



Full wwPDB X-ray Structure Validation Report ⓘ

May 2, 2023 – 02:01 pm BST

PDB ID : 7ZNI
Title : Crystal structure of the light-driven inward proton pump xenorhodopsin BcXeR in the activated state at pH 8.2 at room temperature, 7.5-15-ms-snapshot
Authors : Kovalev, K.; Tsybrov, F.; Alekseev, A.; Bourenkov, G.; Gordeliy, V.
Deposited on : 2022-04-20
Resolution : 2.20 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 : 2.32.2
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) : 2.32.2

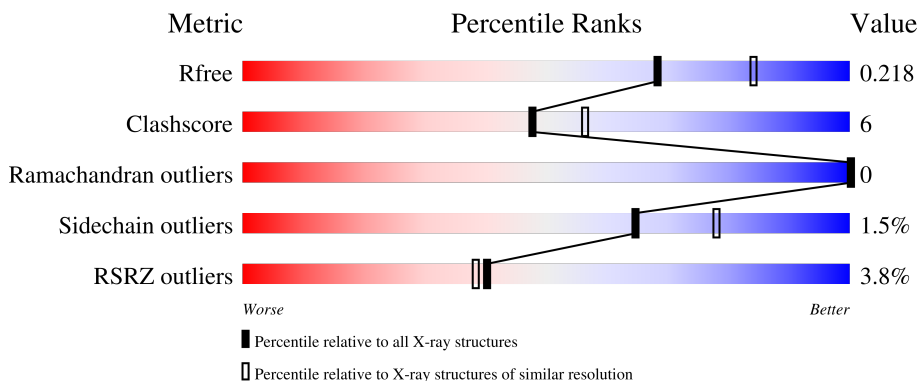
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	C	306	-	-	-	X

2 Entry composition [i](#)

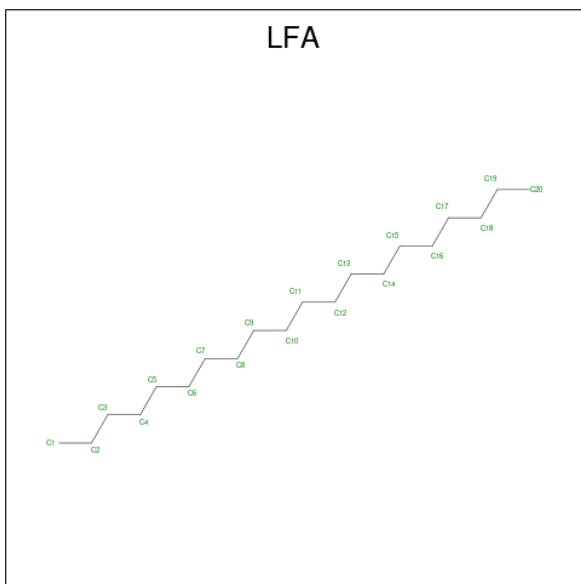
There are 5 unique types of molecules in this entry. The entry contains 6293 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	222	Total 1874	C 1288	N 276	O 304	S 6	0	11	0
1	C	223	Total 1874	C 1288	N 278	O 302	S 6	0	10	0
1	B	221	Total 1879	C 1289	N 281	O 304	S 5	0	13	0

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 7	C 7	0	0
2	A	1	Total 13	C 13	0	0
2	A	1	Total 13	C 13	0	0

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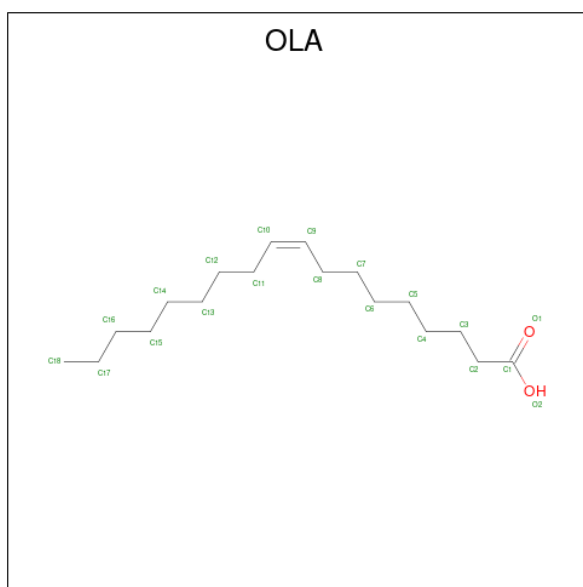
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 11 11	0	0
2	A	1	Total C 14 14	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C 12 12	0	0
2	C	1	Total C 17 17	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 17 17	0	0
2	C	1	Total C 11 11	0	0
2	C	1	Total C 4 4	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 9 9	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C 9 9	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 15 15	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 5 5	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 9 9	0	0

- Molecule 3 is OLEIC ACID (three-letter code: OLA) (formula: C₁₈H₃₄O₂).



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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

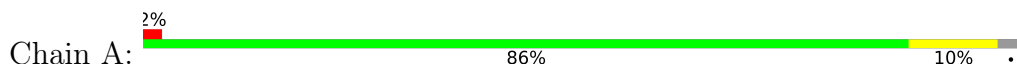
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	11
			36	36		
5	C	30	Total	O	0	10
			31	31		
5	B	27	Total	O	0	11
			28	28		

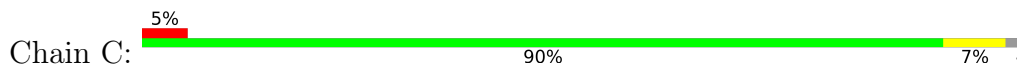
3 Residue-property plots [i](#)

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.

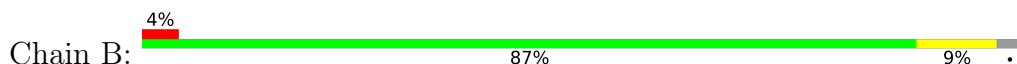
- Molecule 1: xenorhodopsin



- 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	71.50Å 111.50Å 119.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.20) 99.5 (19.88-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.88 (at 2.19Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.184 , 0.214 0.196 , 0.218	Depositor DCC
R_{free} test set	1512 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtrriage
Anisotropy	0.204	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 84.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6293	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.70	0/1856	0.75	0/2539
1	B	0.71	0/1862	0.73	0/2543
1	C	0.70	0/1856	0.74	0/2539
All	All	0.70	0/5574	0.74	0/7621

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	1874	0	1949	27	0
1	B	1879	0	1961	32	0
1	C	1874	0	1950	20	0
2	A	120	0	222	0	0
2	B	121	0	223	3	0
2	C	121	0	223	1	0
3	A	77	0	111	1	0
3	B	61	0	87	2	0
3	C	66	0	95	0	0
4	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	36	0	0	0	0
5	B	28	0	0	1	0
5	C	31	0	0	0	0
All	All	6293	0	6821	80	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 6.

All (80) 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:82:LEU:HD21	1:A:173[C]:TRP:CZ2	2.06	0.90
1:C:82:LEU:HD21	1:C:173[C]:TRP:CZ2	2.09	0.88
1:B:206[A]:SER:O	5:B:401[A]:HOH:O	1.97	0.83
1:A:82:LEU:HD21	1:A:173[C]:TRP:HZ2	1.45	0.81
1:B:82:LEU:HD21	1:B:173[C]:TRP:CZ2	2.19	0.77
1:C:82:LEU:HD21	1:C:173[C]:TRP:HZ2	1.49	0.75
2:C:310:LFA:C12	2:C:312:LFA:H131	2.17	0.74
1:A:165:VAL:HG13	1:A:210:PHE:CE1	2.29	0.67
1:C:82:LEU:CD2	1:C:173[C]:TRP:HZ2	2.09	0.66
1:C:161:HIS:CE1	1:C:217:GLY:HA3	2.31	0.66
1:A:82:LEU:CD2	1:A:173[C]:TRP:HZ2	2.08	0.65
1:A:161:HIS:CE1	1:A:217:GLY:HA3	2.32	0.65
1:B:82:LEU:HD21	1:B:173[C]:TRP:HZ2	1.62	0.65
1:A:203:PRO:HA	1:A:206[C]:SER:OG	1.97	0.64
1:B:161:HIS:CE1	1:B:217:GLY:HA3	2.33	0.63
1:B:207[A]:LYR:H192	1:B:207[A]:LYR:H9	1.82	0.62
1:B:207[C]:LYR:H192	1:B:207[C]:LYR:H9	1.83	0.61
1:C:202:LEU:HB2	1:C:203:PRO:HD3	1.84	0.59
1:B:140:LEU:HD21	1:B:173[C]:TRP:HE3	1.67	0.58
1:A:140:LEU:HD21	1:A:173[C]:TRP:HE3	1.68	0.58
1:B:202:LEU:HB2	1:B:203:PRO:HD3	1.86	0.57
1:A:202:LEU:HB2	1:A:203:PRO:HD3	1.85	0.57
1:C:207[C]:LYR:H9	1:C:207[C]:LYR:H192	1.85	0.57
1:B:82:LEU:CD2	1:B:173[C]:TRP:HZ2	2.17	0.57
1:A:82:LEU:CD2	1:A:173[C]:TRP:CZ2	2.84	0.57
1:C:82:LEU:CD2	1:C:173[C]:TRP:CZ2	2.84	0.56
1:B:194:THR:HG21	3:B:308:OLA:H21	1.87	0.56
1:A:207[A]:LYR:H192	1:A:207[A]:LYR:H9	1.87	0.56
1:A:207[A]:LYR:H9	1:A:207[A]:LYR:H183	1.88	0.56
1:B:203:PRO:HA	1:B:206[C]:SER:OG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207[A]:LYR:H192	1:C:207[A]:LYR:H9	1.87	0.55
1:C:207[A]:LYR:H9	1:C:207[A]:LYR:H183	1.89	0.54
1:C:136[D]:LEU:C	1:C:136[D]:LEU:HD23	2.26	0.54
1:C:203:PRO:HA	1:C:206[C]:SER:OG	2.08	0.53
1:A:207[C]:LYR:H183	1:A:207[C]:LYR:H9	1.90	0.53
1:B:207[A]:LYR:H192	1:B:207[A]:LYR:C9	2.40	0.52
1:A:207[A]:LYR:H192	1:A:207[A]:LYR:C9	2.40	0.51
1:C:207[C]:LYR:H192	1:C:207[C]:LYR:C9	2.41	0.51
1:B:207[C]:LYR:H192	1:B:207[C]:LYR:C9	2.41	0.51
1:C:140:LEU:HD21	1:C:173[C]:TRP:HE3	1.74	0.51
1:B:136[D]:LEU:C	1:B:136[D]:LEU:HD23	2.32	0.50
1:B:82:LEU:CD2	1:B:173[C]:TRP:CZ2	2.91	0.50
1:A:165:VAL:CG1	1:A:210:PHE:CE1	2.95	0.49
1:C:207[A]:LYR:H192	1:C:207[A]:LYR:C9	2.43	0.49
1:B:207[A]:LYR:H9	1:B:207[A]:LYR:H183	1.95	0.48
1:B:198:VAL:HG22	2:B:312:LFA:H81	1.95	0.48
1:A:207[C]:LYR:H9	1:A:207[C]:LYR:H192	1.95	0.48
1:B:140:LEU:HD21	1:B:173[C]:TRP:CE3	2.48	0.47
1:A:136[D]:LEU:C	1:A:136[D]:LEU:HD23	2.35	0.47
1:A:207[C]:LYR:H192	1:A:207[C]:LYR:C9	2.45	0.46
1:B:176:TYR:N	1:B:177:PRO:HD2	2.31	0.46
1:B:195[A]:GLU:HB2	2:B:310:LFA:H11	1.97	0.46
1:A:176:TYR:N	1:A:177:PRO:HD2	2.31	0.45
1:B:203:PRO:O	1:B:207[C]:LYR:N	2.49	0.45
1:C:207[C]:LYR:H9	1:C:207[C]:LYR:H183	1.99	0.45
1:B:194:THR:HG21	3:B:308:OLA:C2	2.47	0.44
1:B:207[A]:LYR:H10	1:B:207[A]:LYR:H81	1.88	0.44
1:A:207[C]:LYR:H6	1:A:207[C]:LYR:H41	1.85	0.44
1:B:206[C]:SER:HB2	1:B:207[C]:LYR:HC2	2.00	0.44
1:C:176:TYR:N	1:C:177:PRO:HD2	2.34	0.43
1:B:170[C]:SER:HA	1:B:173[C]:TRP:CE3	2.53	0.43
1:C:82:LEU:HD23	1:C:82:LEU:HA	1.87	0.43
1:A:78:THR:N	1:A:79:PRO:HD2	2.34	0.42
1:C:78:THR:N	1:C:79:PRO:HD2	2.34	0.42
1:A:207[A]:LYR:H81	1:A:207[A]:LYR:H10	1.83	0.42
1:B:207[C]:LYR:H10	1:B:207[C]:LYR:H81	1.83	0.42
1:C:207[C]:LYR:H10	1:C:207[C]:LYR:H81	1.79	0.42
1:B:21:TYR:CZ	1:B:25:LYS:HE2	2.55	0.42
1:B:195[B]:GLU:HB2	2:B:310:LFA:H11	2.00	0.42
1:B:206[C]:SER:CB	1:B:207[C]:LYR:HC2	2.50	0.42
1:B:140:LEU:CD2	1:B:173[C]:TRP:CE3	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207[C]:LYR:H6	1:B:207[C]:LYR:H41	1.81	0.42
1:A:203:PRO:O	1:A:207[C]:LYR:N	2.53	0.41
1:C:203:PRO:O	1:C:207[C]:LYR:N	2.53	0.41
1:A:56:GLN:HB3	3:A:804:OLA:H51	2.03	0.41
1:A:207[C]:LYR:H81	1:A:207[C]:LYR:H10	1.76	0.41
1:A:193:LEU:O	1:A:197:LEU:HD23	2.21	0.40
1:A:1:FME:O1	1:A:4:ILE:HG12	2.22	0.40
1:A:140:LEU:HD21	1:A:173[C]:TRP:CE3	2.51	0.40
1:B:140:LEU:HD23	1:B:173[C]:TRP:CZ3	2.57	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	231/229 (101%)	227 (98%)	4 (2%)	0	100	100
1	B	230/229 (100%)	228 (99%)	2 (1%)	0	100	100
1	C	231/229 (101%)	227 (98%)	4 (2%)	0	100	100
All	All	692/687 (101%)	682 (99%)	10 (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	186/189 (98%)	183 (98%)	3 (2%)	62	76
1	B	188/189 (100%)	186 (99%)	2 (1%)	73	85
1	C	185/189 (98%)	182 (98%)	3 (2%)	62	76
All	All	559/567 (99%)	551 (99%)	8 (1%)	65	80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	22	LEU
1	A	216	HIS
1	C	18	LEU
1	C	22	LEU
1	C	152	LEU
1	B	22	LEU
1	B	121	ILE

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	191	GLN
1	B	60	GLN
1	B	154	ASN
1	B	191	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](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	C	1	1	8,9,10	0.47	0	7,9,11	0.88	0
1	LYR	B	207[C]	1	27,29,30	1.13	4 (14%)	30,37,39	1.63	4 (13%)
1	LYR	B	207[A]	1	27,29,30	1.27	3 (11%)	30,37,39	1.31	2 (6%)
1	FME	A	1	1	8,9,10	0.50	0	7,9,11	0.84	0
1	LYR	C	207[A]	1	27,29,30	1.24	4 (14%)	30,37,39	1.32	3 (10%)
1	LYR	C	207[C]	1	27,29,30	1.13	2 (7%)	30,37,39	1.46	3 (10%)
1	LYR	A	207[C]	1	27,29,30	1.24	4 (14%)	30,37,39	1.50	3 (10%)
1	FME	B	1	1	5,6,10	0.88	0	3,6,11	1.49	1 (33%)
1	LYR	A	207[A]	1	27,29,30	1.29	4 (14%)	30,37,39	1.33	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	C	1	1	-	2/7/9/11	-
1	LYR	B	207[C]	1	-	4/22/40/42	0/1/1/1
1	LYR	B	207[A]	1	-	3/22/40/42	0/1/1/1
1	FME	A	1	1	-	1/7/9/11	-
1	LYR	C	207[A]	1	-	3/22/40/42	0/1/1/1
1	LYR	C	207[C]	1	-	3/22/40/42	0/1/1/1
1	LYR	A	207[C]	1	-	2/22/40/42	0/1/1/1
1	FME	B	1	1	-	0/2/5/11	-
1	LYR	A	207[A]	1	-	3/22/40/42	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207[A]	LYR	C7-C80	3.77	1.40	1.35
1	A	207[C]	LYR	C7-C80	3.47	1.40	1.35
1	B	207[A]	LYR	C7-C80	2.99	1.39	1.35
1	C	207[A]	LYR	C4-C3	-2.81	1.45	1.50
1	B	207[A]	LYR	C9-C80	-2.80	1.39	1.45
1	C	207[A]	LYR	C9-C80	-2.80	1.39	1.45
1	B	207[C]	LYR	C7-C80	2.67	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	207[A]	LYR	C7-C80	2.61	1.39	1.35
1	A	207[C]	LYR	C4-C3	-2.60	1.45	1.50
1	A	207[A]	LYR	C9-C80	-2.47	1.40	1.45
1	B	207[A]	LYR	C4-C3	-2.42	1.45	1.50
1	C	207[C]	LYR	C4-C3	-2.41	1.45	1.50
1	A	207[A]	LYR	C4-C3	-2.32	1.46	1.50
1	C	207[C]	LYR	C9-C80	-2.32	1.41	1.45
1	B	207[C]	LYR	C16-C15	-2.22	1.47	1.52
1	B	207[C]	LYR	C4-C3	-2.16	1.46	1.50
1	A	207[C]	LYR	C16-C15	-2.14	1.47	1.52
1	B	207[C]	LYR	C10-C9	2.13	1.39	1.33
1	A	207[C]	LYR	C9-C80	-2.12	1.41	1.45
1	A	207[A]	LYR	C6-C5	2.06	1.39	1.34
1	C	207[A]	LYR	C6-C5	2.02	1.39	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207[C]	LYR	C1-NZ-CE	4.90	121.10	113.33
1	B	207[C]	LYR	C1-NZ-CE	4.87	121.06	113.33
1	B	207[C]	LYR	C8-C80-C7	-4.36	116.81	122.92
1	C	207[C]	LYR	C1-NZ-CE	4.31	120.16	113.33
1	C	207[A]	LYR	C8-C80-C7	-4.25	116.97	122.92
1	B	207[A]	LYR	C8-C80-C7	-4.12	117.16	122.92
1	C	207[C]	LYR	C8-C80-C7	-3.96	117.38	122.92
1	A	207[A]	LYR	C8-C80-C7	-3.80	117.59	122.92
1	A	207[A]	LYR	C1-NZ-CE	3.80	119.36	113.33
1	A	207[C]	LYR	C8-C80-C7	-3.73	117.69	122.92
1	B	207[A]	LYR	C1-NZ-CE	3.40	118.71	113.33
1	C	207[A]	LYR	C1-NZ-CE	2.94	117.98	113.33
1	A	207[C]	LYR	C10-C9-C80	-2.61	122.29	126.23
1	B	1	FME	CB-CA-N	2.56	112.46	109.61
1	A	207[A]	LYR	C6-C7-C80	2.54	130.94	127.31
1	B	207[C]	LYR	C1-C2-C3	-2.42	122.33	126.97
1	C	207[C]	LYR	C9-C80-C7	2.36	122.57	118.94
1	B	207[C]	LYR	C9-C80-C7	2.36	122.56	118.94
1	C	207[A]	LYR	C8-C80-C9	2.18	121.51	118.08

There are no chirality outliers.

All (21) torsion outliers are listed below:

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

There are no ring outliers.

