wwPDB X-ray Structure Validation Summary Report (i)

May 2, 2023 – 01:44 pm BST

PDB ID	:	7ZND
Title	:	Crystal structure of the light-driven inward proton pump xenorhodopsin BcXeR in the M state at pH 7.6 in the absence of sodium at 100K
Authors	:	Kovalev, K.; Tsybrov, F.; Alekseev, A.; Bourenkov, G.; Gordeliy, V.
Deposited on	:	2022-04-20
Resolution	:	1.99 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

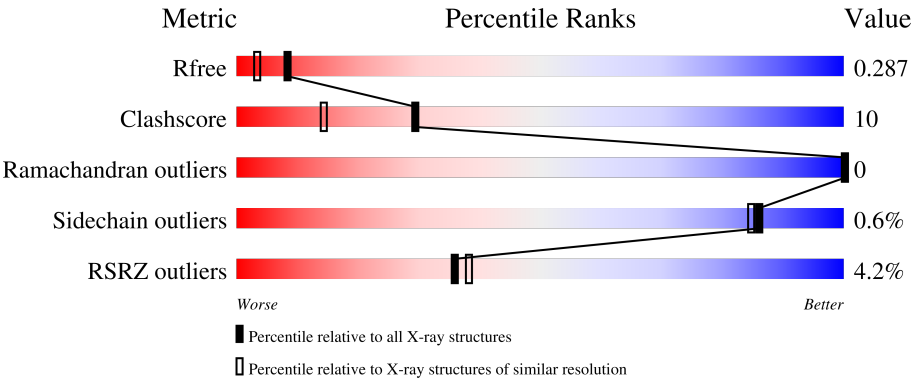
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	3% 80% 16% ·
1	B	229	6% 79% 17% ·
1	C	229	4% 83% 14% ··

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	FME	C	1	X	-	-	-
2	LFA	C	912	-	-	-	X
4	OLC	A	518	-	-	-	X

2 Entry composition (i)

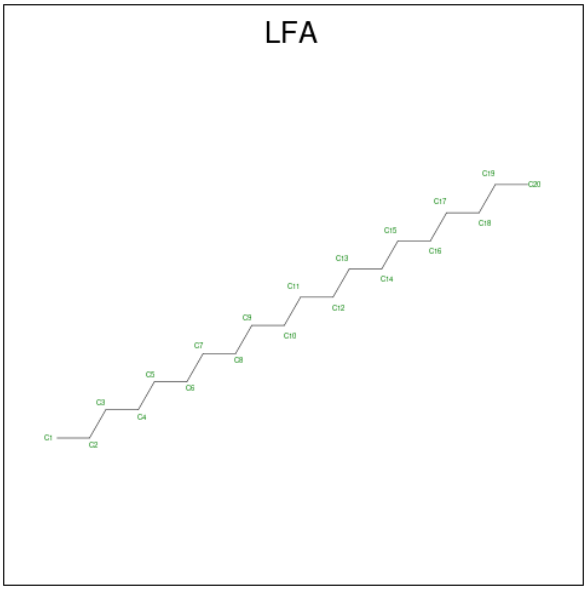
There are 6 unique types of molecules in this entry. The entry contains 6178 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called xenorhodopsin.

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

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



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

Continued on next page...

Continued from previous page...

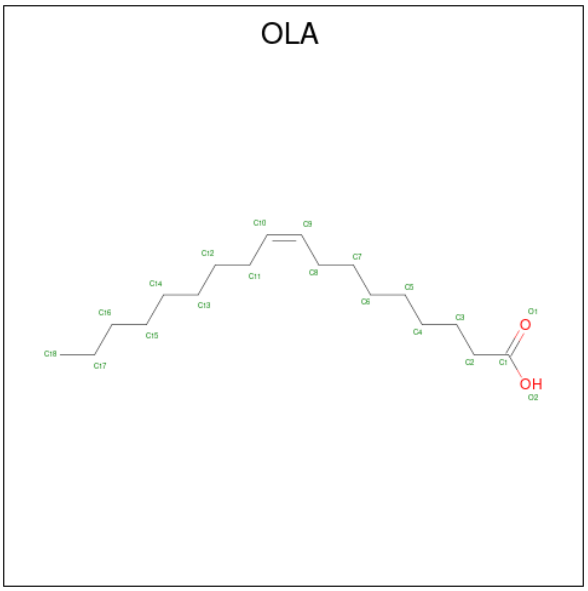
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 9 9	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 4 4	0	0
2	A	1	Total C 20 20	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 10 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 14 14	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 15 15	0	0
2	C	1	Total C 12 12	0	0
2	C	1	Total C 13 13	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 12 12	0	0
2	C	1	Total C 5 5	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 11 11	0	0
2	C	1	Total C 15 15	0	0
2	C	1	Total C 16 16	0	0
2	C	1	Total C 6 6	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 16 16	0	0

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



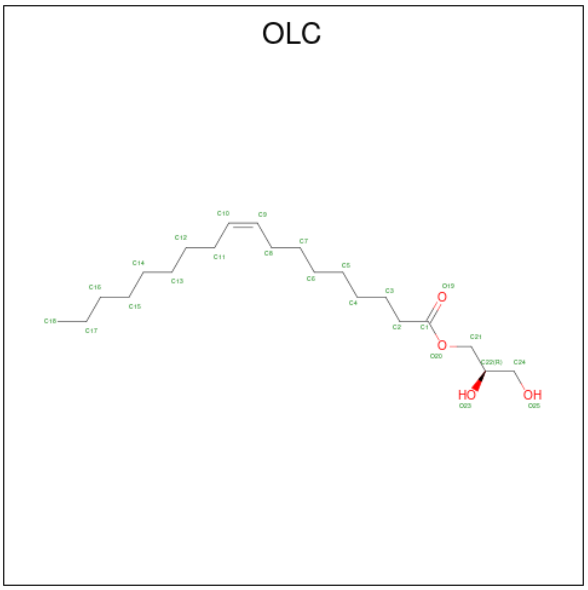
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 10 2	0	0
3	A	1	Total C O 14 12 2	0	0
3	A	1	Total C O 16 14 2	0	0
3	A	1	Total C O 20 18 2	0	0
3	A	1	Total C O 19 17 2	0	0
3	A	1	Total C O 20 18 2	0	0
3	B	1	Total C O 20 18 2	0	0
3	B	1	Total C O 16 14 2	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C O 14 12 2	0	0
3	B	1	Total C O 11 9 2	0	0
3	C	1	Total C O 20 18 2	0	0

Continued on next page...

Continued from previous page...

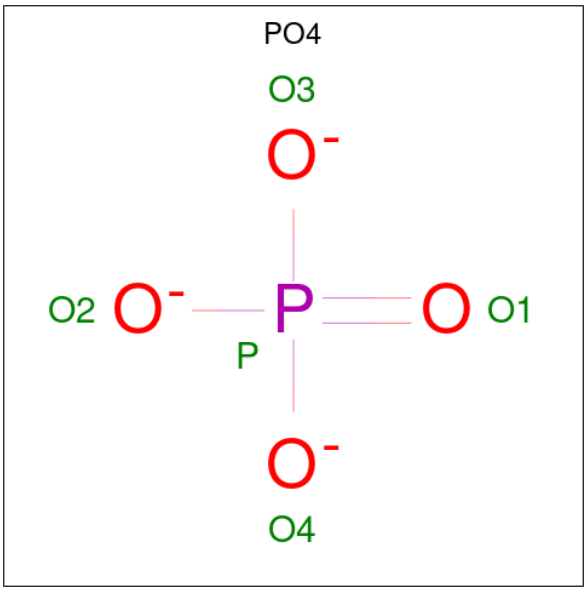
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 9 7 2	0	0

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 17 15 2	0	0
4	A	1	Total C O 19 16 3	0	0
4	A	1	Total C O 19 15 4	0	0
4	B	1	Total C O 19 15 4	0	0
4	B	1	Total C O 20 18 2	0	0
4	B	1	Total C O 19 15 4	0	0
4	B	1	Total C O 13 11 2	0	0
4	C	1	Total C O 17 13 4	0	0
4	C	1	Total C O 15 13 2	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is water.

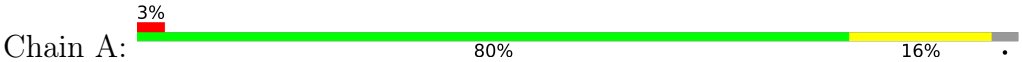
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	28	Total O 28 28	0	1
6	B	22	Total O 22 22	0	1
6	C	25	Total O 25 25	0	0

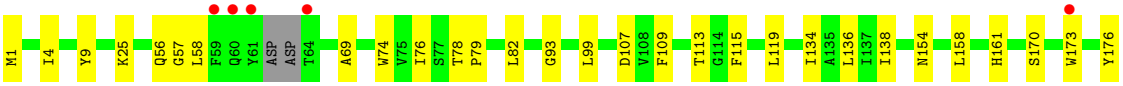
3 Residue-property plots (i)

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

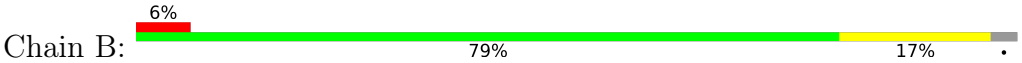
Chain A:

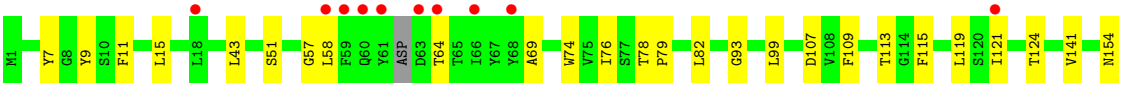




• Molecule 1: xenorhodopsin

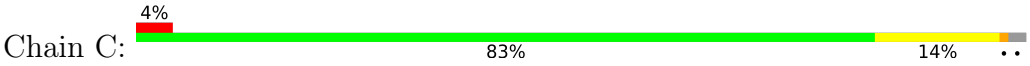
Chain B:

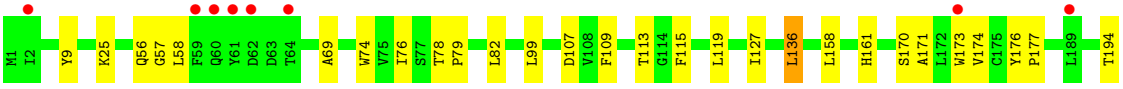


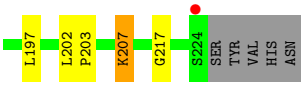


• Molecule 1: xenorhodopsin

Chain C:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.09Å 109.36Å 119.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.99 59.79 – 1.98	Depositor EDS
% Data completeness (in resolution range)	66.9 (20.00-1.99) 67.0 (59.79-1.98)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.249 , 0.282 0.255 , 0.287	Depositor DCC
R_{free} test set	2076 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	20.5	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6178	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, OLC, OLA, FME, LYR, LFA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.63	0/1767	0.62	0/2413
1	B	0.63	0/1778	0.62	0/2430
1	C	0.63	0/1773	0.63	0/2422
All	All	0.63	0/5318	0.62	0/7265

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	1	FME	CA

There are no planarity outliers.

5.2 Too-close contacts

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

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

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

The worst 5 of 123 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:TYR:HE1	1:C:203:PRO:HB2	1.52	0.74
1:A:202:LEU:HB2	1:A:203:PRO:HD3	1.71	0.71
1:B:202:LEU:HB2	1:B:203:PRO:HD3	1.74	0.69
1:B:9:TYR:HE1	1:B:203:PRO:HB2	1.56	0.69
1:C:202:LEU:HB2	1:C:203:PRO:HD3	1.74	0.68

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	218/229 (95%)	217 (100%)	1 (0%)	0	100	100
1	B	219/229 (96%)	219 (100%)	0	0	100	100
1	C	221/229 (96%)	220 (100%)	1 (0%)	0	100	100
All	All	658/687 (96%)	656 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (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	177/189 (94%)	177 (100%)	0	100	100
1	B	178/189 (94%)	176 (99%)	2 (1%)	73	70
1	C	179/189 (95%)	178 (99%)	1 (1%)	86	85
All	All	534/567 (94%)	531 (99%)	3 (1%)	86	85

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

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	B	154	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FME	C	1	1	8,9,10	0.40	0	7,9,11	0.59	0
1	LYR	C	207	1	27,29,30	1.34	2 (7%)	30,37,39	1.17	3 (10%)
1	FME	A	1	1	8,9,10	0.41	0	7,9,11	0.63	0
1	FME	B	1	1	8,9,10	0.40	0	7,9,11	0.67	0
1	LYR	B	207	1	27,29,30	1.33	3 (11%)	30,37,39	1.25	3 (10%)
1	LYR	A	207	1	27,29,30	1.36	4 (14%)	30,37,39	1.19	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	1/1/1/4	3/7/9/11	-
1	LYR	C	207	1	-	4/22/40/42	0/1/1/1
1	FME	A	1	1	-	1/7/9/11	-
1	FME	B	1	1	-	0/7/9/11	-
1	LYR	B	207	1	-	2/22/40/42	0/1/1/1
1	LYR	A	207	1	-	4/22/40/42	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	LYR	C7-C80	4.72	1.42	1.35
1	B	207	LYR	C7-C80	4.62	1.41	1.35
1	C	207	LYR	C7-C80	4.60	1.41	1.35
1	C	207	LYR	C9-C80	-2.53	1.40	1.45
1	A	207	LYR	C9-C80	-2.42	1.40	1.45

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	207	LYR	C8-C80-C7	-4.34	116.85	122.92
1	A	207	LYR	C8-C80-C7	-4.20	117.04	122.92
1	C	207	LYR	C8-C80-C7	-4.10	117.18	122.92
1	B	207	LYR	C9-C80-C7	3.10	123.70	118.94
1	A	207	LYR	C9-C80-C7	3.01	123.57	118.94

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	1	FME	CA

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	1	FME	O1-CN-N-CA
1	C	1	FME	O-C-CA-CB
1	C	207	LYR	O-C-CA-CB
1	C	207	LYR	CG-CD-CE-NZ
1	B	207	LYR	CD-CE-NZ-C1

There are no ring outliers.

4 monomers are involved in 27 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

67 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	LFA	C	915	-	10,10,19	0.09	0	9,9,18	0.06	0
3	OLA	A	503	-	11,11,19	0.66	0	11,11,19	0.59	0
2	LFA	C	902	-	12,12,19	0.08	0	11,11,18	0.07	0
3	OLA	B	1006	-	19,19,19	0.53	0	19,19,19	0.47	0
2	LFA	C	918	-	5,5,19	0.12	0	4,4,18	0.10	0
2	LFA	B	1003	-	8,8,19	0.10	0	7,7,18	0.08	0
3	OLA	A	508	-	15,15,19	0.59	0	15,15,19	0.53	0
2	LFA	C	904	-	5,5,19	0.14	0	4,4,18	0.09	0
2	LFA	A	501	-	5,5,19	0.13	0	4,4,18	0.10	0
3	OLA	B	1013	-	13,13,19	0.61	0	12,13,19	0.59	0
4	OLC	C	913	-	14,14,24	0.27	0	13,14,25	0.15	0
5	PO4	C	914	-	4,4,4	0.66	0	6,6,6	0.44	0
2	LFA	B	1028	-	14,14,19	0.08	0	13,13,18	0.07	0
2	LFA	B	1026	-	13,13,19	0.07	0	12,12,18	0.07	0
2	LFA	C	908	-	4,4,19	0.16	0	3,3,18	0.22	0
2	LFA	B	1019	-	5,5,19	0.13	0	4,4,18	0.08	0
2	LFA	B	1025	-	9,9,19	0.10	0	8,8,18	0.07	0
2	LFA	C	901	-	11,11,19	0.09	0	10,10,18	0.06	0
3	OLA	B	1012	-	13,13,19	0.61	0	12,13,19	0.58	0
3	OLA	B	1009	-	13,13,19	0.62	0	12,13,19	0.58	0
2	LFA	C	910	-	8,8,19	0.10	0	7,7,18	0.08	0
3	OLA	A	506	-	13,13,19	0.61	0	12,13,19	0.57	0
4	OLC	B	1015	-	18,18,24	0.26	0	18,19,25	0.25	0
2	LFA	B	1007	-	9,9,19	0.09	0	8,8,18	0.08	0
3	OLA	A	512	-	18,18,19	0.53	0	18,18,19	0.49	0
2	LFA	B	1020	-	10,10,19	0.09	0	9,9,18	0.07	0
2	LFA	B	1021	-	5,5,19	0.12	0	4,4,18	0.10	0
3	OLA	C	903	-	19,19,19	0.52	0	19,19,19	0.47	0
4	OLC	C	909	-	16,16,24	0.27	0	17,17,25	0.26	0
2	LFA	B	1027	-	9,9,19	0.10	0	8,8,18	0.08	0
2	LFA	C	905	-	7,7,19	0.10	0	6,6,18	0.11	0
3	OLA	B	1014	-	13,13,19	0.60	0	12,13,19	0.59	0
2	LFA	A	505	-	8,8,19	0.10	0	7,7,18	0.08	0
2	LFA	B	1024	-	10,10,19	0.09	0	9,9,18	0.06	0
4	OLC	A	518	-	18,18,24	0.24	0	18,19,25	0.25	0
3	OLA	A	513	-	19,19,19	0.52	0	19,19,19	0.49	0
2	LFA	A	504	-	8,8,19	0.11	0	7,7,18	0.10	0
2	LFA	B	1004	-	10,10,19	0.10	0	9,9,18	0.06	0
4	OLC	A	507	-	16,16,24	0.35	0	16,16,25	0.18	0
2	LFA	B	1023	-	9,9,19	0.10	0	8,8,18	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LFA	B	1022	-	7,7,19	0.11	0	6,6,18	0.09	0
2	LFA	A	514	-	9,9,19	0.11	0	8,8,18	0.06	0
2	LFA	C	917	-	15,15,19	0.07	0	14,14,18	0.05	0
2	LFA	A	515	-	7,7,19	0.11	0	6,6,18	0.07	0
3	OLA	C	911	-	8,8,19	0.75	0	8,8,19	0.71	0
2	LFA	C	916	-	14,14,19	0.08	0	13,13,18	0.05	0
2	LFA	C	920	-	15,15,19	0.07	0	14,14,18	0.06	0
2	LFA	B	1001	-	6,6,19	0.12	0	5,5,18	0.09	0
2	LFA	A	502	-	7,7,19	0.10	0	6,6,18	0.07	0
4	OLC	B	1018	-	18,18,24	0.25	0	18,19,25	0.26	0
2	LFA	A	510	-	10,10,19	0.09	0	9,9,18	0.07	0
3	OLA	B	1016	-	10,10,19	0.67	0	10,10,19	0.65	0
2	LFA	B	1010	-	7,7,19	0.11	0	6,6,18	0.09	0
2	LFA	C	919	-	6,6,19	0.12	0	5,5,18	0.11	0
4	OLC	B	1017	-	19,19,24	0.30	0	19,19,25	0.25	0
3	OLA	A	509	-	19,19,19	0.52	0	19,19,19	0.47	0
2	LFA	A	516	-	3,3,19	0.24	0	2,2,18	0.45	0
2	LFA	B	1002	-	6,6,19	0.10	0	5,5,18	0.11	0
3	OLA	B	1008	-	15,15,19	0.58	0	15,15,19	0.53	0
2	LFA	C	912	-	6,6,19	0.12	0	5,5,18	0.08	0
4	OLC	A	511	-	18,18,24	0.29	0	18,18,25	0.21	0
2	LFA	C	907	-	11,11,19	0.09	0	10,10,18	0.07	0
2	LFA	B	1005	-	8,8,19	0.09	0	7,7,18	0.08	0
2	LFA	A	517	-	19,19,19	0.07	0	18,18,18	0.04	0
4	OLC	B	1029	-	12,12,24	1.32	2 (16%)	12,12,25	1.45	2 (16%)
2	LFA	C	906	-	9,9,19	0.09	0	8,8,18	0.09	0
2	LFA	B	1011	-	10,10,19	0.09	0	9,9,18	0.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	C	915	-	-	2/8/8/17	-
3	OLA	A	503	-	-	5/9/9/17	-
2	LFA	C	902	-	-	4/10/10/17	-
3	OLA	B	1006	-	-	3/17/17/17	-
2	LFA	C	918	-	-	0/3/3/17	-
2	LFA	B	1003	-	-	1/6/6/17	-
3	OLA	A	508	-	-	8/13/13/17	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	C	904	-	-	0/3/3/17	-
2	LFA	A	501	-	-	0/3/3/17	-
3	OLA	B	1013	-	-	1/11/11/17	-
4	OLC	C	913	-	-	8/13/13/24	-
2	LFA	B	1028	-	-	5/12/12/17	-
2	LFA	B	1026	-	-	1/11/11/17	-
2	LFA	C	908	-	-	1/2/2/17	-
2	LFA	B	1019	-	-	0/3/3/17	-
2	LFA	B	1025	-	-	2/7/7/17	-
2	LFA	C	901	-	-	4/9/9/17	-
3	OLA	B	1012	-	-	6/11/11/17	-
3	OLA	B	1009	-	-	7/11/11/17	-
2	LFA	C	910	-	-	1/6/6/17	-
3	OLA	A	506	-	-	6/11/11/17	-
4	OLC	B	1015	-	-	11/18/18/24	-
2	LFA	B	1007	-	-	4/7/7/17	-
3	OLA	A	512	-	-	9/16/16/17	-
2	LFA	B	1020	-	-	0/8/8/17	-
2	LFA	B	1021	-	-	2/3/3/17	-
3	OLA	C	903	-	-	7/17/17/17	-
4	OLC	C	909	-	-	2/16/16/24	-
2	LFA	B	1027	-	-	1/7/7/17	-
2	LFA	C	905	-	-	1/5/5/17	-
3	OLA	B	1014	-	-	6/11/11/17	-
2	LFA	A	505	-	-	2/6/6/17	-
2	LFA	B	1024	-	-	7/8/8/17	-
4	OLC	A	518	-	-	6/18/18/24	-
3	OLA	A	513	-	-	6/17/17/17	-
2	LFA	A	504	-	-	1/6/6/17	-
2	LFA	B	1004	-	-	3/8/8/17	-
4	OLC	A	507	-	-	10/15/15/24	-
2	LFA	B	1023	-	-	0/7/7/17	-
2	LFA	B	1022	-	-	0/5/5/17	-
2	LFA	A	514	-	-	1/7/7/17	-
2	LFA	C	917	-	-	5/13/13/17	-
2	LFA	A	515	-	-	1/5/5/17	-
3	OLA	C	911	-	-	2/6/6/17	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	C	916	-	-	6/12/12/17	-
2	LFA	C	920	-	-	7/13/13/17	-
2	LFA	B	1001	-	-	1/4/4/17	-
2	LFA	A	502	-	-	2/5/5/17	-
4	OLC	B	1018	-	-	7/18/18/24	-
2	LFA	A	510	-	-	5/8/8/17	-
3	OLA	B	1016	-	-	6/8/8/17	-
2	LFA	B	1010	-	-	3/5/5/17	-
2	LFA	C	919	-	-	0/4/4/17	-
4	OLC	B	1017	-	-	7/17/17/24	-
3	OLA	A	509	-	-	4/17/17/17	-
2	LFA	A	516	-	-	0/1/1/17	-
2	LFA	B	1002	-	-	1/4/4/17	-
3	OLA	B	1008	-	-	6/13/13/17	-
2	LFA	C	912	-	-	1/4/4/17	-
4	OLC	A	511	-	-	3/17/17/24	-
2	LFA	C	907	-	-	4/9/9/17	-
2	LFA	B	1005	-	-	4/6/6/17	-
2	LFA	A	517	-	-	6/17/17/17	-
4	OLC	B	1029	-	-	2/10/10/24	-
2	LFA	C	906	-	-	1/7/7/17	-
2	LFA	B	1011	-	-	0/8/8/17	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1029	OLC	O19-C1	3.39	1.33	1.22
4	B	1029	OLC	O20-C1	-2.97	1.20	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1029	OLC	O19-C1-C2	-3.56	111.64	123.08
4	B	1029	OLC	O20-C1-C2	3.43	125.06	114.03

There are no chirality outliers.

5 of 228 torsion outliers are listed below:

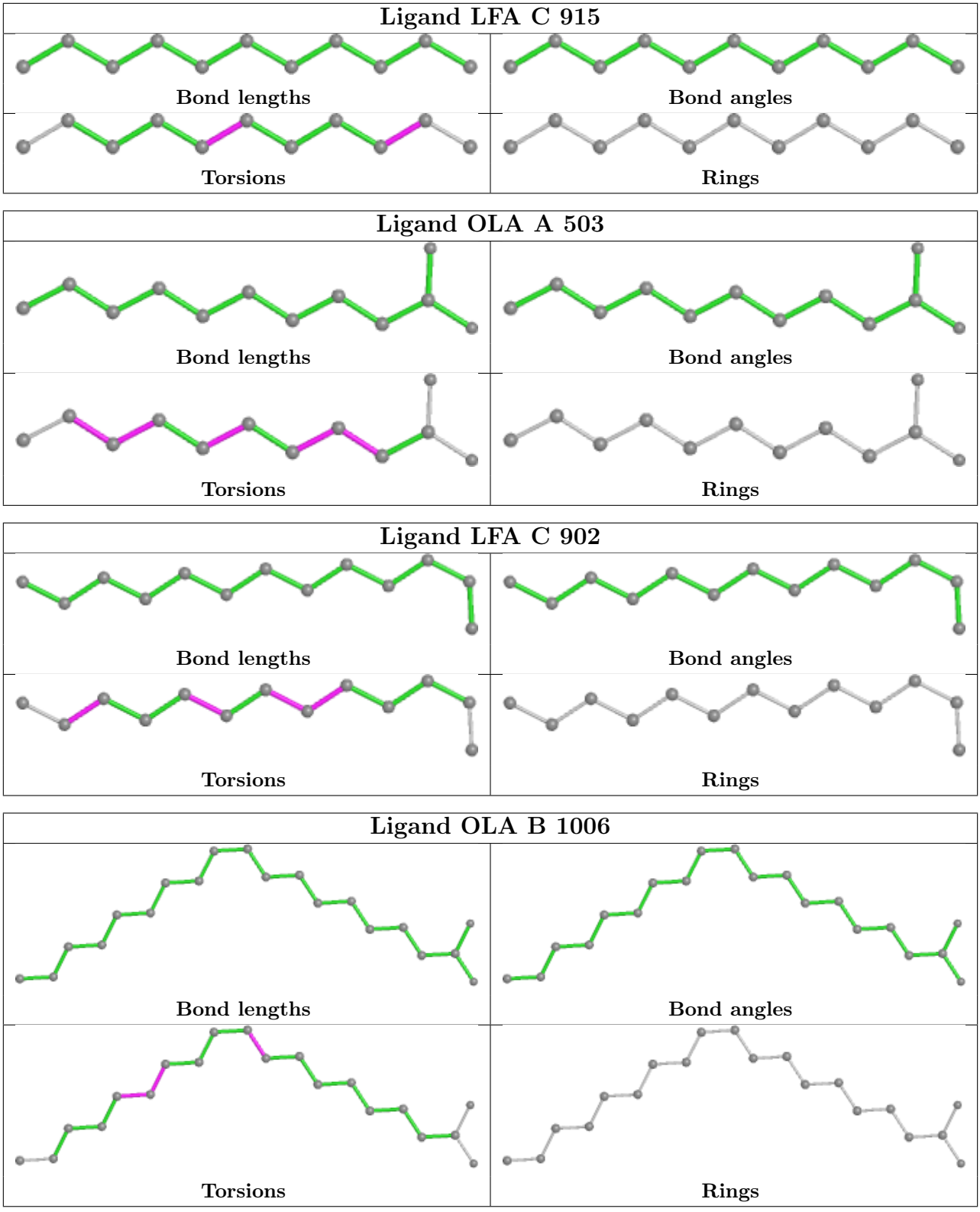
Mol	Chain	Res	Type	Atoms
4	B	1015	OLC	O20-C21-C22-C24
4	B	1018	OLC	O20-C21-C22-C24
4	C	913	OLC	C9-C10-C11-C12
4	A	518	OLC	O19-C1-O20-C21
4	B	1015	OLC	C2-C1-O20-C21

There are no ring outliers.

