



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2023 – 02:00 am BST

PDB ID : 7ZMY
Title : Crystal structure of the light-driven inward proton pump xenorhodopsin BcXeR in the ground state at pH 8.2 in the presence of sodium at 100K
Authors : Kovalev, K.; Tsybrov, F.; Alekseev, A.; Bourenkov, G.; Gordeliy, V.
Deposited on : 2022-04-20
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

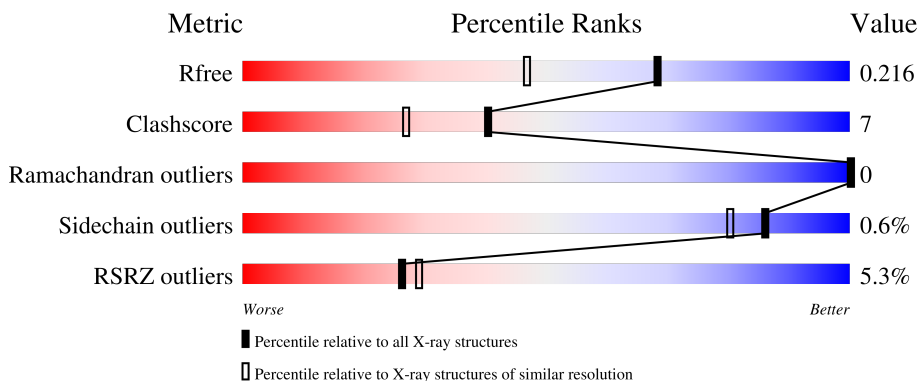
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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% 87% 10% .
1	B	229	 3% 86% 10% .
1	C	229	 6% 88% 8% ..

2 Entry composition [i](#)

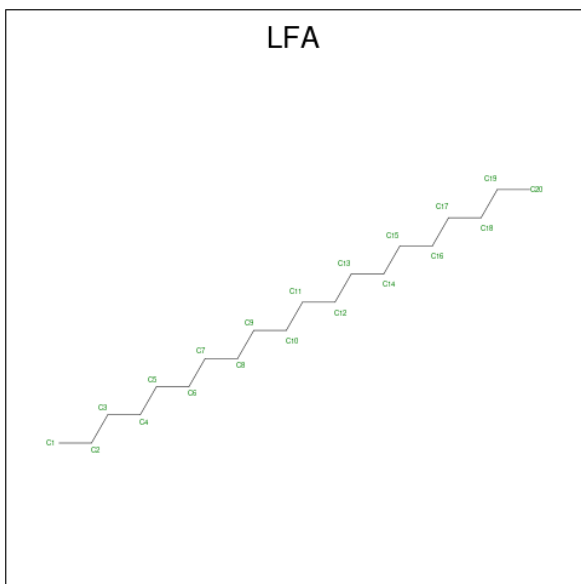
There are 7 unique types of molecules in this entry. The entry contains 6394 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	224	Total 1800	C 1223	N 272	O 298	S 7	0	5	0
1	B	221	Total 1782	C 1212	N 270	O 293	S 7	0	5	0
1	C	222	Total 1779	C 1212	N 267	O 293	S 7	0	4	0

- Molecule 2 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 12 12	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 3 3	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 4 4	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 13 13	0	0
2	A	1	Total C 13 13	0	0
2	A	1	Total C 17 17	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 4 4	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 6 6	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 7 7	0	0

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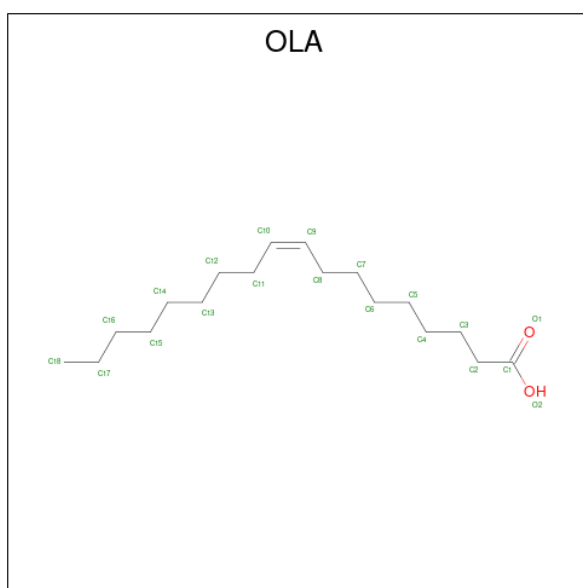
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 5 5	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 15 15	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 4 4	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 9 9	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 16 16	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 12 12	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C 15 15	0	0
2	C	1	Total C 12 12	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 7 7	0	0

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



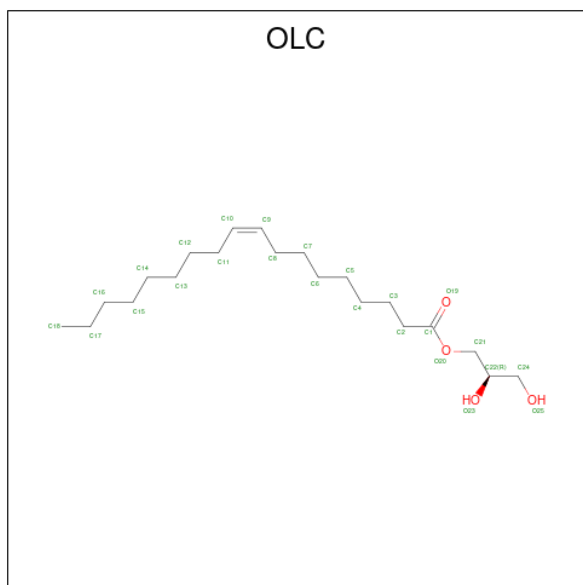
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 14 12 2	0	0
3	A	1	Total C O 11 9 2	0	0
3	A	1	Total C O 14 12 2	0	0
3	B	1	Total C O 13 11 2	0	0
3	B	1	Total C O 16 14 2	0	0

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

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).

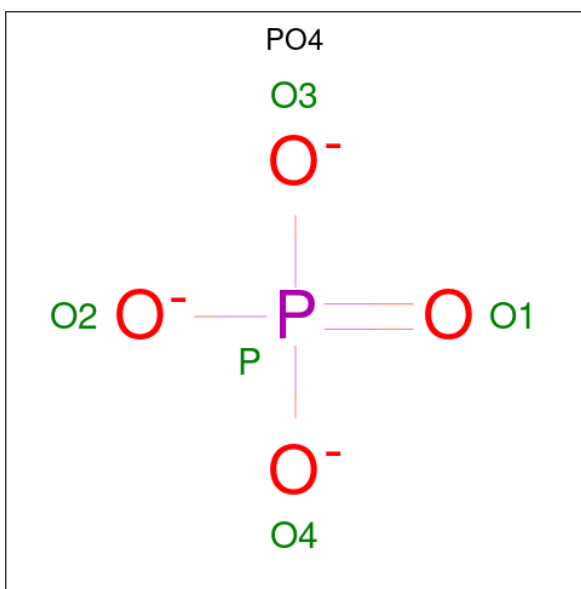


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			25	21	4		

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

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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

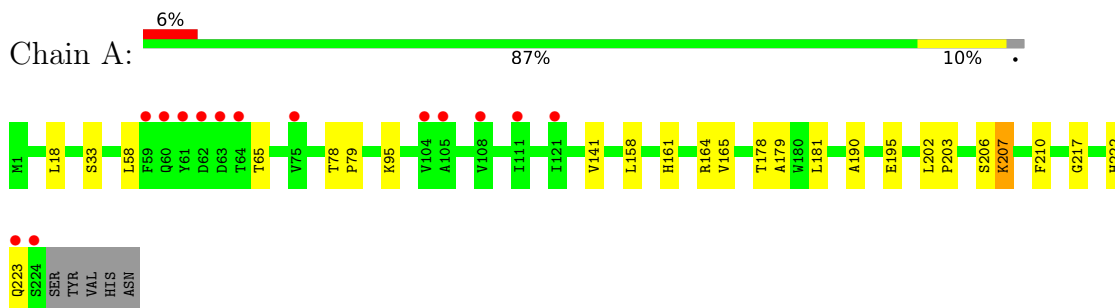
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	94	Total O 95 95	0	1
7	B	82	Total O 83 83	0	1
7	C	104	Total O 105 105	0	1

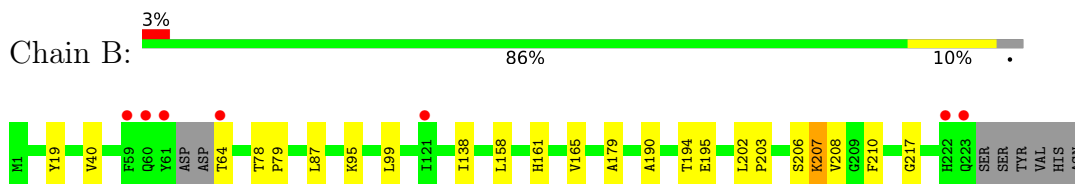
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

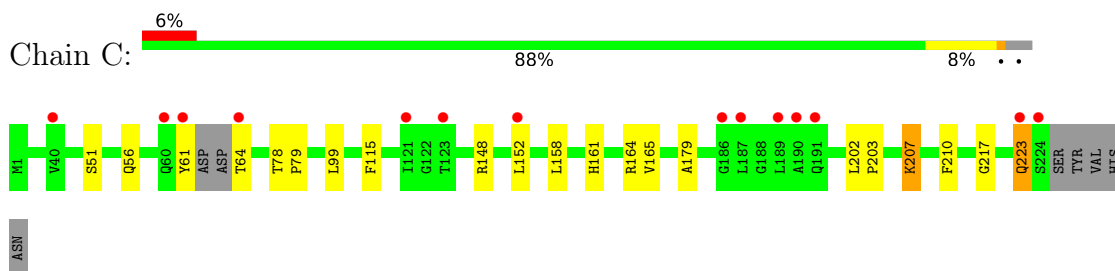
- Molecule 1: xenorhodopsin



- 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	68.24Å 109.57Å 119.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 49.80 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.9 (20.00-1.70) 92.0 (49.80-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.174 , 0.203 0.189 , 0.216	Depositor DCC
R_{free} test set	4506 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtrriage
Anisotropy	0.061	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6394	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.14% 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: OLC, OLA, PO4, LYR, FME, NA, LFA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.63	0/1807	0.62	0/2469
1	B	0.62	0/1788	0.61	0/2441
1	C	0.64	0/1785	0.62	0/2438
All	All	0.63	0/5380	0.62	0/7348

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	1800	0	1873	29	0
1	B	1782	0	1867	27	0
1	C	1779	0	1857	22	0
2	A	170	0	318	14	0
2	B	140	0	246	10	0
2	C	148	0	281	8	0
3	A	59	0	83	3	0
3	B	109	0	149	10	0
3	C	86	0	125	3	0
4	A	25	0	40	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
7	A	95	0	0	5	0
7	B	83	0	0	1	0
7	C	105	0	0	0	0
All	All	6394	0	6839	94	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 (94) 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:A:222:HIS:ND1	7:A:801:HOH:O	1.89	1.04
1:C:148:ARG:O	1:C:152:LEU:HD23	1.72	0.88
2:A:716:LFA:H203	2:B:316:LFA:H131	1.64	0.78
1:A:95:LYS:HE2	4:A:705:OLC:H21	1.74	0.69
1:B:190:ALA:CB	2:B:320:LFA:H192	2.26	0.66
3:B:307:OLA:H131	2:B:319:LFA:C10	2.26	0.66
1:C:56:GLN:HB3	3:C:704:OLA:H31	1.78	0.65
4:A:705:OLC:H21A	3:B:306:OLA:H32	1.79	0.65
1:A:190:ALA:CB	2:A:722:LFA:H72	2.28	0.64
1:A:222:HIS:CE1	7:A:801:HOH:O	2.44	0.63
1:A:181:LEU:HD23	2:A:720:LFA:H81	1.82	0.61
1:A:223:GLN:O	7:A:802:HOH:O	2.16	0.60
1:C:165[A]:VAL:HG13	1:C:210:PHE:CE1	2.36	0.60
3:B:304:OLA:H10	3:B:304:OLA:C14	2.32	0.60
2:C:711:LFA:C8	2:C:721:LFA:C7	2.79	0.60
1:A:165[A]:VAL:HG13	1:A:210:PHE:CE1	2.37	0.59
1:B:190:ALA:HB1	2:B:320:LFA:H192	1.84	0.59
4:A:705:OLC:H24A	3:B:306:OLA:C3	2.33	0.59
2:A:716:LFA:H203	2:B:316:LFA:C13	2.31	0.59
1:B:64:THR:OG1	7:B:401:HOH:O	2.16	0.58
2:A:716:LFA:H172	1:B:138:ILE:HG23	1.84	0.58
1:A:95:LYS:HE2	4:A:705:OLC:H22	1.85	0.57
1:B:99[B]:LEU:HD23	1:B:99[B]:LEU:C	2.26	0.56
1:C:99[B]:LEU:C	1:C:99[B]:LEU:HD23	2.26	0.56
4:A:705:OLC:H24A	3:B:306:OLA:H31	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LYR:H9	1:A:207:LYR:H183	1.89	0.55
1:A:161:HIS:CE1	1:A:217:GLY:HA3	2.42	0.55
1:A:207:LYR:H9	1:A:207:LYR:H192	1.88	0.54
1:B:165[B]:VAL:HG13	1:B:210:PHE:CE1	2.43	0.54
1:B:202:LEU:HB2	1:B:203:PRO:HD3	1.90	0.54
4:A:705:OLC:H22	7:A:846:HOH:O	2.07	0.53
1:B:194:THR:HG21	3:B:305:OLA:H21	1.91	0.53
1:A:33:SER:OG	4:A:705:OLC:H24	2.09	0.53
1:C:115:PHE:CZ	2:C:713:LFA:H152	2.43	0.53
1:B:161:HIS:CE1	1:B:217:GLY:HA3	2.44	0.52
1:C:207:LYR:H183	1:C:207:LYR:H9	1.91	0.52
1:B:207:LYR:H183	1:B:207:LYR:H9	1.90	0.52
1:A:95:LYS:HE2	4:A:705:OLC:C21	2.38	0.52
1:C:164:ARG:HD3	2:C:719:LFA:H201	1.91	0.52
1:C:161:HIS:CE1	1:C:217:GLY:HA3	2.44	0.52
1:A:95:LYS:HE2	4:A:705:OLC:C22	2.40	0.52
2:A:719:LFA:C13	2:A:720:LFA:H51	2.40	0.51
3:B:304:OLA:C14	3:B:304:OLA:C10	2.89	0.51
1:C:164:ARG:CD	2:C:719:LFA:H192	2.41	0.51
1:A:158:LEU:C	1:A:158:LEU:HD13	2.31	0.51
1:A:207:LYR:H1	1:A:207:LYR:HG2	1.91	0.50
1:B:208:VAL:HG11	2:B:319:LFA:H111	1.93	0.50
1:C:158:LEU:C	1:C:158:LEU:HD13	2.31	0.50
1:C:223:GLN:HE21	1:C:223:GLN:HA	1.76	0.50
1:C:202:LEU:HB2	1:C:203:PRO:HD3	1.93	0.50
1:B:207:LYR:H9	1:B:207:LYR:H192	1.94	0.50
1:B:40:VAL:HG13	3:C:702:OLA:H132	1.92	0.50
1:C:207:LYR:H9	1:C:207:LYR:H192	1.93	0.49
1:A:207:LYR:H192	1:A:207:LYR:C9	2.42	0.49
1:A:202:LEU:HB2	1:A:203:PRO:HD3	1.93	0.49
1:B:207:LYR:HG2	1:B:207:LYR:H1	1.93	0.49
1:B:158:LEU:C	1:B:158:LEU:HD13	2.33	0.49
1:C:99[B]:LEU:HD23	1:C:99[B]:LEU:O	2.13	0.48
1:B:87:LEU:HD21	3:B:308:OLA:H22	1.95	0.48
1:A:58:LEU:C	1:A:58:LEU:HD12	2.34	0.48
1:B:19:TYR:CZ	2:B:319:LFA:H172	2.48	0.48
1:B:78:THR:N	1:B:79:PRO:HD2	2.29	0.47
1:A:190:ALA:HB1	2:A:722:LFA:H72	1.97	0.47
2:C:713:LFA:H102	2:C:718:LFA:C9	2.46	0.46
1:A:178:THR:HG21	2:A:712:LFA:H12	1.97	0.46
1:A:78:THR:N	1:A:79:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:705:OLC:H24A	3:B:306:OLA:H32	1.97	0.45
1:C:78:THR:N	1:C:79:PRO:HD2	2.32	0.45
2:A:725:LFA:H201	2:C:717:LFA:H121	1.97	0.45
1:C:179:ALA:O	2:C:712:LFA:H13	2.16	0.45
1:B:207:LYR:H192	1:B:207:LYR:C9	2.47	0.45
1:C:207:LYR:H192	1:C:207:LYR:C9	2.47	0.44
1:B:165[B]:VAL:CG1	1:B:210:PHE:CE1	3.01	0.44
1:B:195:GLU:HA	2:B:320:LFA:H191	2.00	0.44
1:C:207:LYR:HG2	1:C:207:LYR:H1	1.99	0.44
1:A:179:ALA:O	2:A:722:LFA:C8	2.66	0.43
1:C:61:TYR:O	1:C:64:THR:HG22	2.19	0.43
1:C:51:SER:HB2	3:C:704:OLA:H71	1.99	0.43
1:A:141:VAL:HA	3:A:706:OLA:H51	2.01	0.43
1:A:195:GLU:HA	2:A:722:LFA:H71	2.01	0.43
3:A:706:OLA:H10	2:A:708:LFA:H22	2.01	0.42
1:A:58:LEU:HD12	1:A:58:LEU:O	2.19	0.42
1:C:164:ARG:HD3	2:C:719:LFA:C19	2.49	0.42
1:B:95:LYS:HE2	3:B:308:OLA:C1	2.50	0.42
1:A:206:SER:HB3	1:A:207:LYR:H42	2.01	0.42
1:B:194:THR:HG23	2:B:312:LFA:H41	2.03	0.41
1:B:206:SER:HB3	1:B:207:LYR:H42	2.03	0.41
3:A:703:OLA:H81	2:A:718:LFA:H132	2.01	0.41
1:C:207:LYR:H1	1:C:207:LYR:CG	2.50	0.41
1:A:190:ALA:HB3	2:A:722:LFA:H72	2.00	0.41
1:B:99[B]:LEU:HD23	1:B:99[B]:LEU:O	2.19	0.41
1:B:179:ALA:O	2:B:320:LFA:C20	2.69	0.41
1:A:164:ARG:NH1	7:A:807:HOH:O	2.54	0.40
1:B:207:LYR:H6	1:B:207:LYR:H41	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	226/229 (99%)	223 (99%)	3 (1%)	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%)	663 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/189 (97%)	180 (98%)	3 (2%)	62	48
1	B	183/189 (97%)	183 (100%)	0	100	100
1	C	181/189 (96%)	180 (99%)	1 (1%)	86	80
All	All	547/567 (96%)	543 (99%)	4 (1%)	86	77

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18[A]	LEU
1	A	18[B]	LEU
1	A	65	THR
1	C	223	GLN

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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LYR	A	207	1	27,29,30	1.10	3 (11%)	30,37,39	1.25	4 (13%)
1	FME	C	1	1	8,9,10	0.43	0	7,9,11	0.85	0
1	LYR	C	207	1	27,29,30	1.05	4 (14%)	30,37,39	1.44	4 (13%)
1	FME	A	1	1	8,9,10	0.40	0	7,9,11	0.79	0
1	FME	B	1	1	8,9,10	0.48	0	7,9,11	0.68	0
1	LYR	B	207	1	27,29,30	1.04	1 (3%)	30,37,39	1.38	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	LYR	A	207	1	-	3/22/40/42	0/1/1/1
1	FME	C	1	1	-	0/7/9/11	-
1	LYR	C	207	1	-	3/22/40/42	0/1/1/1
1	FME	A	1	1	-	0/7/9/11	-
1	FME	B	1	1	-	0/7/9/11	-
1	LYR	B	207	1	-	3/22/40/42	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	LYR	C7-C80	2.87	1.39	1.35
1	A	207	LYR	C7-C80	2.76	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	LYR	C9-C80	-2.45	1.40	1.45
1	C	207	LYR	C5-C3	-2.29	1.41	1.45
1	C	207	LYR	C7-C80	2.28	1.38	1.35
1	A	207	LYR	C5-C3	-2.25	1.41	1.45
1	C	207	LYR	C9-C80	-2.08	1.41	1.45
1	C	207	LYR	C16-C15	-2.06	1.47	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	207	LYR	C8-C80-C7	-4.30	116.89	122.92
1	B	207	LYR	C8-C80-C7	-4.05	117.25	122.92
1	A	207	LYR	C8-C80-C7	-3.84	117.54	122.92
1	C	207	LYR	C1-NZ-CE	-3.77	107.35	113.33
1	B	207	LYR	C8-C80-C9	3.42	123.47	118.08
1	B	207	LYR	C1-NZ-CE	-3.05	108.49	113.33
1	C	207	LYR	C8-C80-C9	3.03	122.85	118.08
1	A	207	LYR	C1-NZ-CE	-2.94	108.67	113.33
1	A	207	LYR	C8-C80-C9	2.68	122.29	118.08
1	C	207	LYR	C4-C3-C2	2.13	127.77	123.59
1	A	207	LYR	C4-C3-C2	2.08	127.68	123.59
1	B	207	LYR	C4-C3-C2	2.08	127.67	123.59