7 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	207[C]	LYR	7	0
1	B	207[A]	LYR	4	0
1	A	1	FME	1	0
1	C	207[A]	LYR	3	0
1	C	207[C]	LYR	5	0
1	A	207[C]	LYR	6	0
1	A	207[A]	LYR	4	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

52 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	OLA	B	307	-	15,15,19	0.71	0	15,15,19	0.52	0
3	OLA	C	305	-	15,15,19	0.66	0	15,15,19	0.57	0
2	LFA	A	810	-	13,13,19	0.21	0	12,12,18	0.10	0
4	PO4	C	306	-	4,4,4	0.68	0	6,6,6	0.44	0
2	LFA	B	317	-	8,8,19	0.52	0	7,7,18	0.21	0
2	LFA	C	312	-	10,10,19	0.23	0	9,9,18	0.15	0
2	LFA	C	314	-	7,7,19	0.30	0	6,6,18	0.21	0
2	LFA	B	304	-	8,8,19	0.24	0	7,7,18	0.12	0
2	LFA	A	812	-	8,8,19	0.25	0	7,7,18	0.14	0
2	LFA	C	315	-	5,5,19	0.31	0	4,4,18	0.17	0
3	OLA	A	803	-	19,19,19	0.73	1 (5%)	19,19,19	0.45	0
2	LFA	C	309	-	9,9,19	0.27	0	8,8,18	0.18	0
2	LFA	A	813	-	5,5,19	0.33	0	4,4,18	0.21	0
2	LFA	B	302	-	6,6,19	0.30	0	5,5,18	0.51	0
3	OLA	A	804	-	15,15,19	0.55	0	15,15,19	0.62	0
3	OLA	A	802	-	10,10,19	0.80	0	10,10,19	0.71	0
2	LFA	C	307	-	8,8,19	0.32	0	7,7,18	0.31	0
2	LFA	A	814	-	11,11,19	0.21	0	10,10,18	0.14	0
3	OLA	B	301	-	19,19,19	0.54	0	19,19,19	0.62	0
2	LFA	C	317	-	8,8,19	0.37	0	7,7,18	0.23	0
2	LFA	B	303	-	14,14,19	0.33	0	13,13,18	0.27	0
3	OLA	A	806	-	18,18,19	0.58	0	18,18,19	0.55	0
2	LFA	A	808	-	12,12,19	0.26	0	11,11,18	0.21	0
3	OLA	C	302	-	13,13,19	0.59	0	12,13,19	0.65	0
3	OLA	C	304	-	19,19,19	0.67	0	19,19,19	0.73	0
3	OLA	B	306	-	13,13,19	0.75	0	12,13,19	0.46	0
3	OLA	A	805	-	10,10,19	1.04	1 (10%)	10,10,19	0.35	0
2	LFA	A	801	-	6,6,19	0.35	0	5,5,18	0.39	0
2	LFA	A	817	-	11,11,19	0.30	0	10,10,18	0.21	0
2	LFA	C	318	-	8,8,19	0.51	0	7,7,18	0.16	0
2	LFA	B	314	-	6,6,19	0.38	0	5,5,18	0.23	0
2	LFA	C	316	-	5,5,19	0.29	0	4,4,18	0.13	0
3	OLA	B	308	-	10,10,19	0.84	1 (10%)	10,10,19	0.80	0
2	LFA	C	308	-	5,5,19	0.39	0	4,4,18	0.26	0
2	LFA	B	311	-	13,13,19	0.29	0	12,12,18	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LFA	C	301	-	16,16,19	0.31	0	15,15,18	0.22	0
2	LFA	C	313	-	3,3,19	0.29	0	2,2,18	0.48	0
2	LFA	A	807	-	12,12,19	0.25	0	11,11,18	0.24	0
2	LFA	A	816	-	5,5,19	0.23	0	4,4,18	0.09	0
2	LFA	B	305	-	6,6,19	0.44	0	5,5,18	0.16	0
2	LFA	B	312	-	8,8,19	0.31	0	7,7,18	0.33	0
3	OLA	C	303	-	15,15,19	0.60	0	15,15,19	0.56	0
2	LFA	B	309	-	9,9,19	0.13	0	8,8,18	0.14	0
2	LFA	B	316	-	13,13,19	0.22	0	12,12,18	0.28	0
2	LFA	A	809	-	10,10,19	0.33	0	9,9,18	0.17	0
2	LFA	A	811	-	8,8,19	0.19	0	7,7,18	0.22	0
2	LFA	B	315	-	4,4,19	0.32	0	3,3,18	0.32	0
2	LFA	A	815	-	7,7,19	0.21	0	6,6,18	0.10	0
2	LFA	C	310	-	8,8,19	0.28	0	7,7,18	0.25	0
2	LFA	B	310	-	7,7,19	0.18	0	6,6,18	0.16	0
2	LFA	B	313	-	6,6,19	0.39	0	5,5,18	0.20	0
2	LFA	C	311	-	16,16,19	0.27	0	15,15,18	0.19	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	B	307	-	-	7/13/13/17	-
3	OLA	C	305	-	-	7/13/13/17	-
2	LFA	A	810	-	-	2/11/11/17	-
2	LFA	B	317	-	-	0/6/6/17	-
2	LFA	C	312	-	-	2/8/8/17	-
2	LFA	C	314	-	-	3/5/5/17	-
2	LFA	B	304	-	-	0/6/6/17	-
2	LFA	A	812	-	-	3/6/6/17	-
2	LFA	C	315	-	-	2/3/3/17	-
3	OLA	A	803	-	-	9/17/17/17	-
2	LFA	C	309	-	-	1/7/7/17	-
2	LFA	A	813	-	-	0/3/3/17	-
2	LFA	B	302	-	-	0/4/4/17	-
3	OLA	A	804	-	-	3/13/13/17	-
3	OLA	A	802	-	-	2/8/8/17	-
2	LFA	C	307	-	-	1/6/6/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	A	814	-	-	2/9/9/17	-
3	OLA	B	301	-	-	8/17/17/17	-
2	LFA	C	317	-	-	1/6/6/17	-
2	LFA	B	303	-	-	4/12/12/17	-
3	OLA	A	806	-	-	3/16/16/17	-
2	LFA	A	808	-	-	3/10/10/17	-
3	OLA	C	302	-	-	5/11/11/17	-
3	OLA	C	304	-	-	7/17/17/17	-
3	OLA	B	306	-	-	9/11/11/17	-
3	OLA	A	805	-	-	1/8/8/17	-
2	LFA	A	801	-	-	0/4/4/17	-
2	LFA	A	817	-	-	3/9/9/17	-
2	LFA	C	318	-	-	1/6/6/17	-
2	LFA	B	314	-	-	2/4/4/17	-
2	LFA	C	316	-	-	2/3/3/17	-
3	OLA	B	308	-	-	4/8/8/17	-
2	LFA	C	308	-	-	0/3/3/17	-
2	LFA	B	311	-	-	1/11/11/17	-
2	LFA	C	301	-	-	2/14/14/17	-
2	LFA	C	313	-	-	0/1/1/17	-
2	LFA	A	807	-	-	4/10/10/17	-
2	LFA	A	816	-	-	0/3/3/17	-
2	LFA	B	305	-	-	1/4/4/17	-
2	LFA	B	312	-	-	0/6/6/17	-
3	OLA	C	303	-	-	4/13/13/17	-
2	LFA	B	309	-	-	3/7/7/17	-
2	LFA	B	316	-	-	1/11/11/17	-
2	LFA	A	809	-	-	2/8/8/17	-
2	LFA	A	811	-	-	3/6/6/17	-
2	LFA	B	315	-	-	1/2/2/17	-
2	LFA	A	815	-	-	1/5/5/17	-
2	LFA	C	310	-	-	1/6/6/17	-
2	LFA	B	310	-	-	1/5/5/17	-
2	LFA	B	313	-	-	1/4/4/17	-
2	LFA	C	311	-	-	1/14/14/17	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	OLA	O1-C1	2.44	1.30	1.22
3	A	805	OLA	O1-C1	2.24	1.29	1.22
3	B	308	OLA	O1-C1	2.06	1.29	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	302	OLA	C9-C10-C11-C12
3	B	307	OLA	C11-C10-C9-C8
2	C	318	LFA	C15-C16-C17-C18
3	B	308	OLA	C1-C2-C3-C4
2	A	812	LFA	C4-C5-C6-C7
3	B	306	OLA	C3-C4-C5-C6
2	B	316	LFA	C11-C10-C9-C8
3	C	304	OLA	C11-C10-C9-C8
3	A	805	OLA	C4-C5-C6-C7
3	A	803	OLA	C5-C6-C7-C8
2	C	311	LFA	C11-C10-C9-C8
2	B	313	LFA	C2-C3-C4-C5
3	A	804	OLA	C11-C10-C9-C8
3	B	301	OLA	C11-C10-C9-C8
2	B	303	LFA	C4-C5-C6-C7
2	B	314	LFA	C3-C4-C5-C6
3	C	305	OLA	C1-C2-C3-C4
2	B	303	LFA	C3-C4-C5-C6
3	C	304	OLA	C5-C6-C7-C8
3	A	803	OLA	C10-C11-C12-C13
3	A	806	OLA	C6-C7-C8-C9
3	A	803	OLA	C3-C4-C5-C6
2	C	301	LFA	C11-C10-C9-C8
2	B	303	LFA	C6-C7-C8-C9
3	C	303	OLA	C4-C5-C6-C7
3	C	302	OLA	C5-C6-C7-C8
2	B	311	LFA	C12-C13-C14-C15
3	C	302	OLA	C11-C10-C9-C8
3	B	301	OLA	C6-C7-C8-C9
3	A	803	OLA	C4-C5-C6-C7
2	A	811	LFA	C11-C12-C13-C14
3	B	301	OLA	C11-C12-C13-C14
3	B	308	OLA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	B	306	OLA	C5-C6-C7-C8
3	B	307	OLA	C5-C6-C7-C8
2	A	812	LFA	C6-C7-C8-C9
2	C	314	LFA	C17-C18-C19-C20
3	B	307	OLA	C6-C7-C8-C9
2	C	301	LFA	C9-C10-C11-C12
2	C	314	LFA	C16-C17-C18-C19
3	B	306	OLA	C11-C10-C9-C8
3	C	304	OLA	C1-C2-C3-C4
3	B	301	OLA	C1-C2-C3-C4
3	C	304	OLA	C2-C3-C4-C5
2	A	817	LFA	C10-C11-C12-C13
2	C	315	LFA	C4-C5-C6-C7
2	A	807	LFA	C5-C6-C7-C8
2	A	815	LFA	C3-C4-C5-C6
2	A	811	LFA	C14-C15-C16-C17
3	B	306	OLA	C9-C10-C11-C12
3	C	305	OLA	C3-C4-C5-C6
3	B	306	OLA	C1-C2-C3-C4
2	A	808	LFA	C6-C7-C8-C9
2	B	309	LFA	C4-C5-C6-C7
2	A	811	LFA	C13-C14-C15-C16
3	C	303	OLA	C2-C3-C4-C5
2	C	314	LFA	C13-C14-C15-C16
3	A	803	OLA	C14-C15-C16-C17
2	A	809	LFA	C15-C16-C17-C18
2	A	807	LFA	C7-C8-C9-C10
3	A	806	OLA	C11-C12-C13-C14
3	B	306	OLA	C4-C5-C6-C7
2	A	809	LFA	C10-C11-C12-C13
3	A	806	OLA	C5-C6-C7-C8
2	C	316	LFA	C3-C4-C5-C6
3	B	301	OLA	C15-C16-C17-C18
2	C	312	LFA	C10-C11-C12-C13
2	A	810	LFA	C13-C14-C15-C16
3	C	303	OLA	C5-C6-C7-C8
3	B	307	OLA	C7-C8-C9-C10
3	C	305	OLA	C2-C3-C4-C5
3	C	305	OLA	O1-C1-C2-C3
3	B	308	OLA	O1-C1-C2-C3
3	A	804	OLA	O1-C1-C2-C3
2	C	315	LFA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	C	303	OLA	C11-C10-C9-C8
2	A	814	LFA	C9-C10-C11-C12
2	A	808	LFA	C11-C10-C9-C8
3	B	307	OLA	O2-C1-C2-C3
3	B	307	OLA	O1-C1-C2-C3
3	C	302	OLA	O1-C1-C2-C3
3	C	302	OLA	O2-C1-C2-C3
3	B	308	OLA	O2-C1-C2-C3
2	C	307	LFA	C15-C16-C17-C18
3	A	802	OLA	O1-C1-C2-C3
3	A	803	OLA	O2-C1-C2-C3
3	C	305	OLA	O2-C1-C2-C3
2	B	309	LFA	C6-C7-C8-C9
2	A	807	LFA	C11-C12-C13-C14
3	B	307	OLA	C3-C4-C5-C6
3	A	802	OLA	O2-C1-C2-C3
3	B	301	OLA	O2-C1-C2-C3
3	B	306	OLA	O2-C1-C2-C3
3	A	803	OLA	O1-C1-C2-C3
3	C	305	OLA	C10-C11-C12-C13
2	A	817	LFA	C17-C18-C19-C20
3	B	306	OLA	O1-C1-C2-C3
2	B	314	LFA	C2-C3-C4-C5
3	A	803	OLA	C13-C14-C15-C16
2	C	312	LFA	C11-C12-C13-C14
2	A	817	LFA	C9-C10-C11-C12
2	A	810	LFA	C11-C12-C13-C14
2	C	316	LFA	C2-C3-C4-C5
3	A	803	OLA	C7-C8-C9-C10
3	C	304	OLA	C7-C8-C9-C10
2	A	812	LFA	C5-C6-C7-C8
2	B	310	LFA	C2-C3-C4-C5
3	A	804	OLA	O2-C1-C2-C3
3	B	301	OLA	O1-C1-C2-C3
2	A	814	LFA	C4-C5-C6-C7
3	B	306	OLA	C7-C8-C9-C10
2	B	303	LFA	C11-C10-C9-C8
2	B	309	LFA	C7-C8-C9-C10
2	A	808	LFA	C9-C10-C11-C12
3	C	305	OLA	C5-C6-C7-C8
2	C	317	LFA	C6-C7-C8-C9
2	B	315	LFA	C16-C17-C18-C19

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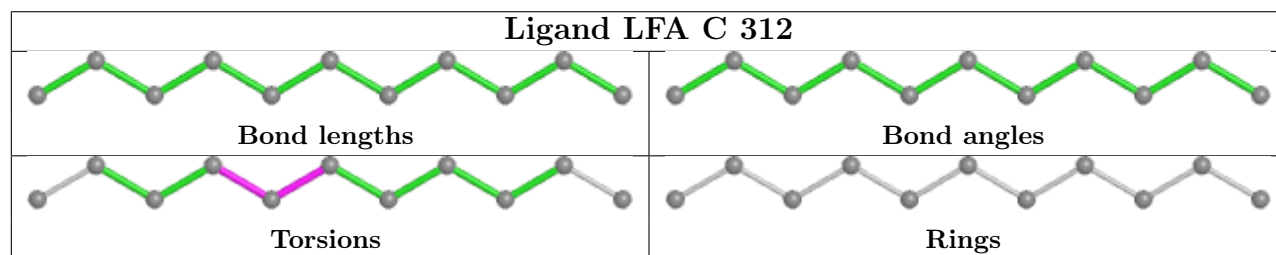
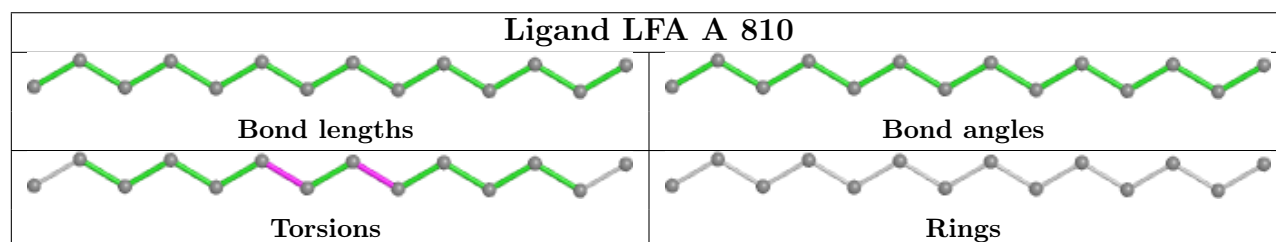
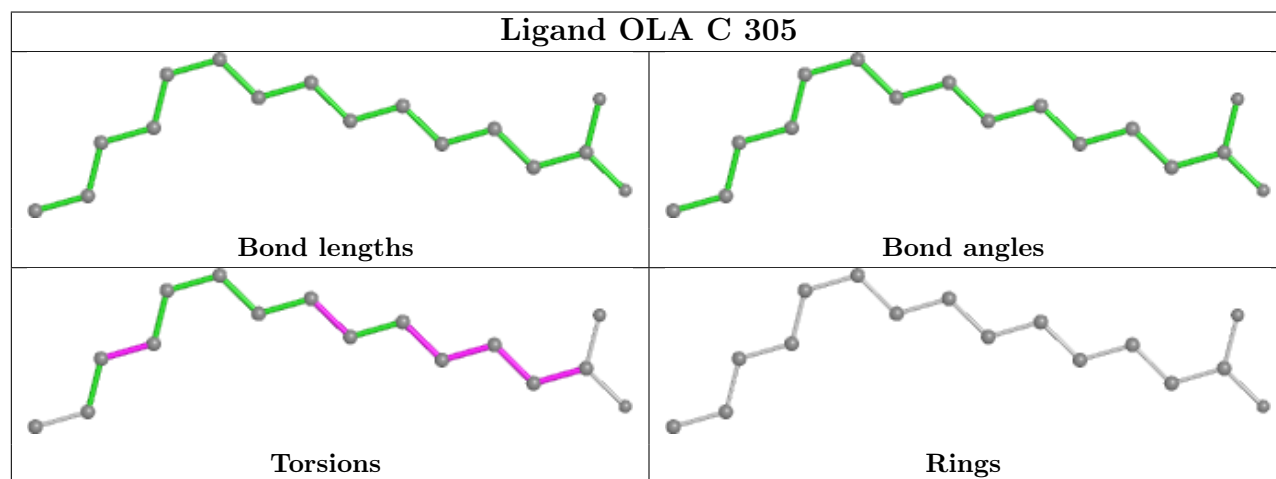
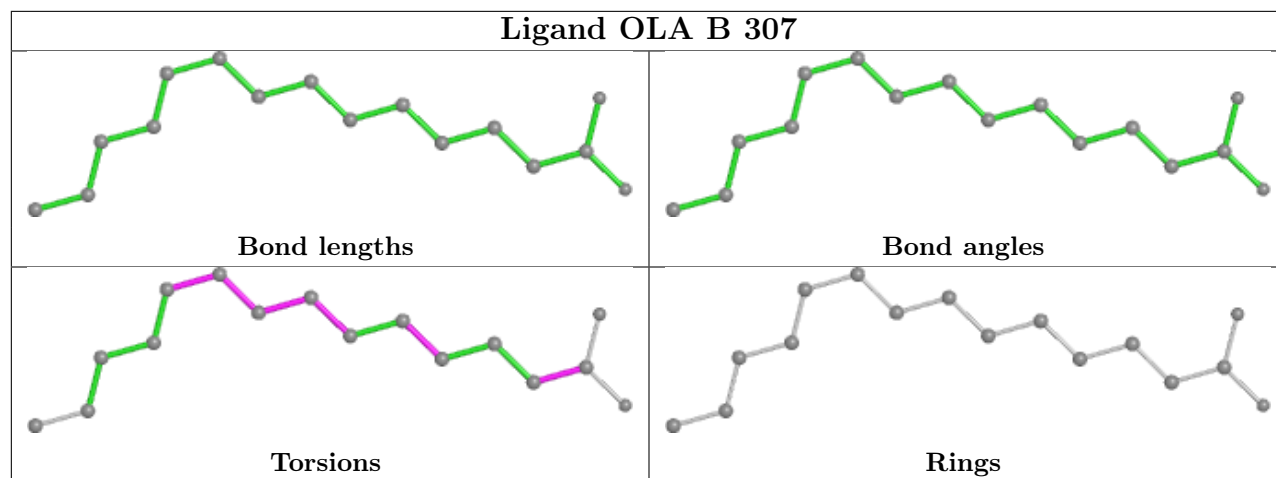
Mol	Chain	Res	Type	Atoms
3	C	304	OLA	O2-C1-C2-C3
2	B	305	LFA	C1-C2-C3-C4
2	A	807	LFA	C9-C10-C11-C12
2	C	310	LFA	C17-C18-C19-C20
3	B	301	OLA	C12-C13-C14-C15
2	C	309	LFA	C3-C4-C5-C6
3	C	304	OLA	O1-C1-C2-C3

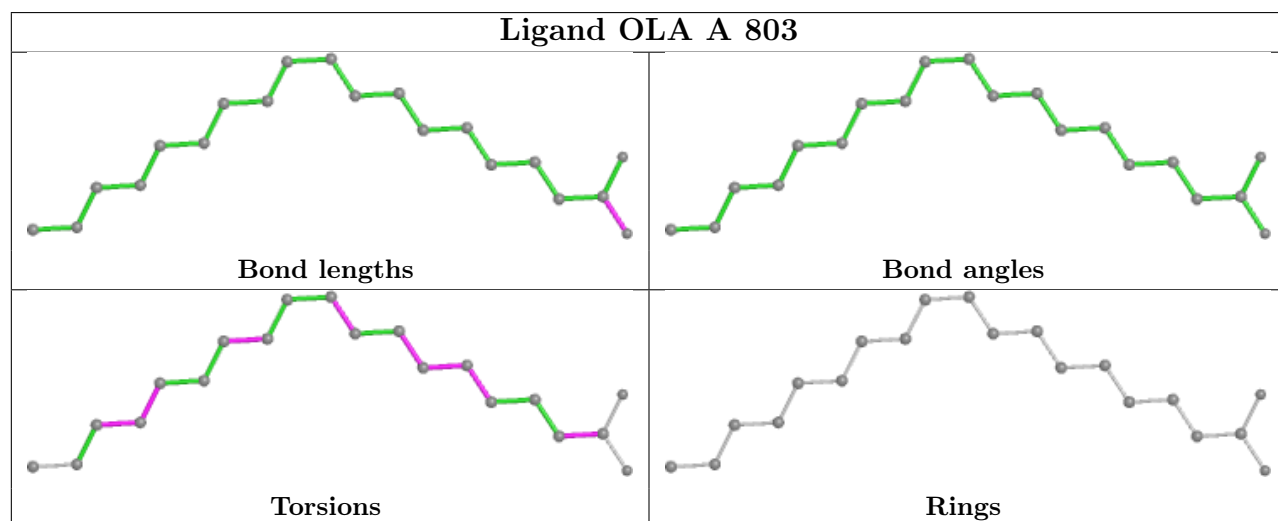
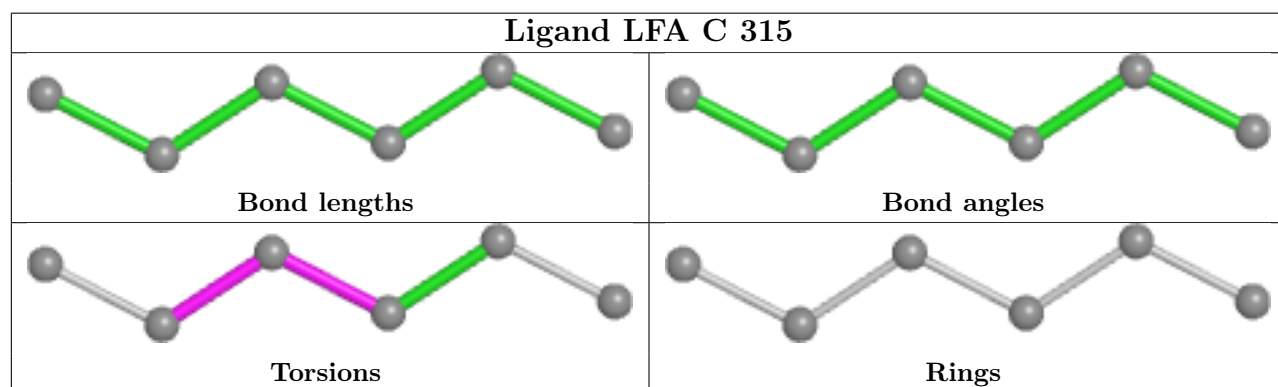
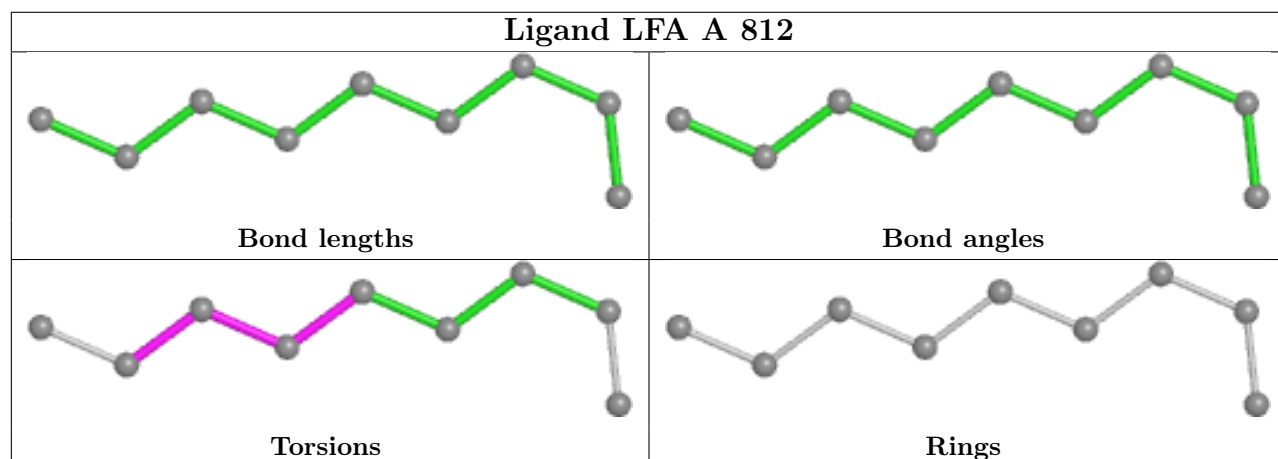
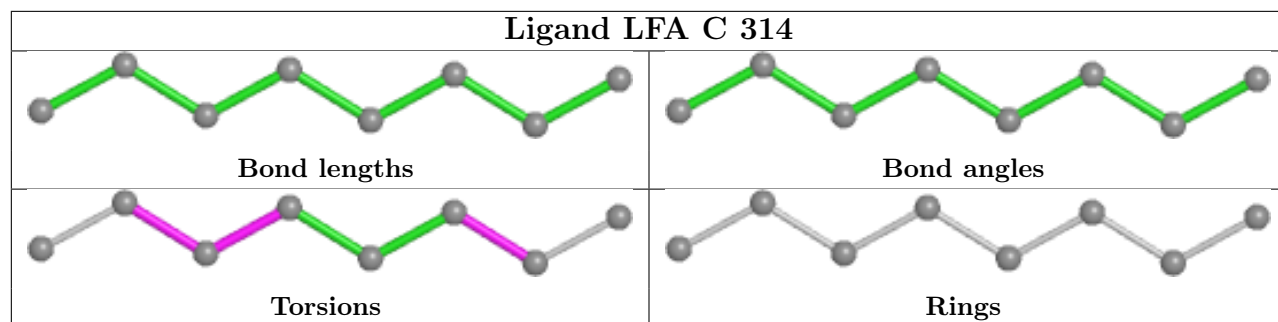
There are no ring outliers.

