wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2026 – 07:43 AM UTC

PDB ID	:	4XTN / pdb_00004xtn
Title	:	Crystal structure of the light-driven sodium pump KR2 in the pentameric red form, pH 4.9
Authors	:	Gushchin, I.; Shevchenko, V.; Polovinkin, V.; Gordeliy, V.
Deposited on	:	2015-01-23
Resolution	:	2.20 Å(reported)

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

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

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

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

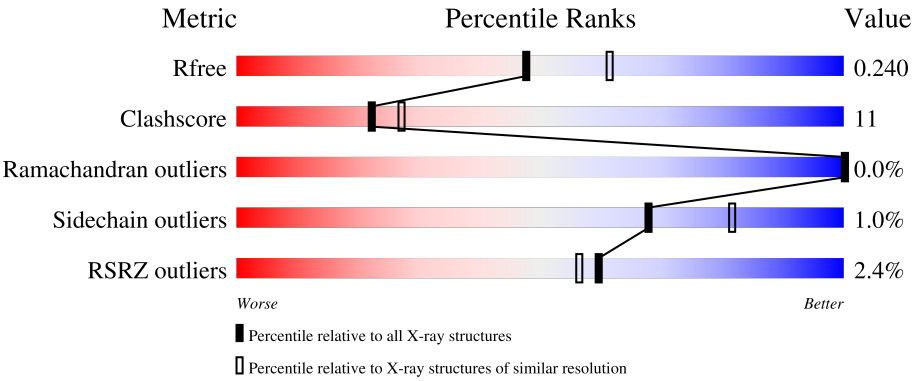
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	288	2% 81% 14% • 5%
1	B	288	5% 73% 20% • 6%
1	C	288	2% 79% 15% 6%
1	D	288	2% 82% 12% 6%
1	E	288	% 77% 16% • 6%

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Mol	Chain	Length	Quality of chain
1	F	288	2% 75% 19% • 6%
1	G	288	% 77% 16% • 6%
1	H	288	2% 78% 15% • 5%
1	I	288	2% 77% 17% • 6%
1	J	288	3% 78% 16% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 23361 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	273	Total	C	N	O	S	0	0	0
			2174	1458	329	378	9			
1	B	270	Total	C	N	O	S	0	1	0
			2158	1449	324	376	9			
1	C	271	Total	C	N	O	S	0	2	0
			2170	1457	326	378	9			
1	D	271	Total	C	N	O	S	0	0	0
			2161	1449	326	377	9			
1	E	272	Total	C	N	O	S	0	0	0
			2166	1451	326	380	9			
1	F	271	Total	C	N	O	S	0	1	0
			2166	1454	326	377	9			
1	G	271	Total	C	N	O	S	0	3	0
			2178	1462	328	379	9			
1	H	273	Total	C	N	O	S	0	1	0
			2186	1464	331	382	9			
1	I	271	Total	C	N	O	S	0	0	0
			2152	1444	322	377	9			
1	J	272	Total	C	N	O	S	0	2	0
			2175	1458	328	380	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	281	LEU	-	expression tag	UNP N0DKS8
A	282	GLU	-	expression tag	UNP N0DKS8
A	283	HIS	-	expression tag	UNP N0DKS8
A	284	HIS	-	expression tag	UNP N0DKS8
A	285	HIS	-	expression tag	UNP N0DKS8
A	286	HIS	-	expression tag	UNP N0DKS8
A	287	HIS	-	expression tag	UNP N0DKS8
A	288	HIS	-	expression tag	UNP N0DKS8
B	281	LEU	-	expression tag	UNP N0DKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	282	GLU	-	expression tag	UNP N0DKS8
B	283	HIS	-	expression tag	UNP N0DKS8
B	284	HIS	-	expression tag	UNP N0DKS8
B	285	HIS	-	expression tag	UNP N0DKS8
B	286	HIS	-	expression tag	UNP N0DKS8
B	287	HIS	-	expression tag	UNP N0DKS8
B	288	HIS	-	expression tag	UNP N0DKS8
C	281	LEU	-	expression tag	UNP N0DKS8
C	282	GLU	-	expression tag	UNP N0DKS8
C	283	HIS	-	expression tag	UNP N0DKS8
C	284	HIS	-	expression tag	UNP N0DKS8
C	285	HIS	-	expression tag	UNP N0DKS8
C	286	HIS	-	expression tag	UNP N0DKS8
C	287	HIS	-	expression tag	UNP N0DKS8
C	288	HIS	-	expression tag	UNP N0DKS8
D	281	LEU	-	expression tag	UNP N0DKS8
D	282	GLU	-	expression tag	UNP N0DKS8
D	283	HIS	-	expression tag	UNP N0DKS8
D	284	HIS	-	expression tag	UNP N0DKS8
D	285	HIS	-	expression tag	UNP N0DKS8
D	286	HIS	-	expression tag	UNP N0DKS8
D	287	HIS	-	expression tag	UNP N0DKS8
D	288	HIS	-	expression tag	UNP N0DKS8
E	281	LEU	-	expression tag	UNP N0DKS8
E	282	GLU	-	expression tag	UNP N0DKS8
E	283	HIS	-	expression tag	UNP N0DKS8
E	284	HIS	-	expression tag	UNP N0DKS8
E	285	HIS	-	expression tag	UNP N0DKS8
E	286	HIS	-	expression tag	UNP N0DKS8
E	287	HIS	-	expression tag	UNP N0DKS8
E	288	HIS	-	expression tag	UNP N0DKS8
F	281	LEU	-	expression tag	UNP N0DKS8
F	282	GLU	-	expression tag	UNP N0DKS8
F	283	HIS	-	expression tag	UNP N0DKS8
F	284	HIS	-	expression tag	UNP N0DKS8
F	285	HIS	-	expression tag	UNP N0DKS8
F	286	HIS	-	expression tag	UNP N0DKS8
F	287	HIS	-	expression tag	UNP N0DKS8
F	288	HIS	-	expression tag	UNP N0DKS8
G	281	LEU	-	expression tag	UNP N0DKS8
G	282	GLU	-	expression tag	UNP N0DKS8
G	283	HIS	-	expression tag	UNP N0DKS8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	284	HIS	-	expression tag	UNP N0DKS8
G	285	HIS	-	expression tag	UNP N0DKS8
G	286	HIS	-	expression tag	UNP N0DKS8
G	287	HIS	-	expression tag	UNP N0DKS8
G	288	HIS	-	expression tag	UNP N0DKS8
H	281	LEU	-	expression tag	UNP N0DKS8
H	282	GLU	-	expression tag	UNP N0DKS8
H	283	HIS	-	expression tag	UNP N0DKS8
H	284	HIS	-	expression tag	UNP N0DKS8
H	285	HIS	-	expression tag	UNP N0DKS8
H	286	HIS	-	expression tag	UNP N0DKS8
H	287	HIS	-	expression tag	UNP N0DKS8
H	288	HIS	-	expression tag	UNP N0DKS8
I	281	LEU	-	expression tag	UNP N0DKS8
I	282	GLU	-	expression tag	UNP N0DKS8
I	283	HIS	-	expression tag	UNP N0DKS8
I	284	HIS	-	expression tag	UNP N0DKS8
I	285	HIS	-	expression tag	UNP N0DKS8
I	286	HIS	-	expression tag	UNP N0DKS8
I	287	HIS	-	expression tag	UNP N0DKS8
I	288	HIS	-	expression tag	UNP N0DKS8
J	281	LEU	-	expression tag	UNP N0DKS8
J	282	GLU	-	expression tag	UNP N0DKS8
J	283	HIS	-	expression tag	UNP N0DKS8
J	284	HIS	-	expression tag	UNP N0DKS8
J	285	HIS	-	expression tag	UNP N0DKS8
J	286	HIS	-	expression tag	UNP N0DKS8
J	287	HIS	-	expression tag	UNP N0DKS8
J	288	HIS	-	expression tag	UNP N0DKS8

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0

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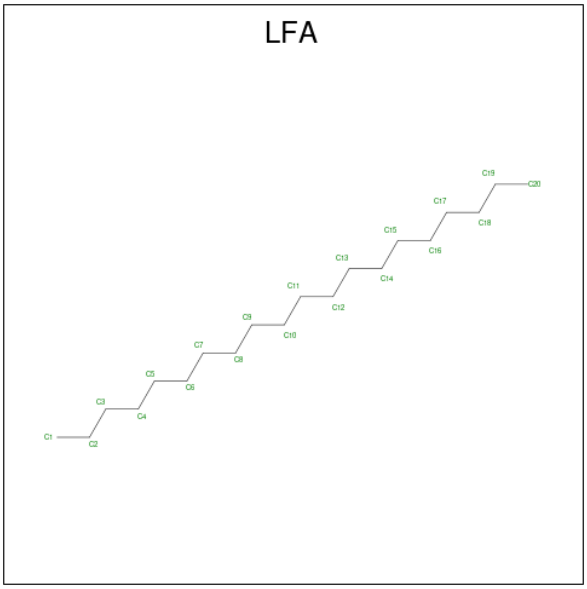
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total Na 1 1	0	0
2	G	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0
2	I	1	Total Na 1 1	0	0
2	J	1	Total Na 1 1	0	0