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	207	LYR	5	0
1	C	207	LYR	5	0
1	B	207	LYR	6	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 3 are monoatomic - leaving 69 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	OLA	C	704	-	14,14,19	0.56	0	14,14,19	0.62	0
2	LFA	B	312	-	8,8,19	0.15	0	7,7,18	0.17	0
2	LFA	A	714	-	9,9,19	0.09	0	8,8,18	0.16	0
2	LFA	A	716	-	9,9,19	0.13	0	8,8,18	0.09	0
3	OLA	A	706	-	13,13,19	0.76	0	12,13,19	0.49	0
2	LFA	B	316	-	14,14,19	0.14	0	13,13,18	0.14	0
3	OLA	B	305	-	11,11,19	0.66	0	11,11,19	0.69	0
3	OLA	B	309	-	13,13,19	0.63	0	12,13,19	0.51	0
2	LFA	C	717	-	14,14,19	0.12	0	13,13,18	0.08	0
3	OLA	C	702	-	18,18,19	0.56	0	18,18,19	0.52	0
3	OLA	A	703	-	13,13,19	0.57	0	12,13,19	0.70	0
2	LFA	B	323	-	10,10,19	0.15	0	9,9,18	0.08	0
2	LFA	C	709	-	7,7,19	0.10	0	6,6,18	0.08	0
3	OLA	B	308	-	18,18,19	0.56	0	18,18,19	0.72	0
3	OLA	B	303	-	12,12,19	0.68	0	12,12,19	0.64	0
2	LFA	B	319	-	9,9,19	0.13	0	8,8,18	0.15	0
2	LFA	A	713	-	2,2,19	0.04	0	0,1,18	-	-
2	LFA	B	317	-	7,7,19	0.10	0	6,6,18	0.16	0
2	LFA	A	724	-	5,5,19	0.13	0	4,4,18	0.14	0
2	LFA	C	711	-	7,7,19	0.14	0	6,6,18	0.10	0
2	LFA	C	710	-	8,8,19	0.13	0	7,7,18	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LFA	B	320	-	8,8,19	0.22	0	7,7,18	0.12	0
2	LFA	A	715	-	3,3,19	0.16	0	2,2,18	0.54	0
2	LFA	C	713	-	11,11,19	0.10	0	10,10,18	0.10	0
2	LFA	C	708	-	15,15,19	0.11	0	14,14,18	0.13	0
2	LFA	A	722	-	7,7,19	0.20	0	6,6,18	0.13	0
2	LFA	B	324	-	8,8,19	0.10	0	7,7,18	0.14	0
2	LFA	A	701	-	8,8,19	0.19	0	7,7,18	0.24	0
3	OLA	C	705	-	19,19,19	0.53	0	19,19,19	0.49	0
2	LFA	C	716	-	6,6,19	0.14	0	5,5,18	0.12	0
2	LFA	B	314	-	4,4,19	0.14	0	3,3,18	0.29	0
2	LFA	C	720	-	8,8,19	0.11	0	7,7,18	0.10	0
2	LFA	C	719	-	8,8,19	0.12	0	7,7,18	0.10	0
3	OLA	A	702	-	19,19,19	0.54	0	19,19,19	0.54	0
2	LFA	B	313	-	6,6,19	0.11	0	5,5,18	0.12	0
2	LFA	B	311	-	5,5,19	0.15	0	4,4,18	0.11	0
6	PO4	A	726	-	4,4,4	0.74	0	6,6,6	0.43	0
2	LFA	A	725	-	3,3,19	0.23	0	2,2,18	0.45	0
2	LFA	A	721	-	10,10,19	0.12	0	9,9,18	0.16	0
2	LFA	C	707	-	9,9,19	0.11	0	8,8,18	0.10	0
2	LFA	A	712	-	5,5,19	0.14	0	4,4,18	0.09	0
2	LFA	B	321	-	13,13,19	0.11	0	12,12,18	0.19	0
3	OLA	B	304	-	15,15,19	0.60	0	15,15,19	0.62	0
2	LFA	B	315	-	5,5,19	0.11	0	4,4,18	0.13	0
2	LFA	A	723	-	7,7,19	0.14	0	6,6,18	0.10	0
2	LFA	B	318	-	10,10,19	0.11	0	9,9,18	0.11	0
2	LFA	C	714	-	9,9,19	0.11	0	8,8,18	0.13	0
2	LFA	C	712	-	7,7,19	0.15	0	6,6,18	0.17	0
3	OLA	C	701	-	15,15,19	0.55	0	15,15,19	0.59	0
2	LFA	A	711	-	7,7,19	0.13	0	6,6,18	0.16	0
2	LFA	A	709	-	8,8,19	0.13	0	7,7,18	0.13	0
2	LFA	A	717	-	9,9,19	0.12	0	8,8,18	0.12	0
2	LFA	A	710	-	11,11,19	0.12	0	10,10,18	0.05	0
2	LFA	C	715	-	7,7,19	0.12	0	6,6,18	0.10	0
2	LFA	C	721	-	6,6,19	0.14	0	5,5,18	0.16	0
3	OLA	C	703	-	15,15,19	0.62	0	15,15,19	0.50	0
2	LFA	C	718	-	11,11,19	0.10	0	10,10,18	0.06	0
3	OLA	B	306	-	18,18,19	0.54	0	18,18,19	0.60	0
3	OLA	B	307	-	15,15,19	0.53	0	15,15,19	0.58	0
4	OLC	A	705	-	24,24,24	0.31	0	25,25,25	0.27	0
2	LFA	A	718	-	12,12,19	0.10	0	11,11,18	0.09	0
3	OLA	A	704	-	10,10,19	0.72	0	10,10,19	0.68	0
2	LFA	A	719	-	12,12,19	0.13	0	11,11,18	0.10	0
2	LFA	A	720	-	16,16,19	0.12	0	15,15,18	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LFA	B	301	-	6,6,19	0.14	0	5,5,18	0.12	0
2	LFA	A	708	-	8,8,19	0.09	0	7,7,18	0.08	0
6	PO4	C	722	-	4,4,4	0.67	0	6,6,6	0.43	0
2	LFA	B	302	-	8,8,19	0.10	0	7,7,18	0.15	0
2	LFA	B	322	-	3,3,19	0.21	0	2,2,18	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLA	C	704	-	-	8/12/12/17	-
2	LFA	B	312	-	-	0/6/6/17	-
2	LFA	A	714	-	-	1/7/7/17	-
2	LFA	A	716	-	-	2/7/7/17	-
3	OLA	A	706	-	-	8/11/11/17	-
2	LFA	B	316	-	-	2/12/12/17	-
3	OLA	B	305	-	-	2/9/9/17	-
3	OLA	B	309	-	-	6/11/11/17	-
2	LFA	C	717	-	-	6/12/12/17	-
3	OLA	C	702	-	-	11/16/16/17	-
3	OLA	A	703	-	-	1/11/11/17	-
2	LFA	B	323	-	-	4/8/8/17	-
2	LFA	C	709	-	-	1/5/5/17	-
3	OLA	B	308	-	-	4/16/16/17	-
3	OLA	B	303	-	-	1/10/10/17	-
2	LFA	B	319	-	-	1/7/7/17	-
2	LFA	B	317	-	-	1/5/5/17	-
2	LFA	A	724	-	-	0/3/3/17	-
2	LFA	C	711	-	-	3/5/5/17	-
2	LFA	C	710	-	-	0/6/6/17	-
2	LFA	B	320	-	-	2/6/6/17	-
2	LFA	A	715	-	-	1/1/1/17	-
2	LFA	C	713	-	-	2/9/9/17	-
2	LFA	C	708	-	-	3/13/13/17	-
2	LFA	A	722	-	-	3/5/5/17	-
2	LFA	B	324	-	-	2/6/6/17	-
2	LFA	A	701	-	-	2/6/6/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLA	C	705	-	-	3/17/17/17	-
2	LFA	C	716	-	-	0/4/4/17	-
2	LFA	B	314	-	-	0/2/2/17	-
2	LFA	C	720	-	-	1/6/6/17	-
2	LFA	C	719	-	-	0/6/6/17	-
3	OLA	A	702	-	-	10/17/17/17	-
2	LFA	B	313	-	-	2/4/4/17	-
2	LFA	B	311	-	-	0/3/3/17	-
2	LFA	A	725	-	-	0/1/1/17	-
2	LFA	A	721	-	-	0/8/8/17	-
2	LFA	C	707	-	-	2/7/7/17	-
2	LFA	A	712	-	-	2/3/3/17	-
2	LFA	B	321	-	-	2/11/11/17	-
3	OLA	B	304	-	-	6/13/13/17	-
2	LFA	B	315	-	-	2/3/3/17	-
2	LFA	A	723	-	-	1/5/5/17	-
2	LFA	B	318	-	-	3/8/8/17	-
2	LFA	C	714	-	-	0/7/7/17	-
2	LFA	C	712	-	-	1/5/5/17	-
3	OLA	C	701	-	-	7/13/13/17	-
2	LFA	A	711	-	-	1/5/5/17	-
2	LFA	A	709	-	-	1/6/6/17	-
2	LFA	A	717	-	-	2/7/7/17	-
2	LFA	A	710	-	-	6/9/9/17	-
2	LFA	C	715	-	-	1/5/5/17	-
2	LFA	C	721	-	-	0/4/4/17	-
3	OLA	C	703	-	-	8/13/13/17	-
2	LFA	C	718	-	-	2/9/9/17	-
3	OLA	B	306	-	-	3/16/16/17	-
3	OLA	B	307	-	-	8/13/13/17	-
4	OLC	A	705	-	-	16/24/24/24	-
2	LFA	A	718	-	-	5/10/10/17	-
3	OLA	A	704	-	-	5/8/8/17	-
2	LFA	A	719	-	-	3/10/10/17	-
2	LFA	A	720	-	-	4/14/14/17	-
2	LFA	B	301	-	-	2/4/4/17	-
2	LFA	A	708	-	-	2/6/6/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	B	302	-	-	2/6/6/17	-
2	LFA	B	322	-	-	0/1/1/17	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (190) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	715	LFA	C1-C2-C3-C4
3	B	303	OLA	C11-C10-C9-C8
3	B	309	OLA	C9-C10-C11-C12
3	C	701	OLA	C11-C10-C9-C8
4	A	705	OLC	C21-C22-C24-O25
4	A	705	OLC	O23-C22-C24-O25
4	A	705	OLC	O20-C21-C22-O23
2	B	319	LFA	C11-C12-C13-C14
3	B	307	OLA	C11-C10-C9-C8
3	B	304	OLA	C11-C10-C9-C8
3	B	304	OLA	C1-C2-C3-C4
3	C	702	OLA	C1-C2-C3-C4
4	A	705	OLC	C1-C2-C3-C4
2	A	720	LFA	C4-C5-C6-C7
4	A	705	OLC	O20-C21-C22-C24
3	C	702	OLA	C4-C5-C6-C7
2	B	318	LFA	C13-C14-C15-C16
2	C	712	LFA	C4-C5-C6-C7
2	A	708	LFA	C4-C5-C6-C7
3	A	704	OLA	C3-C4-C5-C6
3	C	703	OLA	C3-C4-C5-C6
2	A	719	LFA	C5-C6-C7-C8
2	B	323	LFA	C4-C5-C6-C7
2	C	708	LFA	C9-C10-C11-C12
3	C	703	OLA	C5-C6-C7-C8
3	B	305	OLA	C1-C2-C3-C4
3	A	704	OLA	C4-C5-C6-C7
3	C	702	OLA	C11-C12-C13-C14
3	C	703	OLA	C4-C5-C6-C7
2	A	722	LFA	C3-C4-C5-C6
3	C	701	OLA	C10-C11-C12-C13
2	B	313	LFA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	B	307	OLA	C2-C3-C4-C5
3	C	702	OLA	C5-C6-C7-C8
4	A	705	OLC	C3-C4-C5-C6
2	A	710	LFA	C4-C5-C6-C7
2	C	717	LFA	C5-C6-C7-C8
3	C	702	OLA	C6-C7-C8-C9
3	A	706	OLA	C1-C2-C3-C4
3	A	704	OLA	C5-C6-C7-C8
3	C	705	OLA	C11-C12-C13-C14
2	A	723	LFA	C3-C4-C5-C6
2	A	716	LFA	C15-C16-C17-C18
2	C	711	LFA	C2-C3-C4-C5
2	A	718	LFA	C13-C14-C15-C16
3	C	703	OLA	C11-C10-C9-C8
3	C	704	OLA	C11-C10-C9-C8
3	B	304	OLA	C11-C12-C13-C14
3	A	702	OLA	C10-C11-C12-C13
3	B	305	OLA	C4-C5-C6-C7
3	C	705	OLA	C12-C13-C14-C15
3	A	703	OLA	C2-C3-C4-C5
4	A	705	OLC	C13-C14-C15-C16
3	C	701	OLA	C4-C5-C6-C7
3	A	702	OLA	C11-C10-C9-C8
3	B	309	OLA	C11-C10-C9-C8
2	C	717	LFA	C6-C7-C8-C9
4	A	705	OLC	C4-C5-C6-C7
4	A	705	OLC	C9-C10-C11-C12
3	A	702	OLA	C14-C15-C16-C17
2	A	720	LFA	C7-C8-C9-C10
2	C	708	LFA	C7-C8-C9-C10
3	B	306	OLA	C11-C10-C9-C8
3	C	702	OLA	C2-C3-C4-C5
3	C	702	OLA	C12-C13-C14-C15
2	A	708	LFA	C6-C7-C8-C9
2	A	710	LFA	C9-C10-C11-C12
3	C	703	OLA	C6-C7-C8-C9
4	A	705	OLC	C6-C7-C8-C9
2	A	710	LFA	C6-C7-C8-C9
2	A	717	LFA	C11-C12-C13-C14
2	A	718	LFA	C11-C10-C9-C8
3	C	702	OLA	C13-C14-C15-C16
2	B	315	LFA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	B	315	LFA	C4-C5-C6-C7
3	B	309	OLA	C2-C3-C4-C5
2	C	707	LFA	C1-C2-C3-C4
2	A	701	LFA	C2-C3-C4-C5
4	A	705	OLC	C11-C12-C13-C14
4	A	705	OLC	C2-C3-C4-C5
2	B	323	LFA	C11-C10-C9-C8
3	B	307	OLA	C3-C4-C5-C6
2	A	712	LFA	C1-C2-C3-C4
3	B	304	OLA	C3-C4-C5-C6
3	A	706	OLA	C11-C10-C9-C8
2	C	717	LFA	C11-C12-C13-C14
2	B	316	LFA	C4-C5-C6-C7
3	C	702	OLA	C11-C10-C9-C8
2	C	709	LFA	C17-C18-C19-C20
3	C	702	OLA	C3-C4-C5-C6
2	A	722	LFA	C2-C3-C4-C5
2	B	313	LFA	C4-C5-C6-C7
2	C	711	LFA	C1-C2-C3-C4
2	A	710	LFA	C1-C2-C3-C4
2	B	321	LFA	C5-C6-C7-C8
2	A	712	LFA	C2-C3-C4-C5
4	A	705	OLC	C5-C6-C7-C8
3	A	702	OLA	C2-C3-C4-C5
3	A	706	OLA	C3-C4-C5-C6
2	A	720	LFA	C11-C10-C9-C8
3	C	703	OLA	C11-C12-C13-C14
2	B	318	LFA	C15-C16-C17-C18
2	C	715	LFA	C16-C17-C18-C19
3	A	706	OLA	C2-C3-C4-C5
3	C	704	OLA	C3-C4-C5-C6
2	C	717	LFA	C10-C11-C12-C13
2	C	717	LFA	C1-C2-C3-C4
3	B	307	OLA	C11-C12-C13-C14
2	B	323	LFA	C5-C6-C7-C8
2	B	321	LFA	C11-C10-C9-C8
2	C	708	LFA	C11-C12-C13-C14
2	C	713	LFA	C17-C18-C19-C20
2	B	301	LFA	C14-C15-C16-C17
2	C	711	LFA	C3-C4-C5-C6
2	A	718	LFA	C12-C13-C14-C15
2	C	713	LFA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	B	316	LFA	C10-C11-C12-C13
3	B	309	OLA	C7-C8-C9-C10
3	C	701	OLA	C3-C4-C5-C6
2	B	324	LFA	C7-C8-C9-C10
4	A	705	OLC	C14-C15-C16-C17
2	B	320	LFA	C14-C15-C16-C17
2	A	719	LFA	C1-C2-C3-C4
2	A	701	LFA	C6-C7-C8-C9
3	C	705	OLA	C6-C7-C8-C9
3	C	704	OLA	O2-C1-C2-C3
3	C	704	OLA	C2-C3-C4-C5
4	A	705	OLC	C10-C11-C12-C13
2	B	324	LFA	C6-C7-C8-C9
2	B	301	LFA	C13-C14-C15-C16
2	B	318	LFA	C14-C15-C16-C17
2	B	320	LFA	C16-C17-C18-C19
3	A	704	OLA	O1-C1-C2-C3
3	A	706	OLA	C7-C8-C9-C10
3	B	308	OLA	O1-C1-C2-C3
4	A	705	OLC	C7-C8-C9-C10
3	C	704	OLA	C5-C6-C7-C8
2	C	707	LFA	C4-C5-C6-C7
3	B	308	OLA	O2-C1-C2-C3
3	A	704	OLA	O2-C1-C2-C3
3	A	702	OLA	C13-C14-C15-C16
3	C	704	OLA	O1-C1-C2-C3
3	C	701	OLA	O2-C1-C2-C3
2	A	717	LFA	C12-C13-C14-C15
2	A	718	LFA	C17-C18-C19-C20
3	C	701	OLA	O1-C1-C2-C3
2	A	722	LFA	C5-C6-C7-C8
3	C	701	OLA	C11-C12-C13-C14
3	B	308	OLA	C9-C10-C11-C12
3	A	702	OLA	O2-C1-C2-C3
3	A	702	OLA	O1-C1-C2-C3
2	B	323	LFA	C2-C3-C4-C5
2	C	717	LFA	C7-C8-C9-C10
3	A	702	OLA	C7-C8-C9-C10
3	C	704	OLA	C9-C10-C11-C12
3	C	704	OLA	C1-C2-C3-C4
3	A	706	OLA	O2-C1-C2-C3
2	A	709	LFA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	A	718	LFA	C15-C16-C17-C18
3	B	307	OLA	C7-C8-C9-C10
2	A	720	LFA	C5-C6-C7-C8
3	A	706	OLA	O1-C1-C2-C3
3	A	702	OLA	C6-C7-C8-C9
2	B	302	LFA	C3-C4-C5-C6
3	A	702	OLA	C15-C16-C17-C18
2	C	720	LFA	C1-C2-C3-C4
2	A	719	LFA	C3-C4-C5-C6
2	B	317	LFA	C1-C2-C3-C4
2	C	718	LFA	C17-C18-C19-C20
3	C	703	OLA	C2-C3-C4-C5
3	B	304	OLA	O1-C1-C2-C3
2	A	710	LFA	C2-C3-C4-C5
3	A	706	OLA	C6-C7-C8-C9
3	B	306	OLA	O2-C1-C2-C3
3	B	309	OLA	O2-C1-C2-C3
2	A	716	LFA	C11-C12-C13-C14
2	B	302	LFA	C1-C2-C3-C4
2	A	710	LFA	C3-C4-C5-C6
3	B	307	OLA	O2-C1-C2-C3
2	C	718	LFA	C11-C12-C13-C14
3	B	308	OLA	C1-C2-C3-C4
3	C	703	OLA	C7-C8-C9-C10
3	B	304	OLA	O2-C1-C2-C3
2	A	711	LFA	C4-C5-C6-C7
3	B	309	OLA	C5-C6-C7-C8
2	A	714	LFA	C6-C7-C8-C9
3	C	702	OLA	C7-C8-C9-C10
3	B	307	OLA	O1-C1-C2-C3
3	B	306	OLA	O1-C1-C2-C3
3	B	307	OLA	C4-C5-C6-C7

There are no ring outliers.

29 monomers are involved in 48 short contacts:

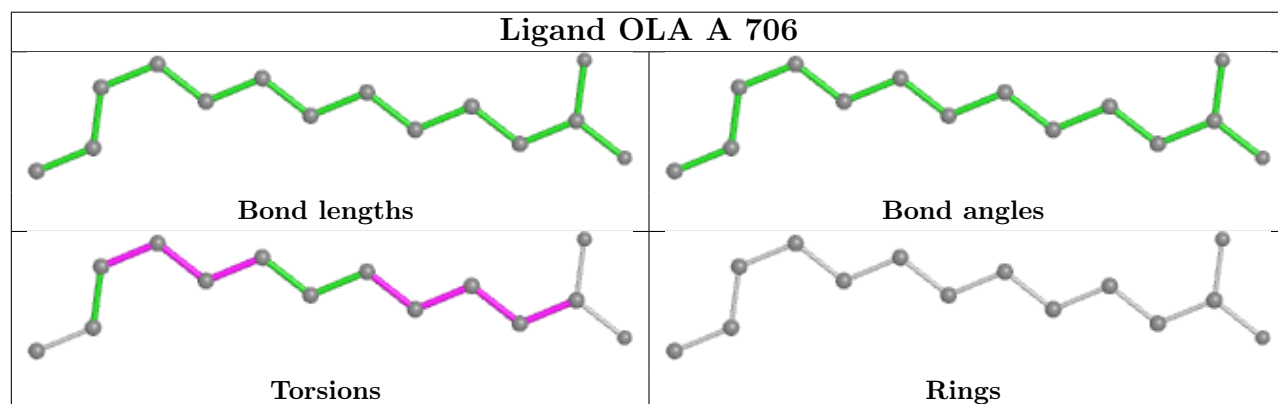
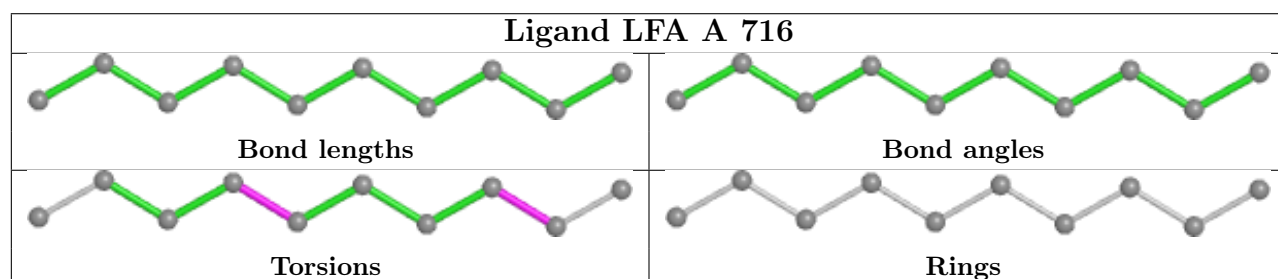
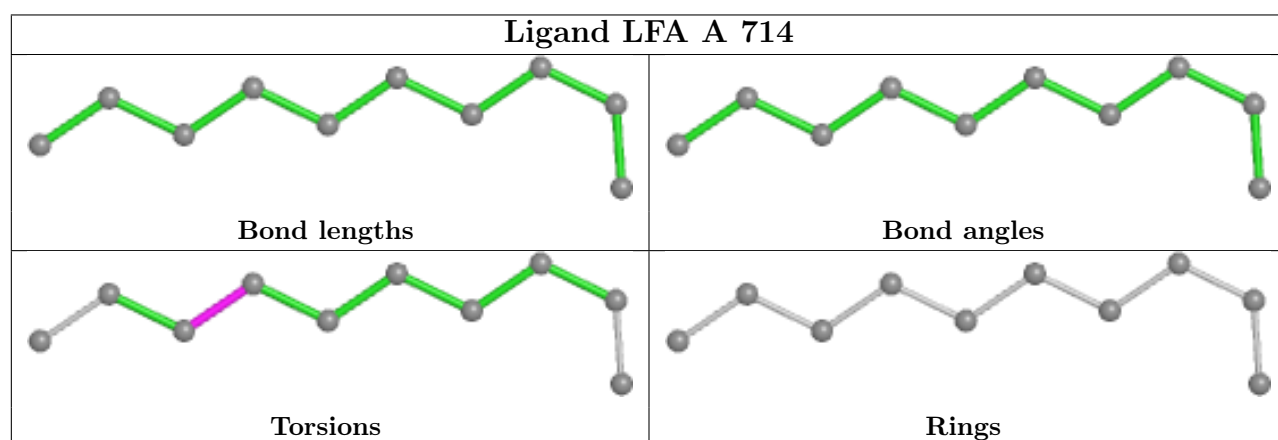
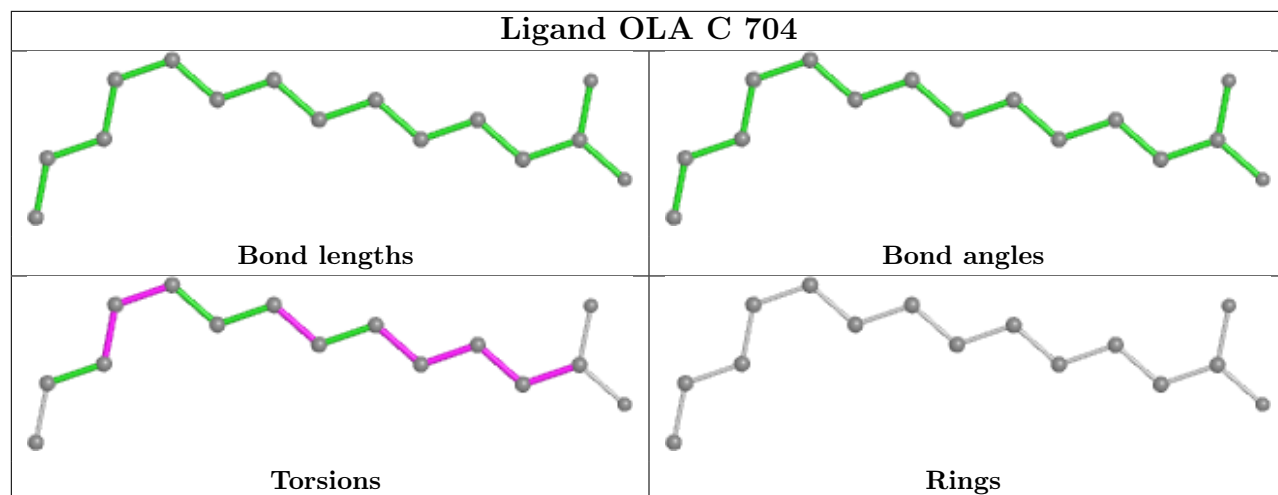
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	704	OLA	2	0
2	B	312	LFA	1	0
2	A	716	LFA	3	0
3	A	706	OLA	2	0
2	B	316	LFA	2	0

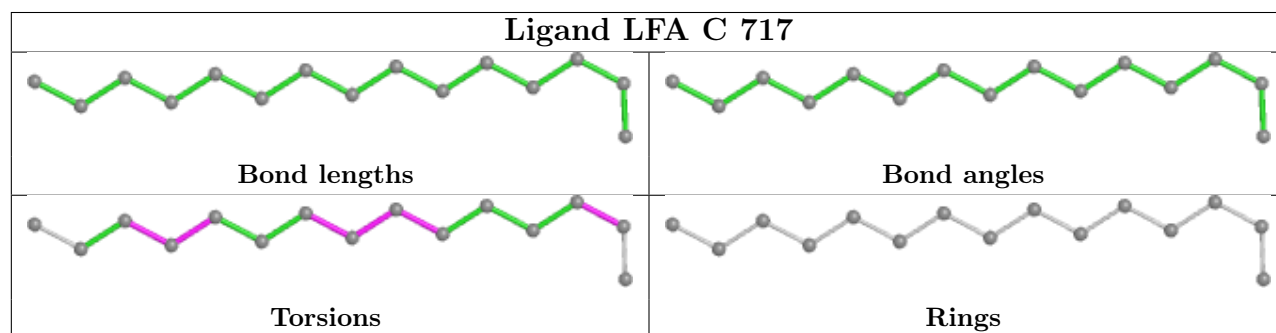
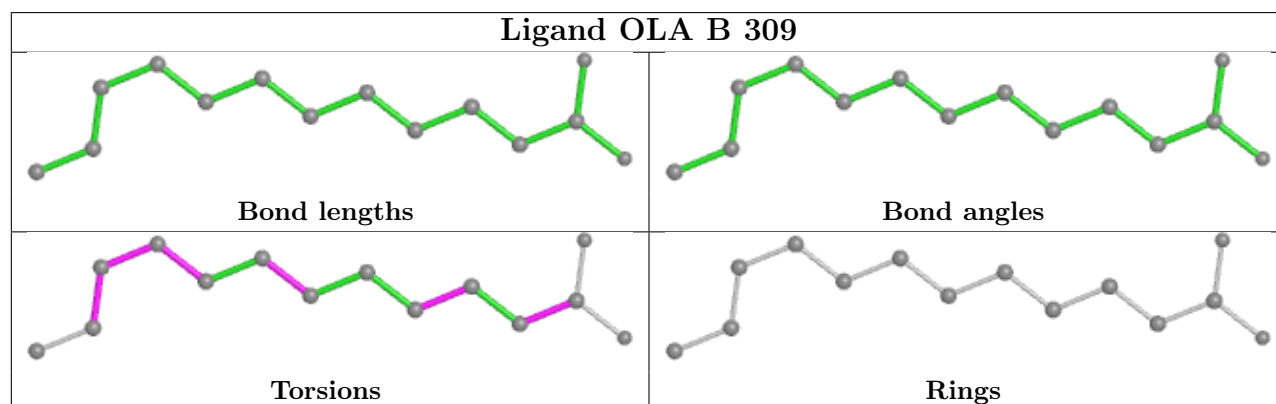
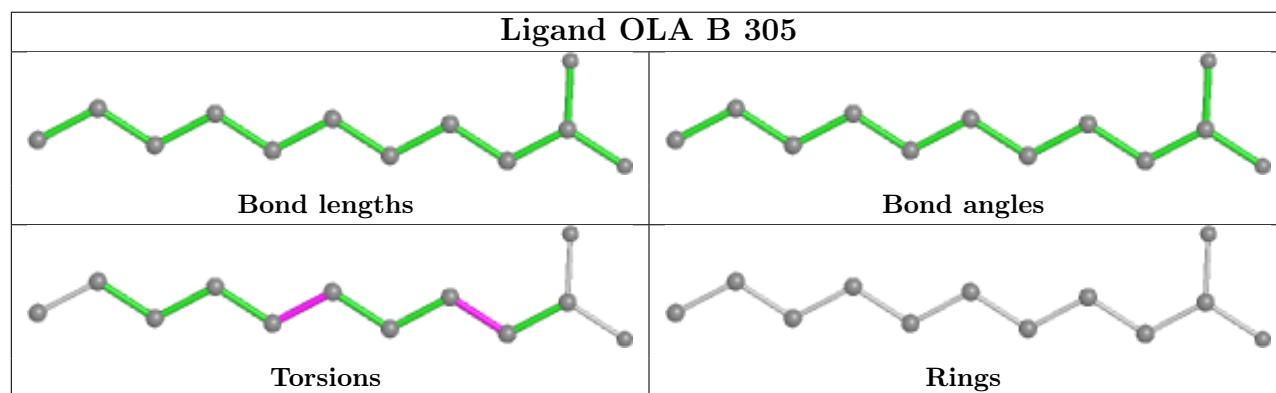
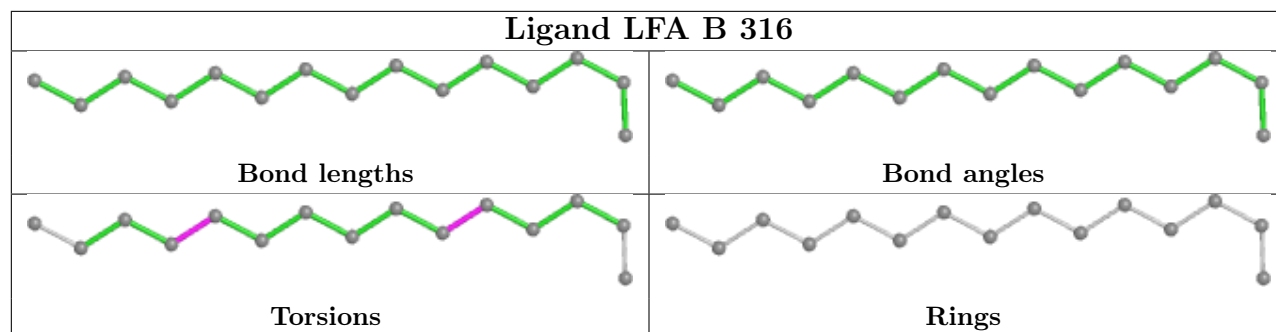
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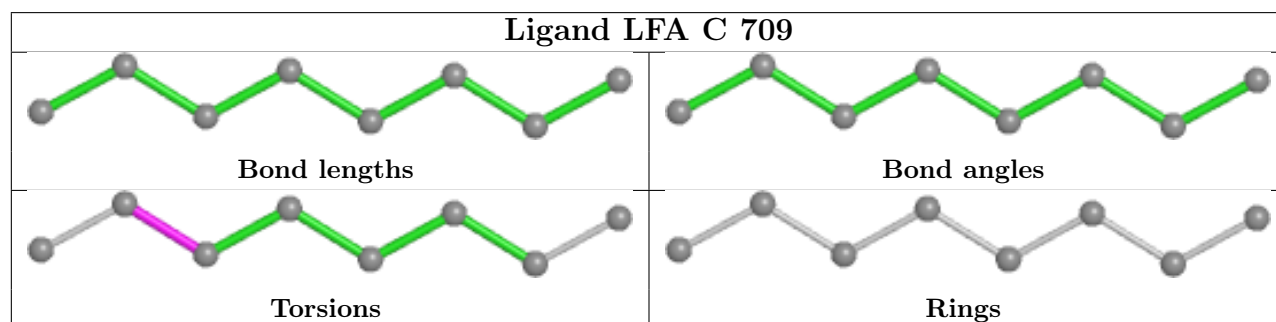
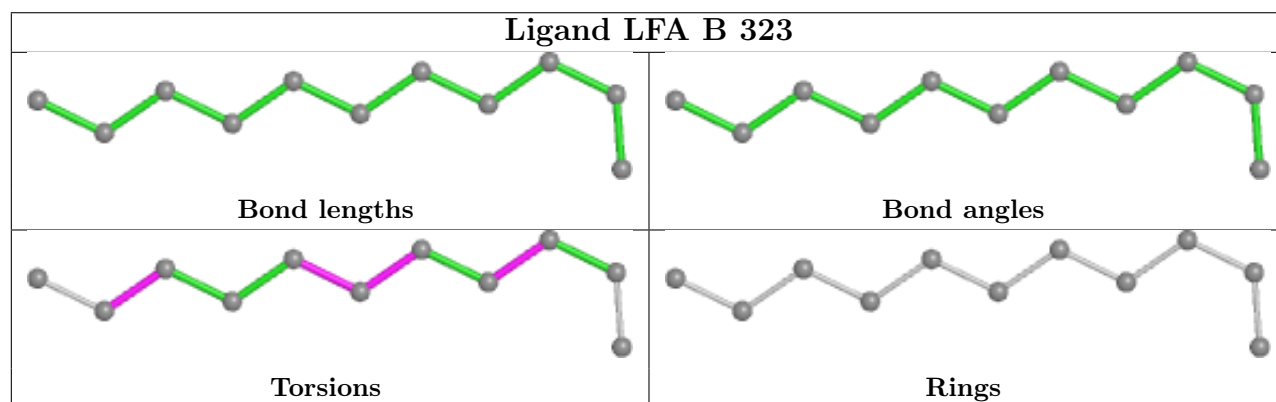
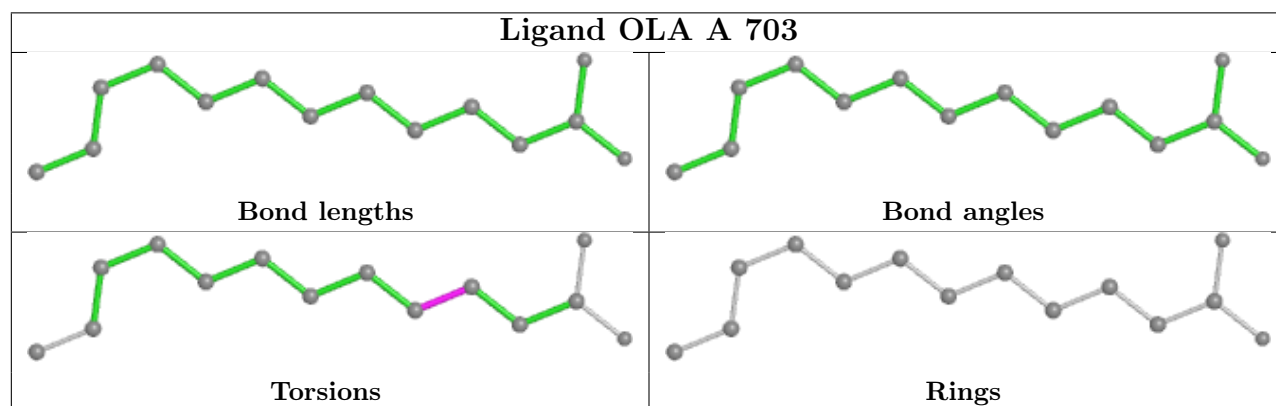
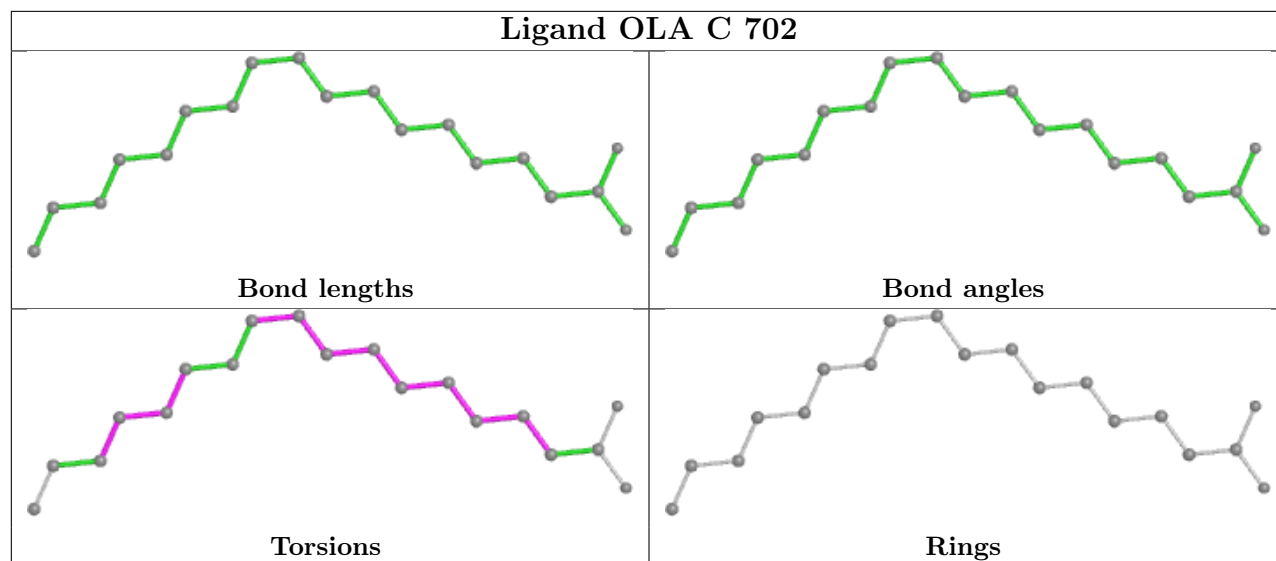
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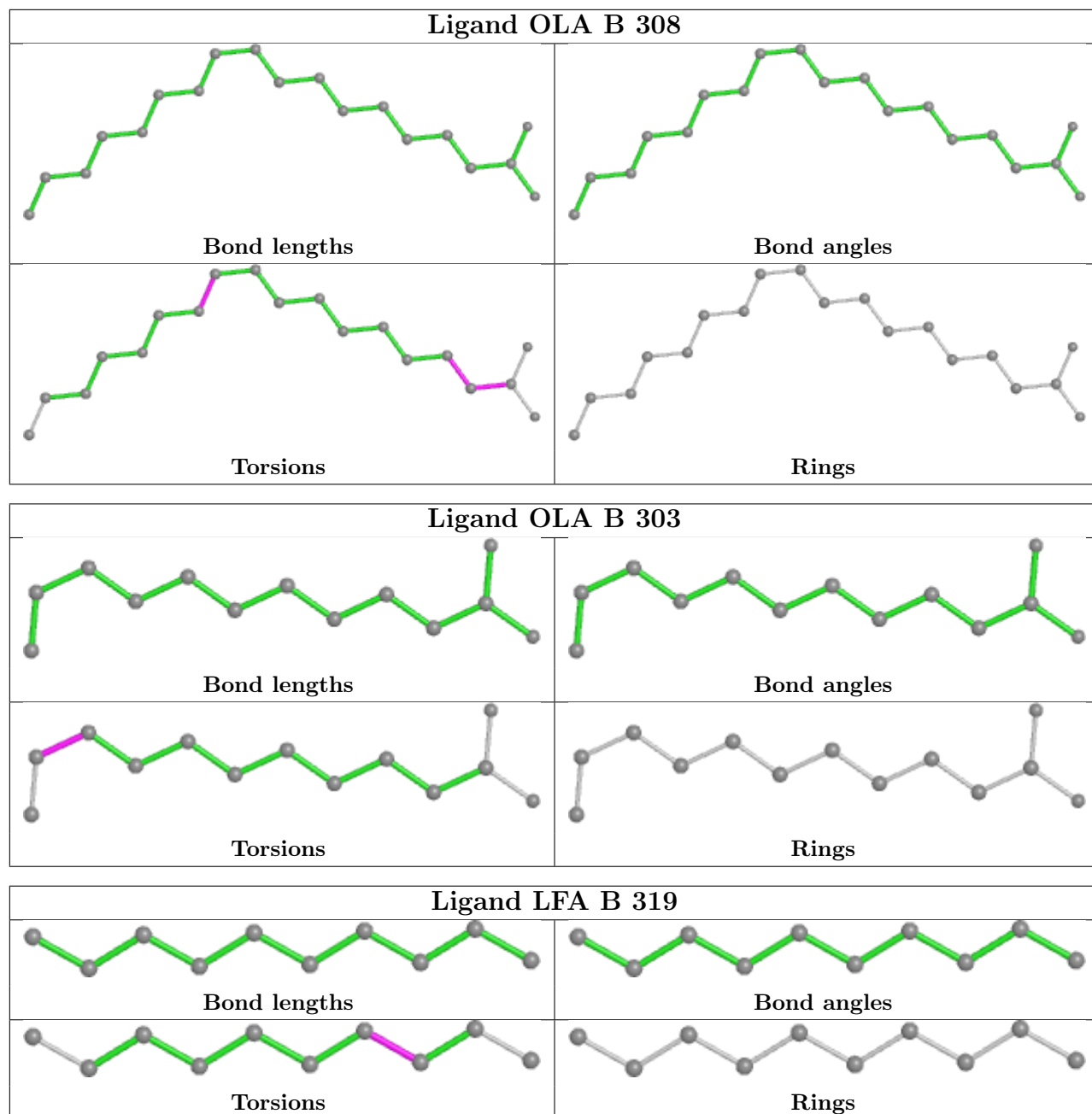
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	305	OLA	1	0
2	C	717	LFA	1	0
3	C	702	OLA	1	0
3	A	703	OLA	1	0
3	B	308	OLA	2	0
2	B	319	LFA	3	0
2	C	711	LFA	1	0
2	B	320	LFA	4	0
2	C	713	LFA	2	0
2	A	722	LFA	5	0
2	C	719	LFA	3	0
2	A	725	LFA	1	0
2	A	712	LFA	1	0
3	B	304	OLA	2	0
2	C	712	LFA	1	0
2	C	721	LFA	1	0
2	C	718	LFA	1	0
3	B	306	OLA	4	0
3	B	307	OLA	1	0
4	A	705	OLC	10	0
2	A	718	LFA	1	0
2	A	719	LFA	1	0
2	A	720	LFA	2	0
2	A	708	LFA	1	0

