Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2023 – 01:57 am BST

PDB ID	:	7ZN9
Title	:	Crystal structure of the light-driven inward proton pump xenorhodopsin BcXeR in the M state at pH 7.0 in the presence of sodium at 100K
Authors	:	Kovalev, K.; Tsybrov, F.; Alekseev, A.; Bourenkov, G.; Gordeliy, V.
Deposited on	:	2022-04-20
Resolution	:	2.30 Å(reported)

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

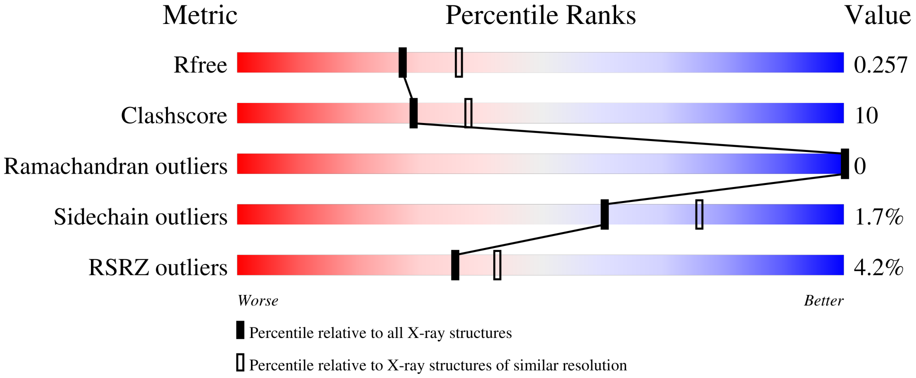
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

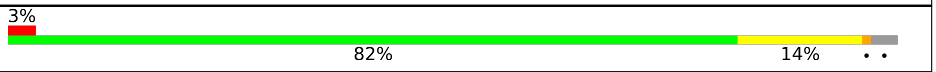
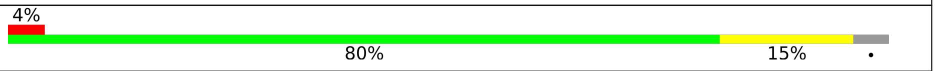
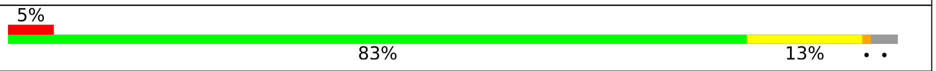
The reported resolution of this entry is 2.30 Å.

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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
2	LFA	A	516	-	-	-	X
2	LFA	B	323	-	-	-	X
2	LFA	C	312	-	-	-	X
2	LFA	C	317	-	-	-	X

2 Entry composition

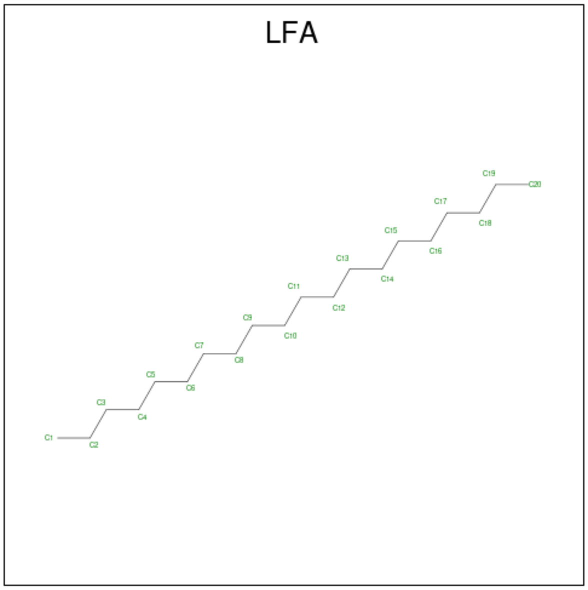
There are 5 unique types of molecules in this entry. The entry contains 6281 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called xenorhodopsin.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	223	Total C N O S 1810 1235 273 295 7	0	6	0
1	B	220	Total C N O S 1785 1215 271 292 7	0	6	0
1	C	223	Total C N O S 1807 1234 270 296 7	0	6	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 6 6	0	0
2	A	1	Total C 7 7	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 9 9	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 7 7	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 5 5	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 6 6	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 6 6	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 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 8 8	0	0

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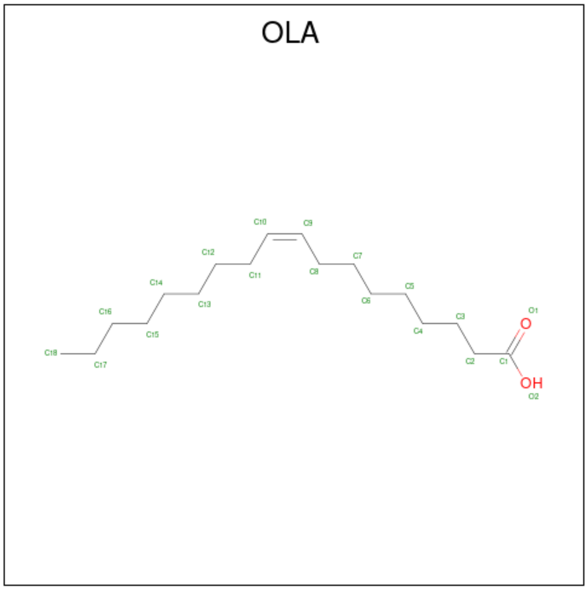
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 16 16	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C 13 13	0	0
2	C	1	Total C 17 17	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 11 11	0	0
2	C	1	Total C 4 4	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 4 4	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 16 16	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 9 9	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 11 11	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 11 9 2	0	0
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 19 17 2	0	0
3	A	1	Total C O 13 11 2	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C O 17 15 2	0	0
3	B	1	Total C O 16 14 2	0	0
3	B	1	Total C O 19 17 2	0	0
3	C	1	Total C O 16 14 2	0	0
3	C	1	Total C O 16 14 2	0	0

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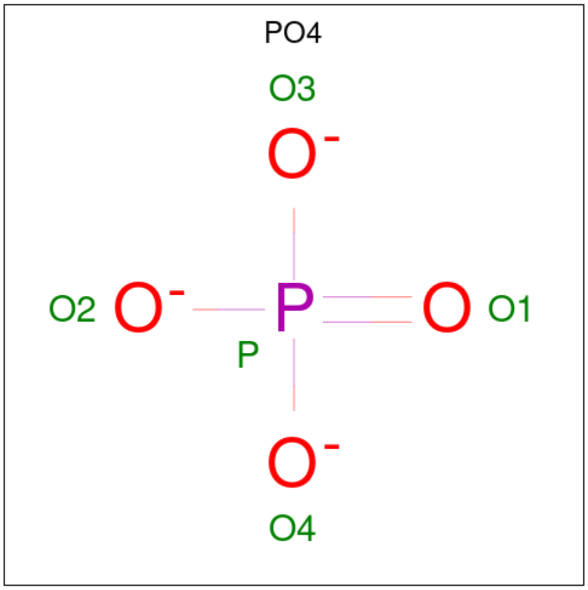
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 13 11 2	0	0
3	C	1	Total C O 15 13 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is water.

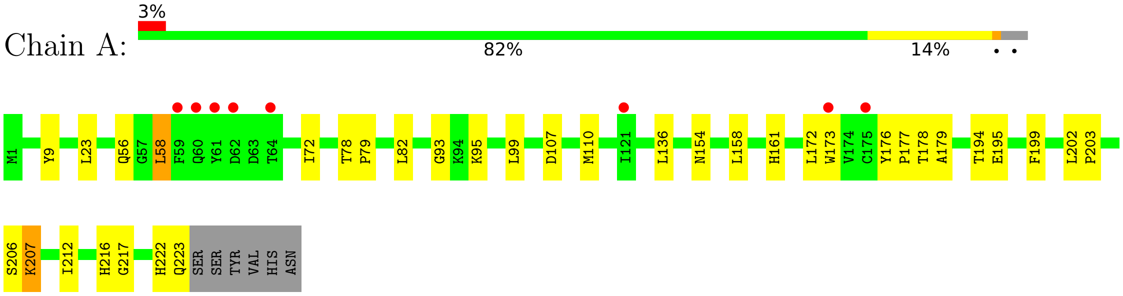
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	80	Total O 80 80	0	2
5	B	81	Total O 81 81	0	3
5	C	82	Total O 82 82	0	1

3 Residue-property plots ⓘ

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.

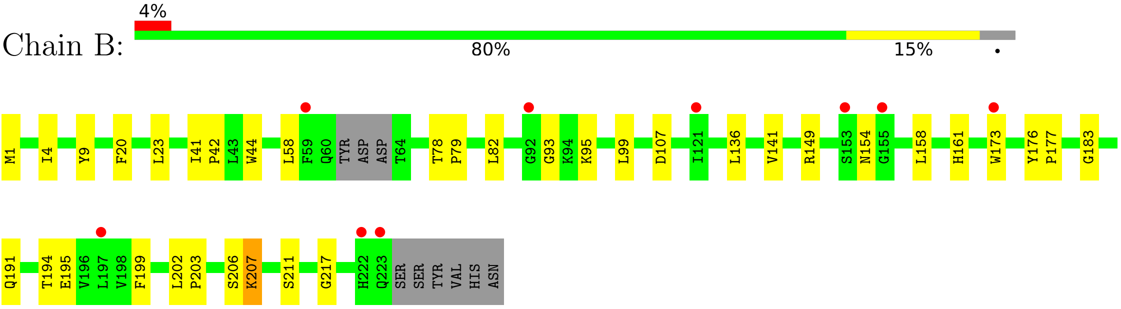
- Molecule 1: xenorhodopsin

Chain A:



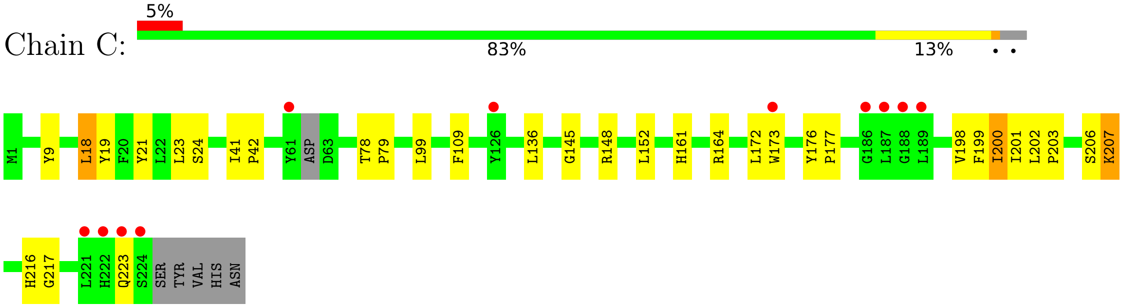
- Molecule 1: xenorhodopsin

Chain B:



- Molecule 1: xenorhodopsin

Chain C:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.90Å 109.50Å 119.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 49.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.4 (20.00-2.30) 93.6 (49.77-2.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.214 , 0.253 0.219 , 0.257	Depositor DCC
R_{free} test set	1897 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.4	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6281	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.64	0/1817	0.63	0/2480
1	B	0.64	0/1791	0.62	0/2444
1	C	0.64	0/1814	0.63	0/2476
All	All	0.64	0/5422	0.63	0/7400

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 ⓘ

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	1810	0	1889	45	0
1	B	1785	0	1865	33	0
1	C	1807	0	1886	30	0
2	A	99	0	181	10	0
2	B	159	0	292	6	0
2	C	130	0	241	7	0
3	A	88	0	123	10	0
3	B	90	0	125	6	0
3	C	60	0	80	5	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	5	0	0	0	0
5	A	80	0	0	2	0
5	B	81	0	0	2	0
5	C	82	0	0	1	0
All	All	6281	0	6682	122	0

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

All (122) 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:B:207:LYR:H192	1:B:207:LYR:H9	1.66	0.78
1:C:161:HIS:CE1	1:C:217:GLY:HA3	2.23	0.73
1:A:161:HIS:CE1	1:A:217:GLY:HA3	2.23	0.73
1:A:202:LEU:HB2	1:A:203:PRO:HD3	1.71	0.73
1:A:56:GLN:HB3	3:A:505:OLA:H51	1.71	0.72
2:A:519:LFA:H202	2:B:314:LFA:H132	1.70	0.72
1:B:161:HIS:CE1	1:B:217:GLY:HA3	2.25	0.72
1:C:148:ARG:O	1:C:152:LEU:HD23	1.90	0.71
1:C:207:LYR:H192	1:C:207:LYR:H9	1.73	0.71
1:B:183:GLY:HA3	1:B:195[A]:GLU:OE2	1.91	0.70
1:A:207:LYR:H192	1:A:207:LYR:H9	1.72	0.69
1:C:202:LEU:HB2	1:C:203:PRO:HD3	1.74	0.68
1:A:58:LEU:HD22	1:A:58:LEU:C	2.16	0.65
3:C:305:OLA:C3	2:C:309:LFA:H203	2.27	0.65
3:B:304:OLA:H41	2:B:319:LFA:H21	1.79	0.65
1:B:207:LYR:H192	1:B:207:LYR:C9	2.26	0.64
3:A:503:OLA:H72	2:A:512:LFA:H72	1.78	0.64
1:B:202:LEU:HB2	1:B:203:PRO:HD3	1.78	0.64
1:A:207:LYR:H192	1:A:207:LYR:C9	2.29	0.63
1:C:207:LYR:H192	1:C:207:LYR:C9	2.29	0.62
1:A:93:GLY:HA3	1:A:154:ASN:HD21	1.66	0.60
3:B:308:OLA:H121	1:C:109:PHE:HB2	1.83	0.60
1:C:78:THR:N	1:C:79:PRO:HD2	2.17	0.60
1:C:18[A]:LEU:HD12	2:C:312:LFA:H72	1.82	0.59
1:A:203:PRO:HA	1:A:206[A]:SER:OG	2.04	0.57
1:A:78:THR:N	1:A:79:PRO:HD2	2.19	0.57
1:B:78:THR:N	1:B:79:PRO:HD2	2.19	0.57
1:C:99[B]:LEU:C	1:C:99[B]:LEU:HD23	2.25	0.56
1:C:207:LYR:H9	1:C:207:LYR:H183	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:305:OLA:H31	2:C:309:LFA:H203	1.85	0.56
1:C:203:PRO:HA	1:C:206[A]:SER:OG	2.06	0.56
1:C:145:GLY:HA3	3:C:305:OLA:H22	1.89	0.55
1:B:203:PRO:HA	1:B:206[A]:SER:OG	2.06	0.55
1:A:99[B]:LEU:C	1:A:99[B]:LEU:HD23	2.27	0.55
1:C:172:LEU:HD13	1:C:206[B]:SER:OG	2.07	0.55
1:C:9:TYR:HE1	1:C:203:PRO:HB2	1.72	0.54
1:A:99[B]:LEU:HD23	1:A:99[B]:LEU:O	2.08	0.54
1:C:9:TYR:CE1	1:C:203:PRO:HB2	2.44	0.53
1:A:212:ILE:HG21	3:A:508:OLA:H41	1.91	0.52
1:A:58:LEU:HD22	1:A:58:LEU:O	2.10	0.52
1:A:173[B]:TRP:CZ3	1:A:207:LYR:H43	2.43	0.52
1:A:207:LYR:H9	1:A:207:LYR:H183	1.92	0.52
3:C:305:OLA:H32	2:C:309:LFA:H203	1.92	0.52
3:B:305:OLA:H51	2:B:323:LFA:H151	1.93	0.51
1:B:93:GLY:HA3	1:B:154:ASN:HD21	1.76	0.50
3:A:505:OLA:H61	2:A:513:LFA:H51	1.94	0.49
1:C:19:TYR:OH	1:C:216:HIS:CE1	2.65	0.49
1:C:136[B]:LEU:C	1:C:136[B]:LEU:HD23	2.33	0.49
1:B:1:FME:O1	1:B:4:ILE:HG12	2.12	0.49
3:A:504:OLA:H9	2:C:301:LFA:H122	1.94	0.49
2:C:311:LFA:H72	2:C:316:LFA:C19	2.42	0.49
1:C:145:GLY:CA	3:C:305:OLA:H22	2.41	0.49
1:B:207:LYR:H9	1:B:207:LYR:H183	1.95	0.49
1:B:9:TYR:CE1	1:B:203:PRO:HB2	2.47	0.48
1:A:9:TYR:HE1	1:A:203:PRO:HB2	1.78	0.48
1:A:136[B]:LEU:C	1:A:136[B]:LEU:HD23	2.34	0.48
1:A:58:LEU:N	1:A:58:LEU:HD13	2.27	0.48
1:A:222:HIS:C	1:A:223:GLN:N	2.67	0.48
1:C:99[B]:LEU:HD23	1:C:99[B]:LEU:O	2.14	0.48
2:B:321:LFA:C10	2:B:323:LFA:C8	2.92	0.48
1:A:194:THR:HG21	3:A:506:OLA:H31	1.96	0.48
1:B:194:THR:HG21	3:B:305:OLA:H31	1.96	0.48
1:A:9:TYR:CE1	1:A:203:PRO:HB2	2.49	0.48
3:A:503:OLA:H72	2:A:512:LFA:C7	2.43	0.48
1:B:9:TYR:HE1	1:B:203:PRO:HB2	1.78	0.47
1:B:44:TRP:CE3	3:B:308:OLA:H152	2.50	0.47
1:A:58:LEU:HD13	1:A:58:LEU:H	1.80	0.47
1:A:212:ILE:HG22	3:A:508:OLA:H21	1.96	0.47
1:B:154:ASN:ND2	5:B:405:HOH:O	2.47	0.47
1:B:82:LEU:HD12	1:B:107:ASP:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136[B]:LEU:C	1:B:136[B]:LEU:HD23	2.35	0.46
1:B:173[B]:TRP:CZ3	1:B:207:LYR:H43	2.50	0.46
1:A:176:TYR:N	1:A:177:PRO:HD2	2.31	0.46
1:A:173[B]:TRP:CZ3	1:A:207:LYR:C4	2.98	0.46
1:A:95:LYS:HE2	3:A:507:OLA:C1	2.45	0.46
1:A:107:ASP:OD1	1:A:173[B]:TRP:HZ2	1.99	0.46
1:B:195[A]:GLU:HB2	2:B:321:LFA:H11	1.96	0.46
1:A:202:LEU:CB	1:A:203:PRO:HD3	2.44	0.46
1:B:141:VAL:HA	3:B:303:OLA:H41	1.98	0.46
1:C:207:LYR:H6	1:C:207:LYR:H41	1.81	0.46
1:A:199:PHE:O	1:A:203:PRO:HG2	2.16	0.45
1:A:72:ILE:HG13	2:A:518:LFA:H42	1.98	0.45
1:B:207:LYR:H6	1:B:207:LYR:H41	1.82	0.45
1:B:199:PHE:O	1:B:203:PRO:HG2	2.17	0.45
1:C:199:PHE:O	1:C:203:PRO:HG2	2.16	0.45
1:A:207:LYR:C	5:A:608:HOH:O	2.65	0.45
1:B:176:TYR:N	1:B:177:PRO:HD2	2.32	0.45
1:A:179:ALA:O	2:A:517:LFA:H13	2.17	0.44
3:A:508:OLA:H81	3:A:508:OLA:H51	1.88	0.44
1:A:82:LEU:HG	5:A:603[A]:HOH:O	2.17	0.44
1:B:20:PHE:CZ	1:B:211:SER:HB2	2.54	0.43
1:B:82:LEU:HD21	1:B:173[A]:TRP:CZ2	2.54	0.43
1:B:173[B]:TRP:CZ3	1:B:207:LYR:C4	3.02	0.43
1:C:200:ILE:HG22	1:C:201:ILE:HG13	2.00	0.43
1:A:107:ASP:O	1:A:110:MET:HB3	2.19	0.42
1:B:95:LYS:NZ	5:B:412:HOH:O	2.52	0.42
1:C:19:TYR:HH	1:C:216:HIS:CE1	2.36	0.42
1:A:172:LEU:HD13	1:A:206[B]:SER:OG	2.19	0.42
1:A:178:THR:HG21	2:A:515:LFA:H12	2.01	0.42
1:A:212:ILE:HG23	1:A:216:HIS:CE1	2.55	0.42
1:A:207:LYR:H6	1:A:207:LYR:H41	1.82	0.42
1:B:99[B]:LEU:HD23	1:B:99[B]:LEU:C	2.40	0.42
1:B:158:LEU:C	1:B:158:LEU:HD13	2.40	0.42
1:A:207:LYR:H10	1:A:207:LYR:H81	1.88	0.42
1:C:41:ILE:HB	1:C:42:PRO:CD	2.50	0.41
1:A:82:LEU:HD21	1:A:173[A]:TRP:CZ2	2.55	0.41
1:B:41:ILE:HB	1:B:42:PRO:CD	2.51	0.41
1:B:107:ASP:OD1	1:B:173[B]:TRP:HZ2	2.03	0.41
1:C:21:TYR:O	1:C:24:SER:OG	2.33	0.41
1:C:173[A]:TRP:O	1:C:177:PRO:HD2	2.20	0.41
1:A:195:GLU:HG3	2:A:517:LFA:H11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:519:LFA:C20	2:B:314:LFA:H132	2.46	0.41
1:B:207:LYR:H10	1:B:207:LYR:H81	1.91	0.41
1:A:178:THR:HG21	2:A:515:LFA:C1	2.51	0.41
1:B:58:LEU:N	1:B:58:LEU:HD23	2.35	0.41
1:C:41:ILE:HB	1:C:42:PRO:HD3	2.03	0.41
1:A:158:LEU:HD13	1:A:158:LEU:C	2.41	0.41
1:C:176:TYR:N	1:C:177:PRO:HD2	2.36	0.41
1:C:198:VAL:HG21	2:C:310:LFA:H32	2.02	0.41
1:C:164:ARG:HD3	5:C:472:HOH:O	2.21	0.40
1:A:82:LEU:HD12	1:A:107:ASP:HB2	2.02	0.40
1:A:58:LEU:N	1:A:58:LEU:CD1	2.84	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	225/229 (98%)	224 (100%)	1 (0%)	0	100	100
1	B	221/229 (96%)	220 (100%)	1 (0%)	0	100	100
1	C	224/229 (98%)	222 (99%)	2 (1%)	0	100	100
All	All	670/687 (98%)	666 (99%)	4 (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%)	181 (99%)	2 (1%)	73	86
1	B	182/189 (96%)	179 (98%)	3 (2%)	62	78
1	C	183/189 (97%)	178 (97%)	5 (3%)	44	61
All	All	548/567 (97%)	538 (98%)	10 (2%)	60	75

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	58	LEU
1	B	23	LEU
1	B	149	ARG
1	B	191	GLN
1	C	18[A]	LEU
1	C	18[B]	LEU
1	C	23	LEU
1	C	200	ILE
1	C	223	GLN

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

Mol	Chain	Res	Type
1	A	154	ASN
1	A	191	GLN
1	B	154	ASN
1	B	191	GLN
1	C	223	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	**Type**	**Chain**	**Res**	**Link**	**Bond lengths**			**Bond angles**		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
1	FME	C	1	1	8,9,10	0.42	0	7,9,11	0.74	0
1	FME	A	1	1	8,9,10	0.39	0	7,9,11	0.68	0
1	FME	B	1	1	8,9,10	0.38	0	7,9,11	0.71	0
1	LYR	B	207	1	27,29,30	1.30	2 (7%)	30,37,39	1.21	3 (10%)
1	LYR	A	207	1	27,29,30	1.32	3 (11%)	30,37,39	1.23	2 (6%)
1	LYR	C	207	1	27,29,30	1.29	2 (7%)	30,37,39	1.15	2 (6%)

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

All (7) bond length outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(Å)**	**Ideal(Å)**
1	B	207	LYR	C7-C80	4.60	1.41	1.35
1	A	207	LYR	C7-C80	4.45	1.41	1.35
1	C	207	LYR	C7-C80	4.42	1.41	1.35
1	C	207	LYR	C9-C80	-2.54	1.40	1.45
1	B	207	LYR	C9-C80	-2.33	1.40	1.45
1	A	207	LYR	C9-C80	-2.15	1.41	1.45
1	A	207	LYR	C4-C3	-2.13	1.46	1.50

All (7) bond angle outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(^{o})**	**Ideal(^{o})**
1	A	207	LYR	C8-C80-C7	-4.39	116.77	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	LYR	C8-C80-C7	-4.31	116.89	122.92
1	C	207	LYR	C8-C80-C7	-4.12	117.15	122.92
1	A	207	LYR	C9-C80-C7	2.99	123.53	118.94
1	B	207	LYR	C9-C80-C7	2.80	123.24	118.94
1	C	207	LYR	C9-C80-C7	2.73	123.13	118.94
1	B	207	LYR	C7-C6-C5	2.29	130.37	123.22

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1	FME	1	0
1	B	207	LYR	7	0
1	A	207	LYR	8	0
1	C	207	LYR	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

62 ligands are modelled in this entry.