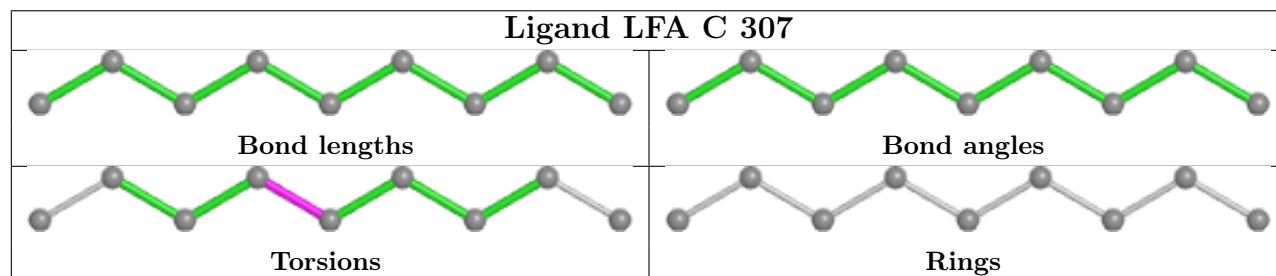
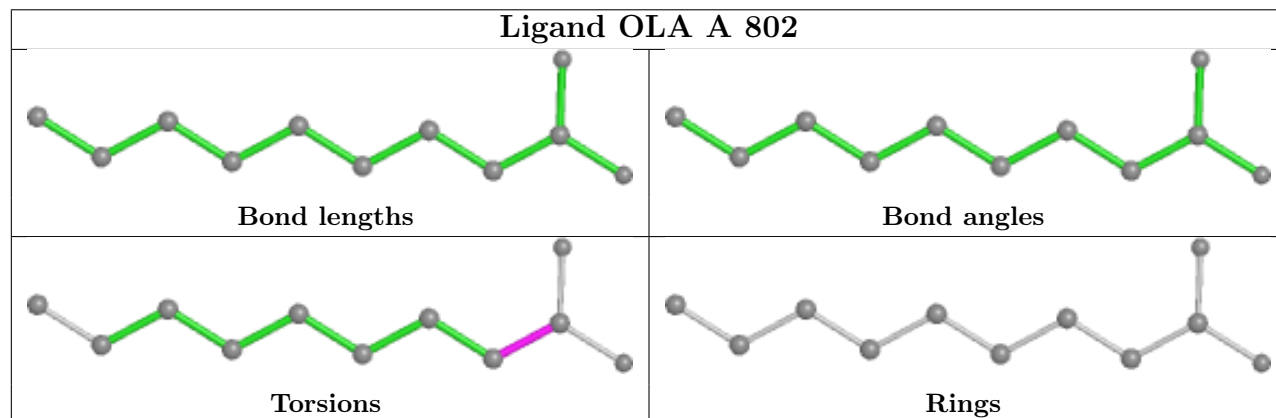
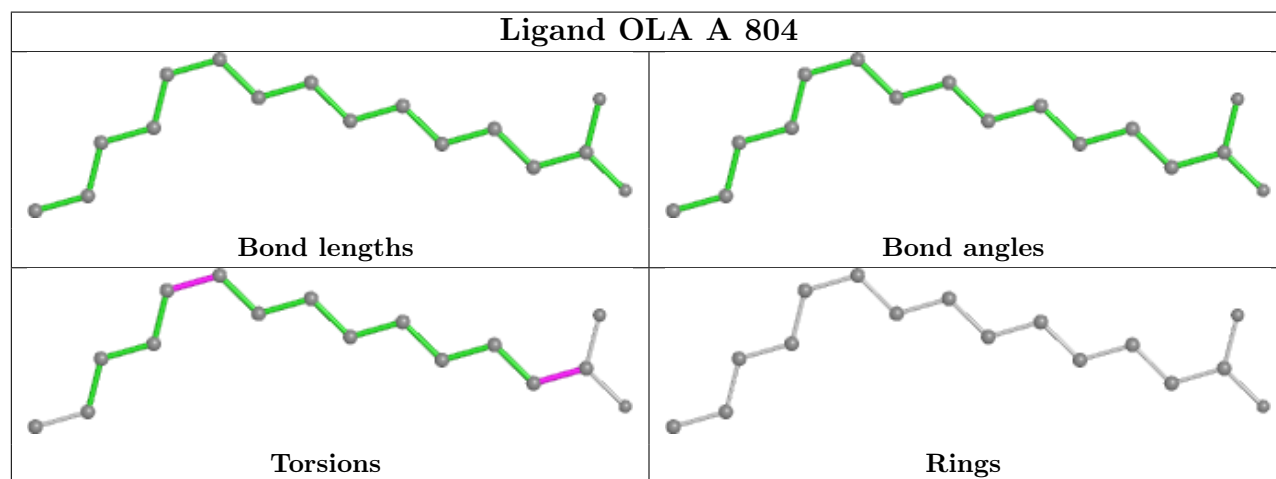
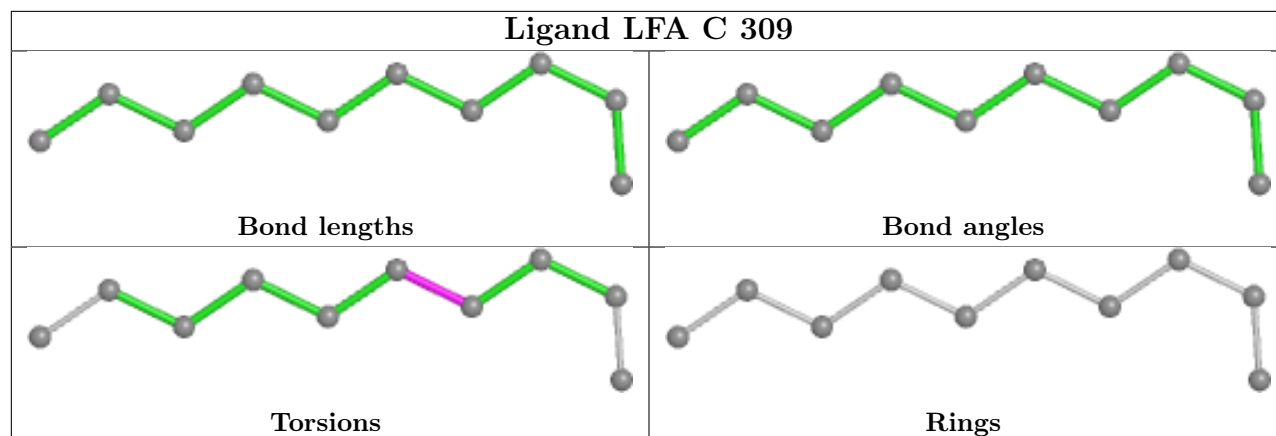
6 monomers are involved in 7 short contacts:

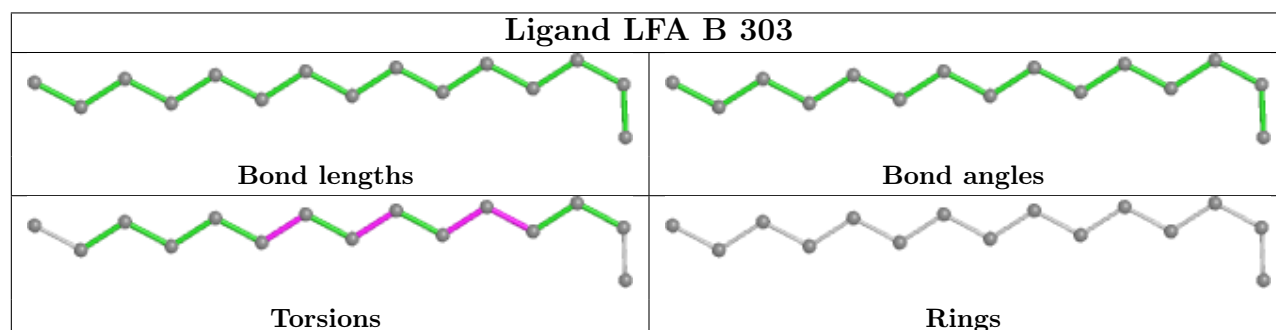
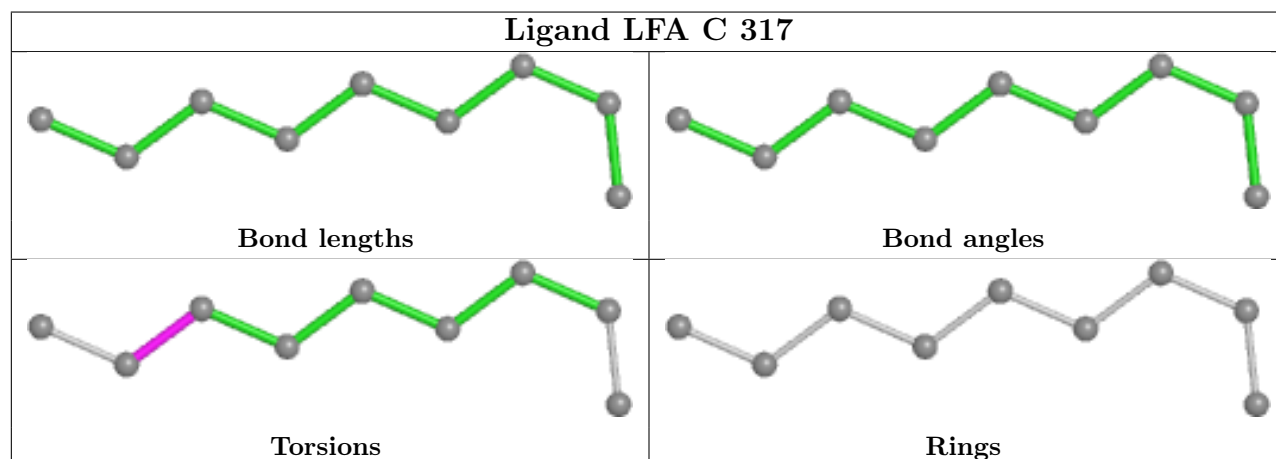
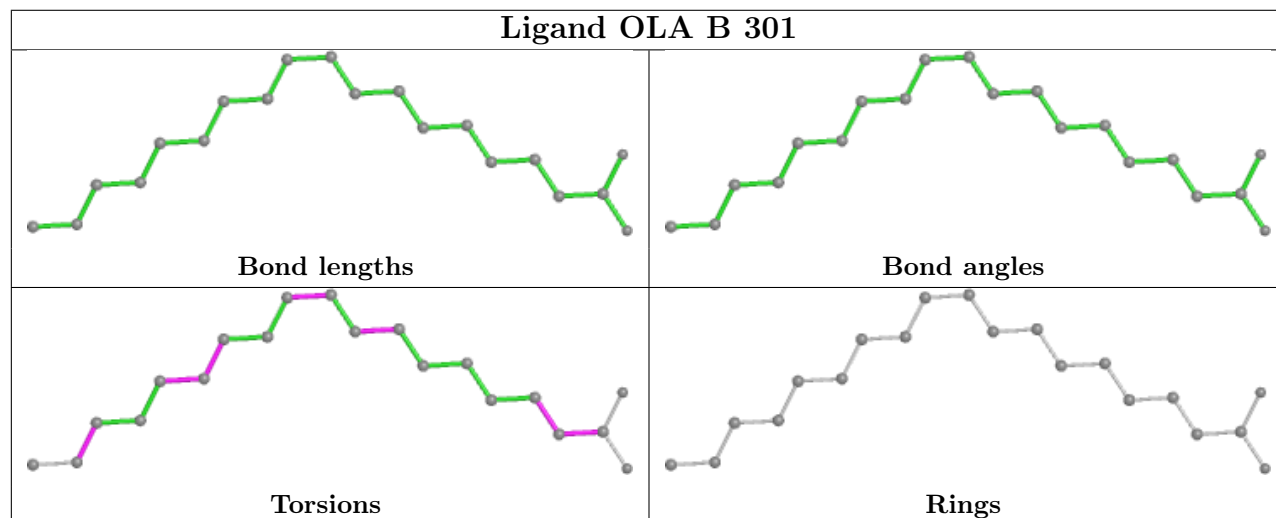
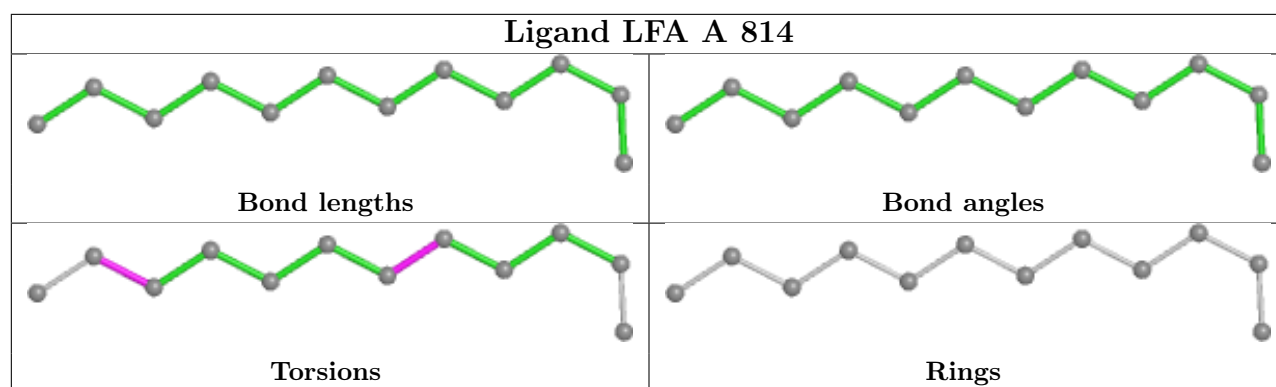
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	312	LFA	1	0
3	A	804	OLA	1	0
3	B	308	OLA	2	0
2	B	312	LFA	1	0
2	C	310	LFA	1	0
2	B	310	LFA	2	0

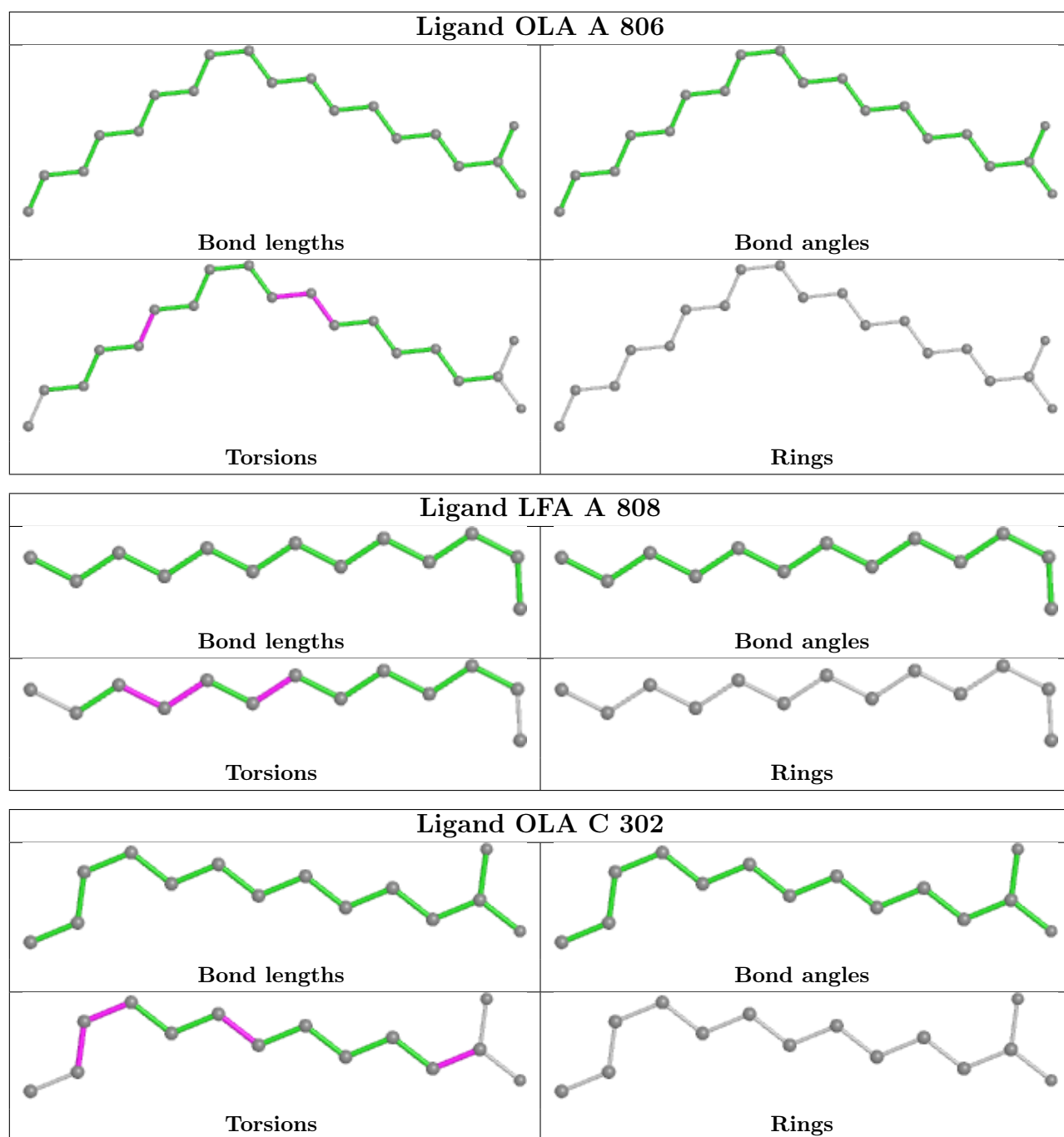
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