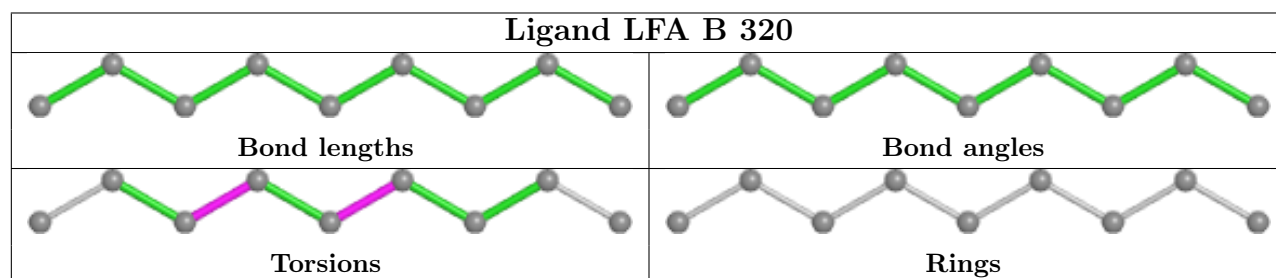
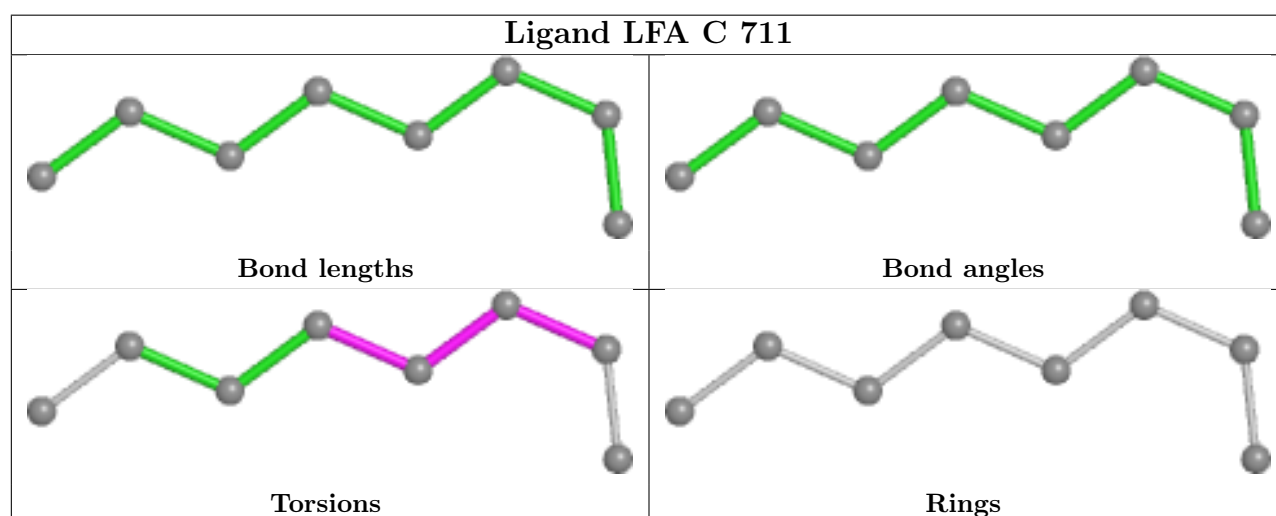
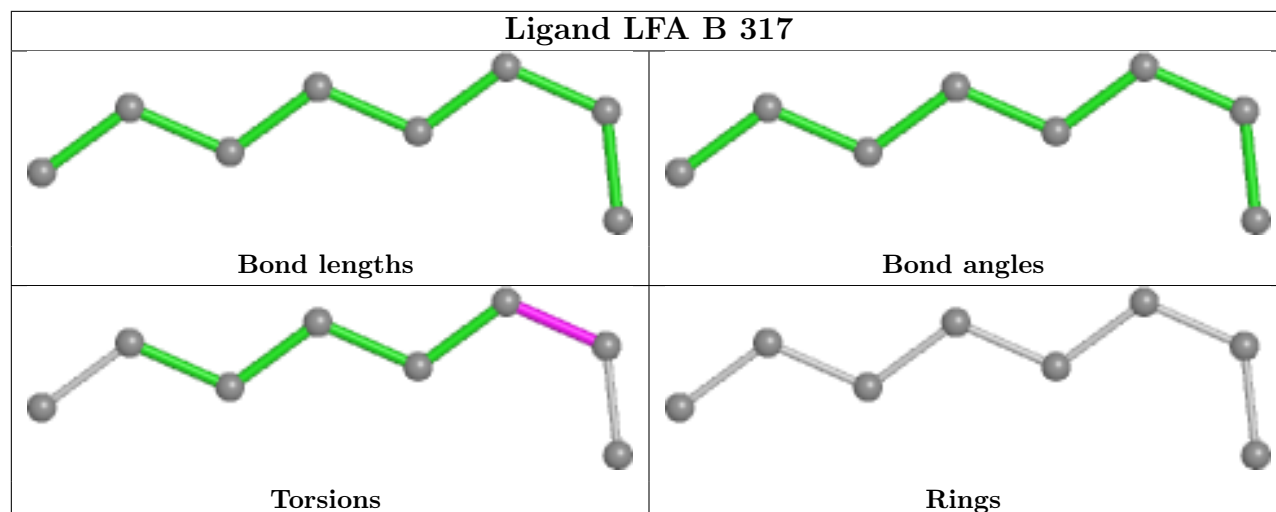
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

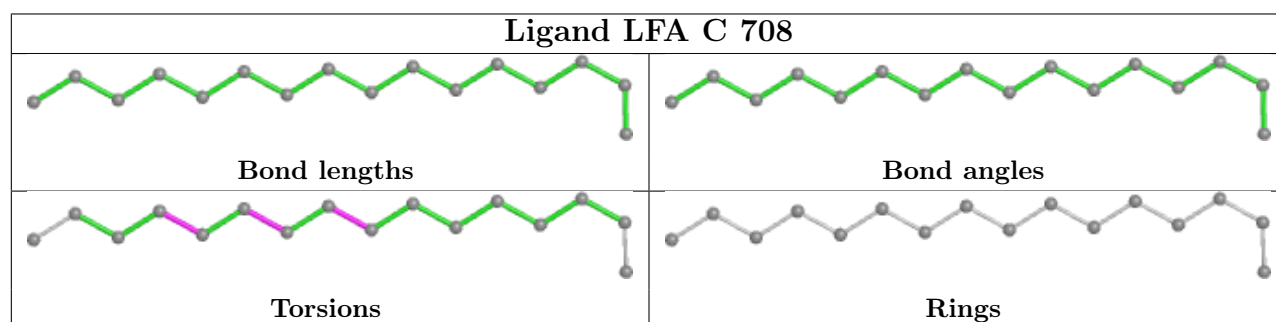
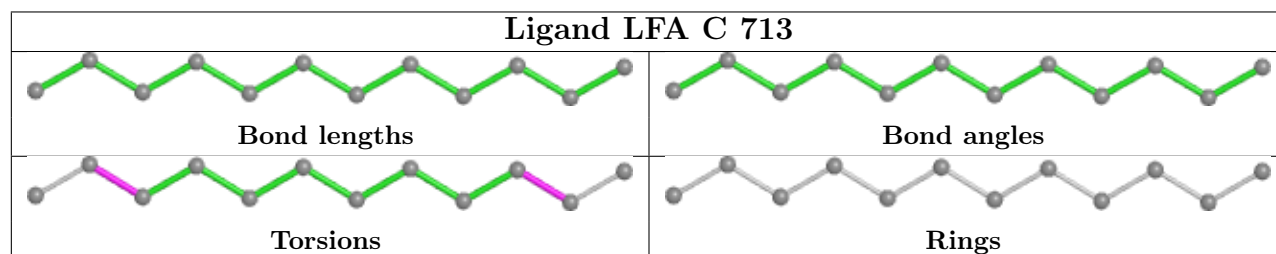
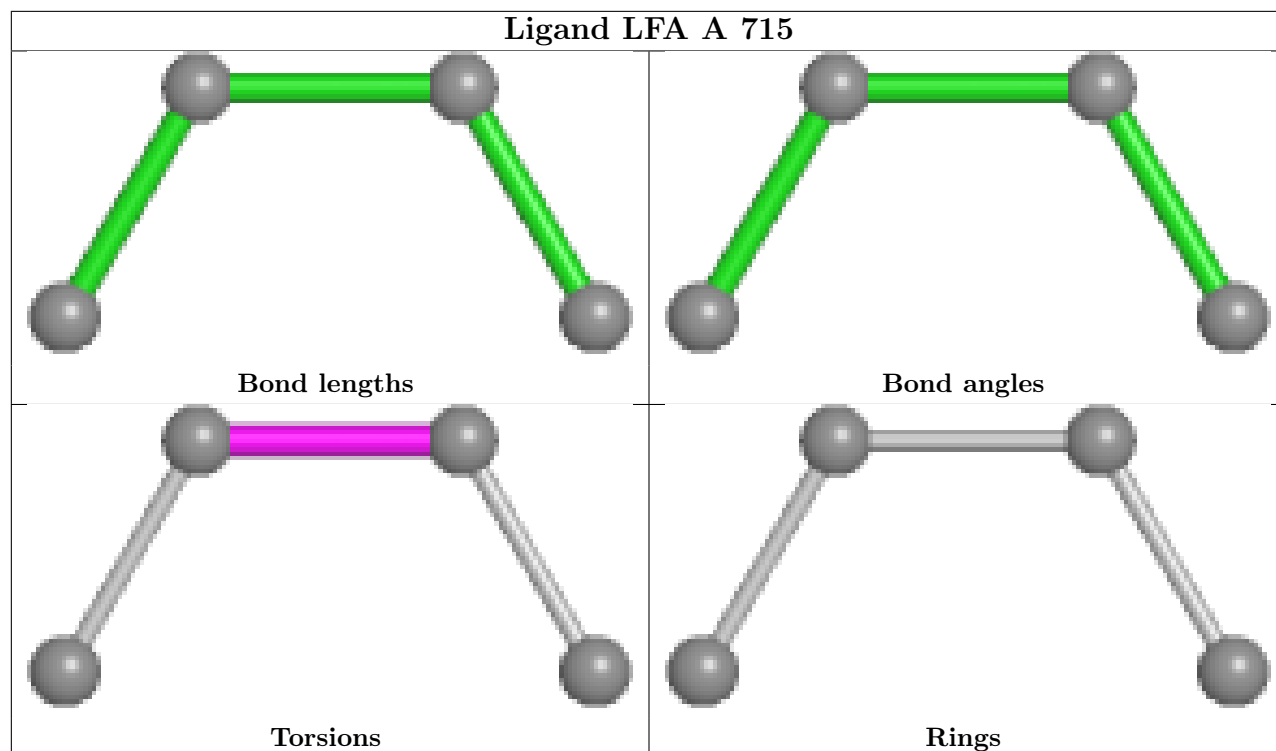


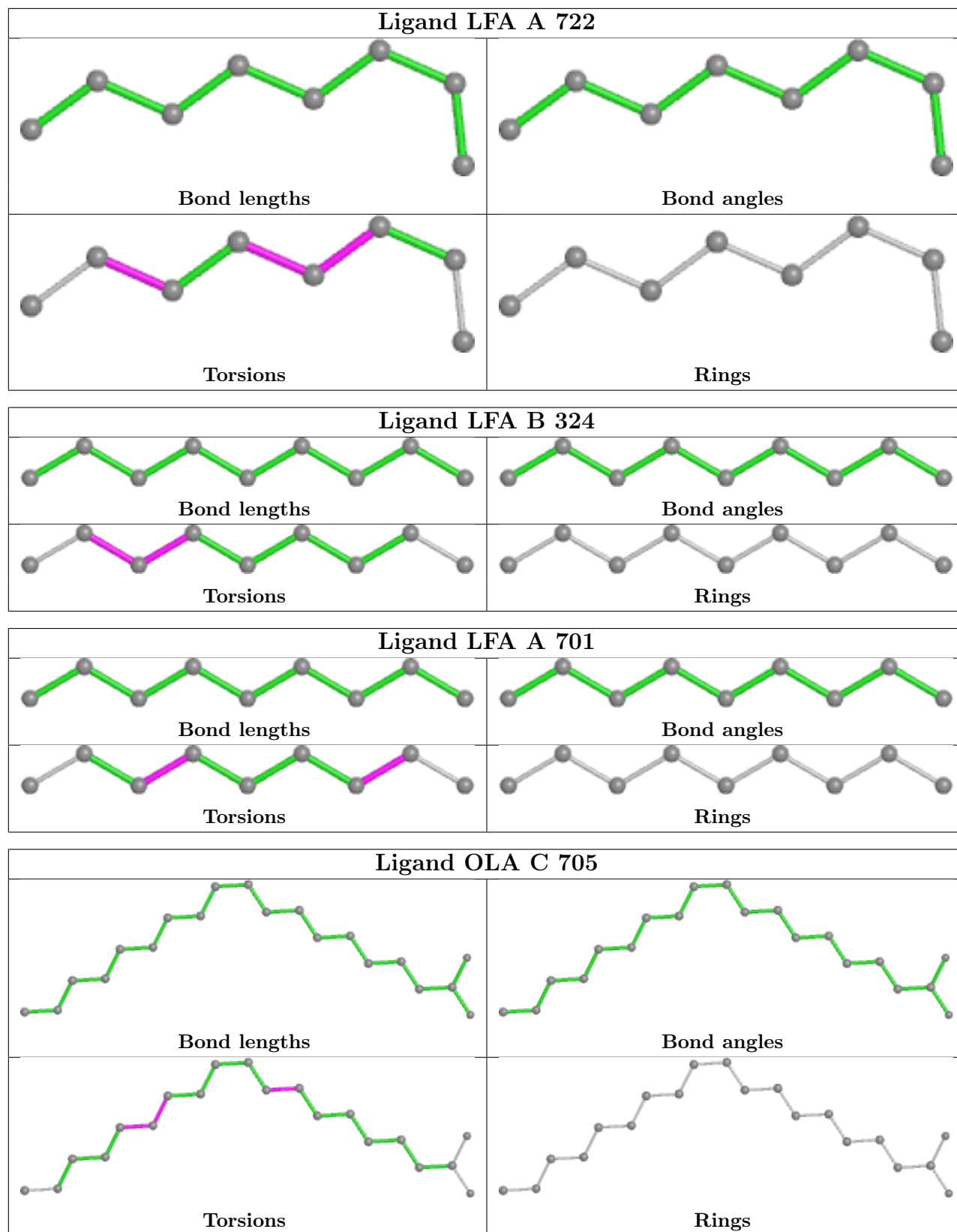


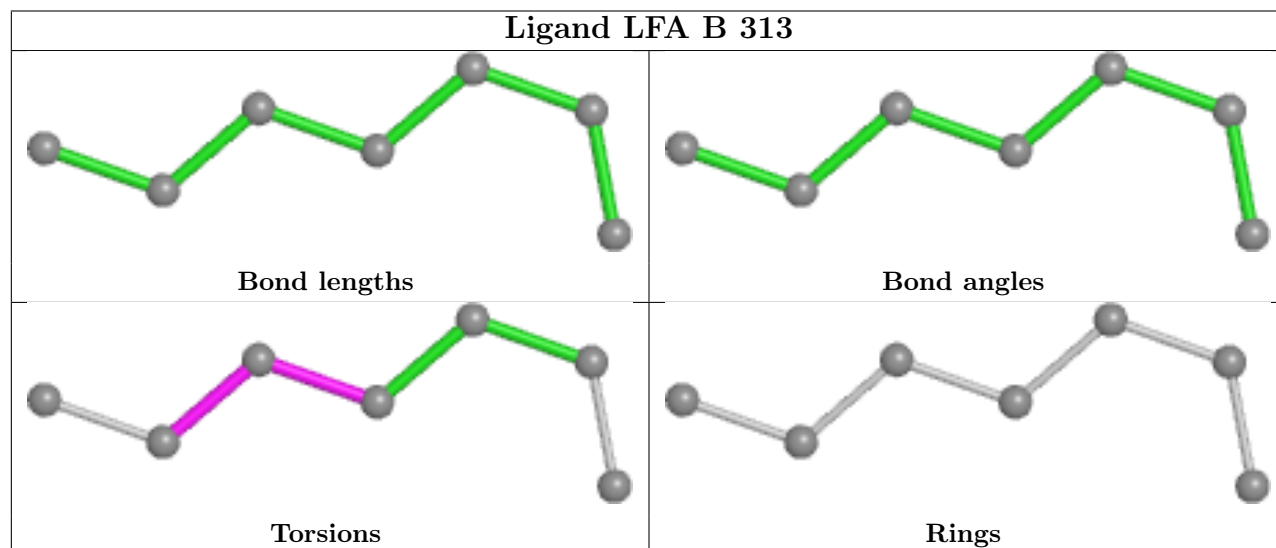
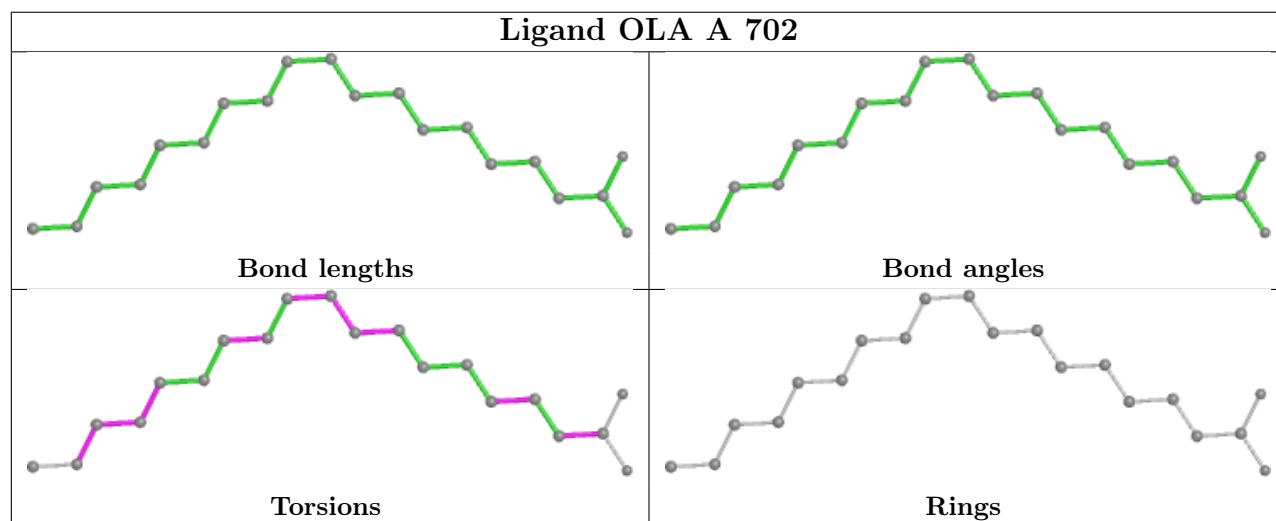
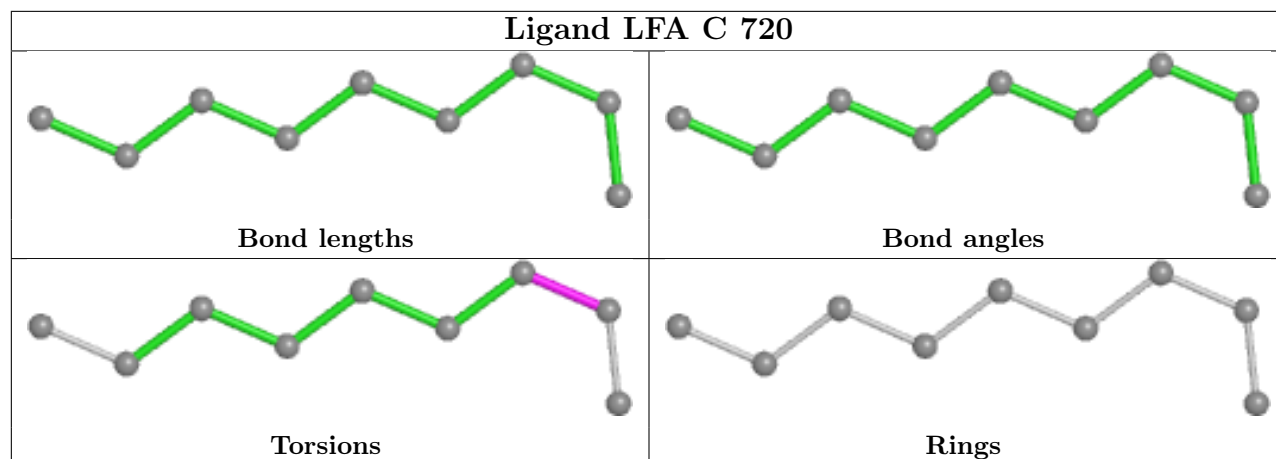