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

Mol	**Type**	**Chain**	**Res**	**Link**	**Bond lengths**			**Bond angles**		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	LFA	B	317	-	15,15,19	0.08	0	14,14,18	0.06	0
2	LFA	A	501	-	5,5,19	0.13	0	4,4,18	0.11	0
2	LFA	C	312	-	15,15,19	0.10	0	14,14,18	0.05	0
3	OLA	C	303	-	15,15,19	0.59	0	15,15,19	0.53	0
2	LFA	C	309	-	7,7,19	0.11	0	6,6,18	0.07	0
2	LFA	A	511	-	6,6,19	0.13	0	5,5,18	0.13	0
2	LFA	B	316	-	7,7,19	0.12	0	6,6,18	0.07	0
2	LFA	C	311	-	7,7,19	0.11	0	6,6,18	0.08	0
3	OLA	B	305	-	9,9,19	0.29	0	8,8,19	0.17	0
2	LFA	B	310	-	6,6,19	0.12	0	5,5,18	0.08	0
4	PO4	A	521	-	4,4,4	0.66	0	6,6,6	0.43	0
2	LFA	A	513	-	6,6,19	0.14	0	5,5,18	0.07	0
2	LFA	B	311	-	4,4,19	0.13	0	3,3,18	0.25	0
2	LFA	B	309	-	5,5,19	0.14	0	4,4,18	0.10	0
2	LFA	A	520	-	5,5,19	0.11	0	4,4,18	0.11	0
2	LFA	A	510	-	8,8,19	0.11	0	7,7,18	0.09	0
2	LFA	A	512	-	11,11,19	0.09	0	10,10,18	0.06	0
2	LFA	C	308	-	3,3,19	0.24	0	2,2,18	0.44	0
2	LFA	B	313	-	5,5,19	0.13	0	4,4,18	0.14	0
2	LFA	A	518	-	6,6,19	0.11	0	5,5,18	0.08	0
3	OLA	A	503	-	10,10,19	0.68	0	10,10,19	0.64	0
3	OLA	B	307	-	15,15,19	0.59	0	15,15,19	0.53	0
3	OLA	C	302	-	15,15,19	0.57	0	15,15,19	0.53	0
2	LFA	B	323	-	12,12,19	0.08	0	11,11,18	0.06	0
2	LFA	C	317	-	10,10,19	0.10	0	9,9,18	0.08	0
2	LFA	C	314	-	9,9,19	0.10	0	8,8,18	0.07	0
3	OLA	B	306	-	16,16,19	0.58	0	16,16,19	0.51	0
2	LFA	B	302	-	8,8,19	0.10	0	7,7,18	0.08	0
2	LFA	B	312	-	4,4,19	0.14	0	3,3,18	0.23	0
2	LFA	C	301	-	16,16,19	0.08	0	15,15,18	0.06	0
2	LFA	A	516	-	2,2,19	0.07	0	0,1,18	-	-
2	LFA	A	519	-	6,6,19	0.12	0	5,5,18	0.09	0
2	LFA	B	321	-	9,9,19	0.10	0	8,8,18	0.08	0
2	LFA	C	306	-	9,9,19	0.10	0	8,8,18	0.07	0
2	LFA	A	514	-	7,7,19	0.11	0	6,6,18	0.07	0
2	LFA	A	509	-	8,8,19	0.11	0	7,7,18	0.09	0
2	LFA	A	517	-	4,4,19	0.14	0	3,3,18	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	OLA	A	508	-	12,12,19	0.63	0	12,12,19	0.60	0
2	LFA	B	318	-	11,11,19	0.10	0	10,10,18	0.06	0
3	OLA	B	303	-	13,13,19	0.62	0	12,13,19	0.58	0
2	LFA	B	314	-	14,14,19	0.09	0	13,13,18	0.06	0
3	OLA	A	506	-	10,10,19	0.64	0	10,10,19	0.67	0
3	OLA	A	507	-	18,18,19	0.53	0	18,18,19	0.48	0
2	LFA	B	301	-	5,5,19	0.14	0	4,4,18	0.11	0
3	OLA	C	304	-	12,12,19	0.62	0	12,12,19	0.63	0
4	PO4	C	318	-	4,4,4	0.65	0	6,6,6	0.43	0
2	LFA	C	313	-	11,11,19	0.10	0	10,10,18	0.06	0
2	LFA	C	315	-	8,8,19	0.11	0	7,7,18	0.12	0
2	LFA	A	515	-	5,5,19	0.13	0	4,4,18	0.10	0
3	OLA	A	505	-	13,13,19	0.61	0	12,13,19	0.59	0
2	LFA	B	322	-	11,11,19	0.09	0	10,10,18	0.06	0
2	LFA	A	502	-	6,6,19	0.13	0	5,5,18	0.10	0
2	LFA	C	307	-	10,10,19	0.10	0	9,9,18	0.08	0
3	OLA	B	304	-	13,13,19	0.60	0	12,13,19	0.63	0
2	LFA	B	319	-	8,8,19	0.11	0	7,7,18	0.08	0
2	LFA	C	316	-	9,9,19	0.09	0	8,8,18	0.08	0
2	LFA	C	310	-	3,3,19	0.24	0	2,2,18	0.44	0
3	OLA	B	308	-	18,18,19	0.54	0	18,18,19	0.51	0
3	OLA	C	305	-	14,14,19	0.60	0	14,14,19	0.53	0
2	LFA	B	320	-	11,11,19	0.09	0	10,10,18	0.06	0
2	LFA	B	315	-	7,7,19	0.11	0	6,6,18	0.10	0
3	OLA	A	504	-	19,19,19	0.50	0	19,19,19	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	B	317	-	-	1/13/13/17	-
2	LFA	A	501	-	-	2/3/3/17	-
2	LFA	C	312	-	-	1/13/13/17	-
3	OLA	C	303	-	-	9/13/13/17	-
2	LFA	C	309	-	-	0/5/5/17	-
2	LFA	A	511	-	-	0/4/4/17	-
2	LFA	B	316	-	-	1/5/5/17	-
2	LFA	C	311	-	-	3/5/5/17	-
3	OLA	B	305	-	-	1/7/7/17	-
2	LFA	B	310	-	-	1/4/4/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	A	513	-	-	1/4/4/17	-
2	LFA	B	311	-	-	0/2/2/17	-
2	LFA	B	309	-	-	2/3/3/17	-
2	LFA	A	520	-	-	2/3/3/17	-
2	LFA	A	510	-	-	5/6/6/17	-
2	LFA	A	512	-	-	8/9/9/17	-
2	LFA	C	308	-	-	0/1/1/17	-
2	LFA	B	313	-	-	2/3/3/17	-
2	LFA	A	518	-	-	0/4/4/17	-
3	OLA	A	503	-	-	3/8/8/17	-
3	OLA	B	307	-	-	4/13/13/17	-
3	OLA	C	302	-	-	8/13/13/17	-
2	LFA	B	323	-	-	0/10/10/17	-
2	LFA	C	317	-	-	2/8/8/17	-
2	LFA	C	314	-	-	5/7/7/17	-
3	OLA	B	306	-	-	5/14/14/17	-
2	LFA	B	302	-	-	1/6/6/17	-
2	LFA	B	312	-	-	1/2/2/17	-
2	LFA	C	301	-	-	10/14/14/17	-
2	LFA	A	519	-	-	2/4/4/17	-
2	LFA	B	321	-	-	2/7/7/17	-
2	LFA	C	306	-	-	3/7/7/17	-
2	LFA	A	514	-	-	0/5/5/17	-
2	LFA	A	509	-	-	1/6/6/17	-
2	LFA	A	517	-	-	2/2/2/17	-
3	OLA	A	508	-	-	3/10/10/17	-
2	LFA	B	318	-	-	2/9/9/17	-
3	OLA	B	303	-	-	6/11/11/17	-
2	LFA	B	314	-	-	5/12/12/17	-
3	OLA	A	506	-	-	3/8/8/17	-
3	OLA	A	507	-	-	6/16/16/17	-
2	LFA	B	301	-	-	2/3/3/17	-
3	OLA	C	304	-	-	6/10/10/17	-
2	LFA	C	313	-	-	4/9/9/17	-
2	LFA	C	315	-	-	1/6/6/17	-
2	LFA	A	515	-	-	1/3/3/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLA	A	505	-	-	5/11/11/17	-
2	LFA	B	322	-	-	1/9/9/17	-
2	LFA	A	502	-	-	0/4/4/17	-
2	LFA	C	307	-	-	1/8/8/17	-
3	OLA	B	304	-	-	3/11/11/17	-
2	LFA	B	319	-	-	0/6/6/17	-
2	LFA	C	316	-	-	0/7/7/17	-
2	LFA	C	310	-	-	0/1/1/17	-
3	OLA	B	308	-	-	9/16/16/17	-
3	OLA	C	305	-	-	7/12/12/17	-
2	LFA	B	320	-	-	1/9/9/17	-
2	LFA	B	315	-	-	0/5/5/17	-
3	OLA	A	504	-	-	11/17/17/17	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (165) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	505	OLA	C9-C10-C11-C12
3	B	307	OLA	C11-C10-C9-C8
3	C	302	OLA	C11-C10-C9-C8
3	A	508	OLA	C5-C6-C7-C8
3	B	306	OLA	C11-C10-C9-C8
3	B	304	OLA	C1-C2-C3-C4
2	C	313	LFA	C11-C10-C9-C8
3	C	304	OLA	C3-C4-C5-C6
3	C	305	OLA	C1-C2-C3-C4
2	B	314	LFA	C9-C10-C11-C12
3	A	508	OLA	C4-C5-C6-C7
3	B	303	OLA	C11-C10-C9-C8
2	C	301	LFA	C11-C12-C13-C14
3	C	303	OLA	C5-C6-C7-C8
3	A	507	OLA	C11-C12-C13-C14
3	B	308	OLA	C11-C12-C13-C14
2	A	510	LFA	C2-C3-C4-C5
2	B	310	LFA	C3-C4-C5-C6
2	B	314	LFA	C4-C5-C6-C7
2	C	314	LFA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	C	314	LFA	C5-C6-C7-C8
2	A	512	LFA	C6-C7-C8-C9
2	C	301	LFA	C13-C14-C15-C16
3	C	304	OLA	C4-C5-C6-C7
3	C	302	OLA	C10-C11-C12-C13
2	A	512	LFA	C4-C5-C6-C7
2	C	301	LFA	C7-C8-C9-C10
2	B	320	LFA	C13-C14-C15-C16
2	C	301	LFA	C10-C11-C12-C13
2	A	512	LFA	C7-C8-C9-C10
2	A	510	LFA	C5-C6-C7-C8
3	B	303	OLA	C3-C4-C5-C6
2	C	317	LFA	C3-C4-C5-C6
2	C	314	LFA	C6-C7-C8-C9
3	C	303	OLA	C4-C5-C6-C7
3	A	508	OLA	C11-C10-C9-C8
3	A	504	OLA	C13-C14-C15-C16
3	A	504	OLA	C10-C11-C12-C13
3	C	304	OLA	C6-C7-C8-C9
3	C	303	OLA	C3-C4-C5-C6
2	B	322	LFA	C11-C10-C9-C8
2	B	314	LFA	C11-C10-C9-C8
2	C	313	LFA	C5-C6-C7-C8
3	C	305	OLA	C11-C10-C9-C8
2	A	513	LFA	C3-C4-C5-C6
2	B	321	LFA	C2-C3-C4-C5
2	B	321	LFA	C6-C7-C8-C9
2	B	314	LFA	C11-C12-C13-C14
3	B	308	OLA	C6-C7-C8-C9
2	C	301	LFA	C6-C7-C8-C9
2	A	512	LFA	C5-C6-C7-C8
2	B	302	LFA	C6-C7-C8-C9
2	C	301	LFA	C3-C4-C5-C6
2	A	501	LFA	C15-C16-C17-C18
2	A	510	LFA	C1-C2-C3-C4
2	C	314	LFA	C3-C4-C5-C6
2	C	313	LFA	C3-C4-C5-C6
3	B	308	OLA	C5-C6-C7-C8
3	C	303	OLA	C1-C2-C3-C4
3	C	304	OLA	C5-C6-C7-C8
2	A	517	LFA	C1-C2-C3-C4
2	A	517	LFA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	A	519	LFA	C14-C15-C16-C17
3	A	503	OLA	C2-C3-C4-C5
3	B	306	OLA	C2-C3-C4-C5
3	A	504	OLA	C15-C16-C17-C18
2	C	301	LFA	C1-C2-C3-C4
3	A	505	OLA	C2-C3-C4-C5
2	B	313	LFA	C3-C4-C5-C6
2	B	309	LFA	C2-C3-C4-C5
2	C	315	LFA	C2-C3-C4-C5
2	C	301	LFA	C2-C3-C4-C5
2	A	512	LFA	C1-C2-C3-C4
3	C	302	OLA	C4-C5-C6-C7
3	A	504	OLA	C4-C5-C6-C7
2	A	512	LFA	C9-C10-C11-C12
2	B	316	LFA	C13-C14-C15-C16
2	C	301	LFA	C5-C6-C7-C8
3	C	303	OLA	C11-C12-C13-C14
3	C	303	OLA	C6-C7-C8-C9
3	C	305	OLA	C2-C3-C4-C5
2	C	311	LFA	C1-C2-C3-C4
2	B	318	LFA	C4-C5-C6-C7
2	C	314	LFA	C7-C8-C9-C10
3	A	506	OLA	C4-C5-C6-C7
3	C	302	OLA	C5-C6-C7-C8
2	C	311	LFA	C2-C3-C4-C5
3	B	305	OLA	C4-C5-C6-C7
3	A	507	OLA	C12-C13-C14-C15
3	B	307	OLA	C5-C6-C7-C8
3	C	304	OLA	C11-C10-C9-C8
3	B	306	OLA	C10-C11-C12-C13
2	B	309	LFA	C1-C2-C3-C4
2	A	520	LFA	C14-C15-C16-C17
2	A	512	LFA	C2-C3-C4-C5
3	B	308	OLA	C10-C11-C12-C13
3	C	304	OLA	C2-C3-C4-C5
2	C	301	LFA	C14-C15-C16-C17
2	A	519	LFA	C15-C16-C17-C18
3	B	303	OLA	C5-C6-C7-C8
2	B	314	LFA	C10-C11-C12-C13
2	B	313	LFA	C4-C5-C6-C7
3	A	504	OLA	C2-C3-C4-C5
3	A	504	OLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	A	504	OLA	C12-C13-C14-C15
3	B	303	OLA	C1-C2-C3-C4
2	B	301	LFA	C14-C15-C16-C17
2	B	312	LFA	C17-C18-C19-C20
2	A	515	LFA	C1-C2-C3-C4
2	C	306	LFA	C3-C4-C5-C6
3	A	507	OLA	C2-C3-C4-C5
2	B	318	LFA	C9-C10-C11-C12
2	A	510	LFA	C6-C7-C8-C9
2	C	306	LFA	C5-C6-C7-C8
3	C	305	OLA	C7-C8-C9-C10
3	C	302	OLA	C1-C2-C3-C4
2	C	307	LFA	C7-C8-C9-C10
3	B	308	OLA	C9-C10-C11-C12
2	A	510	LFA	C3-C4-C5-C6
3	C	305	OLA	C3-C4-C5-C6
2	C	311	LFA	C5-C6-C7-C8
3	B	304	OLA	C11-C10-C9-C8
3	C	303	OLA	C2-C3-C4-C5
3	B	304	OLA	C7-C8-C9-C10
2	C	317	LFA	C6-C7-C8-C9
2	A	509	LFA	C5-C6-C7-C8
3	A	505	OLA	O1-C1-C2-C3
3	C	305	OLA	O1-C1-C2-C3
2	A	520	LFA	C15-C16-C17-C18
2	B	301	LFA	C13-C14-C15-C16
2	C	306	LFA	C4-C5-C6-C7
3	A	506	OLA	O1-C1-C2-C3
3	B	308	OLA	C11-C10-C9-C8
3	A	507	OLA	C3-C4-C5-C6
3	A	505	OLA	C11-C10-C9-C8
3	A	505	OLA	O2-C1-C2-C3
3	C	305	OLA	O2-C1-C2-C3
3	A	506	OLA	O2-C1-C2-C3
3	B	308	OLA	C13-C14-C15-C16
3	A	507	OLA	C5-C6-C7-C8
3	A	503	OLA	C1-C2-C3-C4
3	A	504	OLA	O1-C1-C2-C3
3	A	503	OLA	C6-C7-C8-C9
3	A	504	OLA	O2-C1-C2-C3
3	B	303	OLA	C6-C7-C8-C9
3	A	507	OLA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
3	C	303	OLA	C7-C8-C9-C10
3	C	303	OLA	C9-C10-C11-C12
2	C	313	LFA	C7-C8-C9-C10
3	B	308	OLA	O2-C1-C2-C3
3	A	504	OLA	C6-C7-C8-C9
3	C	302	OLA	C11-C12-C13-C14
3	B	306	OLA	C7-C8-C9-C10
3	C	302	OLA	O2-C1-C2-C3
3	B	303	OLA	C7-C8-C9-C10
3	C	302	OLA	O1-C1-C2-C3
2	A	512	LFA	C11-C10-C9-C8
2	C	312	LFA	C10-C11-C12-C13
3	B	307	OLA	C9-C10-C11-C12
3	B	307	OLA	C1-C2-C3-C4
3	B	308	OLA	O1-C1-C2-C3
3	B	306	OLA	C1-C2-C3-C4
2	A	501	LFA	C17-C18-C19-C20
2	B	317	LFA	C3-C4-C5-C6
3	A	504	OLA	C9-C10-C11-C12

There are no ring outliers.

27 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	312	LFA	1	0
2	C	309	LFA	3	0
2	C	311	LFA	1	0
3	B	305	OLA	2	0
2	A	513	LFA	1	0
2	A	512	LFA	2	0
2	A	518	LFA	1	0
3	A	503	OLA	2	0
2	B	323	LFA	2	0
2	C	301	LFA	1	0
2	A	519	LFA	2	0
2	B	321	LFA	2	0
2	A	517	LFA	2	0
3	A	508	OLA	3	0
3	B	303	OLA	1	0
2	B	314	LFA	2	0
3	A	506	OLA	1	0
3	A	507	OLA	1	0

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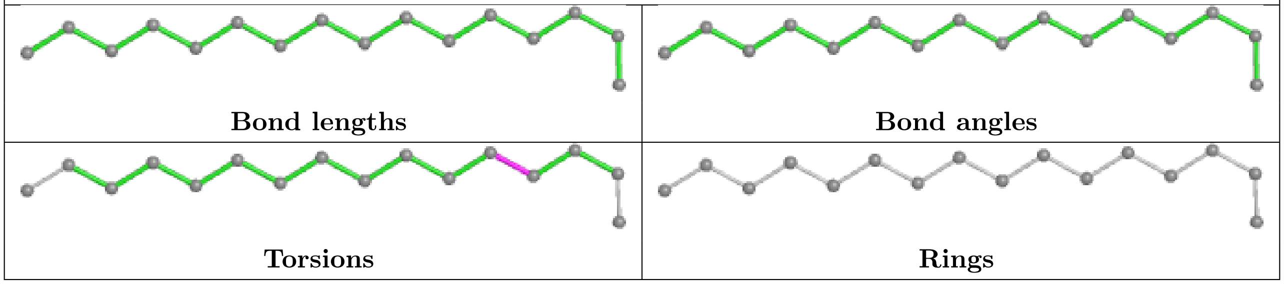
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	515	LFA	2	0
3	A	505	OLA	2	0
3	B	304	OLA	1	0
2	B	319	LFA	1	0
2	C	316	LFA	1	0
2	C	310	LFA	1	0
3	B	308	OLA	2	0
3	C	305	OLA	5	0
3	A	504	OLA	1	0

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

Ligand LFA B 317



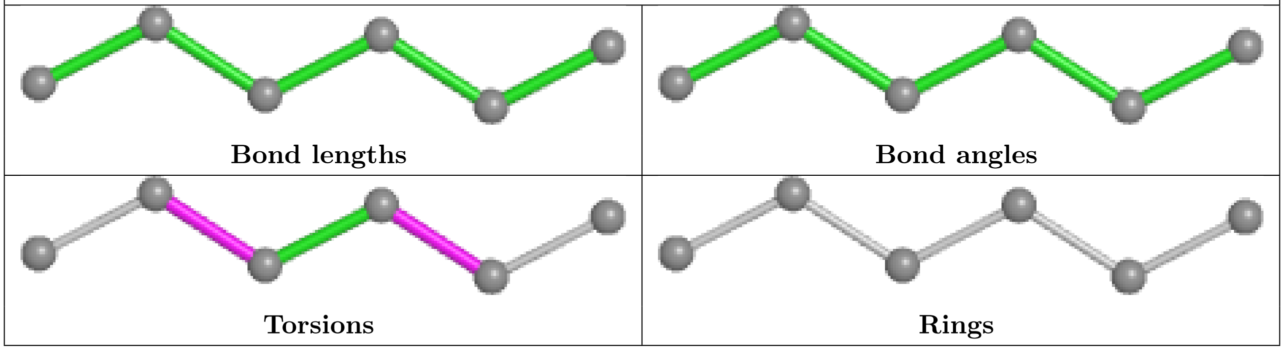
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 501



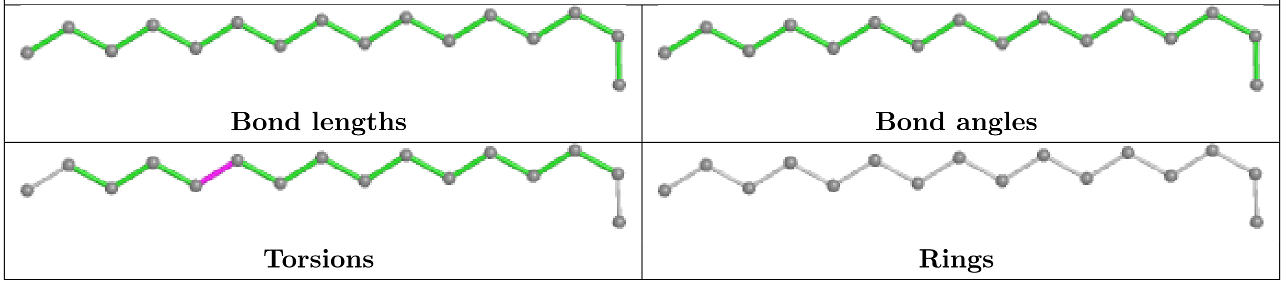
Bond lengths

Bond angles

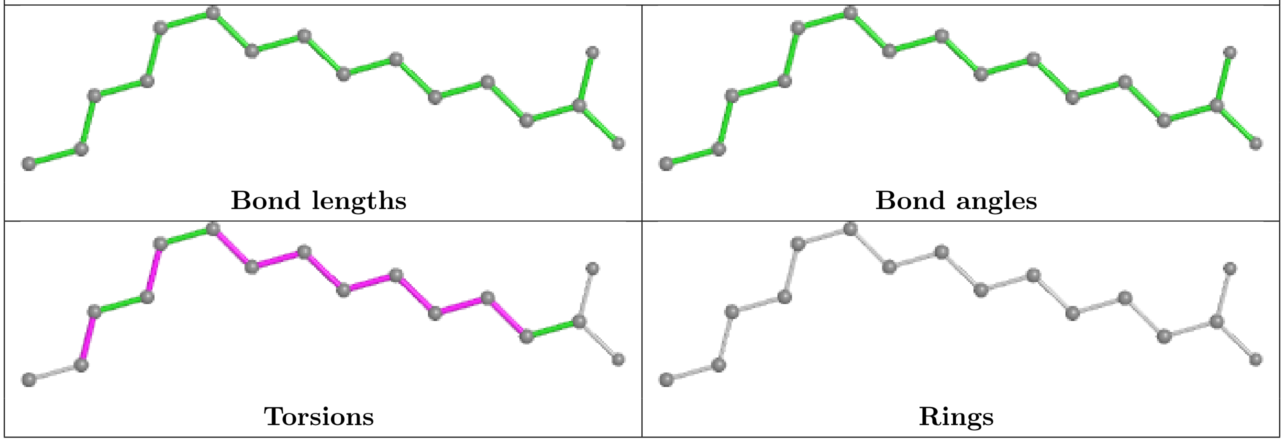
Torsions

Rings

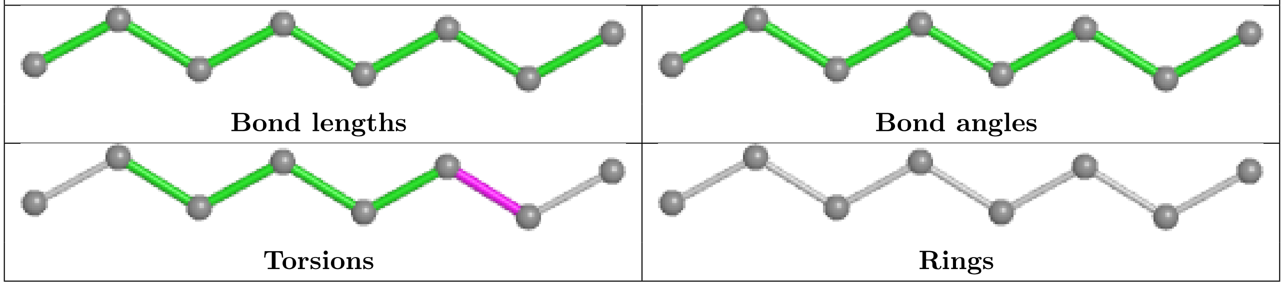
Ligand LFA C 312



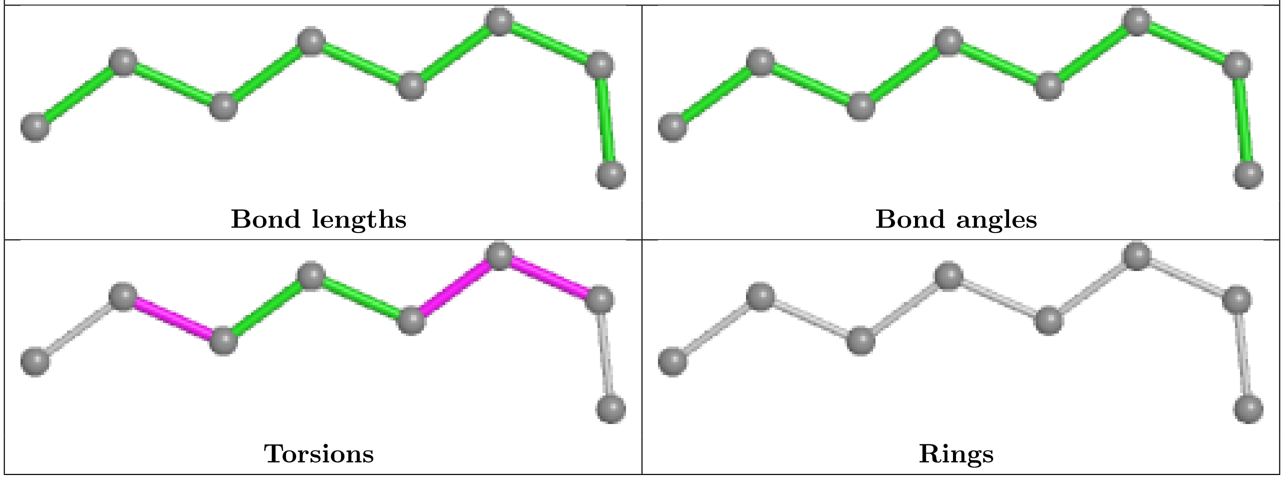
Ligand OLA C 303



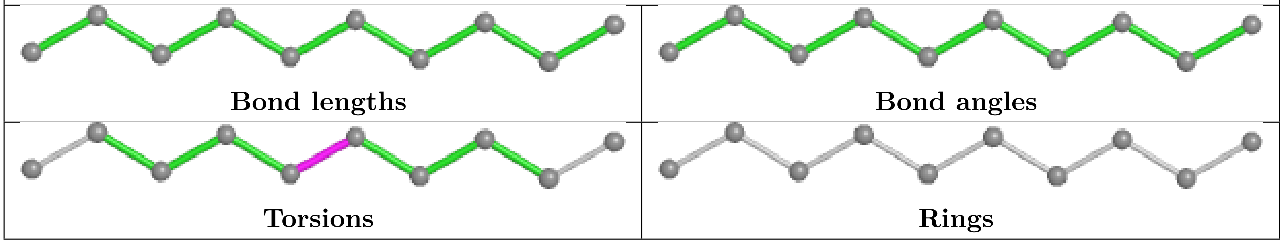
Ligand LFA B 316



Ligand LFA C 311



Ligand OLA B 305



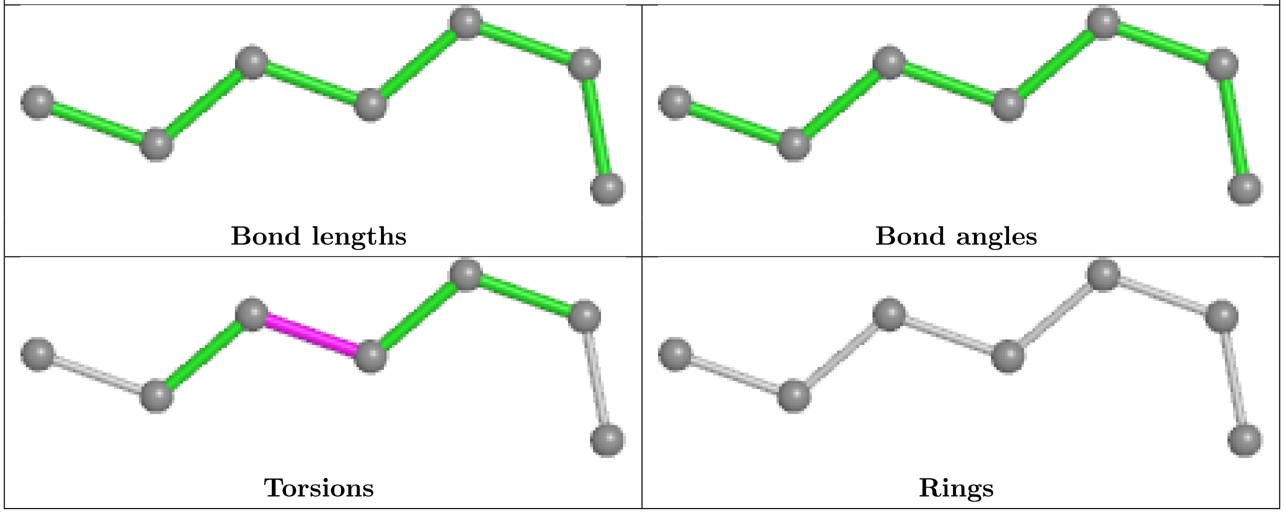
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA B 310



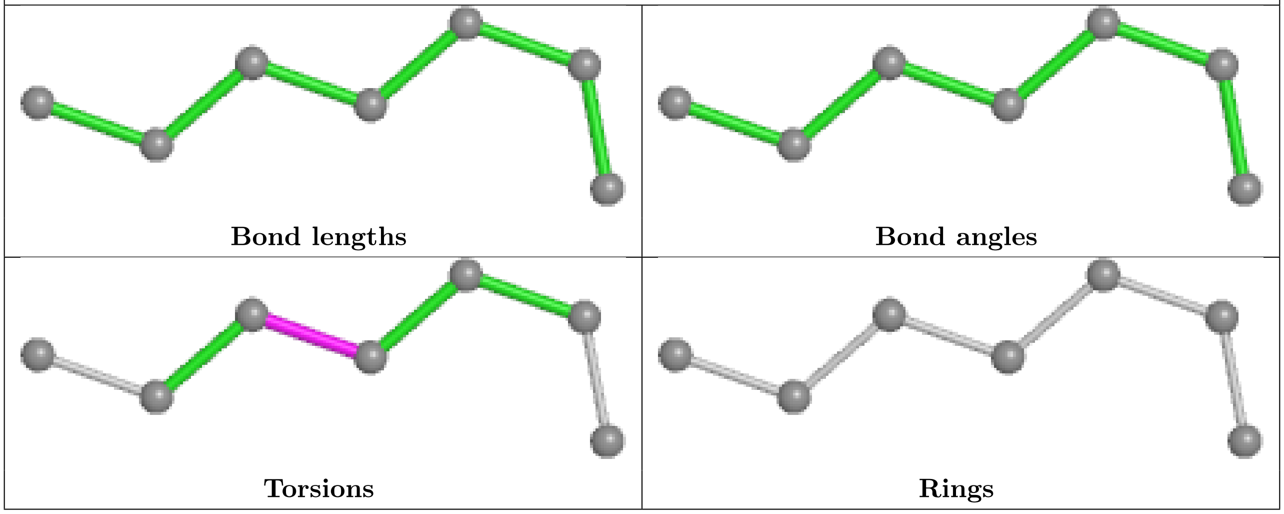
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 513



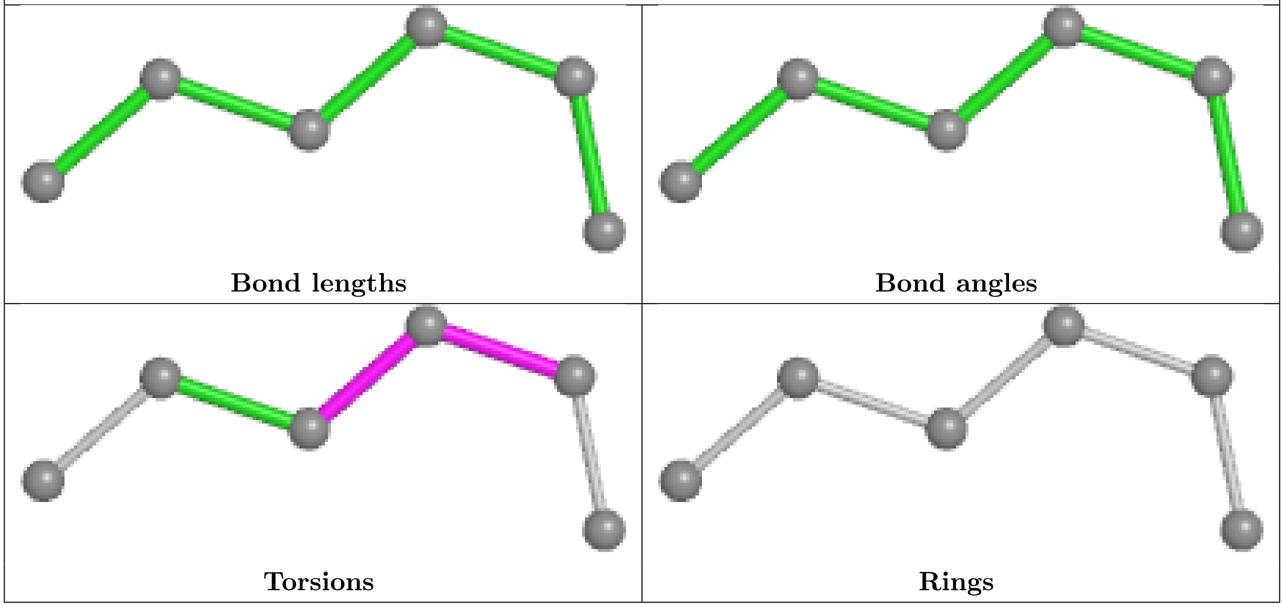
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA B 309



