Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2024 – 03:02 pm GMT

PDB ID	:	6XYT
Title	:	Crystal structure of the O-state of the light-driven sodium pump KR2 in the pentameric form, pH 8.0
Authors	:	Kovalev, K.; Gushchin, I.; Gordeliy, V.
Deposited on	:	2020-01-31
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

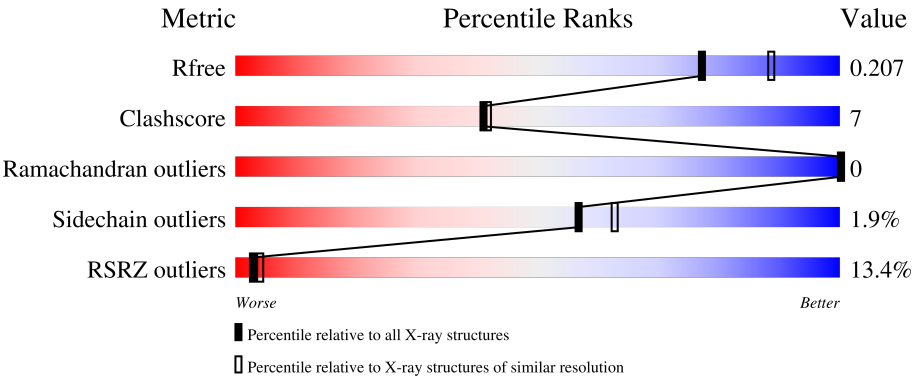
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	273	15% 84% 15%
1	B	273	11% 83% 16%
1	C	273	13% 84% 15%
1	D	273	15% 85% 13%
1	E	273	12% 83% 15%

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	OLC	A	303	-	-	-	X
2	OLC	C	305	-	-	-	X
2	OLC	D	404	-	-	-	X
2	OLC	E	307	-	-	-	X
2	OLC	E	309	-	-	-	X
3	LFA	A	312	-	-	-	X
3	LFA	A	316	-	-	-	X
6	OLA	B	315	-	-	-	X
6	OLA	B	316	-	-	-	X
6	OLA	B	317	-	-	-	X
6	OLA	C	312	-	-	-	X
6	OLA	D	401	-	-	-	X
6	OLA	D	403	-	-	-	X
6	OLA	E	302	-	-	-	X

2 Entry composition

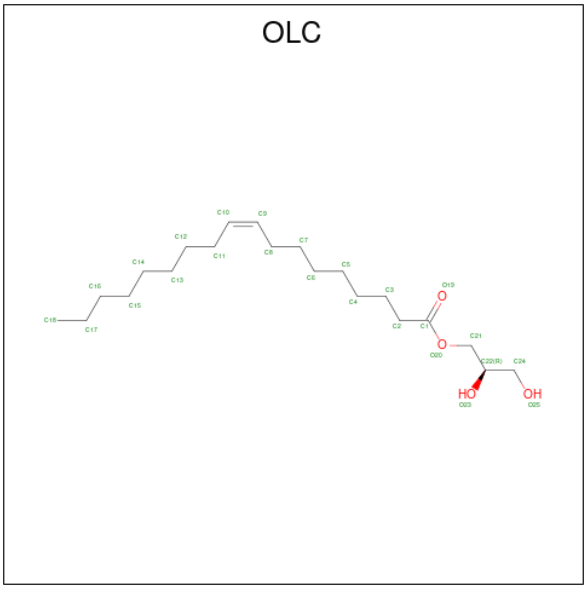
There are 8 unique types of molecules in this entry. The entry contains 12391 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sodium pumping rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	1	0
			2168	1451	325	383	9			
1	B	272	Total	C	N	O	S	0	2	0
			2191	1463	331	388	9			
1	C	273	Total	C	N	O	S	0	1	0
			2198	1470	330	389	9			
1	D	270	Total	C	N	O	S	0	2	0
			2180	1457	328	386	9			
1	E	270	Total	C	N	O	S	0	1	0
			2170	1452	326	383	9			

- Molecule 2 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
2	A	1	Total	C	0	0
			9	9		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 17 15 2	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 13 9 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	A	1	Total C O 15 11 4	0	0
2	A	1	Total C O 20 18 2	0	0
2	B	1	Total C O 22 18 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 21 17 4	0	0
2	B	1	Total C O 20 16 4	0	0
2	B	1	Total C O 21 17 4	0	0
2	B	1	Total C O 16 12 4	0	0
2	C	1	Total C O 20 16 4	0	0
2	C	1	Total C O 23 19 4	0	0
2	C	1	Total C O 22 18 4	0	0
2	C	1	Total C O 20 16 4	0	0
2	C	1	Total C O 22 18 4	0	0
2	C	1	Total C O 16 12 4	0	0
2	C	1	Total C O 18 14 4	0	0
2	D	1	Total C O 13 9 4	0	0
2	D	1	Total C O 25 21 4	0	0

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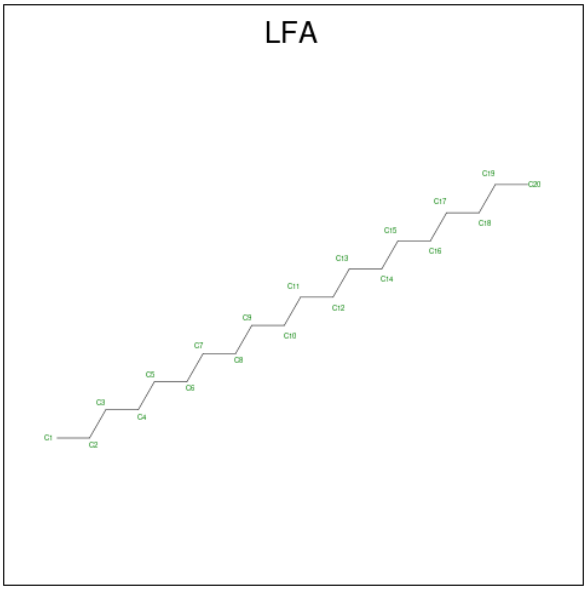
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 18 14 4	0	0
2	D	1	Total C O 18 16 2	0	0
2	D	1	Total C O 14 10 4	0	0
2	E	1	Total C O 19 17 2	0	0
2	E	1	Total C O 25 21 4	0	0
2	E	1	Total C 8 8	0	0
2	E	1	Total C 16 16	0	0
2	E	1	Total C O 20 16 4	0	0
2	E	1	Total C O 15 11 4	0	0
2	E	1	Total C O 15 11 4	0	0
2	E	1	Total C O 20 16 4	0	0

- Molecule 3 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 7 7	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 8 8	0	0
3	A	1	Total C 4 4	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 16 16	0	0
3	A	1	Total C 9 9	0	0
3	B	1	Total C 9 9	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 7 7	0	0
3	C	1	Total C 7 7	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	D	1	Total C 8 8	0	0
3	D	1	Total C 17 17	0	0
3	D	1	Total C 7 7	0	0
3	D	1	Total C 6 6	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 14 14	0	0

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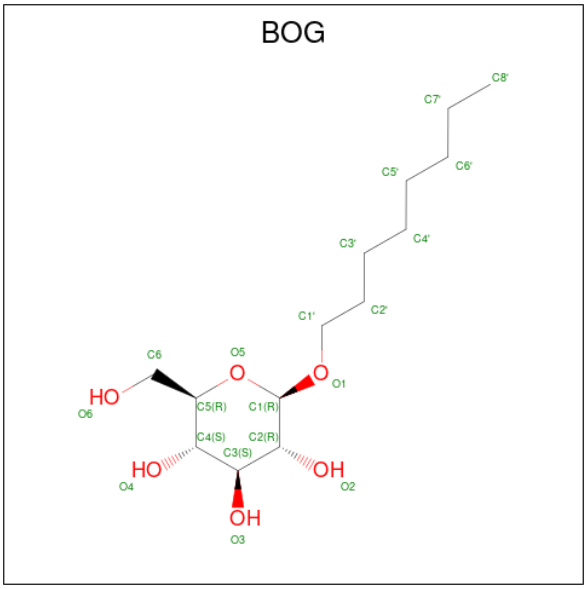
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C 4 4	0	0
3	E	1	Total C 5 5	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Na 2 2	0	0
4	B	2	Total Na 2 2	0	0
4	C	2	Total Na 2 2	0	0
4	D	2	Total Na 2 2	0	0
4	E	2	Total Na 2 2	0	0

- Molecule 5 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 20 14 6	0	0
5	B	1	Total C O 20 14 6	0	0

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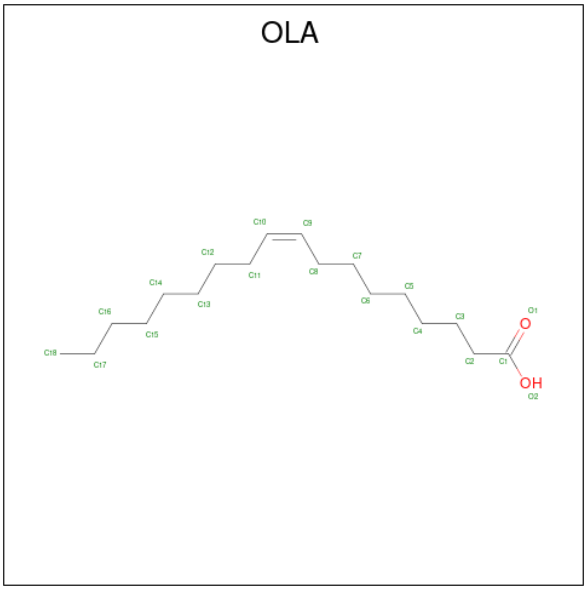
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 20 14 6	0	0
5	D	1	Total C O 20 14 6	0	0
5	E	1	Total C O 20 14 6	0	0

- Molecule 6 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 18 16 2	0	0
6	A	1	Total C O 6 4 2	0	0
6	B	1	Total C O 17 15 2	0	0
6	B	1	Total C O 17 15 2	0	0
6	B	1	Total C O 18 16 2	0	0
6	B	1	Total C O 5 3 2	0	0
6	C	1	Total C O 18 16 2	0	0
6	C	1	Total C O 18 16 2	0	0

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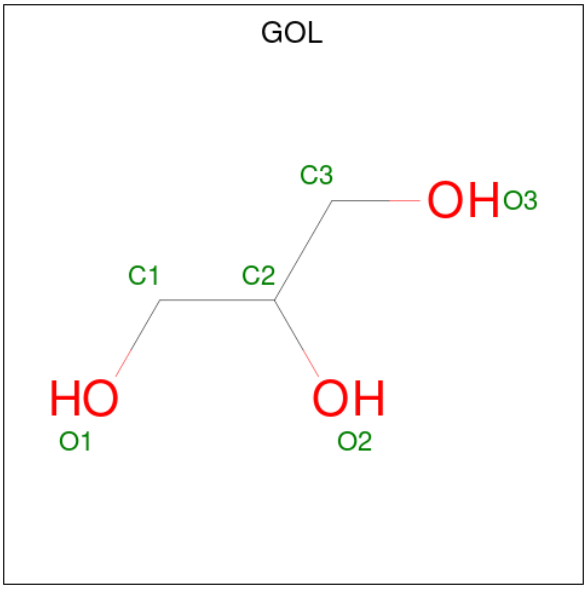
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 20 18 2	0	0
6	D	1	Total C O 15 13 2	0	0
6	D	1	Total C O 18 16 2	0	0
6	E	1	Total C O 17 15 2	0	0
6	E	1	Total C O 7 5 2	0	0
6	E	1	Total C O 17 15 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 4 2 2	0	0
7	C	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

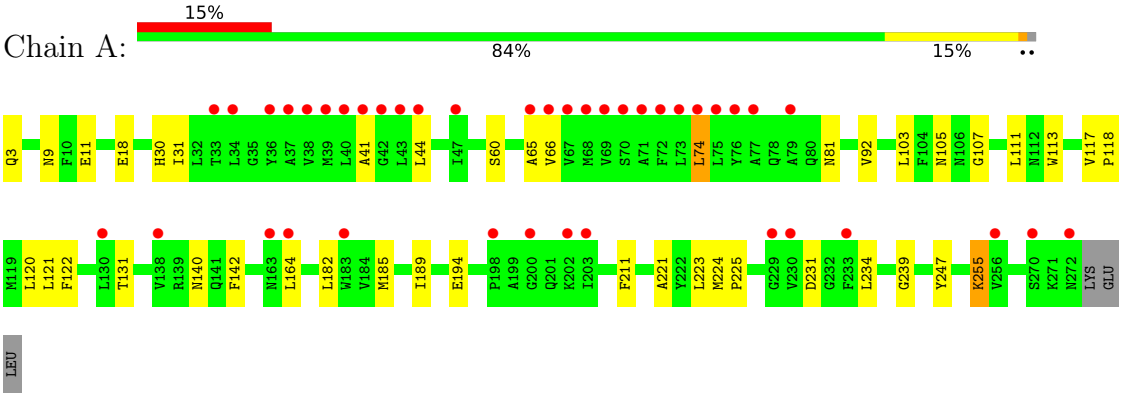
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	59	Total O 59 59	0	0
8	B	56	Total O 56 56	0	0
8	C	59	Total O 60 60	0	1
8	D	61	Total O 62 62	0	1
8	E	61	Total O 62 62	0	1

3 Residue-property plots (i)

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

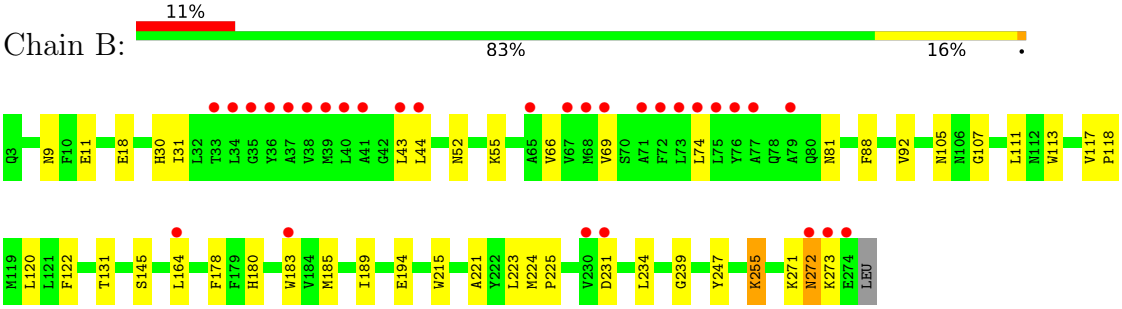
• Molecule 1: Sodium pumping rhodopsin

Chain A:



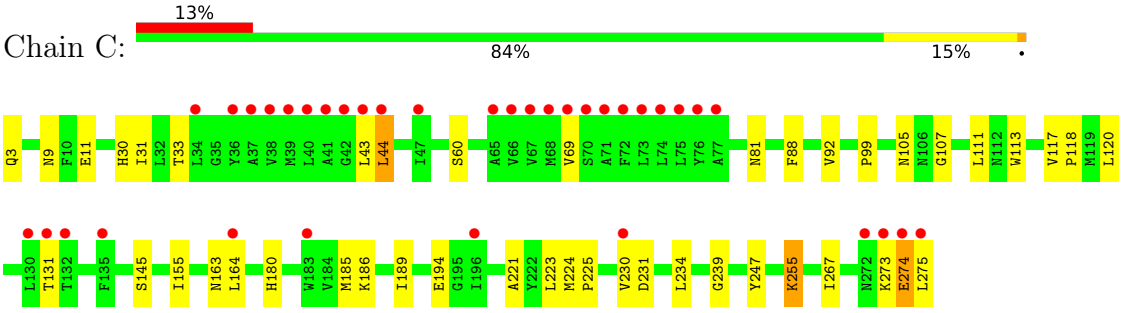
• Molecule 1: Sodium pumping rhodopsin

Chain B:



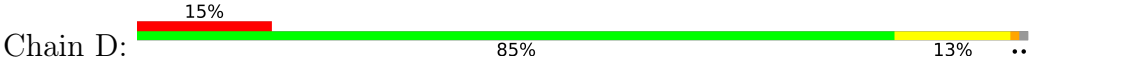
• Molecule 1: Sodium pumping rhodopsin

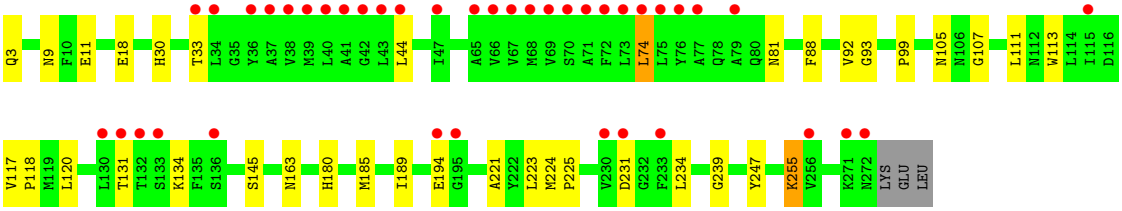
Chain C:



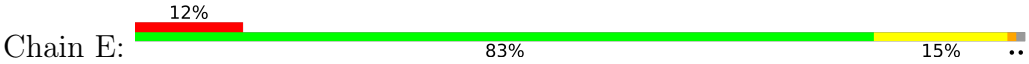
• Molecule 1: Sodium pumping rhodopsin

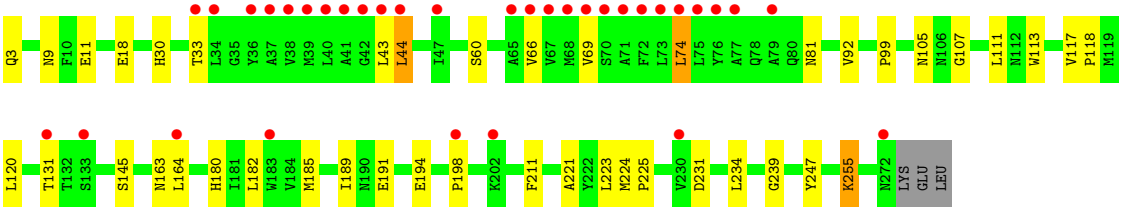
Chain D:





• Molecule 1: Sodium pumping rhodopsin





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	131.16Å 240.63Å 135.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 48.06 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.10) 99.7 (48.06-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.179 , 0.197 0.193 , 0.207	Depositor DCC
R_{free} test set	6240 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 79.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12391	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: GOL, LFA, NA, OLA, BOG, OLC, LYR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.62	0/2196	0.61	0/2987
1	B	0.63	0/2219	0.61	0/3017
1	C	0.63	0/2226	0.61	0/3026
1	D	0.63	0/2208	0.61	0/3002
1	E	0.62	0/2198	0.61	0/2989
All	All	0.63	0/11047	0.61	0/15021

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	2168	0	2143	35	0
1	B	2191	0	2169	38	0
1	C	2198	0	2179	45	0
1	D	2180	0	2160	32	0
1	E	2170	0	2150	37	0
2	A	124	0	183	2	0
2	B	125	0	177	1	0
2	C	141	0	193	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	88	0	121	4	0
2	E	138	0	198	5	0
3	A	58	0	109	0	0
3	B	34	0	64	1	0
3	C	35	0	70	3	0
3	D	78	0	156	4	0
3	E	31	0	58	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
5	A	20	0	28	2	0
5	B	20	0	28	1	0
5	C	20	0	28	2	0
5	D	20	0	28	1	0
5	E	20	0	28	1	0
6	A	24	0	30	2	0
6	B	57	0	76	2	0
6	C	36	0	52	1	0
6	D	53	0	79	3	0
6	E	41	0	54	0	0
7	B	4	0	4	0	0
7	C	4	0	4	0	0
7	D	4	0	3	0	0
8	A	59	0	0	3	0
8	B	56	0	0	1	0
8	C	60	0	0	4	0
8	D	62	0	0	3	0
8	E	62	0	0	7	0
All	All	12391	0	12572	175	0

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

All (175) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:THR:HG21	1:A:194:GLU:OE1	1.80	0.82
1:D:131:THR:HG21	1:D:194:GLU:OE1	1.82	0.79
1:E:131:THR:HG21	1:E:194:GLU:OE1	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:GLU:OE1	8:B:401:HOH:O	2.00	0.78
1:C:131:THR:HG21	1:C:194:GLU:OE1	1.84	0.77
1:B:272:ASN:HD22	1:B:272:ASN:N	1.80	0.77
1:E:60:SER:OG	8:E:401[A]:HOH:O	2.02	0.76
1:D:255:LYR:H183	1:D:255:LYR:H9	1.68	0.76
1:E:198:PRO:HG2	8:E:442:HOH:O	1.85	0.76
1:E:145:SER:OG	1:E:180:HIS:HD2	1.69	0.76
1:C:145:SER:OG	1:C:180:HIS:HD2	1.69	0.74
1:E:231:ASP:N	5:E:315:BOG:O6	2.17	0.74
1:B:255:LYR:H9	1:B:255:LYR:H183	1.68	0.74
1:D:145:SER:OG	1:D:180:HIS:HD2	1.69	0.74
1:A:18:GLU:OE1	8:A:401:HOH:O	2.06	0.73
1:B:145:SER:OG	1:B:180:HIS:HD2	1.69	0.73
1:C:164:LEU:HD21	5:C:311:BOG:H2'1	1.70	0.73
1:A:255:LYR:H9	1:A:255:LYR:H183	1.70	0.73
1:E:255:LYR:H9	1:E:255:LYR:H183	1.71	0.72
1:C:255:LYR:H183	1:C:255:LYR:H9	1.71	0.71
1:B:131:THR:HG21	1:B:194:GLU:OE1	1.91	0.71
1:B:271:LYS:C	1:B:272:ASN:HD22	1.94	0.71
1:E:18:GLU:OE1	8:E:402:HOH:O	2.09	0.69
6:C:314:OLA:H42	6:C:314:OLA:O1	1.91	0.69
1:D:3:GLN:HG2	8:D:509:HOH:O	1.94	0.67
1:B:231:ASP:N	5:B:312:BOG:O6	2.21	0.65
1:D:81:ASN:HD21	1:D:105:ASN:H	1.44	0.65
2:D:404:OLC:O25	3:D:409:LFA:H11	1.97	0.65
1:B:272:ASN:N	1:B:272:ASN:ND2	2.45	0.65
1:C:60:SER:OG	8:C:408[B]:HOH:O	2.13	0.65
1:E:3:GLN:HG2	8:E:410:HOH:O	1.96	0.65
1:B:81:ASN:HD21	1:B:105:ASN:H	1.44	0.64
1:E:81:ASN:HD21	1:E:105:ASN:H	1.46	0.63
1:A:81:ASN:HD21	1:A:105:ASN:H	1.44	0.63
2:C:302:OLC:C16	2:C:315:OLC:C11	2.76	0.63
1:D:231:ASP:N	5:D:416:BOG:O6	2.25	0.62
1:C:81:ASN:HD21	1:C:105:ASN:H	1.45	0.61
1:C:163:ASN:HD22	2:C:306:OLC:C24	2.12	0.61
1:A:231:ASP:N	5:A:314:BOG:O6	2.23	0.59
1:C:231:ASP:N	5:C:311:BOG:O6	2.22	0.58
1:C:180:HIS:CD2	2:C:303:OLC:H7A	2.38	0.58
1:C:3:GLN:HB2	8:C:413:HOH:O	2.02	0.58
1:E:191:GLU:O	8:E:403:HOH:O	2.16	0.58
1:B:30:HIS:CE1	1:C:107:GLY:HA3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HD21	1:B:43:LEU:HD11	1.86	0.57
1:B:255:LYR:H183	1:B:255:LYR:C9	2.34	0.57
1:C:255:LYR:H183	1:C:255:LYR:C9	2.35	0.57
1:D:255:LYR:H183	1:D:255:LYR:C9	2.34	0.57
1:C:186:LYS:HG2	3:C:307:LFA:C5	2.35	0.56
1:E:234:LEU:O	1:E:239:GLY:HA3	2.05	0.56
1:D:234:LEU:O	1:D:239:GLY:HA3	2.06	0.56
3:D:412:LFA:C17	2:E:303:OLC:O25	2.53	0.56
1:C:186:LYS:HG2	3:C:307:LFA:H52	1.87	0.56
1:E:255:LYR:H183	1:E:255:LYR:C9	2.35	0.55
1:E:163:ASN:HD21	2:E:306:OLC:H21A	1.70	0.55
1:D:30:HIS:CE1	1:E:107:GLY:HA3	2.41	0.55
1:A:3:GLN:HG3	8:E:406:HOH:O	2.05	0.55
1:C:234:LEU:O	1:C:239:GLY:HA3	2.07	0.55
1:B:234:LEU:O	1:B:239:GLY:HA3	2.06	0.55
1:C:163:ASN:HD22	2:C:306:OLC:H24A	1.71	0.55
1:A:234:LEU:O	1:A:239:GLY:HA3	2.07	0.54
1:C:30:HIS:CE1	1:D:107:GLY:HA3	2.42	0.54
1:A:107:GLY:HA3	1:E:30:HIS:CE1	2.44	0.53
1:A:255:LYR:H183	1:A:255:LYR:C9	2.35	0.52
8:D:517:HOH:O	1:E:99:PRO:HD2	2.10	0.52
1:C:33:THR:HG22	1:D:74:LEU:CD1	2.40	0.51
1:D:224:MET:N	1:D:225:PRO:HD2	2.26	0.51
1:C:224:MET:N	1:C:225:PRO:HD2	2.26	0.51
1:B:224:MET:N	1:B:225:PRO:HD2	2.26	0.51
1:D:117:VAL:HB	1:D:118:PRO:HD3	1.93	0.51
1:E:117:VAL:HB	1:E:118:PRO:HD3	1.93	0.51
1:C:267:ILE:CD1	2:C:302:OLC:H24A	2.41	0.51
1:D:33:THR:HG22	1:E:74:LEU:CD1	2.41	0.50
1:E:224:MET:N	1:E:225:PRO:HD2	2.27	0.50
1:A:224:MET:N	1:A:225:PRO:HD2	2.26	0.50
1:A:120:LEU:HD11	1:A:255:LYR:H11	1.94	0.50
1:E:221:ALA:HB3	1:E:247:TYR:CE1	2.47	0.50
1:E:60:SER:CB	8:E:401[A]:HOH:O	2.59	0.49
1:D:18:GLU:OE2	8:D:501:HOH:O	2.19	0.49
1:D:44:LEU:HD22	1:E:69:VAL:CG2	2.42	0.49
1:E:113:TRP:CD1	1:E:255:LYR:HC2	2.47	0.49
1:E:164:LEU:HD23	2:E:307:OLC:H24A	1.93	0.49
1:A:30:HIS:CE1	1:B:107:GLY:HA3	2.47	0.49
1:A:117:VAL:HB	1:A:118:PRO:HD3	1.95	0.49
1:A:140:ASN:HB3	2:A:303:OLC:C2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:LEU:HD11	1:D:255:LYR:H11	1.95	0.49
1:A:221:ALA:HB3	1:A:247:TYR:CE1	2.47	0.48
1:C:117:VAL:HB	1:C:118:PRO:HD3	1.94	0.48
1:C:120:LEU:HD11	1:C:255:LYR:H11	1.95	0.48
1:A:44:LEU:CD2	1:B:43:LEU:HD11	2.43	0.48
1:E:120:LEU:HD11	1:E:255:LYR:H11	1.95	0.48
1:A:164:LEU:HD21	5:A:314:BOG:H2'1	1.96	0.48
1:B:120:LEU:HD11	1:B:255:LYR:H11	1.96	0.48
6:A:318:OLA:C4	6:D:401:OLA:C18	2.92	0.48
1:C:164:LEU:HB3	2:C:305:OLC:H24A	1.96	0.48
1:C:221:ALA:HB3	1:C:247:TYR:CE1	2.49	0.48
1:B:221:ALA:HB3	1:B:247:TYR:CE1	2.49	0.48
1:C:163:ASN:ND2	2:C:306:OLC:H24A	2.28	0.48
1:B:117:VAL:HB	1:B:118:PRO:HD3	1.95	0.47
6:A:318:OLA:C4	6:D:401:OLA:H181	2.44	0.47
1:C:60:SER:CB	8:C:408[B]:HOH:O	2.63	0.47
1:D:81:ASN:ND2	1:D:105:ASN:H	2.12	0.47
1:D:221:ALA:HB3	1:D:247:TYR:CE1	2.50	0.47
1:A:113:TRP:CD1	1:A:255:LYR:HC2	2.50	0.47
1:C:230:VAL:HG12	8:C:449:HOH:O	2.13	0.47
1:A:66:VAL:HG11	2:E:301:OLC:H8A	1.97	0.47
1:D:113:TRP:CD1	1:D:255:LYR:HC2	2.50	0.46
1:C:81:ASN:ND2	1:C:105:ASN:H	2.14	0.46
1:B:185:MET:O	1:B:189:ILE:HG12	2.17	0.45
1:A:74:LEU:CD1	1:E:33:THR:HG22	2.47	0.45
1:B:183:TRP:CE3	3:B:307:LFA:H182	2.52	0.45
8:A:412:HOH:O	1:B:55:LYS:HE3	2.16	0.45
1:D:88:PHE:CD2	1:E:99:PRO:HB3	2.52	0.45
1:D:44:LEU:HD22	1:E:69:VAL:HG21	1.99	0.44
1:A:81:ASN:ND2	1:A:105:ASN:H	2.12	0.44
1:E:81:ASN:ND2	1:E:105:ASN:H	2.14	0.44
1:D:185:MET:O	1:D:189:ILE:HG12	2.17	0.44
1:B:81:ASN:ND2	1:B:105:ASN:H	2.12	0.44
2:B:301:OLC:H8	2:B:301:OLC:H11	1.86	0.44
1:C:275:LEU:H	1:C:275:LEU:HD23	1.83	0.43
1:B:145:SER:OG	1:B:180:HIS:CD2	2.60	0.43
1:C:223:LEU:C	1:C:225:PRO:HD2	2.39	0.43
1:C:255:LYR:H9	1:C:255:LYR:H192	2.00	0.43
1:C:274:GLU:N	1:C:274:GLU:CD	2.72	0.43
1:E:223:LEU:C	1:E:225:PRO:HD2	2.39	0.43
1:A:185:MET:O	1:A:189:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:MET:O	1:E:189:ILE:HG12	2.17	0.43
1:A:31:ILE:HD12	1:A:31:ILE:HA	1.87	0.43
1:B:52:ASN:O	1:B:273:LYS:HG3	2.19	0.43
1:B:88:PHE:CD2	1:C:99:PRO:HB2	2.54	0.43
1:A:44:LEU:HD22	1:B:69:VAL:CG2	2.49	0.42
1:D:9:ASN:HB3	1:D:11:GLU:OE1	2.19	0.42
1:B:44:LEU:HD21	1:C:43:LEU:HD11	2.01	0.42
1:C:113:TRP:CD1	1:C:255:LYR:HC2	2.54	0.42
1:C:185:MET:O	1:C:189:ILE:HG12	2.18	0.42
1:E:255:LYR:H9	1:E:255:LYR:H192	2.01	0.42
3:D:412:LFA:C15	2:E:303:OLC:H21A	2.49	0.42
1:B:113:TRP:CD1	1:B:255:LYR:HC2	2.54	0.42
1:D:223:LEU:C	1:D:225:PRO:HD2	2.40	0.42
1:A:140:ASN:HD22	2:A:303:OLC:H22	1.85	0.42
1:D:163:ASN:HD22	2:D:408:OLC:H22	1.84	0.42
1:B:9:ASN:HB3	1:B:11:GLU:OE1	2.19	0.42
1:B:44:LEU:HD22	1:C:69:VAL:CG2	2.49	0.42
1:A:223:LEU:C	1:A:225:PRO:HD2	2.40	0.42
1:B:118:PRO:O	1:B:122:PHE:HB2	2.19	0.42
1:E:9:ASN:HB3	1:E:11:GLU:OE1	2.19	0.42
1:A:9:ASN:HB3	1:A:11:GLU:OE1	2.20	0.41
2:D:407:OLC:H8A	2:D:407:OLC:H11A	1.82	0.41
1:C:9:ASN:HB3	1:C:11:GLU:OE1	2.20	0.41
1:C:186:LYS:CG	3:C:307:LFA:H52	2.50	0.41
1:B:31:ILE:HD12	1:B:31:ILE:HA	1.87	0.41
1:B:255:LYR:H10	1:B:255:LYR:H81	1.91	0.41
3:D:412:LFA:H81	1:E:66:VAL:HG11	2.03	0.41
1:D:44:LEU:HD21	1:E:43:LEU:HD11	2.02	0.41
1:B:223:LEU:C	1:B:225:PRO:HD2	2.41	0.41
1:A:118:PRO:O	1:A:122:PHE:HB2	2.20	0.41
1:C:88:PHE:CD2	1:D:99:PRO:HB3	2.56	0.41
1:A:121:LEU:HB3	1:A:142:PHE:CD2	2.56	0.41
1:A:182:LEU:HD23	1:A:211:PHE:HE2	1.86	0.41
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.80	0.41
1:C:145:SER:OG	1:C:180:HIS:CD2	2.61	0.41
1:D:255:LYR:H9	1:D:255:LYR:H192	2.03	0.41
1:A:41:ALA:HB1	1:B:66:VAL:HG13	2.03	0.40
1:B:178:PHE:HE1	1:B:215:TRP:HB3	1.86	0.40
1:A:65:ALA:HB1	1:E:44:LEU:CD1	2.51	0.40
6:B:314:OLA:H142	1:C:155:ILE:HG12	2.02	0.40
1:C:31:ILE:HD12	1:C:31:ILE:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:PHE:CZ	1:D:93:GLY:HA2	2.56	0.40
6:B:315:OLA:H71	6:D:403:OLA:H72	2.02	0.40
1:D:163:ASN:ND2	2:D:408:OLC:H22	2.36	0.40
1:A:60:SER:OG	8:A:402:HOH:O	2.22	0.40
1:A:255:LYR:H9	1:A:255:LYR:H192	2.03	0.40
1:B:44:LEU:CD2	1:C:43:LEU:HD11	2.51	0.40
1:D:255:LYR:H10	1:D:255:LYR:H81	1.91	0.40
1:E:182:LEU:HD23	1:E:211:PHE:HE2	1.87	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	268/273 (98%)	263 (98%)	5 (2%)	0	100	100
1	B	271/273 (99%)	266 (98%)	5 (2%)	0	100	100
1	C	271/273 (99%)	265 (98%)	6 (2%)	0	100	100
1	D	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
1	E	268/273 (98%)	263 (98%)	5 (2%)	0	100	100
All	All	1347/1365 (99%)	1321 (98%)	26 (2%)	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	226/233 (97%)	222 (98%)	4 (2%)	59	65
1	B	230/233 (99%)	225 (98%)	5 (2%)	52	57
1	C	230/233 (99%)	225 (98%)	5 (2%)	52	57
1	D	229/233 (98%)	225 (98%)	4 (2%)	60	67
1	E	227/233 (97%)	223 (98%)	4 (2%)	59	65
All	All	1142/1165 (98%)	1120 (98%)	22 (2%)	57	63

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LEU
1	A	92	VAL
1	A	103	LEU
1	A	111	LEU
1	B	74	LEU
1	B	92	VAL
1	B	111	LEU
1	B	164	LEU
1	B	272	ASN
1	C	44	LEU
1	C	92	VAL
1	C	111	LEU
1	C	273	LYS
1	C	274	GLU
1	D	74	LEU
1	D	92	VAL
1	D	111	LEU
1	D	134	LYS
1	E	44	LEU
1	E	74	LEU
1	E	92	VAL
1	E	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	81	ASN

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Mol	Chain	Res	Type
1	B	78	GLN
1	B	81	ASN
1	B	180	HIS
1	B	272	ASN
1	C	78	GLN
1	C	81	ASN
1	C	180	HIS
1	D	78	GLN
1	D	81	ASN
1	D	141	GLN
1	D	180	HIS
1	E	78	GLN
1	E	81	ASN
1	E	141	GLN
1	E	180	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	LYR	E	255	1	27,29,30	1.21	3 (11%)	30,37,39	1.10	2 (6%)
1	LYR	A	255	1	27,29,30	1.21	3 (11%)	30,37,39	1.08	2 (6%)
1	LYR	D	255	1	27,29,30	1.21	2 (7%)	30,37,39	1.08	2 (6%)
1	LYR	C	255	1	27,29,30	1.24	2 (7%)	30,37,39	1.05	1 (3%)
1	LYR	B	255	1	27,29,30	1.20	2 (7%)	30,37,39	1.08	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	LYR	E	255	1	-	5/22/40/42	0/1/1/1
1	LYR	A	255	1	-	5/22/40/42	0/1/1/1
1	LYR	D	255	1	-	5/22/40/42	0/1/1/1
1	LYR	C	255	1	-	5/22/40/42	0/1/1/1
1	LYR	B	255	1	-	5/22/40/42	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	255	LYR	C7-C80	3.79	1.40	1.35
1	E	255	LYR	C7-C80	3.71	1.40	1.35
1	B	255	LYR	C7-C80	3.61	1.40	1.35
1	A	255	LYR	C7-C80	3.56	1.40	1.35
1	D	255	LYR	C7-C80	3.55	1.40	1.35
1	A	255	LYR	C9-C80	-2.76	1.40	1.45
1	C	255	LYR	C9-C80	-2.74	1.40	1.45
1	D	255	LYR	C9-C80	-2.74	1.40	1.45
1	B	255	LYR	C9-C80	-2.72	1.40	1.45
1	E	255	LYR	C9-C80	-2.60	1.40	1.45
1	E	255	LYR	C5-C3	-2.02	1.41	1.45
1	A	255	LYR	C5-C3	-2.01	1.41	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	255	LYR	C8-C80-C7	-4.04	117.26	122.92
1	D	255	LYR	C8-C80-C7	-4.03	117.28	122.92
1	B	255	LYR	C8-C80-C7	-3.88	117.49	122.92
1	A	255	LYR	C8-C80-C7	-3.85	117.53	122.92
1	C	255	LYR	C8-C80-C7	-3.77	117.64	122.92
1	B	255	LYR	C8-C80-C9	2.30	121.70	118.08
1	E	255	LYR	C8-C80-C9	2.23	121.59	118.08
1	D	255	LYR	C8-C80-C9	2.15	121.47	118.08
1	A	255	LYR	C8-C80-C9	2.14	121.44	118.08

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	255	LYR	C1-C2-C3-C5
1	B	255	LYR	C1-C2-C3-C5
1	C	255	LYR	C1-C2-C3-C4
1	C	255	LYR	C1-C2-C3-C5
1	D	255	LYR	C1-C2-C3-C5
1	E	255	LYR	C1-C2-C3-C5
1	B	255	LYR	C2-C1-NZ-CE
1	C	255	LYR	C2-C1-NZ-CE
1	E	255	LYR	C2-C1-NZ-CE
1	A	255	LYR	C2-C1-NZ-CE
1	D	255	LYR	C2-C1-NZ-CE
1	A	255	LYR	CE-CD-CG-CB
1	B	255	LYR	CE-CD-CG-CB
1	D	255	LYR	CE-CD-CG-CB
1	C	255	LYR	CE-CD-CG-CB
1	E	255	LYR	CE-CD-CG-CB
1	C	255	LYR	CD-CE-NZ-C1
1	D	255	LYR	CD-CE-NZ-C1
1	B	255	LYR	CD-CE-NZ-C1
1	E	255	LYR	CD-CE-NZ-C1
1	A	255	LYR	C1-C2-C3-C4
1	B	255	LYR	C1-C2-C3-C4
1	D	255	LYR	C1-C2-C3-C4
1	E	255	LYR	C1-C2-C3-C4
1	A	255	LYR	CD-CE-NZ-C1

There are no ring outliers.

5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	255	LYR	5	0
1	A	255	LYR	5	0
1	D	255	LYR	6	0
1	C	255	LYR	5	0
1	B	255	LYR	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 89 ligands modelled in this entry, 10 are monoatomic - leaving 79 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	OLC	E	307	-	14,14,24	1.24	1 (7%)	15,15,25	1.10	1 (6%)
7	GOL	B	313	-	3,3,5	0.33	0	2,2,5	0.17	0
3	LFA	D	412	-	16,16,19	0.09	0	15,15,18	0.08	0
3	LFA	C	307	-	6,6,19	0.12	0	5,5,18	0.06	0
2	OLC	C	302	-	22,22,24	0.94	1 (4%)	23,23,25	0.88	2 (8%)
2	OLC	A	303	-	24,24,24	0.97	1 (4%)	25,25,25	0.86	1 (4%)
2	OLC	A	306	-	14,14,24	1.18	1 (7%)	15,15,25	1.05	2 (13%)
2	OLC	D	404	-	12,12,24	1.35	1 (8%)	13,13,25	1.11	1 (7%)
2	OLC	A	304	-	12,12,24	1.34	1 (8%)	13,13,25	1.14	1 (7%)
5	BOG	B	312	-	20,20,20	0.51	0	25,25,25	0.54	0
2	OLC	C	303	-	21,21,24	1.04	1 (4%)	22,22,25	0.90	1 (4%)
3	LFA	E	310	-	7,7,19	0.12	0	6,6,18	0.09	0
6	OLA	A	318	-	5,5,19	0.93	0	5,5,19	0.87	0
2	OLC	C	305	-	21,21,24	1.03	1 (4%)	22,22,25	0.97	1 (4%)
3	LFA	D	413	-	6,6,19	0.13	0	5,5,18	0.07	0
3	LFA	D	414	-	5,5,19	0.12	0	4,4,18	0.09	0
7	GOL	D	402	-	3,3,5	0.34	0	2,2,5	0.18	0
2	OLC	E	309	-	19,19,24	1.08	1 (5%)	20,20,25	1.01	1 (5%)
2	OLC	B	303	-	20,20,24	1.05	1 (5%)	21,21,25	0.90	1 (4%)
6	OLA	B	314	-	16,16,19	0.54	0	16,16,19	0.52	0
3	LFA	A	309	-	7,7,19	0.10	0	6,6,18	0.07	0
2	OLC	D	408	-	13,13,24	1.24	1 (7%)	14,14,25	0.95	2 (14%)
2	OLC	B	304	-	19,19,24	1.07	1 (5%)	20,20,25	0.98	2 (10%)
3	LFA	B	308	-	7,7,19	0.11	0	6,6,18	0.08	0
3	LFA	D	410	-	19,19,19	0.07	0	18,18,18	0.05	0
2	OLC	B	306	-	15,15,24	1.15	1 (6%)	16,16,25	1.02	2 (12%)
2	OLC	B	301	-	21,21,24	1.05	1 (4%)	22,22,25	0.87	1 (4%)
3	LFA	A	316	-	8,8,19	0.14	0	7,7,18	0.12	0
2	OLC	E	304	-	7,7,24	0.29	0	6,6,25	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	OLC	A	305	-	24,24,24	0.97	1 (4%)	25,25,25	0.90	1 (4%)
2	OLC	D	406	-	17,17,24	1.12	1 (5%)	18,18,25	1.11	1 (5%)
3	LFA	A	307	-	6,6,19	0.13	0	5,5,18	0.07	0
6	OLA	E	316	-	6,6,19	0.88	0	6,6,19	0.80	0
3	LFA	C	309	-	19,19,19	0.07	0	18,18,18	0.05	0
6	OLA	D	401	-	19,19,19	0.52	0	19,19,19	0.48	0
2	OLC	E	308	-	14,14,24	1.18	1 (7%)	15,15,25	0.91	2 (13%)
3	LFA	A	311	-	5,5,19	0.13	0	4,4,18	0.11	0
5	BOG	D	416	-	20,20,20	0.54	0	25,25,25	0.58	0
3	LFA	E	312	-	3,3,19	0.24	0	2,2,18	0.43	0
2	OLC	E	303	-	24,24,24	0.92	1 (4%)	25,25,25	0.83	1 (4%)
2	OLC	C	306	-	15,15,24	1.16	1 (6%)	16,16,25	0.91	1 (6%)
5	BOG	A	314	-	20,20,20	0.52	0	25,25,25	0.58	0
6	OLA	B	317	-	4,4,19	0.96	0	4,4,19	0.72	0
3	LFA	E	313	-	4,4,19	0.16	0	3,3,18	0.22	0
2	OLC	A	315	-	19,19,24	1.09	1 (5%)	19,19,25	0.88	1 (5%)
3	LFA	B	307	-	8,8,19	0.11	0	7,7,18	0.06	0
3	LFA	C	308	-	7,7,19	0.13	0	6,6,18	0.09	0
3	LFA	B	309	-	9,9,19	0.11	0	8,8,18	0.09	0
3	LFA	D	411	-	7,7,19	0.10	0	6,6,18	0.07	0
2	OLC	A	301	-	8,8,24	0.35	0	6,7,25	0.41	0
2	OLC	C	301	-	19,19,24	1.11	1 (5%)	20,20,25	0.93	2 (10%)
2	OLC	D	405	-	24,24,24	0.93	1 (4%)	25,25,25	0.81	1 (4%)
6	OLA	C	314	-	17,17,19	0.53	0	17,17,19	0.51	0
6	OLA	D	403	-	14,14,19	0.59	0	14,14,19	0.56	0
2	OLC	A	302	-	16,16,24	1.21	1 (6%)	16,16,25	0.93	1 (6%)
2	OLC	C	315	-	17,17,24	1.11	1 (5%)	18,18,25	1.01	1 (5%)
6	OLA	C	312	-	17,17,19	0.54	0	17,17,19	0.49	0
5	BOG	C	311	-	20,20,20	0.50	0	25,25,25	0.67	0
7	GOL	C	313	-	3,3,5	0.35	0	2,2,5	0.13	0
3	LFA	A	310	-	3,3,19	0.26	0	2,2,18	0.43	0
2	OLC	B	305	-	20,20,24	1.03	1 (5%)	21,21,25	0.88	1 (4%)
2	OLC	E	306	-	19,19,24	1.11	1 (5%)	20,20,25	0.97	1 (5%)
6	OLA	D	417	-	17,17,19	0.56	0	17,17,19	0.51	0
3	LFA	B	310	-	6,6,19	0.11	0	5,5,18	0.08	0
6	OLA	A	317	-	17,17,19	0.55	0	17,17,19	0.50	0
3	LFA	E	311	-	13,13,19	0.09	0	12,12,18	0.06	0
2	OLC	D	407	-	17,17,24	1.15	1 (5%)	17,17,25	0.89	2 (11%)
6	OLA	B	315	-	16,16,19	0.56	0	16,16,19	0.50	0
2	OLC	C	304	-	19,19,24	1.03	1 (5%)	20,20,25	1.03	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	OLC	E	305	-	15,15,24	0.28	0	14,14,25	0.49	0
6	OLA	E	317	-	16,16,19	0.54	0	16,16,19	0.53	0
2	OLC	E	301	-	18,18,24	1.08	1 (5%)	18,18,25	0.87	0
3	LFA	D	409	-	19,19,19	0.08	0	18,18,18	0.03	0
3	LFA	A	308	-	7,7,19	0.13	0	6,6,18	0.06	0
3	LFA	A	312	-	15,15,19	0.08	0	14,14,18	0.06	0
2	OLC	B	302	-	24,24,24	0.97	1 (4%)	25,25,25	0.87	2 (8%)
6	OLA	E	302	-	16,16,19	0.54	0	16,16,19	0.52	0
6	OLA	B	316	-	17,17,19	0.54	0	17,17,19	0.50	0
5	BOG	E	315	-	20,20,20	0.51	0	25,25,25	0.52	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	OLC	E	307	-	-	8/14/14/24	-
7	GOL	B	313	-	-	1/1/1/4	-
3	LFA	D	412	-	-	9/14/14/17	-
3	LFA	C	307	-	-	3/4/4/17	-
2	OLC	C	302	-	-	12/22/22/24	-
2	OLC	A	303	-	-	12/24/24/24	-
2	OLC	A	306	-	-	5/14/14/24	-
2	OLC	D	404	-	-	6/12/12/24	-
2	OLC	A	304	-	-	2/12/12/24	-
5	BOG	B	312	-	-	4/11/31/31	0/1/1/1
2	OLC	C	303	-	-	5/21/21/24	-
3	LFA	E	310	-	-	3/5/5/17	-
6	OLA	A	318	-	-	0/3/3/17	-
2	OLC	C	305	-	-	9/21/21/24	-
3	LFA	D	413	-	-	2/4/4/17	-
3	LFA	D	414	-	-	0/3/3/17	-
7	GOL	D	402	-	-	0/1/1/4	-
2	OLC	E	309	-	-	10/19/19/24	-
2	OLC	B	303	-	-	11/20/20/24	-
6	OLA	B	314	-	-	10/14/14/17	-
3	LFA	A	309	-	-	3/5/5/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	D	408	-	-	5/13/13/24	-
2	OLC	B	304	-	-	4/19/19/24	-
3	LFA	B	308	-	-	2/5/5/17	-
3	LFA	D	410	-	-	8/17/17/17	-
2	OLC	B	306	-	-	2/15/15/24	-
2	OLC	B	301	-	-	7/21/21/24	-
3	LFA	A	316	-	-	4/6/6/17	-
2	OLC	E	304	-	-	2/5/5/24	-
2	OLC	A	305	-	-	14/24/24/24	-
2	OLC	D	406	-	-	5/17/17/24	-
3	LFA	A	307	-	-	1/4/4/17	-
6	OLA	E	316	-	-	3/4/4/17	-
3	LFA	C	309	-	-	8/17/17/17	-
6	OLA	D	401	-	-	9/17/17/17	-
2	OLC	E	308	-	-	4/14/14/24	-
3	LFA	A	311	-	-	2/3/3/17	-
5	BOG	D	416	-	-	3/11/31/31	0/1/1/1
3	LFA	E	312	-	-	1/1/1/17	-
2	OLC	E	303	-	-	9/24/24/24	-
2	OLC	C	306	-	-	5/15/15/24	-
5	BOG	A	314	-	-	3/11/31/31	0/1/1/1
6	OLA	B	317	-	-	2/2/2/17	-
3	LFA	E	313	-	-	1/2/2/17	-
2	OLC	A	315	-	-	7/17/17/24	-
3	LFA	B	307	-	-	3/6/6/17	-
3	LFA	C	308	-	-	3/5/5/17	-
3	LFA	B	309	-	-	6/7/7/17	-
3	LFA	D	411	-	-	4/5/5/17	-
2	OLC	A	301	-	-	2/6/6/24	-
2	OLC	C	301	-	-	11/19/19/24	-
2	OLC	D	405	-	-	12/24/24/24	-
6	OLA	C	314	-	-	11/15/15/17	-
6	OLA	D	403	-	-	9/12/12/17	-
2	OLC	A	302	-	-	4/14/14/24	-
2	OLC	C	315	-	-	10/17/17/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	OLA	C	312	-	-	9/15/15/17	-
5	BOG	C	311	-	-	3/11/31/31	0/1/1/1
7	GOL	C	313	-	-	1/1/1/4	-
3	LFA	A	310	-	-	0/1/1/17	-
2	OLC	B	305	-	-	6/20/20/24	-
2	OLC	E	306	-	-	11/19/19/24	-
6	OLA	D	417	-	-	7/15/15/17	-
3	LFA	B	310	-	-	1/4/4/17	-
6	OLA	A	317	-	-	12/15/15/17	-
3	LFA	E	311	-	-	5/11/11/17	-
2	OLC	D	407	-	-	4/15/15/24	-
6	OLA	B	315	-	-	4/14/14/17	-
2	OLC	C	304	-	-	4/19/19/24	-
2	OLC	E	305	-	-	5/13/13/24	-
6	OLA	E	317	-	-	9/14/14/17	-
2	OLC	E	301	-	-	6/16/16/24	-
3	LFA	D	409	-	-	10/17/17/17	-
3	LFA	A	308	-	-	1/5/5/17	-
3	LFA	A	312	-	-	8/13/13/17	-
2	OLC	B	302	-	-	11/24/24/24	-
6	OLA	E	302	-	-	6/14/14/17	-
6	OLA	B	316	-	-	9/15/15/17	-
5	BOG	E	315	-	-	11/11/31/31	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	OLC	O20-C1	4.72	1.46	1.30
2	E	306	OLC	O20-C1	4.63	1.46	1.33
2	A	315	OLC	O20-C1	4.60	1.46	1.30
2	D	407	OLC	O20-C1	4.56	1.46	1.30
2	C	303	OLC	O20-C1	4.52	1.46	1.33
2	D	404	OLC	O20-C1	4.51	1.46	1.33
2	C	301	OLC	O20-C1	4.50	1.46	1.33
2	A	304	OLC	O20-C1	4.49	1.46	1.33
2	E	309	OLC	O20-C1	4.49	1.46	1.33
2	C	305	OLC	O20-C1	4.48	1.46	1.33
2	A	303	OLC	O20-C1	4.46	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	OLC	O20-C1	4.46	1.46	1.33
2	B	301	OLC	O20-C1	4.45	1.46	1.33
2	E	307	OLC	O20-C1	4.45	1.46	1.33
2	B	303	OLC	O20-C1	4.44	1.46	1.33
2	A	305	OLC	O20-C1	4.43	1.46	1.33
2	E	301	OLC	O20-C1	4.43	1.45	1.30
2	D	406	OLC	O20-C1	4.40	1.46	1.33
2	B	304	OLC	O20-C1	4.39	1.46	1.33
2	C	315	OLC	O20-C1	4.31	1.45	1.33
2	B	305	OLC	O20-C1	4.30	1.45	1.33
2	C	306	OLC	O20-C1	4.30	1.45	1.33
2	C	304	OLC	O20-C1	4.28	1.45	1.33
2	D	408	OLC	O20-C1	4.26	1.45	1.33
2	D	405	OLC	O20-C1	4.25	1.45	1.33
2	E	303	OLC	O20-C1	4.21	1.45	1.33
2	B	306	OLC	O20-C1	4.20	1.45	1.33
2	E	308	OLC	O20-C1	4.16	1.45	1.33
2	C	302	OLC	O20-C1	4.14	1.45	1.33
2	A	306	OLC	O20-C1	4.12	1.45	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	304	OLC	O20-C1-C2	3.13	121.72	111.91
2	D	406	OLC	O20-C1-C2	3.11	121.67	111.91
2	C	305	OLC	O20-C1-C2	3.08	121.57	111.91
2	E	309	OLC	O20-C1-C2	3.07	121.55	111.91
2	E	307	OLC	O20-C1-C2	3.05	121.47	111.91
2	E	306	OLC	O20-C1-C2	3.04	121.44	111.91
2	A	304	OLC	O20-C1-C2	2.99	121.28	111.91
2	B	304	OLC	O20-C1-C2	2.97	121.24	111.91
2	C	301	OLC	O20-C1-C2	2.96	121.19	111.91
2	B	302	OLC	O20-C1-C2	2.92	121.08	111.91
2	A	305	OLC	O20-C1-C2	2.89	120.98	111.91
2	B	303	OLC	O20-C1-C2	2.85	120.86	111.91
2	D	404	OLC	O20-C1-C2	2.85	120.84	111.91
2	A	303	OLC	O20-C1-C2	2.83	120.78	111.91
2	B	301	OLC	O20-C1-C2	2.78	120.64	111.91
2	C	315	OLC	O20-C1-C2	2.77	120.60	111.91
2	A	306	OLC	O20-C1-C2	2.75	120.55	111.91
2	C	302	OLC	O20-C1-C2	2.73	120.47	111.91
2	C	303	OLC	O20-C1-C2	2.72	120.43	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	303	OLC	O20-C1-C2	2.71	120.40	111.91
2	B	306	OLC	O20-C1-C2	2.68	120.32	111.91
2	B	305	OLC	O20-C1-C2	2.57	119.98	111.91
2	A	306	OLC	O20-C1-O19	-2.53	117.22	123.59
2	D	405	OLC	O20-C1-C2	2.48	119.70	111.91
2	D	408	OLC	O20-C1-C2	2.43	119.52	111.91
2	C	306	OLC	O20-C1-C2	2.28	119.06	111.91
2	E	308	OLC	O20-C1-C2	2.26	119.00	111.91
2	D	408	OLC	O20-C1-O19	-2.20	118.05	123.59
2	E	308	OLC	O20-C1-O19	-2.13	118.22	123.59
2	A	315	OLC	O20-C1-C2	2.11	120.80	114.03
2	C	302	OLC	O20-C1-O19	-2.10	118.29	123.59
2	B	304	OLC	O20-C1-O19	-2.10	118.30	123.59
2	D	407	OLC	O20-C1-C2	2.09	120.75	114.03
2	C	301	OLC	O20-C1-O19	-2.08	118.35	123.59
2	A	302	OLC	O20-C1-C2	2.03	120.55	114.03
2	C	304	OLC	O20-C1-O19	-2.01	118.53	123.59
2	B	306	OLC	O20-C1-O19	-2.00	118.53	123.59
2	D	407	OLC	O20-C1-O19	-2.00	118.31	123.30
2	B	302	OLC	O20-C1-O19	-2.00	118.54	123.59

There are no chirality outliers.

