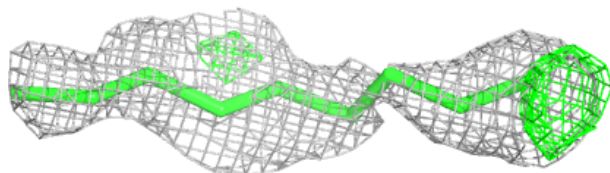
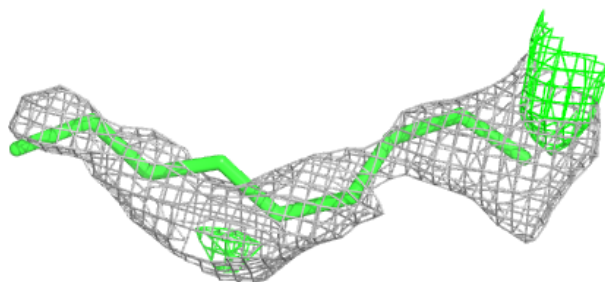
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OLA	B	308	19/20	0.87	0.13	38,46,64,79	0
2	OLA	B	304	16/20	0.87	0.17	44,58,74,77	0
4	LFA	C	701	9/20	0.87	0.12	37,39,45,46	0
4	LFA	C	716	7/20	0.87	0.15	51,54,60,66	0
4	LFA	B	302	9/20	0.88	0.09	46,48,60,66	0
4	LFA	C	711	8/20	0.88	0.12	44,48,54,55	0
5	PO4	A	1024	5/5	0.89	0.09	69,70,74,76	5
2	OLA	A	1002	14/20	0.90	0.12	43,53,70,73	0
4	LFA	B	317	10/20	0.90	0.11	43,52,56,58	0
5	PO4	C	722	5/5	0.90	0.07	63,63,68,70	5
6	NA	B	323[B]	1/1	0.96	0.06	21,21,21,21	1
6	NA	A	1025[B]	1/1	0.97	0.05	29,29,29,29	1
6	NA	C	723[B]	1/1	0.98	0.04	25,25,25,25	1

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

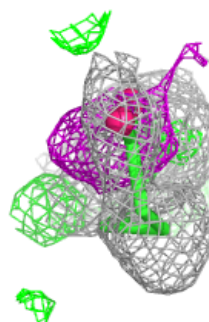
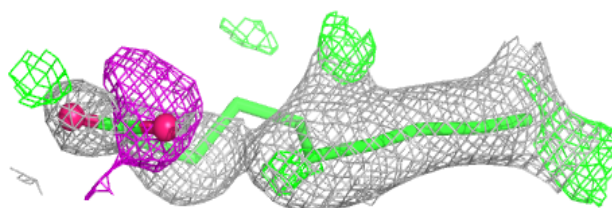
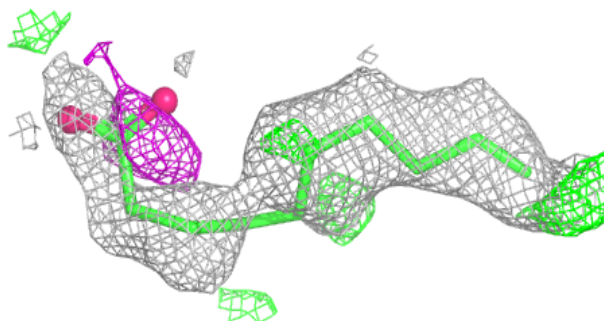
Electron density around LFA C 719:

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

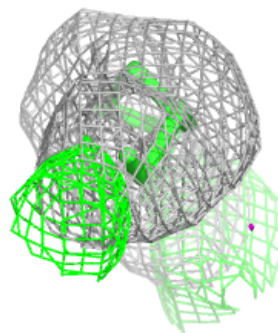
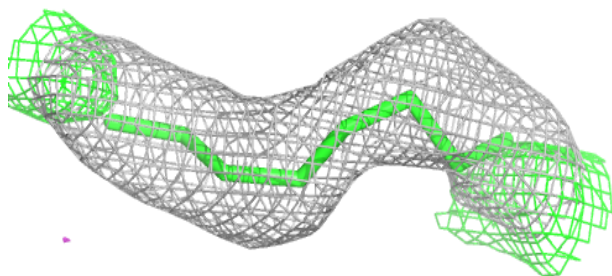
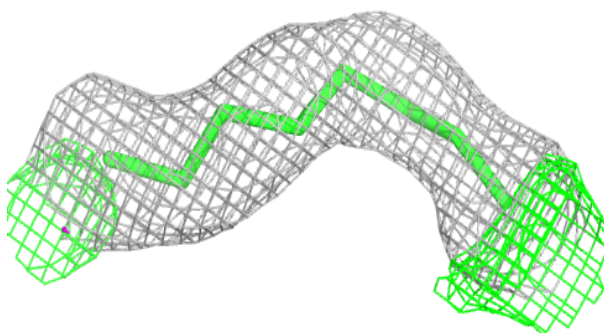


Electron density around OLA B 305:

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

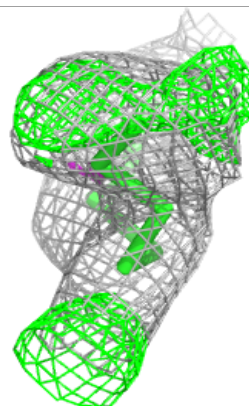
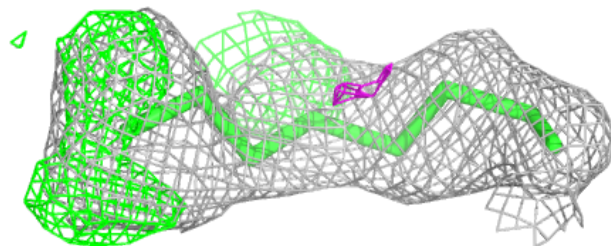
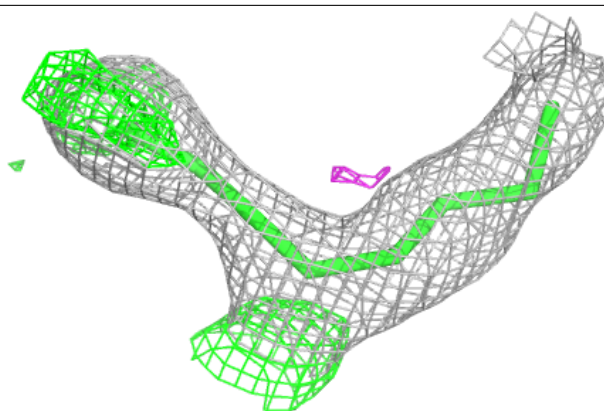
**Electron density around OLA A 1003:**

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

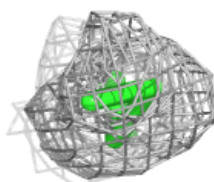
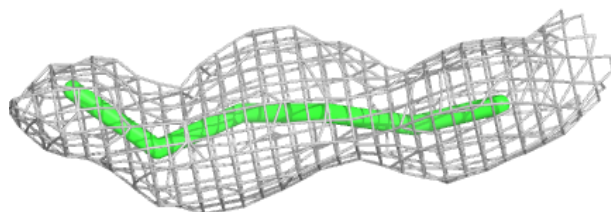
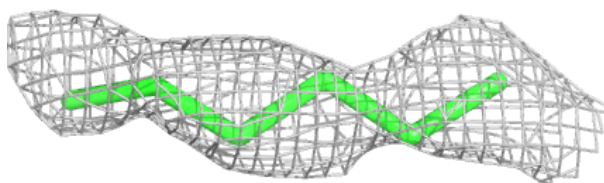


Electron density around LFA A 1020:

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

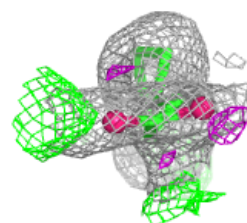
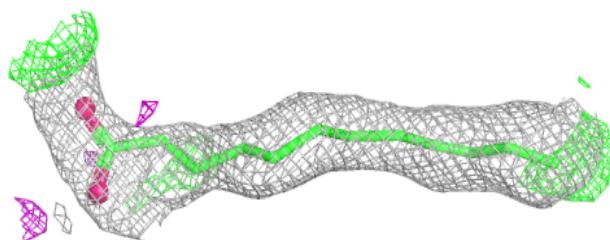
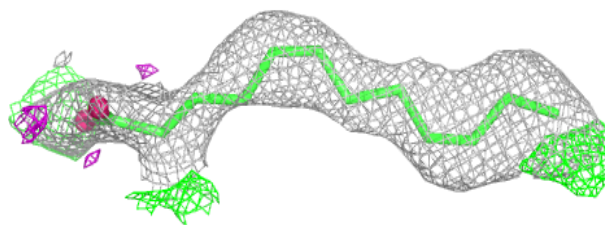
**Electron density around LFA C 710:**