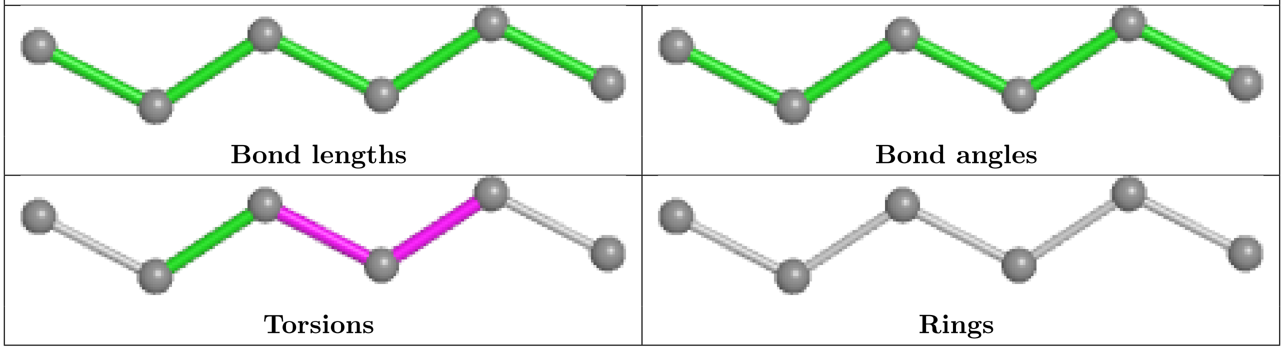
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 520



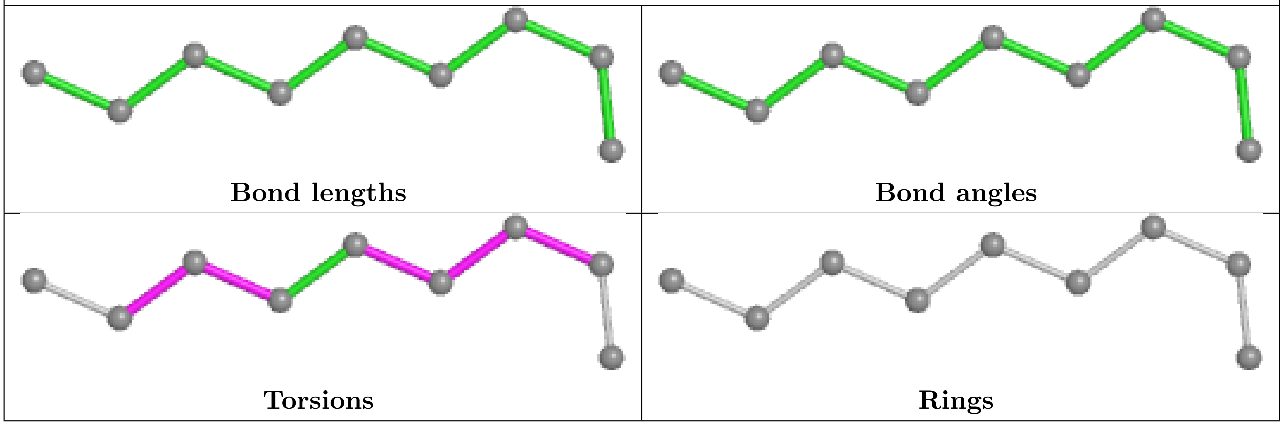
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 510



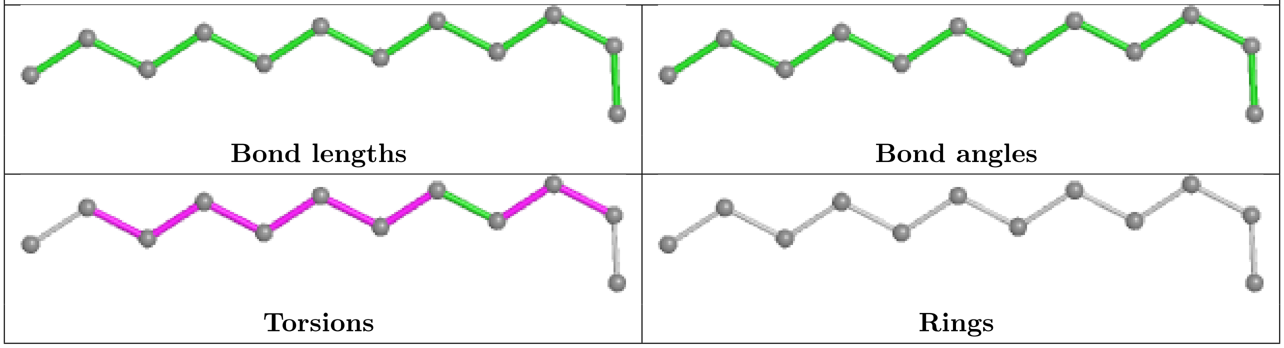
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 512



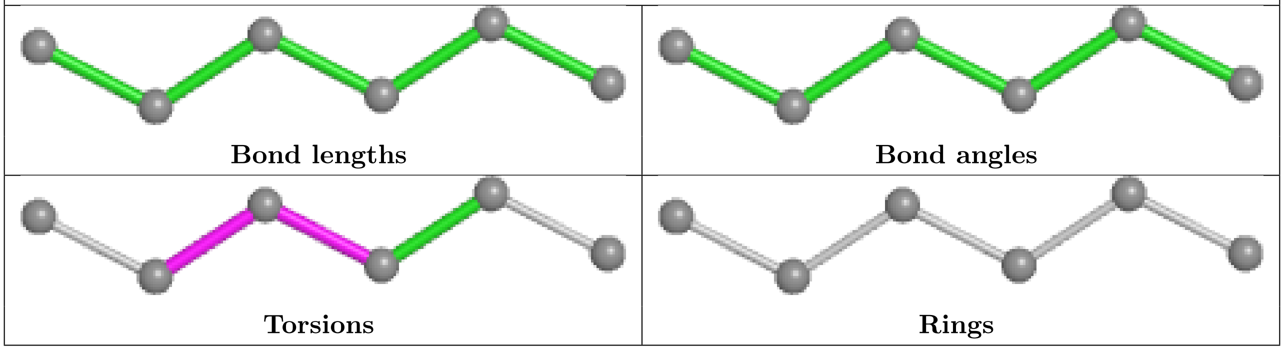
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA B 313



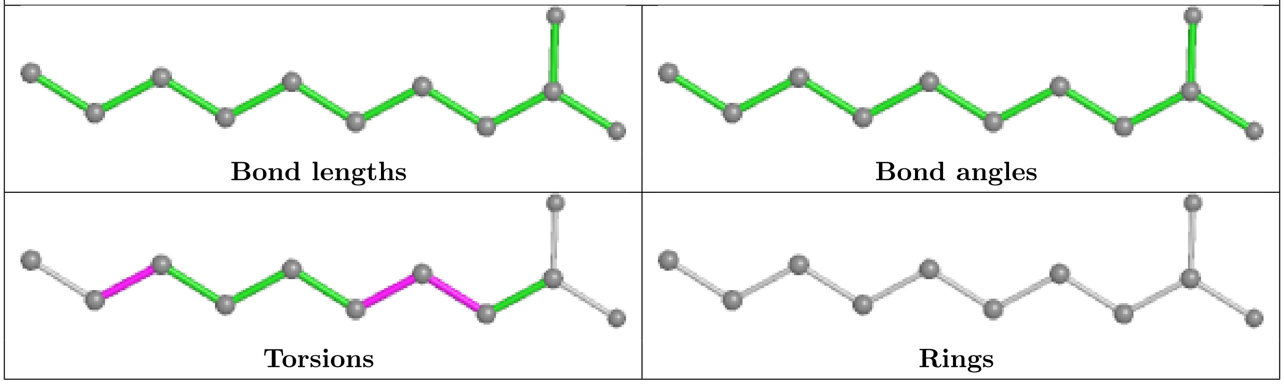
Bond lengths

Bond angles

Torsions

Rings

Ligand OLA A 503



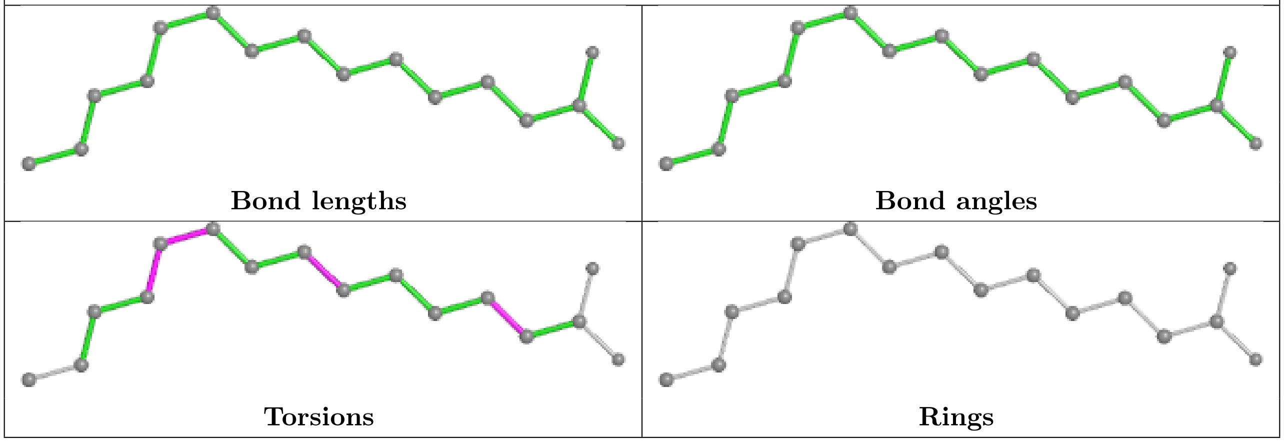
Bond lengths

Bond angles

Torsions

Rings

Ligand OLA B 307



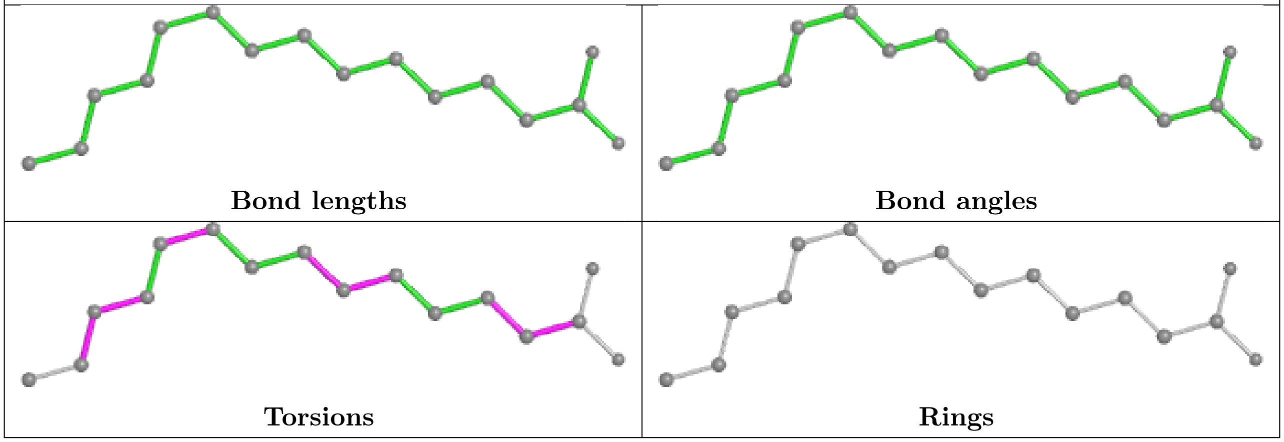
Bond lengths

Bond angles

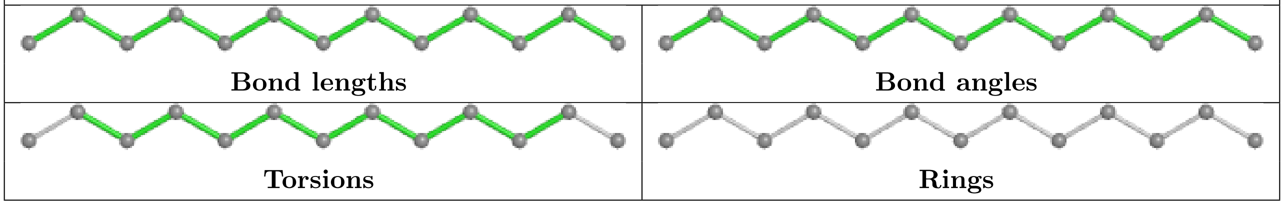
Torsions

Rings

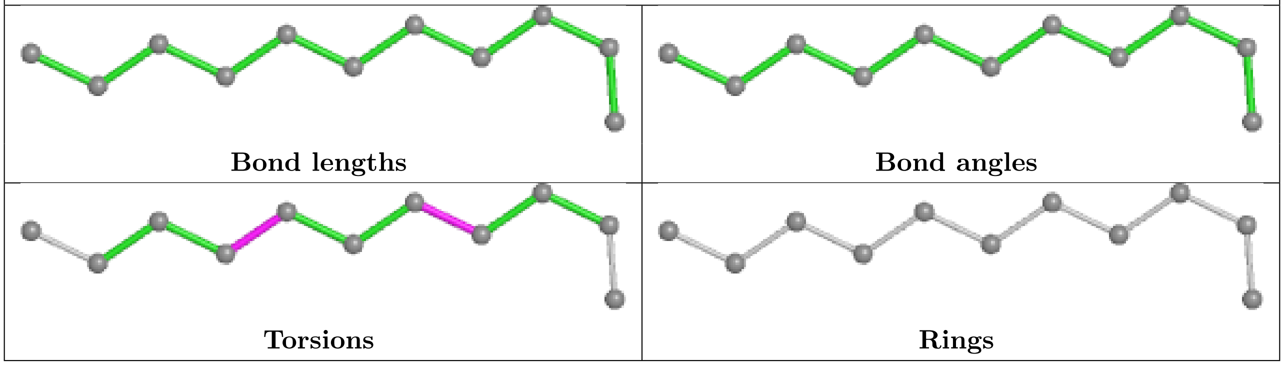
Ligand OLA C 302



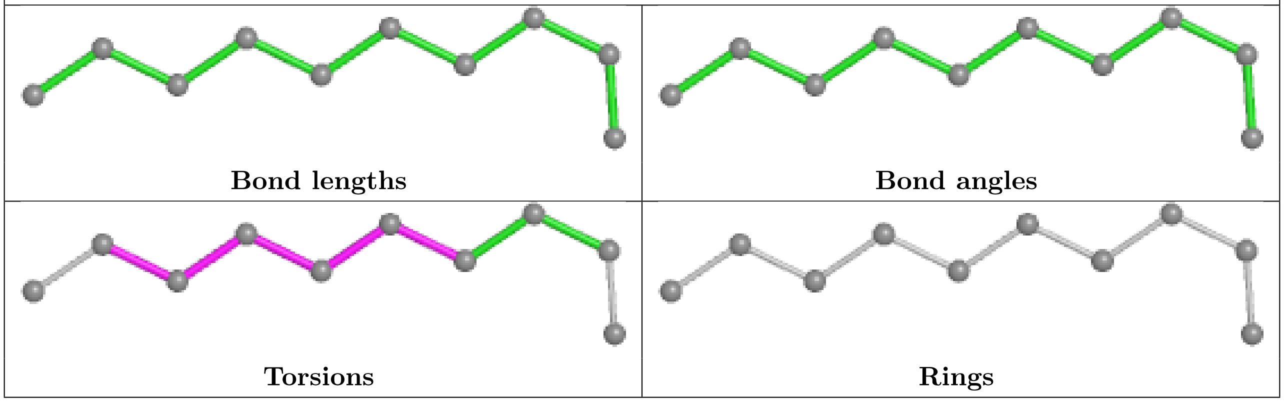
Ligand LFA B 323



Ligand LFA C 317



Ligand LFA C 314



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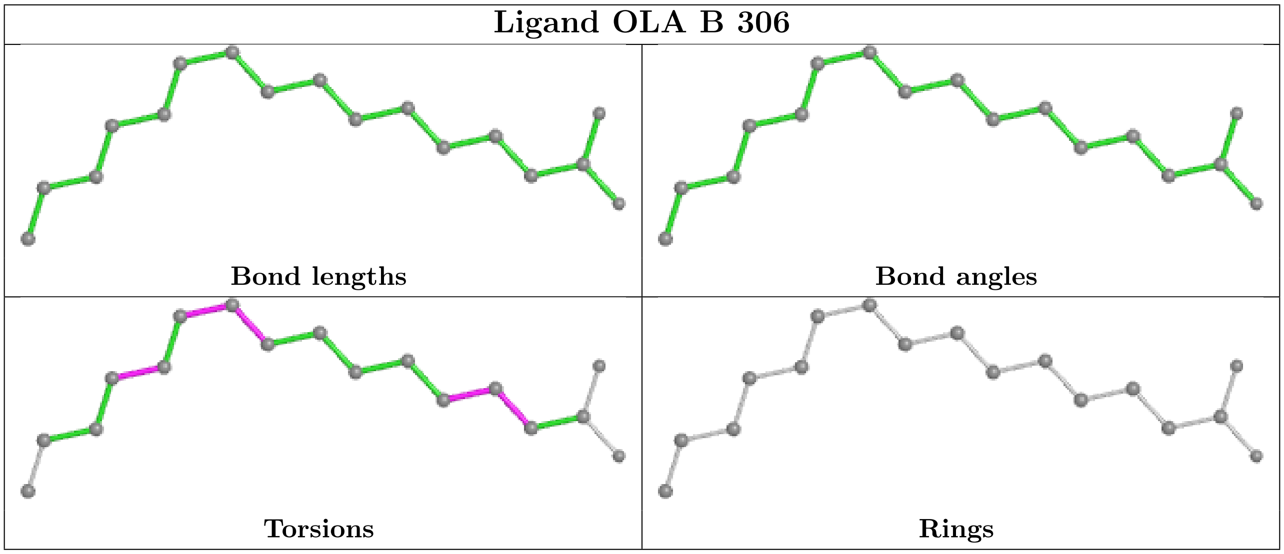

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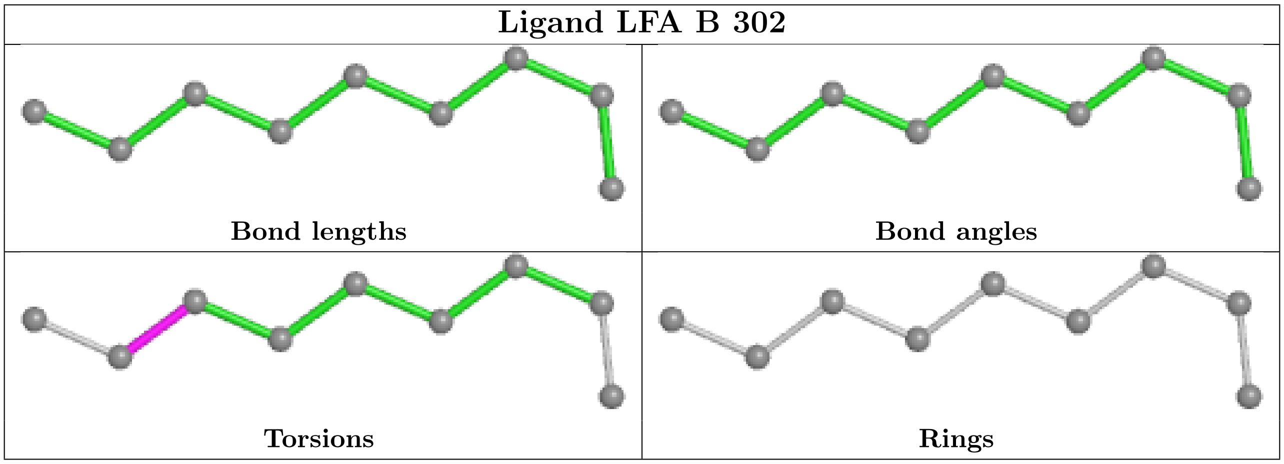

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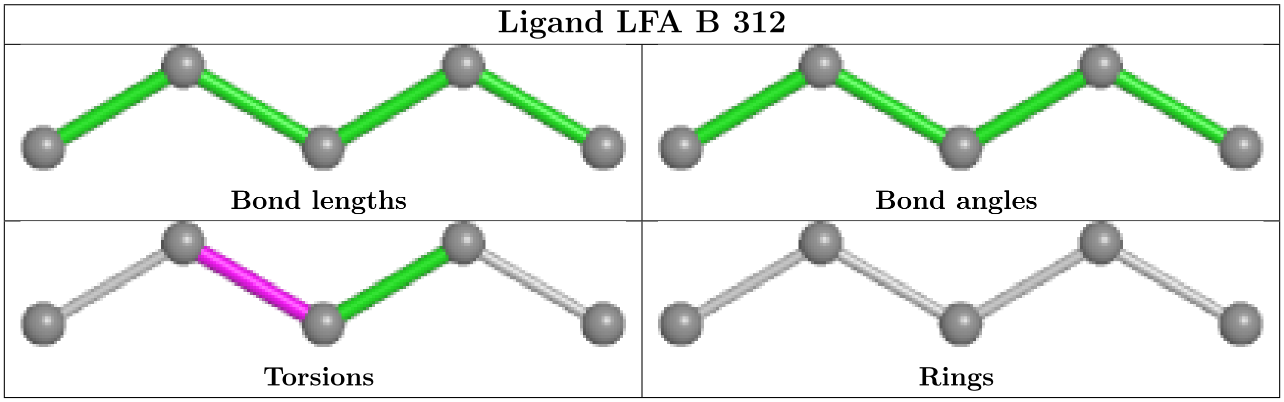

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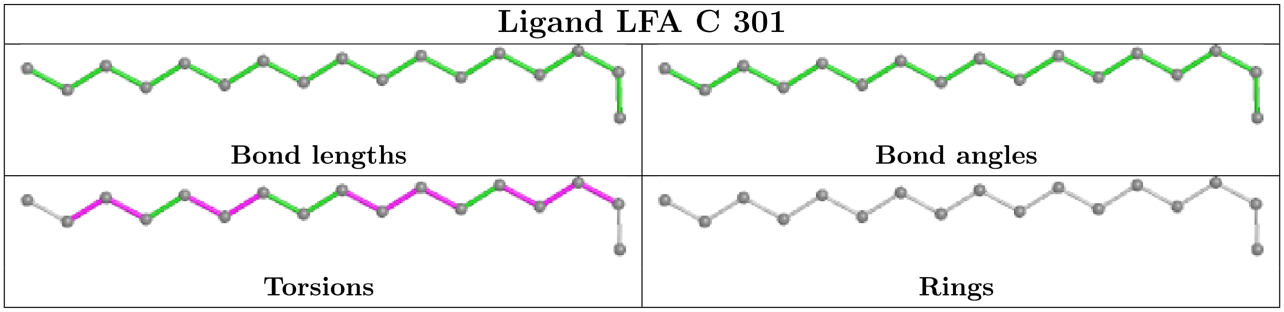
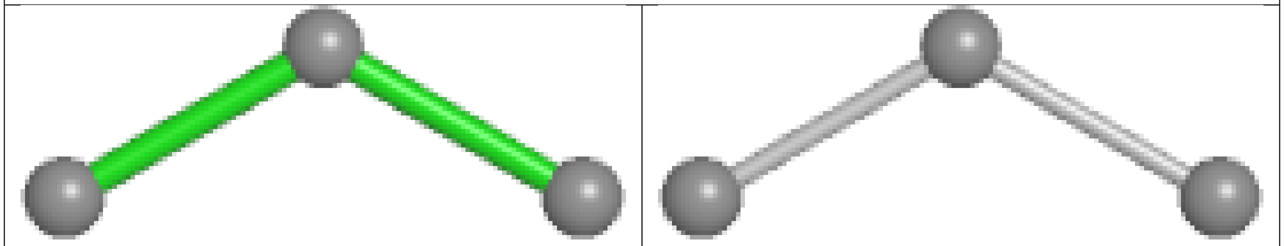
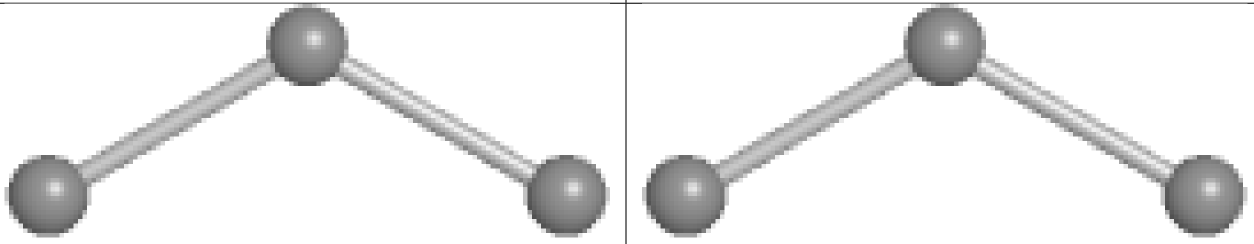