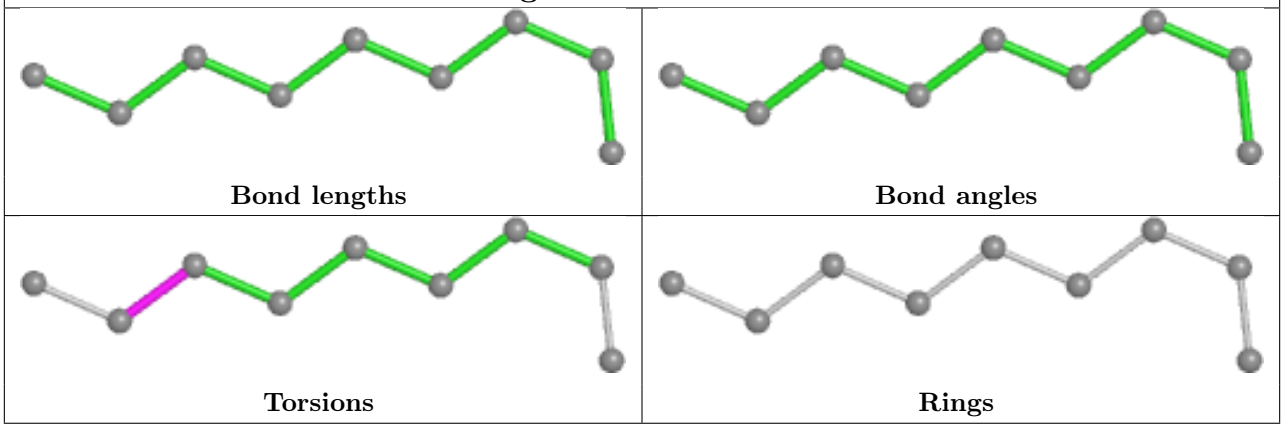
20 monomers are involved in 22 short contacts:

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

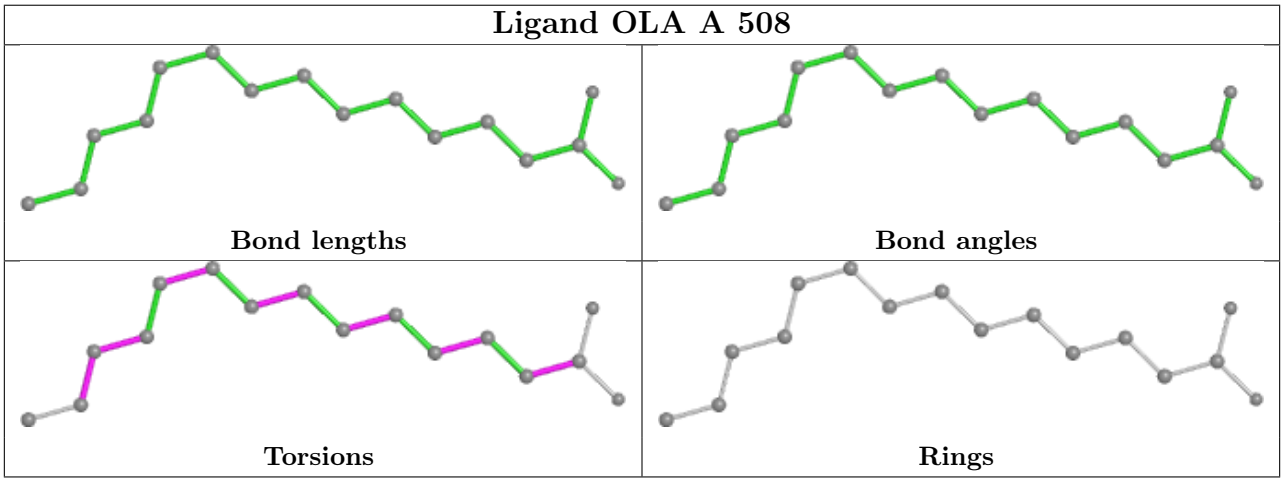
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 C 915
Bond lengths
Bond angles
Torsions
Rings
Ligand OLA A 503
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA C 902
Bond lengths
Bond angles
Torsions
Rings
Ligand OLA B 1006
Bond lengths
Bond angles
Torsions
Rings