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

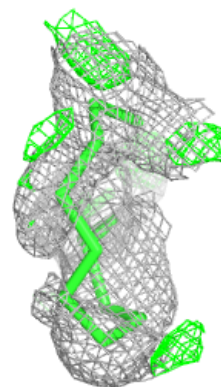
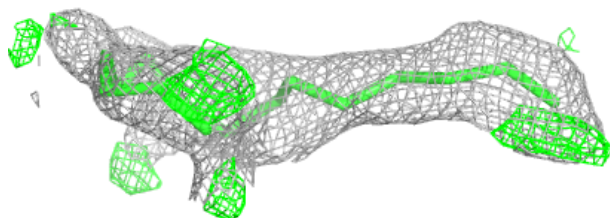
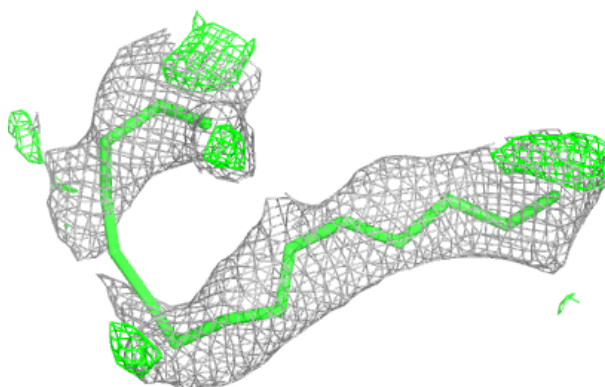


Electron density around OLA B 309:

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

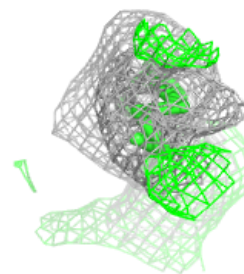
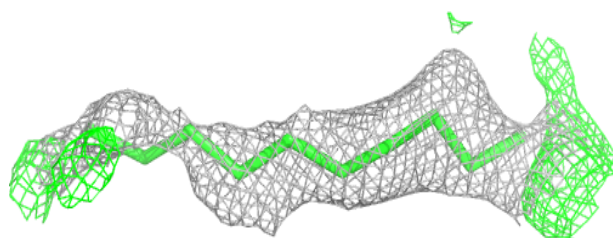
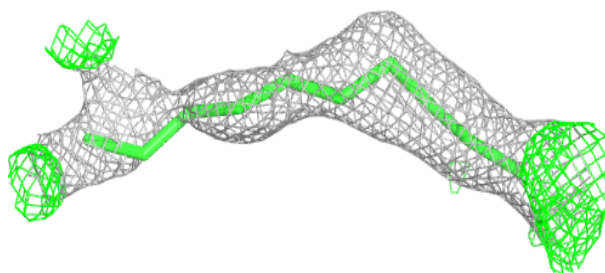
**Electron density around LFA C 717:**

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

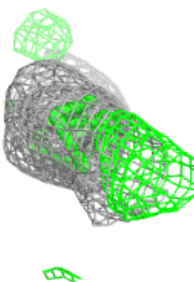
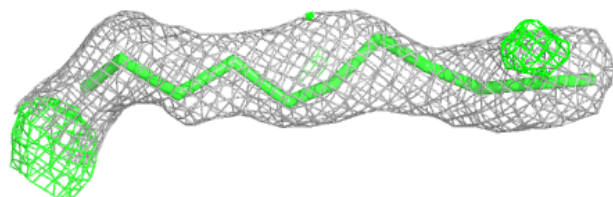
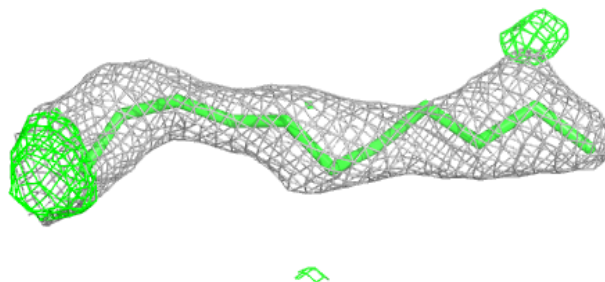


Electron density around LFA A 1014:

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

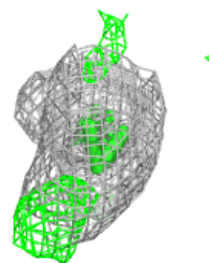
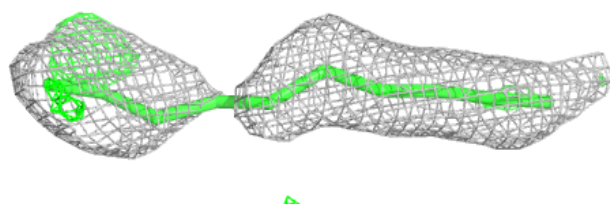
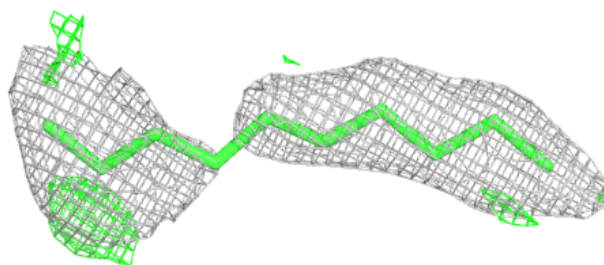
**Electron density around LFA B 321:**

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

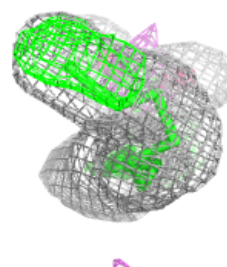
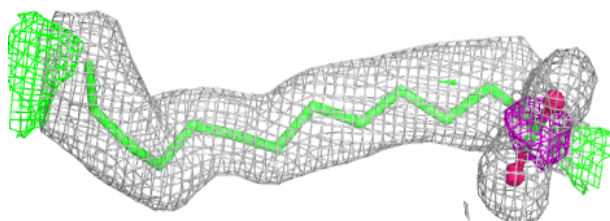
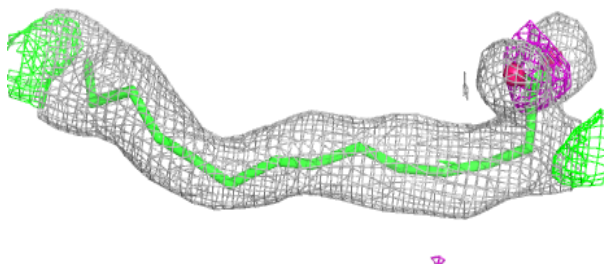


Electron density around LFA A 1012:

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

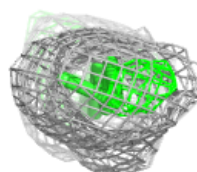
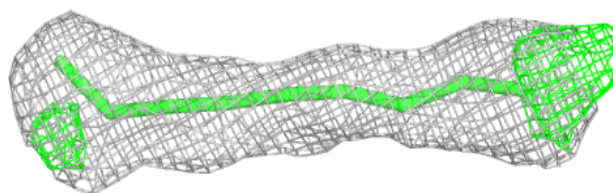
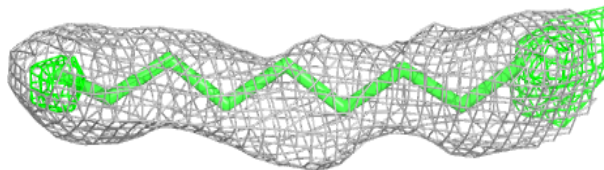
**Electron density around OLA C 702:**

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

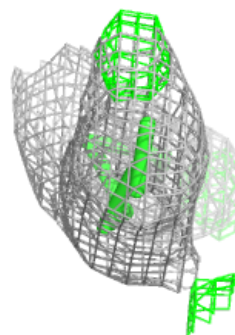
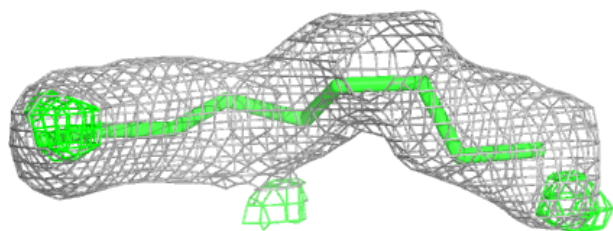
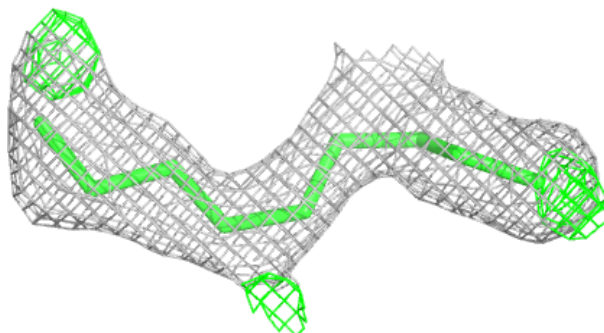


Electron density around LFA B 322:

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

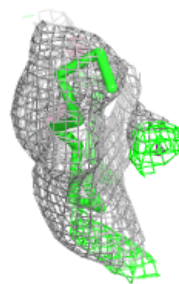
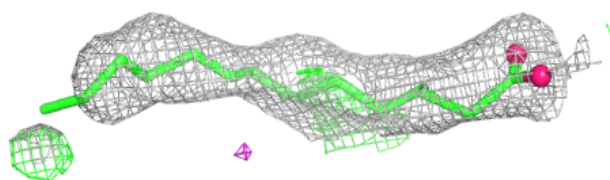
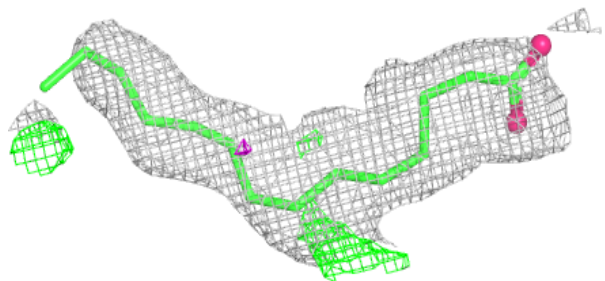
**Electron density around LFA C 720:**