Ligand LFA A 516



Bond lengths

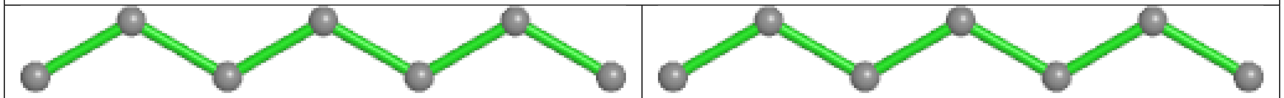
Bond angles



Torsions

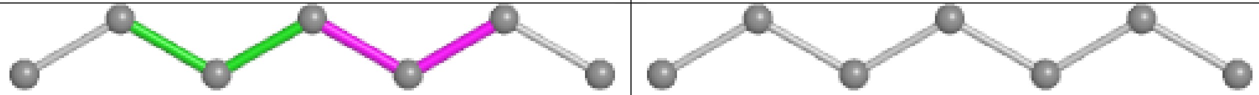
Rings

Ligand LFA A 519



Bond lengths

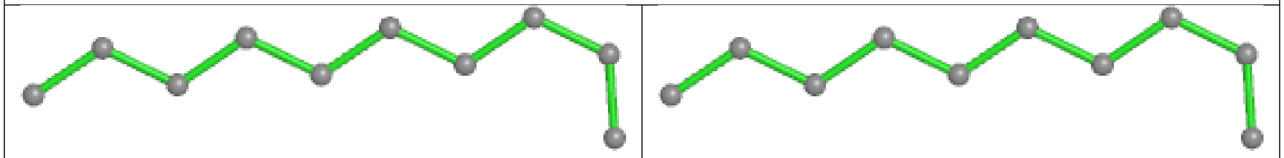
Bond angles



Torsions

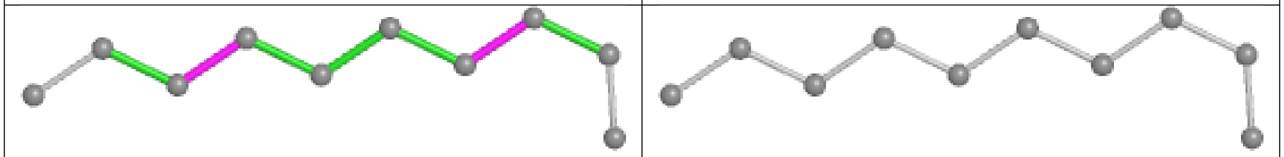
Rings

Ligand LFA B 321



Bond lengths

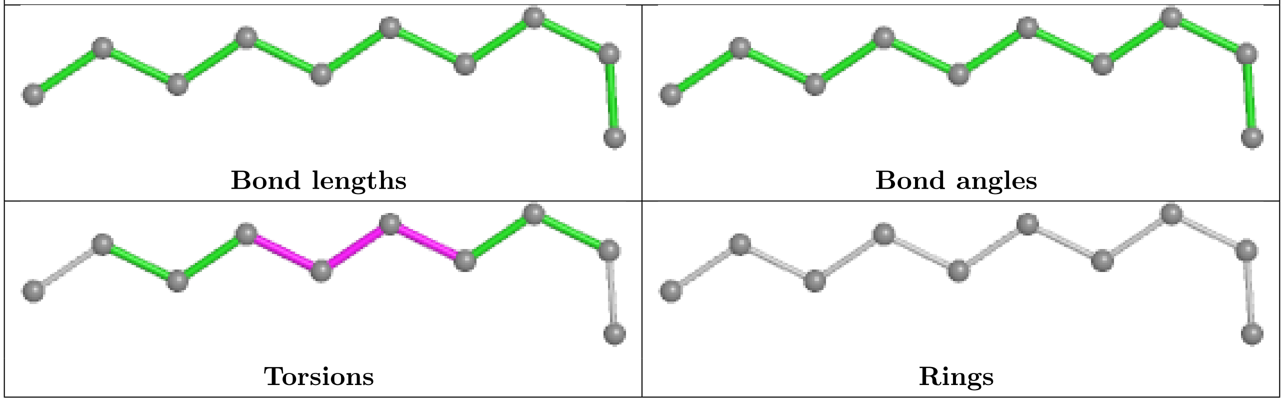
Bond angles



Torsions

Rings

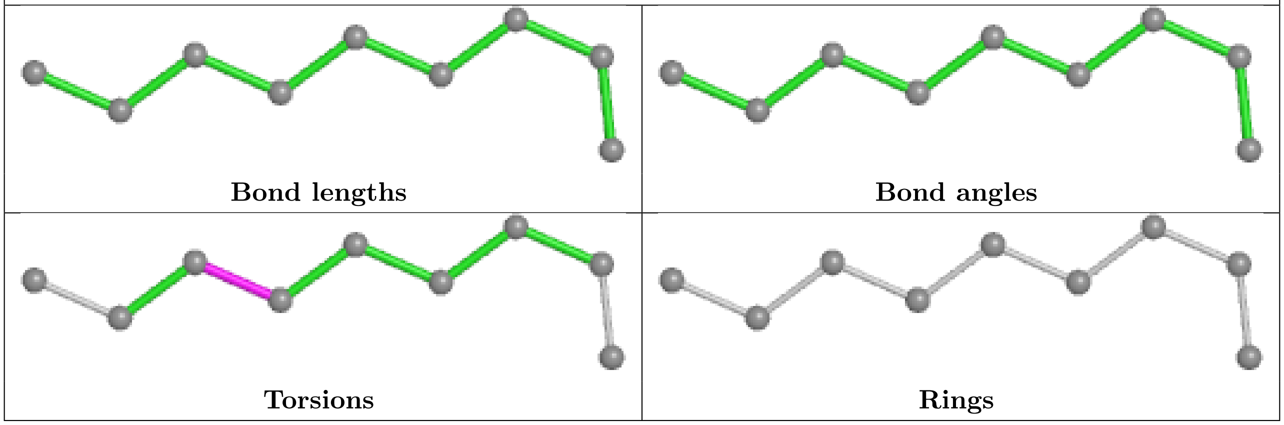
Ligand LFA C 306



Bond lengths Bond angles

Torsions Rings

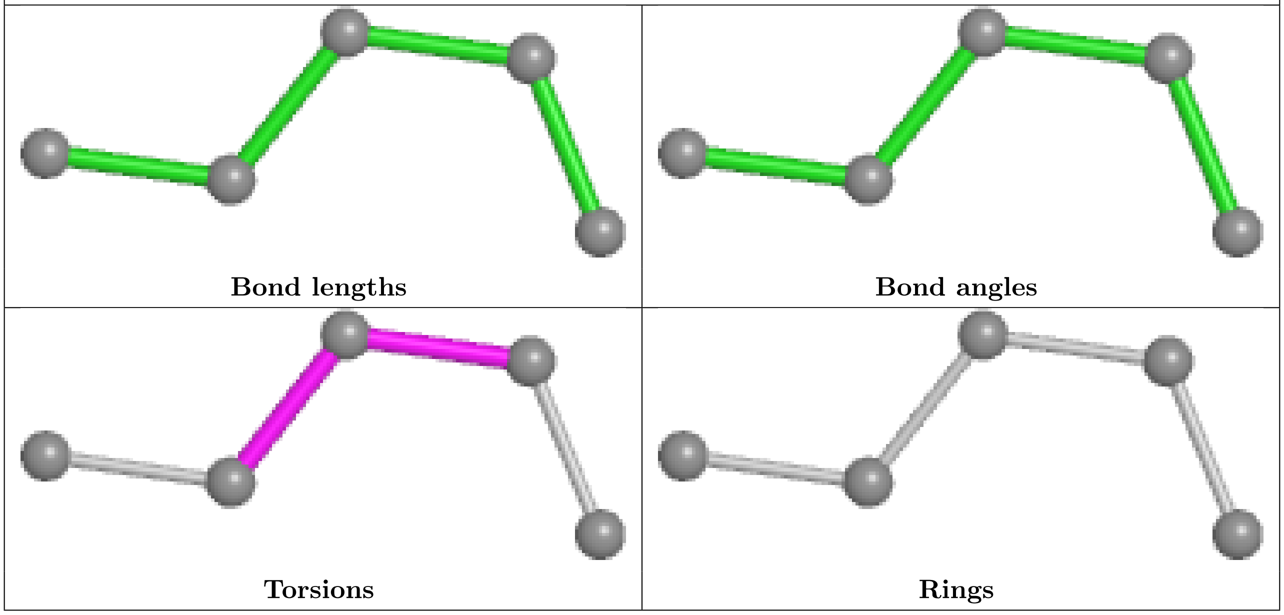
Ligand LFA A 509



Bond lengths Bond angles

Torsions Rings

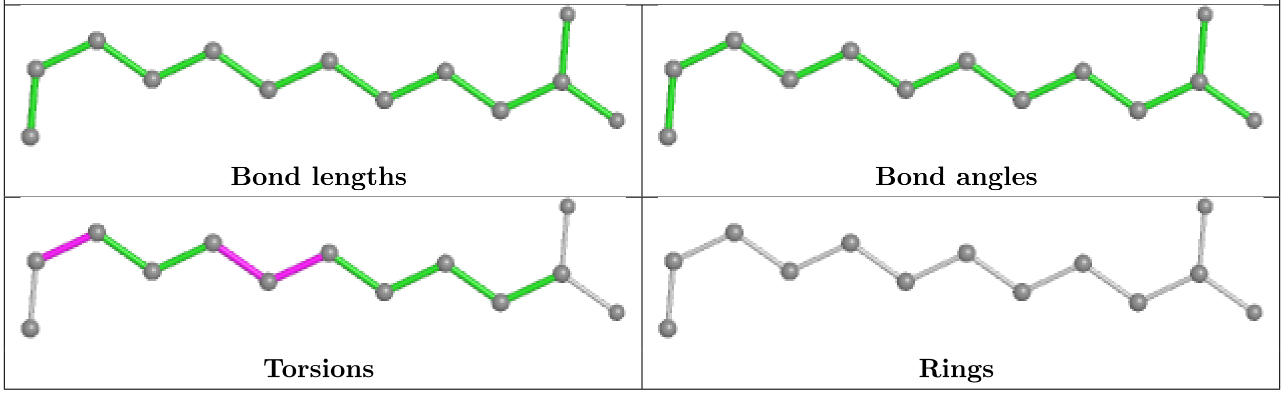
Ligand LFA A 517



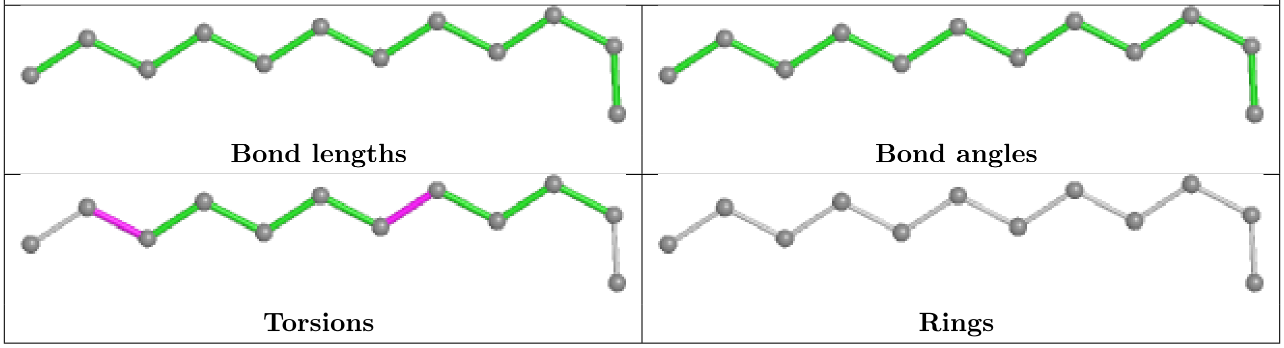
Bond lengths Bond angles

Torsions Rings

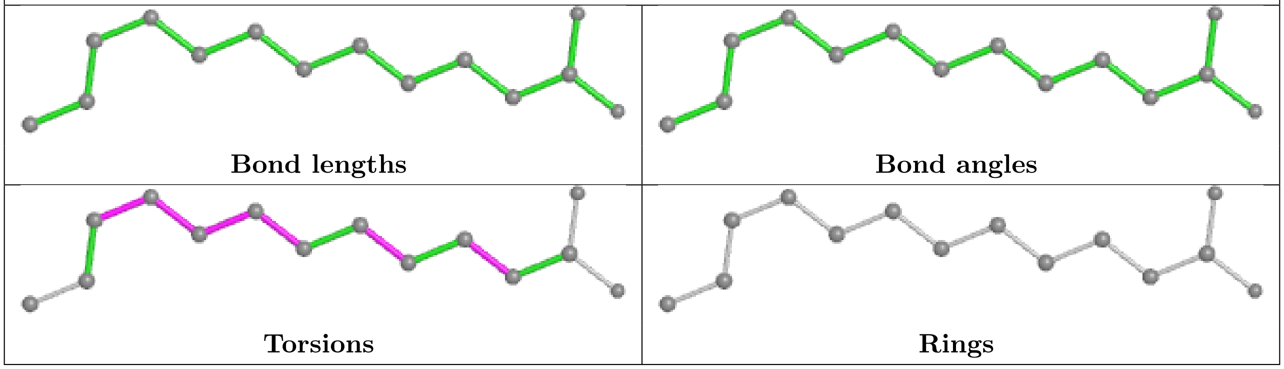
Ligand OLA A 508



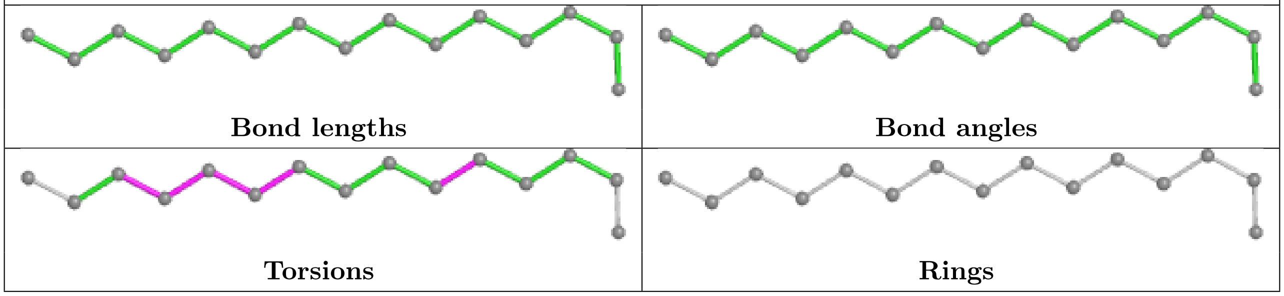
Ligand LFA B 318



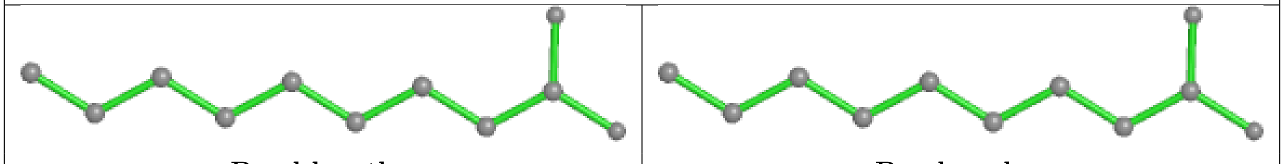
Ligand OLA B 303



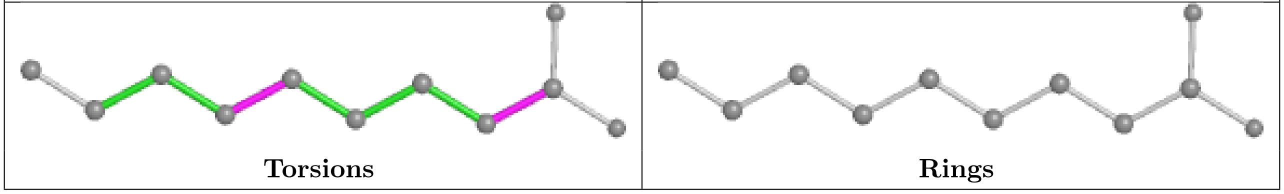
Ligand LFA B 314



Ligand OLA A 506

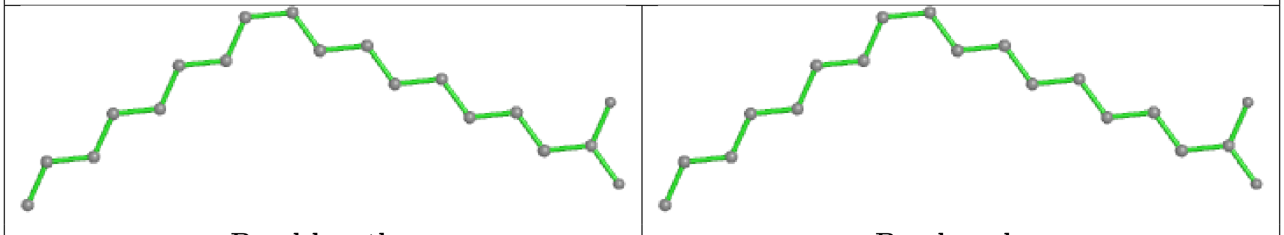


Bond lengths **Bond angles**

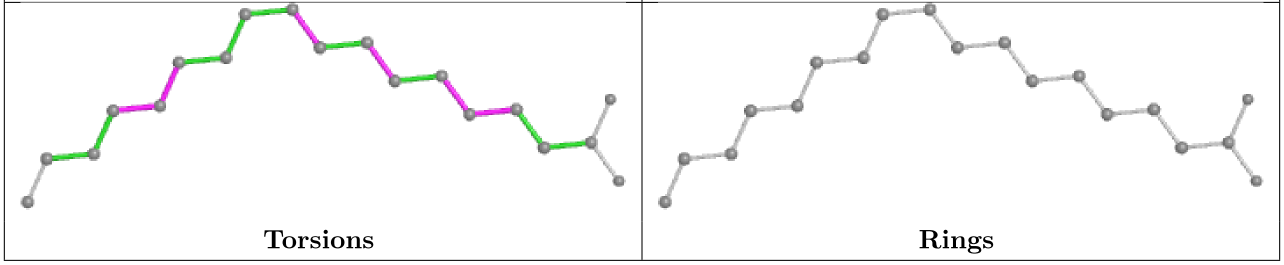


Torsions **Rings**

Ligand OLA A 507

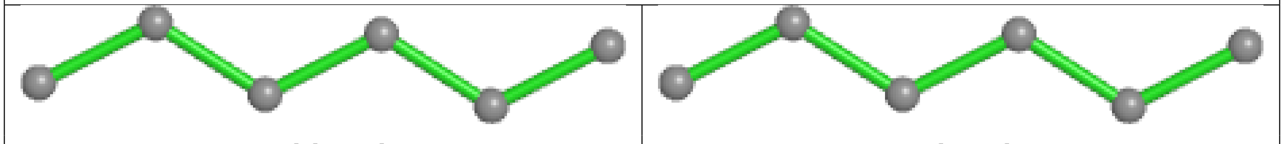


Bond lengths **Bond angles**

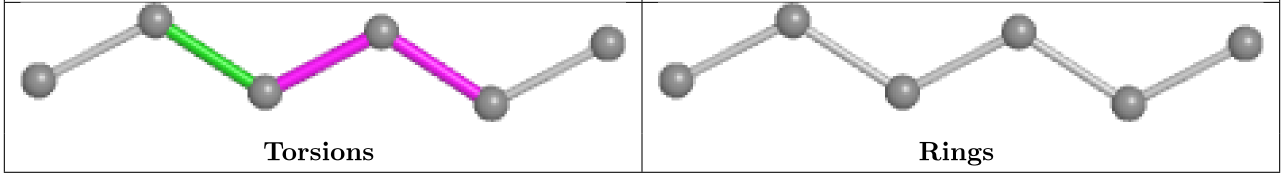


Torsions **Rings**

Ligand LFA B 301

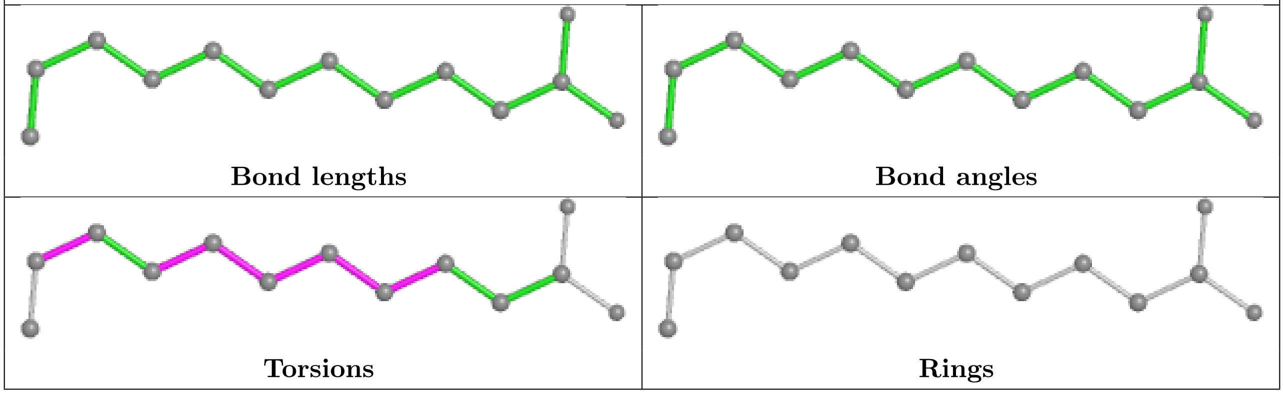


Bond lengths **Bond angles**



Torsions **Rings**

Ligand OLA C 304



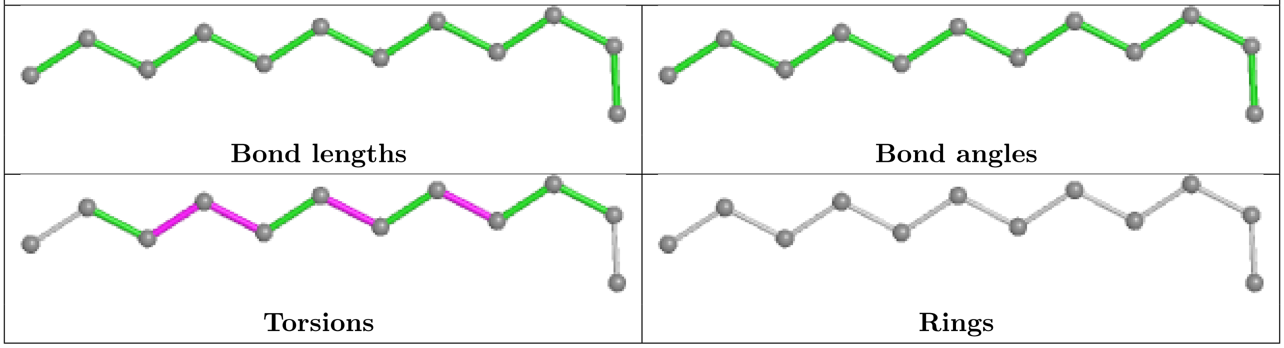
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA C 313



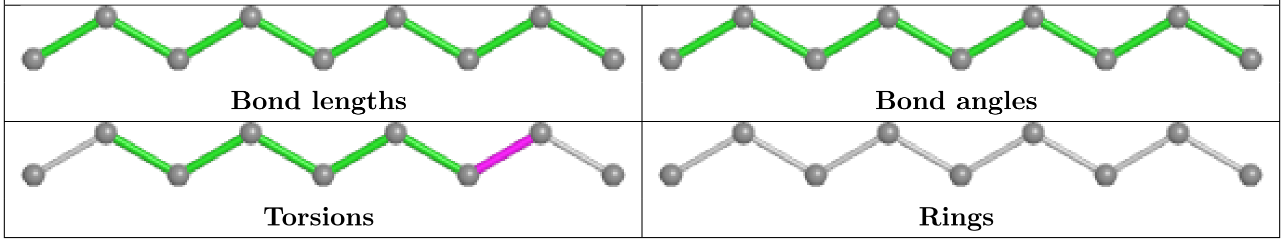
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA C 315



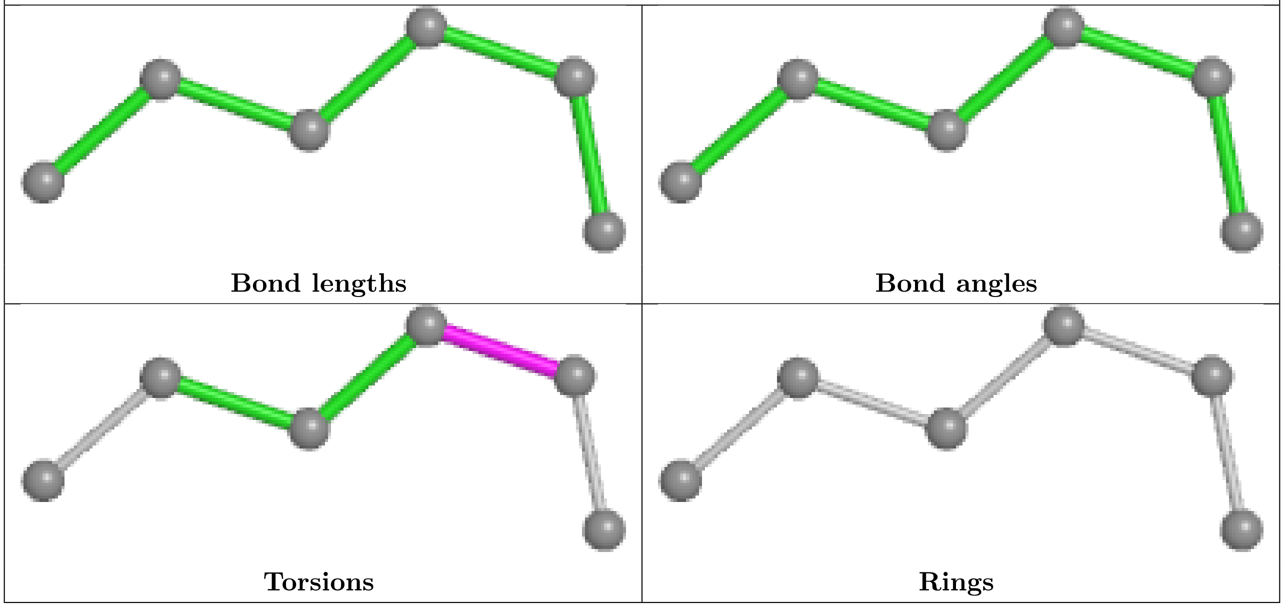
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 515