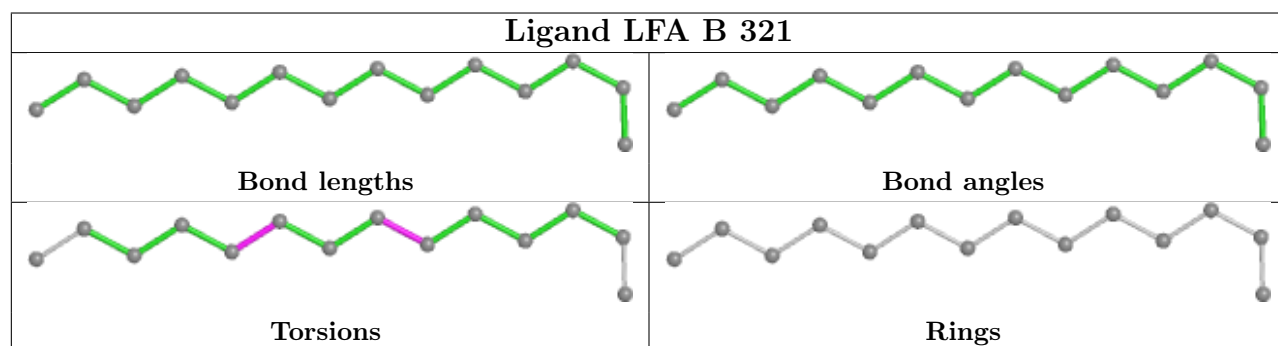
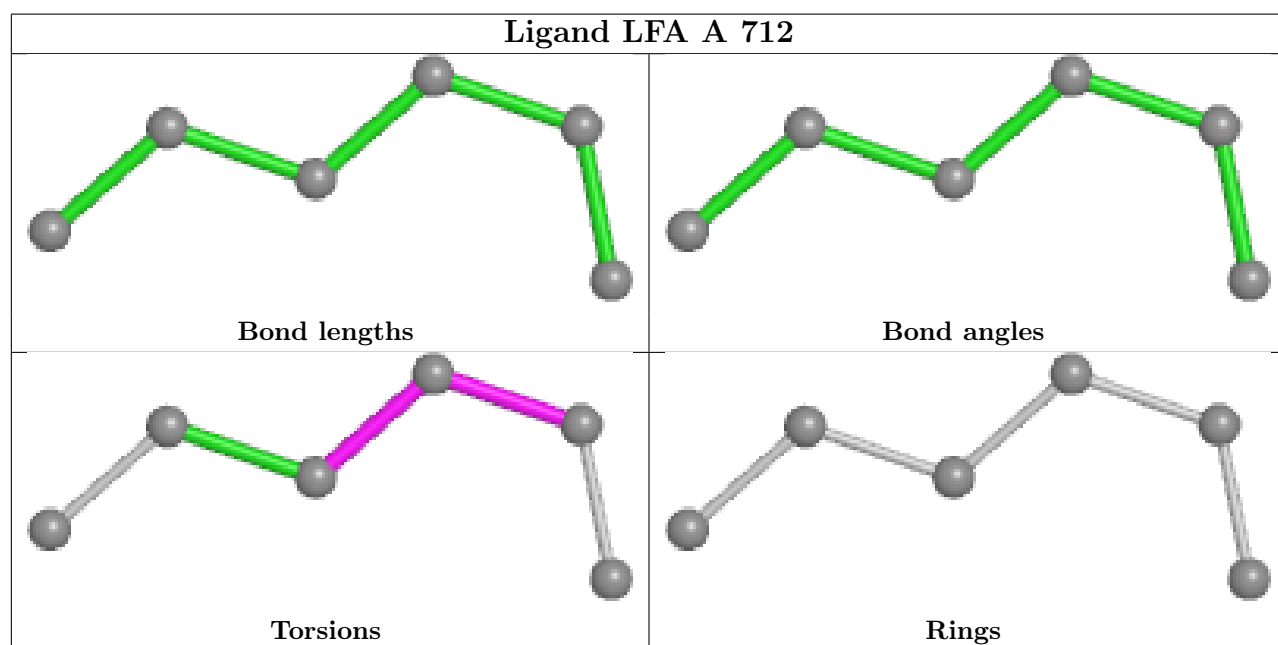
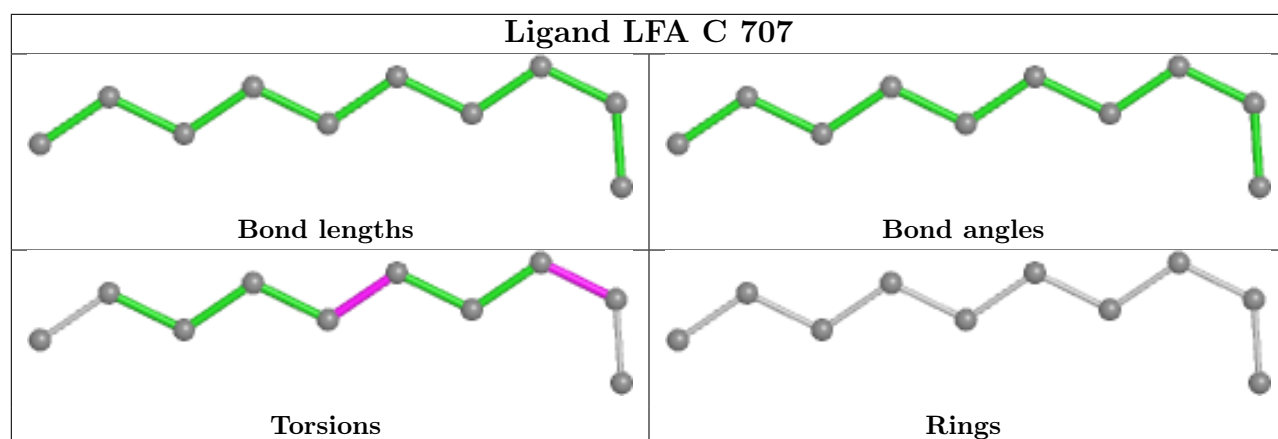


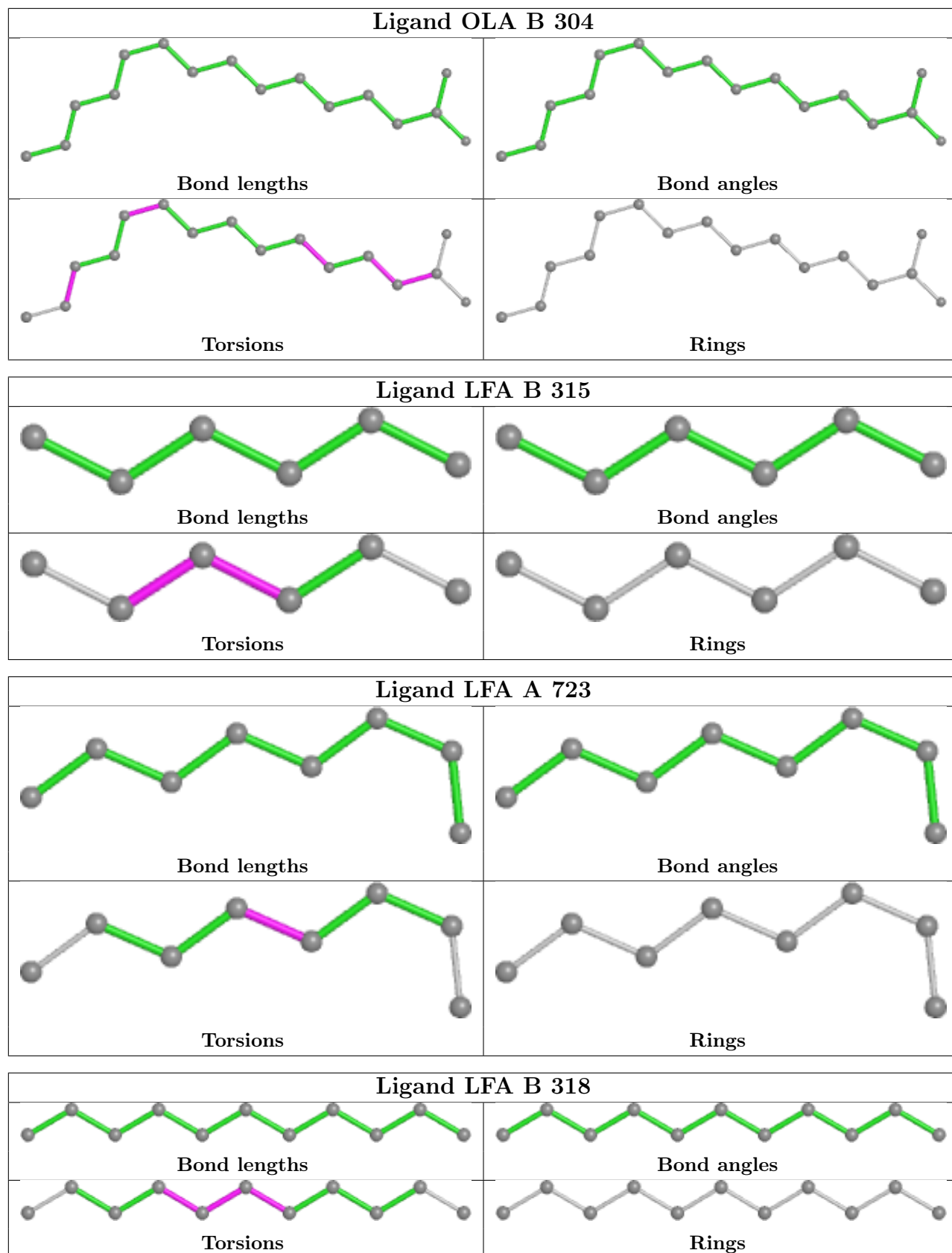


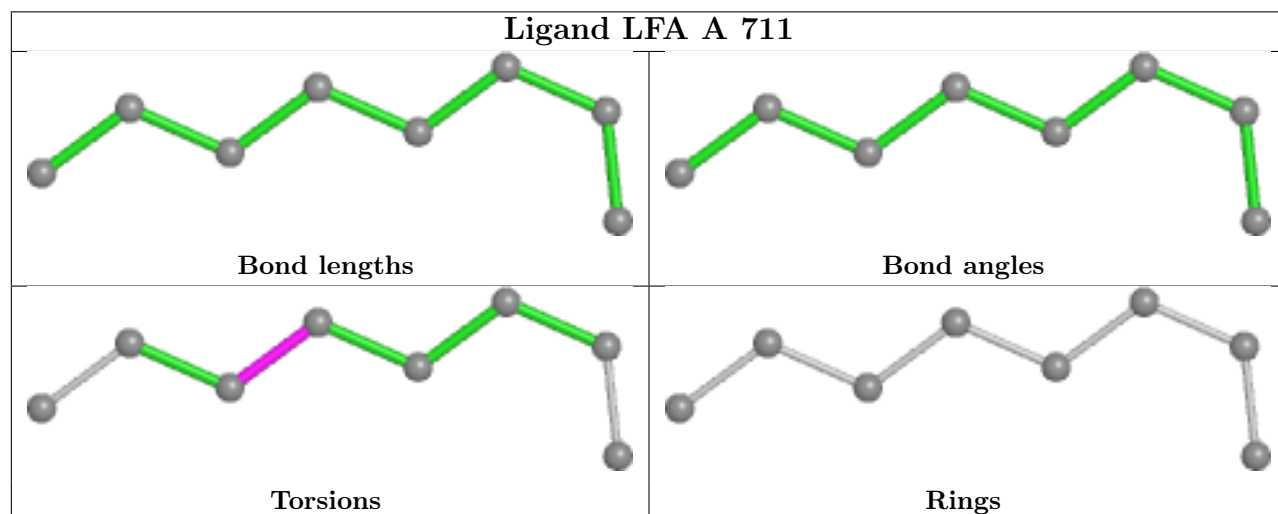
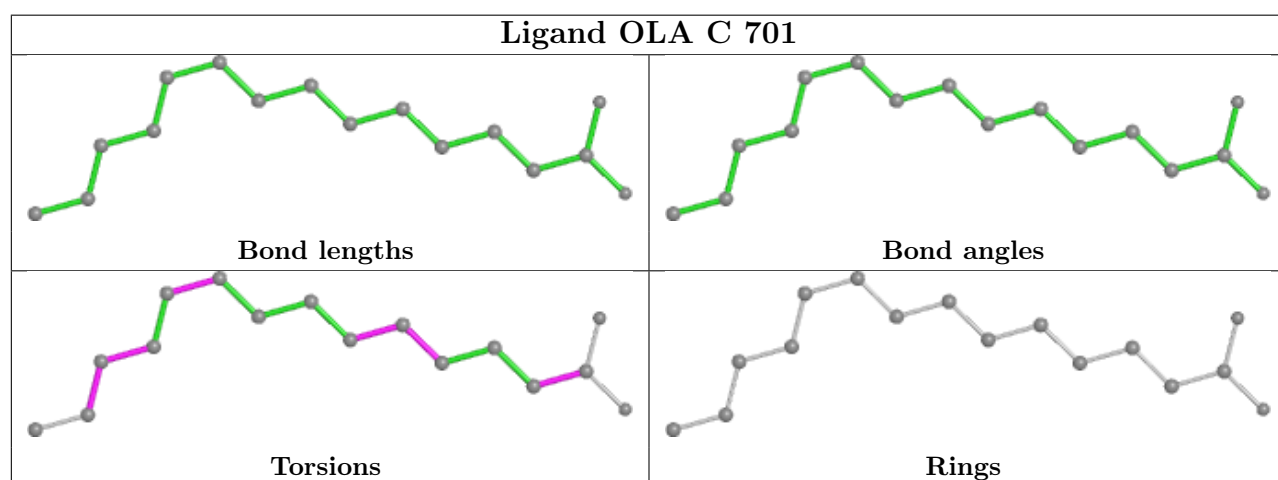
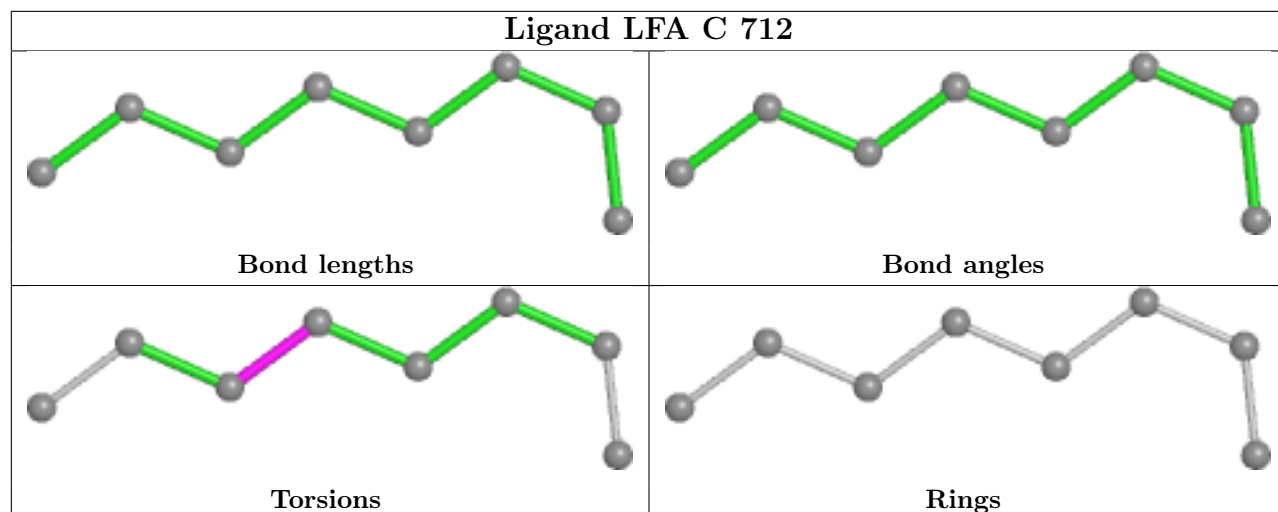


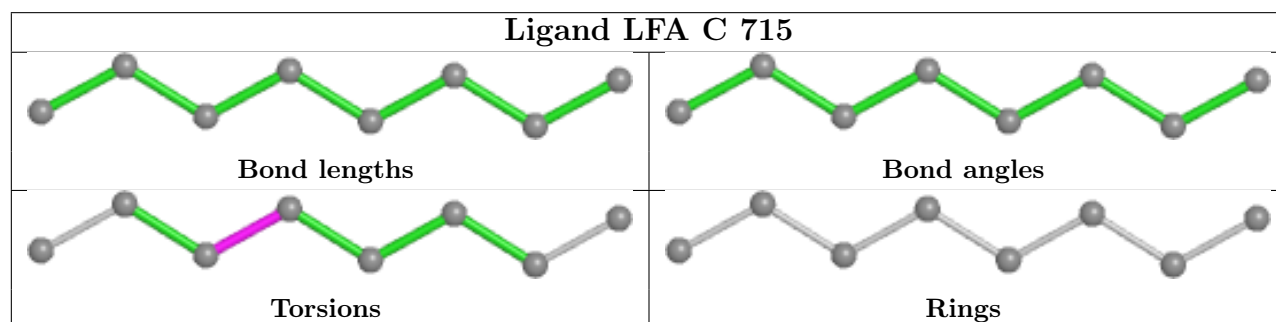
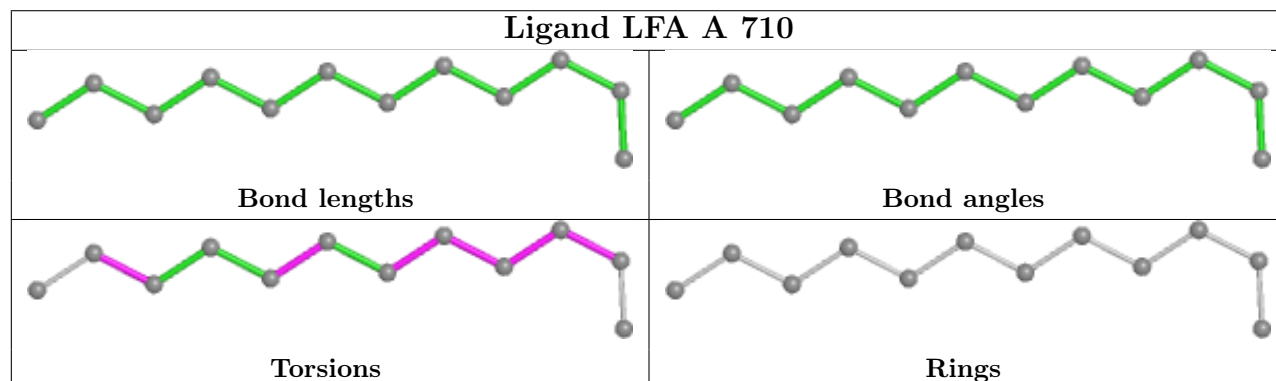
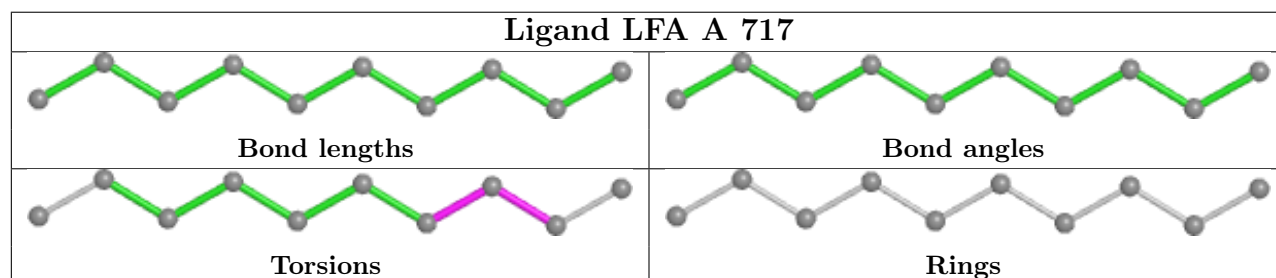
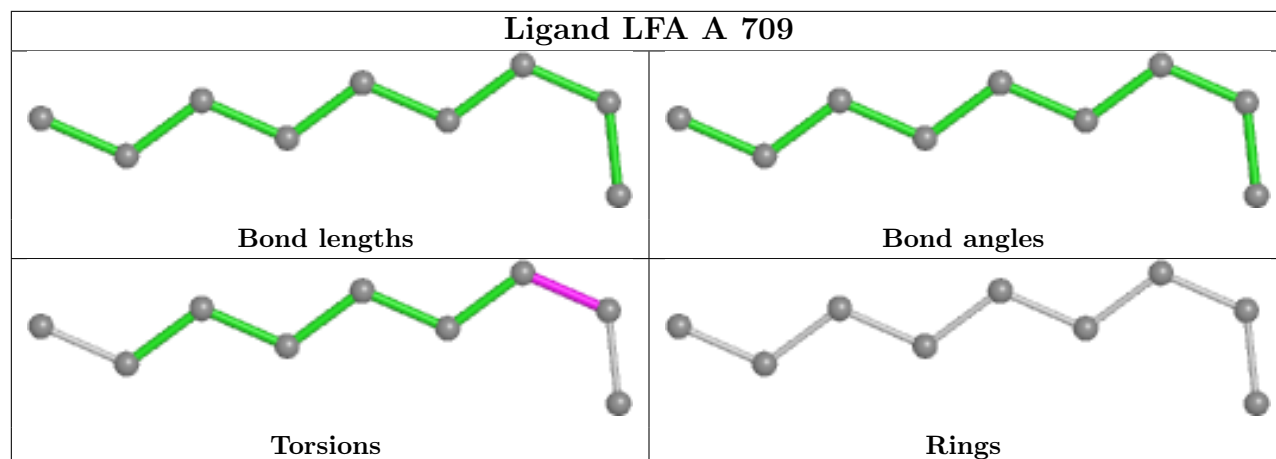


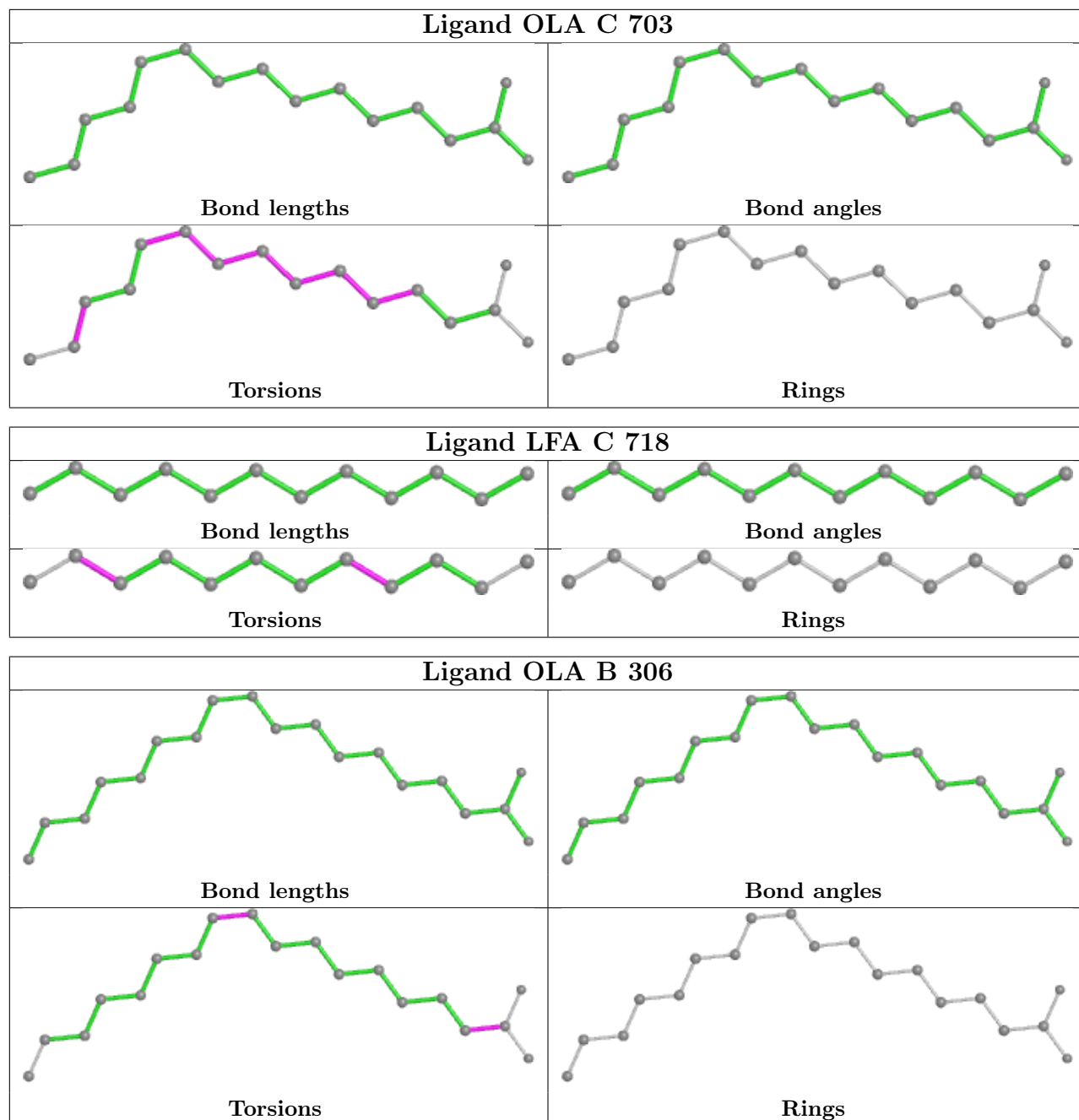


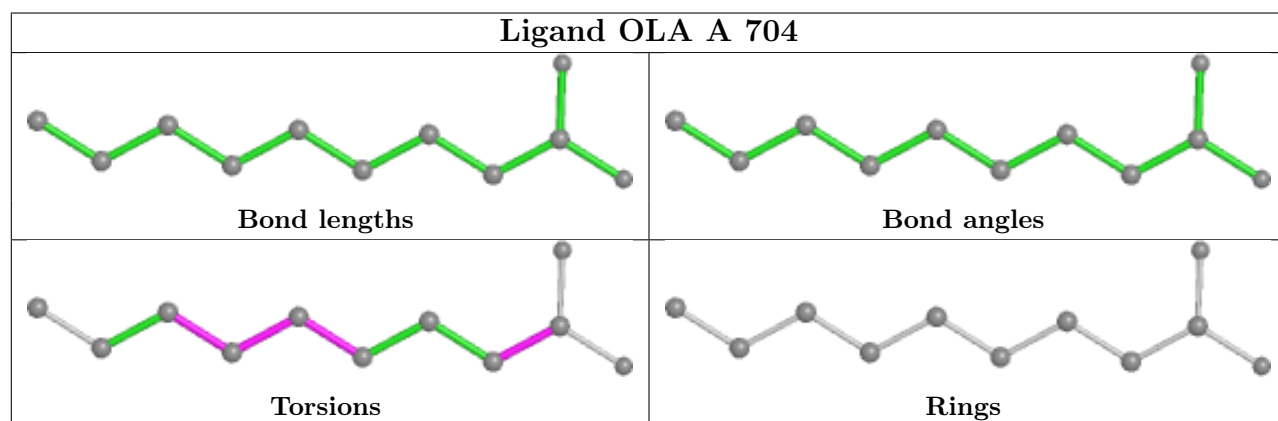
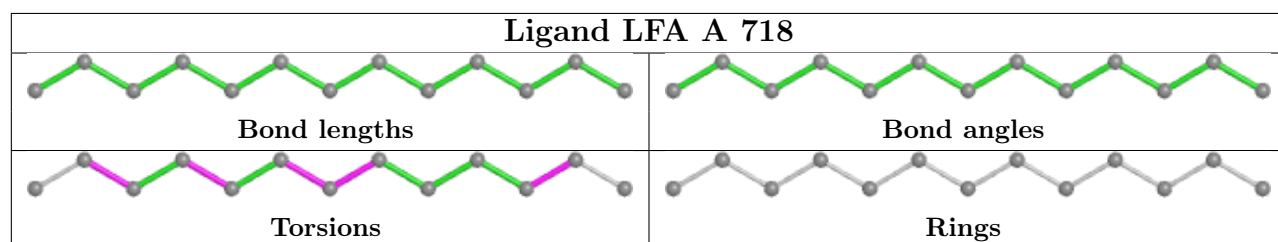
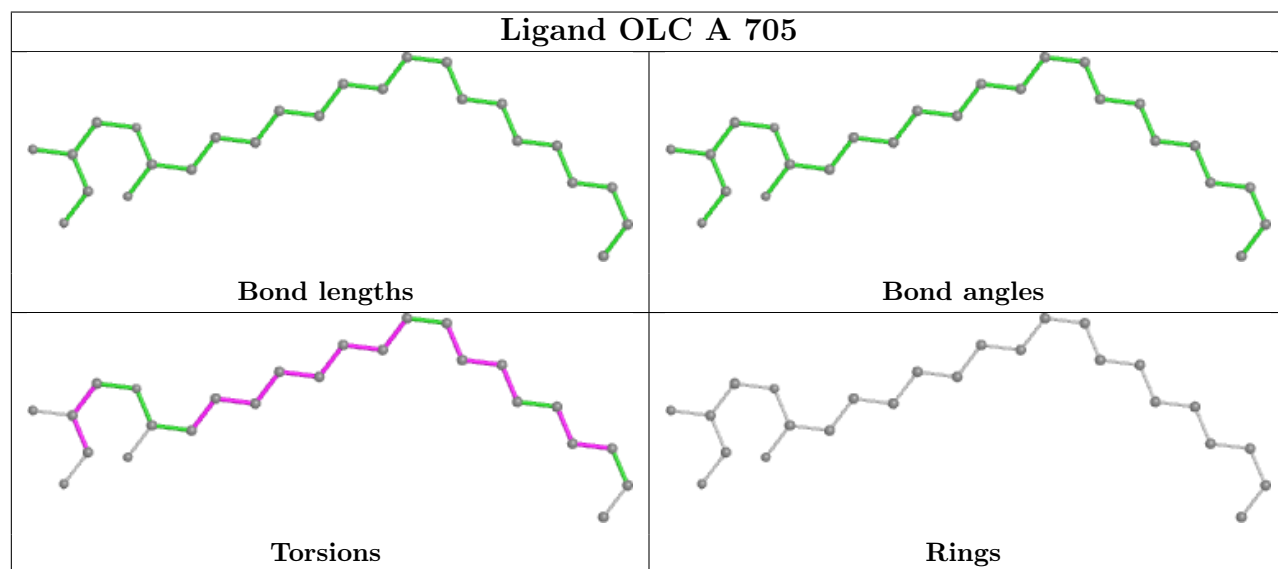
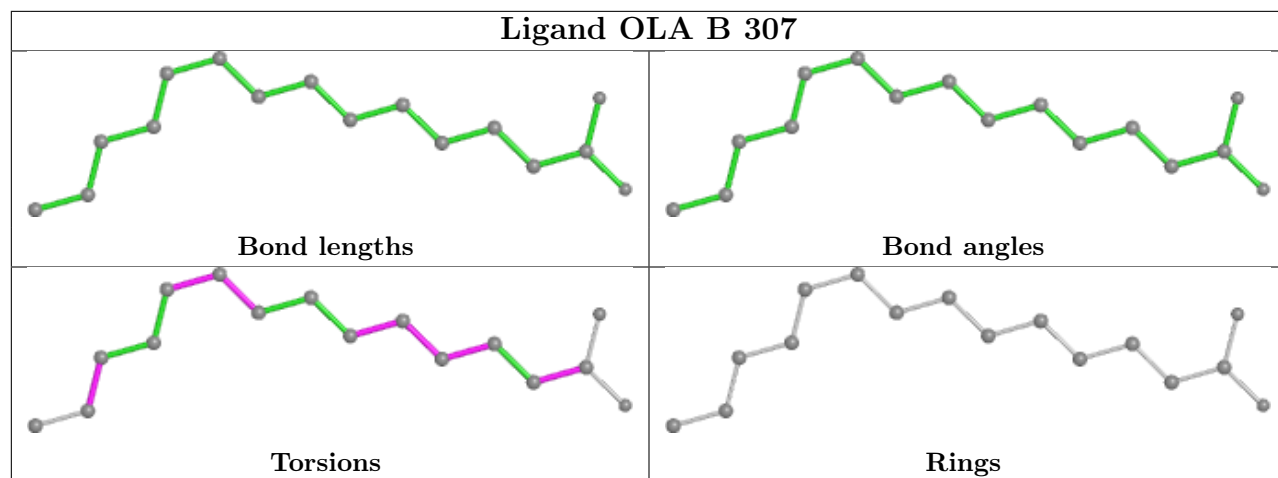