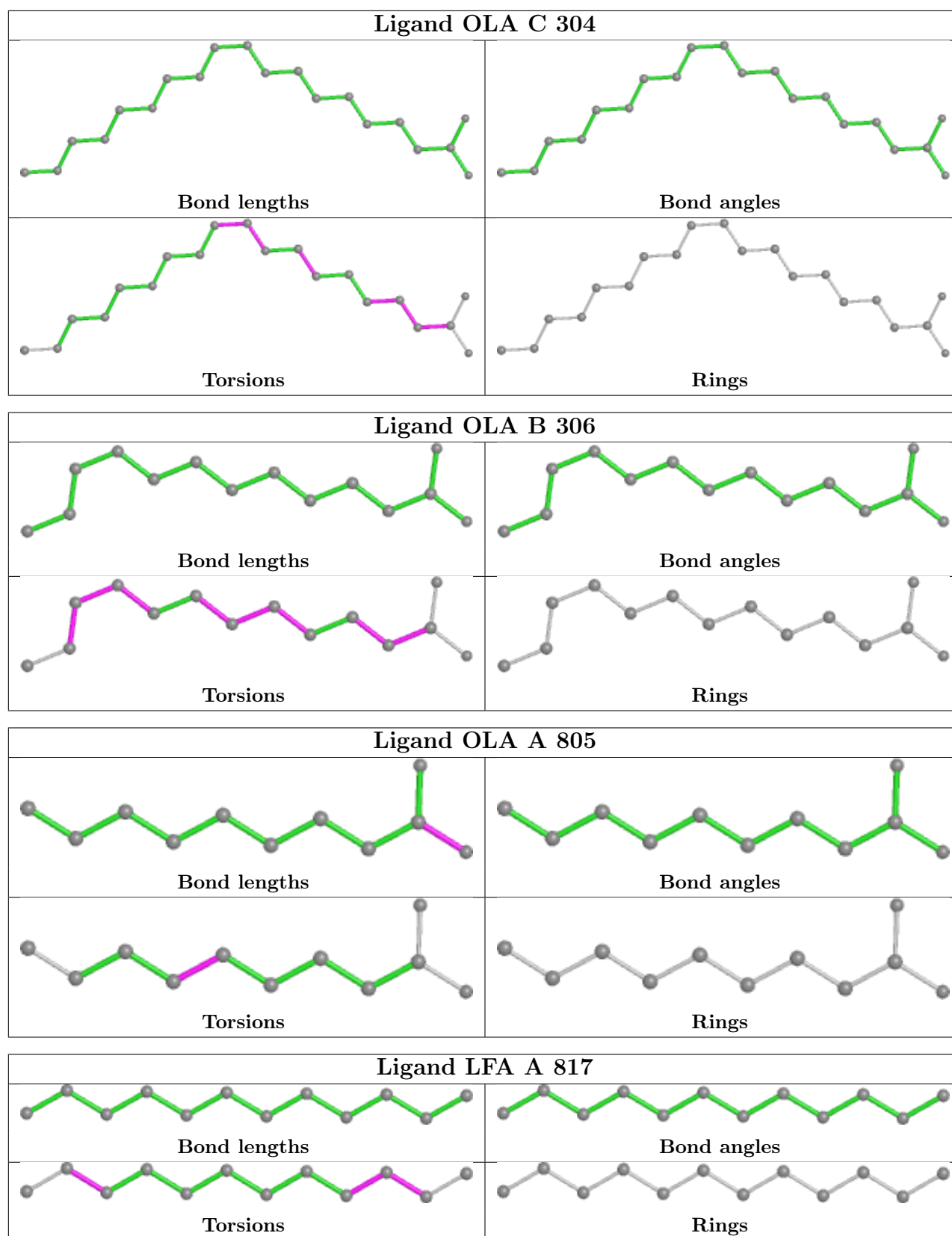


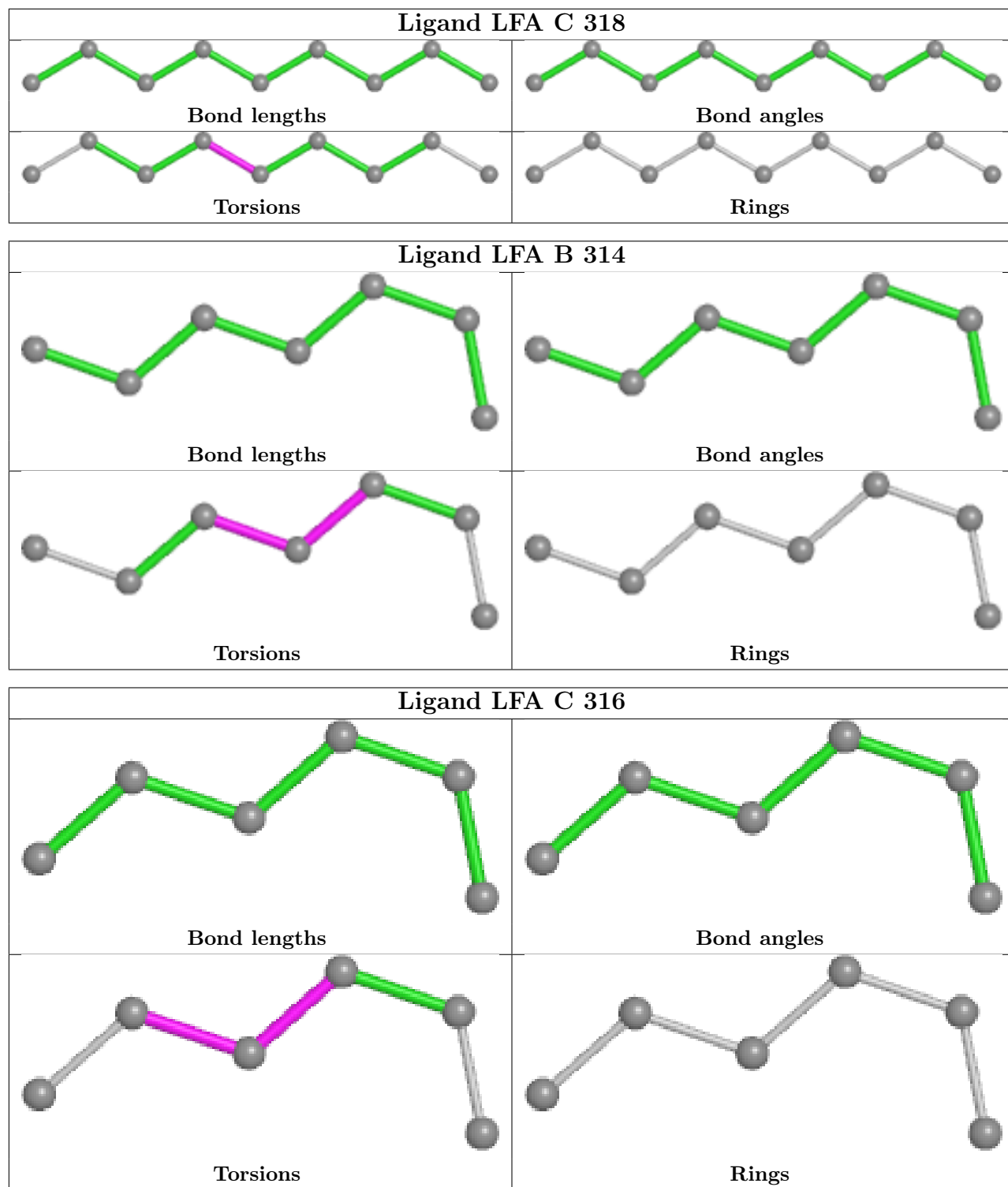


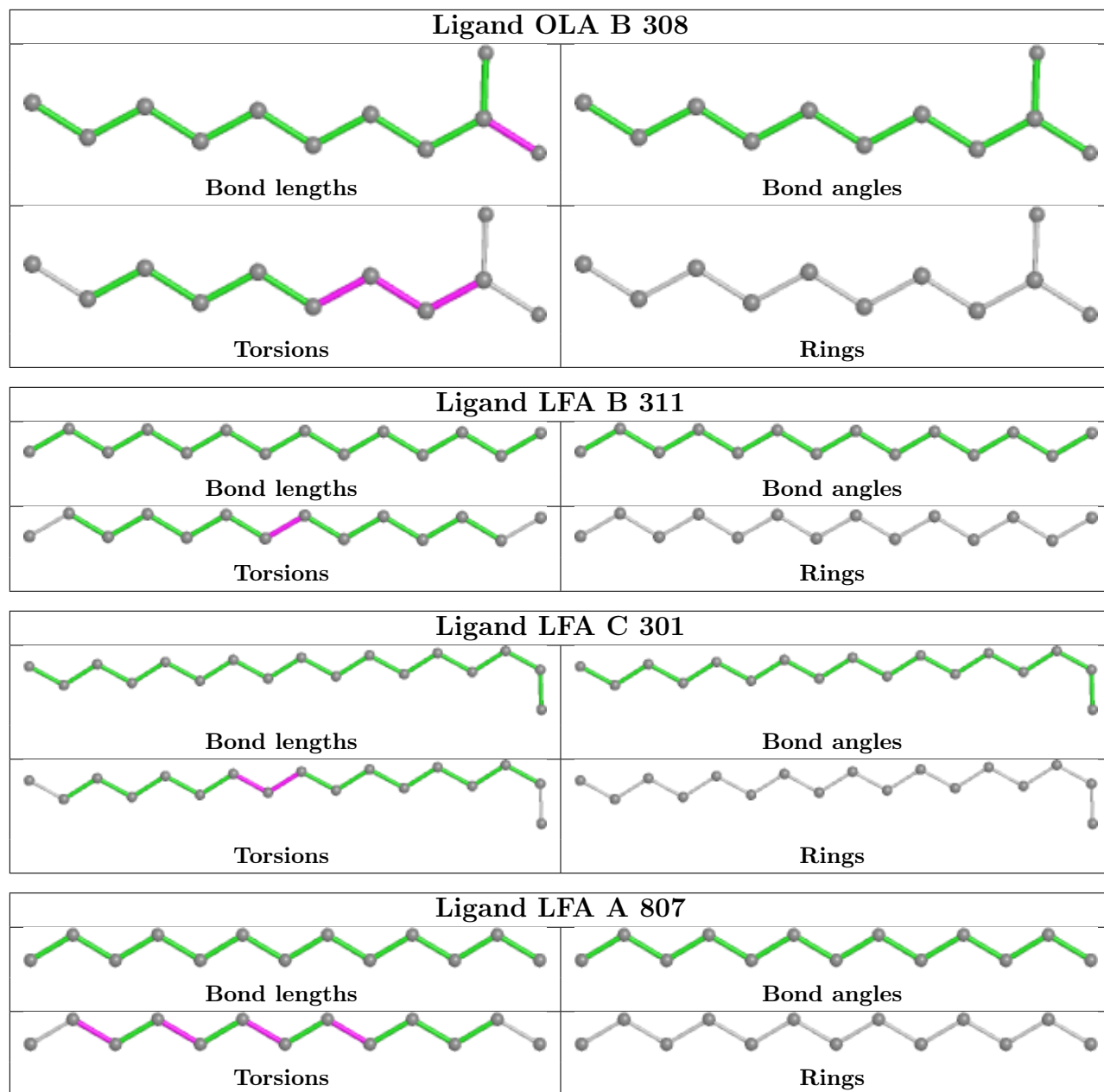


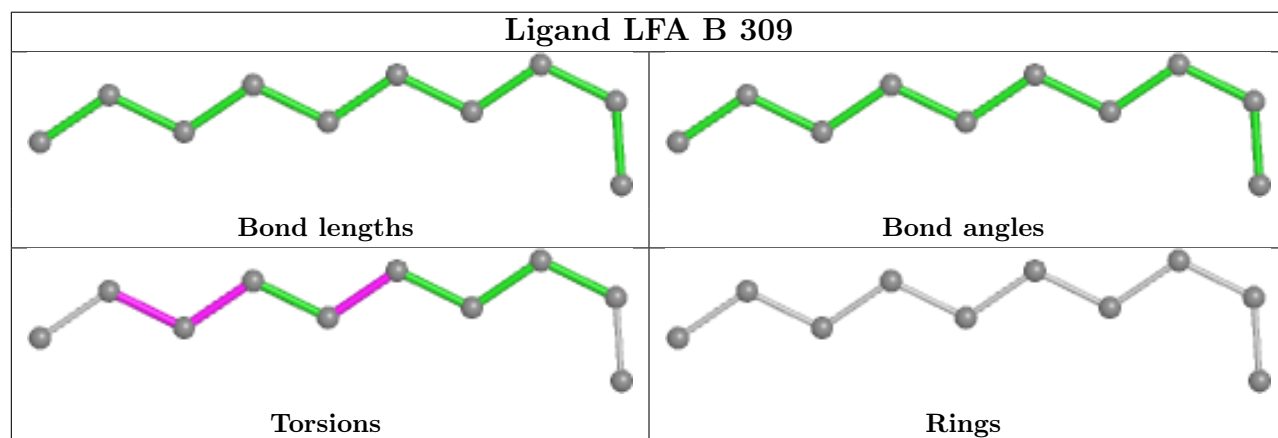
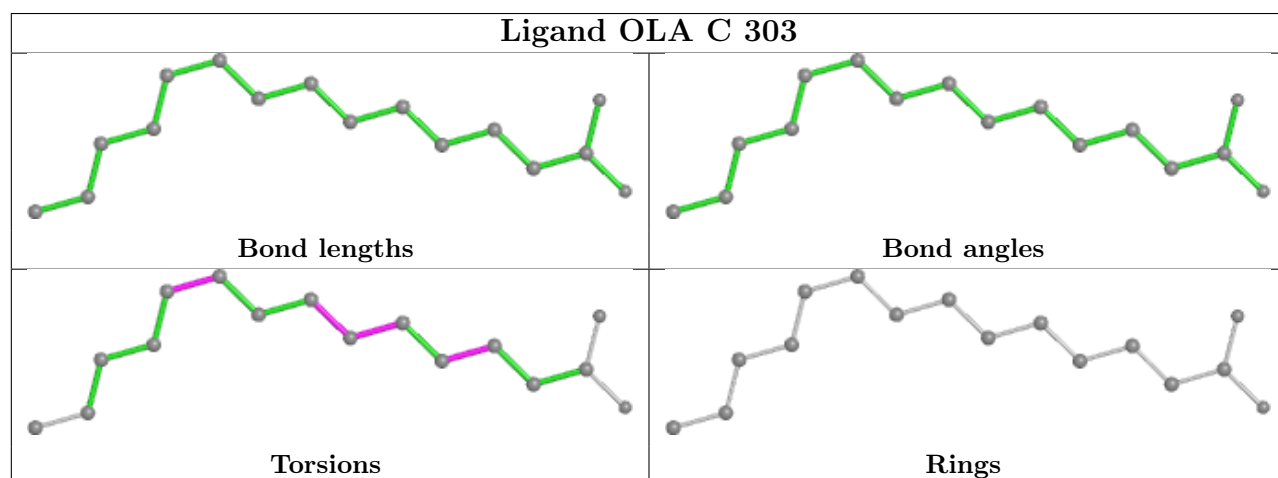
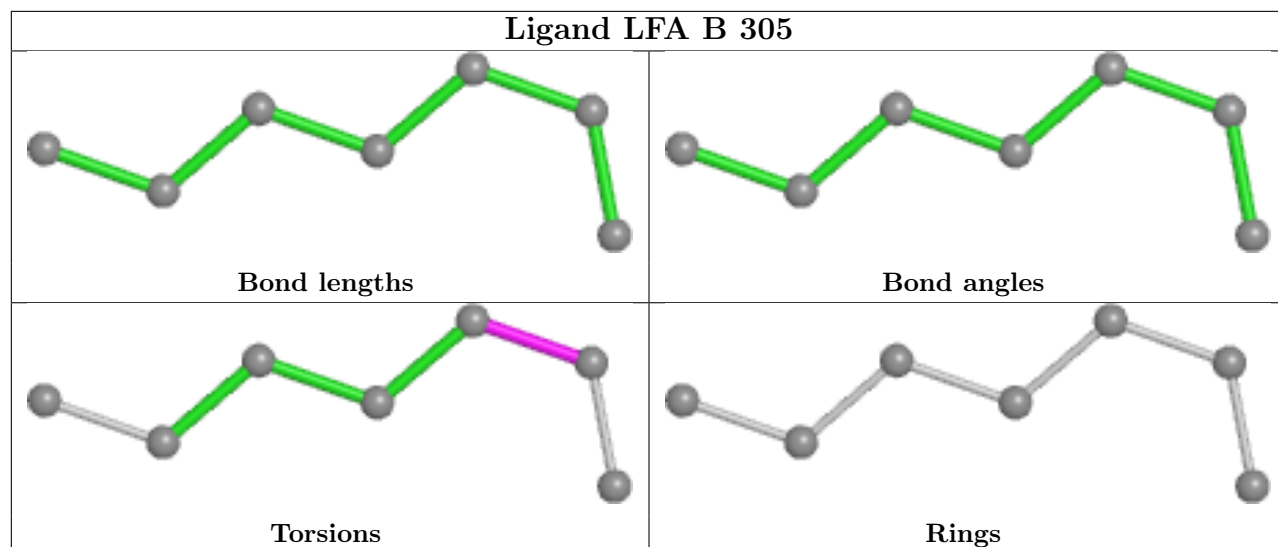


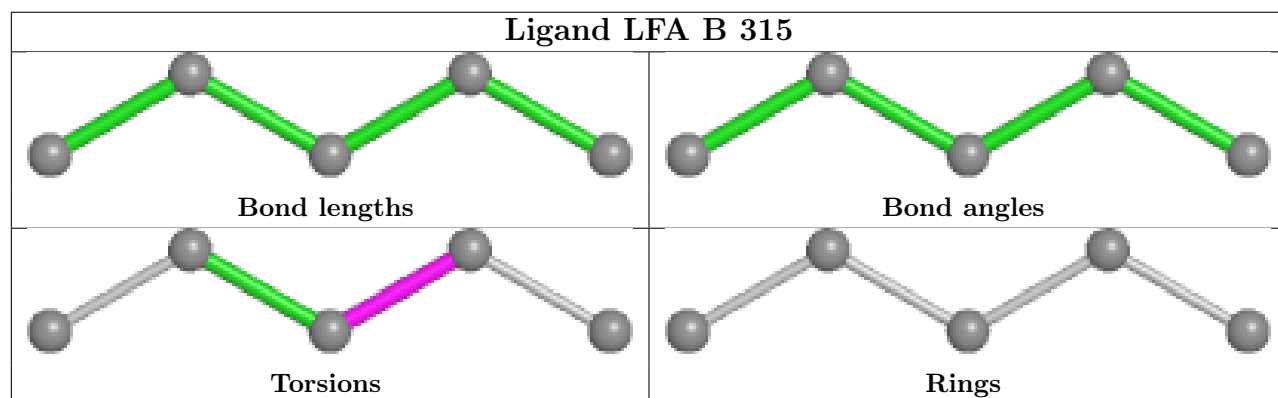
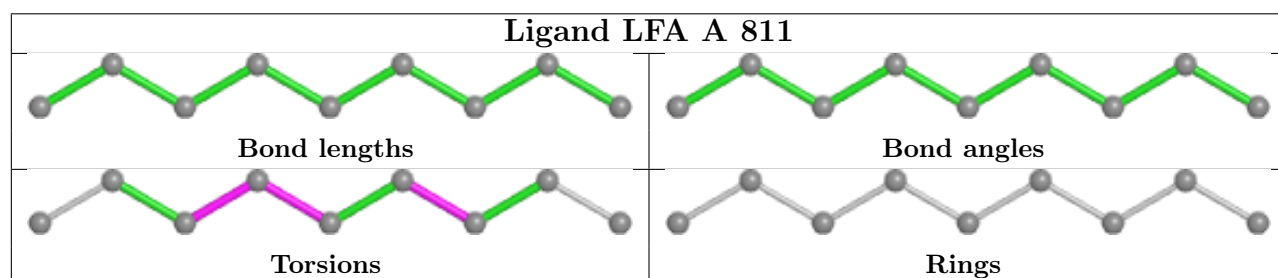
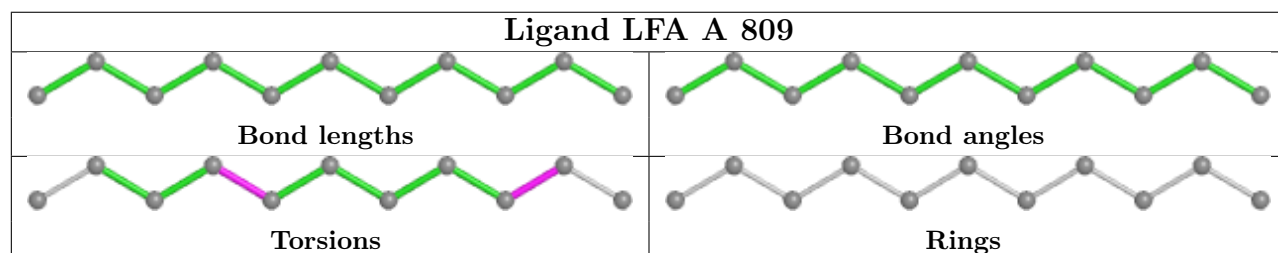
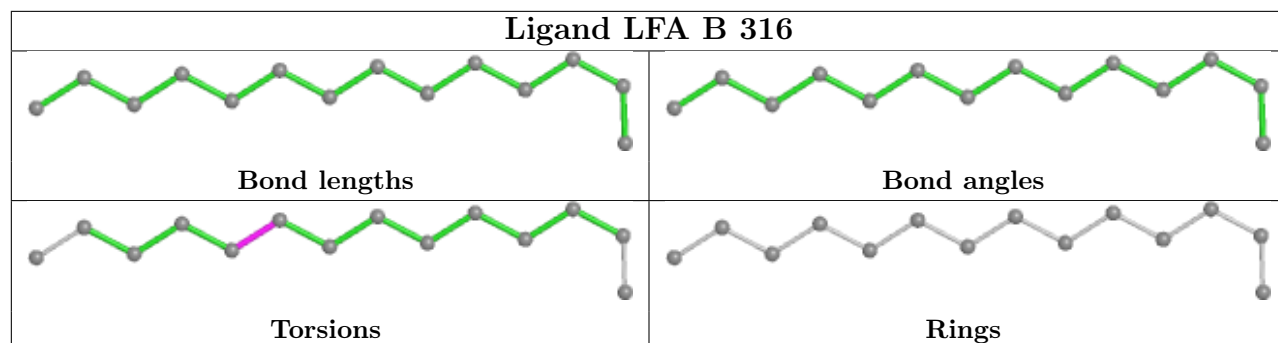