All (444) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	303	OLC	C6-C7-C8-C9
2	A	304	OLC	O20-C21-C22-O23
2	A	305	OLC	C21-C22-C24-O25
2	A	305	OLC	O20-C21-C22-C24
2	A	305	OLC	O20-C21-C22-O23
2	A	306	OLC	O20-C21-C22-C24
2	B	301	OLC	C21-C22-C24-O25
2	B	302	OLC	O20-C21-C22-C24
2	B	303	OLC	C21-C22-C24-O25
2	D	404	OLC	C21-C22-C24-O25
2	D	404	OLC	O20-C21-C22-C24
2	D	405	OLC	O20-C21-C22-C24
2	D	408	OLC	C21-C22-C24-O25
2	D	408	OLC	O23-C22-C24-O25
2	E	307	OLC	C21-C22-C24-O25
2	E	307	OLC	O20-C21-C22-O23
5	E	315	BOG	C2-C1-O1-C1'

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Mol	Chain	Res	Type	Atoms
5	E	315	BOG	O5-C1-O1-C1'
6	B	314	OLA	C11-C10-C9-C8
6	C	314	OLA	C11-C10-C9-C8
6	D	417	OLA	C11-C10-C9-C8
2	A	305	OLC	O19-C1-O20-C21
2	C	302	OLC	O19-C1-O20-C21
2	D	405	OLC	O19-C1-O20-C21
2	A	305	OLC	C2-C1-O20-C21
2	C	302	OLC	C2-C1-O20-C21
2	B	304	OLC	C2-C1-O20-C21
2	C	315	OLC	C2-C1-O20-C21
2	D	405	OLC	C2-C1-O20-C21
6	B	315	OLA	C11-C10-C9-C8
6	B	316	OLA	C11-C10-C9-C8
6	C	312	OLA	C11-C10-C9-C8
2	C	315	OLC	O19-C1-O20-C21
2	A	306	OLC	C2-C1-O20-C21
2	A	306	OLC	O20-C21-C22-O23
2	B	302	OLC	O20-C21-C22-O23
2	C	303	OLC	O20-C21-C22-O23
2	D	404	OLC	O20-C21-C22-O23
2	B	304	OLC	O19-C1-O20-C21
6	C	312	OLA	C2-C3-C4-C5
2	A	306	OLC	O19-C1-O20-C21
2	A	303	OLC	C2-C1-O20-C21
2	E	306	OLC	C2-C1-O20-C21
6	E	302	OLA	C11-C10-C9-C8
2	A	303	OLC	O19-C1-O20-C21
2	B	301	OLC	C2-C1-O20-C21
2	B	306	OLC	C2-C1-O20-C21
2	D	406	OLC	C2-C1-O20-C21
2	E	307	OLC	O20-C21-C22-C24
2	E	309	OLC	O20-C21-C22-C24
2	D	405	OLC	O20-C21-C22-O23
2	E	303	OLC	C1-C2-C3-C4
6	C	314	OLA	C1-C2-C3-C4
6	E	302	OLA	C1-C2-C3-C4
2	B	306	OLC	O19-C1-O20-C21
2	E	307	OLC	C2-C1-O20-C21
2	B	302	OLC	C1-C2-C3-C4
2	D	407	OLC	C1-C2-C3-C4
2	E	303	OLC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
6	D	403	OLA	C1-C2-C3-C4
2	B	301	OLC	O19-C1-O20-C21
2	D	406	OLC	O19-C1-O20-C21
2	E	306	OLC	O19-C1-O20-C21
2	E	307	OLC	O19-C1-O20-C21
2	E	309	OLC	O20-C21-C22-O23
2	C	315	OLC	C1-C2-C3-C4
2	C	304	OLC	C6-C7-C8-C9
2	D	405	OLC	C14-C15-C16-C17
3	A	312	LFA	C7-C8-C9-C10
2	A	303	OLC	C13-C14-C15-C16
2	C	305	OLC	C2-C3-C4-C5
2	D	405	OLC	C4-C5-C6-C7
2	D	406	OLC	C5-C6-C7-C8
2	E	301	OLC	C13-C14-C15-C16
2	E	306	OLC	C5-C6-C7-C8
3	A	309	LFA	C15-C16-C17-C18
6	C	314	OLA	C2-C3-C4-C5
6	D	401	OLA	C14-C15-C16-C17
2	C	306	OLC	C2-C1-O20-C21
2	A	315	OLC	C11-C12-C13-C14
3	D	409	LFA	C3-C4-C5-C6
3	D	411	LFA	C2-C3-C4-C5
6	B	316	OLA	C12-C13-C14-C15
6	D	401	OLA	C12-C13-C14-C15
3	D	409	LFA	C9-C10-C11-C12
3	E	311	LFA	C15-C16-C17-C18
2	A	315	OLC	C5-C6-C7-C8
3	C	308	LFA	C16-C17-C18-C19
2	B	303	OLC	C2-C1-O20-C21
2	C	302	OLC	C11-C12-C13-C14
2	E	306	OLC	C3-C4-C5-C6
3	A	309	LFA	C16-C17-C18-C19
3	D	409	LFA	C11-C10-C9-C8
3	E	311	LFA	C14-C15-C16-C17
2	A	305	OLC	C3-C4-C5-C6
2	B	302	OLC	C3-C4-C5-C6
3	A	312	LFA	C11-C12-C13-C14
3	B	308	LFA	C2-C3-C4-C5
2	B	303	OLC	C4-C5-C6-C7
3	C	308	LFA	C15-C16-C17-C18
2	C	301	OLC	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	E	306	OLC	C4-C5-C6-C7
3	B	309	LFA	C5-C6-C7-C8
3	D	409	LFA	C6-C7-C8-C9
3	D	410	LFA	C11-C12-C13-C14
6	B	316	OLA	C2-C3-C4-C5
2	C	302	OLC	C21-C22-C24-O25
2	E	306	OLC	C21-C22-C24-O25
2	E	303	OLC	C4-C5-C6-C7
3	D	409	LFA	C4-C5-C6-C7
3	D	409	LFA	C11-C12-C13-C14
2	C	302	OLC	C10-C11-C12-C13
6	E	302	OLA	C10-C11-C12-C13
6	A	317	OLA	C1-C2-C3-C4
2	C	302	OLC	C5-C6-C7-C8
2	C	302	OLC	C4-C5-C6-C7
2	C	305	OLC	C3-C4-C5-C6
3	A	312	LFA	C10-C11-C12-C13
3	D	410	LFA	C14-C15-C16-C17
3	D	412	LFA	C13-C14-C15-C16
6	B	314	OLA	C11-C12-C13-C14
2	E	301	OLC	C5-C6-C7-C8
3	B	307	LFA	C16-C17-C18-C19
2	B	303	OLC	C5-C6-C7-C8
2	C	304	OLC	C5-C6-C7-C8
3	B	307	LFA	C15-C16-C17-C18
3	B	310	LFA	C15-C16-C17-C18
3	E	310	LFA	C16-C17-C18-C19
3	E	311	LFA	C13-C14-C15-C16
5	D	416	BOG	C1'-C2'-C3'-C4'
3	A	309	LFA	C14-C15-C16-C17
6	B	314	OLA	C3-C4-C5-C6
5	E	315	BOG	C2'-C1'-O1-C1
2	C	306	OLC	C3-C4-C5-C6
6	B	316	OLA	C1-C2-C3-C4
6	E	317	OLA	C5-C6-C7-C8
3	A	312	LFA	C4-C5-C6-C7
3	E	311	LFA	C9-C10-C11-C12
2	C	306	OLC	C4-C5-C6-C7
2	B	301	OLC	O23-C22-C24-O25
2	B	303	OLC	O23-C22-C24-O25
2	E	307	OLC	O23-C22-C24-O25
2	E	305	OLC	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
6	D	403	OLA	C2-C3-C4-C5
6	D	417	OLA	C5-C6-C7-C8
2	B	303	OLC	C6-C7-C8-C9
2	C	305	OLC	C6-C7-C8-C9
6	A	317	OLA	C10-C11-C12-C13
6	B	315	OLA	C10-C11-C12-C13
5	B	312	BOG	C1'-C2'-C3'-C4'
5	E	315	BOG	C1'-C2'-C3'-C4'
3	A	311	LFA	C2-C3-C4-C5
2	C	306	OLC	O19-C1-O20-C21
3	C	309	LFA	C13-C14-C15-C16
2	B	303	OLC	O19-C1-O20-C21
2	B	302	OLC	C14-C15-C16-C17
2	C	303	OLC	C3-C4-C5-C6
6	E	317	OLA	C3-C4-C5-C6
7	B	313	GOL	O1-C1-C2-O2
2	E	301	OLC	C11-C12-C13-C14
2	B	302	OLC	C13-C14-C15-C16
2	A	305	OLC	C10-C11-C12-C13
2	E	301	OLC	C6-C7-C8-C9
6	B	314	OLA	C6-C7-C8-C9
2	C	305	OLC	C4-C5-C6-C7
3	A	316	LFA	C4-C5-C6-C7
2	B	301	OLC	C3-C4-C5-C6
6	E	317	OLA	C12-C13-C14-C15
6	C	314	OLA	C4-C5-C6-C7
5	D	416	BOG	C3'-C4'-C5'-C6'
5	E	315	BOG	C2'-C3'-C4'-C5'
6	C	312	OLA	C3-C4-C5-C6
2	D	408	OLC	C2-C3-C4-C5
2	E	305	OLC	C11-C12-C13-C14
3	C	309	LFA	C10-C11-C12-C13
2	E	303	OLC	C11-C12-C13-C14
3	D	409	LFA	C10-C11-C12-C13
2	A	315	OLC	C10-C11-C12-C13
2	C	301	OLC	C6-C7-C8-C9
2	E	309	OLC	C6-C7-C8-C9
6	A	317	OLA	C6-C7-C8-C9
2	C	301	OLC	C1-C2-C3-C4
2	E	309	OLC	C4-C5-C6-C7
2	C	302	OLC	C3-C4-C5-C6
5	C	311	BOG	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
2	D	407	OLC	C5-C6-C7-C8
6	C	312	OLA	C4-C5-C6-C7
2	A	303	OLC	C1-C2-C3-C4
6	B	316	OLA	C3-C4-C5-C6
2	D	406	OLC	C4-C5-C6-C7
2	C	305	OLC	C10-C11-C12-C13
2	D	407	OLC	C10-C11-C12-C13
6	E	317	OLA	C10-C11-C12-C13
2	C	301	OLC	C2-C3-C4-C5
2	E	307	OLC	C2-C3-C4-C5
5	A	314	BOG	C1'-C2'-C3'-C4'
6	D	401	OLA	C4-C5-C6-C7
3	C	309	LFA	C12-C13-C14-C15
3	D	410	LFA	C5-C6-C7-C8
3	A	308	LFA	C1-C2-C3-C4
3	D	411	LFA	C4-C5-C6-C7
5	B	312	BOG	C5'-C6'-C7'-C8'
3	D	412	LFA	C1-C2-C3-C4
3	B	309	LFA	C1-C2-C3-C4
3	C	308	LFA	C17-C18-C19-C20
6	C	314	OLA	C13-C14-C15-C16
2	C	302	OLC	O23-C22-C24-O25
2	E	306	OLC	O23-C22-C24-O25
2	B	305	OLC	C4-C5-C6-C7
2	E	303	OLC	C5-C6-C7-C8
3	C	307	LFA	C4-C5-C6-C7
2	A	302	OLC	C10-C11-C12-C13
2	B	302	OLC	C6-C7-C8-C9
2	B	305	OLC	C10-C11-C12-C13
6	C	312	OLA	C10-C11-C12-C13
6	D	417	OLA	C10-C11-C12-C13
2	C	301	OLC	O20-C21-C22-O23
3	D	411	LFA	C5-C6-C7-C8
2	C	315	OLC	O20-C21-C22-C24
2	E	306	OLC	O20-C21-C22-C24
3	D	412	LFA	C5-C6-C7-C8
5	C	311	BOG	C5'-C6'-C7'-C8'
6	B	314	OLA	C2-C3-C4-C5
6	E	316	OLA	C1-C2-C3-C4
2	E	305	OLC	C5-C6-C7-C8
2	B	301	OLC	C2-C3-C4-C5
3	A	316	LFA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	D	410	LFA	C1-C2-C3-C4
2	C	303	OLC	C5-C6-C7-C8
6	D	417	OLA	C7-C8-C9-C10
2	E	301	OLC	C14-C15-C16-C17
3	E	310	LFA	C15-C16-C17-C18
2	A	301	OLC	C11-C12-C13-C14
2	C	315	OLC	C4-C5-C6-C7
3	D	412	LFA	C14-C15-C16-C17
3	D	413	LFA	C14-C15-C16-C17
5	A	314	BOG	C5'-C6'-C7'-C8'
2	D	405	OLC	C15-C16-C17-C18
2	B	305	OLC	O20-C21-C22-O23
5	E	315	BOG	C4-C5-C6-O6
2	A	305	OLC	C12-C13-C14-C15
3	C	309	LFA	C4-C5-C6-C7
3	D	411	LFA	C1-C2-C3-C4
6	B	314	OLA	C12-C13-C14-C15
2	E	309	OLC	C2-C1-O20-C21
3	E	311	LFA	C7-C8-C9-C10
2	A	315	OLC	C12-C13-C14-C15
3	B	308	LFA	C3-C4-C5-C6
2	E	303	OLC	C13-C14-C15-C16
2	A	302	OLC	C2-C3-C4-C5
3	D	412	LFA	C7-C8-C9-C10
6	A	317	OLA	C11-C12-C13-C14
2	D	405	OLC	C3-C4-C5-C6
2	E	304	OLC	C3-C4-C5-C6
2	A	304	OLC	O20-C21-C22-C24
2	C	301	OLC	O20-C21-C22-C24
2	D	408	OLC	C1-C2-C3-C4
2	B	305	OLC	C5-C6-C7-C8
2	E	307	OLC	C4-C5-C6-C7
2	A	305	OLC	O23-C22-C24-O25
2	E	309	OLC	O23-C22-C24-O25
2	E	301	OLC	C10-C11-C12-C13
6	E	317	OLA	C6-C7-C8-C9
2	C	302	OLC	C13-C14-C15-C16
2	C	305	OLC	C5-C6-C7-C8
3	A	316	LFA	C6-C7-C8-C9
2	B	302	OLC	C4-C5-C6-C7
2	C	301	OLC	C2-C1-O20-C21
6	D	403	OLA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
6	C	314	OLA	C5-C6-C7-C8
2	A	315	OLC	C2-C3-C4-C5
6	D	417	OLA	C2-C3-C4-C5
2	E	309	OLC	C3-C4-C5-C6
5	E	315	BOG	O5-C5-C6-O6
3	D	410	LFA	C13-C14-C15-C16
3	D	412	LFA	C4-C5-C6-C7
2	A	305	OLC	C13-C14-C15-C16
6	D	401	OLA	C11-C12-C13-C14
3	A	312	LFA	C3-C4-C5-C6
5	B	312	BOG	C3'-C4'-C5'-C6'
3	D	409	LFA	C14-C15-C16-C17
6	C	312	OLA	C5-C6-C7-C8
2	C	315	OLC	O20-C21-C22-O23
3	D	410	LFA	C11-C10-C9-C8
6	B	315	OLA	C12-C13-C14-C15
2	E	308	OLC	C2-C3-C4-C5
2	C	301	OLC	O19-C1-O20-C21
3	C	309	LFA	C14-C15-C16-C17
6	A	317	OLA	C4-C5-C6-C7
2	D	406	OLC	O23-C22-C24-O25
2	E	309	OLC	O19-C1-O20-C21
6	D	403	OLA	C5-C6-C7-C8
2	B	303	OLC	C11-C12-C13-C14
2	C	315	OLC	C21-C22-C24-O25
5	A	314	BOG	O1-C1'-C2'-C3'
6	B	315	OLA	C3-C4-C5-C6
2	E	306	OLC	O20-C21-C22-O23
6	B	314	OLA	C7-C8-C9-C10
3	D	412	LFA	C3-C4-C5-C6
2	D	407	OLC	C2-C3-C4-C5
5	E	315	BOG	O1-C1'-C2'-C3'
6	A	317	OLA	C11-C10-C9-C8
6	E	317	OLA	C11-C10-C9-C8
2	C	303	OLC	O20-C21-C22-C24
2	C	302	OLC	C12-C13-C14-C15
2	E	306	OLC	C10-C11-C12-C13
6	C	312	OLA	C6-C7-C8-C9
5	D	416	BOG	C4'-C5'-C6'-C7'
6	E	302	OLA	C11-C12-C13-C14
2	C	301	OLC	C3-C4-C5-C6
3	A	307	LFA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
6	E	317	OLA	C2-C3-C4-C5
2	D	404	OLC	C1-C2-C3-C4
3	D	410	LFA	C3-C4-C5-C6
6	C	314	OLA	C3-C4-C5-C6
3	E	312	LFA	C17-C18-C19-C20
3	D	413	LFA	C16-C17-C18-C19
2	C	315	OLC	O23-C22-C24-O25
2	D	404	OLC	O23-C22-C24-O25
2	E	303	OLC	O20-C21-C22-O23
6	D	403	OLA	C4-C5-C6-C7
3	C	309	LFA	C3-C4-C5-C6
6	D	401	OLA	C15-C16-C17-C18
2	B	305	OLC	O20-C21-C22-C24
3	D	409	LFA	C15-C16-C17-C18
5	E	315	BOG	C5'-C6'-C7'-C8'
6	A	317	OLA	C12-C13-C14-C15
2	E	303	OLC	C2-C3-C4-C5
3	D	412	LFA	C11-C12-C13-C14
7	C	313	GOL	O1-C1-C2-O2
2	B	305	OLC	C2-C3-C4-C5
6	D	403	OLA	C9-C10-C11-C12
2	D	405	OLC	C12-C13-C14-C15
3	B	309	LFA	C6-C7-C8-C9
6	B	314	OLA	C5-C6-C7-C8
2	A	303	OLC	C15-C16-C17-C18
3	B	309	LFA	C7-C8-C9-C10
3	E	313	LFA	C17-C18-C19-C20
3	C	307	LFA	C2-C3-C4-C5
2	E	308	OLC	C21-C22-C24-O25
2	A	305	OLC	C9-C10-C11-C12
2	C	305	OLC	C7-C8-C9-C10
6	A	317	OLA	C7-C8-C9-C10
2	A	302	OLC	C6-C7-C8-C9
2	B	301	OLC	C6-C7-C8-C9
6	A	317	OLA	C3-C4-C5-C6
2	C	302	OLC	C7-C8-C9-C10
6	B	314	OLA	O1-C1-C2-C3
3	D	410	LFA	C2-C3-C4-C5
6	D	403	OLA	O1-C1-C2-C3
2	C	304	OLC	C10-C11-C12-C13
3	A	312	LFA	C13-C14-C15-C16
2	A	306	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
6	B	316	OLA	C9-C10-C11-C12
6	D	403	OLA	C7-C8-C9-C10
3	B	307	LFA	C14-C15-C16-C17
3	E	310	LFA	C13-C14-C15-C16
5	E	315	BOG	C4'-C5'-C6'-C7'
6	D	401	OLA	C10-C11-C12-C13
2	D	405	OLC	C13-C14-C15-C16
2	E	308	OLC	C3-C4-C5-C6
6	B	316	OLA	O1-C1-C2-C3
2	B	304	OLC	C9-C10-C11-C12
6	A	317	OLA	O1-C1-C2-C3
6	B	316	OLA	O2-C1-C2-C3
2	C	301	OLC	C4-C5-C6-C7
2	D	408	OLC	C3-C4-C5-C6
6	D	403	OLA	O2-C1-C2-C3
3	D	412	LFA	C6-C7-C8-C9
6	B	314	OLA	O2-C1-C2-C3
2	C	315	OLC	C2-C3-C4-C5
5	B	312	BOG	C4'-C5'-C6'-C7'
2	C	306	OLC	C5-C6-C7-C8
6	A	317	OLA	O2-C1-C2-C3
6	B	316	OLA	C4-C5-C6-C7
2	A	305	OLC	C7-C8-C9-C10
6	B	317	OLA	O1-C1-C2-C3
6	B	317	OLA	O2-C1-C2-C3
6	E	302	OLA	O2-C1-C2-C3
2	A	303	OLC	C21-C22-C24-O25
2	B	302	OLC	C21-C22-C24-O25
2	C	305	OLC	C21-C22-C24-O25
6	E	316	OLA	O2-C1-C2-C3
2	A	301	OLC	C9-C10-C11-C12
2	A	303	OLC	C9-C10-C11-C12
2	B	302	OLC	C7-C8-C9-C10
2	B	303	OLC	C9-C10-C11-C12
2	E	304	OLC	C5-C6-C7-C8
6	E	316	OLA	O1-C1-C2-C3
6	C	314	OLA	O2-C1-C2-C3
2	A	305	OLC	C14-C15-C16-C17
2	B	302	OLC	C10-C11-C12-C13
3	C	309	LFA	C15-C16-C17-C18
2	C	301	OLC	C7-C8-C9-C10
2	D	405	OLC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	A	312	LFA	C11-C10-C9-C8
2	E	308	OLC	C5-C6-C7-C8
3	D	409	LFA	C5-C6-C7-C8
6	C	314	OLA	O1-C1-C2-C3
2	A	315	OLC	C7-C8-C9-C10
2	C	303	OLC	C7-C8-C9-C10
6	C	312	OLA	C7-C8-C9-C10
6	D	401	OLA	C7-C8-C9-C10
3	C	309	LFA	C9-C10-C11-C12
6	E	317	OLA	O2-C1-C2-C3
2	A	305	OLC	C2-C3-C4-C5
6	D	417	OLA	C4-C5-C6-C7
2	A	303	OLC	C7-C8-C9-C10
2	A	315	OLC	C9-C10-C11-C12
2	E	305	OLC	C9-C10-C11-C12
2	B	303	OLC	C10-C11-C12-C13
2	D	404	OLC	C2-C3-C4-C5
6	E	317	OLA	O1-C1-C2-C3
2	A	302	OLC	C7-C8-C9-C10
2	B	303	OLC	C7-C8-C9-C10
6	E	302	OLA	O1-C1-C2-C3
2	D	405	OLC	C6-C7-C8-C9
6	C	314	OLA	C10-C11-C12-C13
3	B	309	LFA	C2-C3-C4-C5
2	A	303	OLC	O20-C1-C2-C3
2	C	305	OLC	C11-C12-C13-C14
2	A	303	OLC	C12-C13-C14-C15
3	A	316	LFA	C1-C2-C3-C4
2	E	309	OLC	C9-C10-C11-C12
2	E	303	OLC	C7-C8-C9-C10
6	D	401	OLA	C6-C7-C8-C9
6	D	417	OLA	C11-C12-C13-C14
2	E	309	OLC	C21-C22-C24-O25
2	E	305	OLC	C7-C8-C9-C10
2	C	304	OLC	C2-C3-C4-C5
2	E	306	OLC	C9-C10-C11-C12
3	A	311	LFA	C1-C2-C3-C4
2	A	303	OLC	O19-C1-C2-C3
2	C	315	OLC	C6-C7-C8-C9
5	E	315	BOG	C3'-C4'-C5'-C6'
6	C	314	OLA	C12-C13-C14-C15
2	B	304	OLC	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
6	C	312	OLA	C11-C12-C13-C14
3	A	312	LFA	C1-C2-C3-C4
3	C	307	LFA	C1-C2-C3-C4
5	C	311	BOG	C2'-C1'-O1-C1
3	B	309	LFA	C4-C5-C6-C7
6	D	401	OLA	O1-C1-C2-C3
6	A	317	OLA	C2-C3-C4-C5

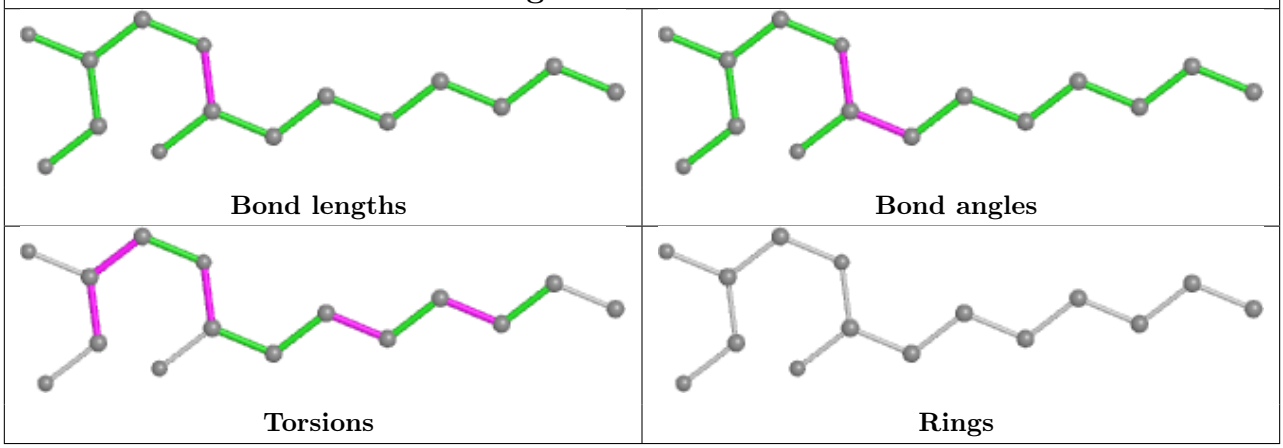
There are no ring outliers.

29 monomers are involved in 36 short contacts:

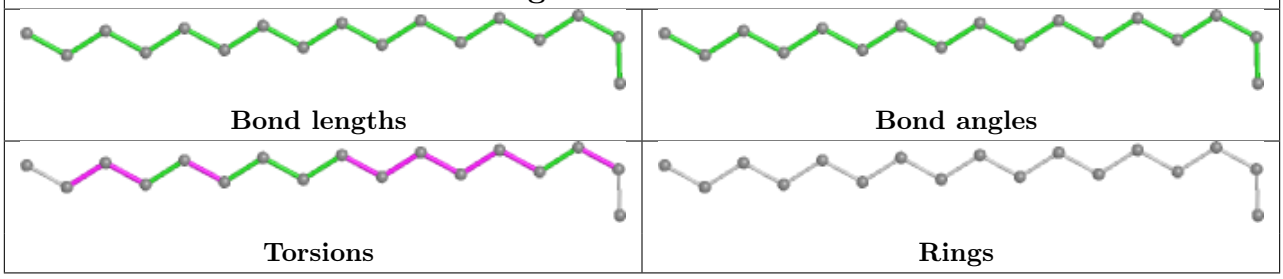
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	307	OLC	1	0
3	D	412	LFA	3	0
3	C	307	LFA	3	0
2	C	302	OLC	2	0
2	A	303	OLC	2	0
2	D	404	OLC	1	0
5	B	312	BOG	1	0
2	C	303	OLC	1	0
6	A	318	OLA	2	0
2	C	305	OLC	1	0
6	B	314	OLA	1	0
2	D	408	OLC	2	0
2	B	301	OLC	1	0
6	D	401	OLA	2	0
5	D	416	BOG	1	0
2	E	303	OLC	2	0
2	C	306	OLC	3	0
5	A	314	BOG	2	0
3	B	307	LFA	1	0
6	C	314	OLA	1	0
6	D	403	OLA	1	0
2	C	315	OLC	1	0
5	C	311	BOG	2	0
2	E	306	OLC	1	0
2	D	407	OLC	1	0
6	B	315	OLA	1	0
2	E	301	OLC	1	0
3	D	409	LFA	1	0
5	E	315	BOG	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.

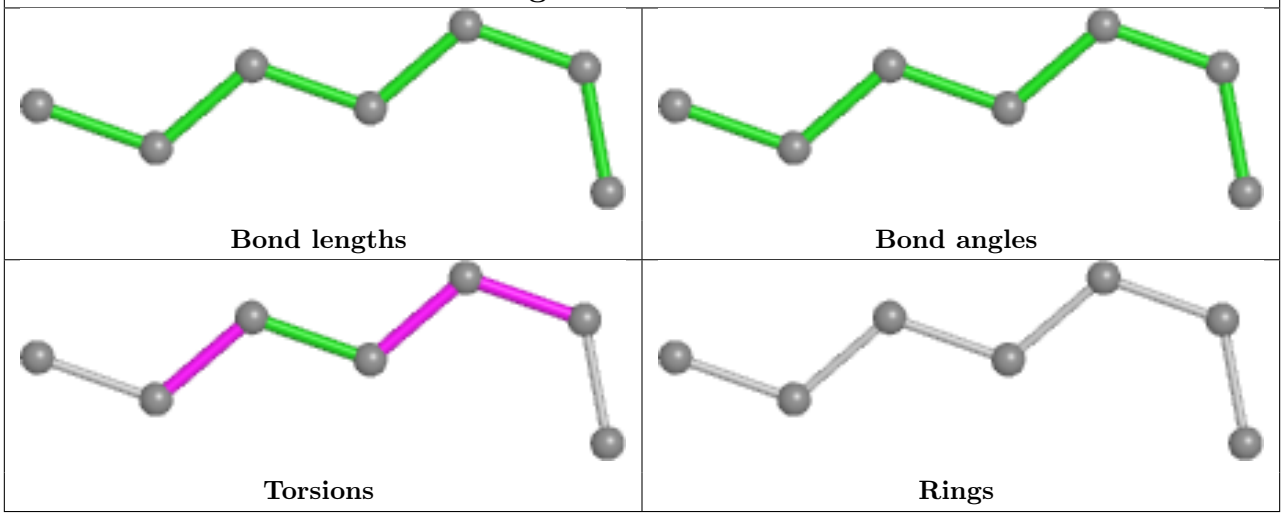
Ligand OLC E 307



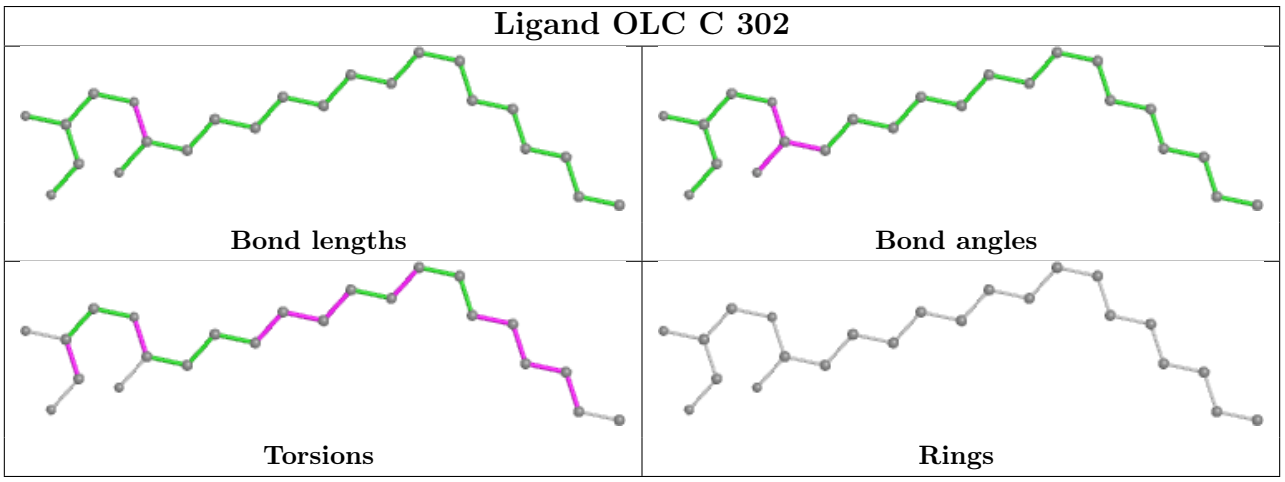
Ligand LFA D 412



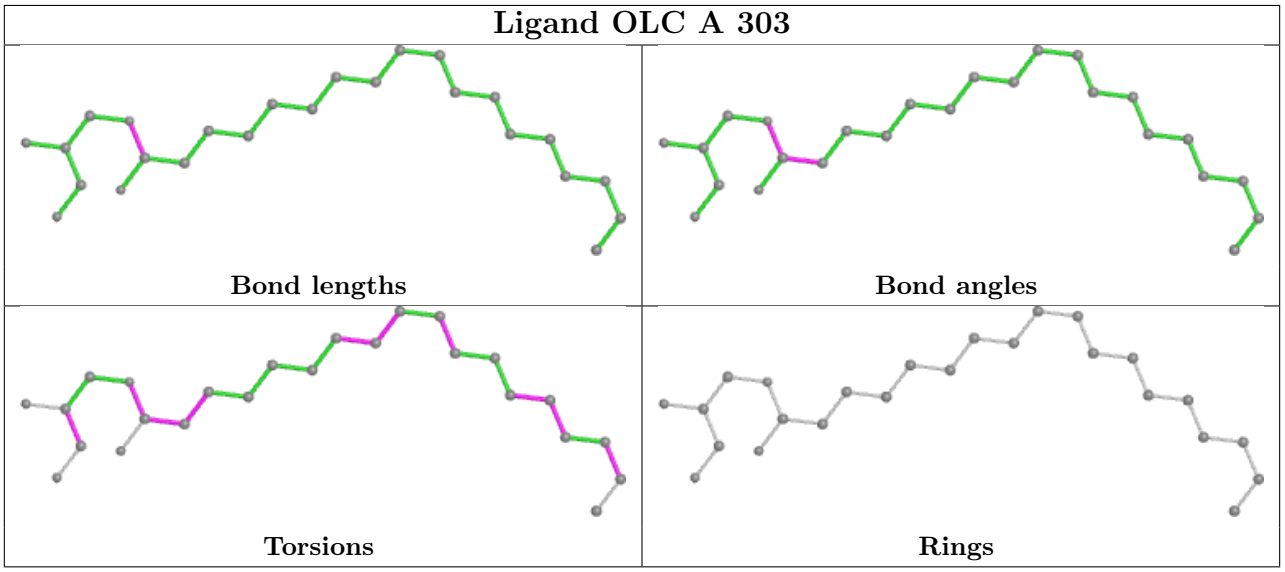
Ligand LFA C 307



Ligand OLC C 302



Ligand OLC A 303



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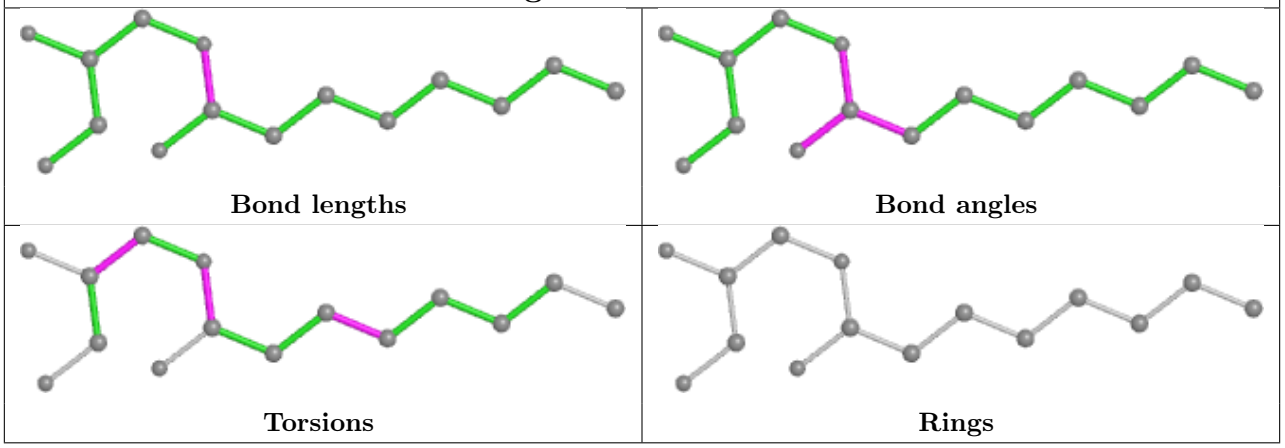

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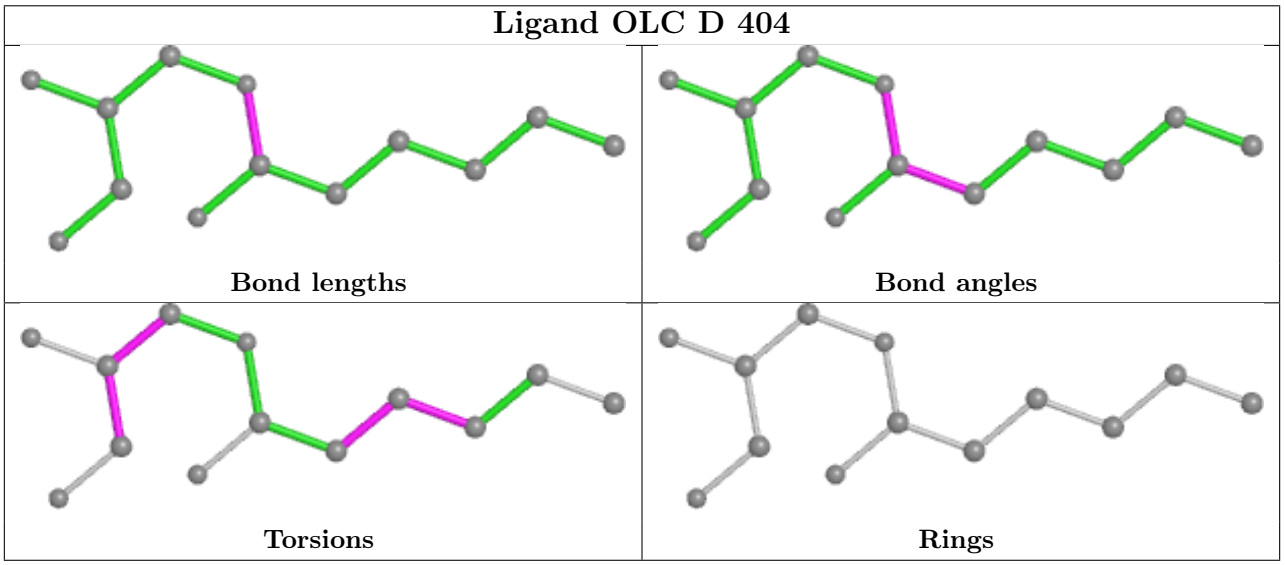

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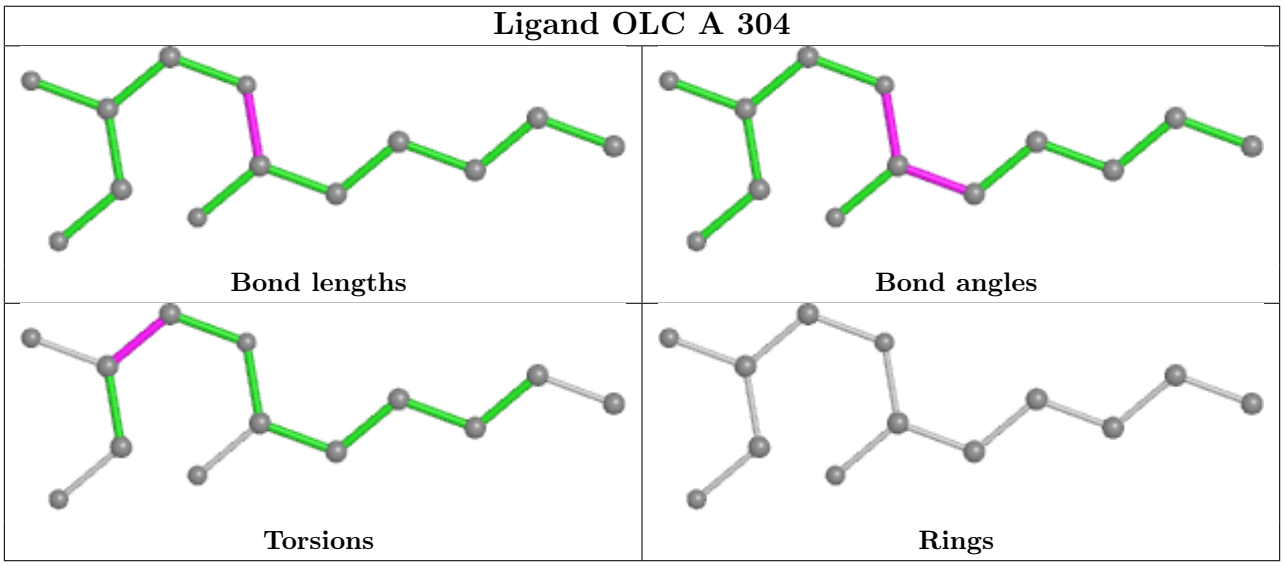
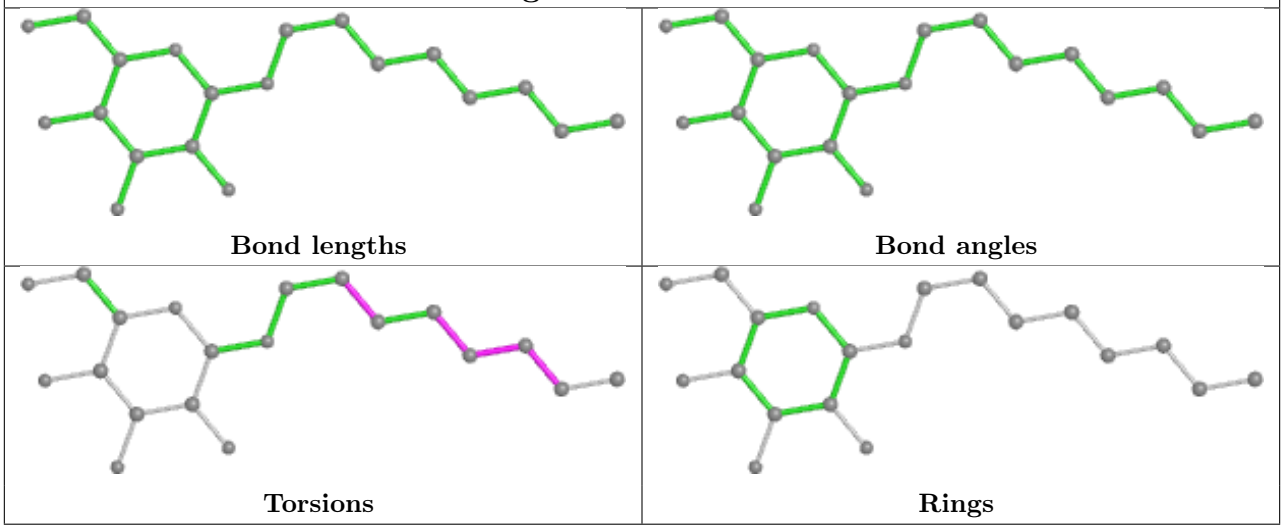


Ligand BOG B 312



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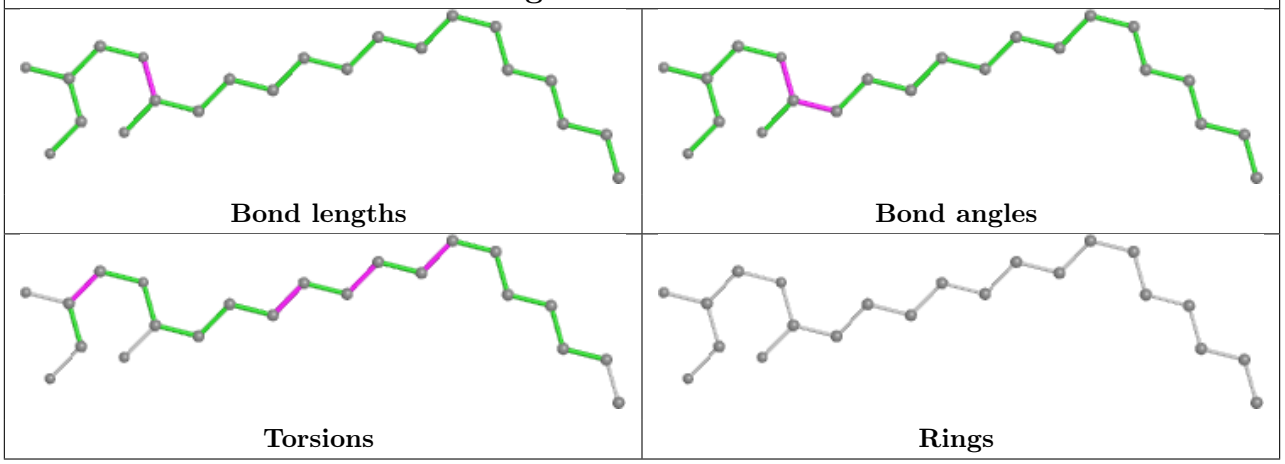
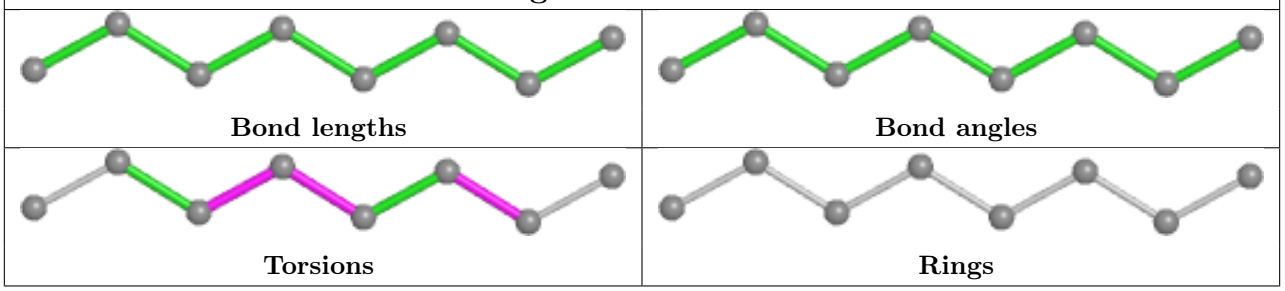


Ligand LFA E 310



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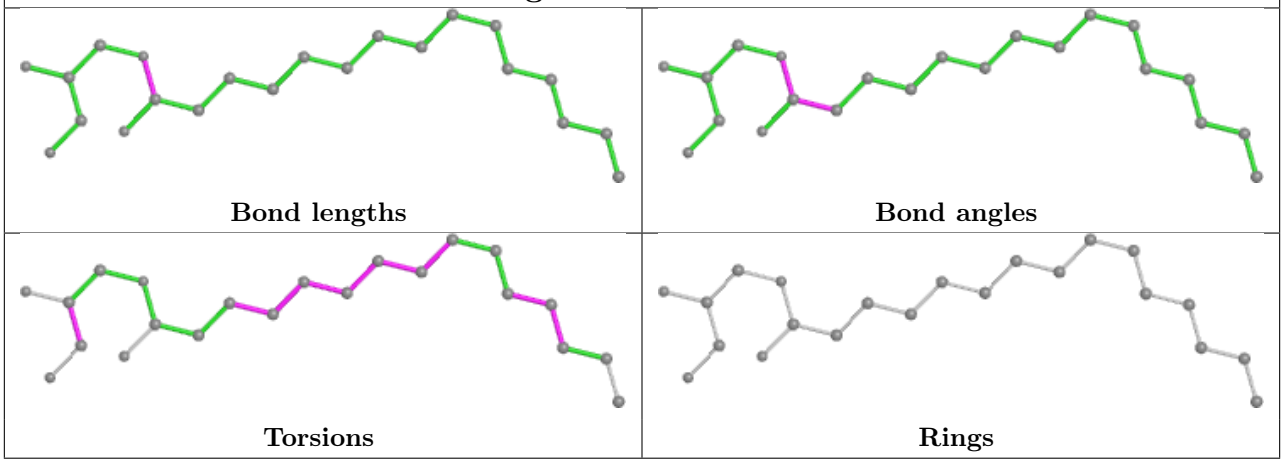

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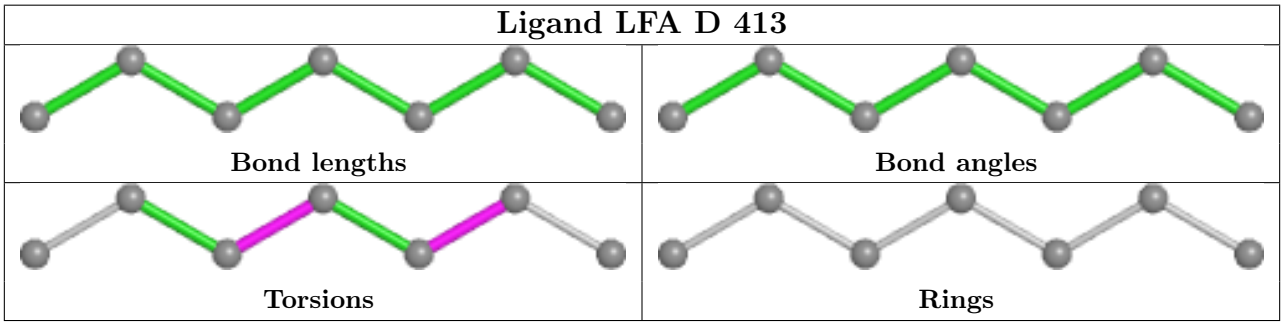

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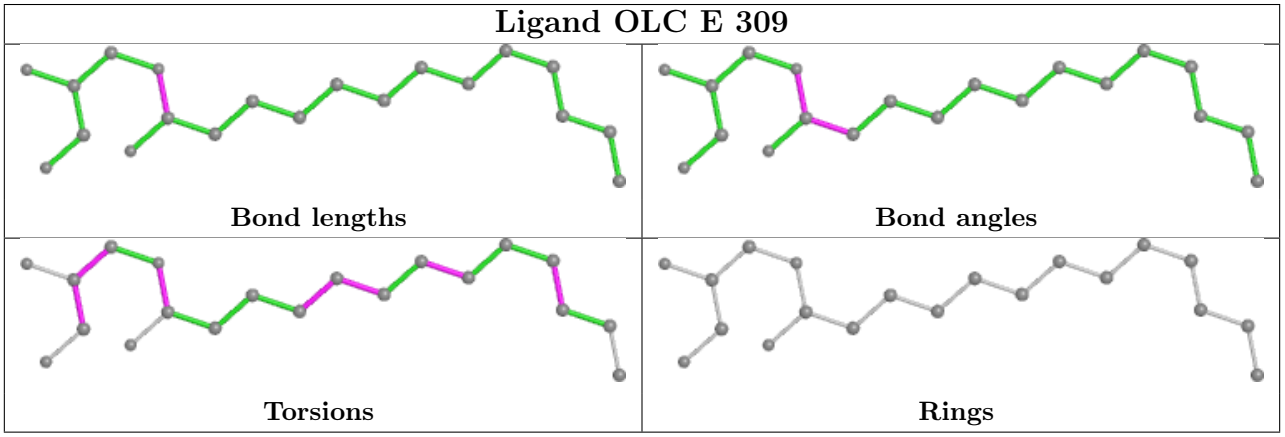

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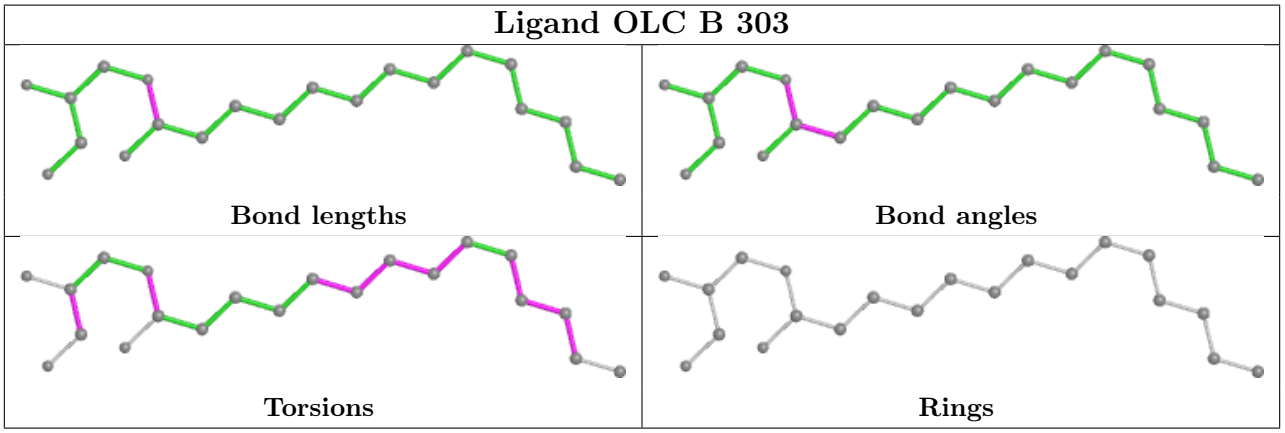
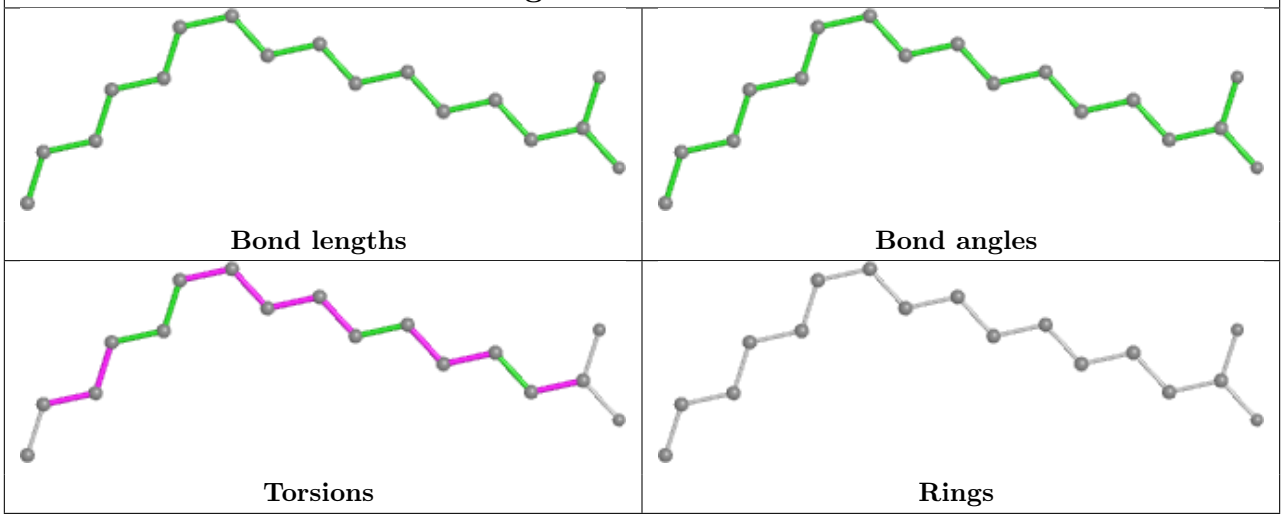


Ligand OLA B 314



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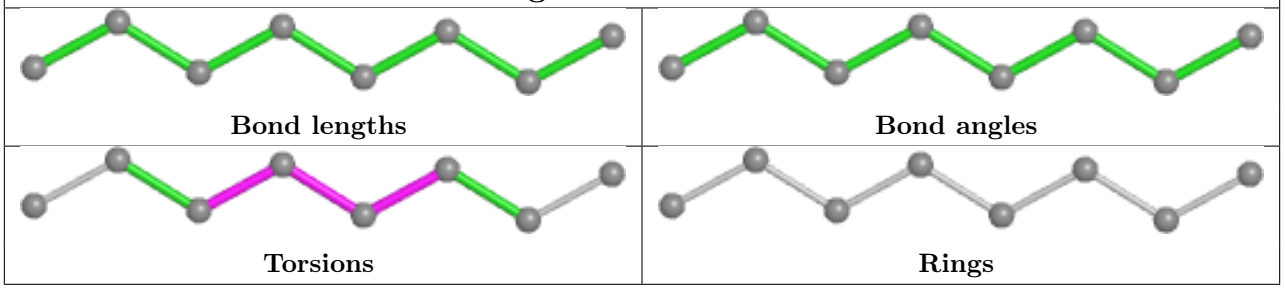

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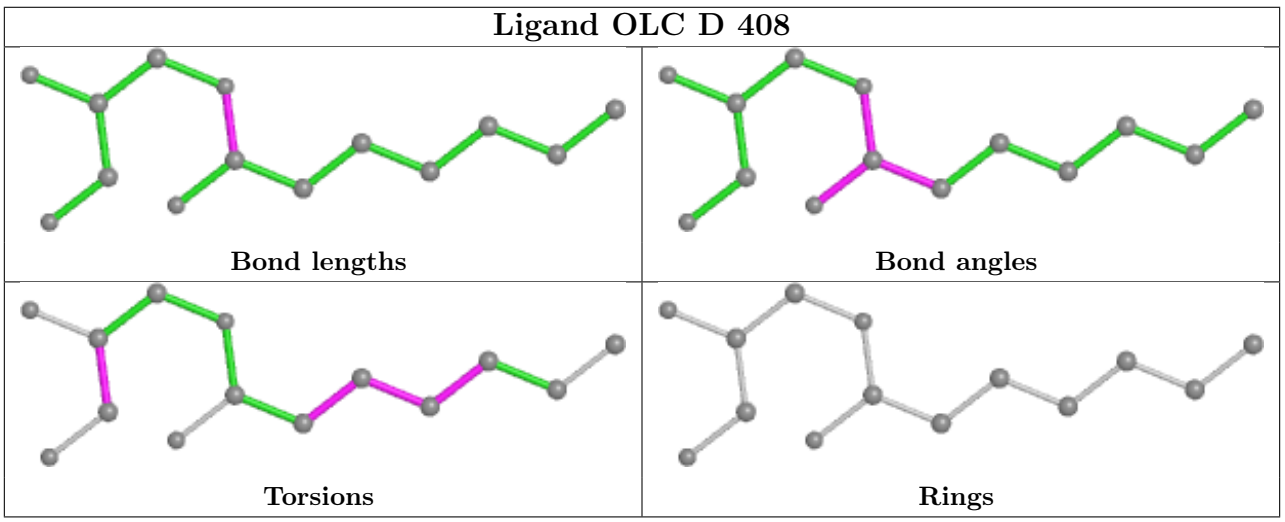