- Molecule 3 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 14 14	0	0
3	A	1	Total C 6 6	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 10 10	0	0
3	A	1	Total C 14 14	0	0
3	A	1	Total C 18 18	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 8 8	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 7 7	0	0
3	A	1	Total C 5 5	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C 7 7	0	0
3	B	1	Total C 14 14	0	0
3	B	1	Total C 6 6	0	0
3	B	1	Total C 8 8	0	0
3	B	1	Total C 16 16	0	0
3	B	1	Total C 18 18	0	0
3	B	1	Total C 13 13	0	0
3	B	1	Total C 11 11	0	0
3	B	1	Total C 8 8	0	0
3	C	1	Total C 7 7	0	0
3	C	1	Total C 10 10	0	0
3	C	1	Total C 6 6	0	0
3	C	1	Total C 10 10	0	0
3	C	1	Total C 16 16	0	0
3	C	1	Total C 18 18	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C 10 10	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 13 13	0	0
3	C	1	Total C 8 8	0	0
3	C	1	Total C 4 4	0	0
3	D	1	Total C 7 7	0	0
3	D	1	Total C 14 14	0	0
3	D	1	Total C 6 6	0	0
3	D	1	Total C 10 10	0	0
3	D	1	Total C 16 16	0	0
3	D	1	Total C 18 18	0	0
3	D	1	Total C 10 10	0	0
3	D	1	Total C 8 8	0	0
3	D	1	Total C 8 8	0	0
3	D	1	Total C 7 7	0	0
3	D	1	Total C 6 6	0	0
3	D	1	Total C 6 6	0	0
3	D	1	Total C 7 7	0	0
3	D	1	Total C 5 5	0	0
3	D	1	Total C 5 5	0	0
3	D	1	Total C 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C 14 14	0	0
3	E	1	Total C 18 18	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 6 6	0	0
3	E	1	Total C 12 12	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 6 6	0	0
3	E	1	Total C 10 10	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C 8 8	0	0
3	F	1	Total C 7 7	0	0
3	F	1	Total C 14 14	0	0
3	F	1	Total C 10 10	0	0
3	F	1	Total C 6 6	0	0
3	F	1	Total C 10 10	0	0
3	F	1	Total C 6 6	0	0
3	F	1	Total C 8 8	0	0
3	F	1	Total C 10 10	0	0
3	F	1	Total C 18 18	0	0
3	F	1	Total C 10 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C 8 8	0	0
3	F	1	Total C 14 14	0	0
3	F	1	Total C 8 8	0	0
3	G	1	Total C 16 16	0	0
3	G	1	Total C 7 7	0	0
3	G	1	Total C 14 14	0	0
3	G	1	Total C 6 6	0	0
3	G	1	Total C 10 10	0	0
3	G	1	Total C 16 16	0	0
3	G	1	Total C 18 18	0	0
3	G	1	Total C 8 8	0	0
3	G	1	Total C 10 10	0	0
3	G	1	Total C 8 8	0	0
3	G	1	Total C 8 8	0	0
3	G	1	Total C 6 6	0	0
3	G	1	Total C 6 6	0	0
3	H	1	Total C 13 13	0	0
3	H	1	Total C 6 6	0	0
3	H	1	Total C 10 10	0	0
3	H	1	Total C 16 16	0	0
3	H	1	Total C 18 18	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C 14 14	0	0
3	H	1	Total C 8 8	0	0
3	H	1	Total C 5 5	0	0
3	H	1	Total C 8 8	0	0
3	H	1	Total C 7 7	0	0
3	H	1	Total C 6 6	0	0
3	I	1	Total C 7 7	0	0
3	I	1	Total C 7 7	0	0
3	I	1	Total C 14 14	0	0
3	I	1	Total C 6 6	0	0
3	I	1	Total C 10 10	0	0
3	I	1	Total C 6 6	0	0
3	I	1	Total C 16 16	0	0
3	I	1	Total C 18 18	0	0
3	I	1	Total C 14 14	0	0
3	I	1	Total C 8 8	0	0
3	I	1	Total C 7 7	0	0
3	I	1	Total C 4 4	0	0
3	J	1	Total C 16 16	0	0
3	J	1	Total C 18 18	0	0
3	J	1	Total C 8 8	0	0

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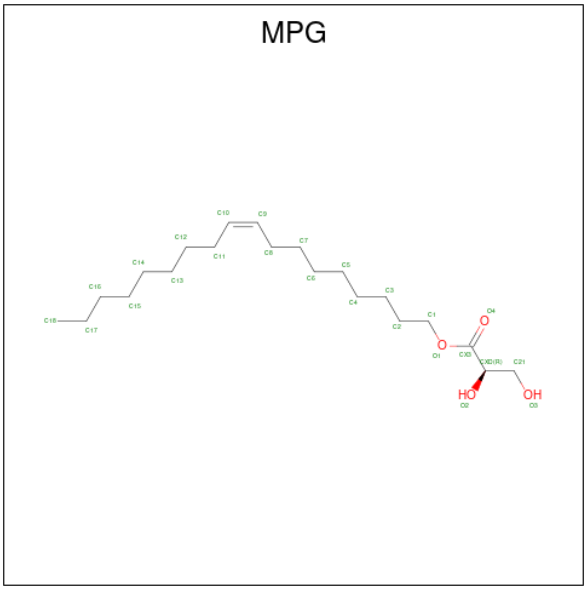
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total C 14 14	0	0
3	J	1	Total C 8 8	0	0
3	J	1	Total C 7 7	0	0
3	J	1	Total C 14 14	0	0
3	J	1	Total C 10 10	0	0
3	J	1	Total C 10 10	0	0
3	J	1	Total C 4 4	0	0

- Molecule 4 is [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (CCD ID: MPG) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 14 11 3	0	0
4	B	1	Total C O 14 11 3	0	0
4	C	1	Total C O 13 10 3	0	0
4	D	1	Total C O 14 11 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 14 11 3	0	0
4	F	1	Total C O 14 11 3	0	0
4	G	1	Total C O 14 11 3	0	0
4	H	1	Total C O 14 11 3	0	0
4	I	1	Total C O 14 11 3	0	0
4	J	1	Total C O 14 11 3	0	0

- Molecule 5 is water.

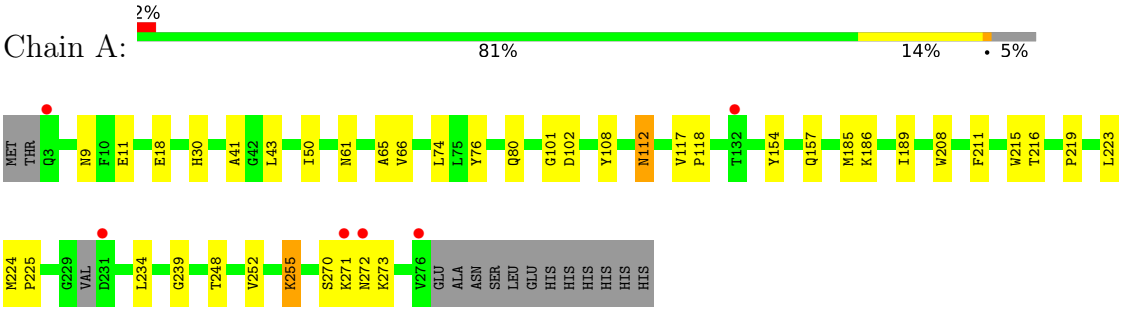
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	39	Total O 39 39	0	0
5	B	30	Total O 30 30	0	0
5	C	31	Total O 31 31	0	0
5	D	34	Total O 34 34	0	0
5	E	30	Total O 30 30	0	0
5	F	30	Total O 30 30	0	0
5	G	35	Total O 35 35	0	0
5	H	45	Total O 45 45	0	0
5	I	40	Total O 40 40	0	0
5	J	37	Total O 37 37	0	0

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.