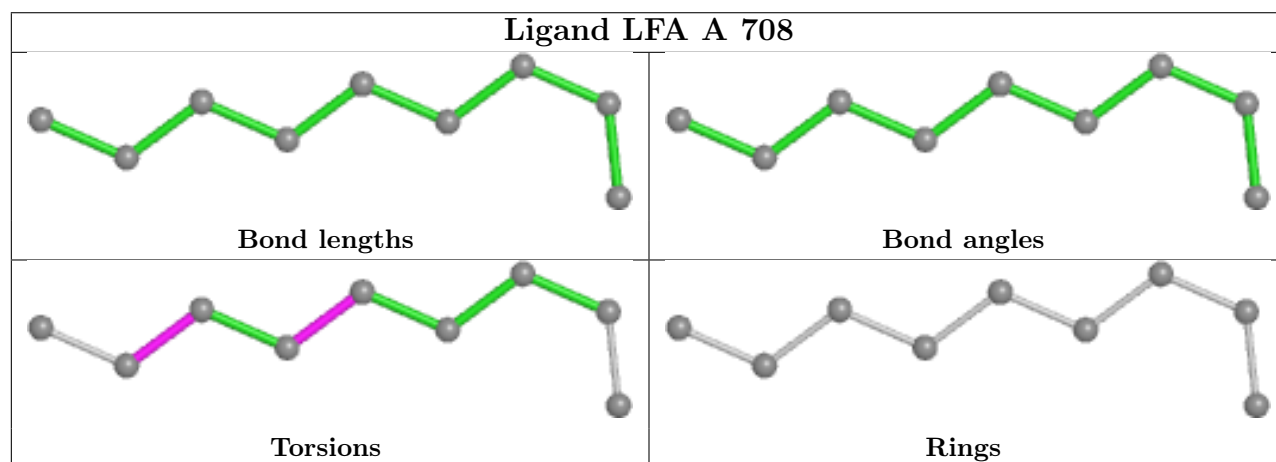
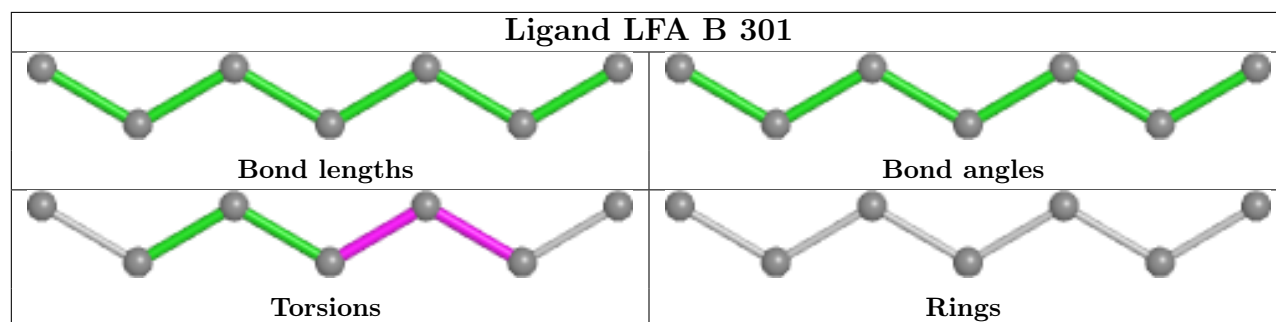
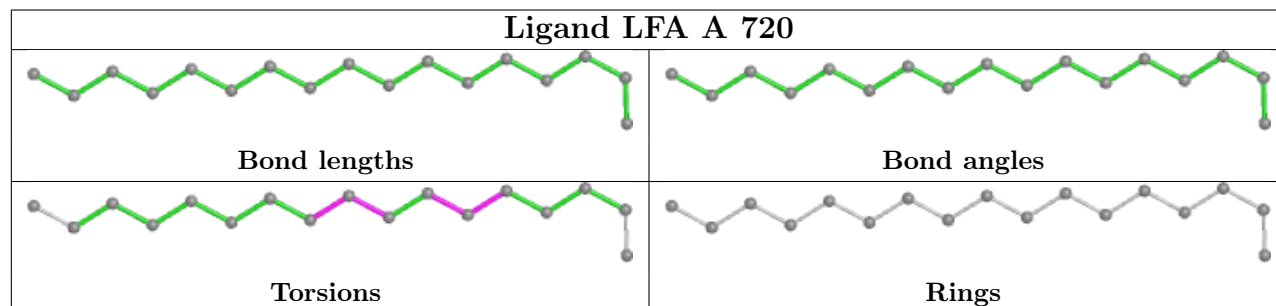
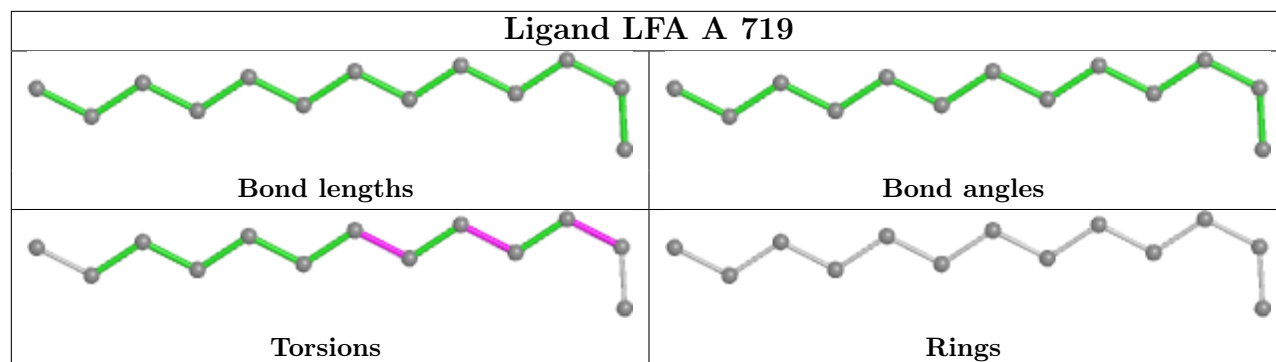


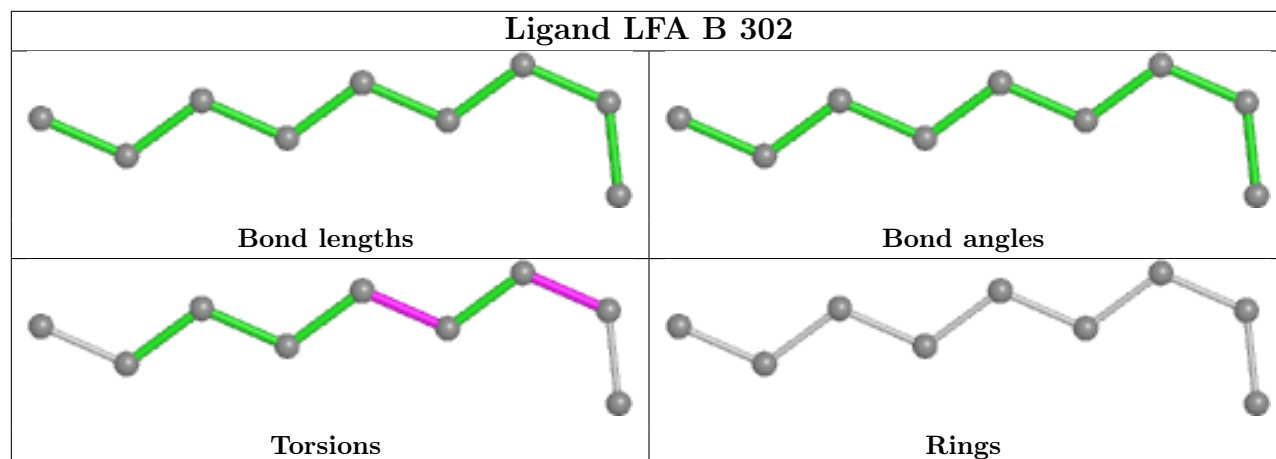












5.7 Other polymers [i](#)

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	222/229 (96%)	0.29	14 (6%) 20 22	23, 29, 46, 97	0
1	B	219/229 (95%)	0.14	7 (3%) 47 52	23, 30, 48, 86	0
1	C	220/229 (96%)	0.15	14 (6%) 19 21	23, 30, 48, 87	0
All	All	661/687 (96%)	0.19	35 (5%) 26 29	23, 29, 48, 97	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	TYR	8.3
1	A	224	SER	7.8
1	A	62	ASP	7.5
1	A	61	TYR	7.5
1	C	189	LEU	6.5
1	B	64	THR	6.1
1	A	63	ASP	6.0
1	C	61	TYR	6.0
1	B	60	GLN	5.9
1	A	64	THR	5.8
1	A	223	GLN	4.4
1	A	60	GLN	4.4
1	C	60	GLN	4.2
1	C	64	THR	4.0
1	B	59	PHE	3.9
1	C	121	ILE	3.8
1	C	187	LEU	3.7
1	C	224	SER	3.5
1	A	121	ILE	3.4
1	A	111	ILE	3.4
1	B	223	GLN	3.2
1	C	123	THR	3.2
1	C	40	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	191	GLN	2.8
1	A	108	VAL	2.7
1	C	190	ALA	2.6
1	C	186	GLY	2.6
1	A	105	ALA	2.5
1	C	152	LEU	2.5
1	C	223	GLN	2.5
1	B	222	HIS	2.5
1	A	104	VAL	2.4
1	A	75	VAL	2.3
1	A	59	PHE	2.2
1	B	121	ILE	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	FME	A	1	10/11	0.88	0.25	37,46,84,92	0
1	FME	C	1	10/11	0.88	0.23	37,45,82,85	0
1	FME	B	1	10/11	0.89	0.15	35,54,71,85	0
1	LYR	B	207	29/30	0.91	0.12	22,27,32,37	0
1	LYR	A	207	29/30	0.92	0.14	23,26,32,39	0
1	LYR	C	207	29/30	0.94	0.09	24,27,32,37	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
3	OLA	A	703	14/20	0.53	0.20	45,57,81,81	0
2	LFA	A	722	8/20	0.55	0.25	40,55,64,65	0
2	LFA	C	718	12/20	0.57	0.32	57,68,76,77	0
2	LFA	B	311	6/20	0.57	0.19	63,68,71,73	0
2	LFA	C	719	9/20	0.58	0.20	64,67,76,77	0
3	OLA	B	306	19/20	0.58	0.29	45,51,67,69	0
3	OLA	C	701	16/20	0.60	0.23	39,53,59,61	0
4	OLC	A	705	25/25	0.62	0.29	45,55,64,73	0
2	LFA	B	324	9/20	0.64	0.18	59,64,69,73	0
2	LFA	B	318	11/20	0.65	0.28	58,64,73,74	0
3	OLA	C	704	15/20	0.65	0.21	50,56,74,78	0
3	OLA	A	702	20/20	0.65	0.28	39,52,62,63	0
3	OLA	B	309	14/20	0.67	0.20	49,57,64,67	0
3	OLA	B	303	13/20	0.68	0.17	46,54,67,84	0
2	LFA	B	313	7/20	0.68	0.14	56,58,65,68	0
2	LFA	B	317	8/20	0.68	0.26	45,49,63,66	0
3	OLA	B	305	12/20	0.69	0.24	55,64,75,89	0
2	LFA	C	717	15/20	0.69	0.19	57,69,77,84	0
2	LFA	A	711	8/20	0.69	0.17	55,64,72,77	0
2	LFA	C	708	16/20	0.71	0.19	57,69,74,78	0
2	LFA	C	720	9/20	0.72	0.17	51,66,69,71	0
3	OLA	B	308	19/20	0.73	0.25	39,49,66,74	0
2	LFA	B	322	4/20	0.74	0.26	56,58,62,62	0
2	LFA	C	713	12/20	0.74	0.23	47,68,75,75	0
3	OLA	C	703	16/20	0.74	0.18	56,63,74,82	0
3	OLA	B	307	16/20	0.74	0.15	62,73,80,84	0
2	LFA	B	315	6/20	0.74	0.14	61,65,72,73	0
3	OLA	B	304	16/20	0.76	0.22	47,57,80,84	0
3	OLA	A	704	11/20	0.76	0.19	51,62,75,77	0
3	OLA	A	706	14/20	0.77	0.16	40,58,67,67	0
3	OLA	C	702	19/20	0.78	0.21	39,55,71,88	0
2	LFA	C	712	8/20	0.78	0.36	38,55,71,78	0
2	LFA	A	716	10/20	0.78	0.18	51,60,72,75	0
2	LFA	C	709	8/20	0.78	0.13	58,63,68,68	0
2	LFA	C	707	10/20	0.79	0.17	59,64,69,70	0
2	LFA	C	721	7/20	0.79	0.16	60,62,71,71	0
2	LFA	B	314	5/20	0.79	0.33	51,52,53,55	0
2	LFA	C	715	8/20	0.80	0.17	53,61,67,68	0
2	LFA	C	710	9/20	0.81	0.13	60,61,65,67	0
2	LFA	A	723	8/20	0.81	0.16	57,62,66,66	0
2	LFA	A	724	6/20	0.81	0.13	53,55,60,62	0
2	LFA	A	718	13/20	0.81	0.23	53,63,74,74	0
2	LFA	B	323	11/20	0.81	0.16	50,58,61,62	0

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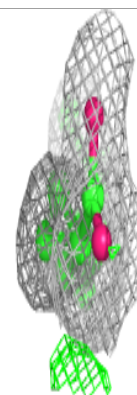
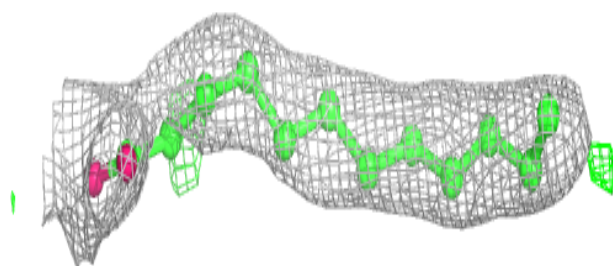
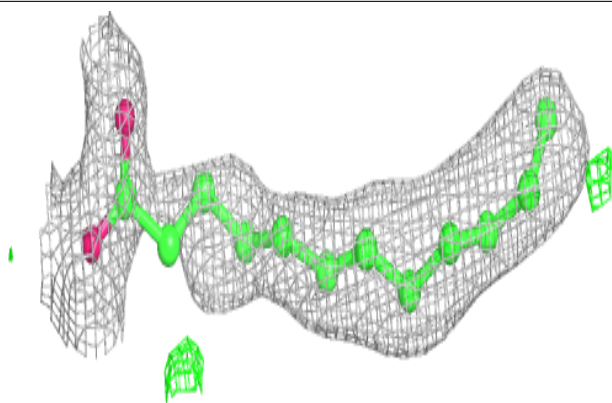
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LFA	B	320	9/20	0.82	0.17	44,48,57,60	0
2	LFA	A	713	3/20	0.82	0.26	55,55,61,66	0
2	LFA	A	717	10/20	0.82	0.28	48,62,67,68	0
2	LFA	A	725	4/20	0.82	0.23	60,64,65,67	0
2	LFA	B	316	15/20	0.83	0.21	41,53,71,72	0
2	LFA	A	710	12/20	0.83	0.14	44,56,64,70	0
2	LFA	C	716	7/20	0.83	0.16	53,57,63,65	0
2	LFA	A	720	17/20	0.83	0.15	42,62,75,78	0
2	LFA	B	321	14/20	0.85	0.14	53,58,63,65	0
2	LFA	A	708	9/20	0.86	0.14	65,72,74,77	0
2	LFA	B	312	9/20	0.86	0.18	52,57,61,63	0
3	OLA	C	705	20/20	0.86	0.23	46,53,62,64	0
2	LFA	A	721	11/20	0.86	0.33	48,50,61,62	0
2	LFA	B	301	7/20	0.87	0.18	41,45,55,61	0
2	LFA	A	712	6/20	0.87	0.20	42,56,59,63	0
2	LFA	C	714	10/20	0.87	0.28	50,56,63,63	0
2	LFA	A	714	10/20	0.89	0.13	46,55,60,61	0
2	LFA	A	719	13/20	0.89	0.13	55,60,72,73	0
2	LFA	C	711	8/20	0.89	0.18	49,53,59,60	0
2	LFA	A	709	9/20	0.90	0.13	42,50,56,61	0
2	LFA	B	319	10/20	0.90	0.10	49,54,62,63	0
2	LFA	A	701	9/20	0.90	0.32	39,43,49,50	0
2	LFA	B	302	9/20	0.94	0.33	48,53,61,64	0
6	PO4	A	726	5/5	0.94	0.30	69,71,81,81	5
6	PO4	C	722	5/5	0.94	0.30	85,89,93,100	5
2	LFA	A	715	4/20	0.95	0.31	45,52,55,61	0
5	NA	A	707	1/1	0.99	0.07	25,25,25,25	0
5	NA	B	310	1/1	0.99	0.04	27,27,27,27	0
5	NA	C	706	1/1	1.00	0.05	25,25,25,25	0

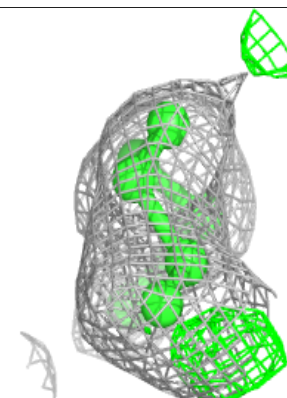
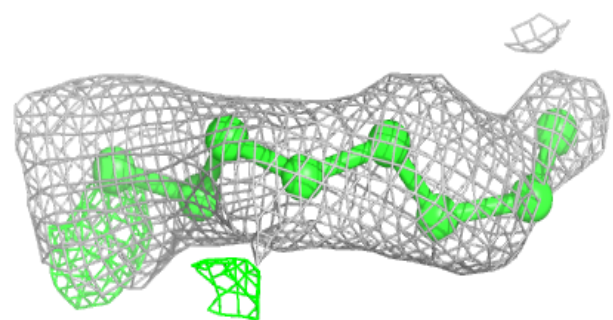
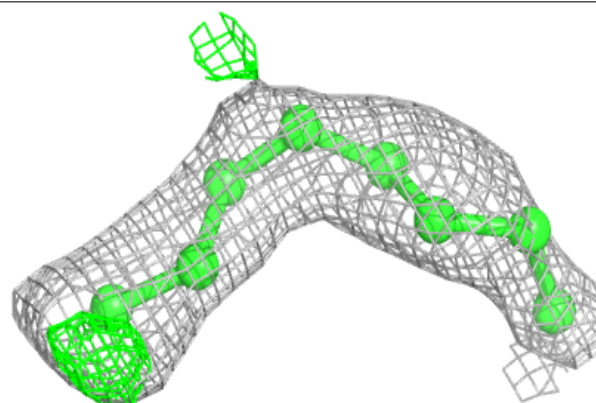
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 703:

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

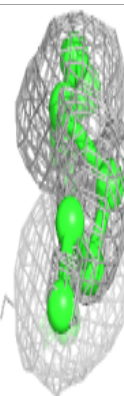
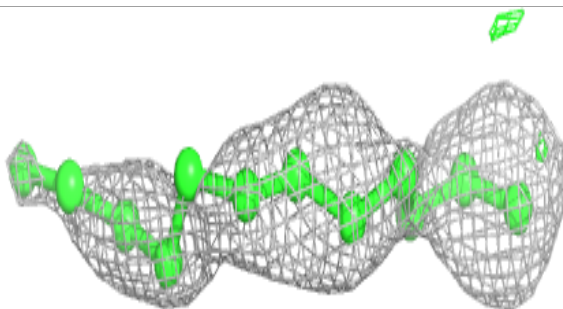
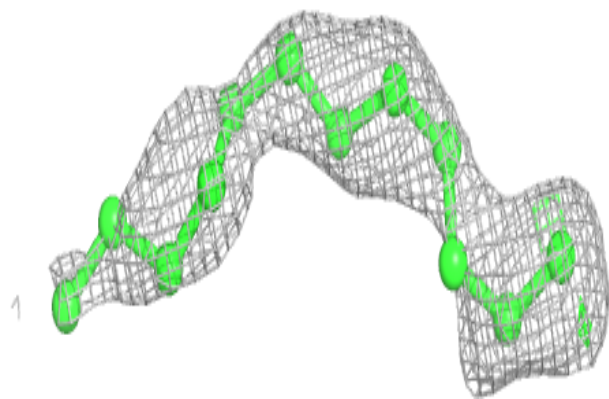
**Electron density around LFA A 722:**

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

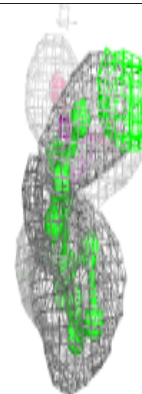
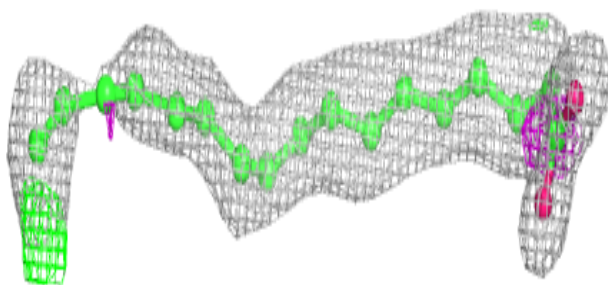
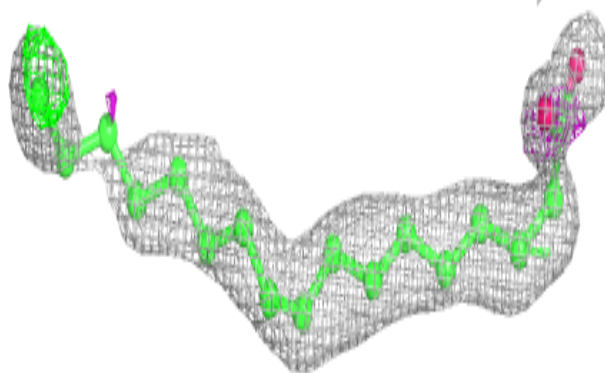


Electron density around LFA C 718:

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

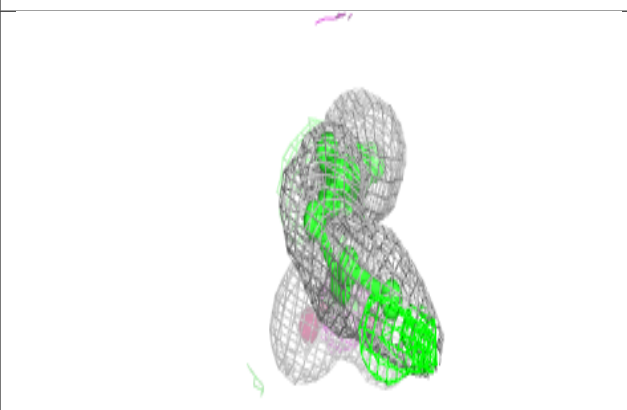
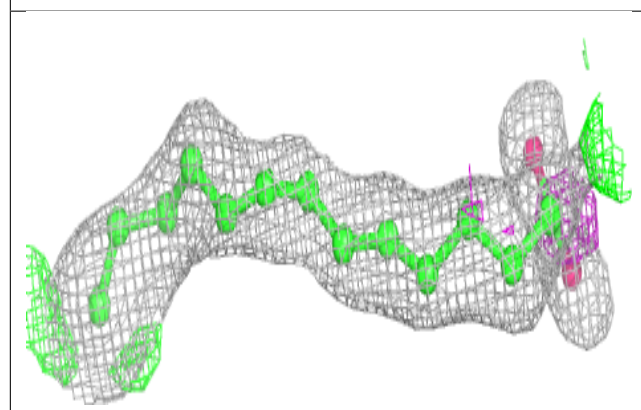
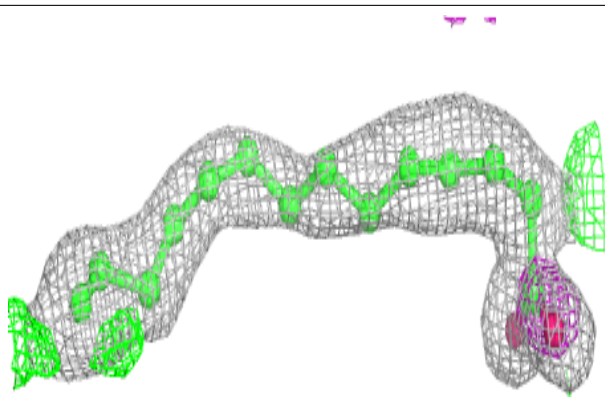
**Electron density around OLA B 306:**

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

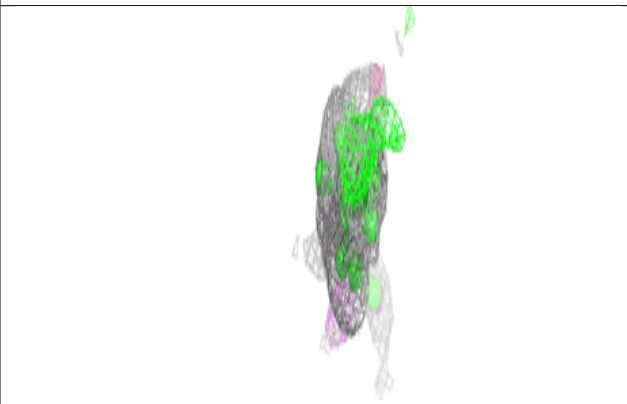
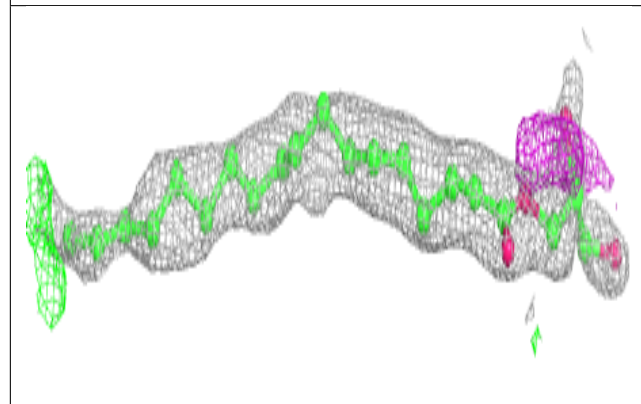
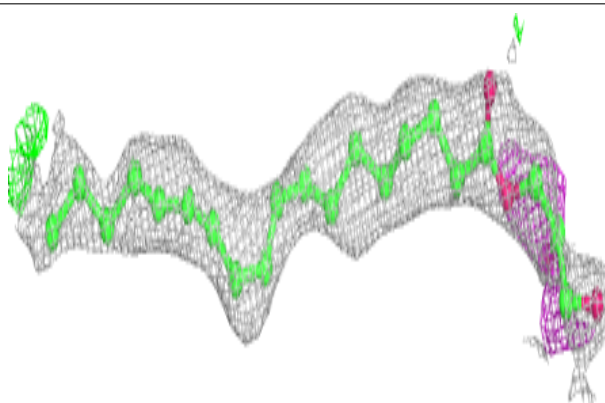


Electron density around OLA C 701:

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

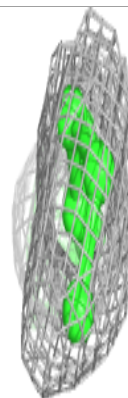
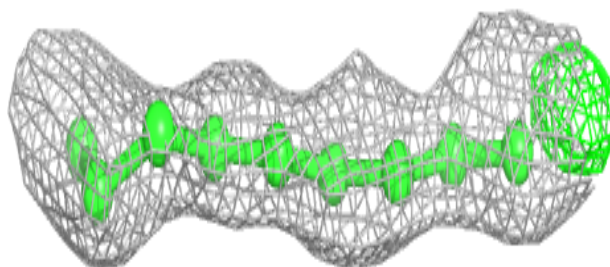
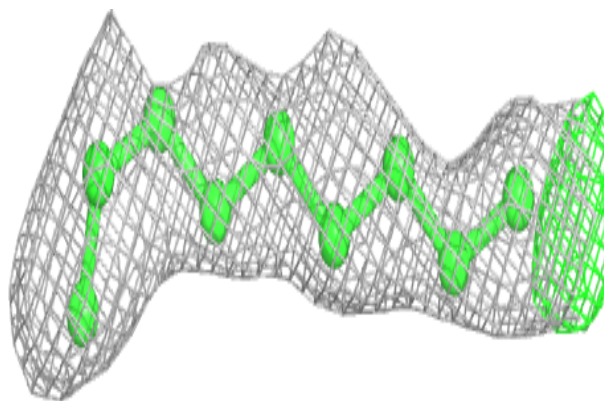
**Electron density around OLC A 705:**