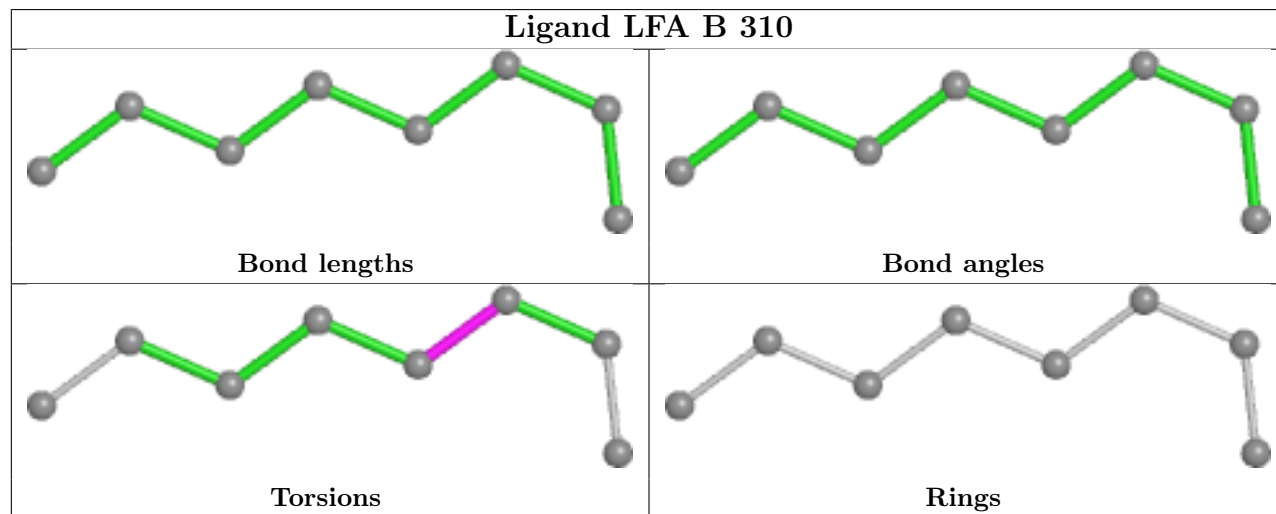
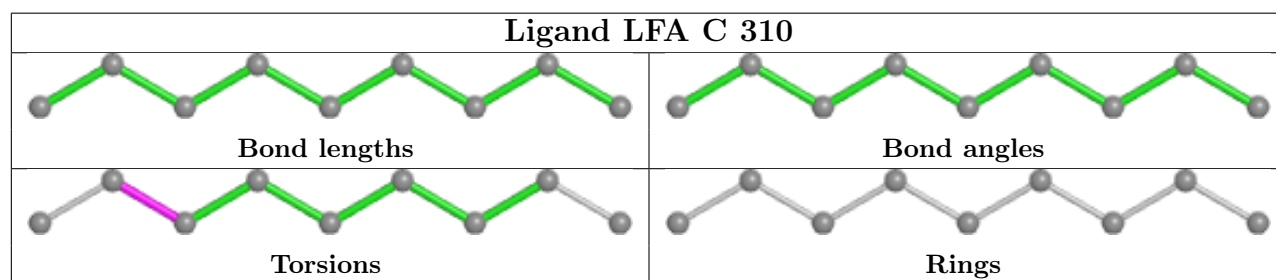
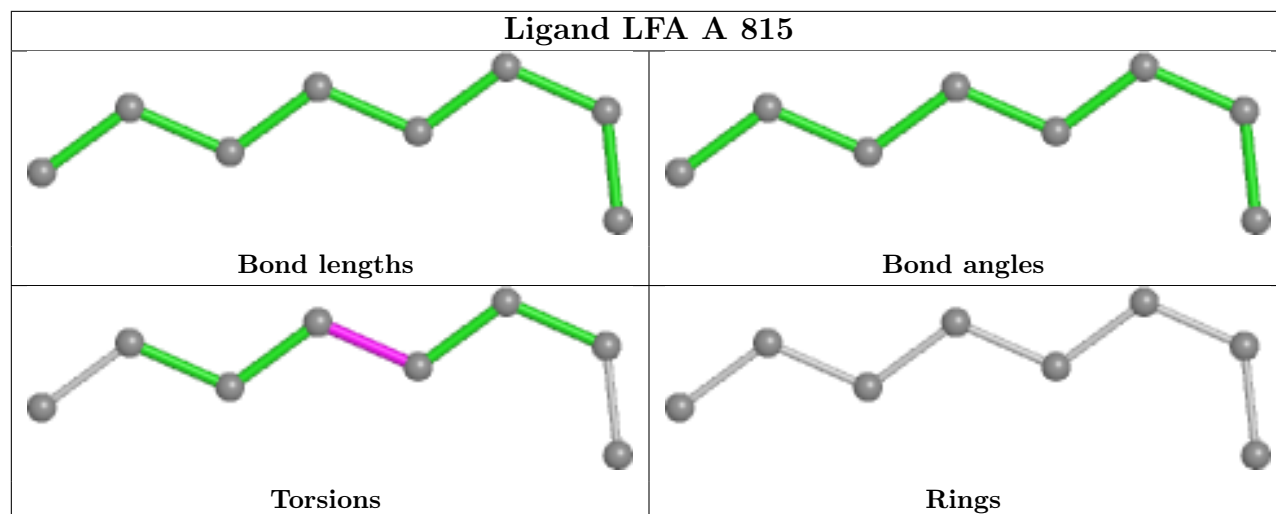


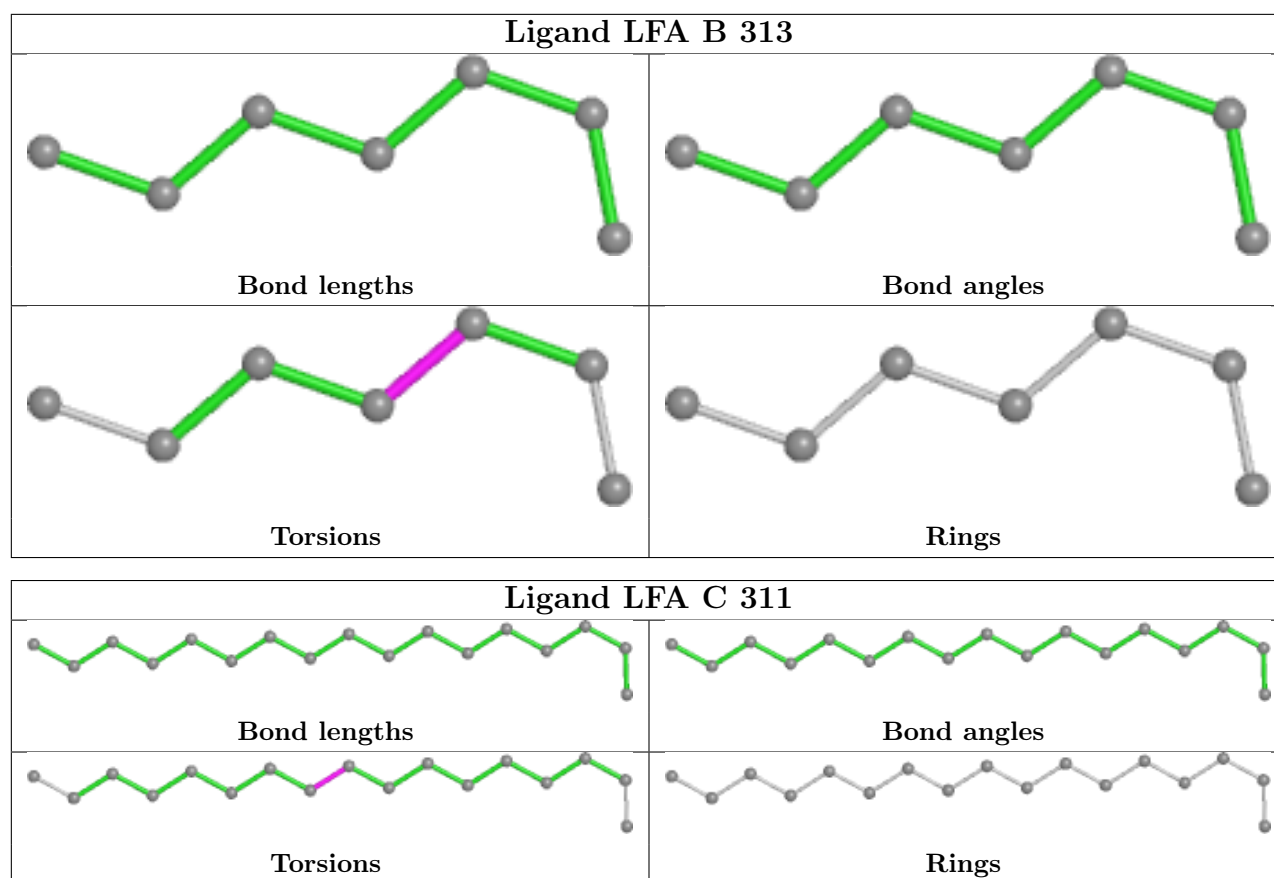












5.7 Other polymers [i](#)

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	220/229 (96%)	-0.34	5 (2%) 60 58	42, 53, 76, 138	0
1	B	219/229 (95%)	-0.13	9 (4%) 37 35	45, 57, 82, 122	0
1	C	221/229 (96%)	-0.19	11 (4%) 28 27	45, 56, 82, 143	0
All	All	660/687 (96%)	-0.22	25 (3%) 40 38	42, 55, 84, 143	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	61	TYR	6.7
1	B	223	GLN	6.6
1	C	223	GLN	6.6
1	A	61	TYR	5.8
1	C	62	ASP	5.3
1	A	62	ASP	5.1
1	B	222	HIS	5.0
1	B	93	GLY	3.6
1	A	60	GLN	3.5
1	B	60	GLN	3.5
1	B	59	PHE	3.2
1	C	64	THR	3.2
1	C	189	LEU	3.1
1	B	85	LEU	2.9
1	B	4	ILE	2.9
1	C	60	GLN	2.8
1	C	94	LYS	2.8
1	B	156	THR	2.7
1	C	222	HIS	2.7
1	A	94	LYS	2.6
1	C	191	GLN	2.4
1	A	64	THR	2.1
1	B	199	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	93	GLY	2.0
1	C	63	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	FME	A	1	10/11	0.88	0.32	72,82,115,124	0
1	FME	C	1	10/11	0.91	0.31	80,90,132,145	0
1	FME	B	1	7/11	0.93	0.27	84,86,108,116	0
1	LYR	A	207[A]	29/30	0.93	0.17	45,52,60,64	29
1	LYR	A	207[C]	29/30	0.93	0.17	33,42,50,51	29
1	LYR	C	207[A]	29/30	0.93	0.20	53,65,75,84	29
1	LYR	C	207[C]	29/30	0.93	0.20	39,45,53,57	29
1	LYR	B	207[A]	29/30	0.94	0.16	50,55,61,65	29
1	LYR	B	207[C]	29/30	0.94	0.16	35,43,52,54	29

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(Å ²)	Q<0.9
2	LFA	B	305	7/20	0.35	0.33	83,97,107,109	0
2	LFA	A	815	8/20	0.52	0.28	93,103,113,120	0
3	OLA	A	802	11/20	0.55	0.17	75,78,115,116	0
2	LFA	C	314	8/20	0.56	0.38	91,107,111,112	0
3	OLA	B	307	16/20	0.61	0.27	69,93,112,123	0
3	OLA	B	301	20/20	0.63	0.23	65,86,118,134	0
2	LFA	B	314	7/20	0.63	0.37	89,100,108,112	0

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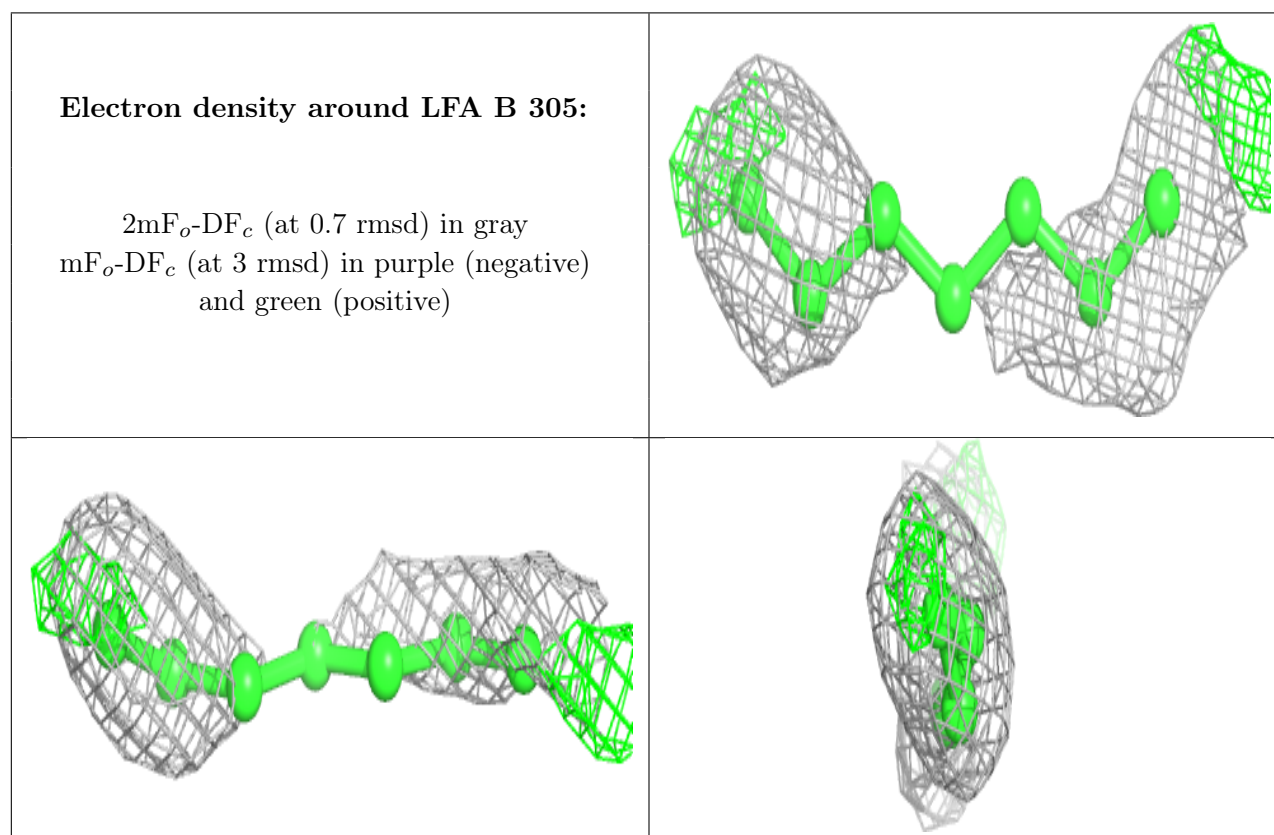
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OLA	C	304	20/20	0.65	0.21	66,87,104,112	0
3	OLA	A	803	20/20	0.65	0.22	70,85,100,110	0
3	OLA	C	303	16/20	0.65	0.26	80,100,135,140	0
4	PO4	C	306	5/5	0.65	0.41	129,130,153,163	0
2	LFA	C	311	17/20	0.66	0.24	79,85,104,106	0
2	LFA	B	309	10/20	0.66	0.29	88,104,113,116	0
2	LFA	B	311	14/20	0.69	0.22	83,91,96,99	0
3	OLA	B	308	11/20	0.70	0.21	89,93,98,102	0
3	OLA	A	806	19/20	0.71	0.17	67,80,111,120	0
2	LFA	A	817	12/20	0.72	0.16	73,82,90,90	0
2	LFA	A	814	12/20	0.73	0.20	75,93,101,106	0
2	LFA	C	308	6/20	0.74	0.26	82,87,90,93	0
2	LFA	C	310	9/20	0.74	0.29	95,100,111,116	0
3	OLA	B	306	14/20	0.74	0.20	81,95,115,117	0
2	LFA	A	813	6/20	0.75	0.29	68,70,74,82	0
2	LFA	A	812	9/20	0.75	0.31	93,96,106,108	0
2	LFA	A	809	11/20	0.77	0.19	83,93,101,106	0
2	LFA	B	315	5/20	0.77	0.16	86,91,98,110	0
2	LFA	B	303	15/20	0.79	0.19	61,68,95,98	0
2	LFA	C	309	10/20	0.79	0.17	86,94,106,109	0
2	LFA	C	312	11/20	0.79	0.27	107,115,131,132	0
3	OLA	A	805	11/20	0.79	0.15	79,92,103,103	0
2	LFA	A	801	7/20	0.79	0.30	71,74,76,78	0
2	LFA	C	315	6/20	0.79	0.39	97,101,104,111	0
2	LFA	B	316	14/20	0.80	0.31	72,85,112,117	0
2	LFA	A	807	13/20	0.80	0.23	92,98,120,122	0
2	LFA	A	816	6/20	0.80	0.22	79,96,97,100	0
2	LFA	A	810	14/20	0.81	0.16	85,100,123,134	0
3	OLA	A	804	16/20	0.82	0.17	75,84,113,116	0
2	LFA	C	301	17/20	0.82	0.19	58,77,89,92	0
3	OLA	C	302	14/20	0.83	0.35	64,82,128,128	0
2	LFA	B	313	7/20	0.83	0.16	68,83,90,92	0
2	LFA	C	316	6/20	0.84	0.26	60,72,76,76	0
2	LFA	C	317	9/20	0.84	0.17	68,71,79,87	0
2	LFA	C	318	9/20	0.84	0.14	69,73,84,94	0
2	LFA	B	312	9/20	0.85	0.11	93,102,106,110	0
2	LFA	A	811	9/20	0.85	0.21	78,85,96,96	0
3	OLA	C	305	16/20	0.86	0.16	67,79,110,112	0
2	LFA	B	317	9/20	0.87	0.14	63,69,75,76	0
2	LFA	B	304	9/20	0.88	0.19	72,79,80,82	0
2	LFA	C	307	9/20	0.89	0.23	66,74,83,84	0
2	LFA	B	302	7/20	0.91	0.13	73,78,84,84	0

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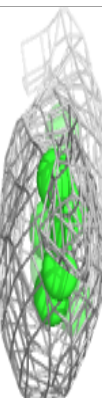
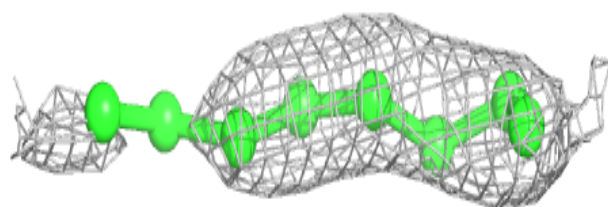
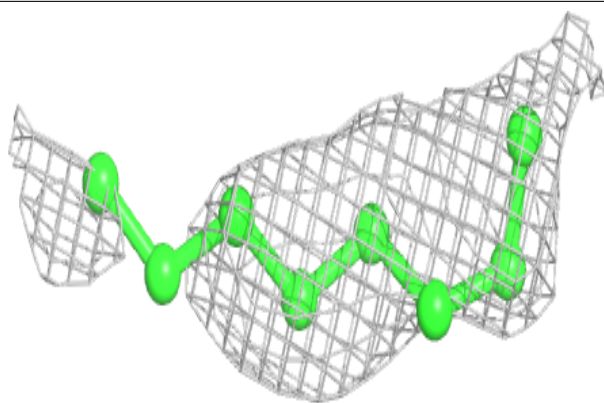
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LFA	A	808	13/20	0.91	0.28	69,72,95,97	0
2	LFA	B	310	8/20	0.93	0.26	76,86,94,98	0
2	LFA	C	313	4/20	0.94	0.17	86,88,89,91	0

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

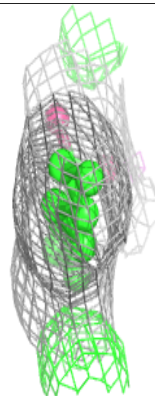
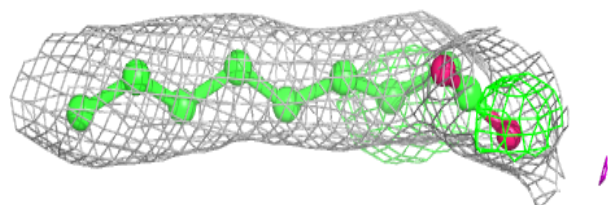
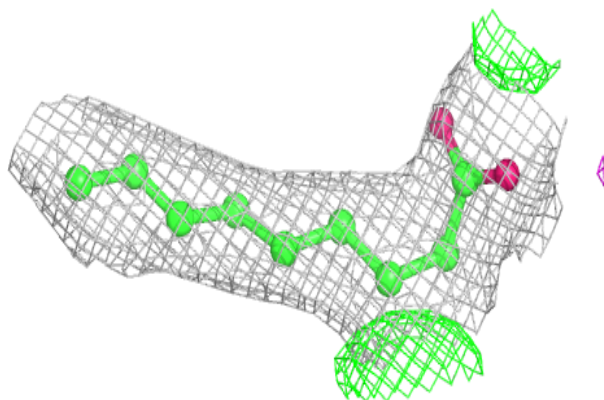


Electron density around LFA A 815:

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

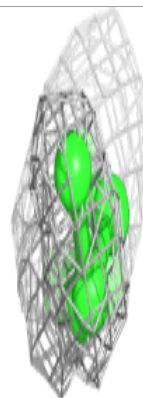
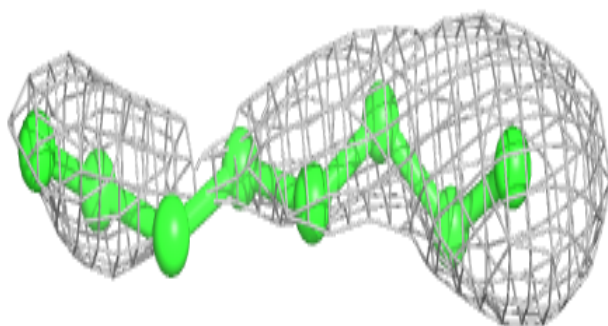
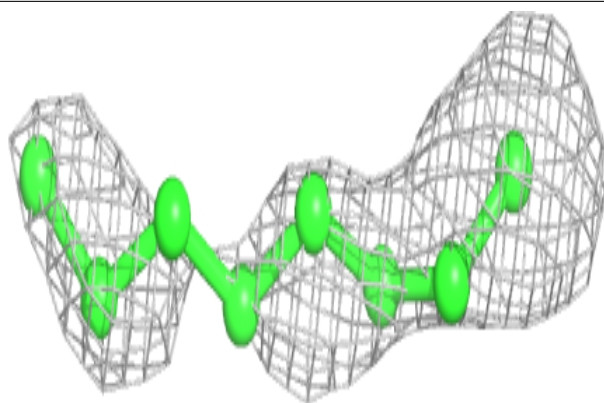
**Electron density around OLA A 802:**