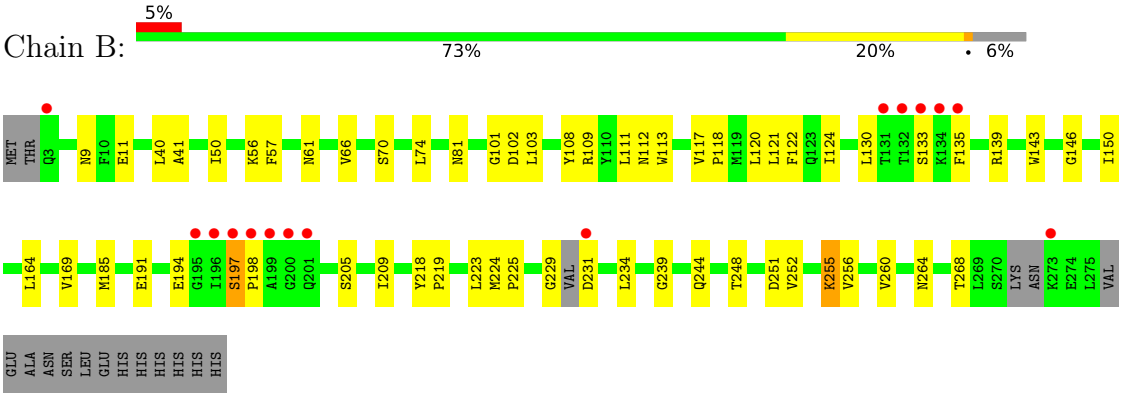
• Molecule 1: Sodium pumping rhodopsin

Chain A:



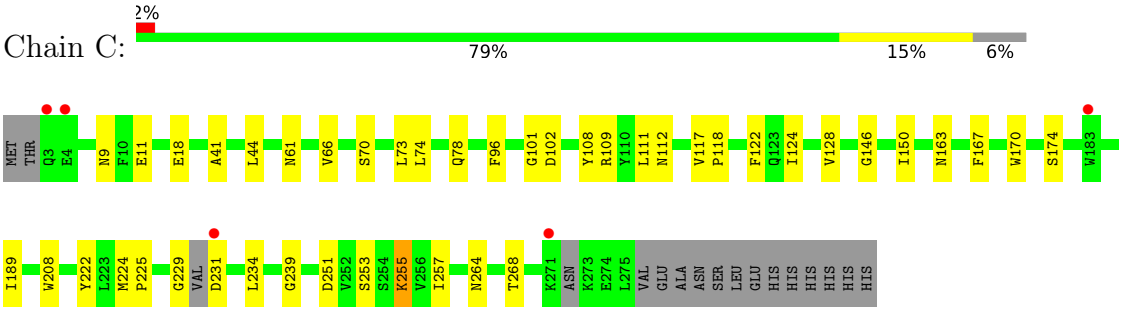
• Molecule 1: Sodium pumping rhodopsin

Chain B:



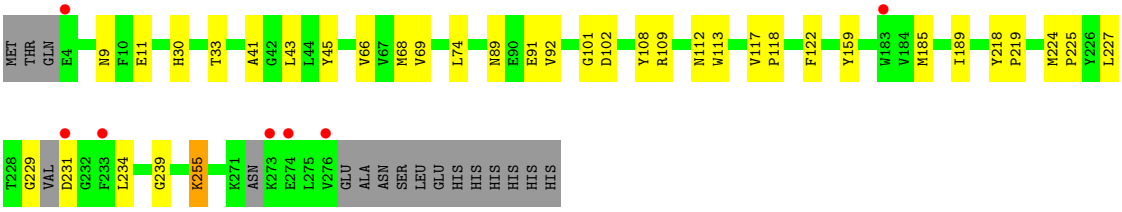
• Molecule 1: Sodium pumping rhodopsin

Chain C:



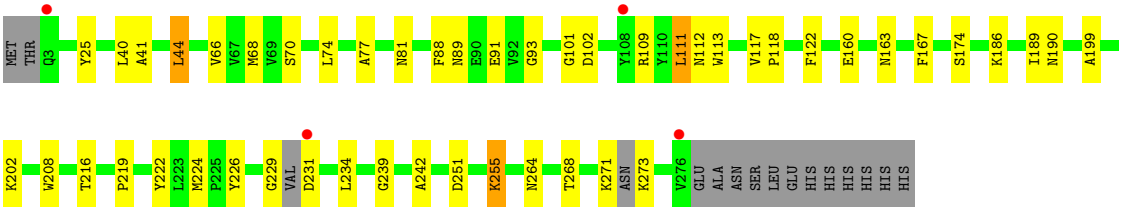
• Molecule 1: Sodium pumping rhodopsin

Chain D:



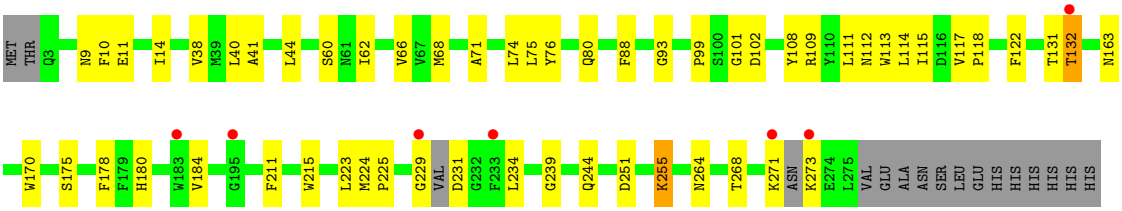
• Molecule 1: Sodium pumping rhodopsin

Chain E:



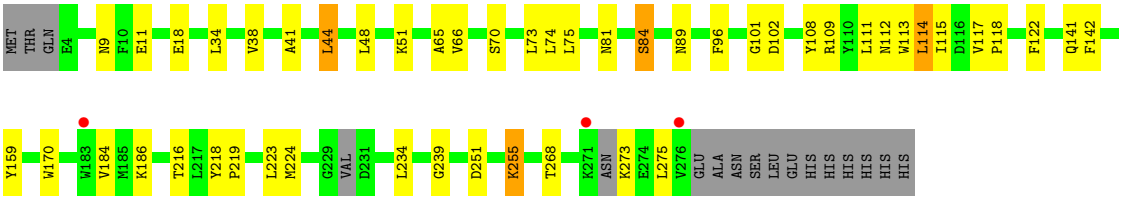
• Molecule 1: Sodium pumping rhodopsin

Chain F:



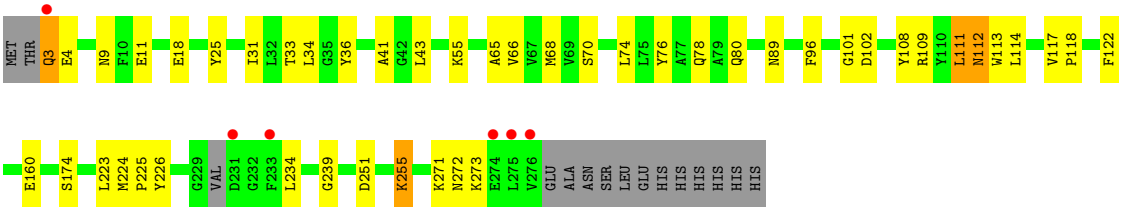
• Molecule 1: Sodium pumping rhodopsin

Chain G:



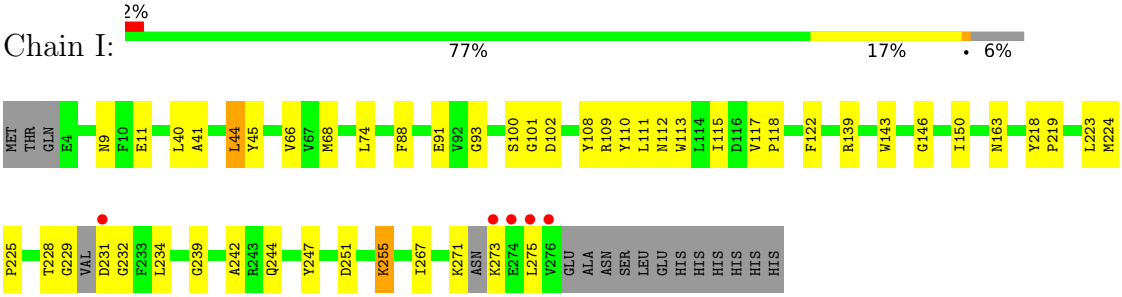
• Molecule 1: Sodium pumping rhodopsin

Chain H:



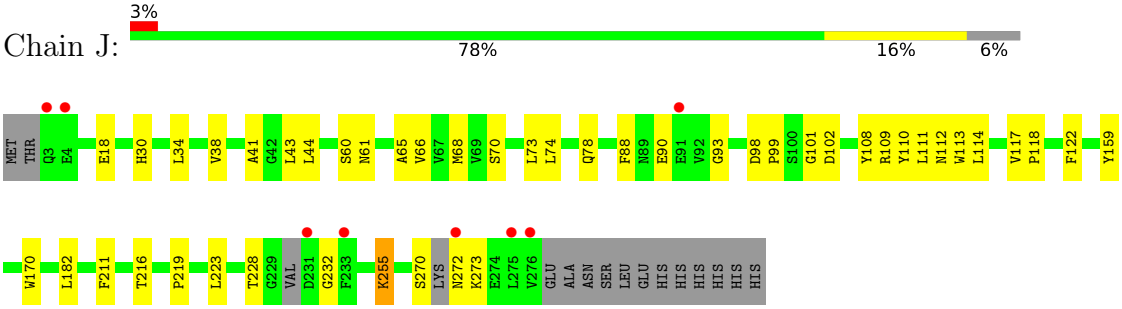
• Molecule 1: Sodium pumping rhodopsin

Chain I:



• Molecule 1: Sodium pumping rhodopsin

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.69Å 107.00Å 240.80Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	48.90 – 2.20 48.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.90-2.20) 96.2 (48.90-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.195 , 0.236 0.203 , 0.240	Depositor DCC
R_{free} test set	9797 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23361	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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: NA, LYR, MPG, LFA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.39	0/2201	0.67	0/2990
1	B	0.36	0/2187	0.67	0/2972
1	C	0.39	0/2202	0.67	0/2992
1	D	0.40	0/2187	0.67	0/2970
1	E	0.39	0/2191	0.70	0/2976
1	F	0.39	0/2195	0.65	0/2982
1	G	0.38	0/2213	0.69	0/3007
1	H	0.40	0/2215	0.66	0/3008
1	I	0.40	0/2178	0.67	0/2963
1	J	0.40	0/2207	0.68	0/3000
All	All	0.39	0/21976	0.67	0/29860

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	2174	0	2164	34	0
1	B	2158	0	2144	58	0
1	C	2170	0	2156	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2161	0	2145	35	0
1	E	2166	0	2140	68	0
1	F	2166	0	2155	62	0
1	G	2178	0	2174	58	0
1	H	2186	0	2177	54	0
1	I	2152	0	2117	54	0
1	J	2175	0	2156	50	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	108	0	199	3	0
3	B	108	0	200	3	0
3	C	110	0	206	6	0
3	D	138	0	260	10	0
3	E	112	0	204	9	0
3	F	129	0	245	7	0
3	G	133	0	250	5	0
3	H	111	0	208	2	0
3	I	117	0	219	7	0
3	J	109	0	205	5	0
4	A	14	0	19	0	0
4	B	14	0	19	0	0
4	C	13	0	17	1	0
4	D	14	0	19	1	0
4	E	14	0	19	3	0
4	F	14	0	19	1	0
4	G	14	0	19	2	0
4	H	14	0	19	0	0
4	I	14	0	19	0	0
4	J	14	0	19	2	0
5	A	39	0	0	3	0
5	B	30	0	0	2	0
5	C	31	0	0	1	0
5	D	34	0	0	0	0
5	E	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	30	0	0	2	0
5	G	35	0	0	3	0
5	H	45	0	0	6	0
5	I	40	0	0	4	0
5	J	37	0	0	6	0
All	All	23361	0	23912	499	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 499 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74[B]:LEU:CD2	1:C:112[B]:ASN:CB	1.81	1.56
1:C:74[B]:LEU:CD2	1:C:112[B]:ASN:HB2	1.03	1.48
1:F:74[B]:LEU:CD2	1:F:112:ASN:HB2	1.41	1.48
1:C:74[B]:LEU:HD22	1:C:112[B]:ASN:CG	1.32	1.48
1:G:74[B]:LEU:CD1	1:G:112[B]:ASN:ND2	1.78	1.28

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	268/288 (93%)	261 (97%)	7 (3%)	0	100	100
1	B	264/288 (92%)	252 (96%)	11 (4%)	1 (0%)	30	34
1	C	266/288 (92%)	261 (98%)	5 (2%)	0	100	100
1	D	264/288 (92%)	258 (98%)	6 (2%)	0	100	100
1	E	265/288 (92%)	259 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	265/288 (92%)	259 (98%)	6 (2%)	0	100	100
1	G	267/288 (93%)	260 (97%)	7 (3%)	0	100	100
1	H	267/288 (93%)	262 (98%)	5 (2%)	0	100	100
1	I	264/288 (92%)	259 (98%)	5 (2%)	0	100	100
1	J	267/288 (93%)	262 (98%)	5 (2%)	0	100	100
All	All	2657/2880 (92%)	2593 (98%)	63 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	197	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/247 (92%)	224 (99%)	2 (1%)	70	84
1	B	224/247 (91%)	221 (99%)	3 (1%)	61	76
1	C	225/247 (91%)	223 (99%)	2 (1%)	70	84
1	D	224/247 (91%)	223 (100%)	1 (0%)	84	92
1	E	224/247 (91%)	222 (99%)	2 (1%)	70	84
1	F	225/247 (91%)	224 (100%)	1 (0%)	84	92
1	G	228/247 (92%)	223 (98%)	5 (2%)	45	61
1	H	228/247 (92%)	223 (98%)	5 (2%)	45	61
1	I	221/247 (90%)	220 (100%)	1 (0%)	81	90
1	J	226/247 (92%)	225 (100%)	1 (0%)	84	92
All	All	2251/2470 (91%)	2228 (99%)	23 (1%)	68	81

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	141	GLN
1	H	55	LYS
1	H	3	GLN
1	H	111	LEU
1	C	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	81	ASN
1	H	3	GLN
1	G	89	ASN
1	I	7	ASN
1	C	244	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)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	LYR	G	255	1	27,29,30	1.15	2 (7%)	30,37,39	2.03	10 (33%)
1	LYR	H	255	1	27,29,30	1.21	2 (7%)	30,37,39	1.96	6 (20%)
1	LYR	E	255	1	27,29,30	1.17	1 (3%)	30,37,39	1.96	6 (20%)
1	LYR	C	255	1	27,29,30	1.15	1 (3%)	30,37,39	2.07	7 (23%)
1	LYR	B	255	1	27,29,30	1.16	1 (3%)	30,37,39	2.00	7 (23%)
1	LYR	D	255	1	27,29,30	1.19	1 (3%)	30,37,39	1.89	8 (26%)
1	LYR	I	255	1	27,29,30	1.07	2 (7%)	30,37,39	2.10	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	LYR	F	255	1	27,29,30	1.21	2 (7%)	30,37,39	1.98	6 (20%)
1	LYR	A	255	1	27,29,30	1.26	2 (7%)	30,37,39	1.85	7 (23%)
1	LYR	J	255	1	27,29,30	1.14	2 (7%)	30,37,39	2.02	8 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LYR	G	255	1	-	3/22/40/42	0/1/1/1
1	LYR	H	255	1	-	3/22/40/42	0/1/1/1
1	LYR	E	255	1	-	3/22/40/42	0/1/1/1
1	LYR	C	255	1	-	3/22/40/42	0/1/1/1
1	LYR	B	255	1	-	3/22/40/42	0/1/1/1
1	LYR	D	255	1	-	3/22/40/42	0/1/1/1
1	LYR	I	255	1	-	3/22/40/42	0/1/1/1
1	LYR	F	255	1	-	4/22/40/42	0/1/1/1
1	LYR	A	255	1	-	4/22/40/42	0/1/1/1
1	LYR	J	255	1	-	3/22/40/42	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	255	LYR	C2-C3	3.16	1.41	1.33
1	B	255	LYR	C2-C3	3.07	1.40	1.33
1	A	255	LYR	C2-C3	3.06	1.40	1.33
1	F	255	LYR	C2-C3	3.04	1.40	1.33
1	D	255	LYR	C2-C3	3.03	1.40	1.33

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	255	LYR	C13-C12-C11	-5.26	118.74	124.48
1	B	255	LYR	C13-C12-C11	-5.13	118.89	124.48
1	J	255	LYR	C13-C12-C11	-5.03	119.00	124.48
1	C	255	LYR	C13-C12-C11	-4.93	119.11	124.48
1	I	255	LYR	C13-C12-C11	-4.88	119.15	124.48

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	255	LYR	C2-C1-NZ-CE
1	E	255	LYR	C2-C1-NZ-CE
1	G	255	LYR	C2-C1-NZ-CE
1	I	255	LYR	C2-C1-NZ-CE
1	B	255	LYR	C2-C1-NZ-CE

There are no ring outliers.