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

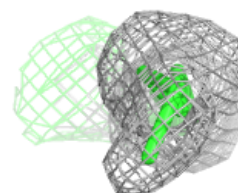
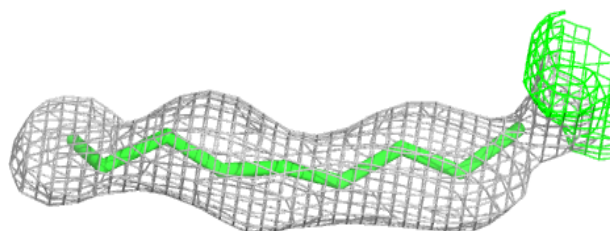
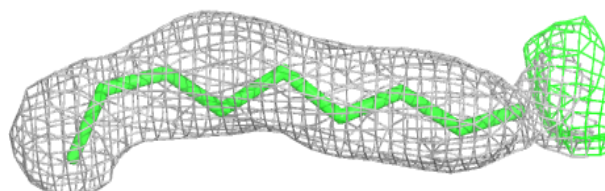


Electron density around OLA B 307:

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

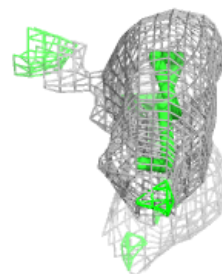
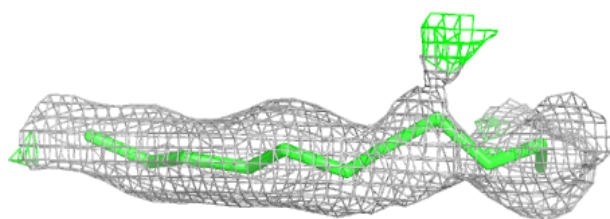
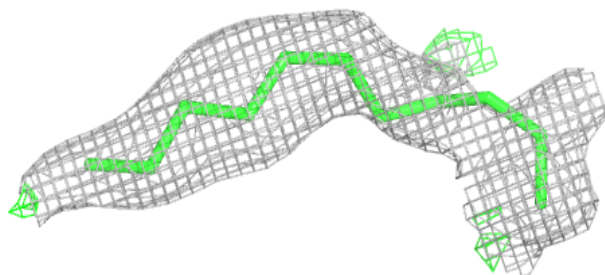
**Electron density around LFA C 709:**

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

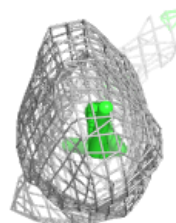
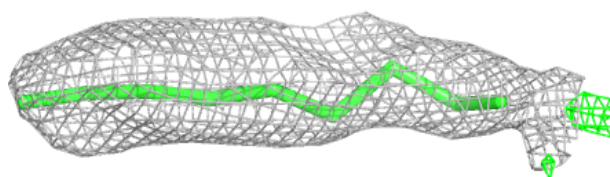
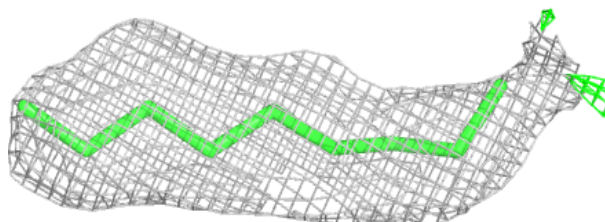


Electron density around LFA B 316:

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

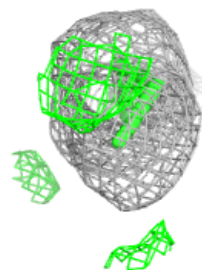
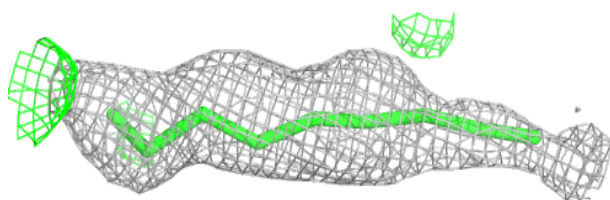
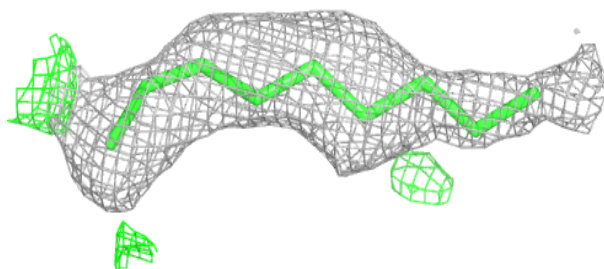
**Electron density around LFA A 1006:**

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

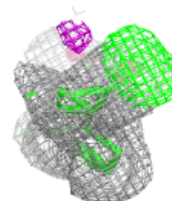
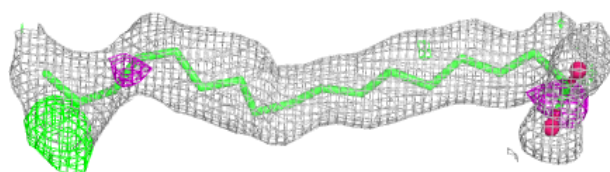
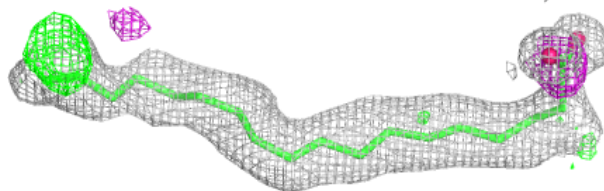


Electron density around LFA B 311:

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

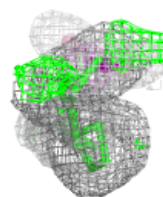
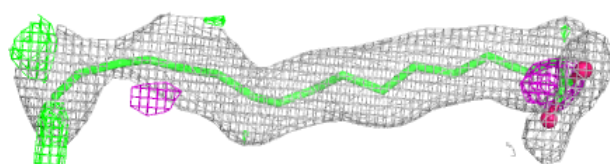
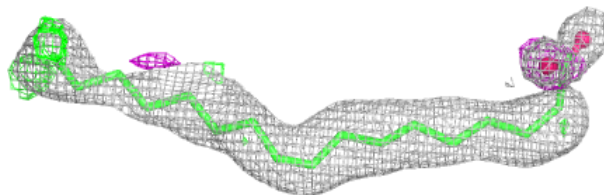
**Electron density around OLA A 1001:**

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

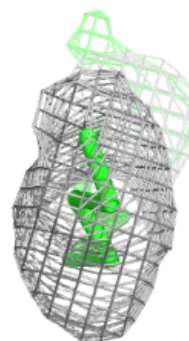
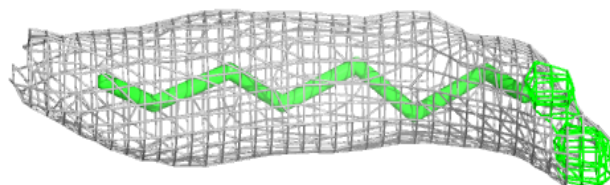
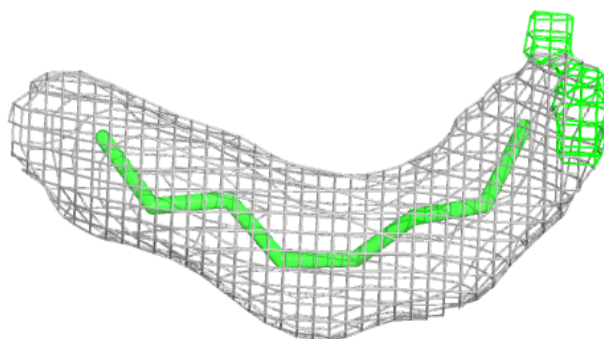


Electron density around OLA B 306:

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

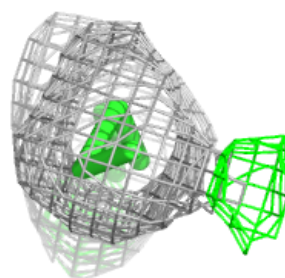
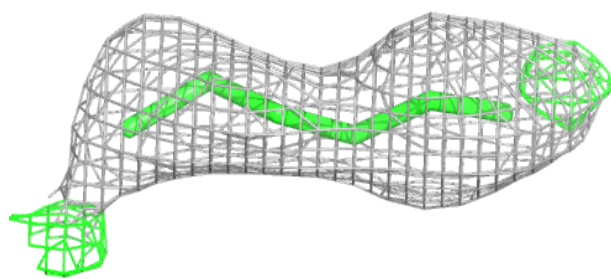
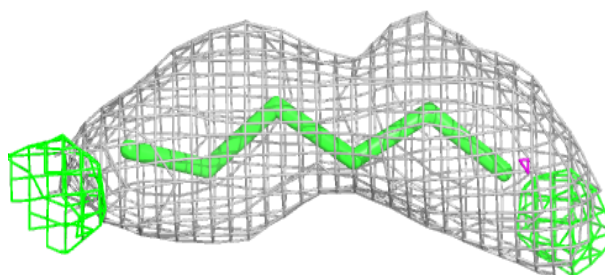
**Electron density around LFA A 1021:**

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

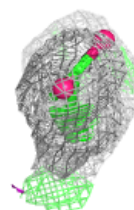
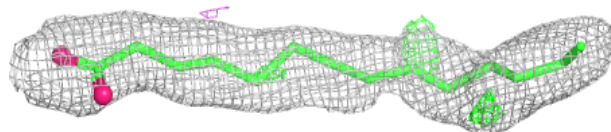
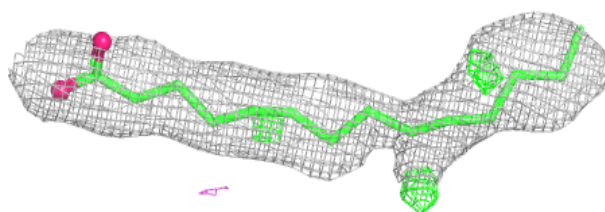