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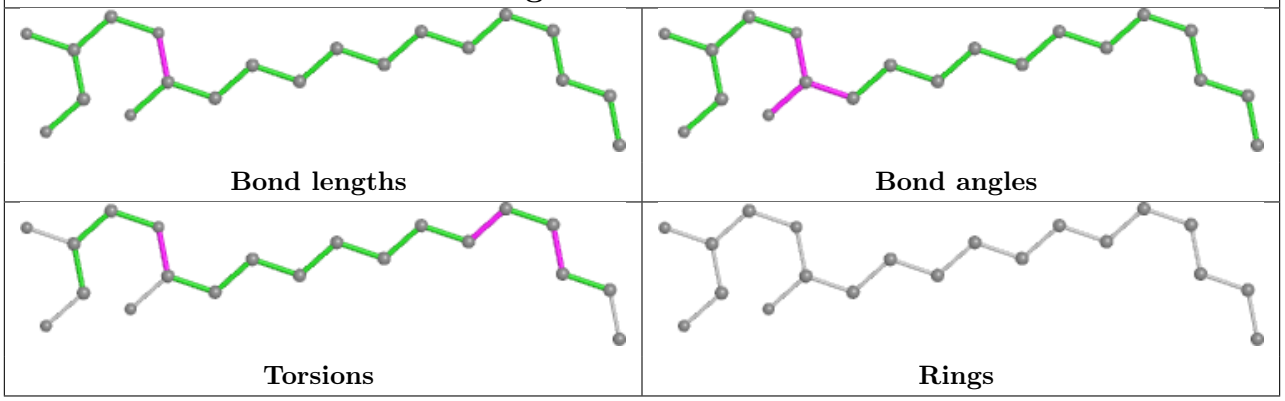

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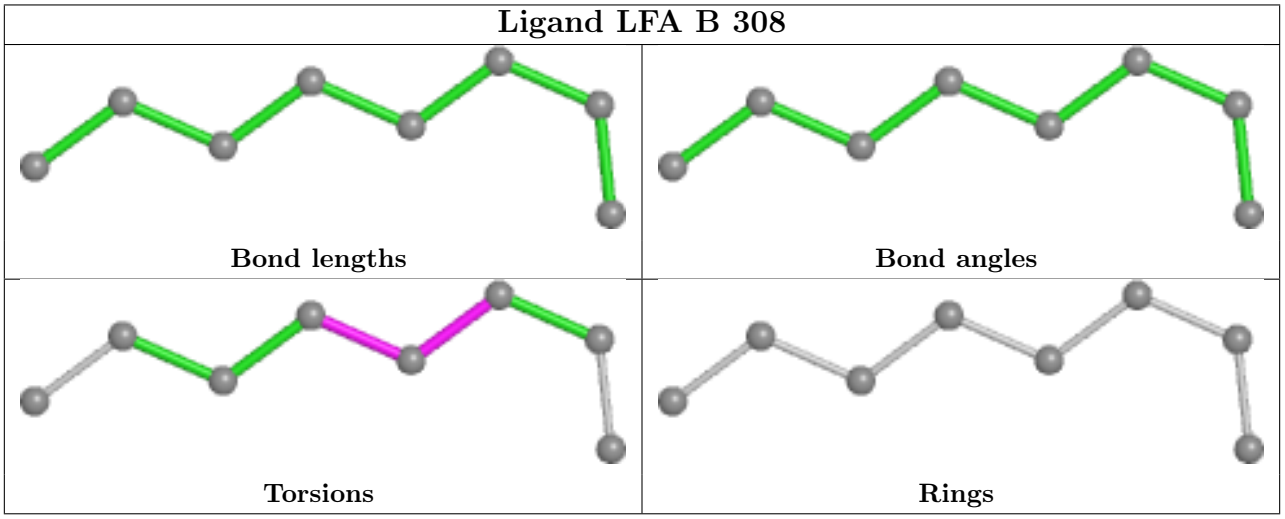

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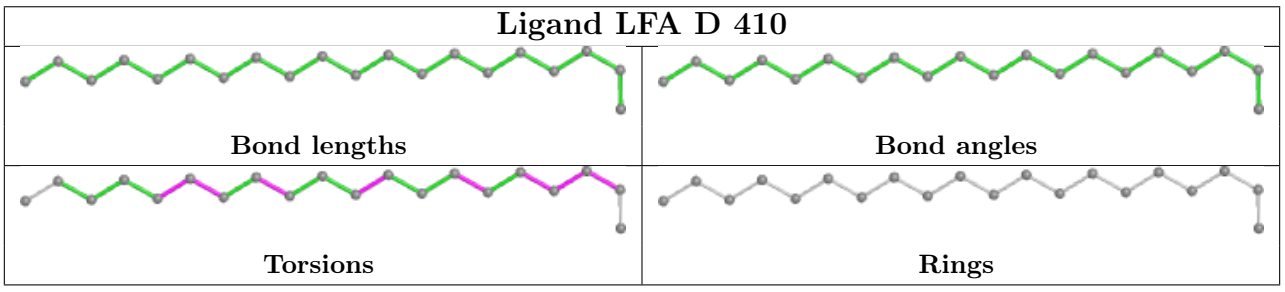

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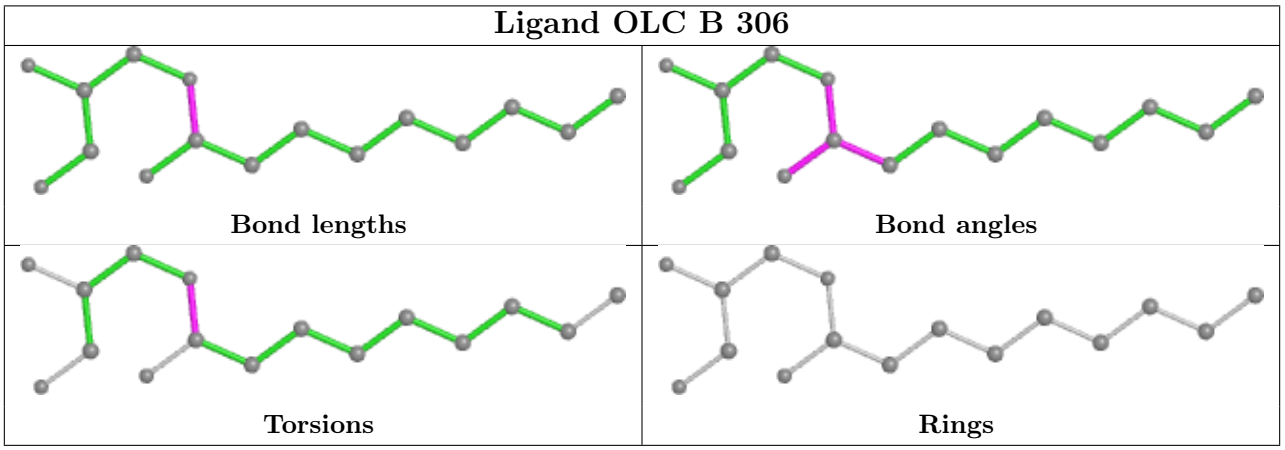

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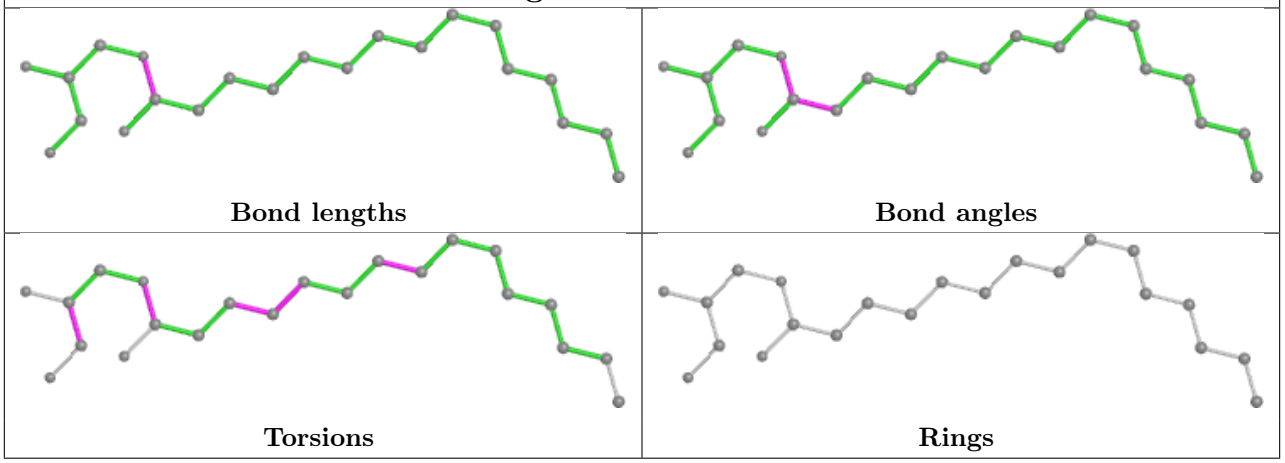
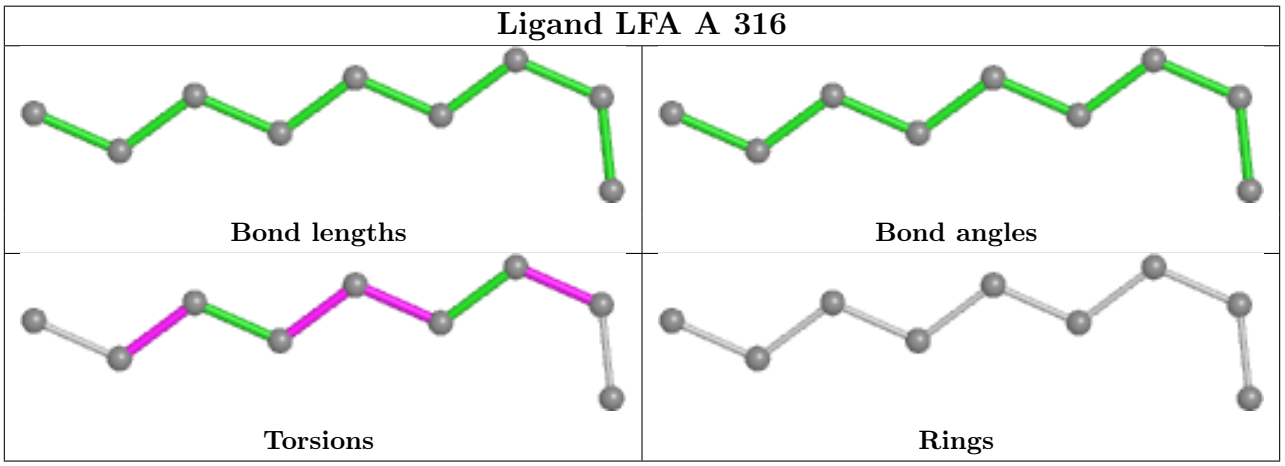
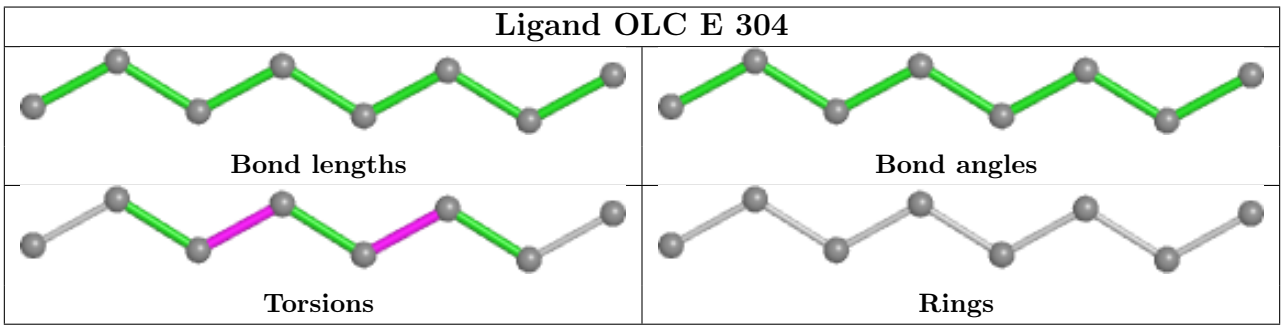