10 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	255	LYR	3	0
1	H	255	LYR	9	0
1	E	255	LYR	8	0
1	C	255	LYR	7	0
1	B	255	LYR	8	0
1	D	255	LYR	7	0
1	I	255	LYR	5	0
1	F	255	LYR	7	0
1	A	255	LYR	5	0
1	J	255	LYR	7	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 138 ligands modelled in this entry, 10 are monoatomic - leaving 128 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	$\#\|Z\| > 2$
3	LFA	I	303	-	6,6,19	0.27	0	5,5,18	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	LFA	I	308	-	15,15,19	0.23	0	14,14,18	0.59	0
3	LFA	A	308	-	7,7,19	0.30	0	6,6,18	0.43	0
3	LFA	B	302	-	6,6,19	0.27	0	5,5,18	0.42	0
3	LFA	G	307	-	15,15,19	0.26	0	14,14,18	0.58	0
3	LFA	D	314	-	6,6,19	0.27	0	5,5,18	0.42	0
3	LFA	D	311	-	6,6,19	0.25	0	5,5,18	0.45	0
3	LFA	C	303	-	9,9,19	0.29	0	8,8,18	0.42	0
3	LFA	C	308	-	9,9,19	0.29	0	8,8,18	0.45	0
3	LFA	D	303	-	13,13,19	0.27	0	12,12,18	0.53	0
3	LFA	D	304	-	5,5,19	0.25	0	4,4,18	0.44	0
3	LFA	I	306	-	9,9,19	0.25	0	8,8,18	0.51	0
3	LFA	D	306	-	15,15,19	0.28	0	14,14,18	0.50	0
3	LFA	G	304	-	13,13,19	0.31	0	12,12,18	0.47	0
3	LFA	B	303	-	6,6,19	0.26	0	5,5,18	0.47	0
3	LFA	I	302	-	6,6,19	0.27	0	5,5,18	0.44	0
3	LFA	E	302	-	13,13,19	0.28	0	12,12,18	0.56	0
3	LFA	F	313	-	13,13,19	0.29	0	12,12,18	0.49	0
4	MPG	E	313	-	13,13,24	0.44	0	13,13,25	1.02	1 (7%)
3	LFA	C	306	-	15,15,19	0.28	0	14,14,18	0.53	0
4	MPG	B	312	-	13,13,24	0.47	0	13,13,25	1.04	1 (7%)
3	LFA	F	305	-	5,5,19	0.27	0	4,4,18	0.37	0
3	LFA	E	312	-	7,7,19	0.26	0	6,6,18	0.44	0
3	LFA	I	313	-	3,3,19	0.38	0	2,2,18	0.64	0
3	LFA	J	302	-	15,15,19	0.26	0	14,14,18	0.54	0
3	LFA	F	309	-	9,9,19	0.32	0	8,8,18	0.41	0
3	LFA	G	306	-	9,9,19	0.28	0	8,8,18	0.43	0
3	LFA	D	317	-	4,4,19	0.27	0	3,3,18	0.38	0
3	LFA	G	315	-	5,5,19	0.28	0	4,4,18	0.38	0
3	LFA	D	309	-	7,7,19	0.26	0	6,6,18	0.46	0
3	LFA	B	305	-	5,5,19	0.31	0	4,4,18	0.31	0
3	LFA	C	305	-	9,9,19	0.26	0	8,8,18	0.49	0
3	LFA	D	313	-	5,5,19	0.27	0	4,4,18	0.37	0
3	LFA	E	307	-	7,7,19	0.25	0	6,6,18	0.49	0
3	LFA	G	308	-	17,17,19	0.28	0	16,16,18	0.48	0
3	LFA	I	305	-	5,5,19	0.29	0	4,4,18	0.34	0
3	LFA	B	311	-	7,7,19	0.28	0	6,6,18	0.44	0
3	LFA	G	313	-	7,7,19	0.29	0	6,6,18	0.45	0
3	LFA	A	305	-	9,9,19	0.28	0	8,8,18	0.45	0
3	LFA	H	310	-	7,7,19	0.28	0	6,6,18	0.44	0
3	LFA	H	307	-	13,13,19	0.26	0	12,12,18	0.52	0
3	LFA	G	314	-	5,5,19	0.26	0	4,4,18	0.40	0
4	MPG	J	312	-	13,13,24	0.44	0	13,13,25	1.10	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	LFA	H	312	-	5,5,19	0.27	0	4,4,18	0.40	0
3	LFA	E	305	-	5,5,19	0.31	0	4,4,18	0.37	0
3	LFA	D	318	-	4,4,19	0.30	0	3,3,18	0.36	0
3	LFA	E	309	-	5,5,19	0.30	0	4,4,18	0.37	0
3	LFA	D	316	-	4,4,19	0.26	0	3,3,18	0.36	0
3	LFA	E	310	-	9,9,19	0.29	0	8,8,18	0.44	0
3	LFA	H	306	-	17,17,19	0.29	0	16,16,18	0.46	0
3	LFA	J	305	-	13,13,19	0.31	0	12,12,18	0.46	0
3	LFA	I	311	-	7,7,19	0.27	0	6,6,18	0.47	0
4	MPG	C	313	-	12,12,24	0.45	0	12,12,25	1.02	1 (8%)
3	LFA	G	302	-	15,15,19	0.25	0	14,14,18	0.57	0
3	LFA	H	302	-	12,12,19	0.29	0	11,11,18	0.50	0
3	LFA	J	310	-	9,9,19	0.27	0	8,8,18	0.48	0
3	LFA	F	307	-	5,5,19	0.31	0	4,4,18	0.34	0
3	LFA	I	304	-	13,13,19	0.29	0	12,12,18	0.50	0
3	LFA	G	311	-	7,7,19	0.25	0	6,6,18	0.49	0
3	LFA	C	302	-	6,6,19	0.28	0	5,5,18	0.41	0
3	LFA	H	305	-	15,15,19	0.26	0	14,14,18	0.52	0
4	MPG	F	315	-	13,13,24	0.41	0	13,13,25	1.08	1 (7%)
3	LFA	J	304	-	7,7,19	0.28	0	6,6,18	0.45	0
3	LFA	G	309	-	7,7,19	0.27	0	6,6,18	0.47	0
3	LFA	H	311	-	6,6,19	0.21	0	5,5,18	0.55	0
3	LFA	B	309	-	12,12,19	0.32	0	11,11,18	0.44	0
3	LFA	G	303	-	6,6,19	0.27	0	5,5,18	0.43	0
3	LFA	H	303	-	5,5,19	0.25	0	4,4,18	0.44	0
3	LFA	H	309	-	4,4,19	0.27	0	3,3,18	0.38	0
3	LFA	F	311	-	9,9,19	0.30	0	8,8,18	0.43	0
3	LFA	H	308	-	7,7,19	0.26	0	6,6,18	0.47	0
4	MPG	G	312	-	13,13,24	0.45	0	13,13,25	1.11	1 (7%)
3	LFA	B	304	-	13,13,19	0.29	0	12,12,18	0.49	0
3	LFA	G	305	-	5,5,19	0.28	0	4,4,18	0.37	0
3	LFA	F	304	-	9,9,19	0.28	0	8,8,18	0.46	0
3	LFA	C	309	-	7,7,19	0.27	0	6,6,18	0.46	0
3	LFA	I	307	-	5,5,19	0.28	0	4,4,18	0.35	0
3	LFA	B	306	-	7,7,19	0.32	0	6,6,18	0.43	0
4	MPG	H	313	-	13,13,24	0.42	0	13,13,25	1.03	1 (7%)
3	LFA	A	312	-	4,4,19	0.35	0	3,3,18	0.33	0
3	LFA	E	303	-	17,17,19	0.26	0	16,16,18	0.50	0
3	LFA	I	309	-	17,17,19	0.30	0	16,16,18	0.45	0
3	LFA	E	308	-	13,13,19	0.27	0	12,12,18	0.50	0
3	LFA	A	304	-	9,9,19	0.27	0	8,8,18	0.48	0
3	LFA	A	309	-	7,7,19	0.27	0	6,6,18	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	LFA	B	310	-	10,10,19	0.27	0	9,9,18	0.49	0
3	LFA	F	310	-	17,17,19	0.27	0	16,16,18	0.48	0
3	LFA	F	312	-	7,7,19	0.25	0	6,6,18	0.49	0
3	LFA	G	310	-	9,9,19	0.31	0	8,8,18	0.44	0
3	LFA	J	303	-	17,17,19	0.27	0	16,16,18	0.50	0
3	LFA	J	309	-	9,9,19	0.24	0	8,8,18	0.51	0
3	LFA	C	304	-	5,5,19	0.28	0	4,4,18	0.36	0
3	LFA	J	308	-	13,13,19	0.32	0	12,12,18	0.42	0
4	MPG	A	313	-	13,13,24	0.47	0	13,13,25	1.09	1 (7%)
3	LFA	I	310	-	13,13,19	0.26	0	12,12,18	0.54	0
3	LFA	A	310	-	7,7,19	0.27	0	6,6,18	0.46	0
3	LFA	A	306	-	13,13,19	0.28	0	12,12,18	0.51	0
3	LFA	C	310	-	12,12,19	0.29	0	11,11,18	0.51	0
3	LFA	I	312	-	6,6,19	0.23	0	5,5,18	0.47	0
3	LFA	A	311	-	6,6,19	0.24	0	5,5,18	0.46	0
3	LFA	D	308	-	9,9,19	0.29	0	8,8,18	0.47	0
