Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 09:03 pm GMT

PDB ID	:	6YC4
Title	:	Crystal structure of the steady-state activated state of the light-driven sodium pump KR2 in the pentameric form at room temperature, pH 8.0
Authors	:	Kovalev, K.; Gushchin, I.; Gordeliy, V.
Deposited on	:	2020-03-18
Resolution	:	2.60 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:

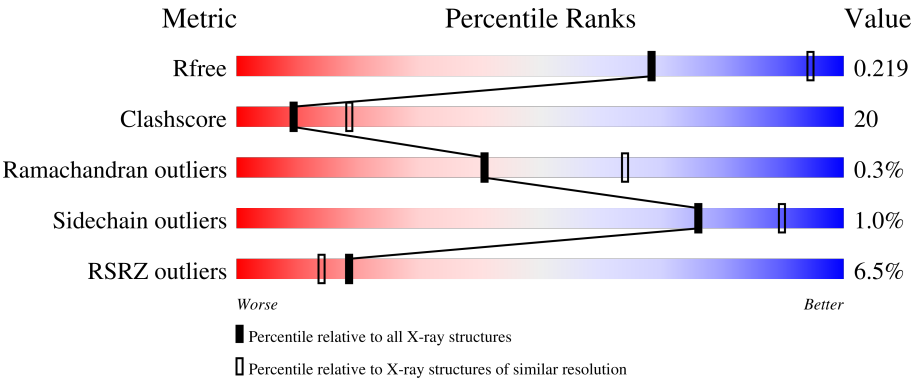
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	5% 74% 24%
1	B	273	4% 72% 26%
1	C	273	8% 73% 25%
1	D	273	7% 72% 26%
1	E	273	8% 73% 25%

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	A	304	-	-	-	X
2	OLC	C	303	-	-	-	X
2	OLC	C	304	-	-	-	X
2	OLC	E	305	-	-	-	X
2	OLC	E	306	-	-	-	X
2	OLC	E	307	-	-	-	X
3	LFA	A	309	-	-	-	X
3	LFA	A	311	-	-	-	X
3	LFA	B	307	-	-	-	X
3	LFA	D	305	-	-	-	X
4	NA	A	317	-	-	X	-
4	NA	B	314	-	-	X	-
4	NA	C	314	-	-	X	-
6	GOL	C	311	-	-	-	X
7	OLA	B	311	-	-	-	X
7	OLA	B	312	-	-	-	X
7	OLA	C	310	-	-	-	X
7	OLA	E	302	-	-	-	X
7	OLA	E	303	-	-	-	X
7	OLA	E	304	-	-	-	X
7	OLA	E	314	-	-	-	X

2 Entry composition

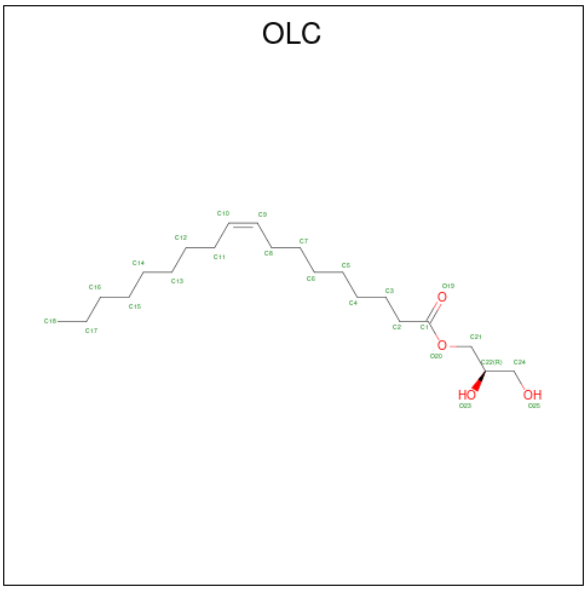
There are 8 unique types of molecules in this entry. The entry contains 13442 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	269	Total	C	N	O	S	0	41	0
			2477	1653	375	438	11			
1	B	269	Total	C	N	O	S	0	41	0
			2475	1651	375	438	11			
1	C	269	Total	C	N	O	S	0	41	0
			2472	1650	375	436	11			
1	D	269	Total	C	N	O	S	0	41	0
			2475	1651	375	438	11			
1	E	269	Total	C	N	O	S	0	41	0
			2475	1652	376	436	11			

- 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 7 7	0	0
2	A	1	Total C O 13 9 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	A	1	Total C O 18 16 2	0	0
2	B	1	Total C O 21 17 4	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C 5 5	0	0
2	B	1	Total C O 12 10 2	0	0
2	B	1	Total C O 20 16 4	0	0
2	C	1	Total C O 19 17 2	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C O 12 10 2	0	0
2	C	1	Total C O 17 15 2	0	0
2	C	1	Total C O 16 12 4	0	0
2	C	1	Total C O 16 13 3	0	0
2	D	1	Total C 5 5	0	0
2	D	1	Total C O 18 14 4	0	0
2	D	1	Total C 5 5	0	0
2	D	1	Total C O 14 10 4	0	0

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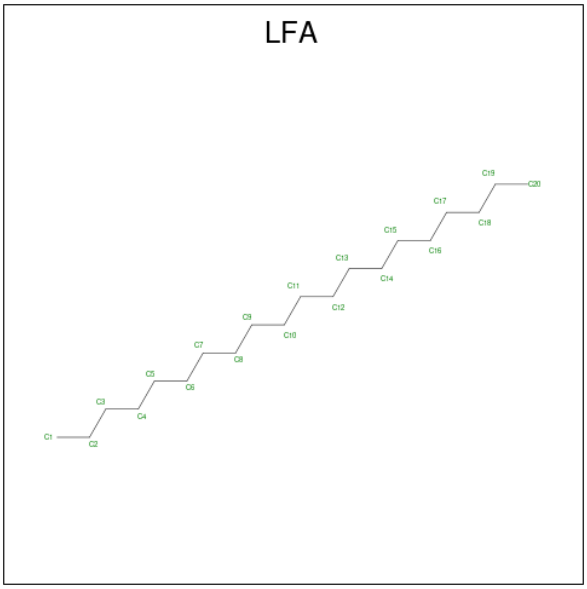
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 20 18 2	0	0
2	E	1	Total C O 19 17 2	0	0
2	E	1	Total C 8 8	0	0
2	E	1	Total C 16 16	0	0
2	E	1	Total C O 20 16 4	0	0
2	E	1	Total C O 15 11 4	0	0

- 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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 7 7	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 4 4	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	E	1	Total C 8 8	0	0
3	E	1	Total C 14 14	0	0
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

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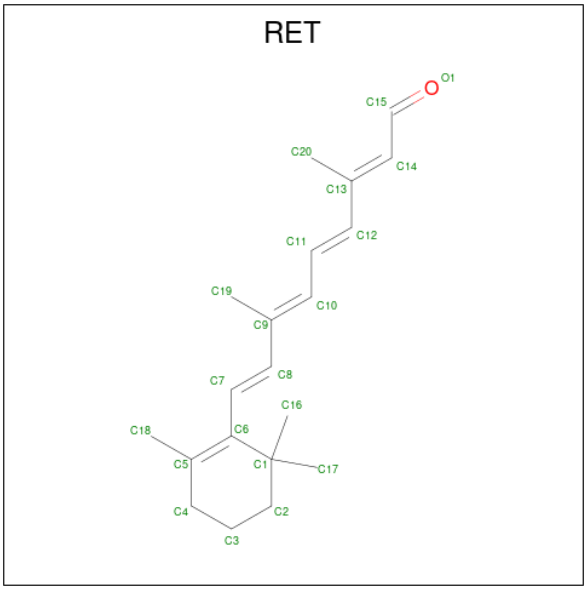
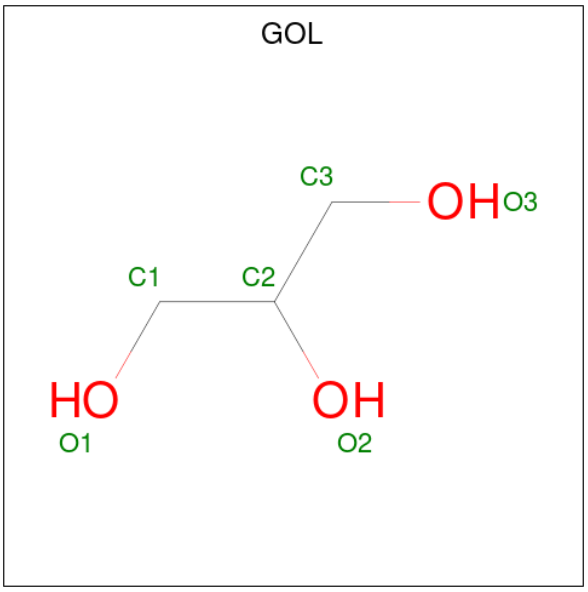
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	2	Total Na 2 2	0	0
4	E	2	Total Na 2 2	0	0

- Molecule 5 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



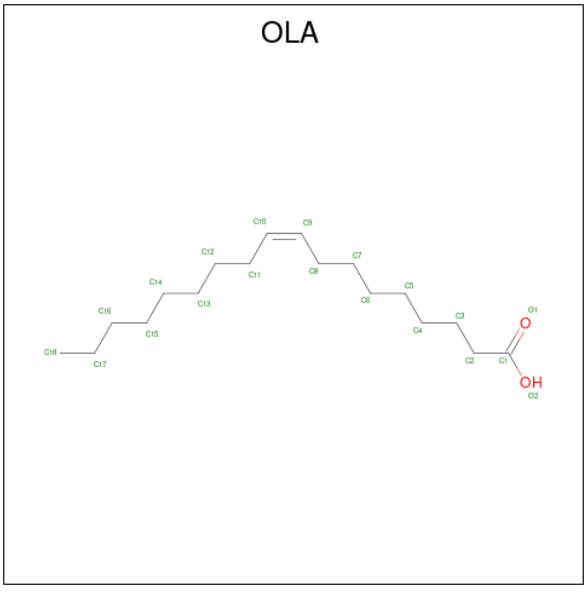
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 20 20	0	0
5	B	1	Total C 20 20	0	0
5	C	1	Total C 20 20	0	0
5	D	1	Total C 20 20	0	0
5	E	1	Total C 20 20	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0

- Molecule 7 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 17 15 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 18 16 2	0	0
7	C	1	Total C O 18 16 2	0	0
7	D	1	Total C O 7 5 2	0	0
7	E	1	Total C O 20 18 2	0	0
7	E	1	Total C O 17 15 2	0	0
7	E	1	Total C O 15 13 2	0	0
7	E	1	Total C O 6 4 2	0	0

- Molecule 8 is water.

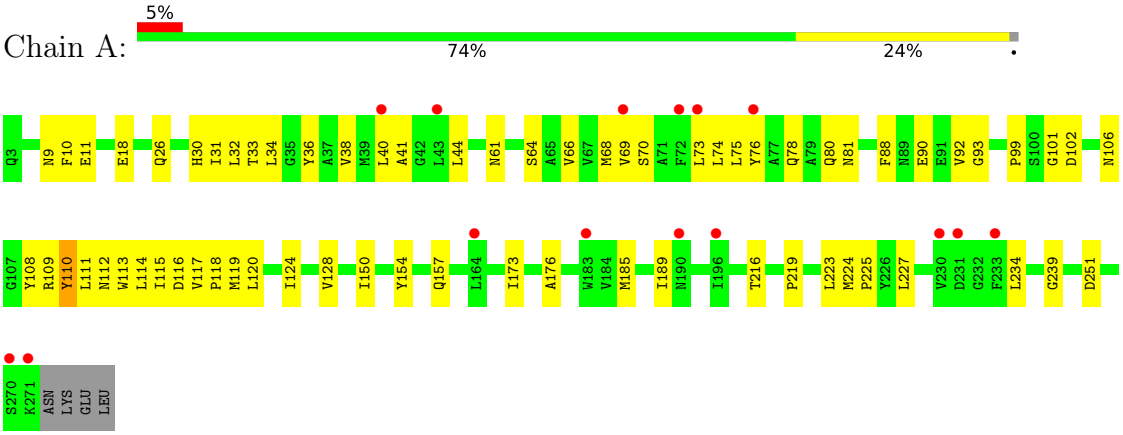
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	42	Total O 42 42	0	0
8	B	50	Total O 50 50	0	0
8	C	47	Total O 47 47	0	0
8	D	45	Total O 45 45	0	0
8	E	43	Total O 43 43	0	0

3 Residue-property plots (i)

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

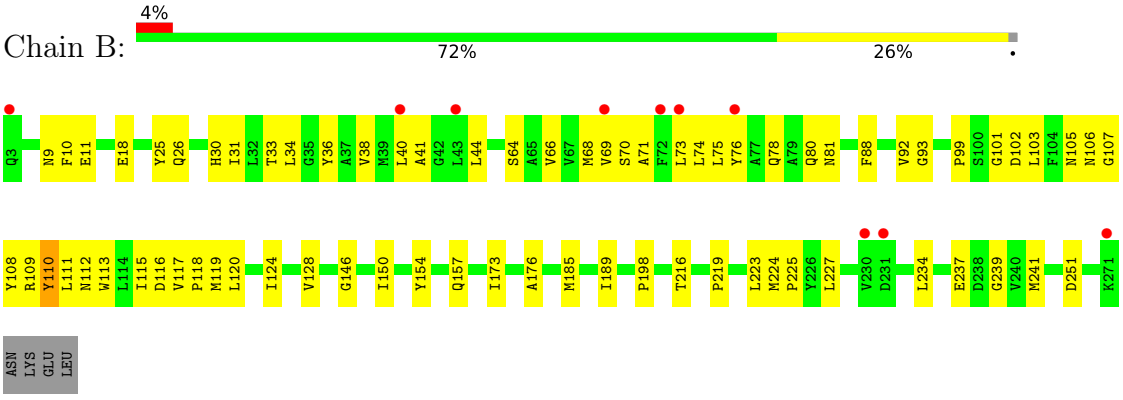
• Molecule 1: Sodium pumping rhodopsin

Chain A:



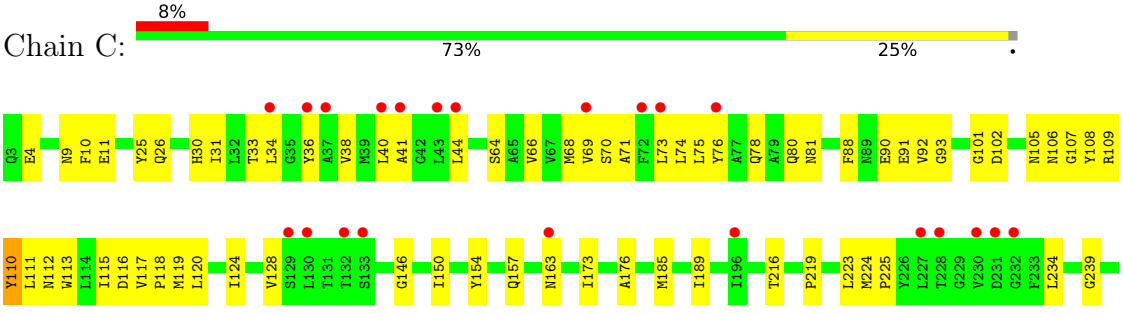
• Molecule 1: Sodium pumping rhodopsin

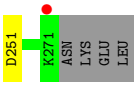
Chain B:



• Molecule 1: Sodium pumping rhodopsin

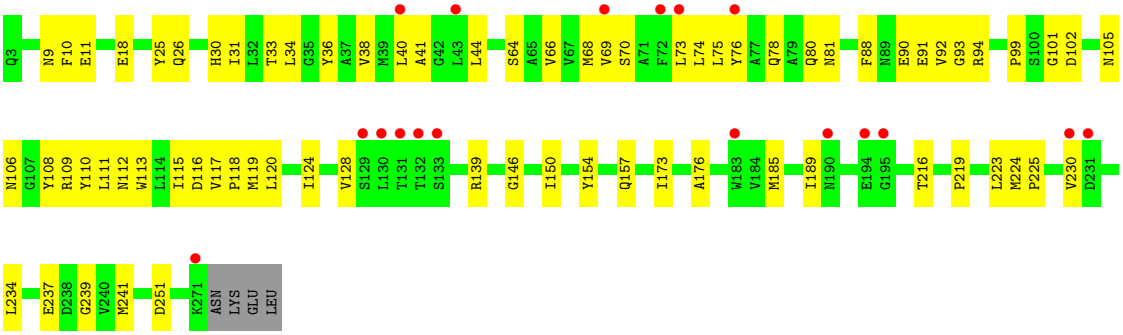
Chain C:





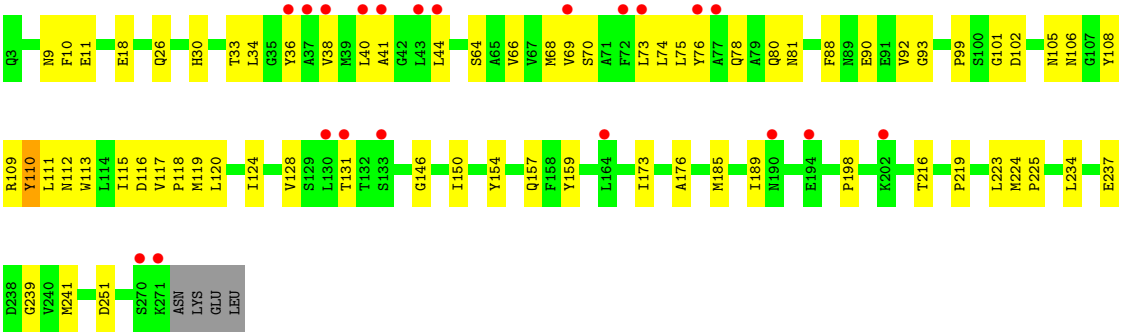
• Molecule 1: Sodium pumping rhodopsin

Chain D:



• Molecule 1: Sodium pumping rhodopsin

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	135.19Å 239.86Å 138.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 48.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.60) 99.9 (48.81-2.60)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.185 , 0.212 0.197 , 0.219	Depositor DCC
R_{free} test set	3492 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 79.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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	0.95	EDS
Total number of atoms	13442	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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, RET, LFA, NA, OLC, OLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.64	0/2546	0.63	0/3467
1	B	0.64	0/2544	0.64	0/3465
1	C	0.64	0/2541	0.63	0/3461
1	D	0.64	0/2544	0.63	0/3465
1	E	0.64	0/2544	0.63	0/3464
All	All	0.64	0/12719	0.63	0/17322

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	2477	0	2434	115	0
1	B	2475	0	2429	116	1
1	C	2472	0	2427	121	0
1	D	2475	0	2429	127	0
1	E	2475	0	2435	112	1
2	A	99	0	135	5	0
2	B	74	0	96	3	0
2	C	88	0	113	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	62	0	85	1	0
2	E	78	0	112	4	0
3	A	40	0	74	0	0
3	B	25	0	47	0	0
3	C	32	0	64	1	0
3	D	72	0	145	3	0
3	E	31	0	58	2	0
4	A	2	0	0	3	0
4	B	2	0	0	3	0
4	C	2	0	0	3	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
5	A	20	0	27	7	0
5	B	20	0	27	8	0
5	C	20	0	27	7	0
5	D	20	0	27	7	0
5	E	20	0	27	8	0
6	A	4	0	4	0	0
6	B	4	0	4	0	0
6	C	4	0	3	0	0
7	B	35	0	50	0	0
7	C	18	0	26	1	0
7	D	7	0	6	0	0
7	E	58	0	81	3	0
8	A	42	0	0	14	0
8	B	50	0	0	12	0
8	C	47	0	0	13	0
8	D	45	0	0	16	0
8	E	43	0	0	13	0
All	All	13442	0	13392	526	1

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 20.

All (526) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:GLY:O	1:B:150[B]:ILE:CD1	1.80	1.29
1:E:112[A]:ASN:HB3	8:E:406:HOH:O	1.35	1.23
1:B:81[A]:ASN:OD1	8:B:403:HOH:O	1.54	1.23
1:D:115[B]:ILE:HG12	8:D:404:HOH:O	1.40	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81[A]:ASN:OD1	8:D:402:HOH:O	1.68	1.08
1:C:4:GLU:CG	8:C:445:HOH:O	2.02	1.07
1:A:112[A]:ASN:HB3	8:A:407:HOH:O	1.54	1.05
1:B:146:GLY:O	1:B:150[B]:ILE:HD12	1.54	1.04
1:B:112[A]:ASN:HB3	8:B:405:HOH:O	1.54	1.04
1:B:146:GLY:O	1:B:150[B]:ILE:HD13	1.57	1.02
5:B:309:RET:H161	5:B:309:RET:H8	1.43	1.00
1:D:112[B]:ASN:O	1:D:115[B]:ILE:HG22	1.61	0.99
5:A:314:RET:H161	5:A:314:RET:H8	1.45	0.98
5:D:311:RET:H161	5:D:311:RET:H8	1.42	0.98
5:C:312:RET:H8	5:C:312:RET:H161	1.43	0.97
1:A:81[A]:ASN:OD1	8:A:402:HOH:O	1.81	0.97
5:E:315:RET:H161	5:E:315:RET:H8	1.45	0.97
1:E:75[B]:LEU:HD22	8:E:432:HOH:O	1.63	0.96
1:D:116[B]:ASP:OD2	8:D:401:HOH:O	1.81	0.96
1:D:115[A]:ILE:HG13	8:D:404:HOH:O	1.66	0.94
3:E:310:LFA:H141	3:E:311:LFA:H201	1.48	0.92
1:D:113[A]:TRP:CD1	5:D:311:RET:H14	2.07	0.90
1:E:115[B]:ILE:HG21	8:E:407:HOH:O	1.70	0.89
1:C:113[A]:TRP:CD1	5:C:312:RET:H14	2.07	0.88
1:B:113[A]:TRP:CD1	5:B:309:RET:H14	2.08	0.88
1:E:117[B]:VAL:HB	1:E:118[B]:PRO:HD3	1.56	0.88
1:E:113[A]:TRP:CD1	5:E:315:RET:H14	2.08	0.87
1:C:30:HIS:HB3	1:D:111[B]:LEU:HD22	1.56	0.87
1:B:117[B]:VAL:HB	1:B:118[B]:PRO:HD3	1.56	0.87
1:D:115[B]:ILE:O	8:D:404:HOH:O	1.93	0.86
1:A:117[B]:VAL:HB	1:A:118[B]:PRO:HD3	1.57	0.86
1:A:113[A]:TRP:CD1	5:A:314:RET:H14	2.10	0.86
1:C:117[B]:VAL:HB	1:C:118[B]:PRO:HD3	1.58	0.85
1:A:116[B]:ASP:OD2	8:A:401:HOH:O	1.95	0.84
1:C:75[B]:LEU:HD22	8:C:443:HOH:O	1.80	0.82
1:E:11:GLU:OE2	8:E:403:HOH:O	1.98	0.81
1:D:78[A]:GLN:HE22	1:D:106[A]:ASN:HA	1.45	0.81
1:B:116[B]:ASP:OD2	8:B:402:HOH:O	2.00	0.80
1:A:61:ASN:OD1	8:A:403:HOH:O	1.99	0.80
1:C:30:HIS:CB	1:D:111[B]:LEU:HD22	2.12	0.80
1:C:70[B]:SER:CB	4:C:314:NA:NA	1.56	0.80
1:C:90:GLU:OE1	1:D:99:PRO:HG3	1.83	0.79
1:D:30:HIS:HB3	1:E:111[A]:LEU:CD1	2.12	0.79
1:C:116[B]:ASP:O	1:C:120[B]:LEU:HG	1.83	0.79
1:D:18:GLU:OE1	8:D:405:HOH:O	2.00	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:HIS:HB3	1:D:111[B]:LEU:CD2	2.14	0.78
1:C:163:ASN:HD22	2:C:305:OLC:H24A	1.48	0.78
1:C:70[B]:SER:HB3	4:C:314:NA:NA	1.13	0.78
1:E:78[A]:GLN:HE22	1:E:106[A]:ASN:HA	1.48	0.77
1:A:111[A]:LEU:CD1	1:E:30:HIS:HB3	2.14	0.77
1:A:81[A]:ASN:CG	8:A:402:HOH:O	2.19	0.77
1:E:115[B]:ILE:CG2	8:E:407:HOH:O	2.31	0.77
1:B:78[A]:GLN:HE22	1:B:106[A]:ASN:HA	1.49	0.76
1:B:70[B]:SER:CB	4:B:314:NA:NA	1.85	0.76
1:C:106[A]:ASN:O	1:C:110[A]:TYR:HD1	1.68	0.76
1:A:81[A]:ASN:ND2	8:A:402:HOH:O	2.19	0.75
1:A:70[B]:SER:CB	4:A:317:NA:NA	1.51	0.75
1:A:106[A]:ASN:O	1:A:110[A]:TYR:HD1	1.69	0.75
1:C:30:HIS:CB	1:D:111[B]:LEU:CD2	2.64	0.75
1:C:112[A]:ASN:HB3	8:C:411:HOH:O	1.85	0.75
1:B:70[B]:SER:HB3	4:B:314:NA:NA	1.40	0.74
1:B:18:GLU:OE1	8:B:404:HOH:O	2.04	0.74
1:D:117[A]:VAL:HB	1:D:118[A]:PRO:HD3	1.71	0.72
1:D:70[B]:SER:OG	1:D:115[B]:ILE:HG21	1.88	0.72
1:E:78[A]:GLN:NE2	1:E:106[A]:ASN:HA	2.04	0.72
1:C:75[A]:LEU:HD22	8:C:443:HOH:O	1.89	0.72
1:D:74[B]:LEU:HD21	1:D:108[B]:TYR:HB3	1.71	0.72
1:D:113[A]:TRP:HD1	5:D:311:RET:H14	1.54	0.72
1:C:113[A]:TRP:HD1	5:C:312:RET:H14	1.54	0.71
1:C:75[B]:LEU:HB3	8:C:443:HOH:O	1.90	0.71
5:D:311:RET:H161	5:D:311:RET:C8	2.20	0.71
1:A:117[A]:VAL:HB	1:A:118[A]:PRO:HD3	1.73	0.71
1:E:117[A]:VAL:HB	1:E:118[A]:PRO:HD3	1.73	0.70
1:B:113[A]:TRP:HD1	5:B:309:RET:H14	1.55	0.70
1:B:76[B]:TYR:O	1:B:80[B]:GLN:HG2	1.90	0.70
1:A:30:HIS:HB3	1:B:111[A]:LEU:CD1	2.22	0.70
1:D:106[A]:ASN:O	1:D:110[A]:TYR:HD1	1.75	0.69
1:C:76[B]:TYR:O	1:C:80[B]:GLN:HG2	1.92	0.69
1:A:119[B]:MET:HE2	1:A:119[B]:MET:HA	1.72	0.69
1:E:113[A]:TRP:HD1	5:E:315:RET:H14	1.56	0.69
1:E:106[A]:ASN:O	1:E:110[A]:TYR:HD1	1.75	0.69
1:D:78[A]:GLN:NE2	1:D:106[A]:ASN:HA	2.07	0.69
5:C:312:RET:H161	5:C:312:RET:C8	2.22	0.68
1:D:40:LEU:HD23	1:E:73[A]:LEU:HD11	1.75	0.68
1:B:30:HIS:HB3	1:C:111[A]:LEU:CD1	2.24	0.68
1:B:117[A]:VAL:HB	1:B:118[A]:PRO:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78[A]:GLN:NE2	1:B:106[A]:ASN:HA	2.09	0.67
1:C:119[B]:MET:HE2	1:C:119[B]:MET:HA	1.75	0.67
1:E:119[B]:MET:HE2	1:E:119[B]:MET:HA	1.75	0.67
1:E:78[A]:GLN:OE1	1:E:78[A]:GLN:HA	1.93	0.67
1:B:106[A]:ASN:O	1:B:110[A]:TYR:HD1	1.78	0.67
1:A:18:GLU:OE1	8:A:404:HOH:O	2.13	0.67
1:C:117[A]:VAL:HB	1:C:118[A]:PRO:HD3	1.75	0.67
1:B:75[B]:LEU:HD22	8:B:439:HOH:O	1.93	0.66
1:A:76[B]:TYR:O	1:A:80[B]:GLN:HG2	1.96	0.66
1:A:113[A]:TRP:HD1	5:A:314:RET:H14	1.55	0.66
1:A:70[B]:SER:HB3	4:A:317:NA:NA	1.15	0.65
1:E:18:GLU:OE1	8:E:405:HOH:O	2.14	0.65
1:C:78[A]:GLN:HE22	1:C:106[A]:ASN:HA	1.61	0.65
1:B:115[B]:ILE:HG21	8:B:416:HOH:O	1.96	0.65
1:B:103:LEU:O	8:B:403:HOH:O	2.15	0.64
1:D:139:ARG:NH2	3:D:306:LFA:C20	2.60	0.64
1:E:76[B]:TYR:O	1:E:80[B]:GLN:HG2	1.98	0.64
1:C:163:ASN:HD22	2:C:305:OLC:C24	2.11	0.64
1:A:116[B]:ASP:O	1:A:120[B]:LEU:HG	1.98	0.63
1:B:234:LEU:O	1:B:239:GLY:HA3	1.99	0.63
1:B:150[B]:ILE:HD12	1:B:150[B]:ILE:H	1.64	0.63
1:D:78[A]:GLN:HA	1:D:78[A]:GLN:OE1	1.99	0.63
1:C:40:LEU:HD23	1:D:73[A]:LEU:HD11	1.79	0.63
1:D:234:LEU:O	1:D:239:GLY:HA3	1.99	0.63
1:E:70[A]:SER:O	1:E:74[A]:LEU:HD23	1.98	0.63
1:B:40:LEU:HD23	1:C:73[A]:LEU:HD11	1.81	0.63
1:D:30:HIS:HB3	1:E:111[A]:LEU:HD11	1.78	0.63
1:C:78[B]:GLN:HA	1:C:78[B]:GLN:OE1	1.99	0.63
1:C:110[B]:TYR:O	1:C:113[B]:TRP:N	2.25	0.63
1:C:234:LEU:O	1:C:239:GLY:HA3	1.99	0.62
1:A:234:LEU:O	1:A:239:GLY:HA3	2.00	0.62
1:B:78[B]:GLN:OE1	1:B:78[B]:GLN:HA	1.97	0.62
1:D:90:GLU:OE1	1:E:99:PRO:HG3	1.99	0.62
1:D:117[B]:VAL:HB	1:D:118[B]:PRO:HD3	1.80	0.62
1:E:74[B]:LEU:HD21	1:E:108[B]:TYR:HB3	1.81	0.62
1:A:111[A]:LEU:HD12	1:E:30:HIS:HB3	1.80	0.62
1:C:30:HIS:HB2	1:D:111[B]:LEU:CD2	2.29	0.62
1:A:68[B]:MET:HE2	1:A:68[B]:MET:HA	1.80	0.62
1:D:44:LEU:HD22	1:E:69[A]:VAL:HG21	1.81	0.62
1:E:78[B]:GLN:OE1	1:E:78[B]:GLN:HA	2.00	0.61
1:E:112[A]:ASN:ND2	8:E:406:HOH:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78[A]:GLN:HA	1:B:78[A]:GLN:OE1	1.99	0.61
1:B:111[A]:LEU:HB2	8:B:437:HOH:O	2.00	0.61
1:C:34:LEU:HD11	1:D:115[A]:ILE:HG21	1.81	0.61
1:E:234:LEU:O	1:E:239:GLY:HA3	1.99	0.61
5:A:314:RET:H161	5:A:314:RET:C8	2.23	0.61
1:C:33:THR:HG22	1:D:74[A]:LEU:CD1	2.29	0.61
1:A:32:LEU:HD22	8:A:437:HOH:O	2.01	0.61
1:C:34:LEU:HD11	1:D:115[A]:ILE:CG2	2.30	0.61
1:D:70[B]:SER:OG	1:D:115[B]:ILE:CG2	2.48	0.61
1:B:105[B]:ASN:OD1	1:B:107[B]:GLY:N	2.32	0.61
1:D:70[B]:SER:HG	1:D:115[B]:ILE:HG21	1.65	0.60
2:B:310:OLC:H11	3:C:308:LFA:H111	1.83	0.60
1:A:119[B]:MET:HA	1:A:119[B]:MET:CE	2.31	0.60
1:D:40:LEU:CD2	1:E:73[A]:LEU:HD11	2.31	0.60
1:C:78[A]:GLN:OE1	1:C:78[A]:GLN:HA	2.02	0.59
1:A:70[B]:SER:OG	4:A:317:NA:NA	1.47	0.59
1:D:115[B]:ILE:HG23	8:D:404:HOH:O	2.03	0.59
1:E:36:TYR:CD2	1:E:76[B]:TYR:HA	2.36	0.59
1:E:112[A]:ASN:CB	8:E:406:HOH:O	2.15	0.59
1:A:110[B]:TYR:O	1:A:113[B]:TRP:N	2.30	0.59
1:D:33:THR:HG22	1:E:74[A]:LEU:CD1	2.33	0.59
1:E:198:PRO:HD2	8:E:441:HOH:O	2.02	0.59
5:B:309:RET:H161	5:B:309:RET:C8	2.22	0.59
1:D:36:TYR:CD2	1:D:76[B]:TYR:HA	2.38	0.59
1:C:40:LEU:CD2	1:D:73[A]:LEU:HD11	2.32	0.58
1:B:112[A]:ASN:CB	8:B:405:HOH:O	2.29	0.58
1:A:109[A]:ARG:NH1	1:A:251:ASP:OD2	2.36	0.58
1:D:115[B]:ILE:CB	8:D:404:HOH:O	2.49	0.58
1:B:110[B]:TYR:HA	1:B:113[B]:TRP:CE3	2.39	0.58
1:C:115[B]:ILE:CG2	8:C:417:HOH:O	2.33	0.58
1:C:119[B]:MET:HA	1:C:119[B]:MET:CE	2.32	0.58
1:B:119[B]:MET:CE	1:B:119[B]:MET:HA	2.33	0.58
1:C:109[A]:ARG:NH1	1:C:251:ASP:OD2	2.37	0.58
1:C:163:ASN:ND2	2:C:305:OLC:H24A	2.16	0.58
1:A:119[A]:MET:HE2	1:A:119[A]:MET:HA	1.86	0.57
1:B:109[A]:ARG:NH1	1:B:251:ASP:OD2	2.36	0.57
1:C:106[A]:ASN:O	1:C:110[A]:TYR:CD1	2.53	0.57
1:A:115[A]:ILE:HG22	2:E:301:OLC:H16A	1.87	0.57
1:A:115[B]:ILE:HG21	8:A:413:HOH:O	2.04	0.57
1:E:109[A]:ARG:NH1	1:E:251:ASP:OD2	2.37	0.57
1:C:116[B]:ASP:OD2	8:C:401:HOH:O	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109[A]:ARG:NH1	1:D:251:ASP:OD2	2.38	0.56
1:A:74[A]:LEU:CD1	1:E:33:THR:HG22	2.36	0.56
1:C:78[A]:GLN:NE2	1:C:106[A]:ASN:HA	2.20	0.56
1:D:110[B]:TYR:O	1:D:113[B]:TRP:HB2	2.05	0.56
1:A:110[B]:TYR:HA	1:A:113[B]:TRP:CE3	2.41	0.56
1:A:78[A]:GLN:HE22	1:A:106[A]:ASN:HA	1.71	0.56
1:A:106[A]:ASN:O	1:A:110[A]:TYR:CD1	2.56	0.56
1:A:119[A]:MET:HA	1:A:119[A]:MET:CE	2.35	0.56
1:B:74[B]:LEU:HD21	1:B:108[B]:TYR:HB3	1.88	0.56
1:A:73[A]:LEU:HD11	1:E:40:LEU:HD23	1.88	0.56
1:A:74[B]:LEU:HB2	1:A:112[B]:ASN:ND2	2.21	0.56
1:D:68[B]:MET:HE2	1:D:68[B]:MET:HA	1.88	0.55
1:E:119[B]:MET:HA	1:E:119[B]:MET:CE	2.36	0.55
1:A:74[B]:LEU:HD23	1:A:112[B]:ASN:ND2	2.22	0.55
1:D:74[B]:LEU:CD2	1:D:108[B]:TYR:HB3	2.36	0.55
1:C:76[A]:TYR:O	1:C:80[A]:GLN:HG2	2.07	0.55
1:D:116[B]:ASP:O	1:D:120[B]:LEU:HG	2.06	0.55
1:C:223:LEU:C	1:C:225:PRO:HD2	2.27	0.55
1:D:112[A]:ASN:ND2	8:D:403:HOH:O	1.80	0.55
1:E:110[B]:TYR:HA	1:E:113[B]:TRP:CE3	2.42	0.55
1:A:70[A]:SER:O	1:A:74[A]:LEU:HD23	2.05	0.55
1:B:36:TYR:CD2	1:B:76[B]:TYR:HA	2.42	0.55
1:B:116[B]:ASP:O	1:B:120[B]:LEU:HG	2.06	0.55
1:C:68[B]:MET:CE	1:C:68[B]:MET:HA	2.37	0.55
1:C:74[B]:LEU:HD21	1:C:108[B]:TYR:HB3	1.89	0.55
5:E:315:RET:H161	5:E:315:RET:C8	2.23	0.55
1:D:74[B]:LEU:HD21	1:D:108[B]:TYR:C	2.27	0.55
1:C:75[B]:LEU:CB	8:C:443:HOH:O	2.50	0.54
1:B:112[A]:ASN:ND2	8:B:405:HOH:O	2.35	0.54
1:A:223:LEU:C	1:A:225:PRO:HD2	2.28	0.54
1:C:90:GLU:OE1	1:D:99:PRO:CG	2.54	0.54
1:C:117[B]:VAL:HB	1:C:118[B]:PRO:CD	2.36	0.54
7:E:303:OLA:C15	7:E:314:OLA:C4	2.86	0.54
1:B:111[B]:LEU:HD13	1:B:154:TYR:CD1	2.42	0.54
1:B:33:THR:HG22	1:C:74[A]:LEU:CD1	2.37	0.54
2:C:301:OLC:H12	1:D:115[B]:ILE:HG13	1.90	0.54
1:A:40:LEU:HD23	1:B:73[A]:LEU:HD11	1.90	0.54
1:D:68[B]:MET:HA	1:D:68[B]:MET:CE	2.38	0.54
1:B:44:LEU:HD22	1:C:69[A]:VAL:HG21	1.90	0.53
2:B:301:OLC:H13A	1:C:115[A]:ILE:HG22	1.90	0.53
1:C:70[B]:SER:OG	4:C:314:NA:NA	1.58	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:HIS:CB	1:E:111[A]:LEU:HD11	2.38	0.53
1:A:115[A]:ILE:HG21	1:E:34:LEU:HD11	1.90	0.53
1:D:30:HIS:HB3	1:E:111[A]:LEU:HD12	1.90	0.53
1:D:64:SER:O	1:D:68[B]:MET:HG2	2.07	0.53
1:E:115[B]:ILE:O	1:E:119[B]:MET:HG2	2.09	0.53
1:B:40:LEU:CD2	1:C:73[A]:LEU:HD11	2.38	0.53
1:D:216:THR:O	1:D:219:PRO:HG2	2.09	0.53
1:E:81[A]:ASN:HD21	1:E:105[A]:ASN:H	1.54	0.53
1:A:36:TYR:CD2	1:A:76[B]:TYR:HA	2.44	0.53
1:B:223:LEU:C	1:B:225:PRO:HD2	2.28	0.53
1:C:90:GLU:CD	1:D:99:PRO:HG3	2.28	0.53
1:A:44:LEU:HD22	1:B:69[A]:VAL:HG21	1.89	0.53
1:C:119[A]:MET:CE	1:C:119[A]:MET:HA	2.39	0.53
1:E:223:LEU:C	1:E:225:PRO:HD2	2.29	0.53
1:A:117[B]:VAL:HB	1:A:118[B]:PRO:CD	2.35	0.53
1:C:44:LEU:HD22	1:D:69[A]:VAL:HG21	1.90	0.53
1:D:119[A]:MET:HE2	1:D:119[A]:MET:HA	1.91	0.53
1:E:64:SER:O	1:E:68[A]:MET:HG2	2.09	0.53
1:A:68[B]:MET:HA	1:A:68[B]:MET:CE	2.39	0.53
1:A:154:TYR:O	1:A:157:GLN:HG3	2.09	0.52
1:B:119[A]:MET:HA	1:B:119[A]:MET:CE	2.39	0.52
1:D:80[B]:GLN:NE2	8:D:410:HOH:O	2.42	0.52
1:D:115[B]:ILE:CG1	8:D:404:HOH:O	2.19	0.52
3:E:310:LFA:C14	3:E:311:LFA:H201	2.31	0.52
1:B:30:HIS:HB3	1:C:111[A]:LEU:HD12	1.91	0.52
1:B:68[B]:MET:HA	1:B:68[B]:MET:CE	2.39	0.52
1:D:33:THR:HG22	1:E:74[A]:LEU:HD13	1.92	0.52
1:D:223:LEU:C	1:D:225:PRO:HD2	2.28	0.52
1:A:216:THR:O	1:A:219:PRO:HG2	2.10	0.52
1:C:64:SER:O	1:C:68[A]:MET:HG2	2.09	0.52
1:E:74[B]:LEU:HB2	1:E:112[B]:ASN:ND2	2.25	0.52
1:A:69[A]:VAL:HG21	1:E:44:LEU:HD22	1.90	0.52
1:B:33:THR:HG22	1:C:74[A]:LEU:HD13	1.91	0.52
1:B:115[B]:ILE:O	1:B:119[B]:MET:HG2	2.09	0.52
1:C:154:TYR:O	1:C:157:GLN:HG3	2.09	0.52
1:D:70[A]:SER:HB2	1:D:115[A]:ILE:HD11	1.92	0.52
1:E:119[A]:MET:HA	1:E:119[A]:MET:CE	2.39	0.52
1:E:216:THR:O	1:E:219:PRO:HG2	2.09	0.52
1:A:111[A]:LEU:HD11	1:E:30:HIS:HB3	1.90	0.52
1:B:216:THR:O	1:B:219:PRO:HG2	2.10	0.52
1:A:110[B]:TYR:O	1:A:113[B]:TRP:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:LEU:HD22	1:E:69[A]:VAL:CG2	2.39	0.52
1:D:119[A]:MET:HA	1:D:119[A]:MET:CE	2.40	0.52
1:D:154:TYR:O	1:D:157:GLN:HG3	2.10	0.52
1:E:64:SER:O	1:E:68[B]:MET:HG2	2.10	0.52
1:E:68[B]:MET:HA	1:E:68[B]:MET:CE	2.40	0.52
1:C:110[B]:TYR:HA	1:C:113[B]:TRP:CE3	2.45	0.52
1:C:117[B]:VAL:CB	1:C:118[B]:PRO:HD3	2.37	0.52
1:D:110[B]:TYR:HA	1:D:113[B]:TRP:CE3	2.44	0.52
1:C:64:SER:O	1:C:68[B]:MET:HG2	2.09	0.52
1:E:115[A]:ILE:HB	8:E:424:HOH:O	2.09	0.52
1:B:110[B]:TYR:O	1:B:113[B]:TRP:HB2	2.10	0.51
1:D:115[B]:ILE:C	8:D:404:HOH:O	2.43	0.51
1:A:111[B]:LEU:HD13	1:A:154:TYR:CD1	2.45	0.51
1:D:76[A]:TYR:CZ	1:D:80[A]:GLN:NE2	2.76	0.51
1:D:81[A]:ASN:HD21	1:D:105[A]:ASN:H	1.57	0.51
1:B:64:SER:O	1:B:68[A]:MET:HG2	2.11	0.51
1:D:224:MET:N	1:D:225:PRO:HD2	2.26	0.51
1:E:154:TYR:O	1:E:157:GLN:HG3	2.11	0.51
1:B:150[B]:ILE:HD12	1:B:150[B]:ILE:N	2.25	0.51
1:D:119[B]:MET:HA	1:D:119[B]:MET:CE	2.41	0.51
1:B:154:TYR:O	1:B:157:GLN:HG3	2.10	0.51
1:C:71[B]:ALA:O	1:C:75[B]:LEU:HG	2.10	0.51
1:D:112[A]:ASN:HB3	8:D:403:HOH:O	2.09	0.51
1:E:9:ASN:HB3	1:E:11:GLU:OE1	2.10	0.51
1:A:33:THR:HG22	1:B:74[A]:LEU:CD1	2.41	0.51
1:A:64:SER:O	1:A:68[A]:MET:HG2	2.09	0.51
1:B:117[B]:VAL:CB	1:B:118[B]:PRO:HD3	2.36	0.51
1:A:115[B]:ILE:CG2	8:A:411:HOH:O	0.81	0.51
1:D:76[B]:TYR:O	1:D:80[B]:GLN:HG2	2.11	0.51
1:C:38:VAL:HG22	1:D:115[B]:ILE:HD12	1.92	0.51
1:D:64:SER:O	1:D:68[A]:MET:HG2	2.10	0.51
1:A:115[A]:ILE:CG2	1:E:34:LEU:HD11	2.41	0.50
1:A:117[B]:VAL:HG21	1:A:150[B]:ILE:HD11	1.93	0.50
1:B:70[B]:SER:OG	4:B:314:NA:NA	1.74	0.50
1:B:224:MET:N	1:B:225:PRO:HD2	2.26	0.50
1:C:111[B]:LEU:HD13	1:C:154:TYR:CE1	2.46	0.50
1:A:111[B]:LEU:HD13	1:A:154:TYR:CE1	2.46	0.50
1:B:119[B]:MET:HA	1:B:119[B]:MET:HE2	1.93	0.50
1:C:115[B]:ILE:HG21	8:C:417:HOH:O	2.06	0.50
1:B:64:SER:O	1:B:68[B]:MET:HG2	2.11	0.50
1:D:25:TYR:OH	1:E:102:ASP:OD2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74[B]:LEU:C	1:E:74[B]:LEU:HD13	2.32	0.50
1:B:9:ASN:HB3	1:B:11:GLU:OE1	2.12	0.50
1:D:94:ARG:NH1	8:D:409:HOH:O	2.41	0.50
1:E:34:LEU:O	1:E:38:VAL:HG23	2.12	0.50
1:E:111[B]:LEU:HD13	1:E:154:TYR:CE1	2.46	0.50
1:B:74[B]:LEU:HB2	1:B:112[B]:ASN:ND2	2.27	0.50
1:C:9:ASN:HB3	1:C:11:GLU:OE1	2.12	0.50
1:C:216:THR:O	1:C:219:PRO:HG2	2.11	0.50
1:A:224:MET:N	1:A:225:PRO:HD2	2.26	0.50
1:C:33:THR:HG22	1:D:74[A]:LEU:HD13	1.92	0.50
1:C:111[B]:LEU:HD13	1:C:154:TYR:CD1	2.46	0.50
1:C:224:MET:N	1:C:225:PRO:HD2	2.26	0.50
1:A:74[A]:LEU:HD13	1:E:33:THR:HG22	1.94	0.50
1:A:64:SER:O	1:A:68[B]:MET:HG2	2.11	0.50
1:D:139:ARG:NH2	3:D:306:LFA:H202	2.26	0.50
1:A:30:HIS:HB3	1:B:111[A]:LEU:HD12	1.93	0.50
1:E:111[B]:LEU:HD13	1:E:154:TYR:CD1	2.47	0.50
2:A:302:OLC:H14	1:B:115[A]:ILE:HG22	1.94	0.49
1:B:109[B]:ARG:NH1	1:B:251:ASP:OD2	2.45	0.49
1:B:111[B]:LEU:HD13	1:B:154:TYR:CE1	2.46	0.49
1:C:74[B]:LEU:C	1:C:74[B]:LEU:HD13	2.32	0.49
1:C:110[B]:TYR:O	1:C:113[B]:TRP:HB2	2.11	0.49
1:E:224:MET:N	1:E:225:PRO:HD2	2.26	0.49
1:C:115[B]:ILE:O	1:C:119[B]:MET:HG2	2.12	0.49
1:E:70[A]:SER:O	1:E:74[A]:LEU:CD2	2.61	0.49
1:A:111[A]:LEU:CD1	1:E:30:HIS:CB	2.89	0.49
1:E:109[B]:ARG:NH1	1:E:251:ASP:OD2	2.44	0.49
1:E:113[A]:TRP:CG	5:E:315:RET:H12	2.48	0.49
1:A:34:LEU:HD11	1:B:115[A]:ILE:HG21	1.94	0.49
1:B:38:VAL:HG22	1:C:115[B]:ILE:HD11	1.94	0.49
1:D:74[B]:LEU:HD13	1:D:74[B]:LEU:C	2.33	0.49
1:E:117[B]:VAL:HB	1:E:118[B]:PRO:CD	2.35	0.49
1:B:115[B]:ILE:CG2	8:B:416:HOH:O	2.59	0.49
1:D:30:HIS:O	1:E:111[A]:LEU:HD12	2.13	0.49
1:A:9:ASN:HB3	1:A:11:GLU:OE1	2.13	0.49
1:C:74[B]:LEU:HB2	1:C:112[B]:ASN:ND2	2.28	0.49
1:A:99:PRO:HG3	1:E:90:GLU:OE1	2.13	0.49
1:A:113[A]:TRP:CG	5:A:314:RET:H12	2.48	0.49
1:A:117[B]:VAL:CB	1:A:118[B]:PRO:HD3	2.36	0.49
1:E:68[B]:MET:HA	1:E:68[B]:MET:HE2	1.94	0.49
1:B:110[B]:TYR:O	1:B:113[B]:TRP:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70[A]:SER:O	1:C:74[A]:LEU:HD23	2.13	0.48
1:D:113[A]:TRP:CG	5:D:311:RET:H12	2.48	0.48
1:E:117[B]:VAL:CB	1:E:118[B]:PRO:HD3	2.35	0.48
1:A:34:LEU:O	1:A:38:VAL:HG23	2.14	0.48
1:C:109[B]:ARG:NH1	1:C:251:ASP:OD2	2.45	0.48
1:A:90:GLU:OE1	1:B:99:PRO:HG3	2.13	0.48
1:C:117[B]:VAL:HG21	1:C:150[B]:ILE:HD11	1.95	0.48
1:D:9:ASN:HB3	1:D:11:GLU:OE1	2.13	0.48
1:A:33:THR:HG22	1:B:74[A]:LEU:HD13	1.95	0.48
1:A:78[A]:GLN:OE1	1:A:78[A]:GLN:HA	2.12	0.48
1:C:34:LEU:O	1:C:38:VAL:HG23	2.13	0.48
1:D:34:LEU:O	1:D:38:VAL:HG23	2.14	0.48
1:B:113[A]:TRP:CG	5:B:309:RET:H12	2.48	0.48
1:D:115[B]:ILE:CG2	8:D:404:HOH:O	2.61	0.48
1:E:116[B]:ASP:O	1:E:120[B]:LEU:HG	2.14	0.48
5:E:315:RET:H8	5:E:315:RET:C16	2.29	0.48
2:A:313:OLC:H15A	2:E:301:OLC:H16	1.94	0.48
1:C:36:TYR:CD2	1:C:76[B]:TYR:HA	2.48	0.48
1:A:68[A]:MET:HA	1:A:68[A]:MET:CE	2.43	0.48
1:A:73[A]:LEU:HD11	1:E:40:LEU:CD2	2.44	0.48
1:C:113[A]:TRP:CG	5:C:312:RET:H12	2.49	0.47
1:D:30:HIS:CB	1:E:111[A]:LEU:CD1	2.90	0.47
1:A:115[A]:ILE:HG22	2:E:301:OLC:H14	1.96	0.47
1:A:115[B]:ILE:O	1:A:119[B]:MET:HG2	2.14	0.47
2:C:301:OLC:H13	2:C:313:OLC:H4A	1.96	0.47
1:A:30:HIS:O	1:B:111[A]:LEU:HD12	2.14	0.47
1:A:78[B]:GLN:HA	1:A:78[B]:GLN:OE1	2.15	0.47
1:B:68[B]:MET:HA	1:B:68[B]:MET:HE2	1.97	0.47
1:C:119[A]:MET:HA	1:C:119[A]:MET:HE2	1.97	0.47
1:A:109[B]:ARG:NH1	1:A:251:ASP:OD2	2.46	0.47
1:A:111[A]:LEU:HD11	1:E:30:HIS:CB	2.44	0.47
1:D:109[B]:ARG:NH1	1:D:251:ASP:OD2	2.44	0.47
1:A:40:LEU:CD2	1:B:73[A]:LEU:HD11	2.45	0.47
1:D:68[A]:MET:CE	1:D:68[A]:MET:HA	2.45	0.47
1:A:33:THR:HA	1:A:36:TYR:CE2	2.50	0.46
1:A:44:LEU:HD22	1:B:69[A]:VAL:CG2	2.45	0.46
1:A:74[B]:LEU:HD13	1:A:74[B]:LEU:C	2.36	0.46
1:A:113[B]:TRP:CD1	5:A:314:RET:H14	2.49	0.46
1:B:34:LEU:O	1:B:38:VAL:HG23	2.16	0.46
1:A:74[B]:LEU:HD21	1:A:108[B]:TYR:HB3	1.97	0.46
1:B:113[B]:TRP:CD1	5:B:309:RET:H14	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:THR:HA	1:B:36:TYR:CE2	2.51	0.46
1:B:68[A]:MET:HA	1:B:68[A]:MET:CE	2.45	0.46
1:C:30:HIS:CB	1:D:111[B]:LEU:HD23	2.44	0.46
1:A:41:ALA:HB1	1:B:66:VAL:HG13	1.98	0.46
1:C:74[B]:LEU:HD13	1:C:74[B]:LEU:O	2.15	0.46
1:D:68[A]:MET:HA	1:D:68[A]:MET:HE2	1.97	0.46
1:C:30:HIS:HB2	1:D:111[B]:LEU:HD22	1.92	0.46
1:B:81[A]:ASN:ND2	8:B:401:HOH:O	0.61	0.46
1:A:115[B]:ILE:HD11	1:E:38:VAL:HG22	1.98	0.46
1:B:117[B]:VAL:HB	1:B:118[B]:PRO:CD	2.36	0.46
1:C:185:MET:O	1:C:189:ILE:HG12	2.16	0.46
1:D:185:MET:O	1:D:189:ILE:HG12	2.16	0.46
1:B:74[B]:LEU:C	1:B:74[B]:LEU:HD13	2.37	0.45
1:D:75[B]:LEU:HD22	8:D:429:HOH:O	2.15	0.45
1:B:106[A]:ASN:O	1:B:110[A]:TYR:CD1	2.65	0.45
1:C:68[A]:MET:HA	1:C:68[A]:MET:CE	2.47	0.45
1:D:33:THR:HA	1:D:36:TYR:CE2	2.51	0.45
1:D:106[A]:ASN:O	1:D:110[A]:TYR:CD1	2.62	0.45
1:A:30:HIS:HB3	1:B:111[A]:LEU:HD11	1.95	0.45
1:D:90:GLU:CD	1:E:99:PRO:HG3	2.37	0.45
1:E:106[A]:ASN:O	1:E:110[A]:TYR:CD1	2.63	0.45
1:B:44:LEU:HD22	1:C:69[A]:VAL:CG2	2.47	0.45
1:C:116[B]:ASP:O	1:C:120[B]:LEU:CG	2.58	0.45
1:D:119[B]:MET:HA	1:D:119[B]:MET:HE2	1.99	0.45
1:E:110[B]:TYR:O	1:E:113[B]:TRP:HB2	2.16	0.45
7:E:303:OLA:H42	7:E:304:OLA:H42	1.99	0.45
1:C:36:TYR:HB3	1:C:75[B]:LEU:HB2	1.99	0.45
1:E:159:TYR:CE1	2:E:308:OLC:H24A	2.52	0.45
1:B:31:ILE:HD12	1:B:31:ILE:HA	1.87	0.45
1:C:33:THR:HA	1:C:36:TYR:CE2	2.51	0.45
1:A:185:MET:O	1:A:189:ILE:HG12	2.17	0.45
1:B:185:MET:O	1:B:189:ILE:HG12	2.17	0.45
1:C:41:ALA:HB1	1:D:66:VAL:HG13	1.99	0.45
1:D:38:VAL:HG22	1:E:115[B]:ILE:HD11	1.99	0.44
1:B:119[A]:MET:HA	1:B:119[A]:MET:HE2	1.99	0.44
1:C:31:ILE:HD12	1:C:31:ILE:HA	1.88	0.44
1:A:69[A]:VAL:CG2	1:E:44:LEU:HD22	2.47	0.44
1:A:75[B]:LEU:HD22	8:A:437:HOH:O	2.17	0.44
2:C:301:OLC:H8A	2:C:301:OLC:H11	1.72	0.44
1:D:78[B]:GLN:OE1	1:D:78[B]:GLN:HA	2.16	0.44
1:E:68[A]:MET:HA	1:E:68[A]:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:HIS:CE1	1:C:107[A]:GLY:HA3	2.53	0.44
1:E:185:MET:O	1:E:189:ILE:HG12	2.17	0.44
1:A:115[B]:ILE:HG22	8:A:411:HOH:O	0.74	0.44
1:B:25:TYR:OH	1:C:102:ASP:OD2	2.35	0.44
1:E:124:ILE:O	1:E:128:VAL:HG22	2.18	0.44
1:A:70[A]:SER:O	1:A:74[A]:LEU:CD2	2.65	0.44
1:C:30:HIS:HB3	1:D:111[B]:LEU:HD23	1.97	0.44
1:C:113[A]:TRP:NE1	8:C:406:HOH:O	2.36	0.44
1:E:113[B]:TRP:CD1	5:E:315:RET:H14	2.52	0.44
1:C:44:LEU:HD22	1:D:69[A]:VAL:CG2	2.46	0.44
1:E:33:THR:HA	1:E:36:TYR:CE2	2.52	0.44
1:D:31:ILE:HD12	1:D:31:ILE:HA	1.88	0.44
1:A:101:GLY:O	1:A:102:ASP:HB2	2.18	0.43
1:A:227:LEU:HB2	1:A:234:LEU:HD12	1.99	0.43
7:C:310:OLA:H42	7:E:304:OLA:H21	2.00	0.43
1:B:30:HIS:O	1:C:111[A]:LEU:HD12	2.18	0.43
1:D:34:LEU:HD11	1:E:115[A]:ILE:HG21	1.99	0.43
1:E:74[B]:LEU:HD13	1:E:74[B]:LEU:O	2.18	0.43
1:E:101:GLY:O	1:E:102:ASP:HB2	2.18	0.43
1:A:26:GLN:HB3	1:A:30:HIS:CE1	2.54	0.43
1:A:38:VAL:HG22	1:B:115[B]:ILE:HD11	1.99	0.43
1:E:76[A]:TYR:O	1:E:80[A]:GLN:HG2	2.19	0.43
1:A:115[A]:ILE:C	8:A:411:HOH:O	2.56	0.43
1:E:115[B]:ILE:CG2	8:E:424:HOH:O	0.76	0.43
1:D:90:GLU:OE1	1:E:99:PRO:CG	2.66	0.43
1:B:101:GLY:O	1:B:102:ASP:HB2	2.18	0.43
1:C:124:ILE:O	1:C:128:VAL:HG22	2.19	0.43
1:D:146:GLY:O	1:D:150[A]:ILE:HG12	2.19	0.43
1:A:66:VAL:HG13	1:E:41:ALA:HB1	2.01	0.43
1:B:88:PHE:CZ	1:B:93:GLY:HA2	2.54	0.43
2:B:302:OLC:H11	2:B:302:OLC:H8	1.76	0.43
1:C:26:GLN:HB3	1:C:30:HIS:CE1	2.53	0.43
1:E:146:GLY:O	1:E:150[B]:ILE:HG13	2.19	0.43
1:B:124:ILE:O	1:B:128:VAL:HG22	2.19	0.43
1:C:146:GLY:O	1:C:150[A]:ILE:HG12	2.19	0.43
1:D:237:GLU:O	1:D:241:MET:HG3	2.19	0.43
5:E:315:RET:H181	5:E:315:RET:H7	1.80	0.43
1:A:68[A]:MET:HA	1:A:68[A]:MET:HE2	2.00	0.42
2:A:302:OLC:H11	2:A:302:OLC:H8A	1.73	0.42
1:B:146:GLY:O	1:B:150[A]:ILE:HG12	2.19	0.42
1:E:119[A]:MET:HA	1:E:119[A]:MET:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:GLY:O	1:E:150[A]:ILE:HG12	2.18	0.42
1:C:111[A]:LEU:HB2	8:C:434:HOH:O	2.18	0.42
1:D:26:GLN:HB3	1:D:30:HIS:CE1	2.54	0.42
2:A:315:OLC:H11	2:A:315:OLC:H8	1.84	0.42
1:B:26:GLN:HB3	1:B:30:HIS:CE1	2.54	0.42
5:C:312:RET:H181	5:C:312:RET:H7	1.80	0.42
1:D:74[B]:LEU:HD13	1:D:74[B]:LEU:O	2.19	0.42
1:D:101:GLY:O	1:D:102:ASP:HB2	2.18	0.42
1:D:113[B]:TRP:C	1:D:115[B]:ILE:H	2.22	0.42
1:A:31:ILE:HD12	1:A:31:ILE:HA	1.83	0.42
1:C:38:VAL:HG22	1:D:115[B]:ILE:CD1	2.49	0.42
1:D:70[A]:SER:CB	1:D:115[A]:ILE:HD11	2.49	0.42
1:A:34:LEU:HD11	1:B:115[A]:ILE:CG2	2.50	0.42
1:B:237:GLU:O	1:B:241:MET:HG3	2.20	0.42
1:D:88:PHE:CZ	1:D:93:GLY:HA2	2.54	0.42
1:A:117[B]:VAL:CG2	1:A:150[B]:ILE:HD11	2.48	0.42
1:C:101:GLY:O	1:C:102:ASP:HB2	2.20	0.42
1:D:34:LEU:HD11	1:E:115[A]:ILE:CG2	2.49	0.42
5:D:311:RET:H7	5:D:311:RET:H181	1.81	0.42
1:E:88:PHE:CZ	1:E:93:GLY:HA2	2.54	0.42
1:A:173:ILE:O	1:A:176:ALA:HB3	2.20	0.42
1:C:173:ILE:O	1:C:176:ALA:HB3	2.20	0.42
1:E:26:GLN:HB3	1:E:30:HIS:CE1	2.55	0.42
5:B:309:RET:H11	5:B:309:RET:H191	1.92	0.42
1:D:41:ALA:HB1	1:E:66:VAL:HG13	2.01	0.42
1:D:173:ILE:O	1:D:176:ALA:HB3	2.20	0.42
1:E:173:ILE:O	1:E:176:ALA:HB3	2.20	0.42
1:A:30:HIS:CB	1:B:111[A]:LEU:CD1	2.96	0.42
1:A:30:HIS:CB	1:B:111[A]:LEU:HD11	2.50	0.42
1:A:111[A]:LEU:HB2	8:E:437:HOH:O	2.19	0.42
1:B:30:HIS:HB3	1:C:111[A]:LEU:HD11	2.00	0.42
1:E:81[A]:ASN:ND2	1:E:105[A]:ASN:H	2.17	0.42
1:C:109[A]:ARG:HG3	8:C:406:HOH:O	2.20	0.41
3:D:305:LFA:H203	3:D:307:LFA:H11	2.02	0.41
1:A:88:PHE:CZ	1:A:93:GLY:HA2	2.55	0.41
1:B:227:LEU:HB2	1:B:234:LEU:HD12	2.01	0.41
5:B:309:RET:H181	5:B:309:RET:H7	1.82	0.41
1:A:124:ILE:O	1:A:128:VAL:HG22	2.20	0.41
1:C:81[A]:ASN:HD21	1:C:105[A]:ASN:H	1.69	0.41
1:B:68[A]:MET:HA	1:B:68[A]:MET:HE2	2.03	0.41
1:C:113[B]:TRP:CD1	5:C:312:RET:H14	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ALA:HB1	1:C:66:VAL:HG13	2.03	0.41
1:B:117[A]:VAL:HG21	1:B:150[A]:ILE:HD11	2.03	0.41
1:D:30:HIS:C	1:E:111[A]:LEU:HD12	2.41	0.41
1:A:114[B]:LEU:HD22	2:A:313:OLC:H15	2.03	0.41
1:B:34:LEU:HD11	1:C:115[A]:ILE:CG2	2.51	0.41
1:C:25:TYR:OH	1:D:102:ASP:OD2	2.39	0.41
1:D:91:GLU:OE1	1:D:91:GLU:N	2.51	0.41
2:D:312:OLC:H13	2:D:312:OLC:H10	1.84	0.41
1:A:76[A]:TYR:O	1:A:80[A]:GLN:HG2	2.21	0.41
1:A:99:PRO:HG3	1:E:90:GLU:HG2	2.02	0.41
1:C:91:GLU:OE1	1:C:91:GLU:N	2.52	0.41
1:B:70[A]:SER:O	1:B:74[A]:LEU:HD23	2.20	0.40
1:C:119[B]:MET:CE	1:C:119[B]:MET:CA	2.99	0.40
1:D:90:GLU:HG2	1:E:99:PRO:HG3	2.03	0.40
1:E:237:GLU:O	1:E:241:MET:HG3	2.21	0.40
1:B:173:ILE:O	1:B:176:ALA:HB3	2.21	0.40
1:C:68[B]:MET:HA	1:C:68[B]:MET:HE2	2.04	0.40
1:D:90:GLU:CG	1:E:99:PRO:HG3	2.51	0.40
1:E:115[B]:ILE:HG23	8:E:424:HOH:O	0.55	0.40
1:A:30:HIS:C	1:B:111[A]:LEU:HD12	2.41	0.40
5:A:314:RET:H11	5:A:314:RET:H191	1.91	0.40
1:B:71[A]:ALA:O	1:B:75[A]:LEU:HG	2.21	0.40
1:B:80[A]:GLN:OE1	1:B:80[A]:GLN:HA	2.21	0.40
1:D:117[B]:VAL:HG21	1:D:150[B]:ILE:HD11	2.04	0.40
1:D:124:ILE:O	1:D:128:VAL:HG22	2.21	0.40
1:A:32:LEU:CD2	8:A:437:HOH:O	2.67	0.40
1:B:81[A]:ASN:HD21	1:B:105[A]:ASN:H	1.68	0.40
1:C:66:VAL:HG12	8:C:417:HOH:O	2.22	0.40
1:C:88:PHE:CZ	1:C:93:GLY:HA2	2.56	0.40
1:D:113[B]:TRP:CD1	5:D:311:RET:H14	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:PRO:CB	1:E:131:THR:O[8_445]	2.17	0.03