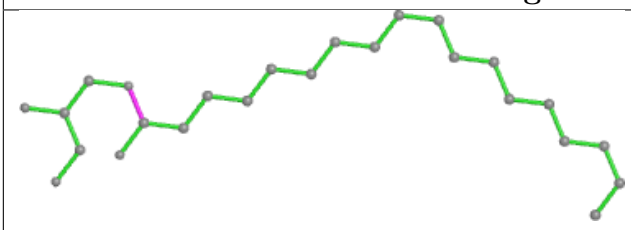
Ligand LFA A 316



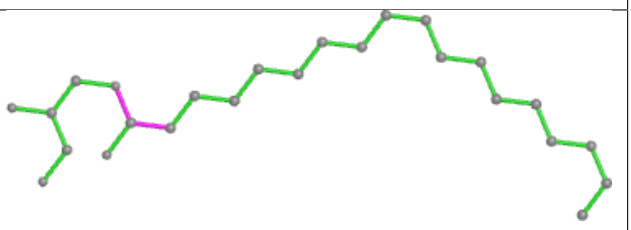
Ligand OLC E 304



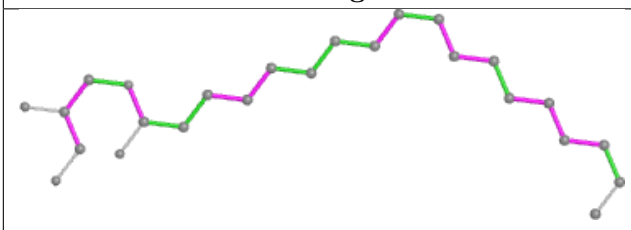
Ligand OLC A 305



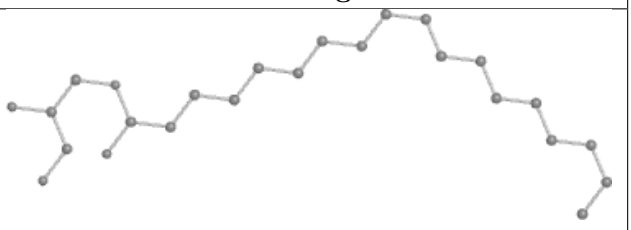
Bond lengths



Bond angles

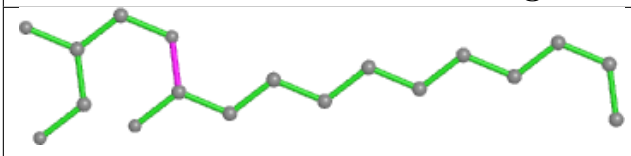


Torsions

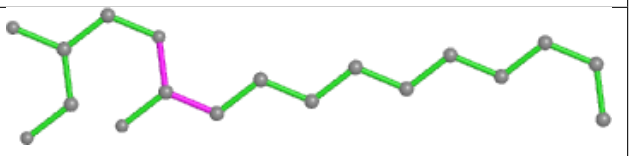


Rings

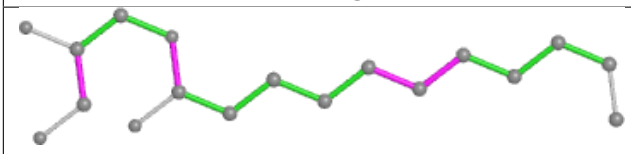
Ligand OLC D 406



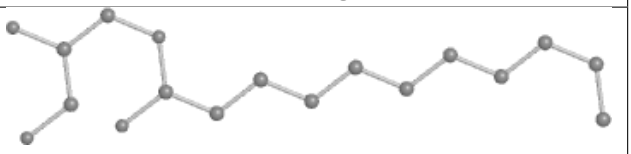
Bond lengths



Bond angles

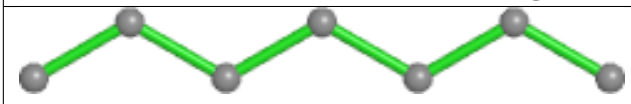


Torsions

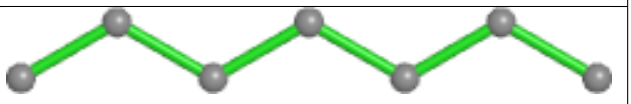


Rings

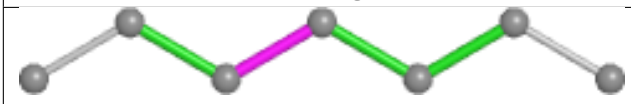
Ligand LFA A 307



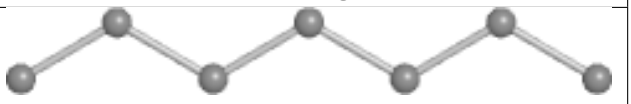
Bond lengths



Bond angles

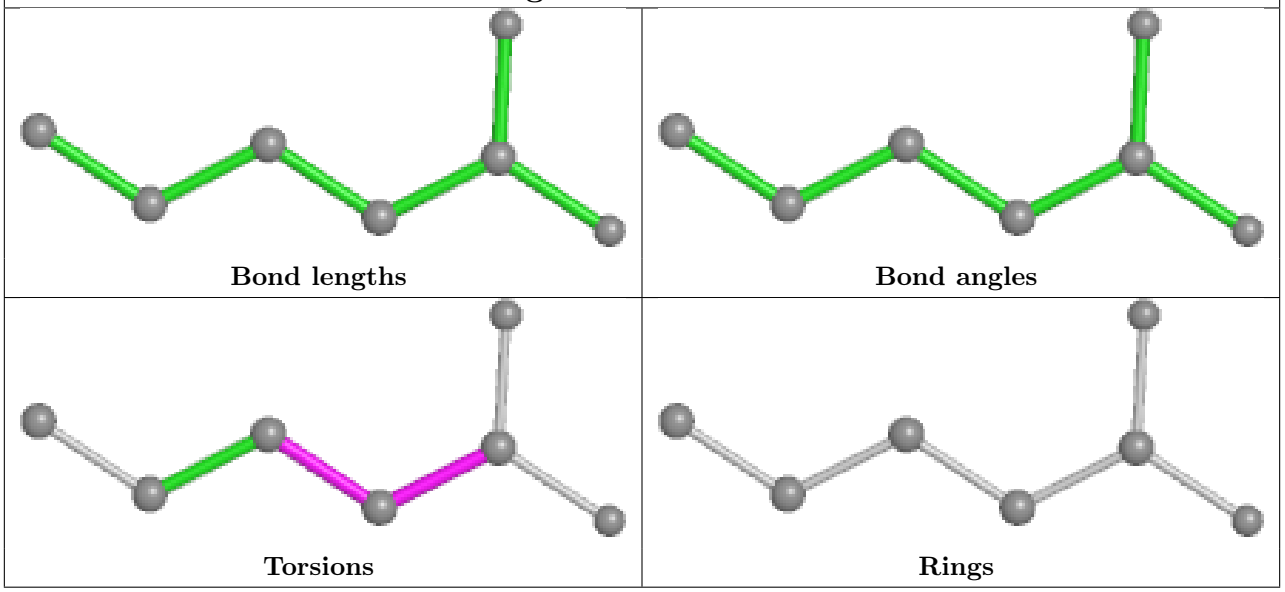


Torsions

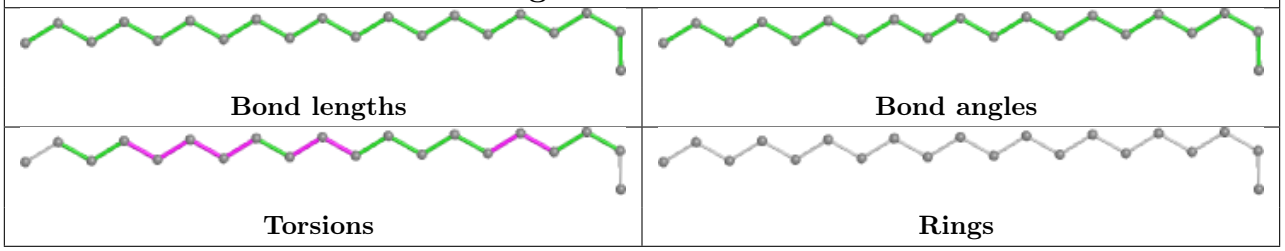


Rings

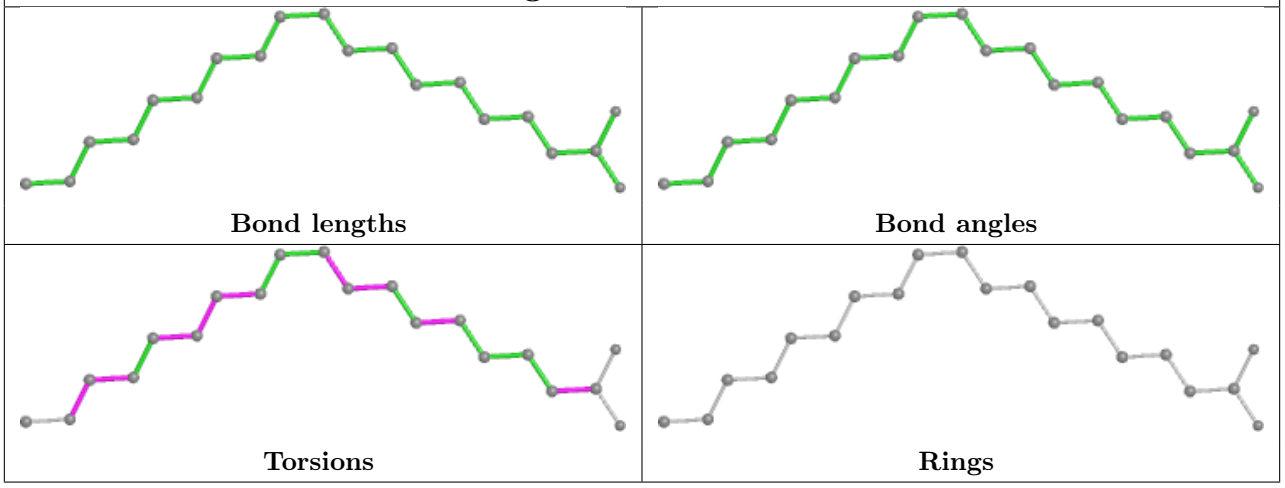
Ligand OLA E 316



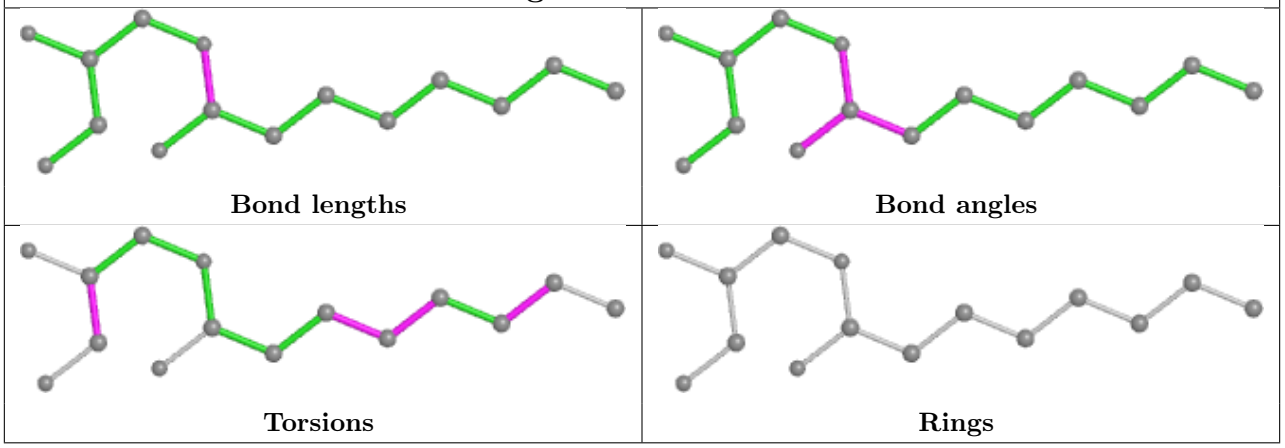
Ligand LFA C 309



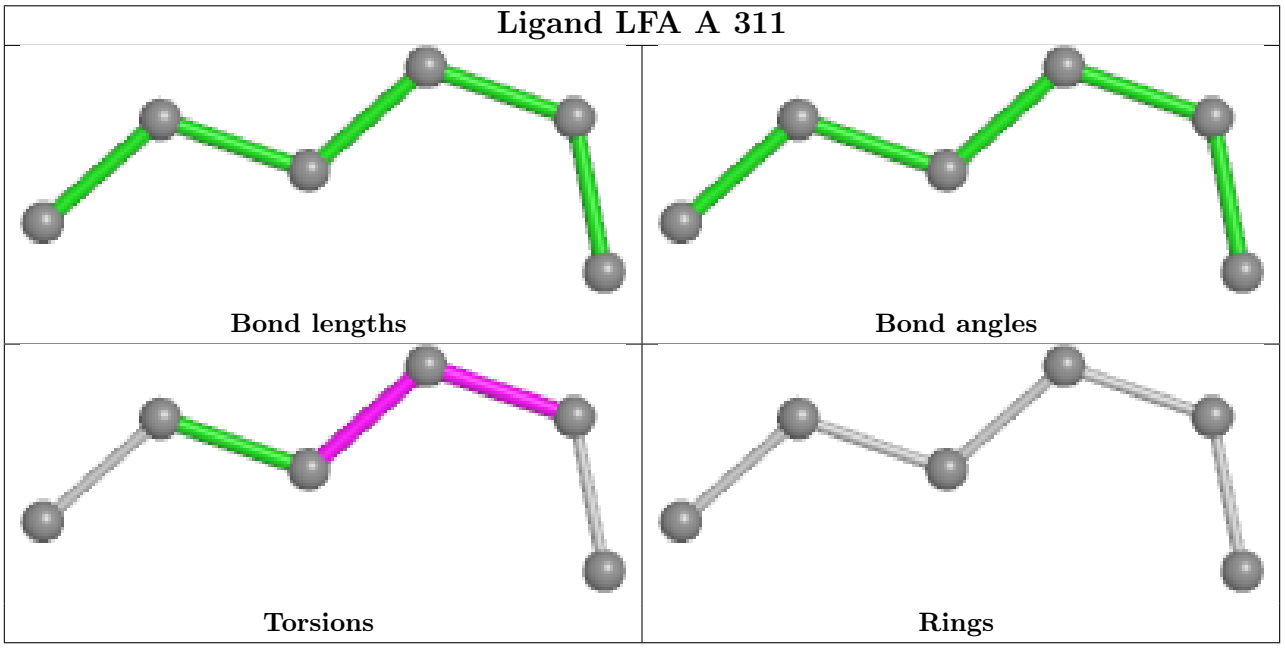
Ligand OLA D 401



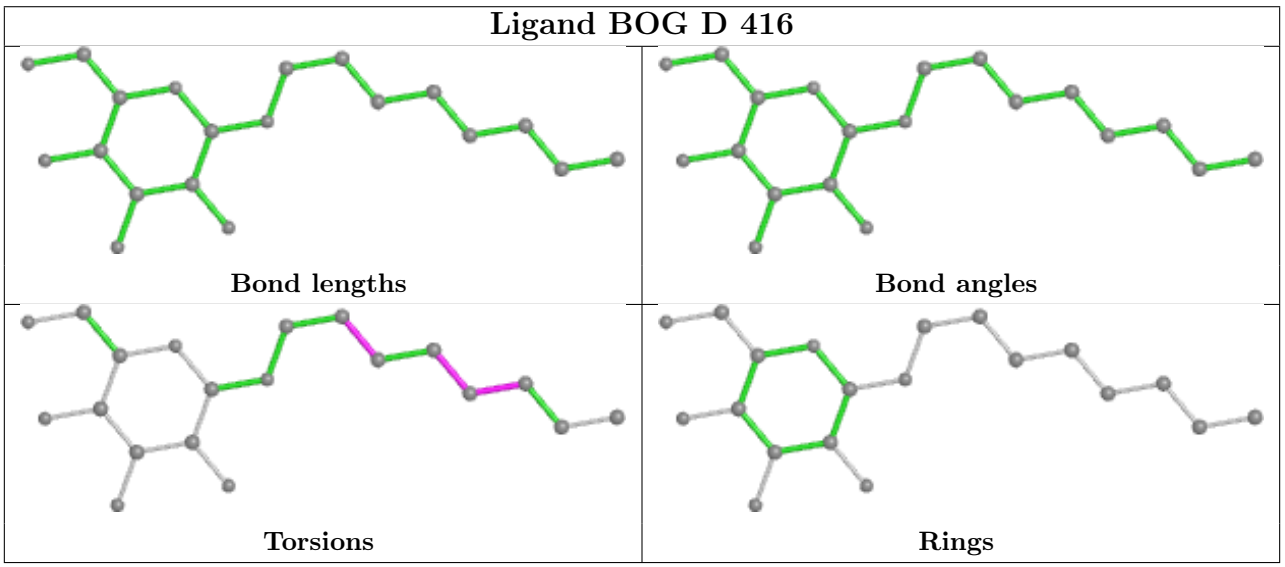
Ligand OLC E 308



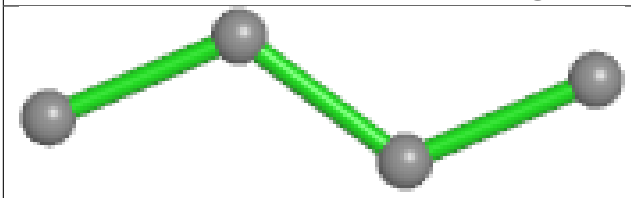
Ligand LFA A 311



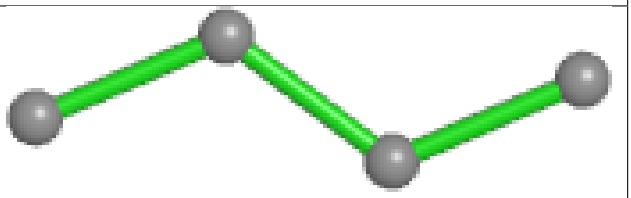
Ligand BOG D 416



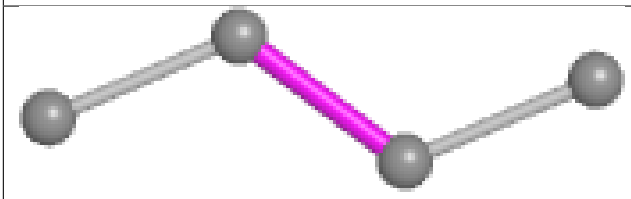
Ligand LFA E 312



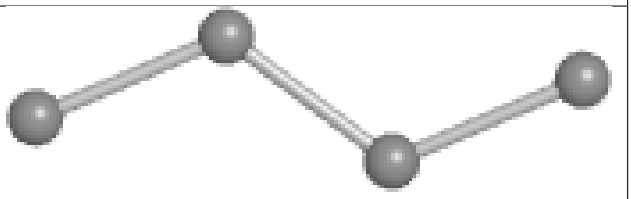
Bond lengths



Bond angles

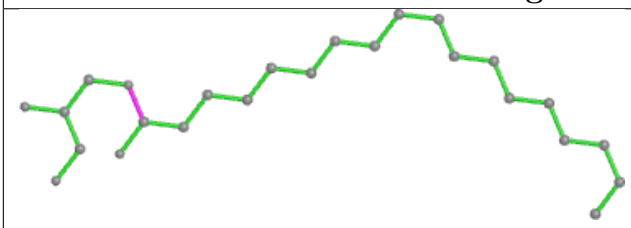


Torsions

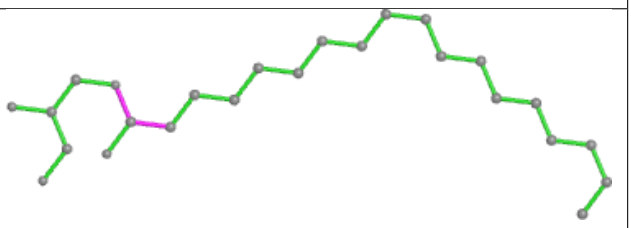


Rings

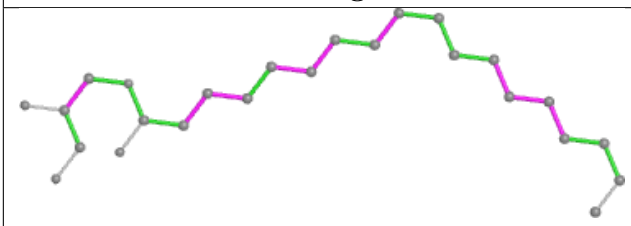
Ligand OLC E 303



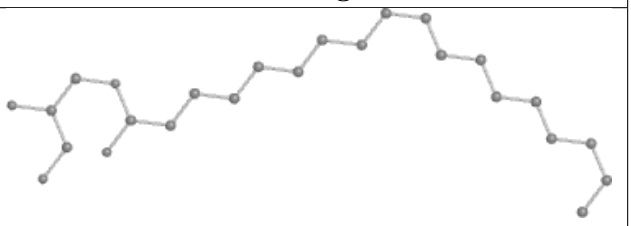
Bond lengths



Bond angles

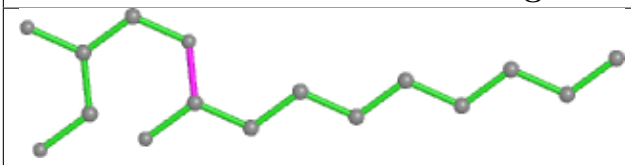


Torsions

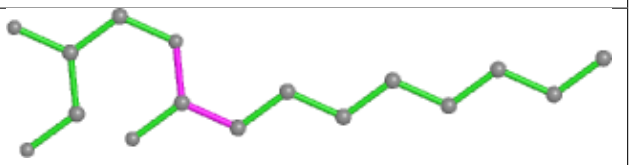


Rings

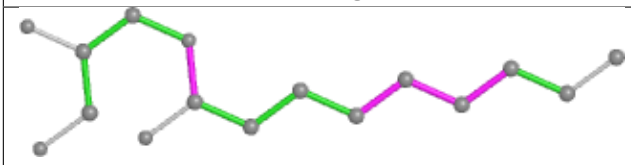
Ligand OLC C 306



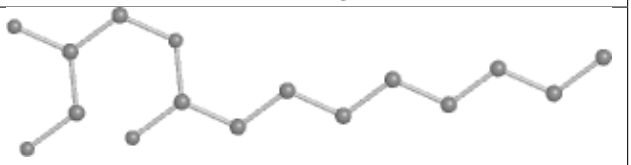
Bond lengths



Bond angles

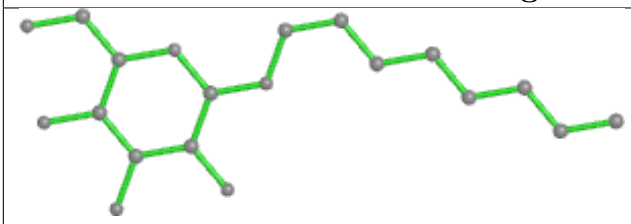


Torsions

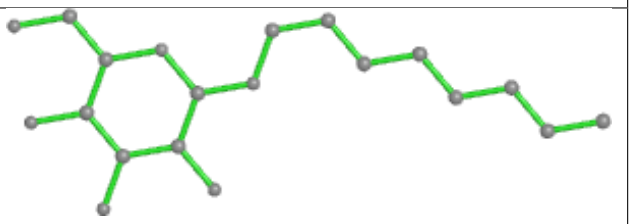


Rings

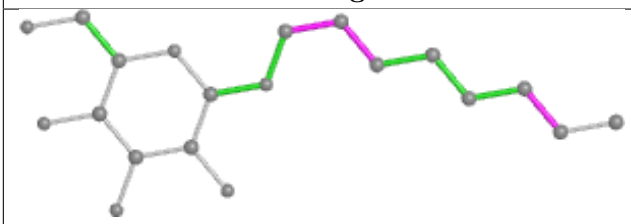
Ligand BOG A 314



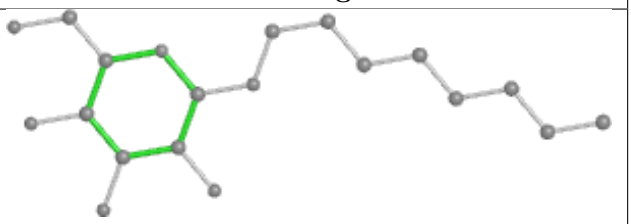
Bond lengths



Bond angles

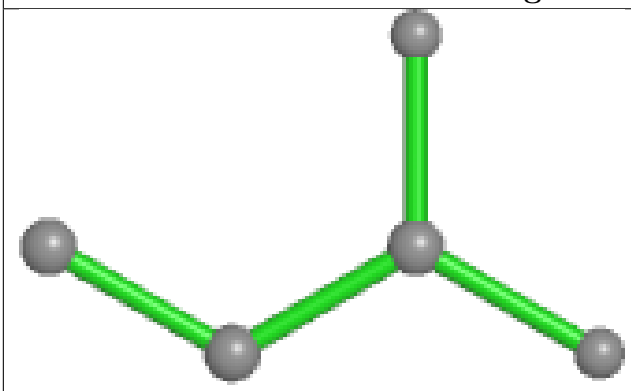


Torsions

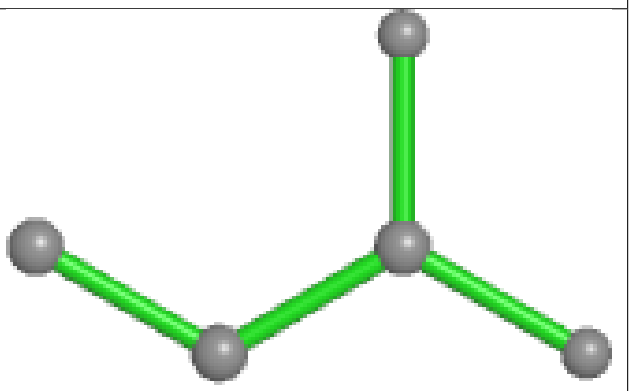


Rings

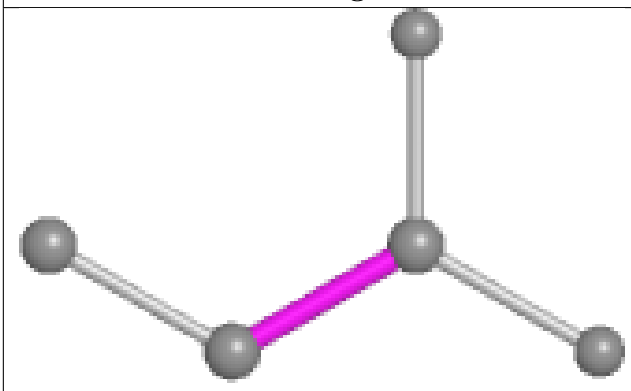
Ligand OLA B 317



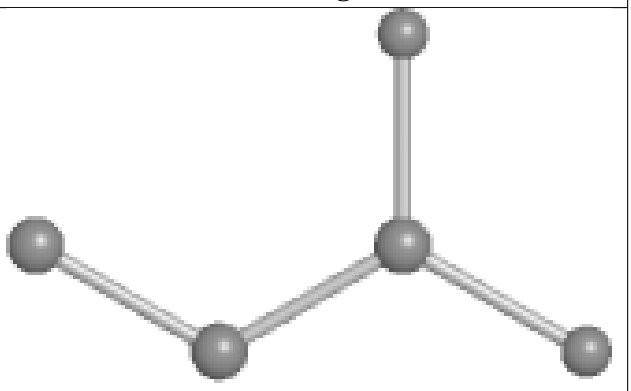
Bond lengths



Bond angles

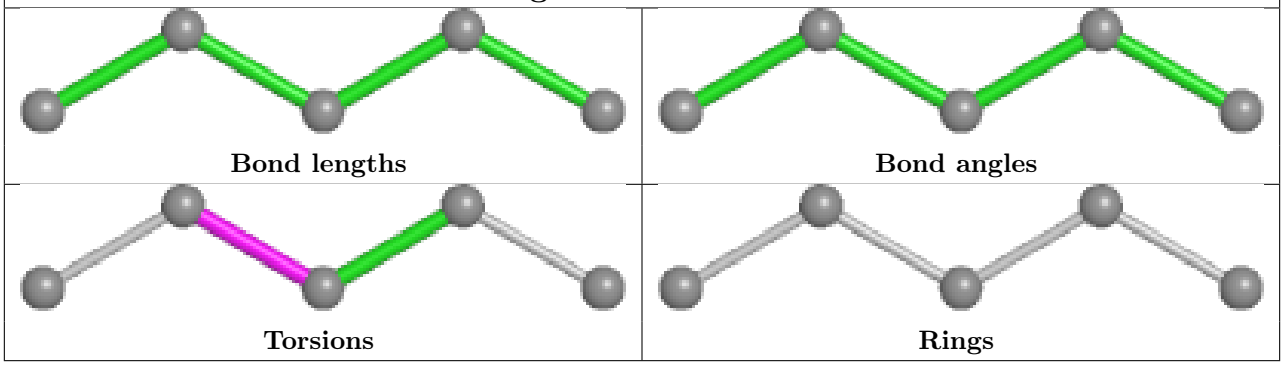


Torsions

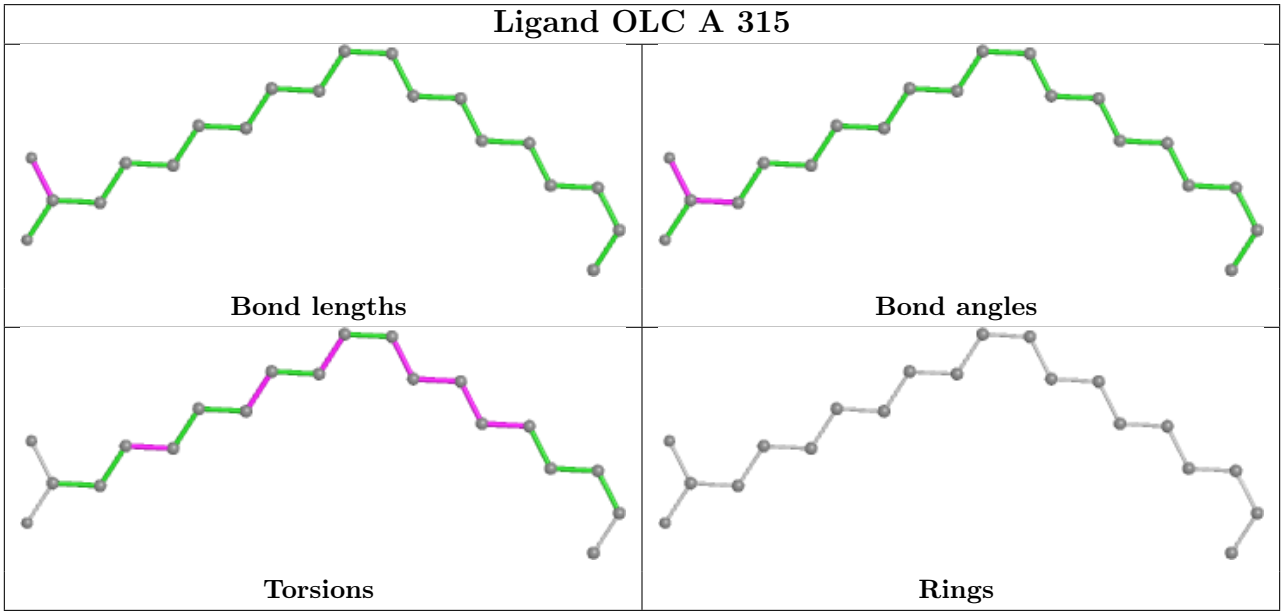


Rings

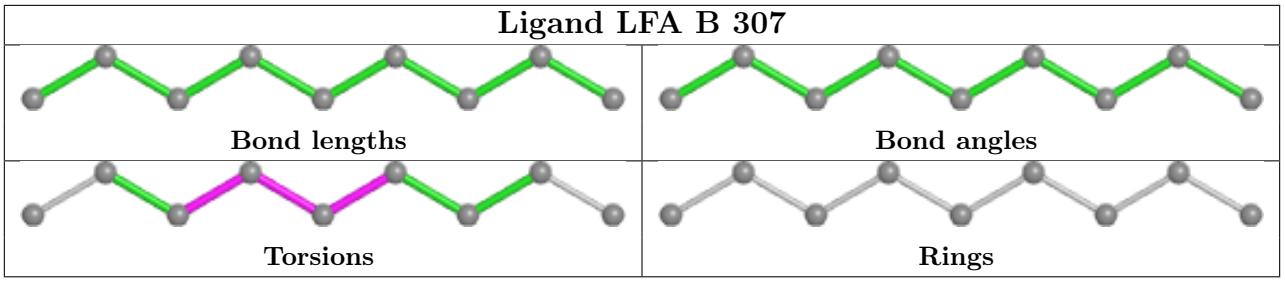
Ligand LFA E 313



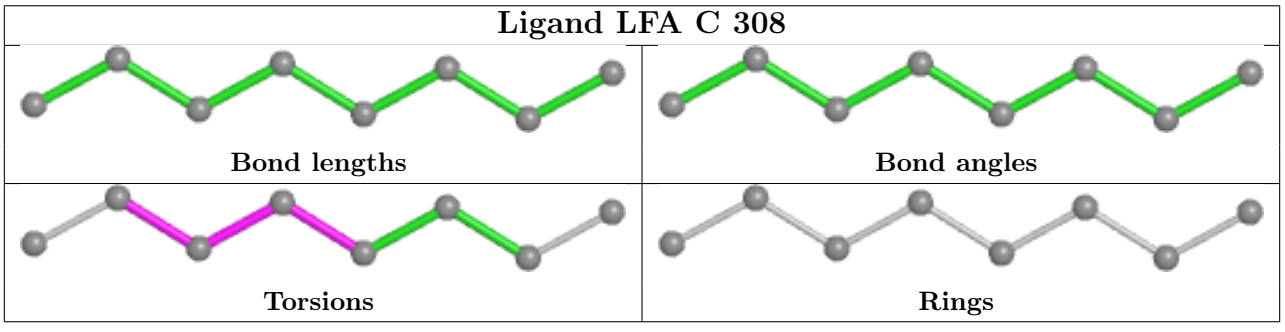
Ligand OLC A 315



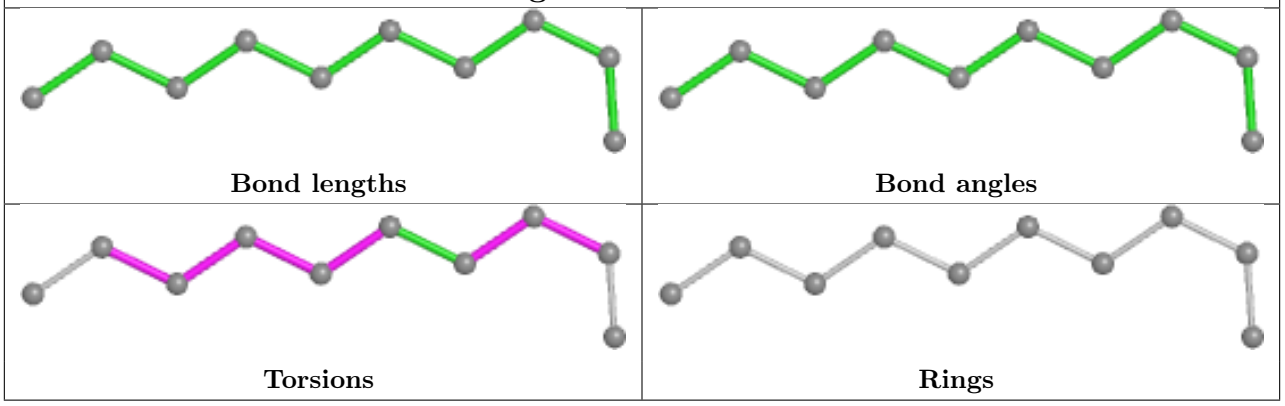
Ligand LFA B 307



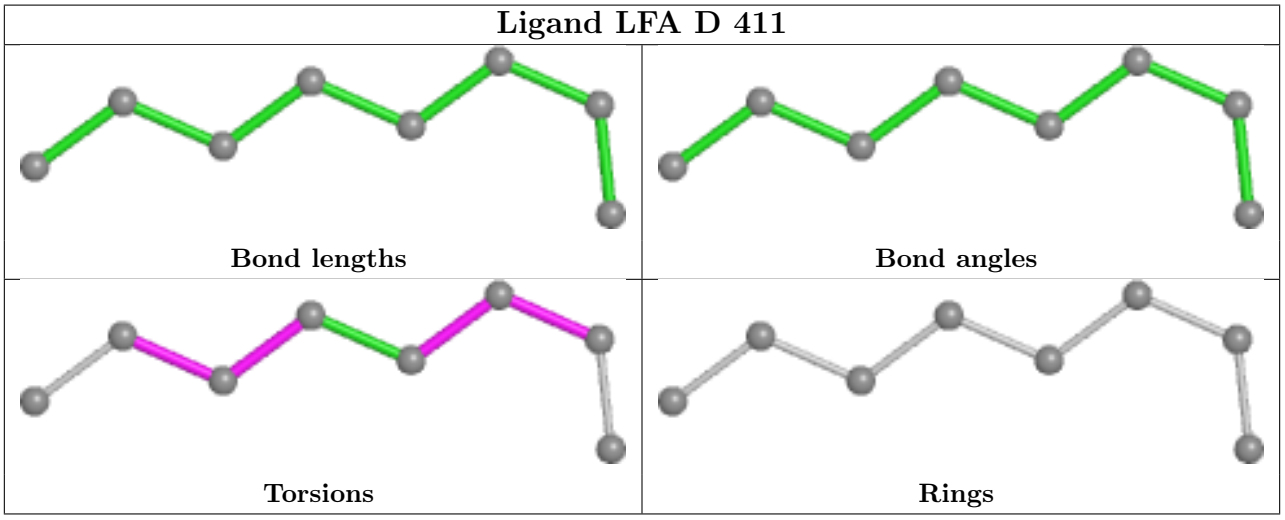
Ligand LFA C 308



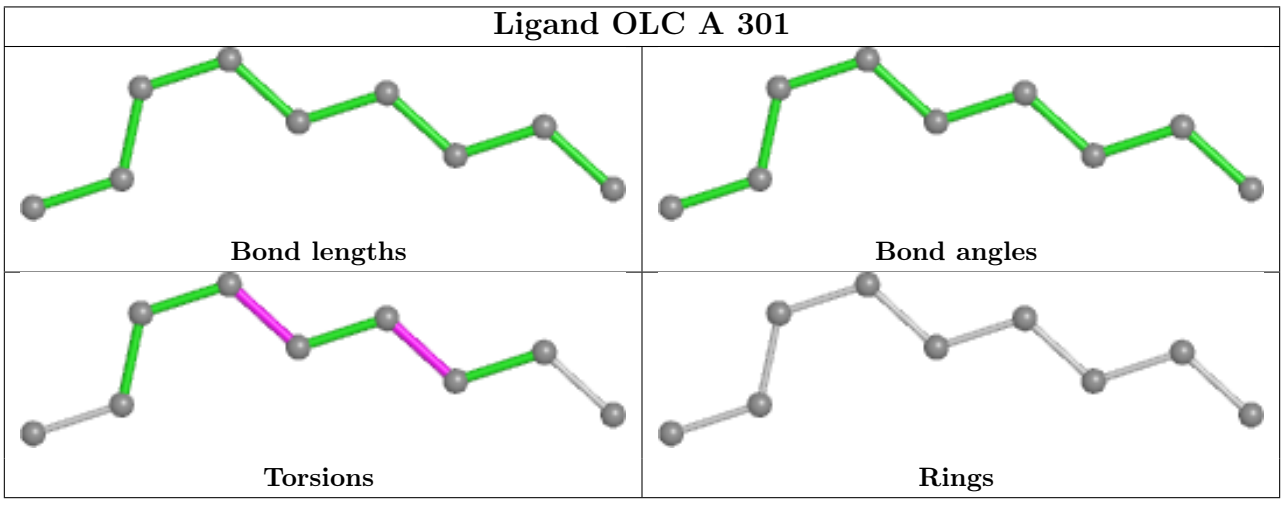
Ligand LFA B 309



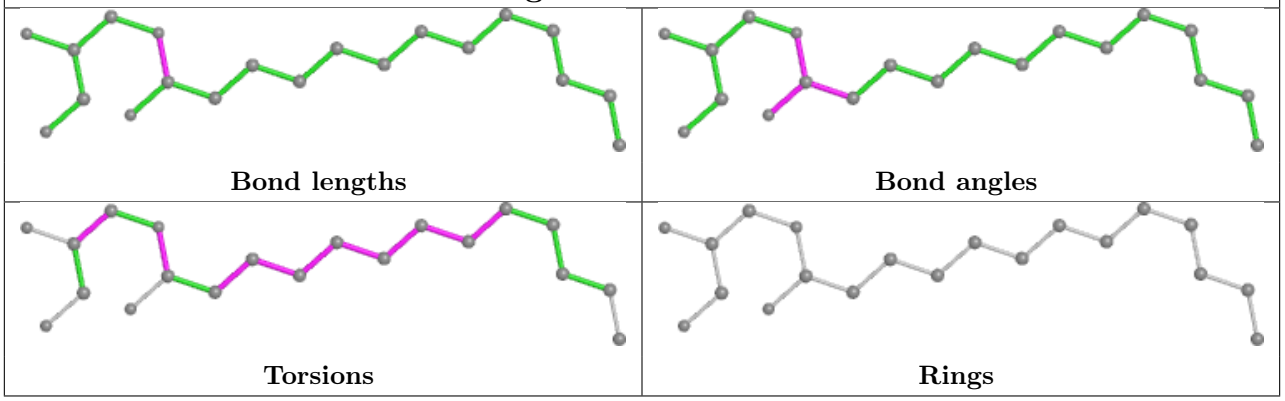
Ligand LFA D 411



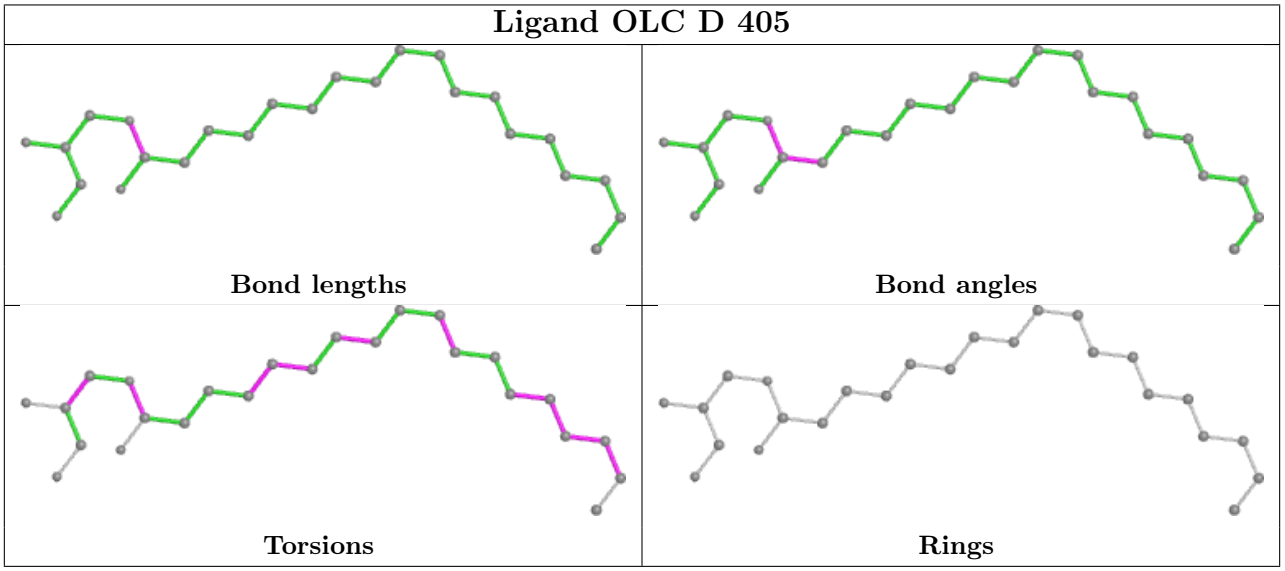
Ligand OLC A 301



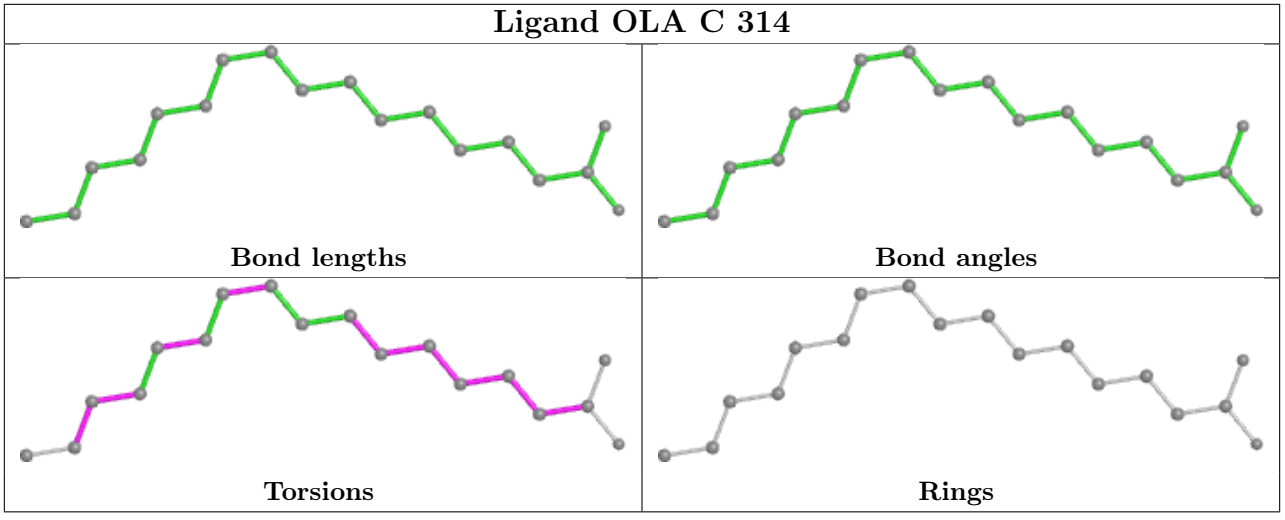
Ligand OLC C 301



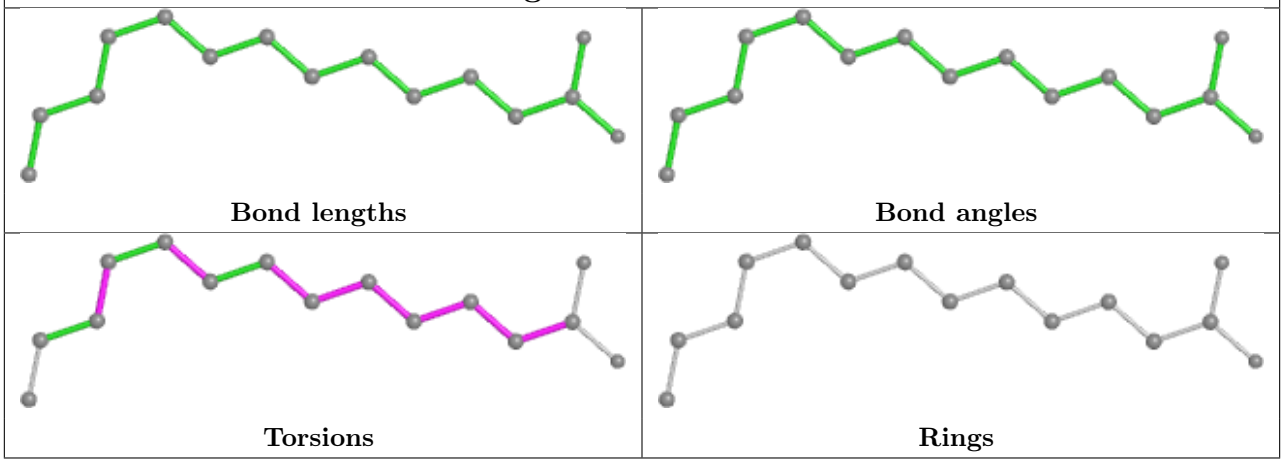
Ligand OLC D 405



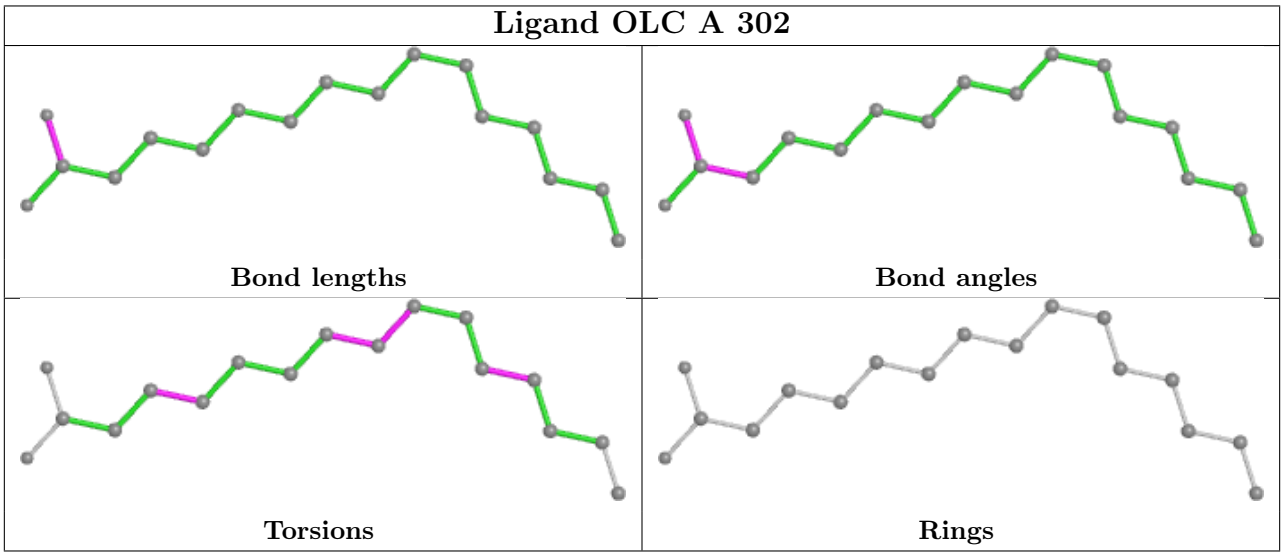
Ligand OLA C 314



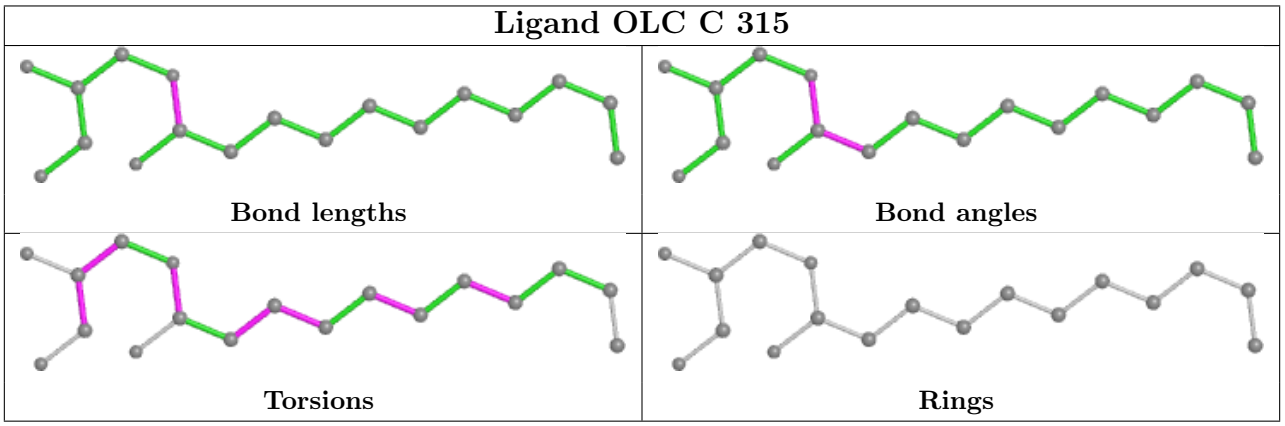
Ligand OLA D 403



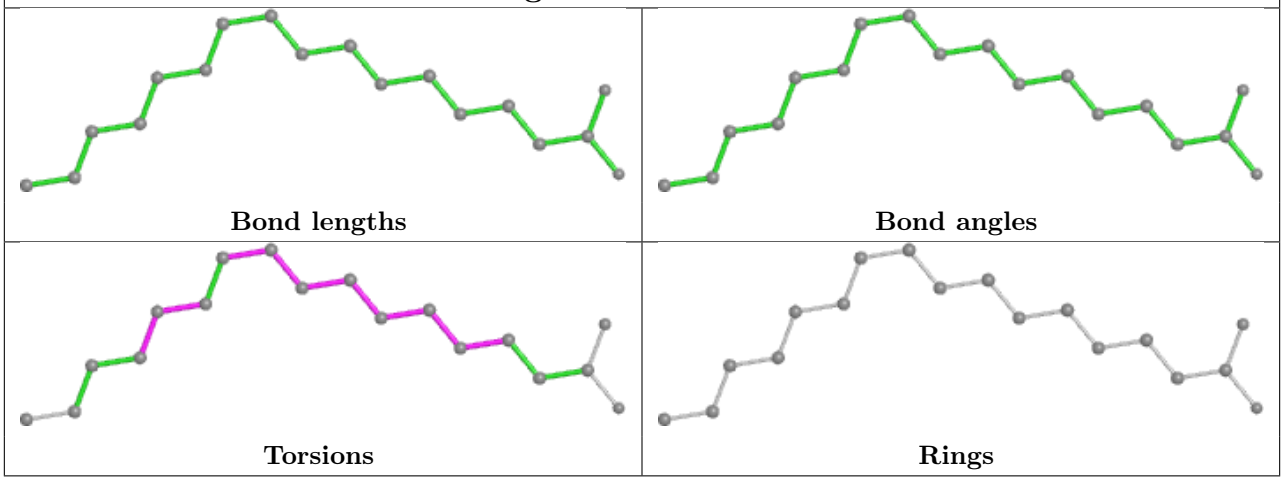
Ligand OLC A 302



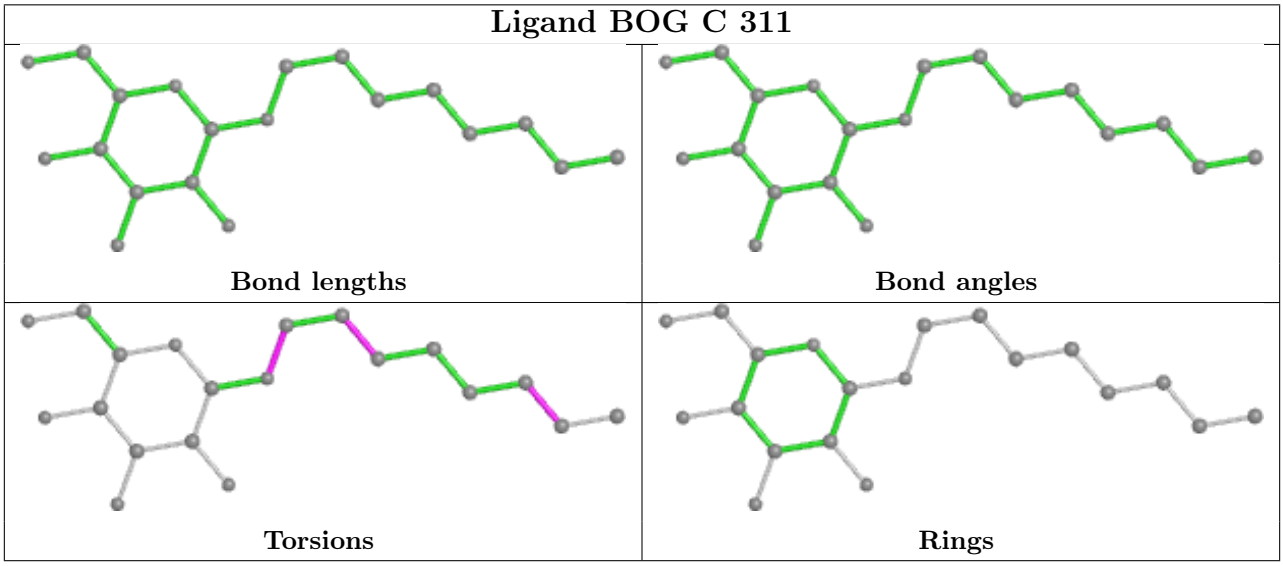
Ligand OLC C 315



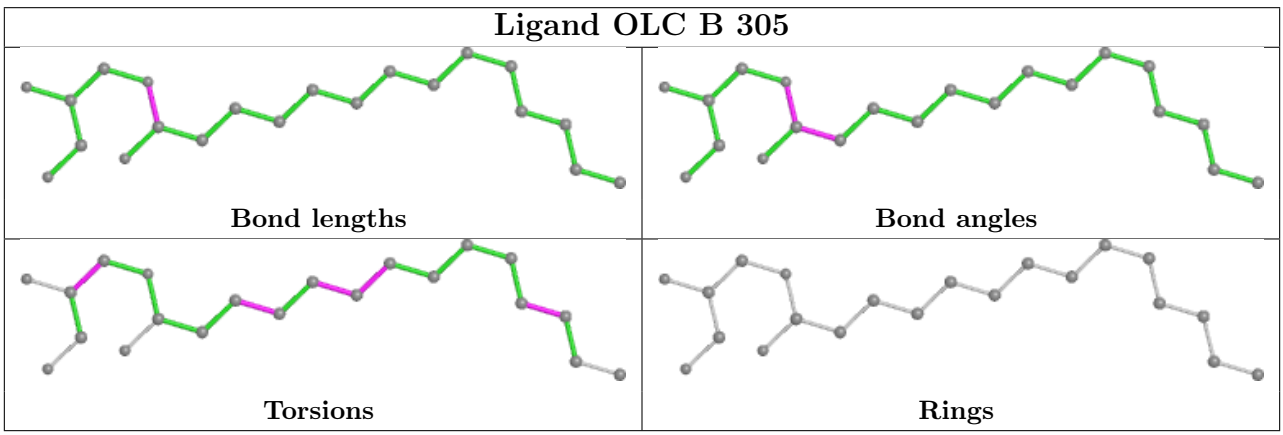
Ligand OLA C 312



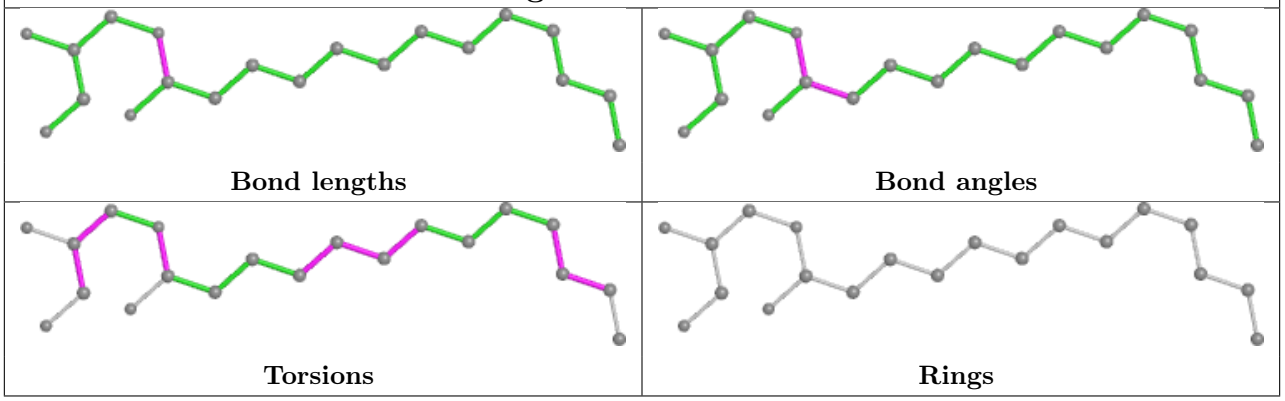
Ligand BOG C 311



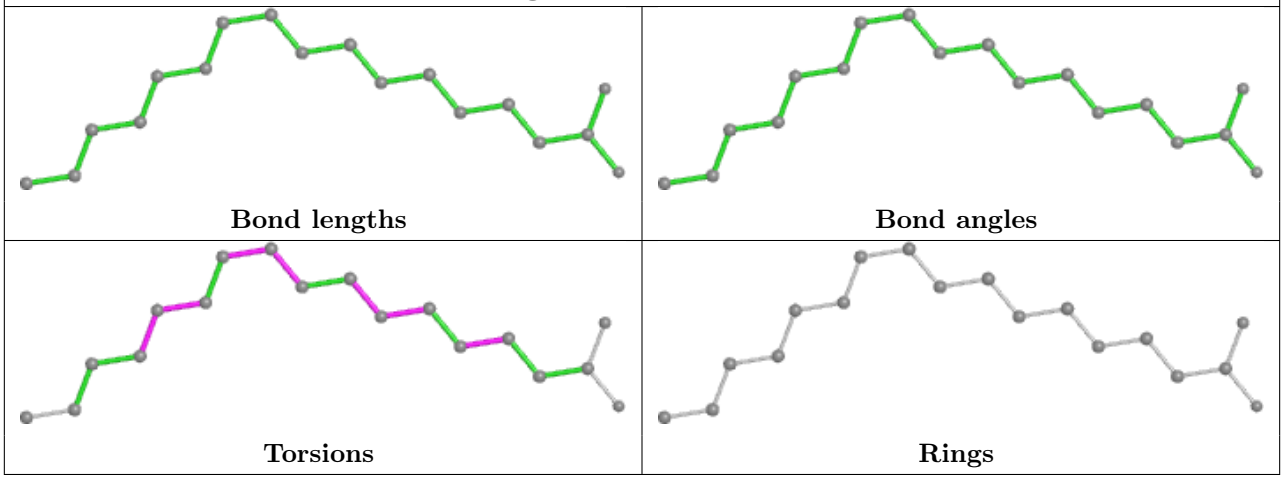
Ligand OLC B 305



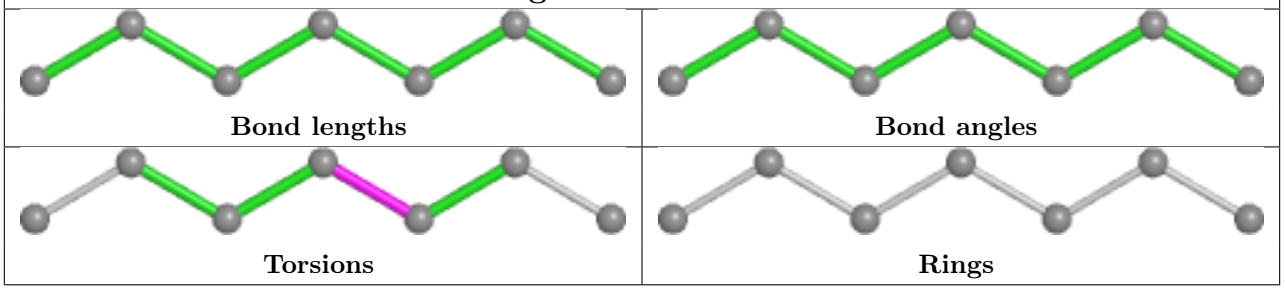
Ligand OLC E 306



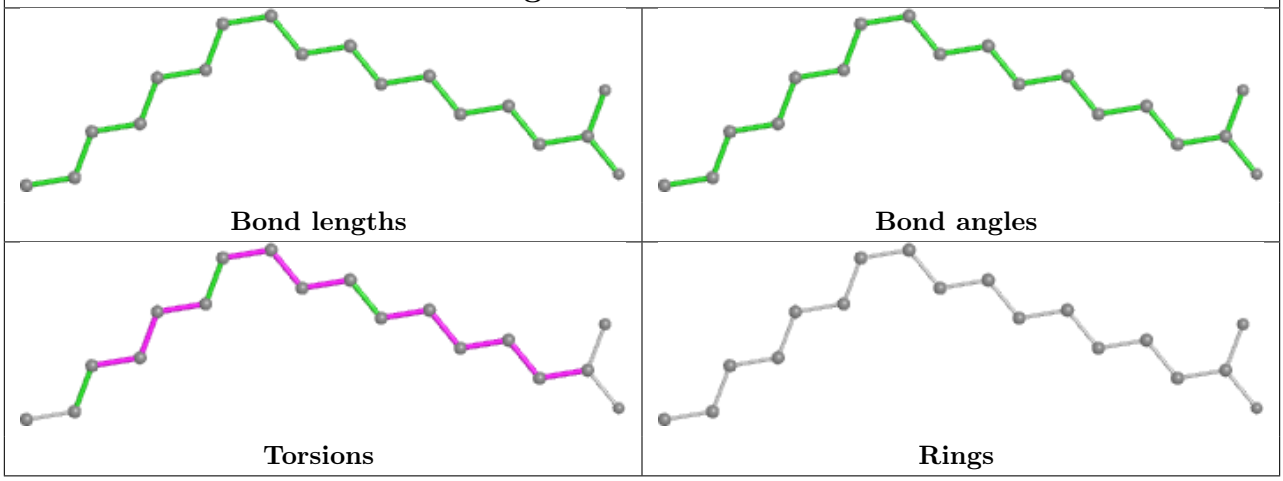
Ligand OLA D 417



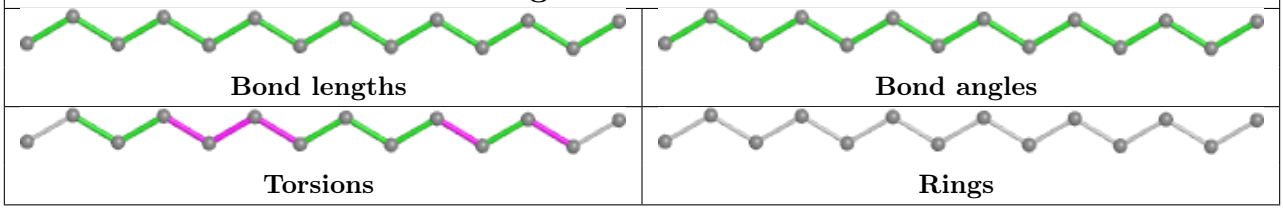
Ligand LFA B 310



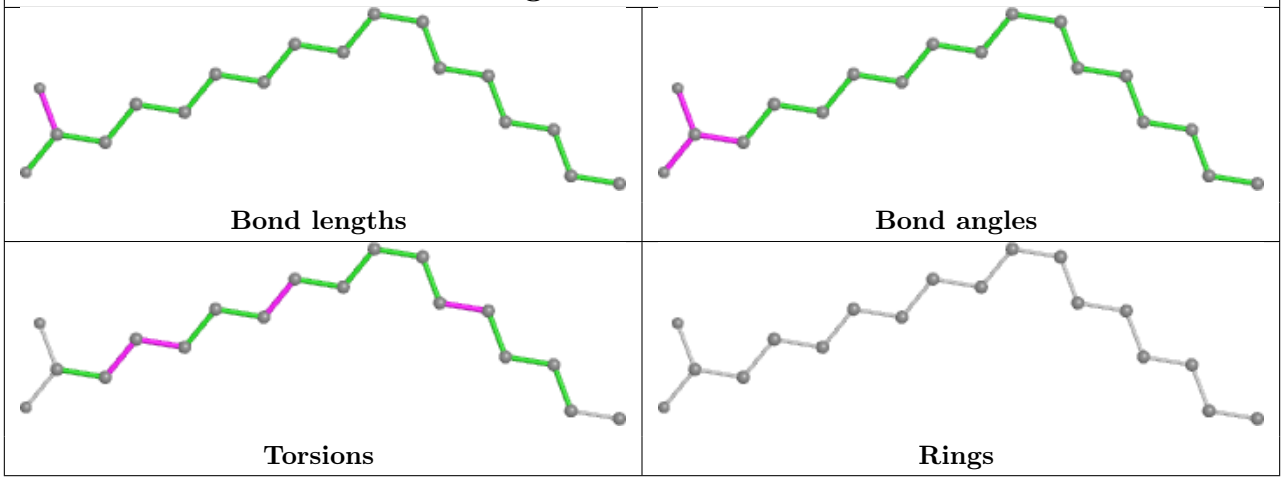
Ligand OLA A 317



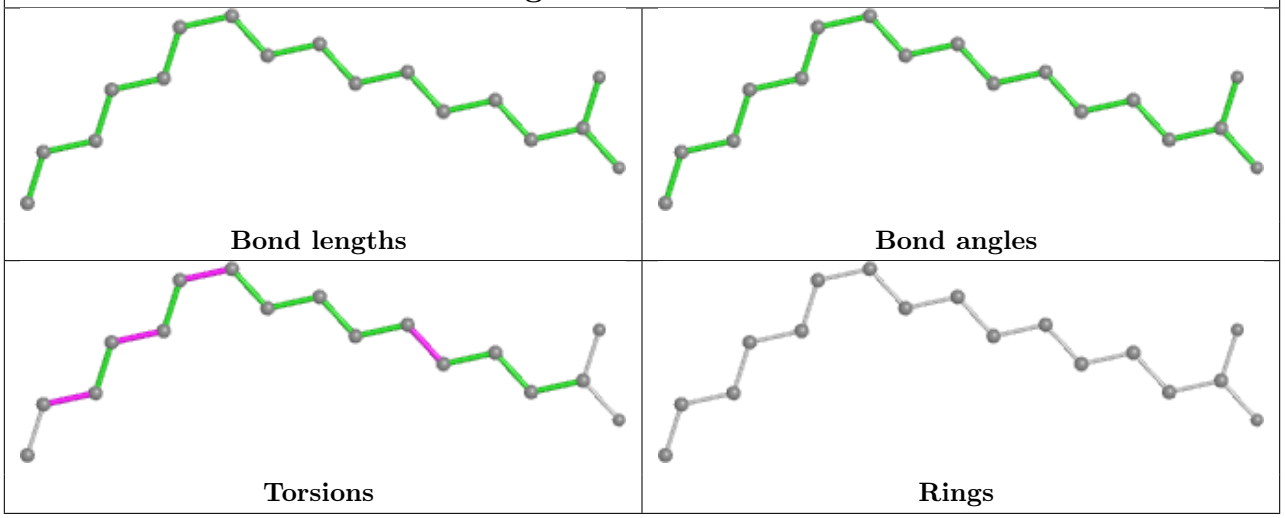
Ligand LFA E 311



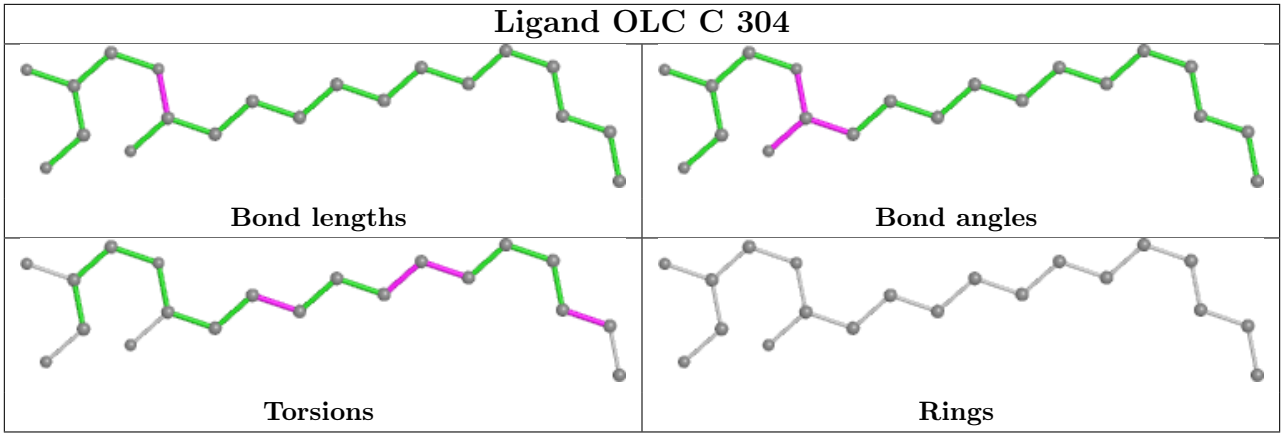
Ligand OLC D 407



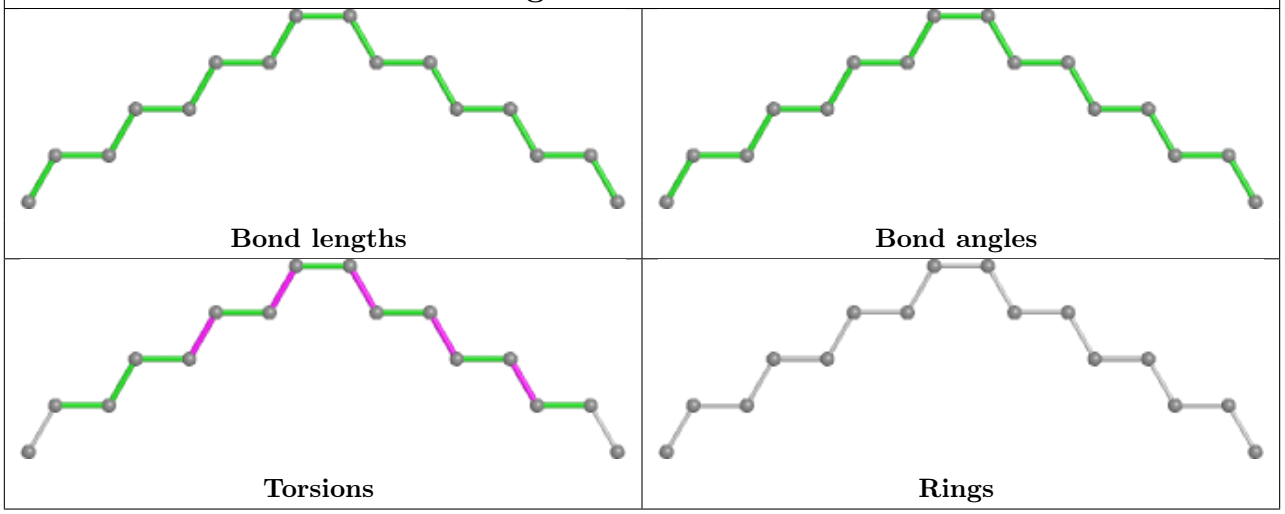
Ligand OLA B 315



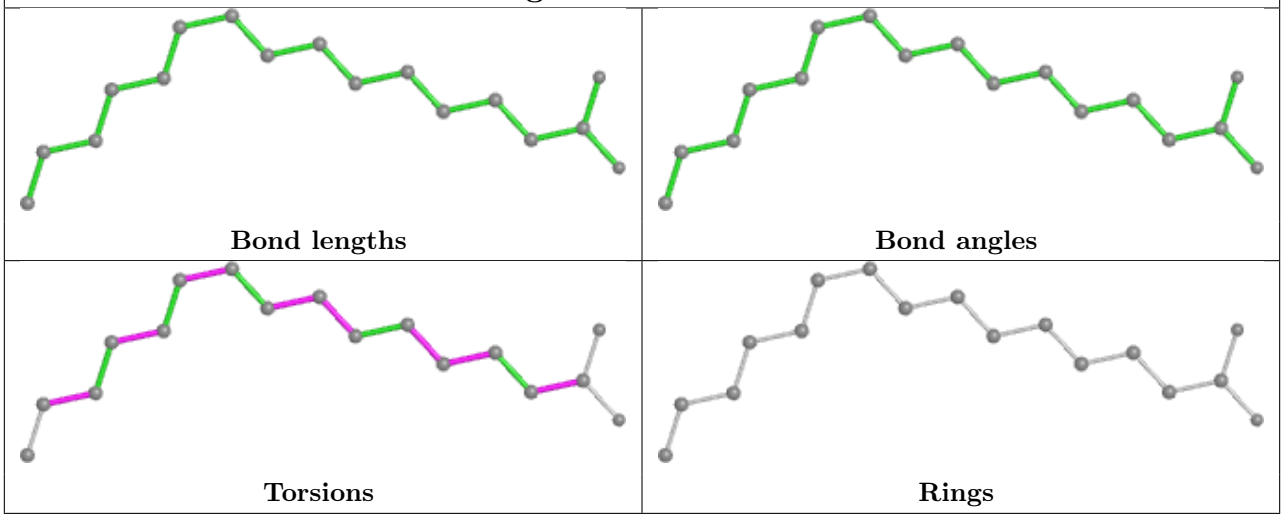
Ligand OLC C 304



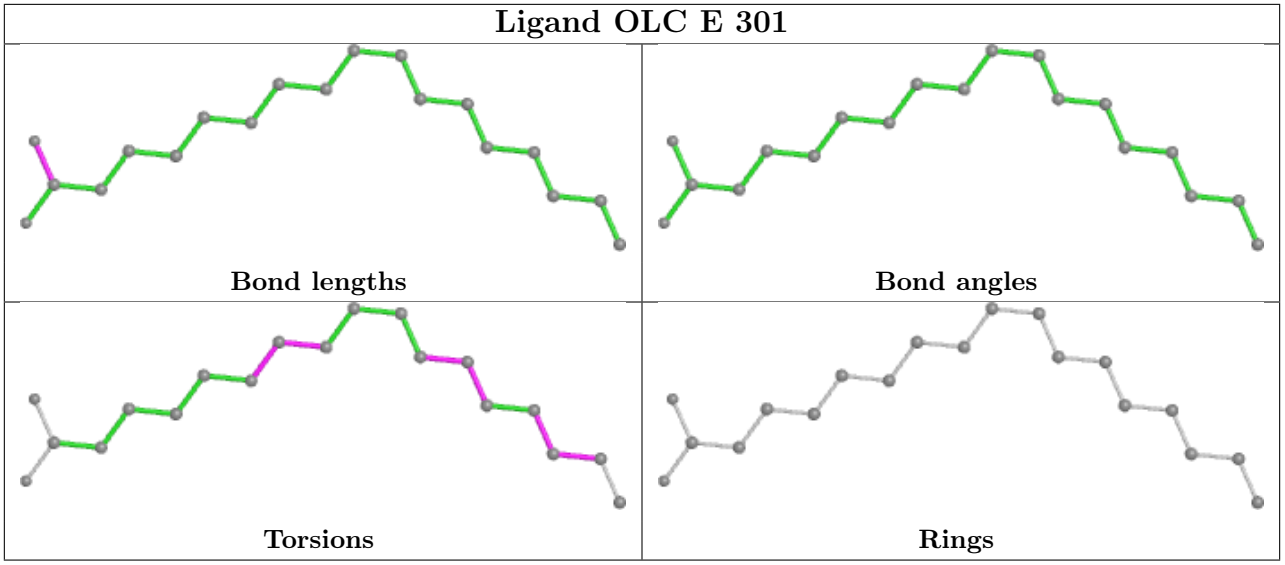
Ligand OLC E 305



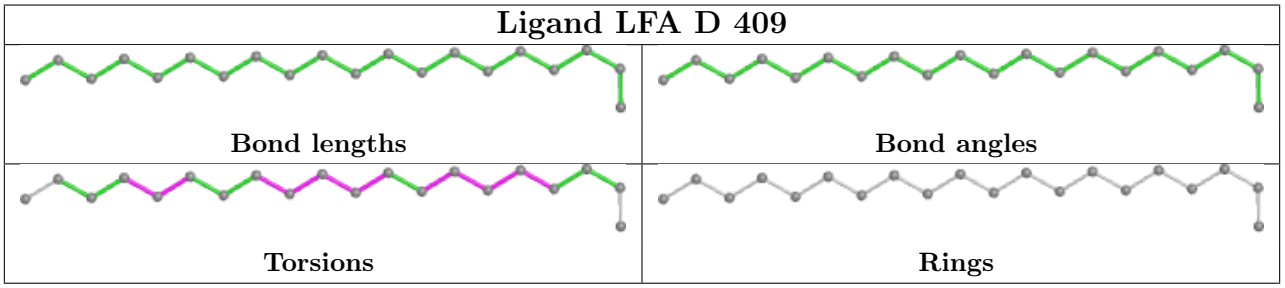
Ligand OLA E 317



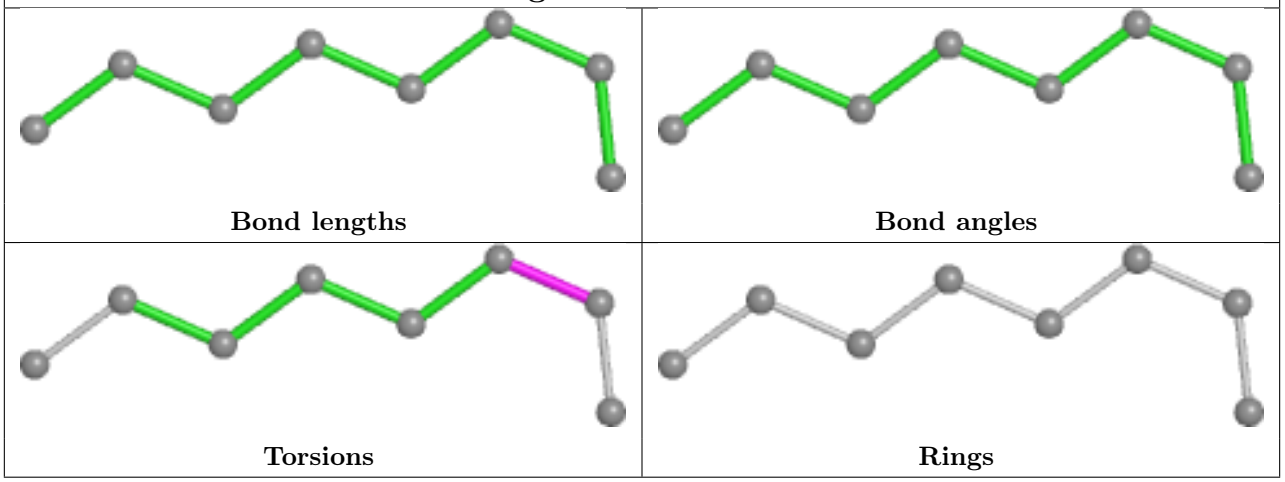
Ligand OLC E 301



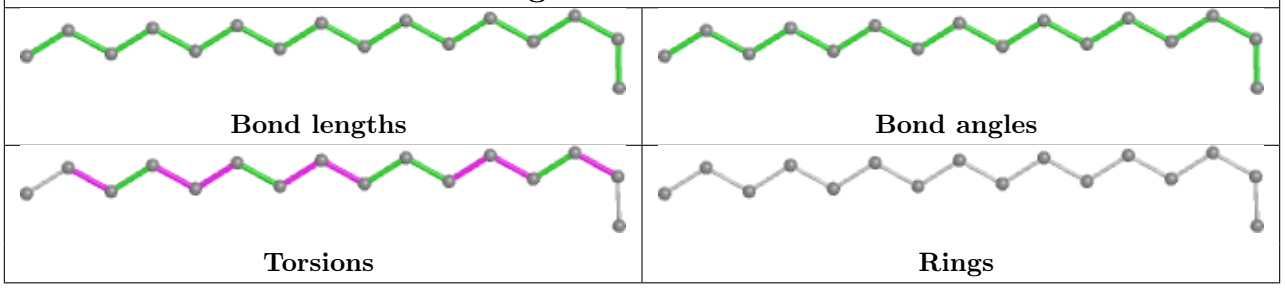
Ligand LFA D 409



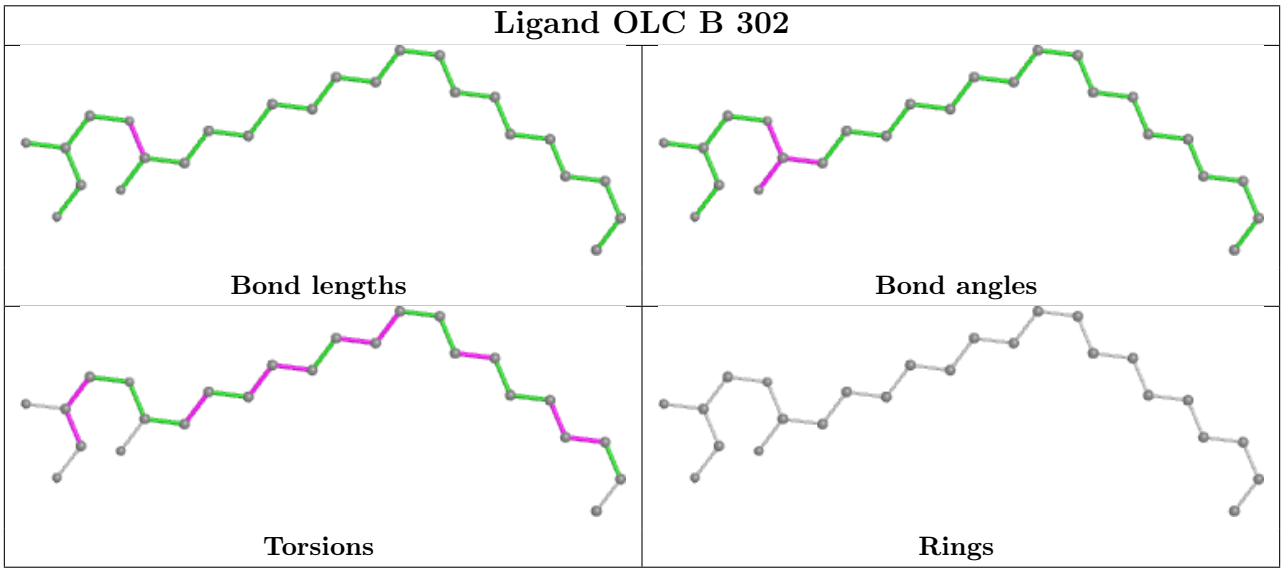
Ligand LFA A 308



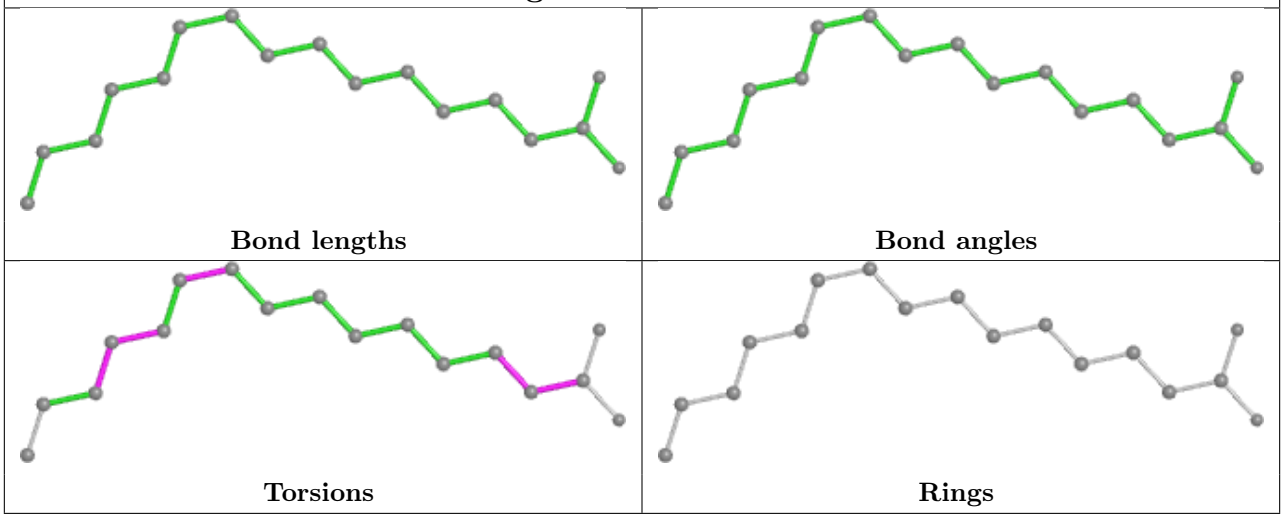
Ligand LFA A 312



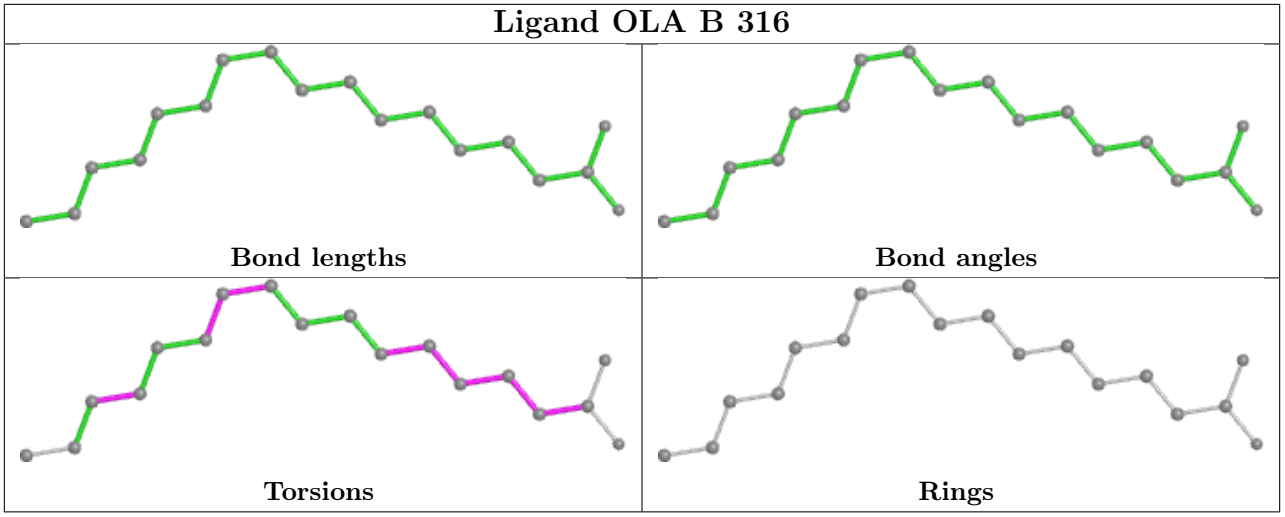
Ligand OLC B 302



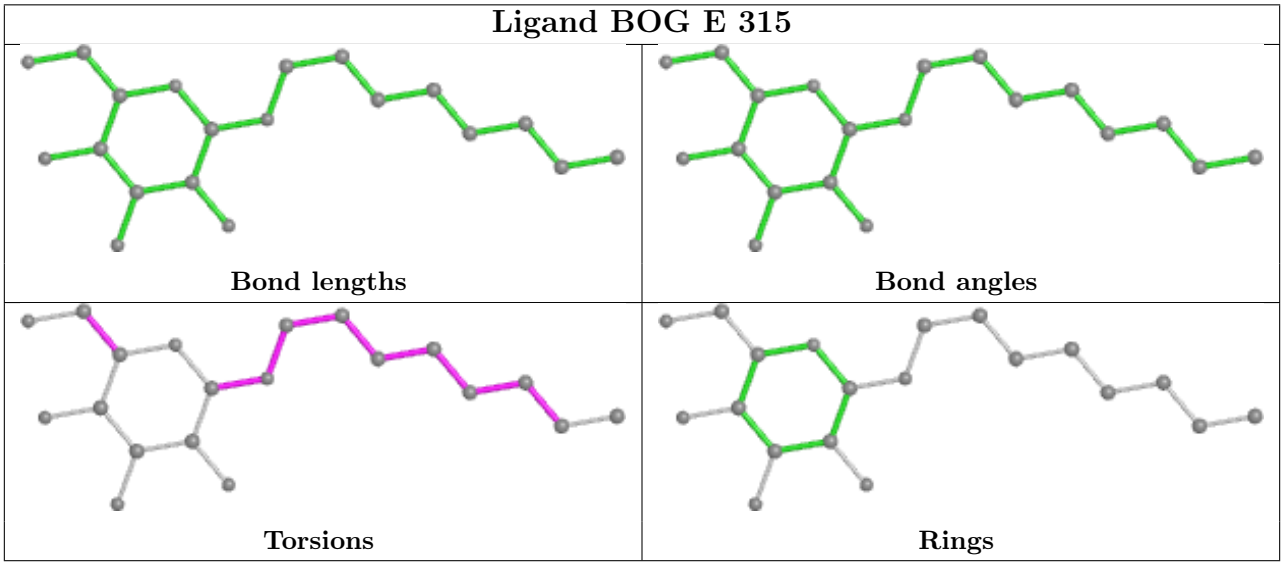
Ligand OLA E 302



Ligand OLA B 316



Ligand BOG E 315



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	269/273 (98%)	0.63	41 (15%)	2 3	46, 56, 75, 123	0
1	B	271/273 (99%)	0.50	30 (11%)	5 7	44, 56, 81, 143	0
1	C	272/273 (99%)	0.53	36 (13%)	3 4	45, 55, 82, 160	0
1	D	269/273 (98%)	0.63	40 (14%)	2 3	45, 56, 83, 140	0
1	E	269/273 (98%)	0.60	34 (12%)	3 5	46, 56, 76, 115	0
All	All	1350/1365 (98%)	0.58	181 (13%)	3 4	44, 56, 80, 160	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	LEU	6.9
1	A	272	ASN	6.4
1	A	40	LEU	6.4
1	D	272	ASN	6.4
1	C	73	LEU	6.2
1	E	40	LEU	6.2
1	B	73	LEU	6.1
1	D	40	LEU	6.1
1	A	76	TYR	6.1
1	C	273	LYS	6.1
1	E	272	ASN	6.0
1	E	43	LEU	5.9
1	E	72	PHE	5.9
1	A	72	PHE	5.9
1	D	73	LEU	5.8
1	B	72	PHE	5.8
1	B	40	LEU	5.8
1	E	73	LEU	5.7
1	C	272	ASN	5.7
1	A	43	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	43	LEU	5.5
1	D	69	VAL	5.4
1	C	76	TYR	5.4
1	D	72	PHE	5.3
1	B	273	LYS	5.3
1	C	72	PHE	5.3
1	C	40	LEU	5.2
1	D	76	TYR	5.2
1	B	272	ASN	5.2
1	B	76	TYR	5.1
1	E	44	LEU	5.1
1	A	69	VAL	5.0
1	B	69	VAL	5.0
1	C	69	VAL	4.9
1	B	274	GLU	4.8
1	A	36	TYR	4.8
1	A	230	VAL	4.8
1	E	76	TYR	4.7
1	C	74	LEU	4.7
1	D	38	VAL	4.5
1	C	44	LEU	4.4
1	D	230	VAL	4.4
1	D	131	THR	4.3
1	C	43	LEU	4.3
1	E	69	VAL	4.3
1	E	36	TYR	4.3
1	D	36	TYR	4.2
1	C	230	VAL	4.2
1	A	77	ALA	4.2
1	D	271	LYS	4.1
1	E	37	ALA	4.1
1	A	74	LEU	4.1
1	D	130	LEU	4.1
1	B	36	TYR	4.0
1	D	41	ALA	4.0
1	D	44	LEU	4.0
1	E	74	LEU	3.8
1	B	44	LEU	3.8
1	B	37	ALA	3.8
1	B	43	LEU	3.8
1	D	74	LEU	3.8
1	C	41	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	130	LEU	3.7
1	B	230	VAL	3.7
1	A	37	ALA	3.6
1	A	164	LEU	3.6
1	B	74	LEU	3.6
1	A	38	VAL	3.6
1	B	77	ALA	3.5
1	E	77	ALA	3.5
1	B	75	LEU	3.5
1	B	164	LEU	3.5
1	E	230	VAL	3.4
1	A	203	ILE	3.4
1	A	66	VAL	3.4
1	B	41	ALA	3.3
1	C	132	THR	3.3
1	C	66	VAL	3.3
1	E	65	ALA	3.3
1	D	37	ALA	3.3
1	B	38	VAL	3.2
1	C	38	VAL	3.2
1	E	41	ALA	3.2
1	D	132	THR	3.2
1	E	38	VAL	3.2
1	D	65	ALA	3.2
1	A	44	LEU	3.2
1	D	34	LEU	3.2
1	A	39	MET	3.1
1	C	77	ALA	3.1
1	E	39	MET	3.1
1	A	75	LEU	3.1
1	C	274	GLU	3.1
1	B	79	ALA	3.0
1	A	33	THR	3.0
1	B	33	THR	3.0
1	A	65	ALA	3.0
1	D	75	LEU	3.0
1	C	75	LEU	3.0
1	C	36	TYR	2.9
1	A	233	PHE	2.9
1	E	34	LEU	2.9
1	A	41	ALA	2.9
1	C	37	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	47	ILE	2.9
1	D	39	MET	2.8
1	A	183	TRP	2.8
1	C	183	TRP	2.8
1	E	79	ALA	2.8
1	B	39	MET	2.8
1	E	71	ALA	2.8
1	C	71	ALA	2.7
1	E	33	THR	2.7
1	C	67	VAL	2.7
1	A	71	ALA	2.7
1	D	71	ALA	2.7
1	E	183	TRP	2.7
1	D	66	VAL	2.6
1	A	79	ALA	2.6
1	C	39	MET	2.6
1	D	67	VAL	2.6
1	E	75	LEU	2.6
1	D	42	GLY	2.6
1	A	68	MET	2.6
1	D	194	GLU	2.6
1	A	198	PRO	2.6
1	C	275	LEU	2.6
1	E	66	VAL	2.5
1	E	47	ILE	2.5
1	D	256	VAL	2.5
1	D	68	MET	2.5
1	A	42	GLY	2.5
1	C	68	MET	2.5
1	C	65	ALA	2.5
1	E	164	LEU	2.5
1	E	68	MET	2.4
1	D	195	GLY	2.4
1	A	47	ILE	2.4
1	D	77	ALA	2.4
1	D	70	SER	2.4
1	B	71	ALA	2.4
1	C	70	SER	2.4
1	D	115	ILE	2.4
1	C	47	ILE	2.3
1	E	42	GLY	2.3
1	D	33	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	202	LYS	2.3
1	C	34	LEU	2.3
1	A	34	LEU	2.3
1	A	138	VAL	2.3
1	E	67	VAL	2.3
1	A	70	SER	2.3
1	C	196	ILE	2.3
1	B	68	MET	2.2
1	A	200	GLY	2.2
1	B	35	GLY	2.2
1	B	183	TRP	2.2
1	D	79	ALA	2.2
1	C	135	PHE	2.2
1	B	67	VAL	2.2
1	A	229	GLY	2.2
1	E	198	PRO	2.2
1	A	67	VAL	2.2
1	D	133	SER	2.2
1	C	42	GLY	2.2
1	D	233	PHE	2.2
1	B	231	ASP	2.2
1	D	231	ASP	2.2
1	E	133	SER	2.2
1	B	34	LEU	2.1
1	A	163	ASN	2.1
1	E	131	THR	2.1
1	E	202	LYS	2.1
1	B	65	ALA	2.1
1	A	270	SER	2.0
1	D	136	SER	2.0
1	C	164	LEU	2.0
1	E	70	SER	2.0
1	A	130	LEU	2.0
1	C	131	THR	2.0
1	A	256	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	LYR	C	255	29/30	0.89	0.14	48,57,67,78	0
1	LYR	A	255	29/30	0.90	0.17	46,56,64,66	0
1	LYR	B	255	29/30	0.93	0.13	44,54,62,67	0
1	LYR	D	255	29/30	0.94	0.14	48,57,64,72	0
1	LYR	E	255	29/30	0.95	0.14	48,54,63,67	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OLC	D	404	13/25	0.32	0.51	109,125,161,171	0
6	OLA	B	316	18/20	0.43	0.78	70,89,105,109	0
3	LFA	A	316	9/20	0.45	0.53	88,91,100,100	0
6	OLA	B	317	5/20	0.48	1.17	115,128,145,169	0
6	OLA	D	403	15/20	0.52	1.11	89,122,139,142	0
3	LFA	A	309	8/20	0.56	0.27	74,101,109,115	0
3	LFA	B	310	7/20	0.57	0.25	80,87,102,114	0
2	OLC	B	302	25/25	0.58	0.27	76,100,135,139	0
2	OLC	A	305	25/25	0.58	0.33	85,107,125,125	0
3	LFA	A	308	8/20	0.58	0.21	75,88,91,94	0
6	OLA	A	317	18/20	0.60	0.27	79,95,101,119	0
3	LFA	B	309	10/20	0.61	0.20	83,110,119,119	0
6	OLA	C	312	18/20	0.63	0.77	69,79,106,108	0
2	OLC	D	407	18/25	0.63	0.33	68,101,114,115	0
2	OLC	D	405	25/25	0.64	0.32	91,107,119,126	0
3	LFA	D	413	7/20	0.65	0.21	86,93,102,115	0
2	OLC	A	303	25/25	0.65	0.50	90,115,138,151	0
2	OLC	C	303	22/25	0.65	0.35	83,107,131,143	0
2	OLC	B	305	21/25	0.66	0.39	62,97,127,147	0
6	OLA	E	302	17/20	0.66	0.84	71,84,96,108	0
3	LFA	E	311	14/20	0.67	0.21	83,101,114,116	0
2	OLC	E	309	20/25	0.67	0.52	59,106,129,130	0
6	OLA	C	314	18/20	0.67	0.23	79,94,109,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	OLA	B	315	17/20	0.67	0.71	64,80,95,100	0
3	LFA	E	310	8/20	0.67	0.23	77,93,104,105	0
2	OLC	E	303	25/25	0.68	0.25	74,110,131,134	0
3	LFA	C	307	7/20	0.69	0.36	80,91,96,100	0
2	OLC	B	301	22/25	0.69	0.33	84,116,134,144	0
2	OLC	B	304	20/25	0.69	0.23	72,103,121,131	0
3	LFA	B	308	8/20	0.71	0.23	80,88,103,104	0
6	OLA	E	317	17/20	0.71	0.18	81,93,116,123	0
2	OLC	C	301	20/25	0.72	0.29	88,103,119,122	0
2	OLC	C	305	22/25	0.73	0.47	69,92,117,143	0
3	LFA	A	312	16/20	0.73	0.47	96,108,120,122	0
6	OLA	D	401	20/20	0.73	0.77	67,90,105,112	0
2	OLC	A	304	13/25	0.74	0.22	72,82,102,105	0
3	LFA	D	414	6/20	0.74	0.39	100,109,111,114	0
6	OLA	D	417	18/20	0.76	0.18	77,94,105,106	0
3	LFA	D	409	20/20	0.76	0.20	89,102,113,116	0
3	LFA	D	411	8/20	0.76	0.22	82,88,107,113	0
2	OLC	E	307	15/25	0.77	0.60	85,104,120,142	0
2	OLC	E	305	16/25	0.79	0.29	78,99,107,114	0
6	OLA	B	314	17/20	0.79	0.19	74,92,105,109	0
3	LFA	B	307	9/20	0.79	0.31	88,101,110,118	0
3	LFA	C	308	8/20	0.79	0.20	75,95,98,106	0
2	OLC	A	315	20/25	0.80	0.25	80,100,122,122	0
2	OLC	E	306	20/25	0.80	0.32	77,94,106,110	0
2	OLC	C	302	23/25	0.81	0.26	63,85,120,132	0
3	LFA	A	307	7/20	0.81	0.23	85,90,98,102	0
3	LFA	D	410	20/20	0.82	0.15	87,97,109,111	0
5	BOG	B	312	20/20	0.82	0.37	75,91,102,113	0
5	BOG	E	315	20/20	0.82	0.37	72,92,105,116	0
6	OLA	E	316	7/20	0.83	1.02	94,96,105,114	0
2	OLC	D	406	18/25	0.83	0.26	78,92,119,120	0
5	BOG	A	314	20/20	0.84	0.46	76,91,99,100	0
2	OLC	E	304	8/25	0.84	0.18	84,87,94,95	0
2	OLC	A	302	17/25	0.84	0.23	60,76,96,102	0
2	OLC	B	303	21/25	0.84	0.29	62,86,109,126	0
2	OLC	C	315	18/25	0.84	0.21	84,105,116,134	0
2	OLC	E	308	15/25	0.84	0.18	65,85,93,108	0
2	OLC	A	301	9/25	0.84	0.29	76,84,98,100	0
3	LFA	E	313	5/20	0.84	0.20	75,77,98,102	0
3	LFA	A	310	4/20	0.85	0.36	82,95,97,98	0
6	OLA	A	318	6/20	0.86	1.11	82,98,107,116	0
7	GOL	C	313	4/6	0.86	1.31	85,85,95,101	0