Electron density around LFA A 1010:

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

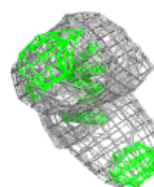
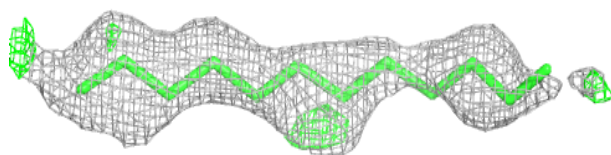
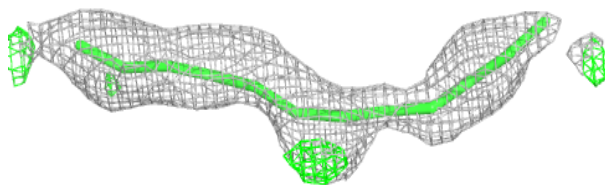
**Electron density around OLA C 704:**

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

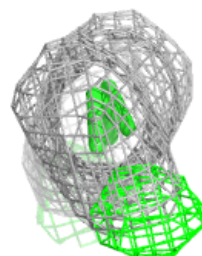
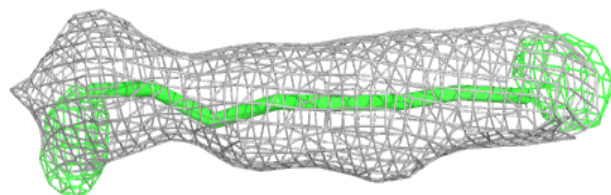
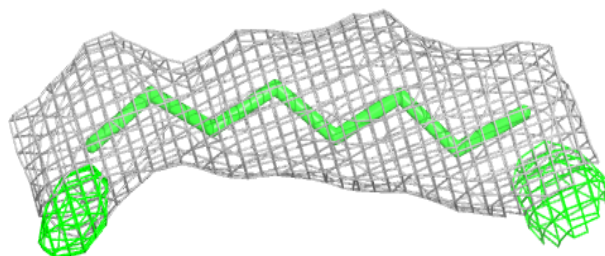


Electron density around LFA C 707:

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

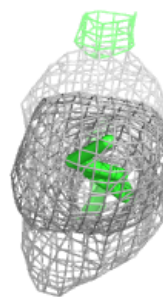
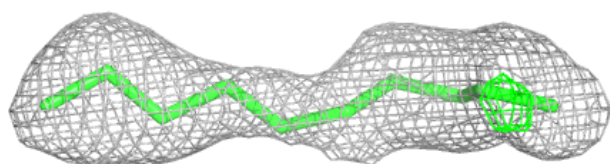
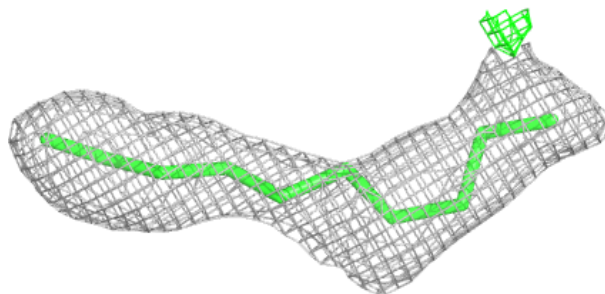
**Electron density around LFA A 1009:**

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

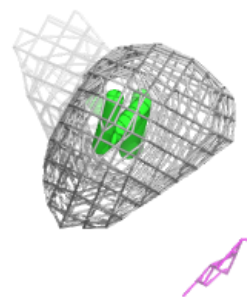
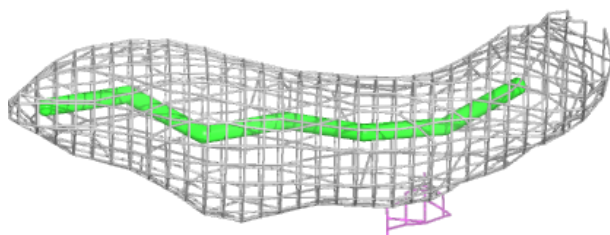
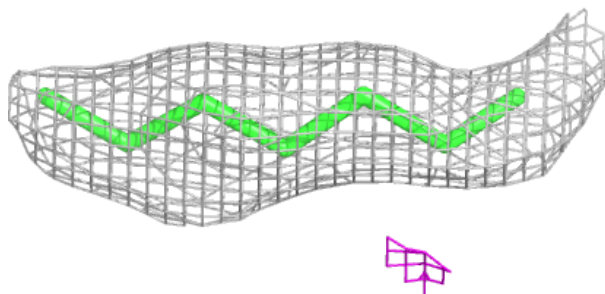


Electron density around LFA A 1015:

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

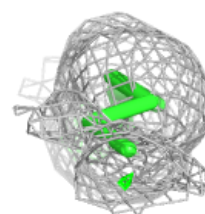
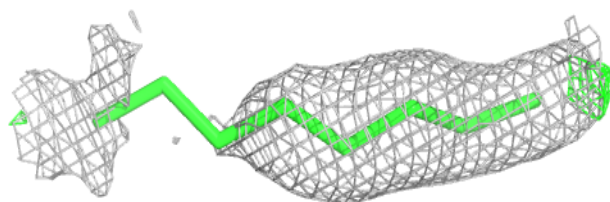
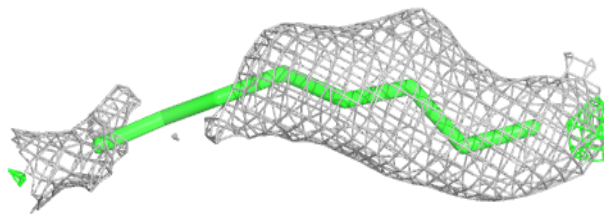
**Electron density around LFA C 721:**

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

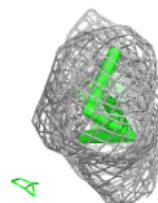
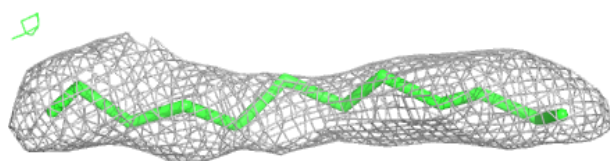
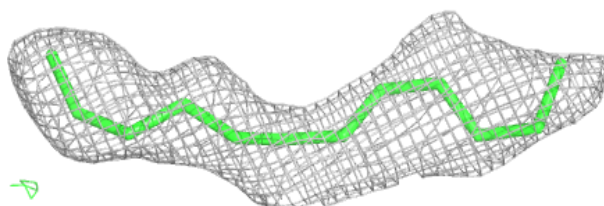


Electron density around LFA C 712:

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

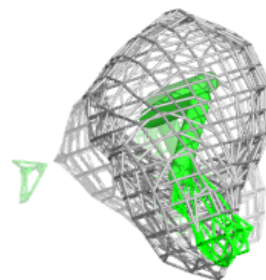
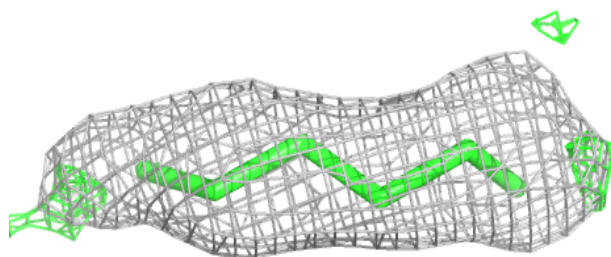
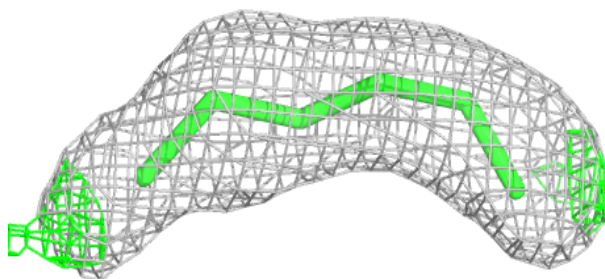
**Electron density around LFA C 713:**

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

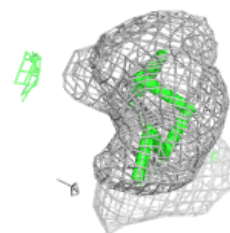
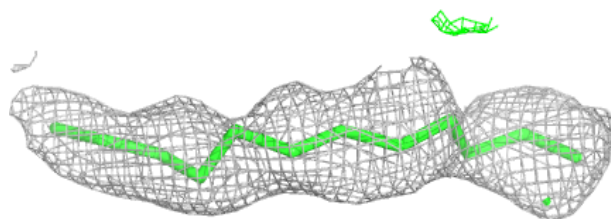
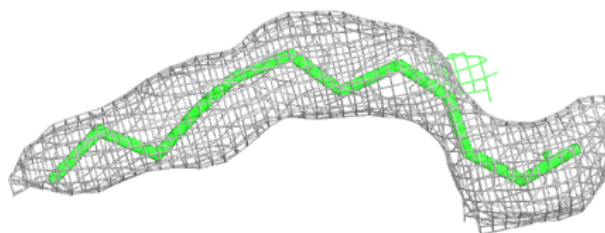


Electron density around LFA A 1022:

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

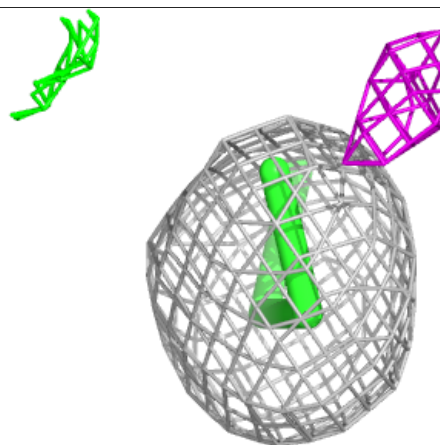
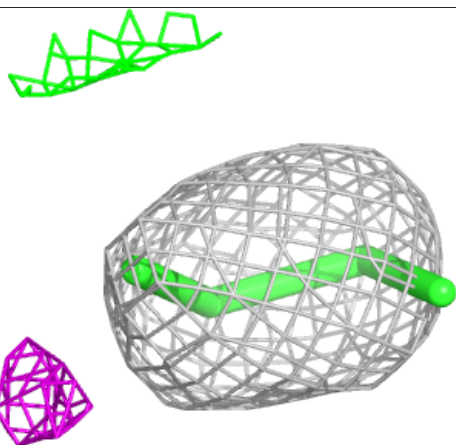
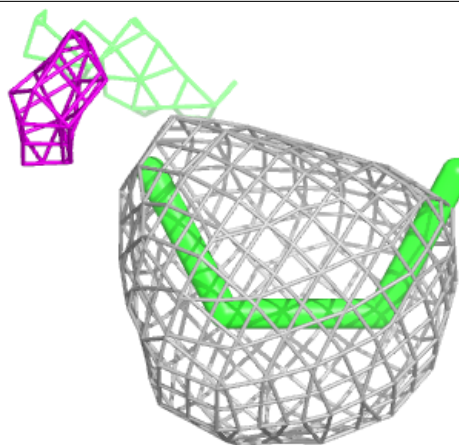
**Electron density around LFA C 718:**

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

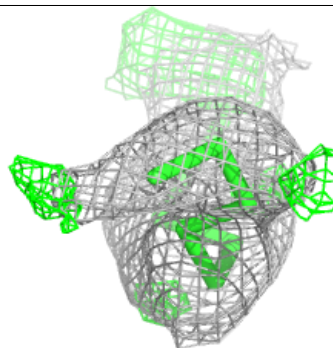
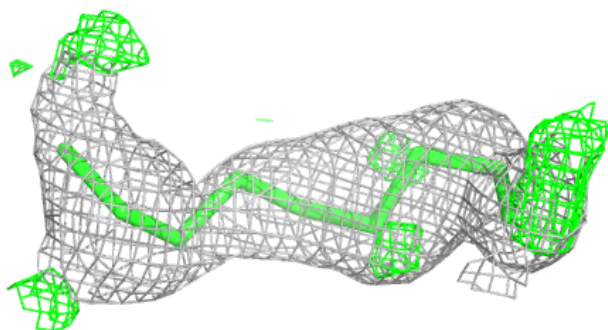
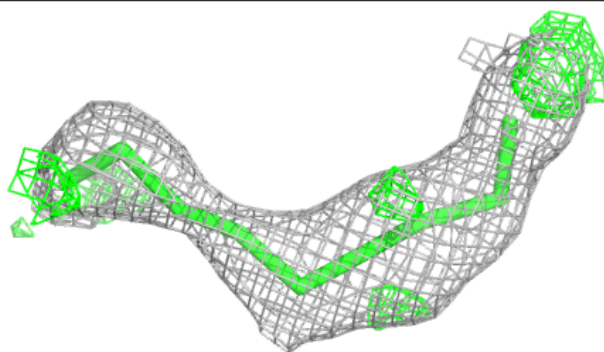


Electron density around LFA A 1013:

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

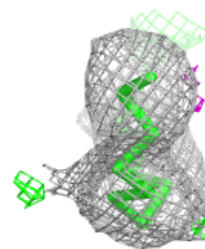
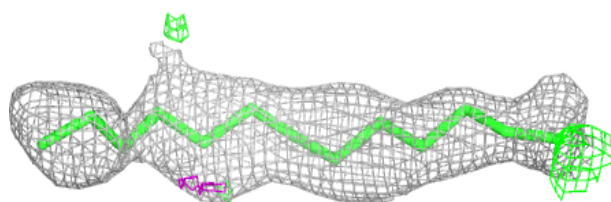
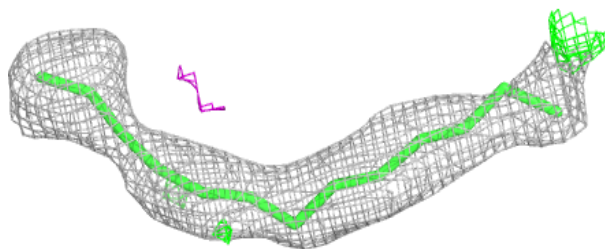
**Electron density around LFA B 318:**

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

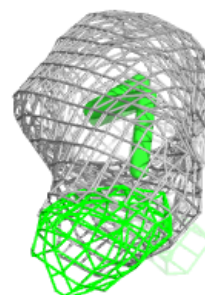
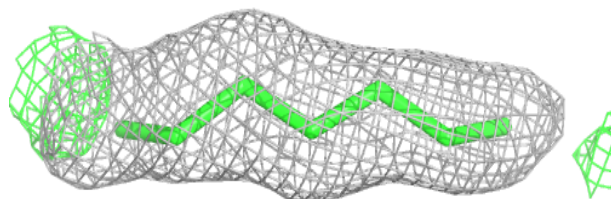
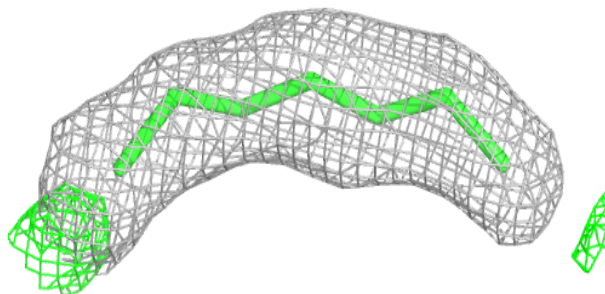


Electron density around LFA A 1016:

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

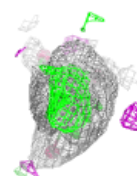
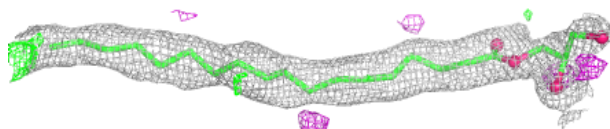
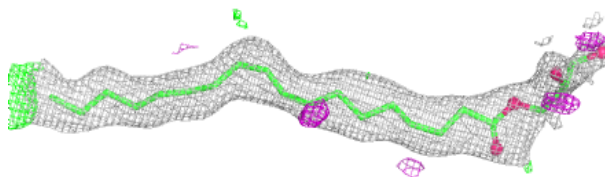
**Electron density around LFA B 301:**

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

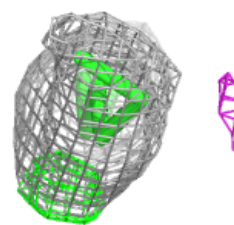
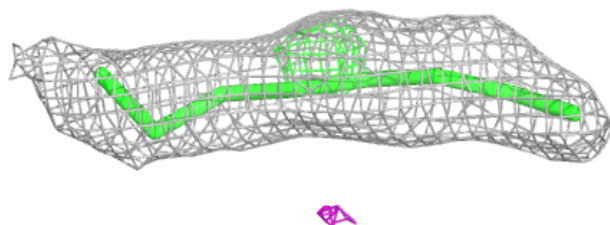
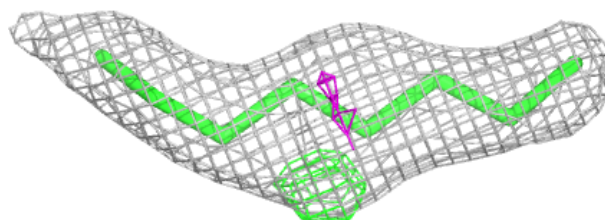


Electron density around OLC A 1004:

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

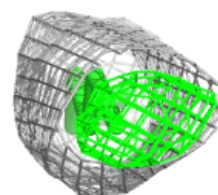
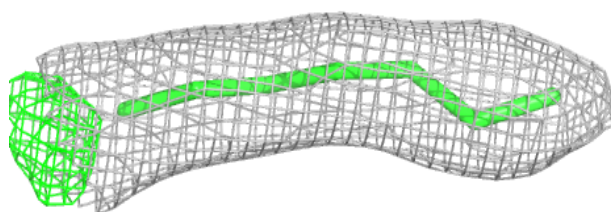
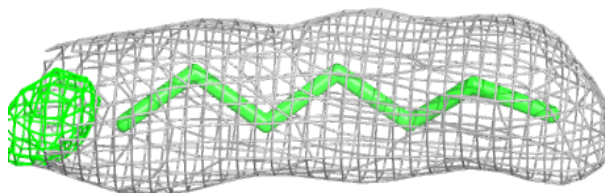
**Electron density around LFA C 715:**