3	LFA	C	312	-	3,3,19	0.35	0	2,2,18	0.61	0
3	LFA	F	314	-	7,7,19	0.28	0	6,6,18	0.44	0
3	LFA	D	310	-	7,7,19	0.27	0	6,6,18	0.47	0
3	LFA	C	311	-	7,7,19	0.27	0	6,6,18	0.46	0
3	LFA	F	303	-	13,13,19	0.27	0	12,12,18	0.50	0
3	LFA	B	307	-	15,15,19	0.27	0	14,14,18	0.56	0
4	MPG	D	315	-	13,13,24	0.44	0	13,13,25	1.08	1 (7%)
4	MPG	I	314	-	13,13,24	0.34	0	13,13,25	1.03	1 (7%)
3	LFA	D	302	-	6,6,19	0.24	0	5,5,18	0.49	0
3	LFA	E	304	-	7,7,19	0.31	0	6,6,18	0.45	0
3	LFA	A	302	-	13,13,19	0.26	0	12,12,18	0.51	0
3	LFA	D	312	-	5,5,19	0.27	0	4,4,18	0.40	0
3	LFA	E	306	-	11,11,19	0.28	0	10,10,18	0.49	0
3	LFA	E	311	-	7,7,19	0.27	0	6,6,18	0.46	0
3	LFA	C	307	-	17,17,19	0.27	0	16,16,18	0.47	0
3	LFA	H	304	-	9,9,19	0.29	0	8,8,18	0.51	0
3	LFA	F	302	-	6,6,19	0.23	0	5,5,18	0.49	0
3	LFA	D	307	-	17,17,19	0.26	0	16,16,18	0.48	0
3	LFA	J	306	-	7,7,19	0.26	0	6,6,18	0.48	0
3	LFA	F	306	-	9,9,19	0.27	0	8,8,18	0.50	0
3	LFA	A	307	-	17,17,19	0.23	0	16,16,18	0.56	0
3	LFA	J	311	-	3,3,19	0.37	0	2,2,18	0.62	0
3	LFA	B	308	-	17,17,19	0.28	0	16,16,18	0.50	0
3	LFA	A	303	-	5,5,19	0.27	0	4,4,18	0.40	0
3	LFA	F	308	-	7,7,19	0.30	0	6,6,18	0.41	0
3	LFA	D	305	-	9,9,19	0.27	0	8,8,18	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	LFA	J	307	-	6,6,19	0.26	0	5,5,18	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	I	303	-	-	3/4/4/17	-
3	LFA	I	308	-	-	5/13/13/17	-
3	LFA	A	308	-	-	2/5/5/17	-
3	LFA	B	302	-	-	2/4/4/17	-
3	LFA	G	307	-	-	6/13/13/17	-
3	LFA	D	314	-	-	1/4/4/17	-
3	LFA	D	311	-	-	2/4/4/17	-
3	LFA	C	303	-	-	3/7/7/17	-
3	LFA	C	308	-	-	3/7/7/17	-
3	LFA	D	303	-	-	3/11/11/17	-
3	LFA	D	304	-	-	0/3/3/17	-
3	LFA	I	306	-	-	4/7/7/17	-
3	LFA	D	306	-	-	8/13/13/17	-
3	LFA	G	304	-	-	5/11/11/17	-
3	LFA	B	303	-	-	3/4/4/17	-
3	LFA	I	302	-	-	2/4/4/17	-
3	LFA	E	302	-	-	2/11/11/17	-
3	LFA	F	313	-	-	4/11/11/17	-
4	MPG	E	313	-	-	10/12/12/25	-
3	LFA	C	306	-	-	5/13/13/17	-
4	MPG	B	312	-	-	7/12/12/25	-
3	LFA	F	305	-	-	1/3/3/17	-
3	LFA	E	312	-	-	4/5/5/17	-
3	LFA	I	313	-	-	0/1/1/17	-
3	LFA	J	302	-	-	9/13/13/17	-
3	LFA	F	309	-	-	4/7/7/17	-
3	LFA	G	306	-	-	6/7/7/17	-
3	LFA	D	317	-	-	0/2/2/17	-
3	LFA	G	315	-	-	0/3/3/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	D	309	-	-	3/5/5/17	-
3	LFA	B	305	-	-	1/3/3/17	-
3	LFA	C	305	-	-	6/7/7/17	-
3	LFA	D	313	-	-	0/3/3/17	-
3	LFA	E	307	-	-	4/5/5/17	-
3	LFA	G	308	-	-	9/15/15/17	-
3	LFA	I	305	-	-	1/3/3/17	-
3	LFA	B	311	-	-	3/5/5/17	-
3	LFA	G	313	-	-	4/5/5/17	-
3	LFA	A	305	-	-	5/7/7/17	-
3	LFA	H	310	-	-	3/5/5/17	-
3	LFA	H	307	-	-	7/11/11/17	-
3	LFA	G	314	-	-	1/3/3/17	-
4	MPG	J	312	-	-	8/12/12/25	-
3	LFA	H	312	-	-	1/3/3/17	-
3	LFA	E	305	-	-	1/3/3/17	-
3	LFA	D	318	-	-	0/2/2/17	-
3	LFA	E	309	-	-	2/3/3/17	-
3	LFA	D	316	-	-	1/2/2/17	-
3	LFA	E	310	-	-	3/7/7/17	-
3	LFA	H	306	-	-	9/15/15/17	-
3	LFA	J	305	-	-	5/11/11/17	-
3	LFA	I	311	-	-	4/5/5/17	-
4	MPG	C	313	-	-	7/11/11/25	-
3	LFA	G	302	-	-	5/13/13/17	-
3	LFA	H	302	-	-	8/10/10/17	-
3	LFA	J	310	-	-	3/7/7/17	-
3	LFA	F	307	-	-	2/3/3/17	-
3	LFA	I	304	-	-	5/11/11/17	-
3	LFA	G	311	-	-	1/5/5/17	-
3	LFA	C	302	-	-	3/4/4/17	-
3	LFA	H	305	-	-	5/13/13/17	-
4	MPG	F	315	-	-	9/12/12/25	-
3	LFA	J	304	-	-	1/5/5/17	-
3	LFA	G	309	-	-	2/5/5/17	-
3	LFA	H	311	-	-	1/4/4/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	B	309	-	-	6/10/10/17	-
3	LFA	G	303	-	-	3/4/4/17	-
3	LFA	H	303	-	-	0/3/3/17	-
3	LFA	H	309	-	-	1/2/2/17	-
3	LFA	F	311	-	-	3/7/7/17	-
3	LFA	H	308	-	-	2/5/5/17	-
4	MPG	G	312	-	-	5/12/12/25	-
3	LFA	B	304	-	-	6/11/11/17	-
3	LFA	G	305	-	-	1/3/3/17	-
3	LFA	F	304	-	-	2/7/7/17	-
3	LFA	C	309	-	-	3/5/5/17	-
3	LFA	I	307	-	-	1/3/3/17	-
3	LFA	B	306	-	-	0/5/5/17	-
4	MPG	H	313	-	-	8/12/12/25	-
3	LFA	A	312	-	-	0/2/2/17	-
3	LFA	E	303	-	-	11/15/15/17	-
3	LFA	I	309	-	-	12/15/15/17	-
3	LFA	E	308	-	-	6/11/11/17	-
3	LFA	A	304	-	-	5/7/7/17	-
3	LFA	A	309	-	-	2/5/5/17	-
3	LFA	B	310	-	-	7/8/8/17	-
3	LFA	F	310	-	-	10/15/15/17	-
3	LFA	F	312	-	-	3/5/5/17	-
3	LFA	G	310	-	-	3/7/7/17	-
3	LFA	J	303	-	-	8/15/15/17	-
3	LFA	J	309	-	-	3/7/7/17	-
3	LFA	C	304	-	-	1/3/3/17	-
3	LFA	J	308	-	-	6/11/11/17	-
4	MPG	A	313	-	-	7/12/12/25	-
3	LFA	I	310	-	-	4/11/11/17	-
3	LFA	A	310	-	-	0/5/5/17	-
3	LFA	A	306	-	-	7/11/11/17	-
3	LFA	C	310	-	-	4/10/10/17	-
3	LFA	I	312	-	-	1/4/4/17	-
3	LFA	A	311	-	-	3/4/4/17	-
3	LFA	D	308	-	-	4/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	C	312	-	-	0/1/1/17	-
3	LFA	F	314	-	-	0/5/5/17	-
3	LFA	D	310	-	-	1/5/5/17	-
3	LFA	C	311	-	-	1/5/5/17	-
3	LFA	F	303	-	-	6/11/11/17	-
3	LFA	B	307	-	-	7/13/13/17	-
4	MPG	D	315	-	-	9/12/12/25	-
4	MPG	I	314	-	-	9/12/12/25	-
3	LFA	D	302	-	-	3/4/4/17	-
3	LFA	E	304	-	-	2/5/5/17	-
3	LFA	A	302	-	-	7/11/11/17	-
3	LFA	D	312	-	-	0/3/3/17	-
3	LFA	E	306	-	-	4/9/9/17	-
3	LFA	E	311	-	-	1/5/5/17	-
3	LFA	C	307	-	-	11/15/15/17	-
3	LFA	H	304	-	-	4/7/7/17	-
3	LFA	F	302	-	-	2/4/4/17	-
3	LFA	D	307	-	-	9/15/15/17	-
3	LFA	J	306	-	-	2/5/5/17	-
3	LFA	F	306	-	-	2/7/7/17	-
3	LFA	A	307	-	-	13/15/15/17	-
3	LFA	J	311	-	-	0/1/1/17	-
3	LFA	B	308	-	-	11/15/15/17	-
3	LFA	A	303	-	-	1/3/3/17	-
3	LFA	F	308	-	-	4/5/5/17	-
3	LFA	D	305	-	-	4/7/7/17	-
3	LFA	J	307	-	-	3/4/4/17	-