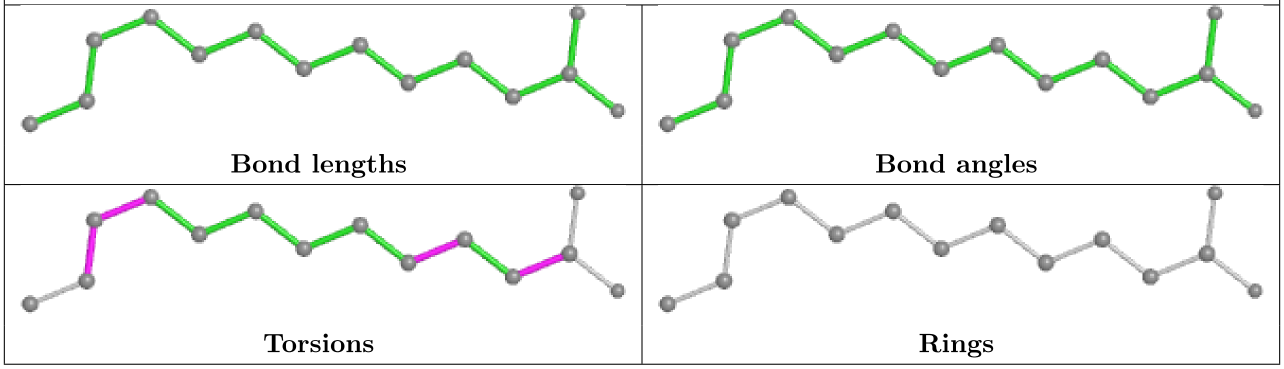
Bond lengths

Bond angles

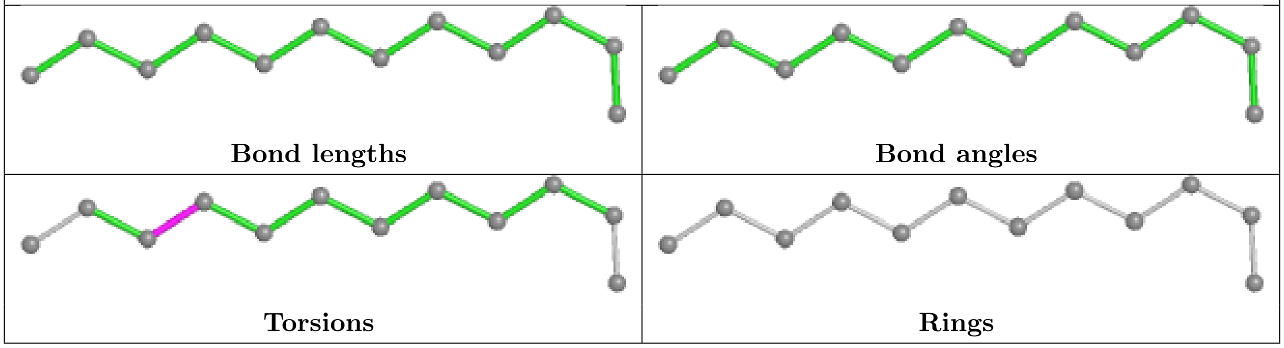
Torsions

Rings

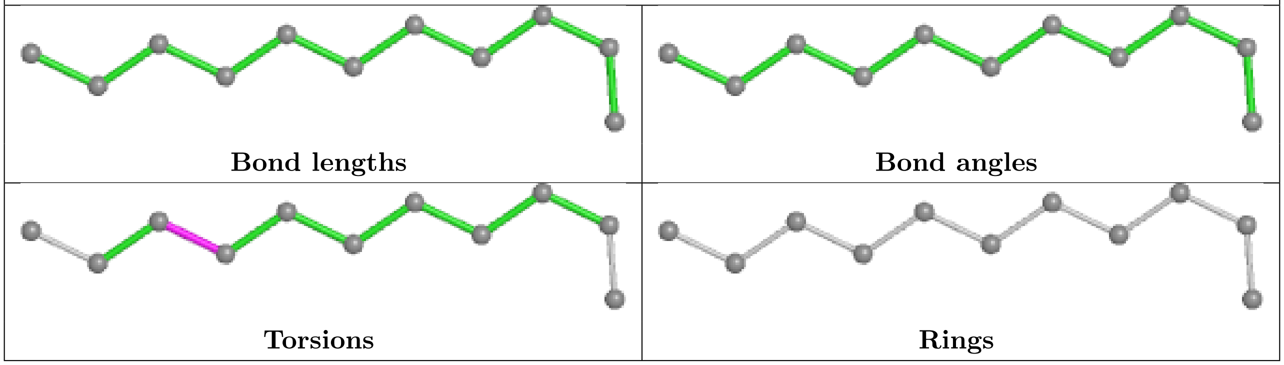
Ligand OLA A 505



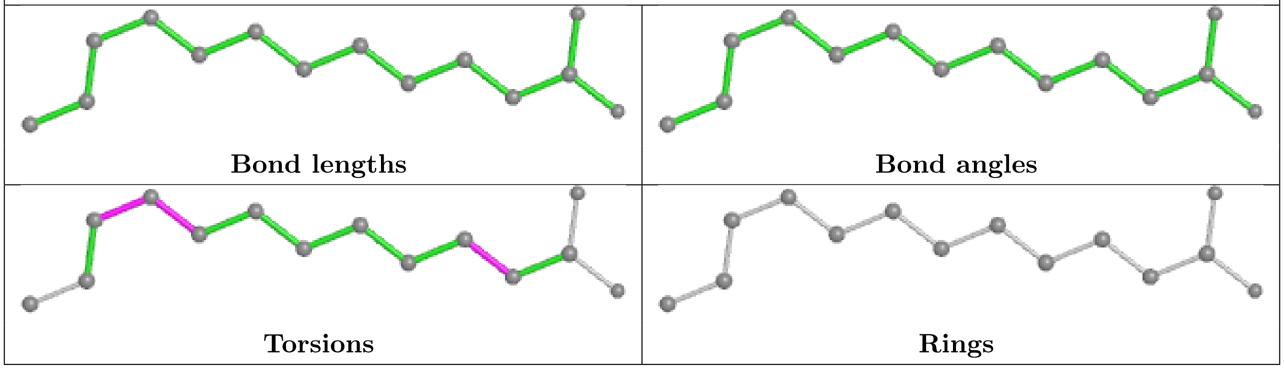
Ligand LFA B 322



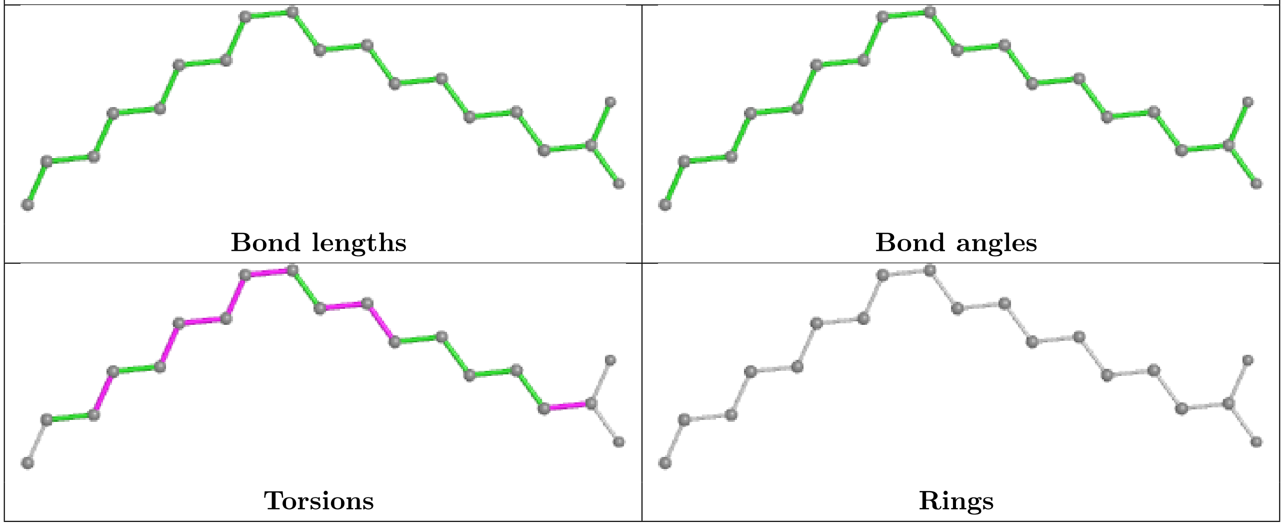
Ligand LFA C 307



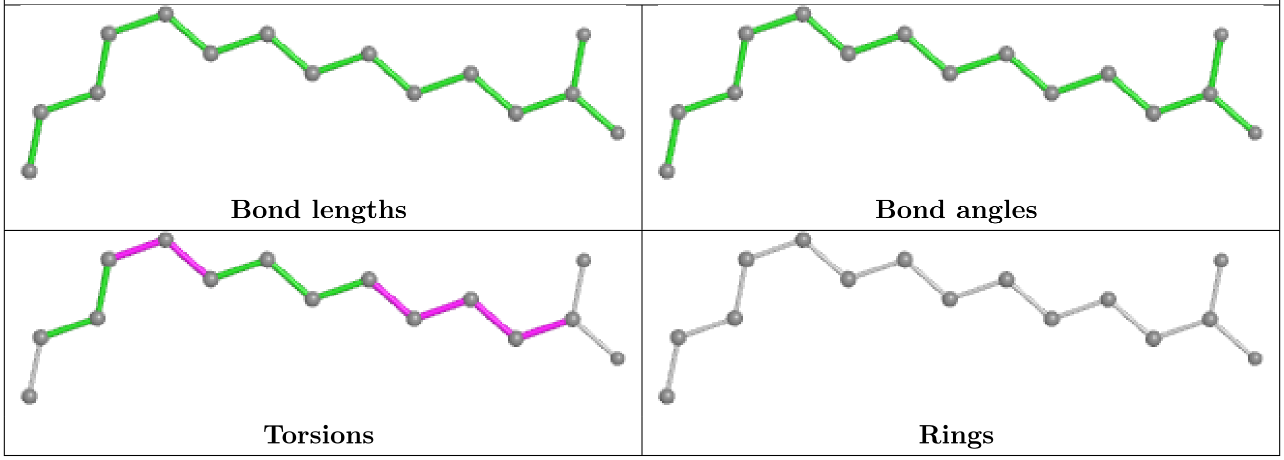
Ligand OLA B 304



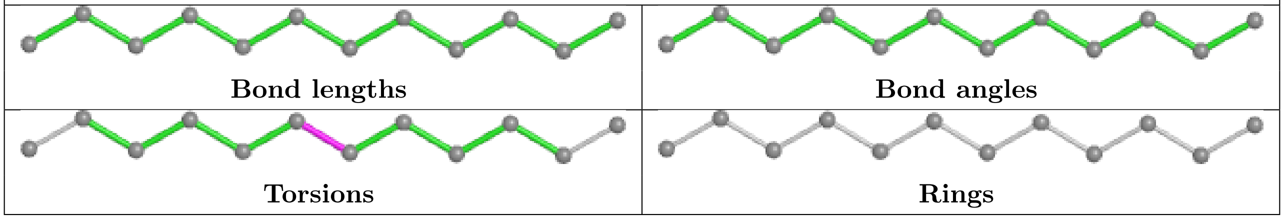
Ligand OLA B 308

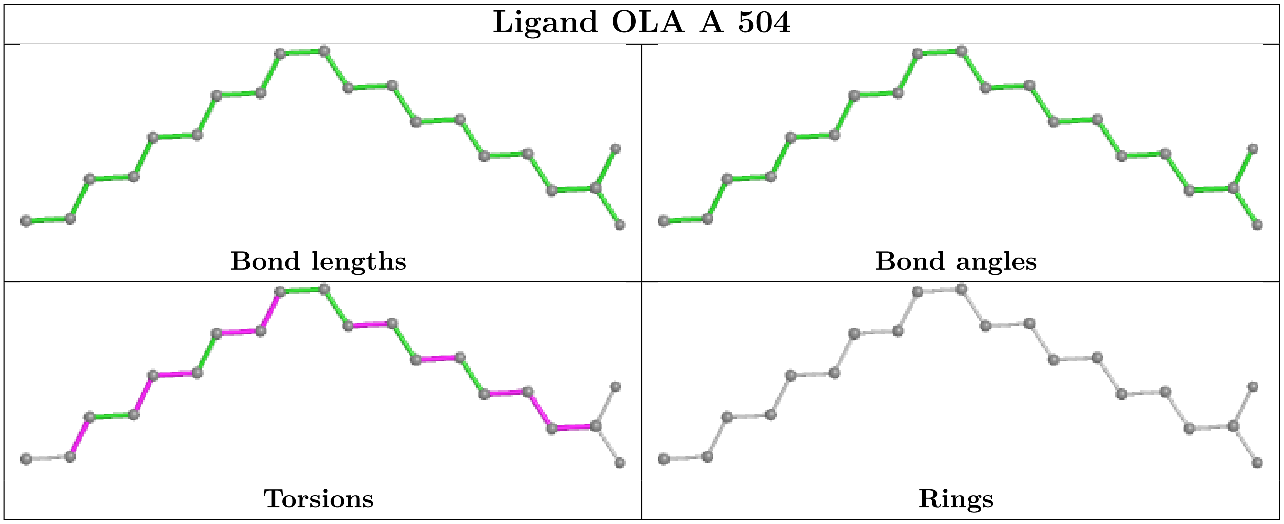


Ligand OLA C 305



Ligand LFA B 320





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	222:HIS	C	223:GLN	N	2.67

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, 95^{th} 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	221/229 (96%)	0.08	8 (3%)	42	49	25, 33, 55, 103	0
1	B	218/229 (95%)	0.07	9 (4%)	37	44	25, 35, 53, 83	0
1	C	221/229 (96%)	0.17	11 (4%)	28	35	26, 36, 57, 94	0
All	All	660/687 (96%)	0.11	28 (4%)	36	43	25, 35, 57, 103	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	224	SER	8.9
1	A	61	TYR	5.6
1	B	223	GLN	5.5
1	C	223	GLN	5.4
1	C	189	LEU	5.1
1	C	61	TYR	4.9
1	A	62	ASP	4.6
1	C	221	LEU	3.4
1	C	187	LEU	3.3
1	A	173[A]	TRP	3.0
1	B	222	HIS	2.7
1	A	64	THR	2.7
1	A	175	CYS	2.6
1	A	59	PHE	2.5
1	B	173[A]	TRP	2.4
1	A	121	ILE	2.4
1	B	155	GLY	2.2
1	C	186	GLY	2.2
1	C	188	GLY	2.2
1	B	121	ILE	2.1
1	B	153	SER	2.1
1	C	173[A]	TRP	2.1
1	B	59	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	197	LEU	2.1
1	C	222	HIS	2.1
1	C	126	TYR	2.0
1	A	60	GLN	2.0
1	B	92	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	FME	C	1	10/11	0.86	0.20	38,53,82,100	0
1	LYR	A	207	29/30	0.89	0.17	26,33,44,53	0
1	LYR	C	207	29/30	0.91	0.14	29,36,42,49	0
1	LYR	B	207	29/30	0.92	0.13	25,30,38,39	0
1	FME	B	1	10/11	0.92	0.22	51,64,105,106	0
1	FME	A	1	10/11	0.93	0.17	50,57,110,120	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	OLA	A	506	11/20	0.61	0.30	47,59,66,77	0
3	OLA	B	305	10/20	0.61	0.29	52,63,73,77	0
2	LFA	C	307	11/20	0.64	0.31	65,76,88,89	0
2	LFA	C	306	10/20	0.65	0.24	59,62,69,70	0
2	LFA	B	323	13/20	0.66	0.41	73,81,97,99	0
2	LFA	B	317	16/20	0.69	0.25	56,71,88,88	0
2	LFA	A	513	7/20	0.69	0.27	49,54,60,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LFA	C	317	11/20	0.70	0.41	53,64,71,79	0
2	LFA	B	310	7/20	0.70	0.28	59,61,64,65	0
2	LFA	C	315	9/20	0.70	0.31	44,60,67,67	0
3	OLA	B	308	19/20	0.70	0.27	47,56,83,88	0
2	LFA	C	312	16/20	0.71	0.42	49,68,76,77	0
3	OLA	B	307	16/20	0.72	0.28	48,57,62,68	0
2	LFA	A	518	7/20	0.72	0.39	46,53,66,66	0
2	LFA	B	315	8/20	0.73	0.32	46,57,62,64	0
2	LFA	A	516	3/20	0.73	0.47	58,58,58,68	0
2	LFA	B	316	8/20	0.74	0.25	56,60,62,66	0
2	LFA	B	309	6/20	0.75	0.28	55,57,60,61	0
3	OLA	A	508	13/20	0.76	0.35	56,69,86,93	0
3	OLA	C	303	16/20	0.76	0.33	59,67,79,85	0
3	OLA	B	306	17/20	0.77	0.26	44,49,62,70	0
2	LFA	A	514	8/20	0.77	0.24	60,63,69,70	0
3	OLA	A	504	20/20	0.78	0.31	42,53,70,74	0
2	LFA	C	308	4/20	0.78	0.27	52,54,55,57	0
3	OLA	A	507	19/20	0.78	0.28	36,52,67,72	0
3	OLA	C	304	13/20	0.78	0.21	45,55,77,77	0
2	LFA	B	319	9/20	0.79	0.25	57,62,66,69	0
3	OLA	C	302	16/20	0.79	0.25	46,53,64,65	0
2	LFA	A	512	12/20	0.79	0.27	45,54,61,64	0
2	LFA	A	517	5/20	0.79	0.26	47,53,54,57	0
3	OLA	B	303	14/20	0.80	0.16	44,54,75,80	0
2	LFA	C	309	8/20	0.80	0.21	58,60,63,67	0
3	OLA	C	305	15/20	0.80	0.38	49,64,70,71	0
2	LFA	C	316	10/20	0.81	0.18	58,64,77,77	0
2	LFA	A	502	7/20	0.81	0.50	50,53,59,62	0
2	LFA	A	519	7/20	0.81	0.32	50,56,62,63	0
2	LFA	B	313	6/20	0.81	0.23	59,64,71,73	0
2	LFA	B	318	12/20	0.81	0.17	46,53,61,63	0
2	LFA	A	509	9/20	0.82	0.31	55,58,62,65	0
2	LFA	B	320	12/20	0.83	0.17	51,68,77,80	0
2	LFA	C	313	12/20	0.83	0.20	38,46,57,57	0
4	PO4	A	521	5/5	0.83	0.36	97,98,102,102	5
2	LFA	C	310	4/20	0.84	0.39	56,58,59,59	0
2	LFA	B	321	10/20	0.84	0.23	52,59,66,70	0
2	LFA	B	312	5/20	0.84	0.36	55,57,60,63	0
2	LFA	B	311	5/20	0.84	0.18	49,51,52,54	0
2	LFA	C	314	10/20	0.85	0.39	49,59,68,70	0
3	OLA	A	503	11/20	0.85	0.15	39,46,60,71	0
2	LFA	A	511	7/20	0.85	0.18	42,46,48,48	0

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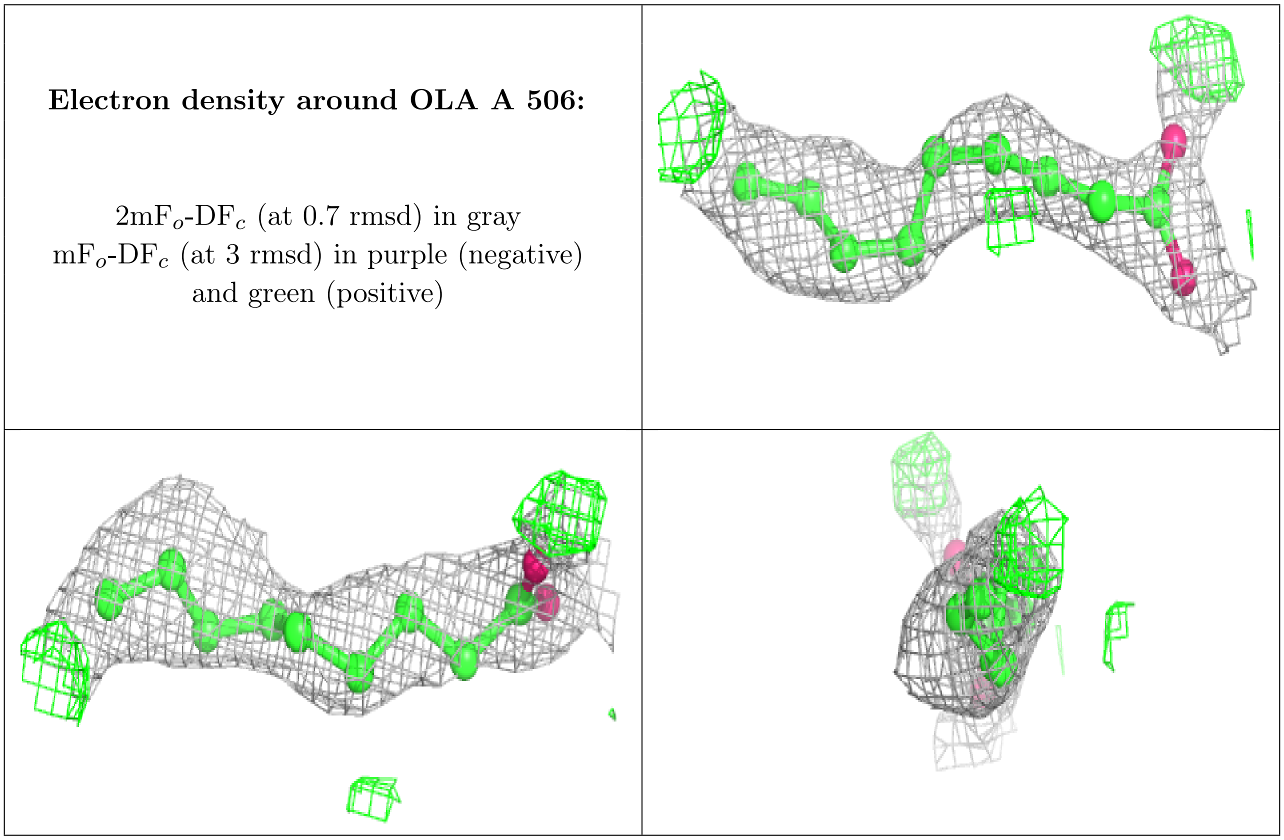
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
2	LFA	B	322	12/20	0.85	0.17	58,60,67,68	0
2	LFA	A	510	9/20	0.86	0.28	44,46,57,61	0
2	LFA	C	311	8/20	0.86	0.28	51,56,57,58	0
3	OLA	B	304	14/20	0.86	0.15	44,47,62,62	0
2	LFA	B	314	15/20	0.87	0.17	46,55,68,69	0
2	LFA	C	301	17/20	0.87	0.30	42,49,54,60	0
3	OLA	A	505	14/20	0.90	0.16	41,53,74,87	0
2	LFA	A	515	6/20	0.90	0.24	39,50,52,54	0
2	LFA	A	520	6/20	0.90	0.21	44,48,53,53	0
4	PO4	C	318	5/5	0.90	0.36	84,84,89,91	5
2	LFA	B	301	6/20	0.91	0.17	42,42,48,52	0
2	LFA	B	302	9/20	0.91	0.33	44,47,50,51	0
2	LFA	A	501	6/20	0.91	0.18	43,45,53,54	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.

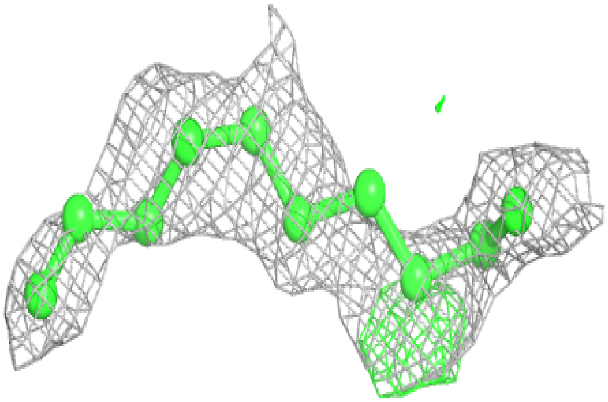


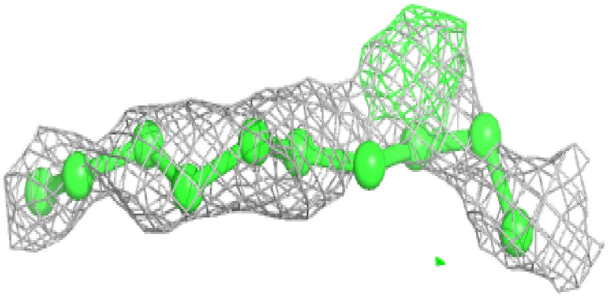
Electron density around OLA A 506:

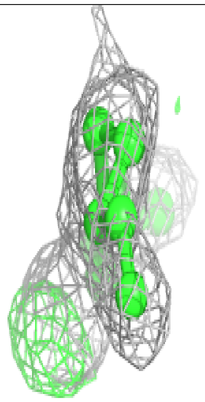
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around 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)

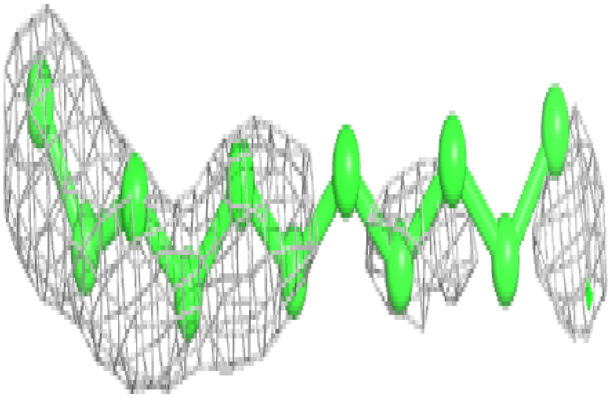


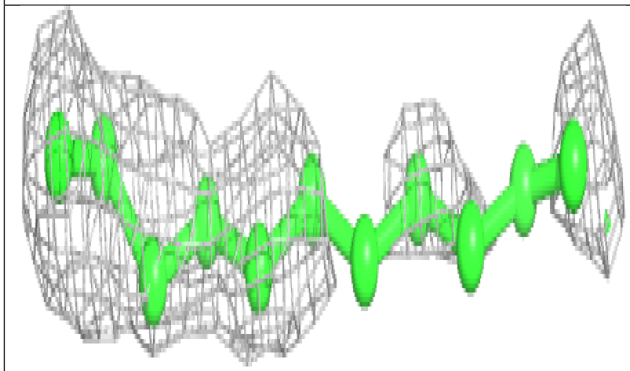


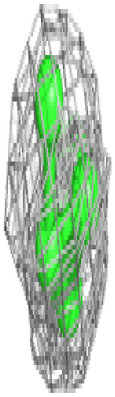


Electron density around LFA C 307:

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

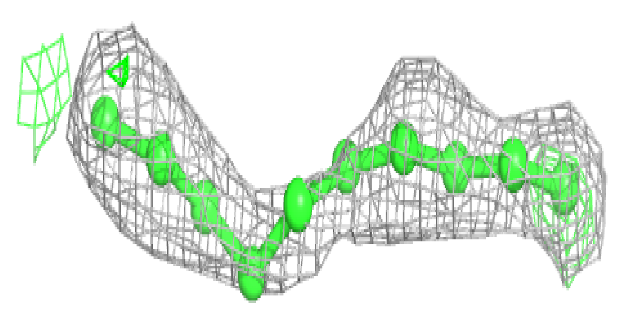


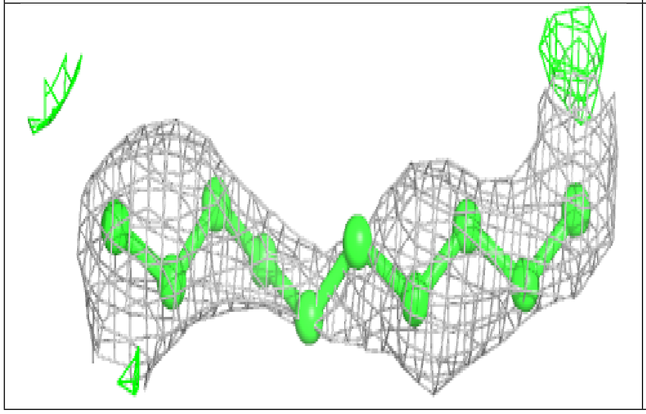


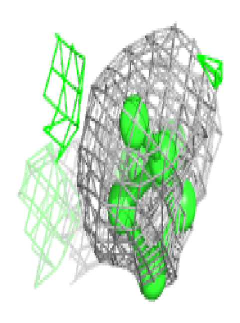


Electron density around LFA C 306:

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 B 323:

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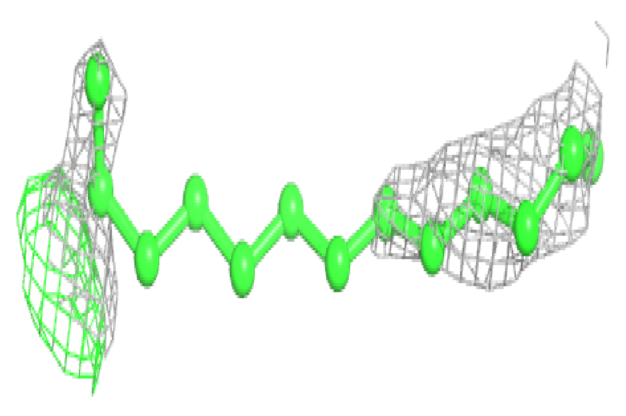
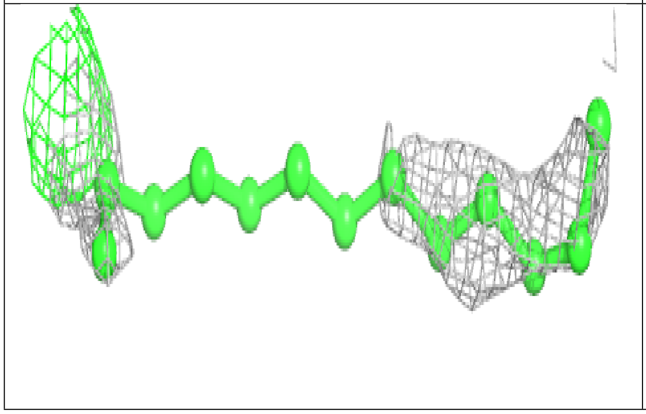
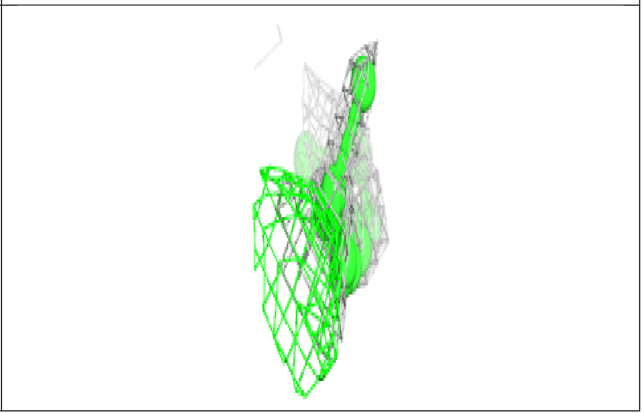
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

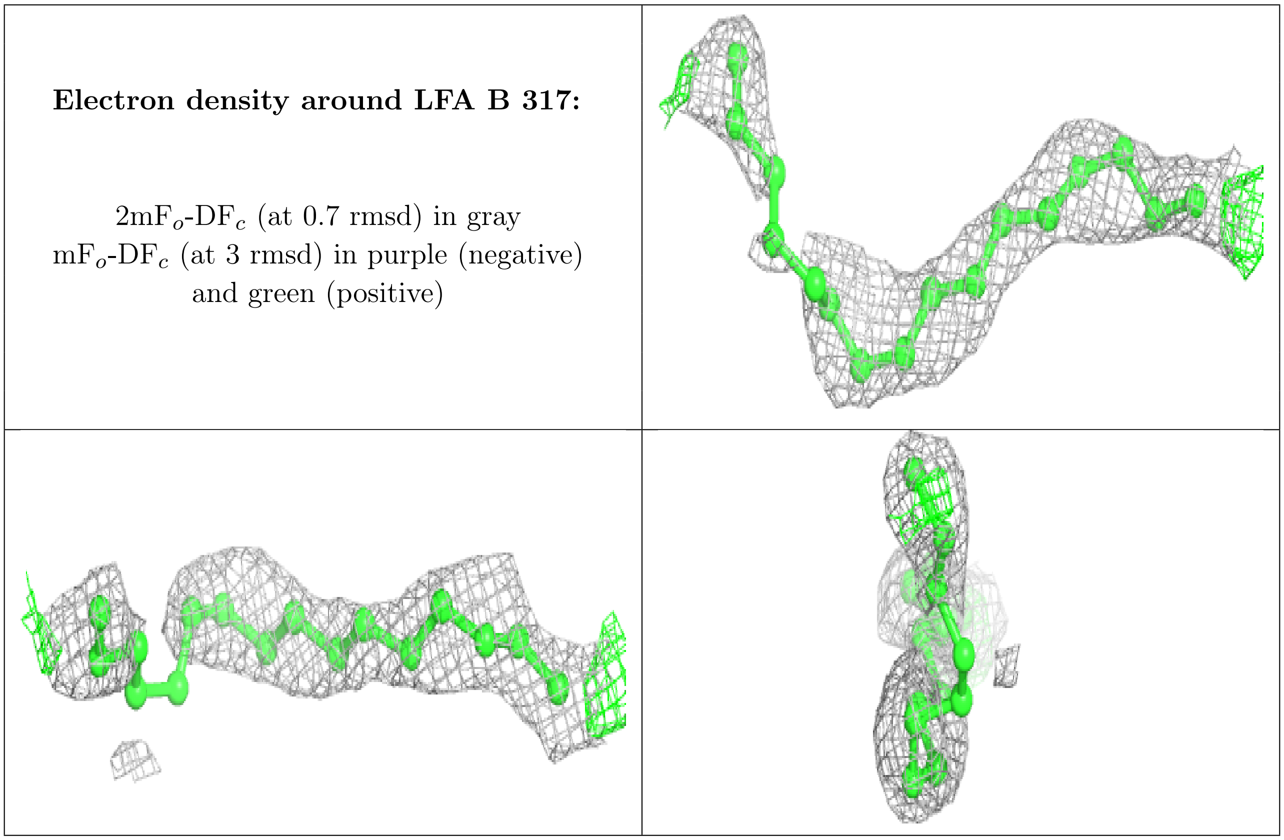






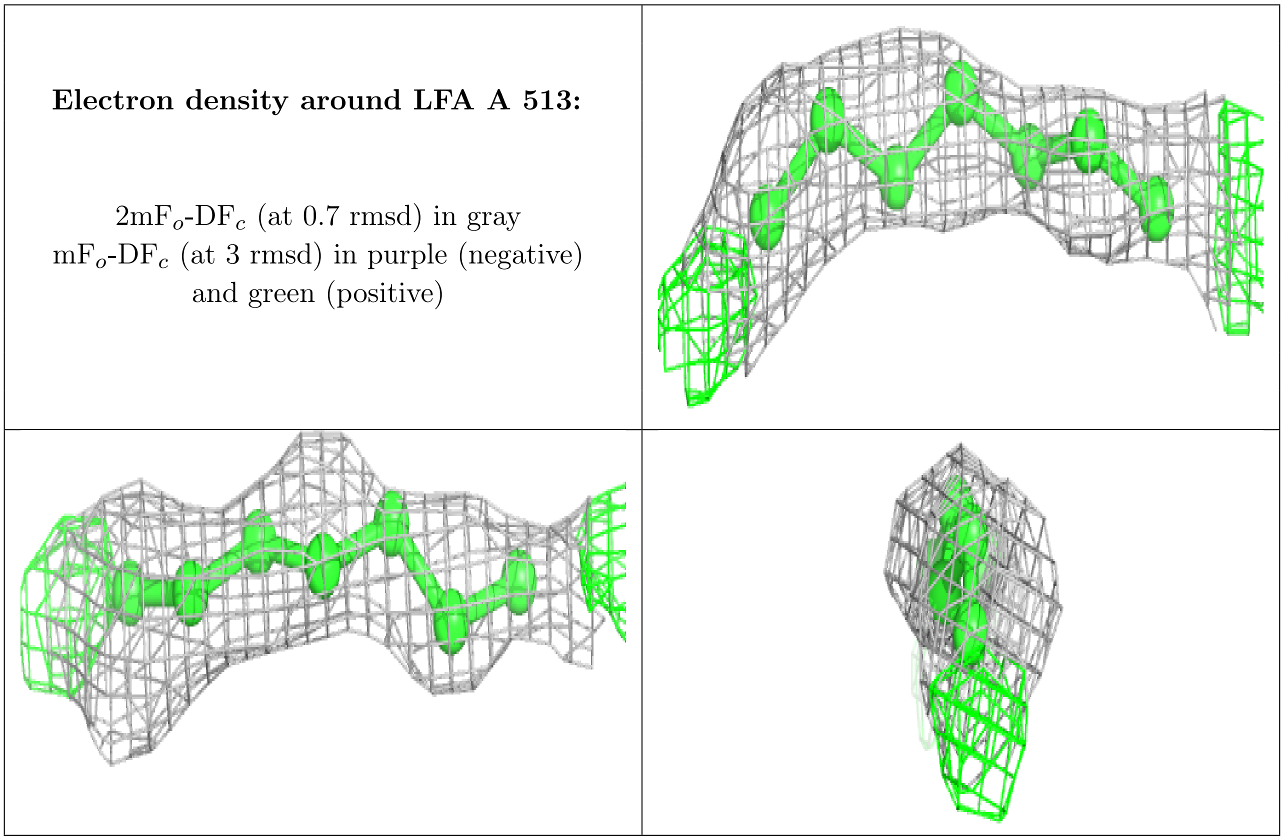
Electron density around LFA B 317:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