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	308/273 (113%)	284 (92%)	22 (7%)	2 (1%)	25 47
1	B	308/273 (113%)	286 (93%)	20 (6%)	2 (1%)	25 47
1	C	308/273 (113%)	287 (93%)	19 (6%)	2 (1%)	25 47
1	D	308/273 (113%)	291 (94%)	17 (6%)	0	100 100
1	E	308/273 (113%)	290 (94%)	16 (5%)	2 (1%)	25 47
All	All	1540/1365 (113%)	1438 (93%)	94 (6%)	8 (0%)	41 52

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	110[A]	TYR
1	C	110[B]	TYR
1	A	110[A]	TYR
1	A	110[B]	TYR
1	B	110[A]	TYR
1	B	110[B]	TYR
1	E	110[A]	TYR
1	E	110[B]	TYR

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	262/234 (112%)	260 (99%)	2 (1%)	81 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	262/234 (112%)	260 (99%)	2 (1%)	81 92
1	C	261/234 (112%)	259 (99%)	2 (1%)	81 92
1	D	262/234 (112%)	259 (99%)	3 (1%)	73 88
1	E	262/234 (112%)	260 (99%)	2 (1%)	81 92
All	All	1309/1170 (112%)	1298 (99%)	11 (1%)	76 92

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PHE
1	A	92	VAL
1	B	10	PHE
1	B	92	VAL
1	C	10	PHE
1	C	92	VAL
1	D	10	PHE
1	D	92	VAL
1	D	230	VAL
1	E	10	PHE
1	E	92	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 75 ligands modelled in this entry, 10 are monoatomic - leaving 65 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	-	19,19,24	1.05	1 (5%)	20,20,25	0.93	1 (5%)
3	LFA	D	309	-	6,6,19	0.12	0	5,5,18	0.08	0
2	OLC	A	315	-	17,17,24	1.06	1 (5%)	17,17,25	0.87	1 (5%)
2	OLC	B	303	-	4,4,24	0.26	0	3,3,25	0.41	0
2	OLC	D	301	-	4,4,24	0.27	0	3,3,25	0.39	0
3	LFA	C	308	-	19,19,19	0.07	0	18,18,18	0.04	0
3	LFA	D	305	-	19,19,19	0.07	0	18,18,18	0.04	0
3	LFA	A	308	-	7,7,19	0.11	0	6,6,18	0.08	0
2	OLC	A	302	-	16,16,24	1.14	1 (6%)	16,16,25	0.91	0
3	LFA	B	306	-	9,9,19	0.10	0	8,8,18	0.08	0
3	LFA	D	308	-	16,16,19	0.07	0	15,15,18	0.05	0
3	LFA	D	307	-	7,7,19	0.10	0	6,6,18	0.08	0
3	LFA	E	310	-	13,13,19	0.07	0	12,12,18	0.06	0
5	RET	E	315	1	20,20,21	1.66	3 (15%)	27,27,28	1.09	1 (3%)
2	OLC	E	306	-	15,15,24	0.27	0	14,14,25	0.51	0
3	LFA	E	312	-	4,4,19	0.15	0	3,3,18	0.22	0
3	LFA	B	307	-	6,6,19	0.11	0	5,5,18	0.08	0
2	OLC	C	305	-	15,15,24	1.16	1 (6%)	16,16,25	0.96	1 (6%)
3	LFA	A	309	-	3,3,19	0.25	0	2,2,18	0.45	0
2	OLC	D	302	-	17,17,24	1.11	1 (5%)	18,18,25	1.01	1 (5%)
3	LFA	E	311	-	3,3,19	0.23	0	2,2,18	0.46	0
5	RET	D	311	1	20,20,21	1.71	3 (15%)	27,27,28	1.11	2 (7%)
7	OLA	B	311	-	16,16,19	0.57	0	16,16,19	0.50	0
2	OLC	D	304	-	13,13,24	1.25	1 (7%)	14,14,25	1.01	2 (14%)
2	OLC	C	313	-	15,15,24	1.19	1 (6%)	15,15,25	1.11	1 (6%)
7	OLA	D	313	-	6,6,19	0.86	0	6,6,19	0.82	0
2	OLC	A	304	-	12,12,24	1.30	1 (8%)	13,13,25	1.08	1 (7%)
3	LFA	A	311	-	6,6,19	0.12	0	5,5,18	0.09	0
2	OLC	C	304	-	16,16,24	1.92	2 (12%)	16,16,25	0.96	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	OLC	B	301	-	20,20,24	1.02	1 (5%)	21,21,25	0.94	1 (4%)
5	RET	A	314	1	20,20,21	1.67	3 (15%)	27,27,28	1.14	2 (7%)
2	OLC	E	308	-	14,14,24	1.20	1 (7%)	15,15,25	0.99	2 (13%)
2	OLC	E	301	-	18,18,24	1.09	1 (5%)	18,18,25	0.90	0
7	OLA	E	302	-	19,19,19	0.52	0	19,19,19	0.47	0
7	OLA	E	304	-	14,14,19	0.59	0	14,14,19	0.54	0
2	OLC	E	305	-	7,7,24	0.27	0	6,6,25	0.46	0
7	OLA	C	310	-	17,17,19	0.54	0	17,17,19	0.50	0
7	OLA	E	314	-	5,5,19	0.94	0	5,5,19	0.87	0
2	OLC	A	301	-	8,8,24	0.33	0	6,7,25	0.47	0
2	OLC	B	310	-	19,19,24	1.05	1 (5%)	20,20,25	0.92	1 (5%)
3	LFA	E	309	-	7,7,19	0.10	0	6,6,18	0.07	0
7	OLA	B	312	-	17,17,19	0.54	0	17,17,19	0.50	0
6	GOL	C	311	-	3,3,5	0.34	0	2,2,5	0.14	0
3	LFA	A	310	-	5,5,19	0.12	0	4,4,18	0.09	0
6	GOL	A	316	-	3,3,5	0.35	0	2,2,5	0.14	0
2	OLC	C	302	-	7,7,24	0.34	0	5,6,25	0.51	0
5	RET	B	309	1	20,20,21	1.69	3 (15%)	27,27,28	1.10	2 (7%)
3	LFA	A	307	-	7,7,19	0.10	0	6,6,18	0.07	0
2	OLC	A	305	-	14,14,24	1.21	1 (7%)	15,15,25	0.99	1 (6%)
2	OLC	C	303	-	11,11,24	1.29	1 (9%)	11,11,25	0.98	1 (9%)
5	RET	C	312	1	20,20,21	1.69	3 (15%)	27,27,28	1.09	1 (3%)
3	LFA	B	305	-	7,7,19	0.11	0	6,6,18	0.08	0
3	LFA	C	306	-	3,3,19	0.24	0	2,2,18	0.44	0
3	LFA	C	307	-	7,7,19	0.11	0	6,6,18	0.08	0
2	OLC	D	303	-	4,4,24	0.30	0	3,3,25	0.37	0
2	OLC	A	303	-	6,6,24	0.36	0	4,5,25	0.45	0
2	OLC	B	302	-	15,15,24	1.13	1 (6%)	15,15,25	0.89	1 (6%)
3	LFA	D	306	-	19,19,19	0.07	0	18,18,18	0.04	0
3	LFA	A	306	-	6,6,19	0.12	0	5,5,18	0.08	0
2	OLC	B	304	-	11,11,24	1.29	1 (9%)	11,11,25	1.01	1 (9%)
2	OLC	D	312	-	19,19,24	1.06	1 (5%)	19,19,25	0.93	1 (5%)
6	GOL	B	313	-	3,3,5	0.34	0	2,2,5	0.16	0
2	OLC	A	313	-	19,19,24	1.06	1 (5%)	19,19,25	0.92	1 (5%)
2	OLC	C	301	-	18,18,24	1.01	1 (5%)	18,18,25	0.81	0
7	OLA	E	303	-	16,16,19	0.56	0	16,16,19	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	-	-	7/19/19/24	-
3	LFA	D	309	-	-	2/4/4/17	-
2	OLC	A	315	-	-	2/16/16/24	-
2	OLC	B	303	-	-	1/2/2/24	-
2	OLC	D	301	-	-	1/2/2/24	-
3	LFA	C	308	-	-	12/17/17/17	-
3	LFA	D	305	-	-	11/17/17/17	-
3	LFA	A	308	-	-	2/5/5/17	-
2	OLC	A	302	-	-	5/14/14/24	-
3	LFA	B	306	-	-	0/7/7/17	-
3	LFA	D	308	-	-	5/14/14/17	-
3	LFA	D	307	-	-	3/5/5/17	-
3	LFA	E	310	-	-	0/11/11/17	-
5	RET	E	315	1	-	0/13/30/31	0/1/1/1
2	OLC	E	306	-	-	9/13/13/24	-
3	LFA	E	312	-	-	0/2/2/17	-
3	LFA	B	307	-	-	2/4/4/17	-
2	OLC	C	305	-	-	7/15/15/24	-
3	LFA	A	309	-	-	0/1/1/17	-
2	OLC	D	302	-	-	6/17/17/24	-
3	LFA	E	311	-	-	1/1/1/17	-
5	RET	D	311	1	-	0/13/30/31	0/1/1/1
7	OLA	B	311	-	-	4/14/14/17	-
2	OLC	D	304	-	-	8/13/13/24	-
2	OLC	C	313	-	-	5/14/14/24	-
7	OLA	D	313	-	-	2/4/4/17	-
2	OLC	A	304	-	-	1/12/12/24	-
3	LFA	A	311	-	-	1/4/4/17	-
2	OLC	C	304	-	-	8/14/14/24	-
2	OLC	B	301	-	-	6/20/20/24	-
5	RET	A	314	1	-	0/13/30/31	0/1/1/1
2	OLC	E	308	-	-	4/14/14/24	-
2	OLC	E	301	-	-	9/16/16/24	-
7	OLA	E	302	-	-	4/17/17/17	-
7	OLA	E	304	-	-	6/12/12/17	-
2	OLC	E	305	-	-	2/5/5/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OLA	C	310	-	-	8/15/15/17	-
7	OLA	E	314	-	-	1/3/3/17	-
2	OLC	A	301	-	-	1/6/6/24	-
2	OLC	B	310	-	-	11/19/19/24	-
3	LFA	E	309	-	-	0/5/5/17	-
7	OLA	B	312	-	-	11/15/15/17	-
6	GOL	C	311	-	-	0/1/1/4	-
3	LFA	A	310	-	-	1/3/3/17	-
6	GOL	A	316	-	-	0/1/1/4	-
2	OLC	C	302	-	-	3/5/5/24	-
5	RET	B	309	1	-	0/13/30/31	0/1/1/1
3	LFA	A	307	-	-	1/5/5/17	-
2	OLC	A	305	-	-	3/14/14/24	-
2	OLC	C	303	-	-	3/10/10/24	-
5	RET	C	312	1	-	0/13/30/31	0/1/1/1
3	LFA	B	305	-	-	2/5/5/17	-
3	LFA	C	306	-	-	0/1/1/17	-
3	LFA	C	307	-	-	4/5/5/17	-
2	OLC	D	303	-	-	0/2/2/24	-
2	OLC	A	303	-	-	2/4/4/24	-
2	OLC	B	302	-	-	2/14/14/24	-
3	LFA	D	306	-	-	9/17/17/17	-
3	LFA	A	306	-	-	2/4/4/17	-
2	OLC	B	304	-	-	5/10/10/24	-
2	OLC	D	312	-	-	7/17/17/24	-
6	GOL	B	313	-	-	1/1/1/4	-
2	OLC	A	313	-	-	9/17/17/24	-
2	OLC	C	301	-	-	5/17/17/24	-
7	OLA	E	303	-	-	6/14/14/17	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	304	OLC	O19-C1	7.20	1.46	1.22
2	D	312	OLC	O20-C1	4.51	1.45	1.30
2	A	313	OLC	O20-C1	4.51	1.45	1.30
2	E	301	OLC	O20-C1	4.49	1.45	1.30
2	A	302	OLC	O20-C1	4.46	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	313	OLC	O20-C1	4.39	1.46	1.33
2	A	305	OLC	O20-C1	4.35	1.46	1.33
2	B	301	OLC	O20-C1	4.34	1.46	1.33
2	A	304	OLC	O20-C1	4.34	1.46	1.33
2	B	310	OLC	O20-C1	4.34	1.46	1.33
2	E	307	OLC	O20-C1	4.33	1.46	1.33
2	D	302	OLC	O20-C1	4.33	1.46	1.33
2	C	305	OLC	O20-C1	4.29	1.45	1.33
2	D	304	OLC	O20-C1	4.28	1.45	1.33
2	E	308	OLC	O20-C1	4.27	1.45	1.33
5	D	311	RET	C14-C13	4.20	1.37	1.33
5	E	315	RET	C10-C9	4.18	1.41	1.35
5	B	309	RET	C10-C9	4.17	1.41	1.35
2	B	302	OLC	O20-C1	4.15	1.46	1.33
2	A	315	OLC	O20-C1	4.14	1.46	1.33
5	D	311	RET	C10-C9	4.14	1.41	1.35
2	C	303	OLC	O20-C1	4.12	1.46	1.33
2	B	304	OLC	O20-C1	4.10	1.46	1.33
2	C	301	OLC	O20-C1	4.08	1.46	1.33
5	C	312	RET	C10-C9	4.07	1.41	1.35
5	A	314	RET	C10-C9	4.07	1.41	1.35
5	B	309	RET	C14-C13	4.05	1.36	1.33
5	C	312	RET	C14-C13	3.93	1.36	1.33
5	A	314	RET	C14-C13	3.90	1.36	1.33
5	E	315	RET	C14-C13	3.85	1.36	1.33
5	C	312	RET	C8-C9	-2.67	1.40	1.45
5	B	309	RET	C8-C9	-2.62	1.40	1.45
5	E	315	RET	C8-C9	-2.60	1.40	1.45
5	D	311	RET	C8-C9	-2.56	1.40	1.45
5	A	314	RET	C8-C9	-2.55	1.40	1.45
2	C	304	OLC	O20-C1	-2.47	1.22	1.30

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	314	RET	C19-C9-C10	-4.15	117.11	122.92
5	D	311	RET	C19-C9-C10	-4.01	117.30	122.92
5	B	309	RET	C19-C9-C10	-3.99	117.34	122.92
5	E	315	RET	C19-C9-C10	-3.96	117.37	122.92
5	C	312	RET	C19-C9-C10	-3.91	117.45	122.92
2	A	304	OLC	O20-C1-C2	2.79	120.67	111.91
2	B	301	OLC	O20-C1-C2	2.78	120.64	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	313	OLC	O20-C1-C2	2.75	120.55	111.91
2	E	307	OLC	O20-C1-C2	2.75	120.53	111.91
2	B	310	OLC	O20-C1-C2	2.72	120.45	111.91
2	D	302	OLC	O20-C1-C2	2.68	120.33	111.91
2	D	304	OLC	O20-C1-C2	2.65	120.21	111.91
2	E	308	OLC	O20-C1-C2	2.64	120.20	111.91
2	A	305	OLC	O20-C1-C2	2.64	120.19	111.91
2	C	305	OLC	O20-C1-C2	2.57	119.98	111.91
5	B	309	RET	C8-C9-C10	2.14	122.22	118.94
2	A	315	OLC	O20-C1-C2	2.13	120.65	112.23
2	B	304	OLC	O20-C1-C2	2.10	120.55	112.23
5	A	314	RET	C8-C9-C10	2.08	122.13	118.94
2	C	303	OLC	O20-C1-C2	2.06	120.39	112.23
2	A	313	OLC	O20-C1-C2	2.06	120.65	114.03
2	D	312	OLC	O20-C1-C2	2.06	120.64	114.03
2	B	302	OLC	O20-C1-C2	2.05	120.34	112.23
2	D	304	OLC	O20-C1-O19	-2.04	118.44	123.59
2	E	308	OLC	O20-C1-O19	-2.03	118.47	123.59
2	C	304	OLC	O20-C1-C2	2.02	120.52	114.03
5	D	311	RET	C8-C9-C10	2.00	122.01	118.94

There are no chirality outliers.

All (233) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	305	OLC	C21-C22-C24-O25
2	A	305	OLC	O23-C22-C24-O25
2	C	302	OLC	C9-C10-C11-C12
2	C	305	OLC	C21-C22-C24-O25
2	C	305	OLC	O20-C21-C22-O23
2	E	308	OLC	O20-C21-C22-O23
3	E	311	LFA	C17-C18-C19-C20
7	B	312	OLA	C11-C10-C9-C8
7	B	311	OLA	C11-C10-C9-C8
7	C	310	OLA	C11-C10-C9-C8
7	E	303	OLA	C11-C10-C9-C8
2	B	304	OLC	C2-C1-O20-C21
3	C	308	LFA	C14-C15-C16-C17
2	D	304	OLC	O20-C21-C22-O23
2	B	304	OLC	O19-C1-O20-C21
2	D	304	OLC	O20-C21-C22-C24
2	E	307	OLC	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	D	312	OLC	C1-C2-C3-C4
2	D	304	OLC	C1-C2-C3-C4
2	E	307	OLC	C2-C1-O20-C21
7	E	304	OLA	C1-C2-C3-C4
3	D	305	LFA	C6-C7-C8-C9
7	E	304	OLA	C2-C3-C4-C5
3	C	308	LFA	C10-C11-C12-C13
3	D	305	LFA	C9-C10-C11-C12
2	C	303	OLC	C5-C6-C7-C8
3	C	308	LFA	C13-C14-C15-C16
2	A	313	OLC	C5-C6-C7-C8
2	A	304	OLC	C1-C2-C3-C4
7	E	303	OLA	C1-C2-C3-C4
2	E	307	OLC	C5-C6-C7-C8
3	A	308	LFA	C14-C15-C16-C17
3	D	308	LFA	C11-C12-C13-C14
3	D	305	LFA	C3-C4-C5-C6
7	B	312	OLA	C12-C13-C14-C15
2	C	301	OLC	C4-C5-C6-C7
3	B	307	LFA	C15-C16-C17-C18
3	D	308	LFA	C6-C7-C8-C9
2	B	310	OLC	O20-C21-C22-O23
2	A	302	OLC	C6-C7-C8-C9
2	C	304	OLC	C6-C7-C8-C9
2	E	301	OLC	C10-C11-C12-C13
2	E	306	OLC	C6-C7-C8-C9
2	C	304	OLC	C4-C5-C6-C7
2	C	304	OLC	C2-C3-C4-C5
7	B	312	OLA	C2-C3-C4-C5
7	C	310	OLA	C3-C4-C5-C6
3	D	306	LFA	C5-C6-C7-C8
2	B	301	OLC	C5-C6-C7-C8
3	D	306	LFA	C14-C15-C16-C17
7	E	302	OLA	C12-C13-C14-C15
3	D	305	LFA	C11-C12-C13-C14
3	C	308	LFA	C12-C13-C14-C15
7	E	304	OLA	C11-C10-C9-C8
2	E	307	OLC	O19-C1-O20-C21
2	C	304	OLC	C3-C4-C5-C6
2	B	301	OLC	C6-C7-C8-C9
2	E	305	OLC	C4-C5-C6-C7
2	D	304	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	D	306	LFA	C12-C13-C14-C15
7	B	312	OLA	C3-C4-C5-C6
7	E	302	OLA	C14-C15-C16-C17
2	A	313	OLC	C2-C3-C4-C5
3	D	305	LFA	C11-C10-C9-C8
2	D	302	OLC	C2-C1-O20-C21
2	E	306	OLC	C4-C5-C6-C7
7	C	310	OLA	C4-C5-C6-C7
2	A	302	OLC	C2-C3-C4-C5
2	B	310	OLC	C6-C7-C8-C9
2	C	304	OLC	C10-C11-C12-C13
7	E	303	OLA	C10-C11-C12-C13
2	C	313	OLC	C2-C1-O20-C21
7	E	302	OLA	C4-C5-C6-C7
3	C	307	LFA	C15-C16-C17-C18
2	E	308	OLC	O20-C21-C22-C24
2	D	304	OLC	C3-C4-C5-C6
3	A	310	LFA	C2-C3-C4-C5
2	D	302	OLC	O19-C1-O20-C21
2	E	301	OLC	C2-C3-C4-C5
2	A	313	OLC	C10-C11-C12-C13
7	B	312	OLA	C10-C11-C12-C13
2	C	313	OLC	C2-C3-C4-C5
3	D	306	LFA	C3-C4-C5-C6
2	C	301	OLC	C12-C13-C14-C15
3	D	306	LFA	C6-C7-C8-C9
2	B	304	OLC	C4-C5-C6-C7
3	C	307	LFA	C16-C17-C18-C19
2	D	312	OLC	C4-C5-C6-C7
3	D	305	LFA	C13-C14-C15-C16
2	C	304	OLC	C11-C12-C13-C14
7	E	303	OLA	C12-C13-C14-C15
2	C	313	OLC	O19-C1-O20-C21
7	D	313	OLA	C2-C3-C4-C5
2	D	302	OLC	C4-C5-C6-C7
2	D	312	OLC	C3-C4-C5-C6
2	C	303	OLC	C6-C7-C8-C9
2	C	305	OLC	O23-C22-C24-O25
7	B	311	OLA	C10-C11-C12-C13
2	B	310	OLC	O20-C21-C22-C24
2	C	305	OLC	O20-C21-C22-C24
2	E	306	OLC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	D	308	LFA	C11-C10-C9-C8
2	B	310	OLC	C2-C3-C4-C5
3	D	306	LFA	C1-C2-C3-C4
3	A	307	LFA	C1-C2-C3-C4
3	D	309	LFA	C14-C15-C16-C17
3	C	308	LFA	C9-C10-C11-C12
3	B	305	LFA	C3-C4-C5-C6
3	D	309	LFA	C16-C17-C18-C19
3	A	311	LFA	C3-C4-C5-C6
3	D	305	LFA	C4-C5-C6-C7
2	E	306	OLC	C2-C3-C4-C5
2	C	301	OLC	C11-C12-C13-C14
2	C	305	OLC	C6-C7-C8-C9
3	B	305	LFA	C2-C3-C4-C5
3	C	308	LFA	C17-C18-C19-C20
7	E	304	OLA	C3-C4-C5-C6
2	E	306	OLC	C13-C14-C15-C16
2	D	304	OLC	C2-C1-O20-C21
2	A	313	OLC	C1-C2-C3-C4
3	D	305	LFA	C14-C15-C16-C17
2	B	301	OLC	C4-C5-C6-C7
2	C	305	OLC	C2-C1-O20-C21
3	C	308	LFA	C11-C10-C9-C8
3	A	306	LFA	C17-C18-C19-C20
2	B	310	OLC	C5-C6-C7-C8
3	C	307	LFA	C17-C18-C19-C20
3	D	307	LFA	C5-C6-C7-C8
2	E	306	OLC	C10-C11-C12-C13
2	A	302	OLC	C11-C12-C13-C14
2	B	310	OLC	C3-C4-C5-C6
3	D	306	LFA	C15-C16-C17-C18
3	D	306	LFA	C4-C5-C6-C7
3	D	308	LFA	C14-C15-C16-C17
2	A	303	OLC	C7-C8-C9-C10
7	E	304	OLA	C4-C5-C6-C7
3	D	307	LFA	C1-C2-C3-C4
3	B	307	LFA	C16-C17-C18-C19
2	E	308	OLC	C3-C4-C5-C6
7	B	311	OLA	C12-C13-C14-C15
3	D	305	LFA	C10-C11-C12-C13
2	E	301	OLC	C6-C7-C8-C9
7	C	310	OLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	B	302	OLC	C2-C3-C4-C5
2	D	304	OLC	O19-C1-O20-C21
2	A	315	OLC	C2-C3-C4-C5
2	E	306	OLC	C5-C6-C7-C8
2	C	305	OLC	O19-C1-O20-C21
2	D	302	OLC	C6-C7-C8-C9
3	A	306	LFA	C16-C17-C18-C19
2	D	301	OLC	C6-C7-C8-C9
2	A	305	OLC	C2-C3-C4-C5
2	C	302	OLC	C5-C6-C7-C8
3	D	305	LFA	C15-C16-C17-C18
3	C	308	LFA	C5-C6-C7-C8
7	B	312	OLA	C11-C12-C13-C14
2	D	312	OLC	C2-C3-C4-C5
3	C	307	LFA	C13-C14-C15-C16
7	C	310	OLA	C12-C13-C14-C15
2	D	302	OLC	O20-C21-C22-O23
7	C	310	OLA	C5-C6-C7-C8
2	E	301	OLC	C5-C6-C7-C8
7	E	302	OLA	C7-C8-C9-C10
3	C	308	LFA	C1-C2-C3-C4
2	D	304	OLC	C4-C5-C6-C7
2	E	301	OLC	C3-C4-C5-C6
7	C	310	OLA	C7-C8-C9-C10
3	C	308	LFA	C4-C5-C6-C7
2	C	313	OLC	C1-C2-C3-C4
2	C	304	OLC	C12-C13-C14-C15
2	D	312	OLC	C5-C6-C7-C8
2	A	313	OLC	C9-C10-C11-C12
2	B	310	OLC	C9-C10-C11-C12
2	D	312	OLC	C7-C8-C9-C10
2	B	310	OLC	C4-C5-C6-C7
2	A	313	OLC	C12-C13-C14-C15
2	E	305	OLC	C2-C3-C4-C5
7	B	312	OLA	C6-C7-C8-C9
7	E	303	OLA	O2-C1-C2-C3
7	B	312	OLA	C4-C5-C6-C7
3	A	308	LFA	C17-C18-C19-C20
2	C	301	OLC	C5-C6-C7-C8
2	B	310	OLC	C2-C1-O20-C21
3	C	308	LFA	C3-C4-C5-C6
2	A	302	OLC	O19-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	D	305	LFA	C5-C6-C7-C8
2	B	301	OLC	C9-C10-C11-C12
2	E	306	OLC	C7-C8-C9-C10
2	B	310	OLC	O19-C1-O20-C21
7	B	312	OLA	O1-C1-C2-C3
2	C	313	OLC	C6-C7-C8-C9
7	D	313	OLA	C1-C2-C3-C4
3	C	308	LFA	C6-C7-C8-C9
2	A	315	OLC	C3-C4-C5-C6
7	E	303	OLA	O1-C1-C2-C3
2	A	302	OLC	O20-C1-C2-C3
2	E	307	OLC	C4-C5-C6-C7
6	B	313	GOL	O1-C1-C2-O2
7	B	311	OLA	C4-C5-C6-C7
3	D	306	LFA	C7-C8-C9-C10
7	B	312	OLA	O2-C1-C2-C3
3	D	307	LFA	C2-C3-C4-C5
2	E	301	OLC	C9-C10-C11-C12
2	D	312	OLC	C9-C10-C11-C12
2	C	303	OLC	C3-C4-C5-C6
2	C	302	OLC	C7-C8-C9-C10
2	E	301	OLC	C14-C15-C16-C17
2	C	301	OLC	C3-C4-C5-C6
2	D	302	OLC	C7-C8-C9-C10
2	E	307	OLC	C7-C8-C9-C10
2	A	301	OLC	C9-C10-C11-C12
2	E	307	OLC	C9-C10-C11-C12
7	E	304	OLA	C7-C8-C9-C10
7	C	310	OLA	C10-C11-C12-C13
2	A	313	OLC	O20-C1-C2-C3
2	B	310	OLC	C7-C8-C9-C10
2	C	304	OLC	C7-C8-C9-C10
2	E	308	OLC	C5-C6-C7-C8
2	A	313	OLC	O19-C1-C2-C3
2	B	303	OLC	C10-C11-C12-C13
2	B	301	OLC	C3-C4-C5-C6
2	A	313	OLC	C7-C8-C9-C10
7	B	312	OLA	C9-C10-C11-C12
2	A	303	OLC	C9-C10-C11-C12
2	B	301	OLC	C7-C8-C9-C10
2	E	301	OLC	C12-C13-C14-C15
3	D	308	LFA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	E	301	OLC	C11-C12-C13-C14
2	E	306	OLC	C11-C12-C13-C14
2	B	302	OLC	C10-C11-C12-C13
2	B	304	OLC	O20-C1-C2-C3
2	B	304	OLC	O19-C1-C2-C3
7	E	314	OLA	O2-C1-C2-C3

There are no ring outliers.