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

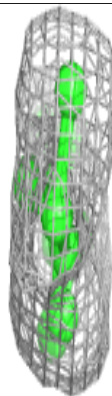
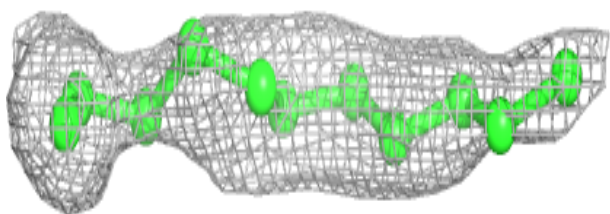
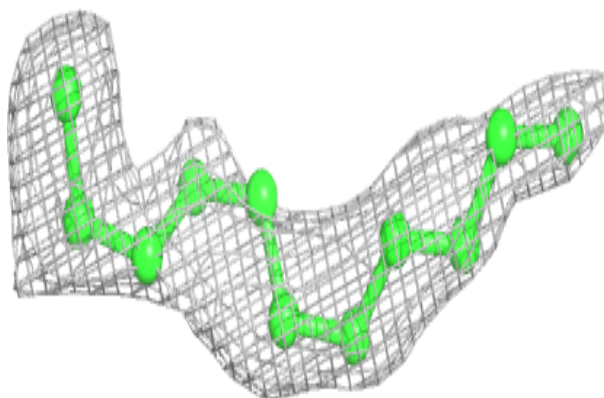


Electron density around LFA B 324:

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

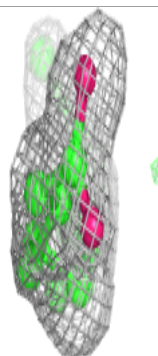
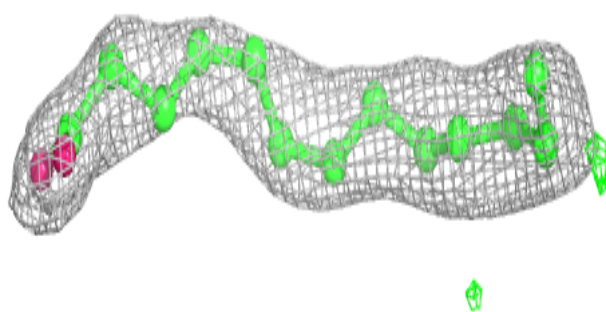
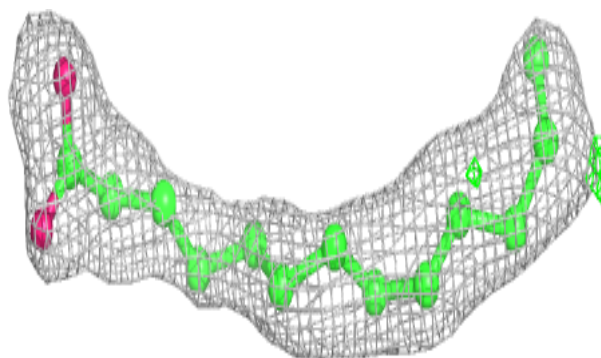
**Electron density around LFA B 318:**

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

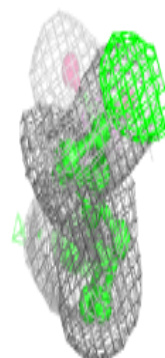
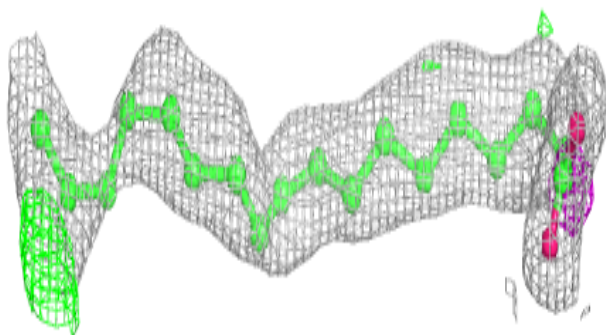
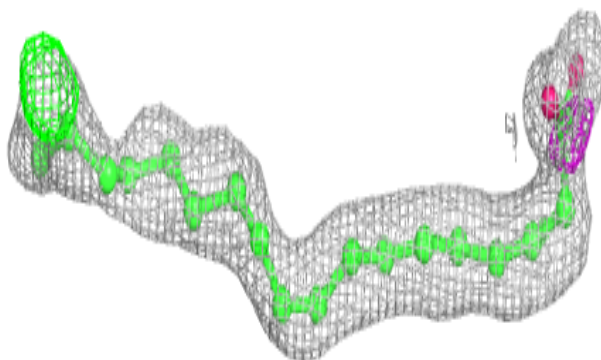


Electron density around OLA C 704:

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

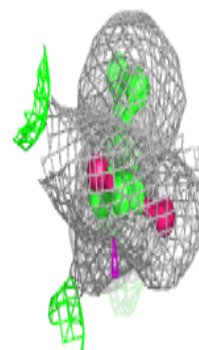
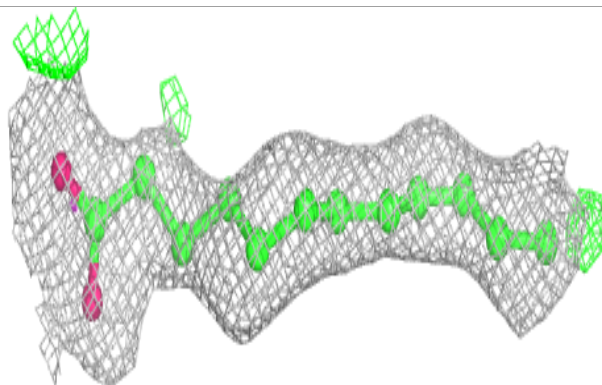
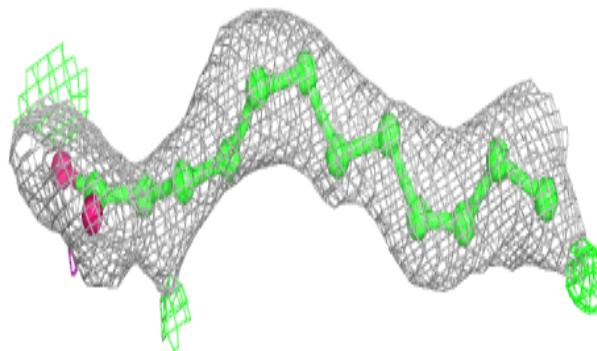
**Electron density around OLA A 702:**

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

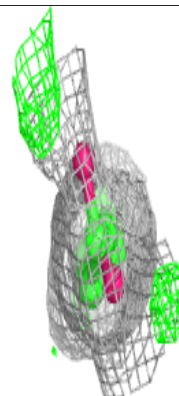
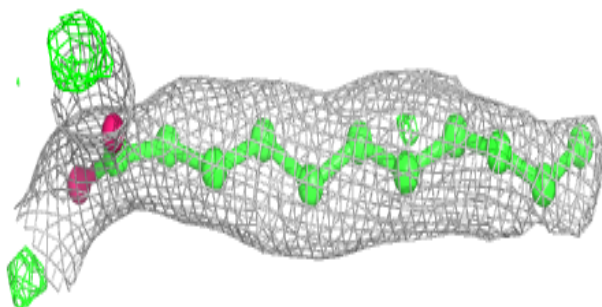
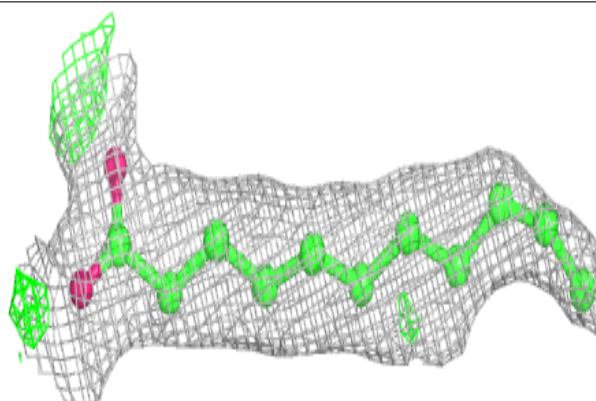


Electron density around OLA B 309:

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

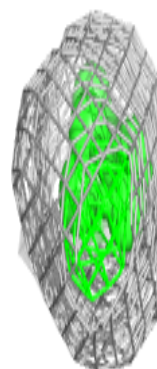
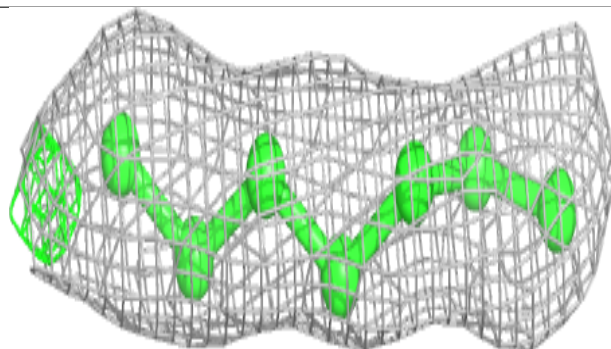
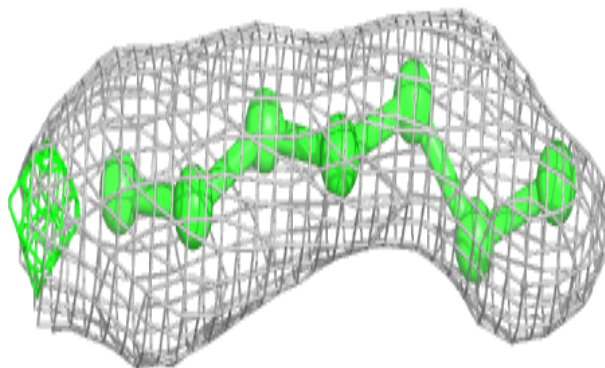
**Electron density around OLA B 303:**

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

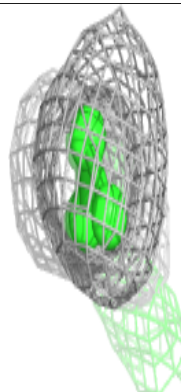
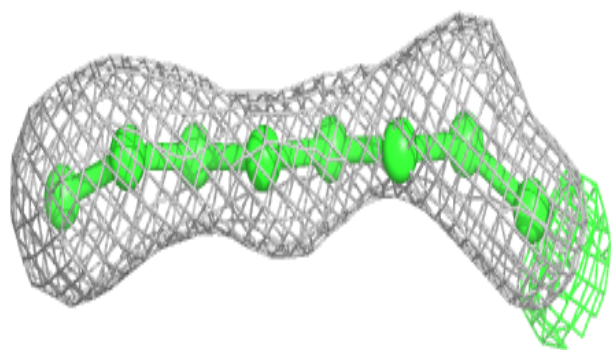
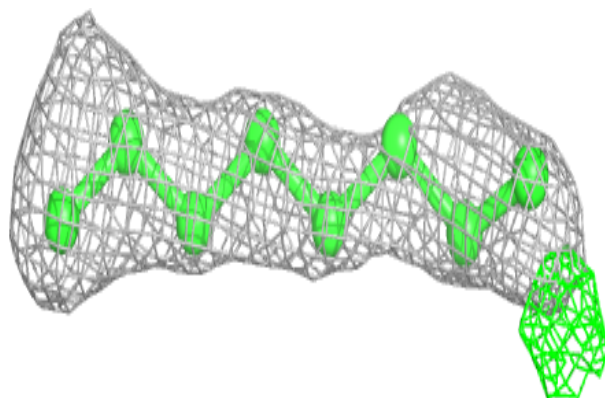


Electron density around LFA B 313:

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

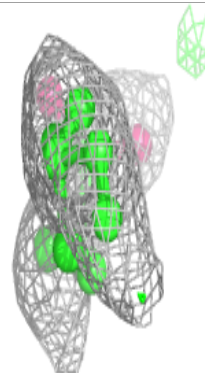
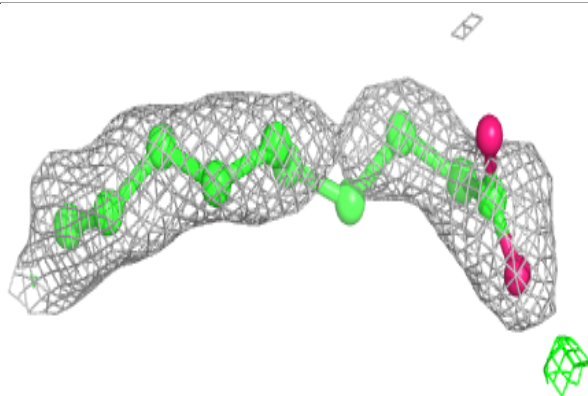
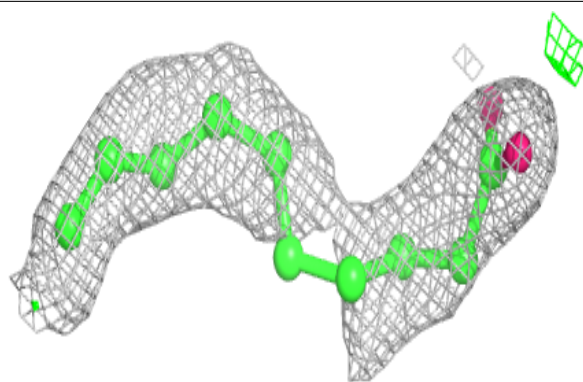
**Electron density around LFA B 317:**

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

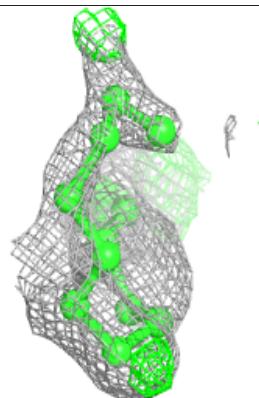
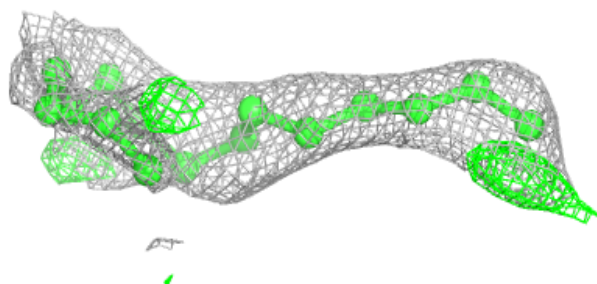
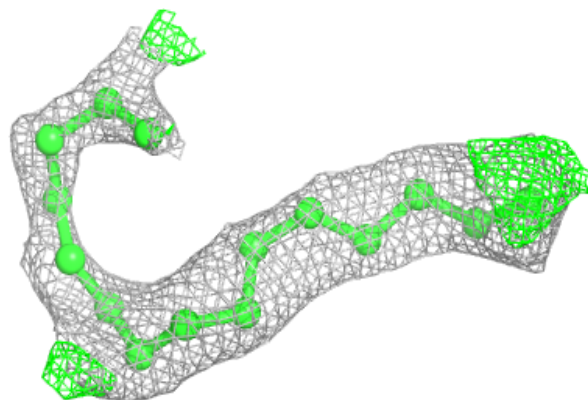


Electron density around OLA B 305:

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

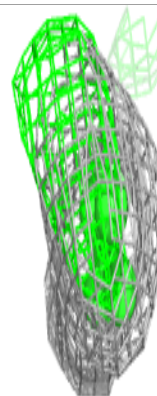
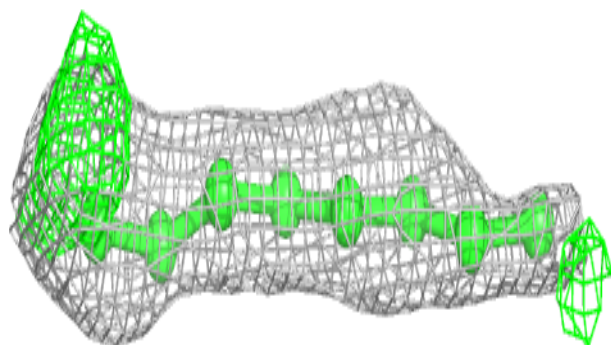
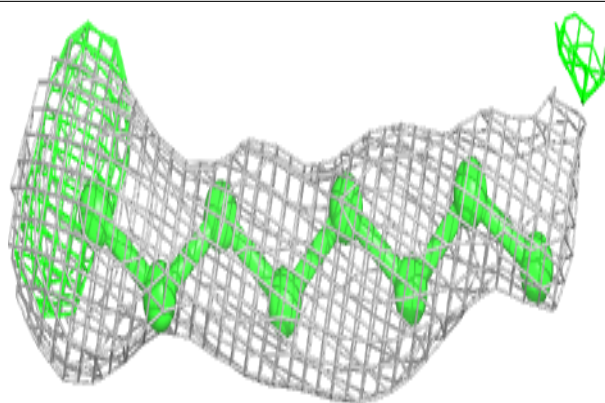
**Electron density around LFA C 717:**

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

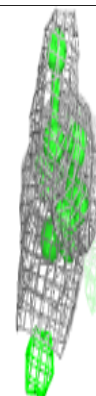
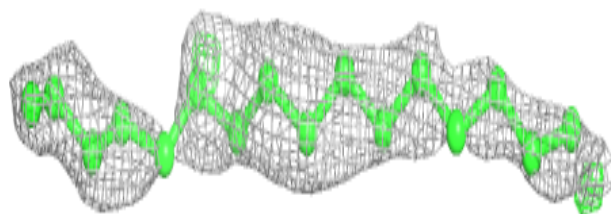
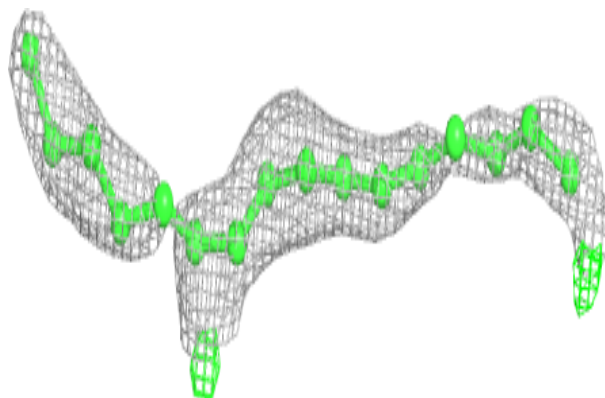


Electron density around LFA A 711:

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

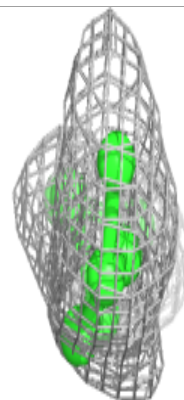
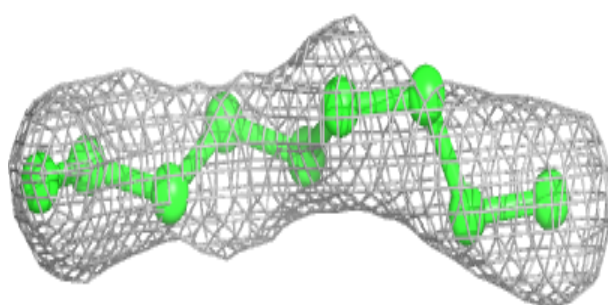
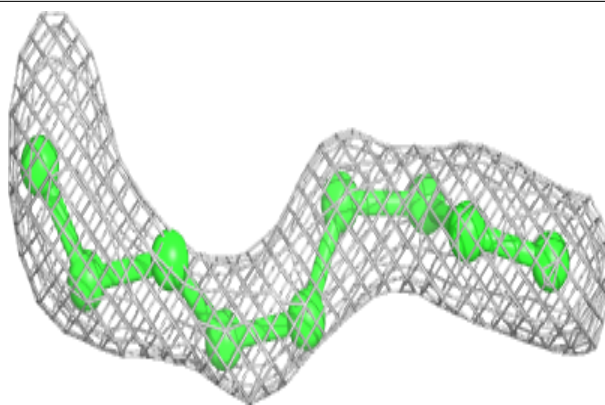
**Electron density around LFA C 708:**

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

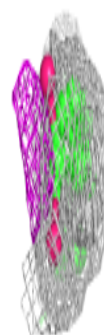
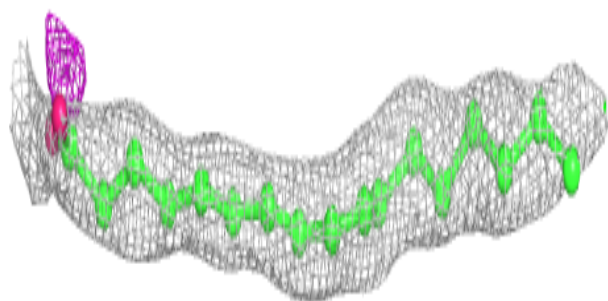
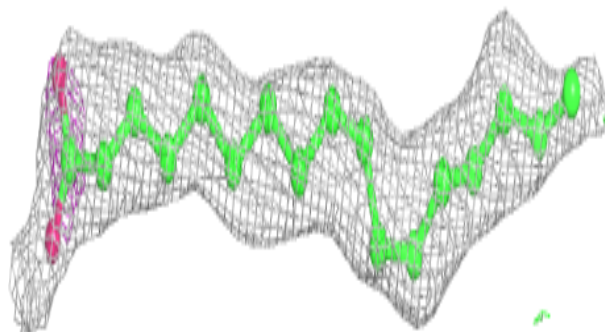


Electron density around LFA C 720:

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

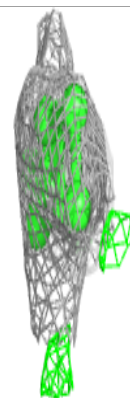
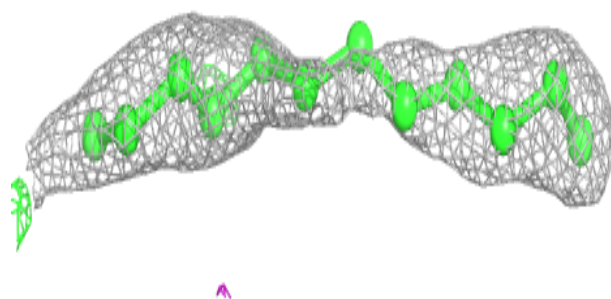
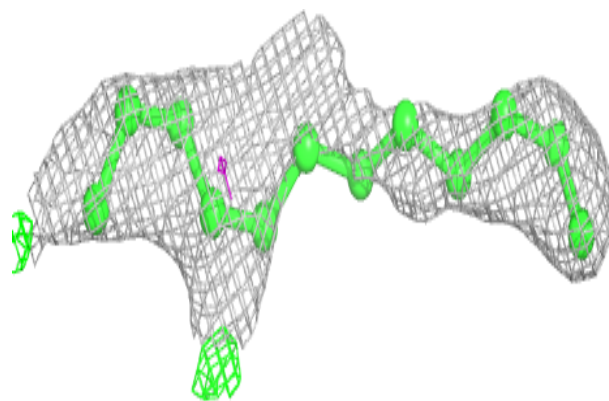
**Electron density around OLA B 308:**

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

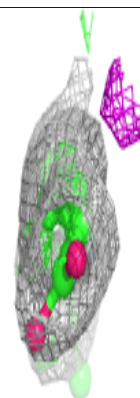
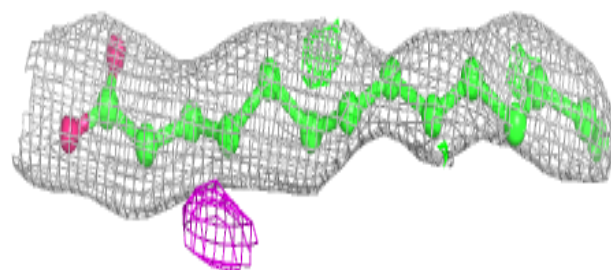
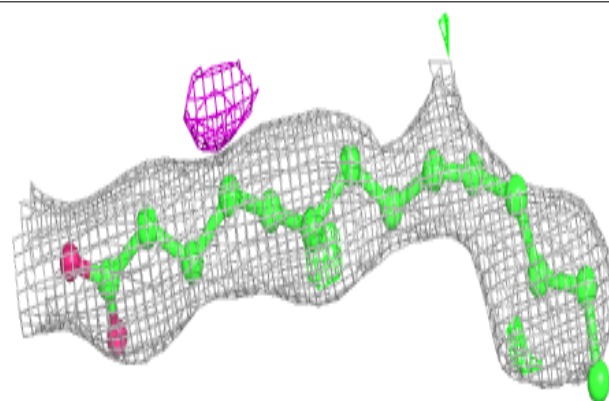


Electron density around LFA C 713:

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

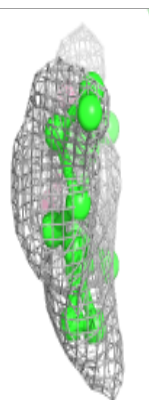
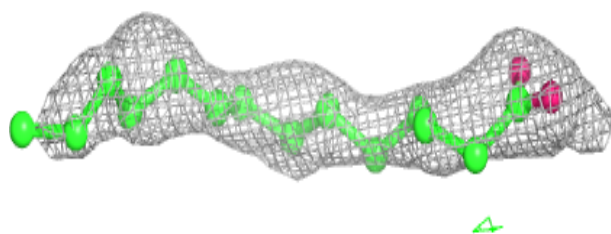
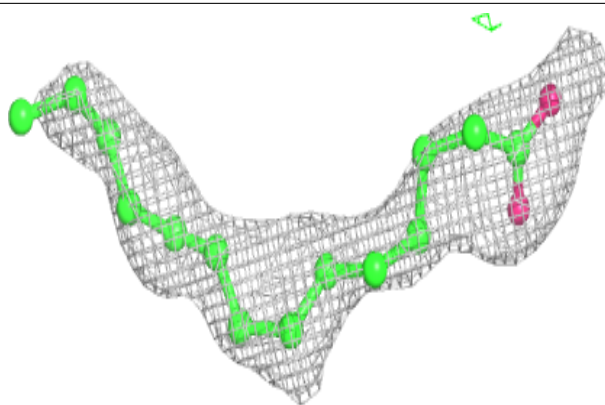
**Electron density around OLA C 703:**

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

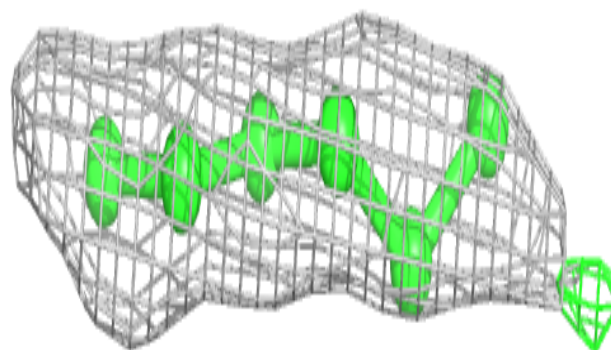
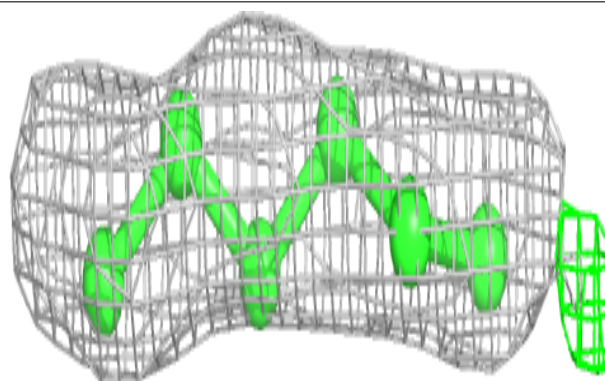


Electron density around OLA B 307:

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

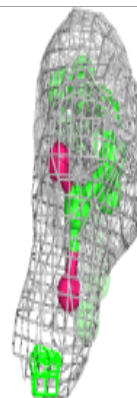
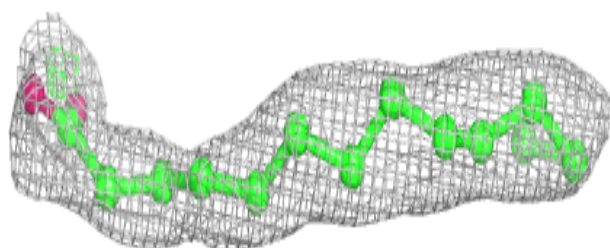
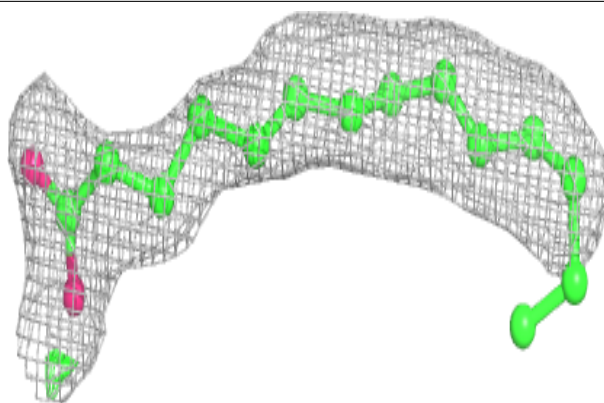
**Electron density around LFA B 315:**