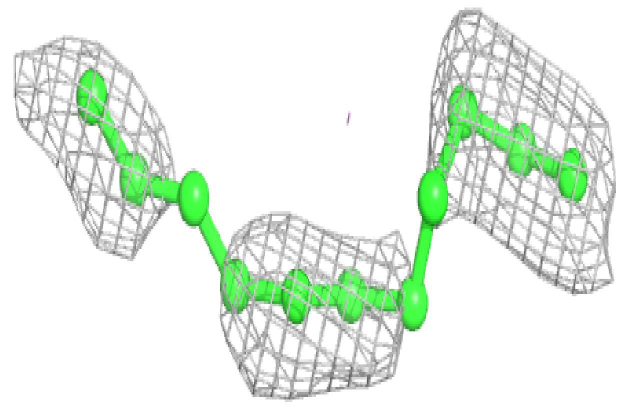
Electron density around LFA A 513:

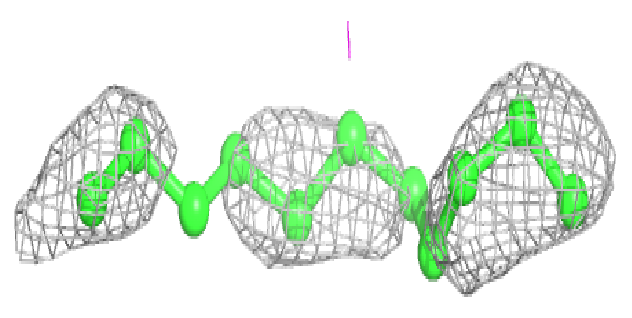
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

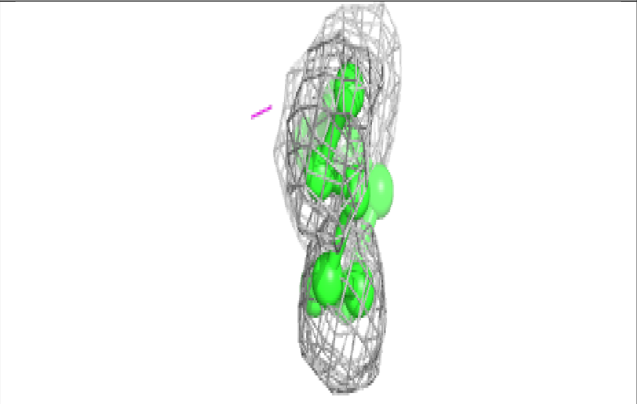


Electron density around LFA C 317:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

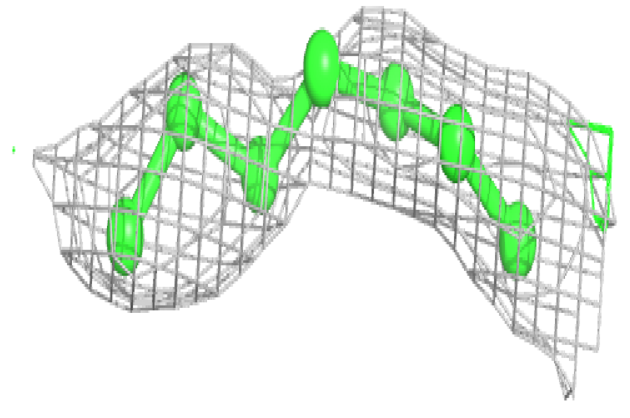


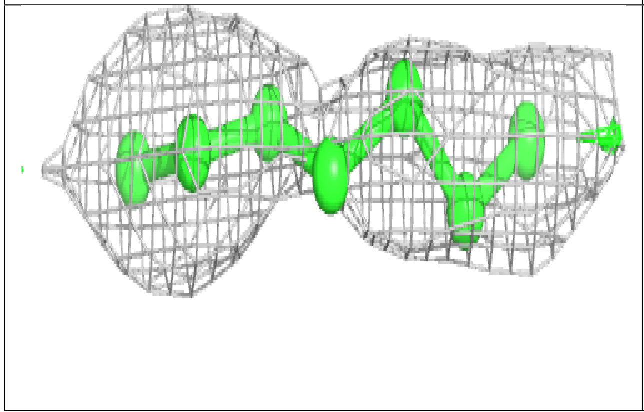


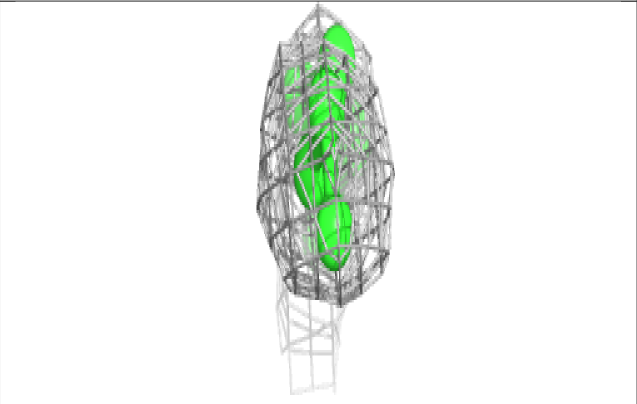


Electron density around LFA B 310:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

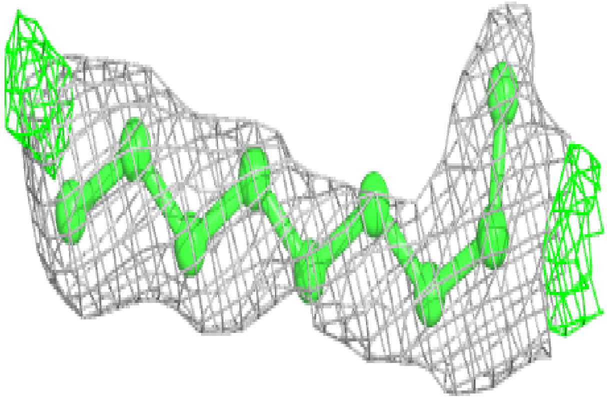


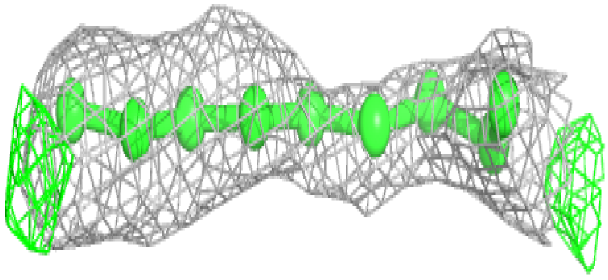


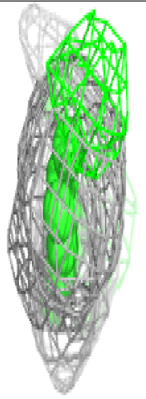


Electron density around LFA C 315:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

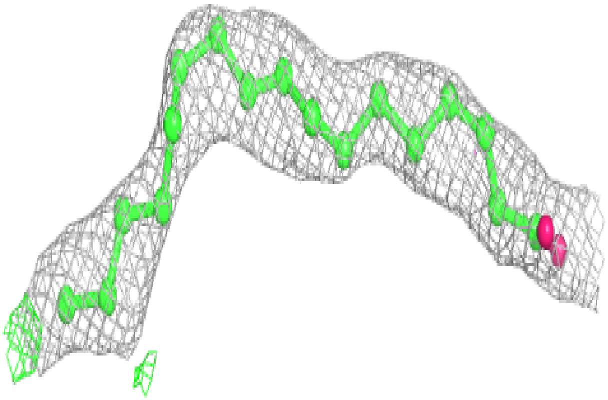


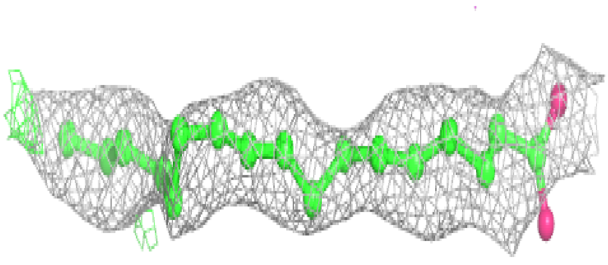


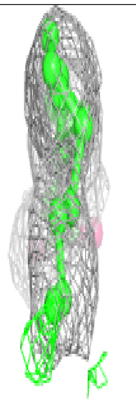


Electron density around OLA B 308:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

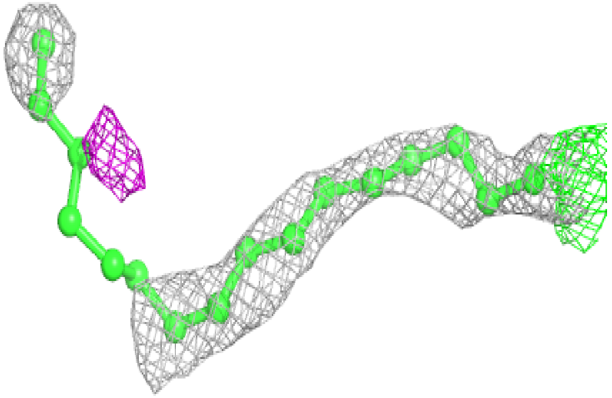


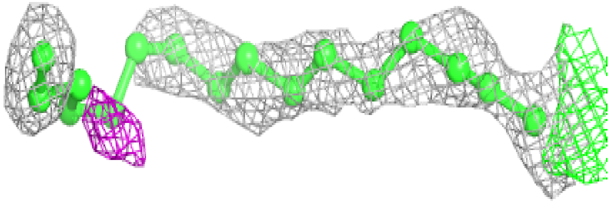


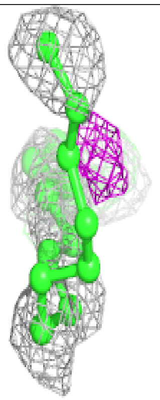


Electron density around LFA C 312:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

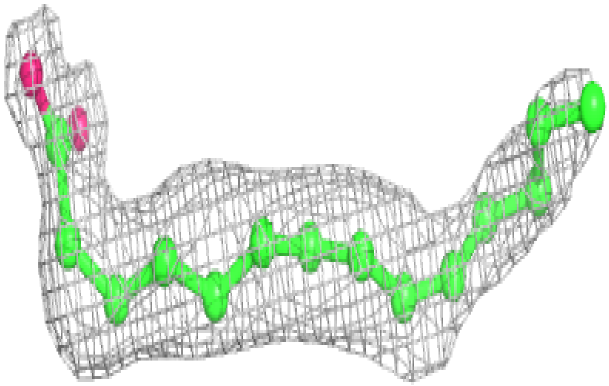


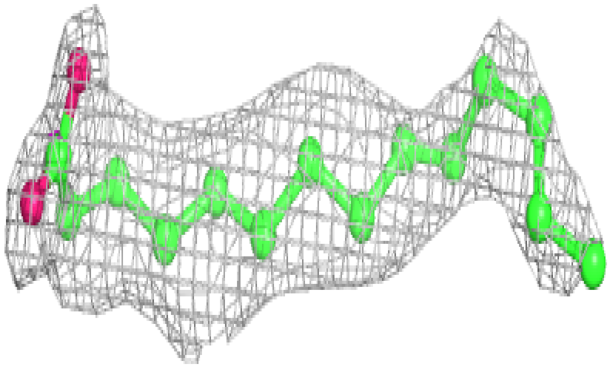


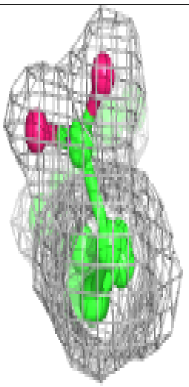


Electron density around OLA B 307:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

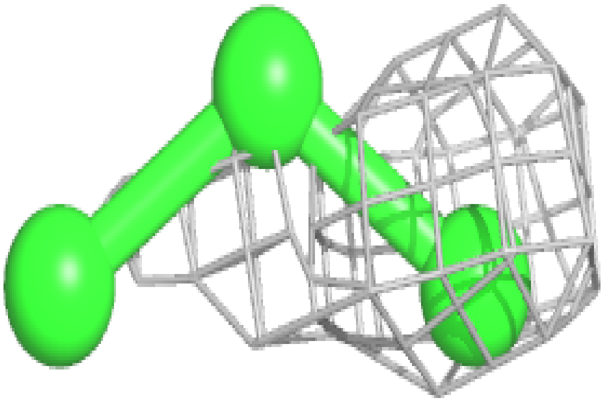


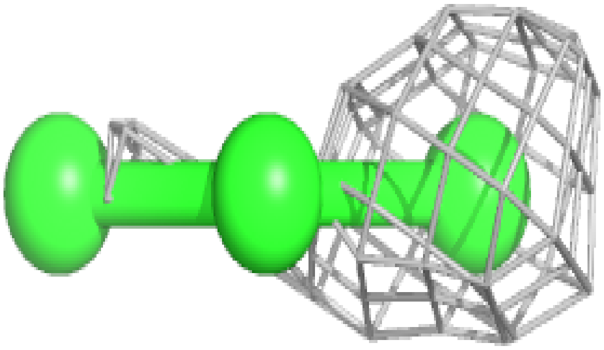


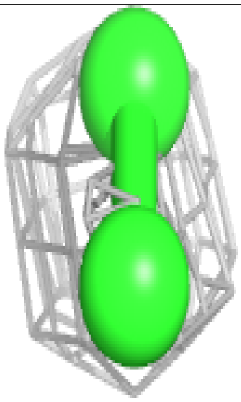


Electron density around LFA A 516:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

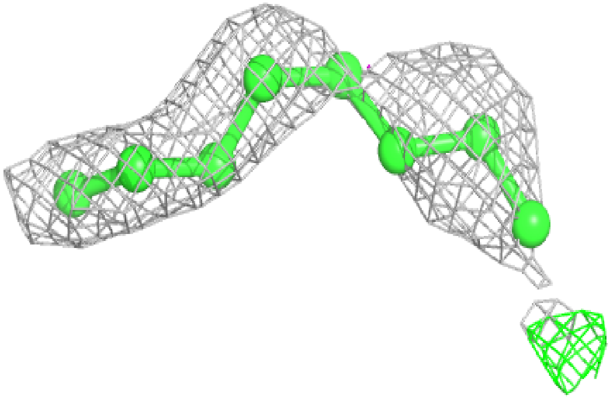


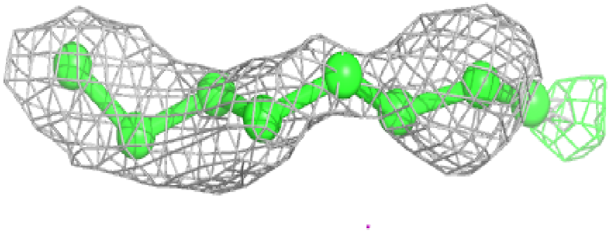


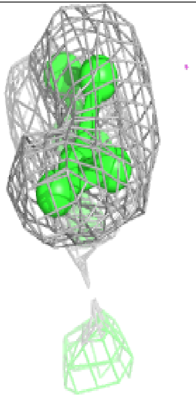


Electron density around LFA B 316:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

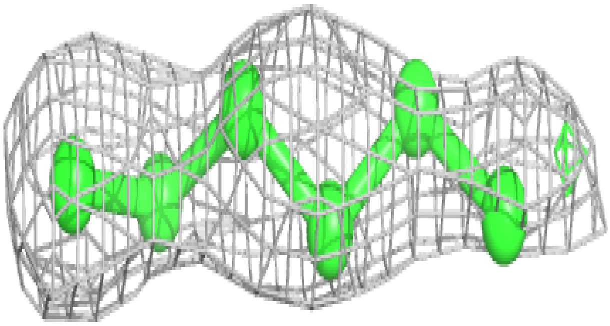


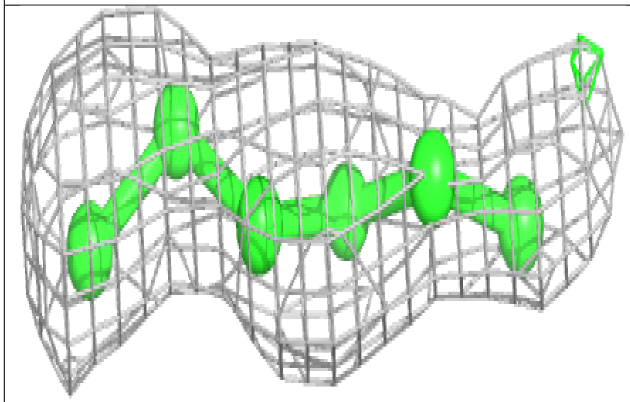


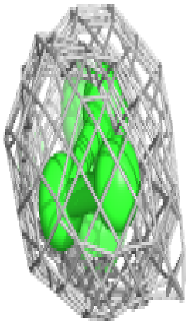


Electron density around LFA B 309:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

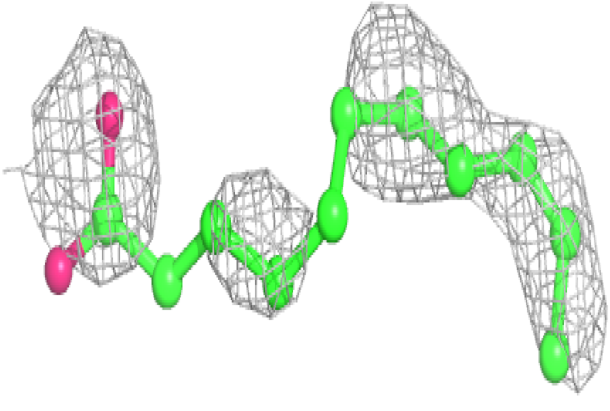


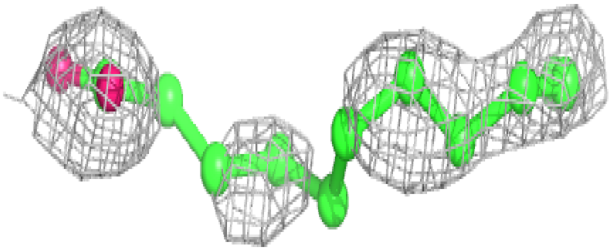




Electron density around OLA A 508:

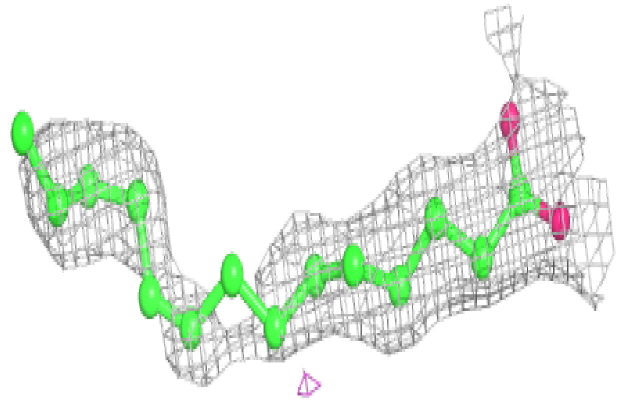
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

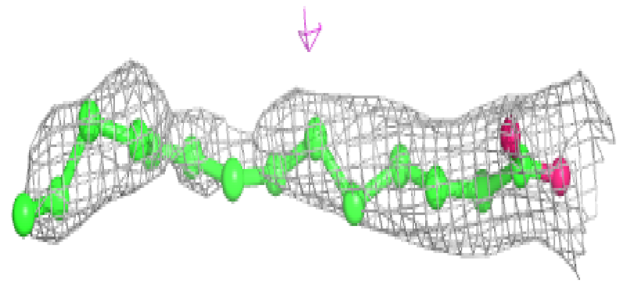


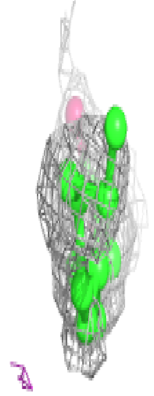


Electron density around OLA C 303:

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

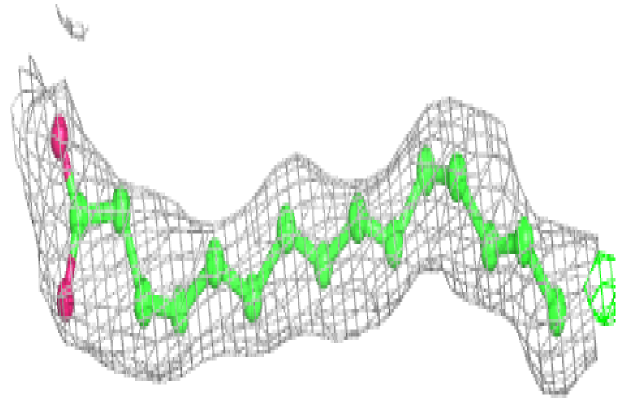


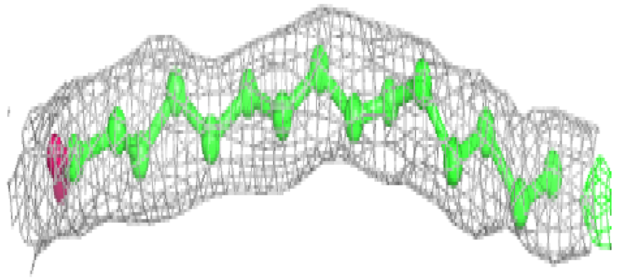




Electron density around OLA B 306:

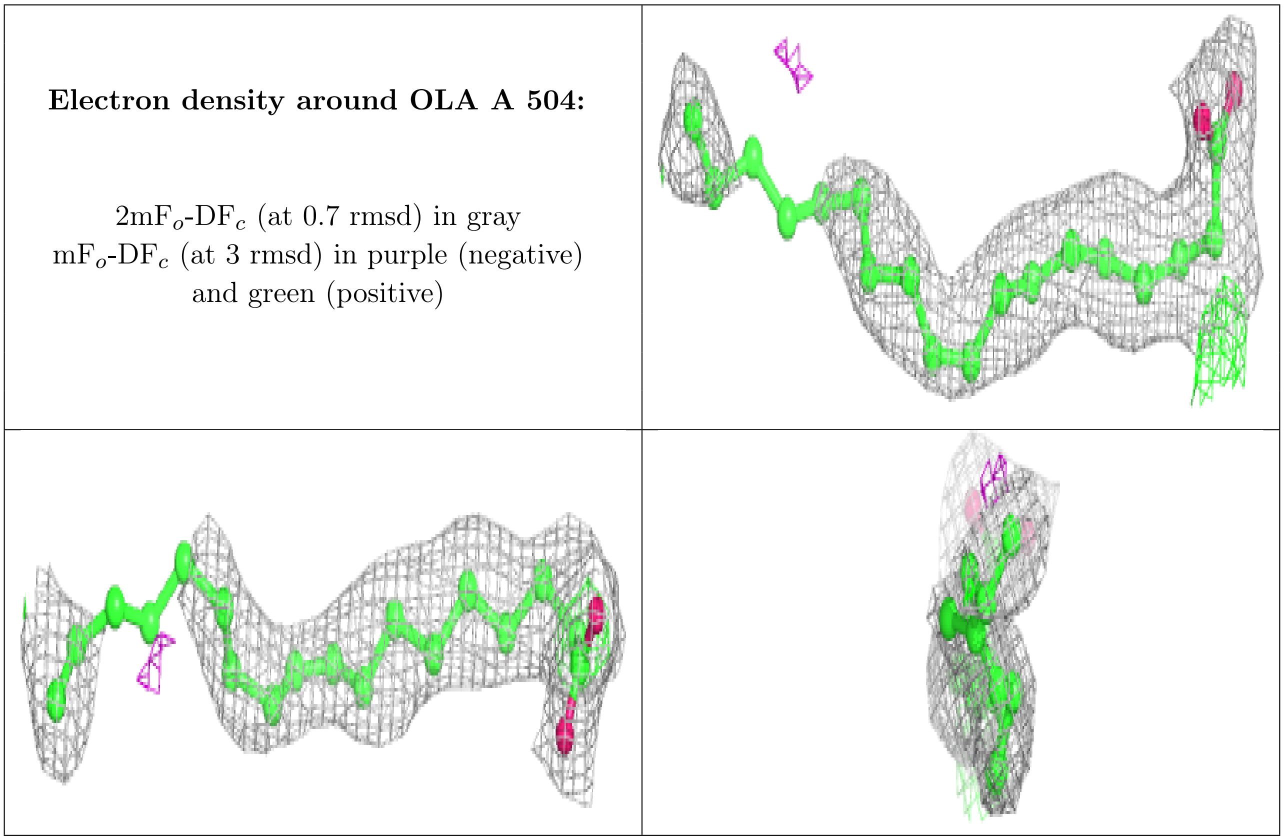
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





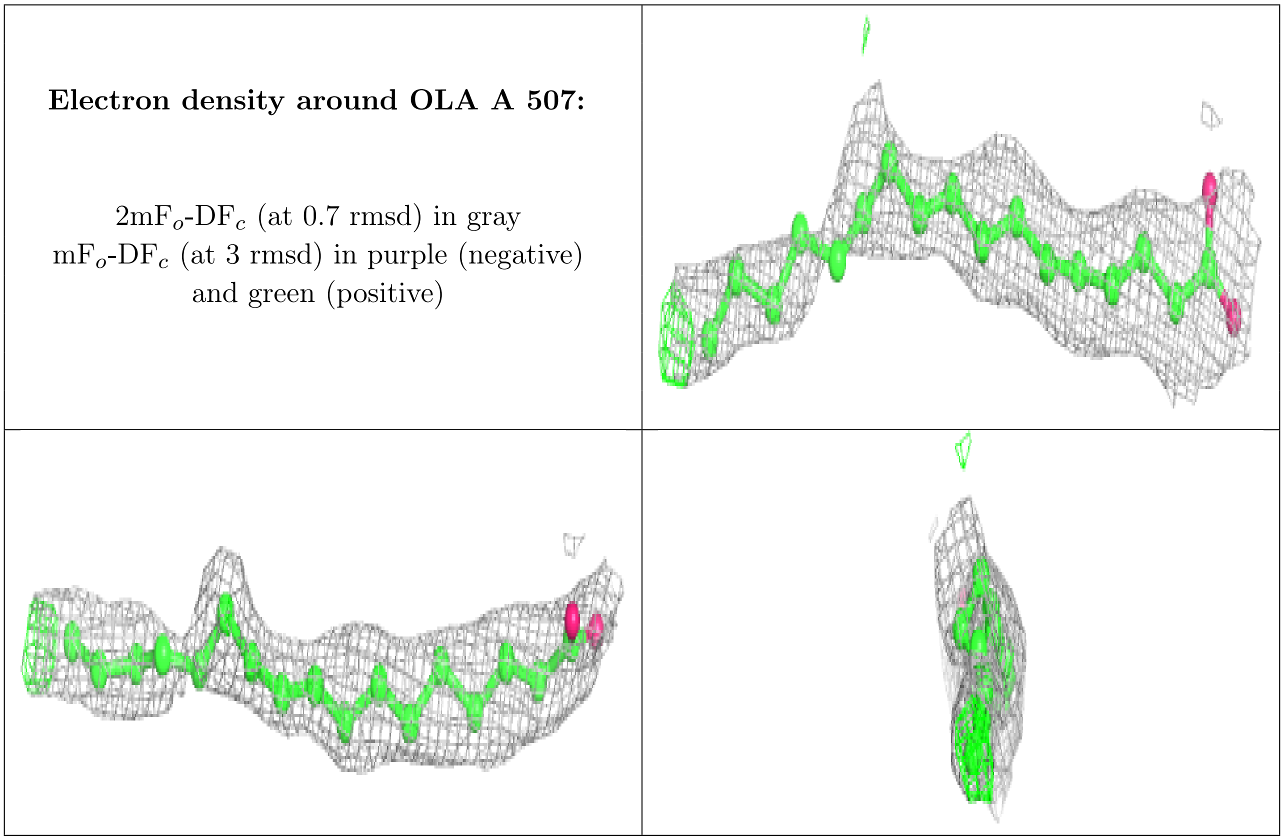
Electron density around OLA A 504:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