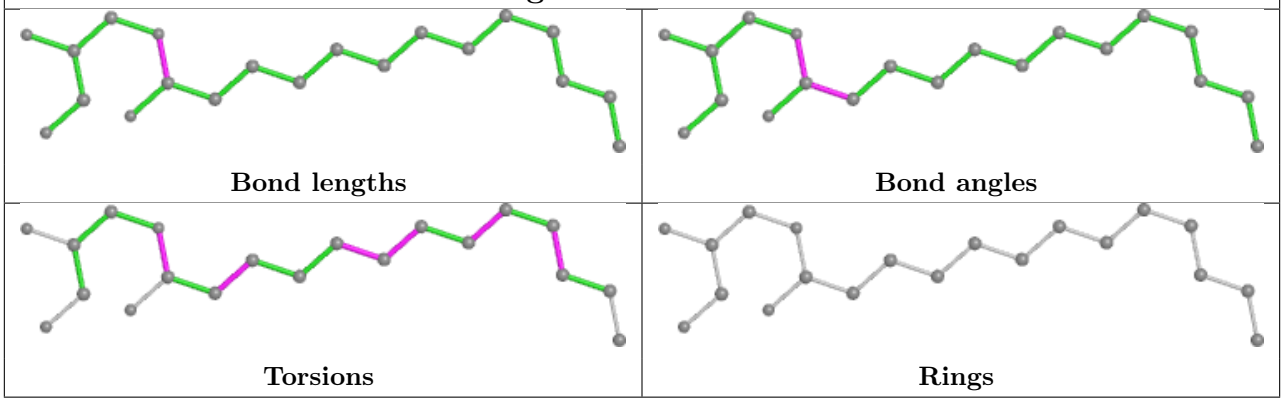
27 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	315	OLC	1	0
3	C	308	LFA	1	0
3	D	305	LFA	1	0
2	A	302	OLC	2	0
3	D	307	LFA	1	0
3	E	310	LFA	2	0
5	E	315	RET	8	0
2	C	305	OLC	3	0
3	E	311	LFA	2	0
5	D	311	RET	7	0
2	C	313	OLC	1	0
2	B	301	OLC	1	0
5	A	314	RET	7	0
2	E	308	OLC	1	0
2	E	301	OLC	3	0
7	E	304	OLA	2	0
7	C	310	OLA	1	0
7	E	314	OLA	1	0
2	B	310	OLC	1	0
5	B	309	RET	8	0
5	C	312	RET	7	0
2	B	302	OLC	1	0
3	D	306	LFA	2	0
2	D	312	OLC	1	0
2	A	313	OLC	2	0
2	C	301	OLC	3	0
7	E	303	OLA	2	0

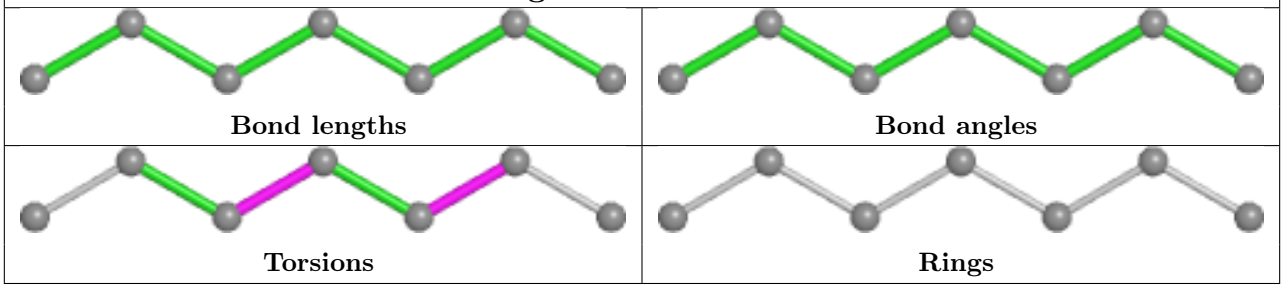
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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.