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

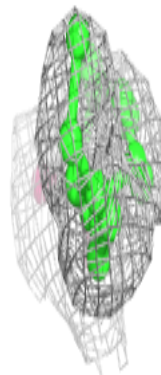
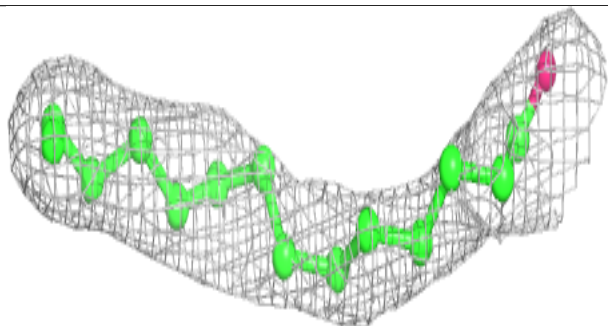
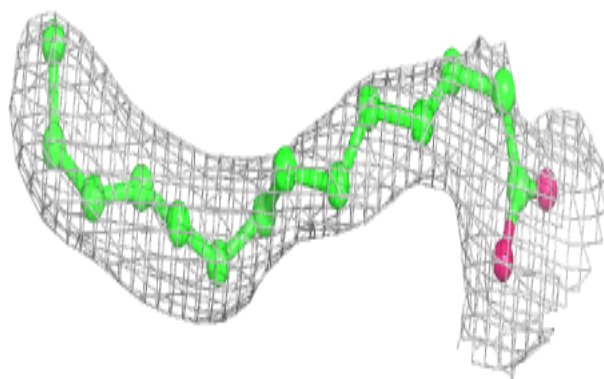


Electron density around LFA C 314:

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

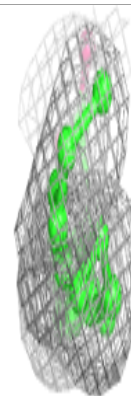
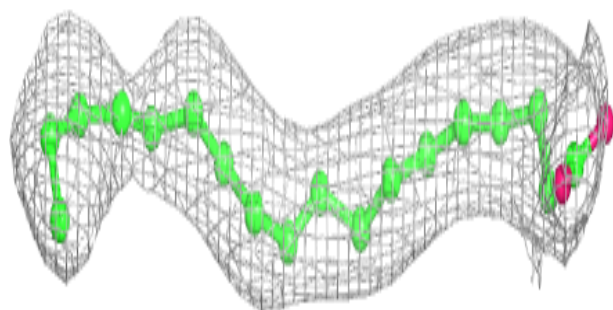
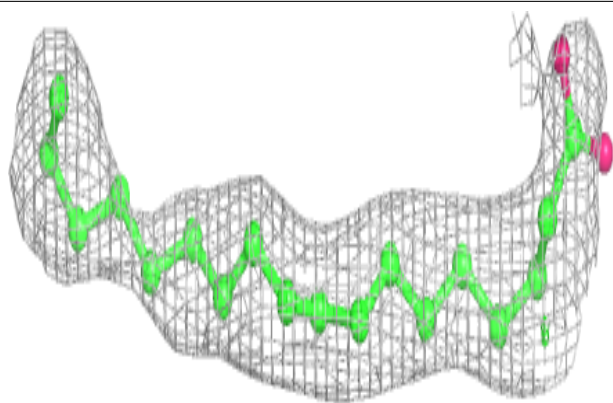
**Electron density around OLA B 307:**

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

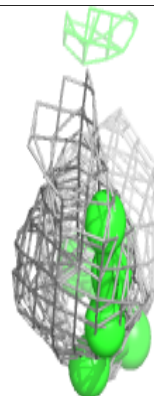
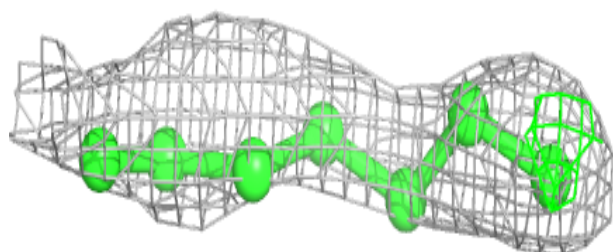
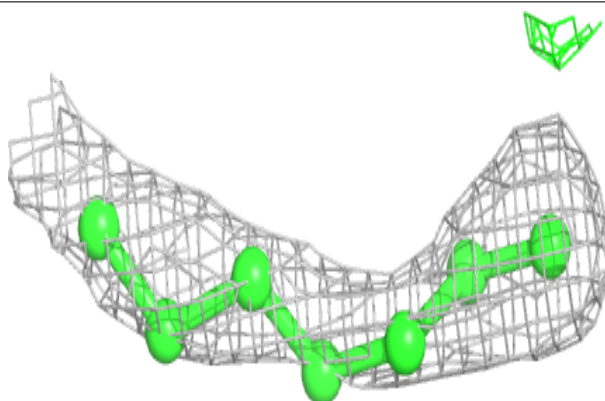


Electron density around OLA B 301:

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

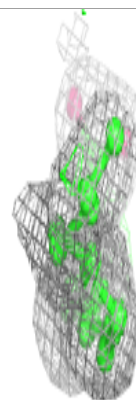
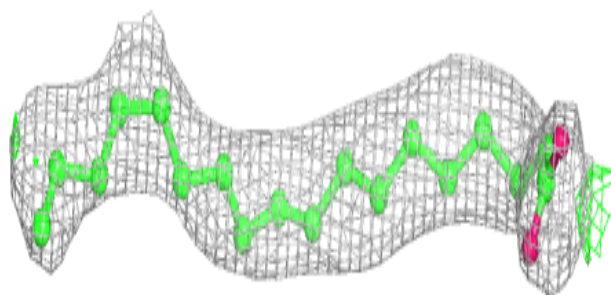
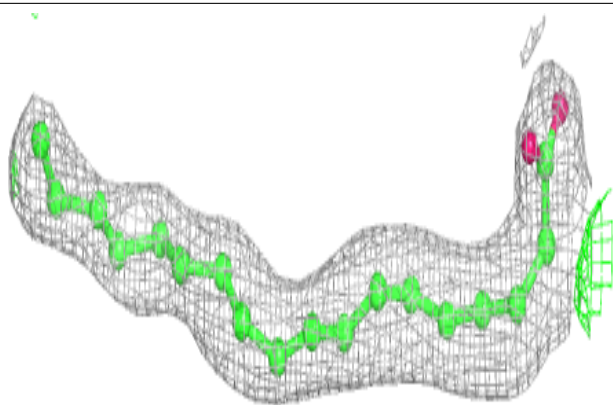
**Electron density around LFA B 314:**

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

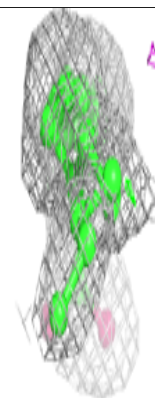
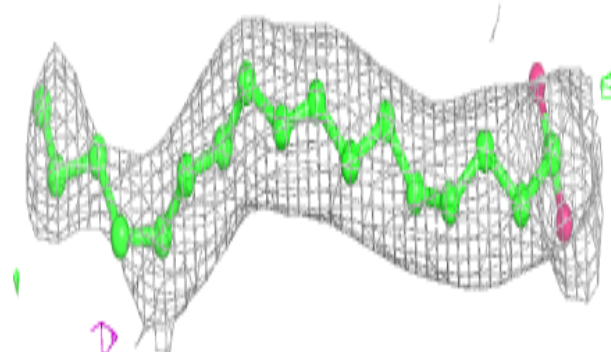
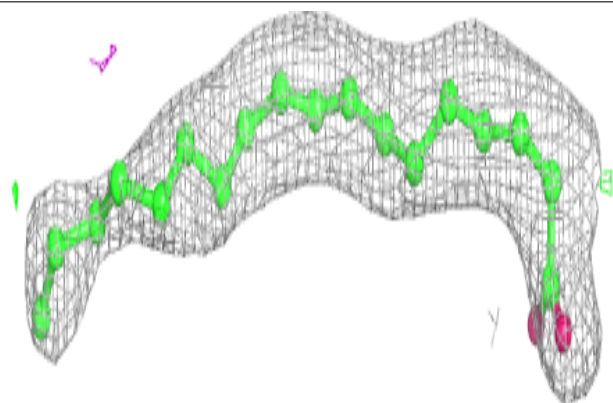


Electron density around OLA C 304:

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

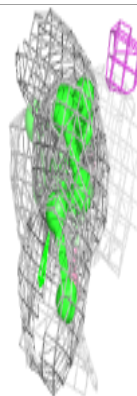
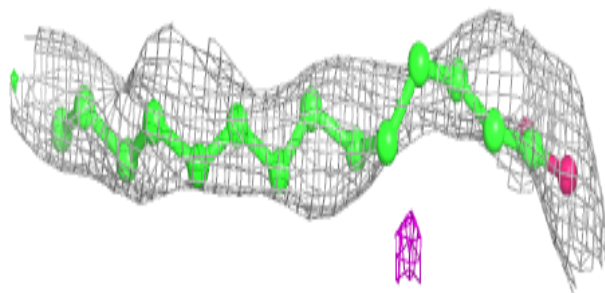
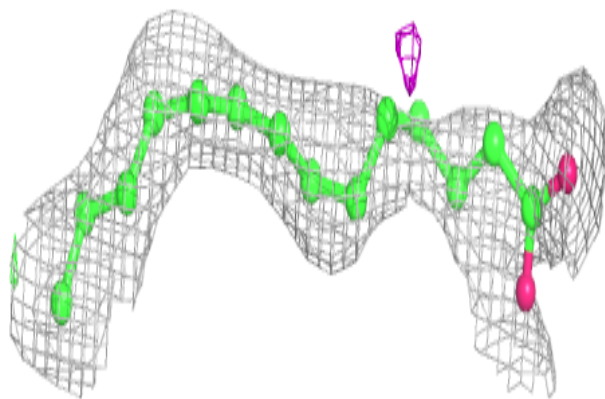
**Electron density around OLA A 803:**

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

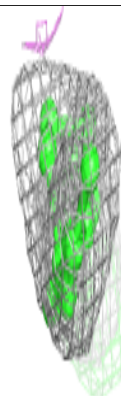
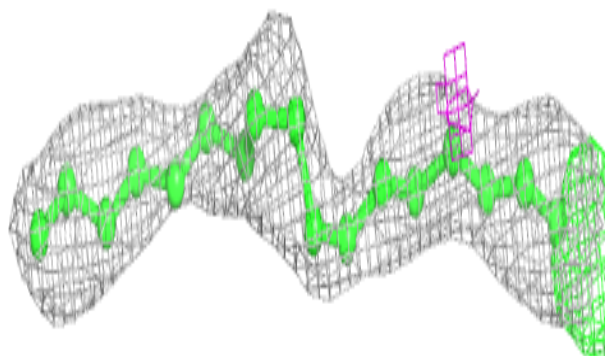
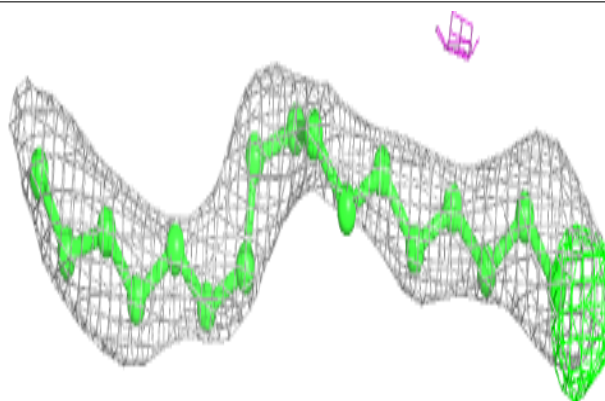


Electron density around OLA C 303:

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

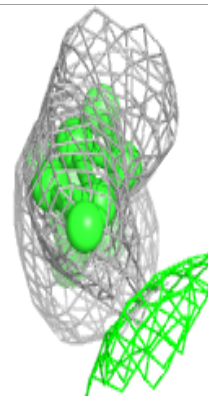
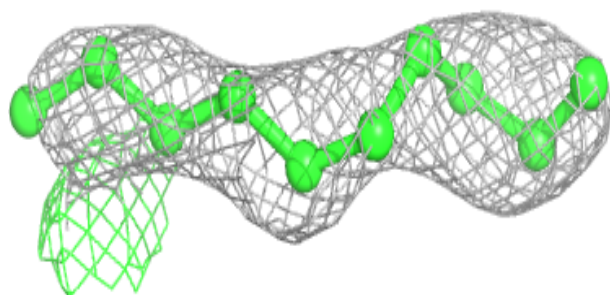
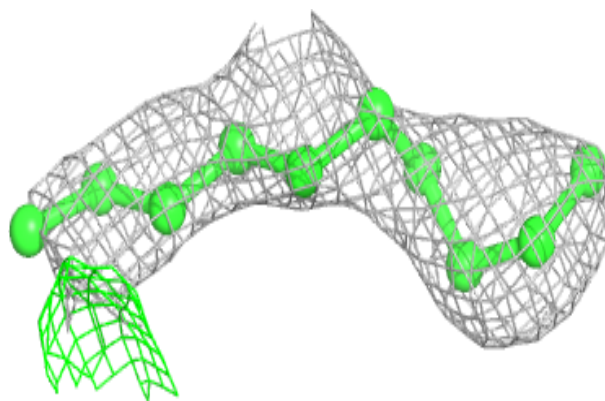
**Electron density around LFA C 311:**

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

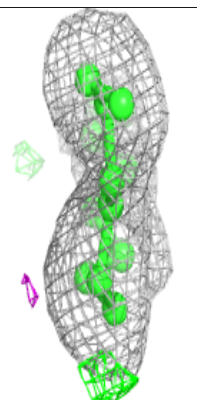
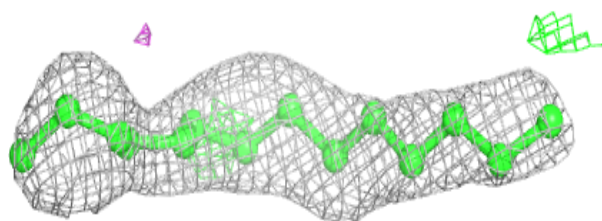
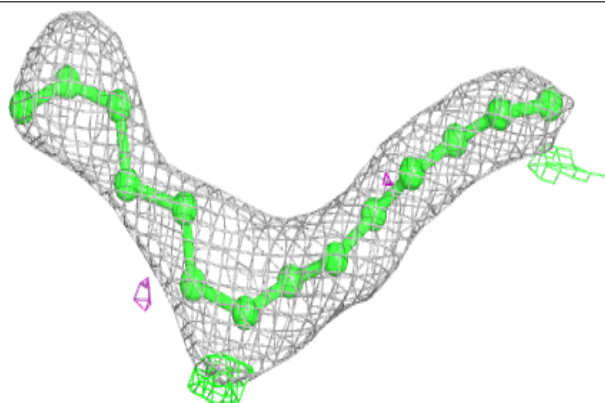


Electron density around LFA B 309:

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

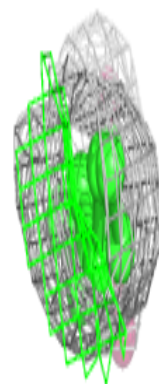
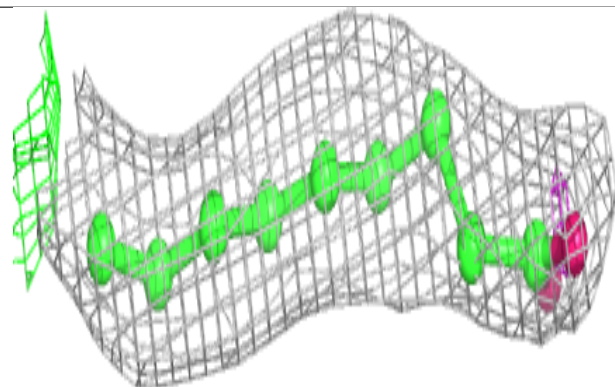
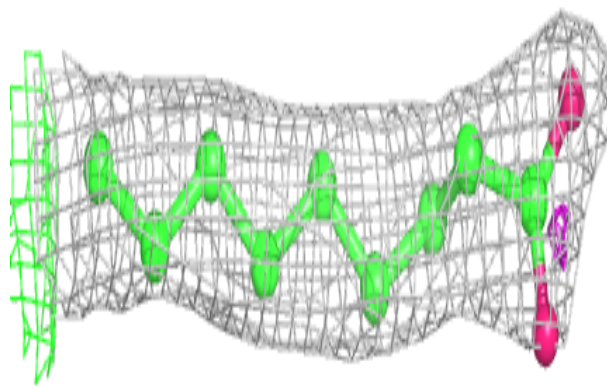
**Electron density around LFA B 311:**

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

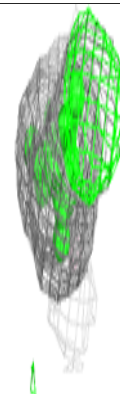
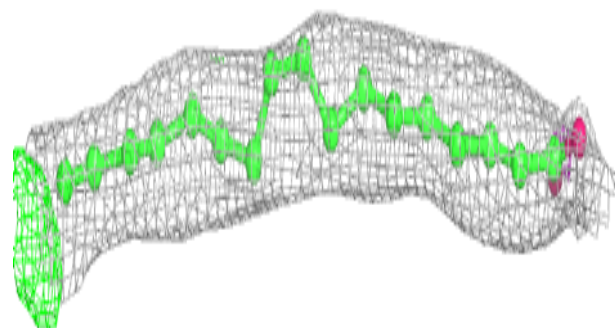
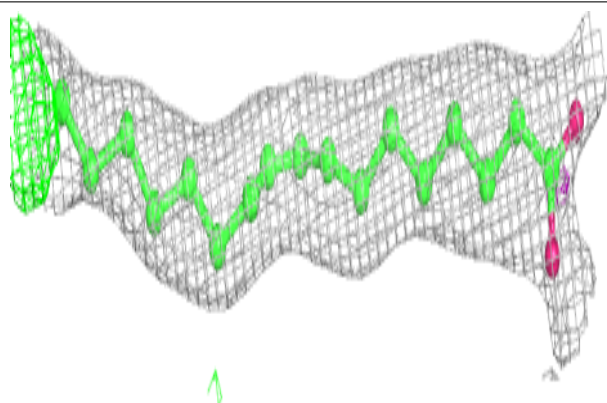


Electron density around OLA B 308:

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

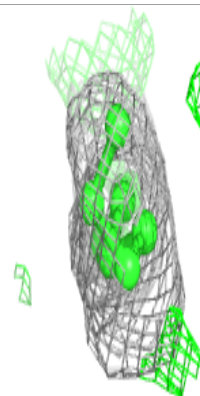
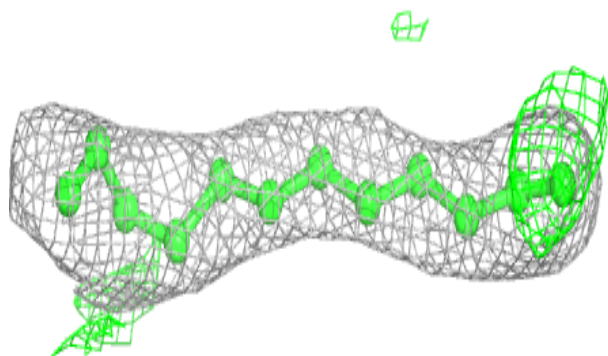
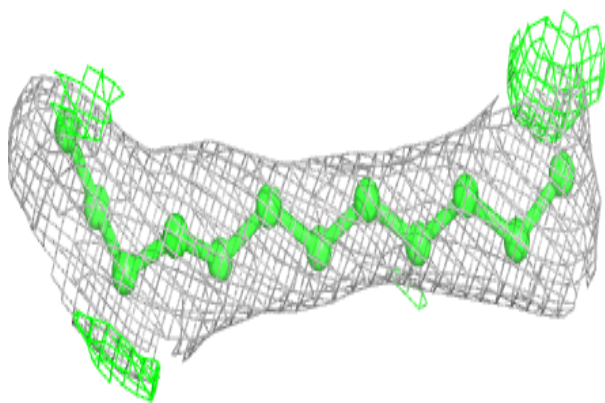
**Electron density around OLA A 806:**

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

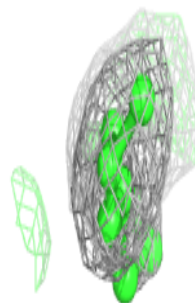
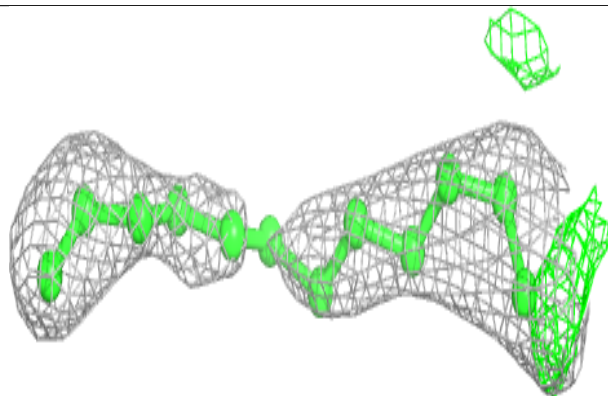
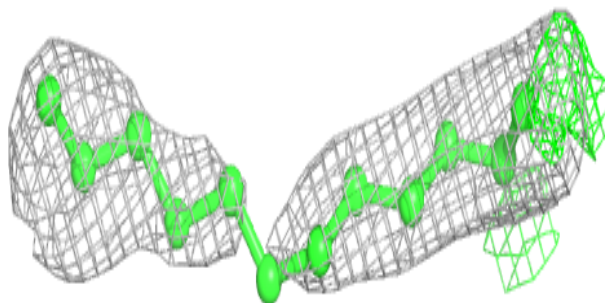