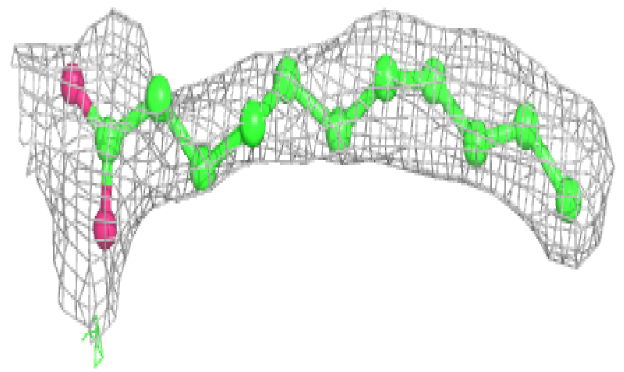
Electron density around OLA A 507:

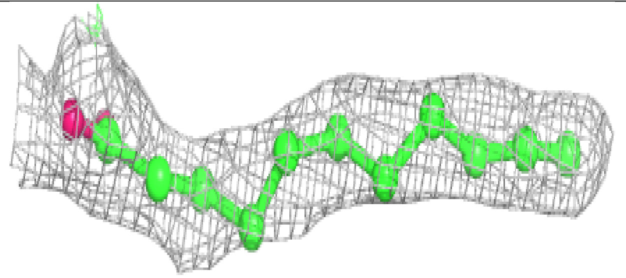
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

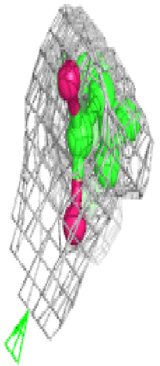


Electron density around OLA C 304:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

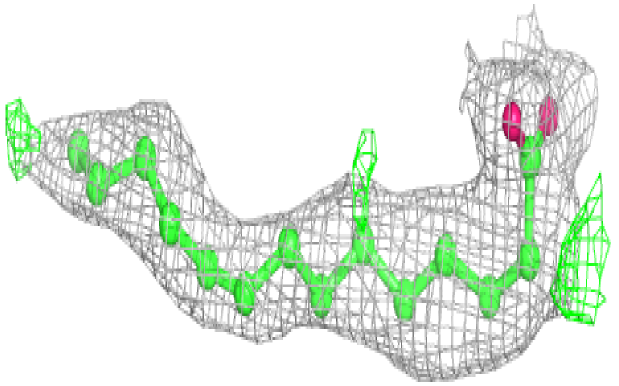


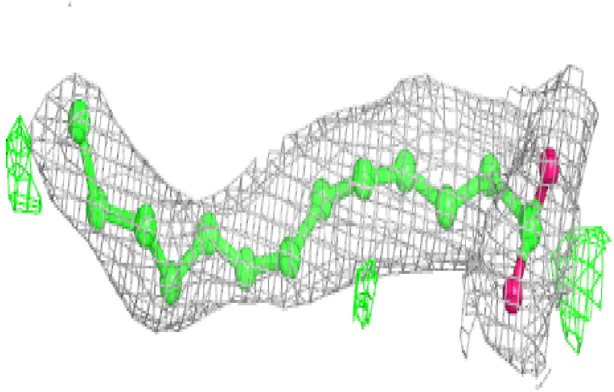


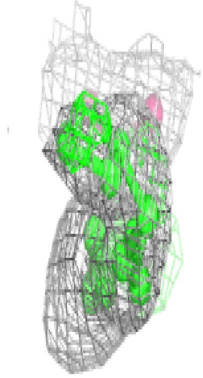


Electron density around OLA C 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

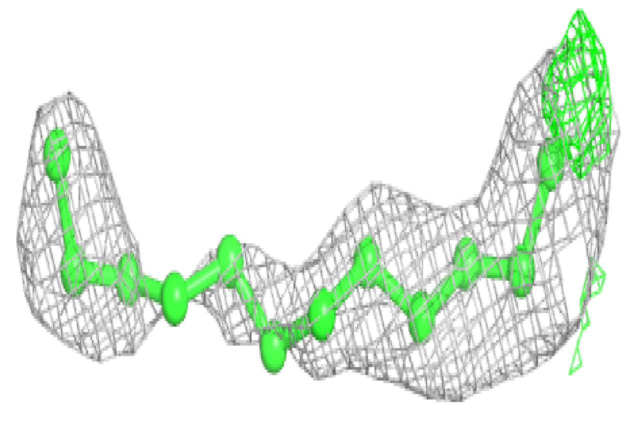


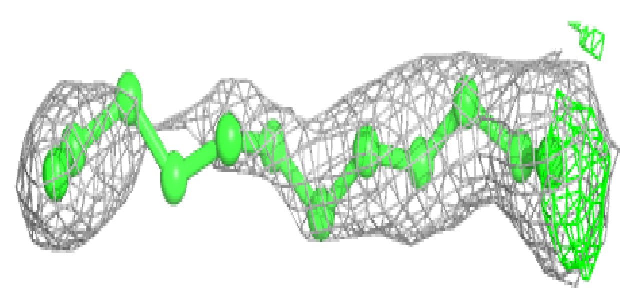


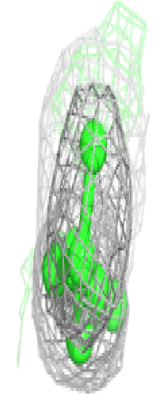


Electron density around LFA A 512:

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

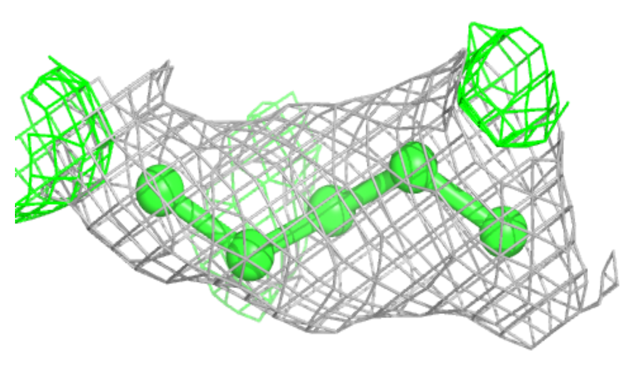


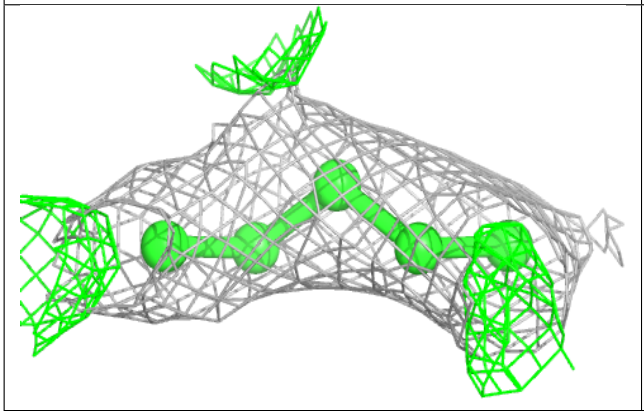


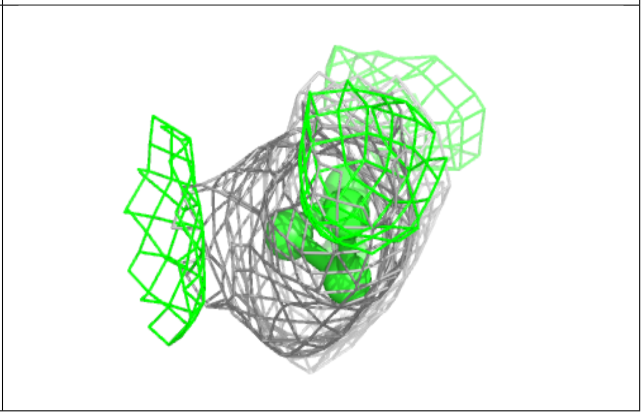


Electron density around LFA A 517:

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

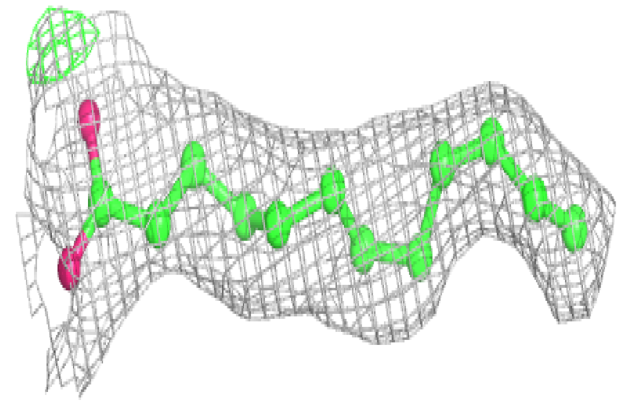


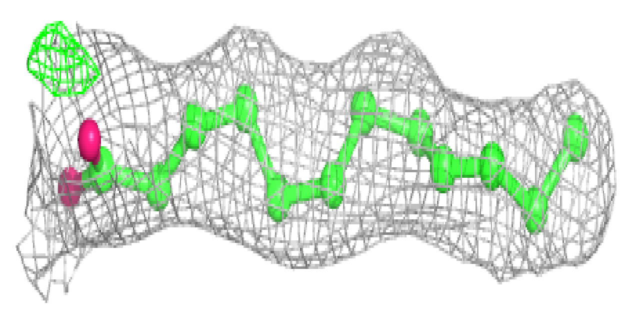


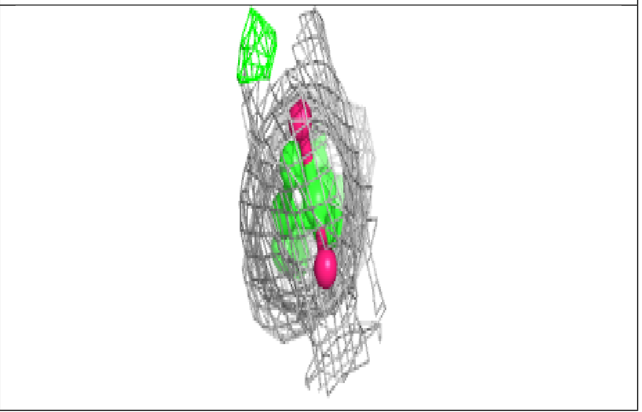


Electron density around OLA B 303:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

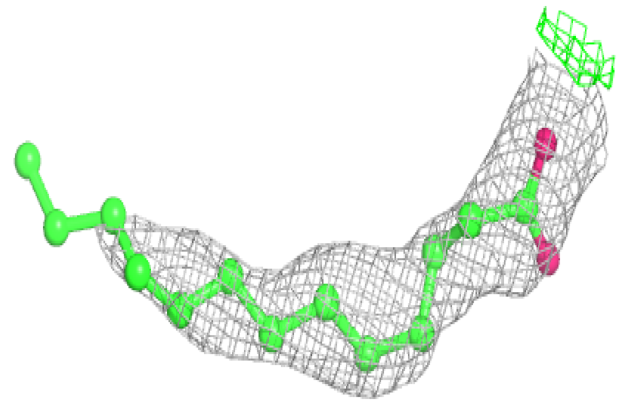


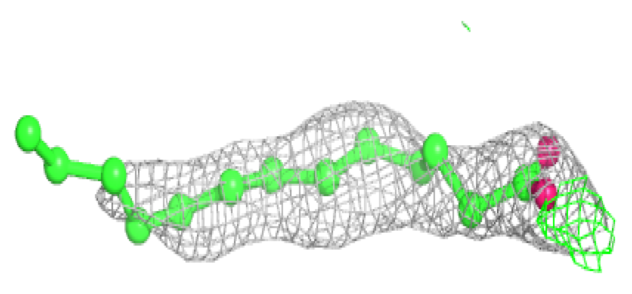


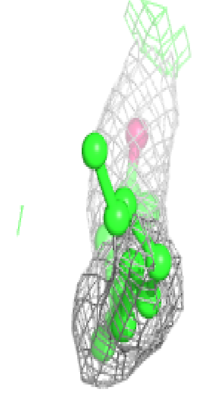


Electron density around OLA C 305:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

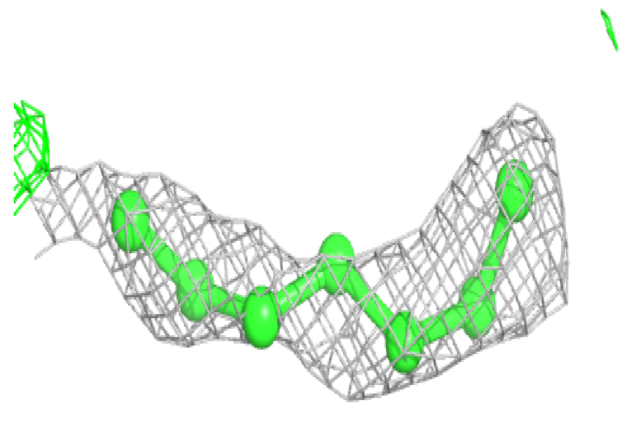


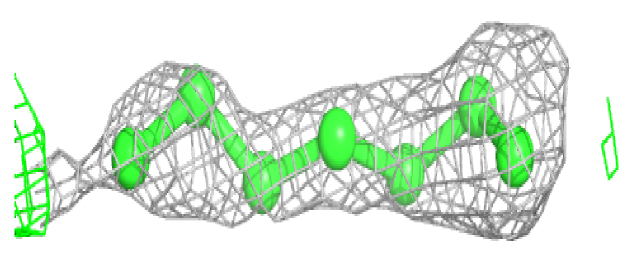


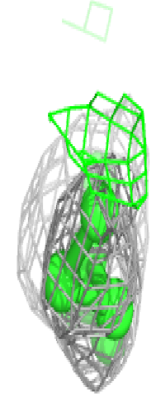


Electron density around LFA A 519:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

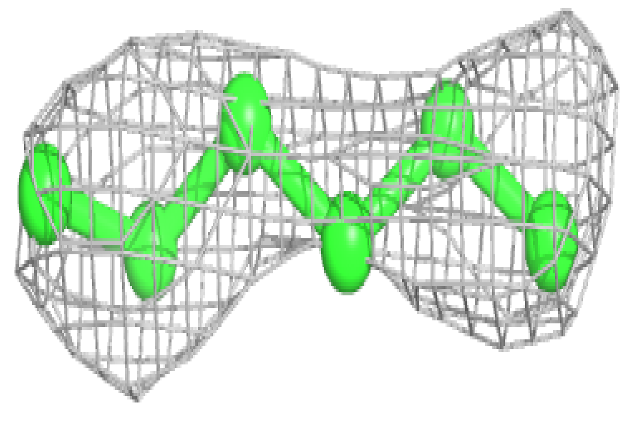


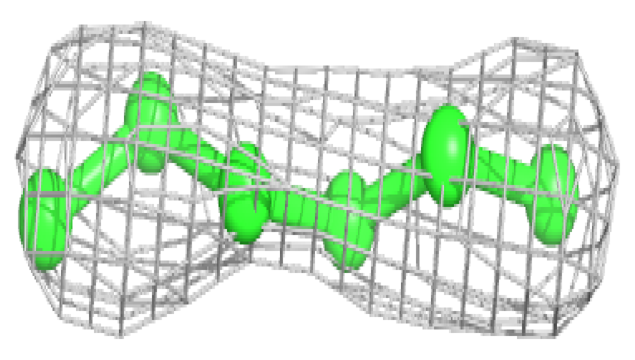


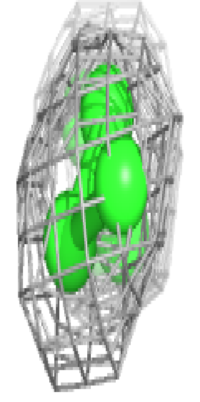


Electron density around LFA B 313:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

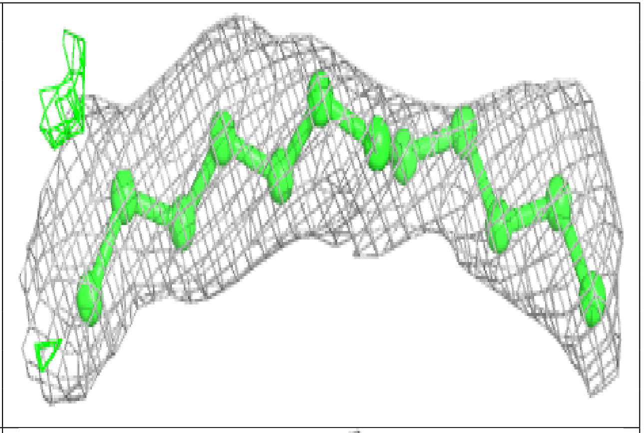


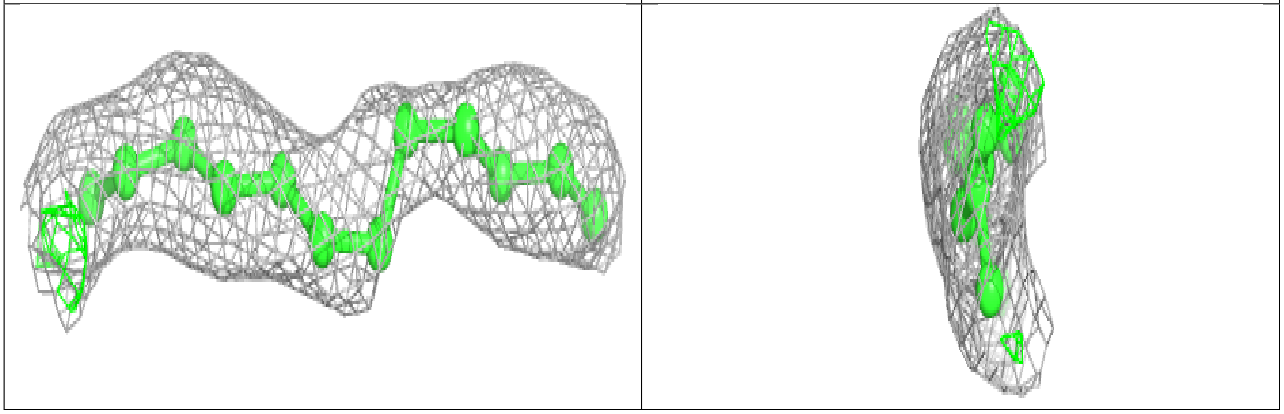




Electron density around LFA B 318:

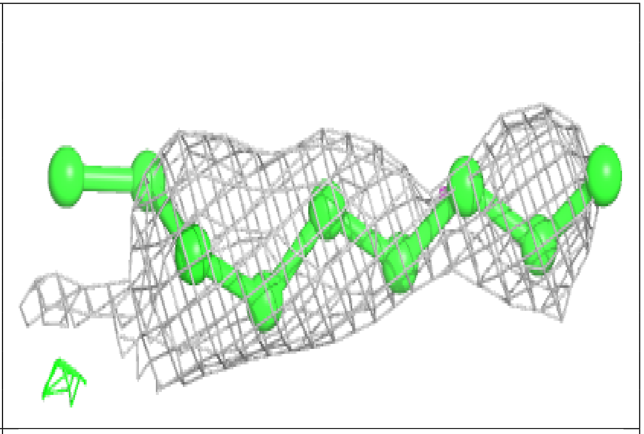
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

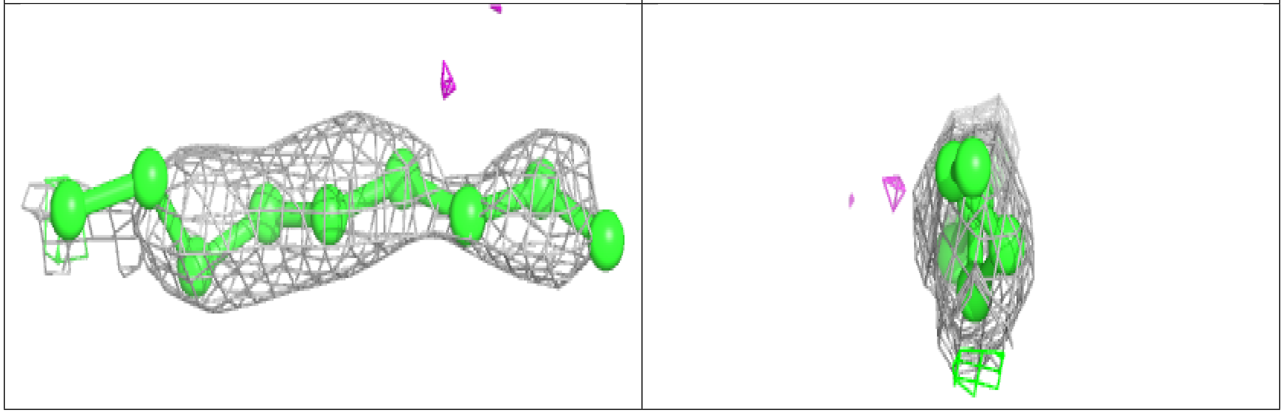




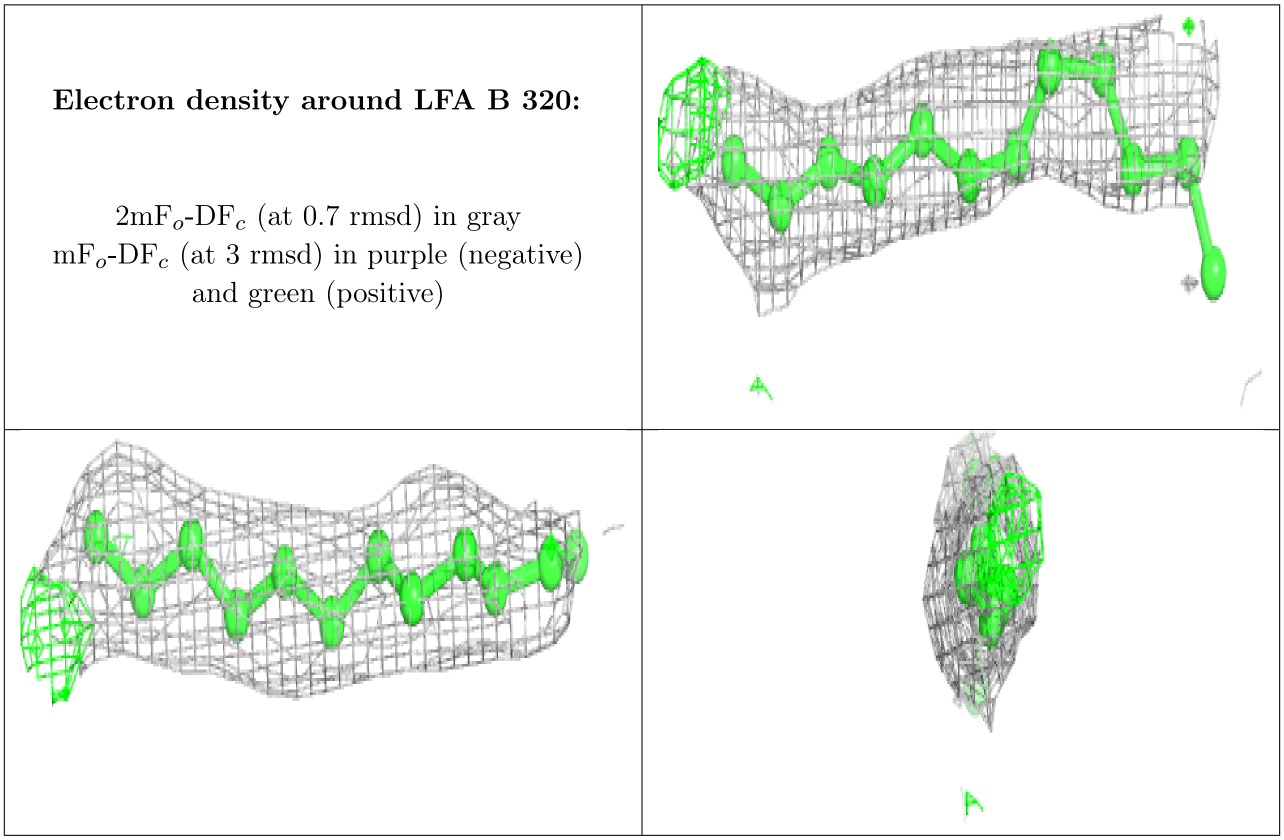
Electron density around LFA A 509:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



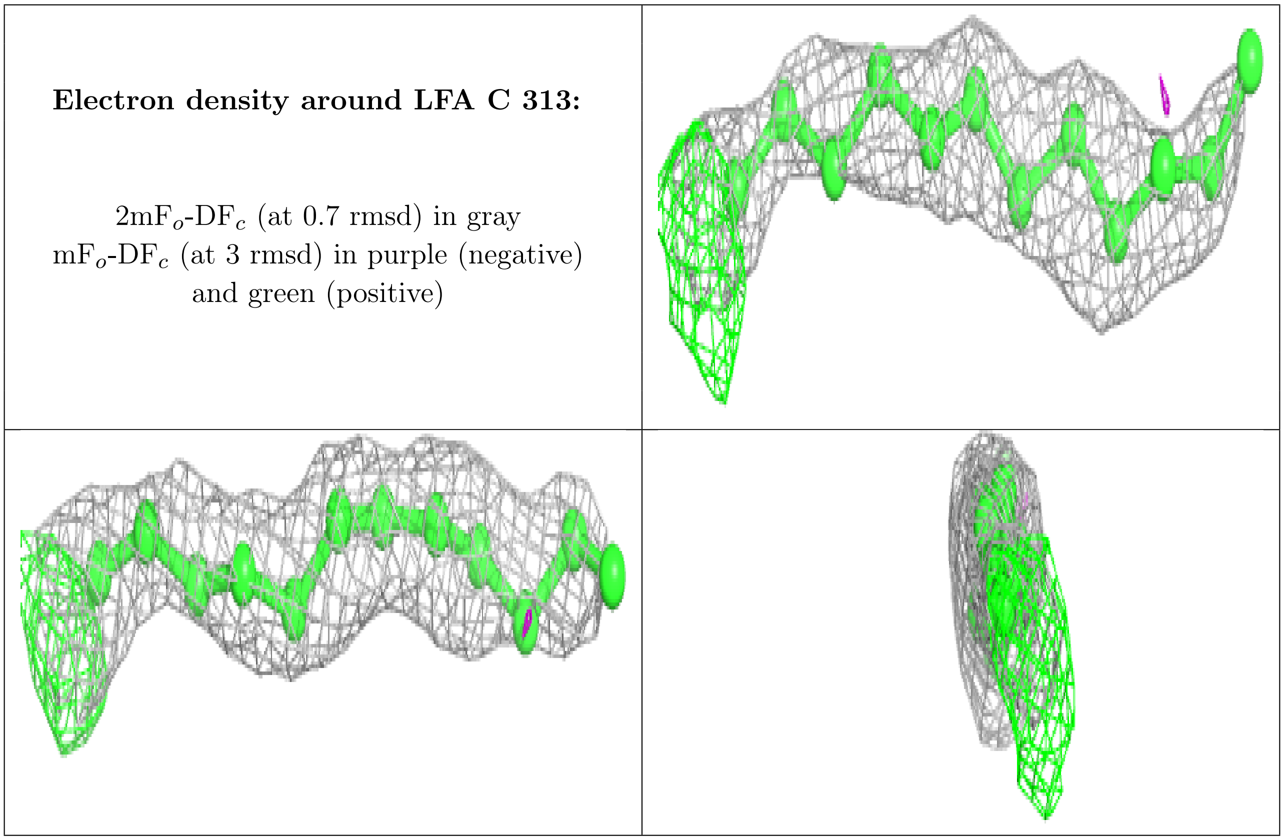


Electron density around LFA B 320:



2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

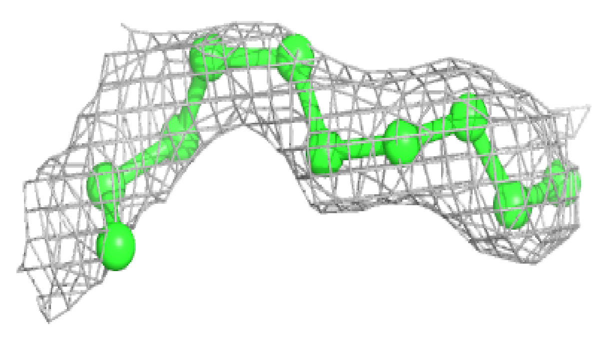
Electron density around LFA C 313:

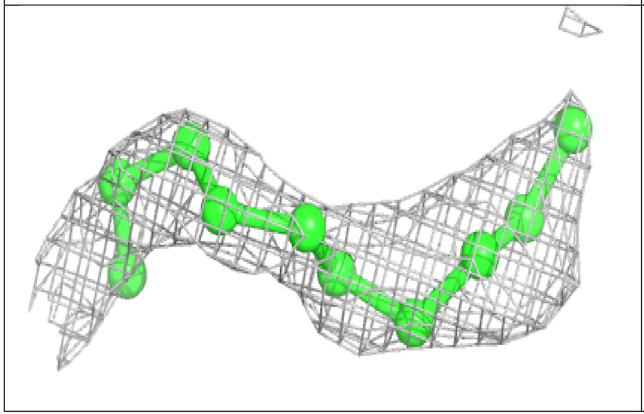


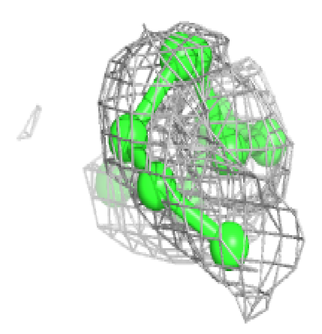
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around LFA B 321:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