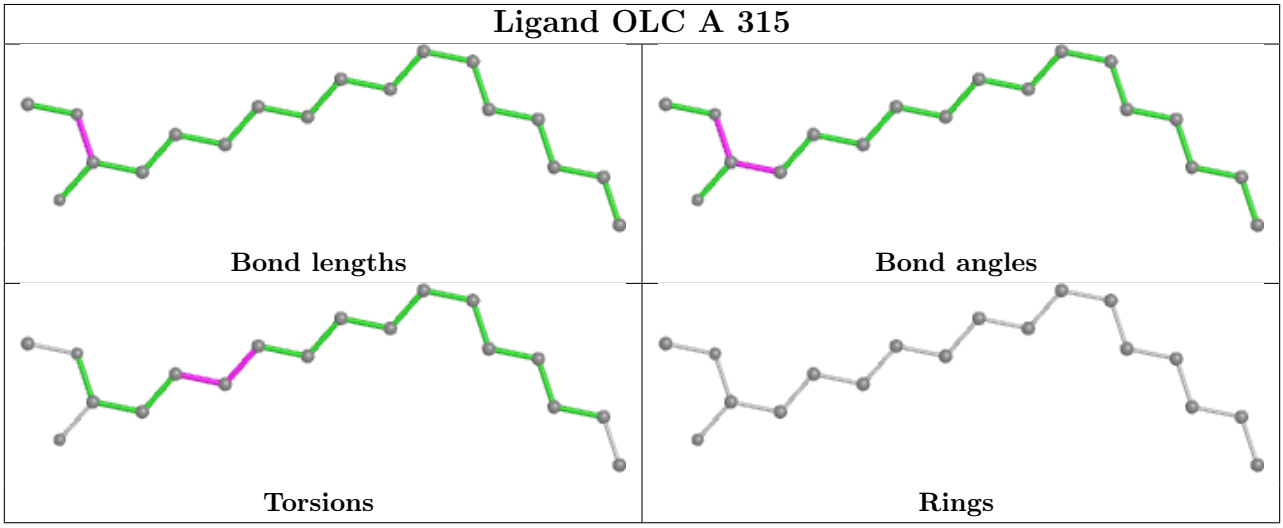
Ligand OLC E 307



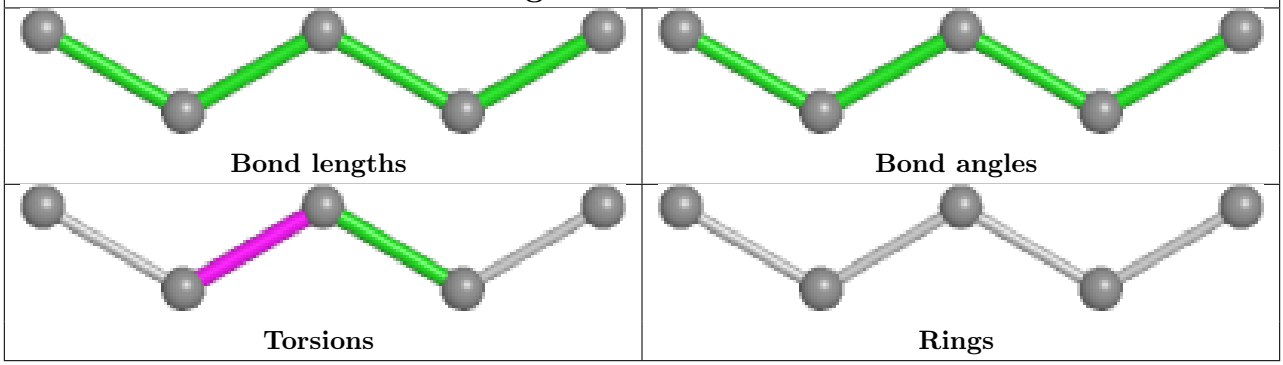
Ligand LFA D 309



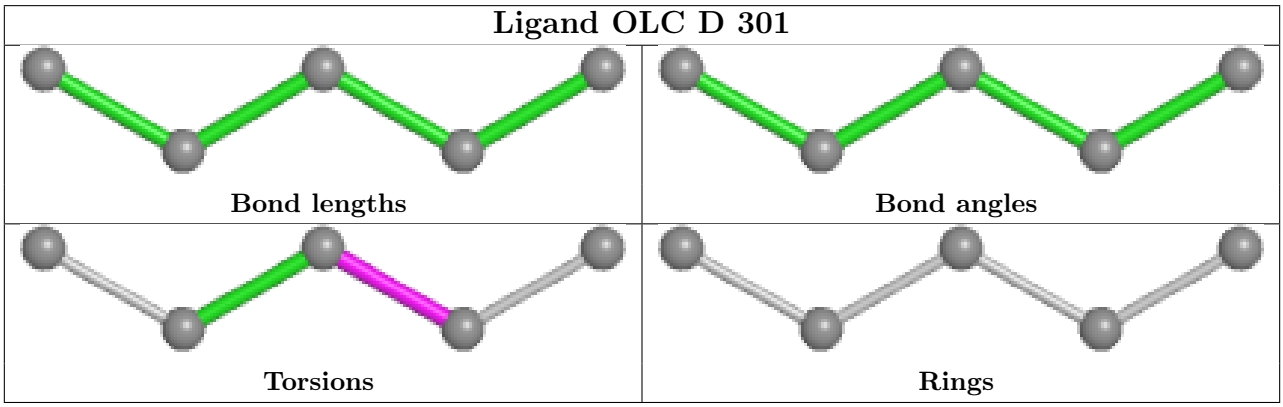
Ligand OLC A 315



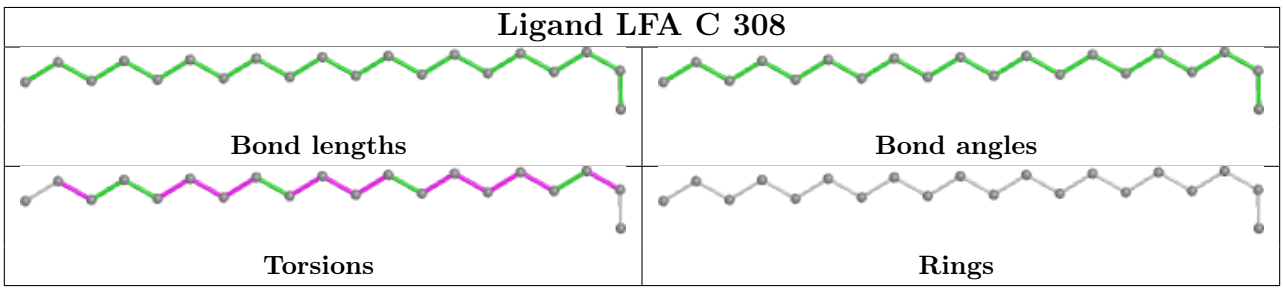
Ligand OLC B 303



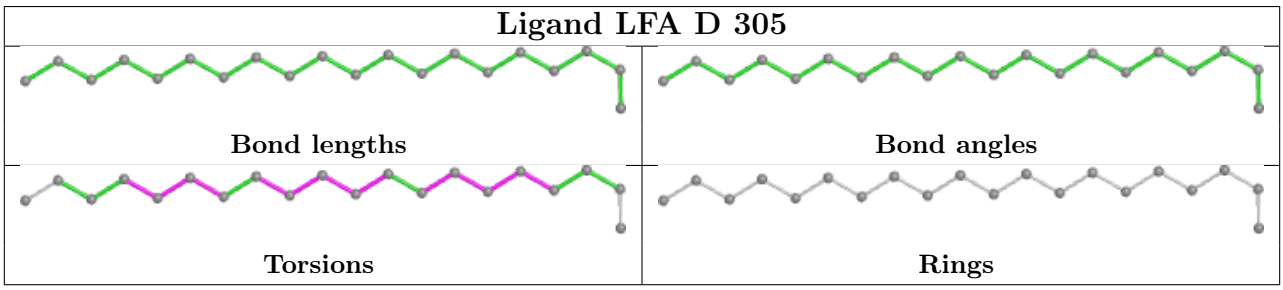
Ligand OLC D 301



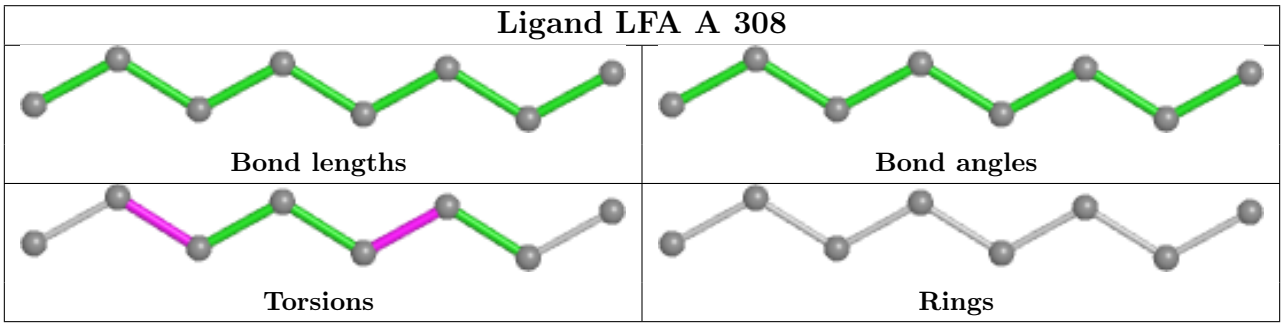
Ligand LFA C 308



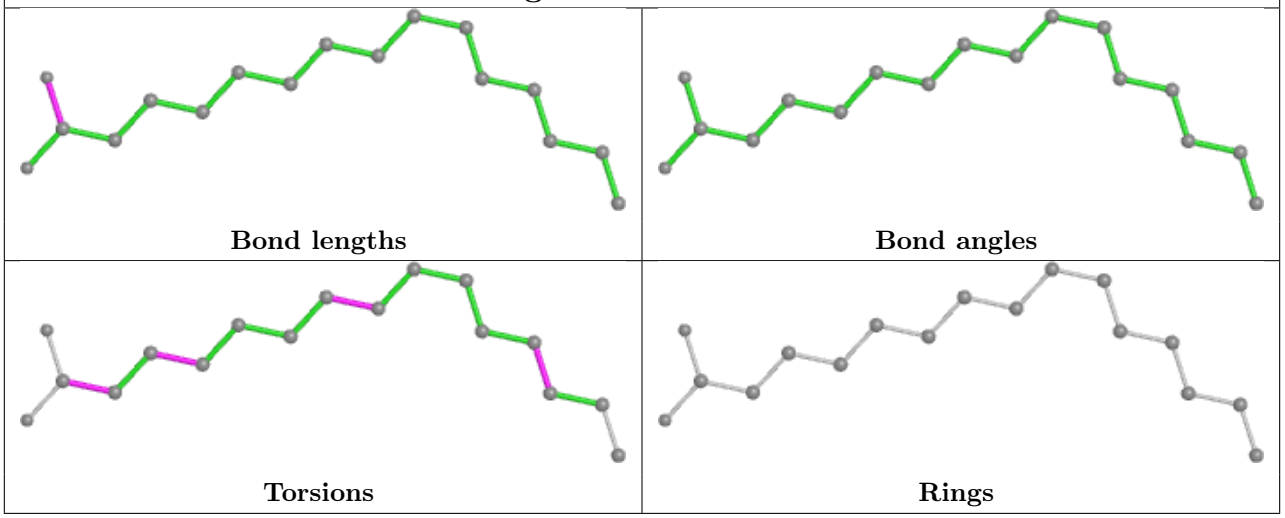
Ligand LFA D 305



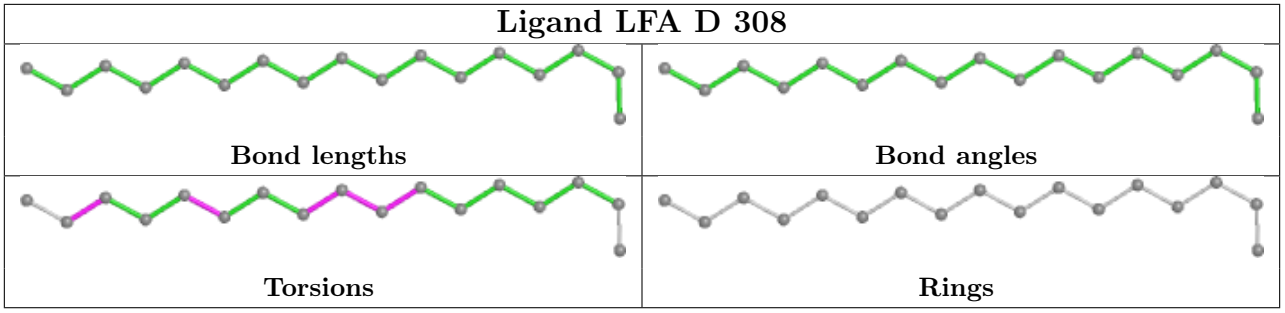
Ligand LFA A 308



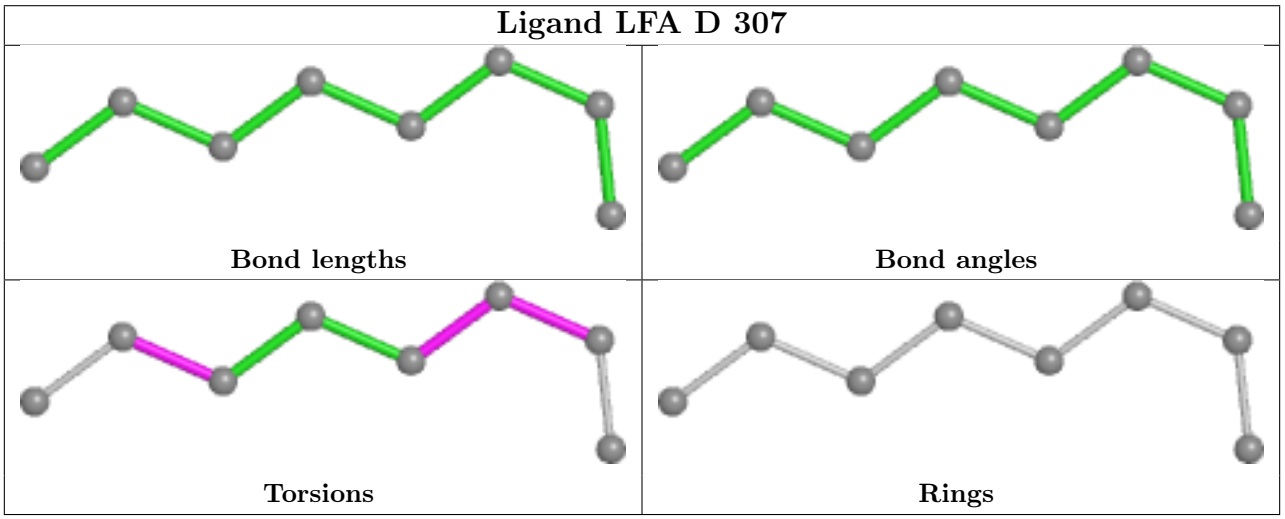
Ligand OLC A 302



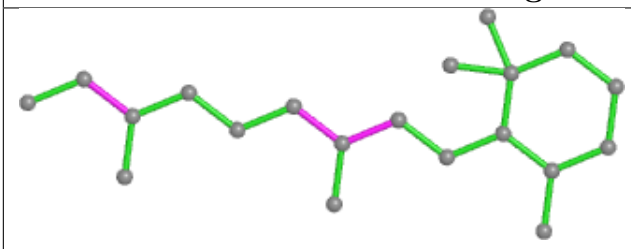
Ligand LFA D 308



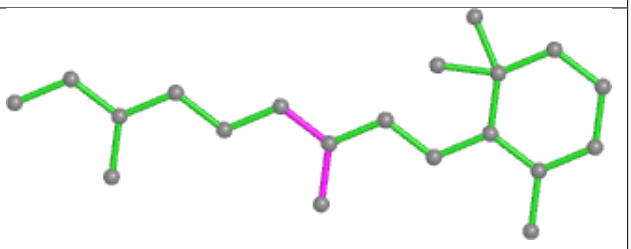
Ligand LFA D 307



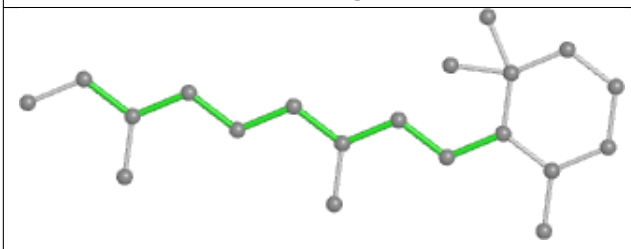
Ligand RET E 315



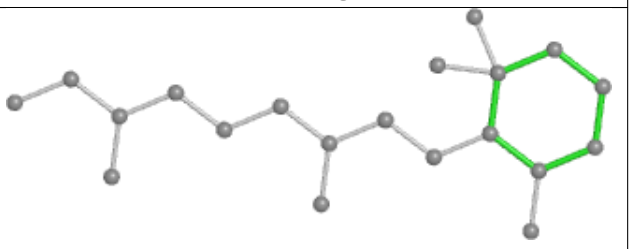
Bond lengths



Bond angles

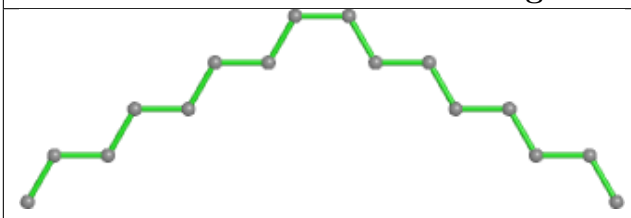


Torsions

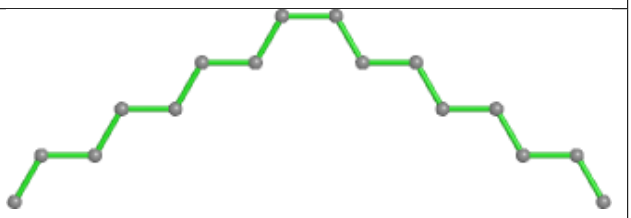


Rings

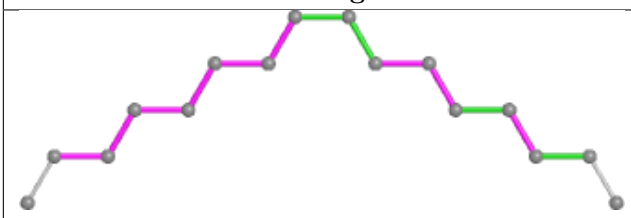
Ligand OLC E 306



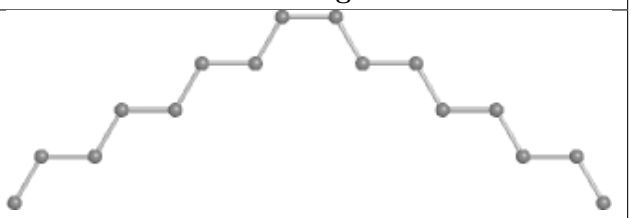
Bond lengths



Bond angles

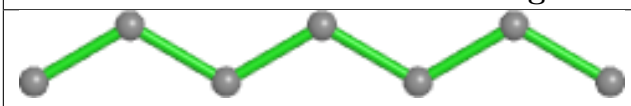


Torsions

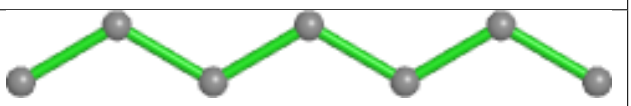


Rings

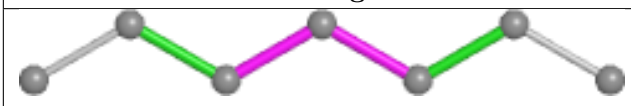
Ligand LFA B 307



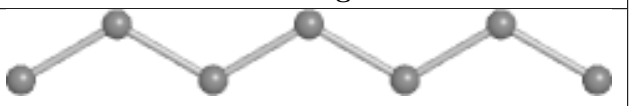
Bond lengths



Bond angles

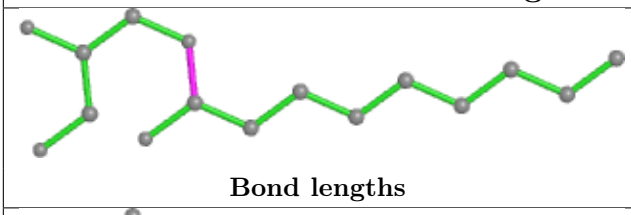


Torsions

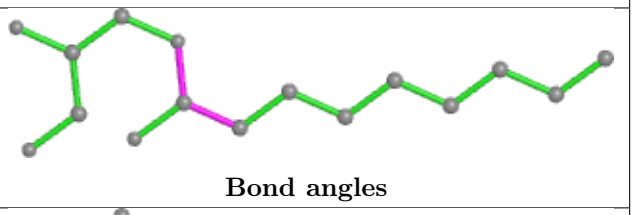


Rings

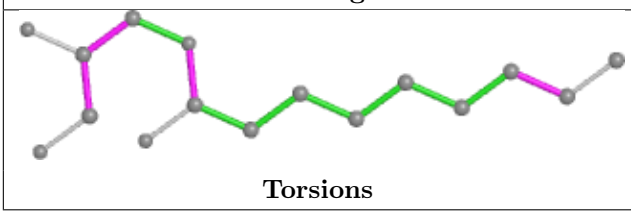
Ligand OLC C 305



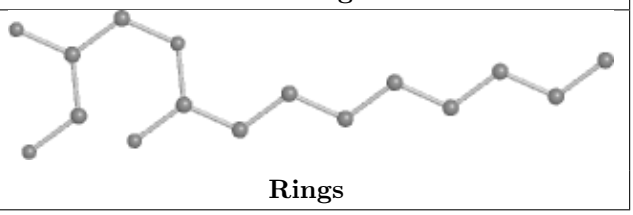
Bond lengths



Bond angles

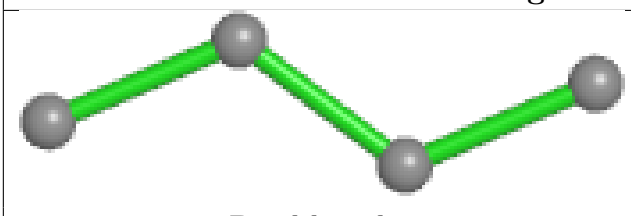


Torsions

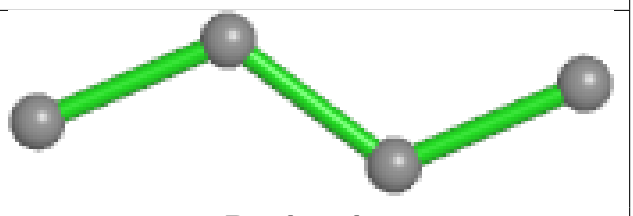


Rings

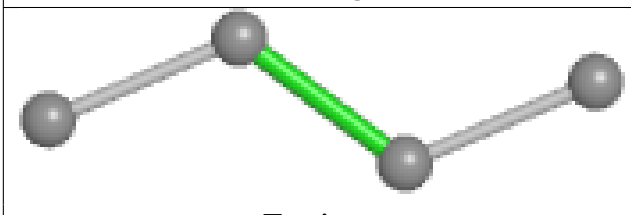
Ligand LFA A 309



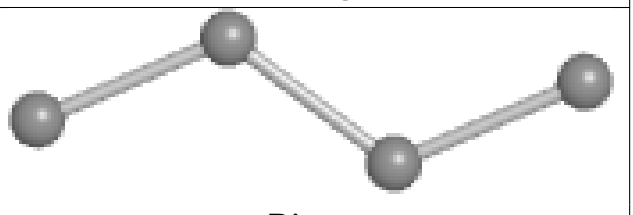
Bond lengths



Bond angles

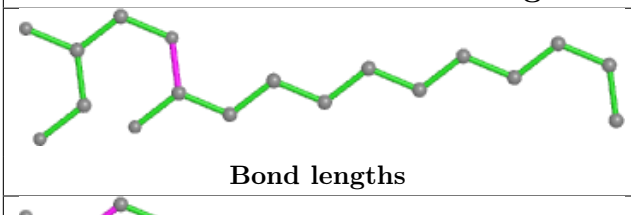


Torsions

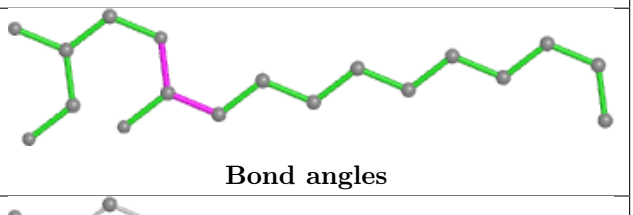


Rings

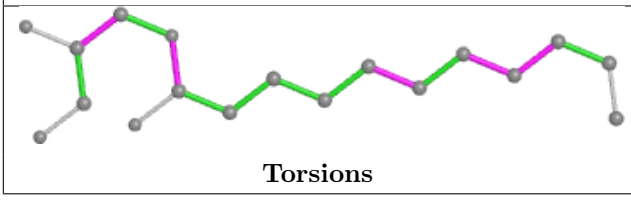
Ligand OLC D 302



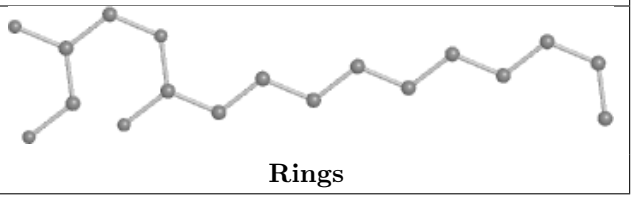
Bond lengths



Bond angles

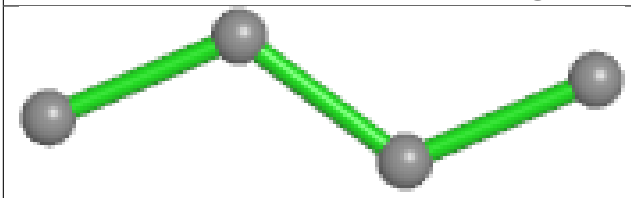


Torsions

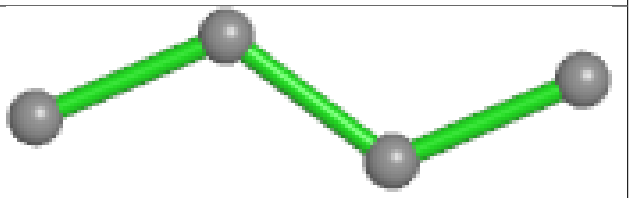


Rings

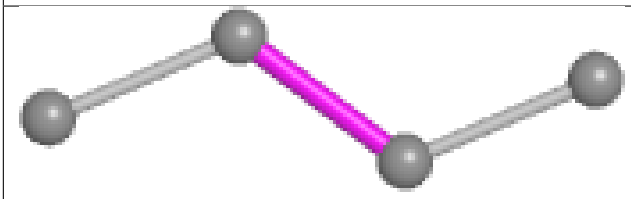
Ligand LFA E 311



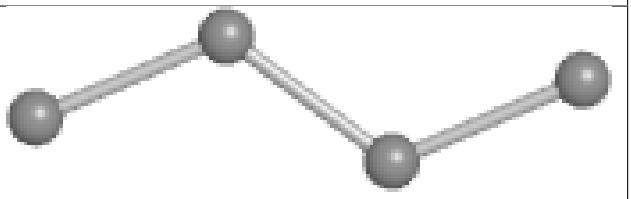
Bond lengths



Bond angles

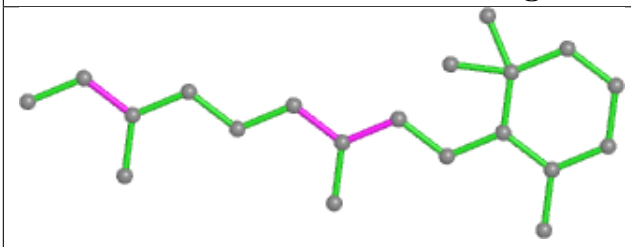


Torsions

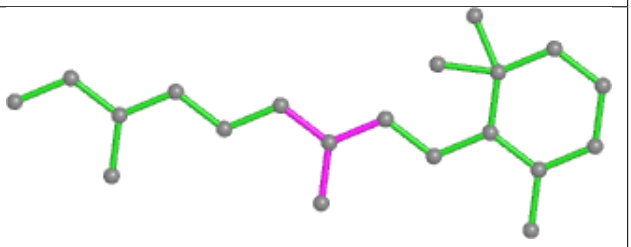


Rings

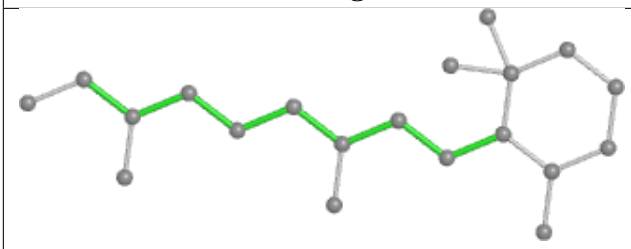
Ligand RET D 311



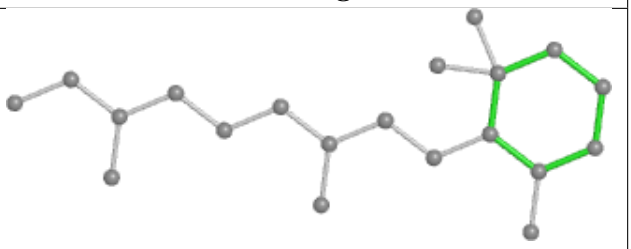
Bond lengths



Bond angles

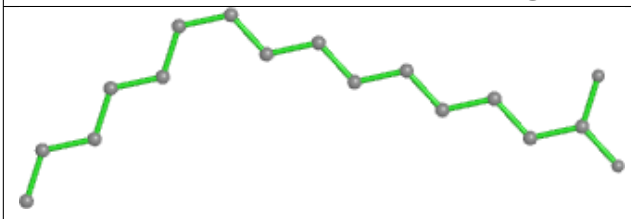


Torsions

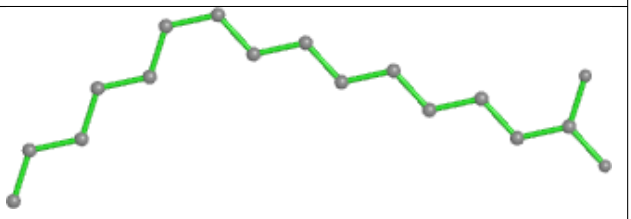


Rings

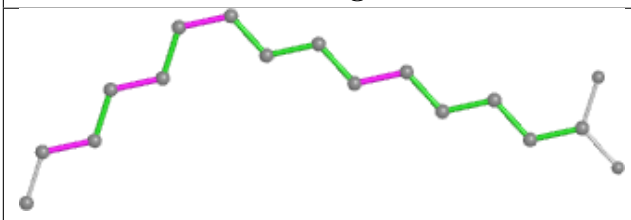
Ligand OLA B 311



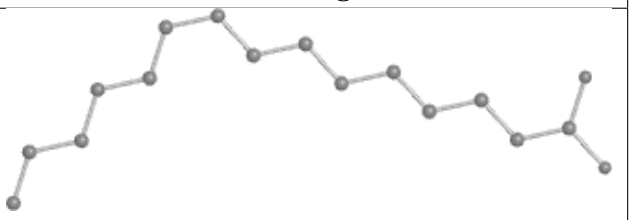
Bond lengths



Bond angles

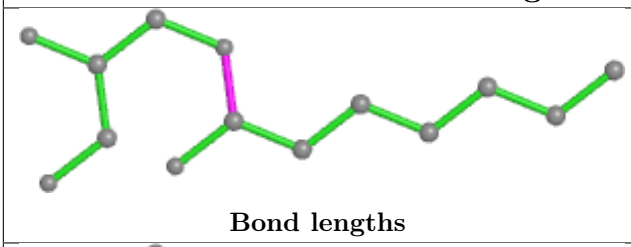


Torsions

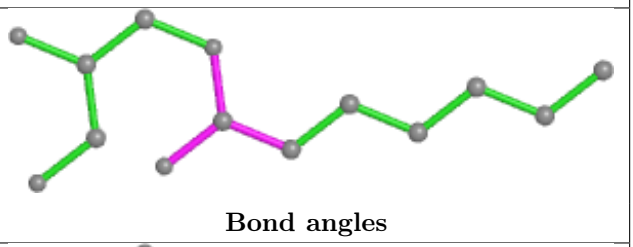


Rings

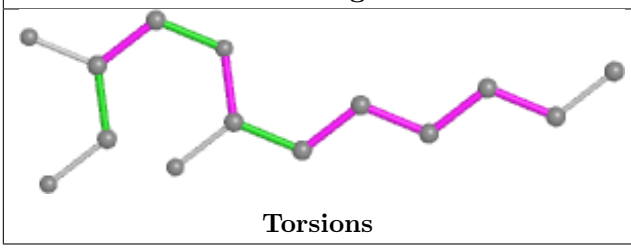
Ligand OLC D 304



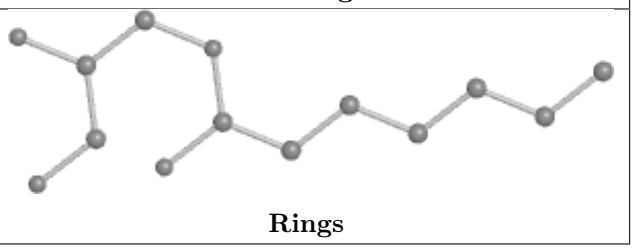
Bond lengths



Bond angles

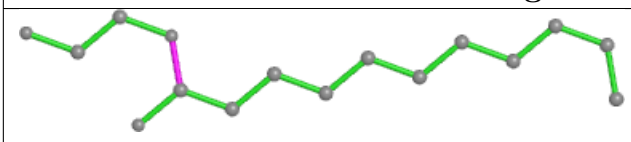


Torsions

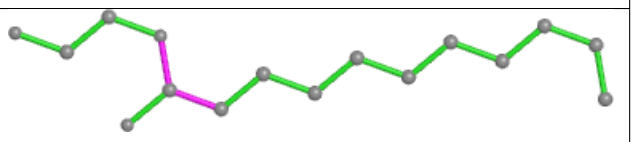


Rings

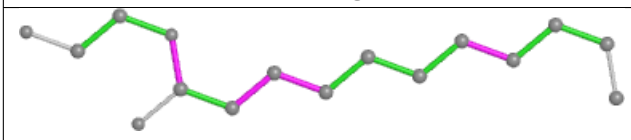
Ligand OLC C 313



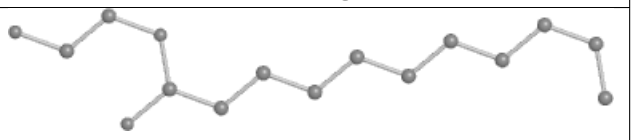
Bond lengths



Bond angles

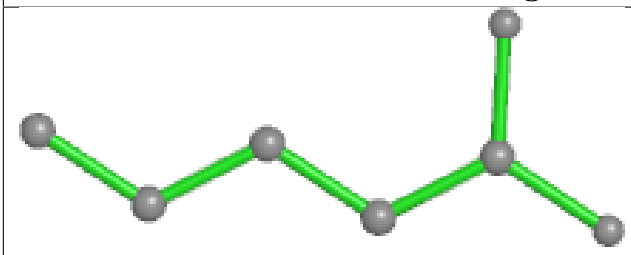


Torsions

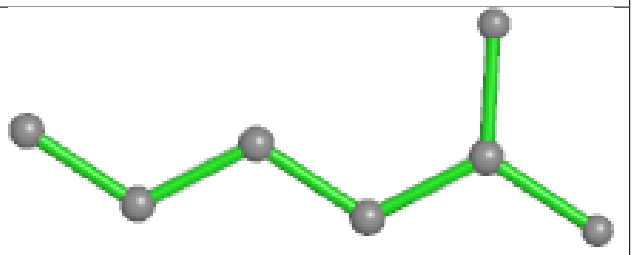


Rings

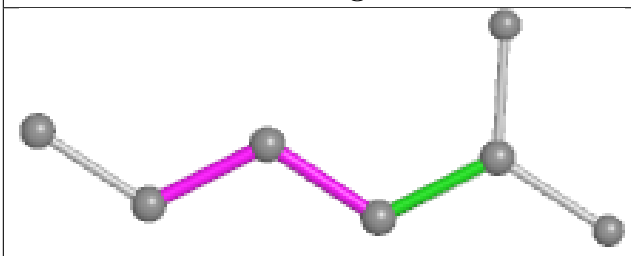
Ligand OLA D 313



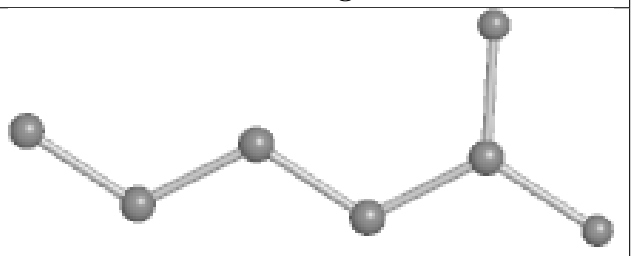
Bond lengths



Bond angles

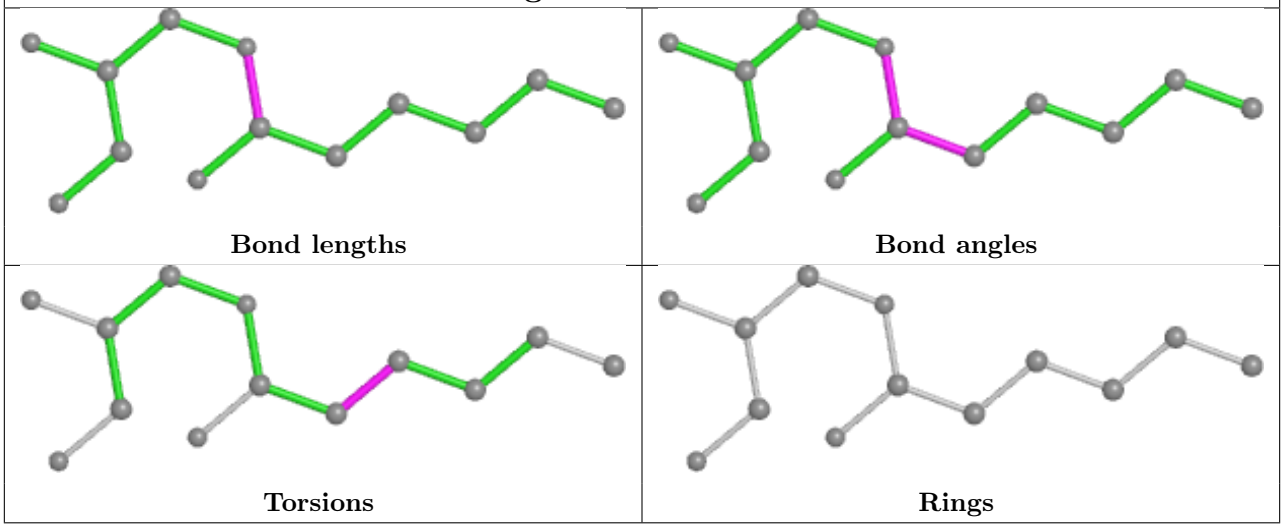


Torsions

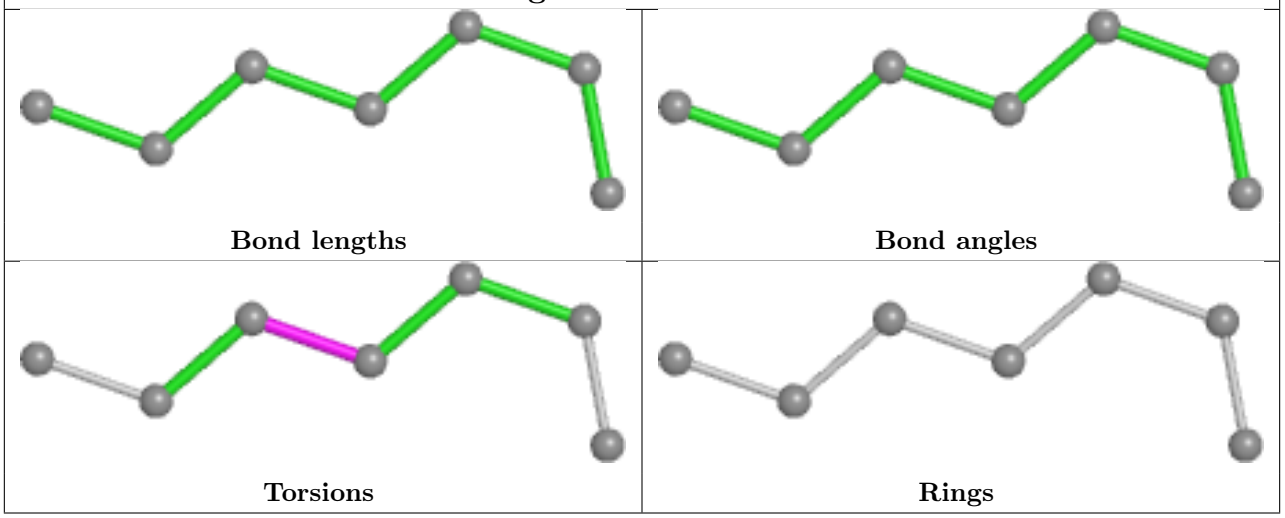


Rings

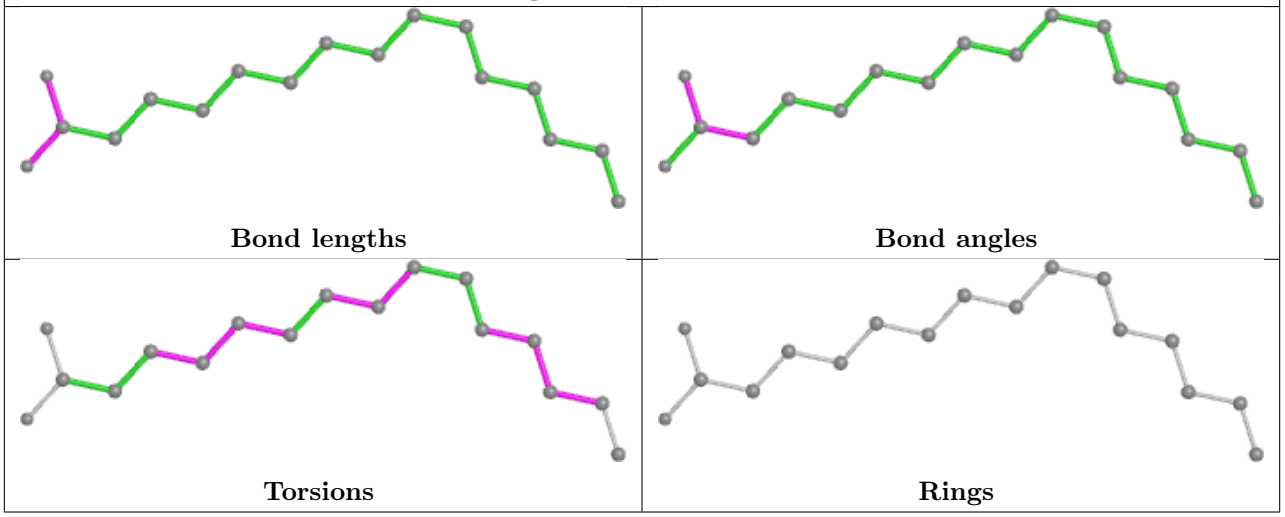
Ligand OLC A 304



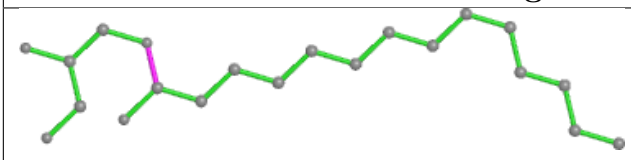
Ligand LFA A 311



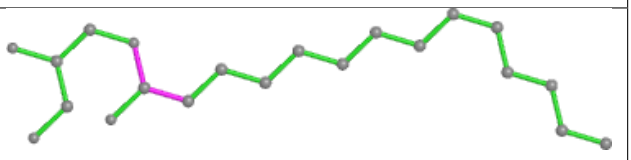
Ligand OLC C 304



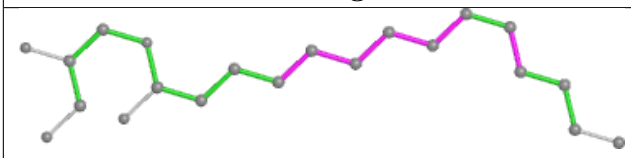
Ligand OLC B 301



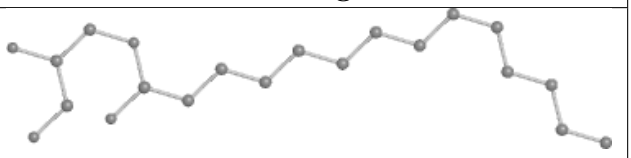
Bond lengths



Bond angles

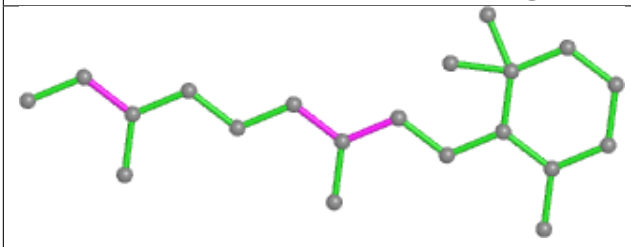


Torsions

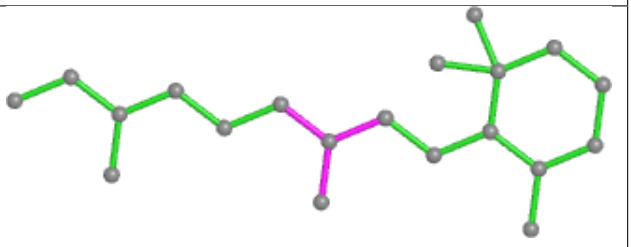


Rings

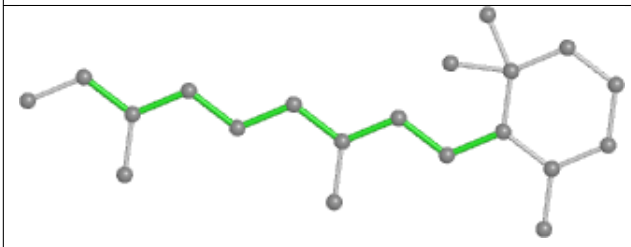
Ligand RET A 314



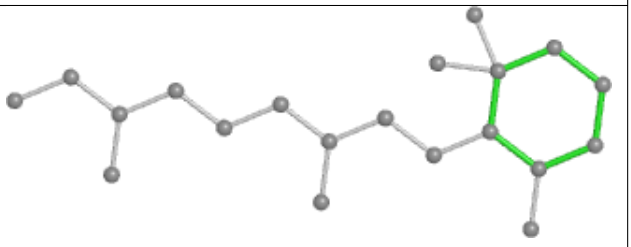
Bond lengths



Bond angles

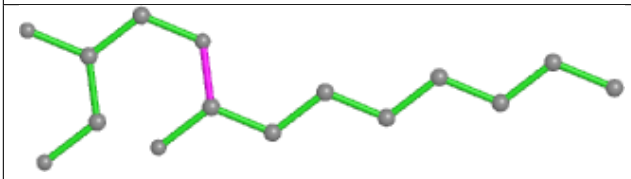


Torsions

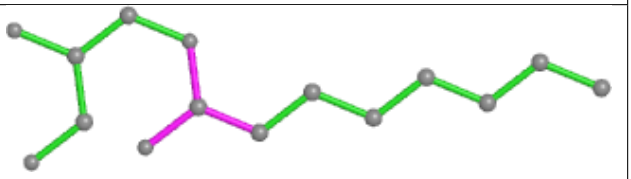


Rings

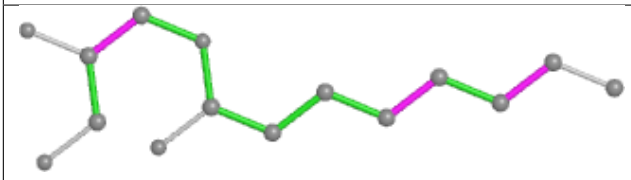
Ligand OLC E 308



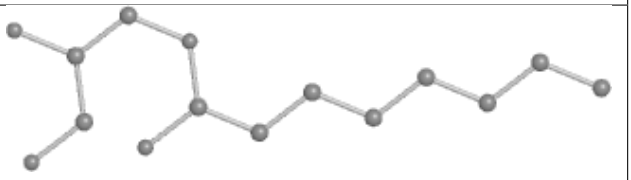
Bond lengths



Bond angles

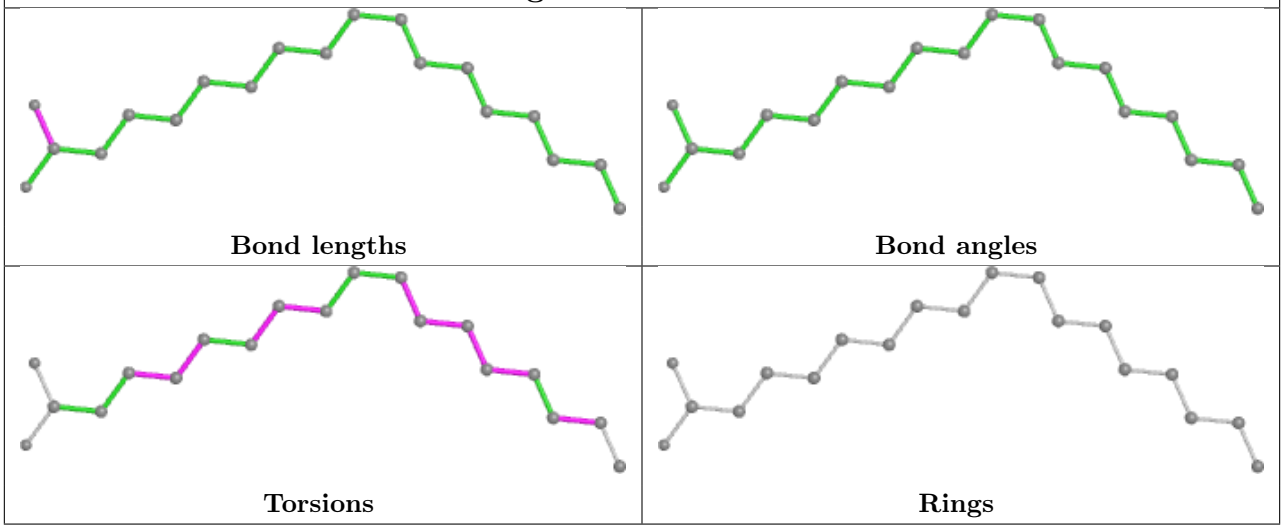


Torsions

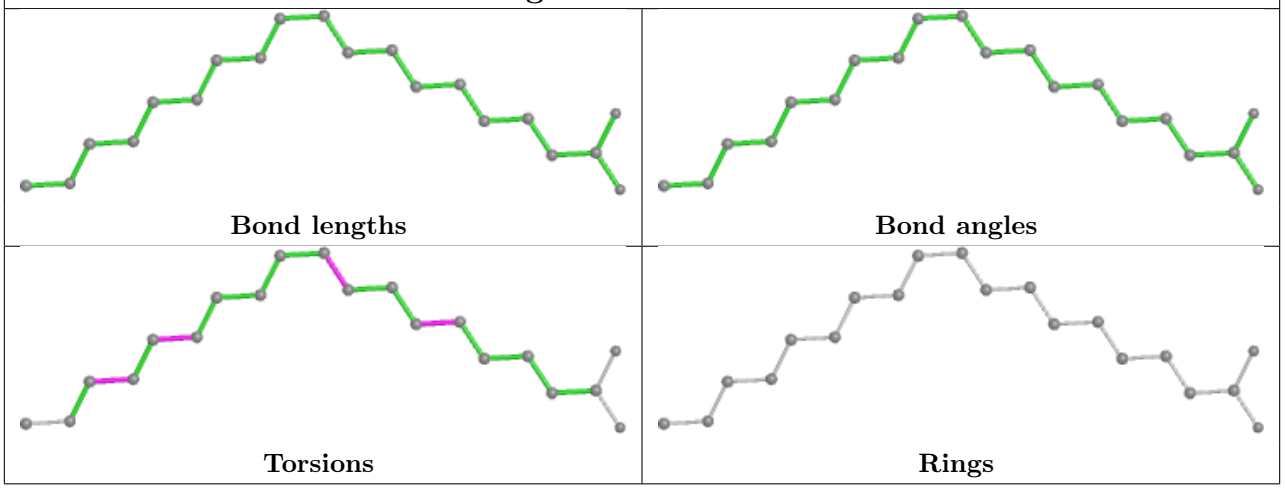


Rings

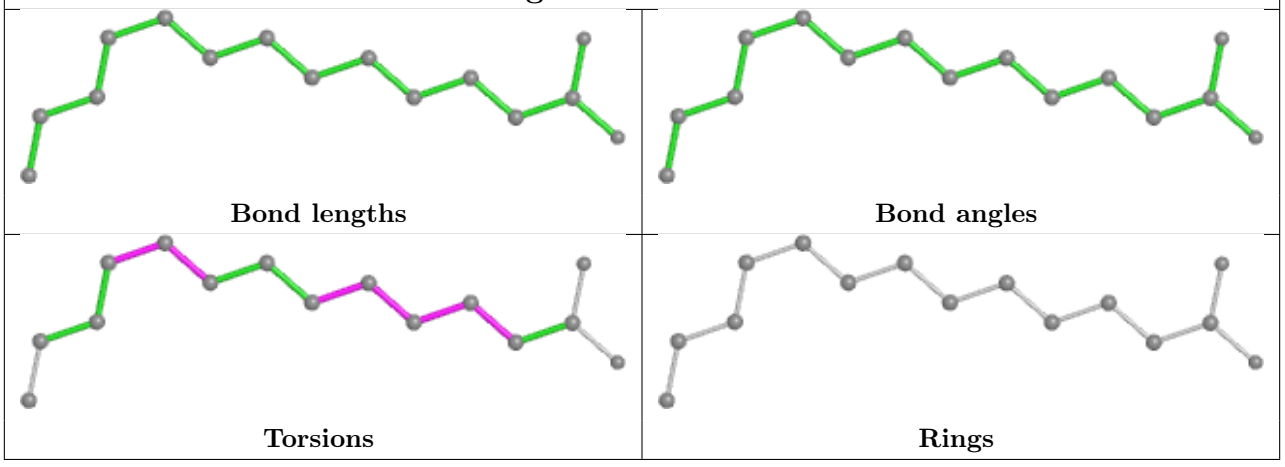
Ligand OLC E 301



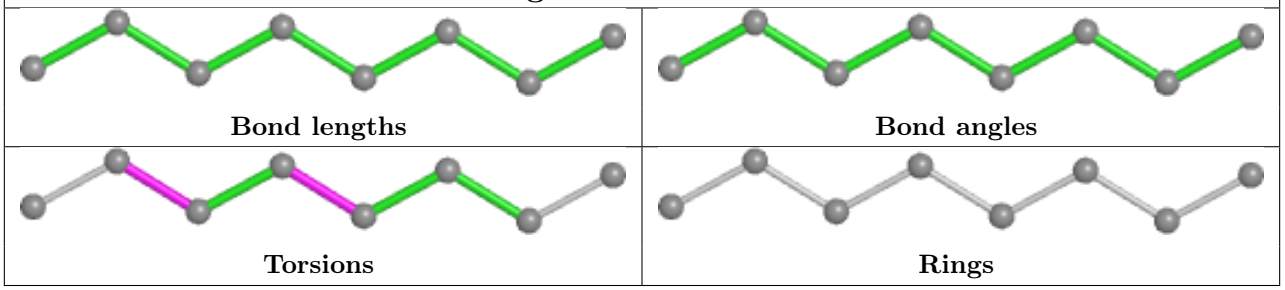
Ligand OLA E 302



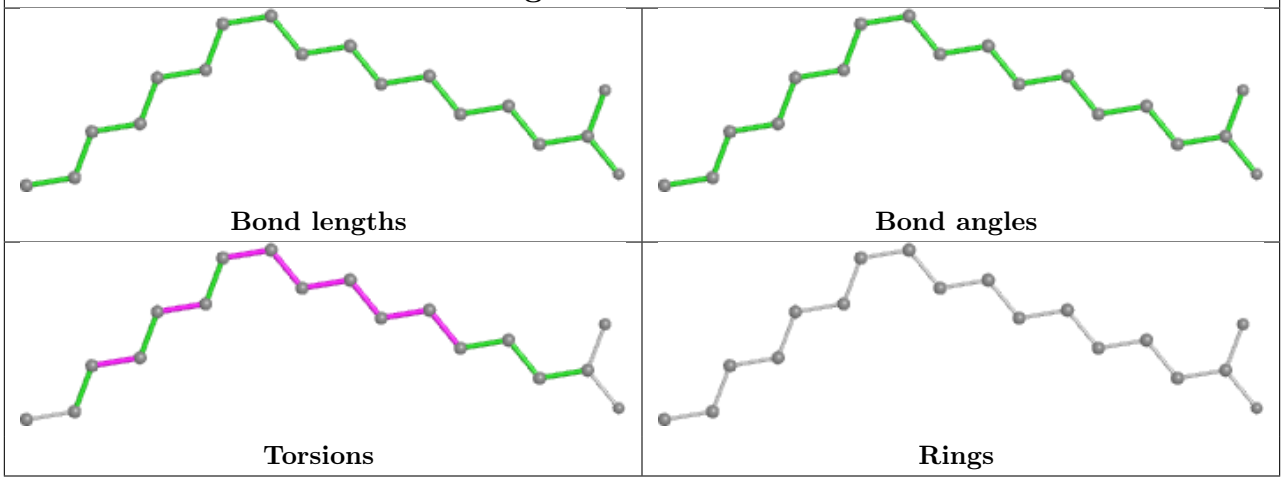
Ligand OLA E 304



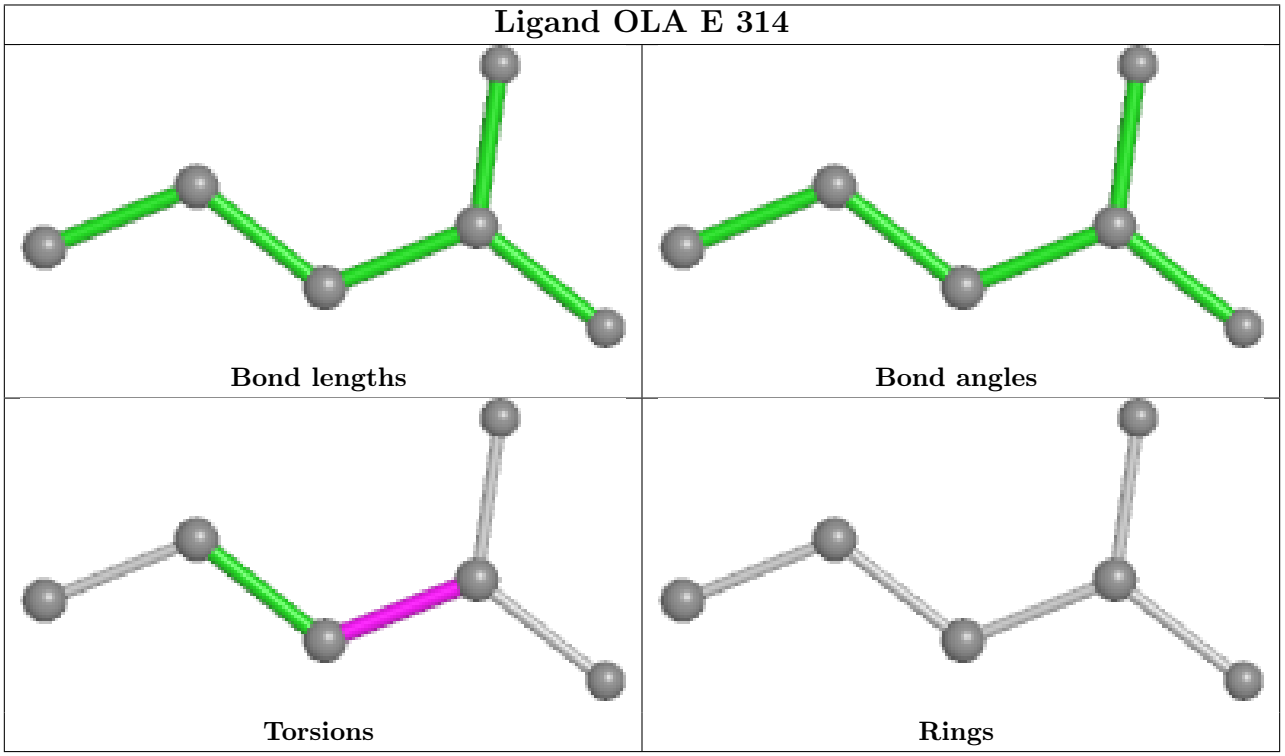
Ligand OLC E 305



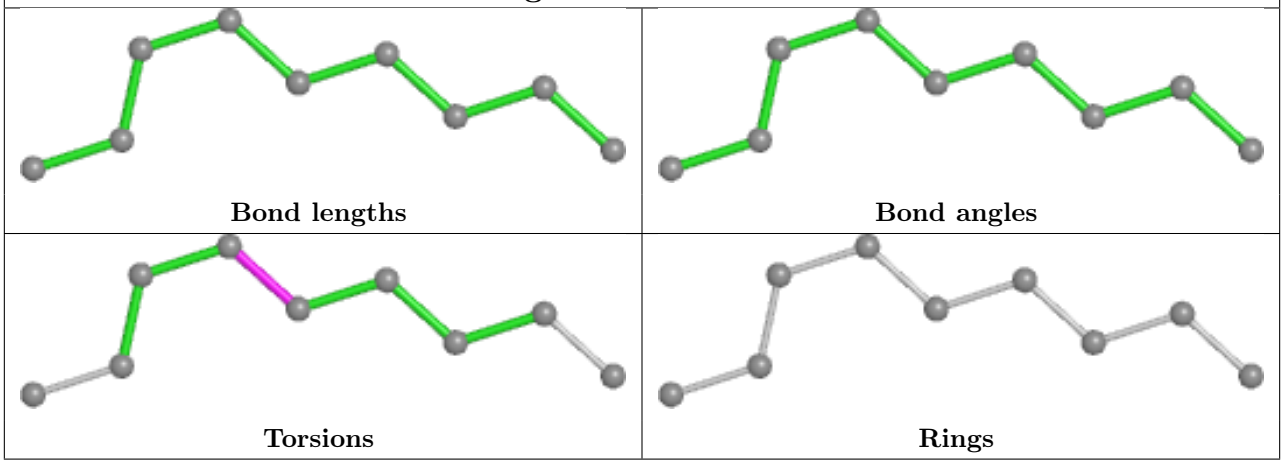
Ligand OLA C 310



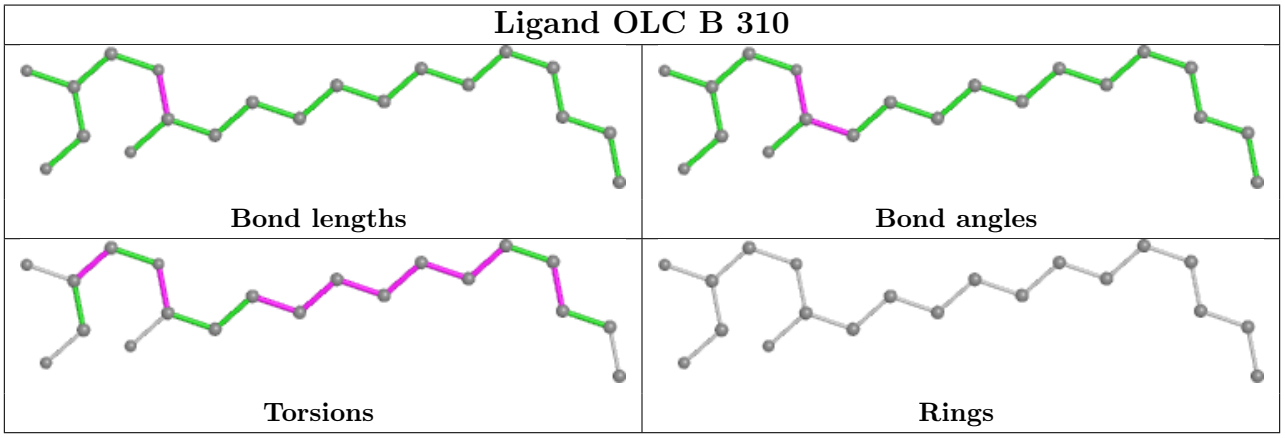
Ligand OLA E 314



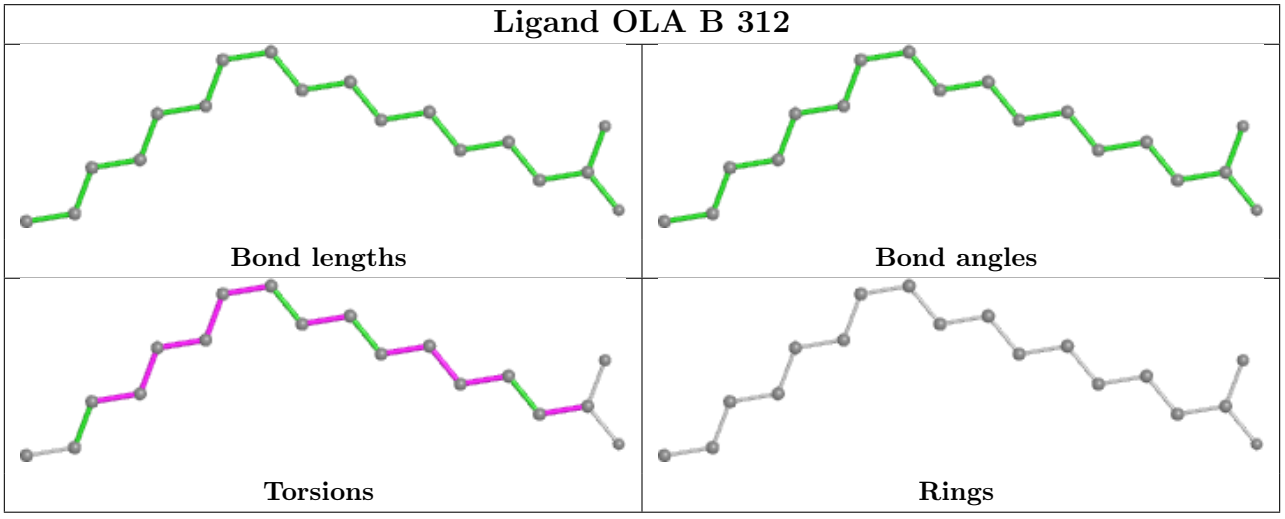
Ligand OLC A 301



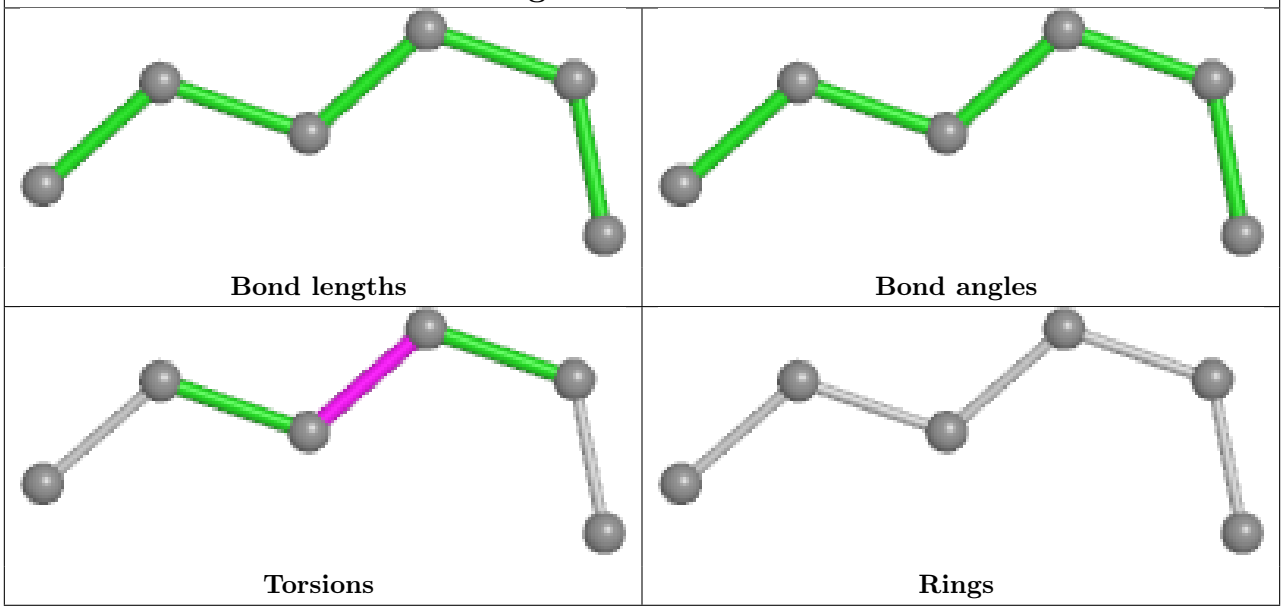
Ligand OLC B 310



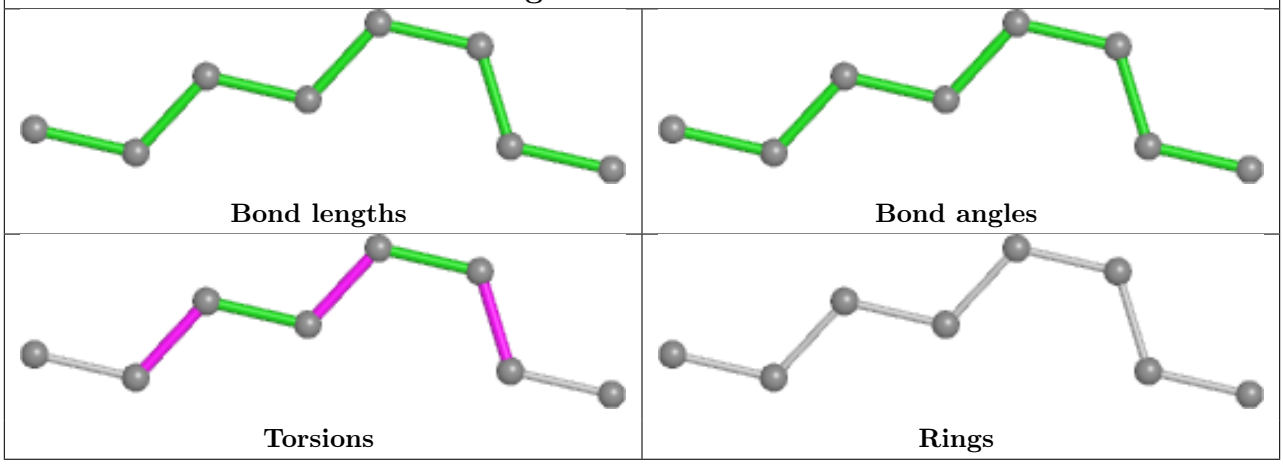
Ligand OLA B 312



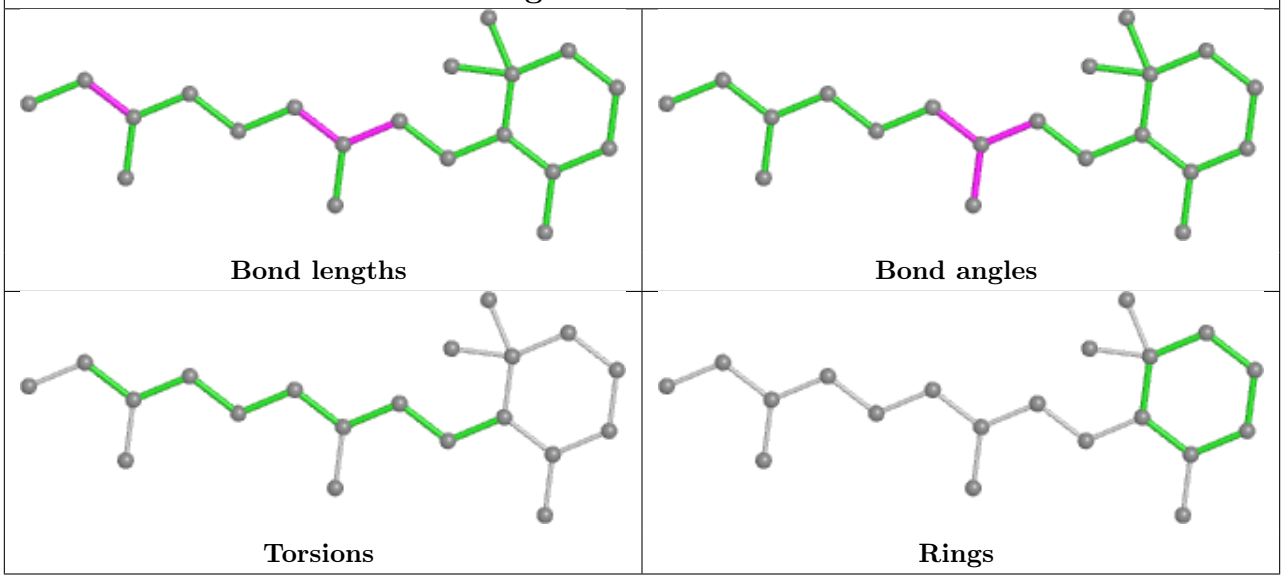
Ligand LFA A 310



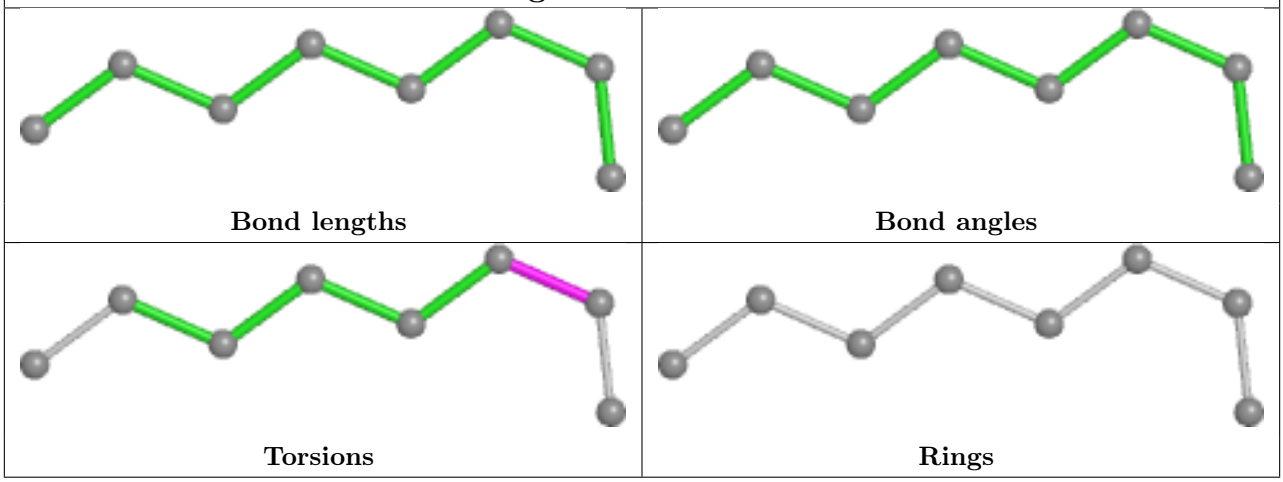
Ligand OLC C 302



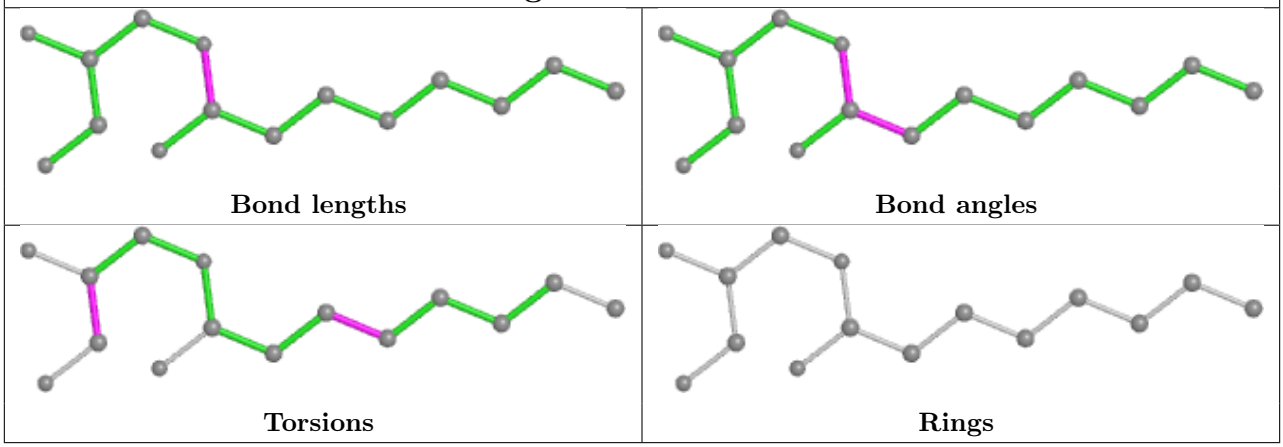
Ligand RET B 309



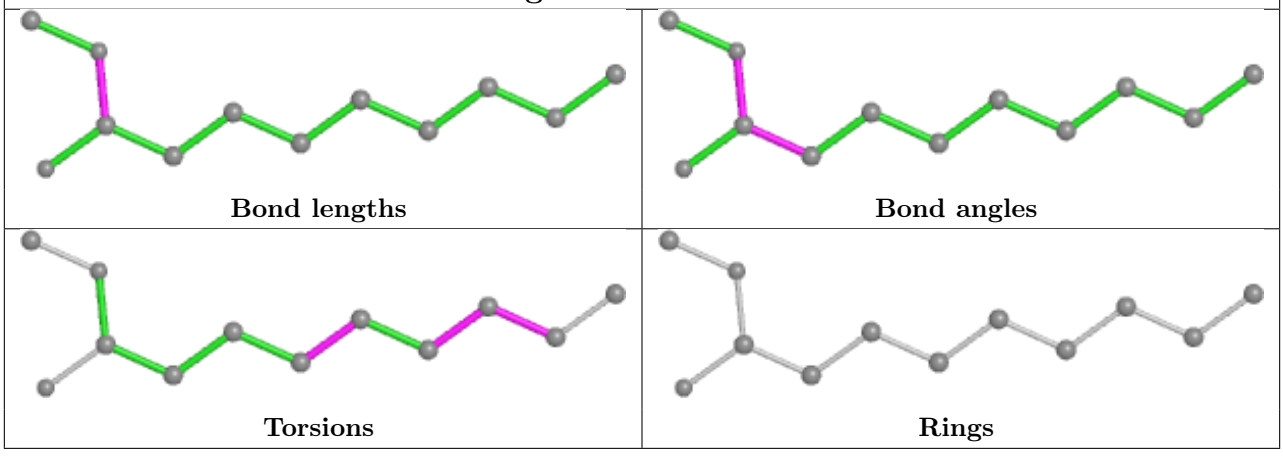
Ligand LFA A 307



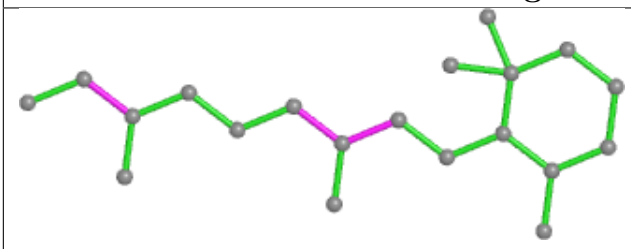
Ligand OLC A 305



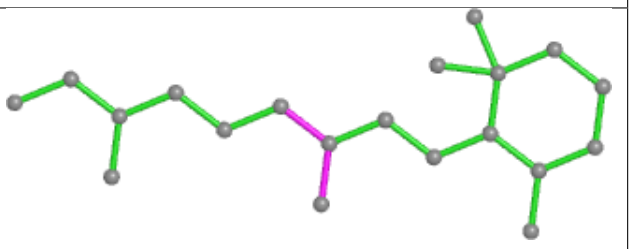
Ligand OLC C 303



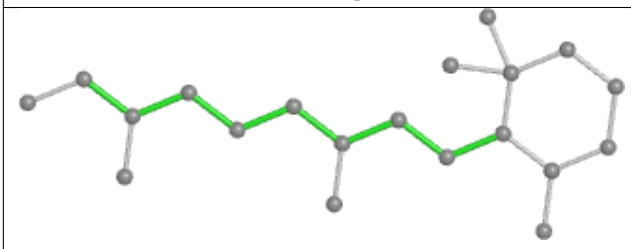
Ligand RET C 312



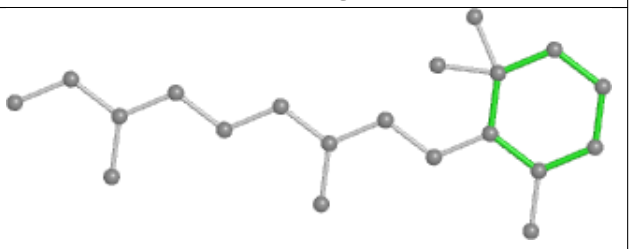
Bond lengths



Bond angles

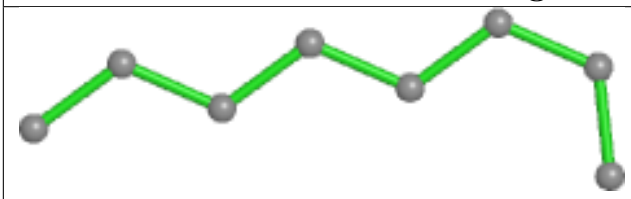


Torsions

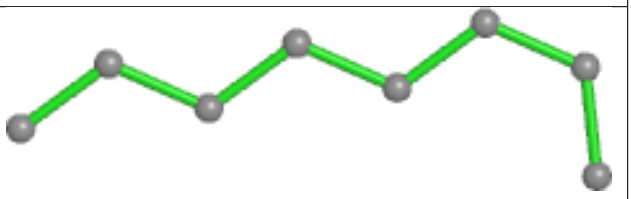


Rings

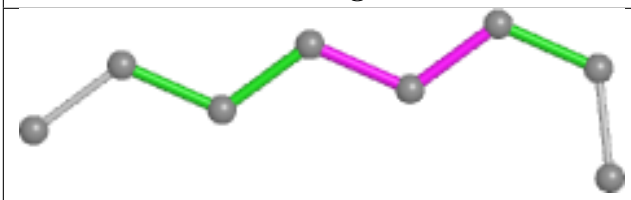
Ligand LFA B 305



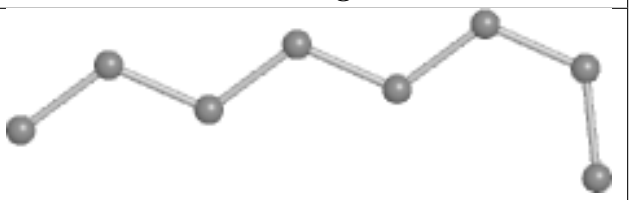
Bond lengths



Bond angles

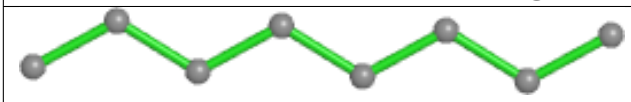


Torsions

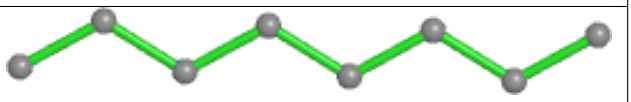


Rings

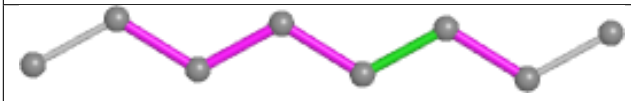
Ligand LFA C 307



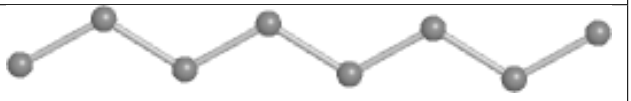
Bond lengths



Bond angles

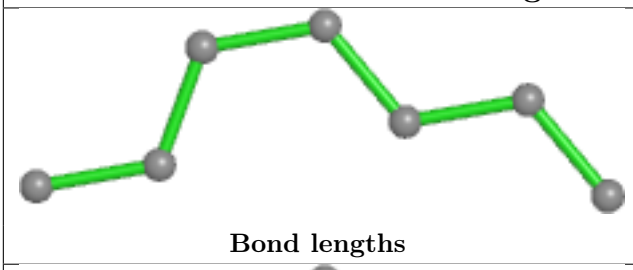


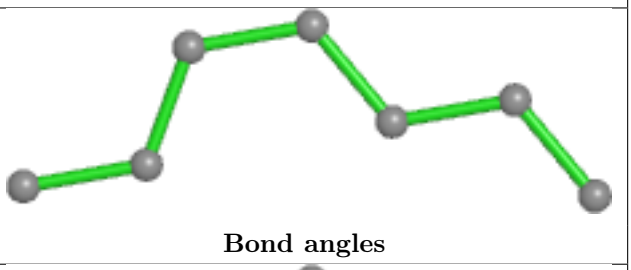
Torsions

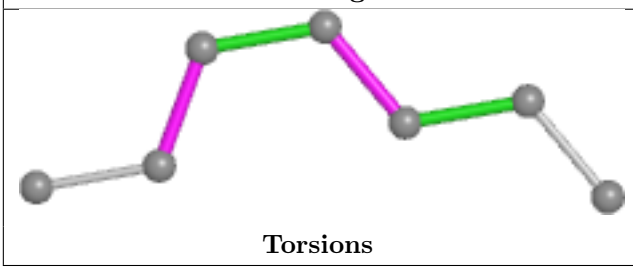


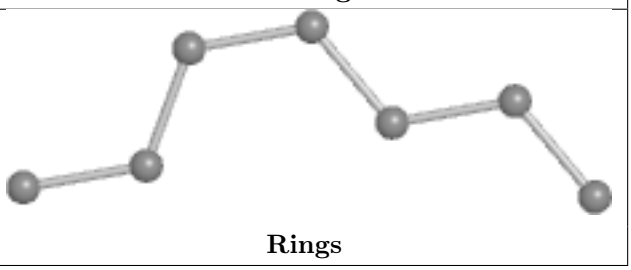
Rings

Ligand OLC A 303

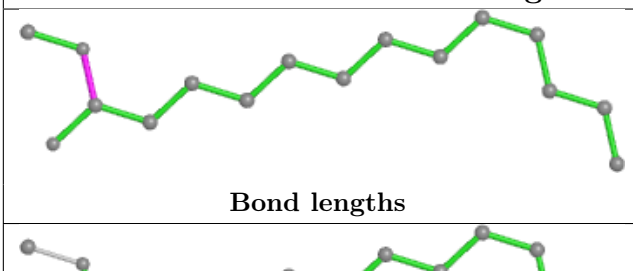

Bond lengths

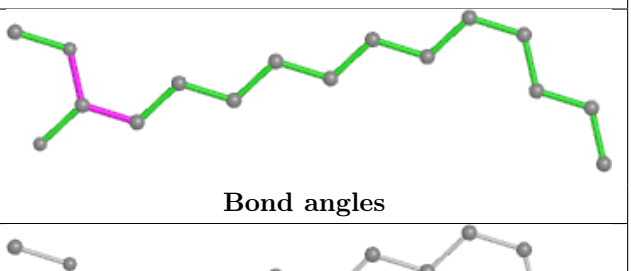

Bond angles

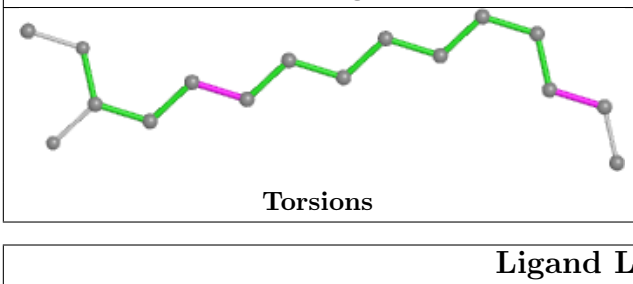

Torsions

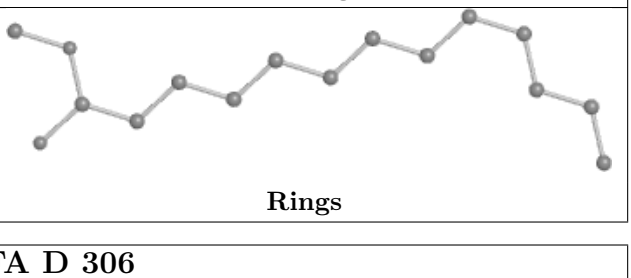

Rings

Ligand OLC B 302

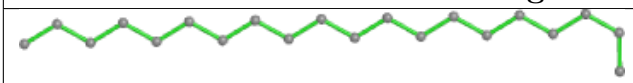

Bond lengths

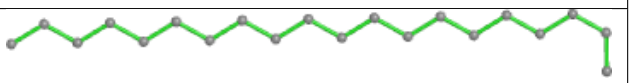

Bond angles

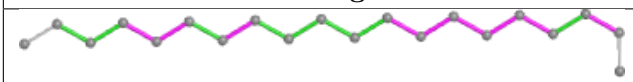

Torsions

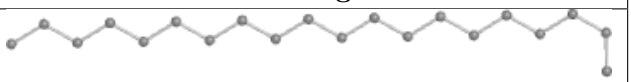

Rings

Ligand LFA D 306

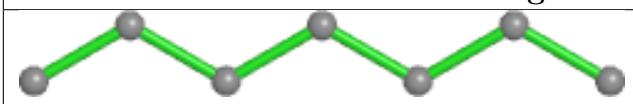

Bond lengths

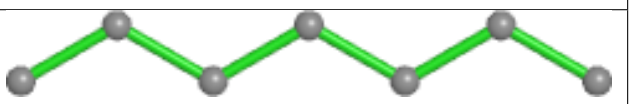

Bond angles

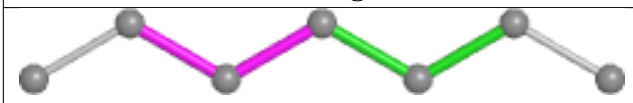

Torsions

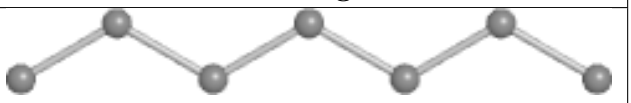

Rings

Ligand LFA A 306

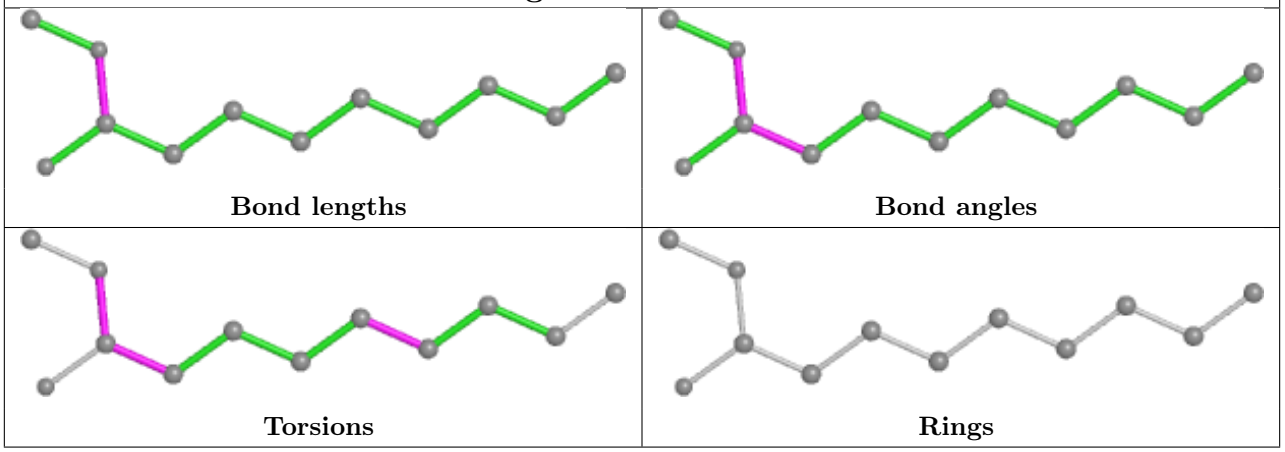

Bond lengths


Bond angles

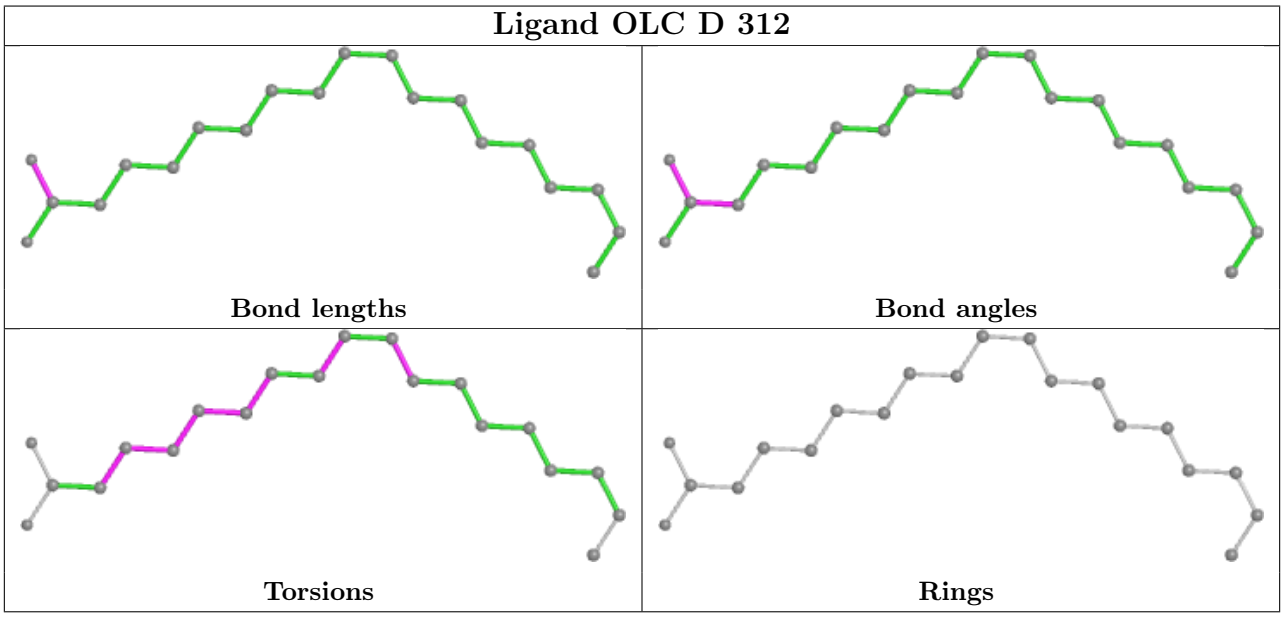

Torsions


Rings

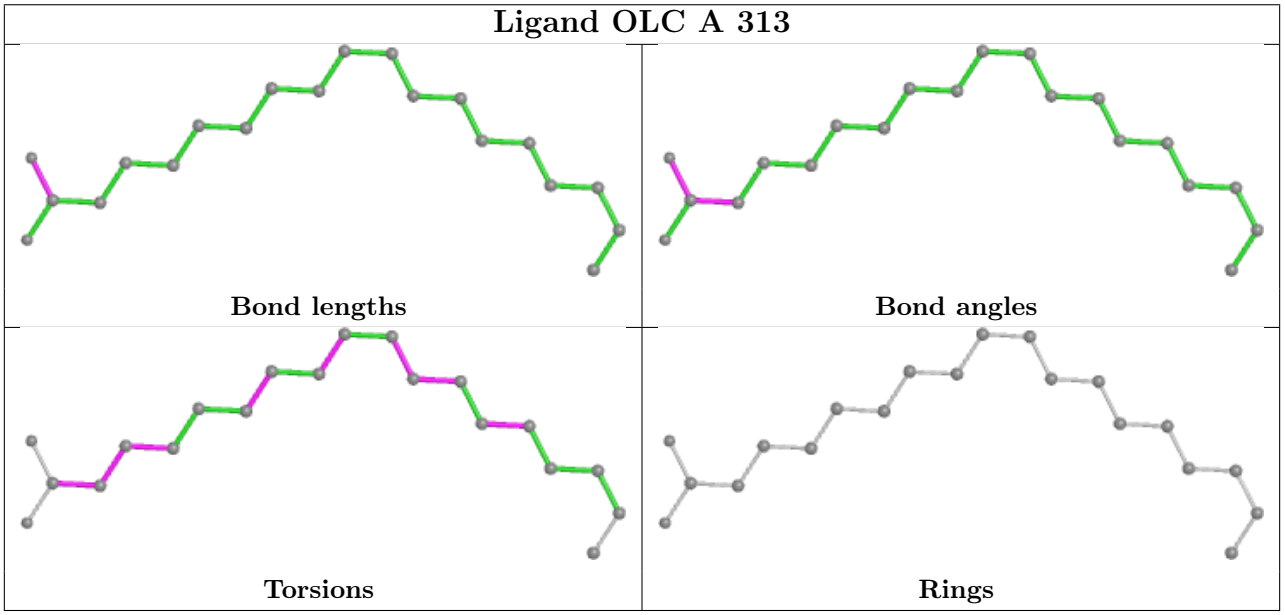
Ligand OLC B 304



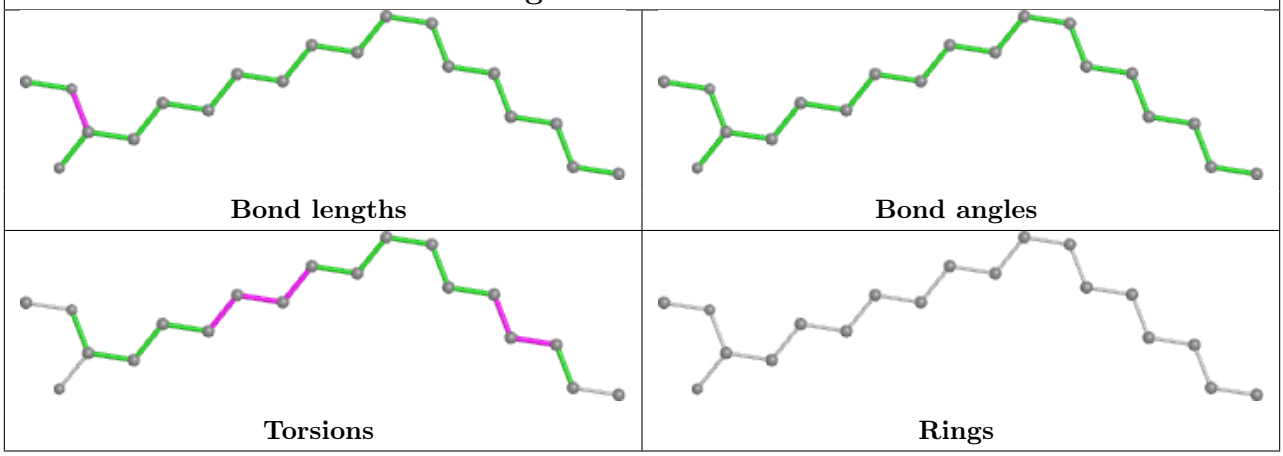
Ligand OLC D 312



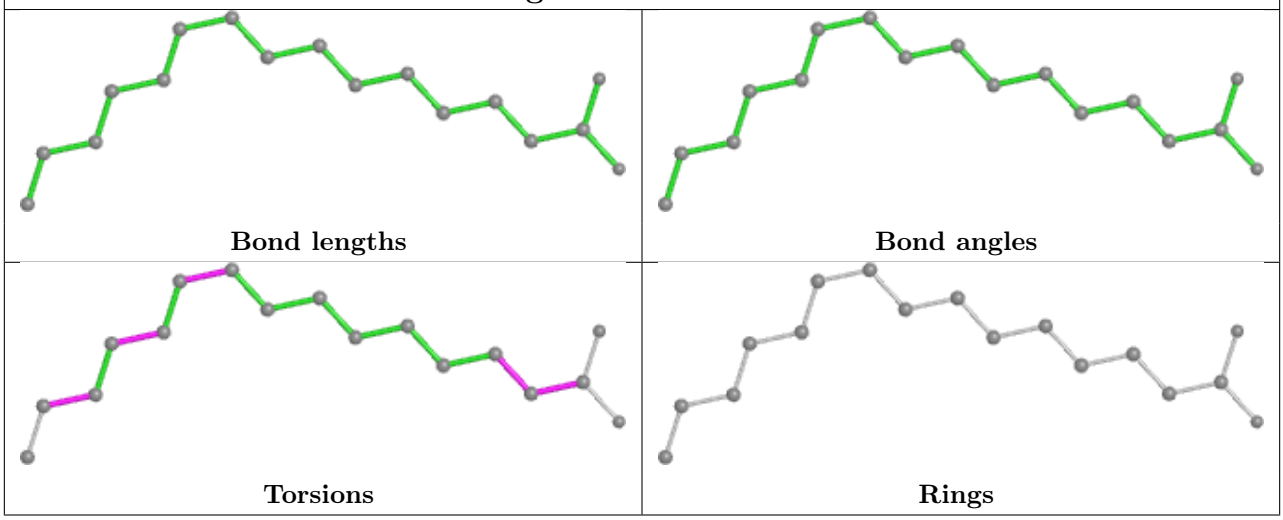
Ligand OLC A 313



Ligand OLC C 301



Ligand OLA E 303



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%)	0.25	15 (5%)	24	19	34, 47, 76, 113	0