Electron density around LFA A 817:

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

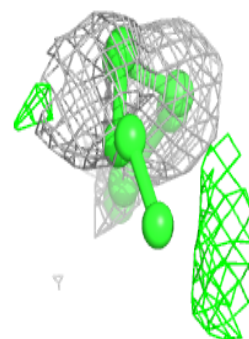
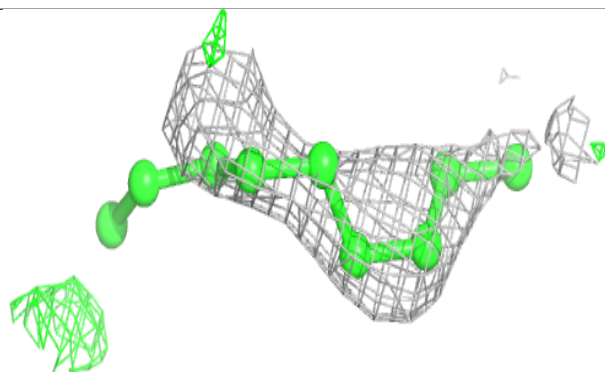
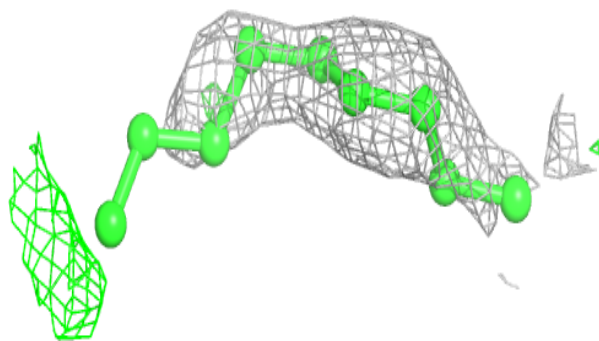
**Electron density around LFA A 814:**

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

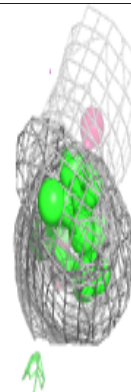
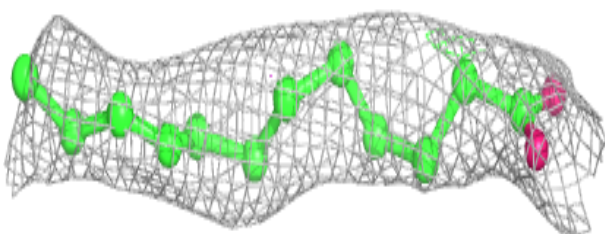
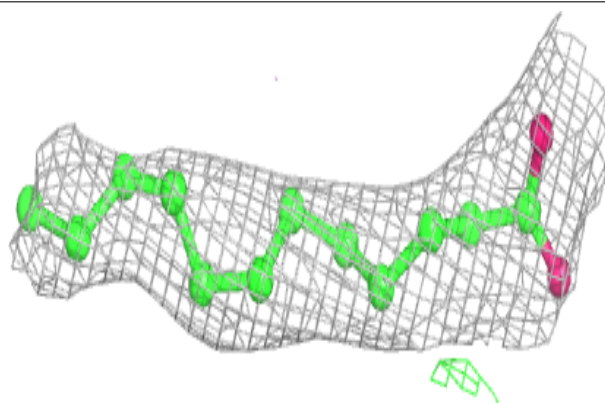


Electron density around LFA C 310:

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

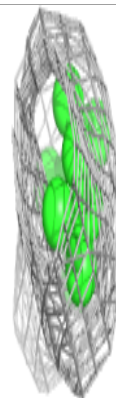
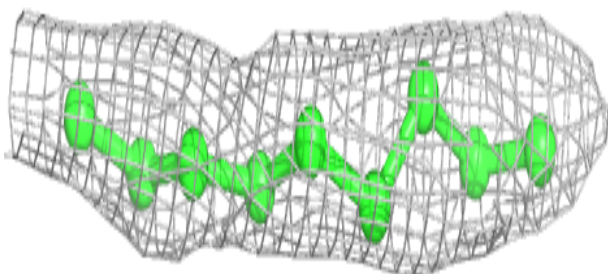
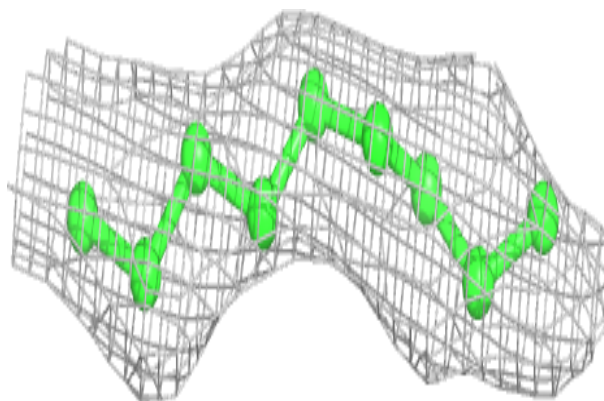
**Electron density around OLA B 306:**

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

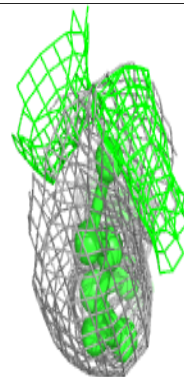
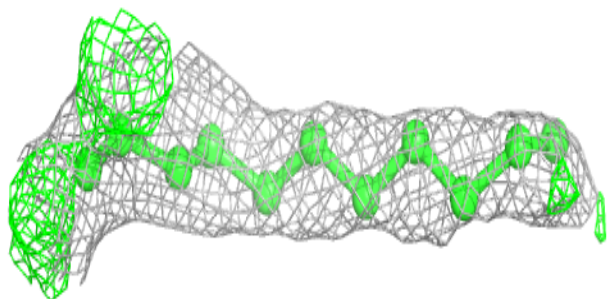
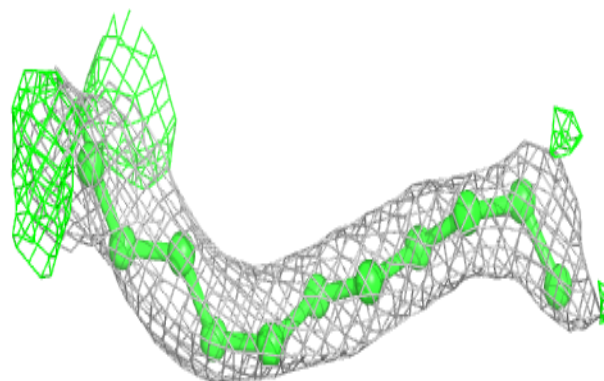


Electron density around LFA A 812:

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

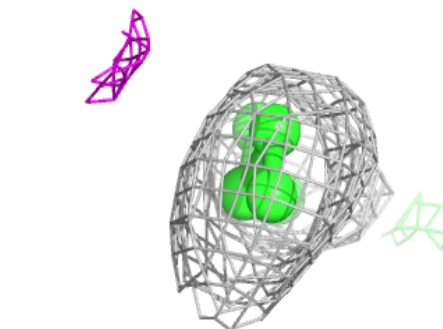
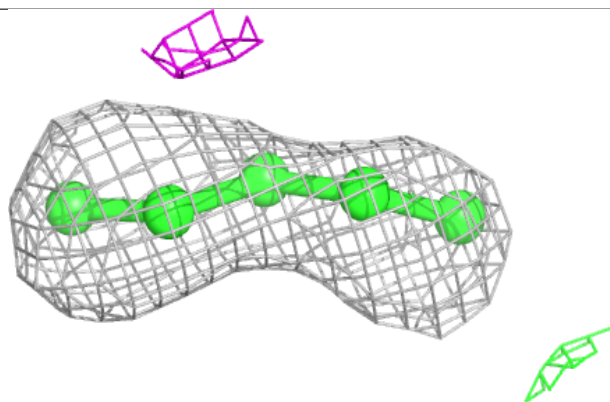
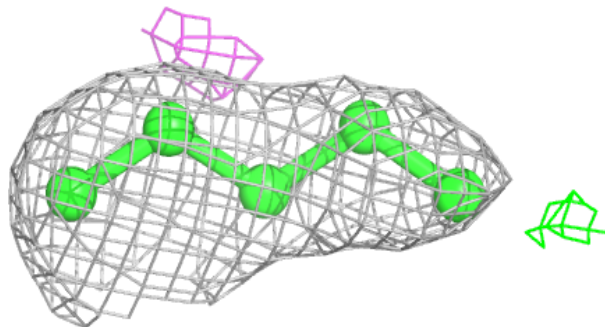
**Electron density around LFA A 809:**

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

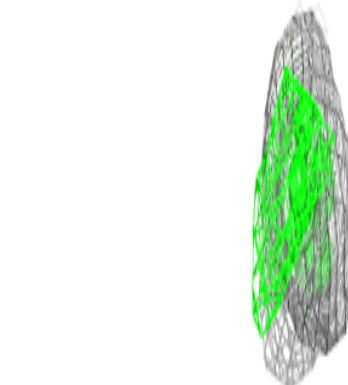
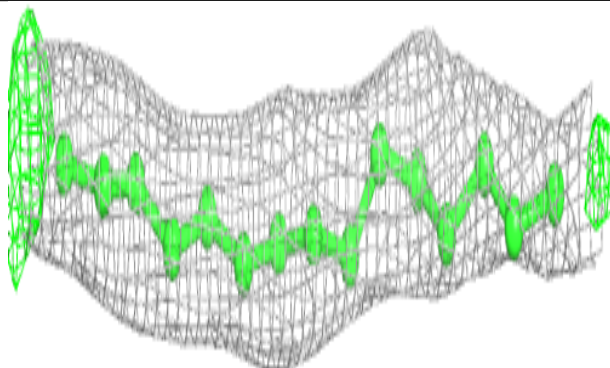
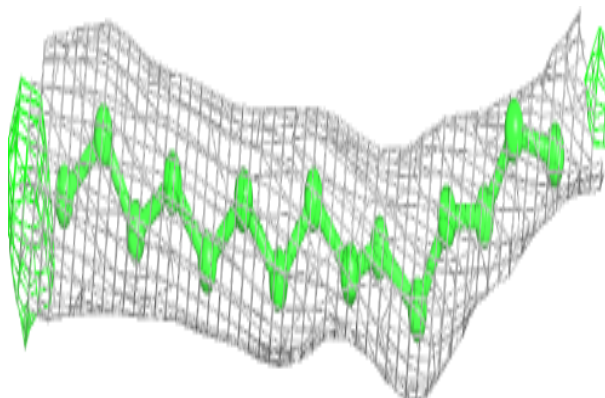


Electron density around LFA B 315:

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

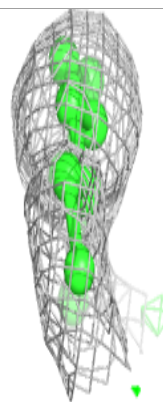
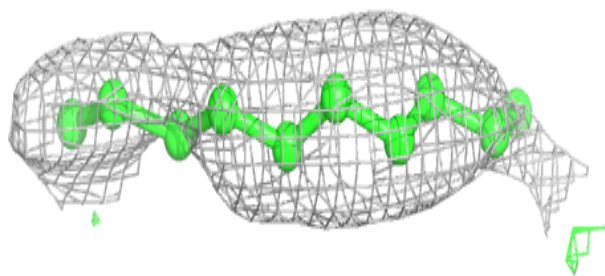
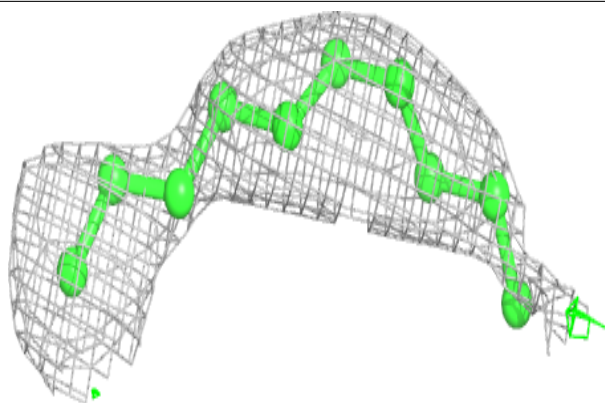
**Electron density around LFA B 303:**

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

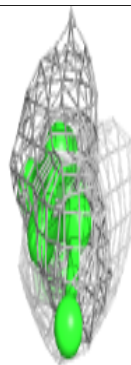
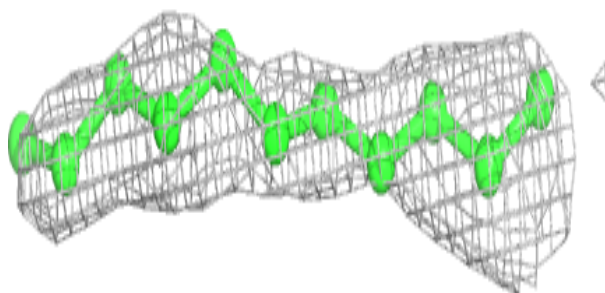
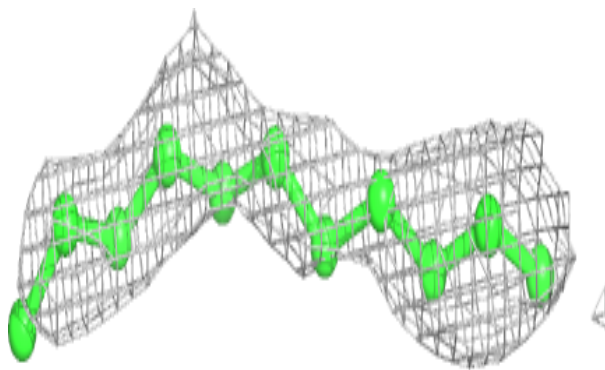


Electron density around LFA C 309:

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

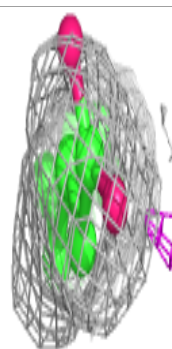
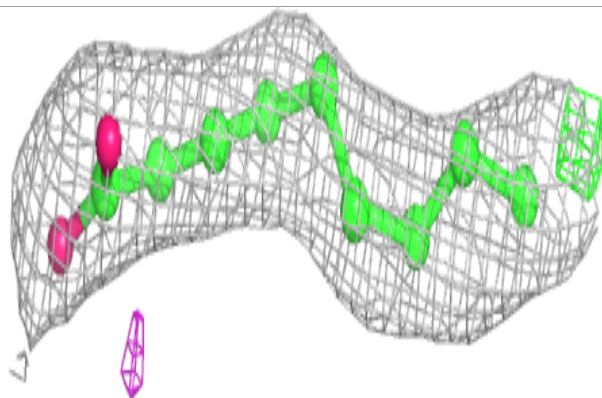
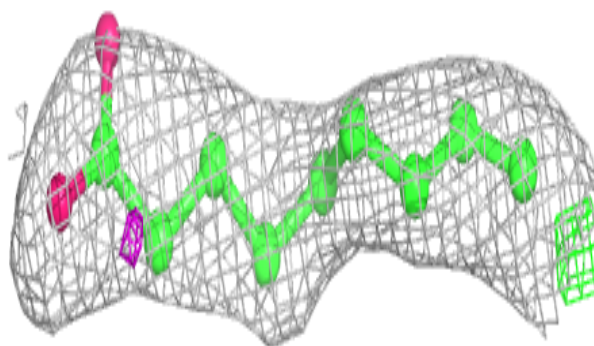
**Electron density around LFA C 312:**

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

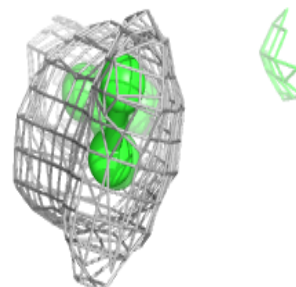
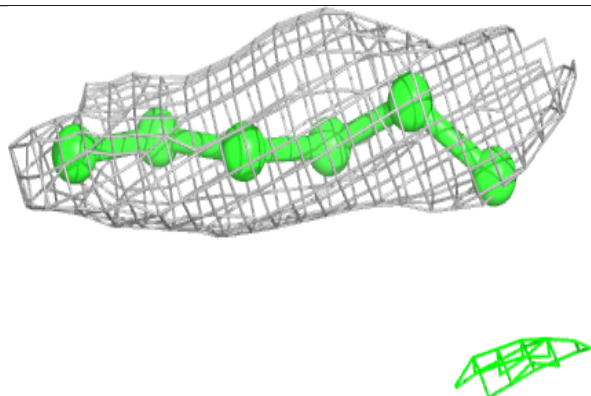
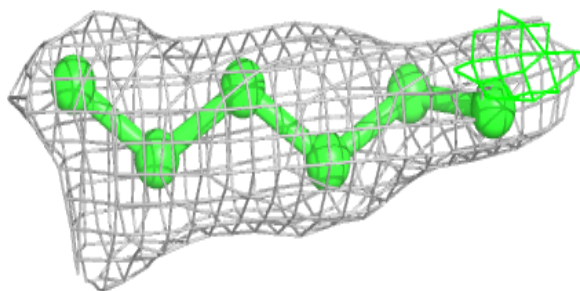


Electron density around OLA A 805:

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

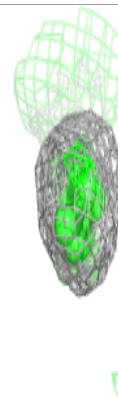
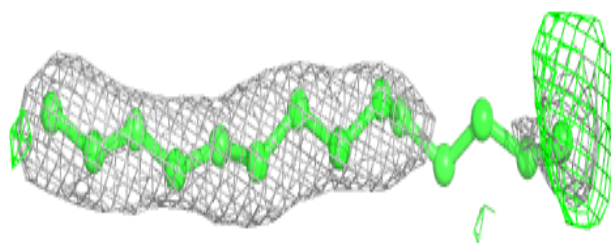
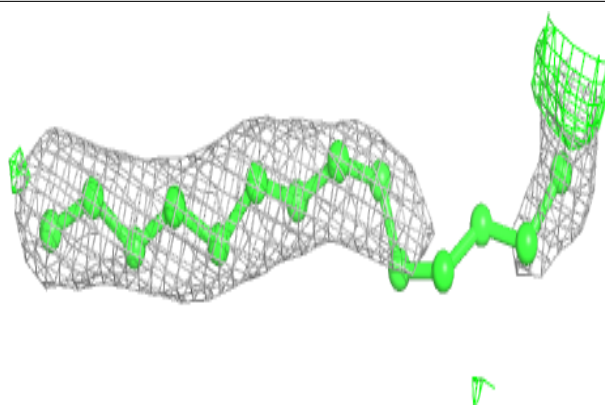
**Electron density around LFA C 315:**

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

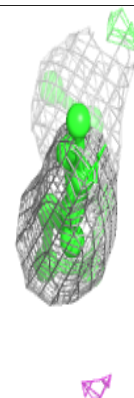
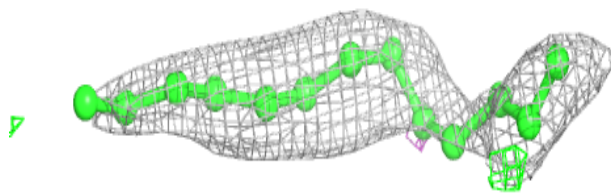
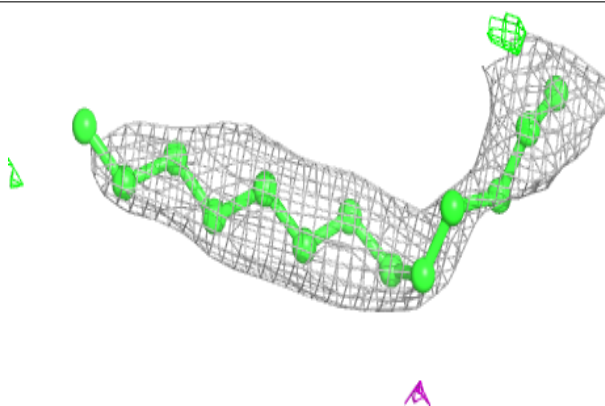


Electron density around LFA B 316:

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

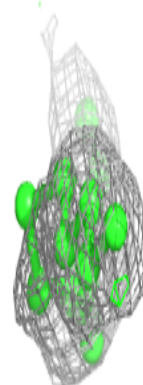
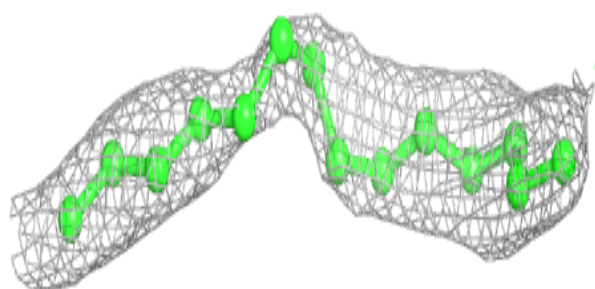
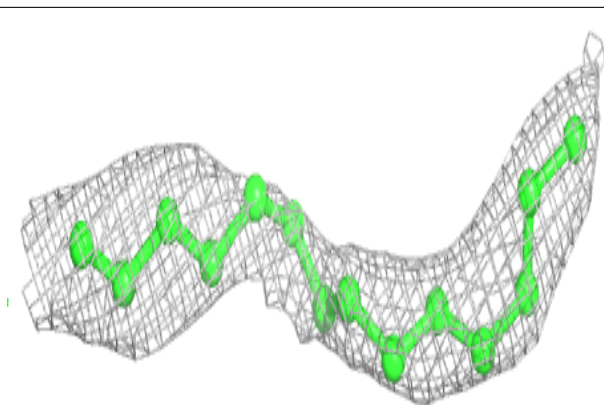
**Electron density around LFA A 807:**