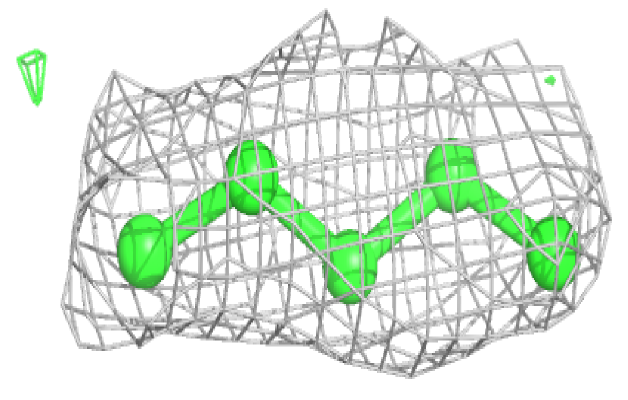


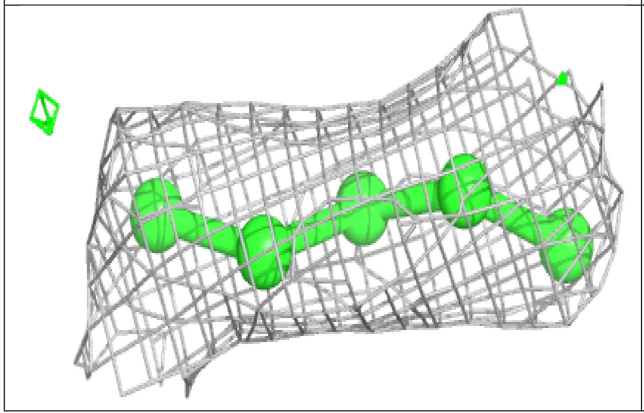


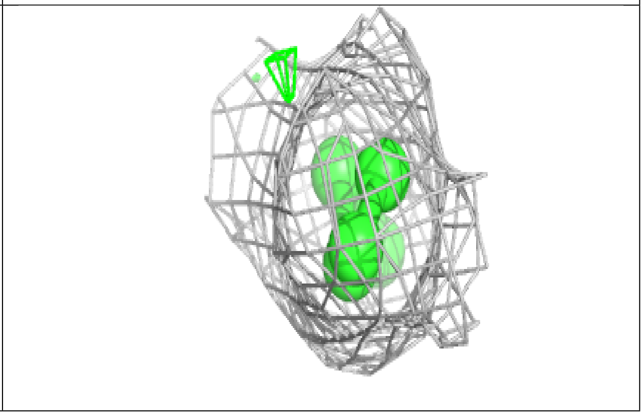


Electron density around LFA B 312:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

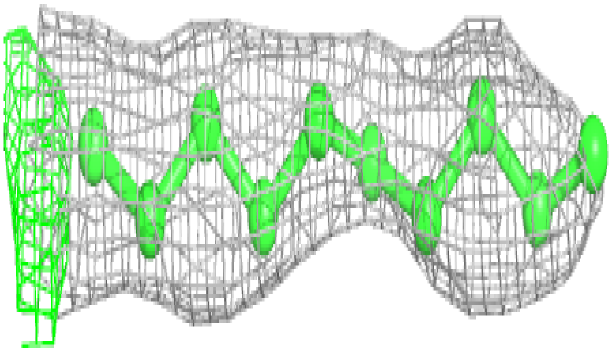


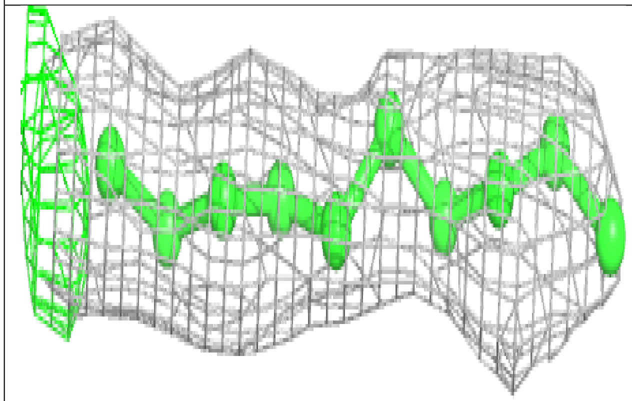


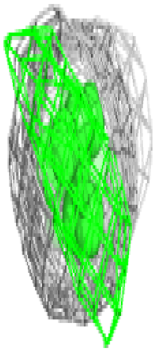


Electron density around LFA C 314:

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

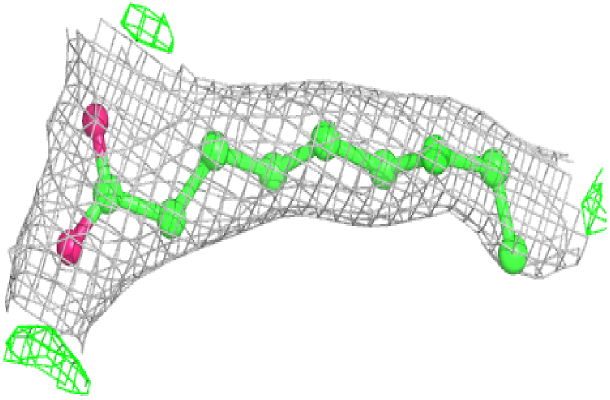


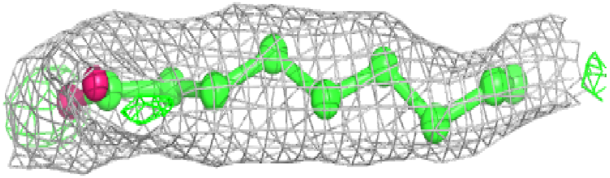


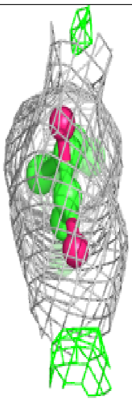


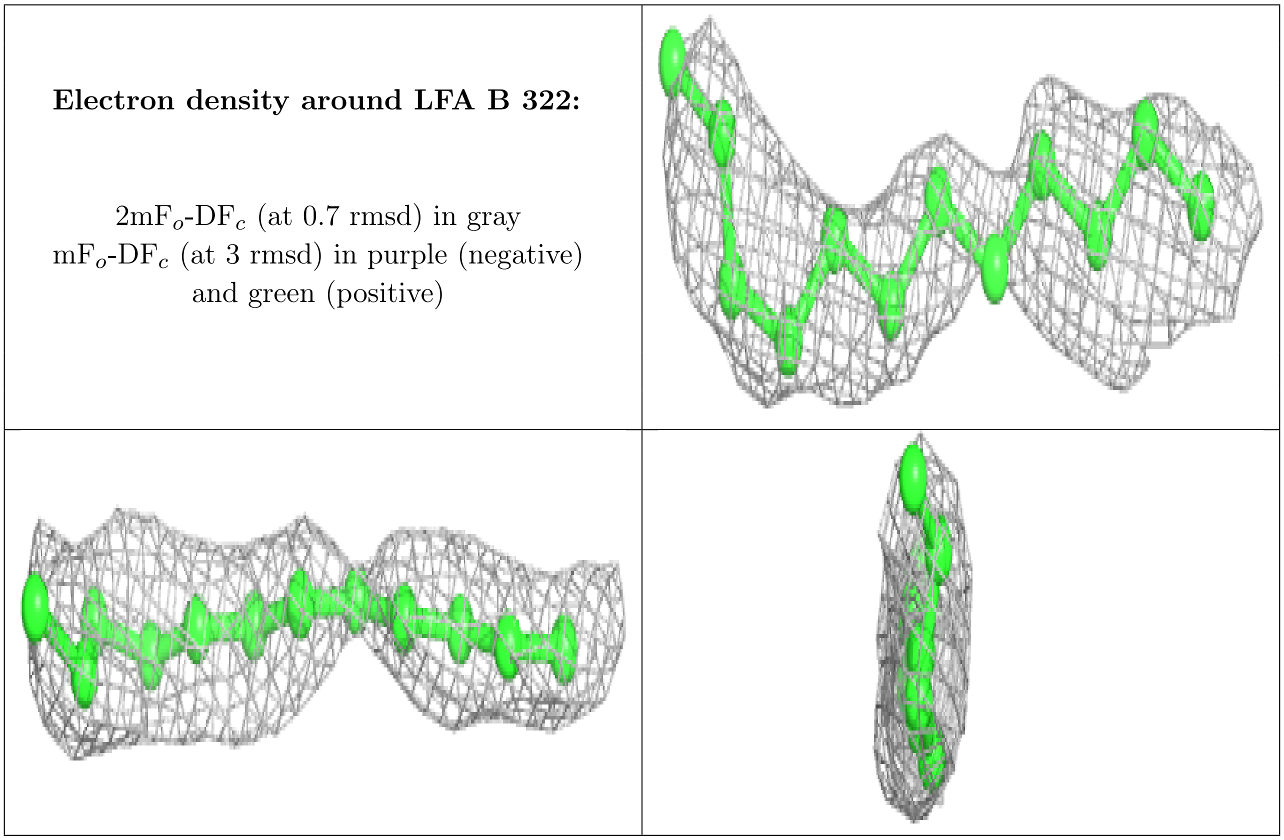
Electron density around OLA A 503:

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



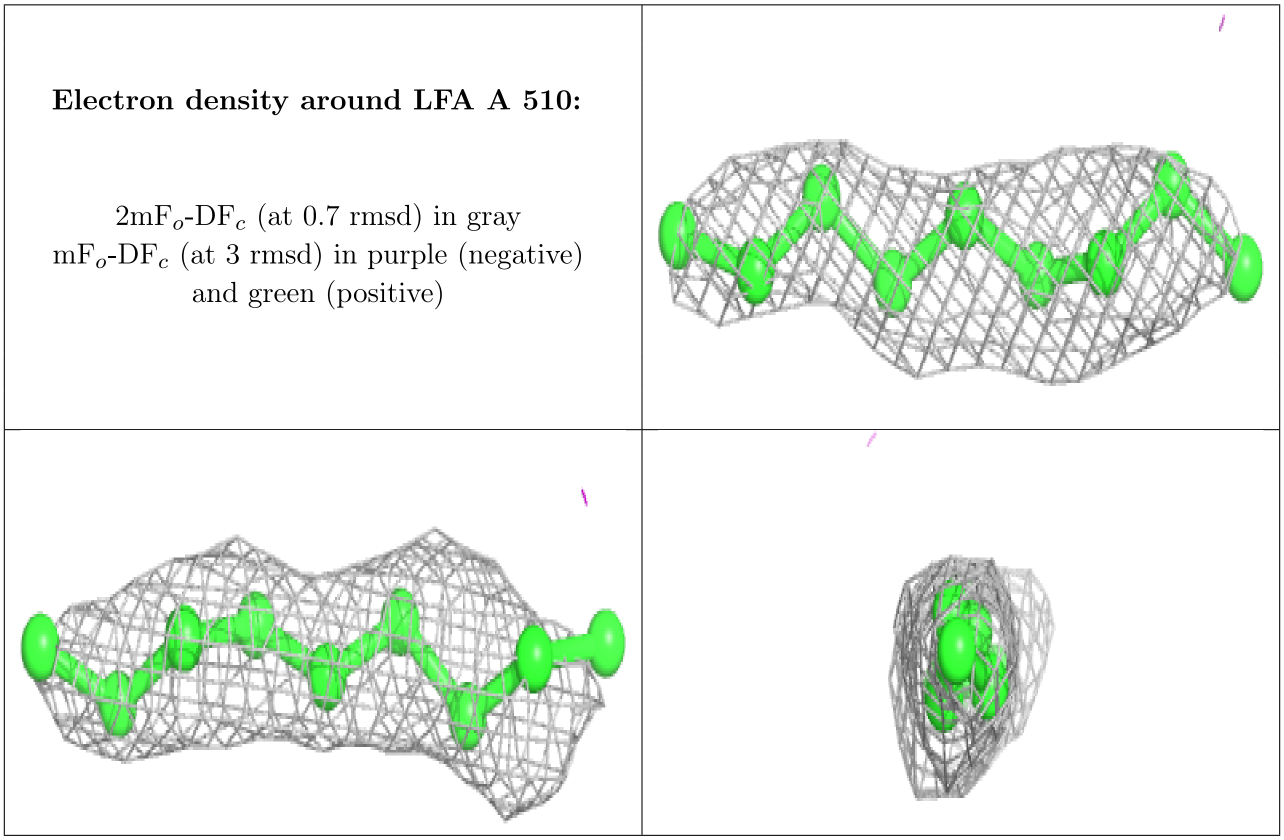






Electron density around LFA B 322:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

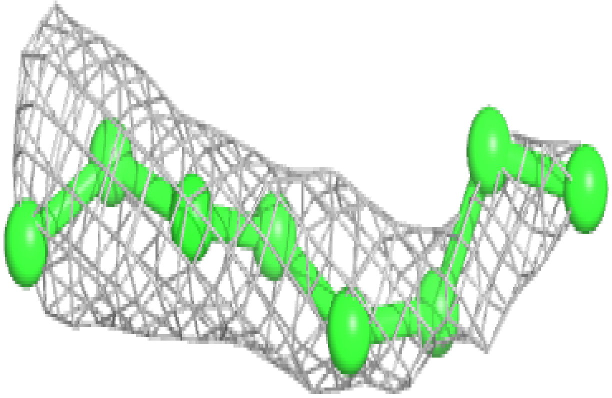


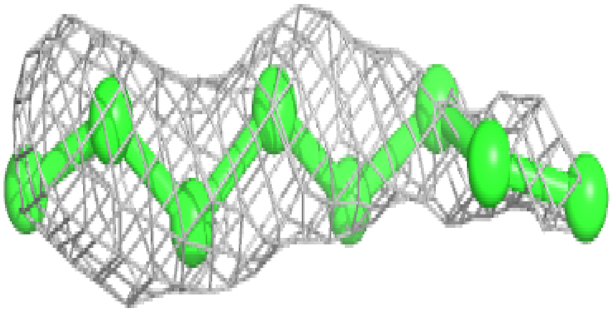
Electron density around LFA A 510:

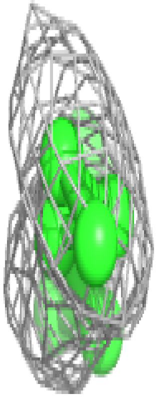
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around LFA C 311:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

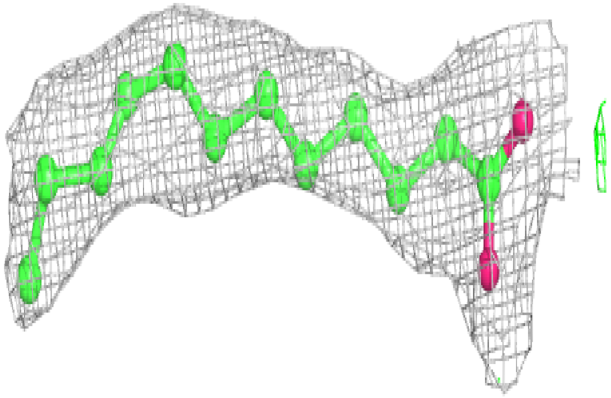


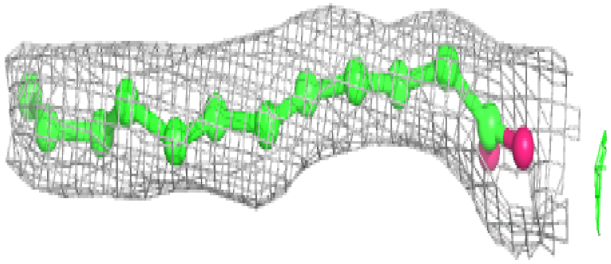


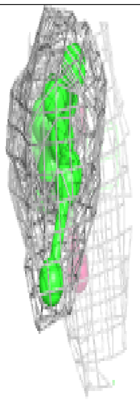


Electron density around OLA B 304:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

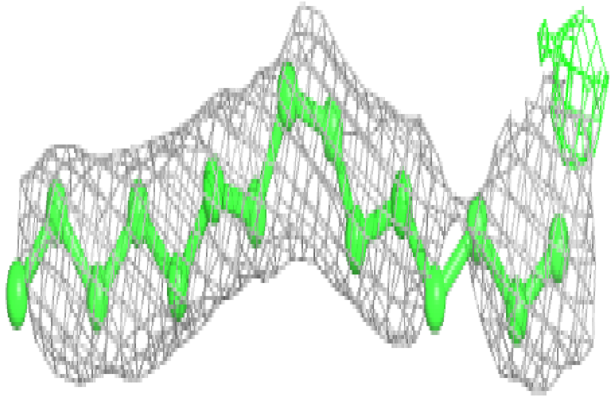


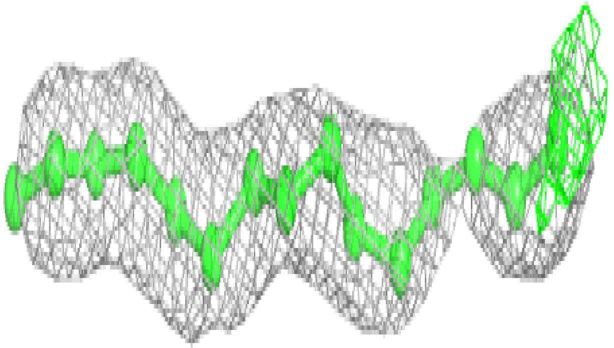




Electron density around LFA B 314:

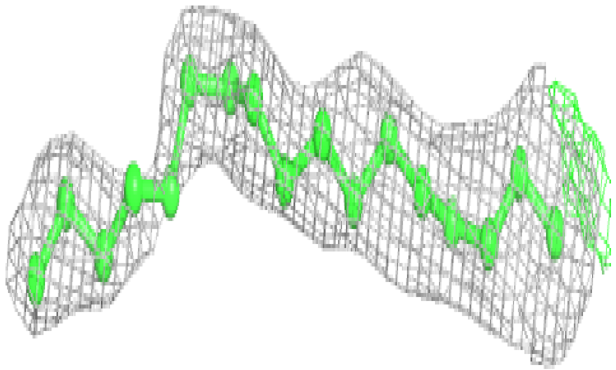
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

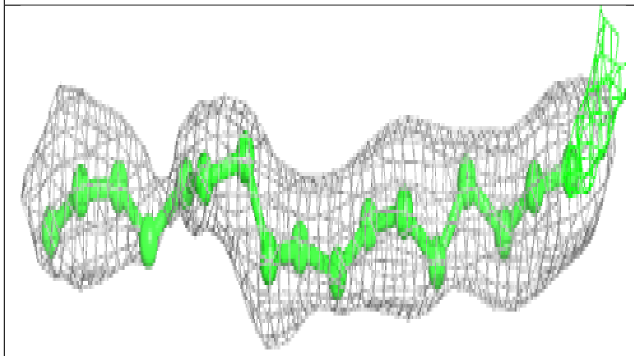


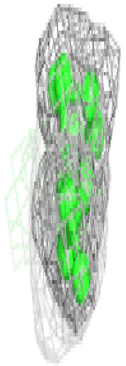


Electron density around LFA C 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

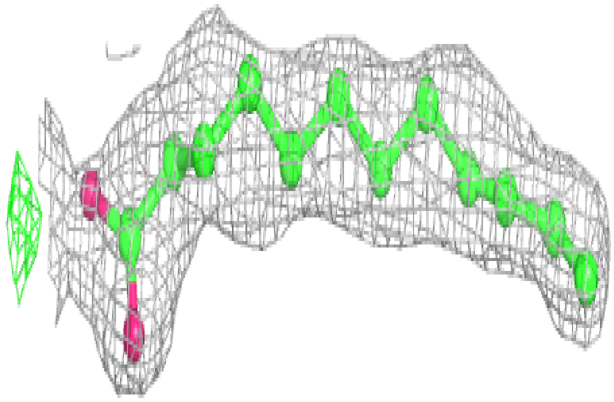


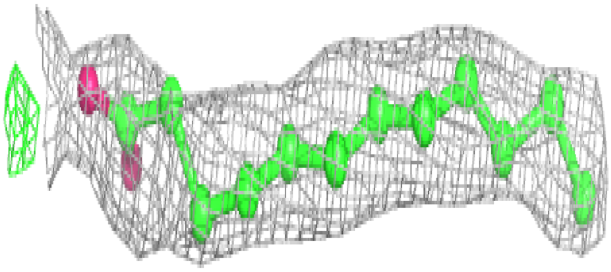


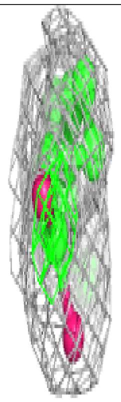


Electron density around OLA A 505:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

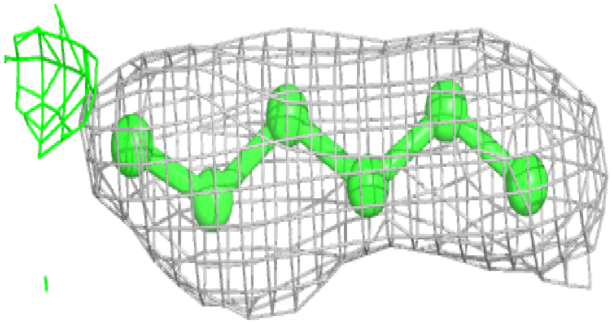


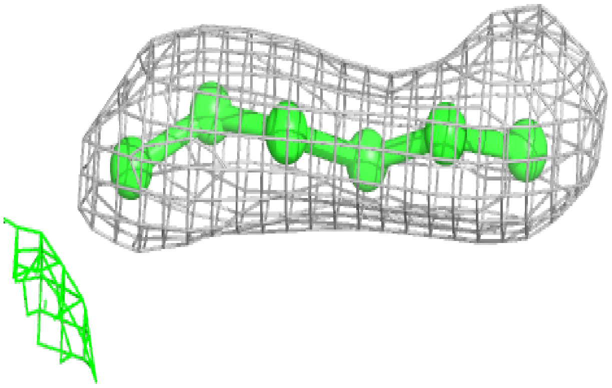


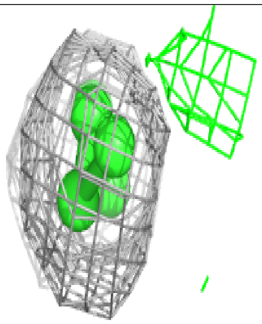


Electron density around LFA A 515:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

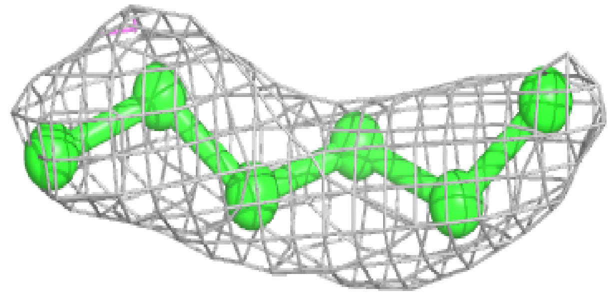


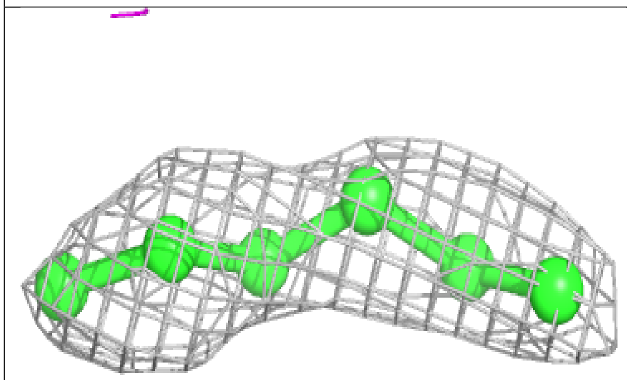


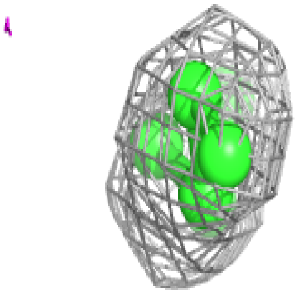


Electron density around LFA A 520:

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

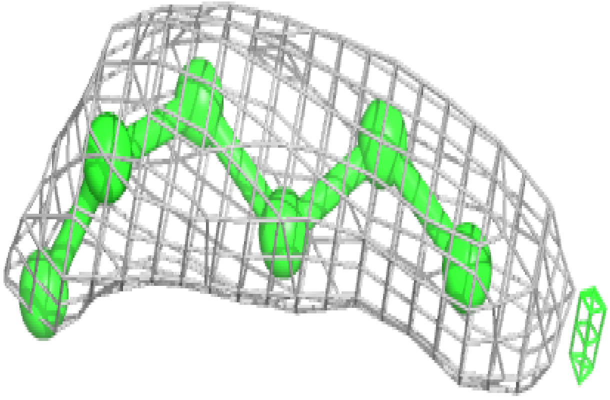


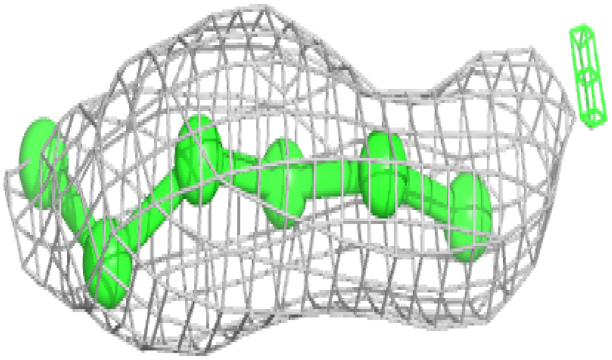


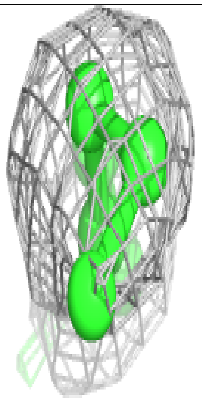


Electron density around LFA B 301:

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

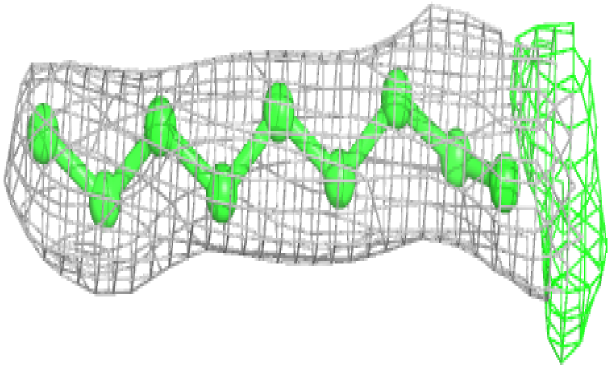


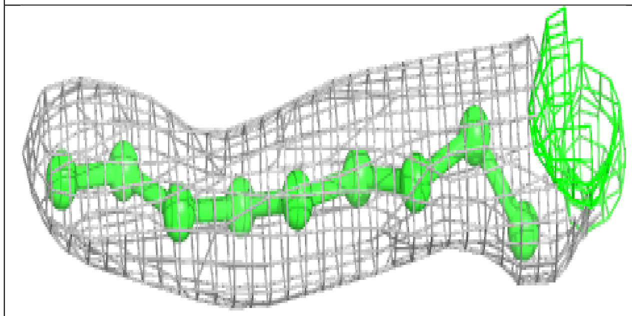


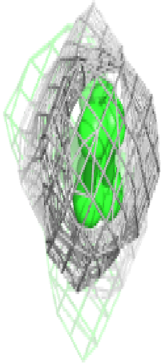


Electron density around LFA B 302:

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

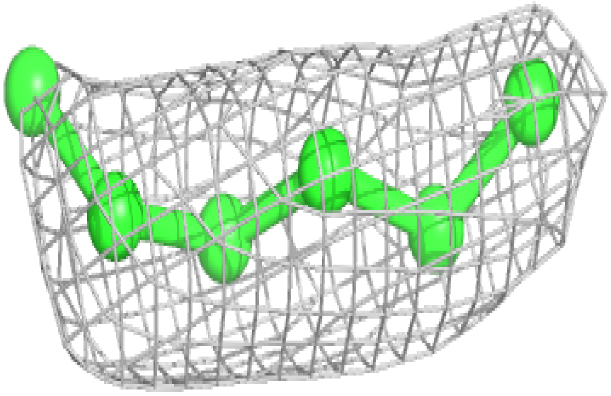


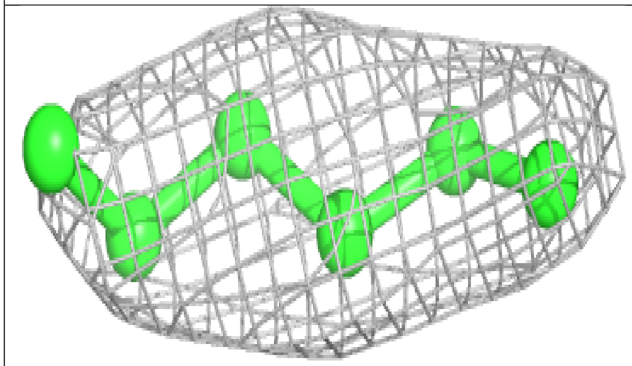


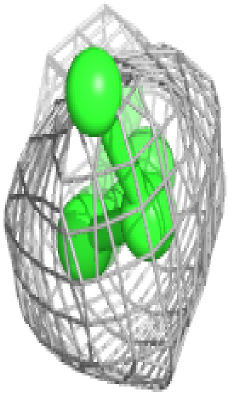


Electron density around LFA A 501:

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







6.5 Other polymers ⓘ

There are no such residues in this entry.