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	312	MPG	O1-CX3-CXD	3.41	120.03	109.56
4	A	313	MPG	O1-CX3-CXD	3.37	119.91	109.56
4	J	312	MPG	O1-CX3-CXD	3.36	119.89	109.56
4	D	315	MPG	O1-CX3-CXD	3.25	119.56	109.56
4	B	312	MPG	O1-CX3-CXD	3.20	119.39	109.56

There are no chirality outliers.

5 of 501 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	313	MPG	O3-C21-CXD-CX3
4	B	312	MPG	O1-CX3-CXD-O2
4	B	312	MPG	O1-CX3-CXD-C21
4	C	313	MPG	O3-C21-CXD-O2
4	C	313	MPG	O3-C21-CXD-CX3

There are no ring outliers.

43 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	303	LFA	1	0
3	I	308	LFA	1	0
3	G	307	LFA	1	0
3	I	306	LFA	1	0
3	D	306	LFA	2	0
3	I	302	LFA	1	0
4	E	313	MPG	3	0
3	C	306	LFA	3	0
3	J	302	LFA	2	0
3	D	317	LFA	2	0
3	C	305	LFA	1	0
3	G	308	LFA	1	0
4	J	312	MPG	2	0
3	E	305	LFA	1	0
3	D	316	LFA	2	0
3	E	310	LFA	1	0
4	C	313	MPG	1	0
3	G	302	LFA	3	0
3	H	302	LFA	1	0
3	C	302	LFA	2	0
3	H	305	LFA	1	0
4	F	315	MPG	1	0
3	J	304	LFA	1	0
3	G	303	LFA	2	0
3	F	311	LFA	3	0
4	G	312	MPG	2	0
3	F	304	LFA	1	0
3	B	306	LFA	2	0
3	I	309	LFA	2	0
3	F	312	LFA	3	0

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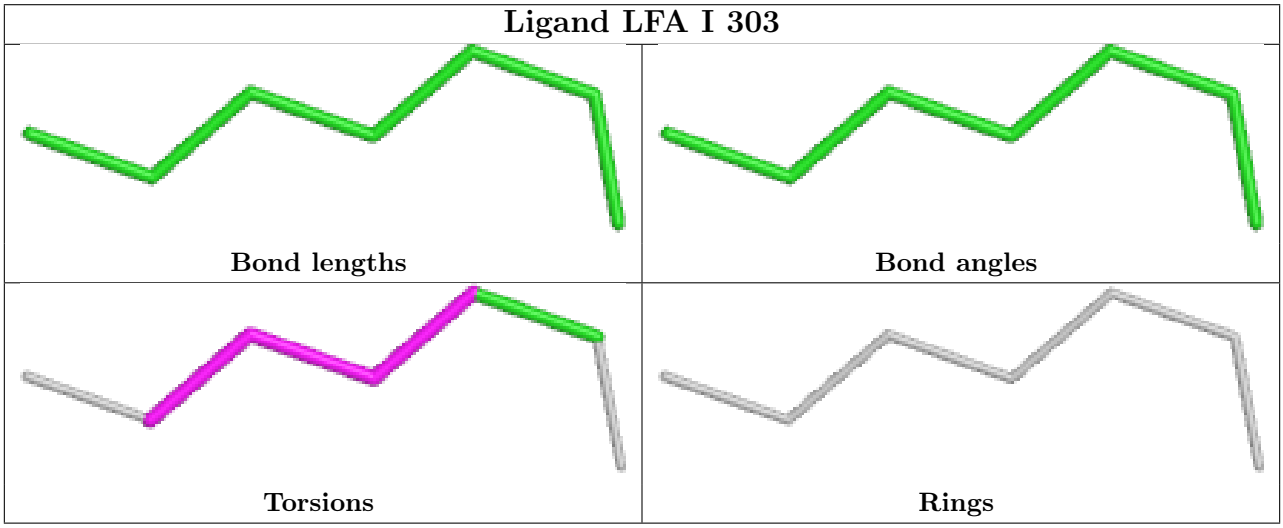
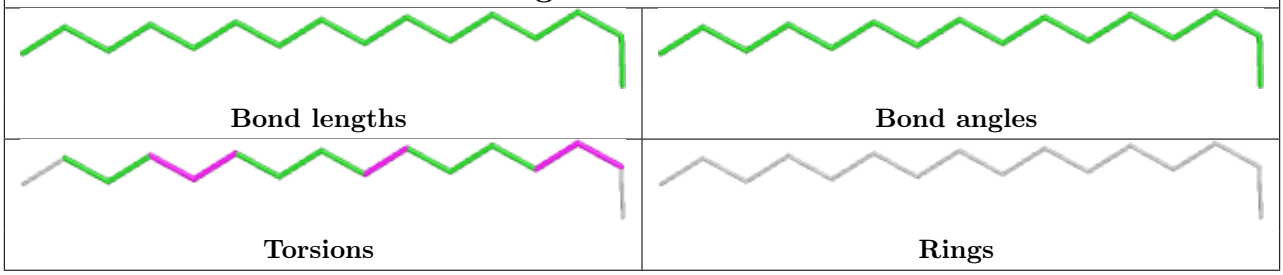
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	312	LFA	1	0
3	A	311	LFA	2	0
3	B	307	LFA	1	0
4	D	315	MPG	1	0
3	D	302	LFA	5	0
3	E	304	LFA	1	0
3	E	311	LFA	7	0
3	F	302	LFA	2	0
3	D	307	LFA	1	0
3	F	306	LFA	1	0
3	A	307	LFA	1	0
3	J	311	LFA	1	0
3	J	307	LFA	1	0

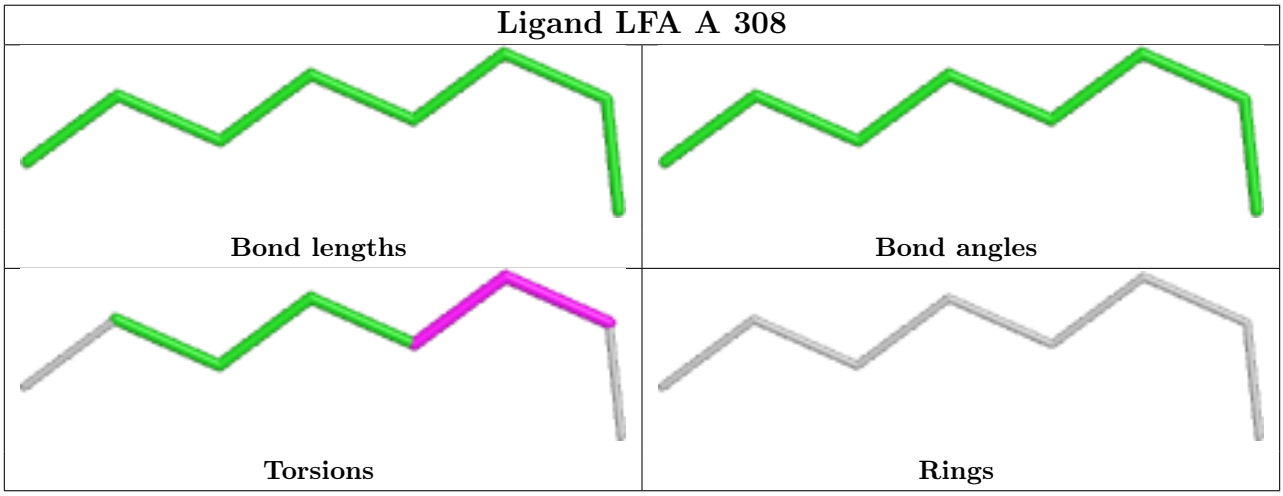
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