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

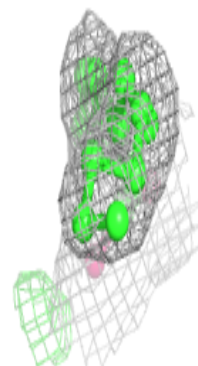
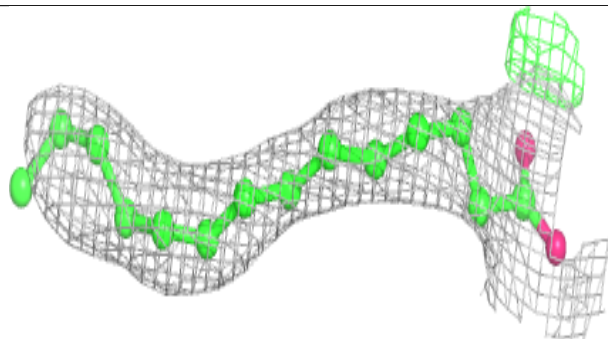
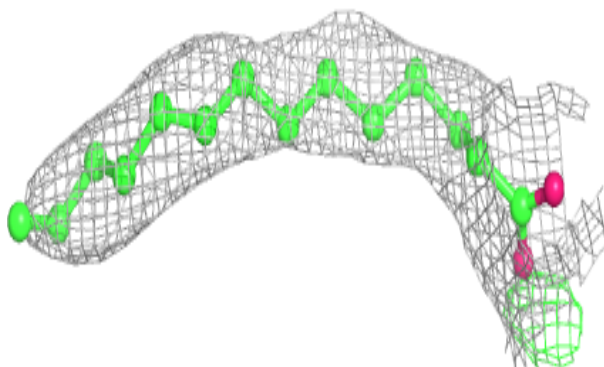


Electron density around LFA A 810:

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

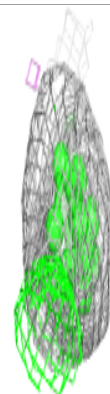
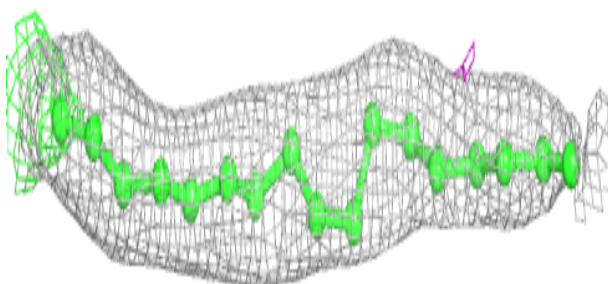
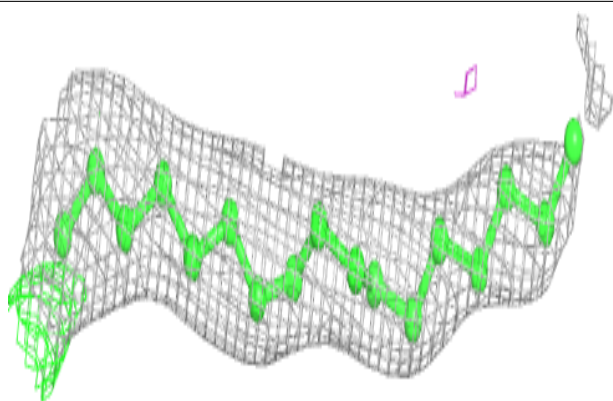
**Electron density around OLA A 804:**

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

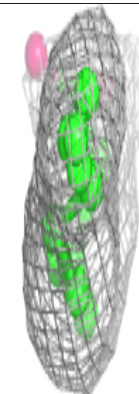
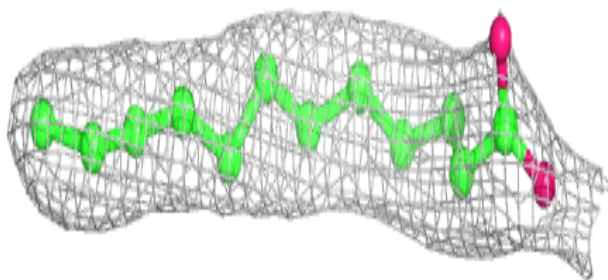
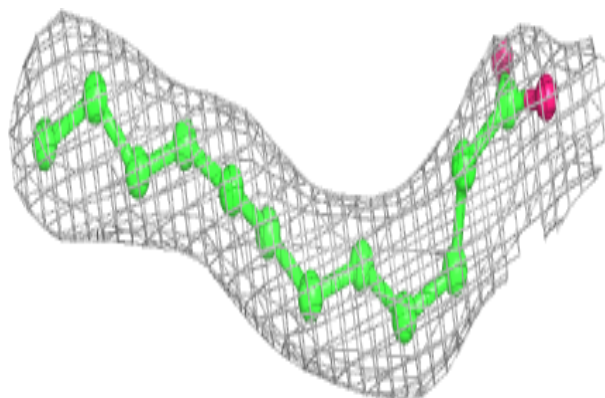


Electron density around LFA C 301:

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

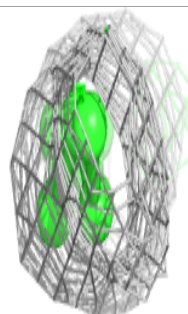
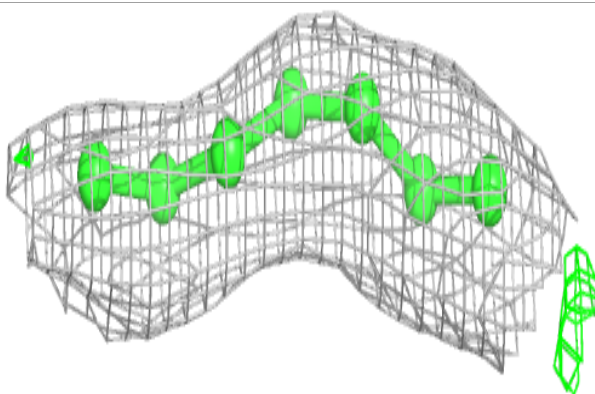
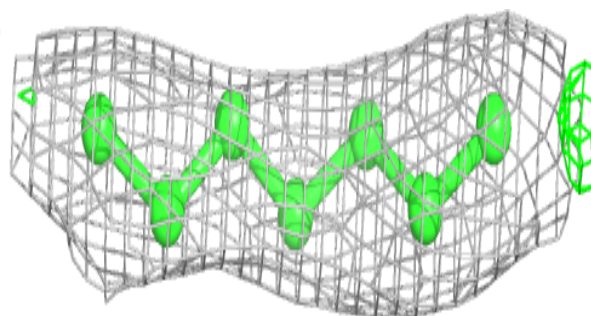
**Electron density around OLA C 302:**

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

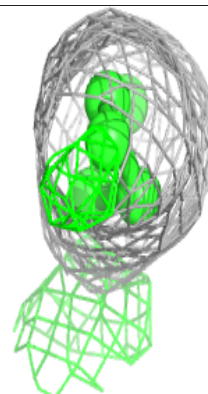
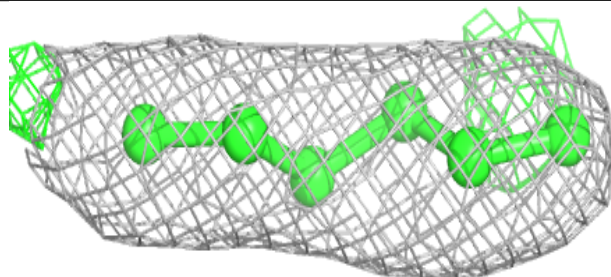
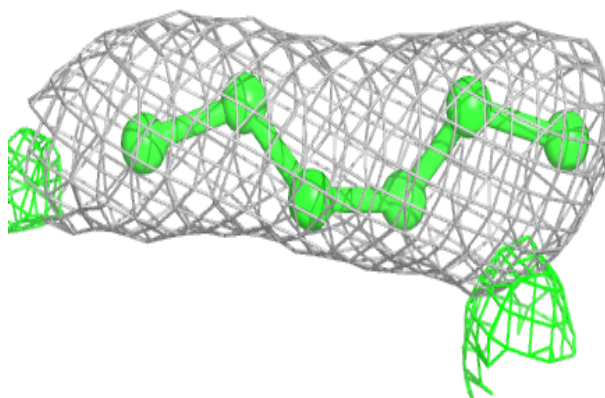


Electron density around LFA B 313:

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

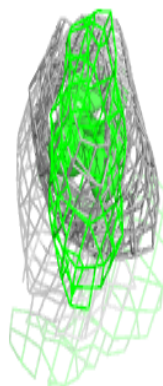
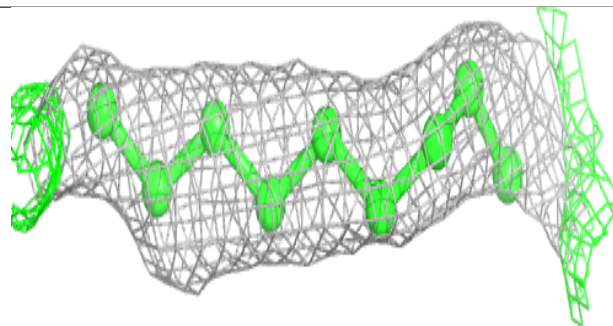
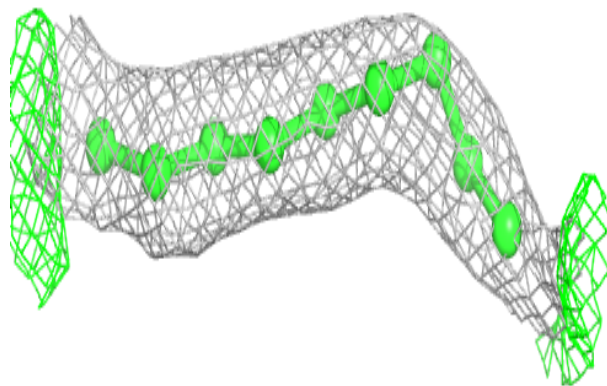
**Electron density around LFA C 316:**

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

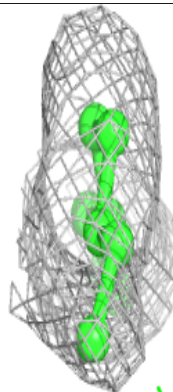
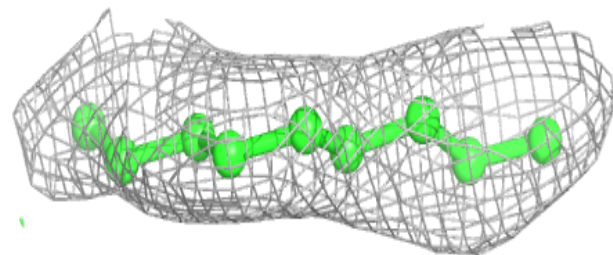
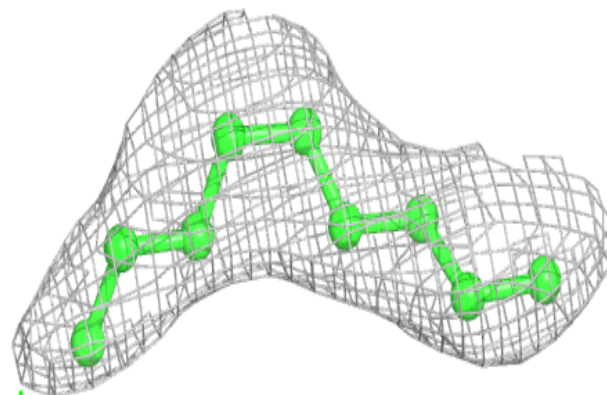


Electron density around LFA C 317:

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

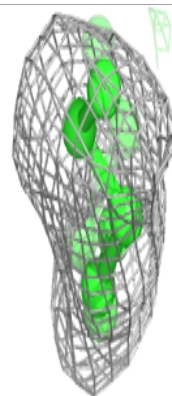
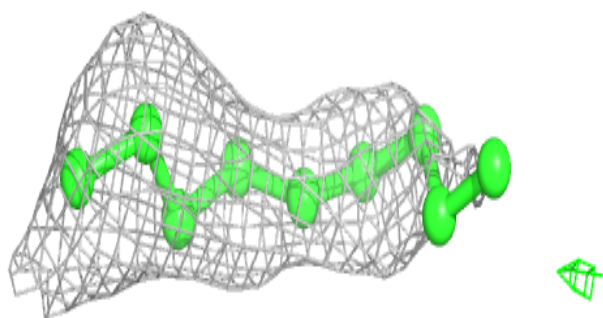
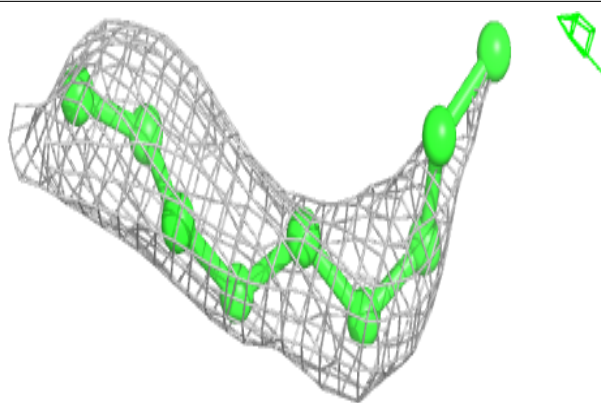
**Electron density around LFA C 318:**

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

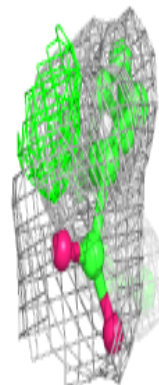
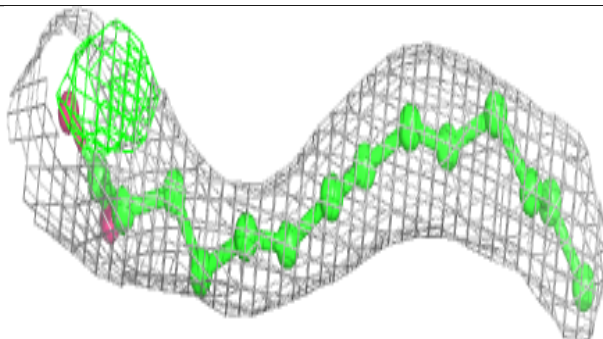
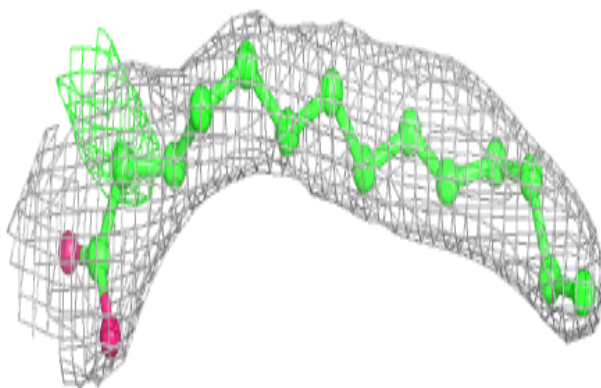


Electron density around LFA A 811:

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

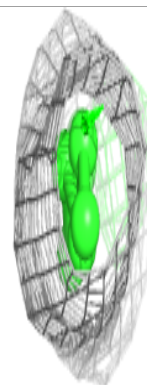
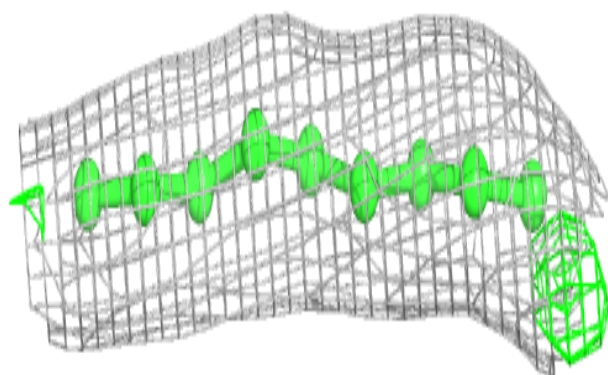
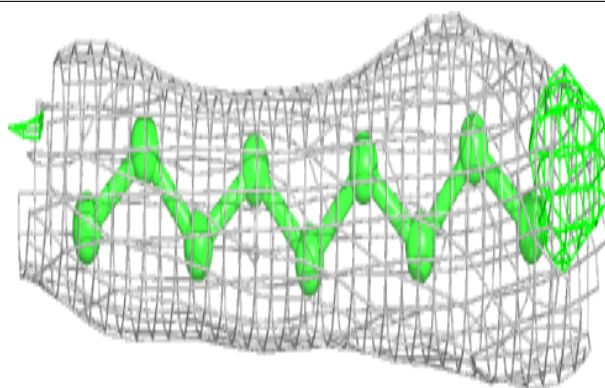
**Electron density around OLA C 305:**

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

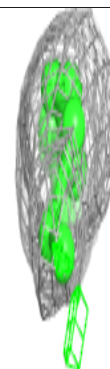
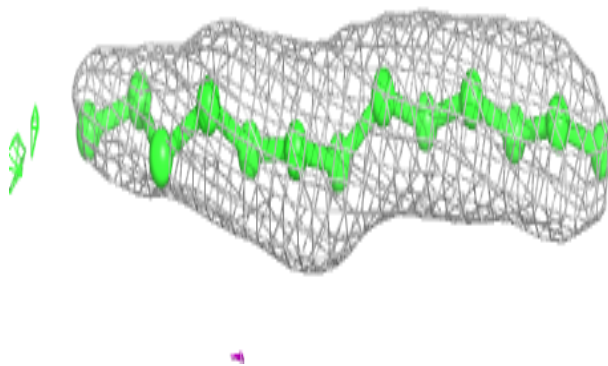
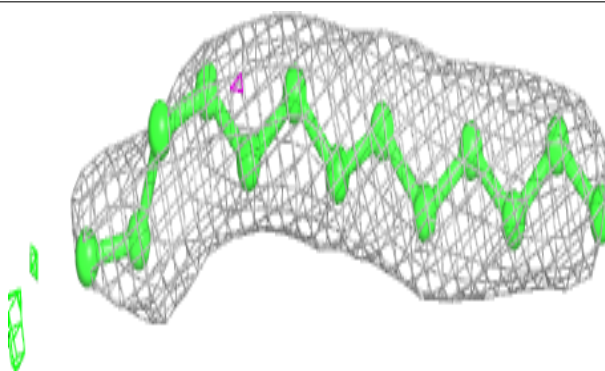


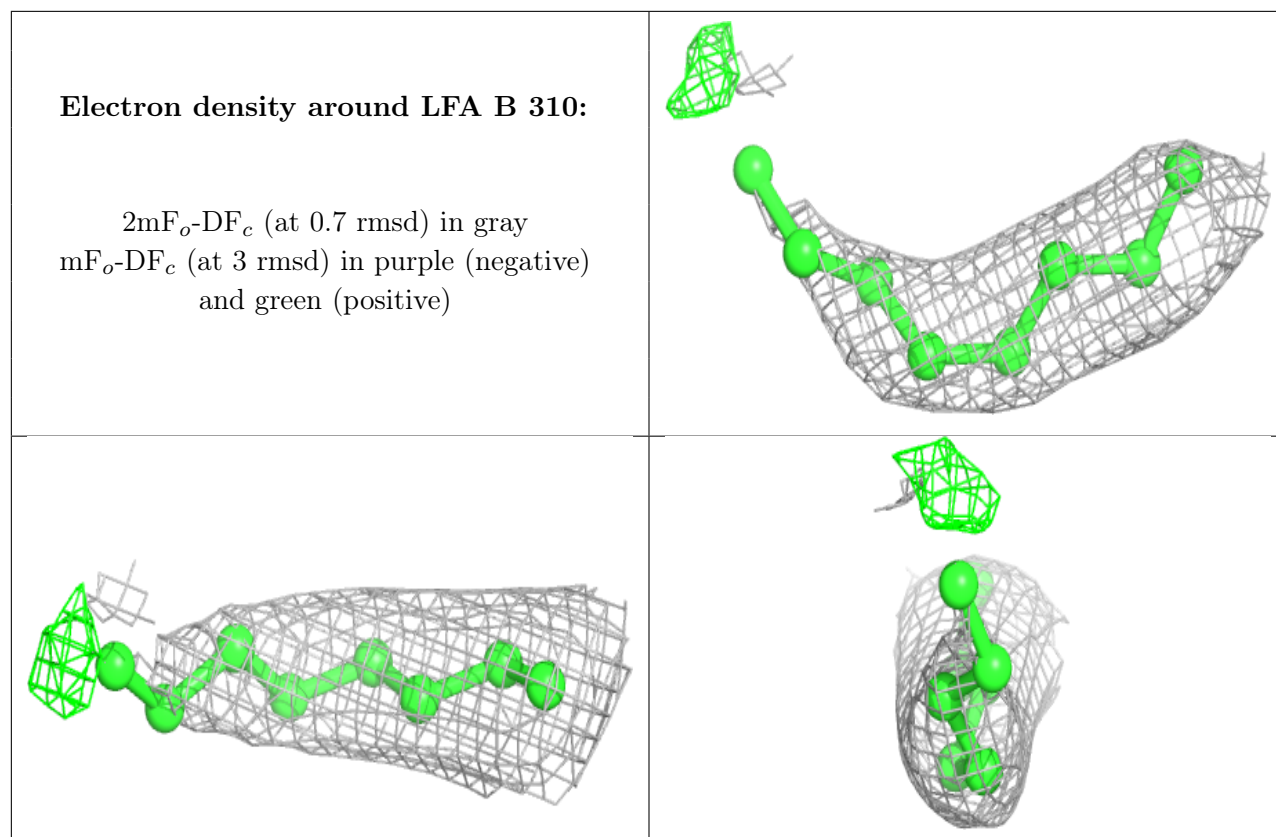
Electron density around LFA C 307:

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

**Electron density around LFA A 808:**

$2mF_o-DF_c$ (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.