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

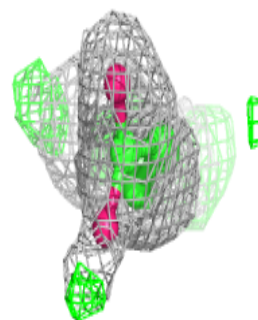
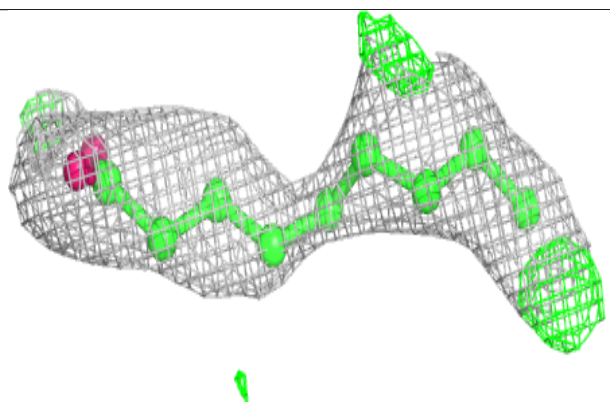
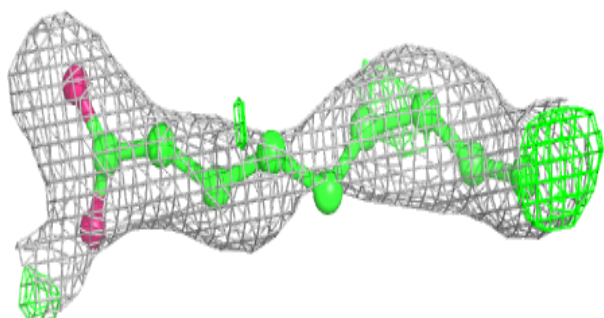


Electron density around OLA B 304:

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

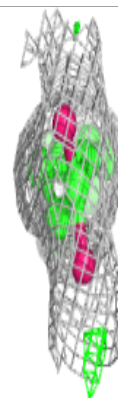
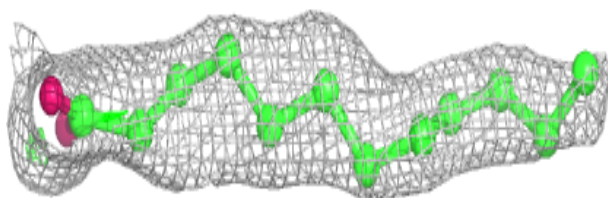
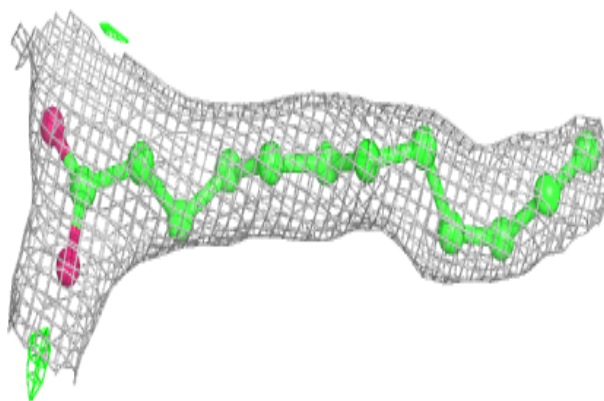
**Electron density around OLA A 704:**

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

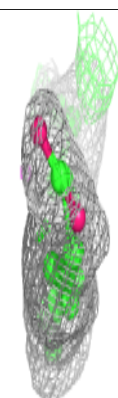
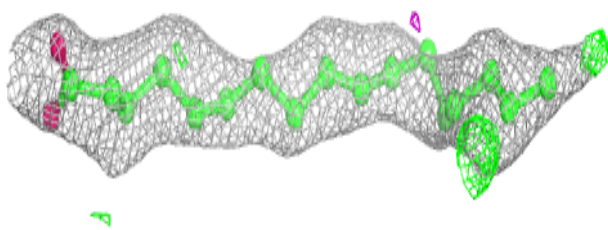
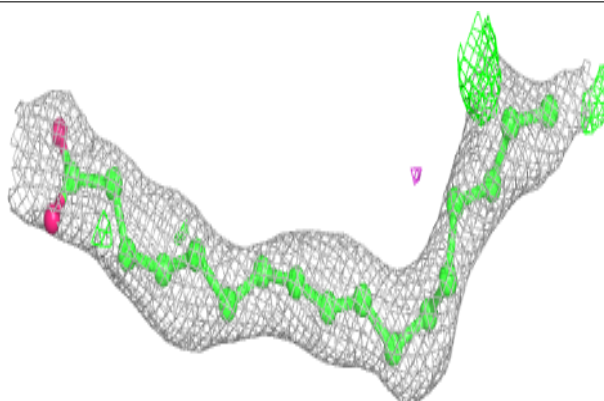


Electron density around OLA A 706:

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

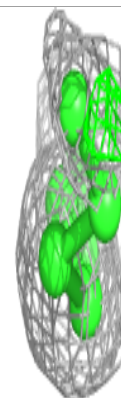
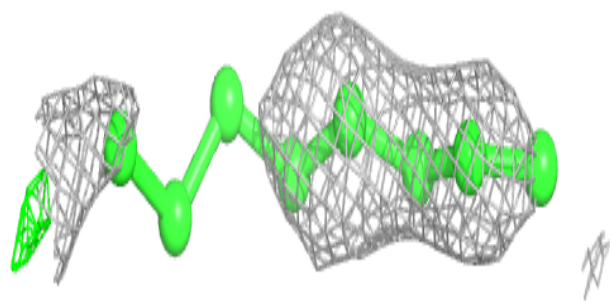
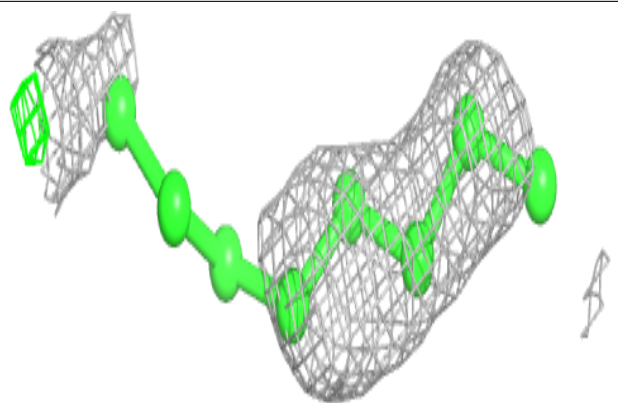
**Electron density around OLA C 702:**

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

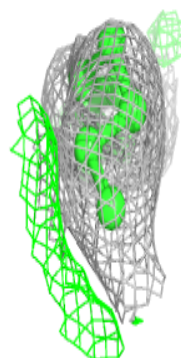
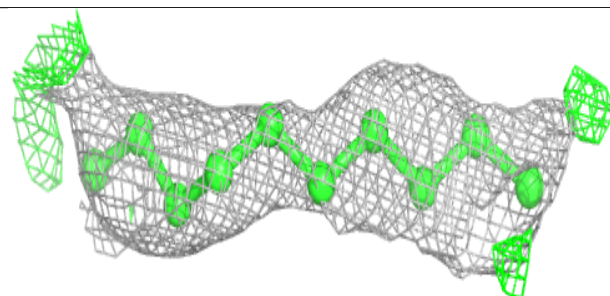
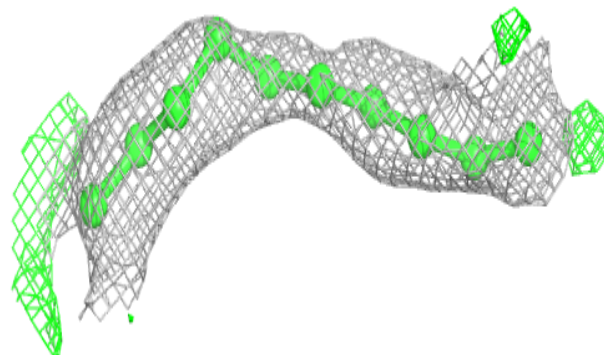


Electron density around LFA C 712:

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

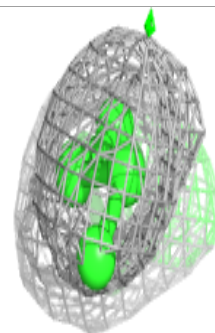
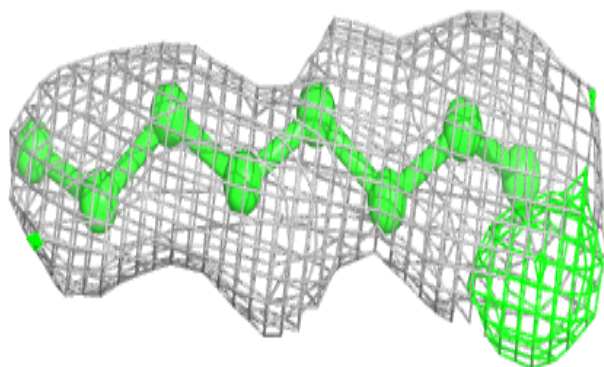
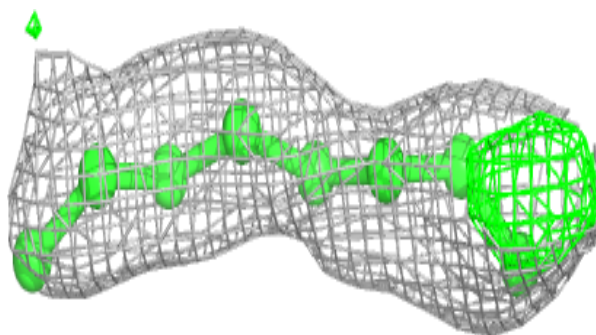
**Electron density around LFA A 716:**

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

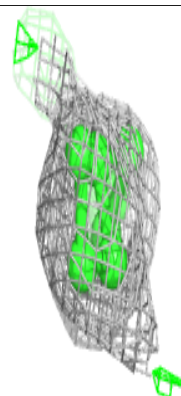
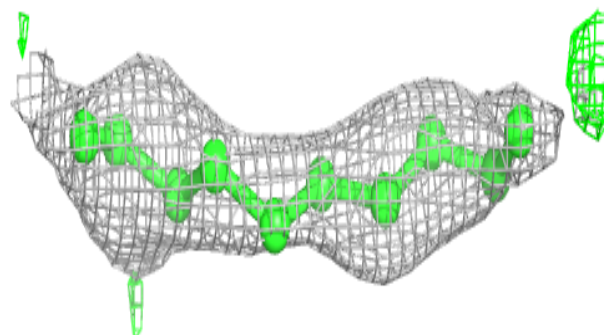
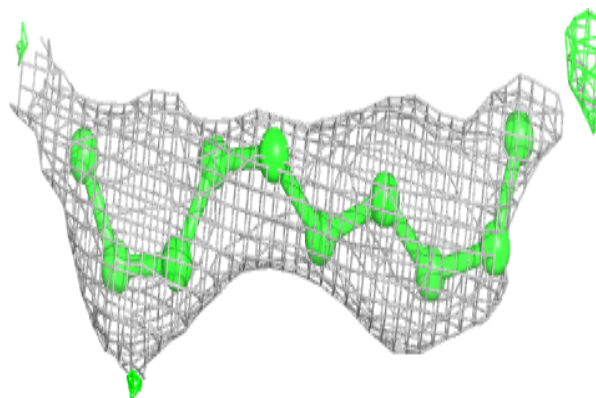


Electron density around LFA C 709:

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

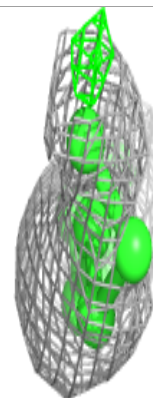
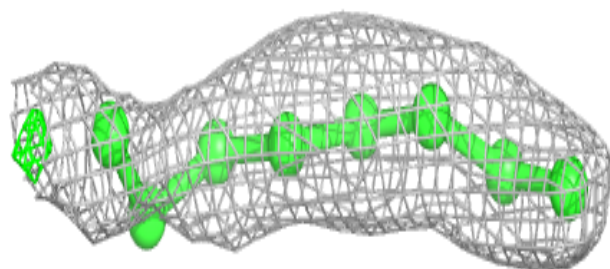
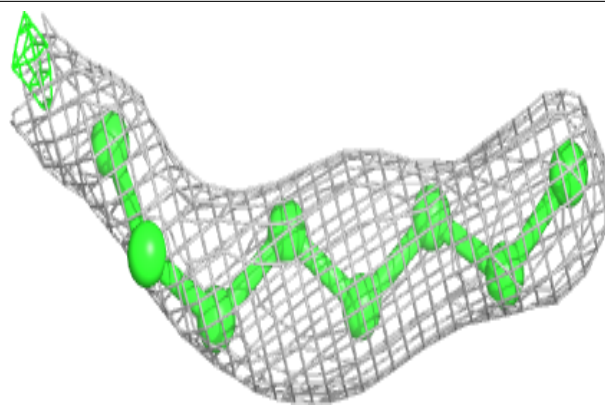
**Electron density around LFA C 707:**

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

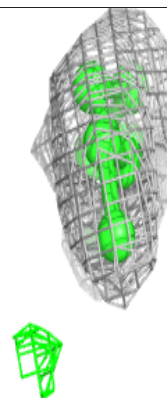
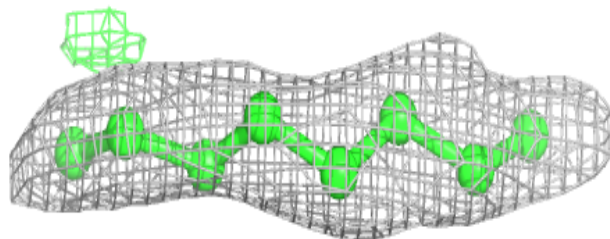
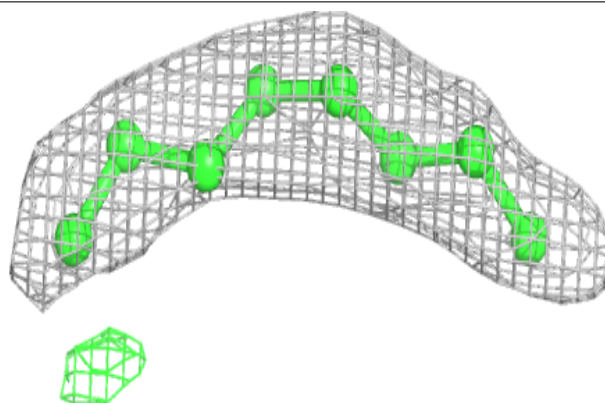


Electron density around LFA C 715:

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

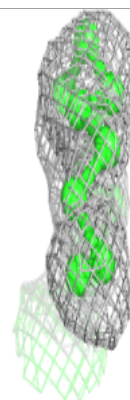
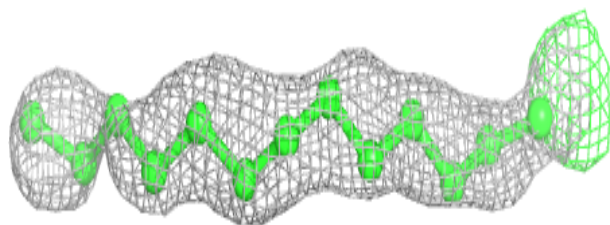
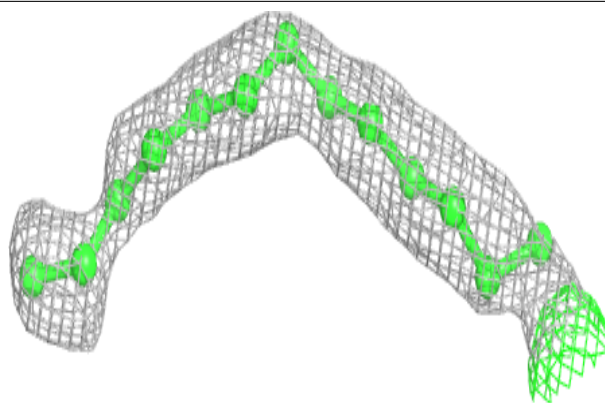
**Electron density around LFA A 723:**

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

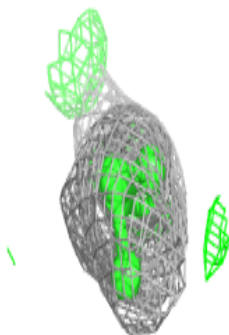
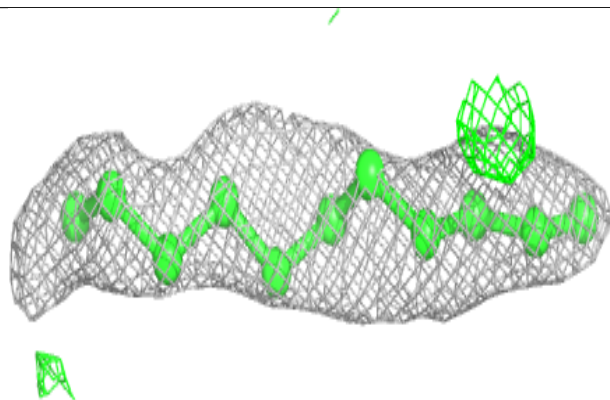
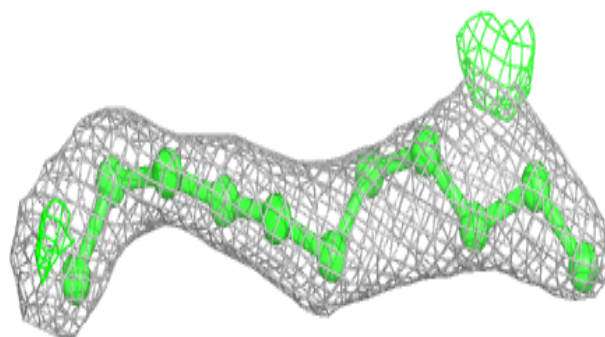


Electron density around LFA A 718:

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

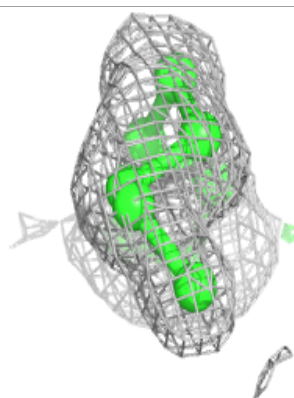
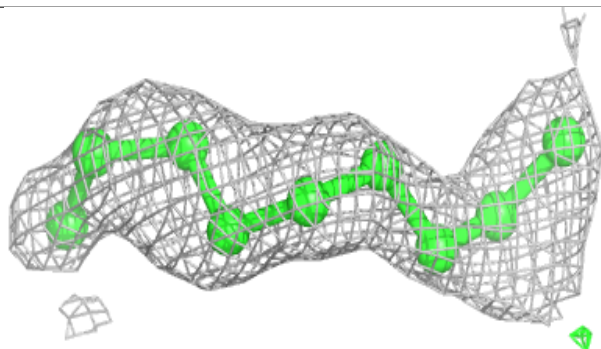
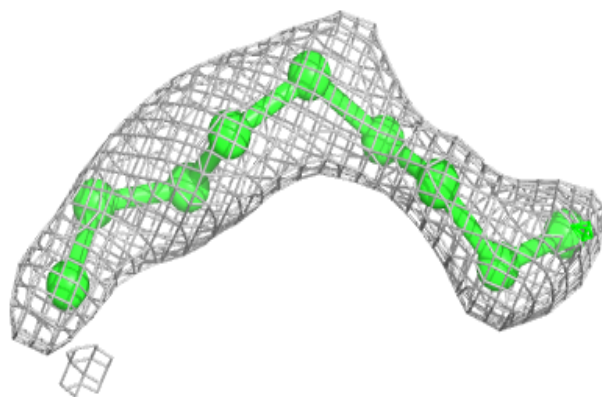
**Electron density around LFA B 323:**

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

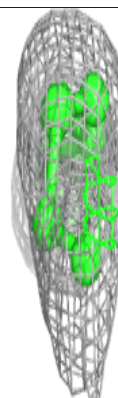
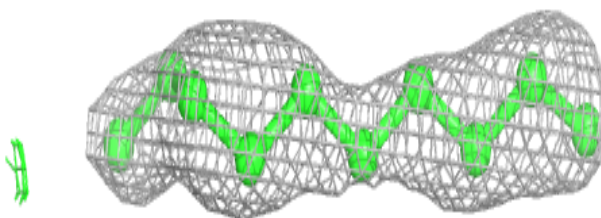
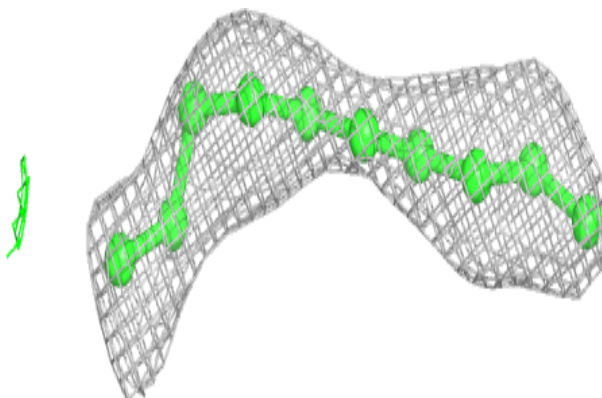


Electron density around LFA B 320:

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

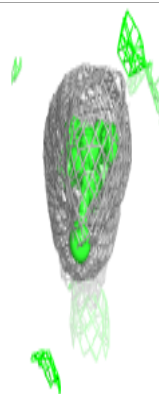
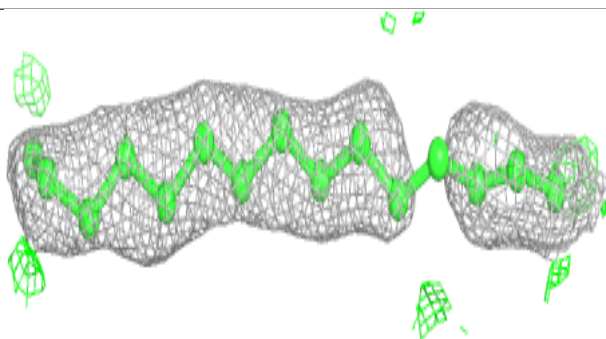
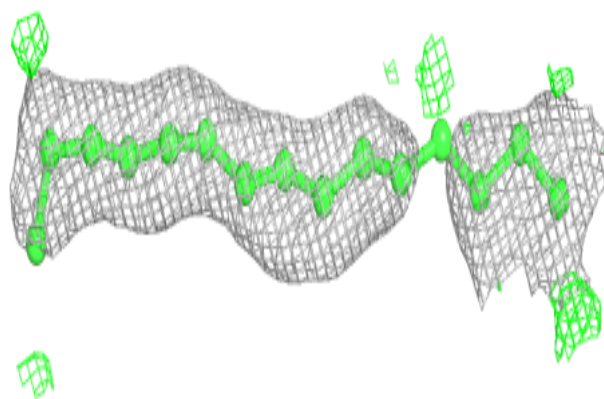
**Electron density around LFA A 717:**

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

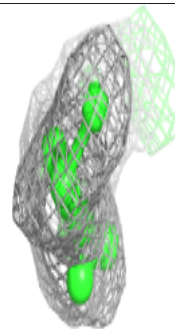
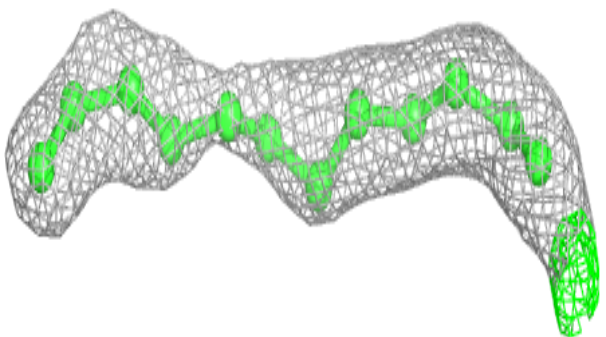
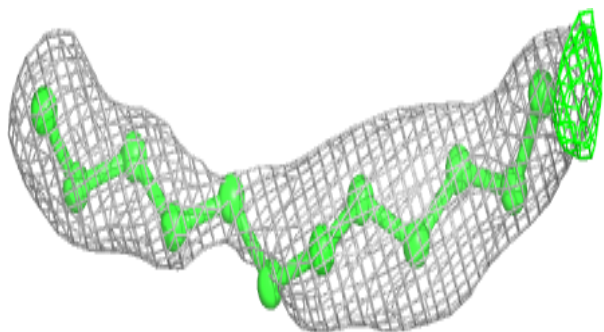


Electron density around LFA B 316:

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

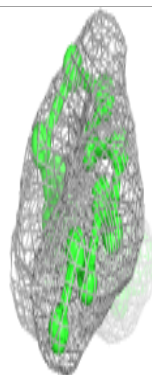
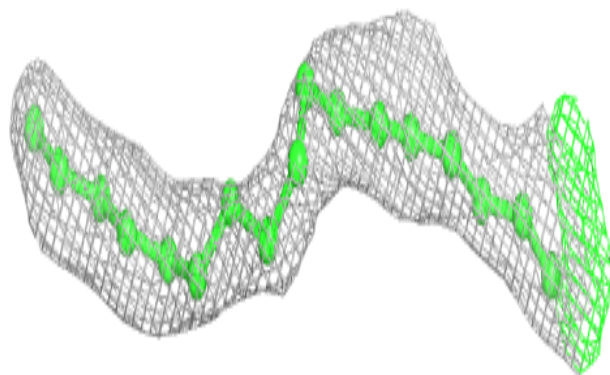
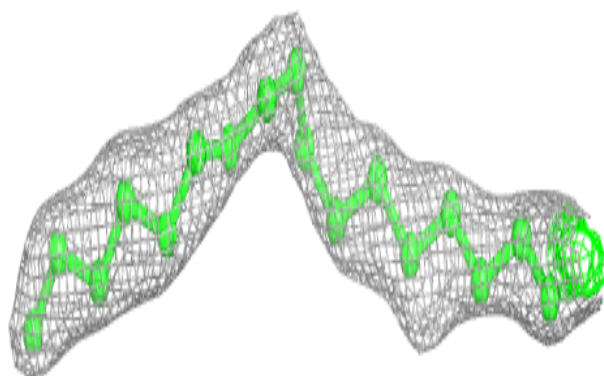
**Electron density around LFA A 710:**

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

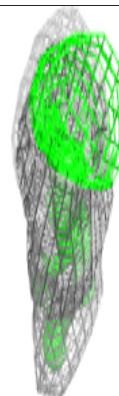
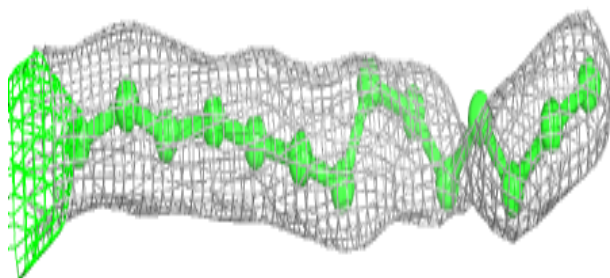
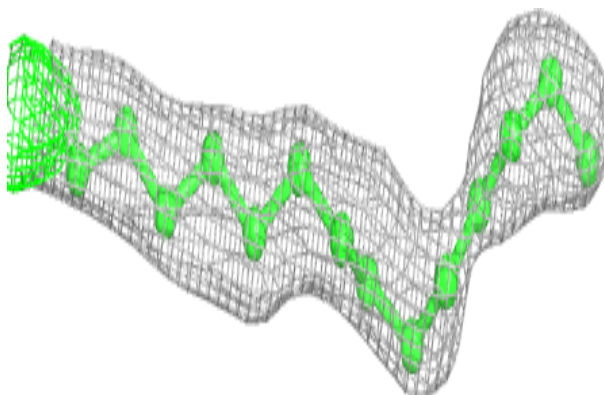


Electron density around LFA A 720:

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

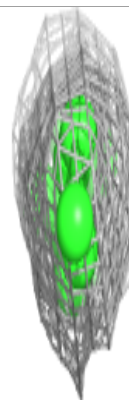
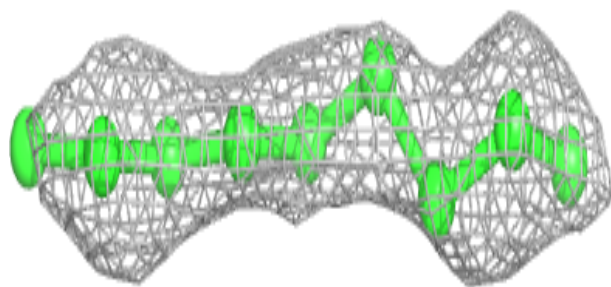
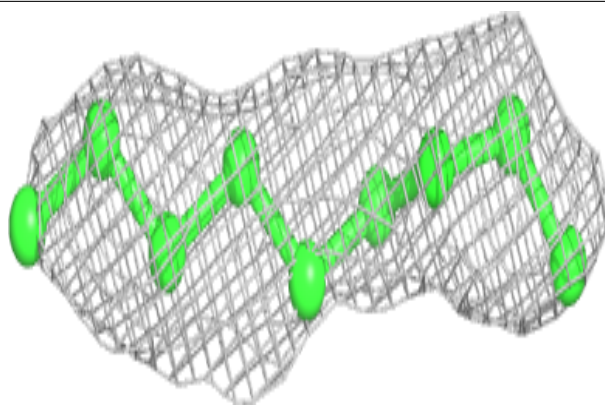
**Electron density around LFA B 321:**

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

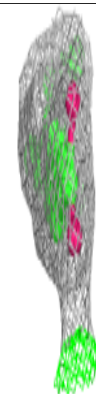
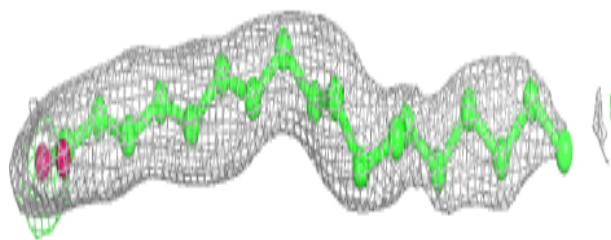
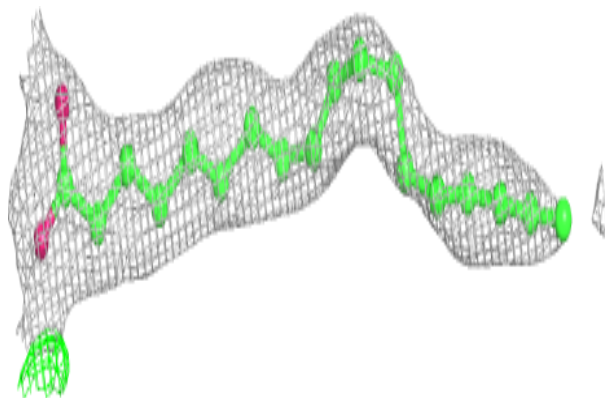