1	B	269/273 (98%)	0.19	10 (3%)	41	34	36, 48, 70, 121	0
1	C	269/273 (98%)	0.20	23 (8%)	10	7	32, 48, 76, 114	0
1	D	269/273 (98%)	0.26	18 (6%)	17	13	36, 50, 84, 107	0
1	E	269/273 (98%)	0.28	21 (7%)	13	9	35, 49, 75, 117	0
All	All	1345/1365 (98%)	0.23	87 (6%)	18	14	32, 49, 78, 121	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	132	THR	4.1
1	B	72[A]	PHE	3.7
1	E	40	LEU	3.7
1	B	230	VAL	3.5
1	B	73[A]	LEU	3.5
1	C	40	LEU	3.5
1	A	73[A]	LEU	3.4
1	B	40	LEU	3.4
1	D	69[A]	VAL	3.4
1	A	271	LYS	3.3
1	B	231	ASP	3.3
1	E	72[A]	PHE	3.3
1	C	76[A]	TYR	3.3
1	D	133	SER	3.3
1	A	40	LEU	3.2
1	C	228	THR	3.2
1	A	230	VAL	3.2
1	E	76[A]	TYR	3.1
1	B	69[A]	VAL	3.1
1	C	130	LEU	3.1

Continued on next page...

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Mol	Chain	Res	Type	RSRZ
1	A	233	PHE	3.0
1	E	37	ALA	3.0
1	C	231	ASP	2.9
1	A	183	TRP	2.9
1	E	271	LYS	2.9
1	D	40	LEU	2.9
1	D	130	LEU	2.9
1	C	72[A]	PHE	2.9
1	A	69[A]	VAL	2.9
1	E	190	ASN	2.9
1	A	72[A]	PHE	2.8
1	D	76[A]	TYR	2.8
1	C	232	GLY	2.8
1	A	270	SER	2.8
1	E	270	SER	2.8
1	A	231	ASP	2.8
1	C	271	LYS	2.8
1	A	76[A]	TYR	2.8
1	D	73[A]	LEU	2.7
1	E	73[A]	LEU	2.7
1	C	69[A]	VAL	2.7
1	B	76[A]	TYR	2.7
1	E	36	TYR	2.7
1	C	230	VAL	2.7
1	E	69[A]	VAL	2.6
1	E	43	LEU	2.6
1	E	130	LEU	2.6
1	D	231	ASP	2.5
1	D	72[A]	PHE	2.5
1	A	190	ASN	2.5
1	D	271	LYS	2.5
1	E	202	LYS	2.4
1	A	164	LEU	2.4
1	C	73[A]	LEU	2.4
1	D	194	GLU	2.4
1	E	44	LEU	2.4
1	C	129	SER	2.4
1	A	196	ILE	2.3
1	C	36	TYR	2.3
1	D	195	GLY	2.3
1	D	183	TRP	2.3
1	C	34	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	132	THR	2.3
1	C	196	ILE	2.3
1	B	3	GLN	2.2
1	C	133	SER	2.2
1	B	43	LEU	2.2
1	C	163	ASN	2.2
1	E	164	LEU	2.2
1	E	133	SER	2.2
1	D	43	LEU	2.2
1	C	37	ALA	2.2
1	E	41	ALA	2.2
1	A	43	LEU	2.2
1	D	230	VAL	2.2
1	C	44	LEU	2.2
1	C	41	ALA	2.2
1	D	190	ASN	2.1
1	C	43	LEU	2.1
1	E	77[A]	ALA	2.1
1	E	194	GLU	2.1
1	E	131	THR	2.1
1	E	38	VAL	2.1
1	D	129	SER	2.1
1	D	131	THR	2.0
1	C	227	LEU	2.0
1	B	271	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	OLA	E	304	15/20	0.32	0.69	109,133,243,256	0
7	OLA	B	311	17/20	0.39	0.94	67,87,115,116	0
7	OLA	E	303	17/20	0.42	1.06	64,94,110,122	0
7	OLA	C	310	18/20	0.44	0.78	76,90,115,119	0
7	OLA	B	312	18/20	0.47	0.94	55,102,118,123	0
7	OLA	E	302	20/20	0.52	0.97	76,108,117,117	0
6	GOL	C	311	4/6	0.60	1.40	89,89,94,104	0
2	OLC	C	304	17/25	0.62	0.51	70,99,116,119	0
3	LFA	A	306	7/20	0.65	0.31	84,91,107,115	0
3	LFA	B	306	10/20	0.66	0.31	76,102,113,120	0
2	OLC	E	305	8/25	0.66	0.61	71,89,101,105	0
3	LFA	D	309	7/20	0.68	0.23	78,99,114,122	0
3	LFA	A	307	8/20	0.68	0.31	62,88,98,103	0
2	OLC	C	303	12/25	0.70	0.47	73,97,118,125	0
3	LFA	A	308	8/20	0.72	0.24	72,93,106,108	0
3	LFA	D	305	20/20	0.72	0.41	94,106,124,129	0
3	LFA	E	310	14/20	0.73	0.36	83,106,122,124	0
2	OLC	E	306	16/25	0.73	0.44	72,103,117,118	0
2	OLC	B	310	20/25	0.74	0.36	83,95,110,117	0
3	LFA	C	307	8/20	0.74	0.35	72,90,109,118	0
3	LFA	A	309	4/20	0.74	0.50	76,81,83,90	0
3	LFA	D	307	8/20	0.75	0.29	93,103,116,120	0
3	LFA	A	311	7/20	0.75	0.71	77,82,87,90	0
7	OLA	E	314	6/20	0.76	1.32	82,89,103,121	0
2	OLC	C	305	16/25	0.77	0.29	80,97,113,118	0
2	OLC	D	304	14/25	0.77	0.38	77,97,106,107	0
3	LFA	E	309	8/20	0.77	0.31	72,97,108,123	0
2	OLC	A	304	13/25	0.77	0.56	66,96,124,125	0
3	LFA	C	308	20/20	0.77	0.30	73,106,137,140	0
2	OLC	A	303	7/25	0.77	0.78	62,82,91,102	0
2	OLC	A	301	9/25	0.78	0.20	67,76,88,90	0
3	LFA	E	312	5/20	0.78	0.22	74,75,82,93	0
2	OLC	E	307	20/25	0.79	0.53	86,105,116,117	0
3	LFA	D	306	20/20	0.79	0.37	88,100,140,144	0
3	LFA	B	307	7/20	0.79	0.42	86,102,126,134	0
3	LFA	A	310	6/20	0.79	0.28	74,81,91,100	0
2	OLC	A	313	20/25	0.79	0.32	72,102,133,138	0
2	OLC	D	302	18/25	0.80	0.56	79,105,117,124	0
2	OLC	B	302	16/25	0.82	0.53	80,103,129,155	0
2	OLC	B	304	12/25	0.82	0.63	78,88,100,104	0
2	OLC	C	313	16/25	0.82	0.25	82,94,104,106	0
2	OLC	A	315	18/25	0.83	0.28	75,92,119,122	0

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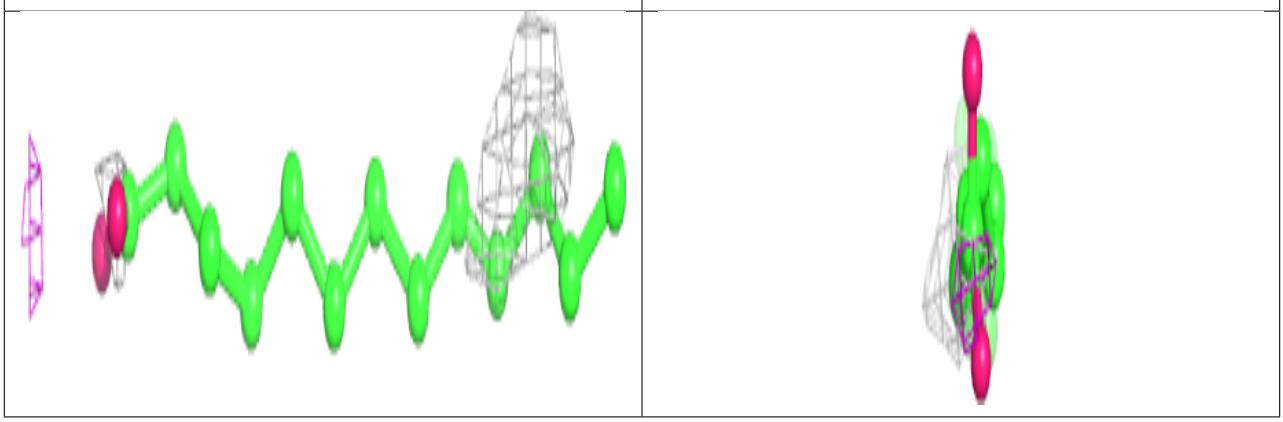
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	B	313	4/6	0.83	1.13	84,91,99,100	0
2	OLC	D	312	20/25	0.84	0.28	77,86,119,127	0
3	LFA	E	311	4/20	0.84	0.20	80,80,84,85	0
2	OLC	A	305	15/25	0.84	0.38	68,85,104,107	0
2	OLC	E	308	15/25	0.84	0.41	75,92,102,116	0
2	OLC	B	301	21/25	0.86	0.28	55,72,87,96	0
2	OLC	E	301	19/25	0.86	0.30	55,67,77,78	0
6	GOL	A	316	4/6	0.86	1.22	83,84,87,93	0
2	OLC	A	302	17/25	0.87	0.25	49,59,76,79	0
3	LFA	B	305	8/20	0.88	0.23	60,77,85,85	0
7	OLA	D	313	7/20	0.88	1.13	84,91,102,109	0
2	OLC	C	301	19/25	0.88	0.33	61,67,87,88	0
2	OLC	C	302	8/25	0.90	0.26	76,79,86,88	0
2	OLC	D	303	5/25	0.91	0.17	66,70,80,83	0
5	RET	D	311	20/21	0.92	0.18	43,61,66,67	0
2	OLC	D	301	5/25	0.92	0.35	64,70,77,78	0
5	RET	B	309	20/21	0.92	0.19	38,45,57,64	0
3	LFA	C	306	4/20	0.93	0.12	71,76,78,81	0
2	OLC	B	303	5/25	0.93	0.19	65,74,75,76	0
5	RET	A	314	20/21	0.93	0.19	39,46,55,63	0
3	LFA	D	308	17/20	0.93	0.38	57,63,71,73	0
5	RET	E	315	20/21	0.94	0.18	35,46,60,69	0
4	NA	C	314	1/1	0.94	0.17	51,51,51,51	1
4	NA	B	308	1/1	0.95	0.14	37,37,37,37	0
4	NA	A	317	1/1	0.95	0.16	32,32,32,32	1
5	RET	C	312	20/21	0.95	0.14	38,53,59,64	0
4	NA	D	310	1/1	0.95	0.11	38,38,38,38	0
4	NA	E	316	1/1	0.96	0.26	50,50,50,50	1
4	NA	C	309	1/1	0.97	0.06	34,34,34,34	0
4	NA	A	312	1/1	0.98	0.10	41,41,41,41	0
4	NA	D	314	1/1	0.98	0.13	40,40,40,40	1
4	NA	E	313	1/1	0.98	0.07	34,34,34,34	0
4	NA	B	314	1/1	0.98	0.18	49,49,49,49	1

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

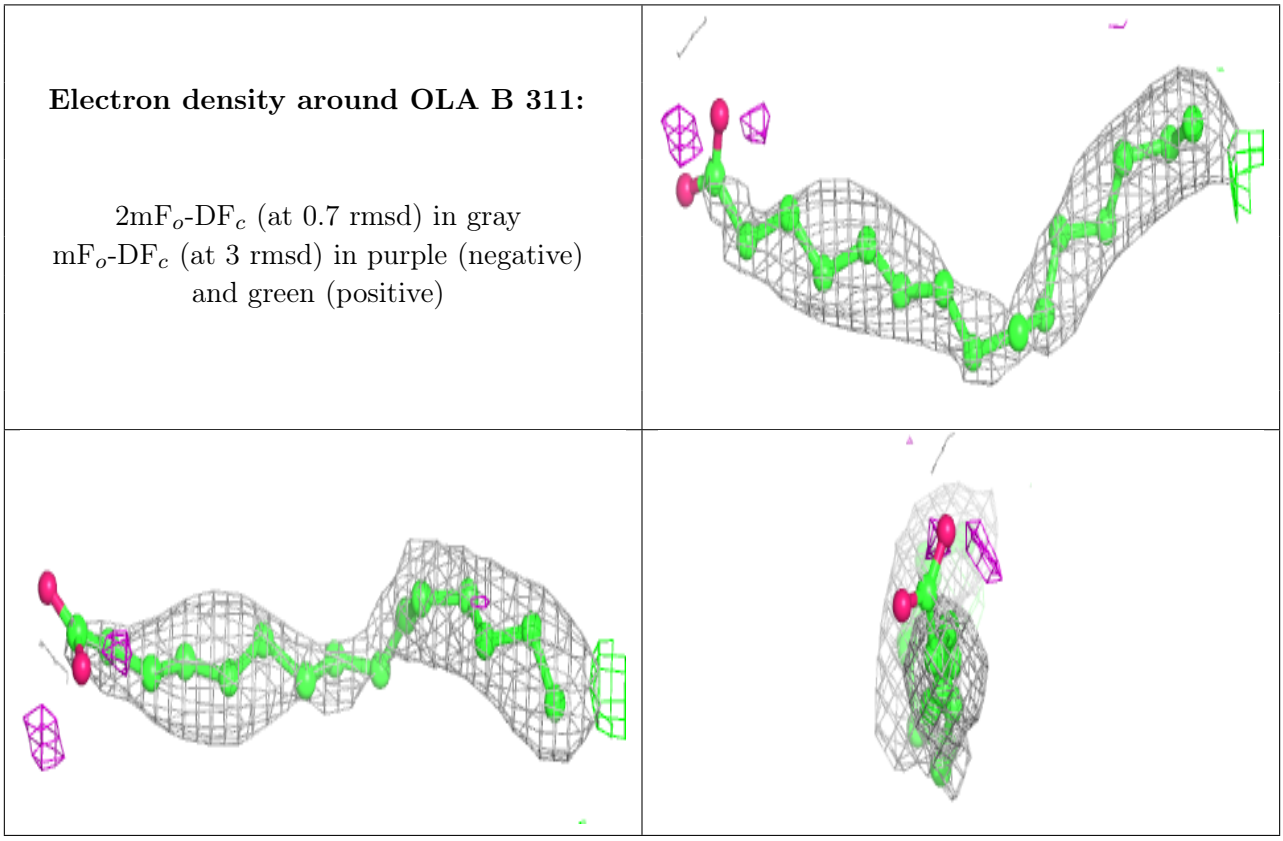
Electron density around OLA E 304:

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



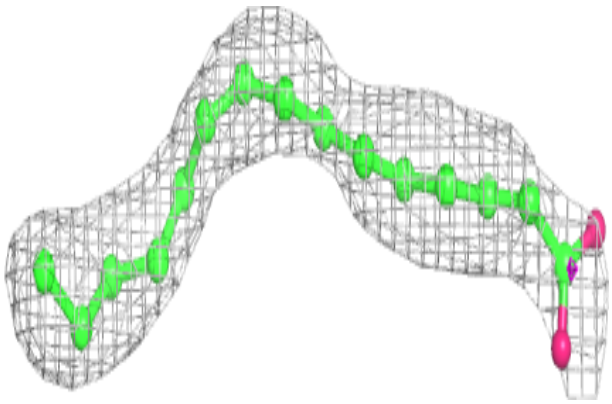
Electron density around OLA B 311:

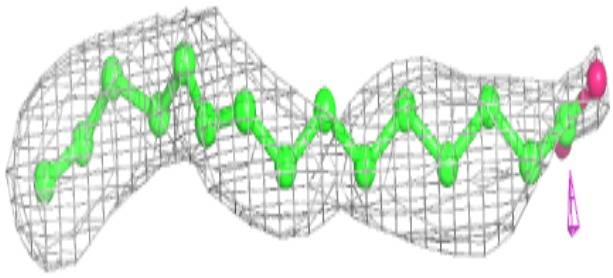
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

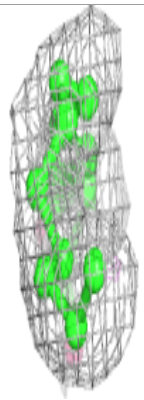


Electron density around OLA E 303:

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

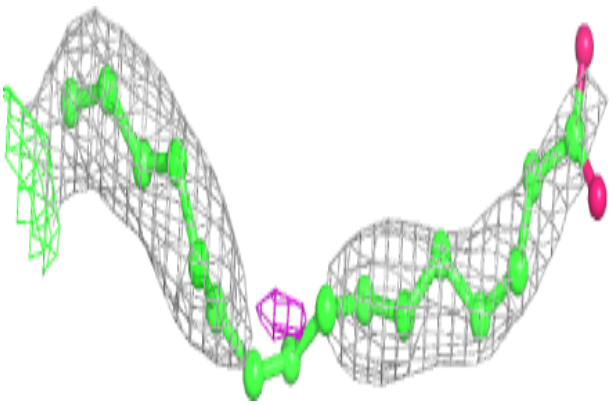


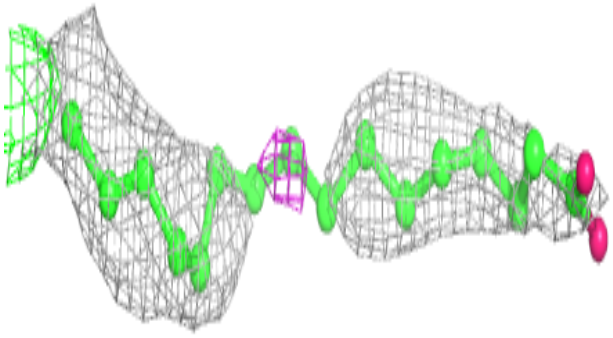


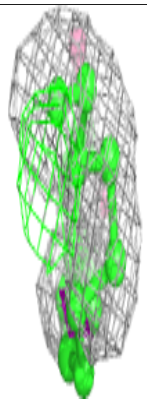


Electron density around OLA C 310:

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

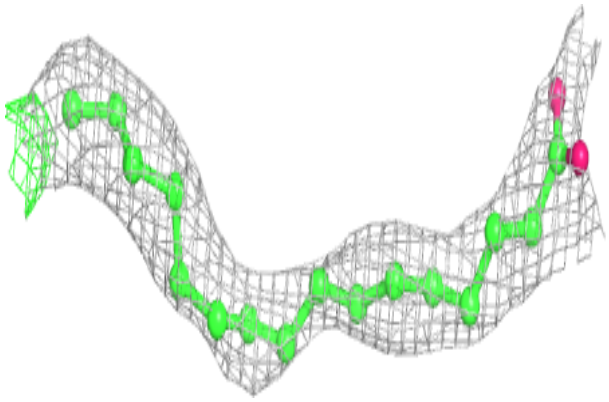


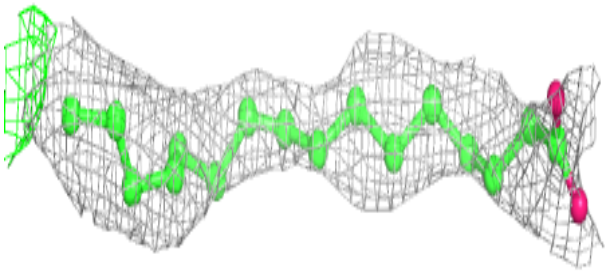


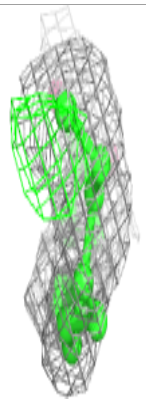


Electron density around OLA B 312:

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

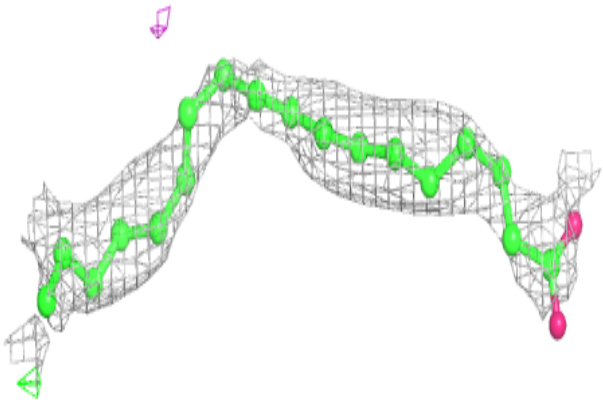


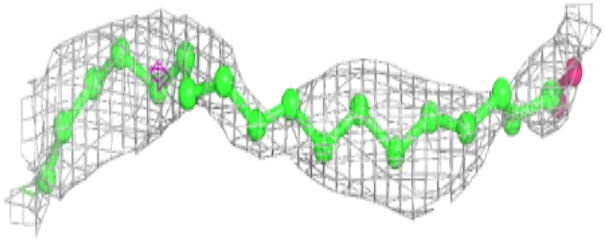


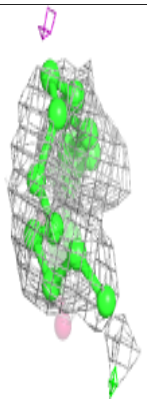


Electron density around OLA E 302:

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

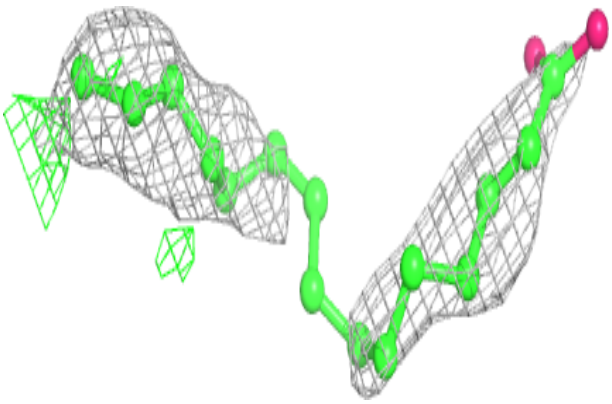


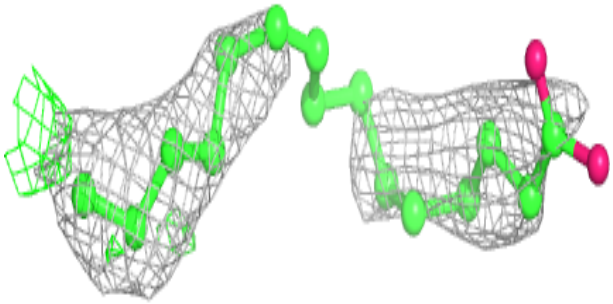


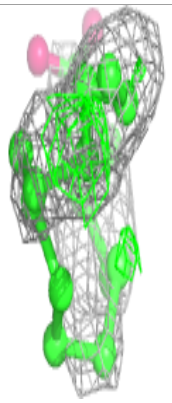


Electron density around OLC C 304:

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

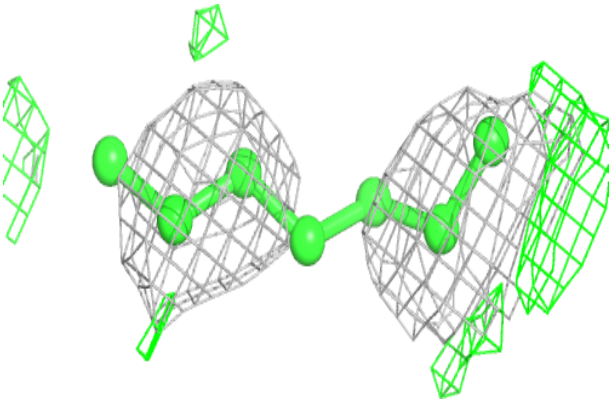


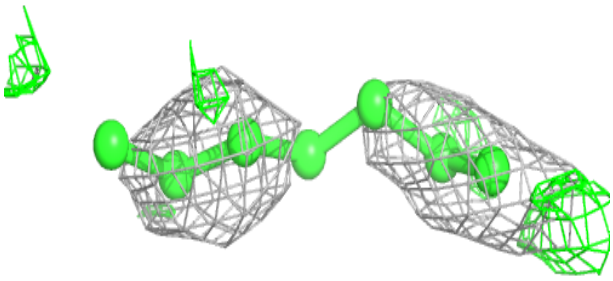


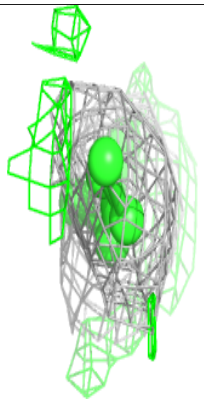


Electron density around LFA A 306:

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

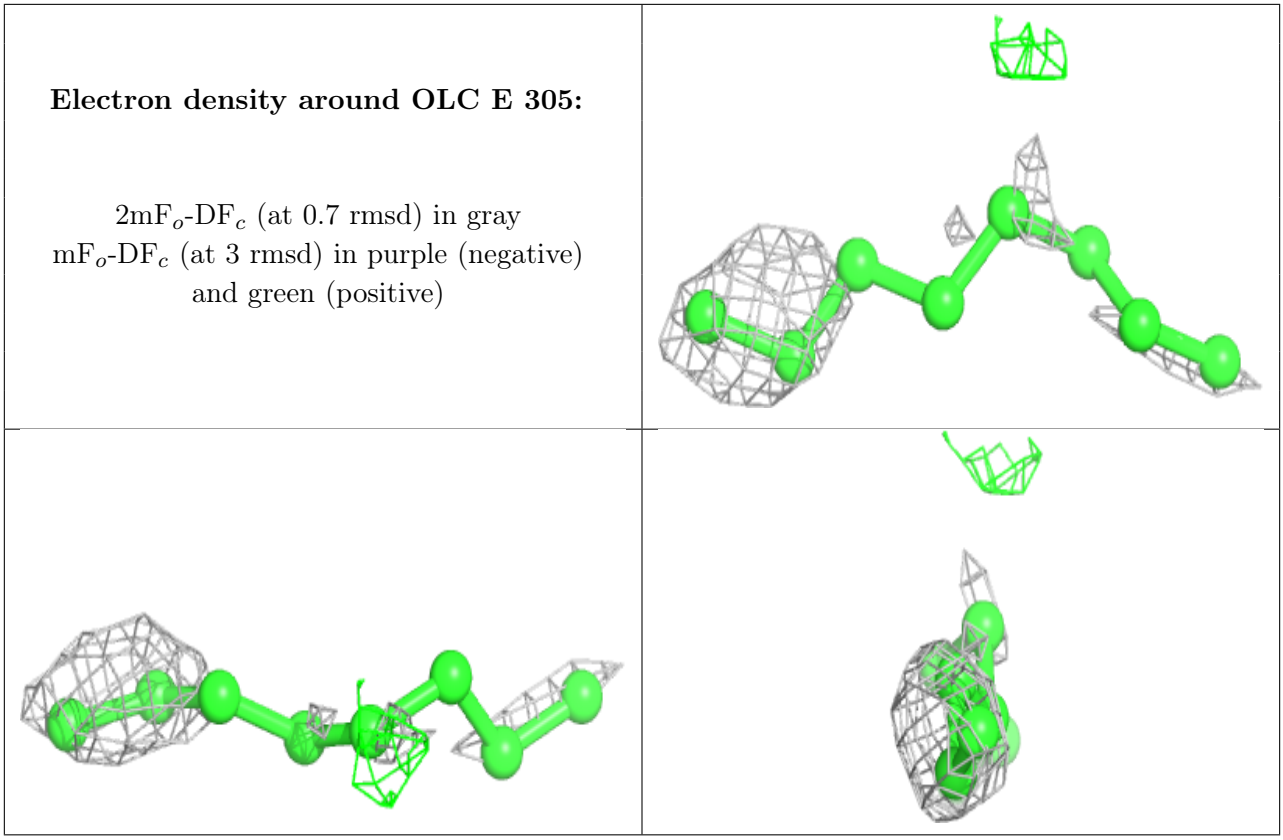






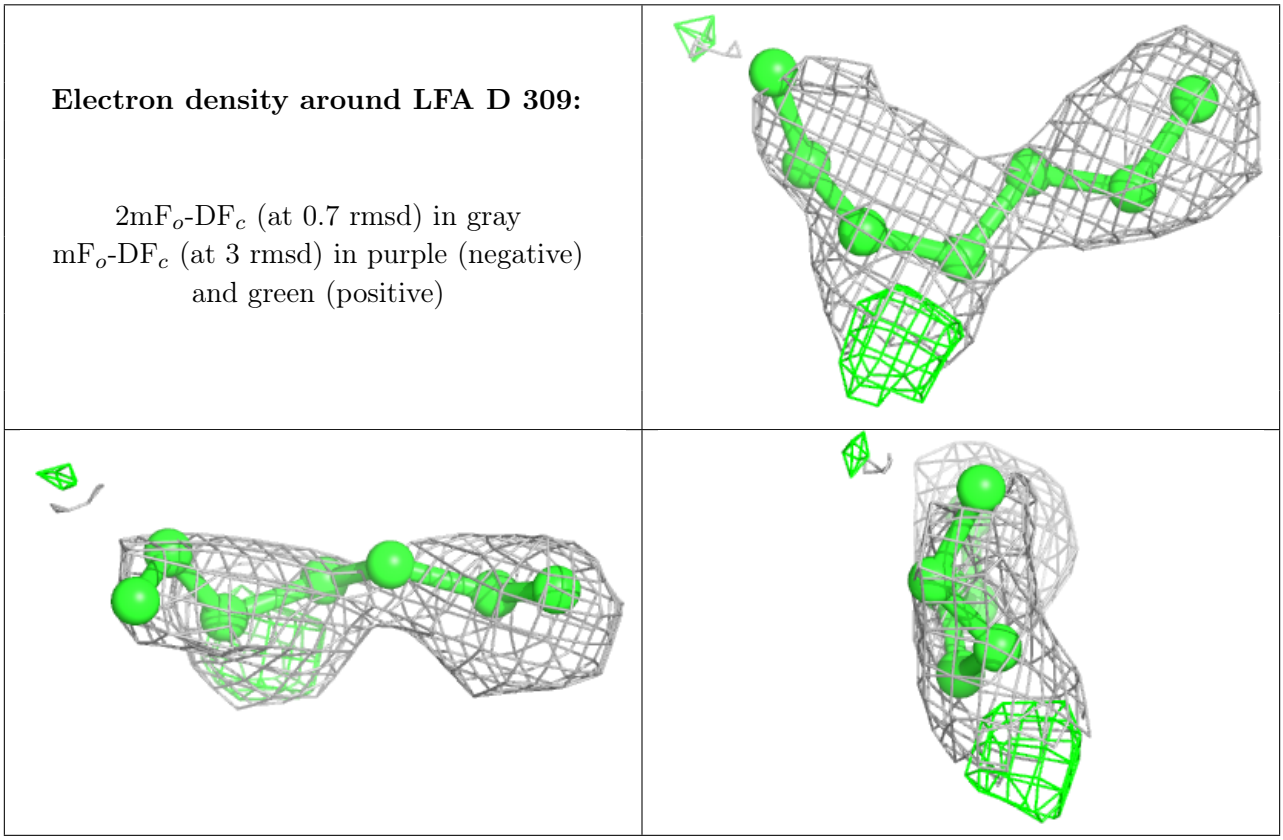
Electron density around OLC E 305:

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



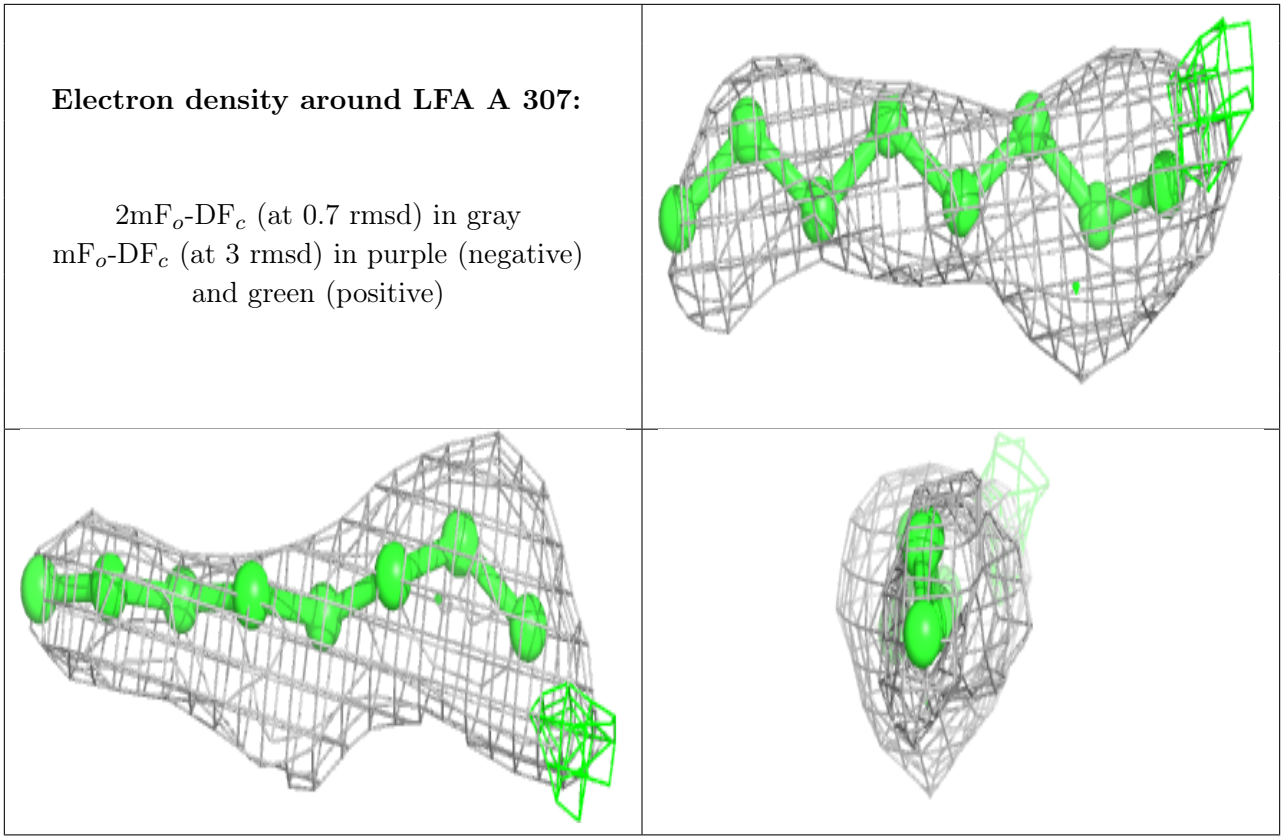
Electron density around LFA D 309:

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



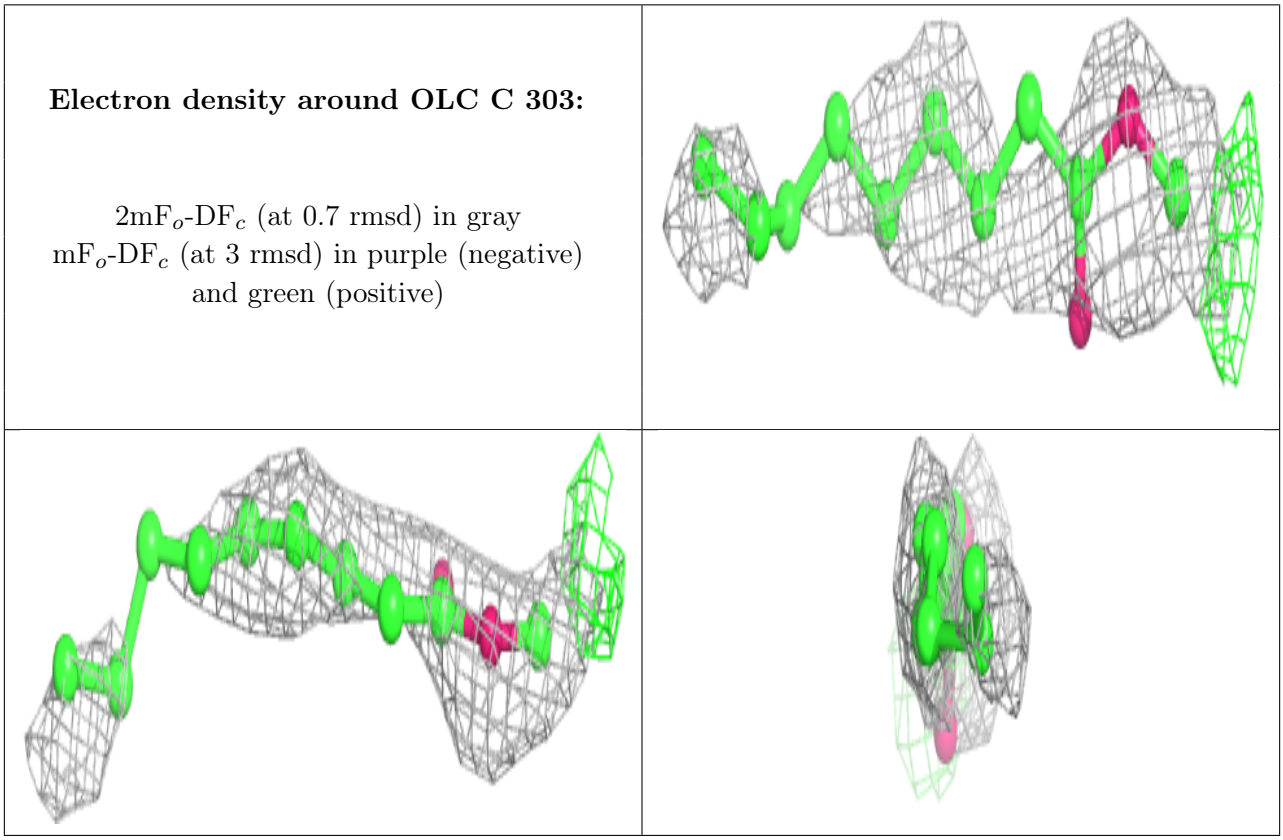
Electron density around LFA A 307:

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



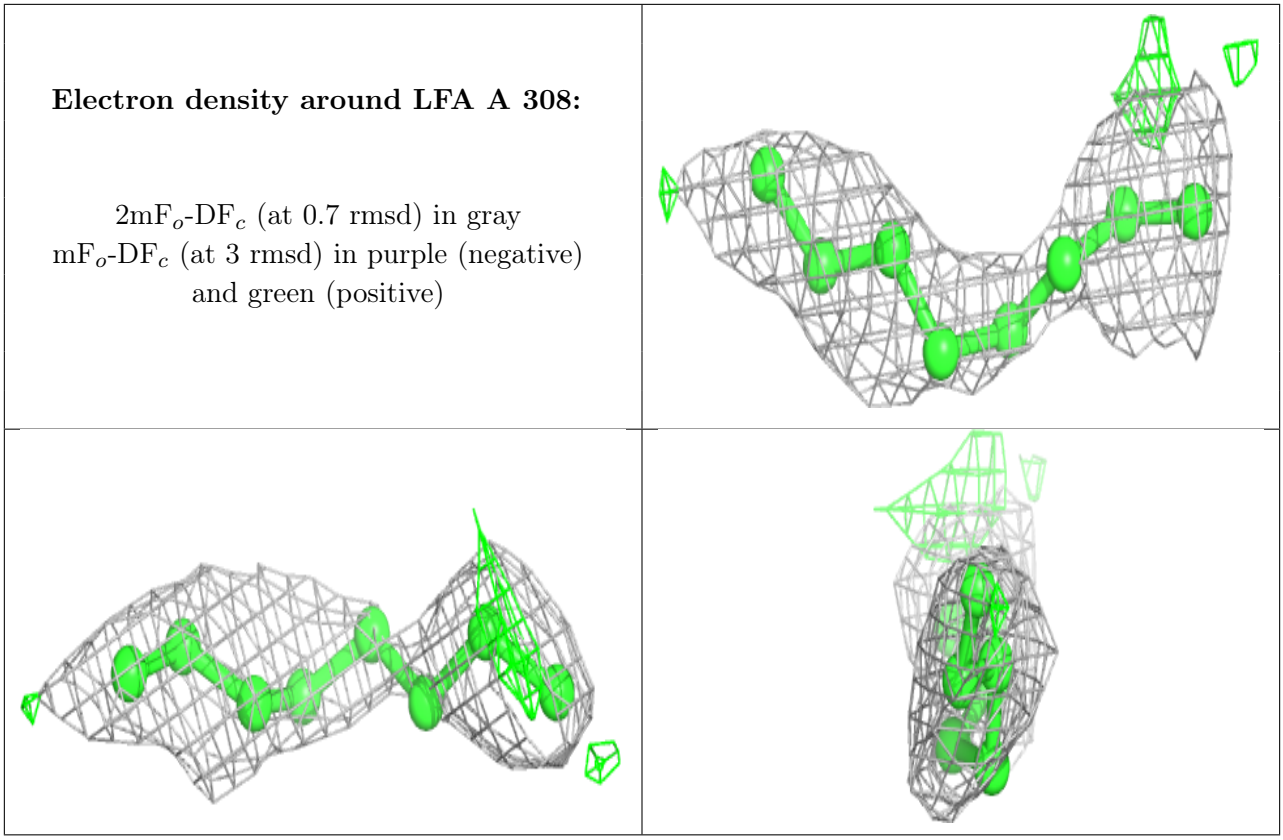
Electron density around OLC C 303:

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



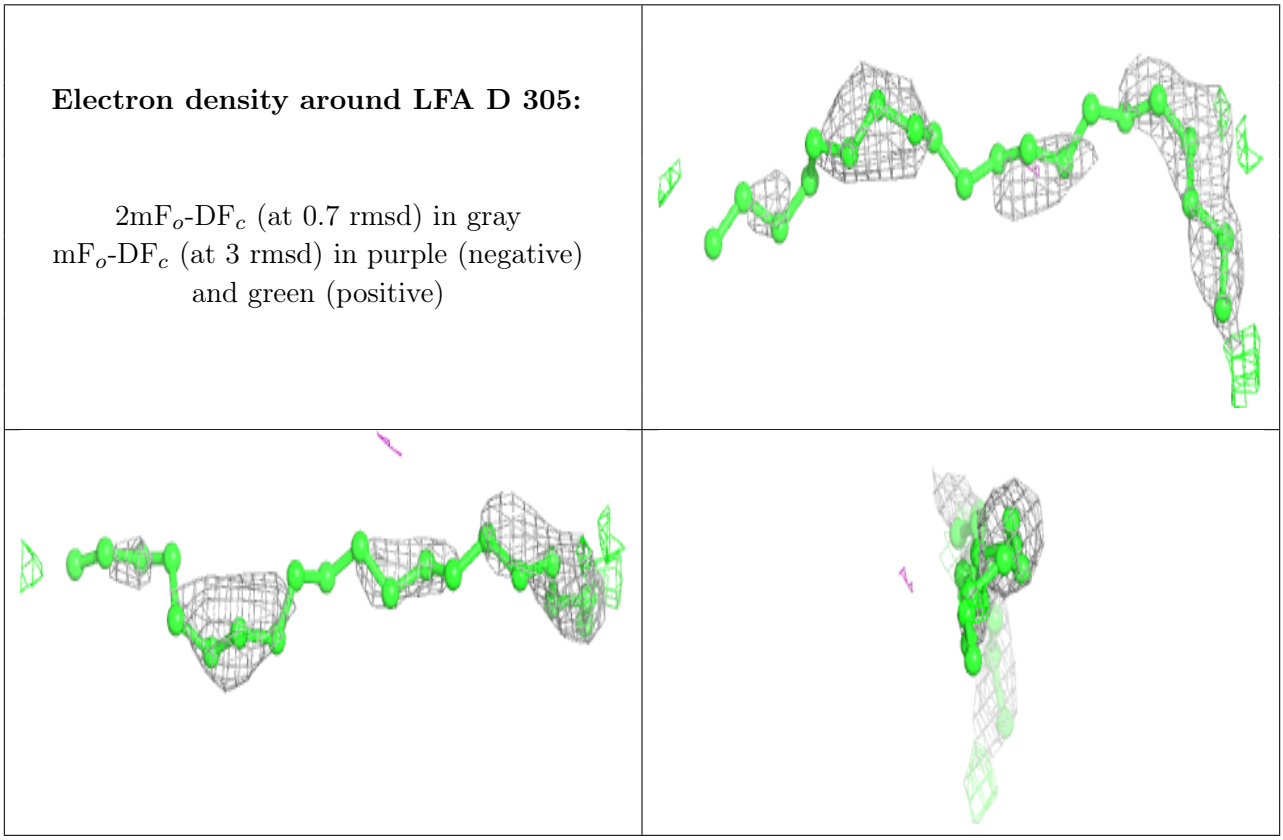
Electron density around LFA A 308:

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



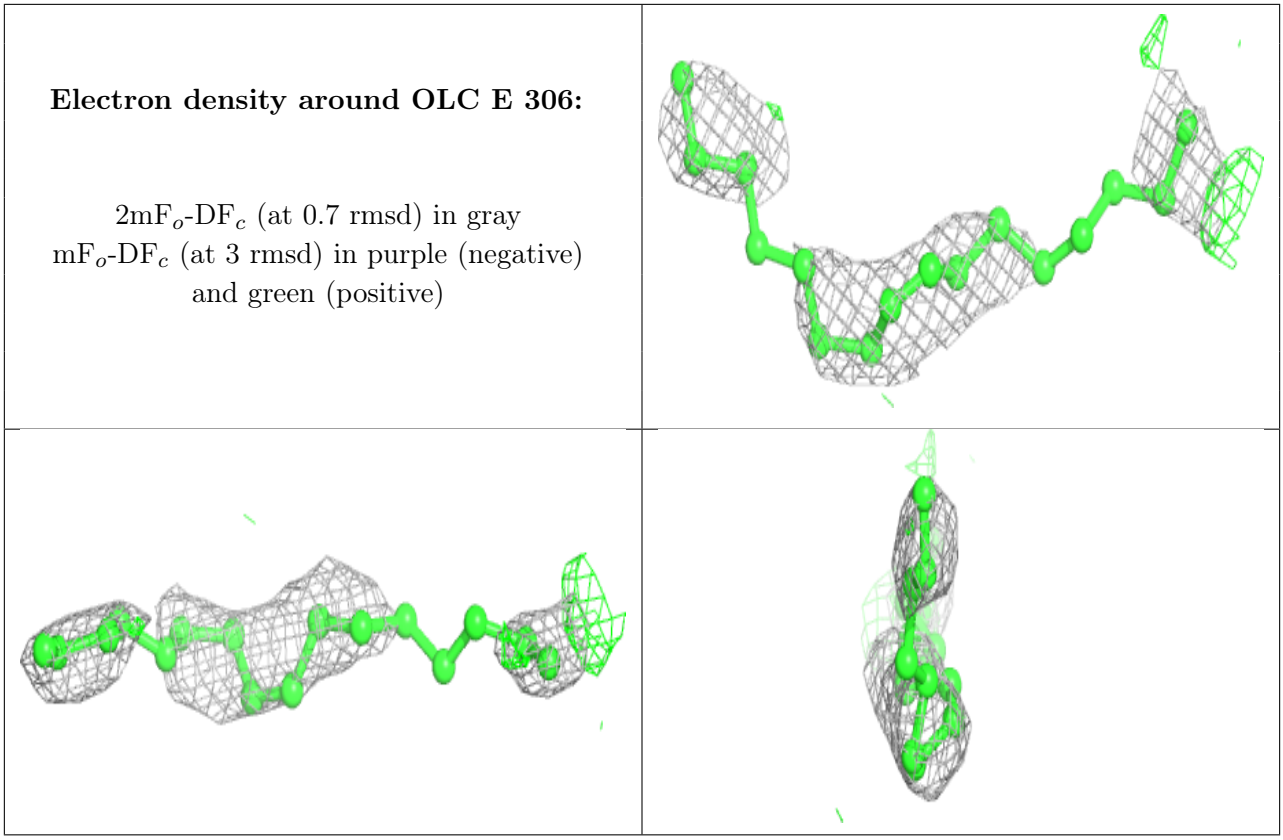
Electron density around LFA D 305:

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



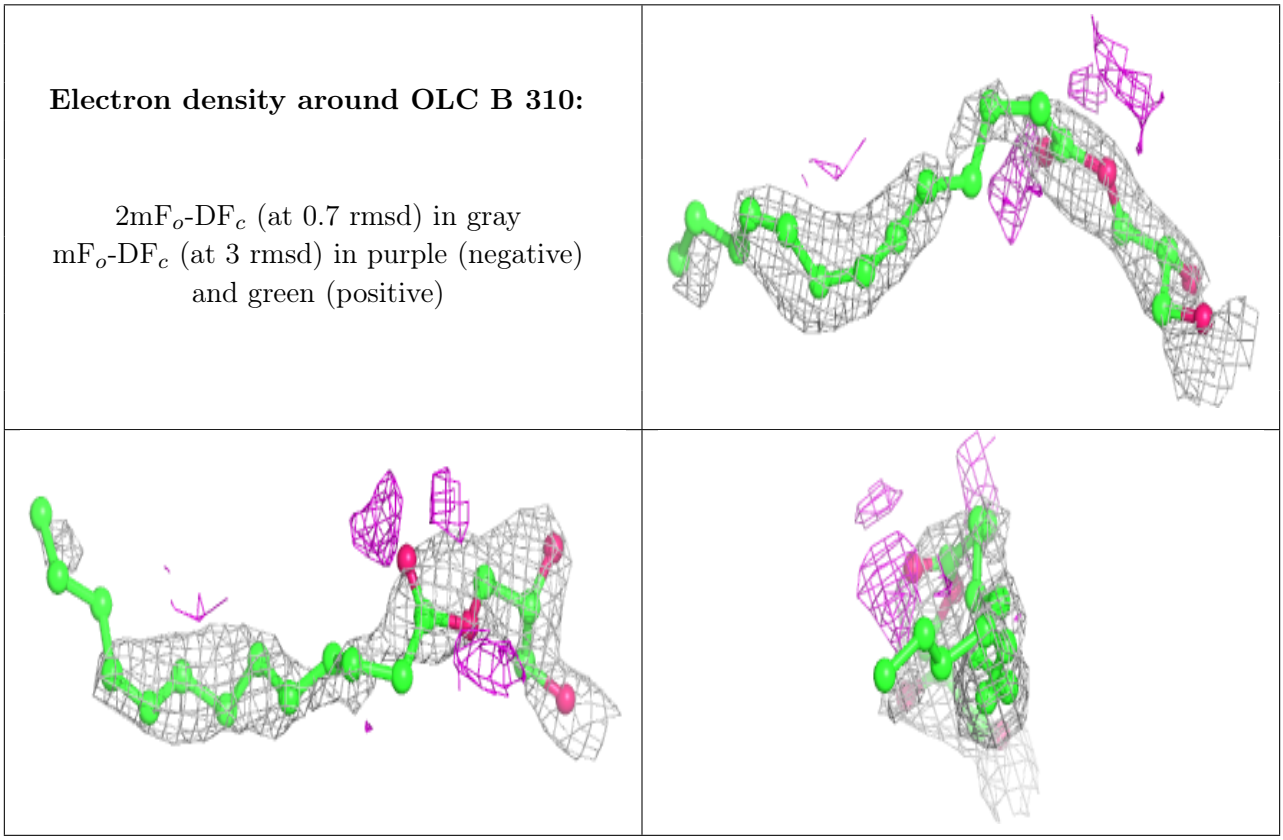
Electron density around OLC E 306:

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



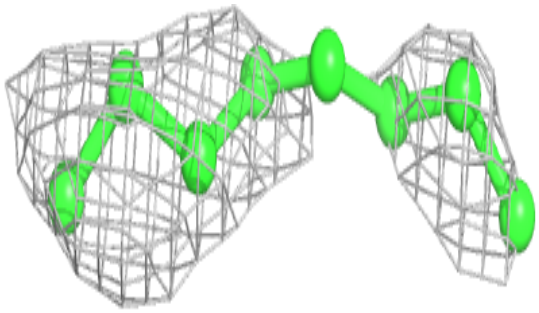
Electron density around OLC B 310:

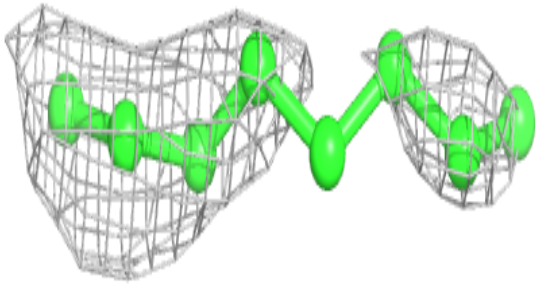
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

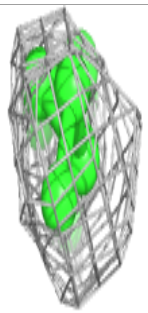


Electron density around LFA C 307:

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

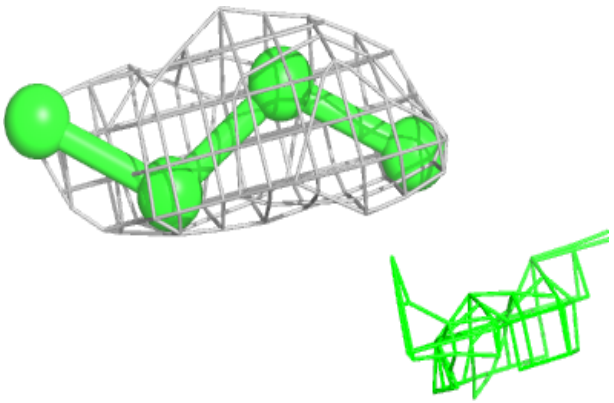


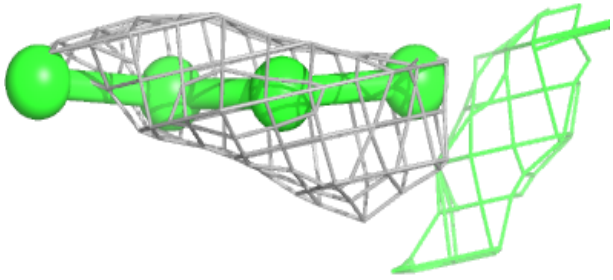


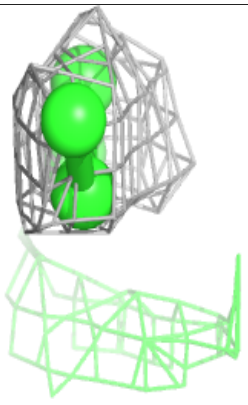


Electron density around LFA A 309:

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

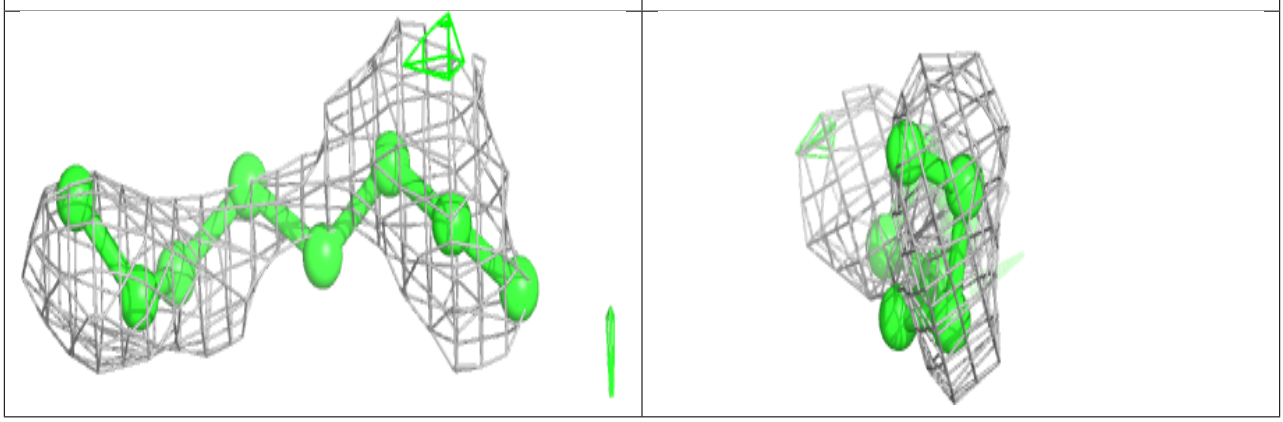






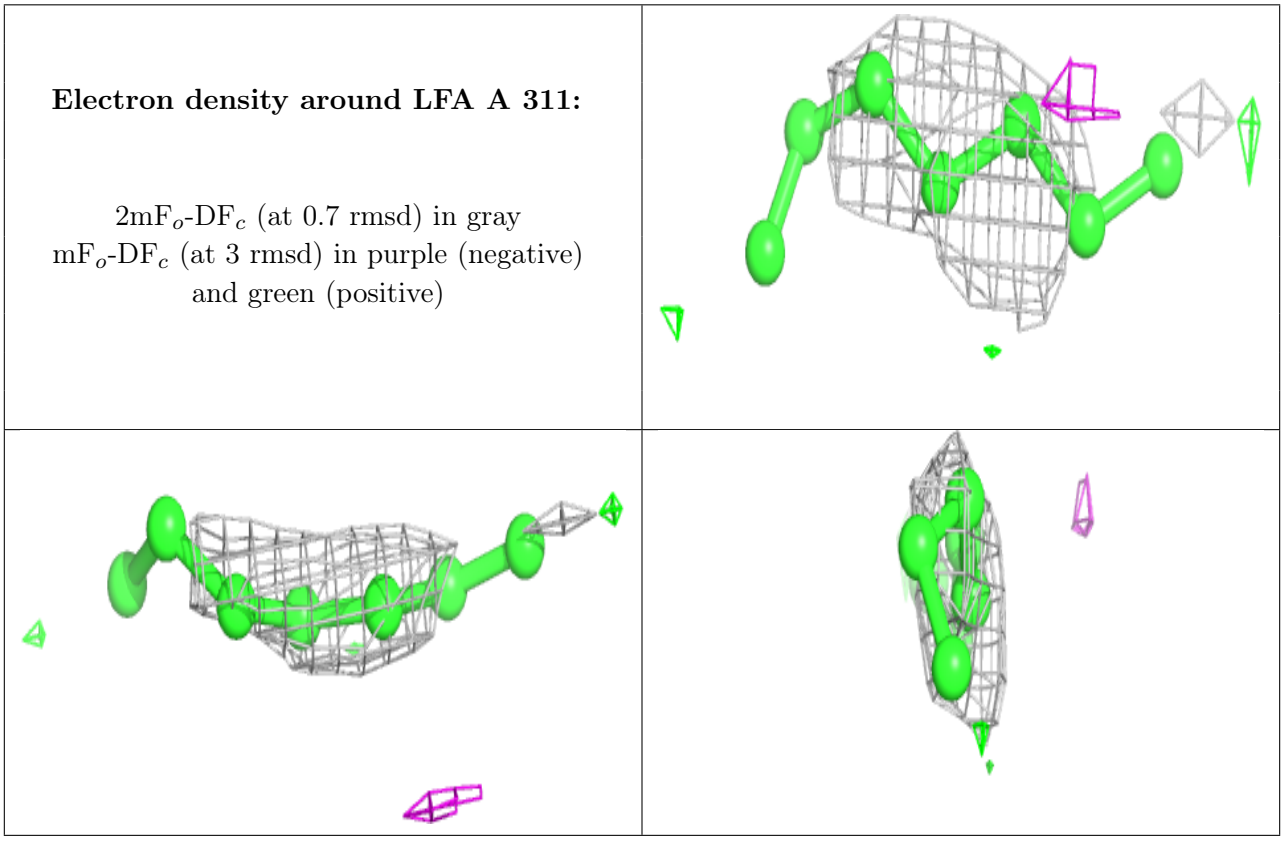
Electron density around LFA D 307:

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



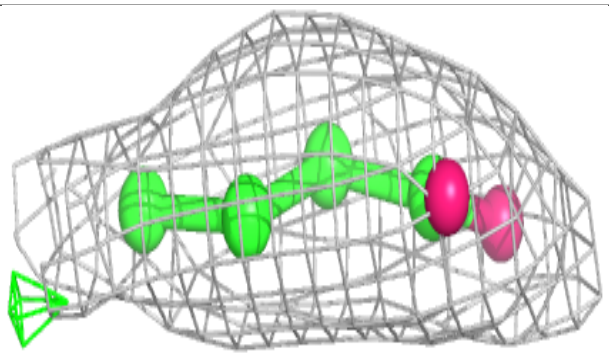
Electron density around LFA A 311:

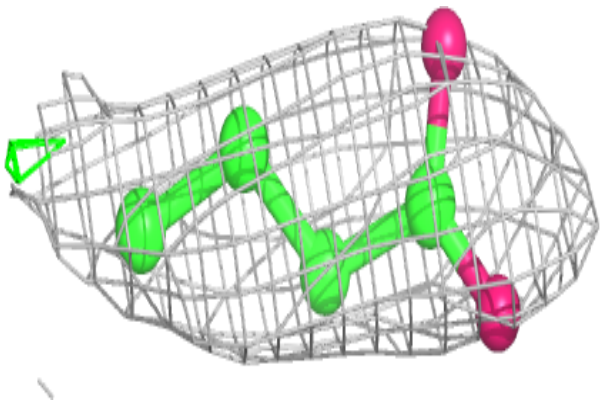
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

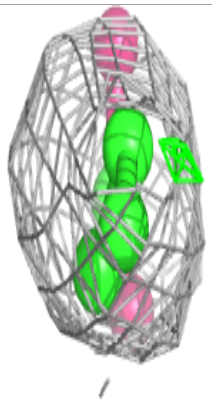


Electron density around OLA E 314:

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

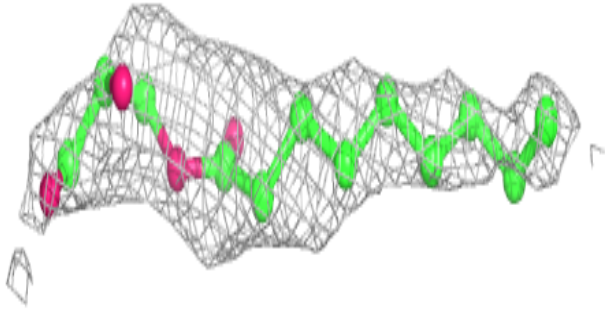


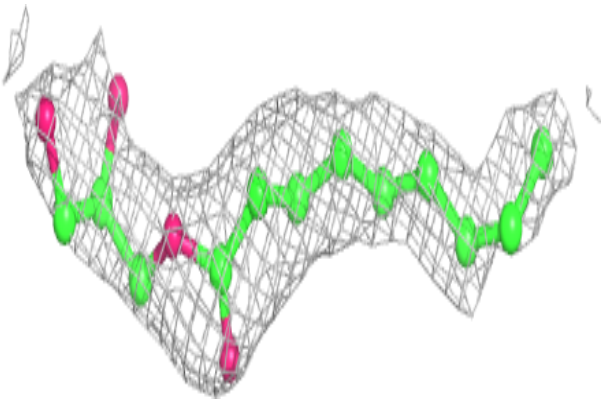


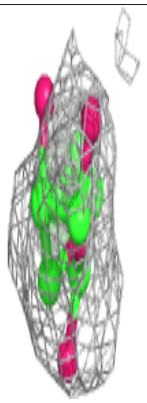


Electron density around OLC C 305:

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

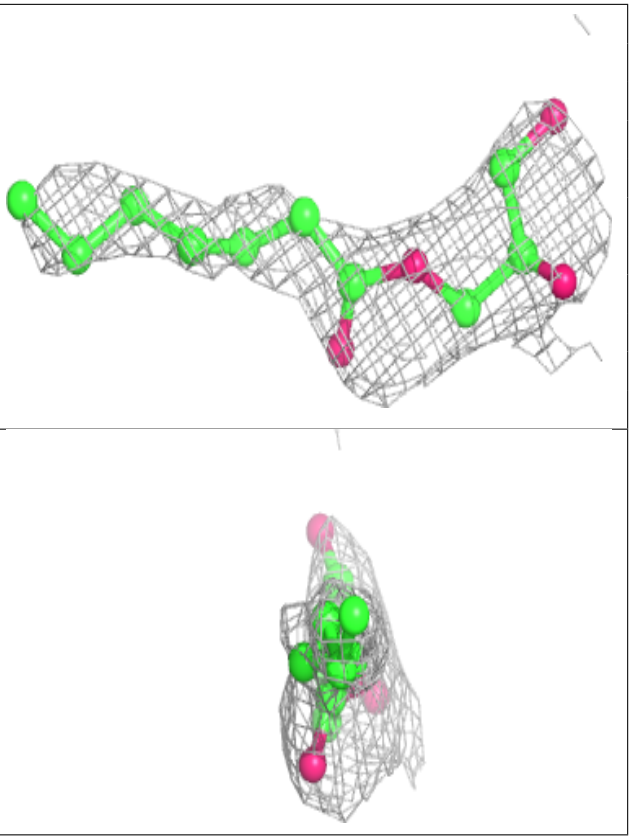






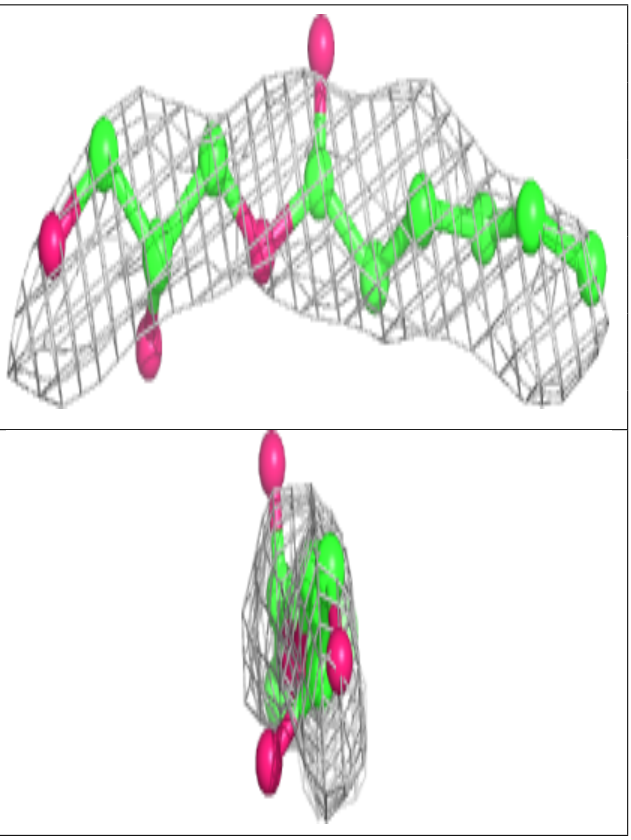
Electron density around OLC D 304:

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



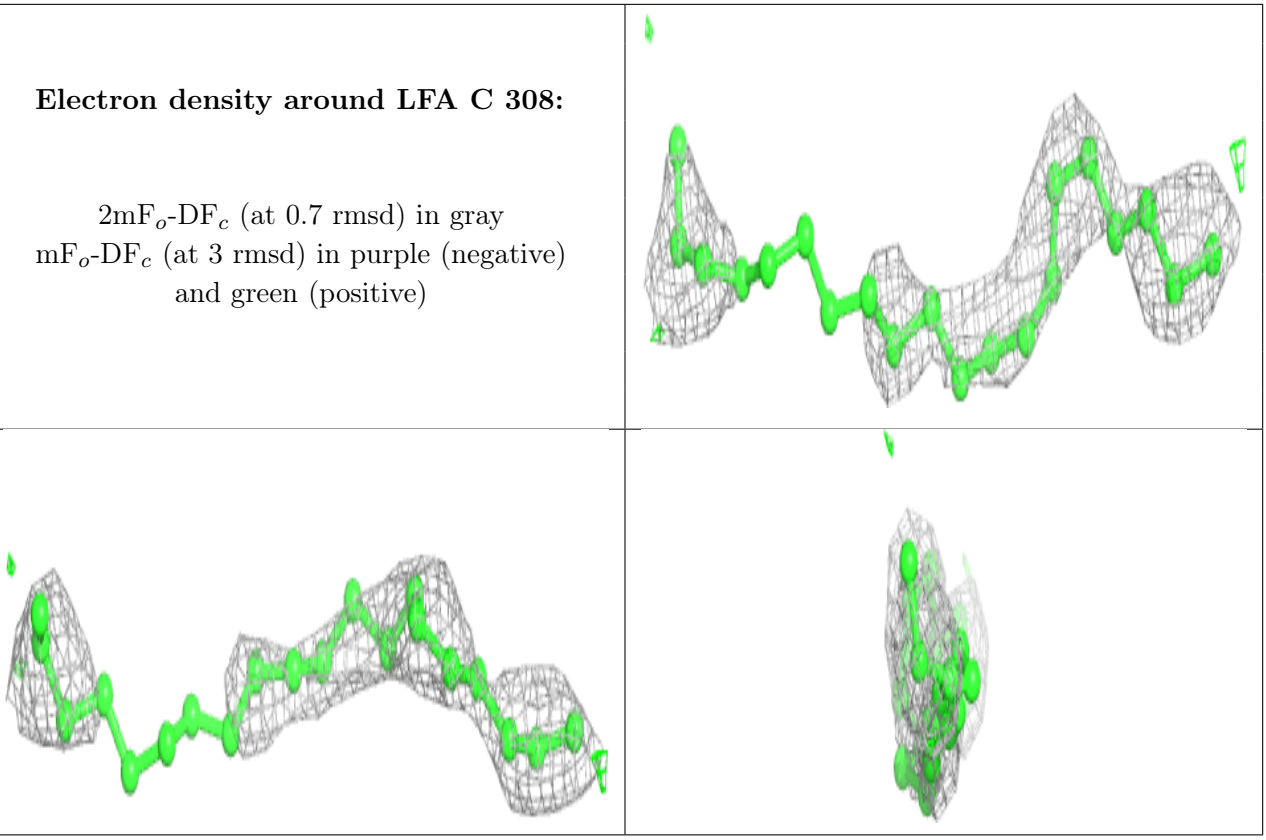
Electron density around OLC A 304:

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



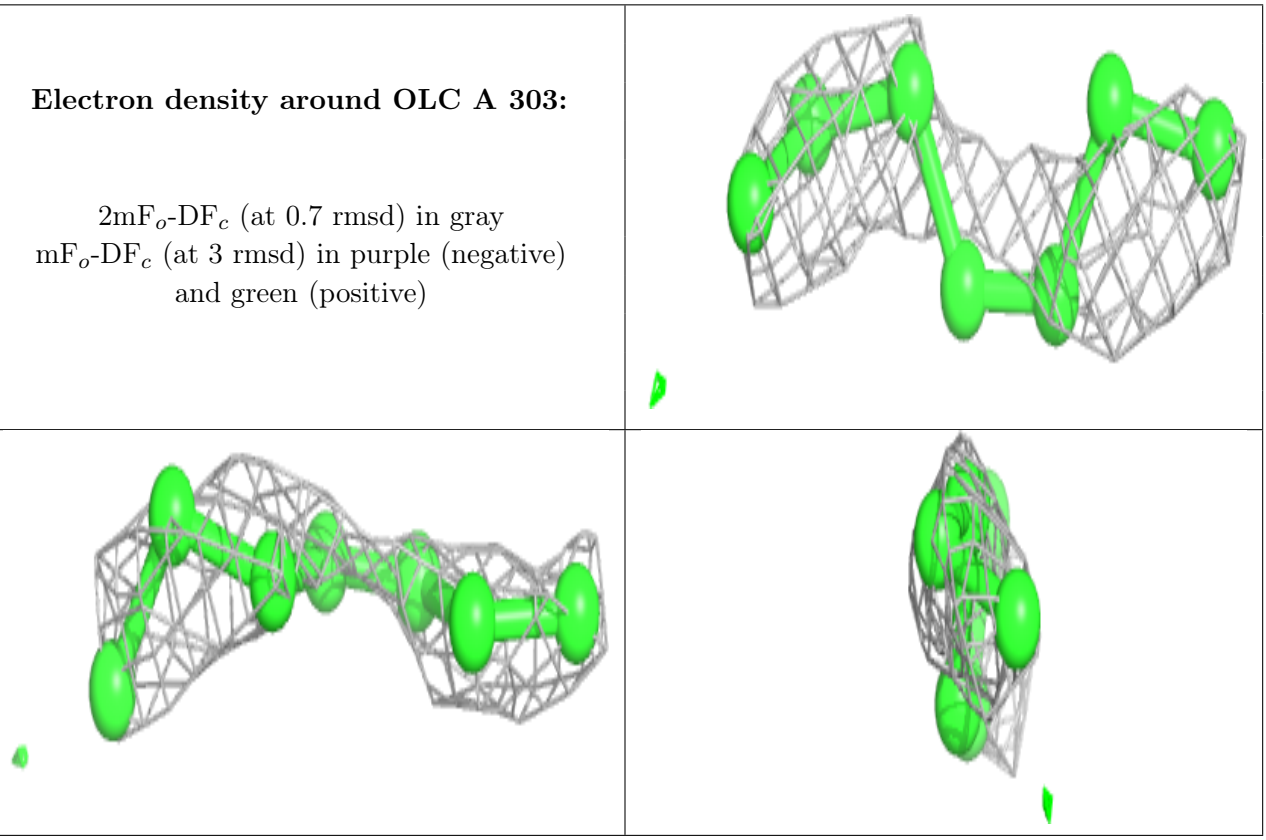
Electron density around LFA C 308:

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



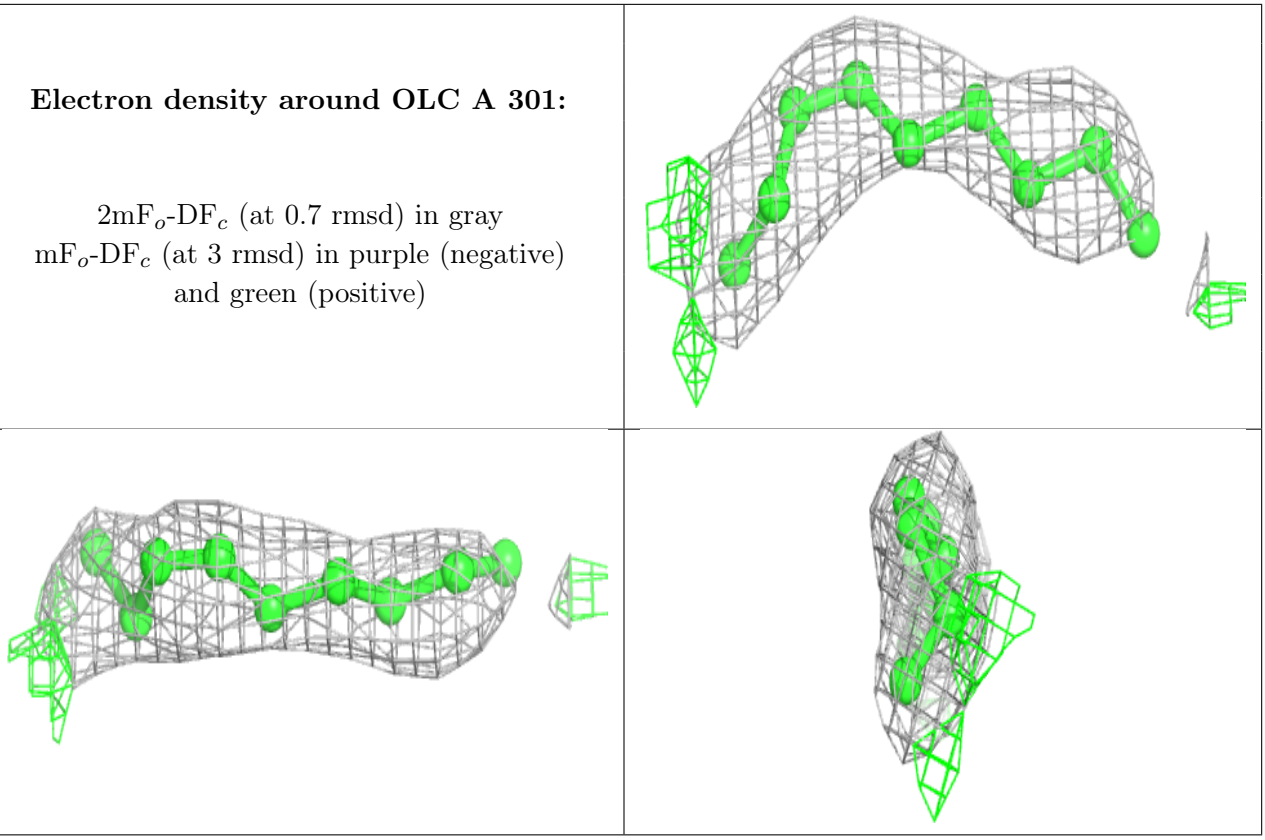
Electron density around OLC A 303:

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



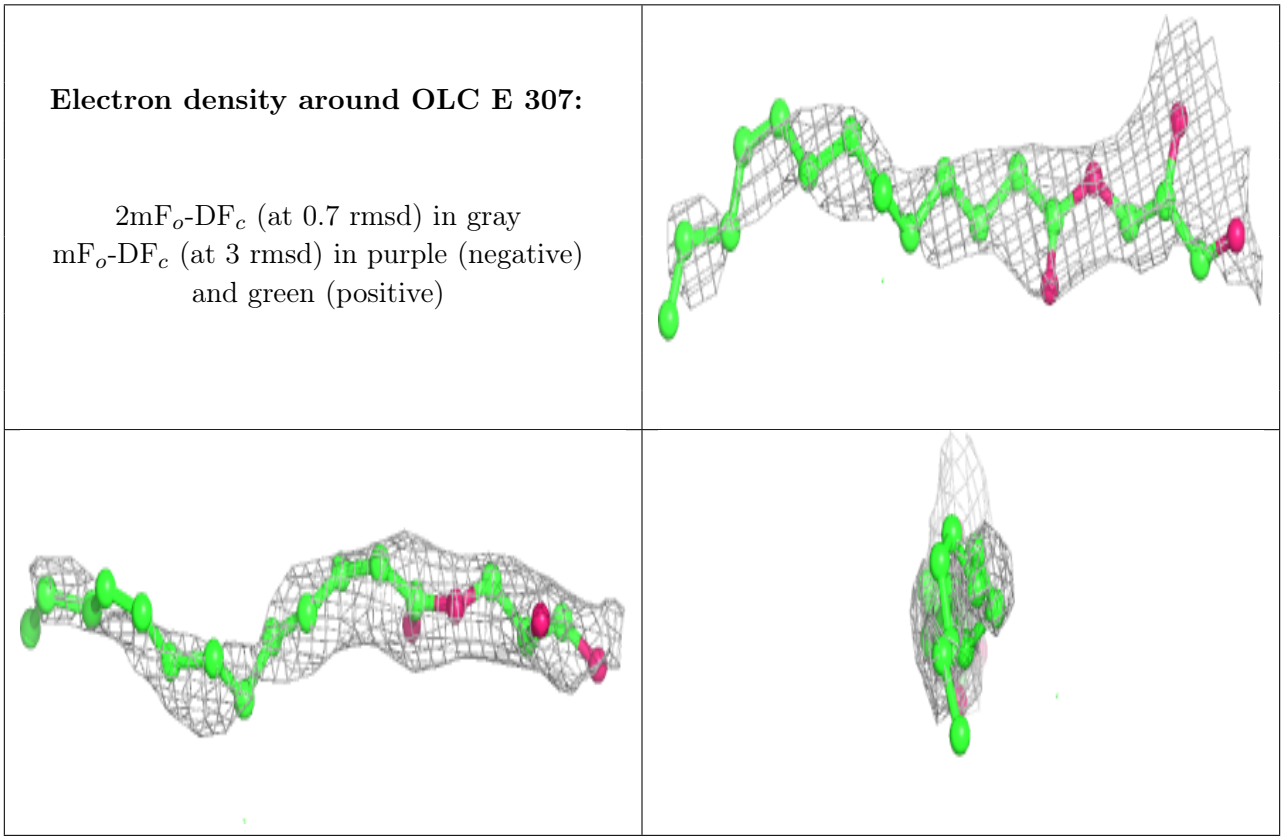
Electron density around OLC A 301:

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



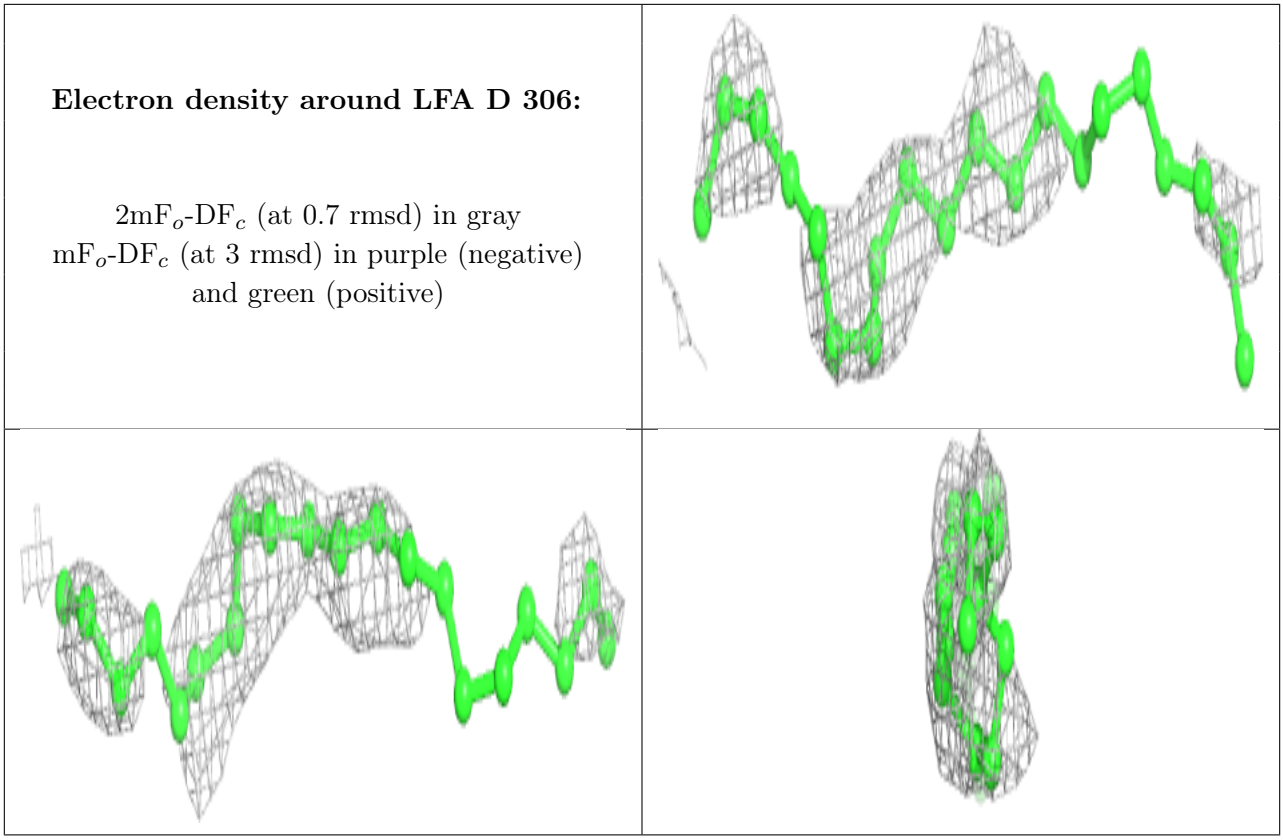
Electron density around OLC E 307:

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



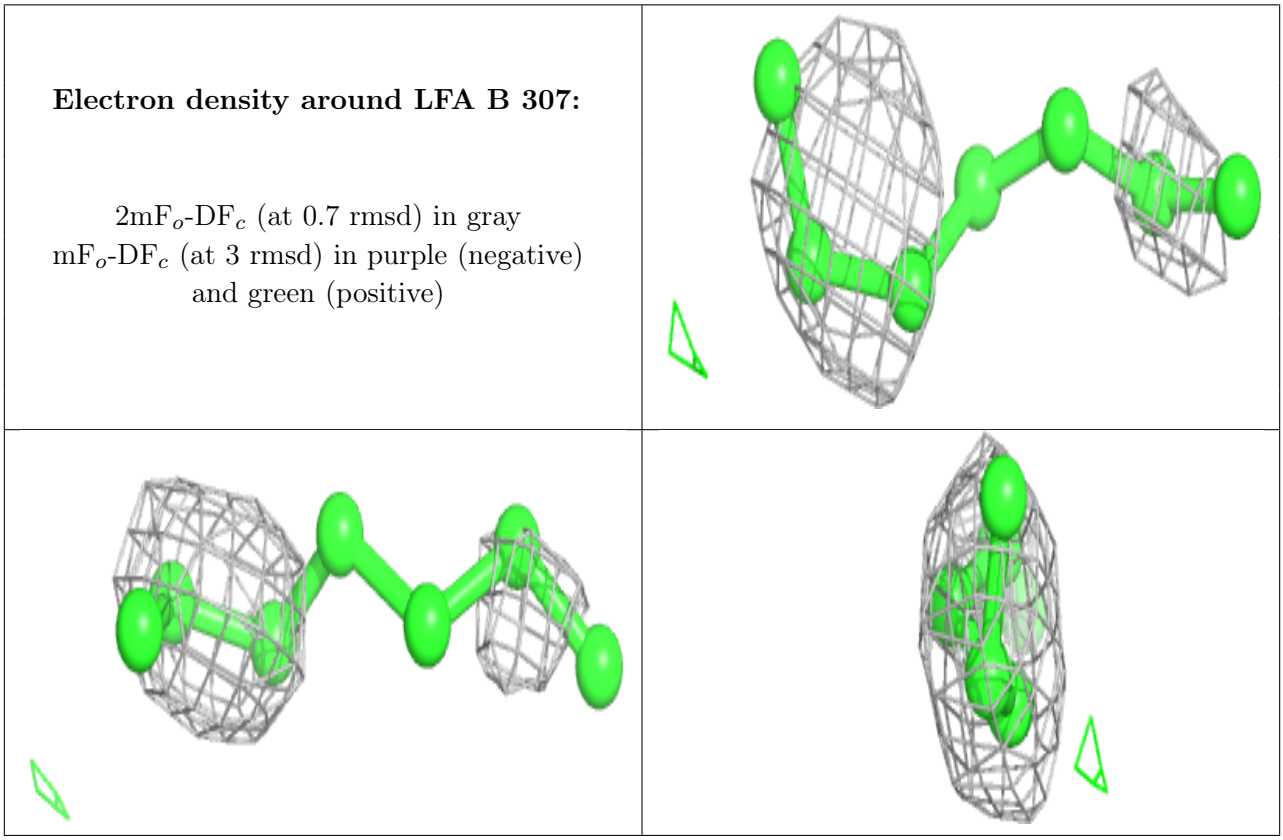
Electron density around LFA D 306:

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



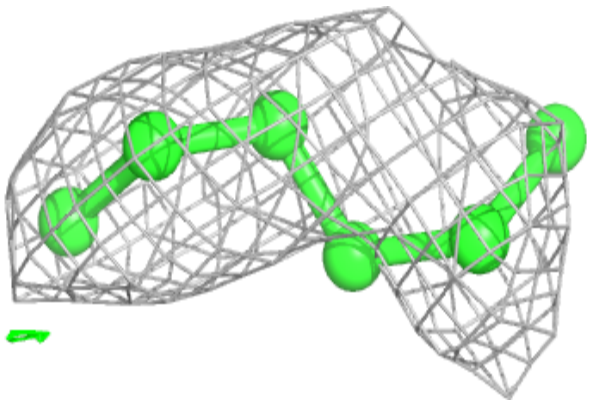
Electron density around LFA B 307:

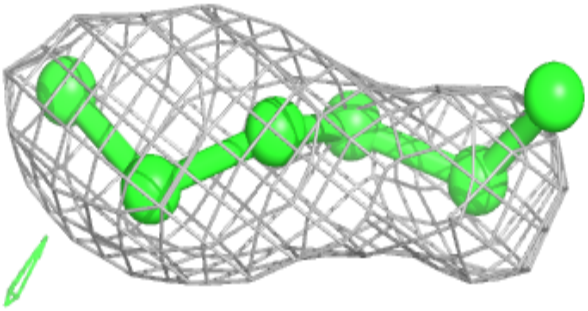
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

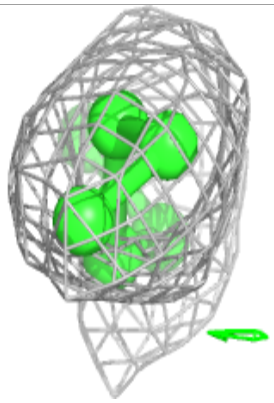


Electron density around LFA A 310:

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

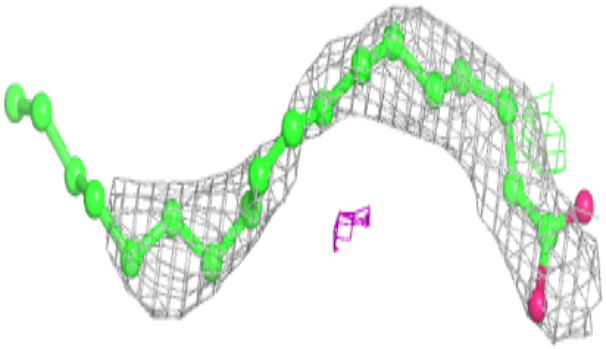


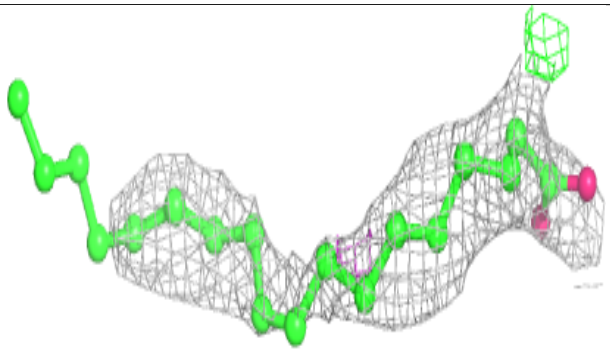


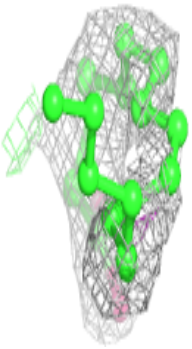


Electron density around OLC A 313:

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

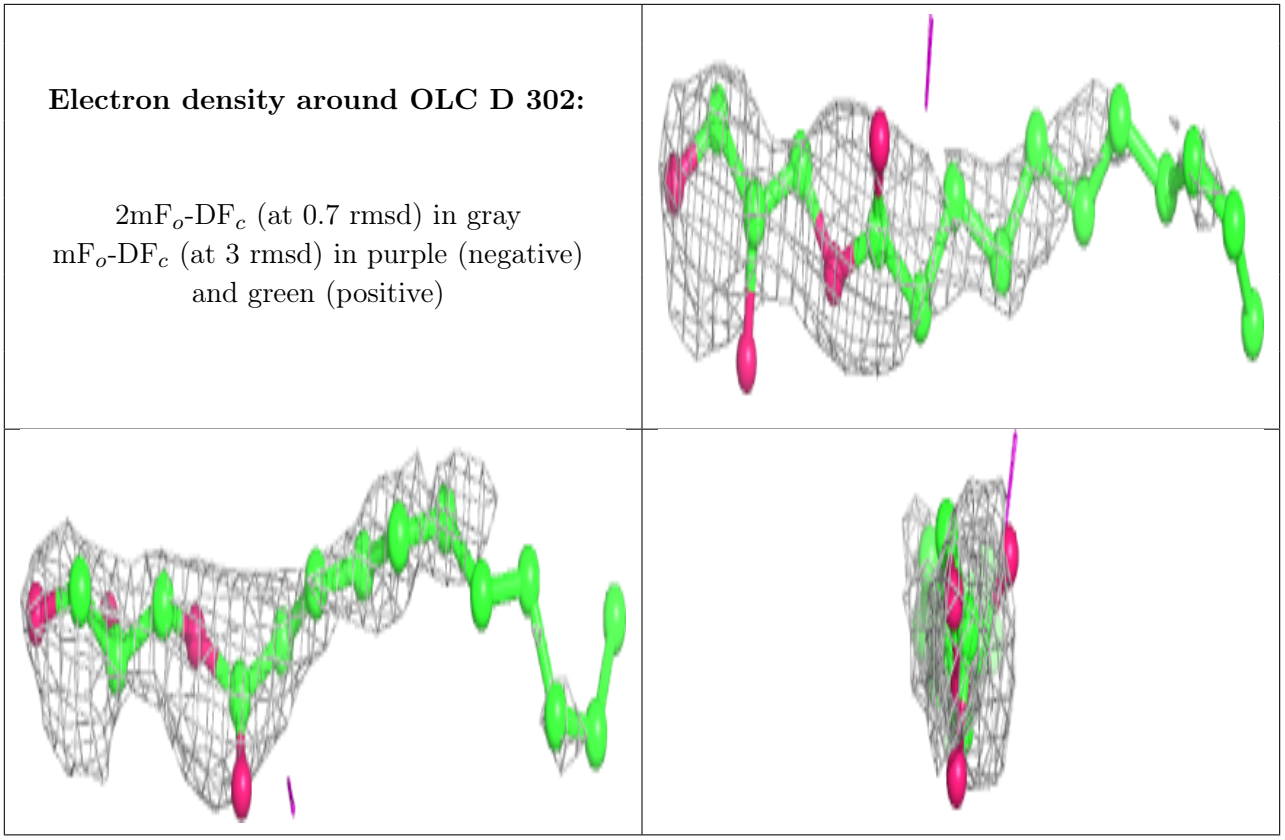






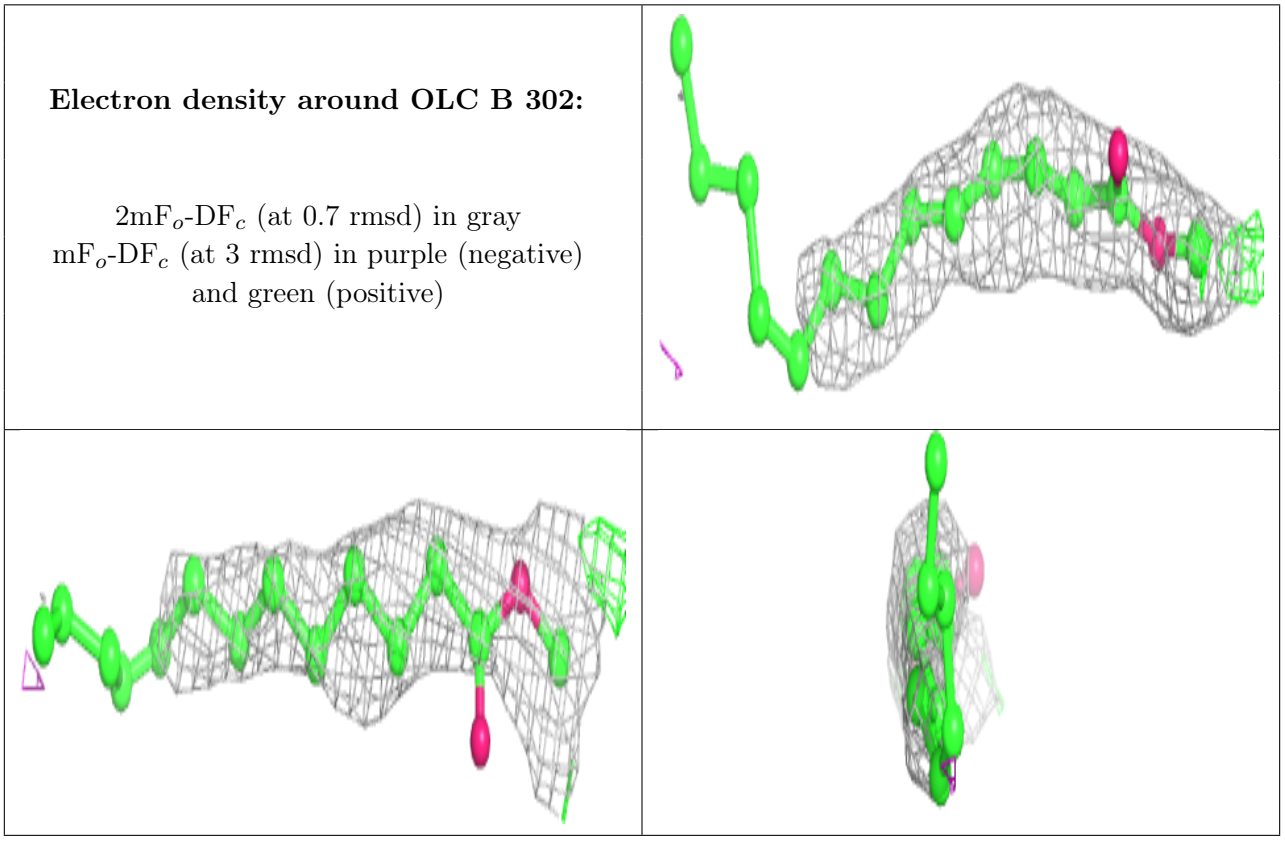
Electron density around OLC D 302:

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



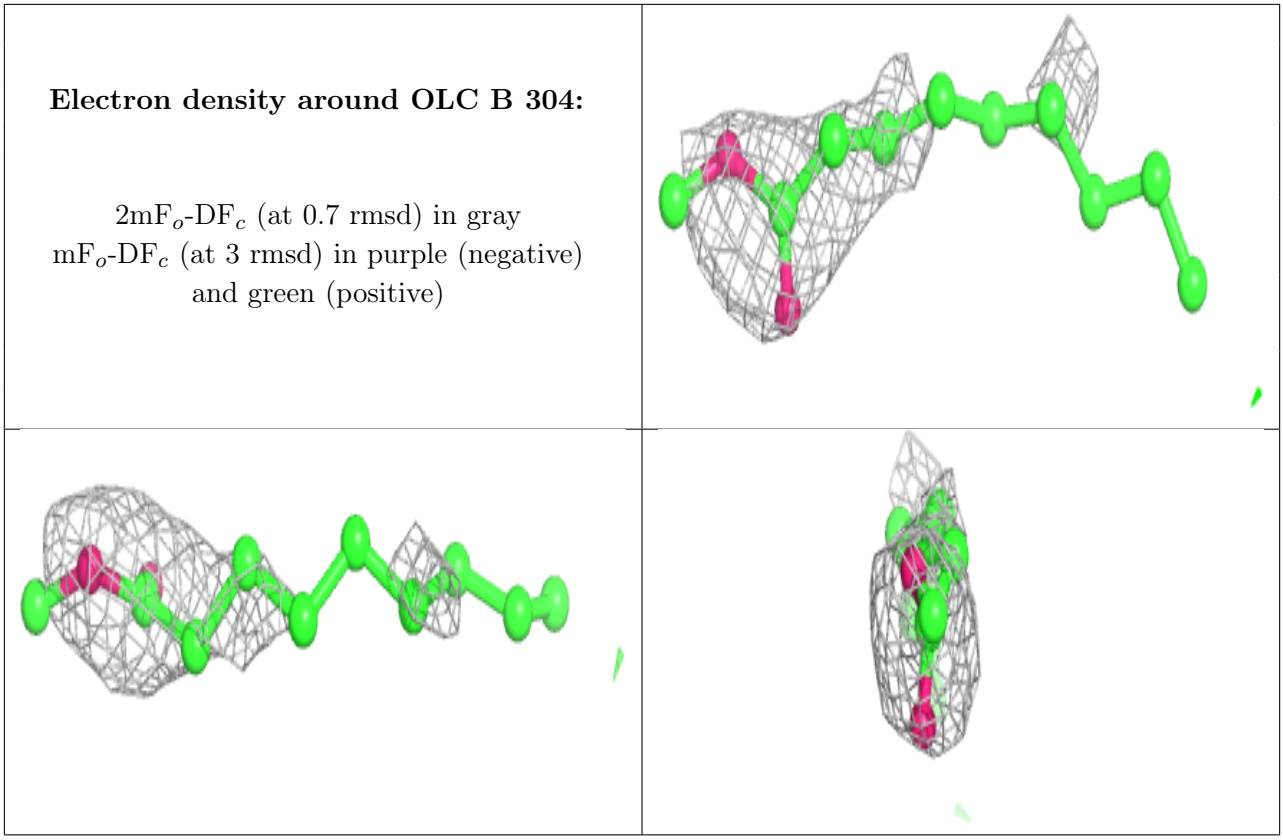
Electron density around OLC B 302:

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



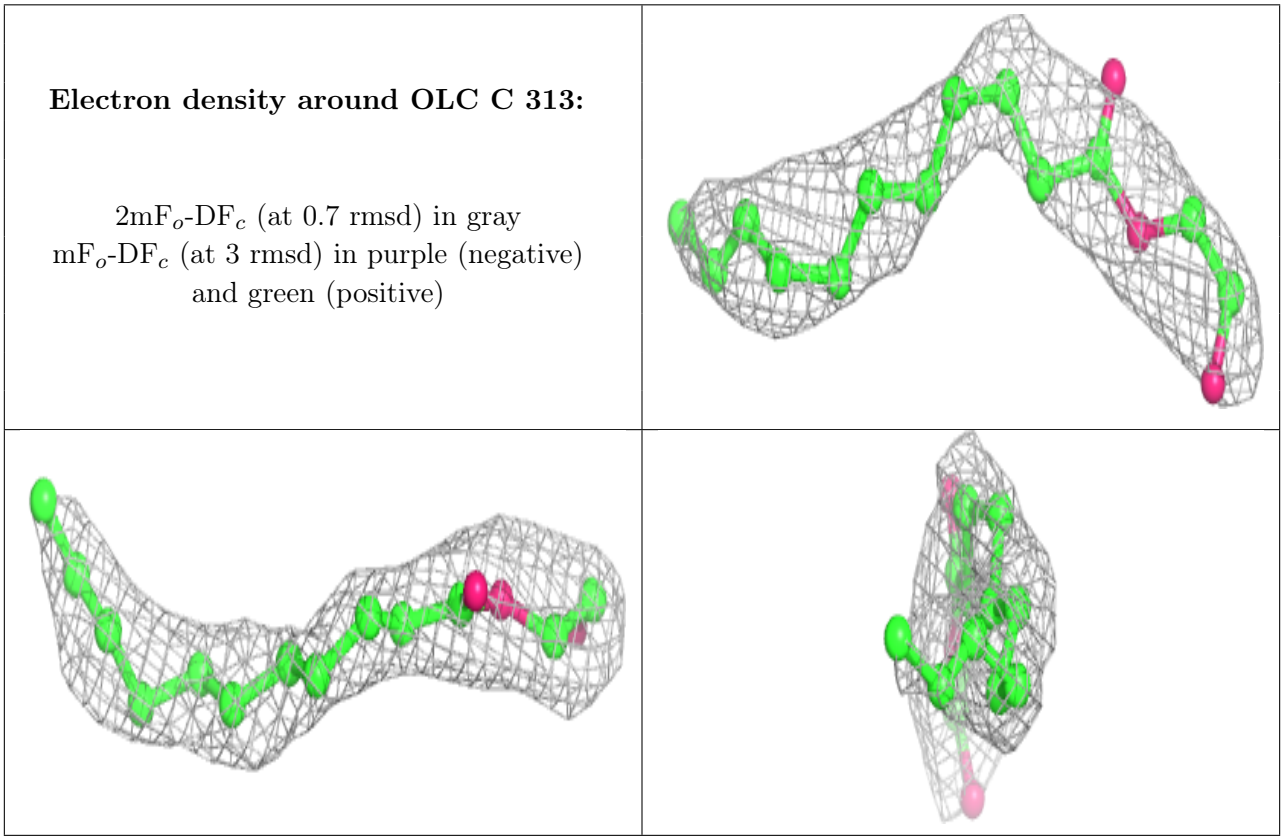
Electron density around OLC B 304:

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



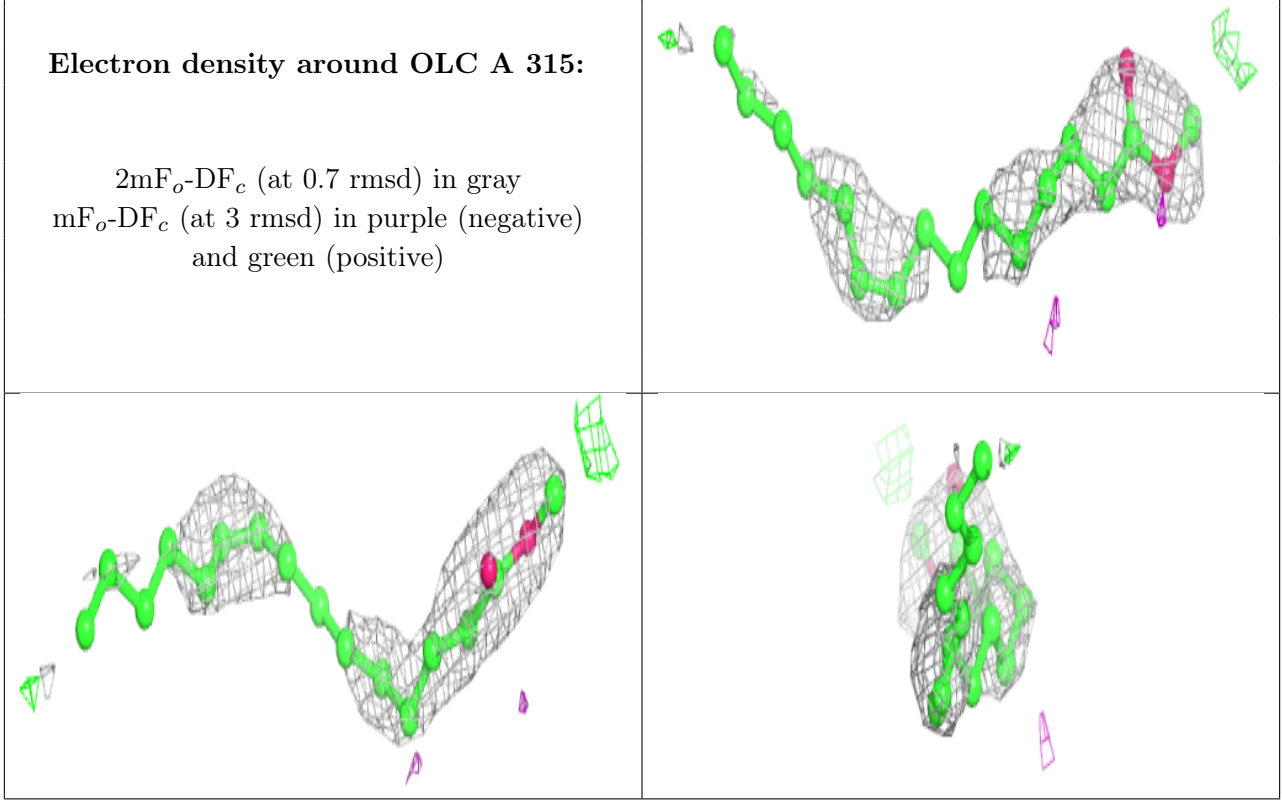
Electron density around OLC C 313:

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



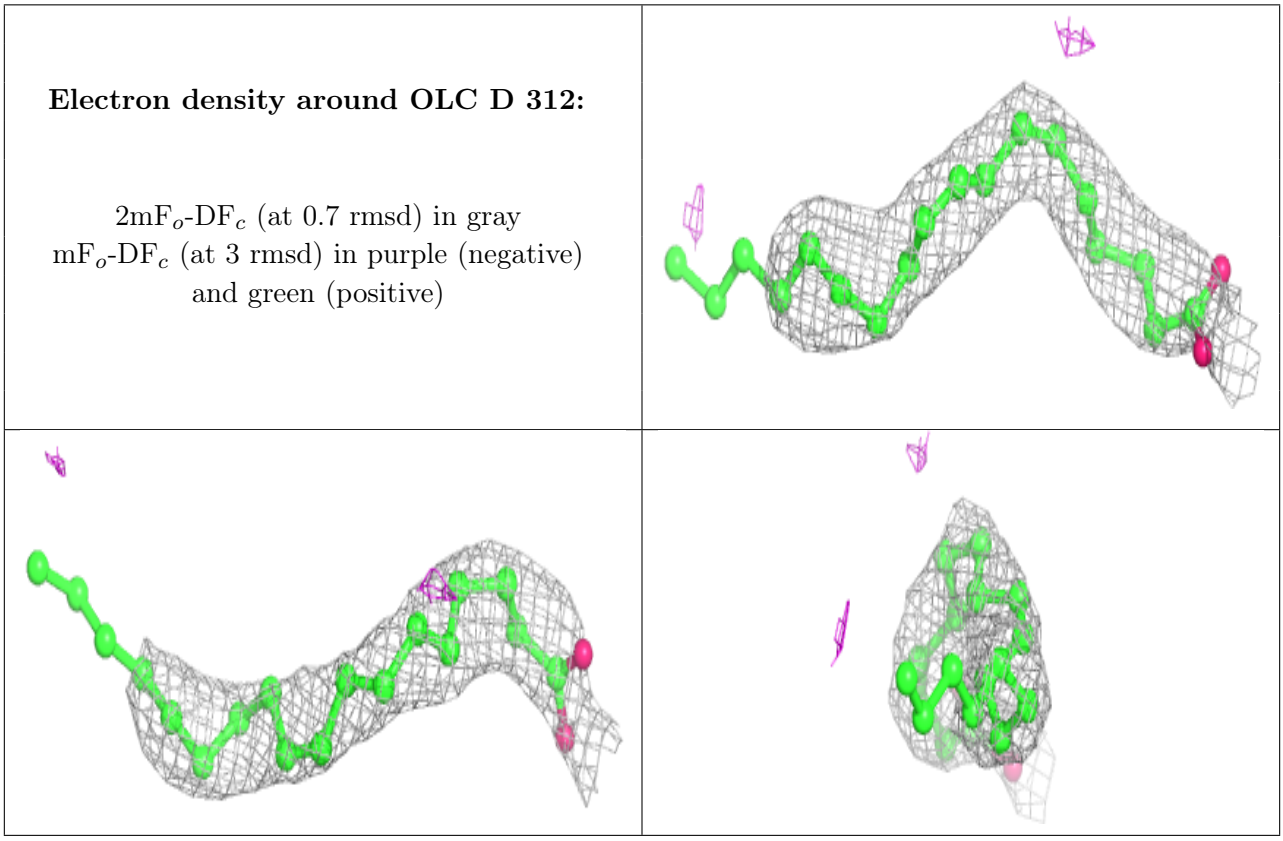
Electron density around OLC A 315:

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



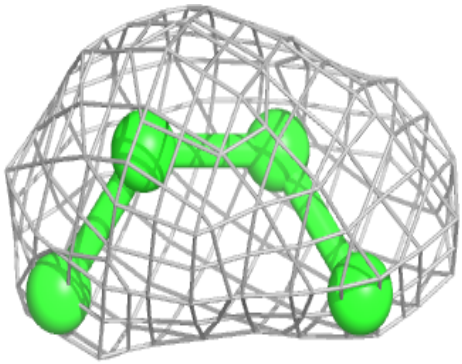
Electron density around OLC D 312:

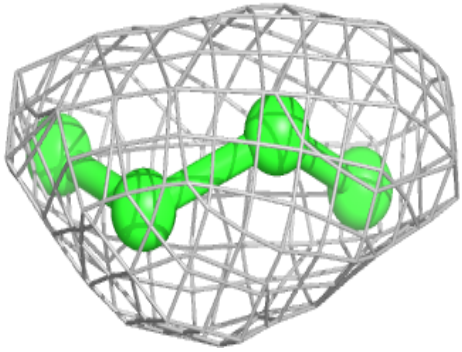
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

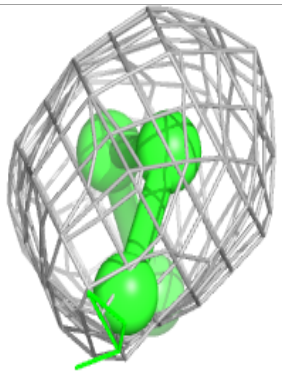


Electron density around LFA E 311:

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

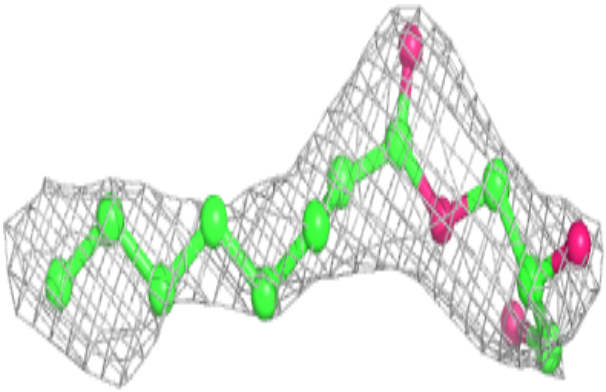


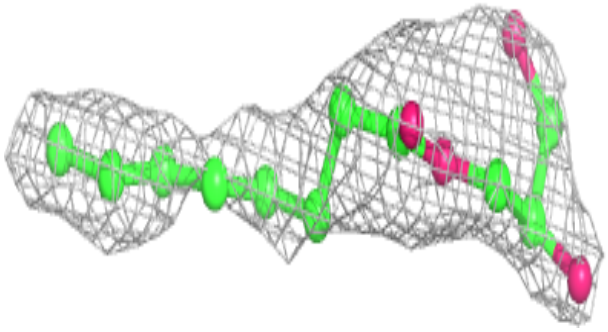


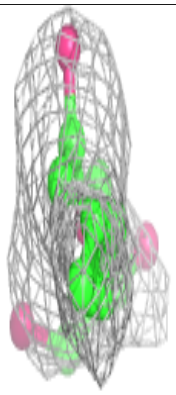


Electron density around OLC A 305:

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

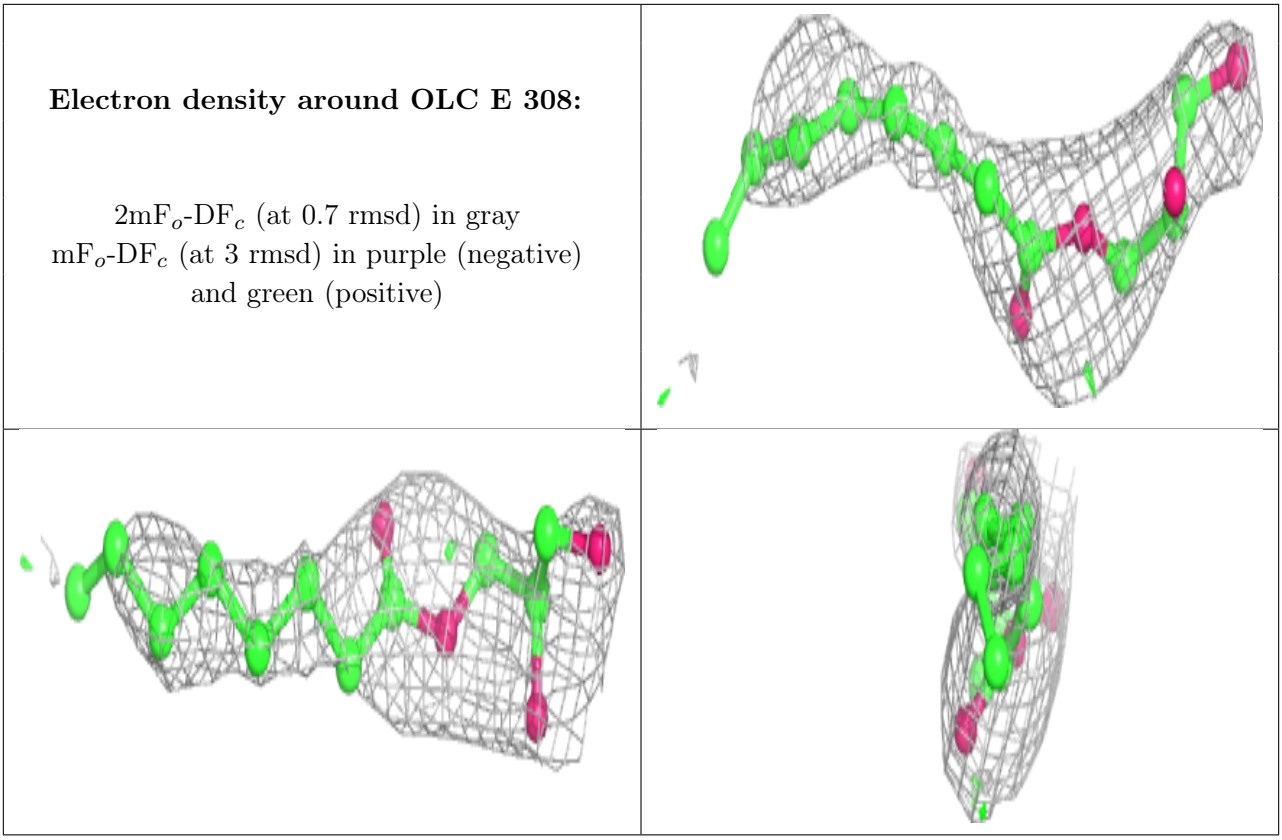






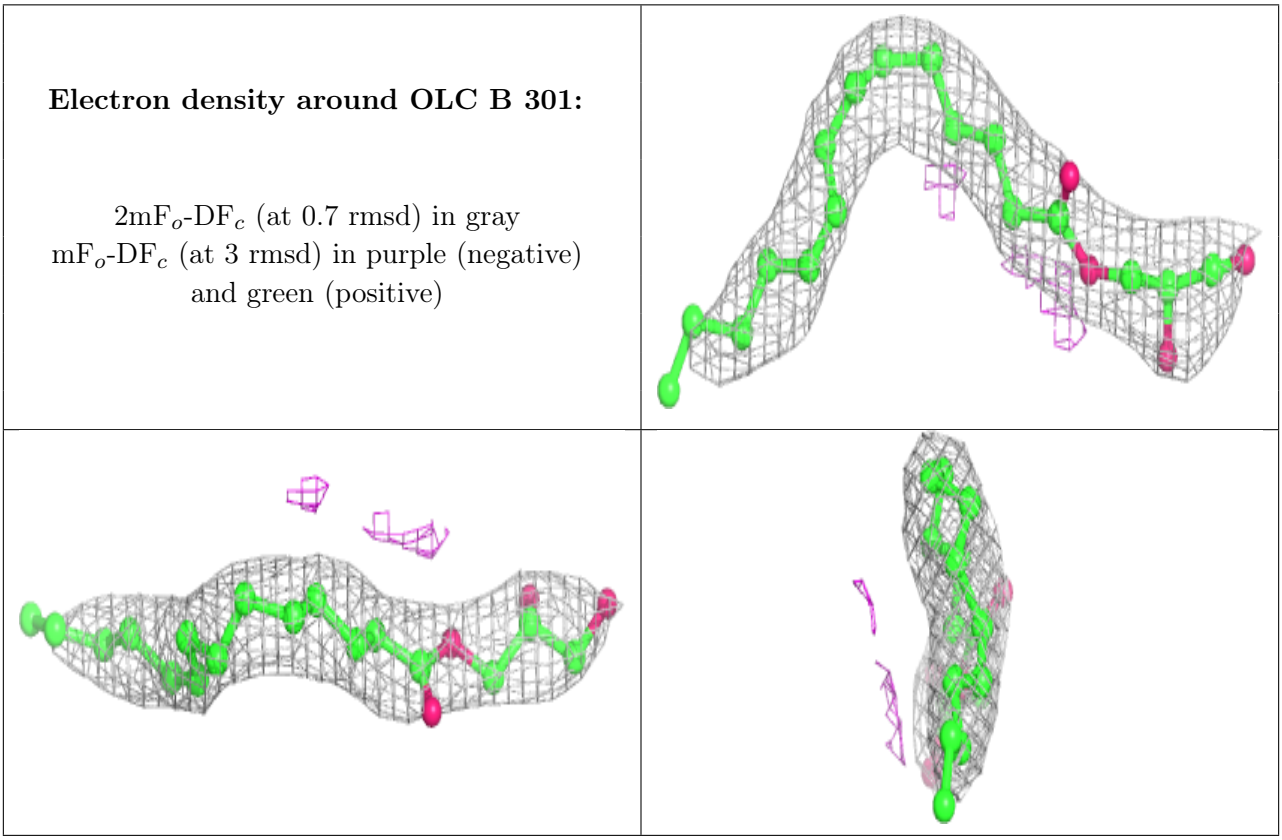
Electron density around OLC E 308:

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



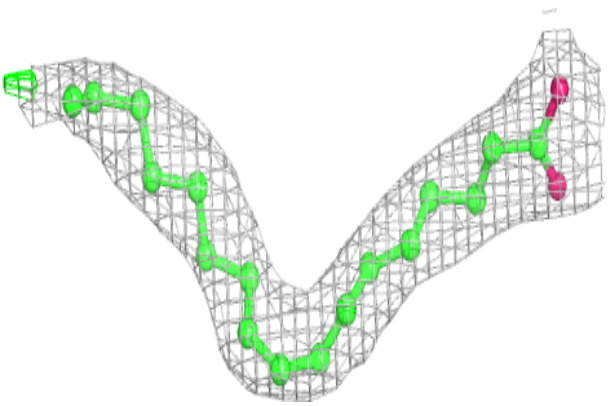
Electron density around OLC B 301:

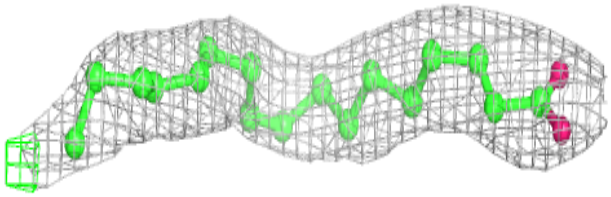
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

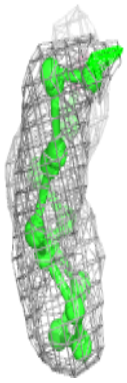


Electron density around OLC E 301:

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

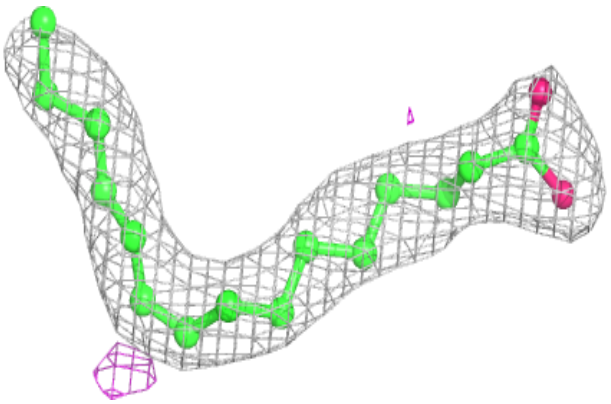


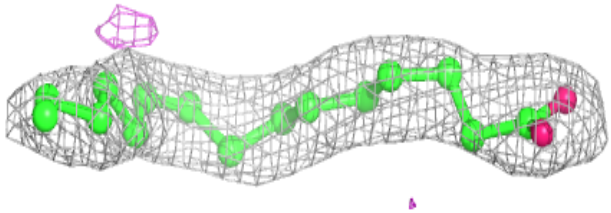


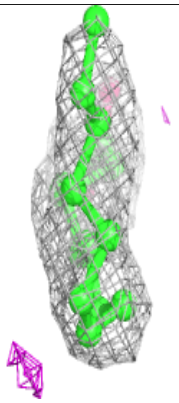


Electron density around OLC A 302:

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

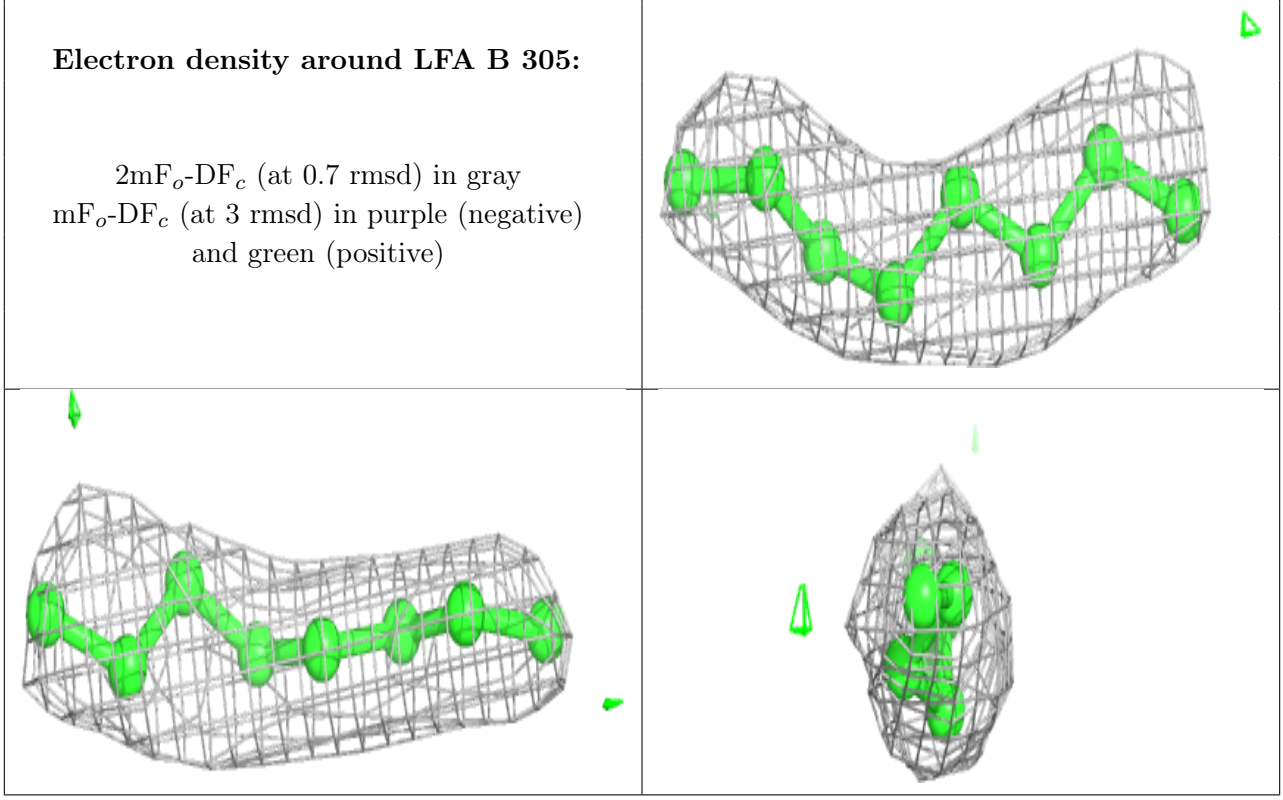






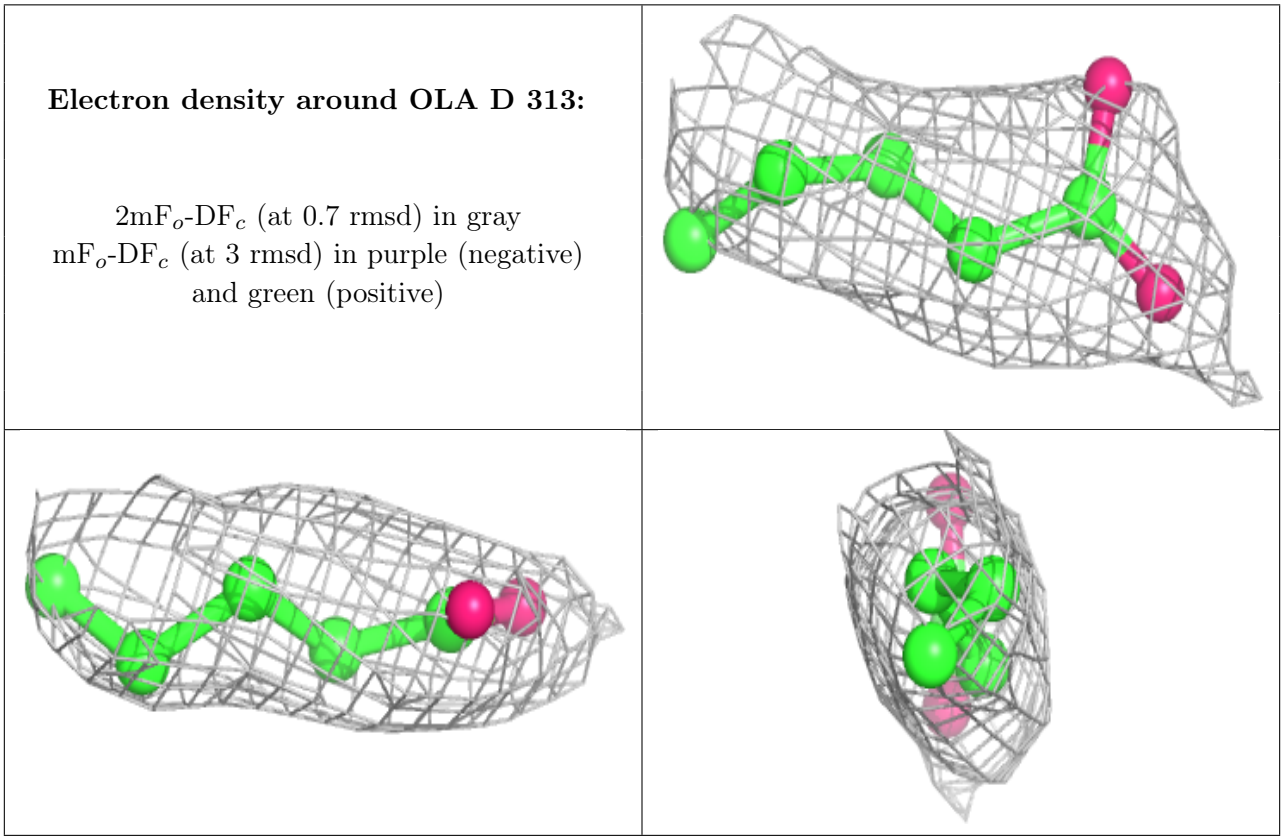
Electron density around LFA B 305:

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



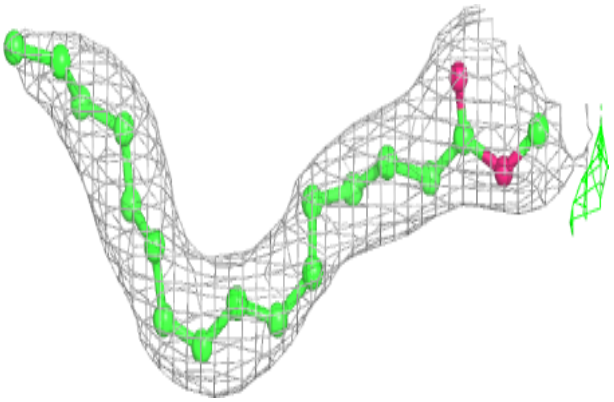
Electron density around OLA D 313:

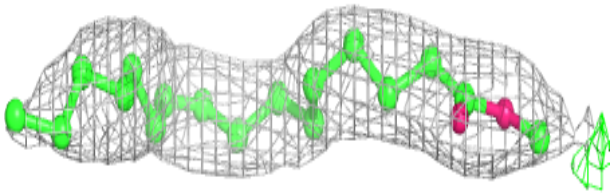
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

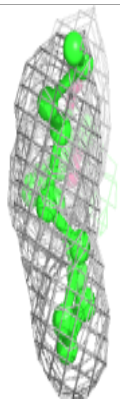


Electron density around OLC C 301:

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

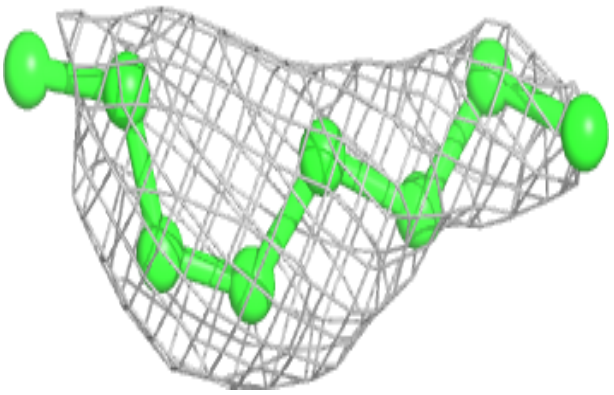


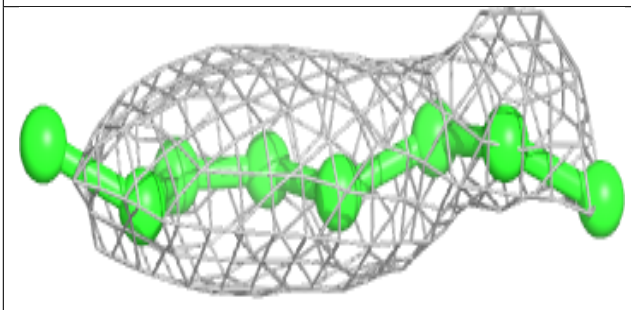


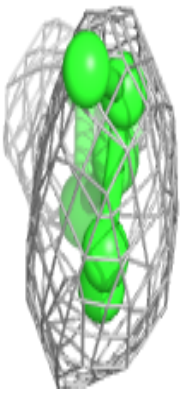


Electron density around OLC C 302:

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

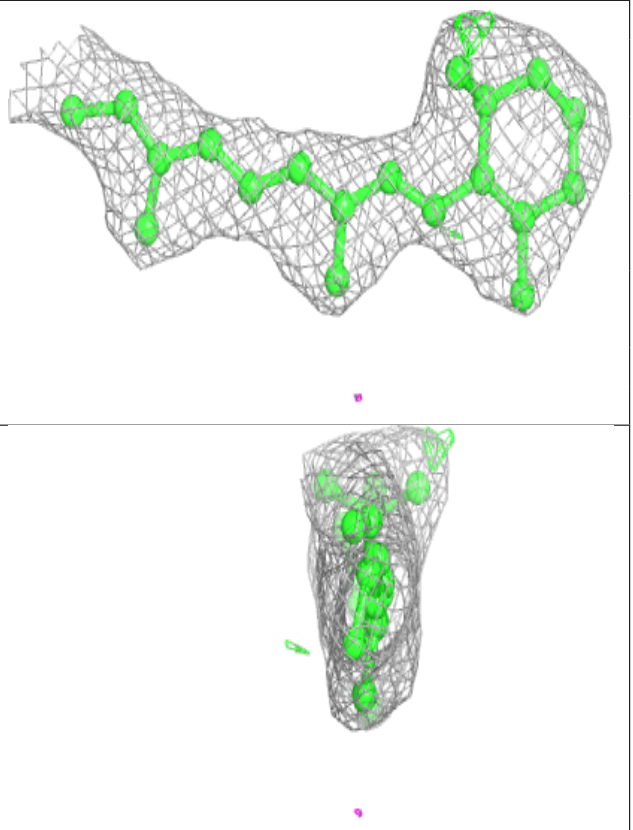






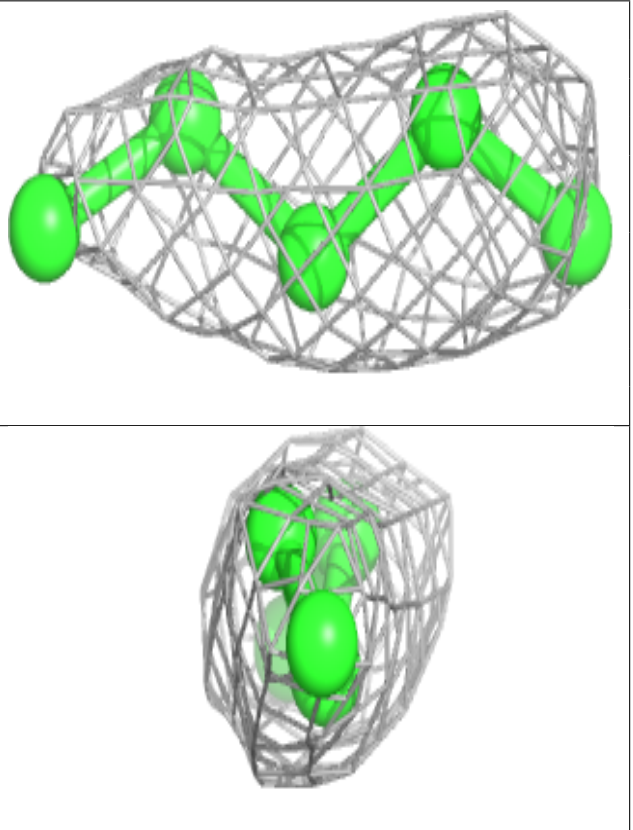
Electron density around RET D 311:

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



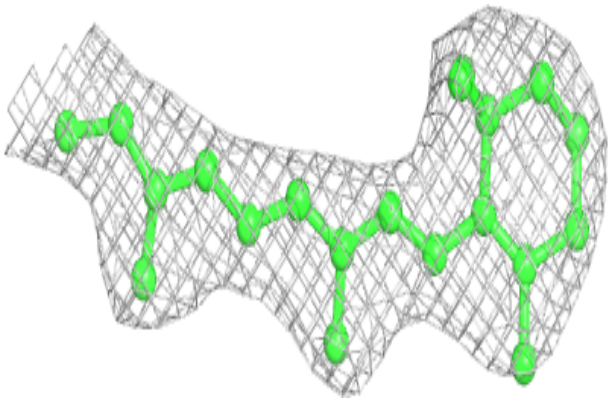
Electron density around OLC D 301:

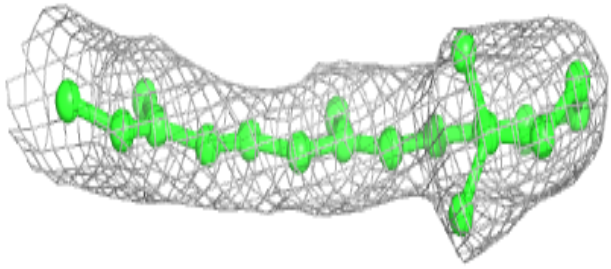
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

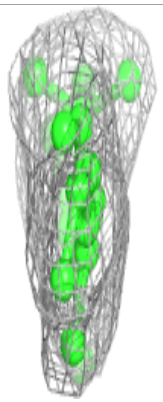


Electron density around RET B 309:

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

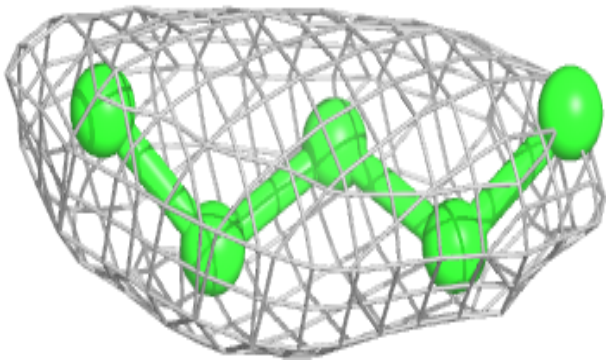


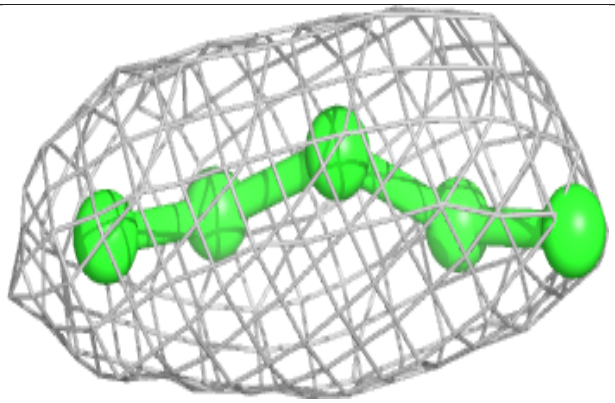


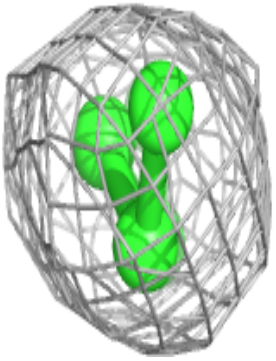


Electron density around OLC B 303:

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

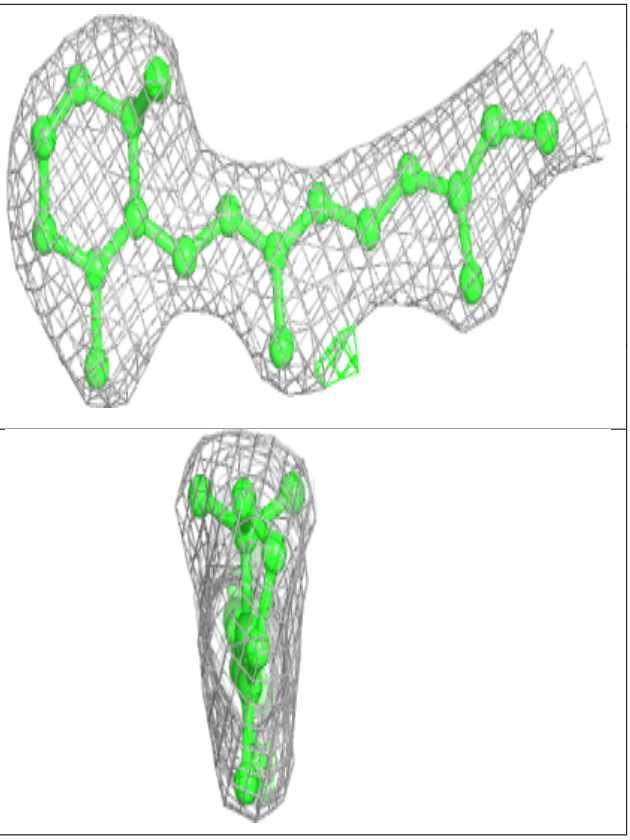






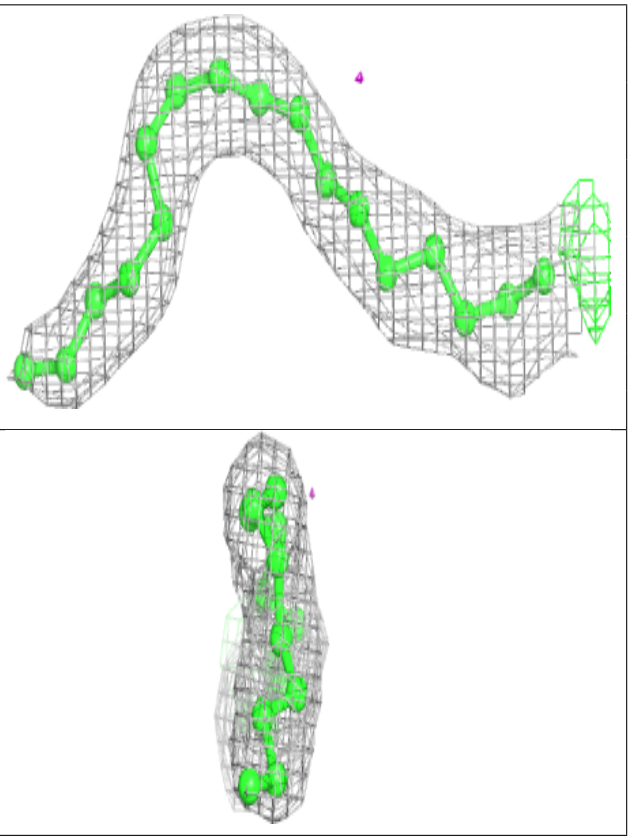
Electron density around RET A 314:

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



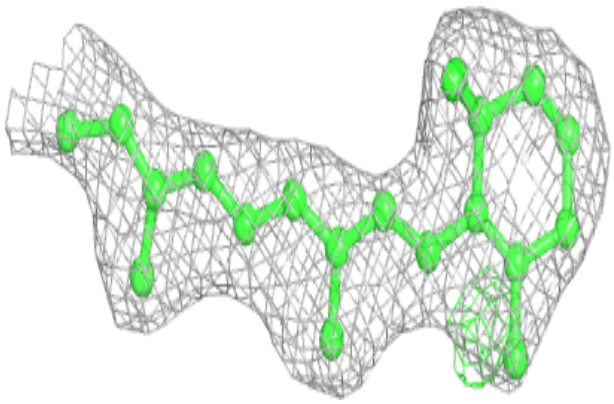
Electron density around LFA D 308:

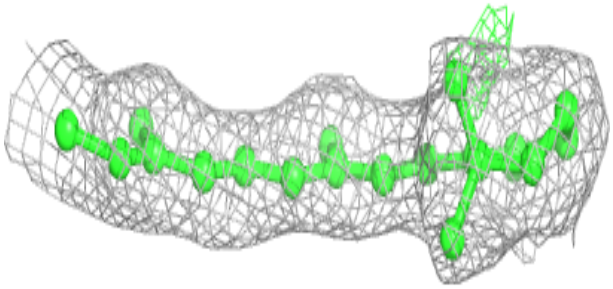
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

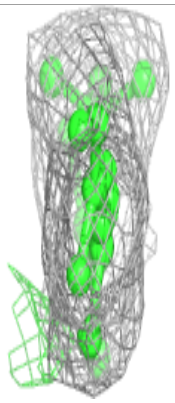


Electron density around RET E 315:

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

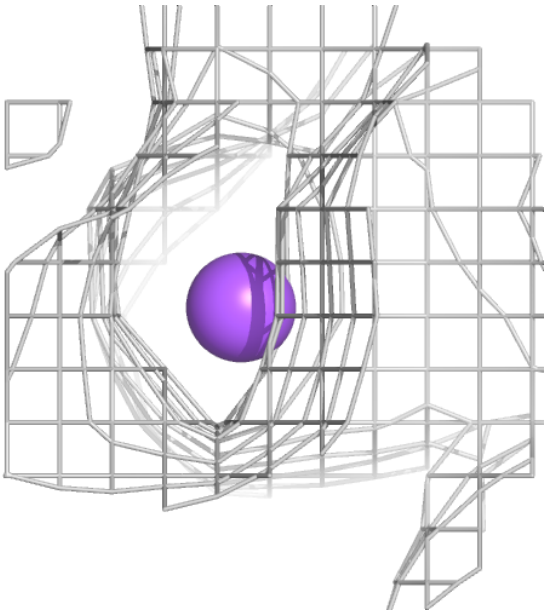


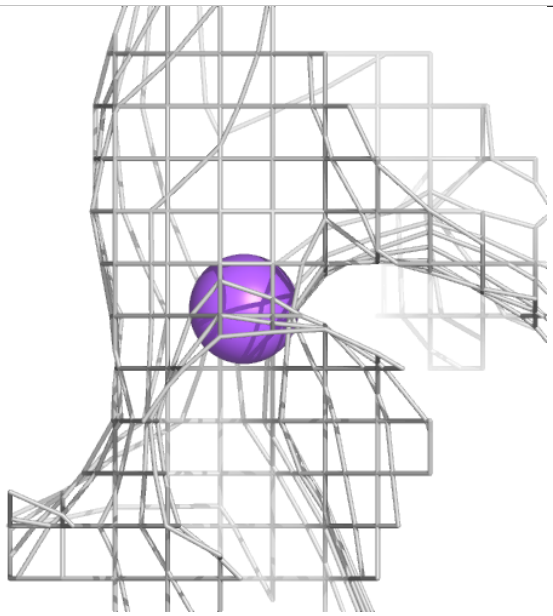


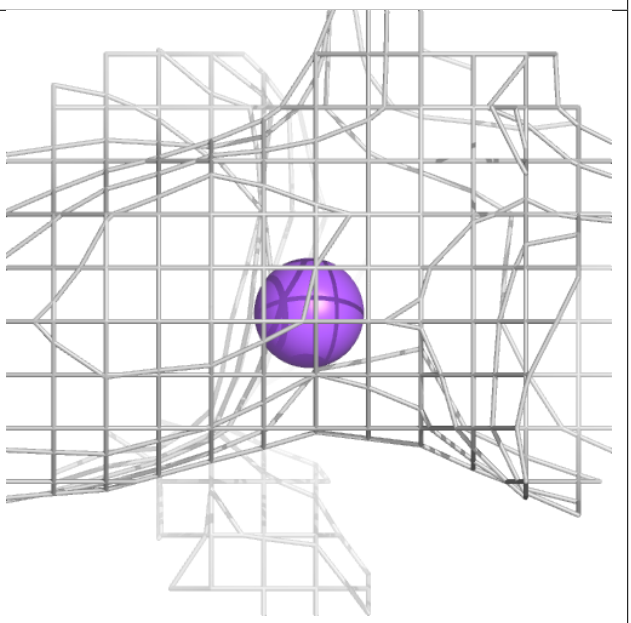


Electron density around NA C 314:

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

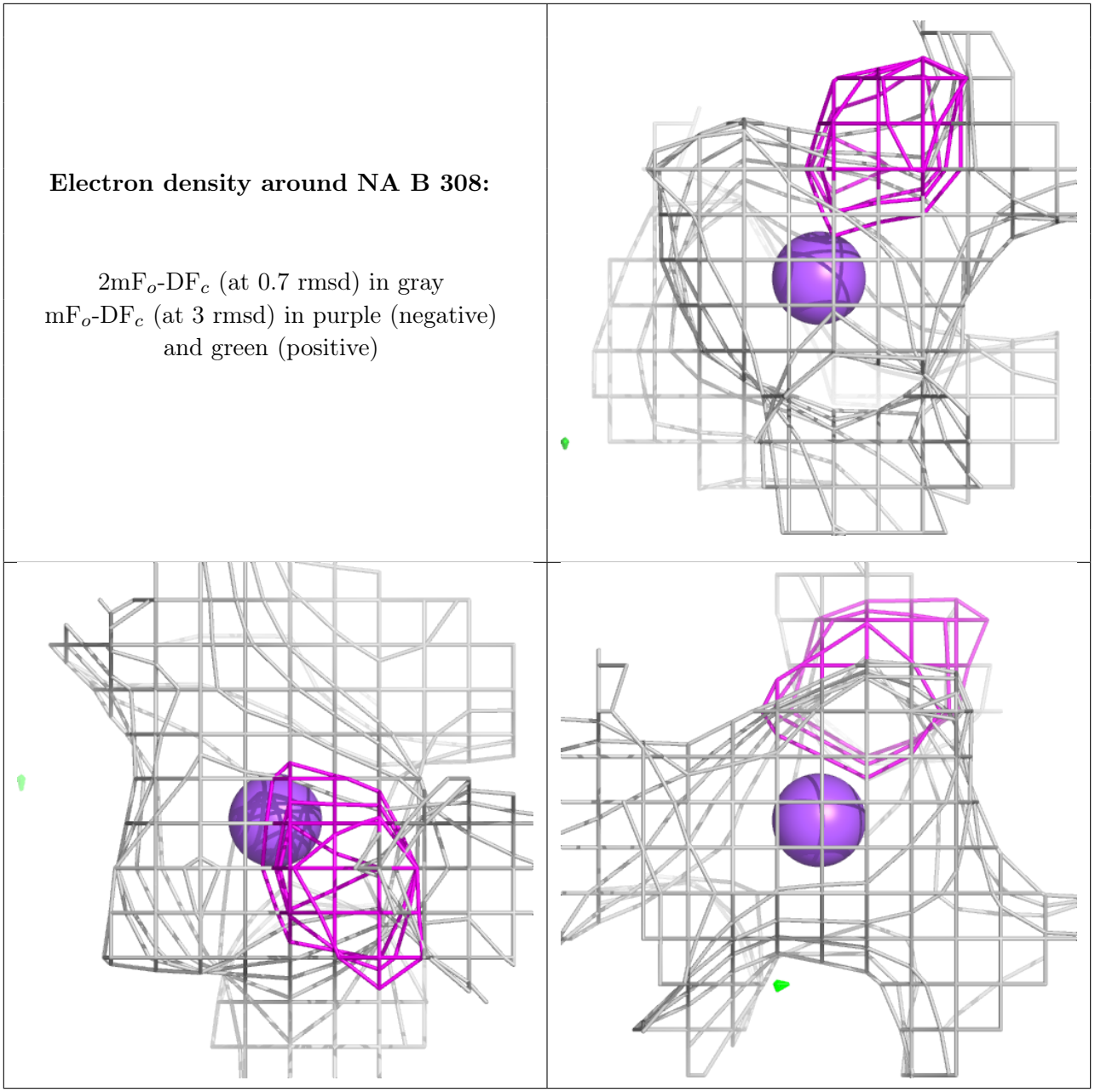






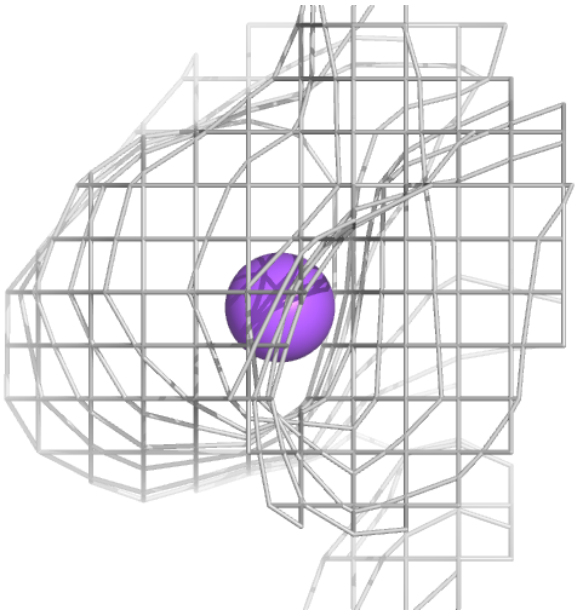
Electron density around NA B 308:

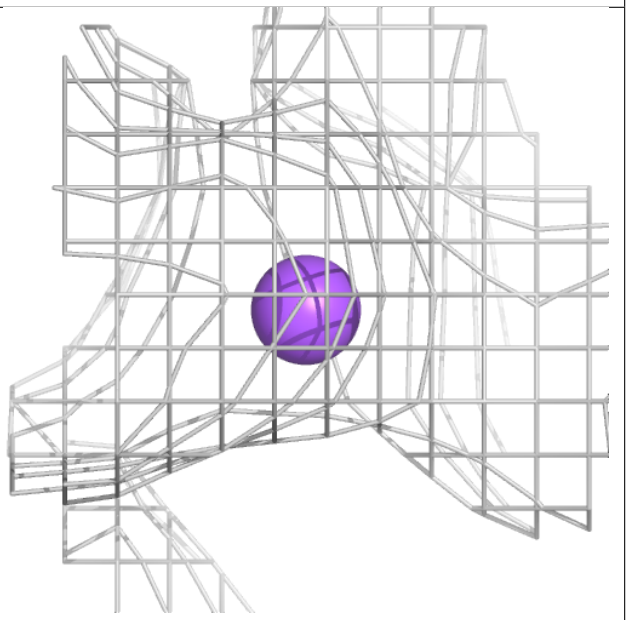
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around NA A 317:

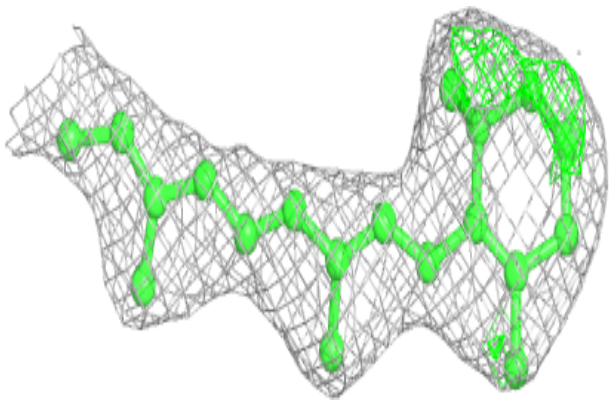
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

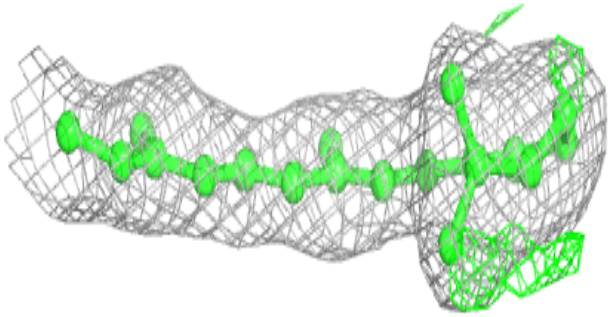


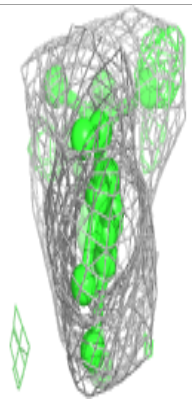


Electron density around RET C 312:

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

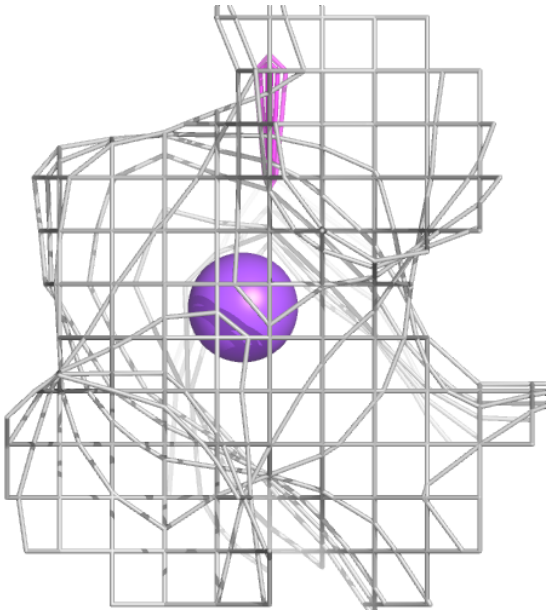


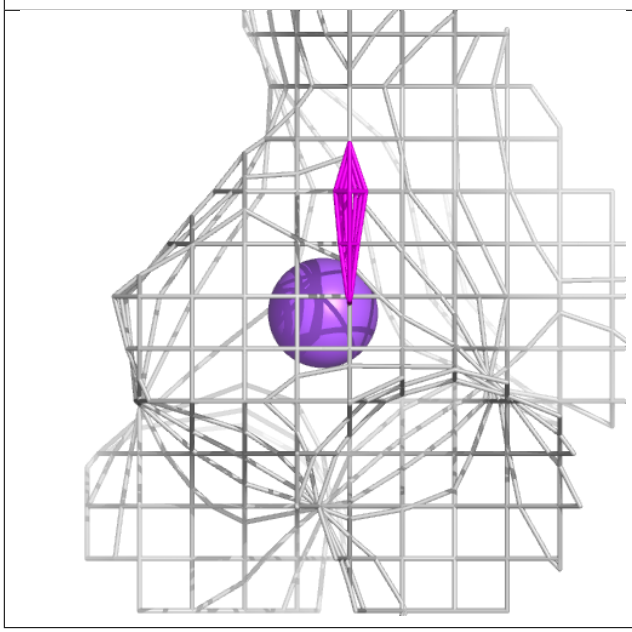


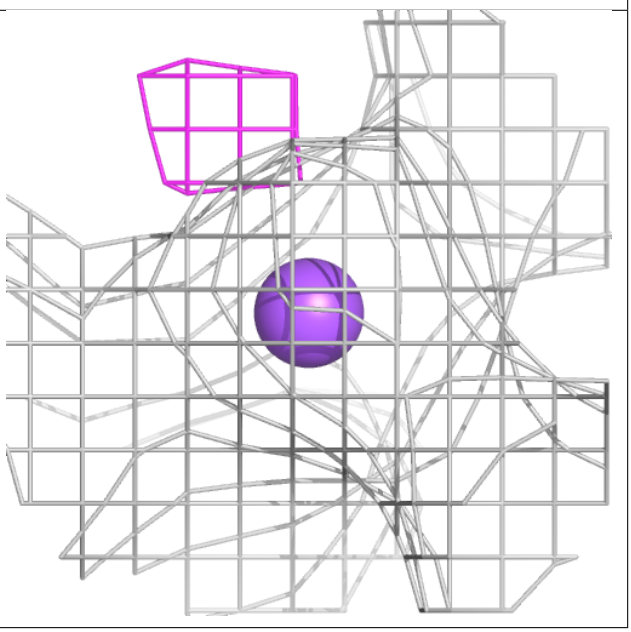


Electron density around NA D 310:

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

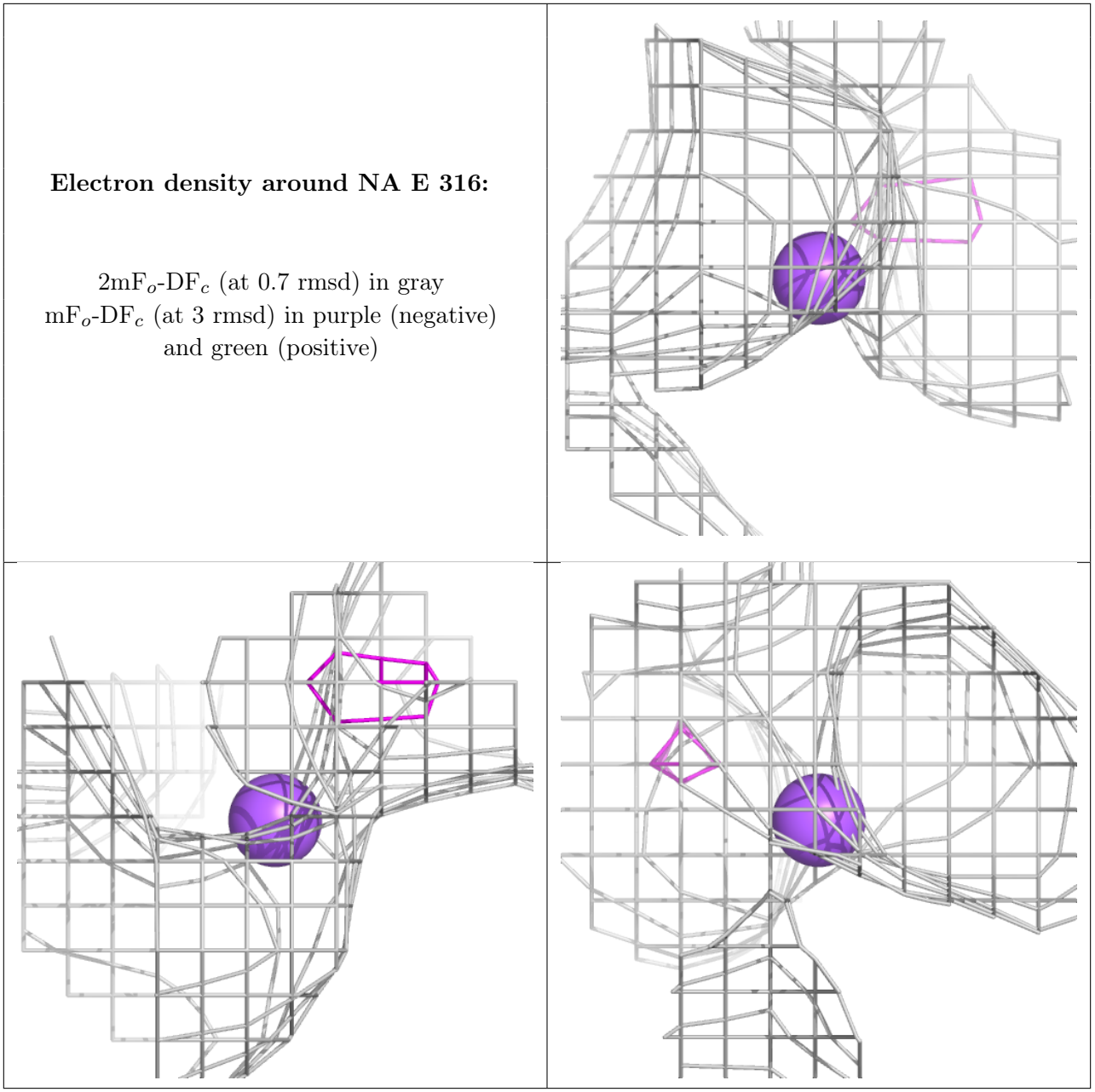






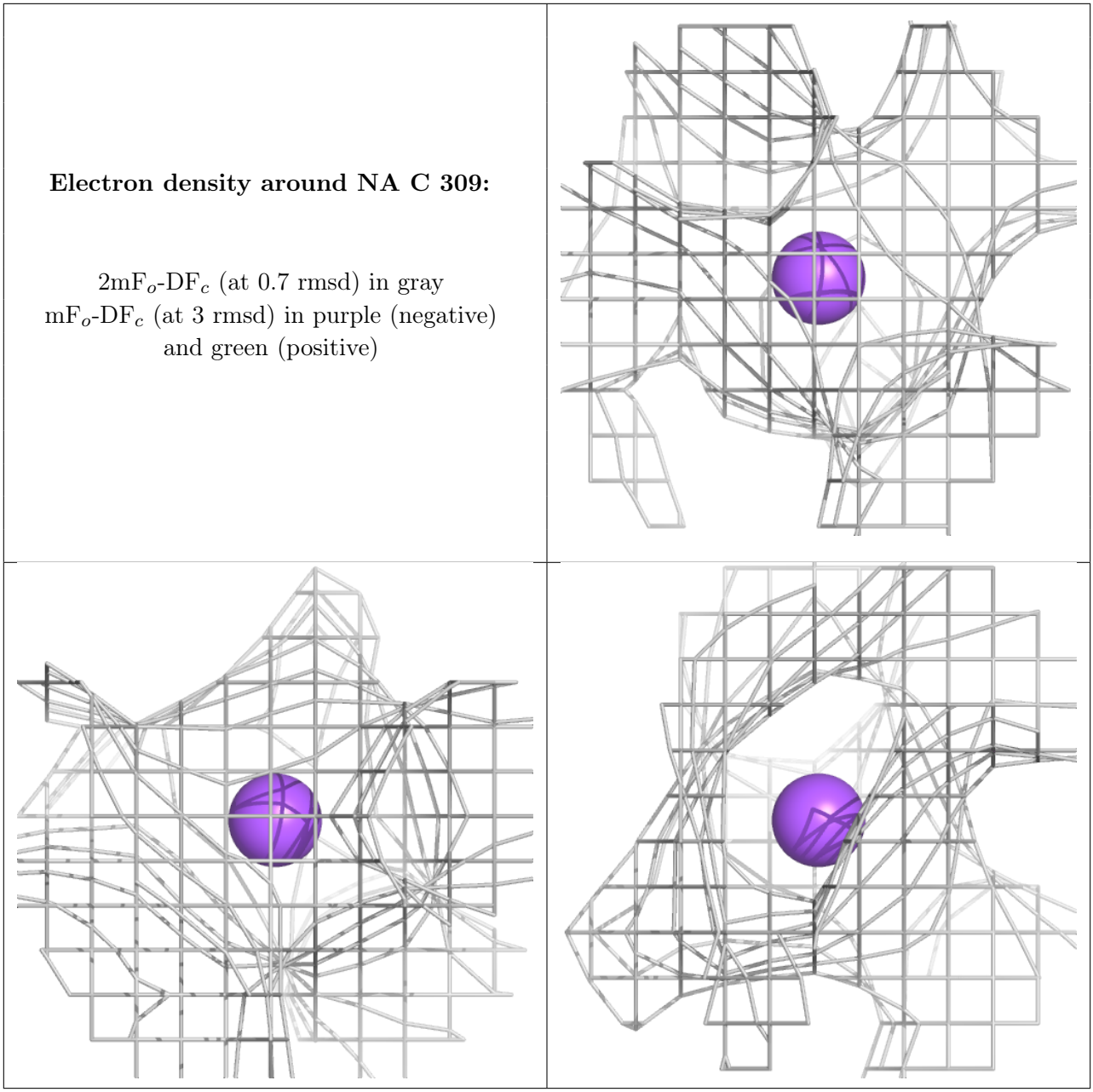
Electron density around NA E 316:

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



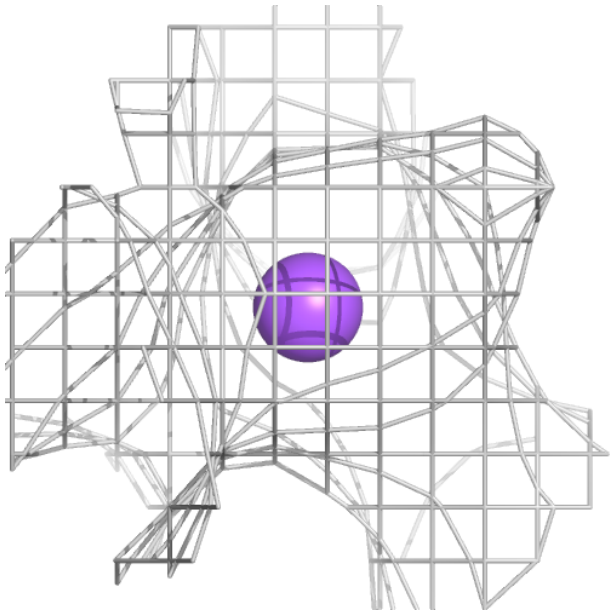
Electron density around NA C 309:

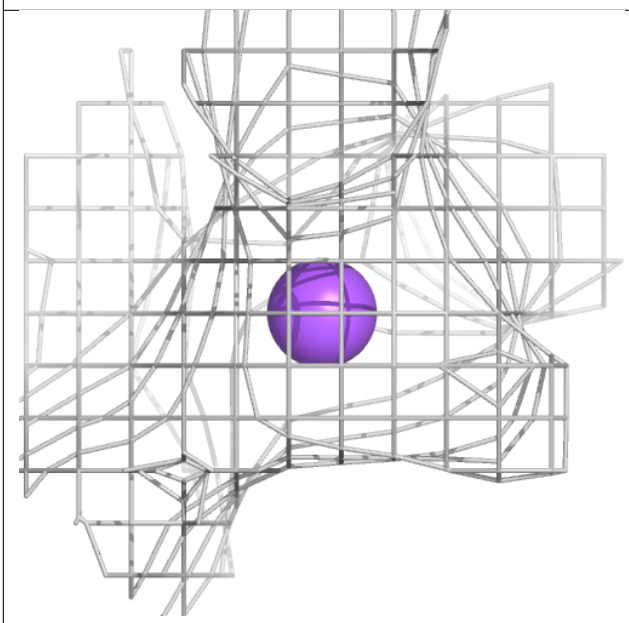
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around NA A 312:

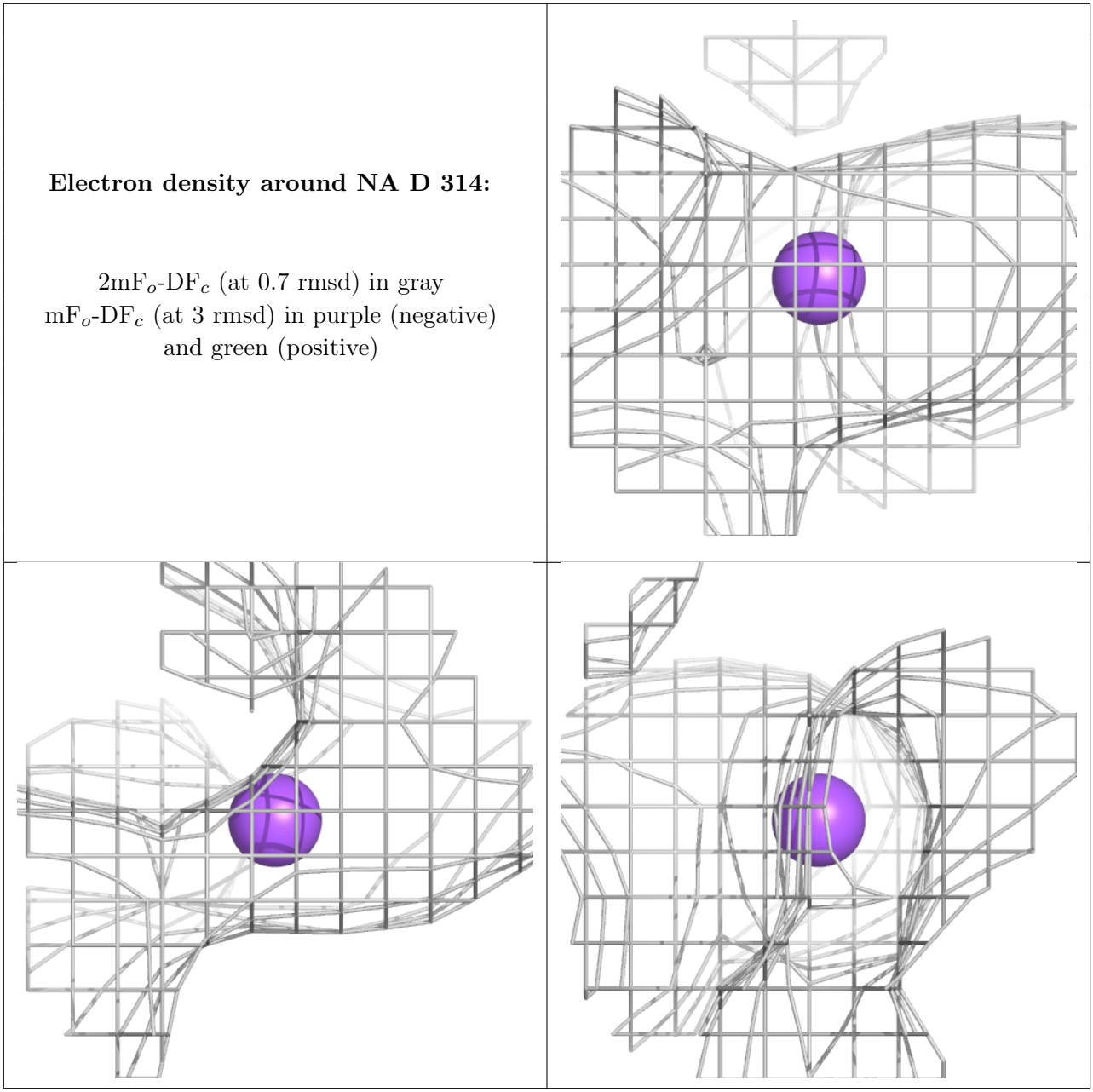
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





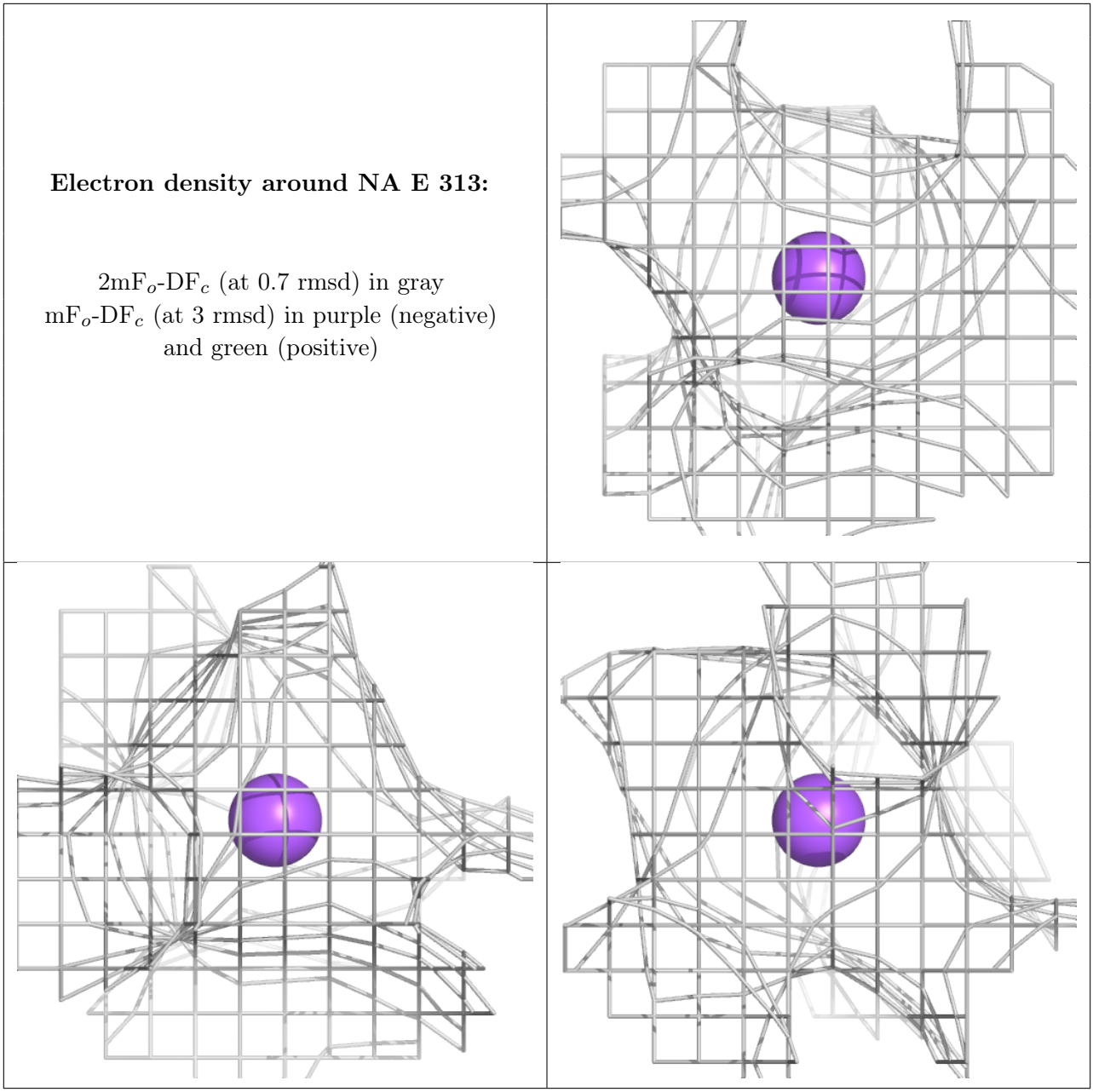
Electron density around NA D 314:

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



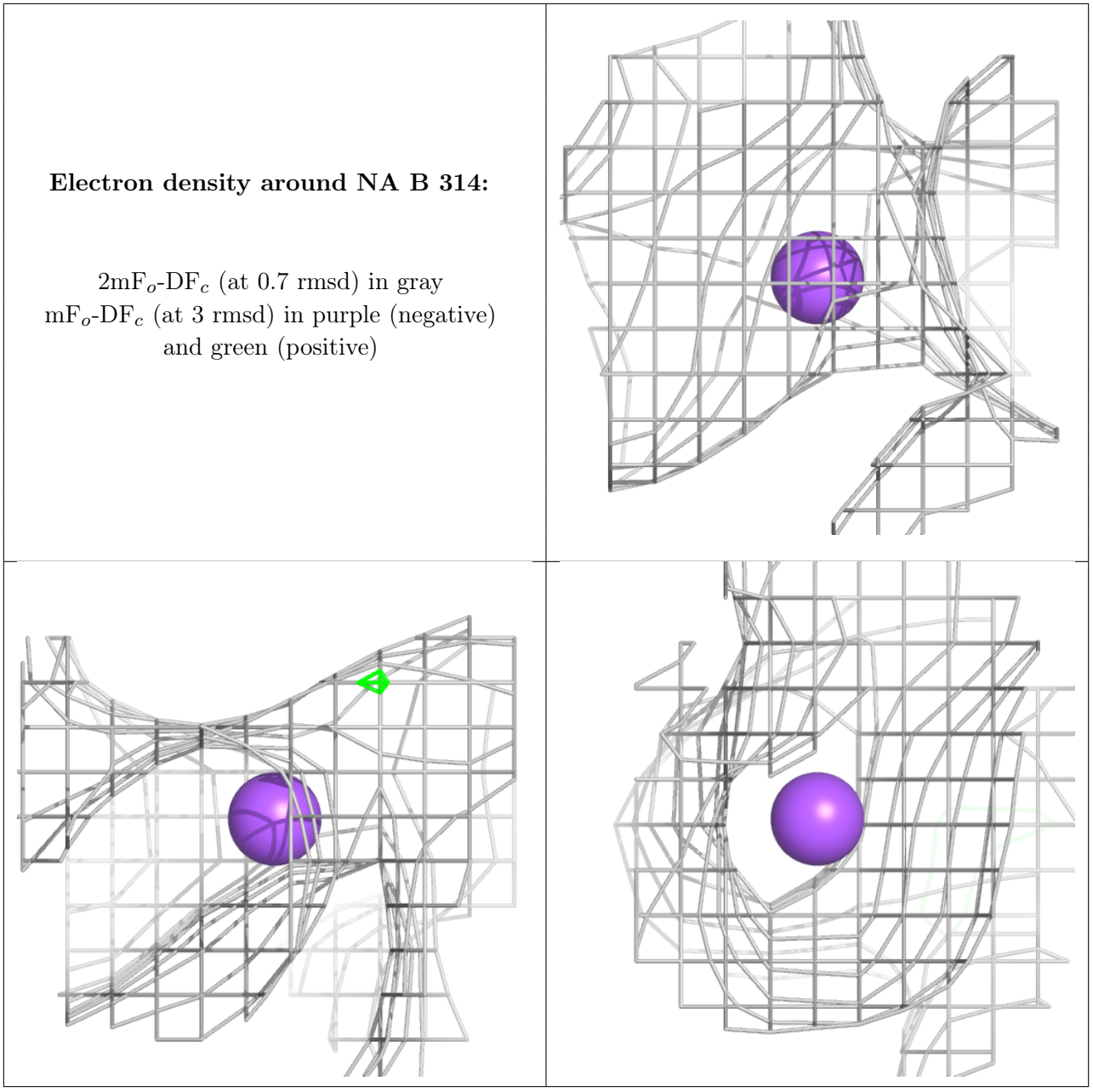
Electron density around NA E 313:

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



Electron density around NA 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)



6.5 Other polymers

There are no such residues in this entry.