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

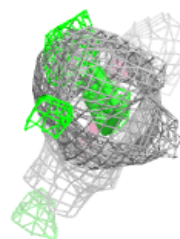
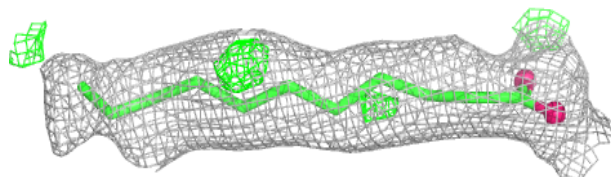
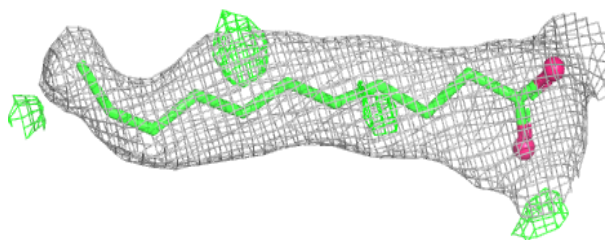


Electron density around LFA B 312:

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

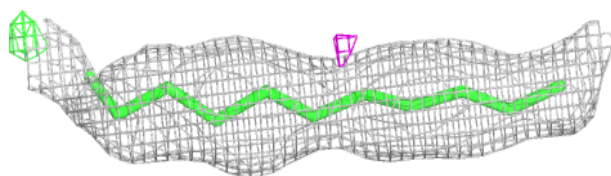
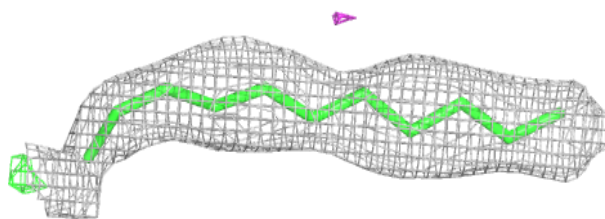
**Electron density around OLA B 303:**

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

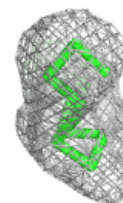
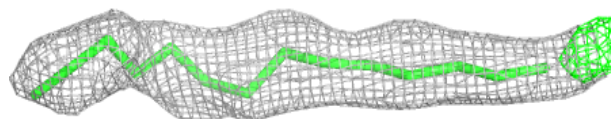
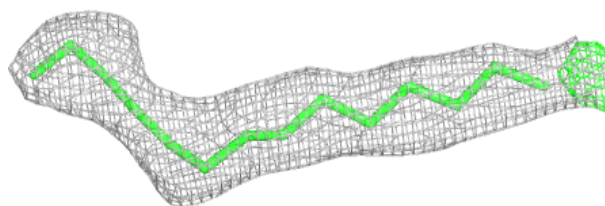


Electron density around LFA A 1019:

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

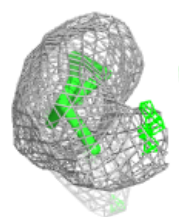
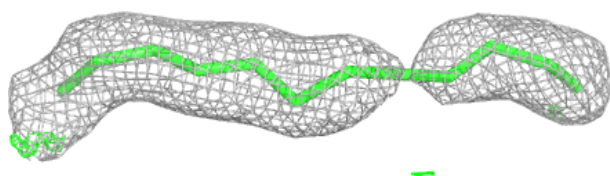
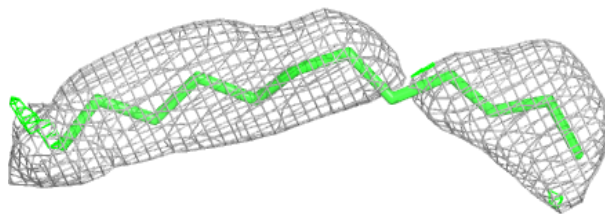
**Electron density around LFA B 319:**

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

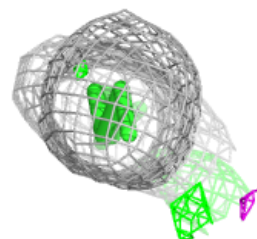
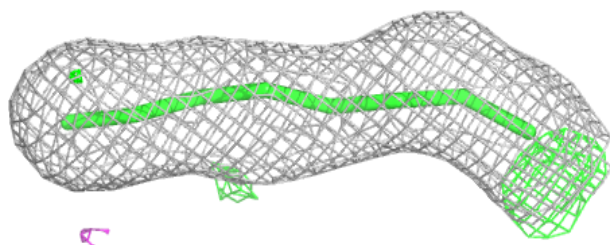
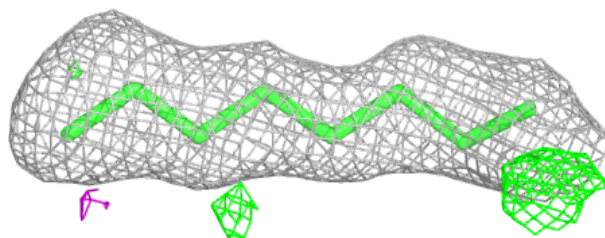


Electron density around LFA A 1008:

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

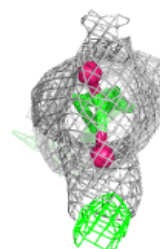
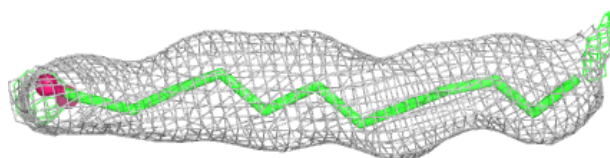
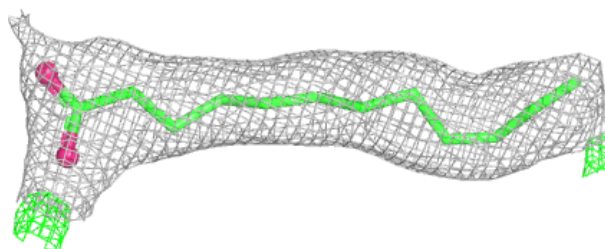
**Electron density around LFA B 315:**

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

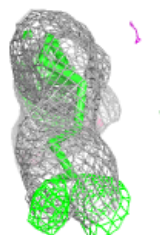
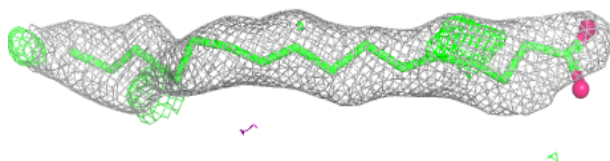
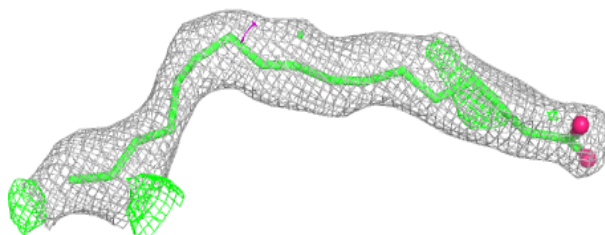


Electron density around OLA A 1005:

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

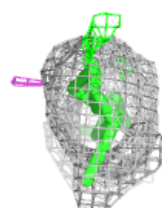
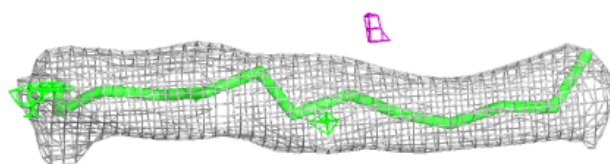
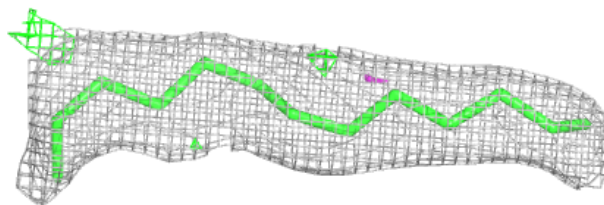
**Electron density around OLA C 703:**

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

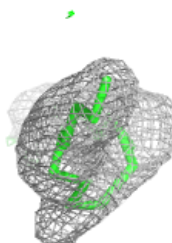
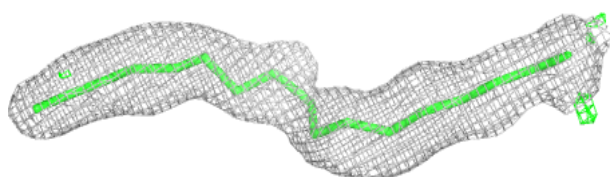
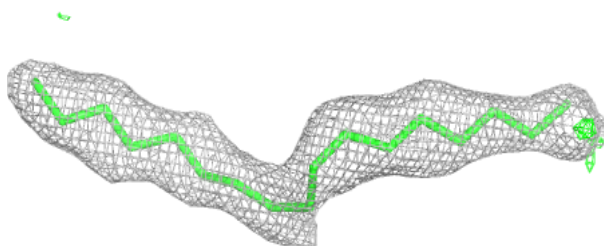


Electron density around LFA A 1017:

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

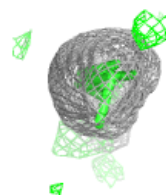
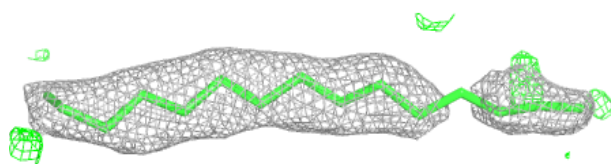
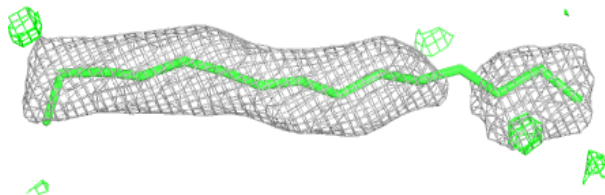
**Electron density around LFA A 1018:**