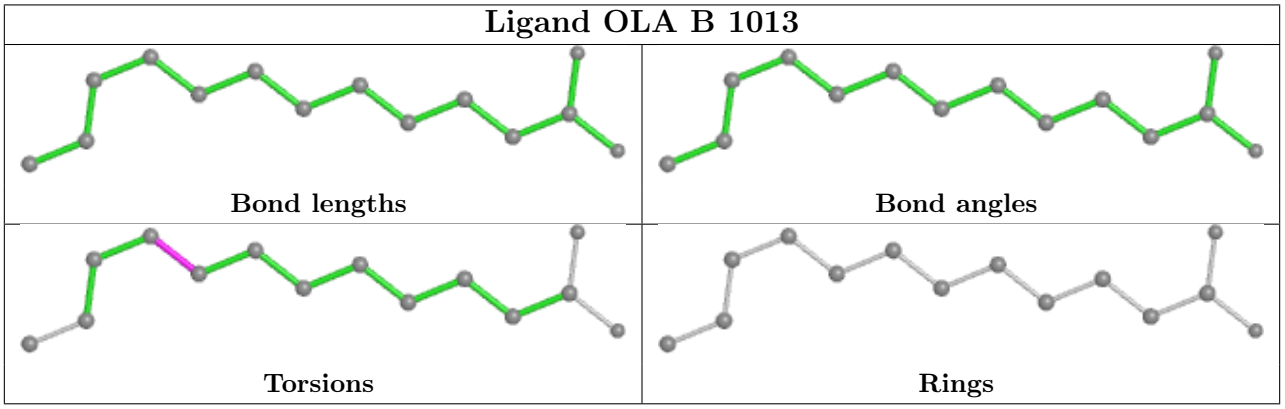
Ligand LFA B 1003



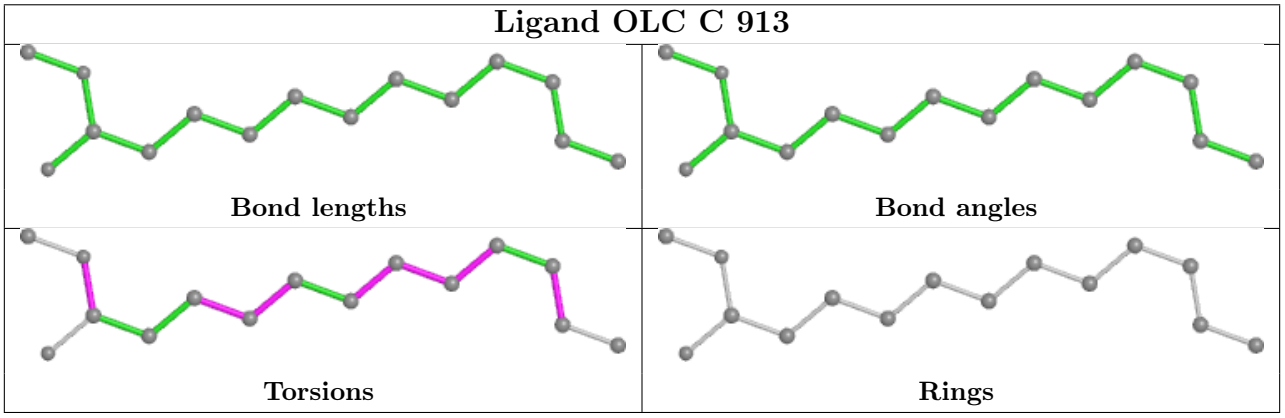
Ligand OLA A 508



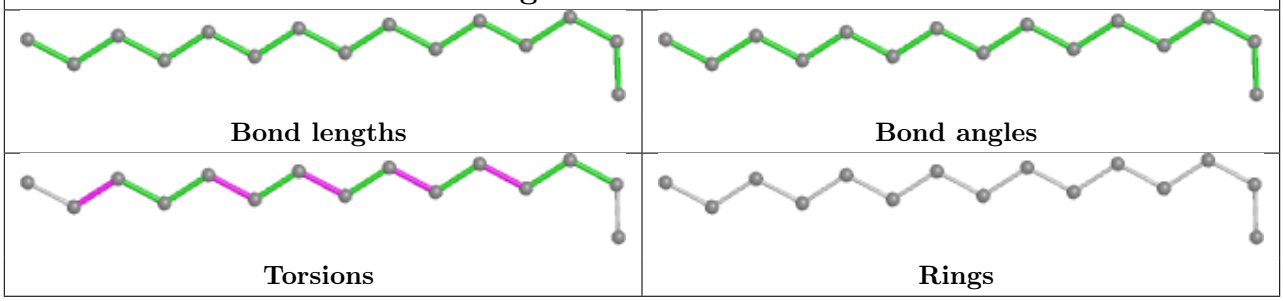
Ligand OLA B 1013



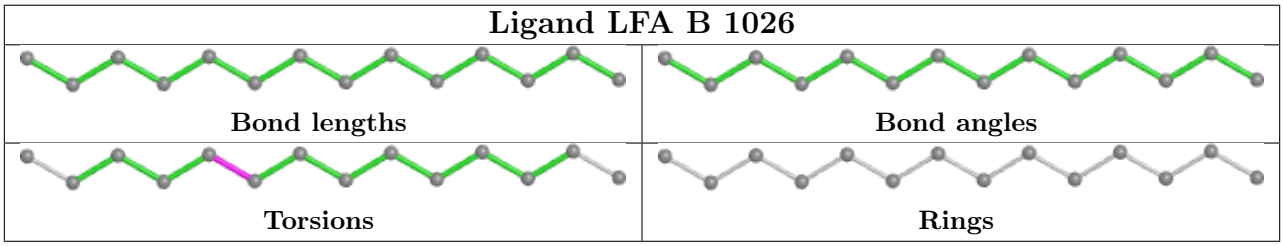
Ligand OLC C 913



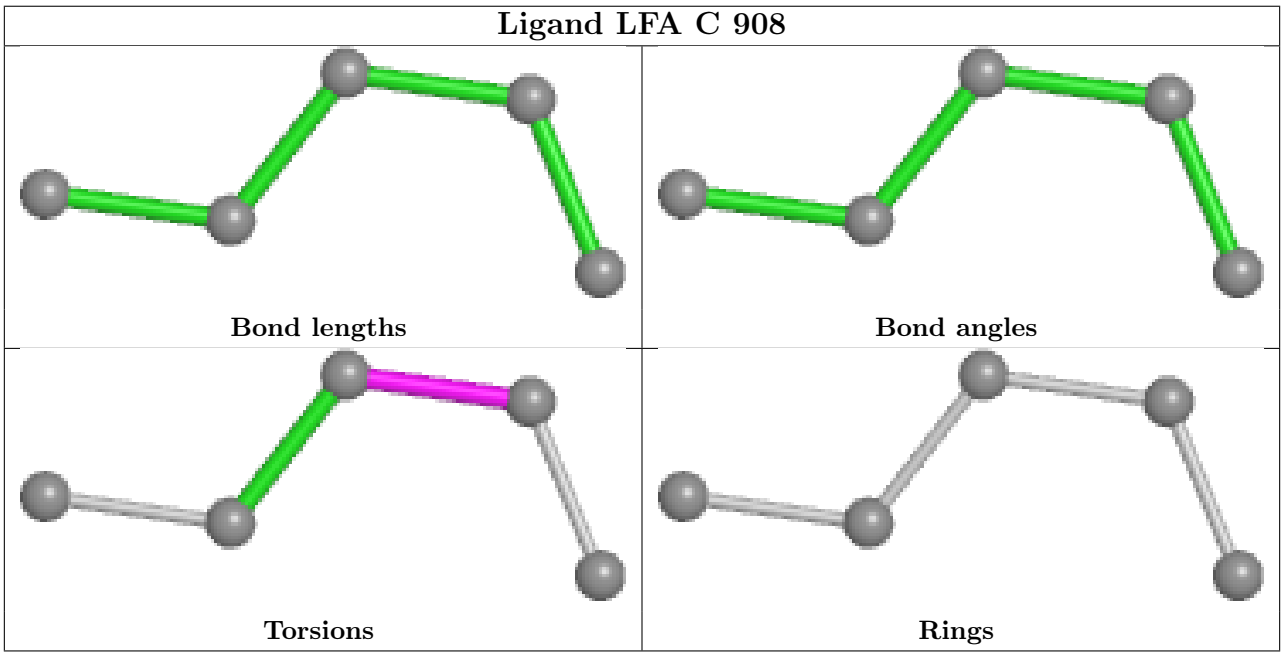
Ligand LFA B 1028



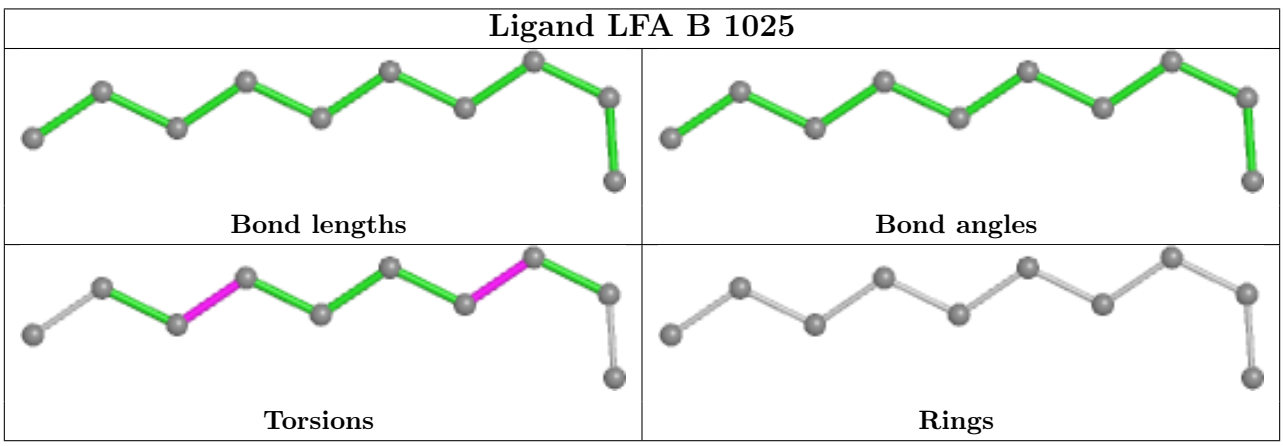
Ligand LFA B 1026



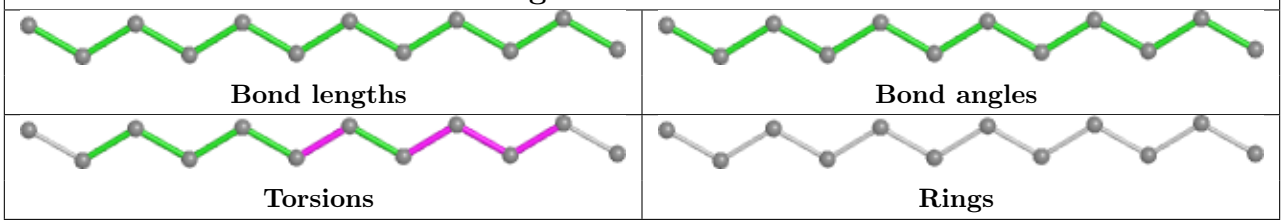
Ligand LFA C 908



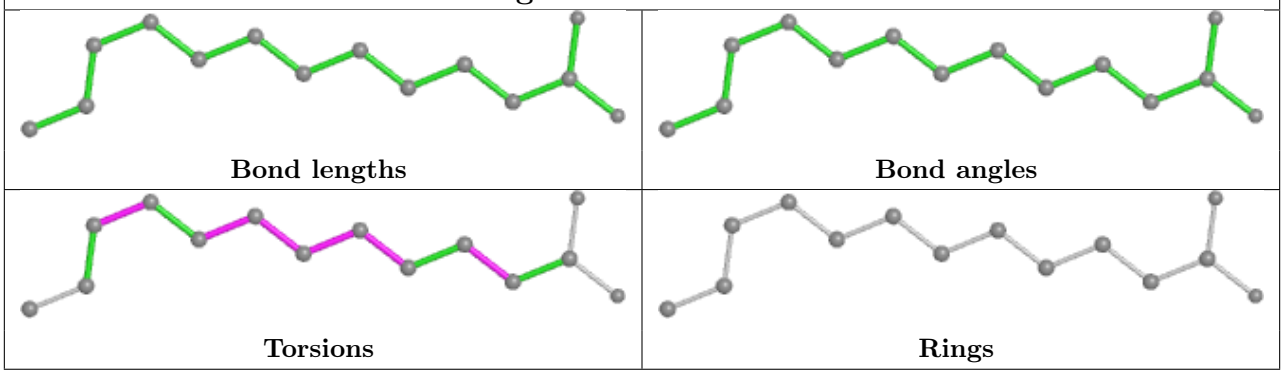
Ligand LFA B 1025



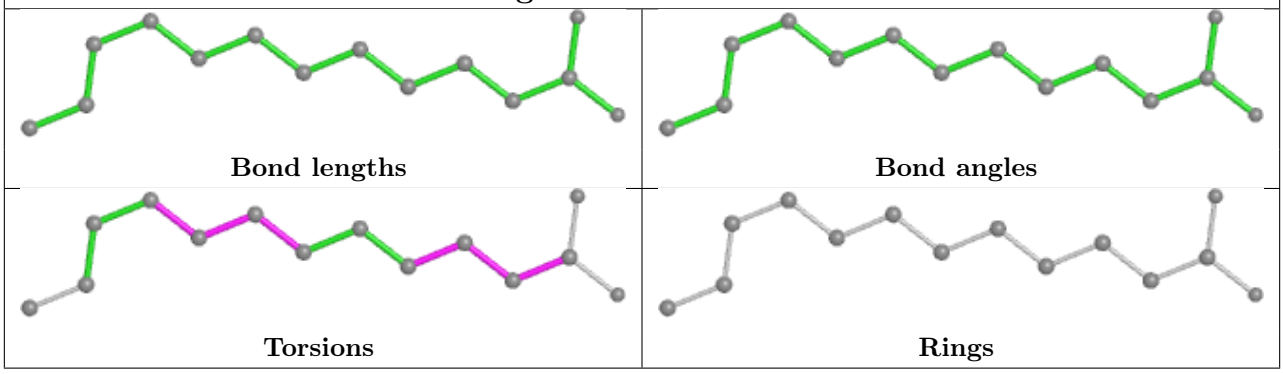
Ligand LFA C 901



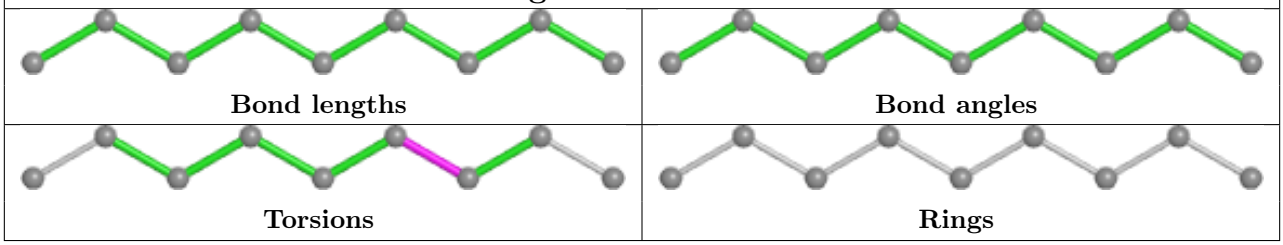
Ligand OLA B 1012



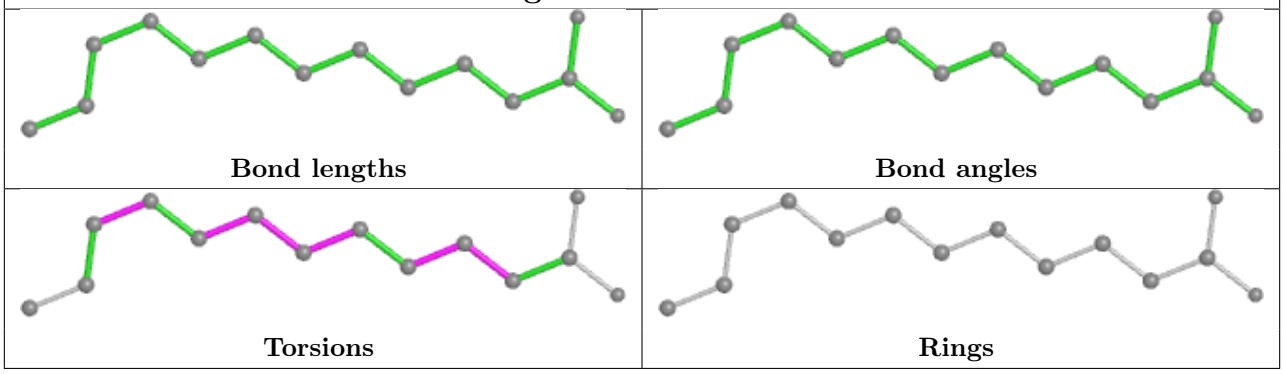
Ligand OLA B 1009



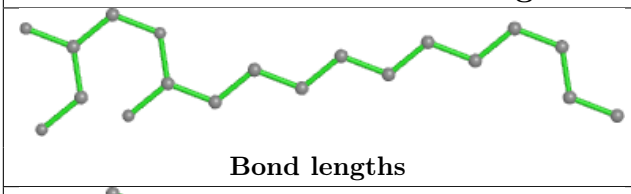
Ligand LFA C 910

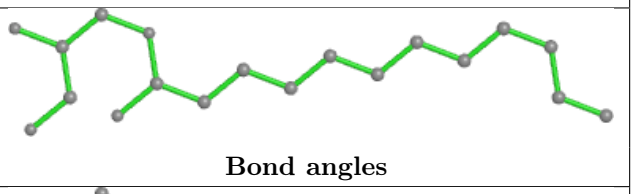


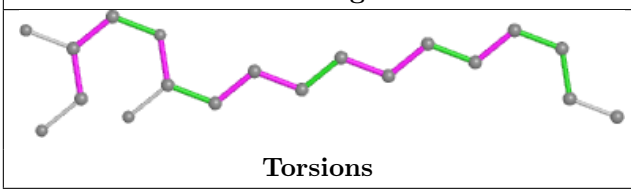
Ligand OLA A 506

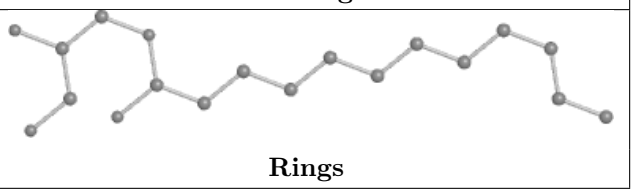


Ligand OLC B 1015

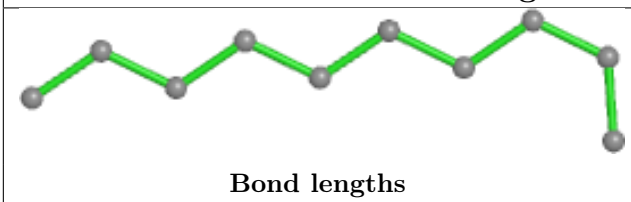

Bond lengths

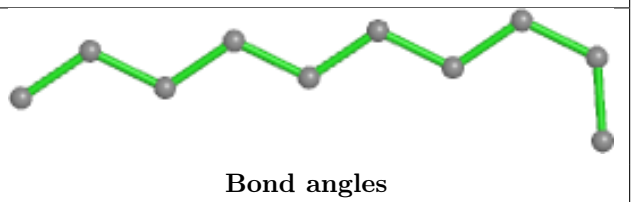

Bond angles

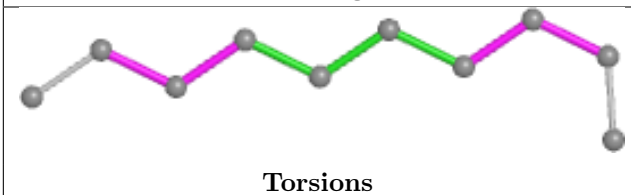

Torsions

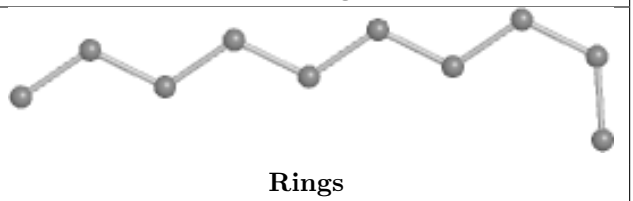

Rings

Ligand LFA B 1007

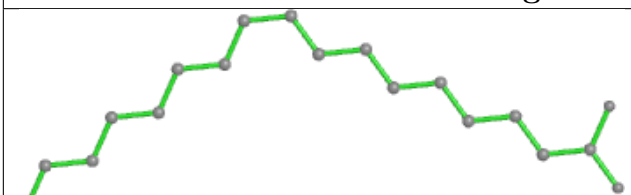

Bond lengths

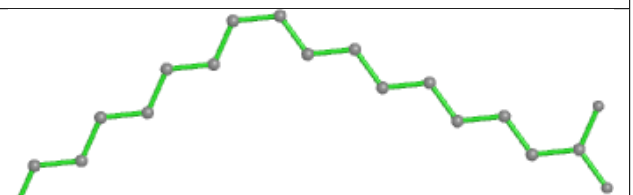

Bond angles

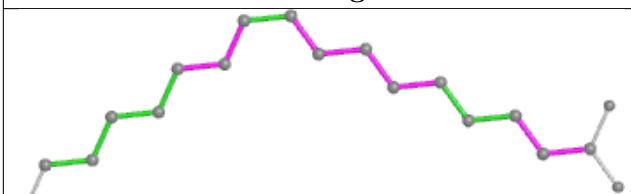

Torsions

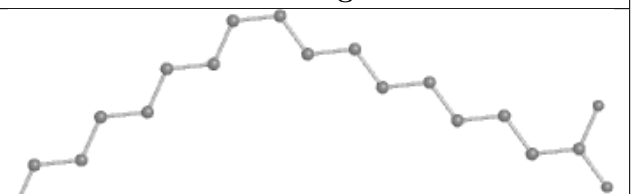

Rings

Ligand OLA A 512

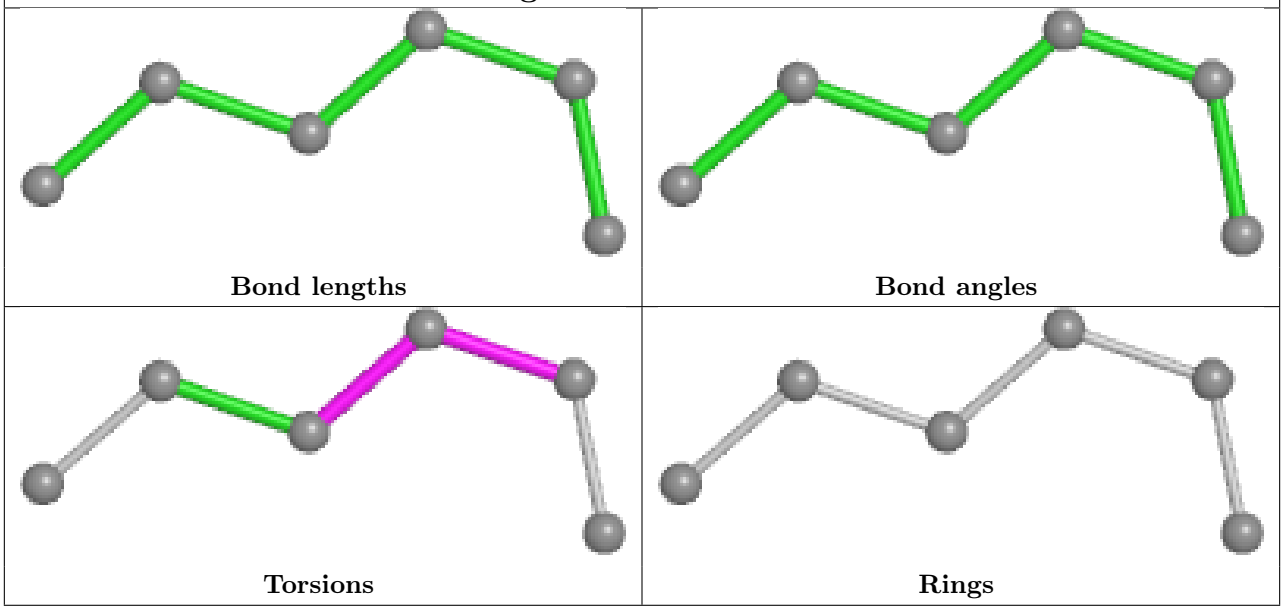

Bond lengths


Bond angles

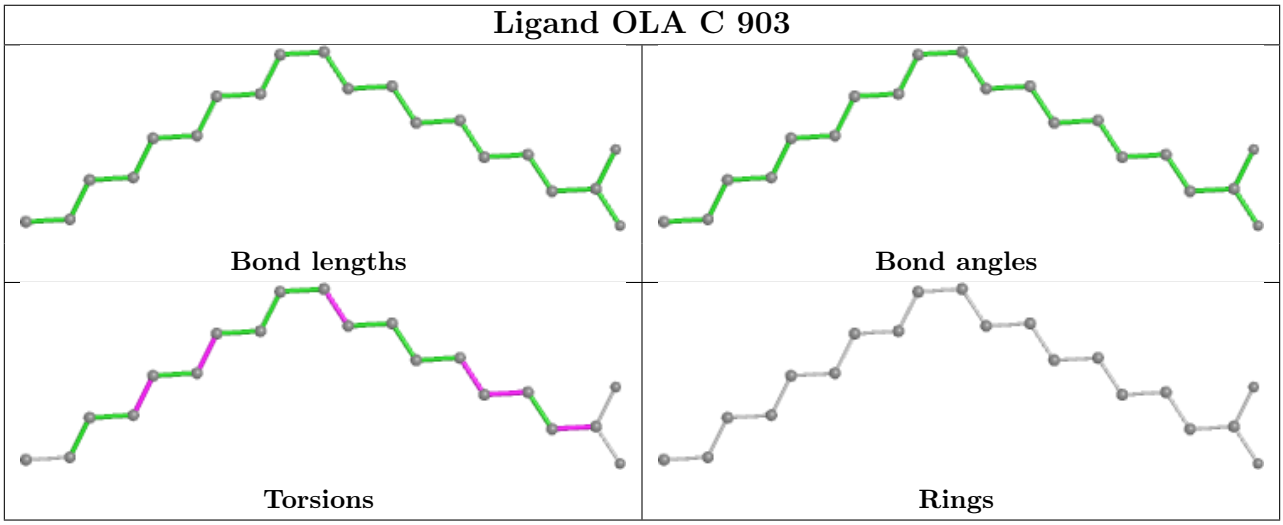

Torsions


Rings

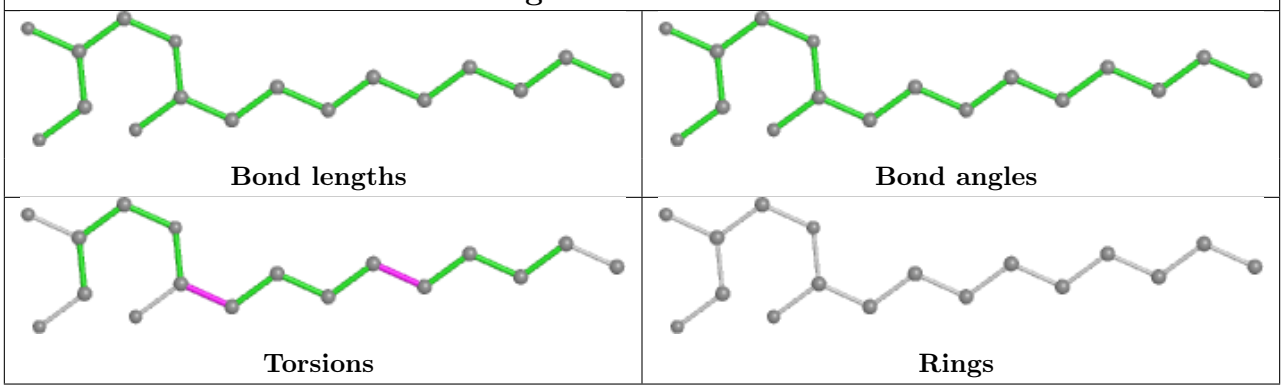
Ligand LFA B 1021



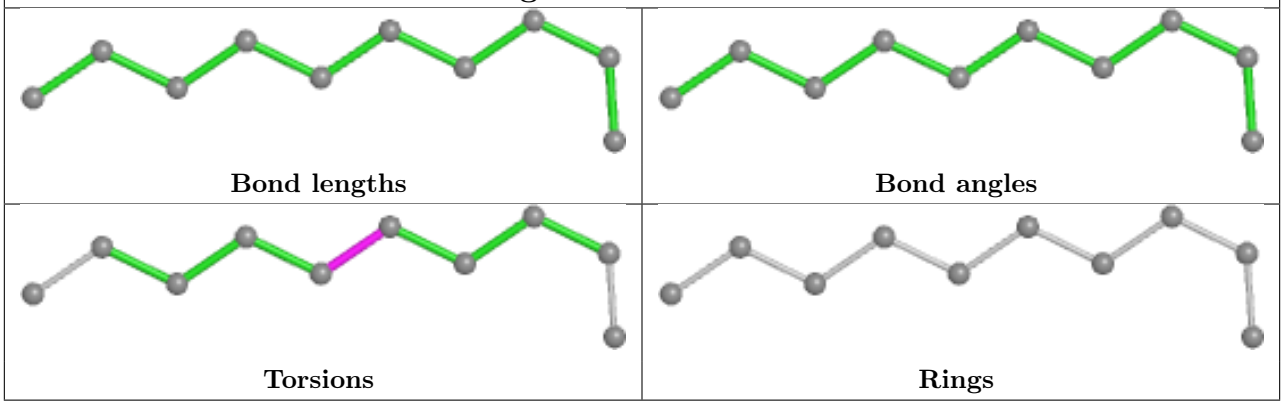
Ligand OLA C 903



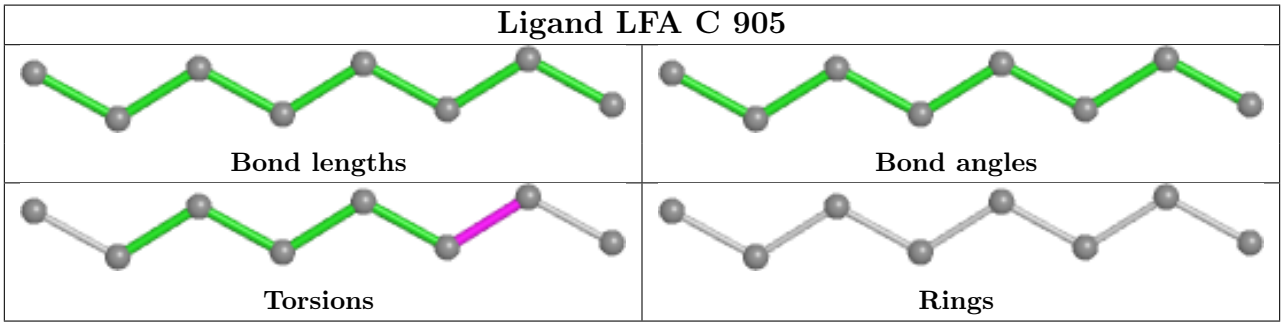
Ligand OLC C 909



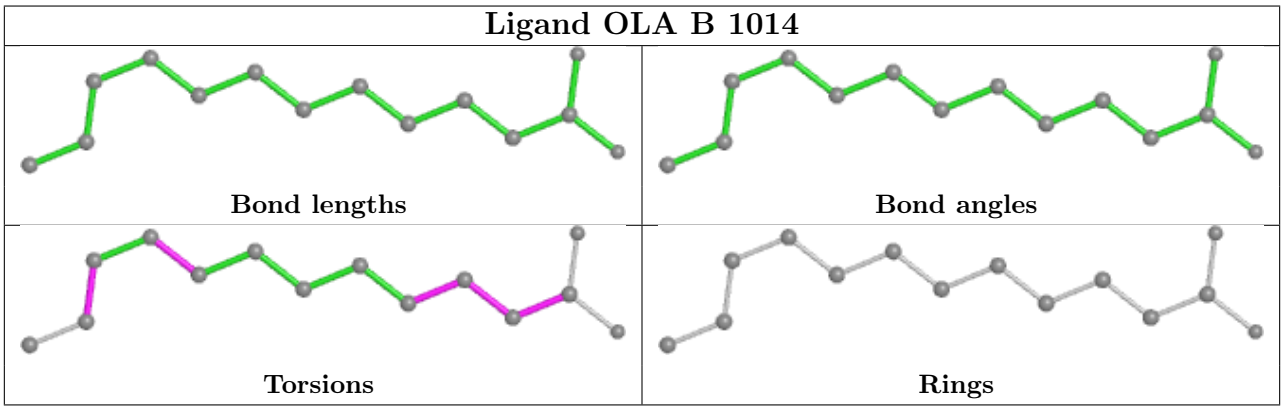
Ligand LFA B 1027



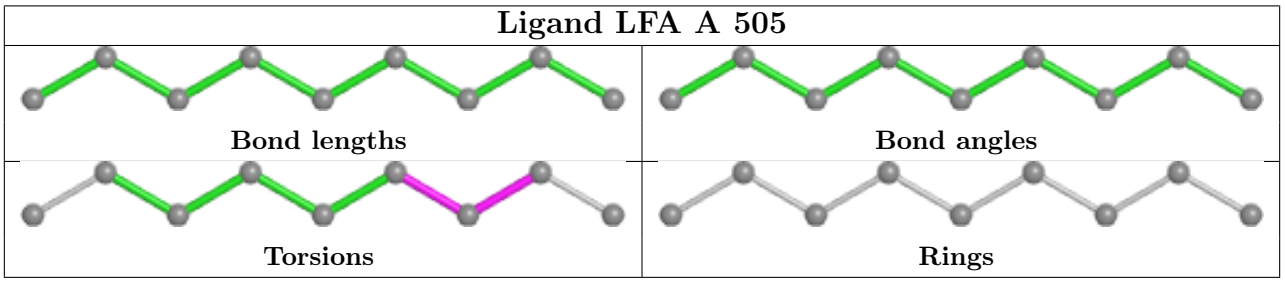
Ligand LFA C 905



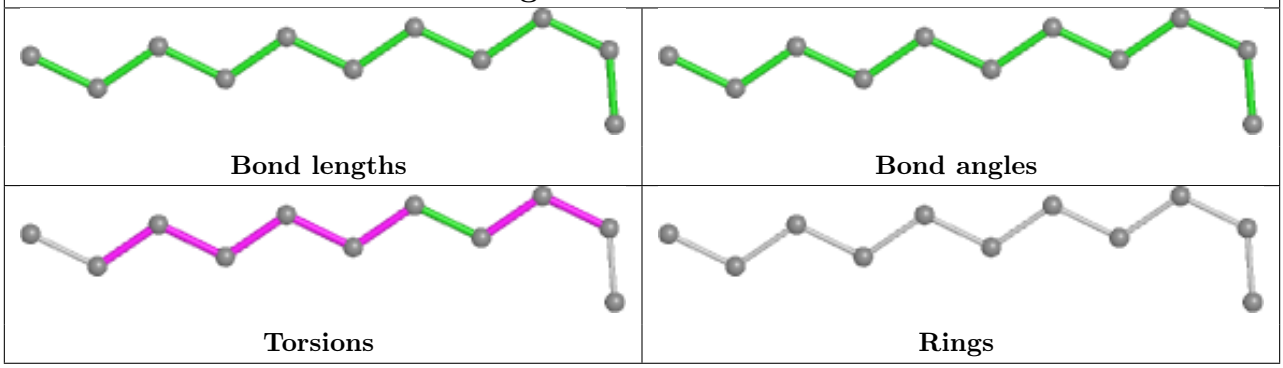
Ligand OLA B 1014



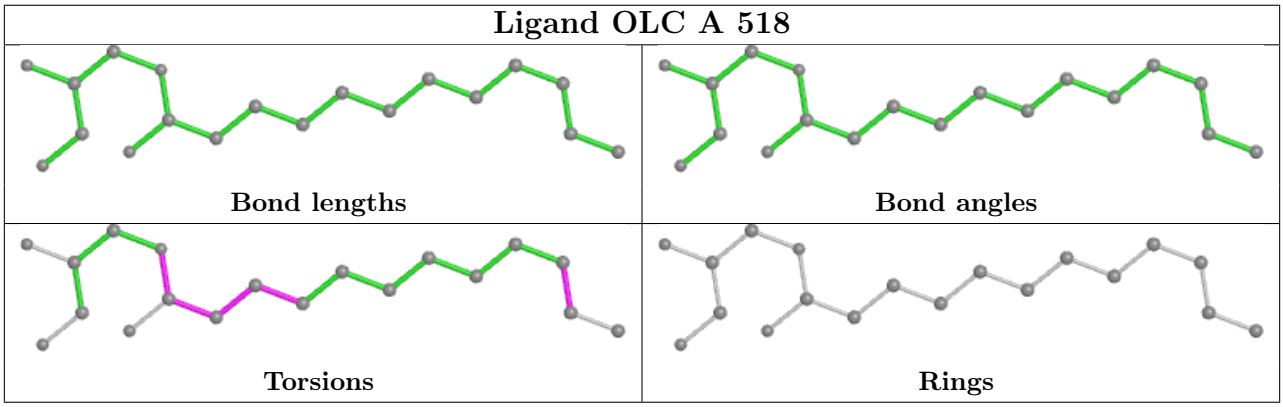
Ligand LFA A 505



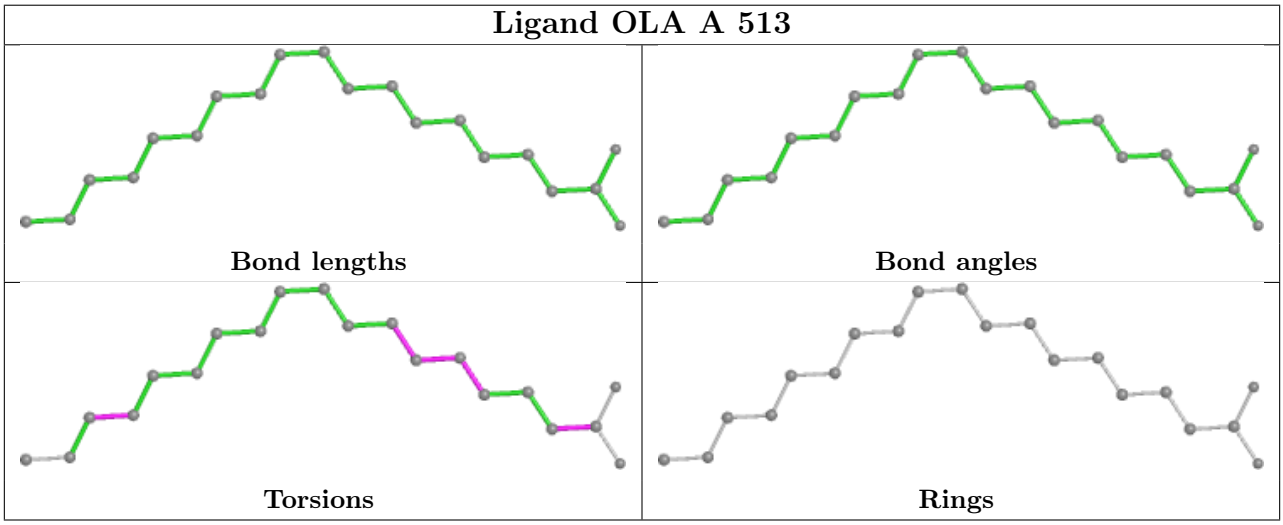
Ligand LFA B 1024



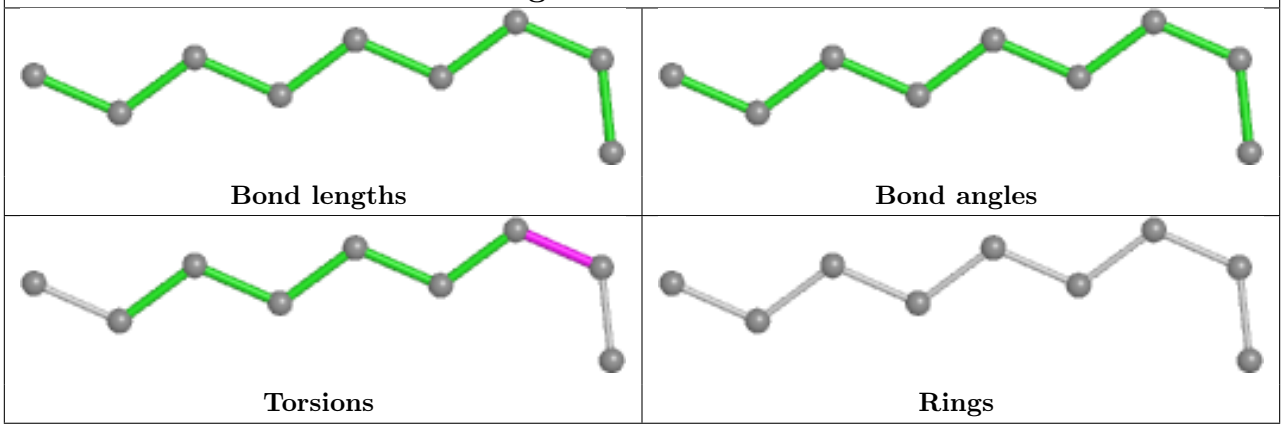
Ligand OLC A 518



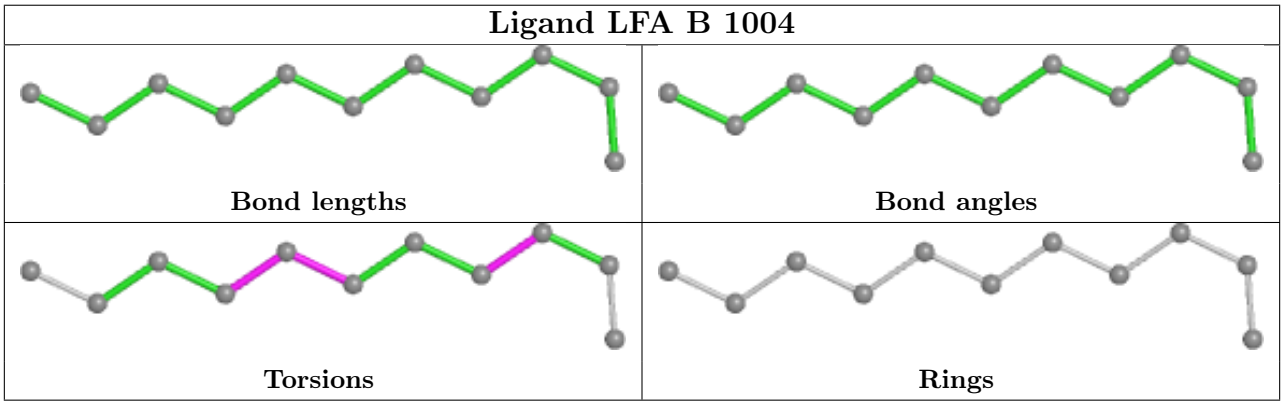
Ligand OLA A 513



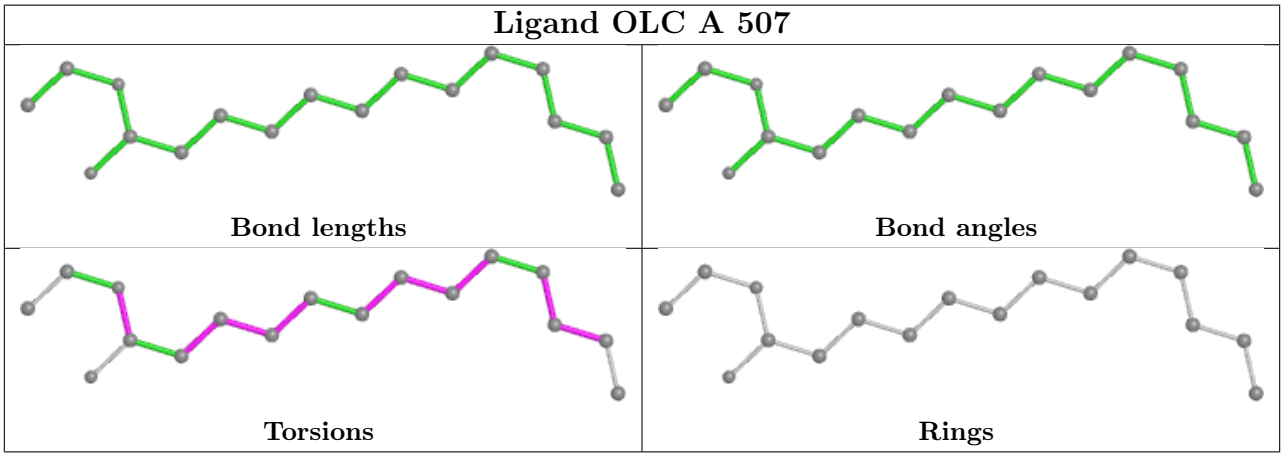
Ligand LFA A 504



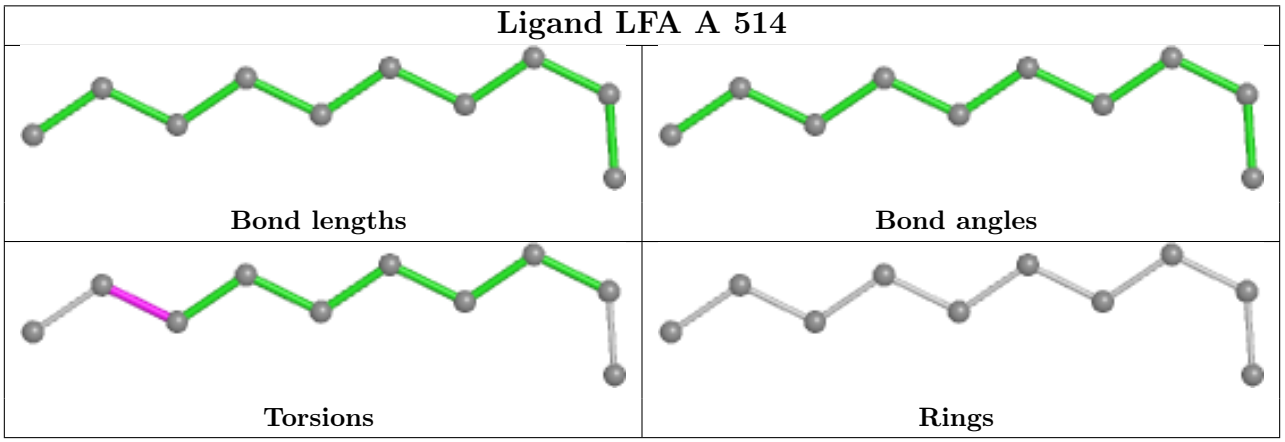
Ligand LFA B 1004



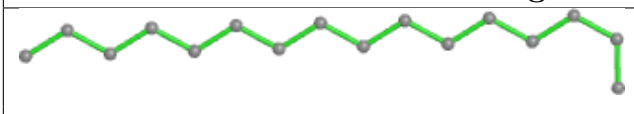
Ligand OLC A 507

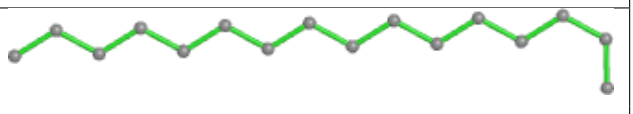


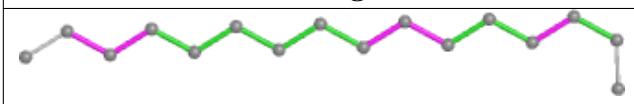
Ligand LFA A 514

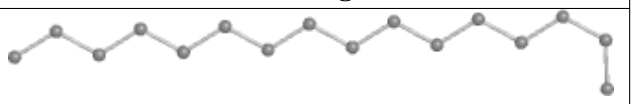


Ligand LFA C 917

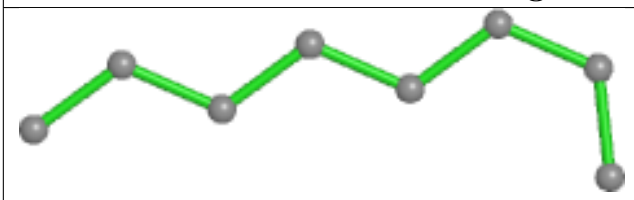

Bond lengths

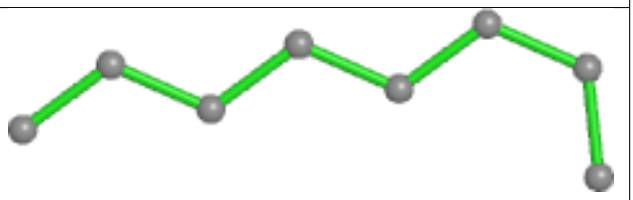

Bond angles

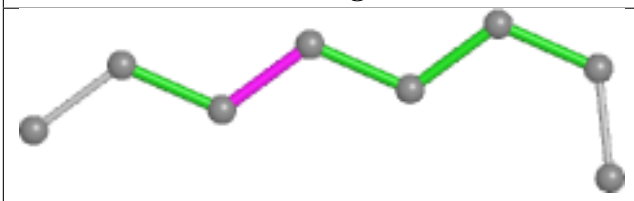

Torsions

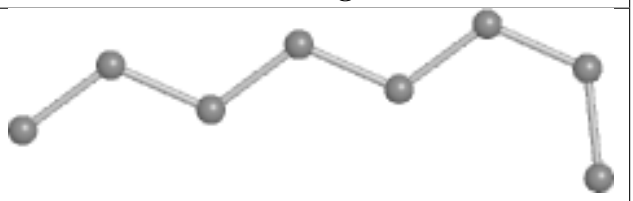

Rings

Ligand LFA A 515

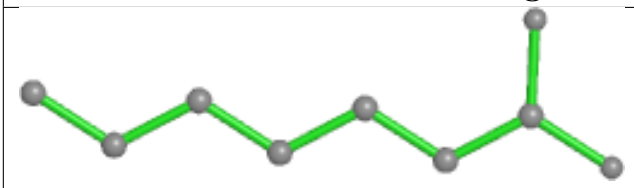

Bond lengths

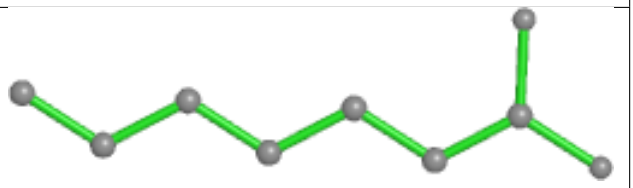

Bond angles

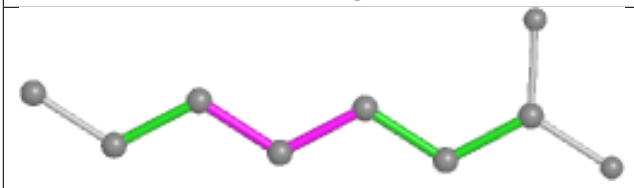

Torsions

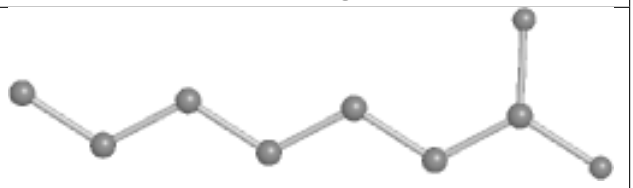

Rings

Ligand OLA C 911

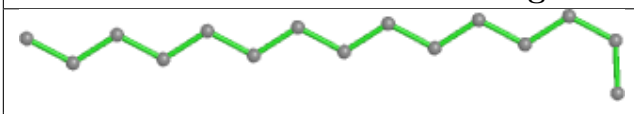

Bond lengths

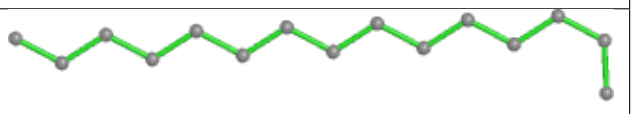

Bond angles

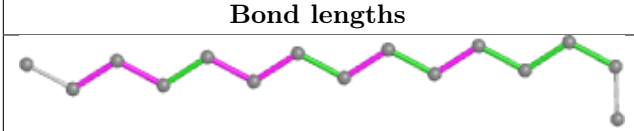

Torsions

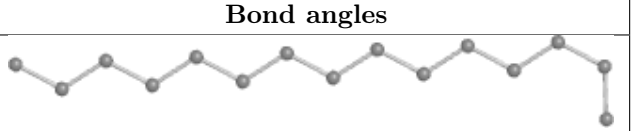

Rings

Ligand LFA C 916

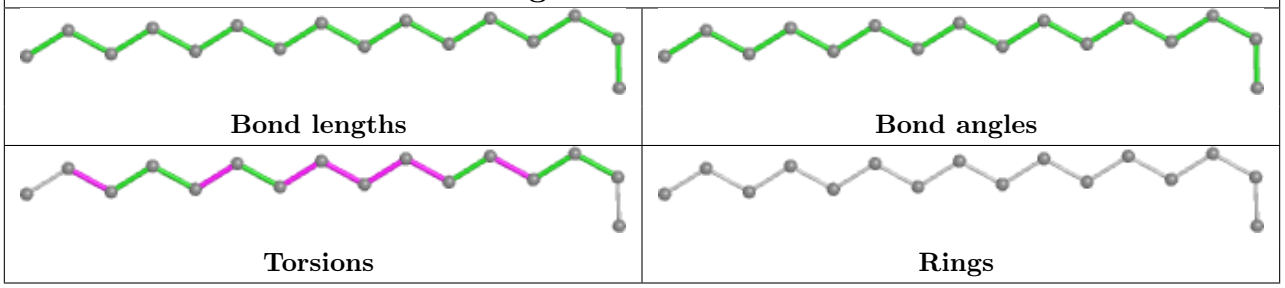

Bond lengths


Bond angles

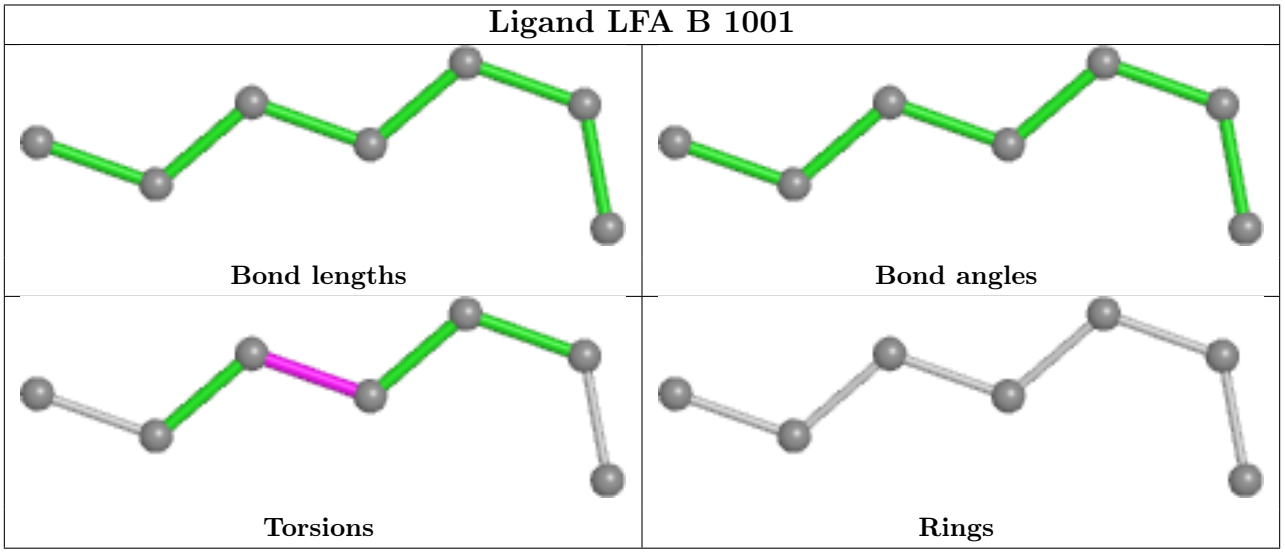

Torsions


Rings

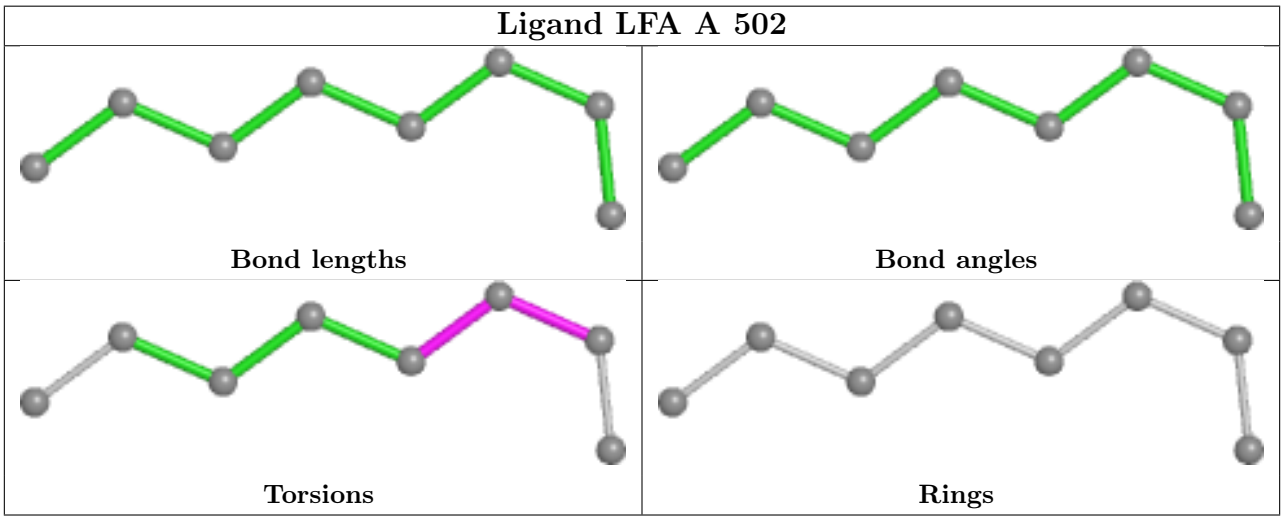