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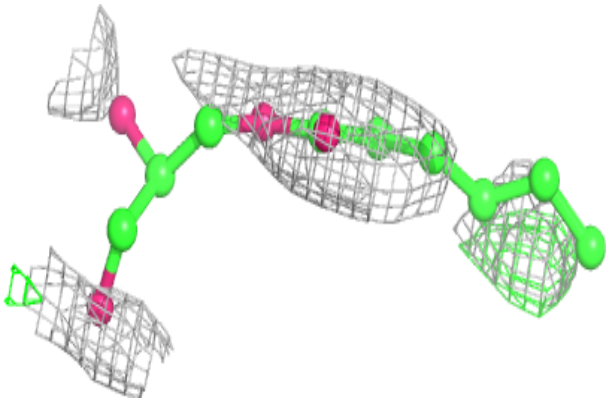
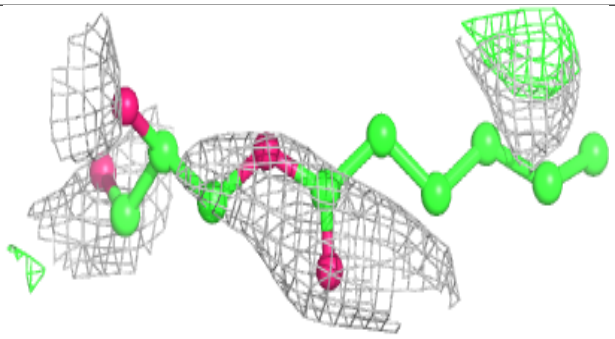
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LFA	D	412	17/20	0.87	0.43	63,80,99,107	0
2	OLC	C	304	20/25	0.87	0.27	76,97,117,117	0
2	OLC	A	306	15/25	0.87	0.20	69,85,111,127	0
2	OLC	C	306	16/25	0.87	0.23	70,89,97,106	0
7	GOL	D	402	4/6	0.87	1.65	94,96,102,107	0
3	LFA	C	309	20/20	0.88	0.17	81,99,112,112	0
5	BOG	D	416	20/20	0.89	0.39	75,85,99,101	0
2	OLC	E	301	19/25	0.89	0.28	65,75,130,136	0
3	LFA	A	311	6/20	0.89	0.14	75,81,86,90	0
2	OLC	D	408	14/25	0.90	0.23	67,85,104,108	0
7	GOL	B	313	4/6	0.90	1.22	83,85,92,96	0
2	OLC	B	306	16/25	0.90	0.22	72,84,89,105	0
5	BOG	C	311	20/20	0.90	0.40	72,88,100,107	0
3	LFA	E	312	4/20	0.92	0.15	79,90,92,106	0
4	NA	B	318	1/1	0.93	0.10	56,56,56,56	0
4	NA	D	418	1/1	0.93	0.14	56,56,56,56	0
4	NA	E	318	1/1	0.94	0.06	61,61,61,61	0
4	NA	A	319	1/1	0.95	0.09	56,56,56,56	0
4	NA	C	316	1/1	0.96	0.13	54,54,54,54	0
4	NA	A	313	1/1	0.97	0.06	53,53,53,53	0
4	NA	C	310	1/1	0.98	0.05	48,48,48,48	0
4	NA	B	311	1/1	0.98	0.04	52,52,52,52	0
4	NA	E	314	1/1	0.99	0.06	49,49,49,49	0
4	NA	D	415	1/1	0.99	0.05	51,51,51,51	0

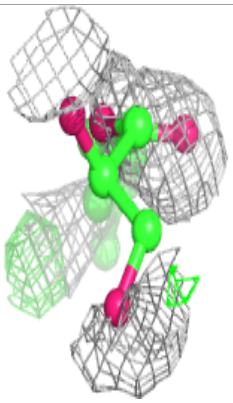
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC D 404:

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

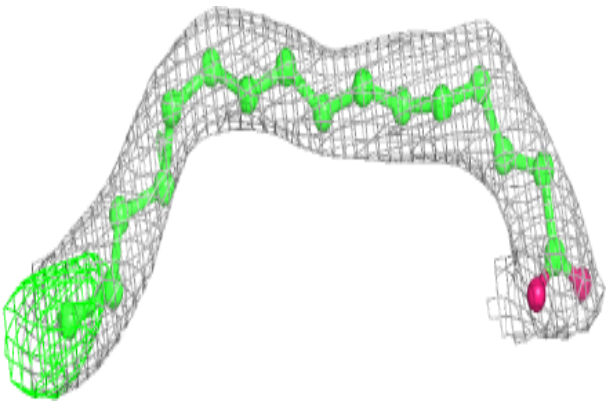


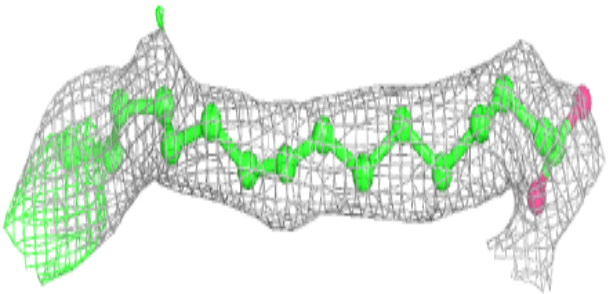


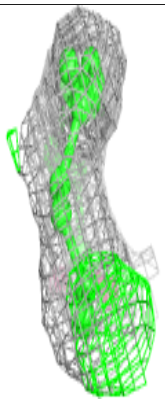


Electron density around OLA B 316:

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

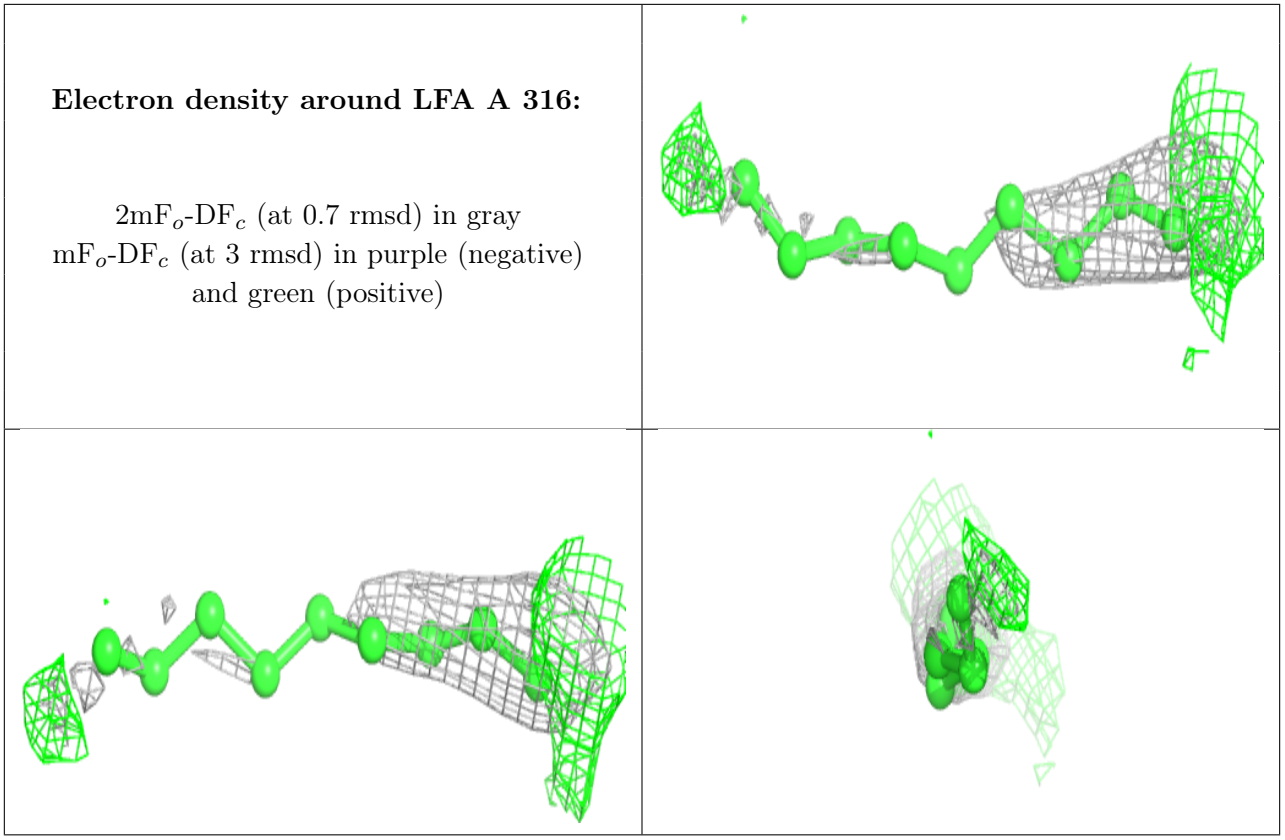






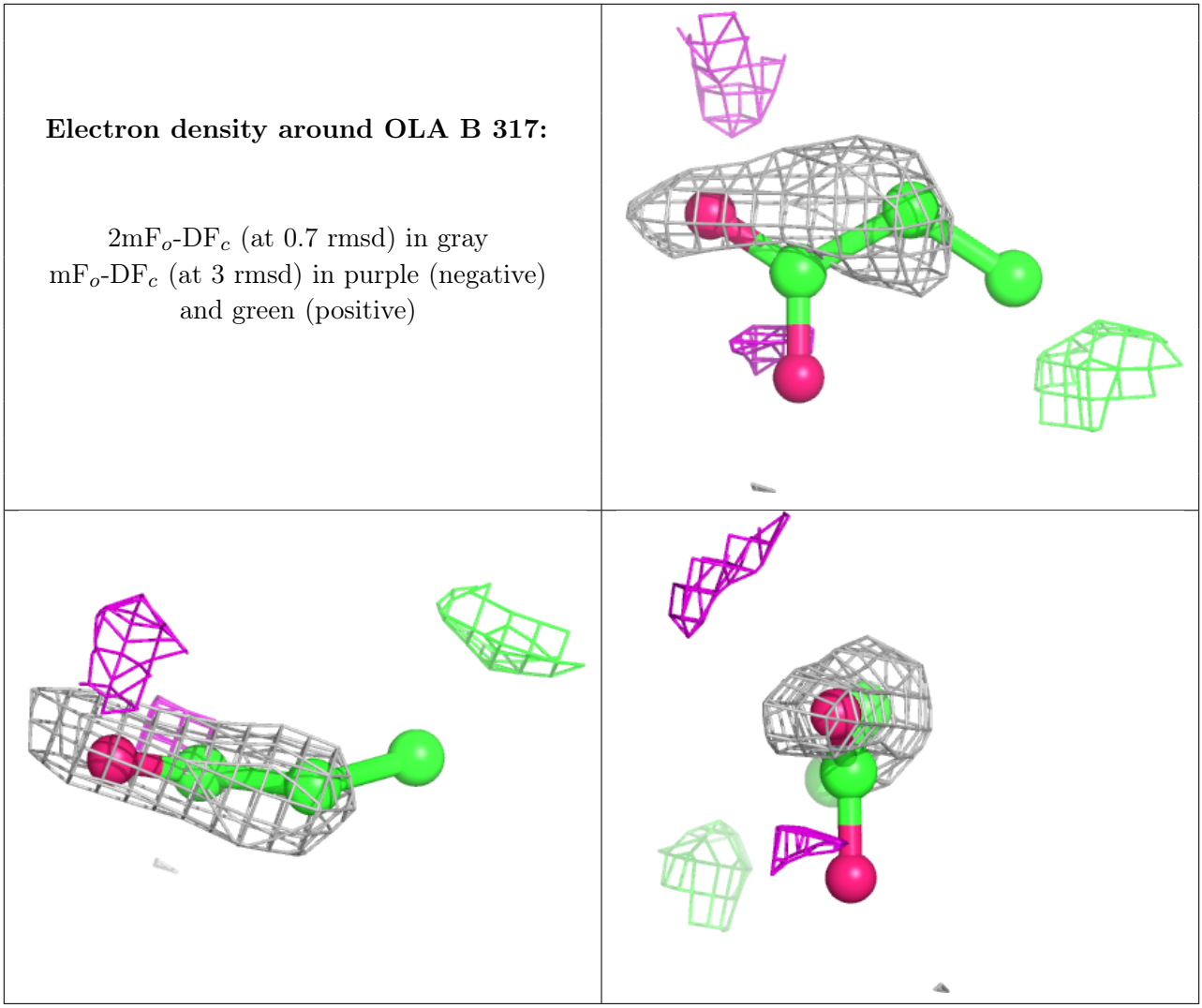
Electron density around LFA A 316:

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



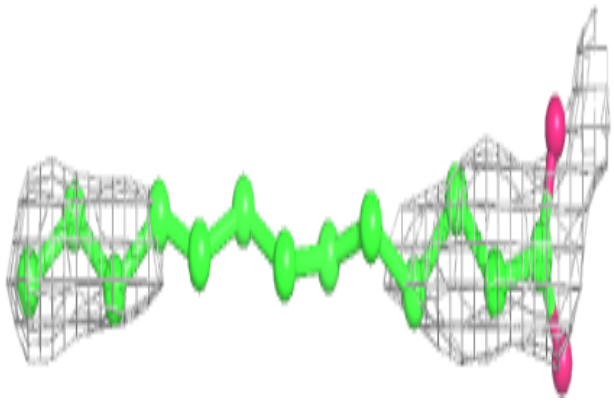
Electron density around OLA B 317:

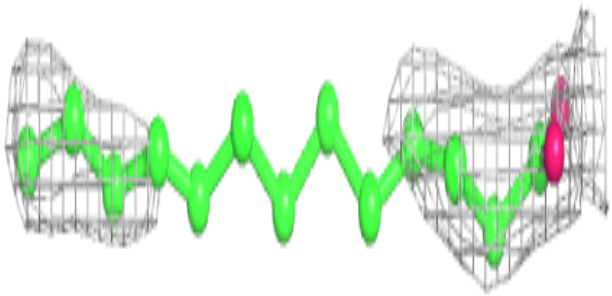
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around OLA D 403:

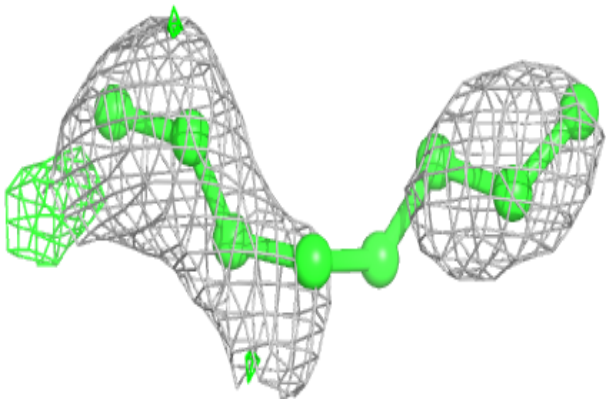
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

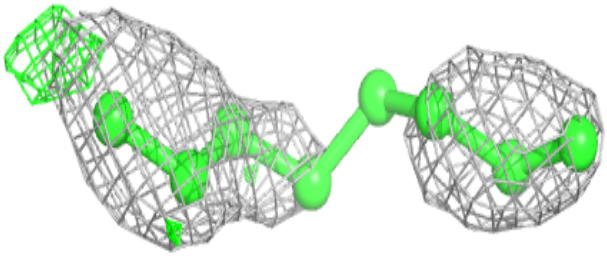


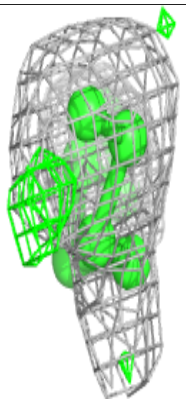


Electron density around LFA A 309:

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

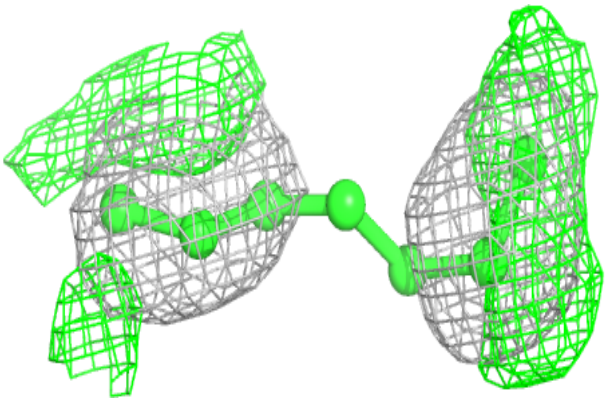


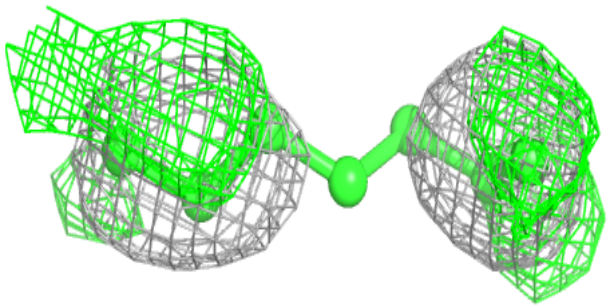


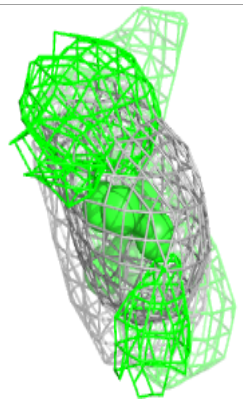


Electron density around LFA B 310:

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

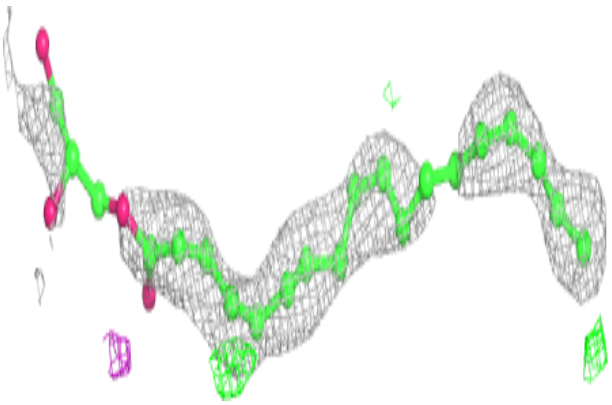


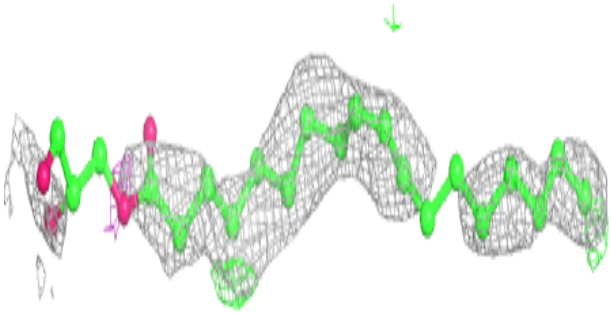


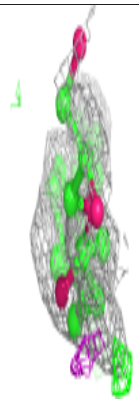


Electron density around OLC B 302:

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

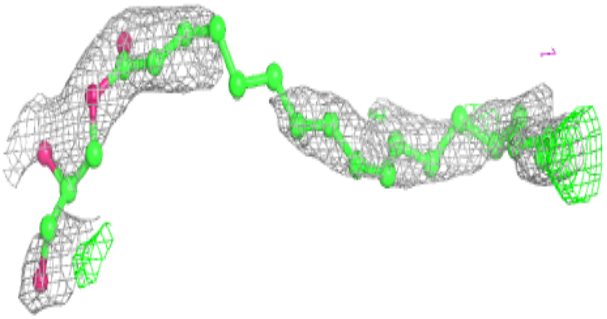


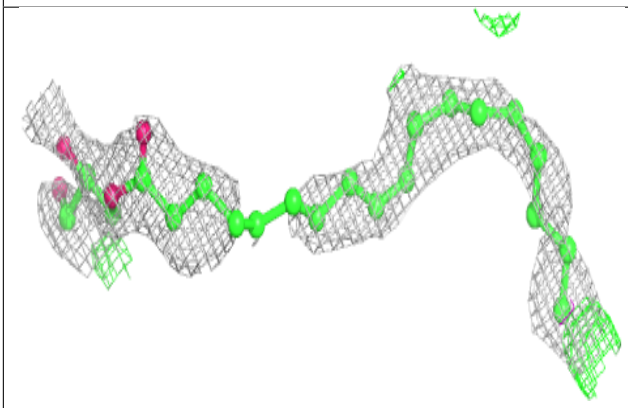


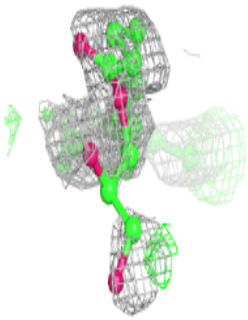


Electron density around OLC A 305:

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

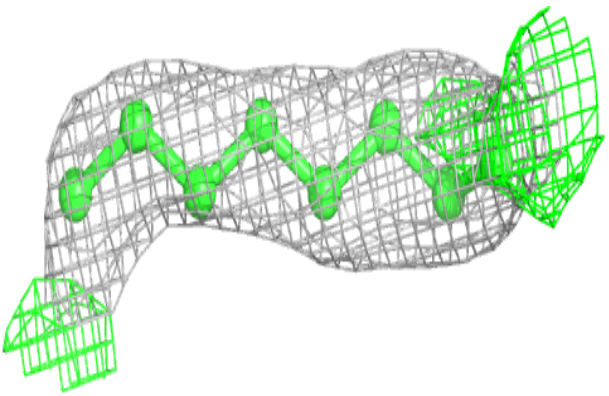


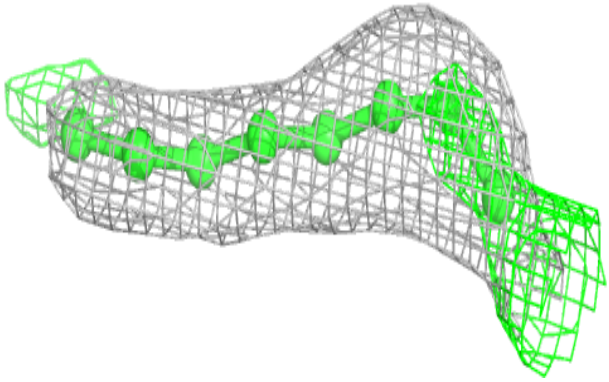


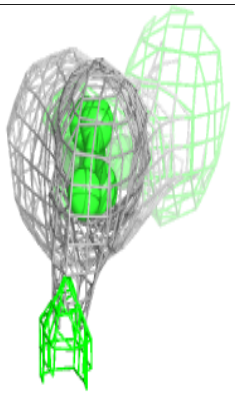


Electron density around LFA A 308:

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

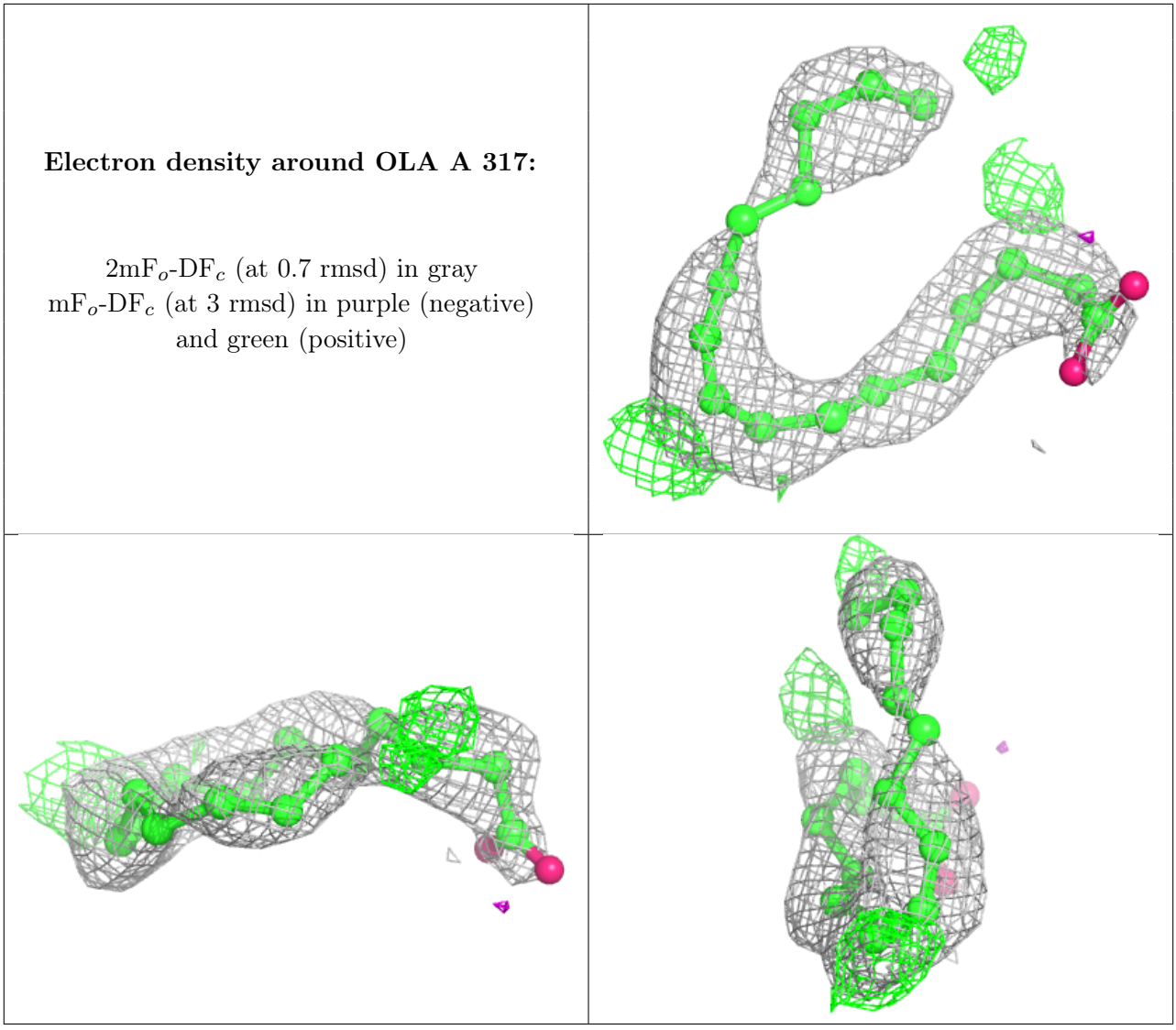






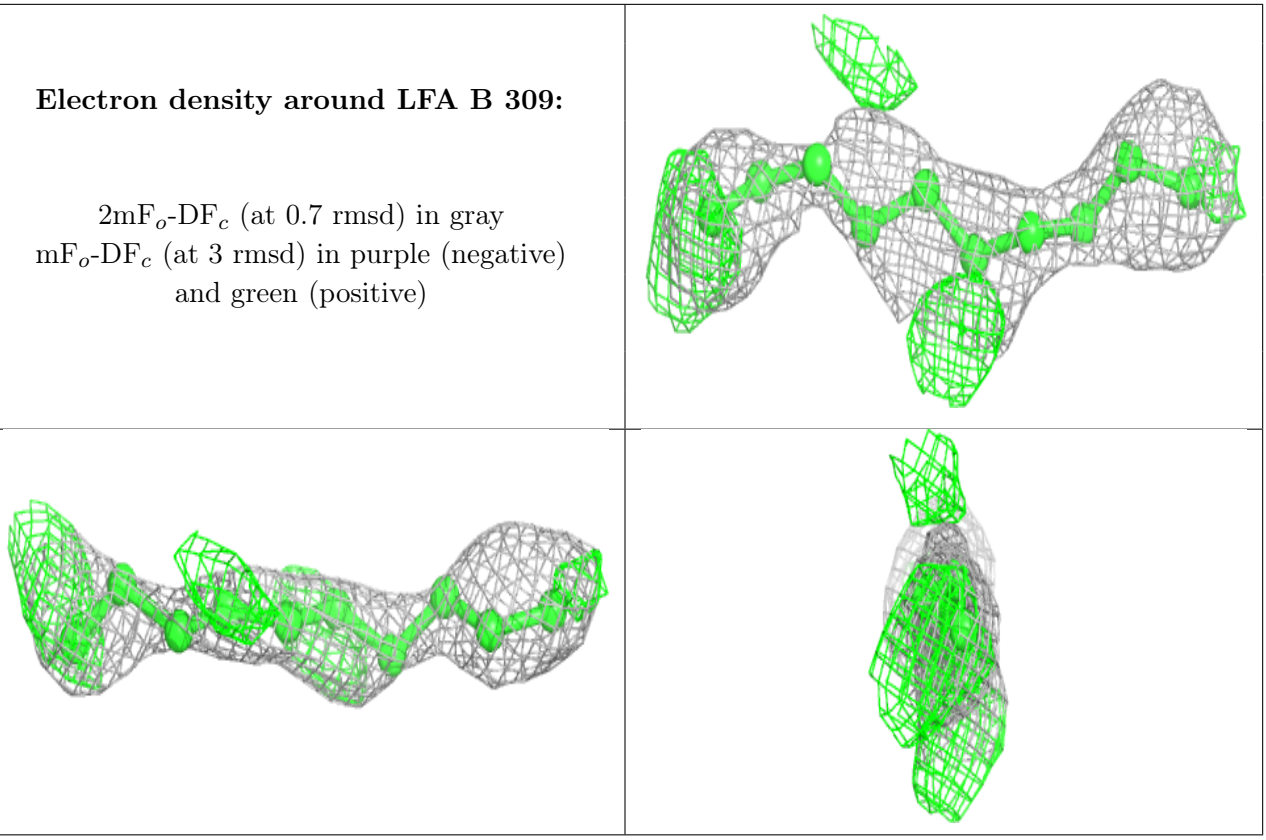
Electron density around OLA A 317:

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



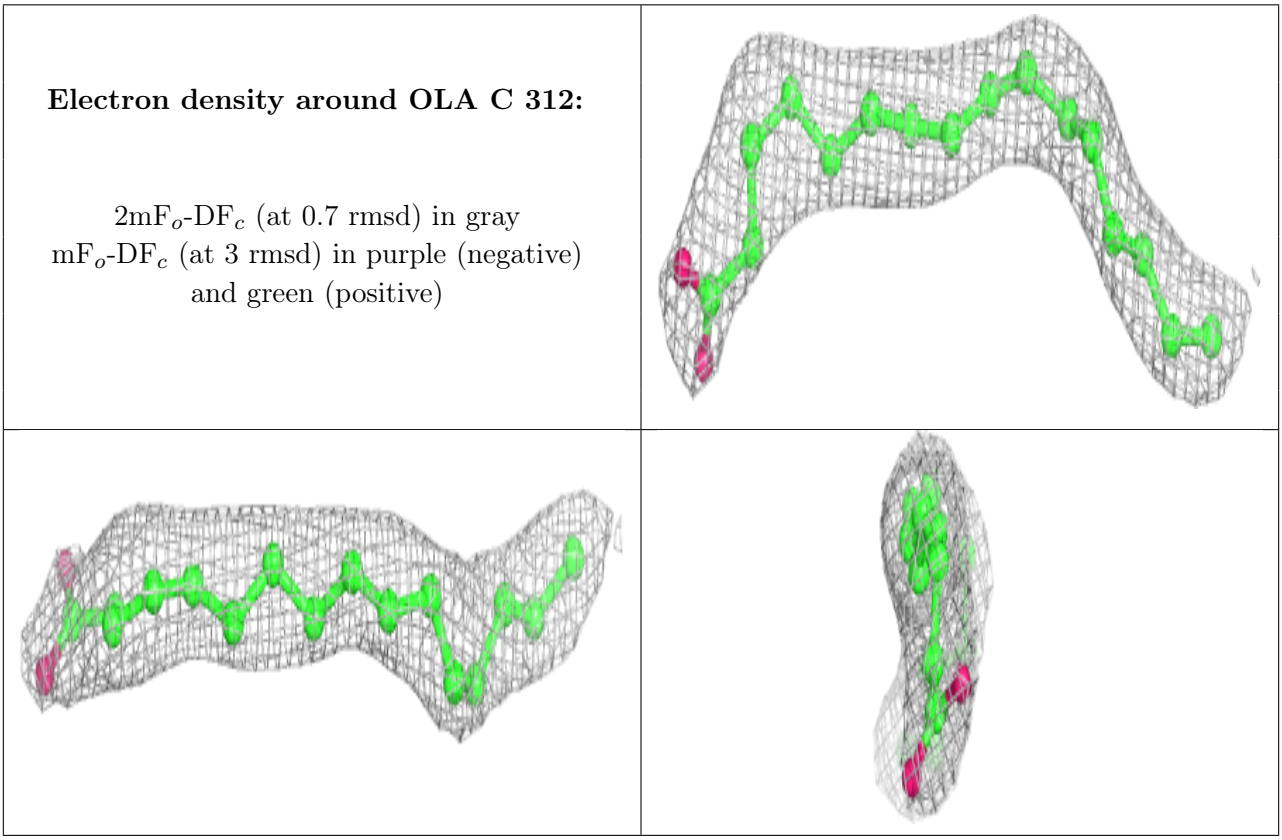
Electron density around LFA B 309:

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



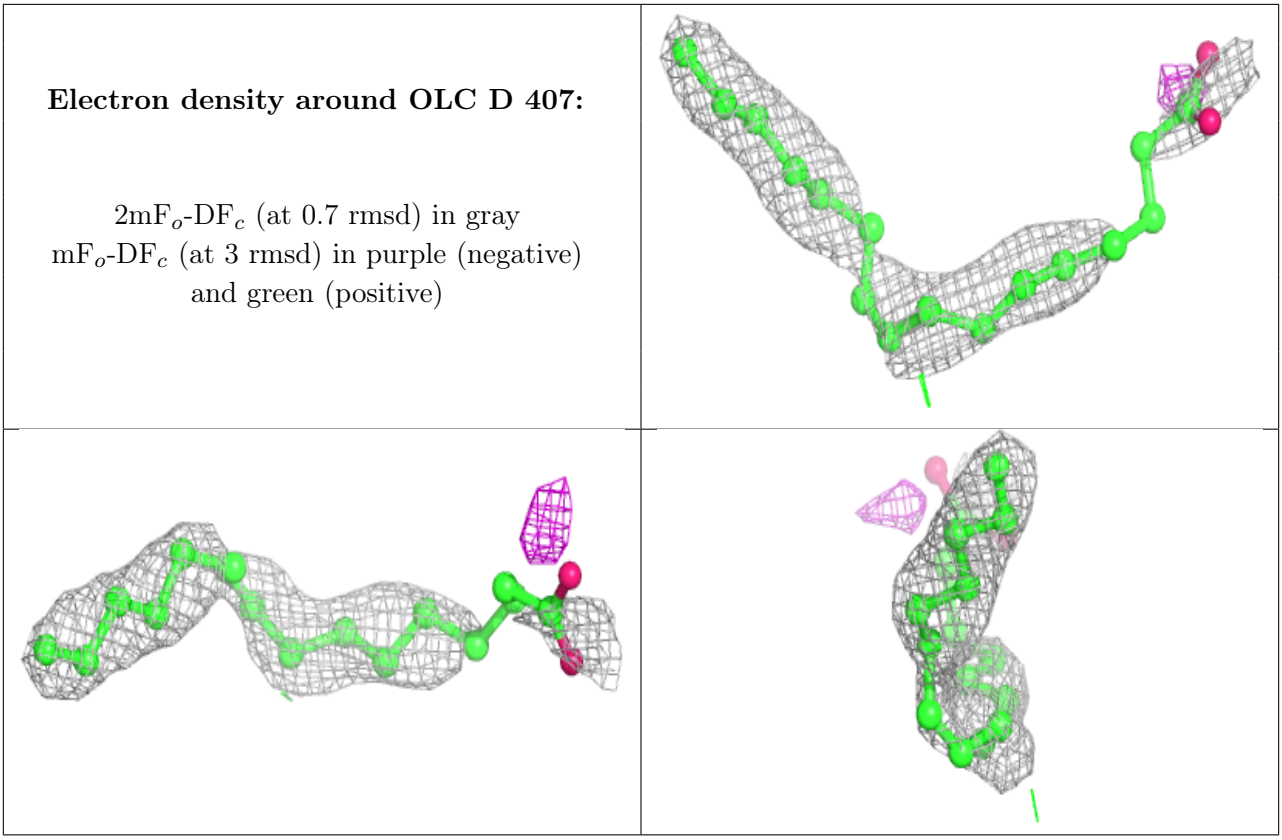
Electron density around OLA C 312:

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



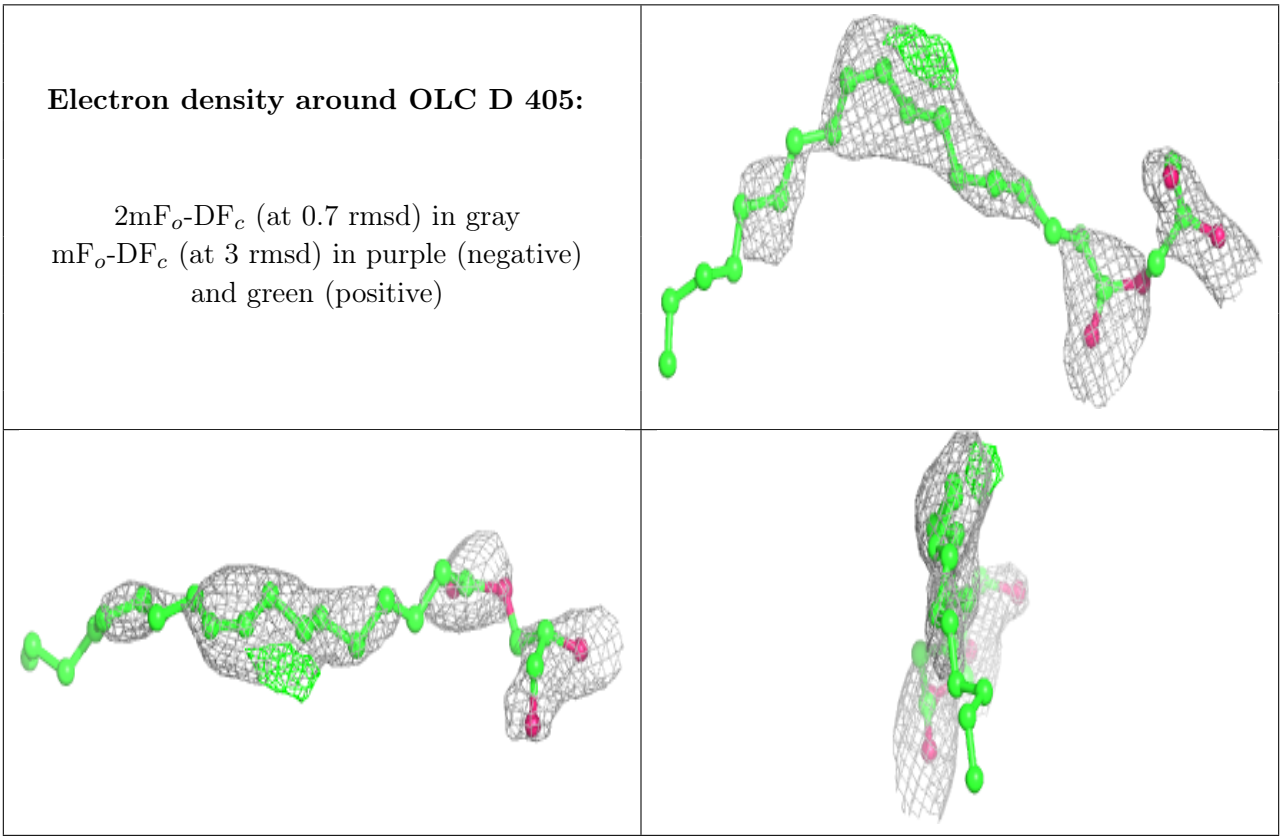
Electron density around OLC D 407:

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



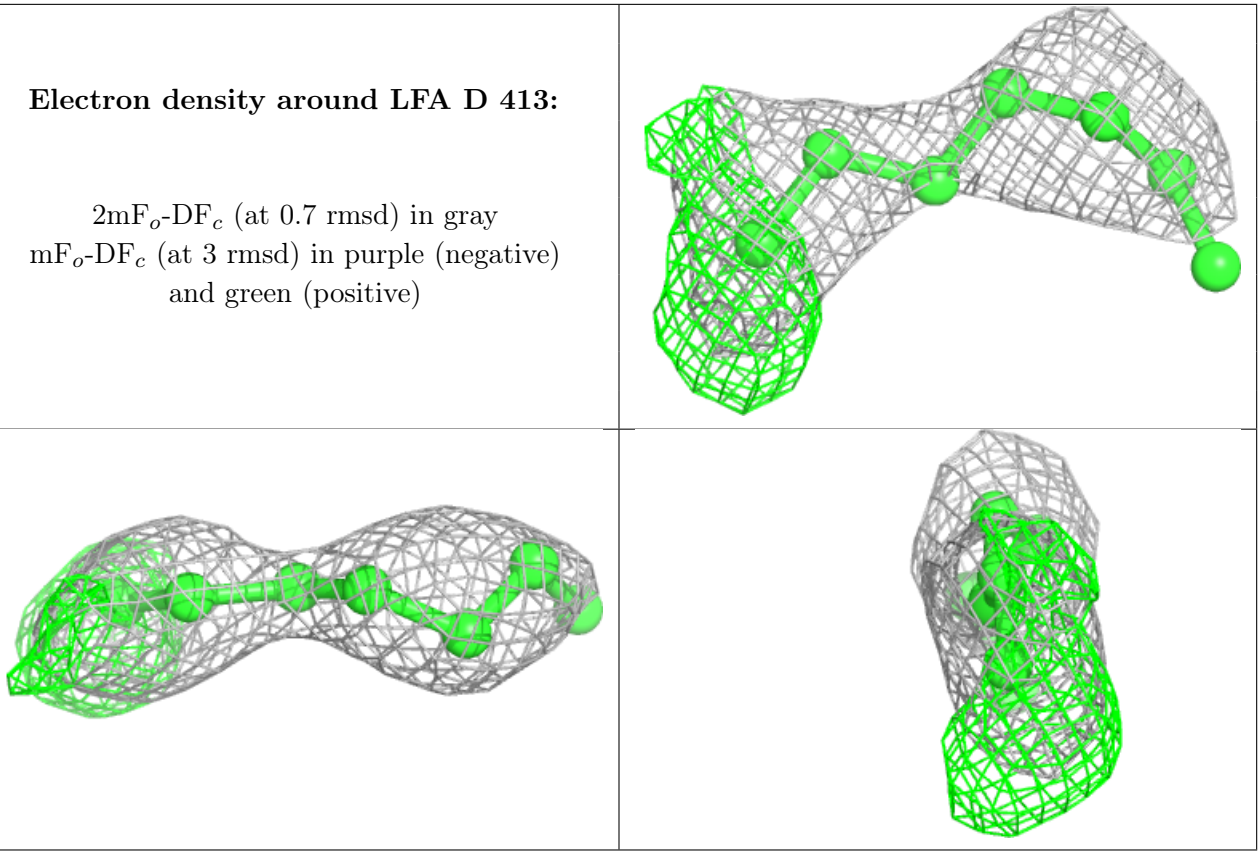
Electron density around OLC D 405:

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



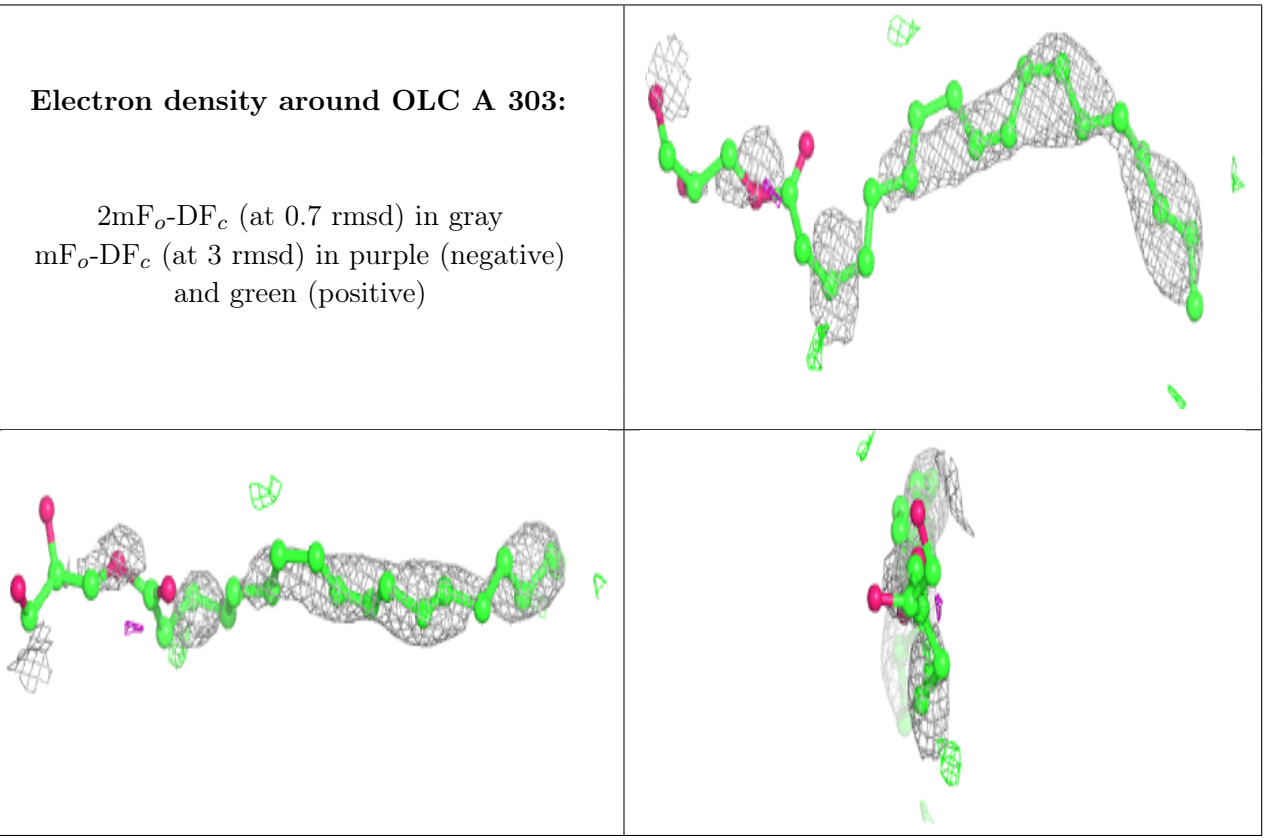
Electron density around LFA D 413:

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



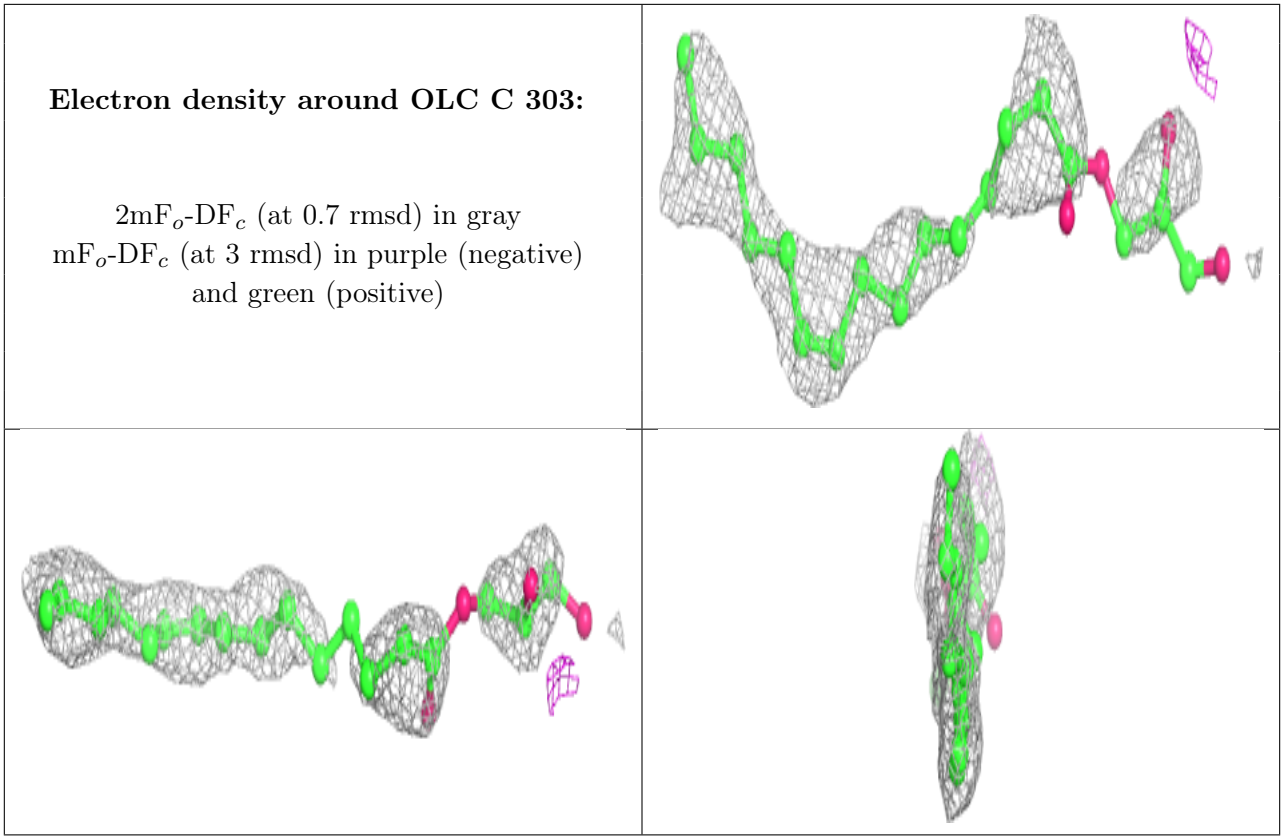
Electron density around OLC A 303:

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



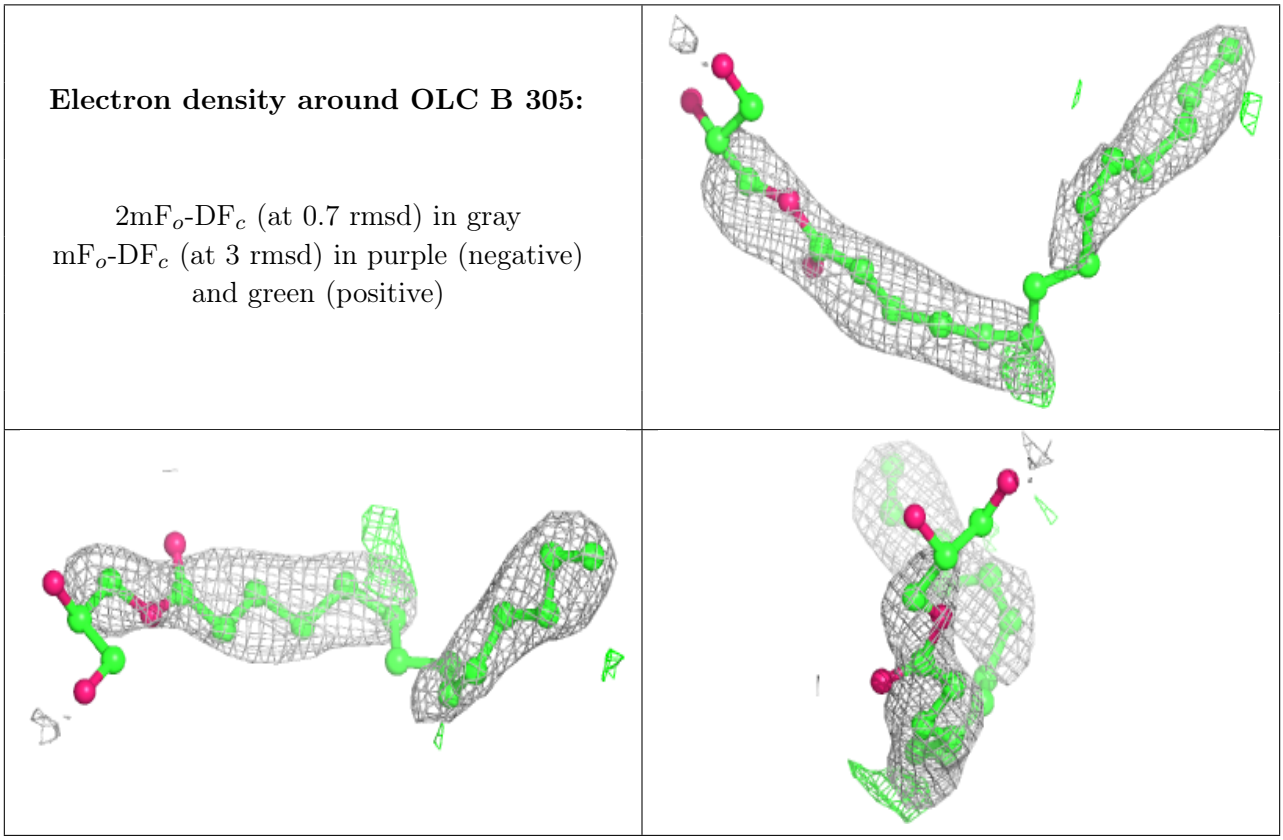
Electron density around OLC C 303:

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



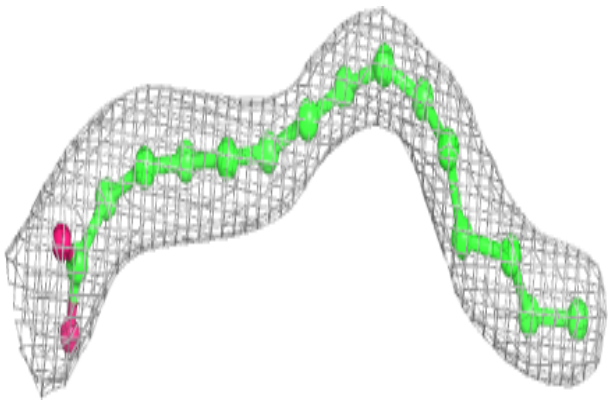
Electron density around OLC B 305:

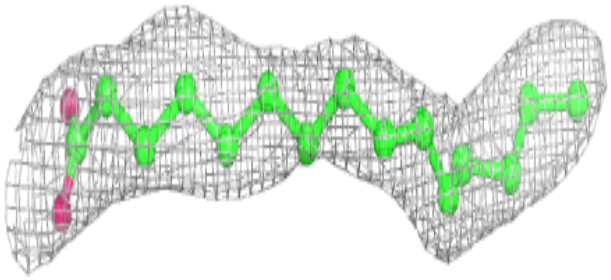
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

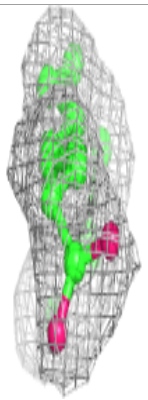


Electron density around OLA E 302:

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

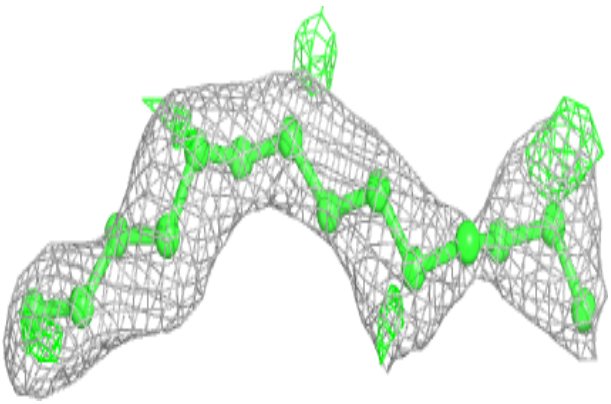


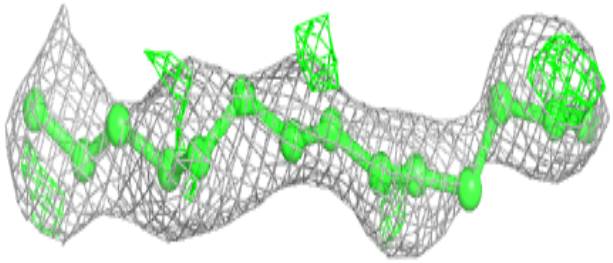


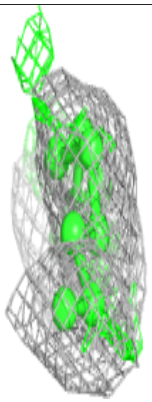


Electron density around LFA E 311:

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

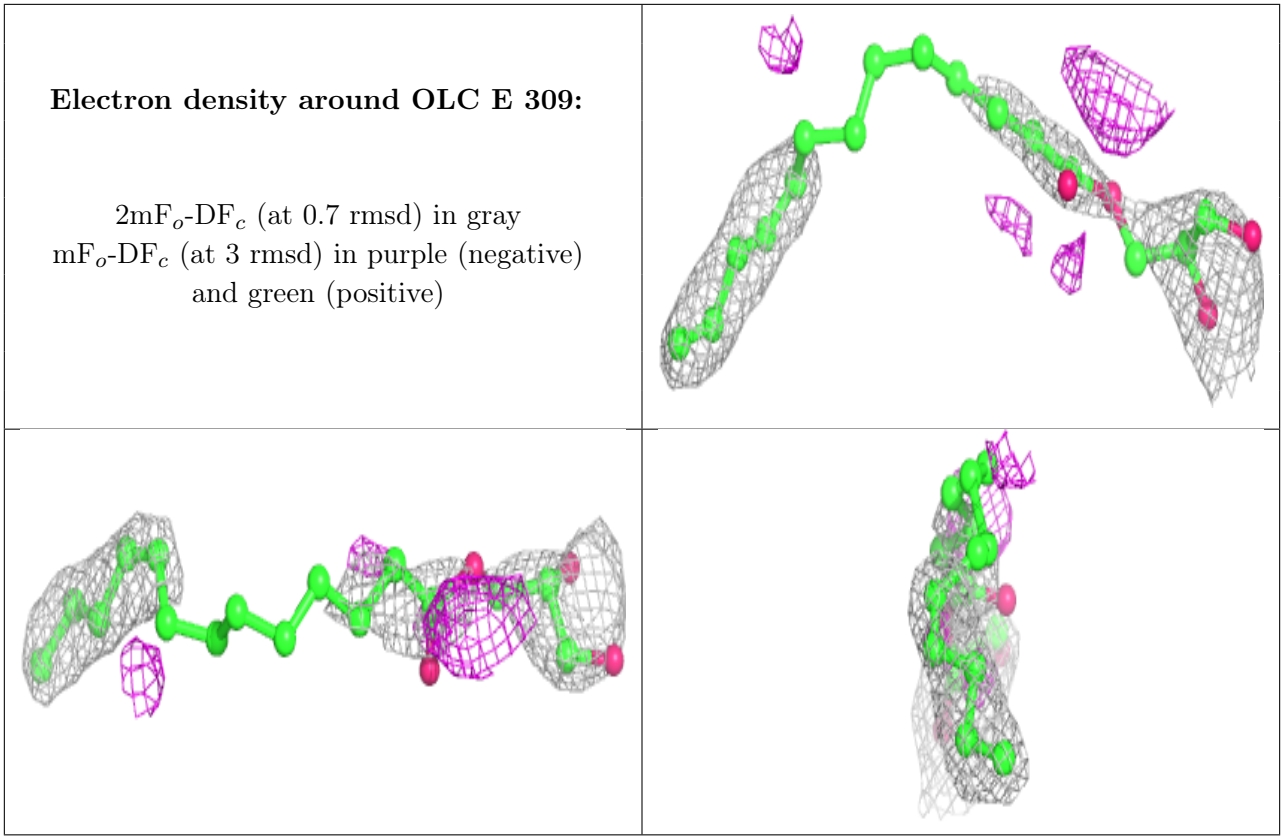






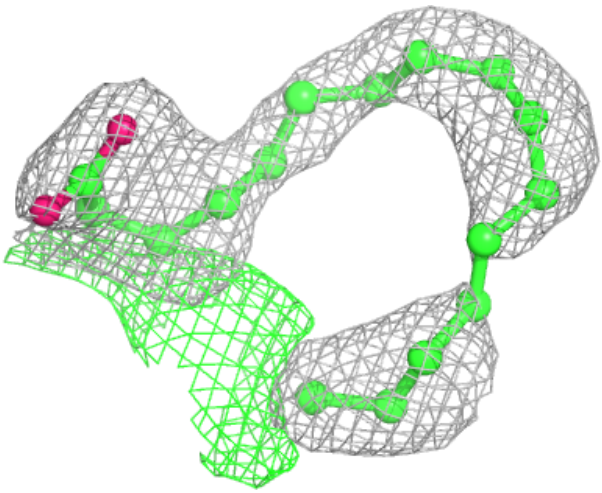
Electron density around OLC E 309:

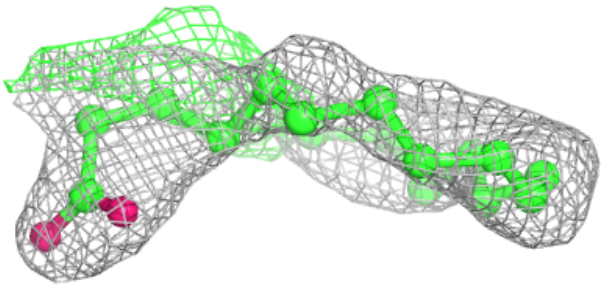
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

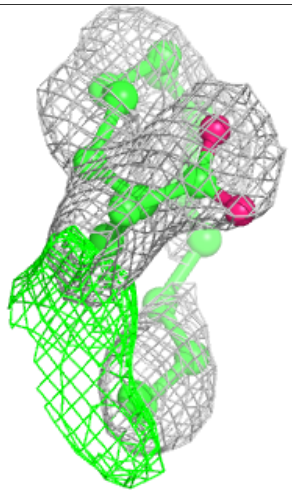


Electron density around OLA C 314:

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

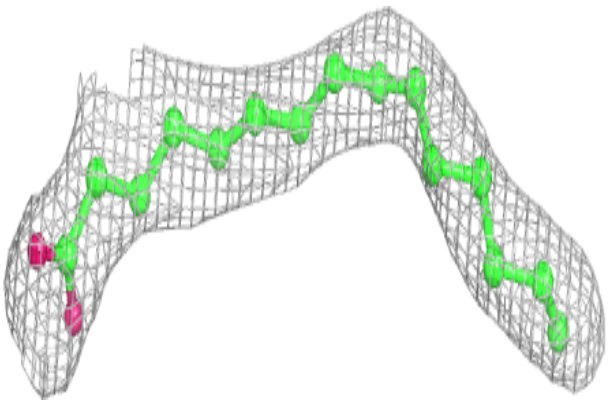


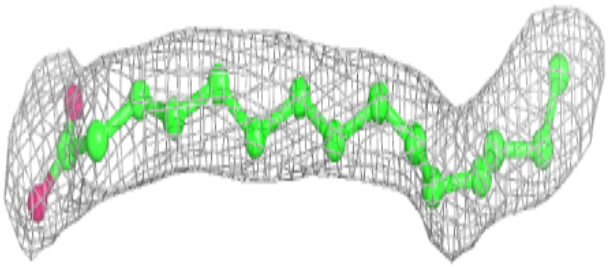


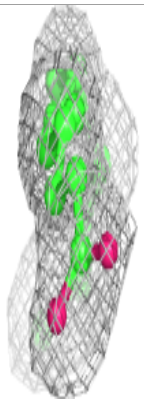


Electron density around OLA B 315:

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

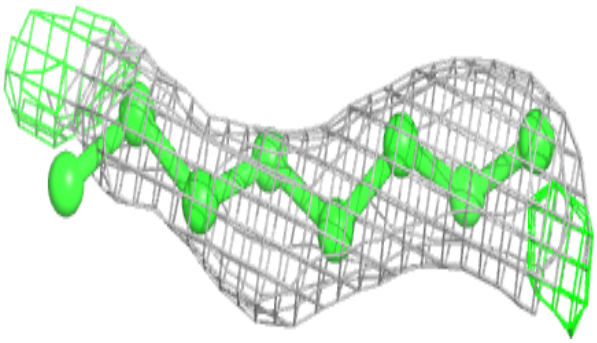


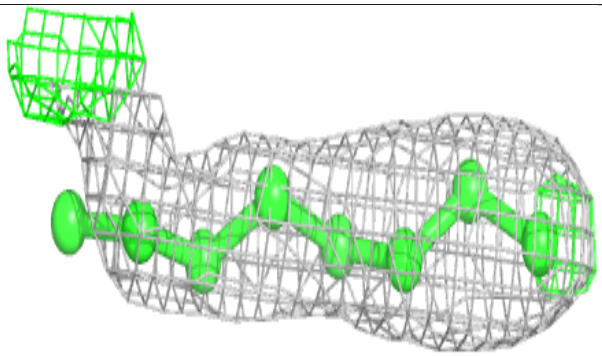


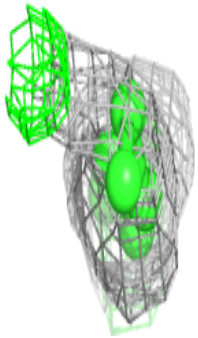


Electron density around LFA E 310:

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

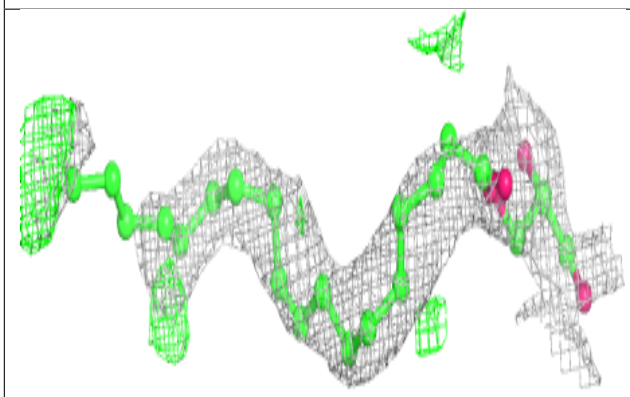


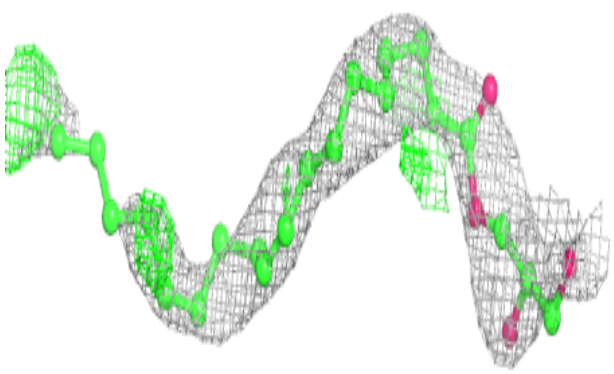


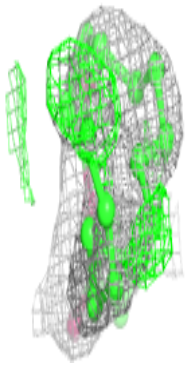


Electron density around OLC E 303:

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

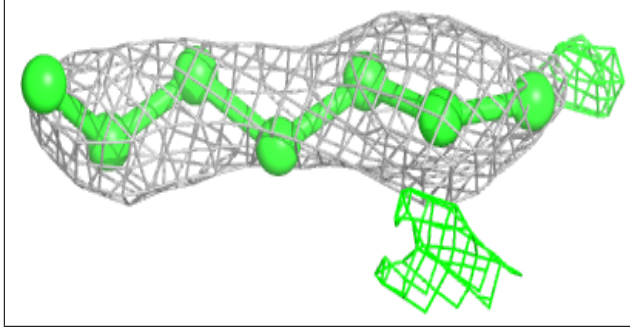


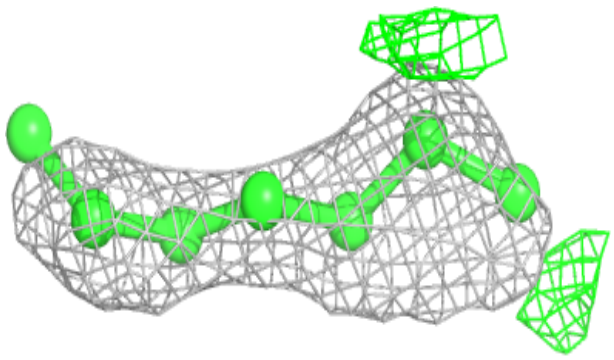


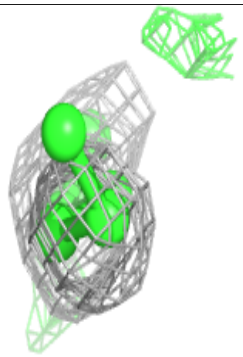


Electron density around LFA C 307:

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

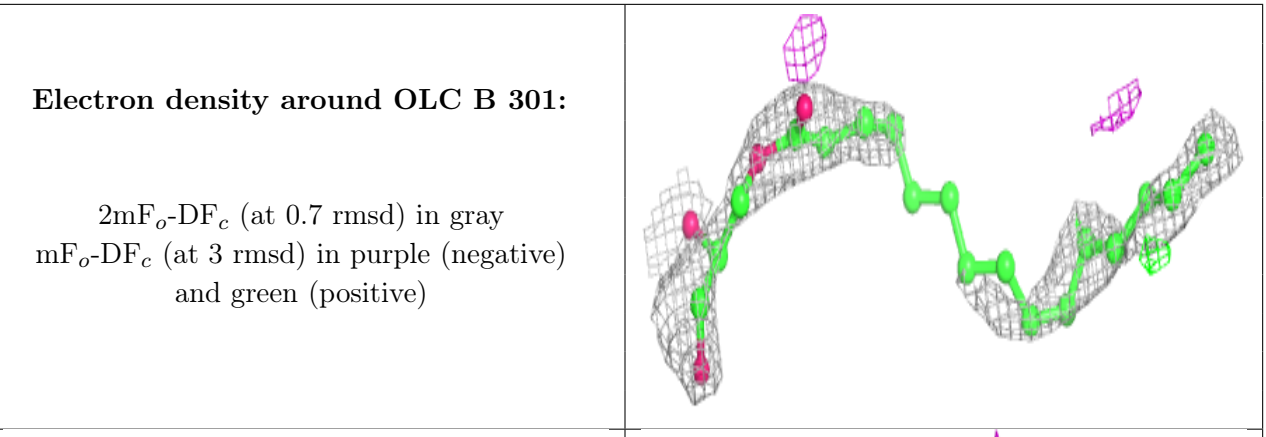






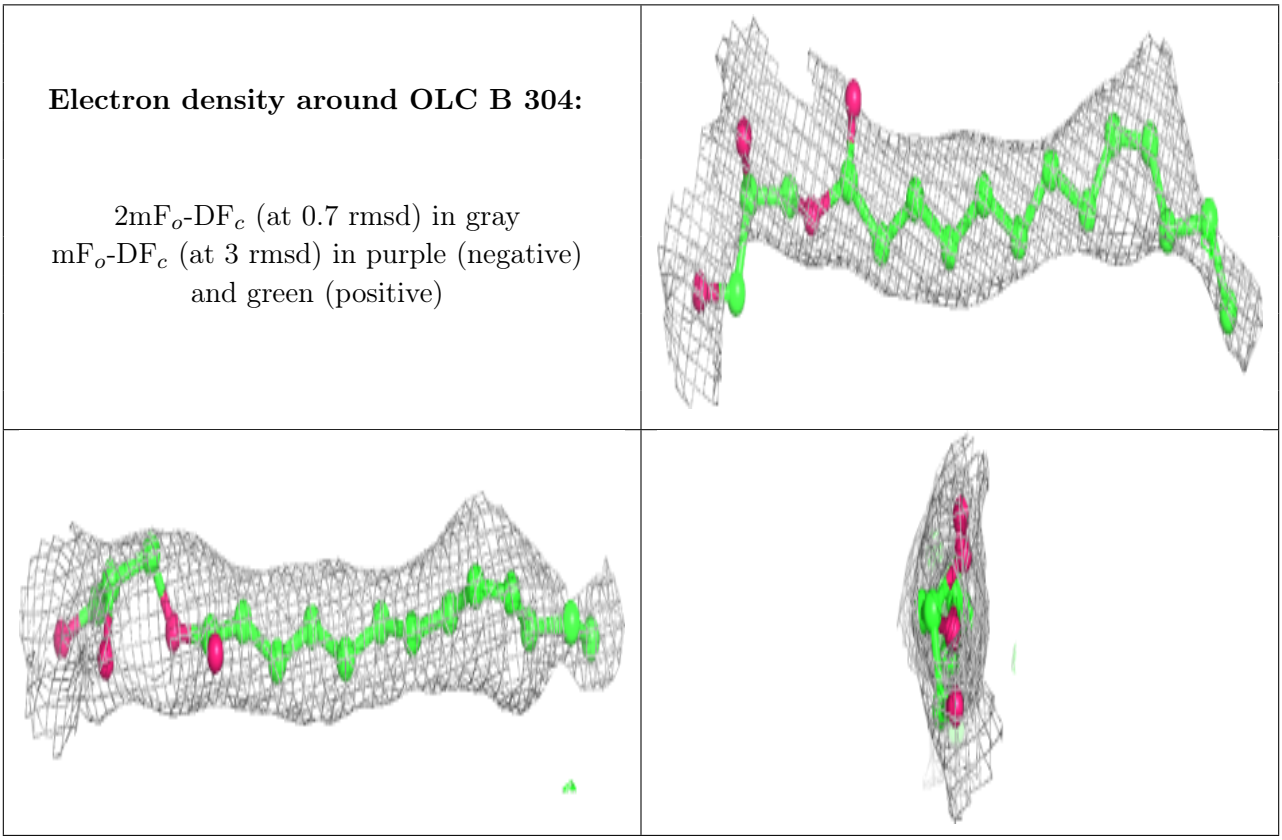
Electron density around OLC B 301:

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



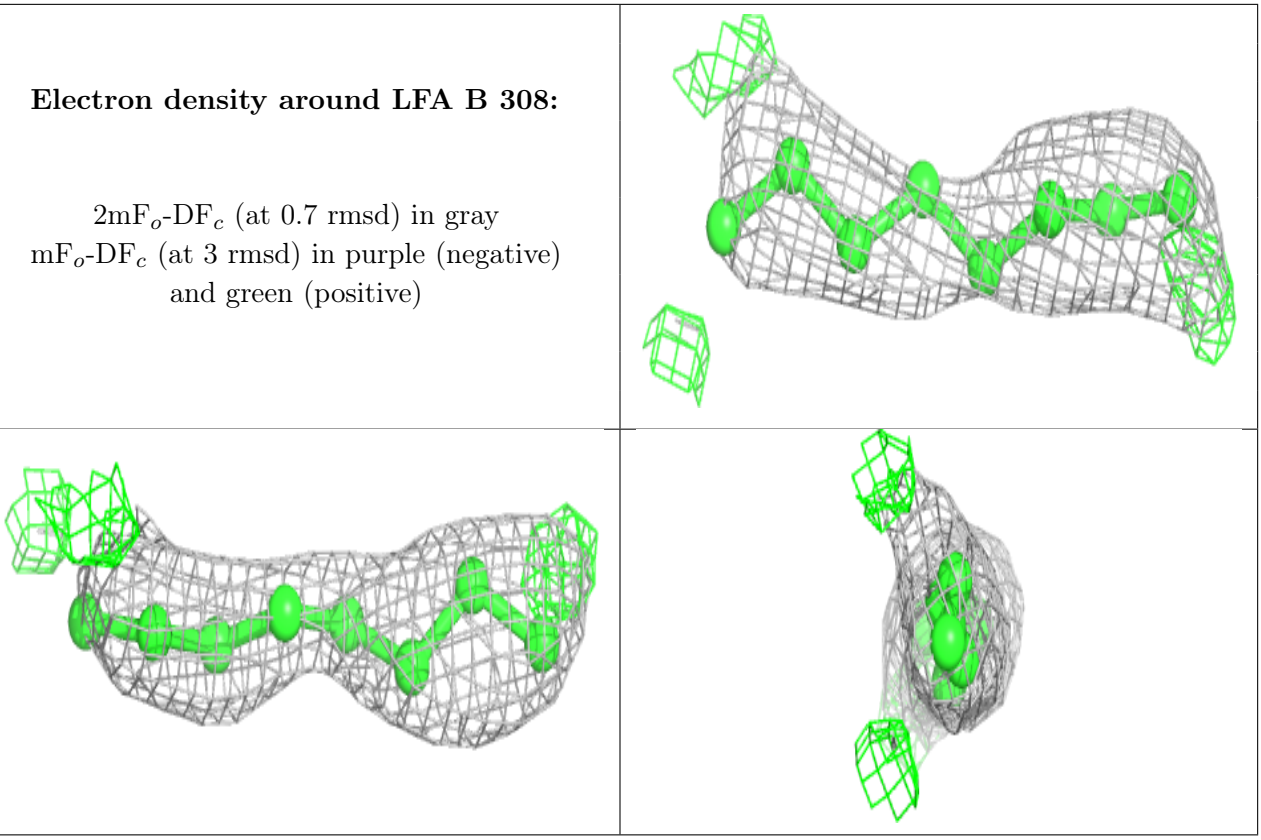
Electron density around OLC B 304:

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



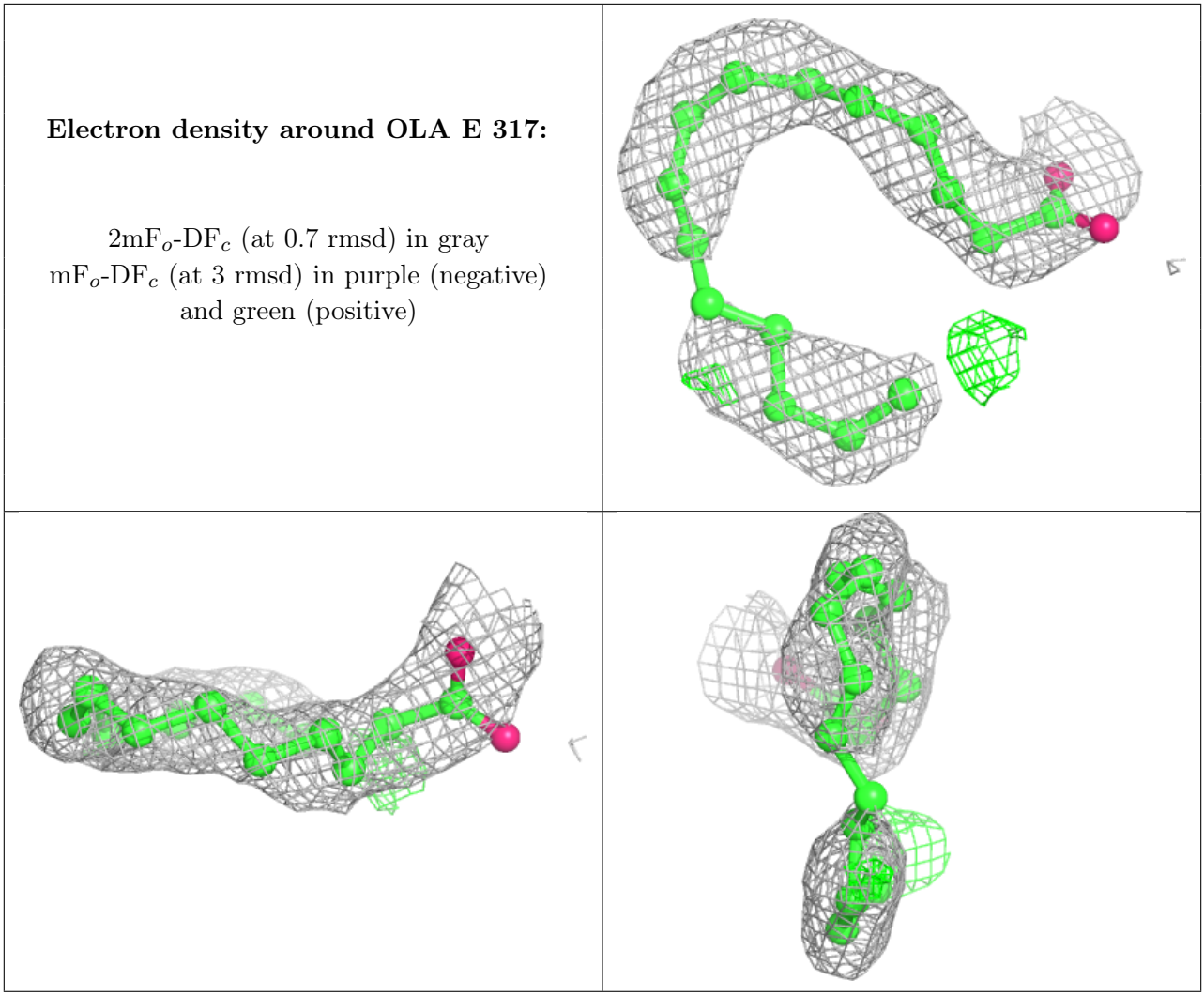
Electron density around LFA B 308:

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



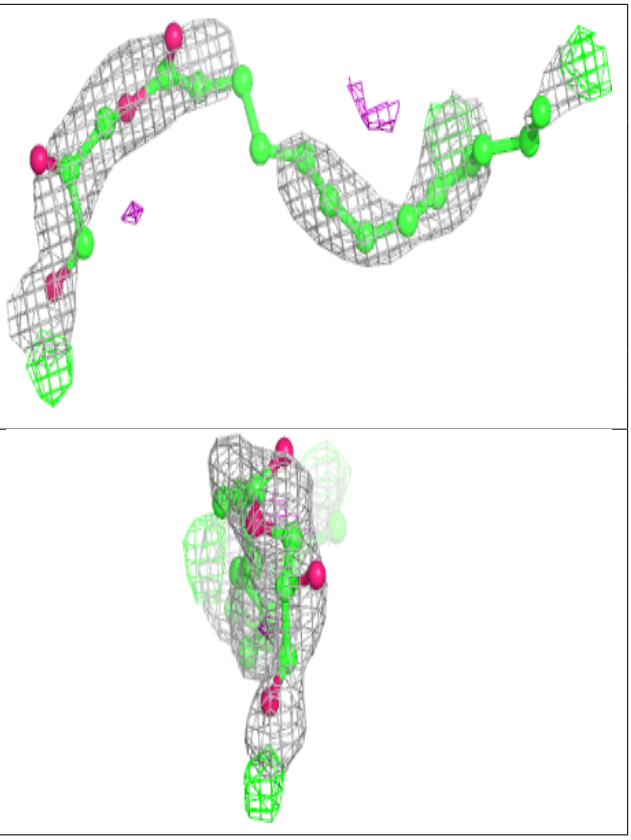
Electron density around OLA E 317:

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



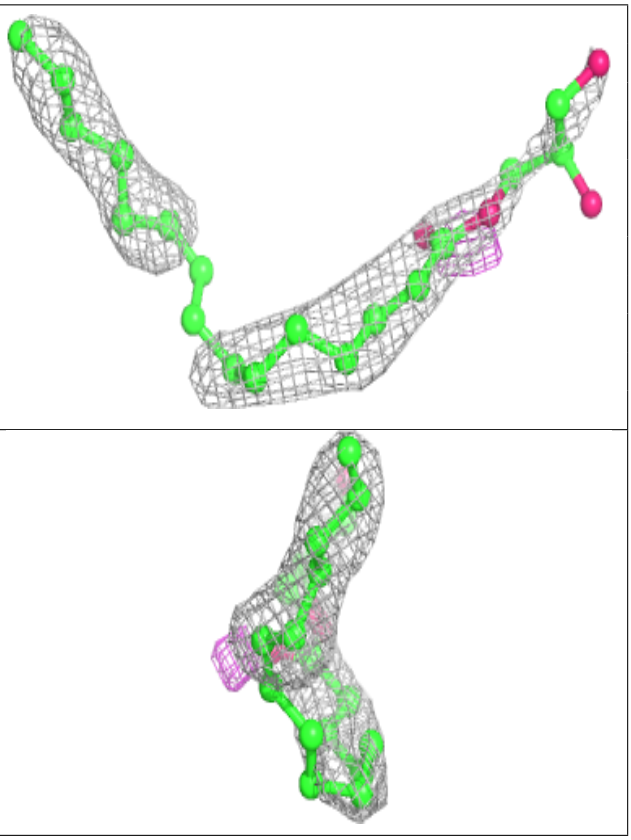
Electron density around OLC C 301:

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



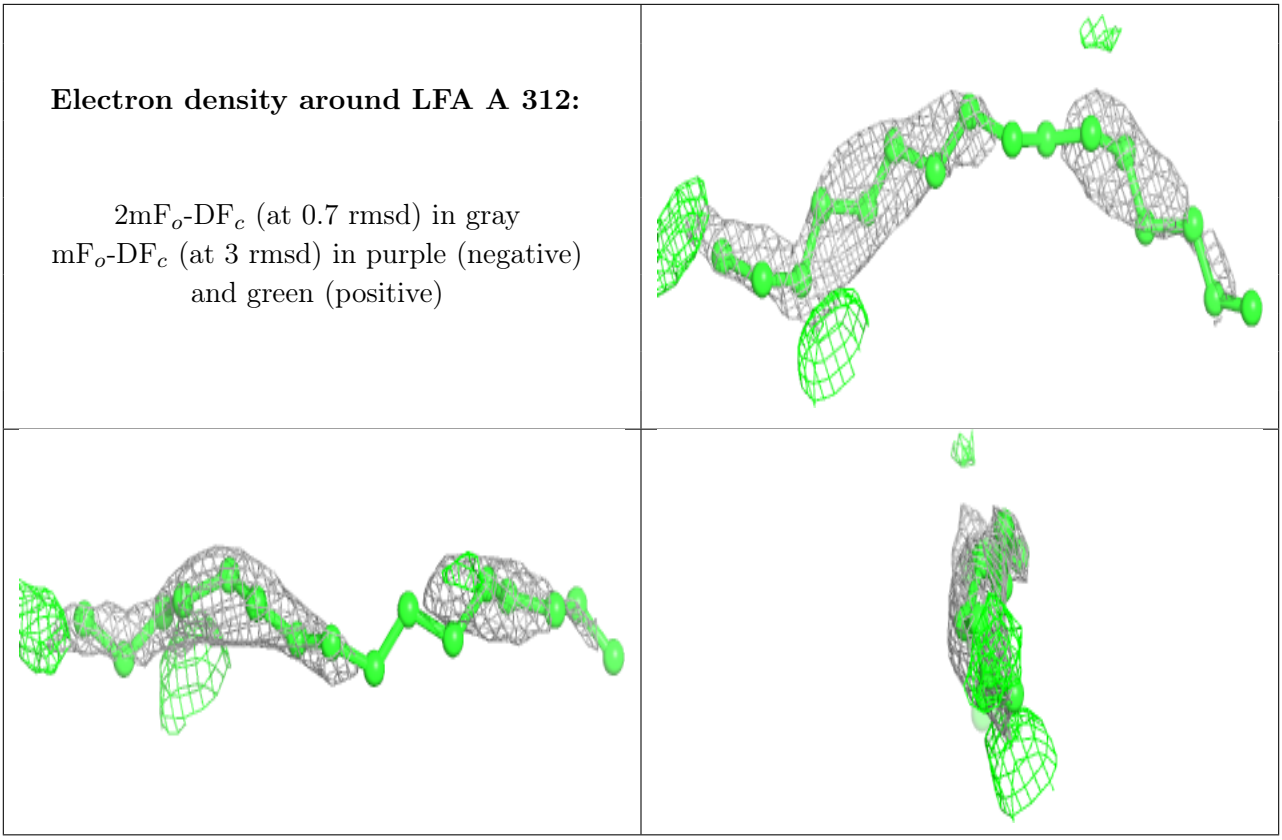
Electron density around OLC C 305:

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



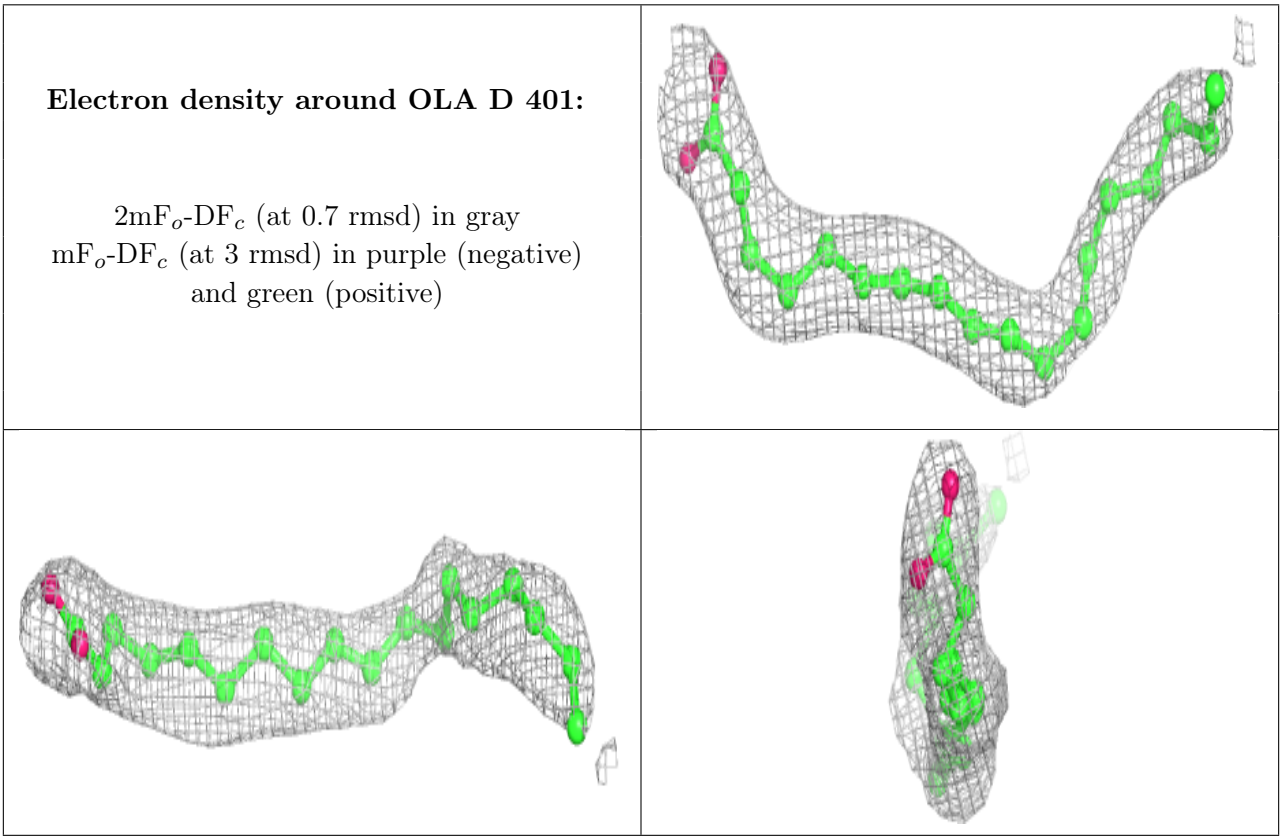
Electron density around LFA A 312:

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



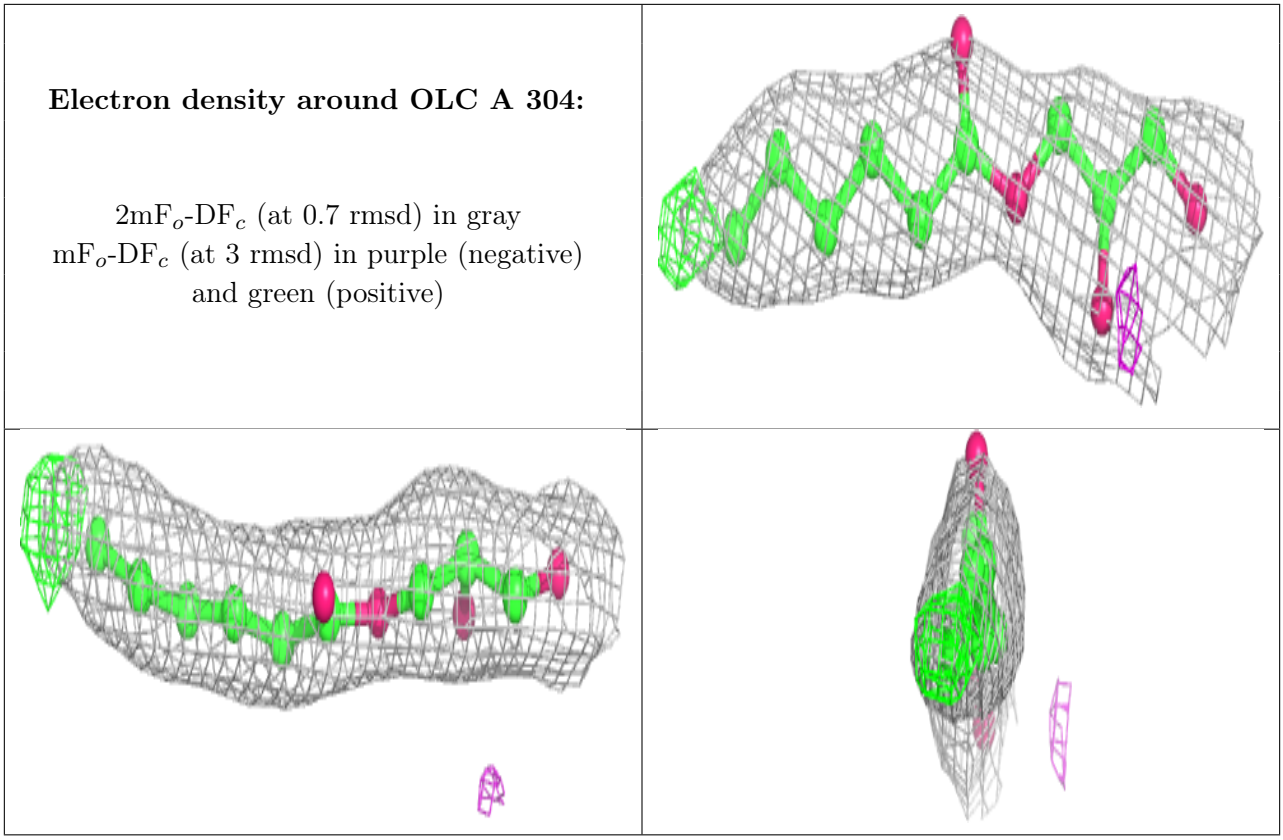
Electron density around OLA D 401:

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



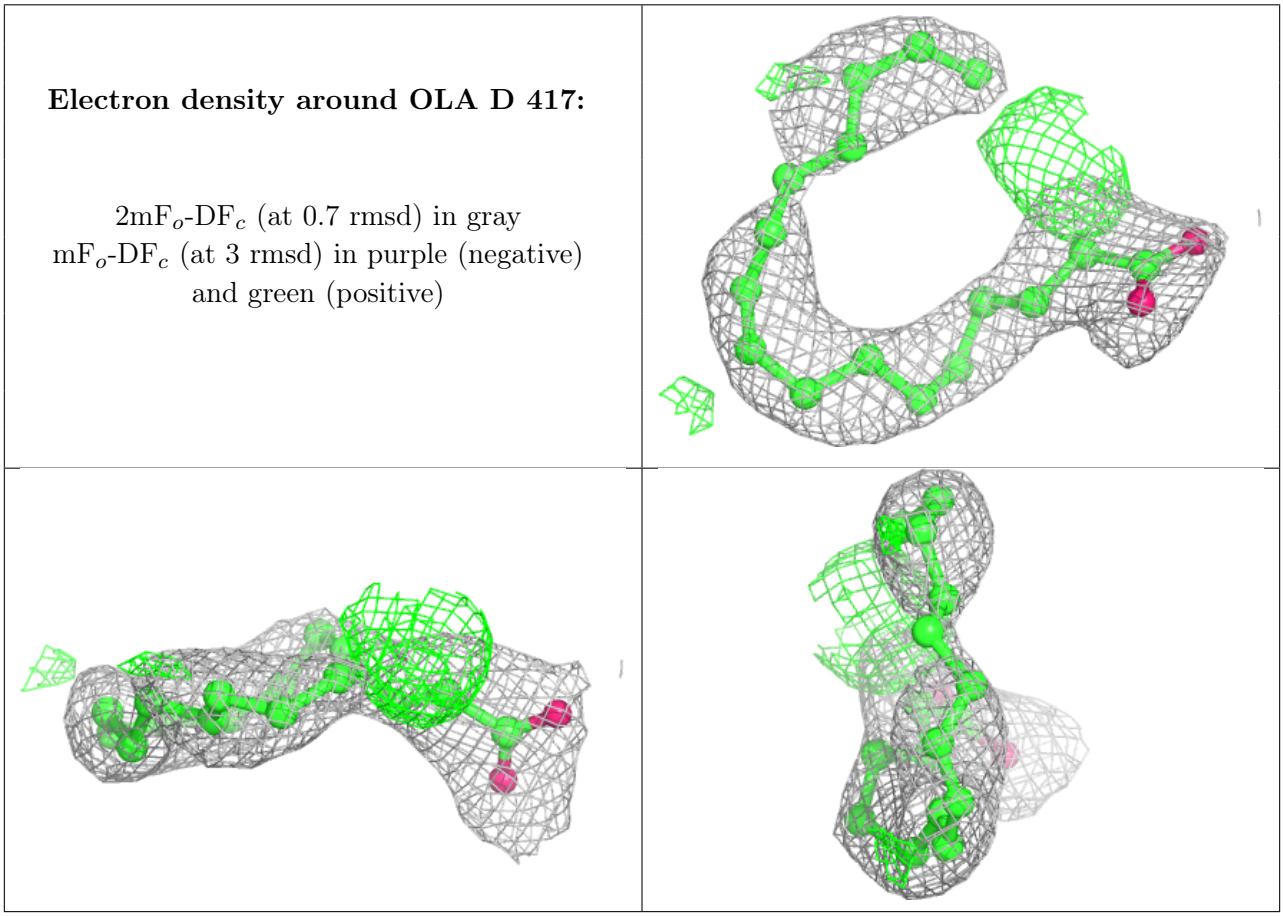
Electron density around OLC A 304:

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



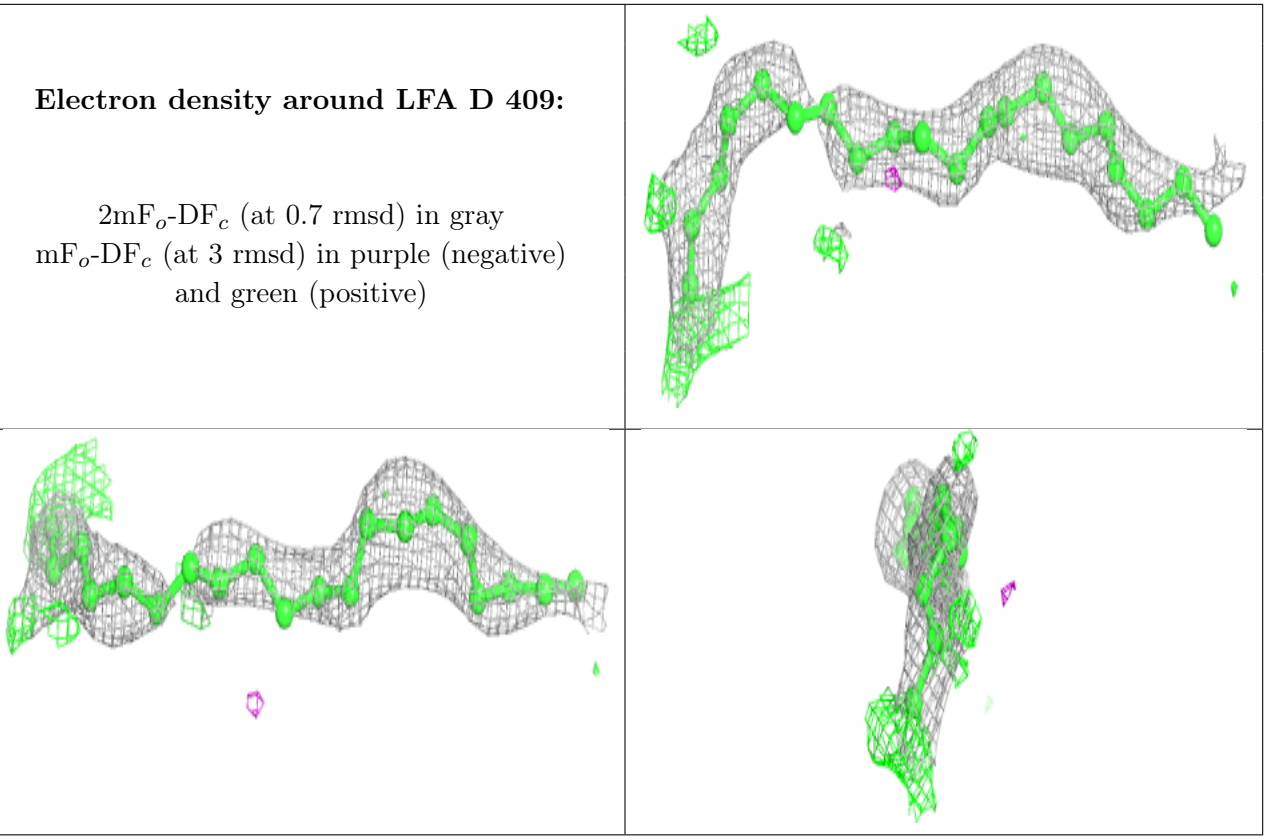
Electron density around OLA D 417:

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



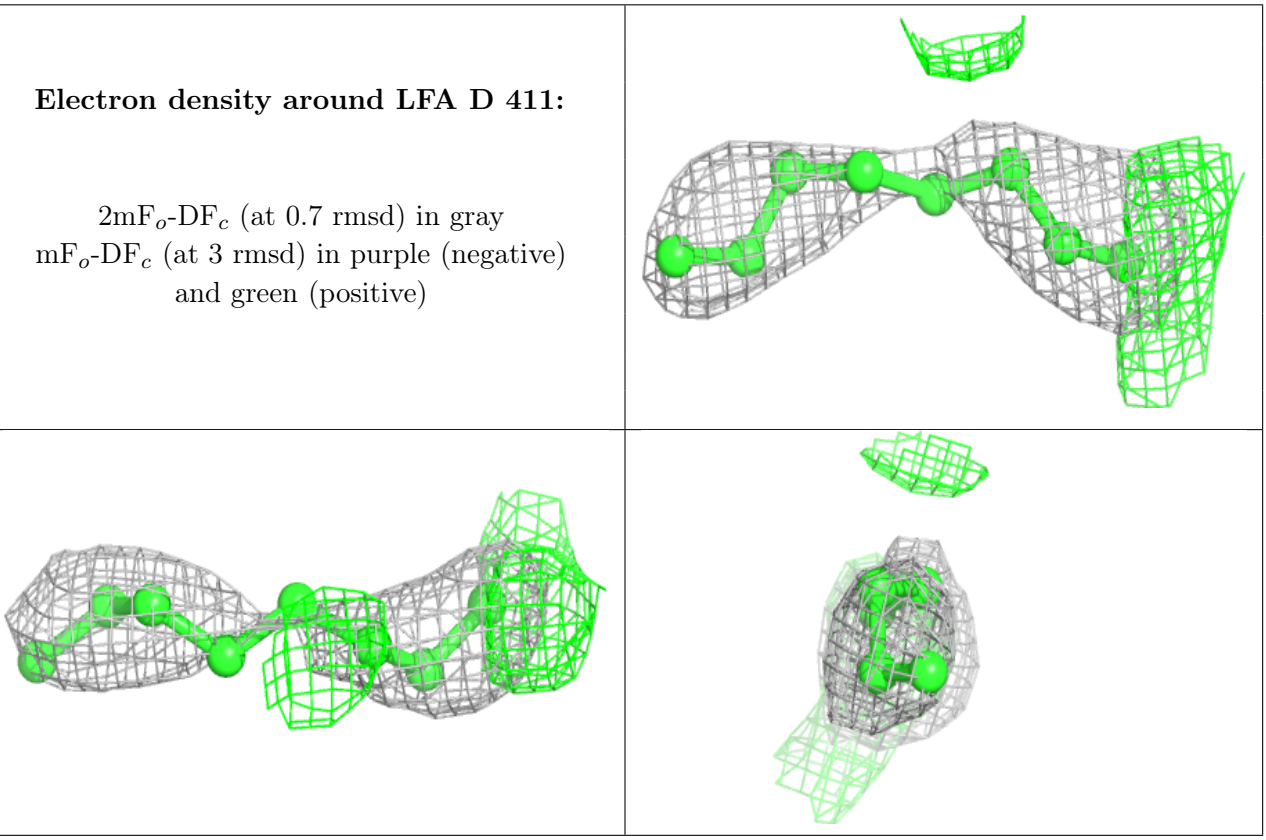
Electron density around LFA D 409:

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



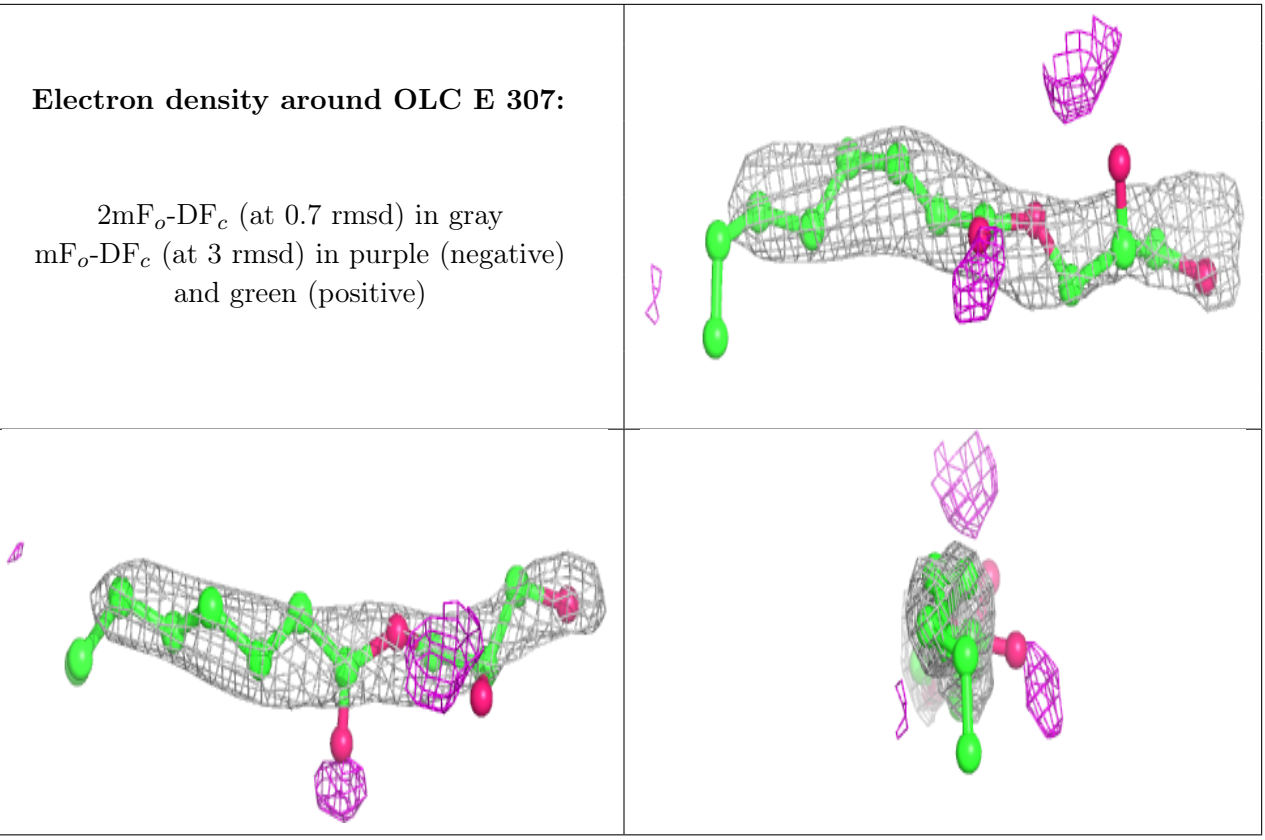
Electron density around LFA D 411:

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



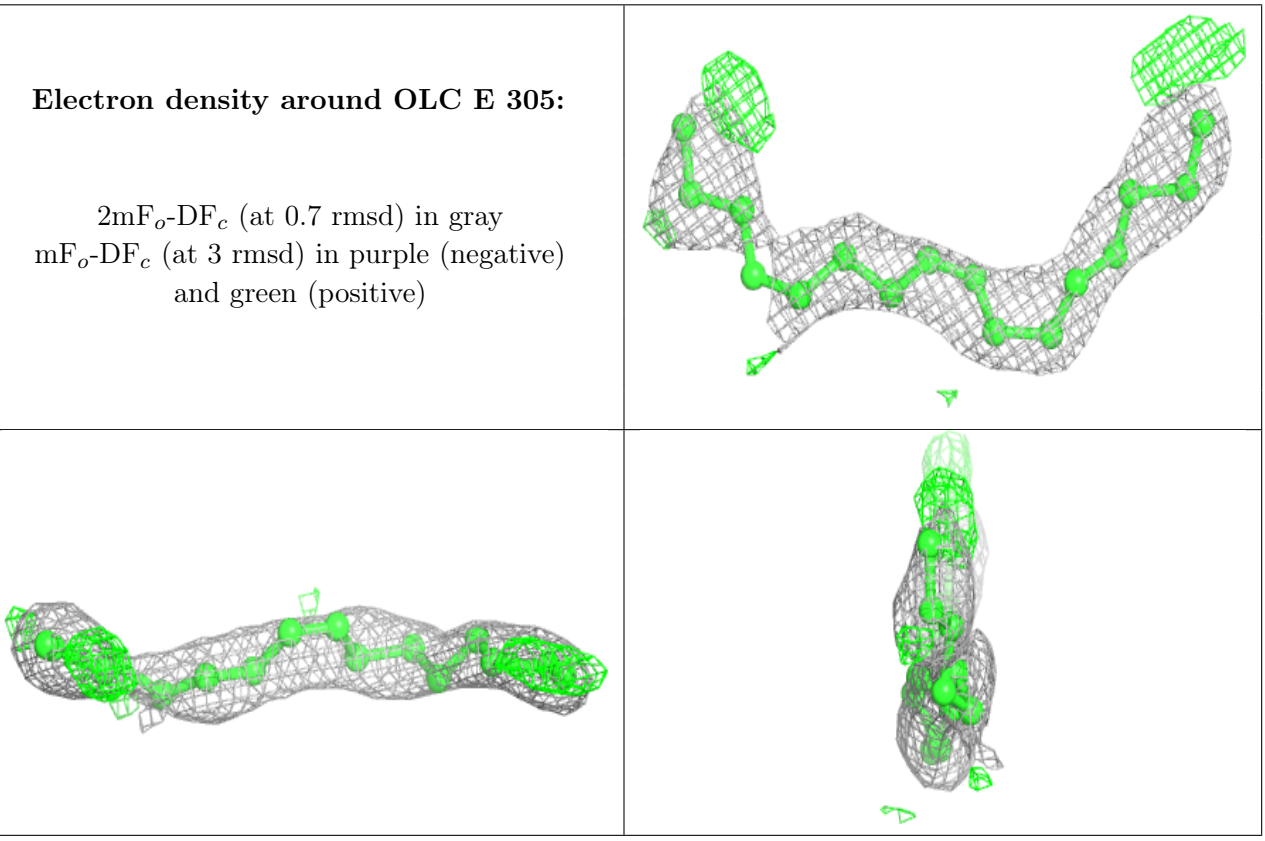
Electron density around OLC E 307:

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



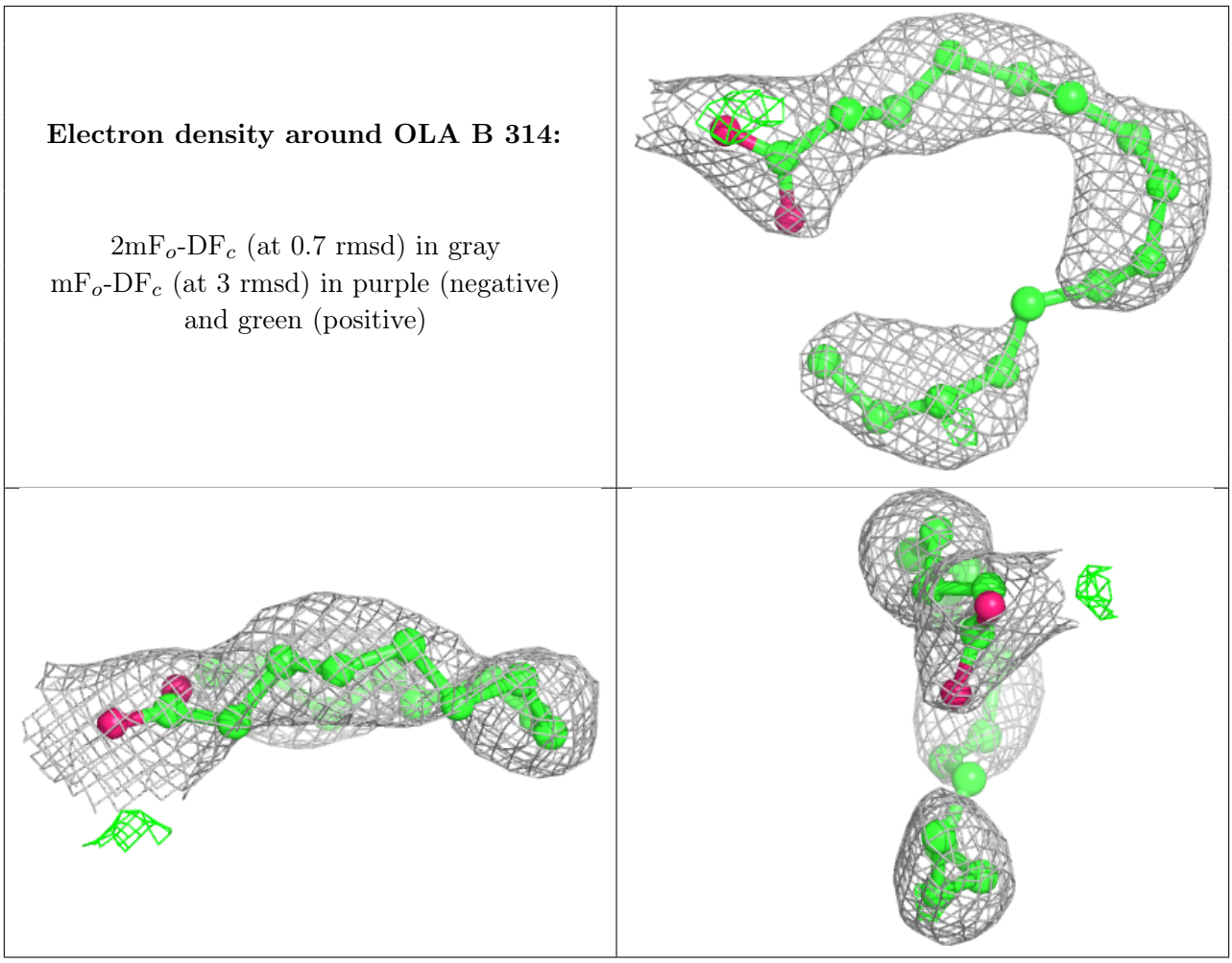
Electron density around OLC E 305:

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



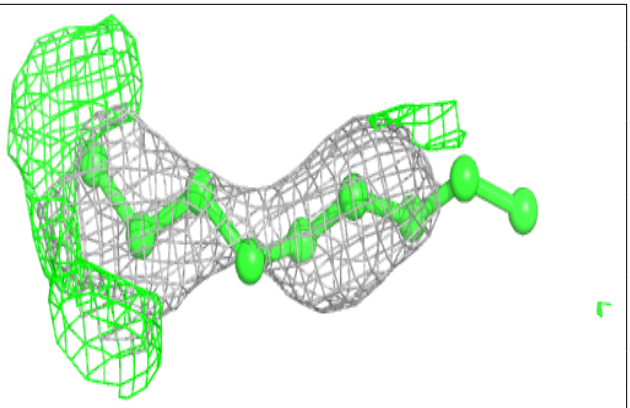
Electron density around OLA B 314:

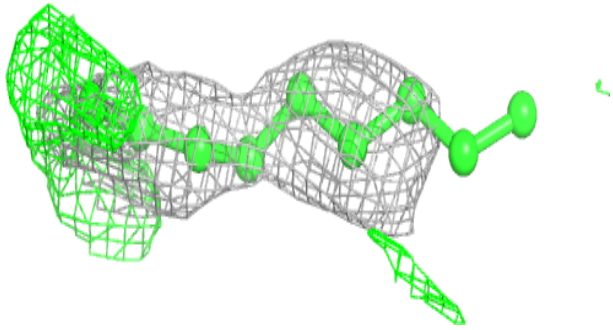
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

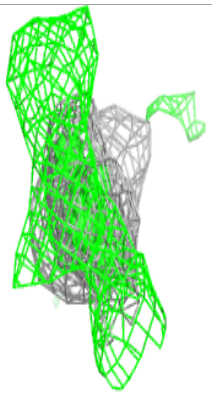


Electron density around LFA B 307:

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

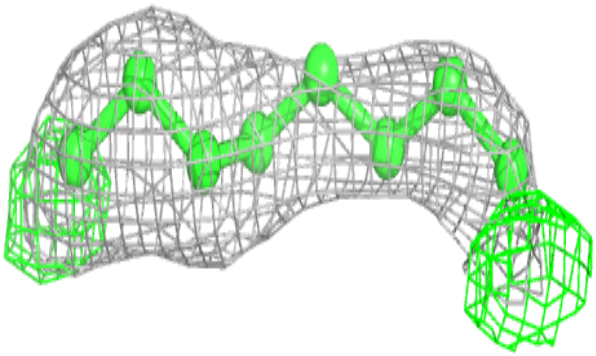


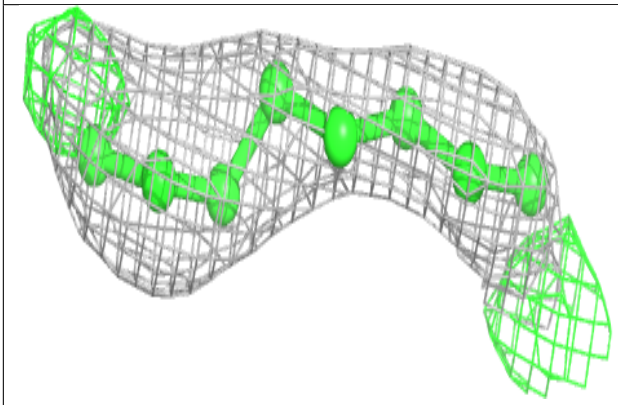


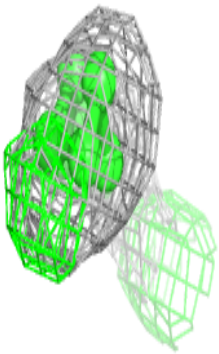


Electron density around LFA C 308:

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

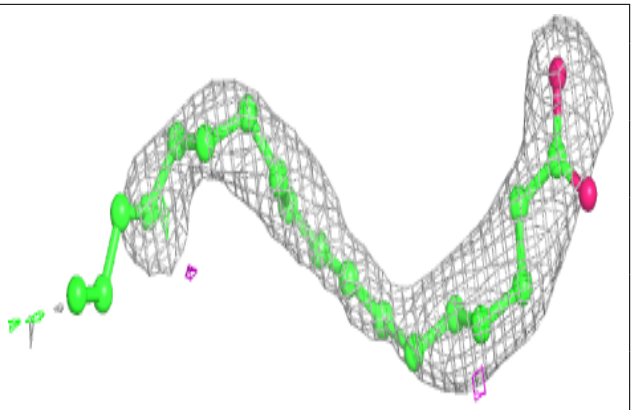


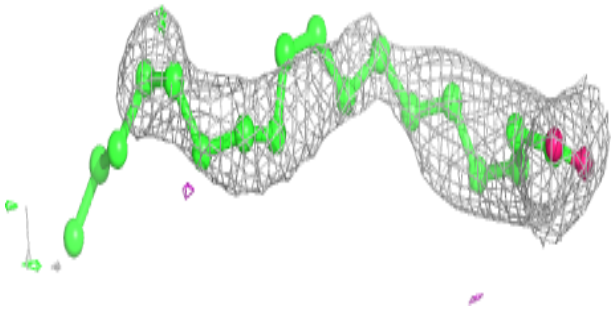


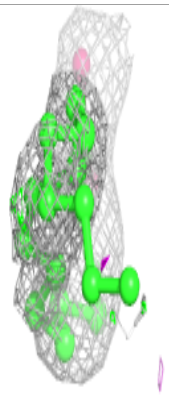


Electron density around OLC A 315:

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

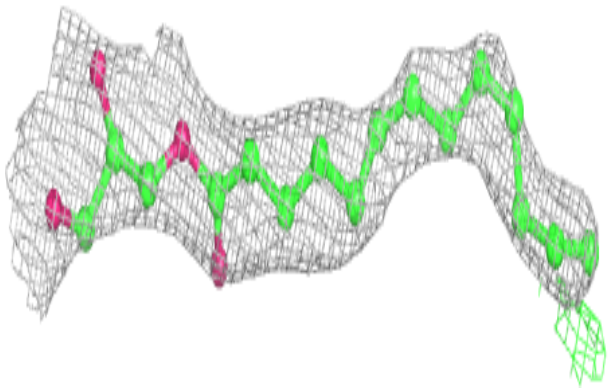


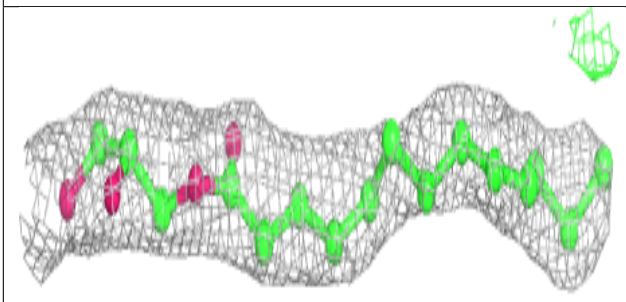


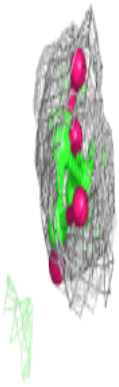


Electron density around OLC E 306:

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

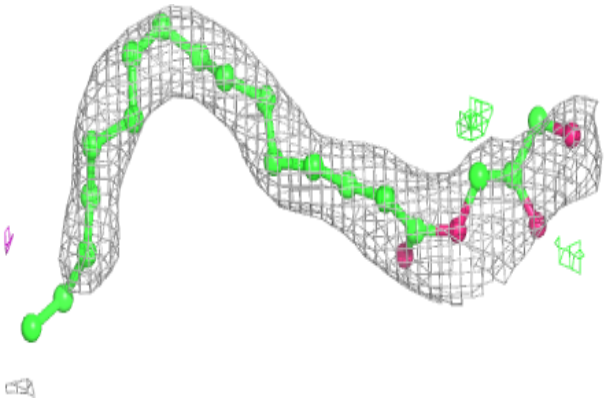


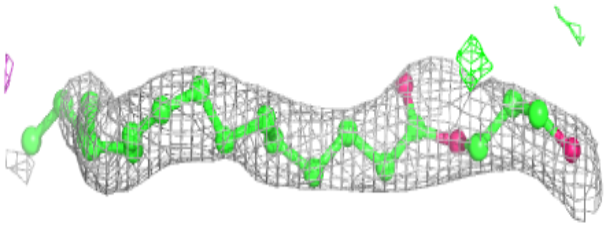


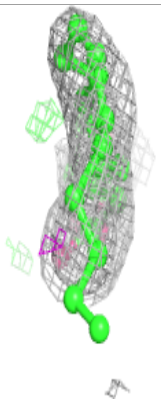


Electron density around OLC C 302:

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

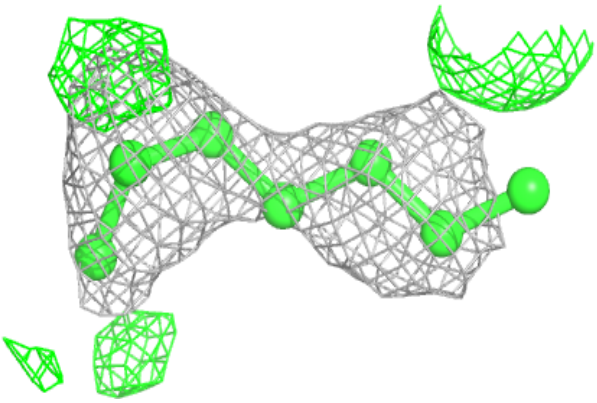


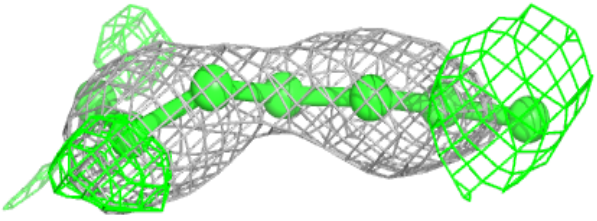


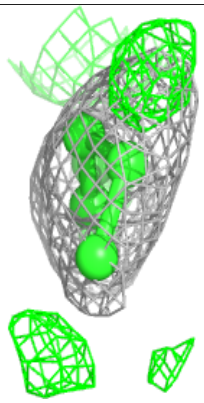


Electron density around LFA A 307:

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

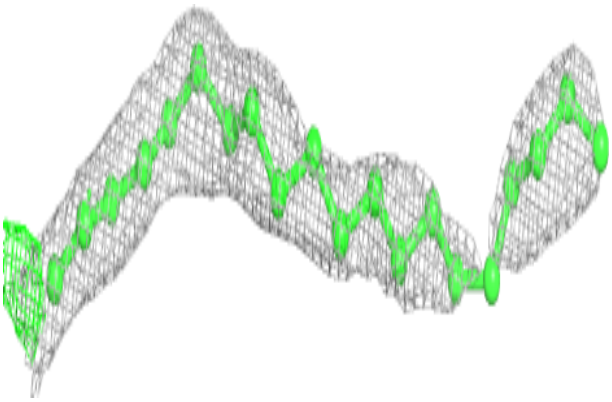


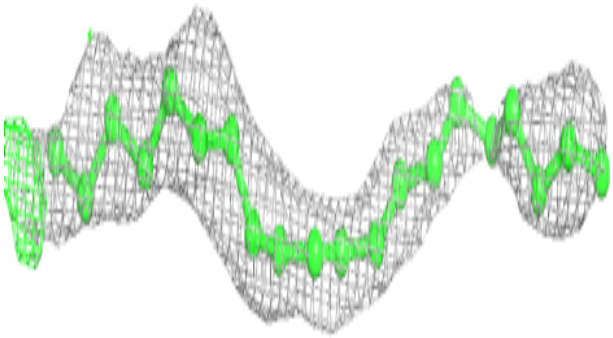


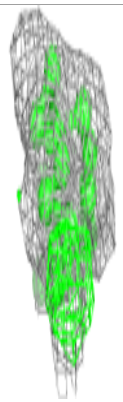


Electron density around LFA D 410:

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

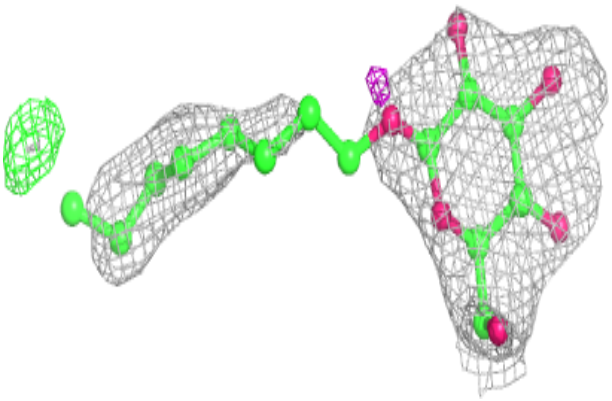


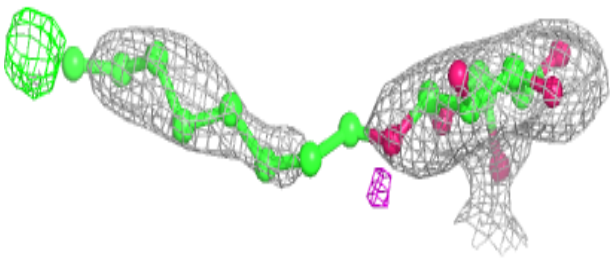


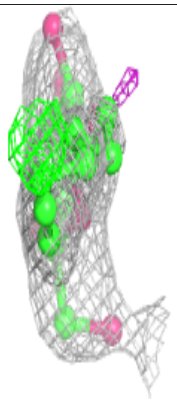


Electron density around BOG B 312:

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

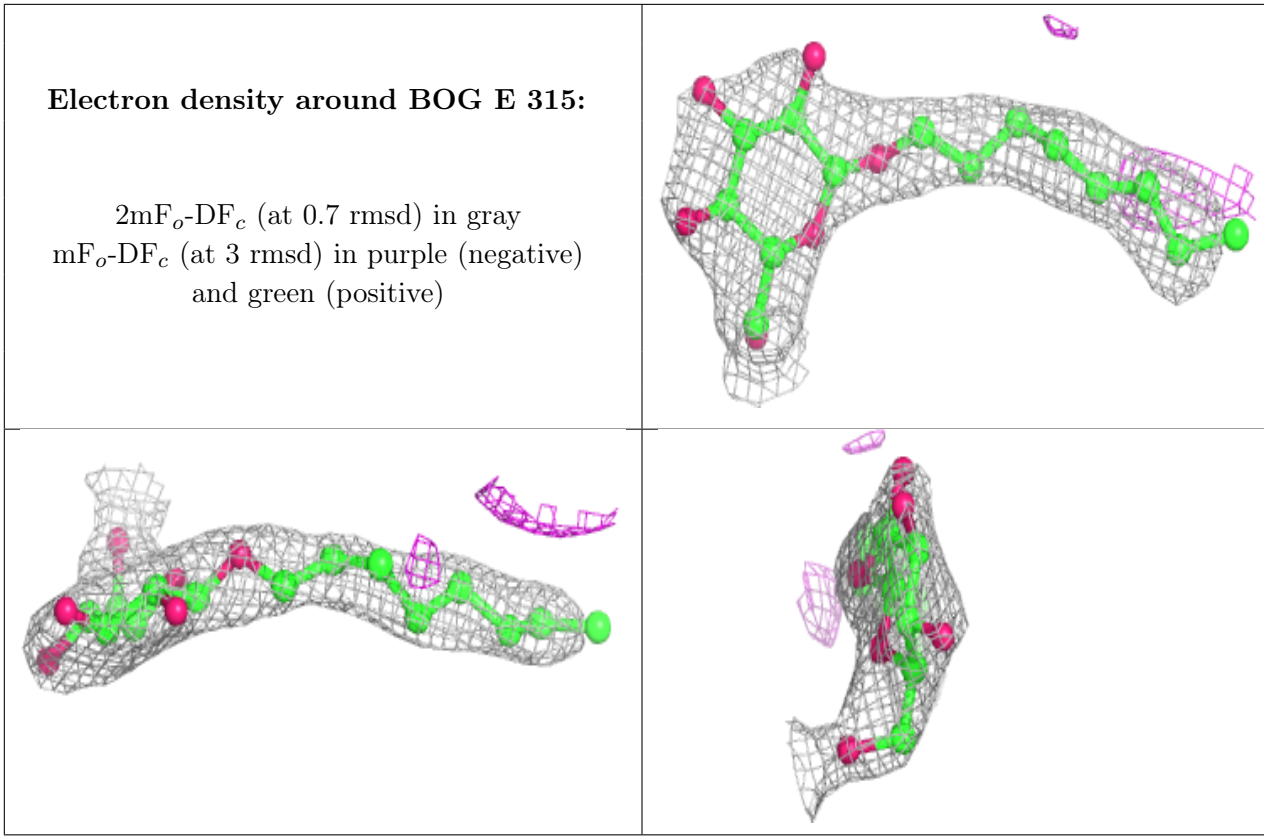






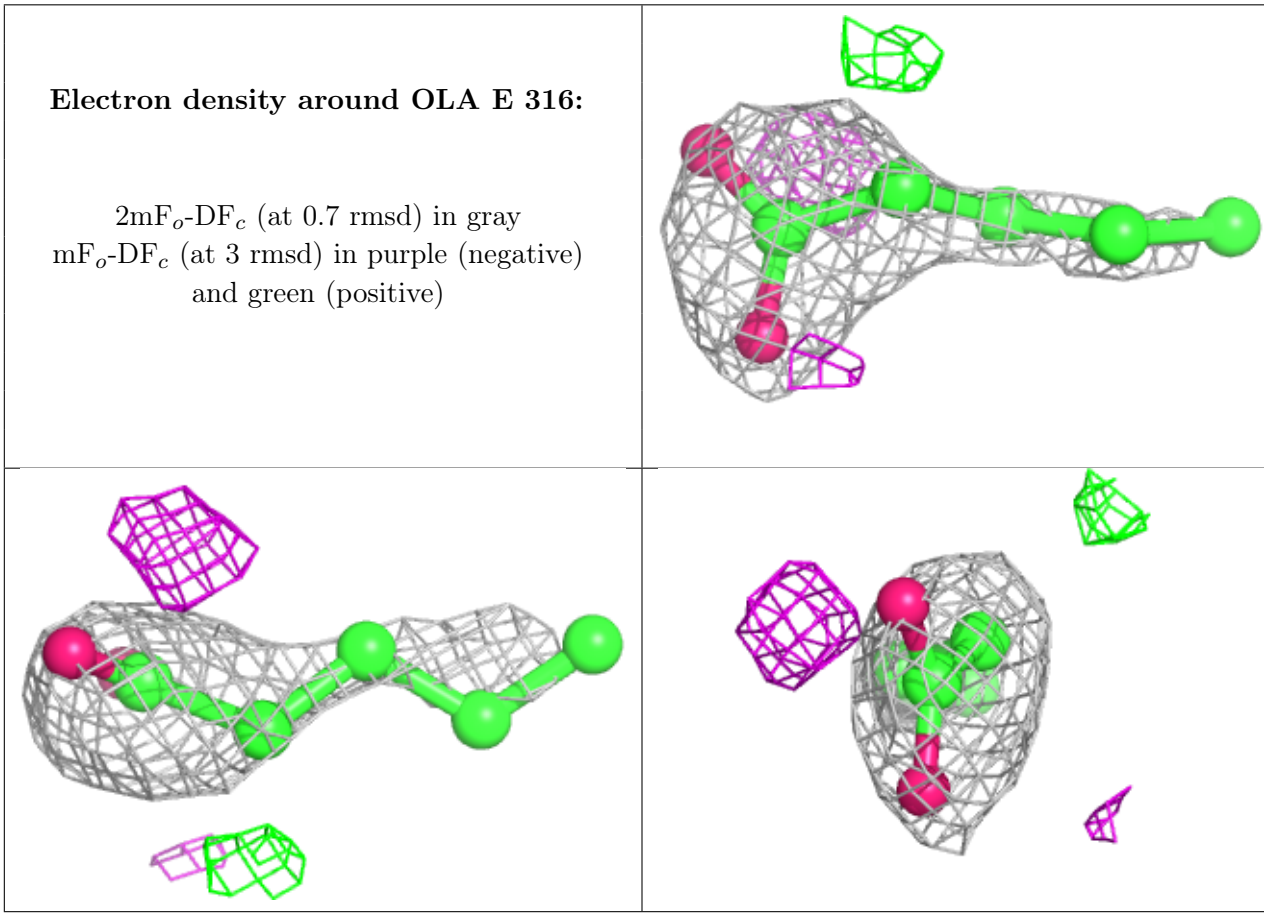
Electron density around BOG E 315:

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



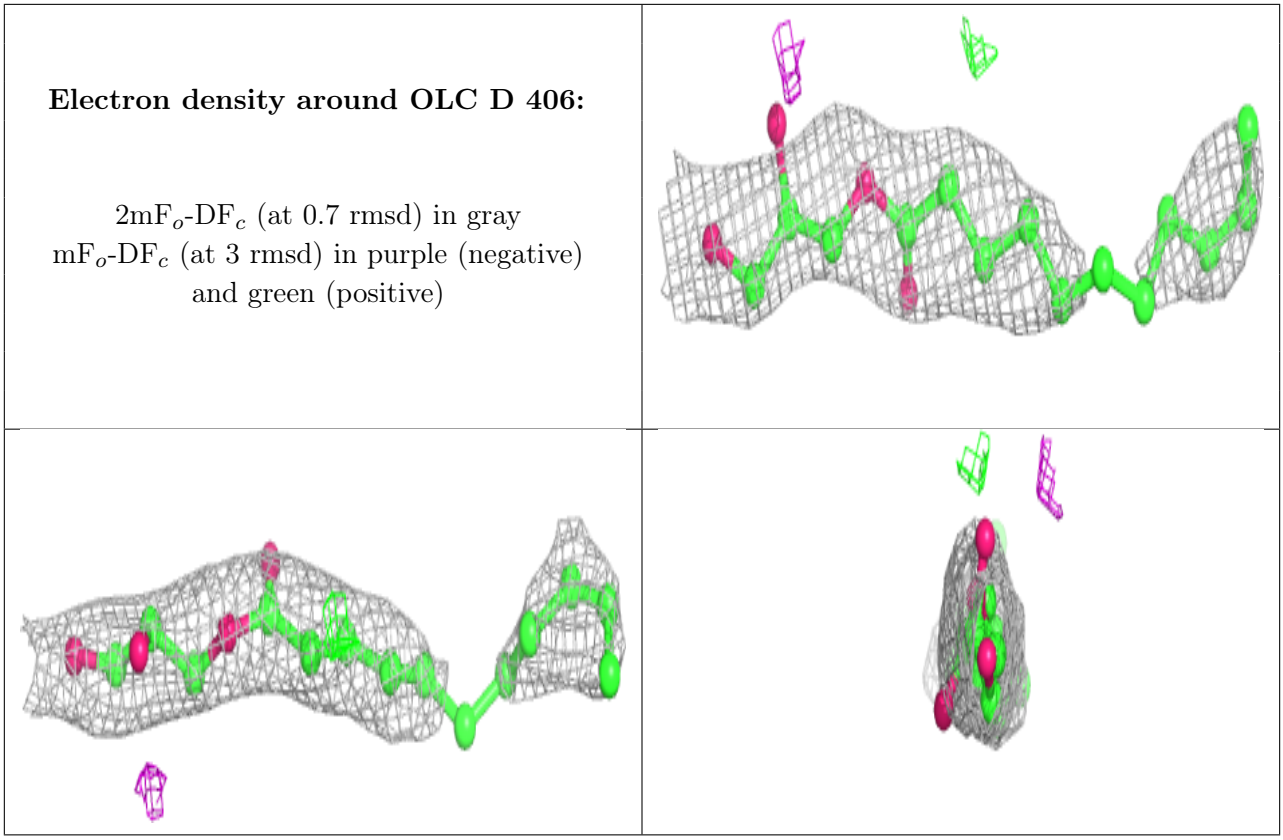
Electron density around OLA E 316:

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



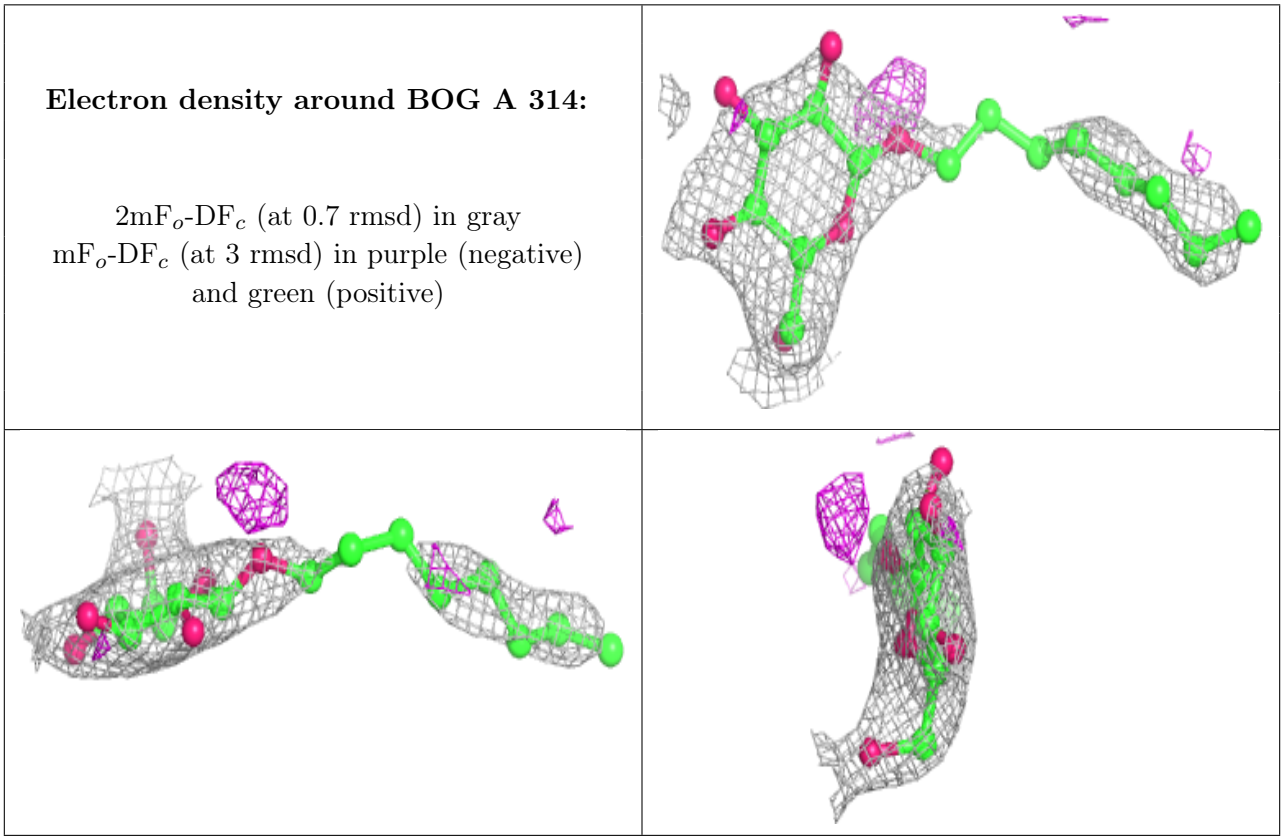
Electron density around OLC D 406:

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



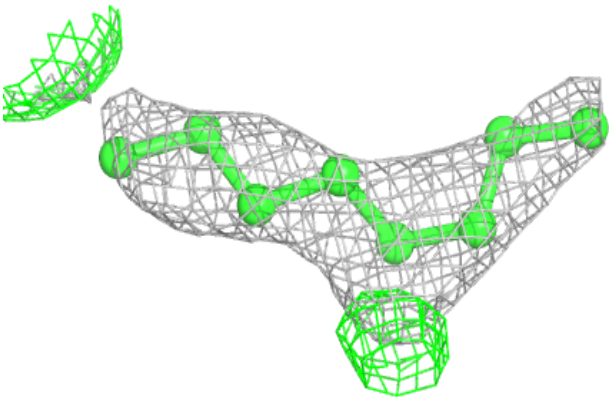
Electron density around BOG A 314:

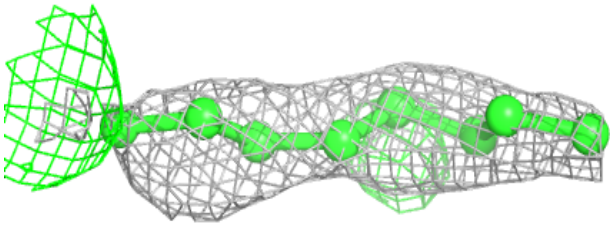
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

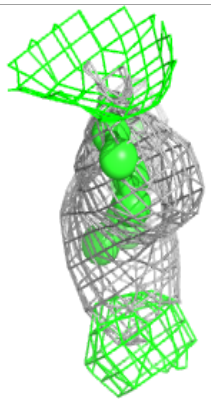


Electron density around OLC E 304:

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

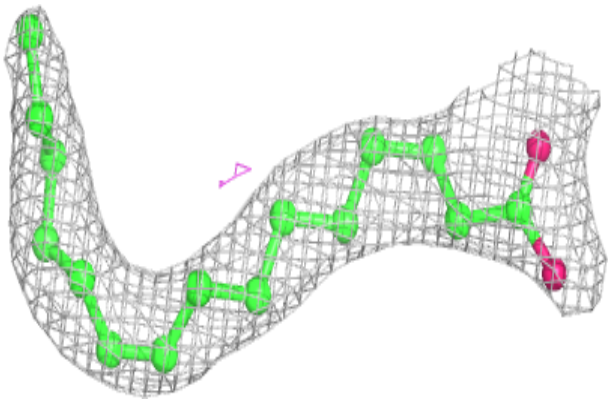


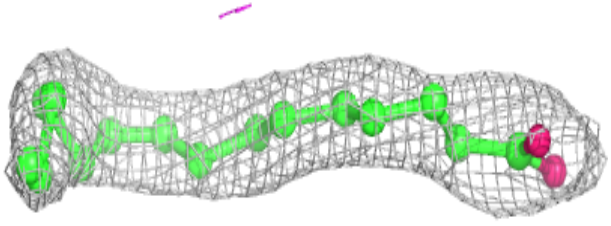


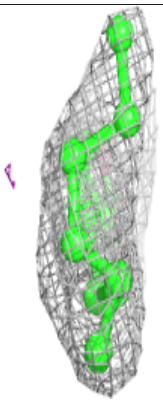


Electron density around OLC A 302:

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

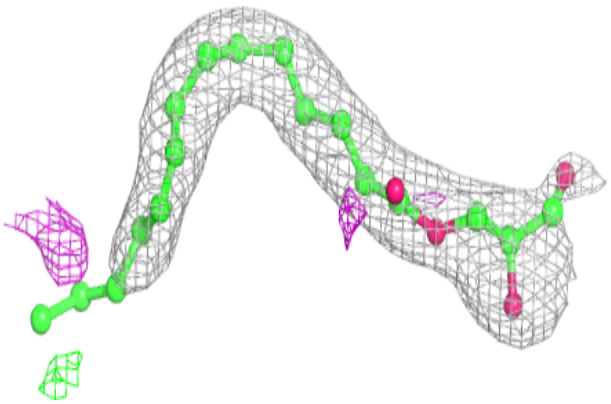


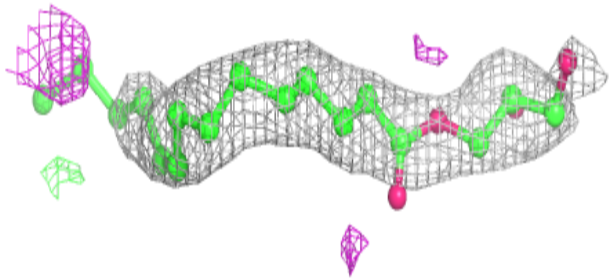


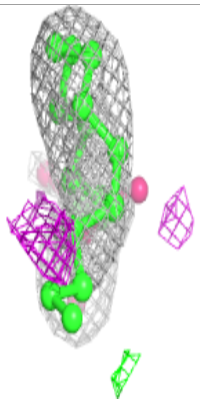


Electron density around OLC B 303:

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

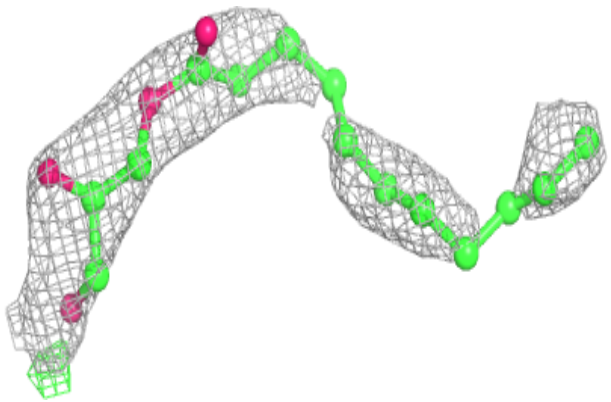


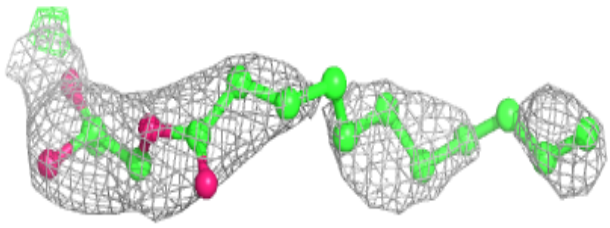


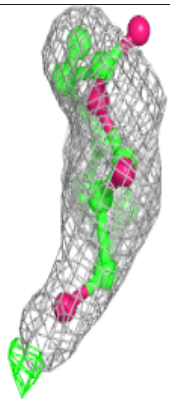


Electron density around OLC C 315:

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

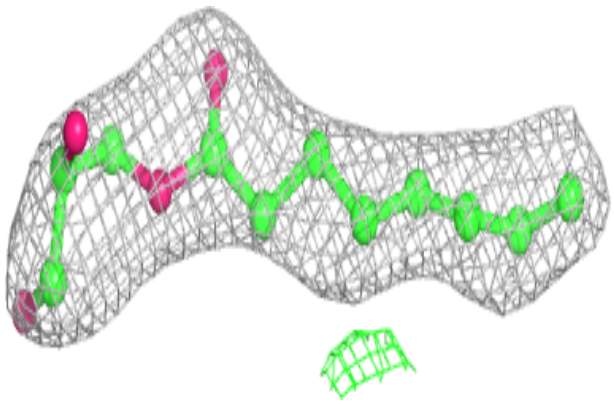


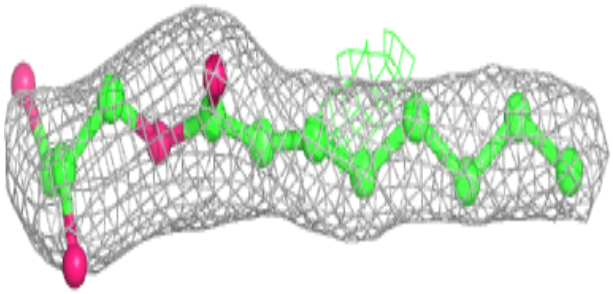


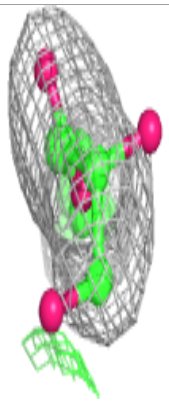


Electron density around OLC E 308:

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

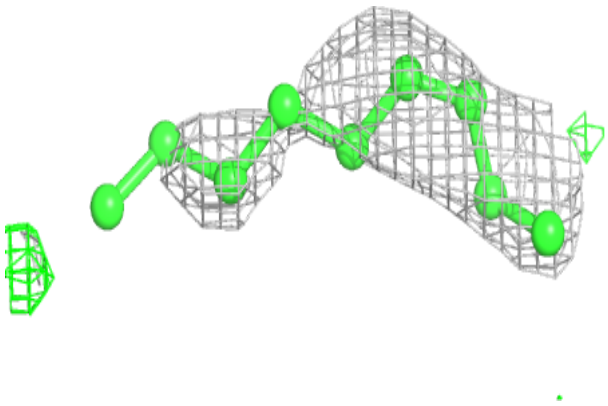


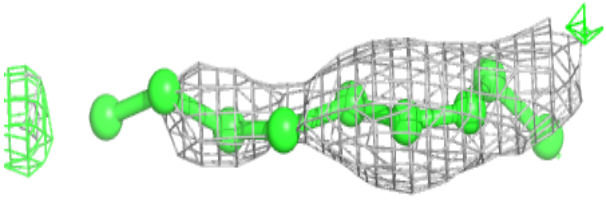


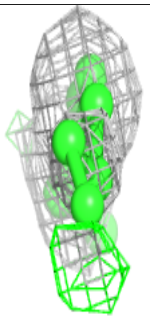


Electron density around OLC A 301:

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

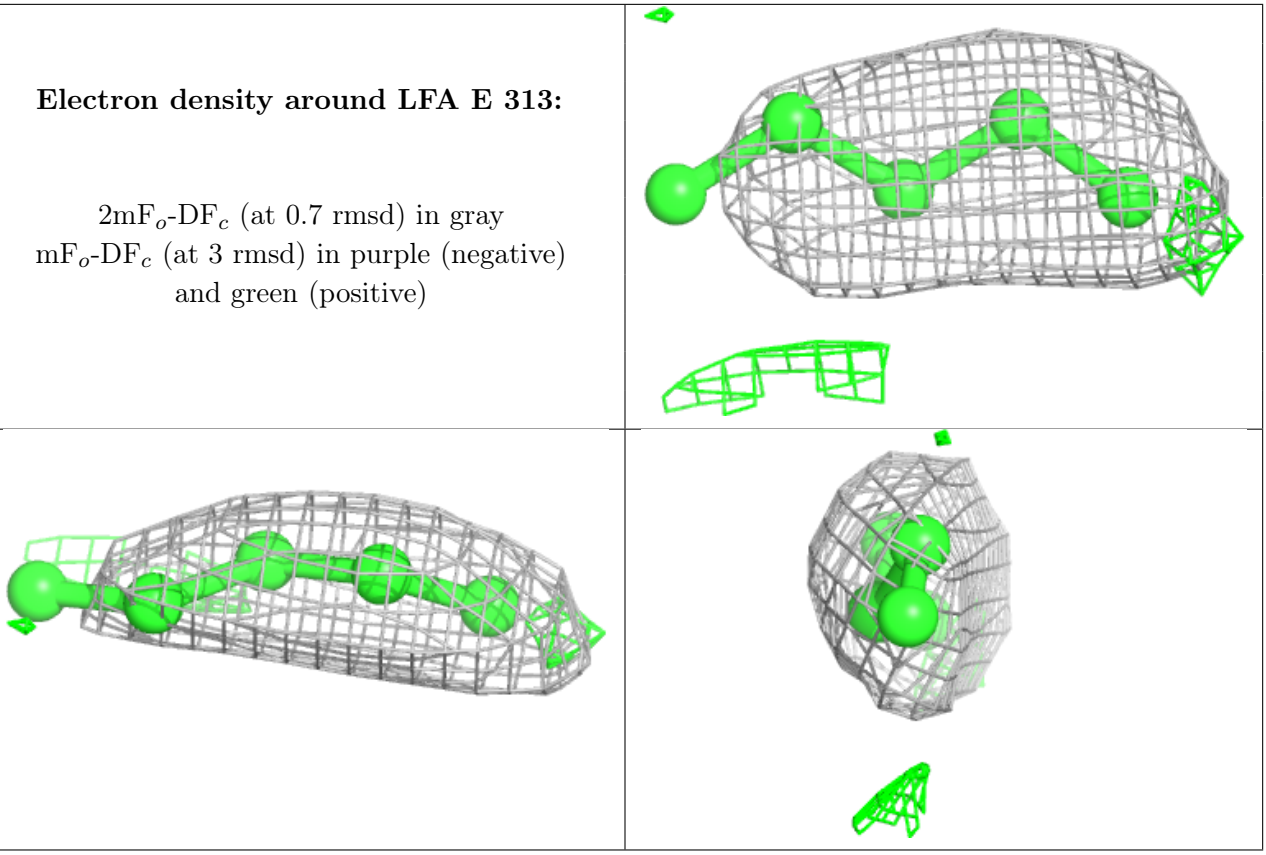






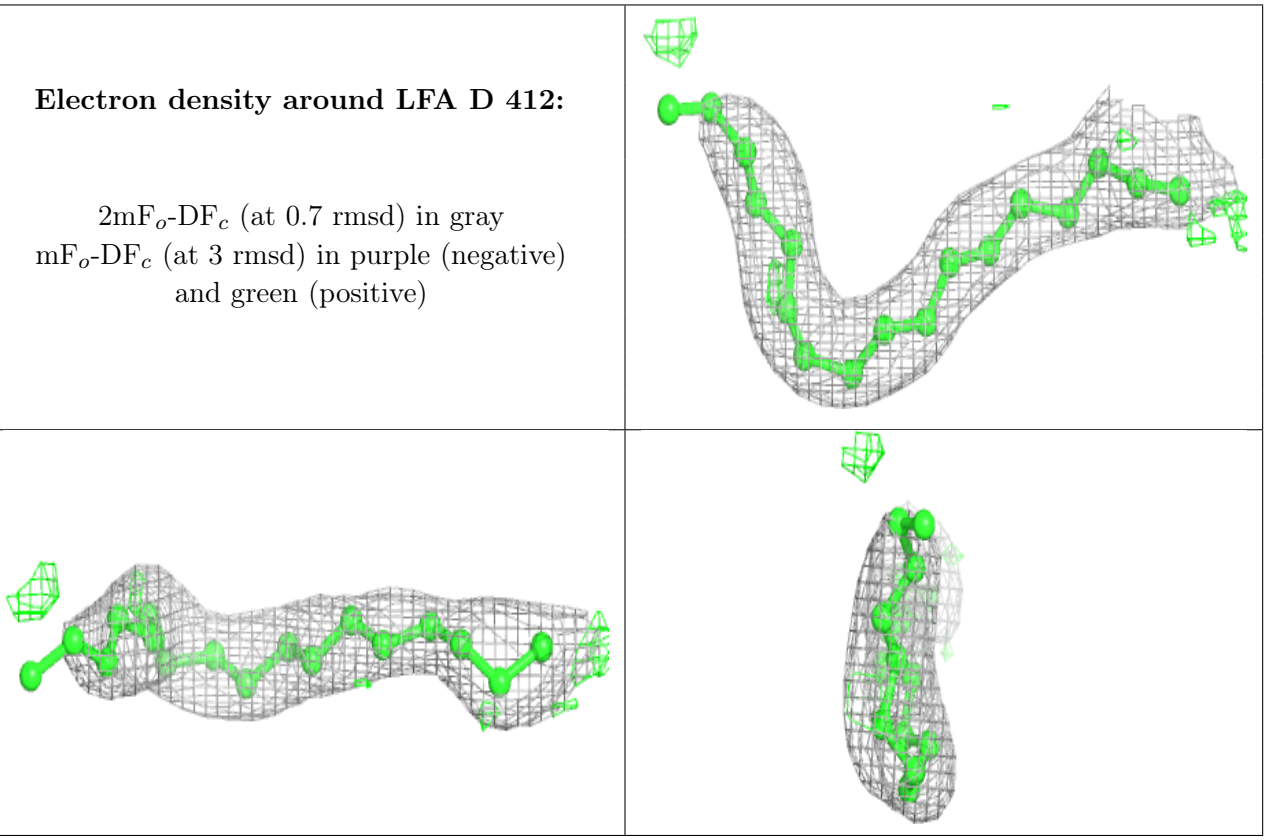
Electron density around LFA E 313:

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



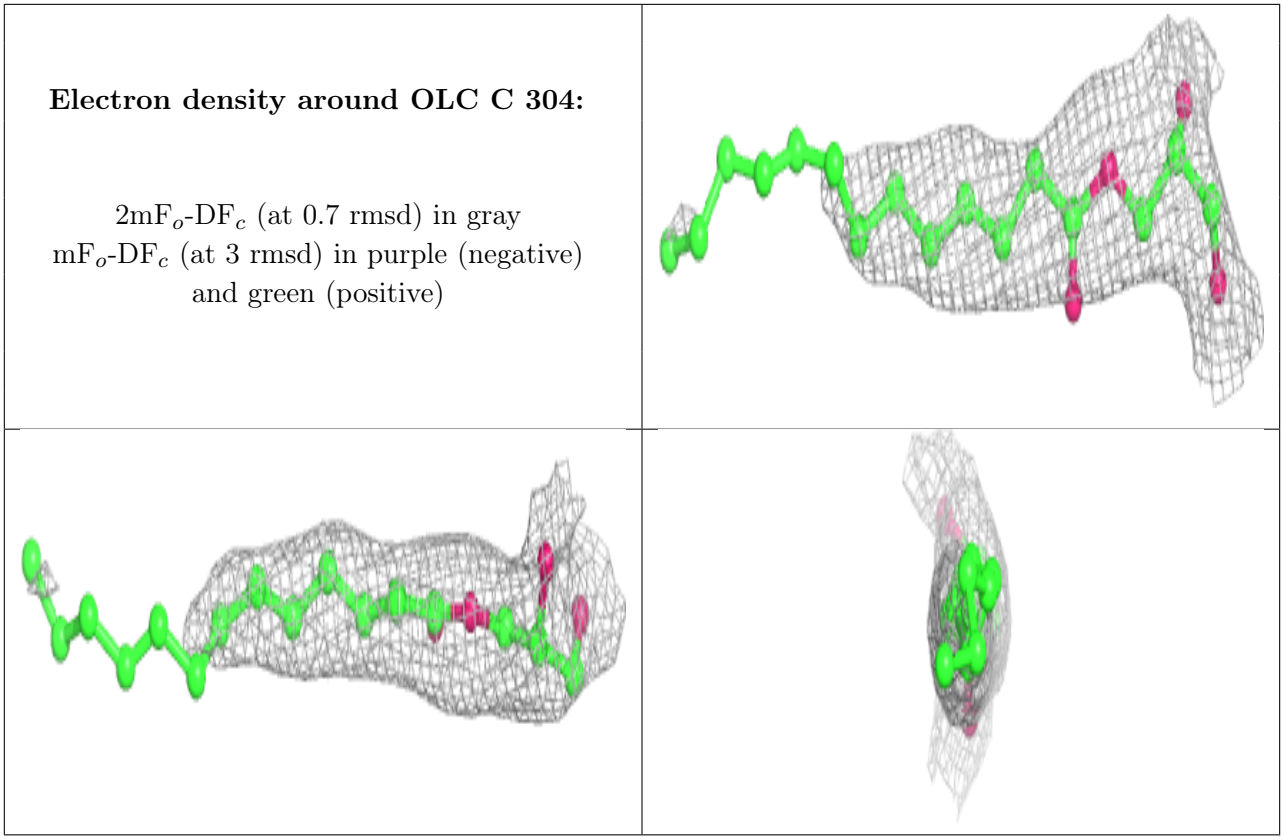
Electron density around LFA D 412:

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



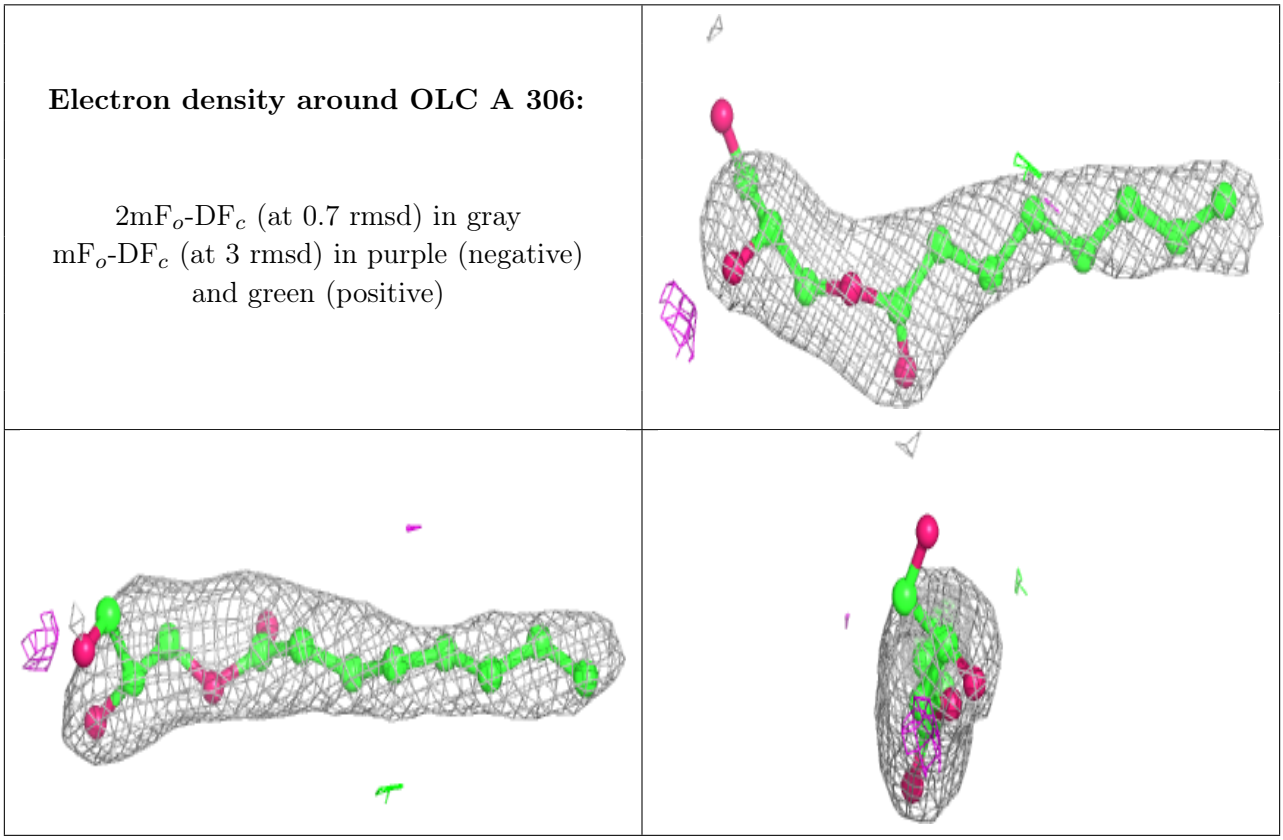
Electron density around OLC C 304:

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



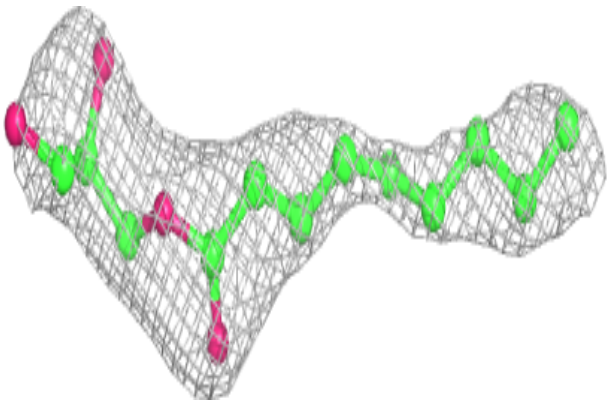
Electron density around OLC A 306:

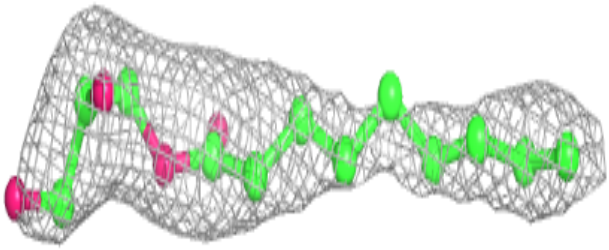
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

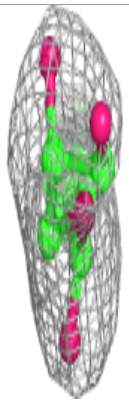


Electron density around OLC C 306:

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

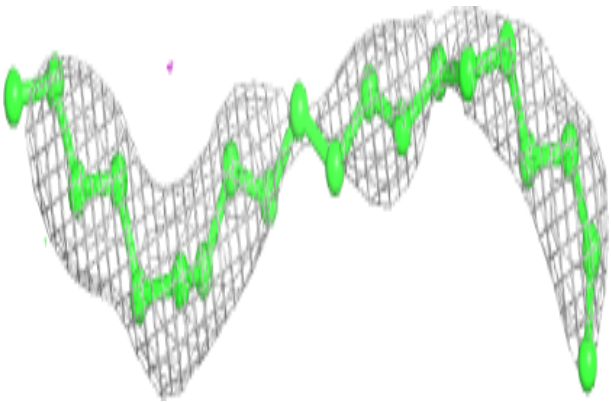


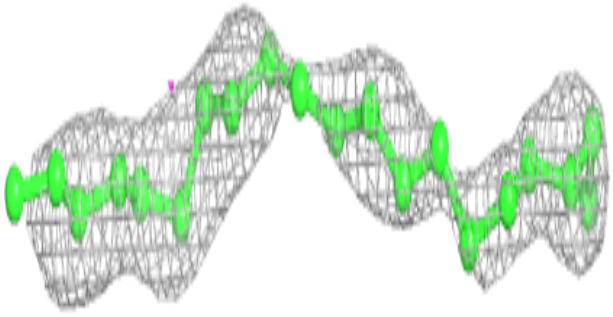


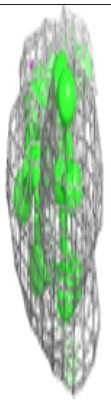


Electron density around LFA C 309:

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

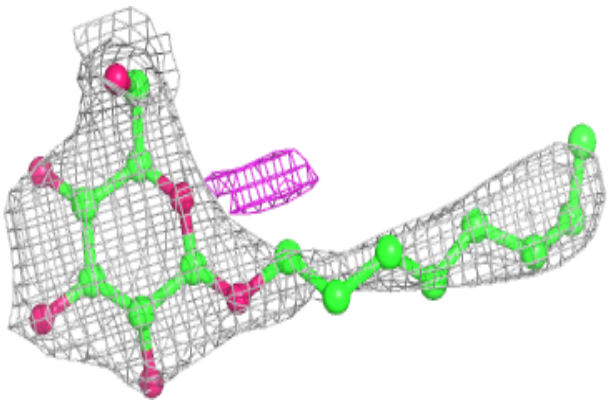


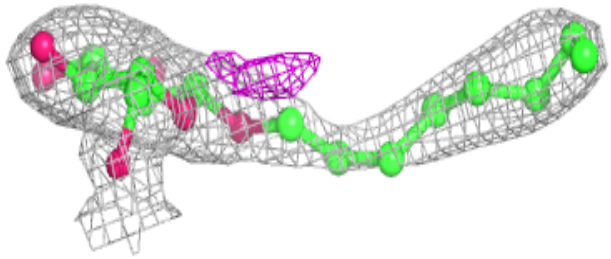


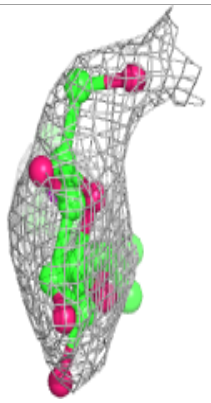


Electron density around BOG D 416:

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

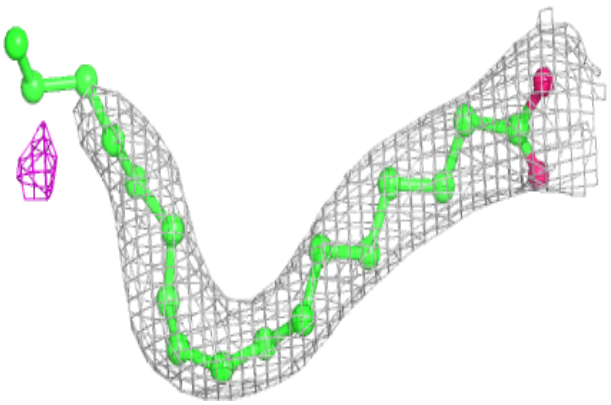


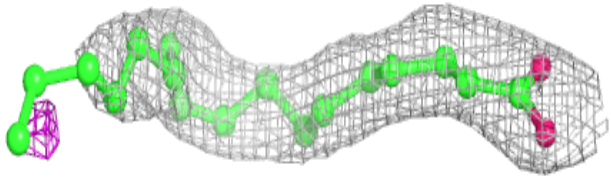


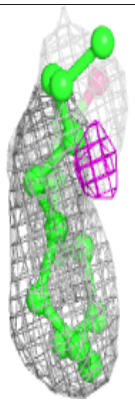


Electron density around OLC E 301:

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

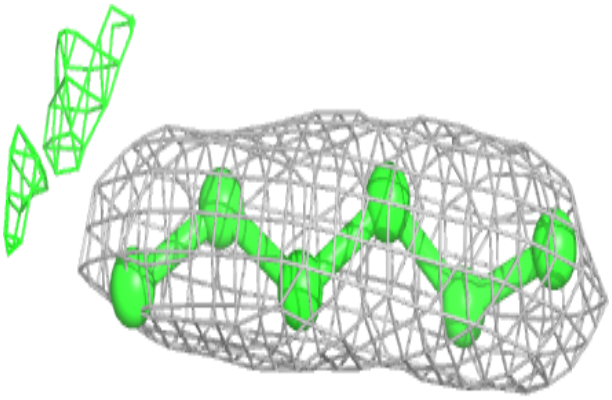


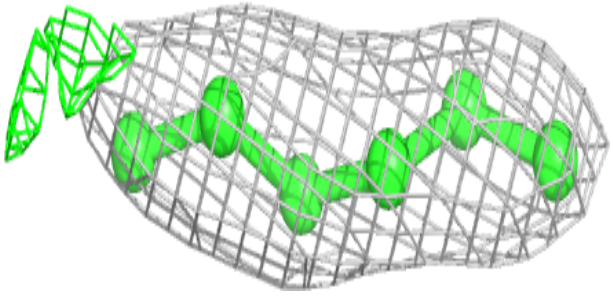


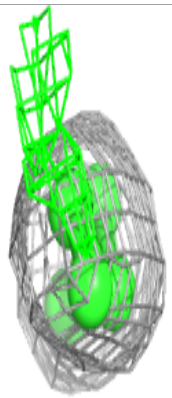


Electron density around LFA A 311:

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

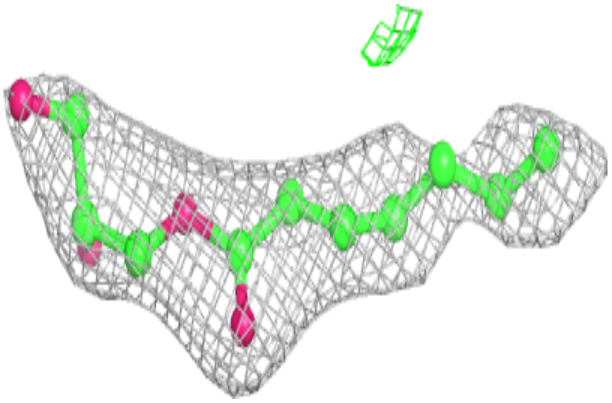


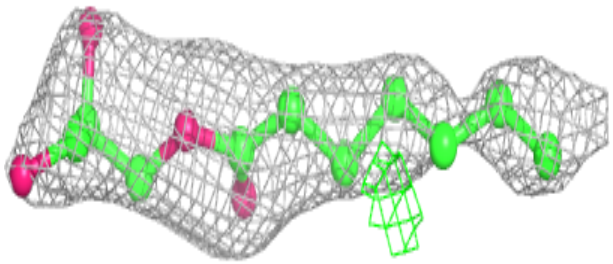


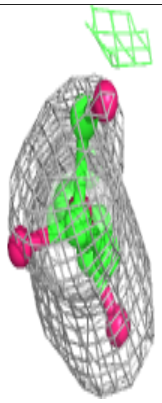


Electron density around OLC D 408:

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

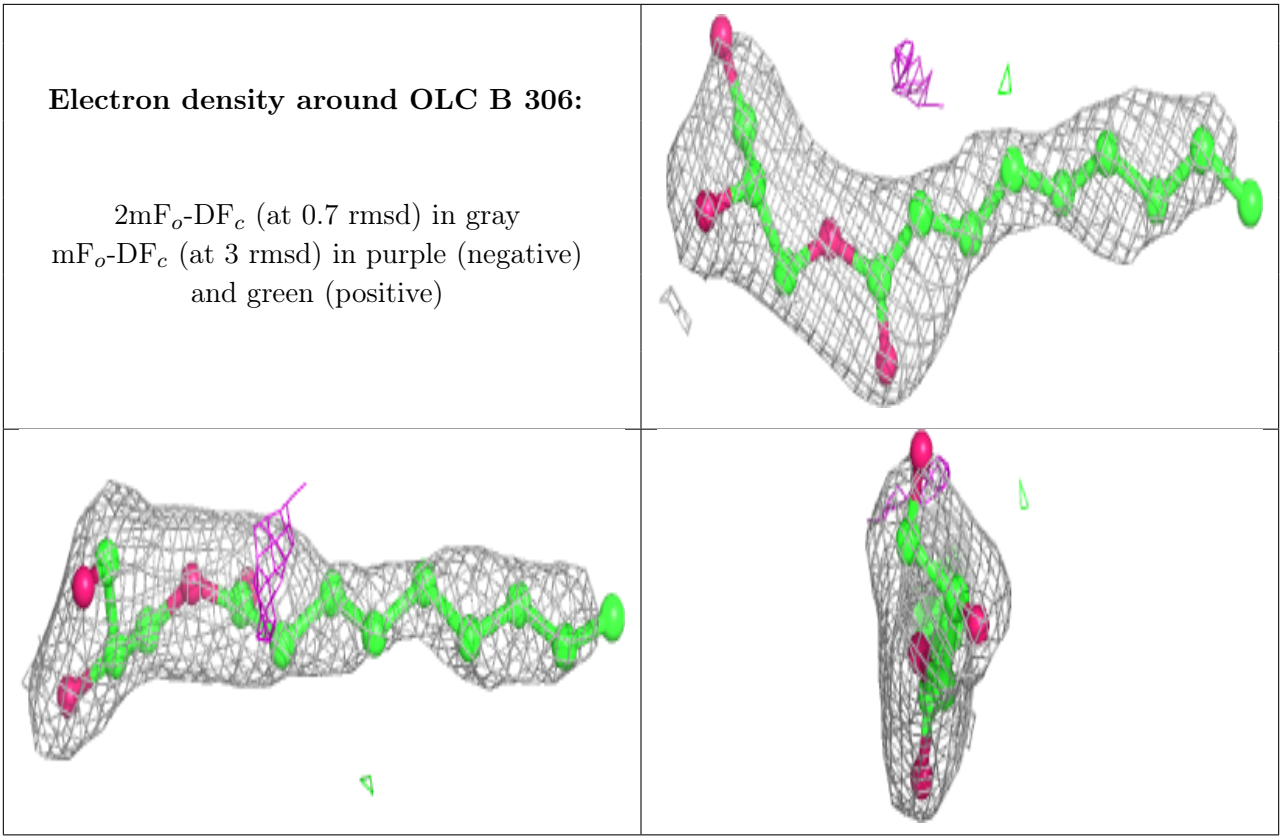






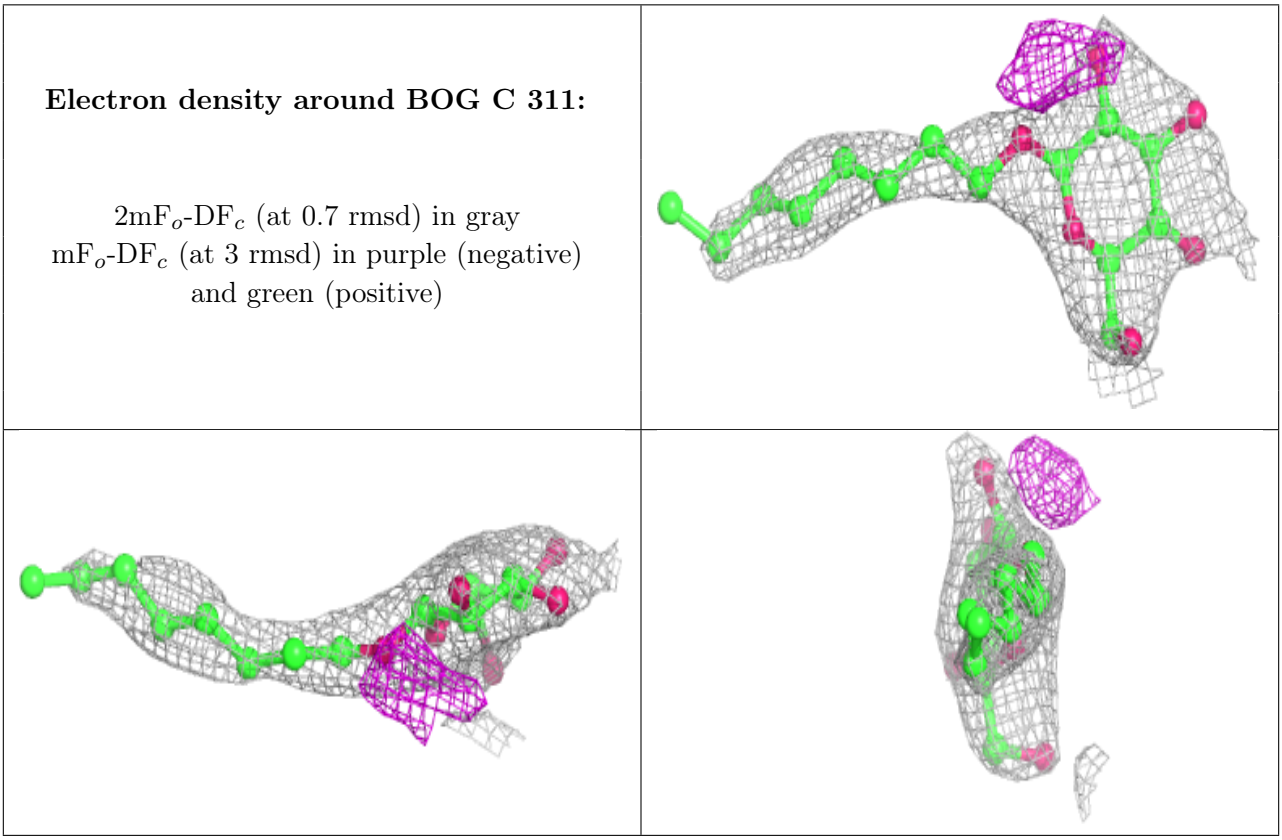
Electron density around OLC B 306:

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



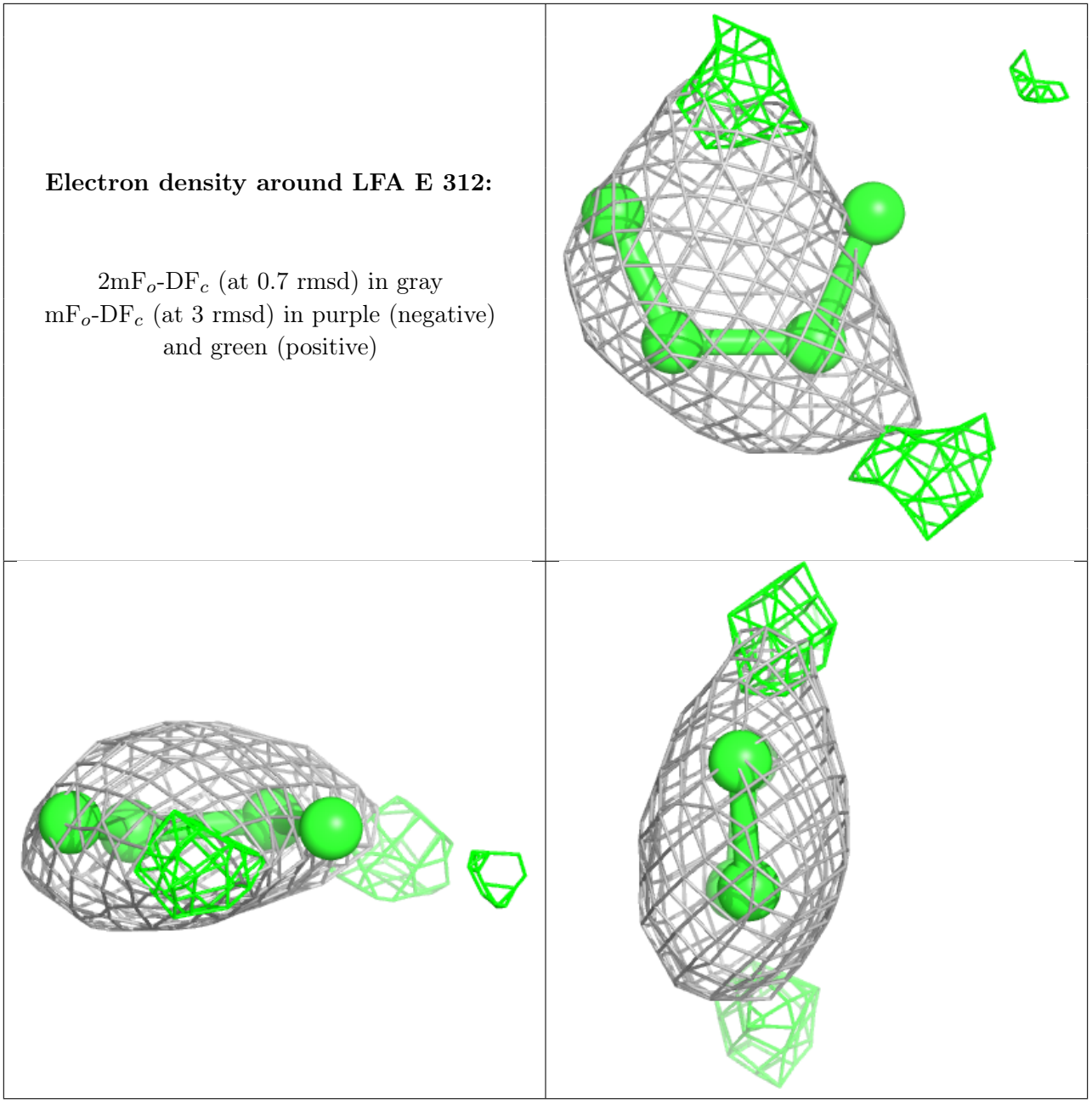
Electron density around BOG C 311:

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



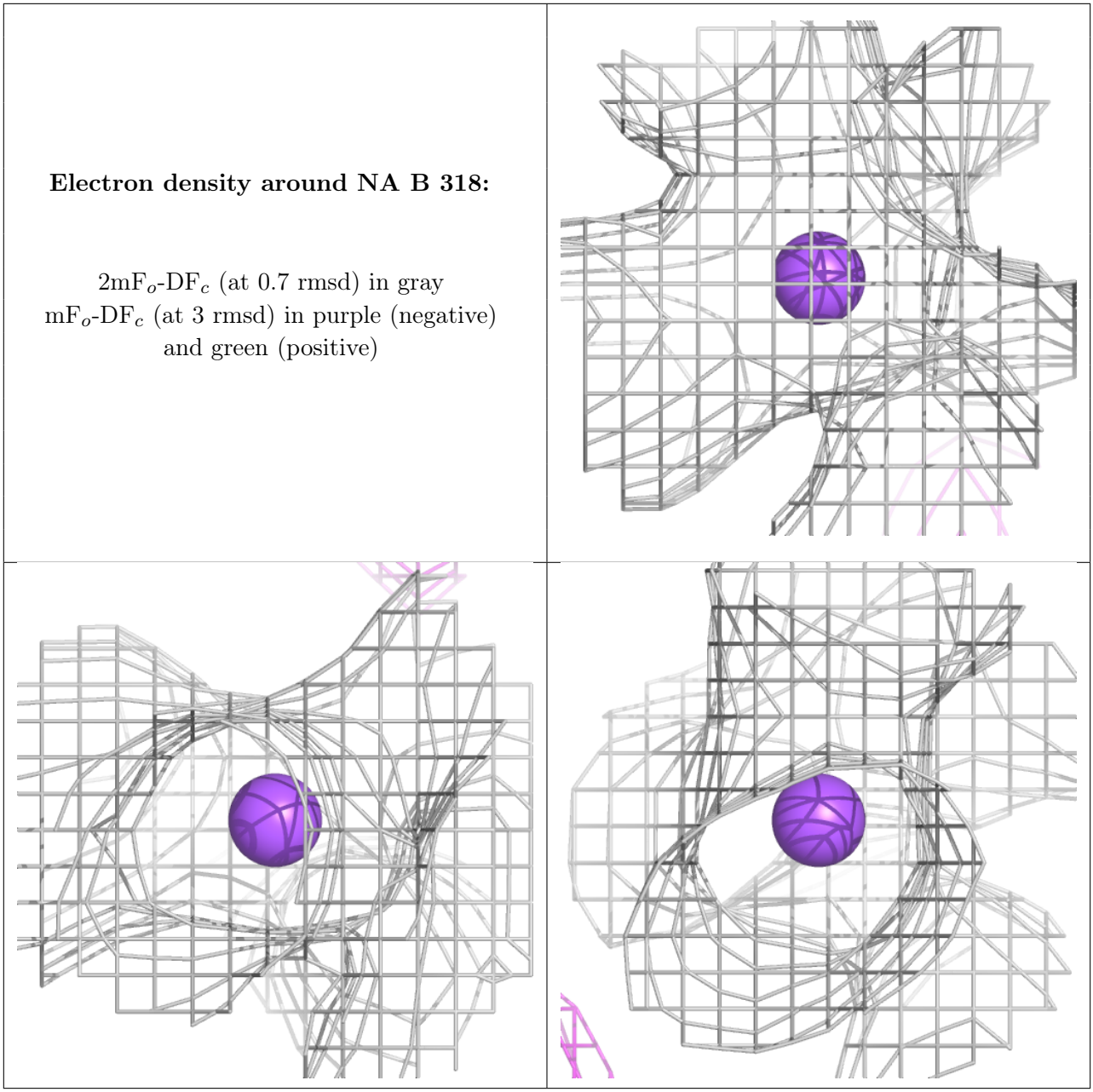
Electron density around LFA E 312:

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



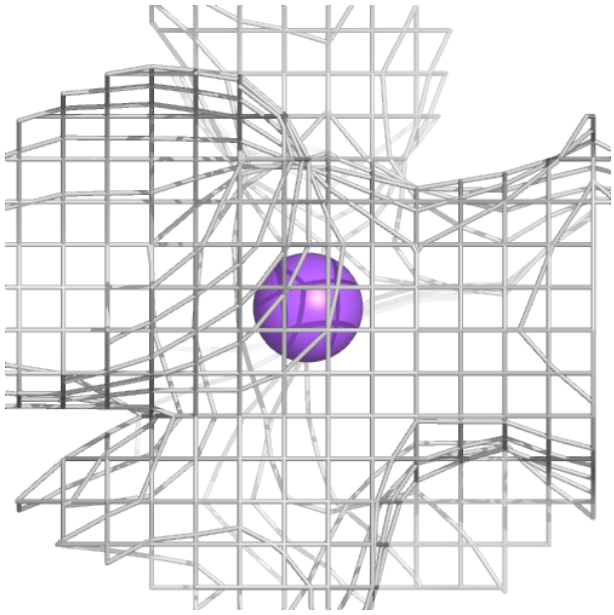
Electron density around NA B 318:

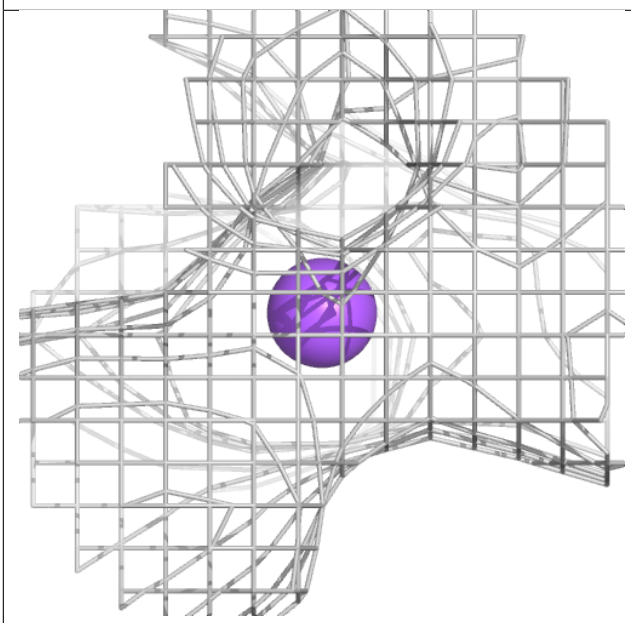
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

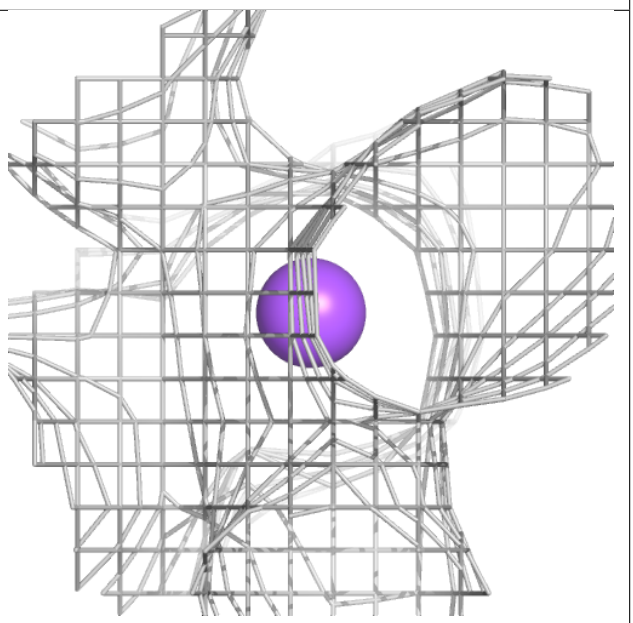


Electron density around NA D 418:

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

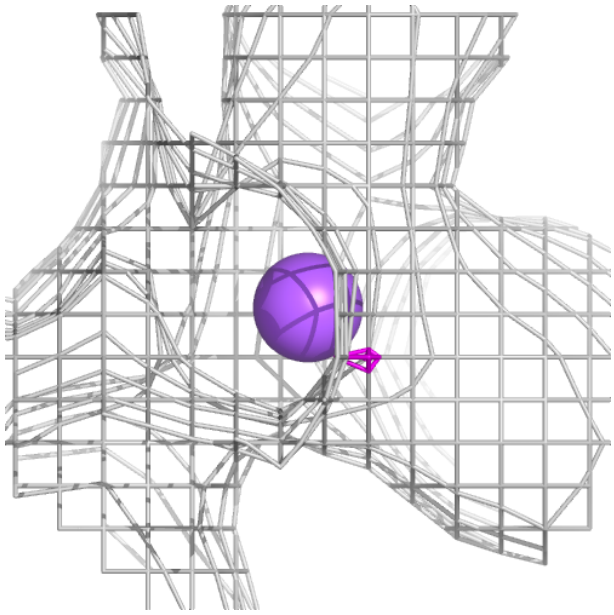


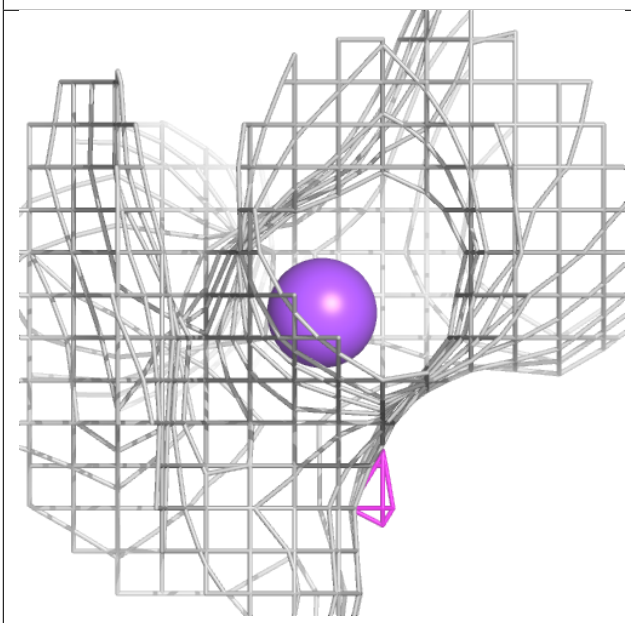


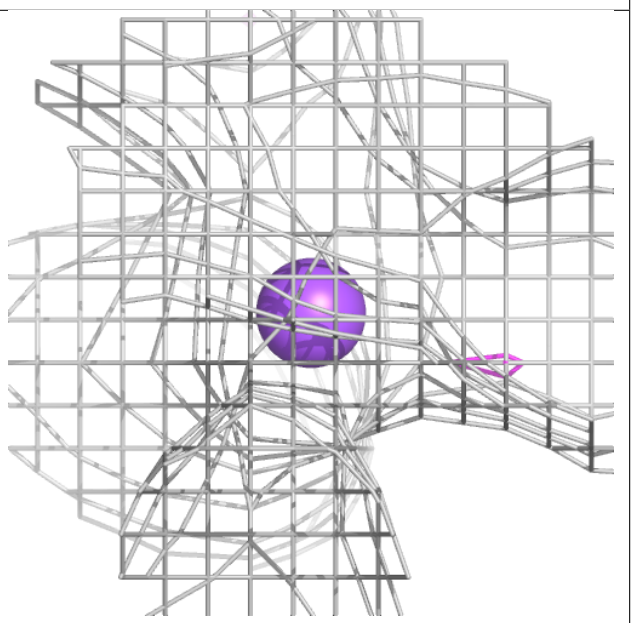


Electron density around NA E 318:

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

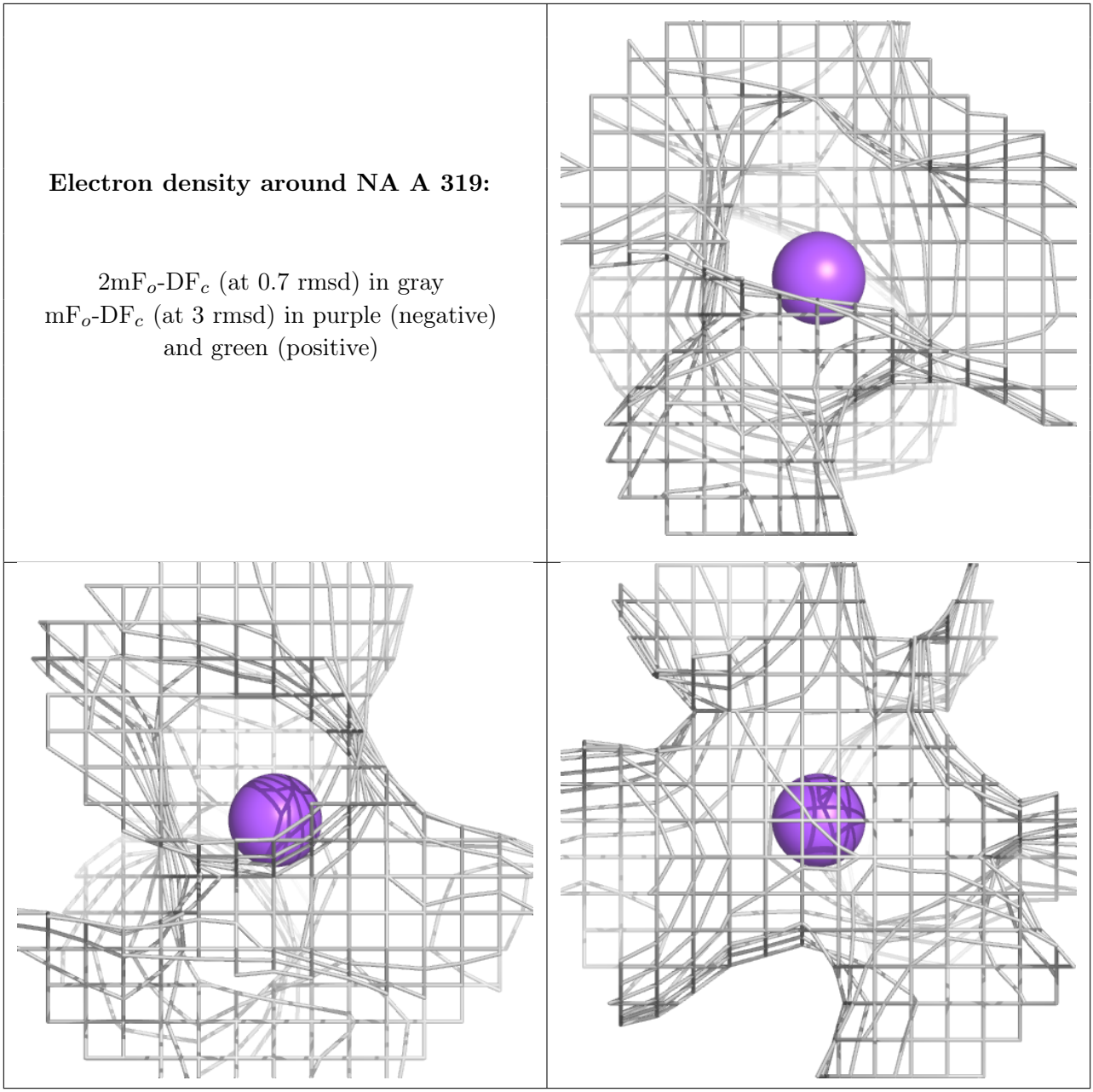






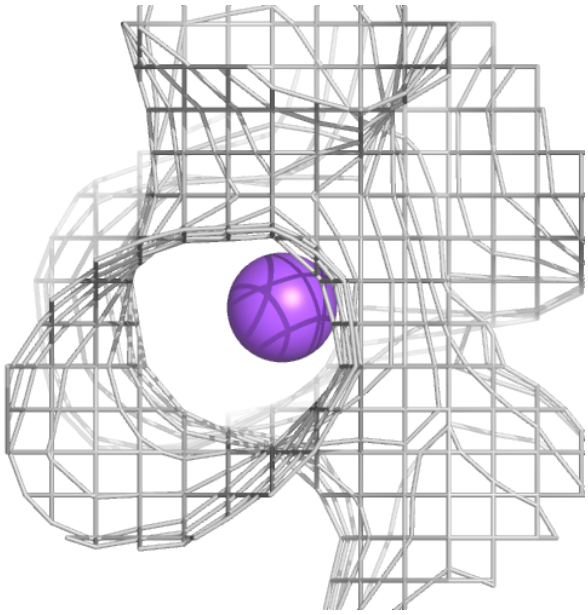
Electron density around NA A 319:

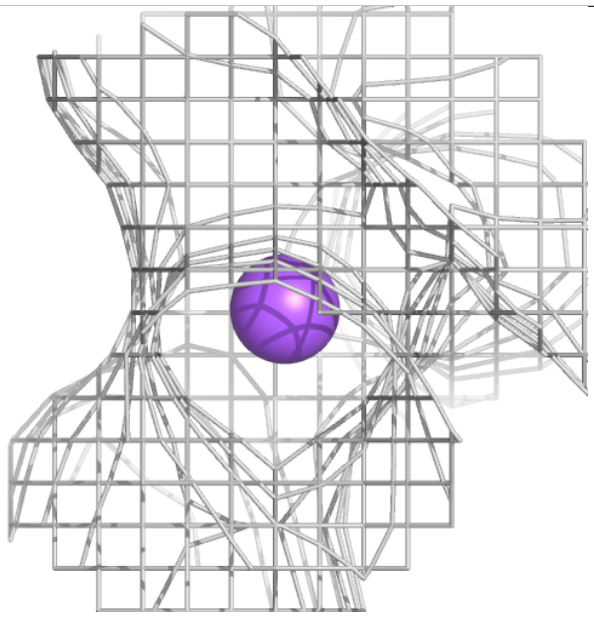
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

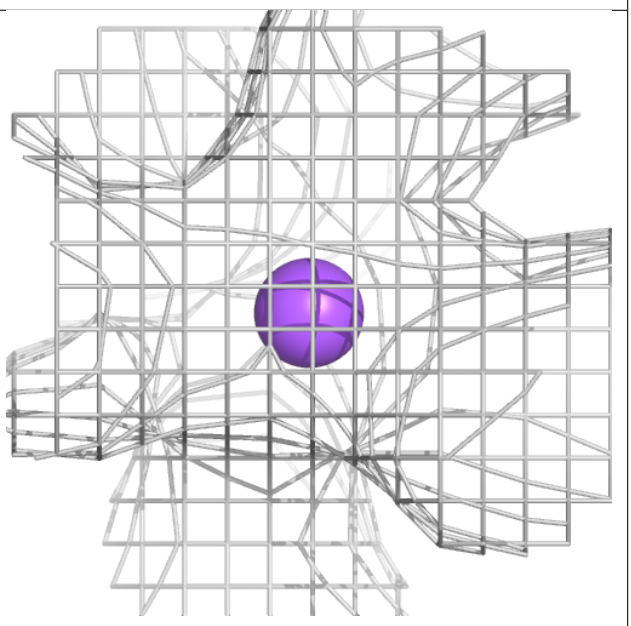


Electron density around NA C 316:

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

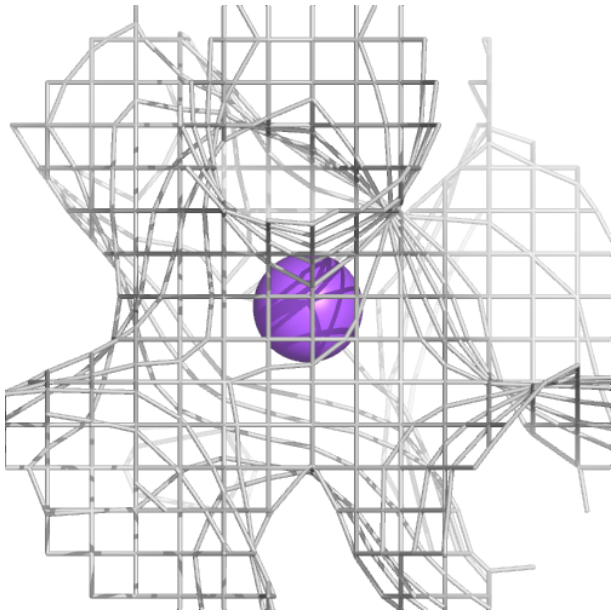


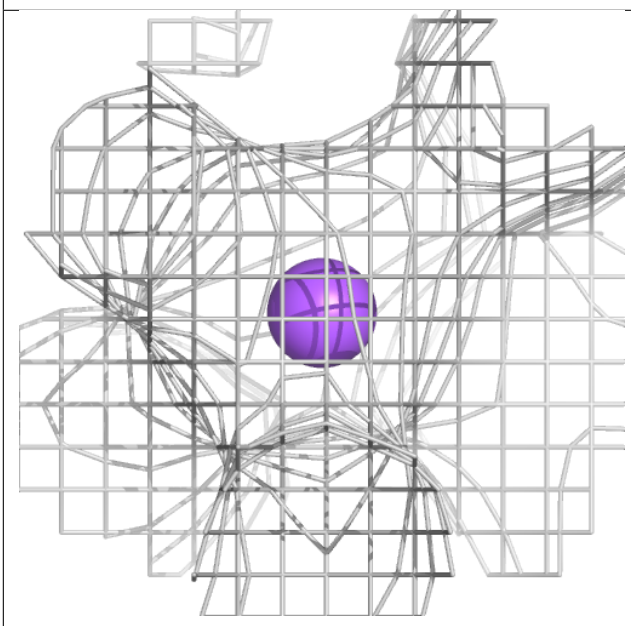


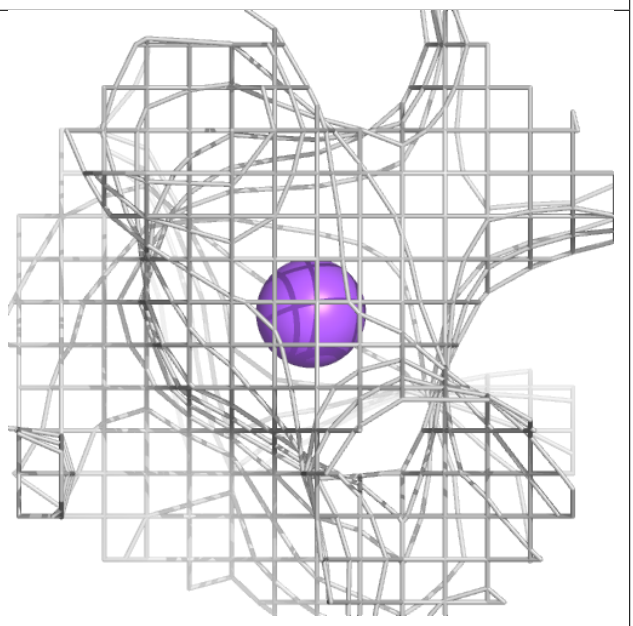


Electron density around NA A 313:

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

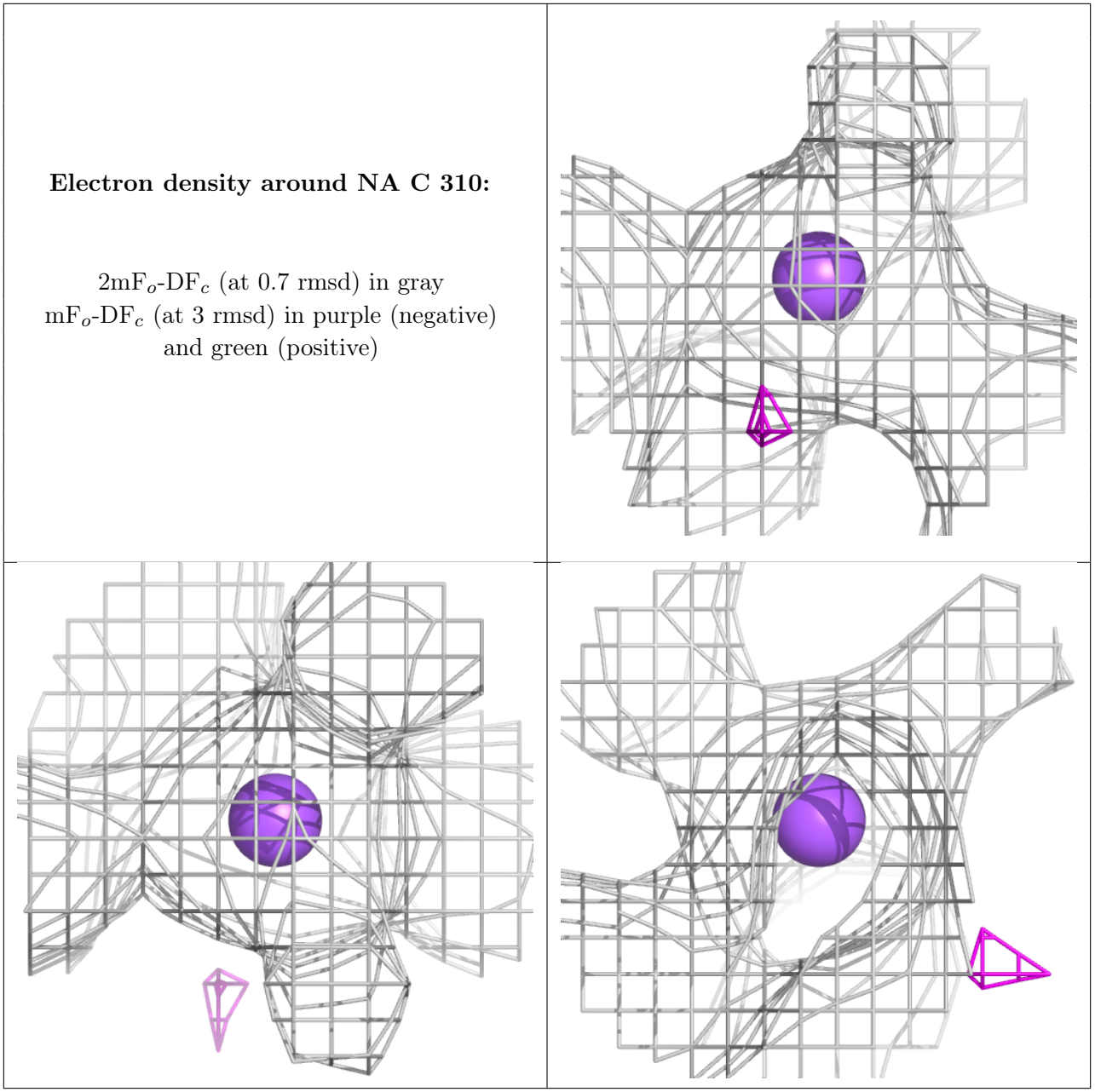






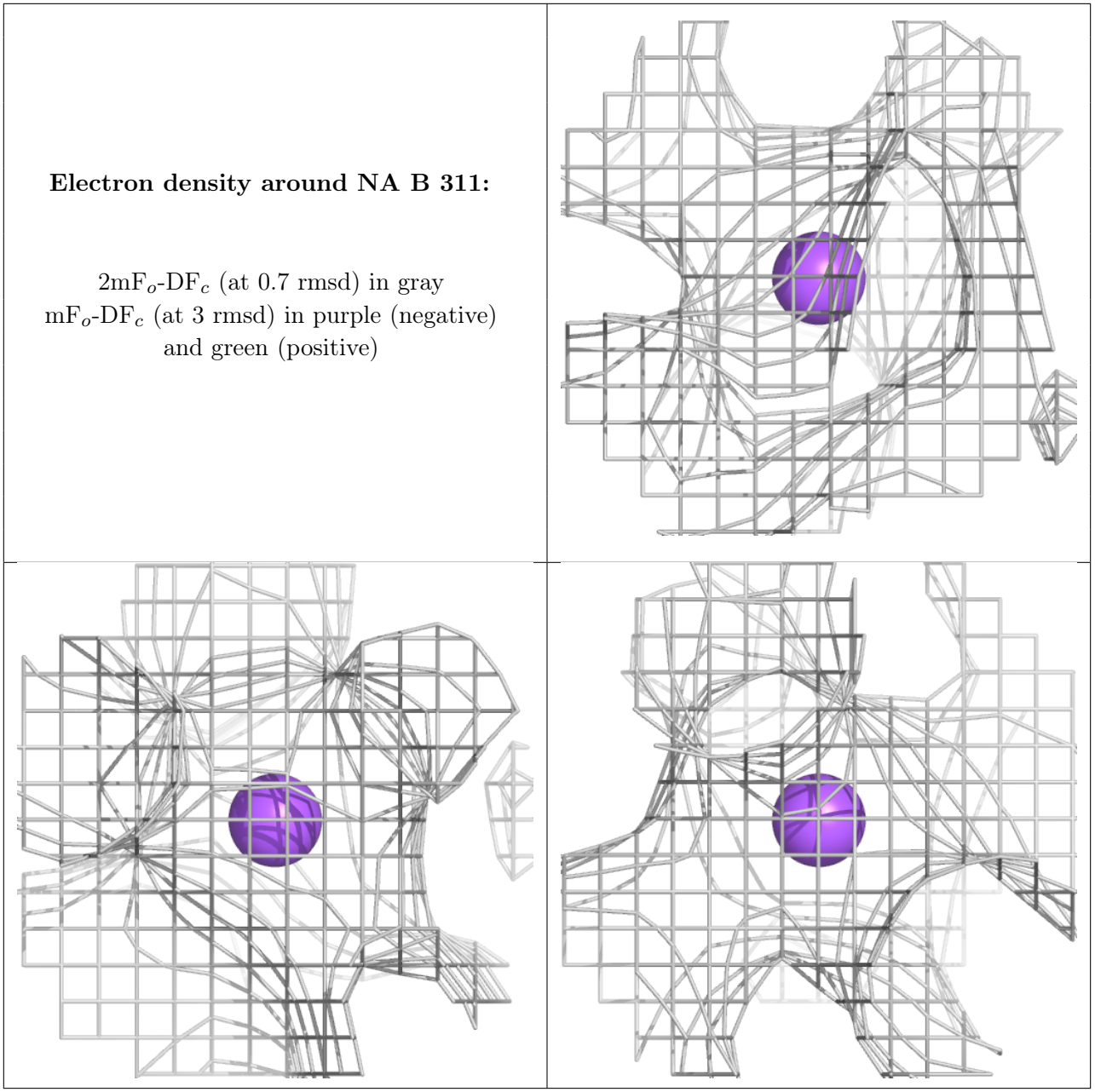
Electron density around NA C 310:

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



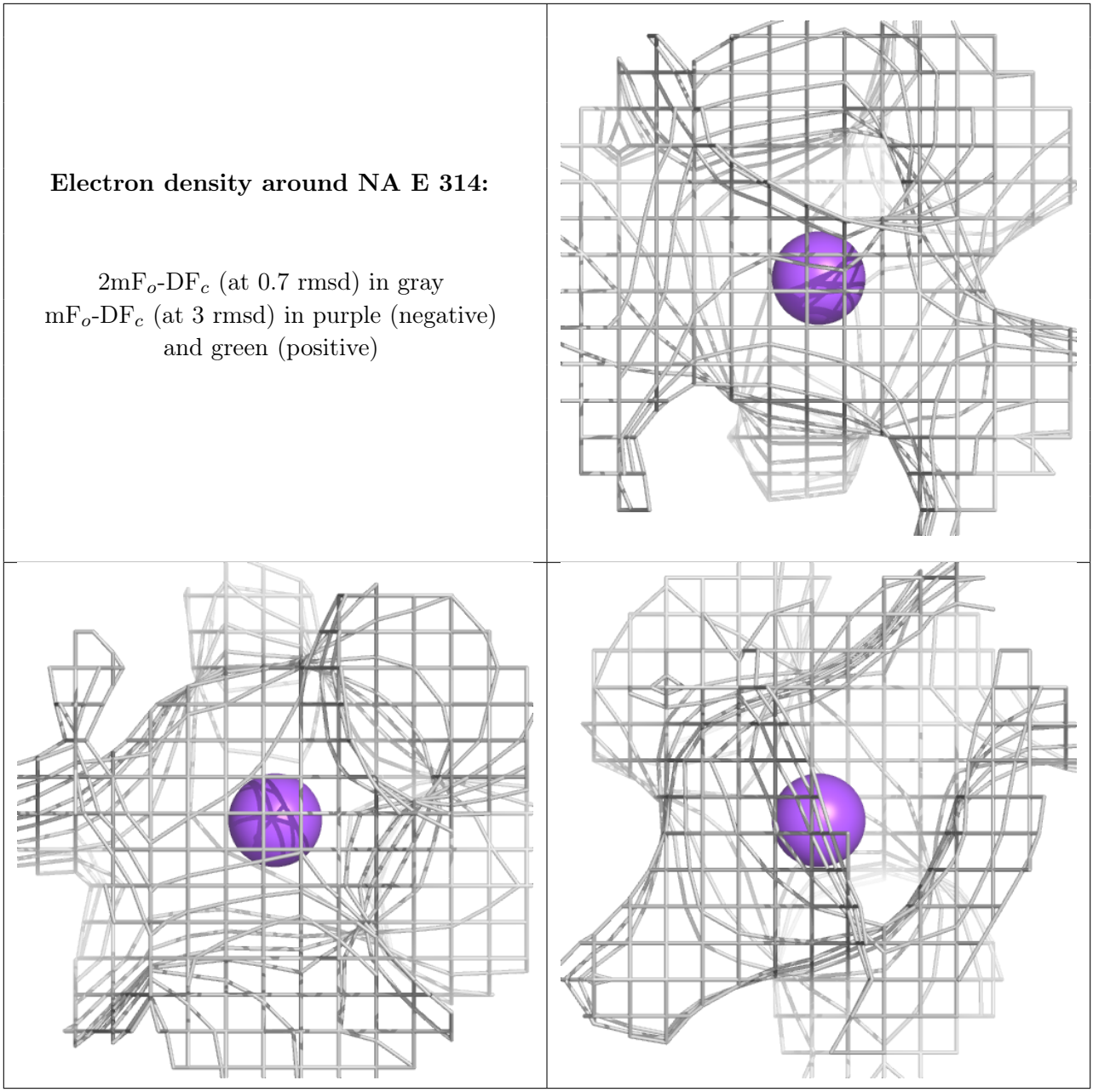
Electron density around NA B 311:

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



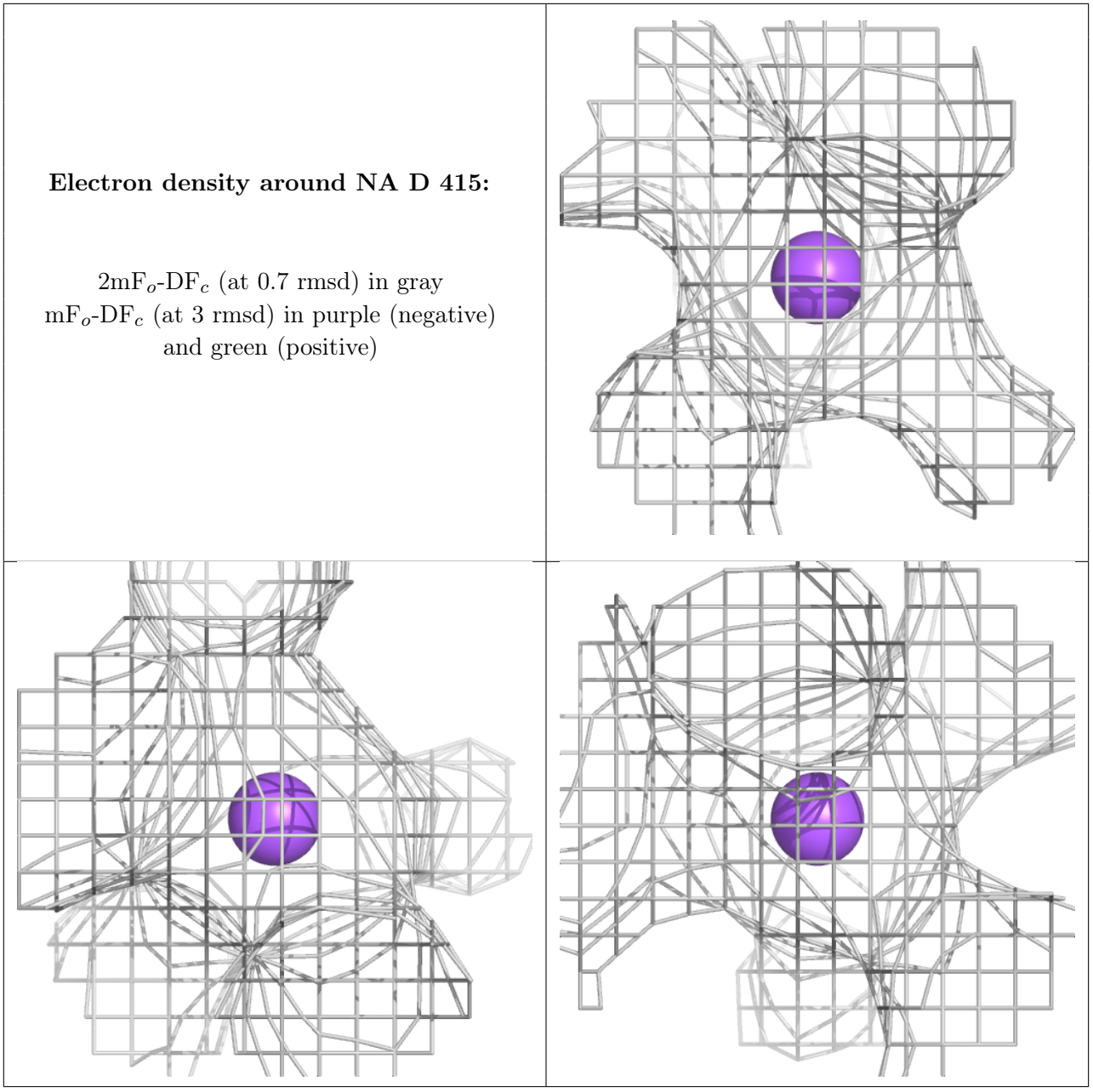
Electron density around NA E 314:

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



Electron density around NA D 415:

$2mF_o$-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.