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

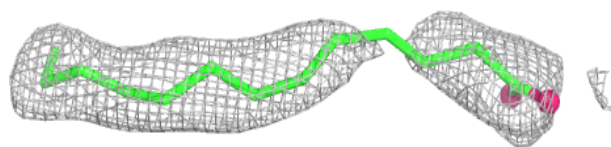
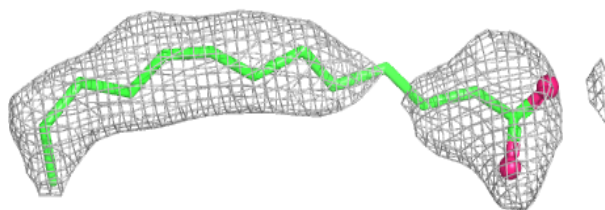


Electron density around LFA B 314:

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

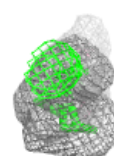
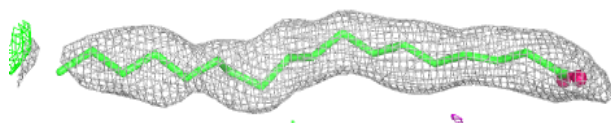
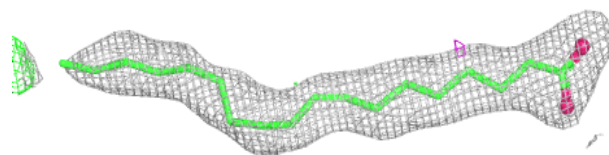
**Electron density around OLA C 705:**

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

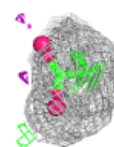
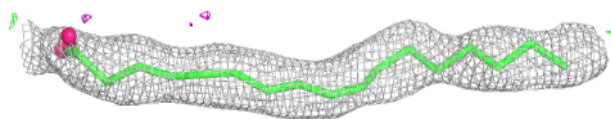
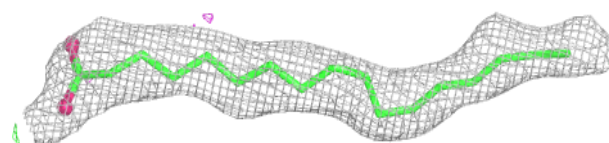


Electron density around OLA C 706:

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

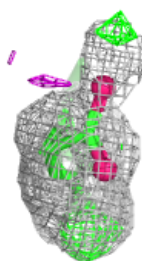
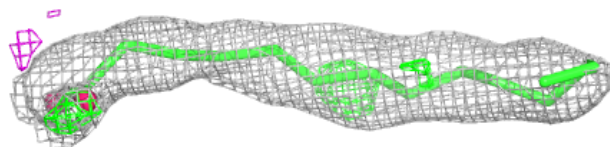
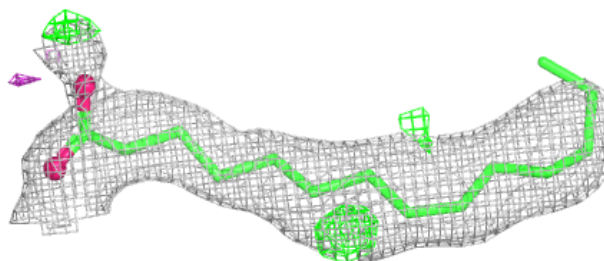
**Electron density around OLA B 308:**

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

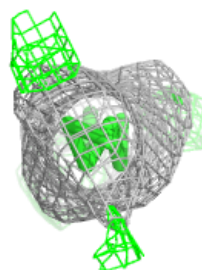
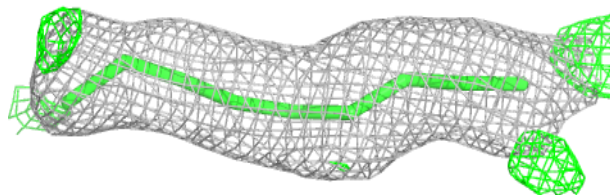
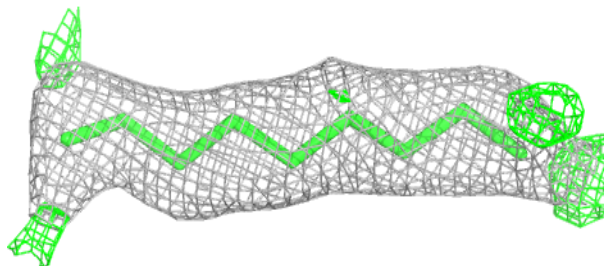


Electron density around OLA B 304:

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

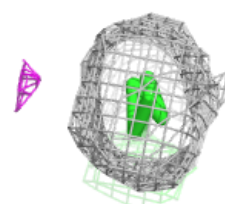
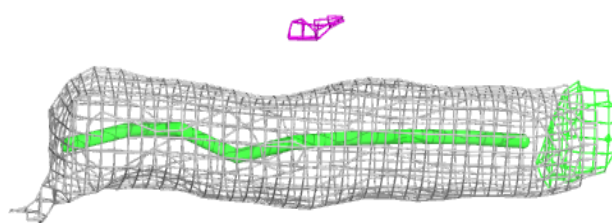
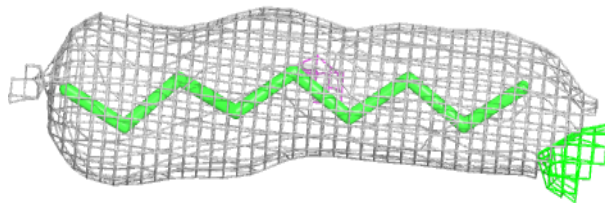
**Electron density around LFA C 701:**

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

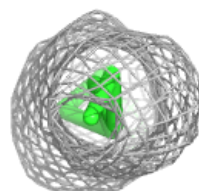
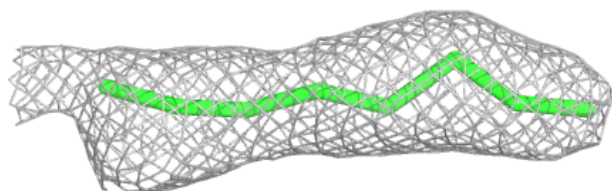
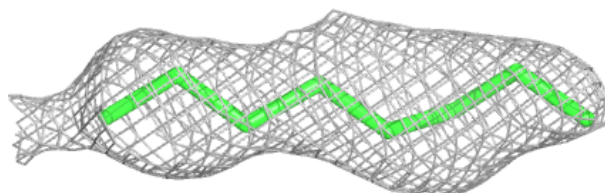


Electron density around LFA B 302:

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

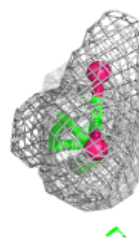
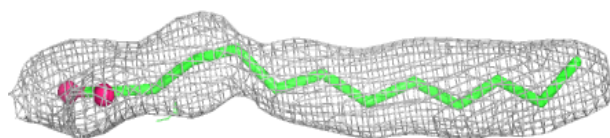
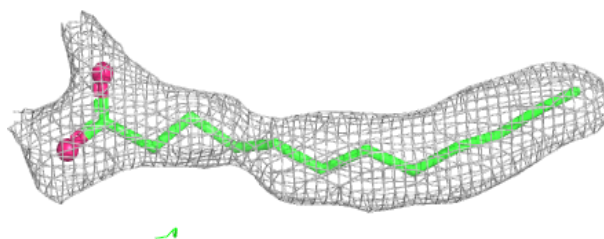
**Electron density around LFA C 711:**

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

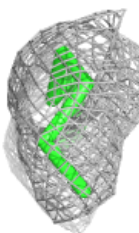
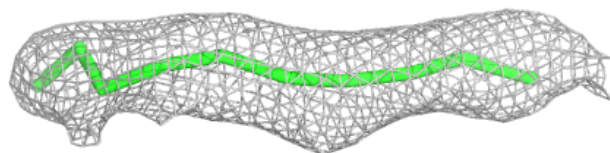
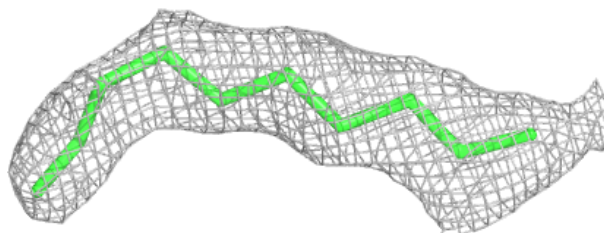


Electron density around OLA A 1002:

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

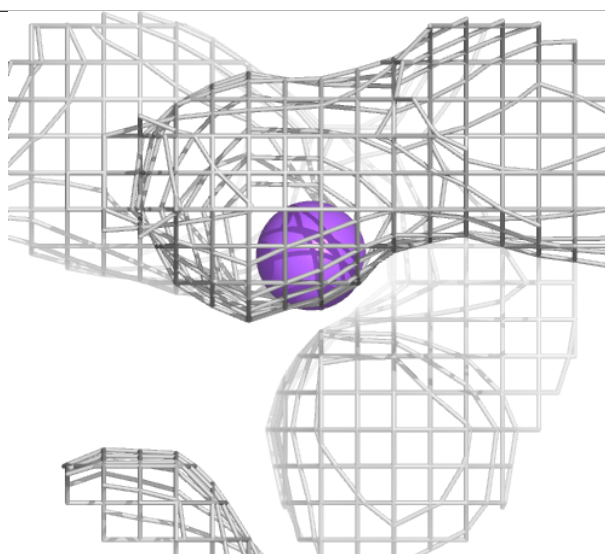
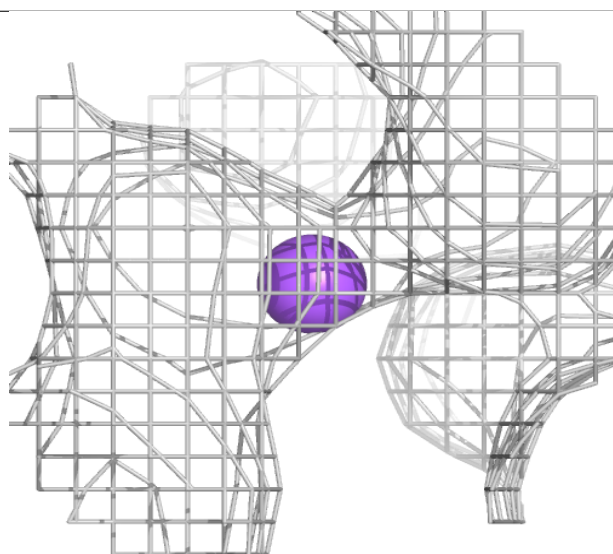
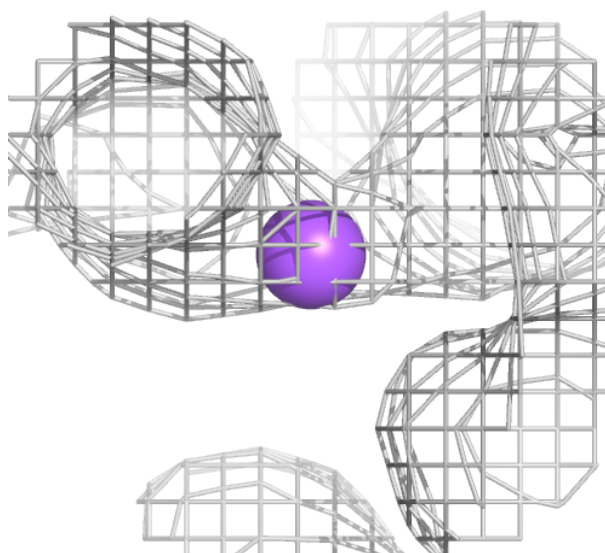
**Electron density around LFA B 317:**

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



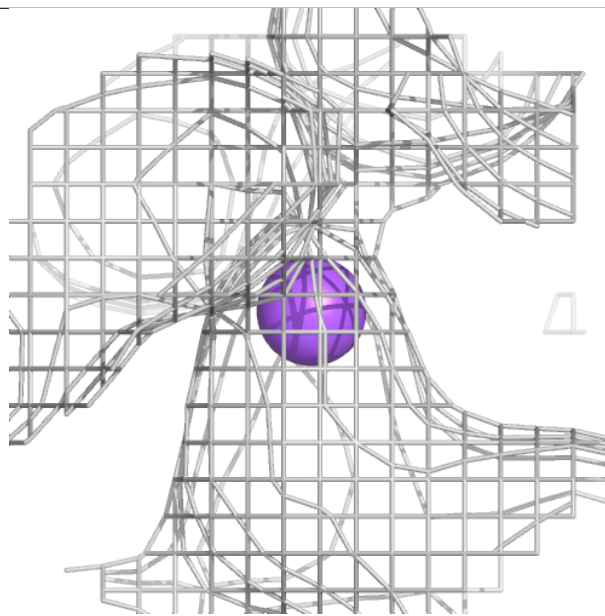
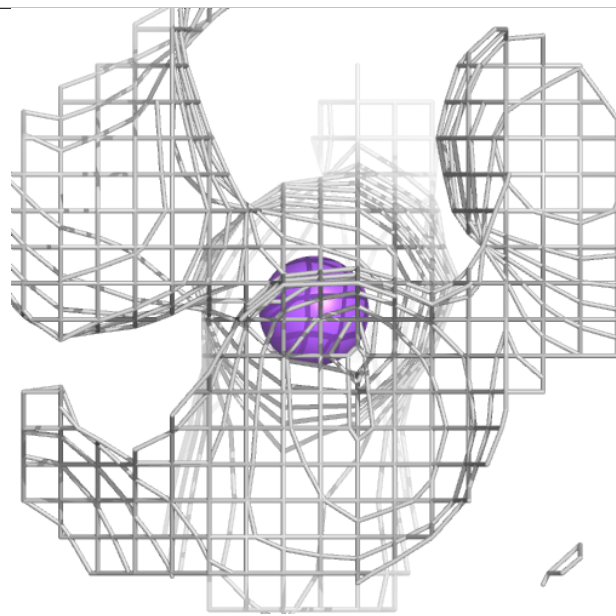
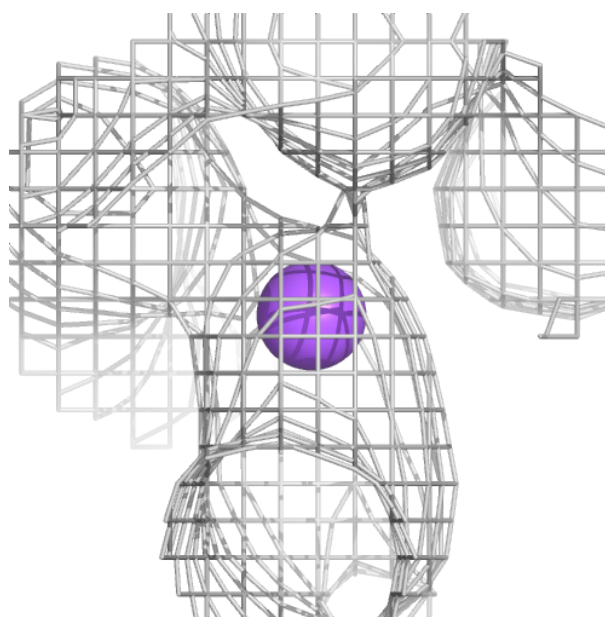
Electron density around NA B 323 (B):

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



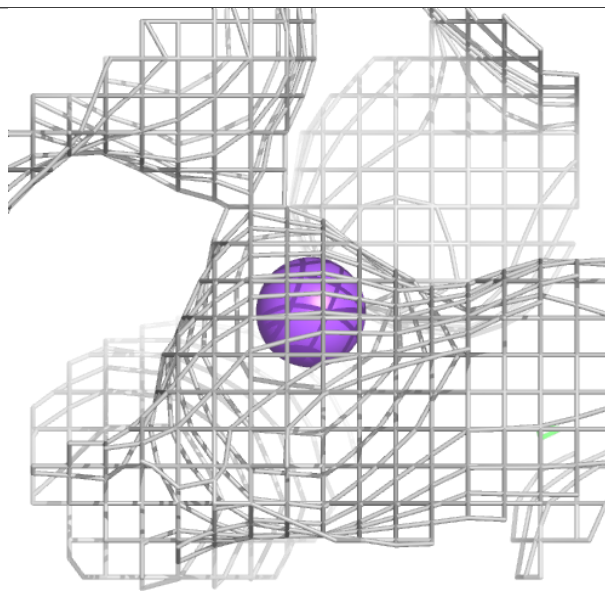
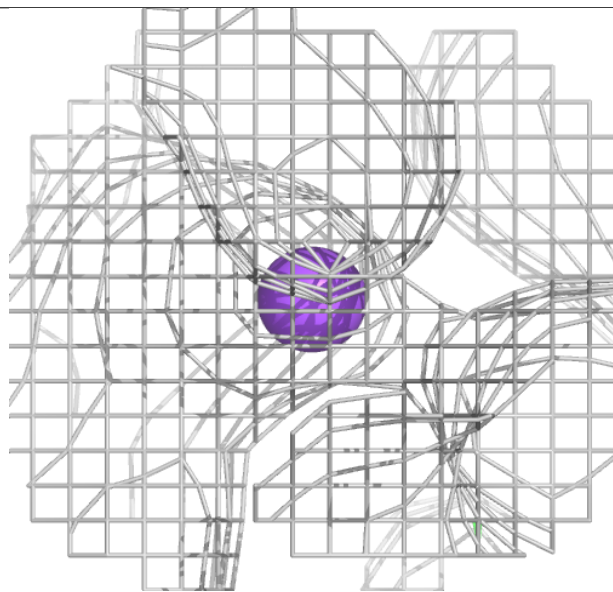
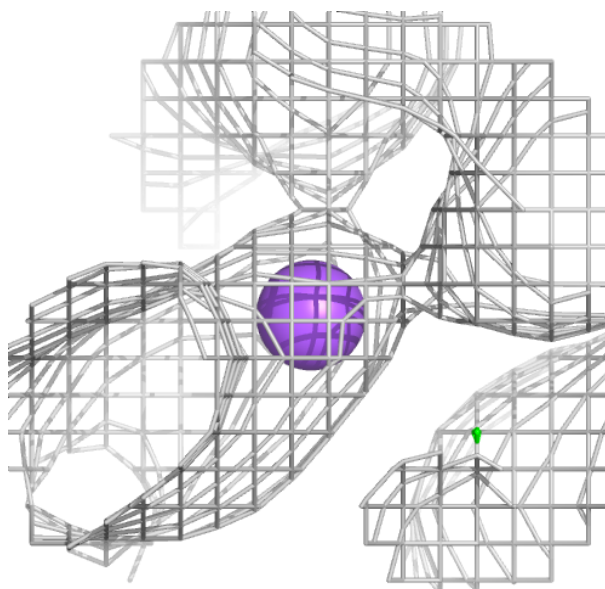
Electron density around NA A 1025 (B):

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



Electron density around NA C 723 (B):

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



6.5 Other polymers ⓘ

There are no such residues in this entry.