Ligand LFA C 920



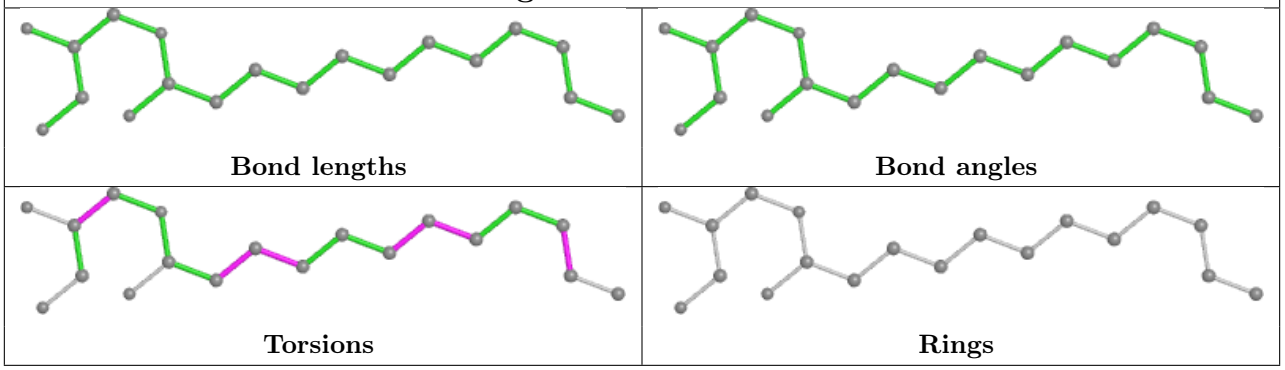
Ligand LFA B 1001



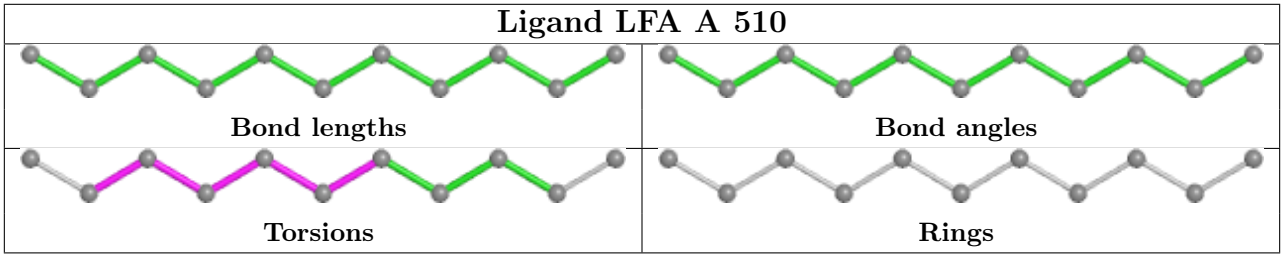
Ligand LFA A 502



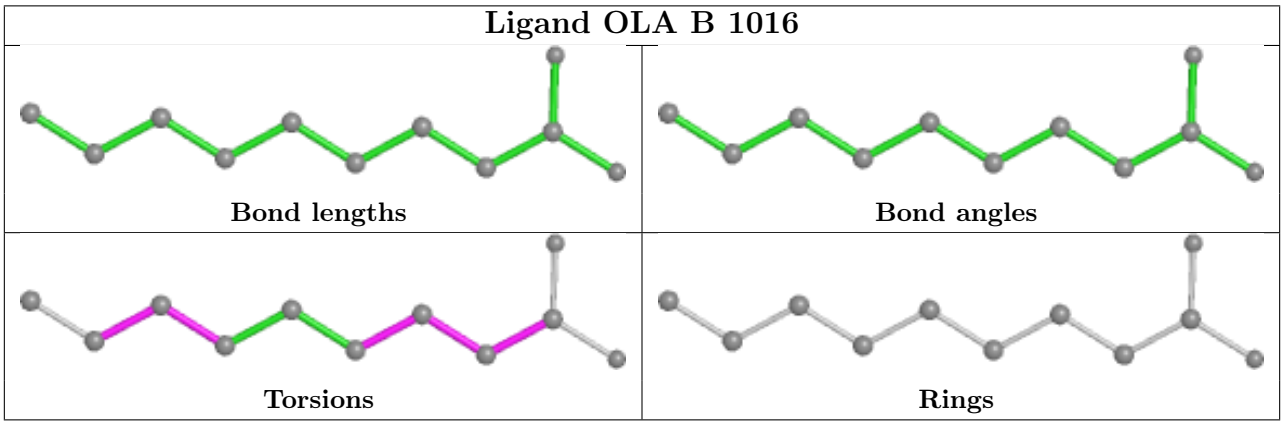
Ligand OLC B 1018



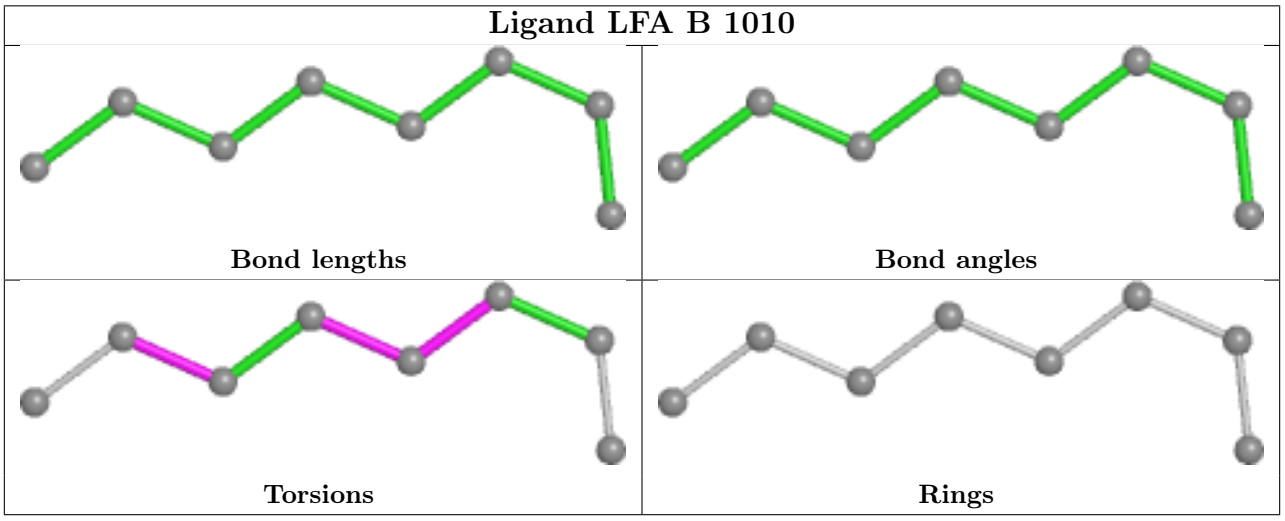
Ligand LFA A 510



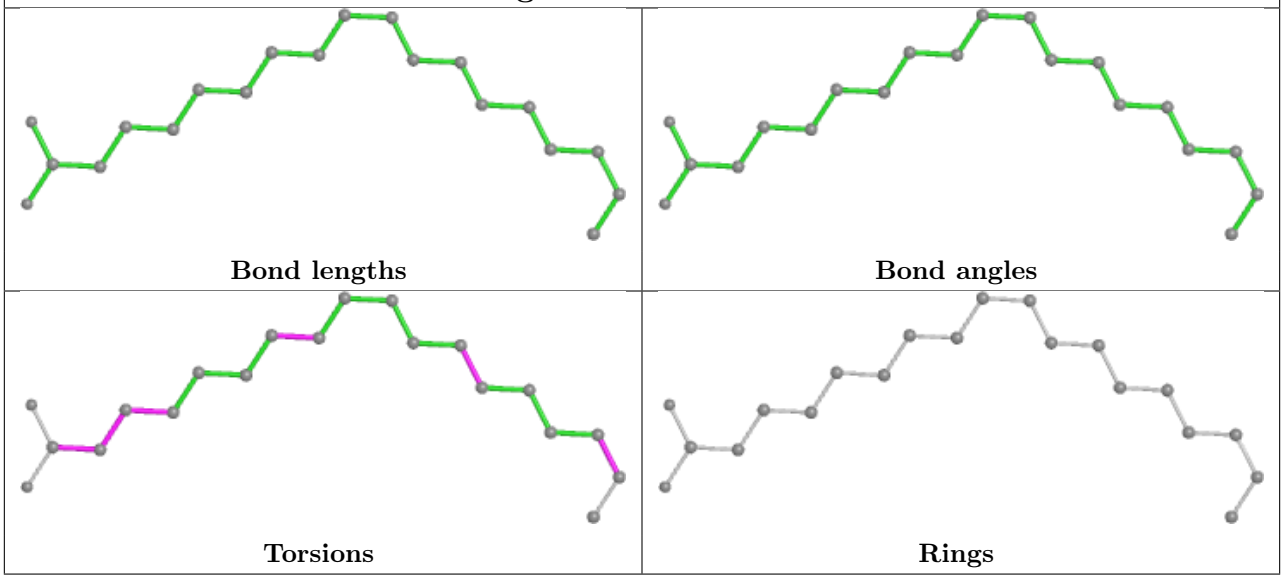
Ligand OLA B 1016



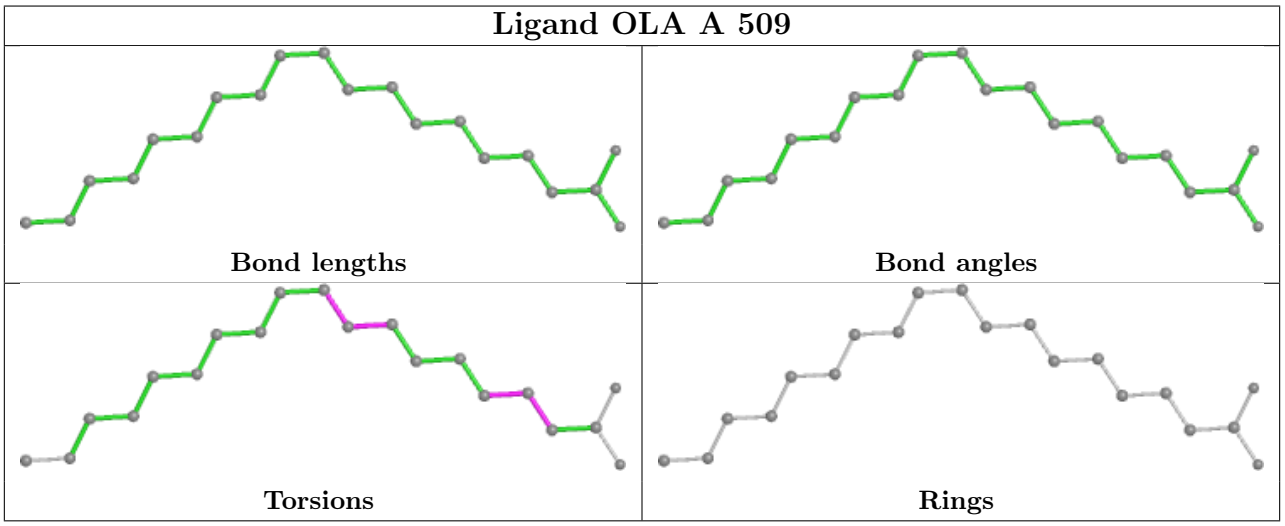
Ligand LFA B 1010



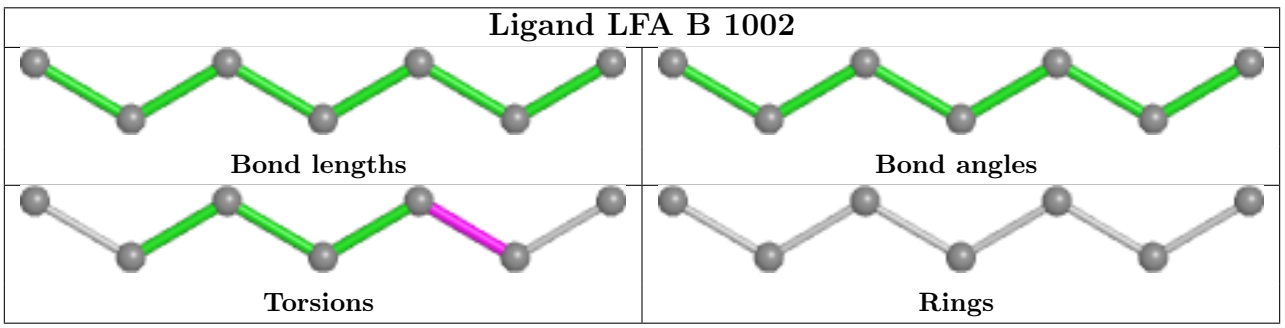
Ligand OLC B 1017



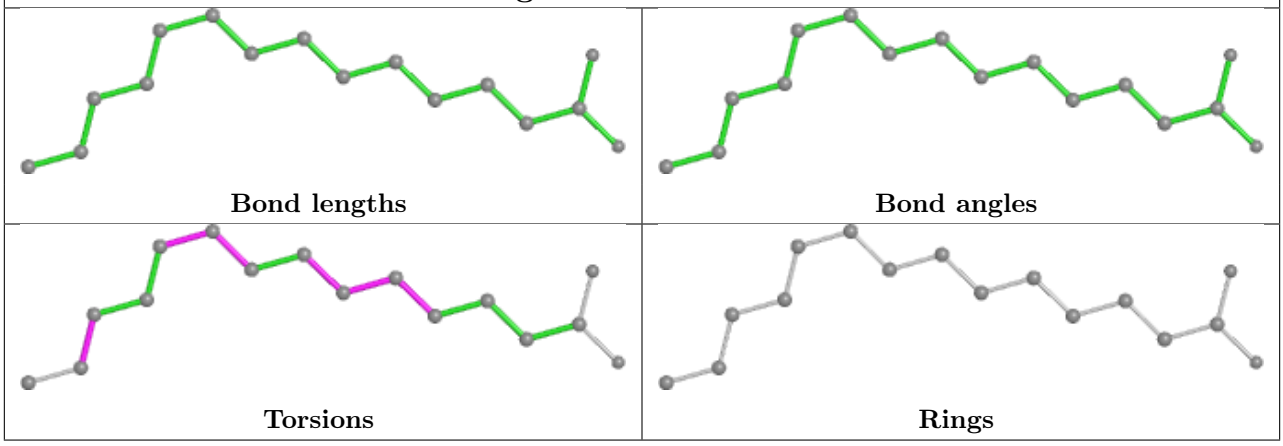
Ligand OLA A 509



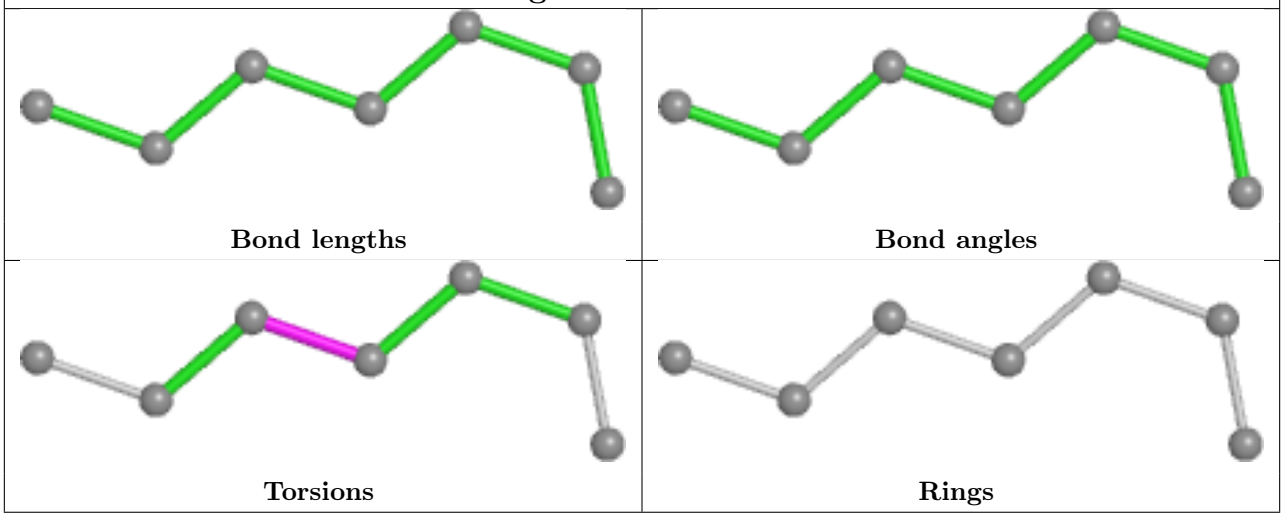
Ligand LFA B 1002



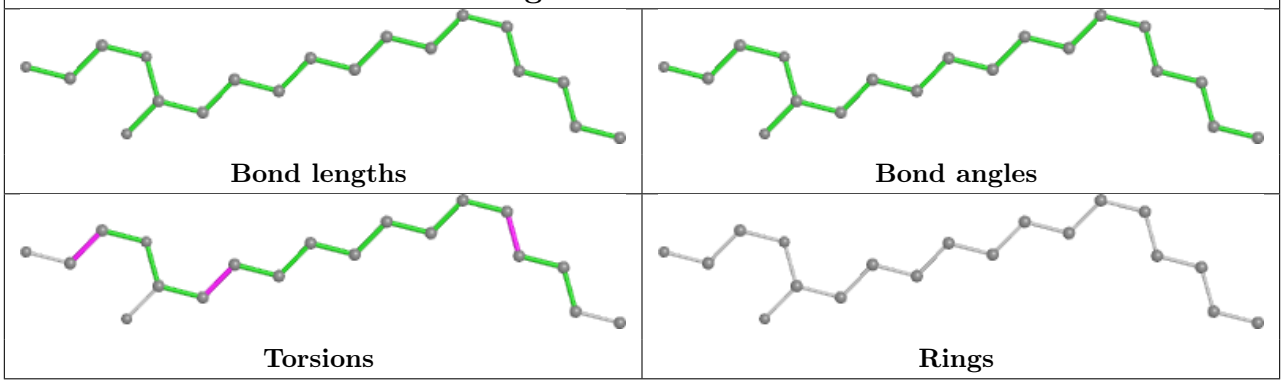
Ligand OLA B 1008



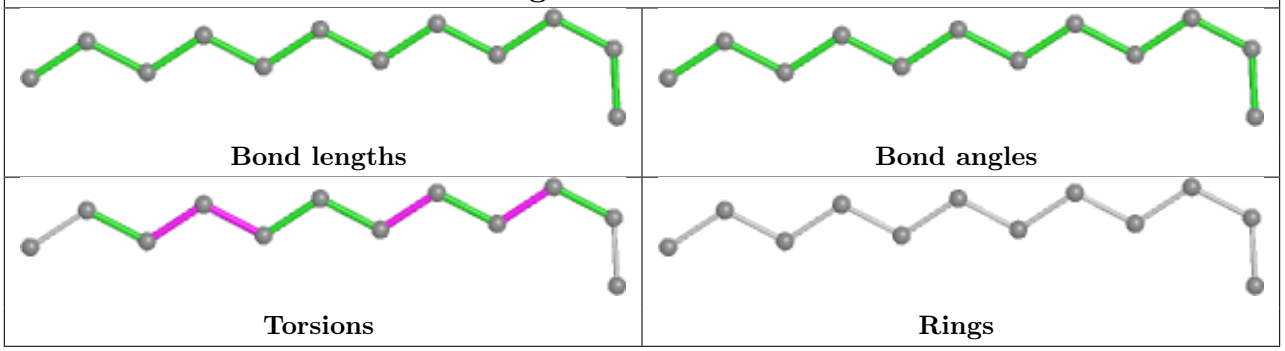
Ligand LFA C 912



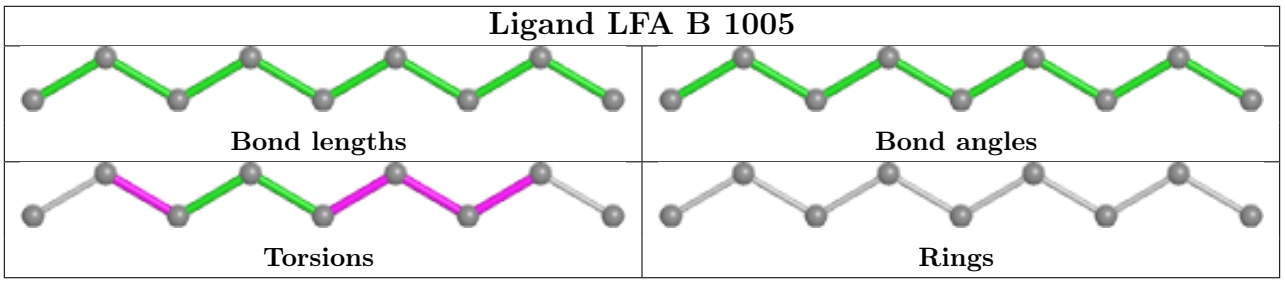
Ligand OLC A 511



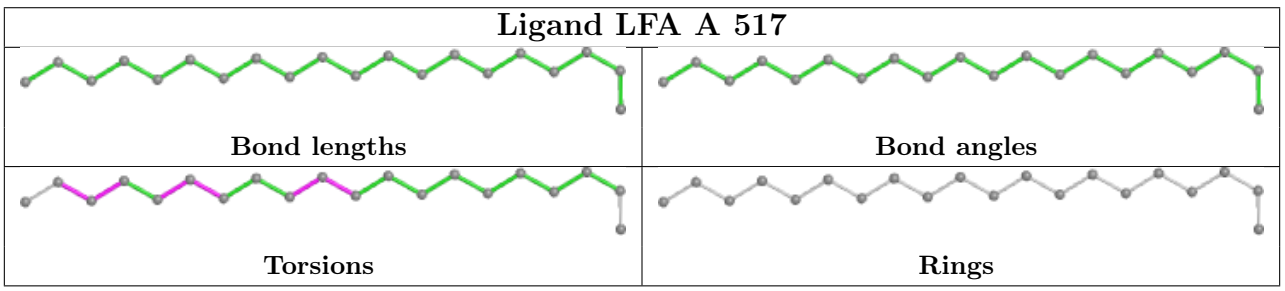
Ligand LFA C 907



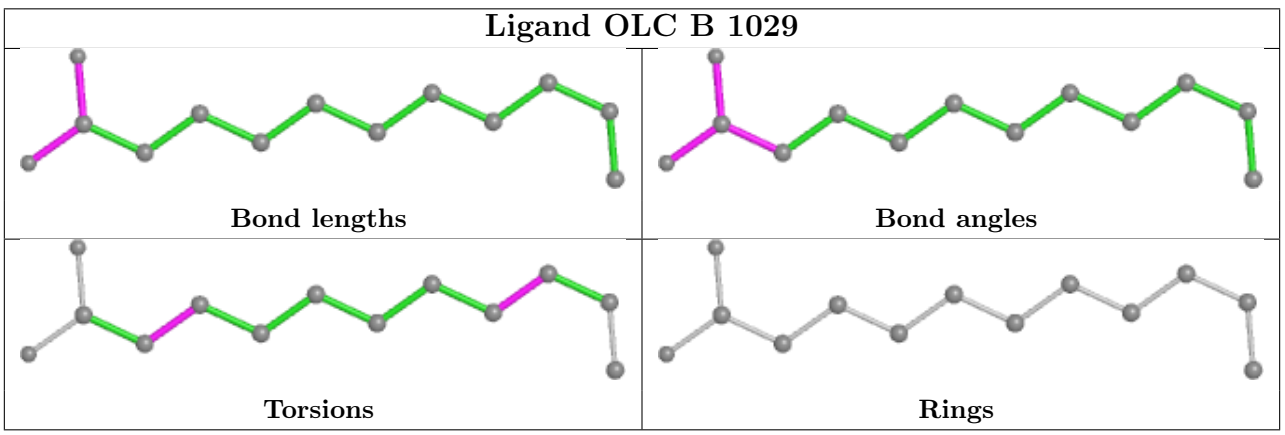
Ligand LFA B 1005



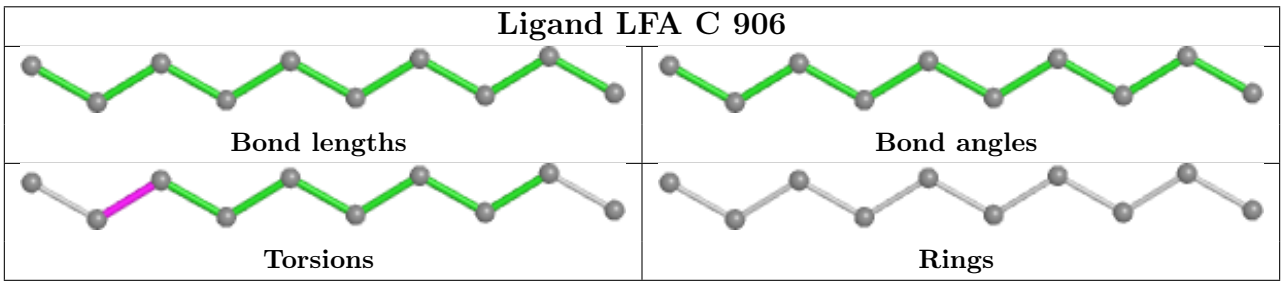
Ligand LFA A 517



Ligand OLC B 1029



Ligand LFA C 906



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, 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	220/229 (96%)	0.39	6 (2%)	54	56	20, 28, 51, 74	0
1	B	220/229 (96%)	0.46	13 (5%)	22	24	21, 30, 48, 86	0
1	C	222/229 (96%)	0.43	9 (4%)	37	39	21, 30, 51, 114	0
All	All	662/687 (96%)	0.43	28 (4%)	36	38	20, 30, 50, 114	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	62	ASP	7.9
1	B	61	TYR	7.6
1	C	61	TYR	5.3
1	B	64	THR	4.9
1	B	59	PHE	4.8

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, 95^{th} 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	0.73	0.29	40,54,83,99	0
1	FME	A	1	10/11	0.81	0.20	45,59,77,90	0
1	FME	B	1	10/11	0.88	0.16	40,58,73,79	0
1	LYR	C	207	29/30	0.88	0.13	21,26,36,43	0
1	LYR	B	207	29/30	0.90	0.13	20,24,36,39	0
1	LYR	A	207	29/30	0.91	0.13	23,28,38,43	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	C	910	9/20	0.39	0.35	47,57,66,68	0
2	LFA	B	1023	10/20	0.52	0.25	65,72,73,75	0
2	LFA	A	517	20/20	0.54	0.37	65,74,86,87	0
4	OLC	A	518	19/25	0.54	0.49	58,84,101,102	0
2	LFA	B	1027	10/20	0.56	0.33	56,61,67,68	0
2	LFA	A	515	8/20	0.59	0.21	47,58,64,65	0
2	LFA	C	904	6/20	0.61	0.33	45,52,55,56	0
2	LFA	C	917	16/20	0.62	0.29	56,60,63,67	0
3	OLA	A	508	16/20	0.63	0.34	59,77,82,84	0
2	LFA	C	912	7/20	0.63	0.41	40,48,62,63	0
4	OLC	B	1029	13/25	0.64	0.33	62,79,87,91	0
2	LFA	B	1004	11/20	0.65	0.25	44,48,50,51	0
4	OLC	B	1018	19/25	0.65	0.31	57,76,91,99	0
2	LFA	B	1025	10/20	0.65	0.23	51,56,64,65	0
3	OLA	A	513	20/20	0.66	0.34	50,62,84,91	0
2	LFA	C	905	8/20	0.66	0.20	52,53,55,55	0
2	LFA	B	1028	15/20	0.67	0.27	47,59,78,79	0
3	OLA	A	506	14/20	0.68	0.32	50,59,70,77	0
2	LFA	A	516	4/20	0.68	0.30	47,47,56,59	0
4	OLC	C	909	17/25	0.68	0.24	50,67,84,86	0
2	LFA	C	901	12/20	0.69	0.19	40,47,54,57	0
2	LFA	B	1026	14/20	0.71	0.28	57,71,76,76	0
3	OLA	A	512	19/20	0.72	0.23	49,58,74,75	0
2	LFA	A	501	6/20	0.72	0.23	40,43,44,45	0
2	LFA	C	918	6/20	0.72	0.23	63,63,64,65	0
4	OLC	B	1015	19/25	0.73	0.20	42,61,83,83	0
3	OLA	B	1016	11/20	0.73	0.31	59,63,85,92	0
3	OLA	C	911	9/20	0.73	0.22	55,72,76,78	0
2	LFA	C	919	7/20	0.73	0.30	56,59,64,65	0
3	OLA	B	1008	16/20	0.74	0.19	38,42,53,54	0
3	OLA	A	509	20/20	0.74	0.24	41,49,65,67	0
2	LFA	B	1020	11/20	0.74	0.21	56,63,74,76	0

Continued on next page...

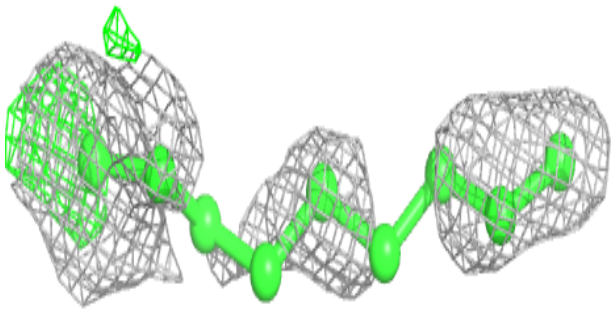
Continued from previous page...