Electron density around LFA A 708:

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

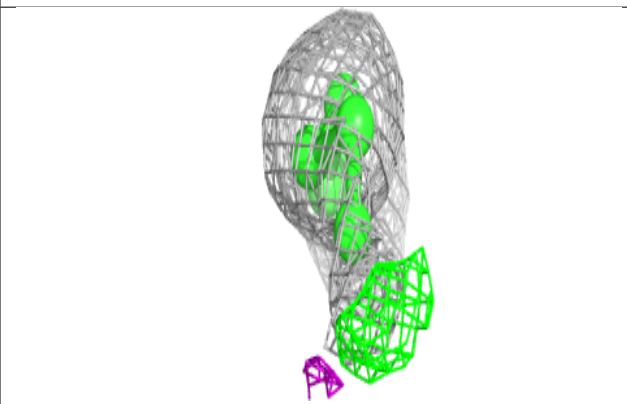
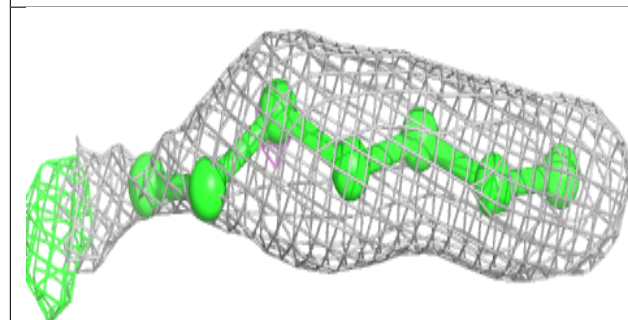
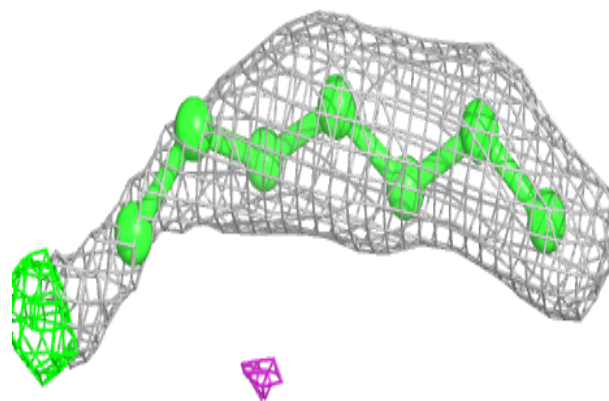
**Electron density around OLA C 705:**

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

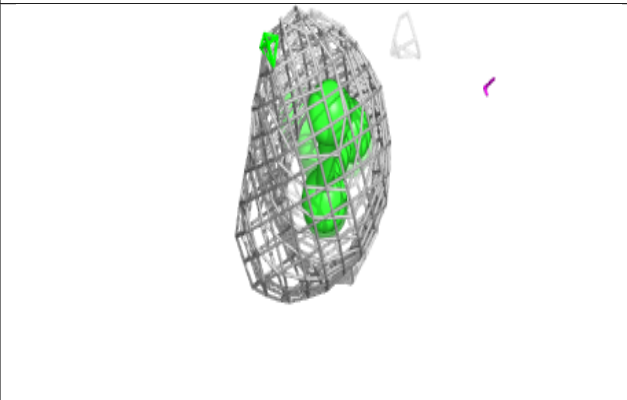
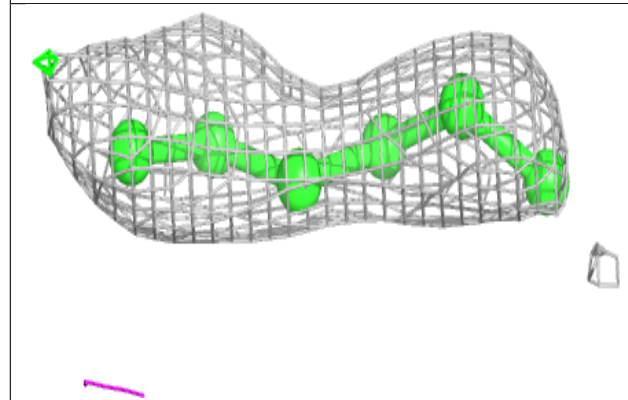
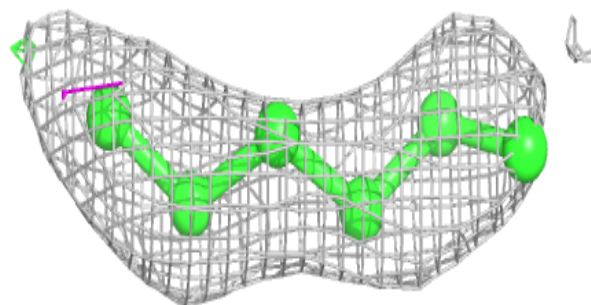


Electron density around LFA B 301:

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

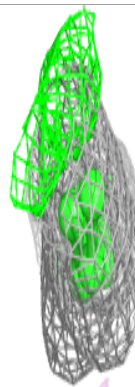
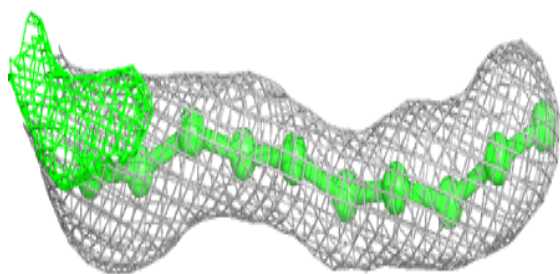
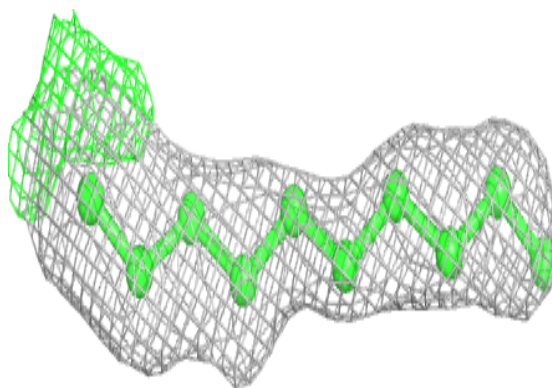
**Electron density around LFA A 712:**

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

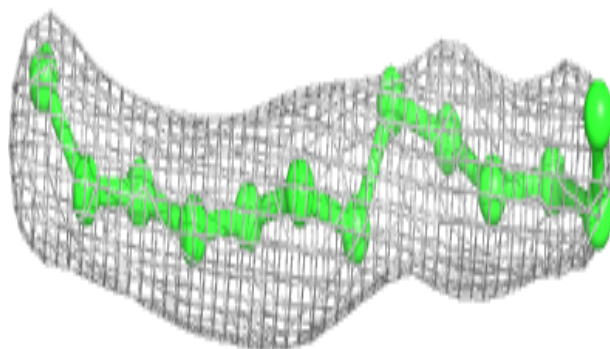
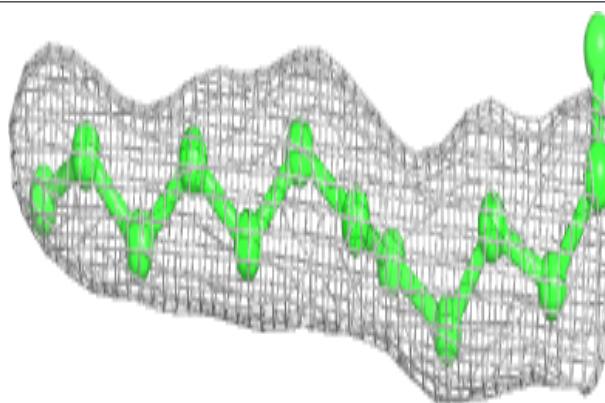


Electron density around LFA A 714:

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

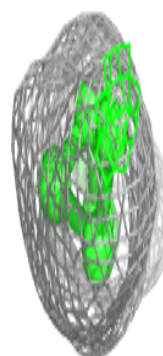
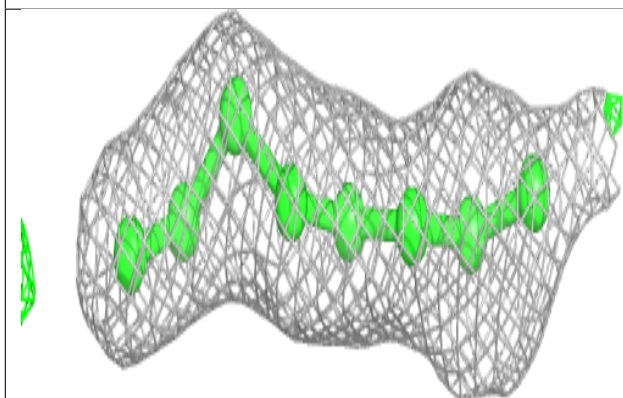
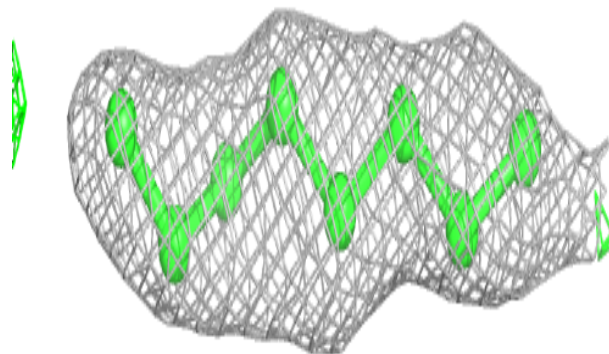
**Electron density around LFA A 719:**

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

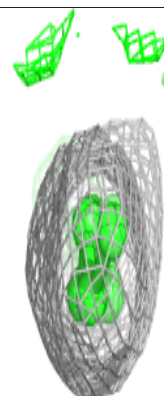
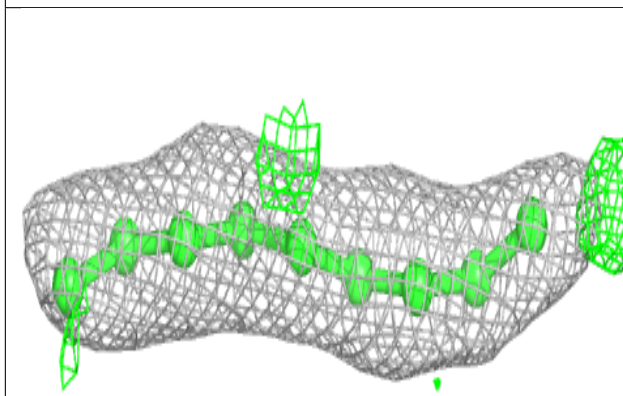
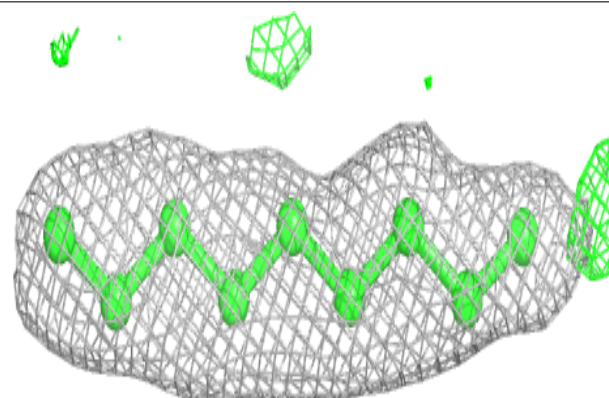


Electron density around LFA C 711:

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

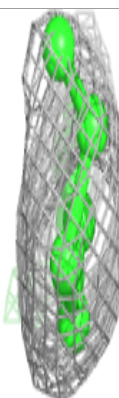
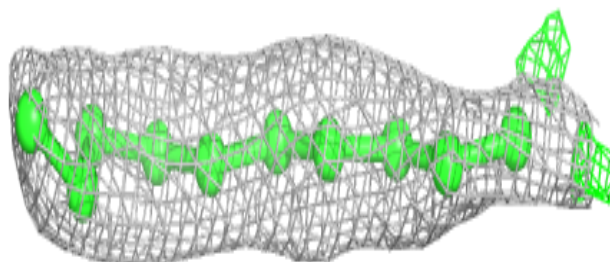
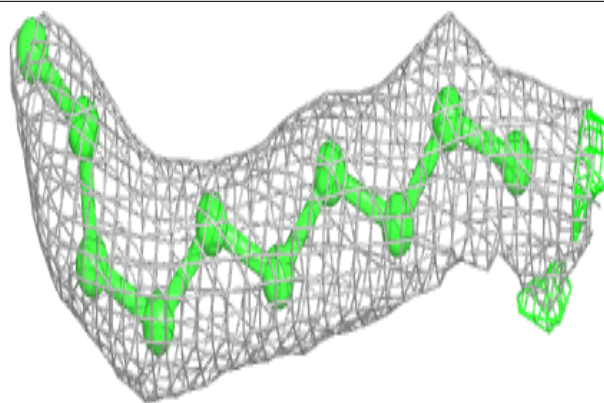
**Electron density around LFA A 709:**

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

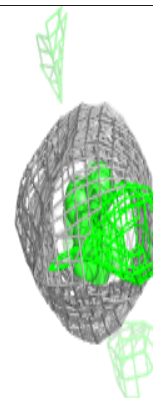
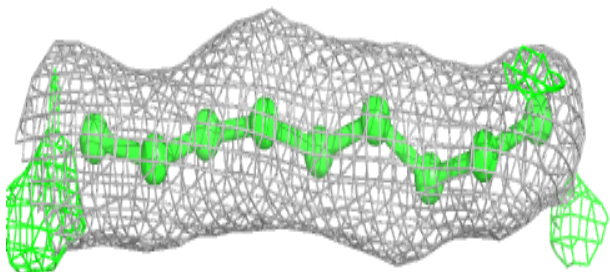
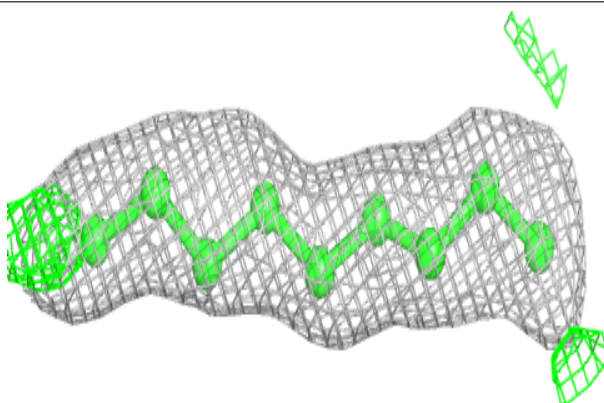


Electron density around LFA B 319:

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

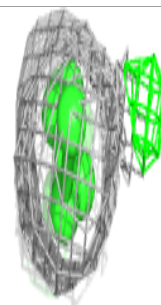
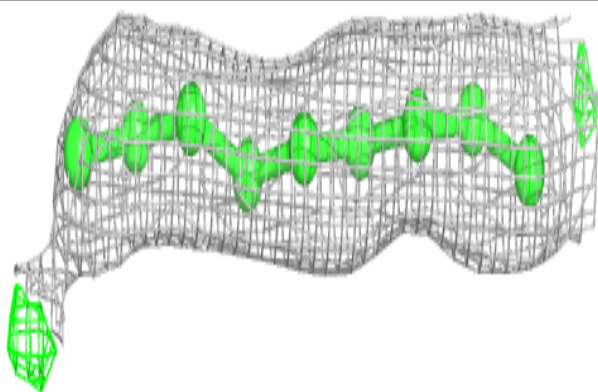
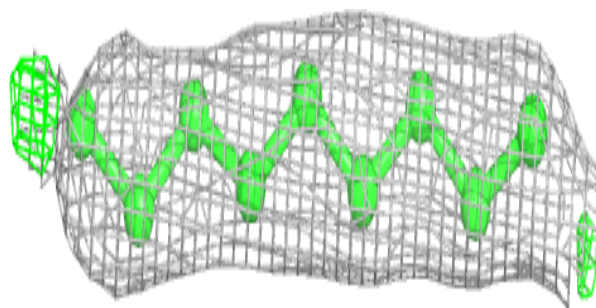
**Electron density around LFA A 701:**

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



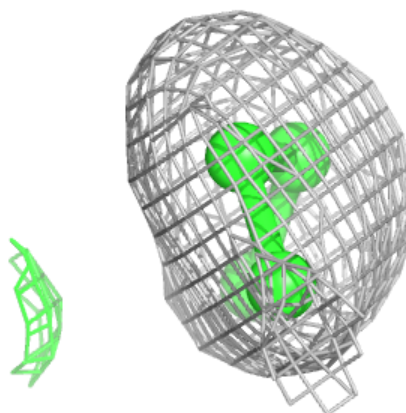
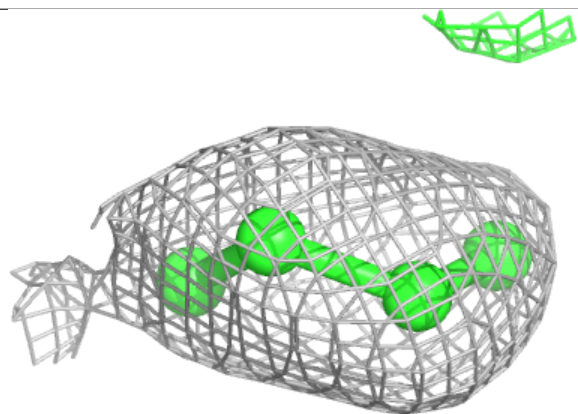
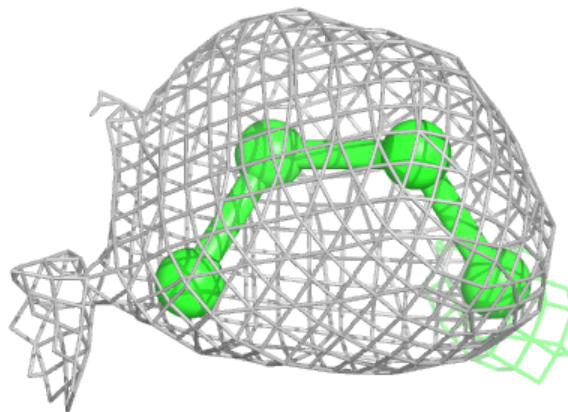
Electron density around LFA B 302:

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



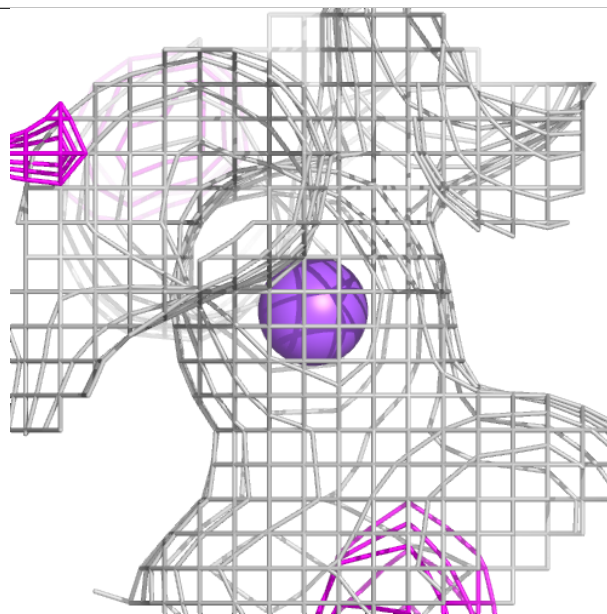
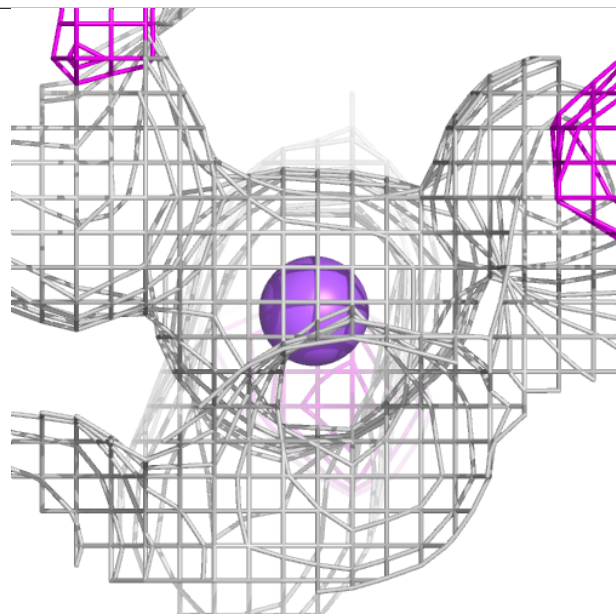
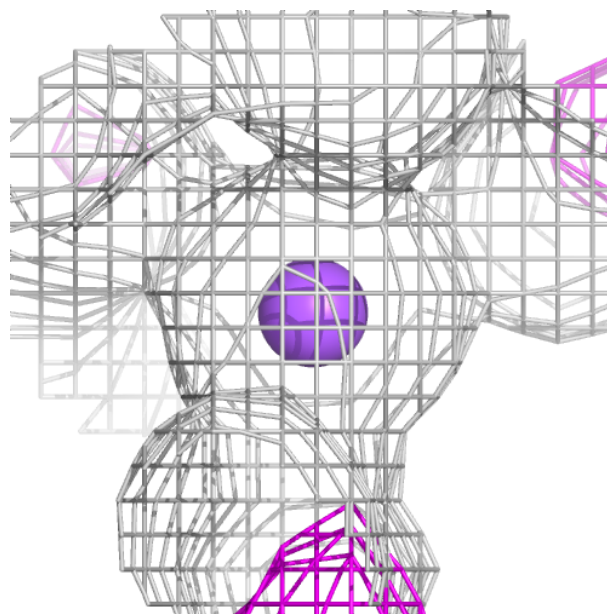
Electron density around LFA A 715:

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



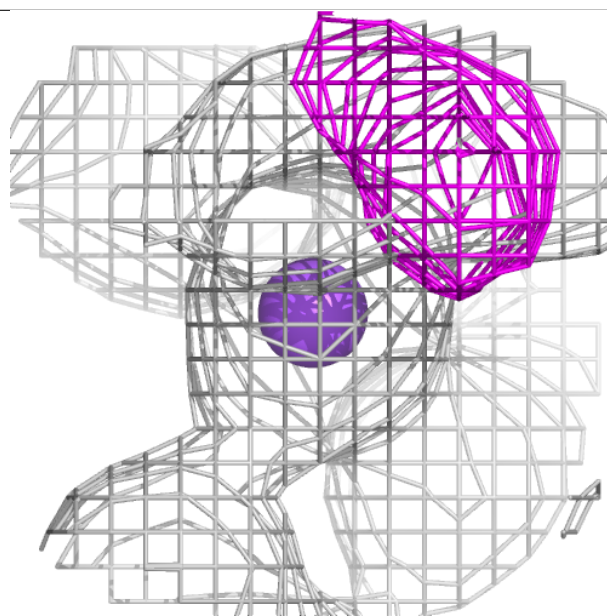
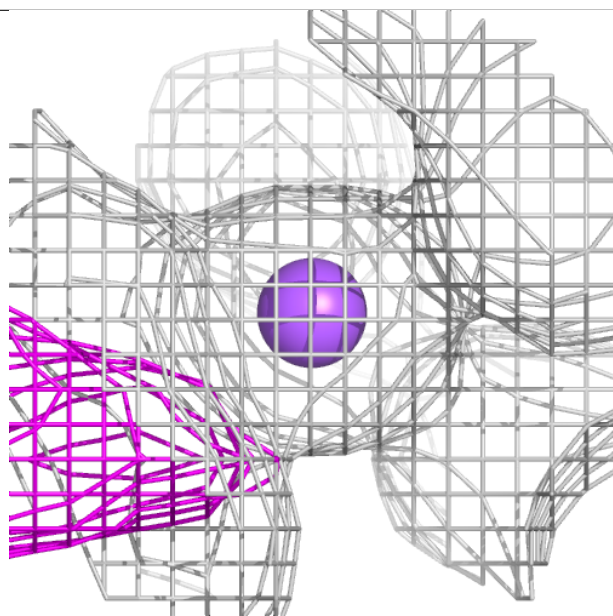
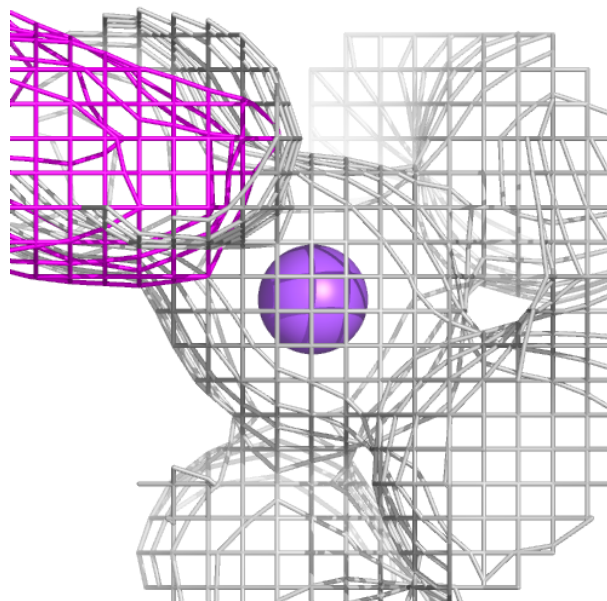
Electron density around NA A 707:

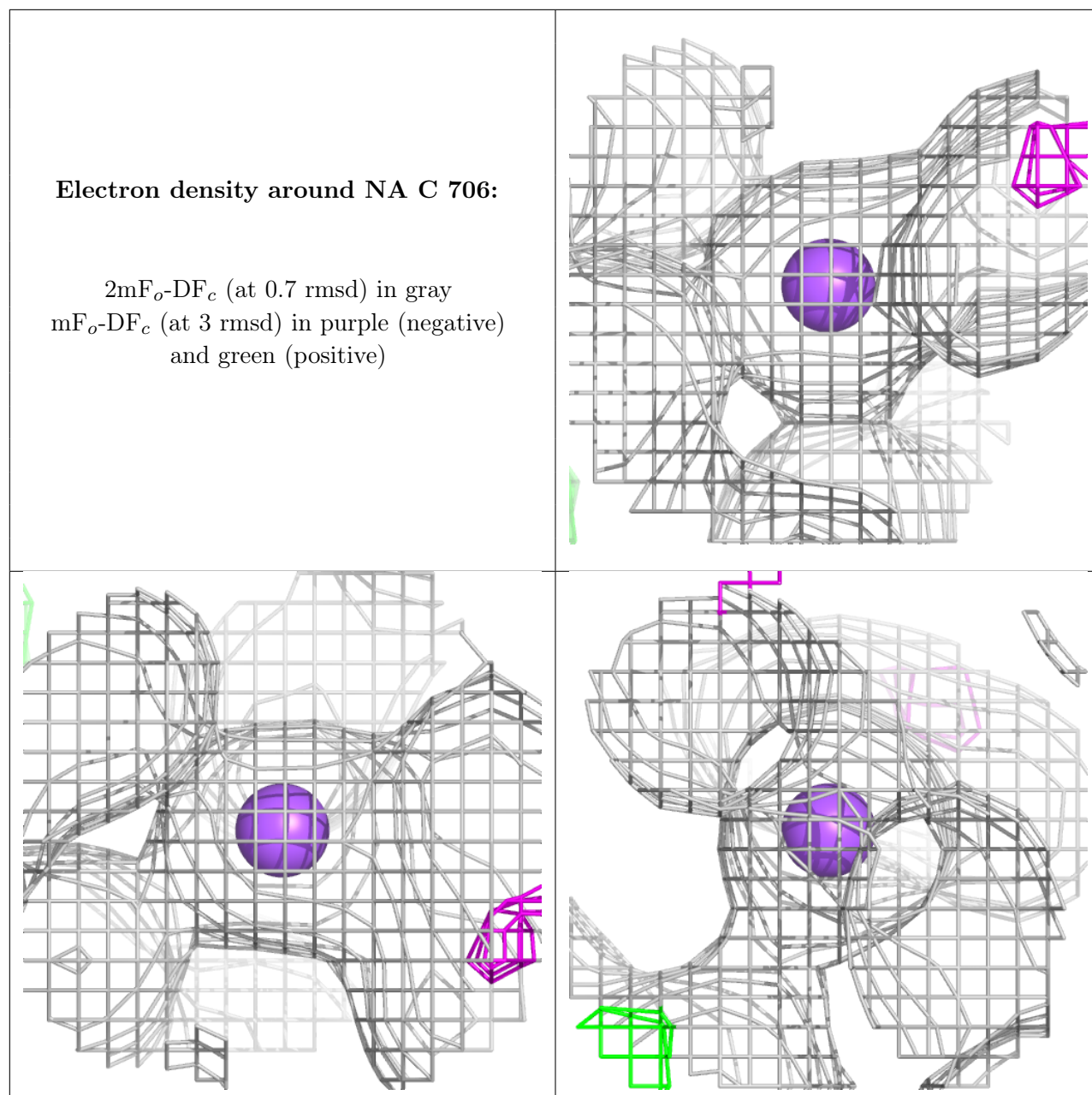
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NA B 310:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.