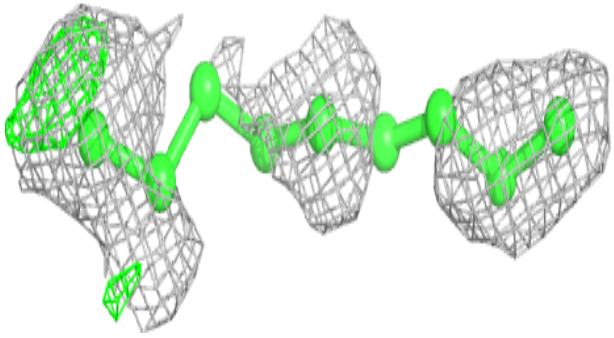
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LFA	A	502	8/20	0.74	0.21	48,54,57,58	0
4	OLC	C	913	15/25	0.74	0.21	44,55,69,73	0
2	LFA	C	902	13/20	0.75	0.32	63,70,78,80	0
4	OLC	A	507	17/25	0.75	0.22	37,54,71,75	0
2	LFA	C	915	11/20	0.75	0.27	43,47,50,50	0
2	LFA	B	1001	7/20	0.75	0.22	43,43,51,52	0
2	LFA	B	1003	9/20	0.76	0.17	39,45,47,50	0
2	LFA	A	505	9/20	0.76	0.31	56,59,61,62	0
2	LFA	C	916	15/20	0.76	0.33	60,62,70,71	0
4	OLC	A	511	19/25	0.76	0.21	50,62,72,73	0
2	LFA	B	1024	11/20	0.76	0.21	49,61,77,78	0
3	OLA	B	1012	14/20	0.77	0.22	47,53,71,73	0
3	OLA	B	1009	14/20	0.78	0.18	44,52,60,68	0
2	LFA	B	1005	9/20	0.78	0.21	41,46,57,58	0
2	LFA	B	1007	10/20	0.78	0.17	40,51,58,59	0
3	OLA	A	503	12/20	0.78	0.18	47,54,63,63	0
4	OLC	B	1017	20/25	0.79	0.21	45,81,93,93	0
3	OLA	B	1013	14/20	0.79	0.19	52,62,73,75	0
3	OLA	B	1014	14/20	0.79	0.21	49,58,73,75	0
2	LFA	B	1010	8/20	0.79	0.23	53,55,57,58	0
2	LFA	A	514	10/20	0.79	0.20	35,37,53,58	0
2	LFA	B	1019	6/20	0.80	0.25	49,60,62,66	0
2	LFA	C	920	16/20	0.80	0.19	44,48,64,64	0
2	LFA	A	504	9/20	0.80	0.20	42,46,55,56	0
2	LFA	C	908	5/20	0.80	0.20	45,47,50,52	0
5	PO4	C	914	5/5	0.80	0.17	97,98,107,112	0
3	OLA	C	903	20/20	0.81	0.23	36,46,83,88	0
2	LFA	C	907	12/20	0.81	0.17	43,45,56,57	0
2	LFA	A	510	11/20	0.81	0.17	43,48,58,59	0
3	OLA	B	1006	20/20	0.81	0.23	37,51,81,82	0
2	LFA	B	1021	6/20	0.82	0.24	56,59,65,66	0
2	LFA	C	906	10/20	0.83	0.25	54,57,57,61	0
2	LFA	B	1022	8/20	0.83	0.18	51,54,57,61	0
2	LFA	B	1002	7/20	0.84	0.28	39,40,43,52	0
2	LFA	B	1011	11/20	0.84	0.16	40,46,60,61	0

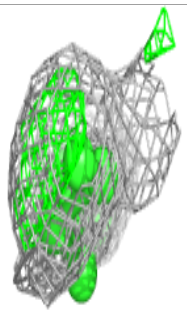
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LFA C 910:

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

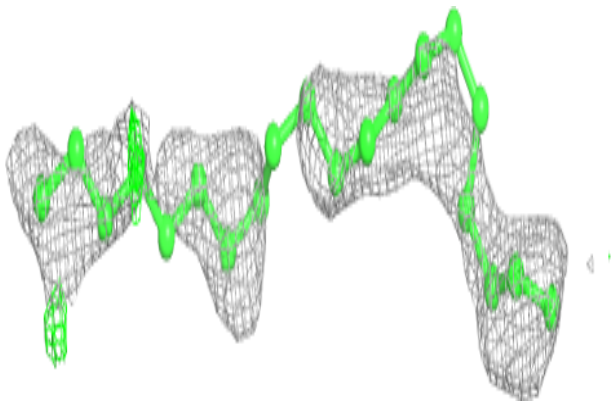


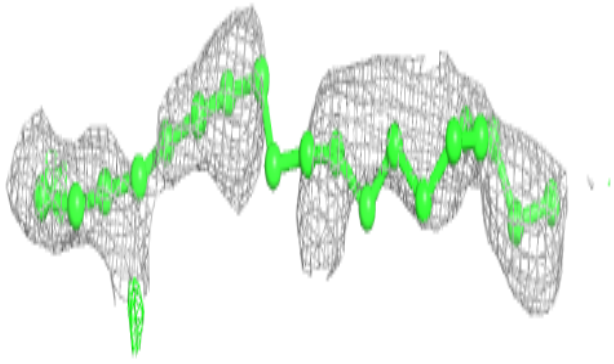


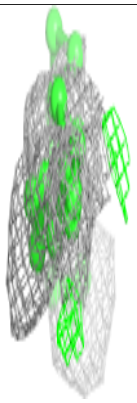


Electron density around LFA A 517:

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

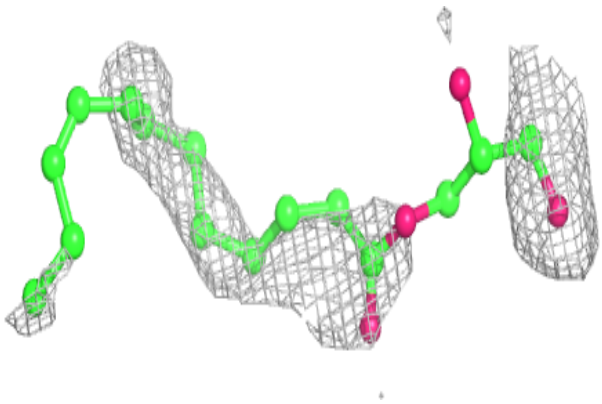


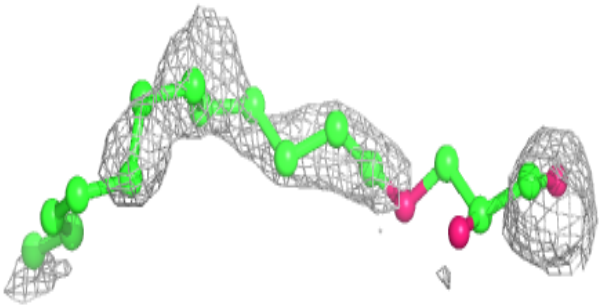


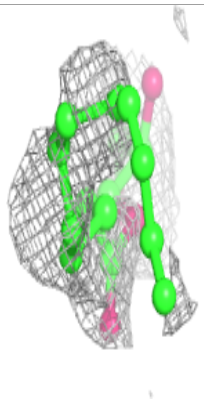


Electron density around OLC A 518:

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

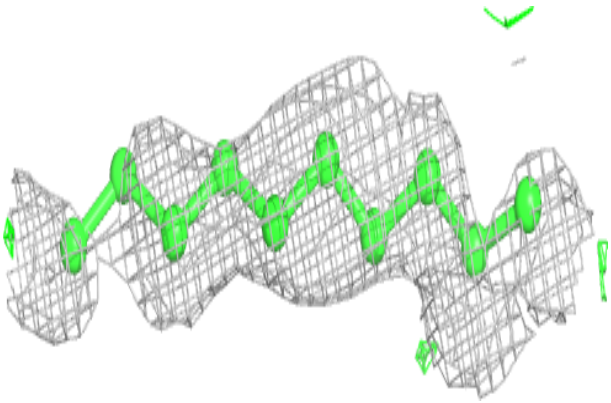


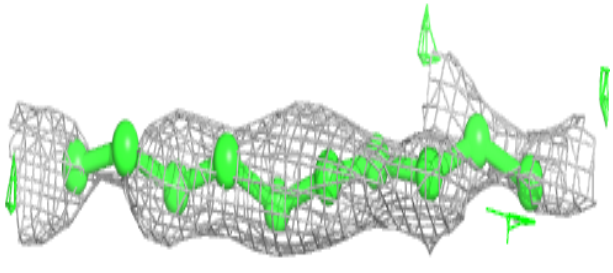


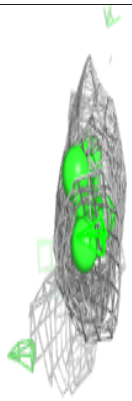


Electron density around LFA B 1027:

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

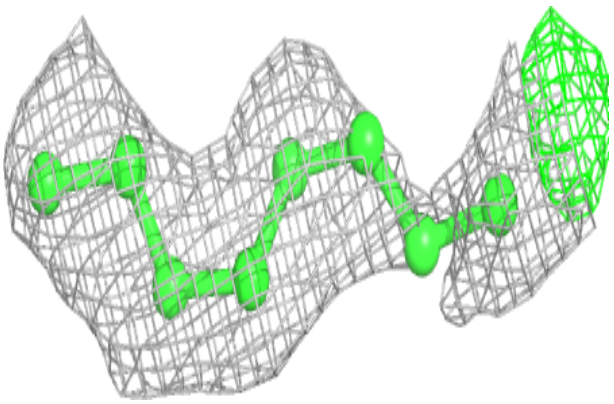


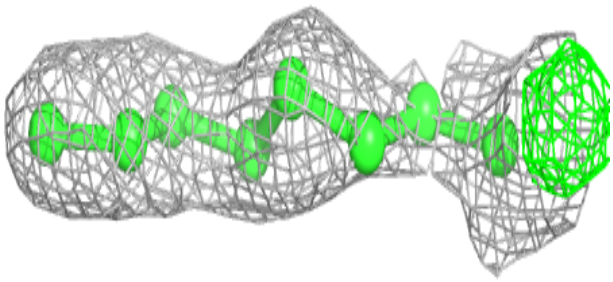


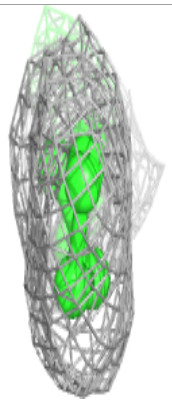


Electron density around LFA A 515:

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

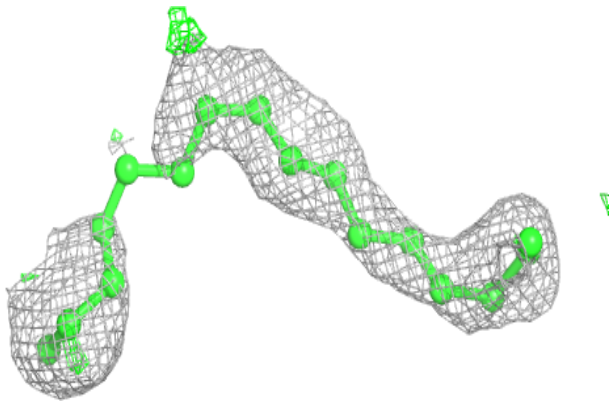


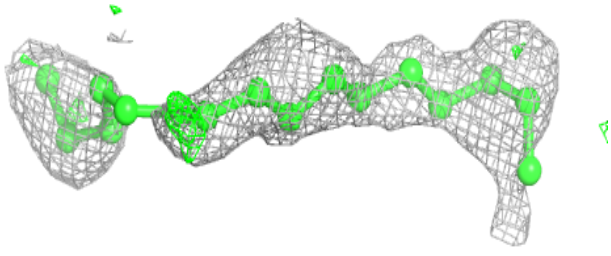


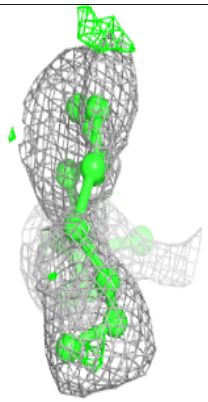


Electron density around LFA C 917:

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

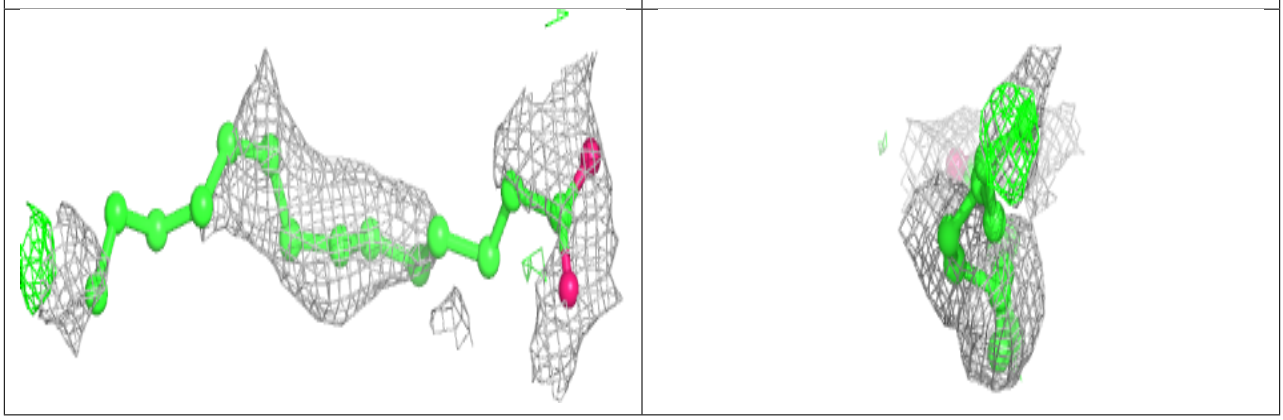






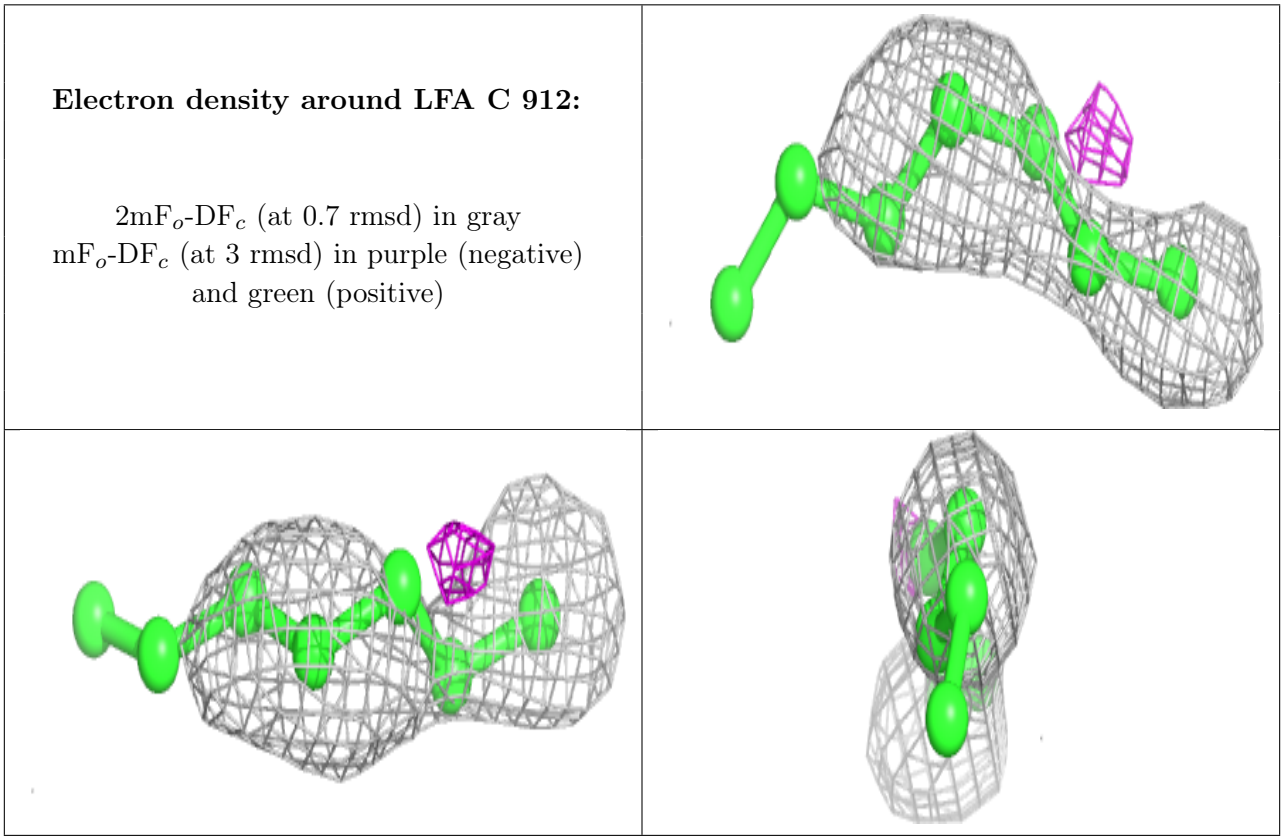
Electron density around OLA A 508:

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



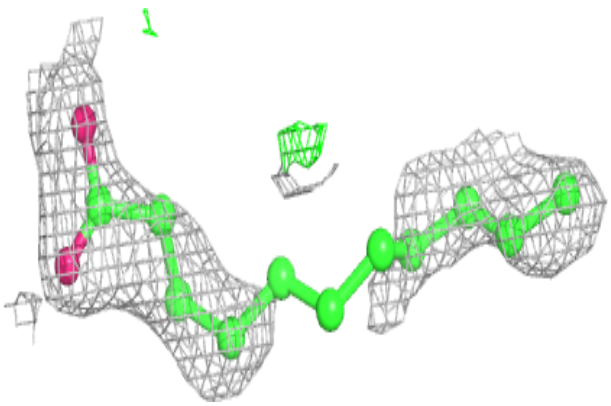
Electron density around LFA C 912:

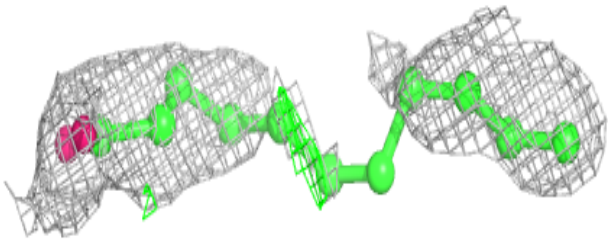
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

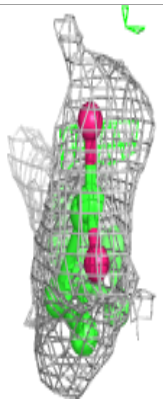


Electron density around OLC B 1029:

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

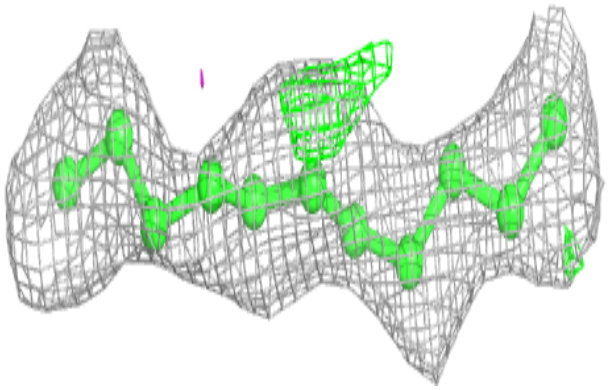


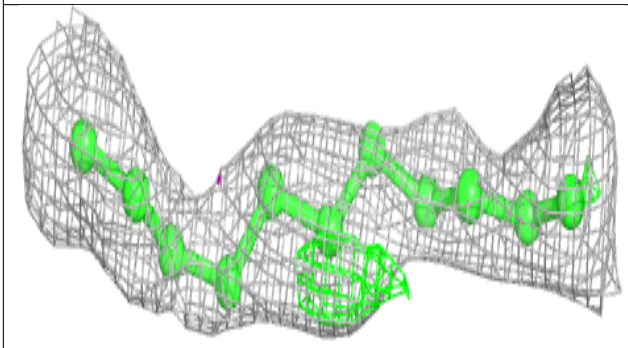


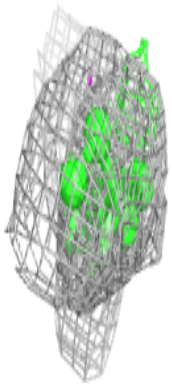


Electron density around LFA B 1004:

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

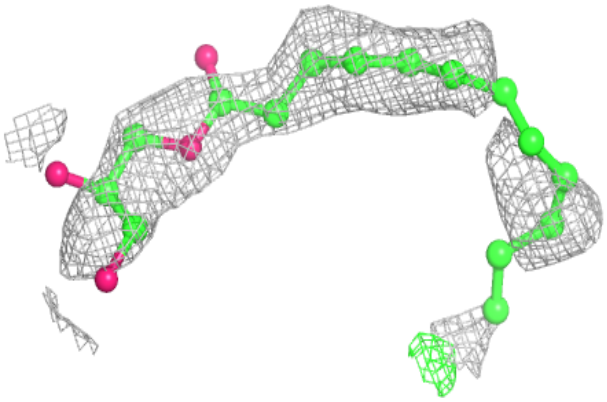


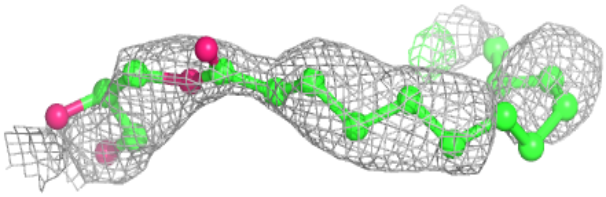


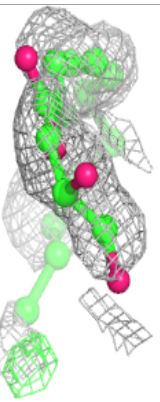


Electron density around OLC B 1018:

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

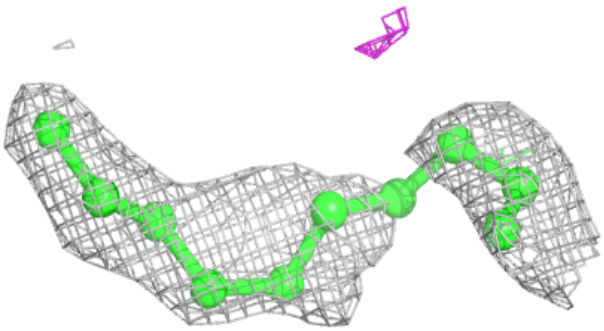


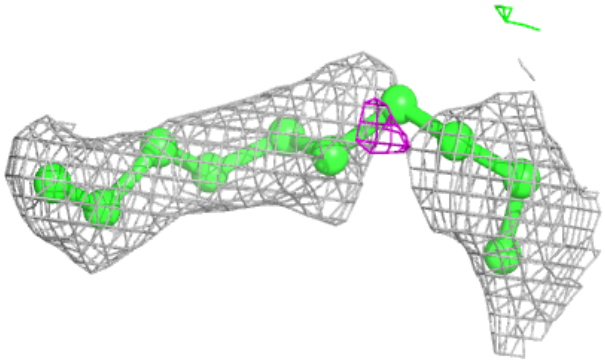


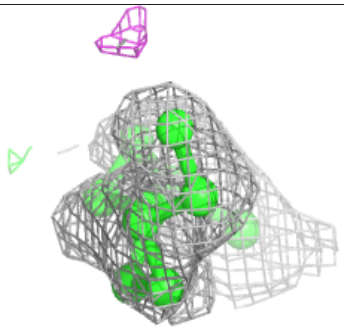


Electron density around LFA B 1025:

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

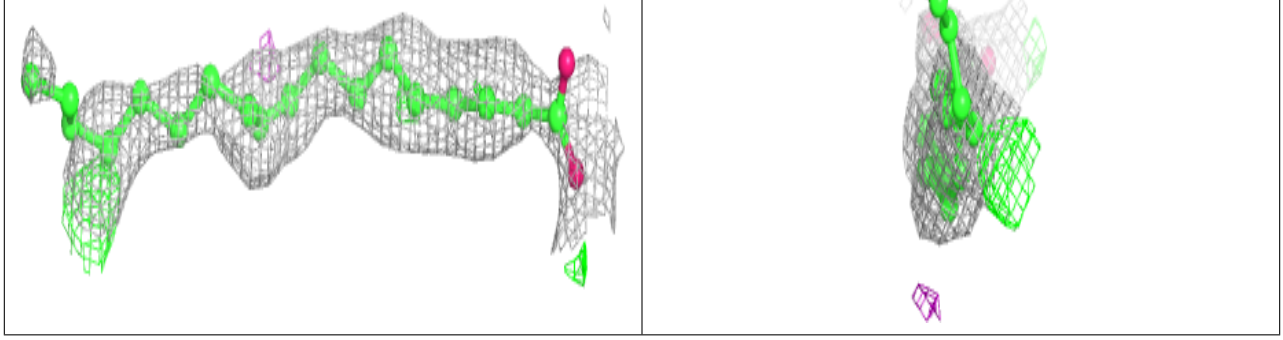






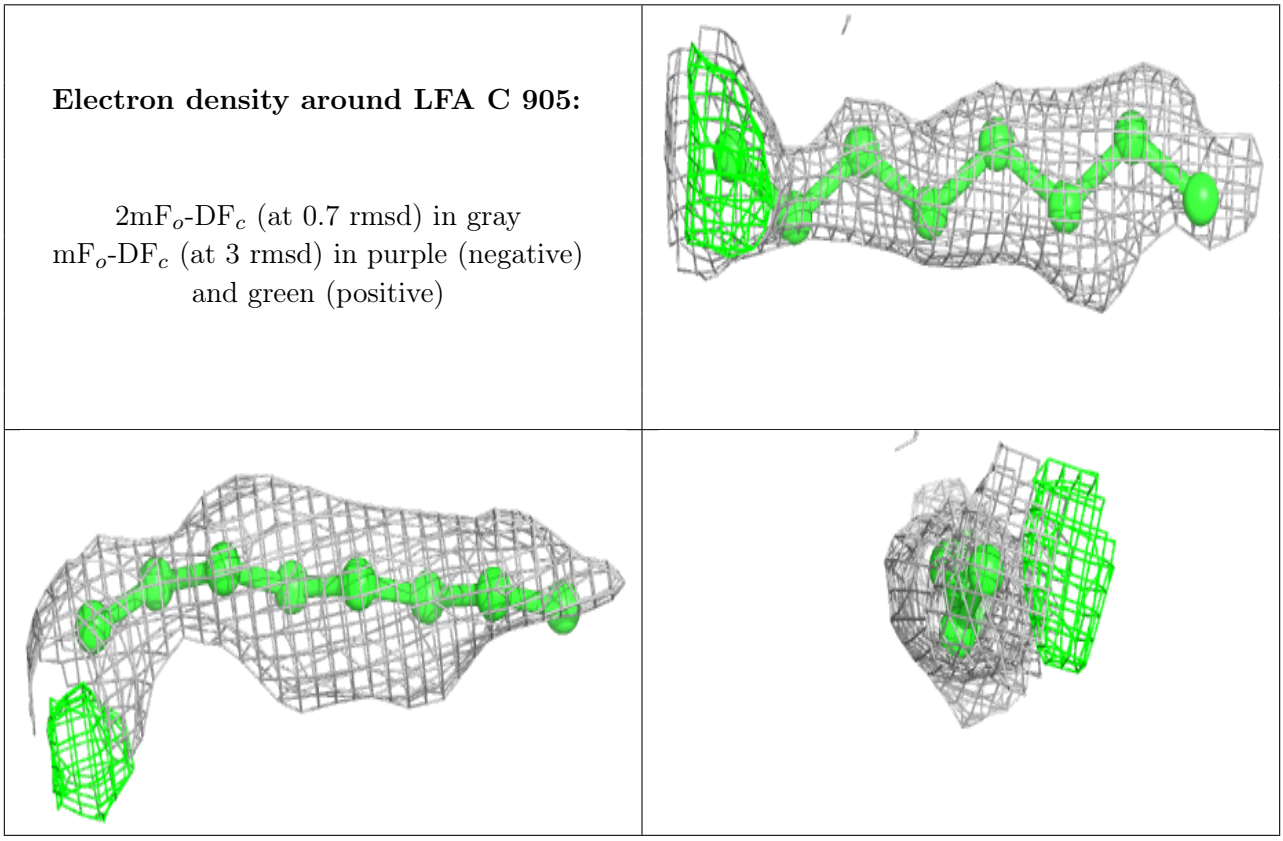
Electron density around OLA A 513:

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



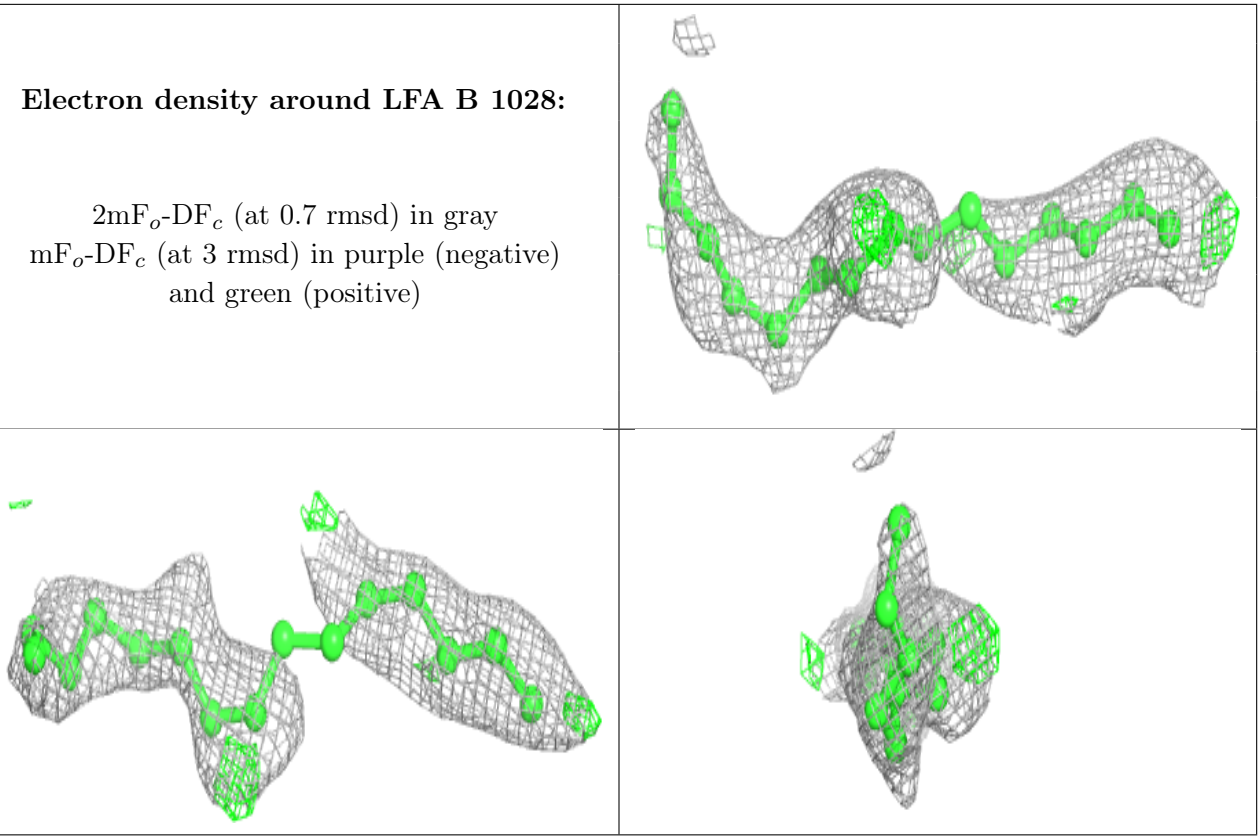
Electron density around LFA C 905:

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



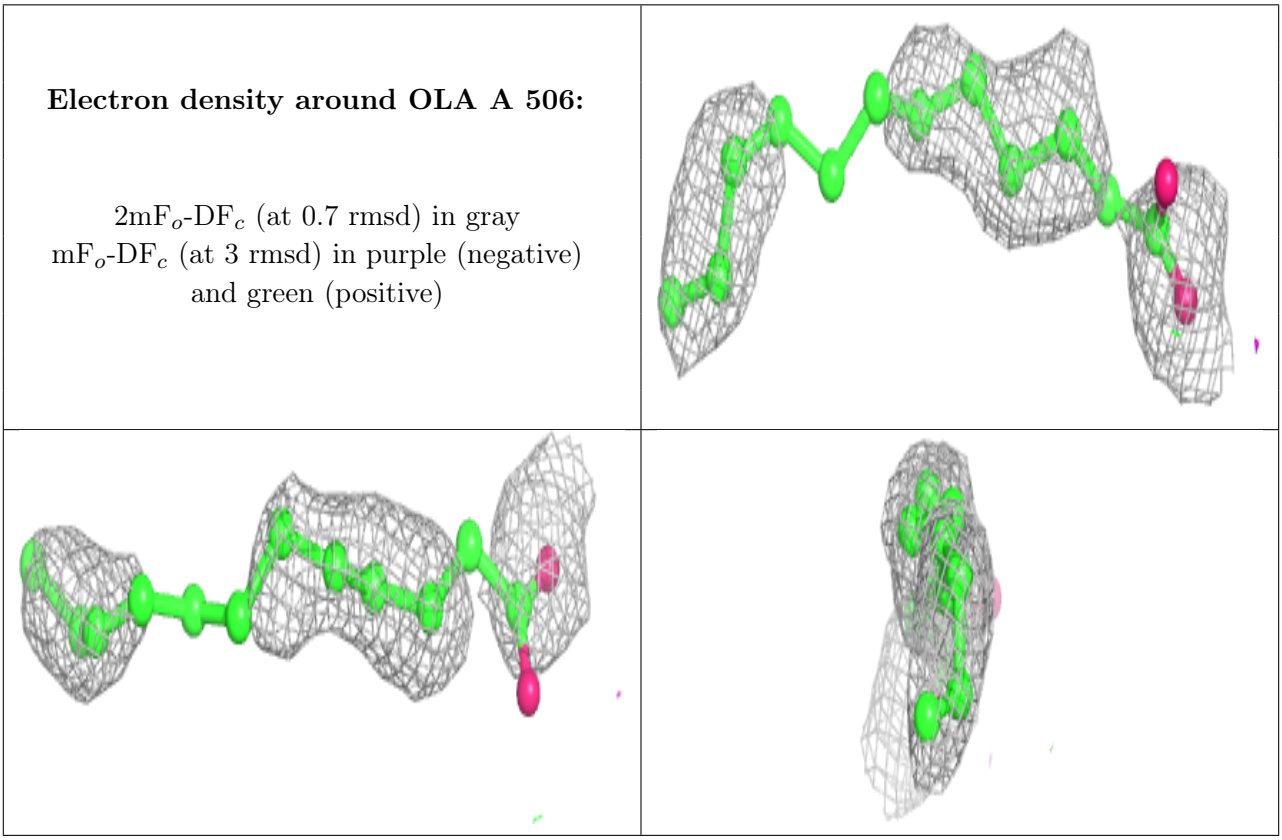
Electron density around LFA B 1028:

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



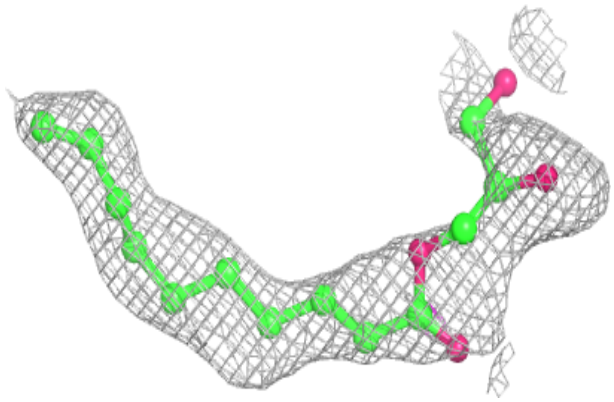
Electron density around OLA A 506:

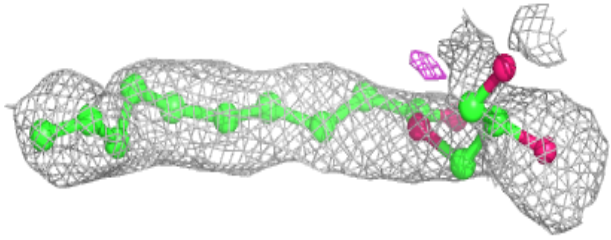
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

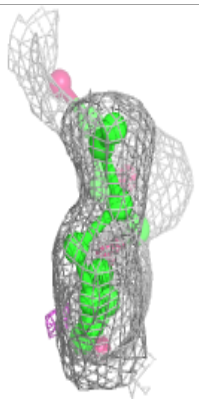


Electron density around OLC C 909:

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

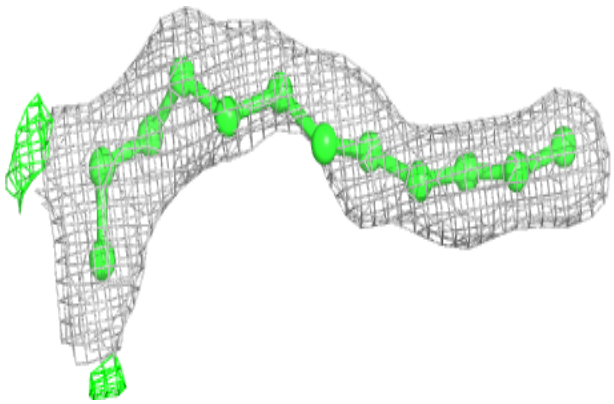


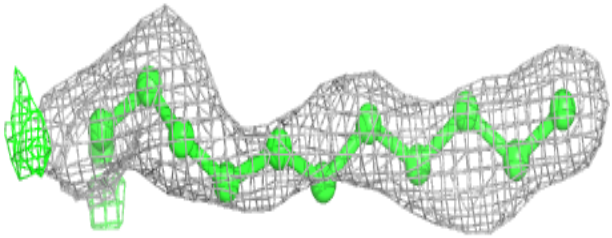


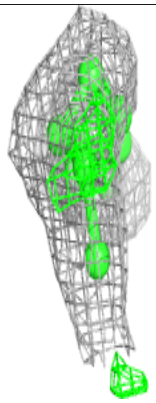


Electron density around LFA C 901:

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

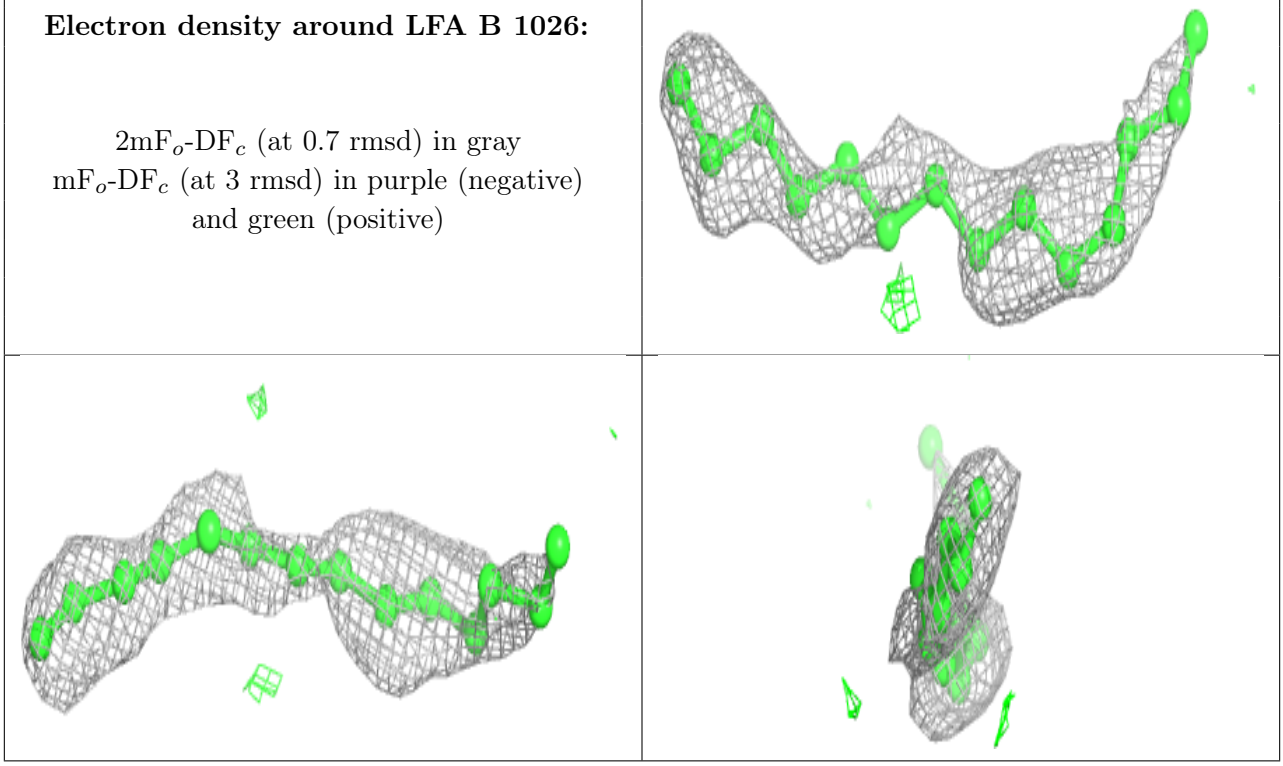






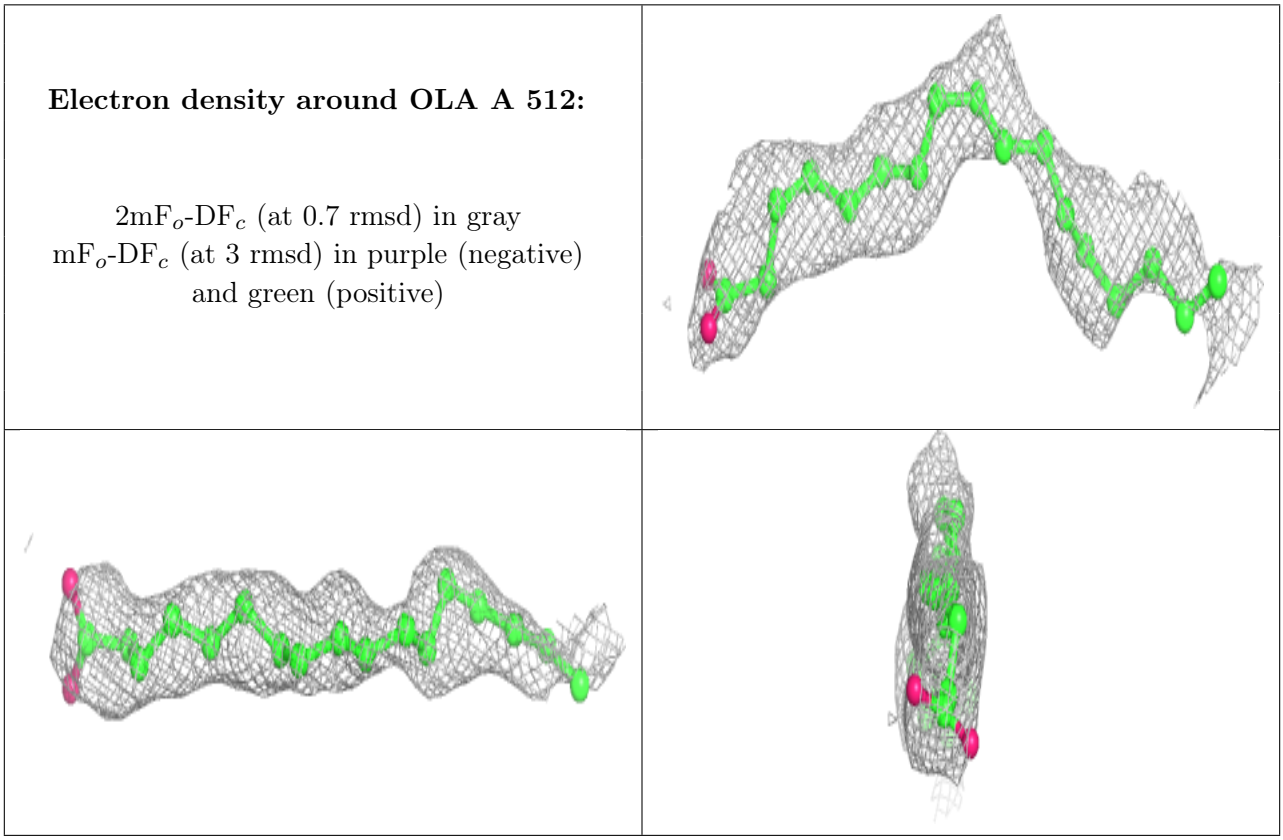
Electron density around LFA B 1026:

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



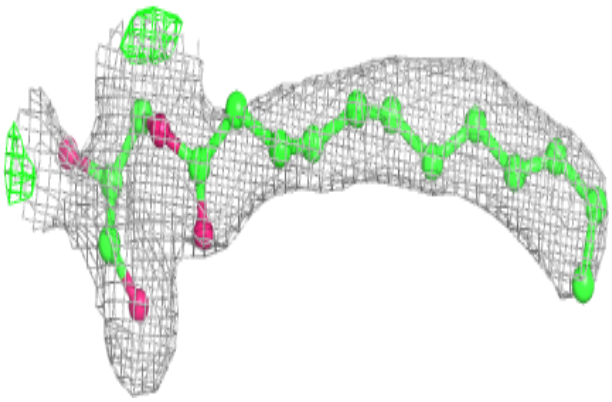
Electron density around OLA A 512:

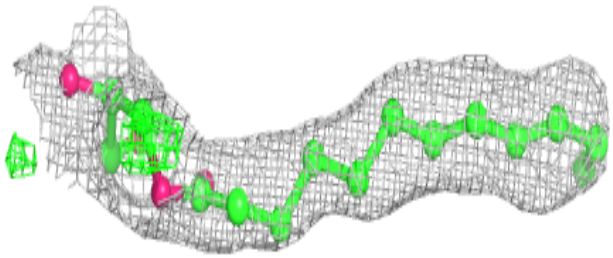
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

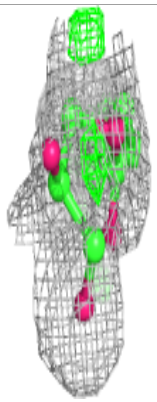


Electron density around OLC B 1015:

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

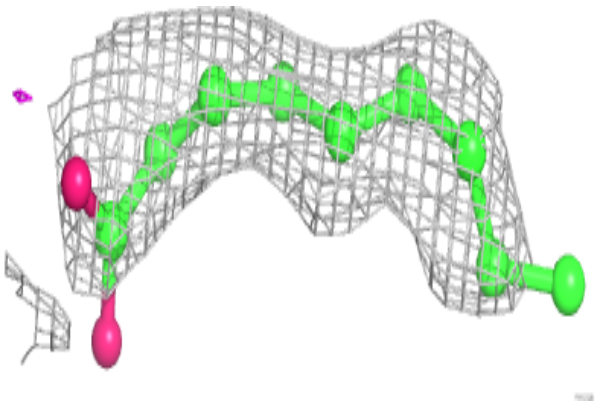


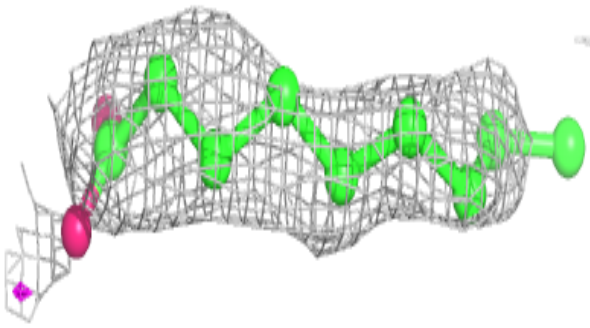


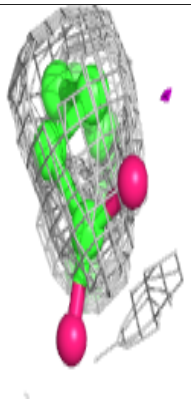


Electron density around OLA B 1016:

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

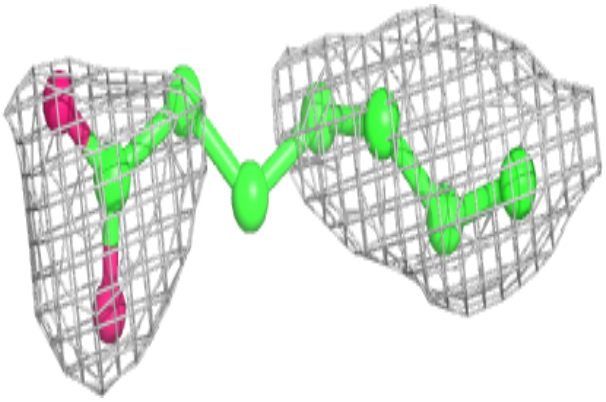


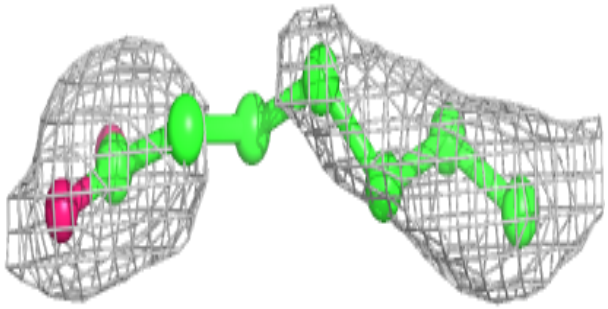


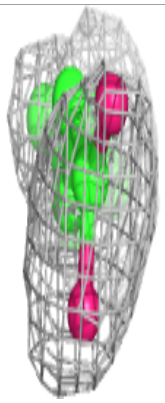


Electron density around OLA C 911:

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

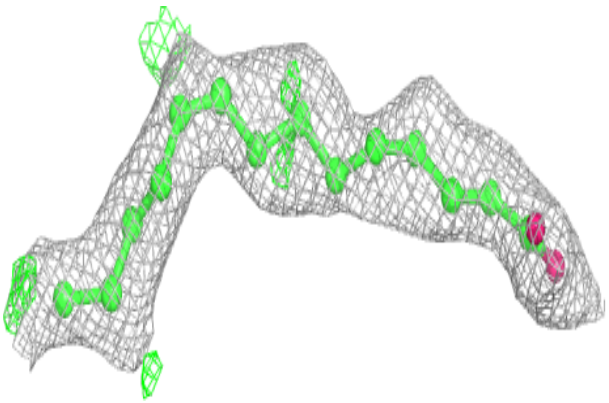


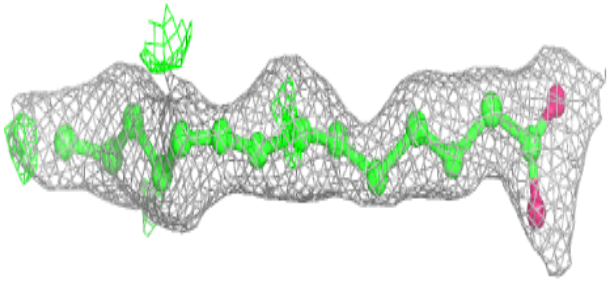


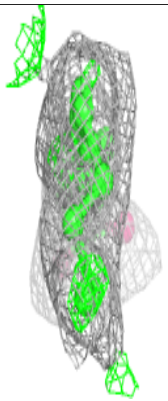


Electron density around OLA B 1008:

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

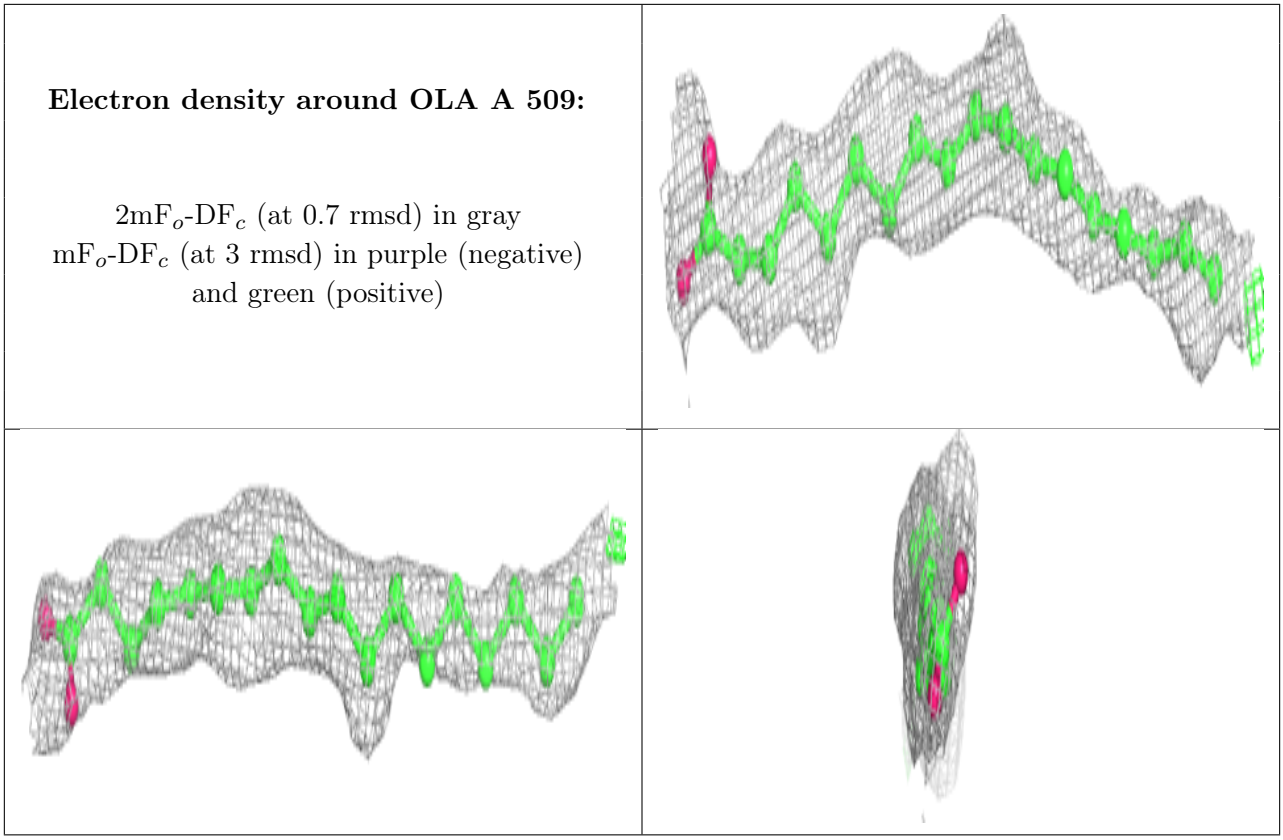






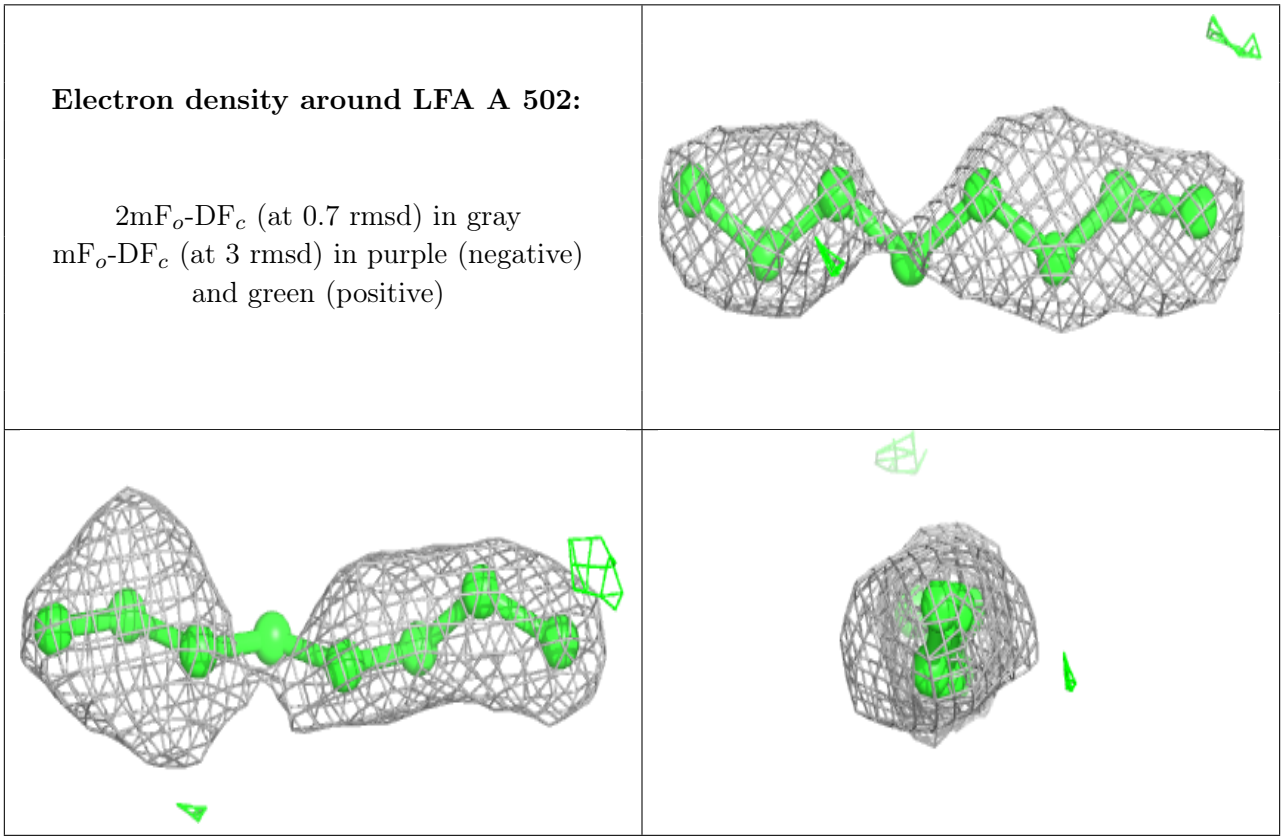
Electron density around OLA A 509:

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



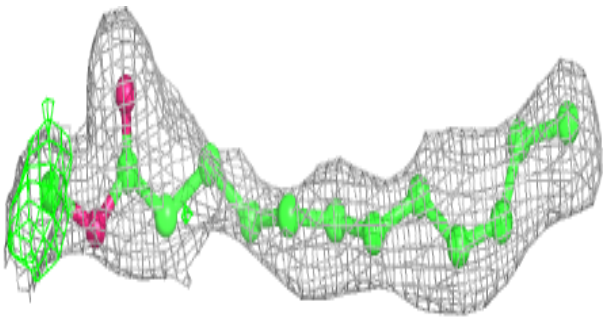
Electron density around LFA A 502:

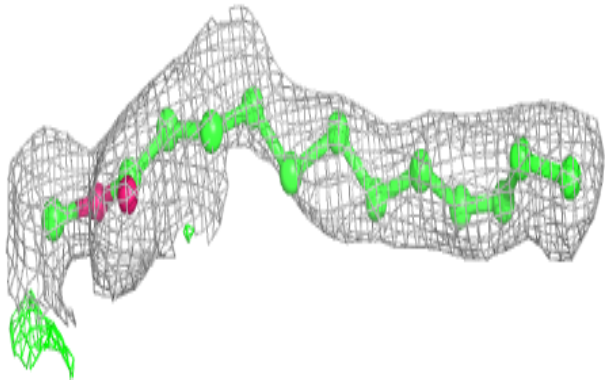
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

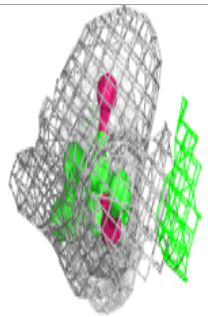


Electron density around OLC C 913:

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

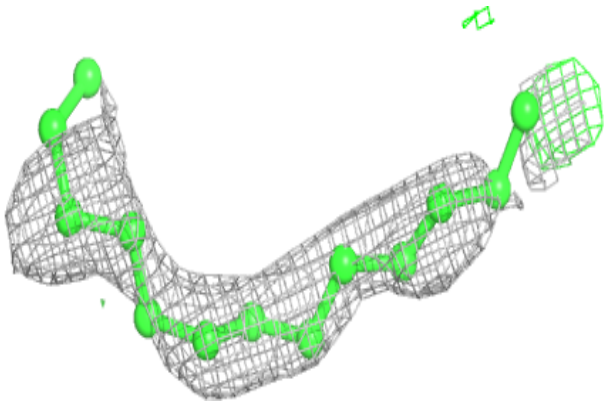


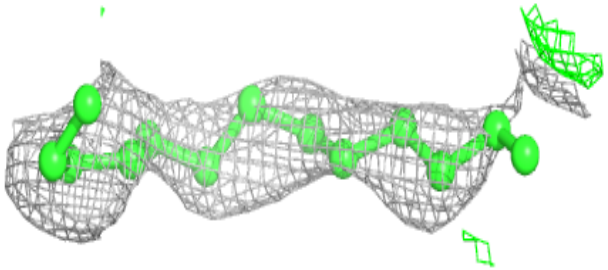


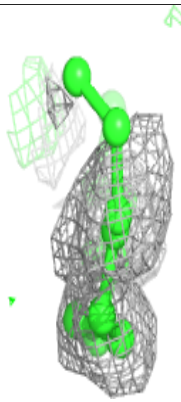


Electron density around LFA C 902:

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

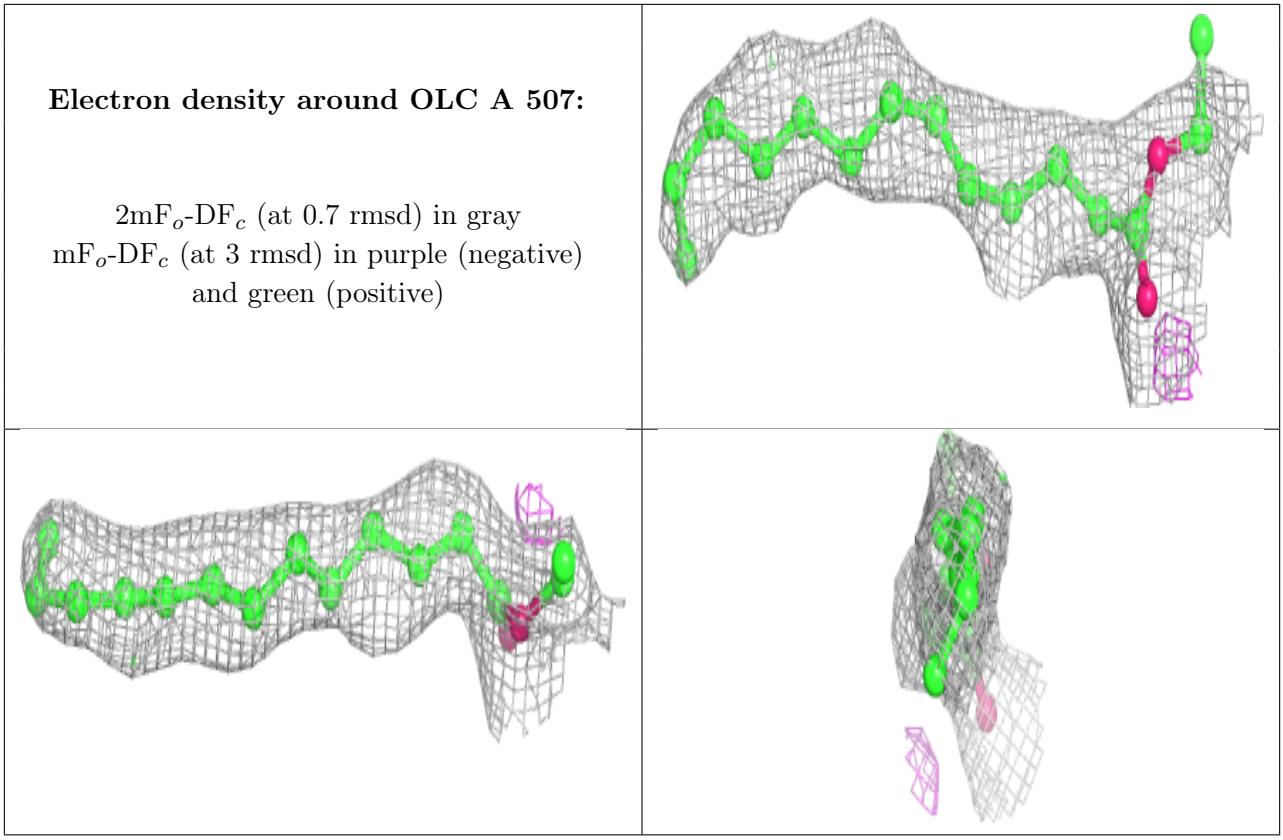






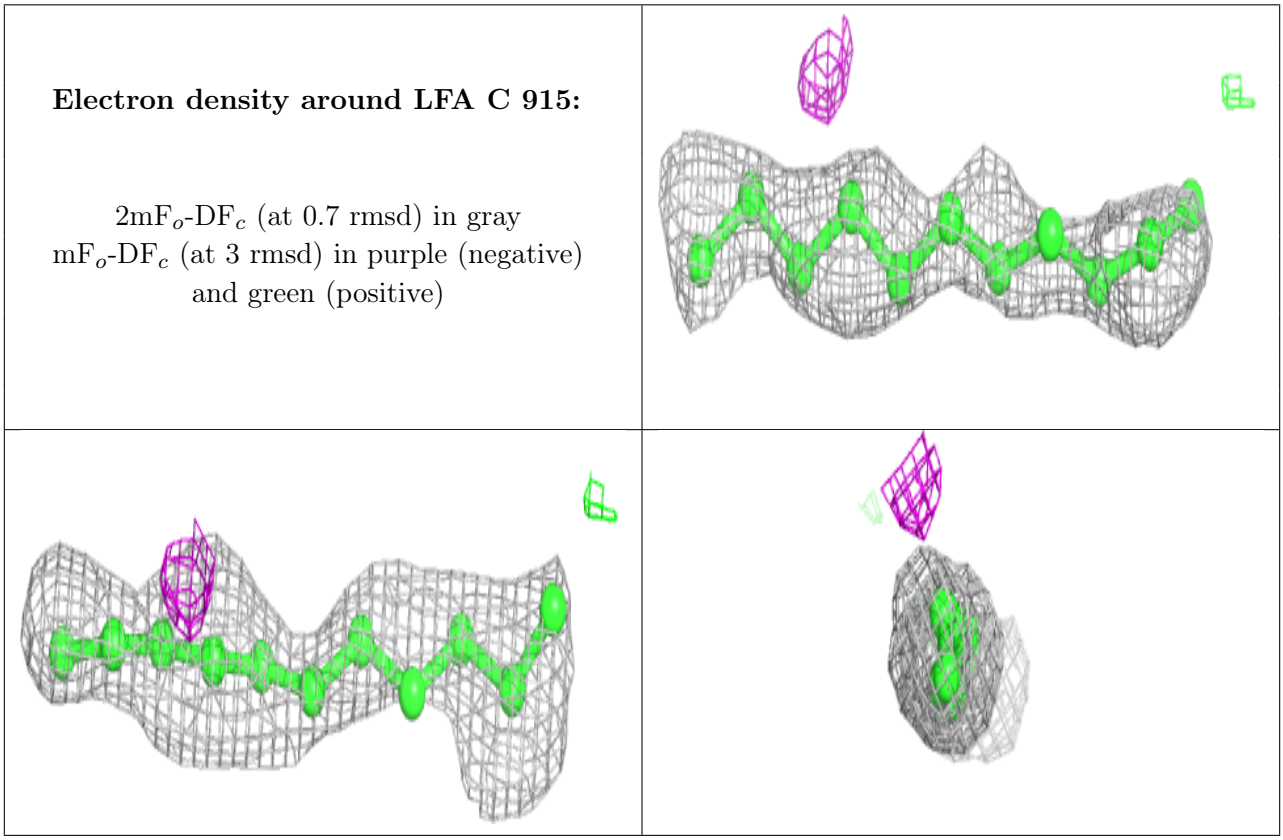
Electron density around OLC A 507:

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



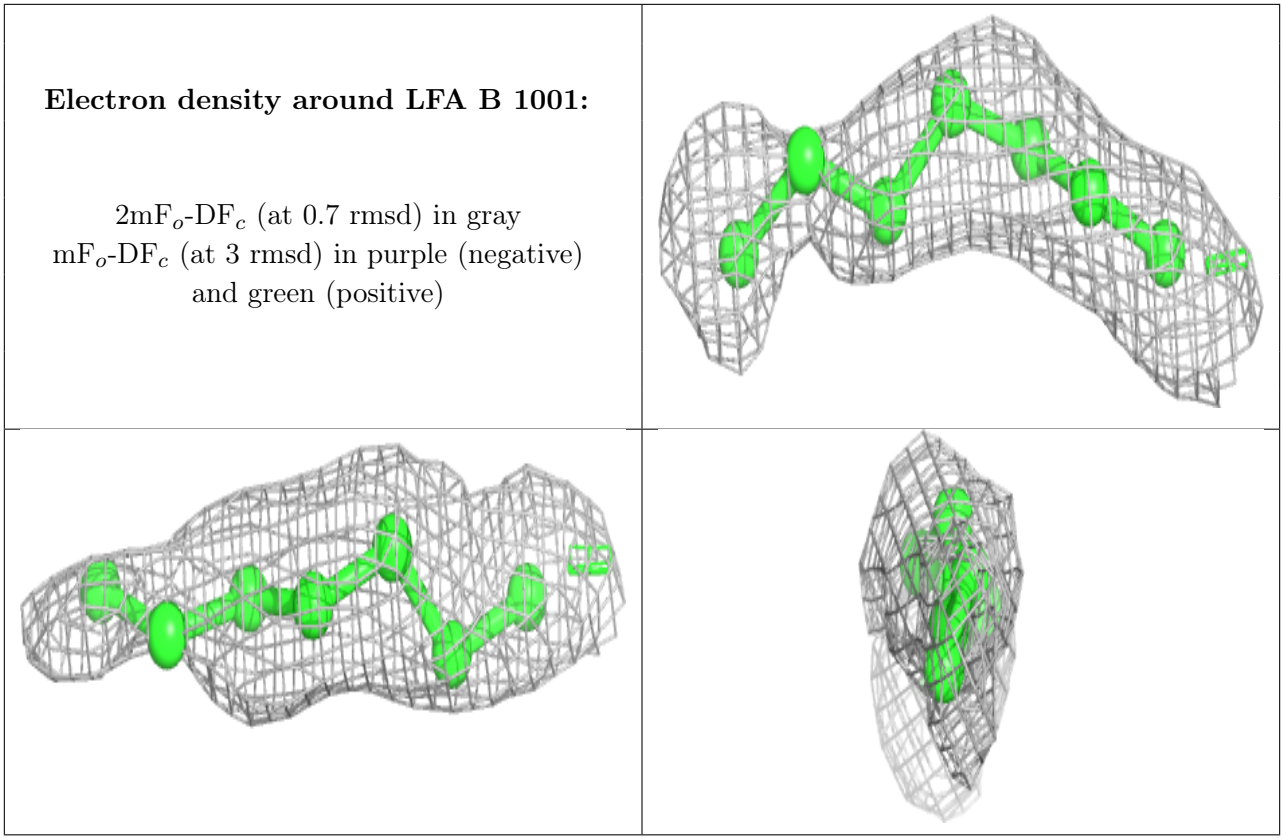
Electron density around LFA C 915:

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



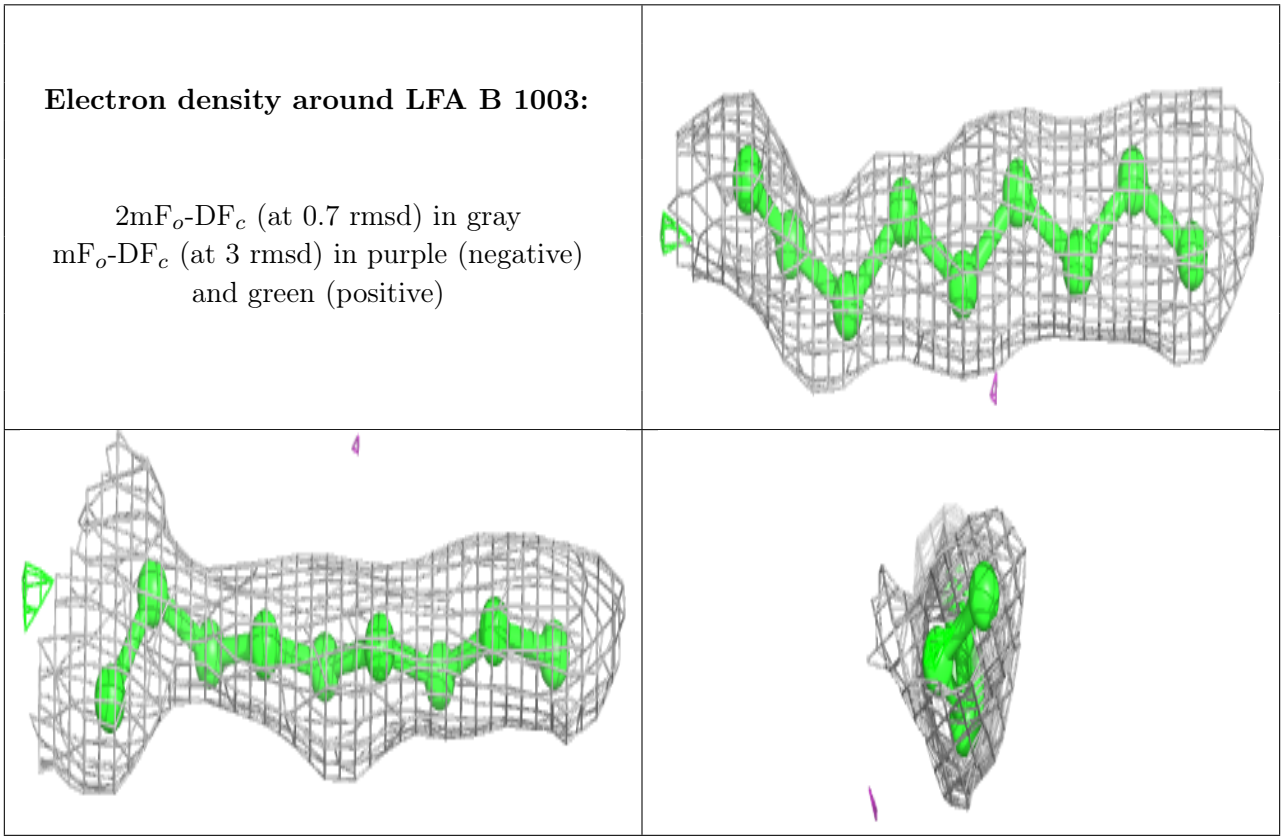
Electron density around LFA B 1001:

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



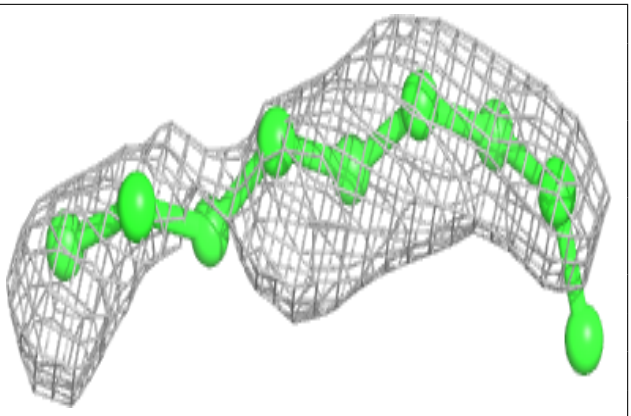
Electron density around LFA B 1003:

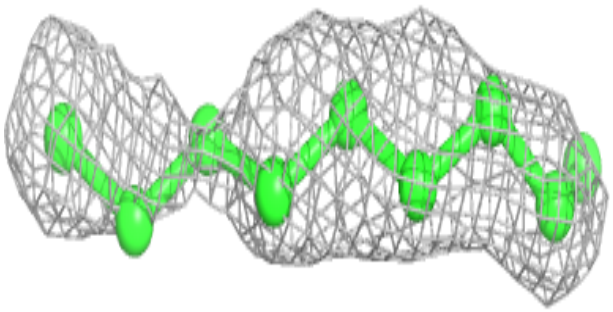
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

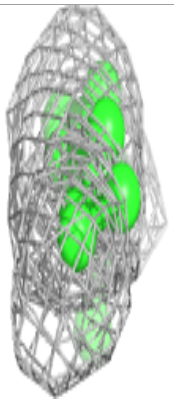


Electron density around LFA A 505:

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

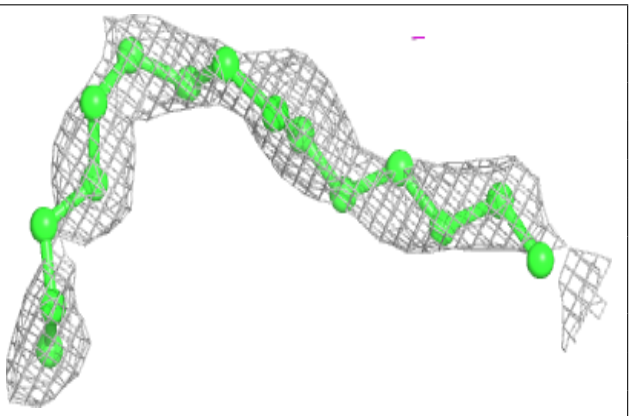


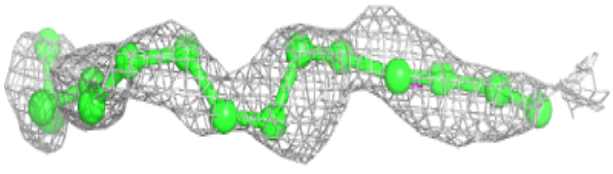


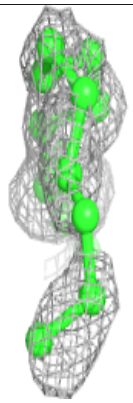


Electron density around LFA C 916:

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

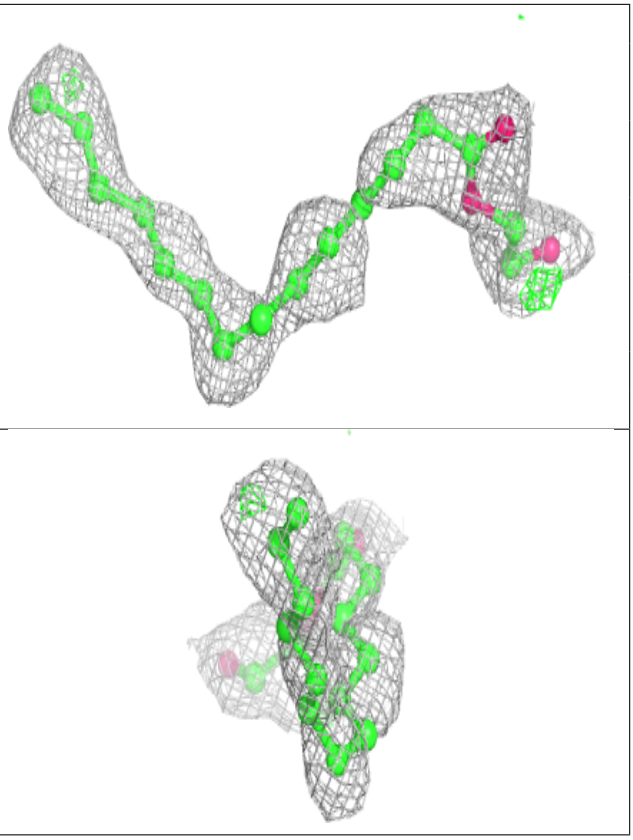






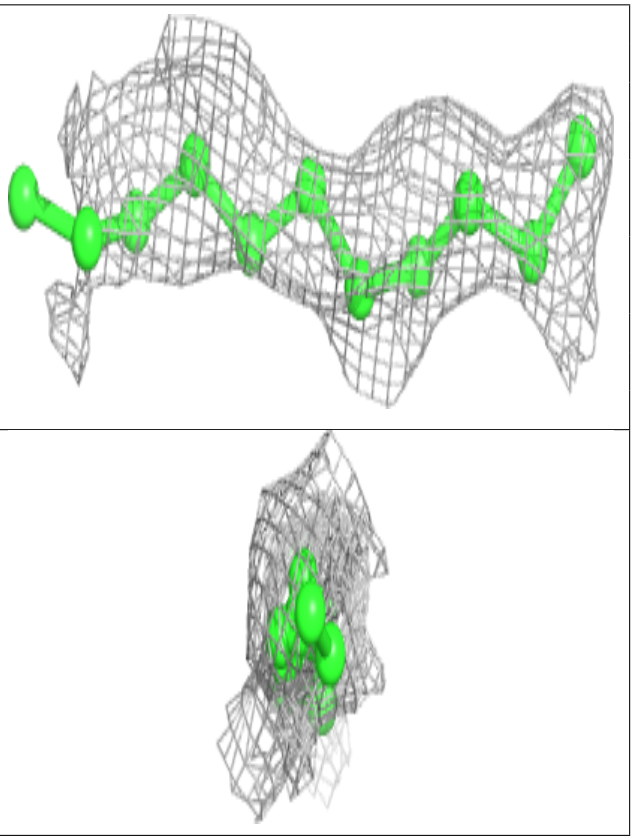
Electron density around OLC A 511:

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



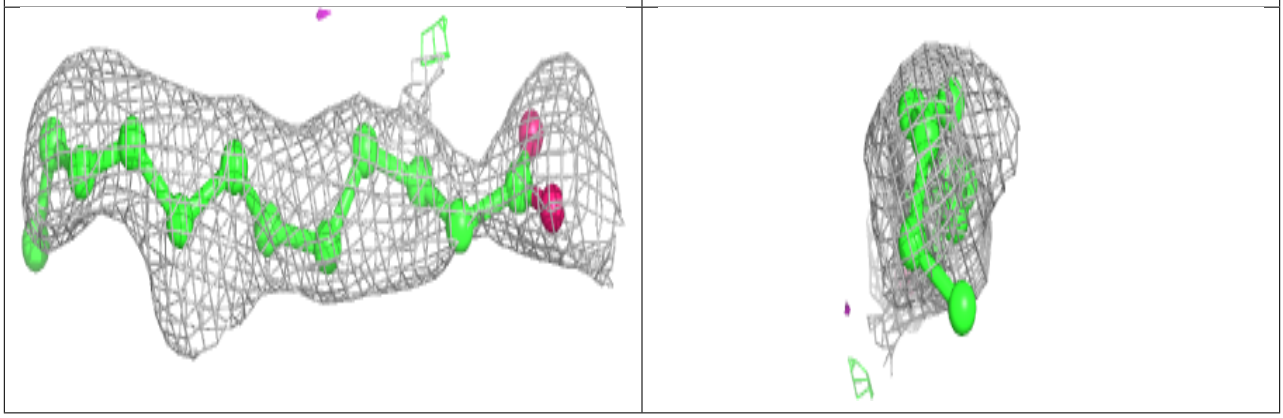
Electron density around LFA B 1024:

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



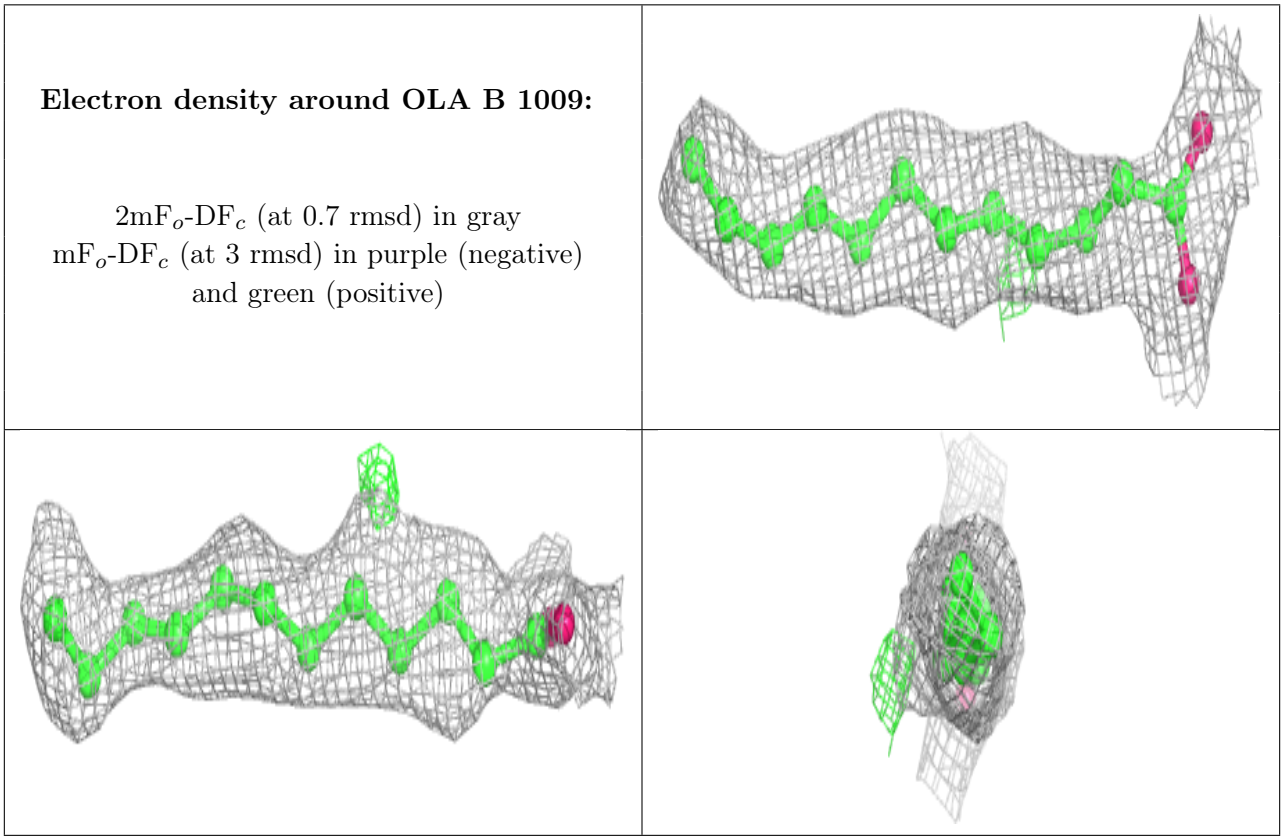
Electron density around OLA B 1012:

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



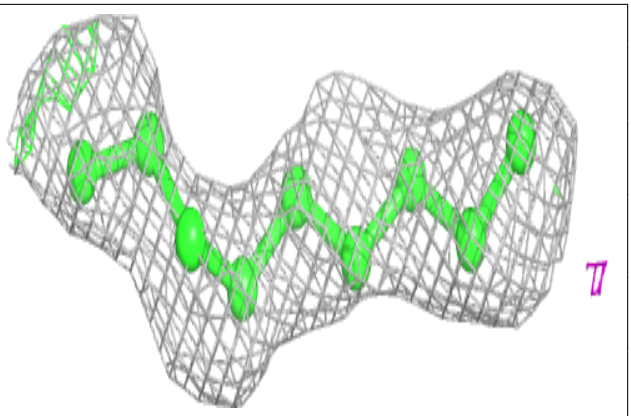
Electron density around OLA B 1009:

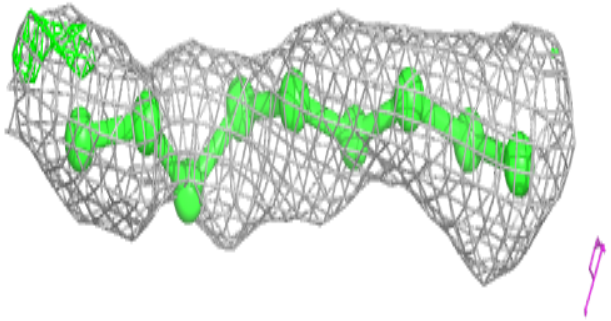
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

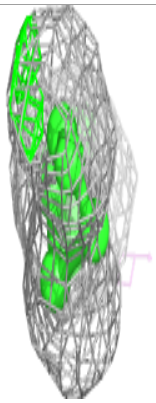


Electron density around LFA B 1005:

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

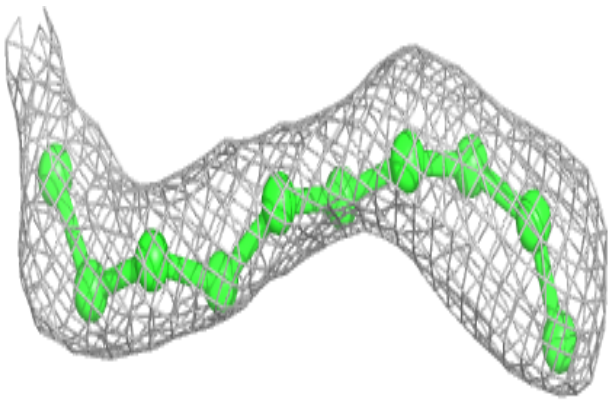


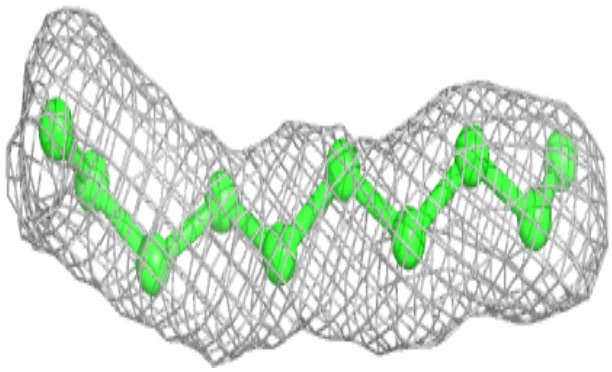


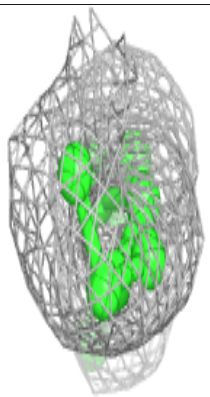


Electron density around LFA B 1007:

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

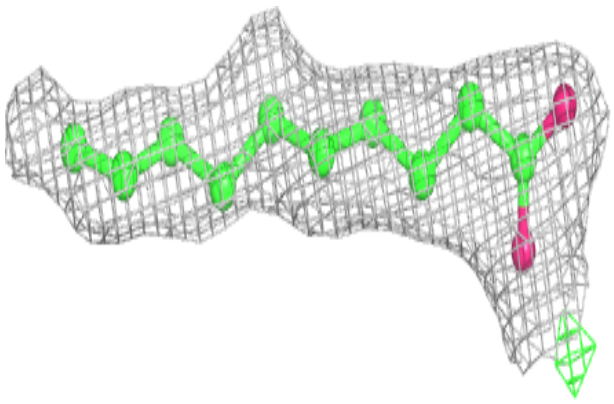


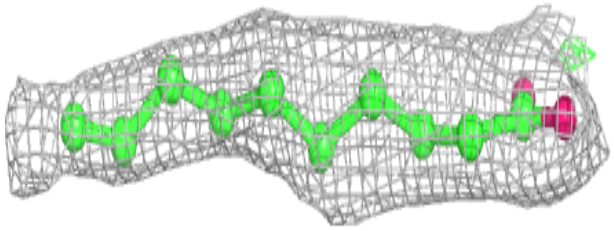


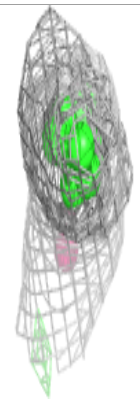


Electron density around OLA A 503:

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

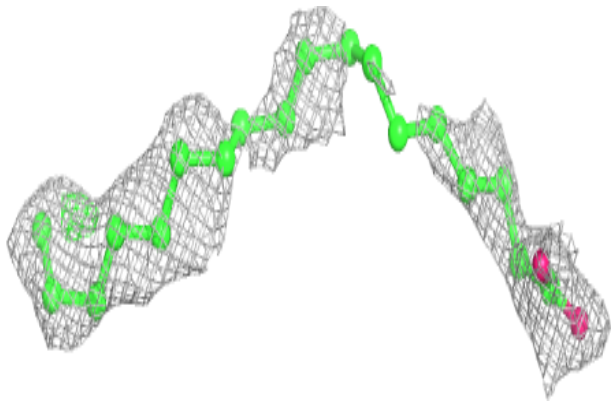


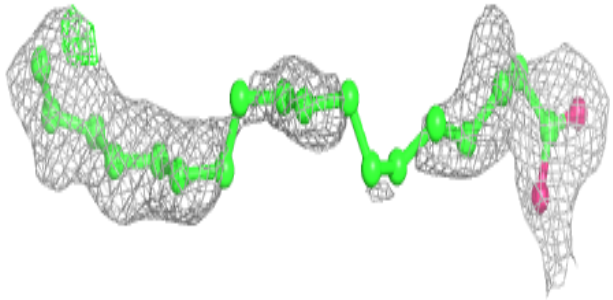


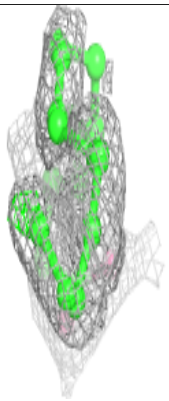


Electron density around OLC B 1017:

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

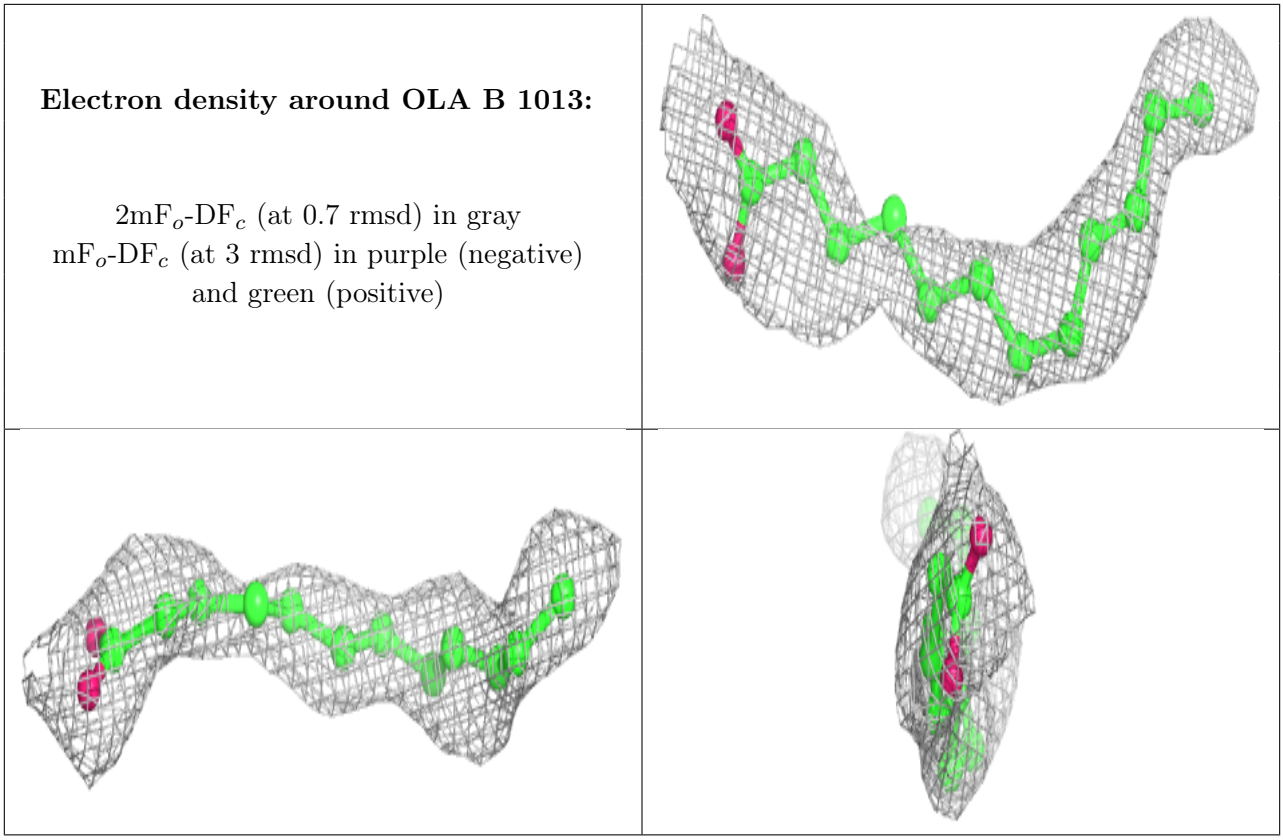






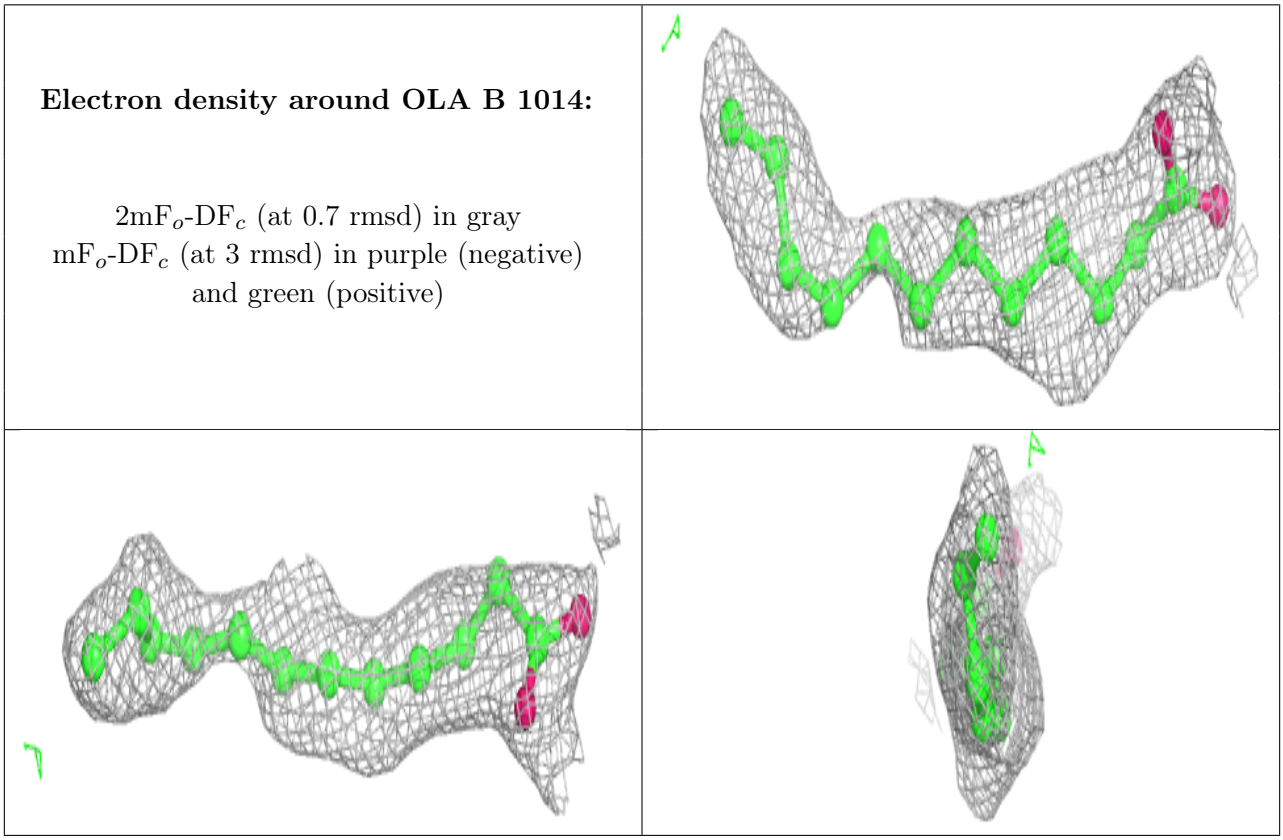
Electron density around OLA B 1013:

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



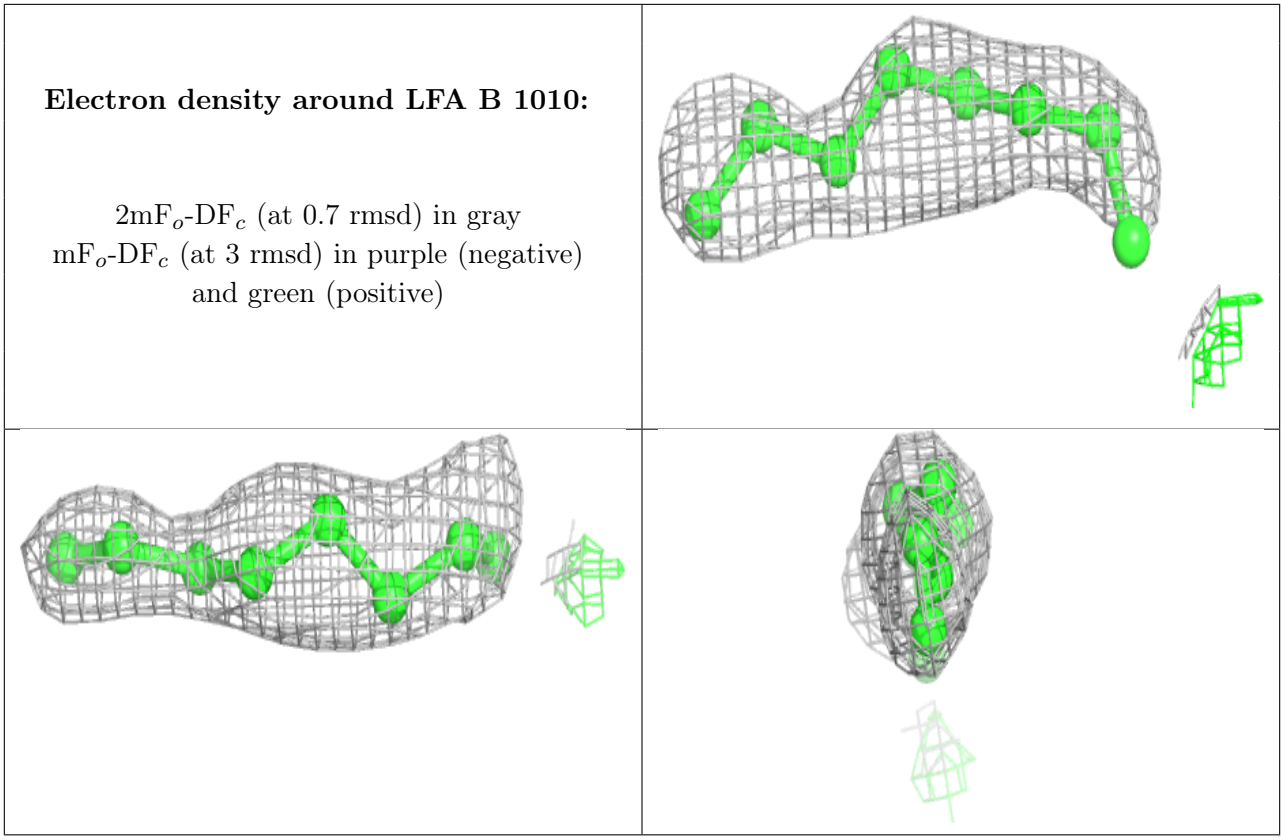
Electron density around OLA B 1014:

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



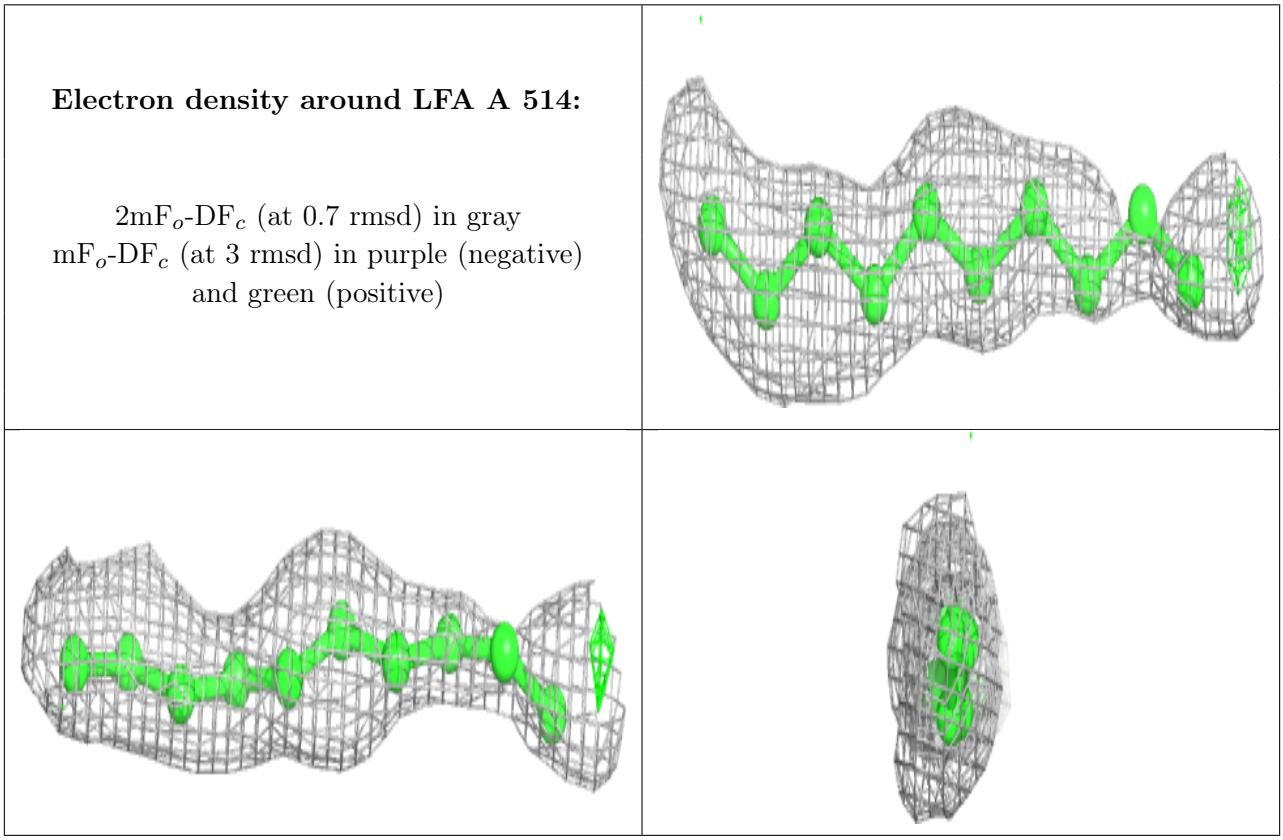
Electron density around LFA B 1010:

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



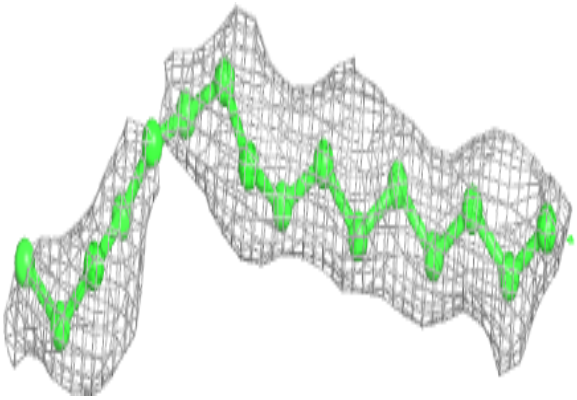
Electron density around LFA A 514:

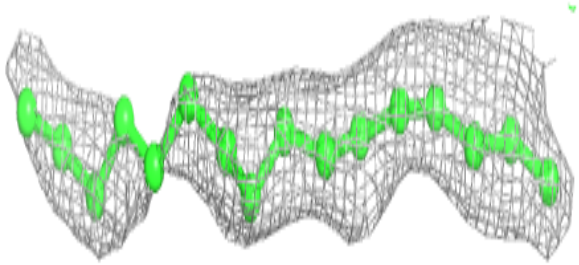
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

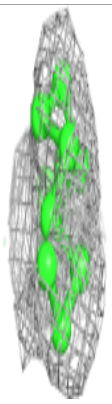


Electron density around LFA C 920:

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

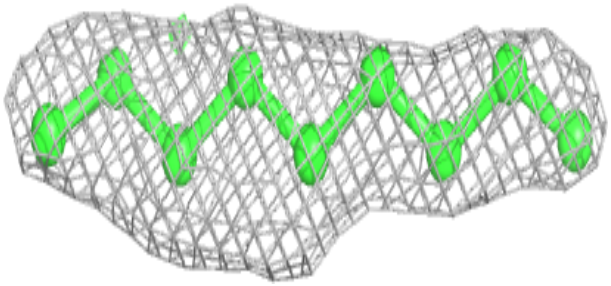


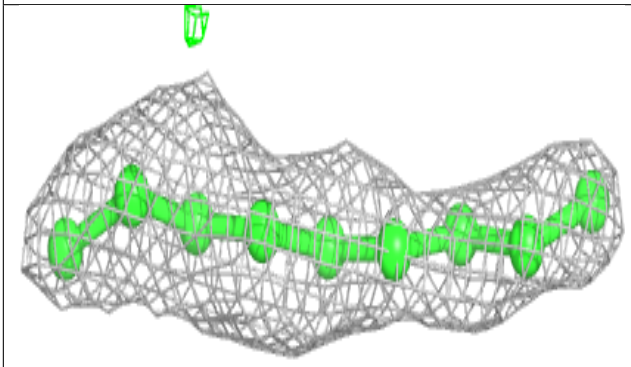


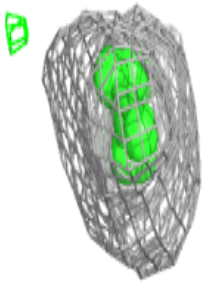


Electron density around LFA A 504:

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

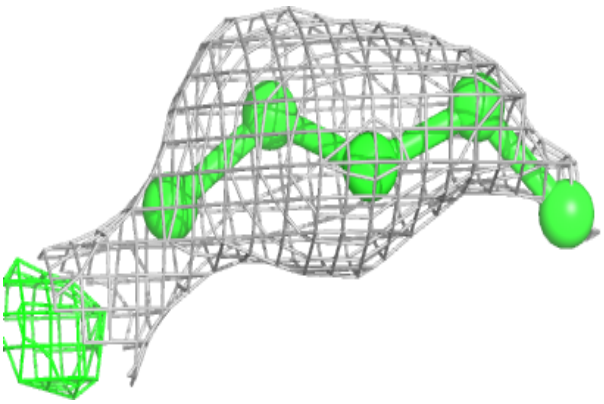


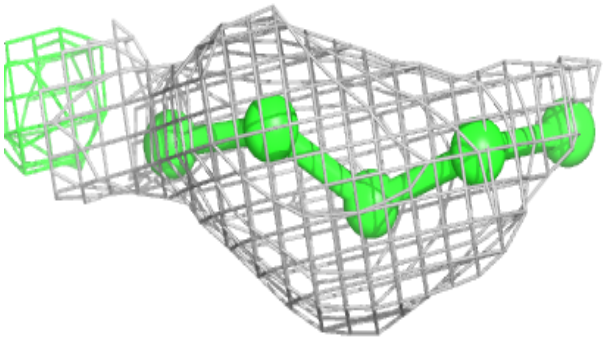


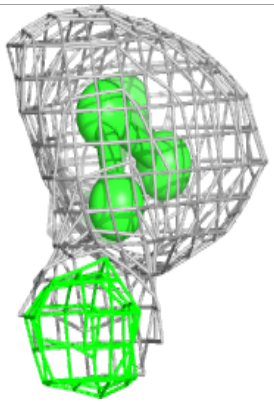


Electron density around LFA C 908:

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

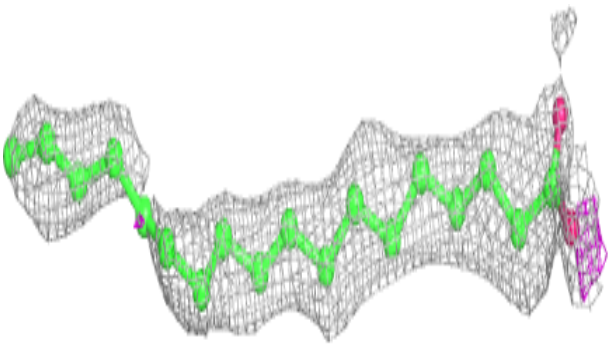


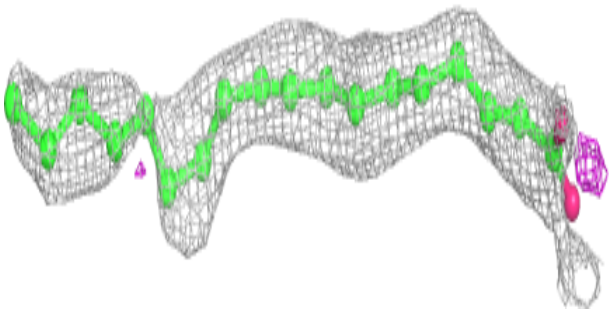


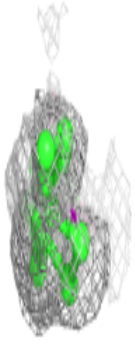


Electron density around OLA C 903:

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

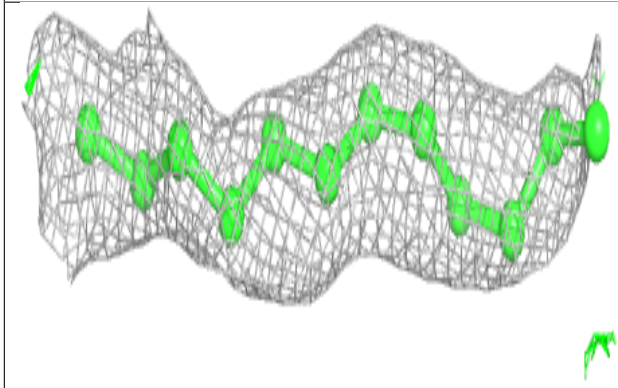


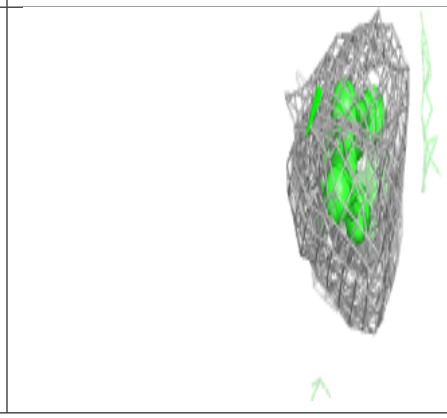




Electron density around LFA C 907:

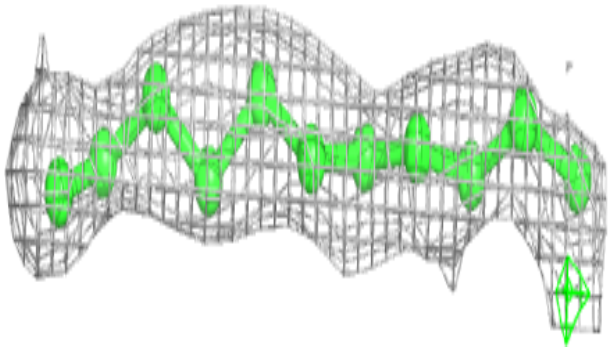
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

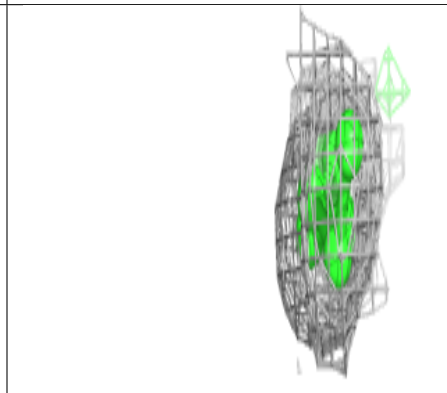




Electron density around LFA A 510:

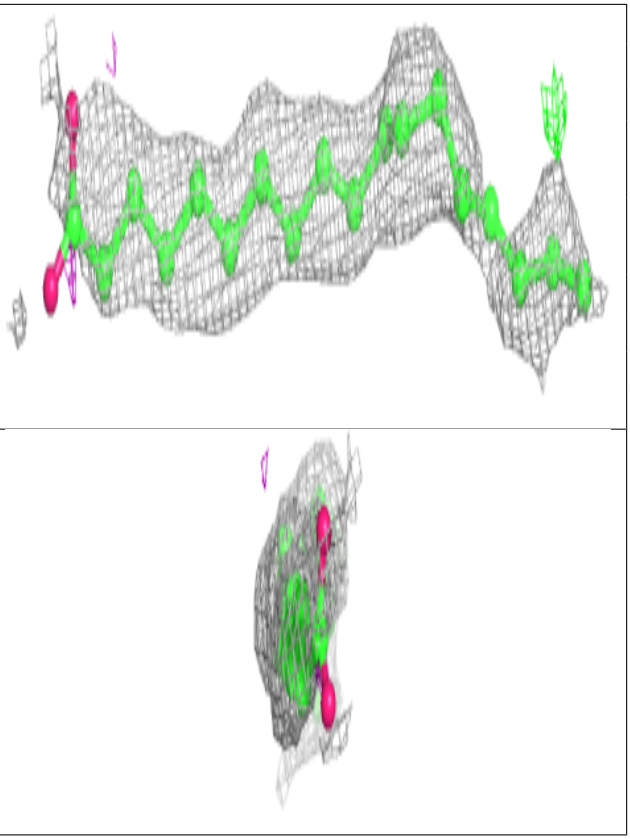
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





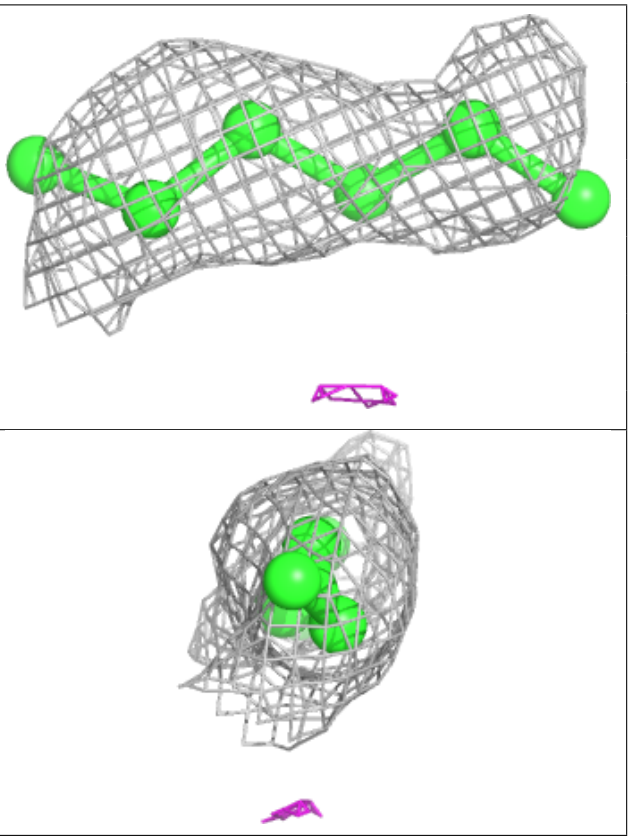
Electron density around OLA B 1006:

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



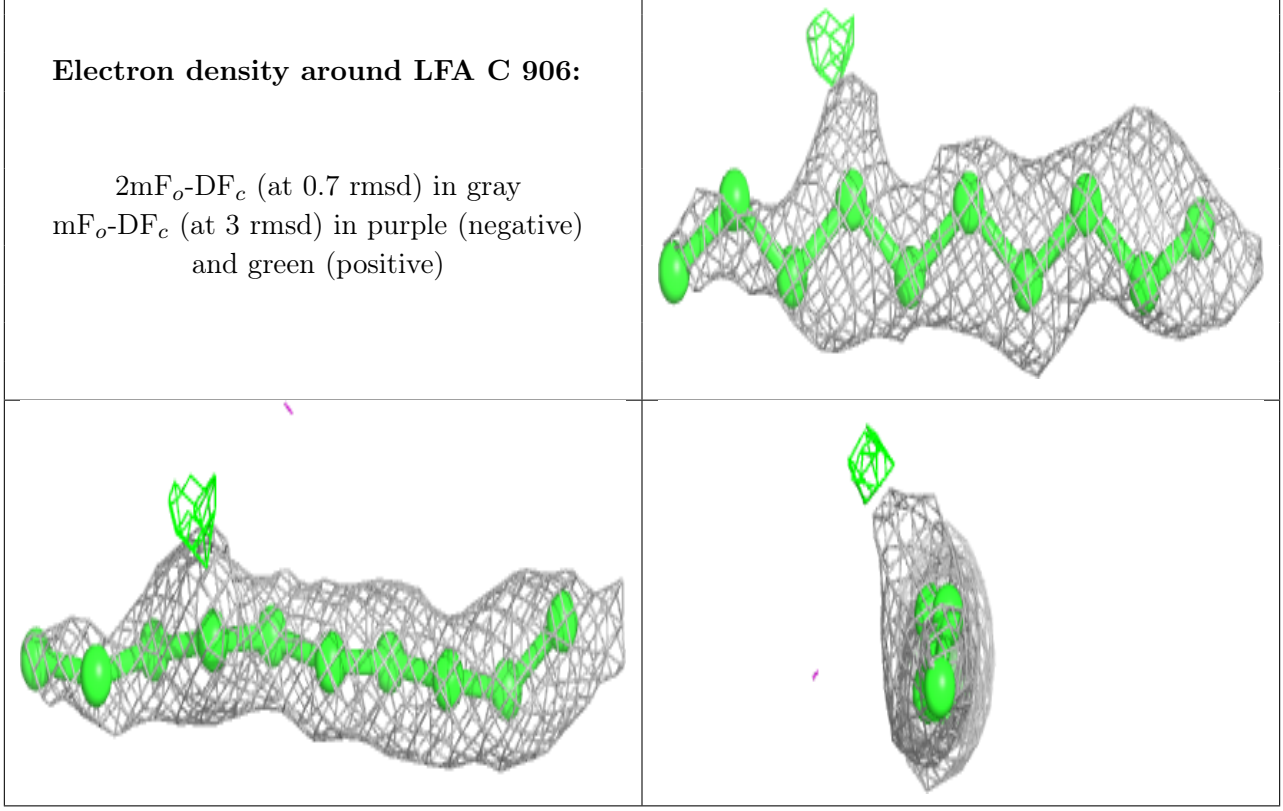
Electron density around LFA B 1021:

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



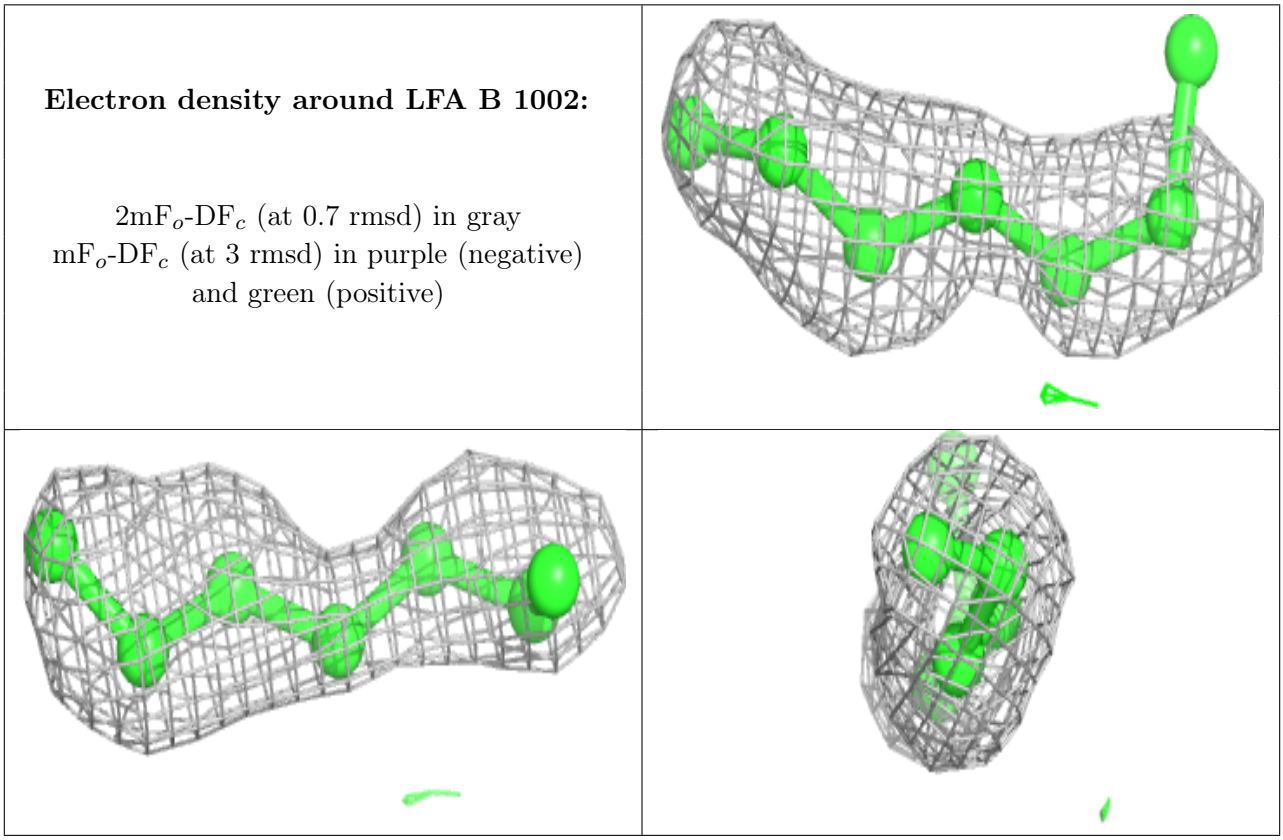
Electron density around LFA C 906:

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



Electron density around LFA B 1002:

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



6.5 Other polymers (i)

There are no such residues in this entry.