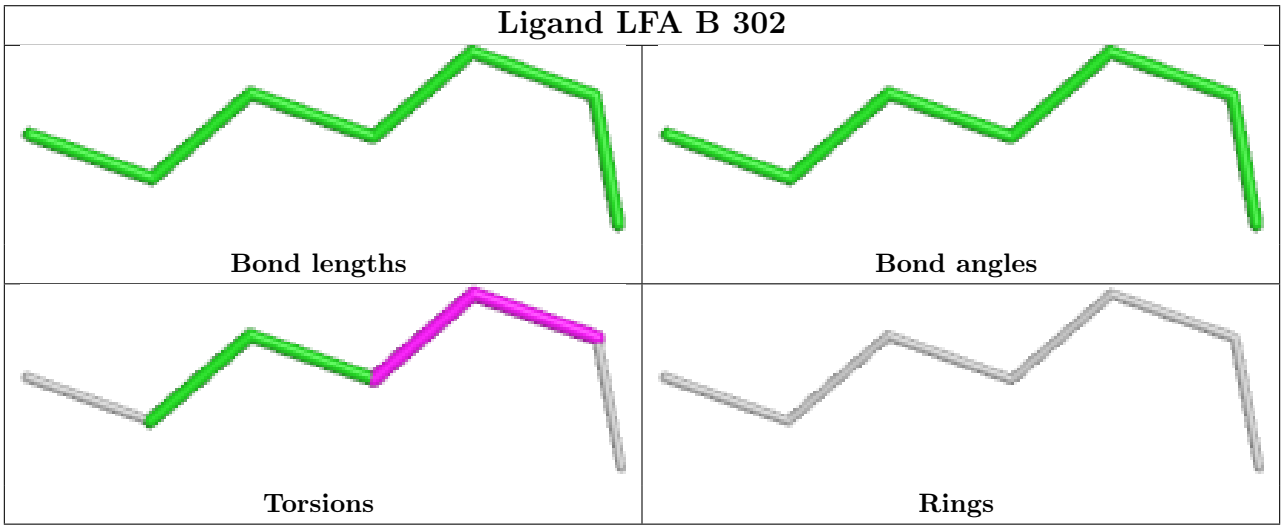
Ligand LFA I 308



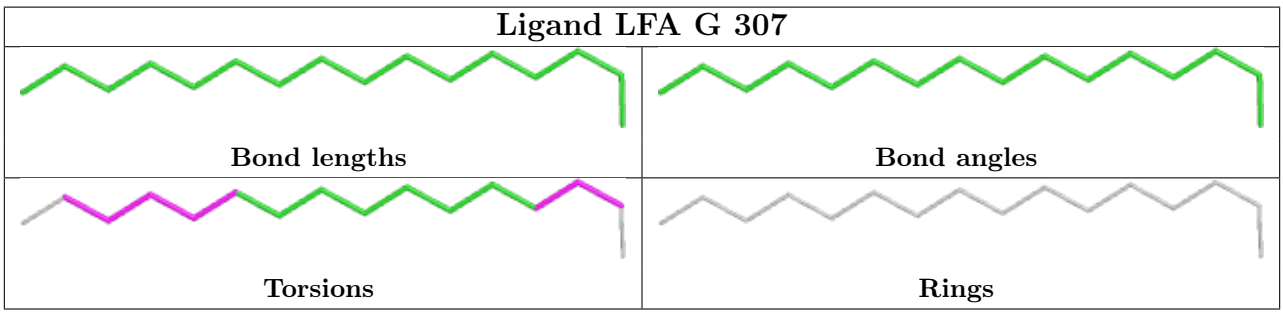
Ligand LFA A 308



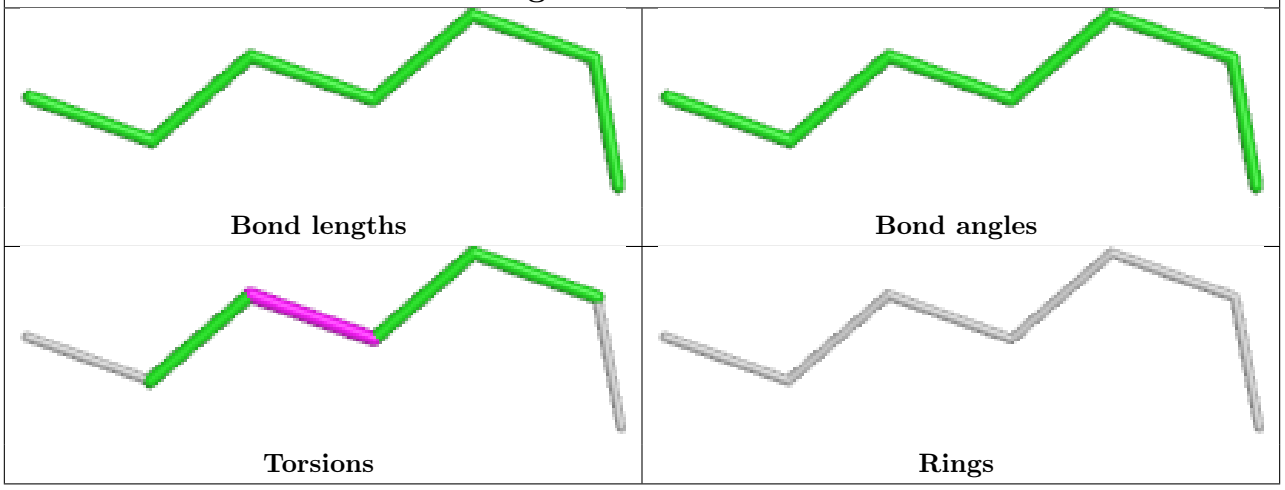
Ligand LFA B 302



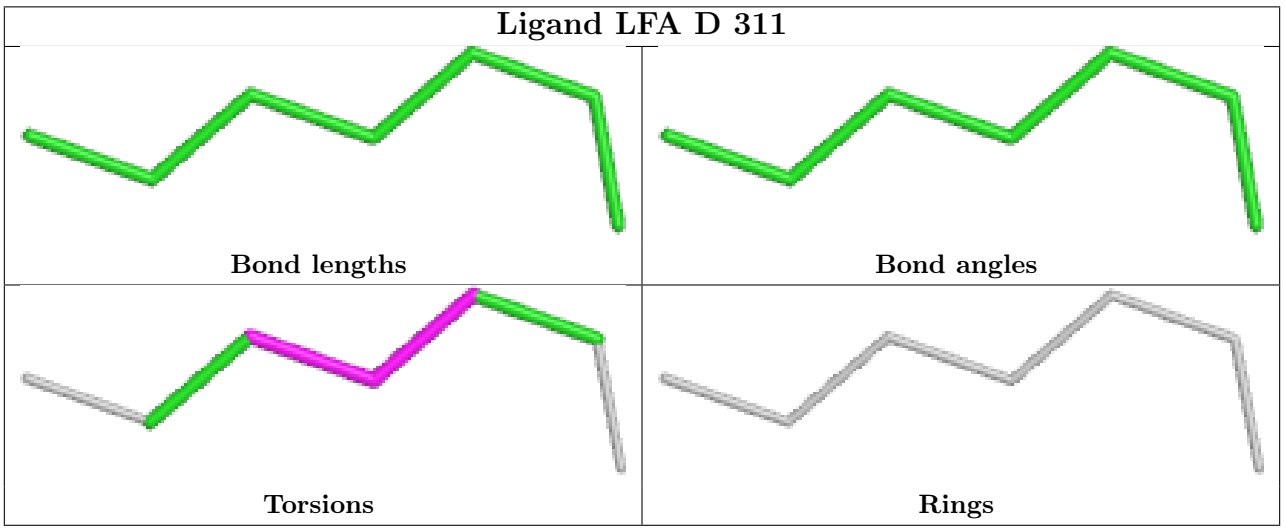
Ligand LFA G 307



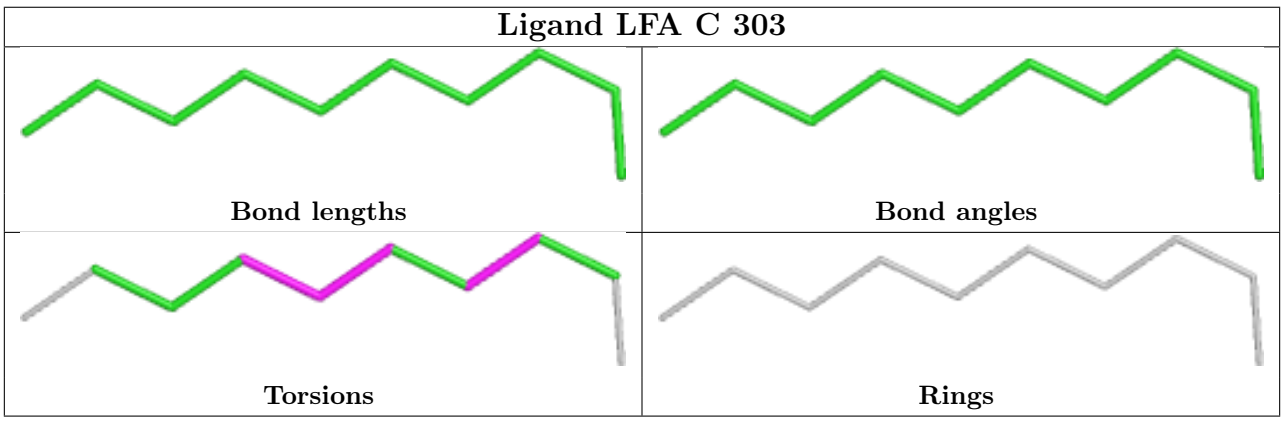
Ligand LFA D 314

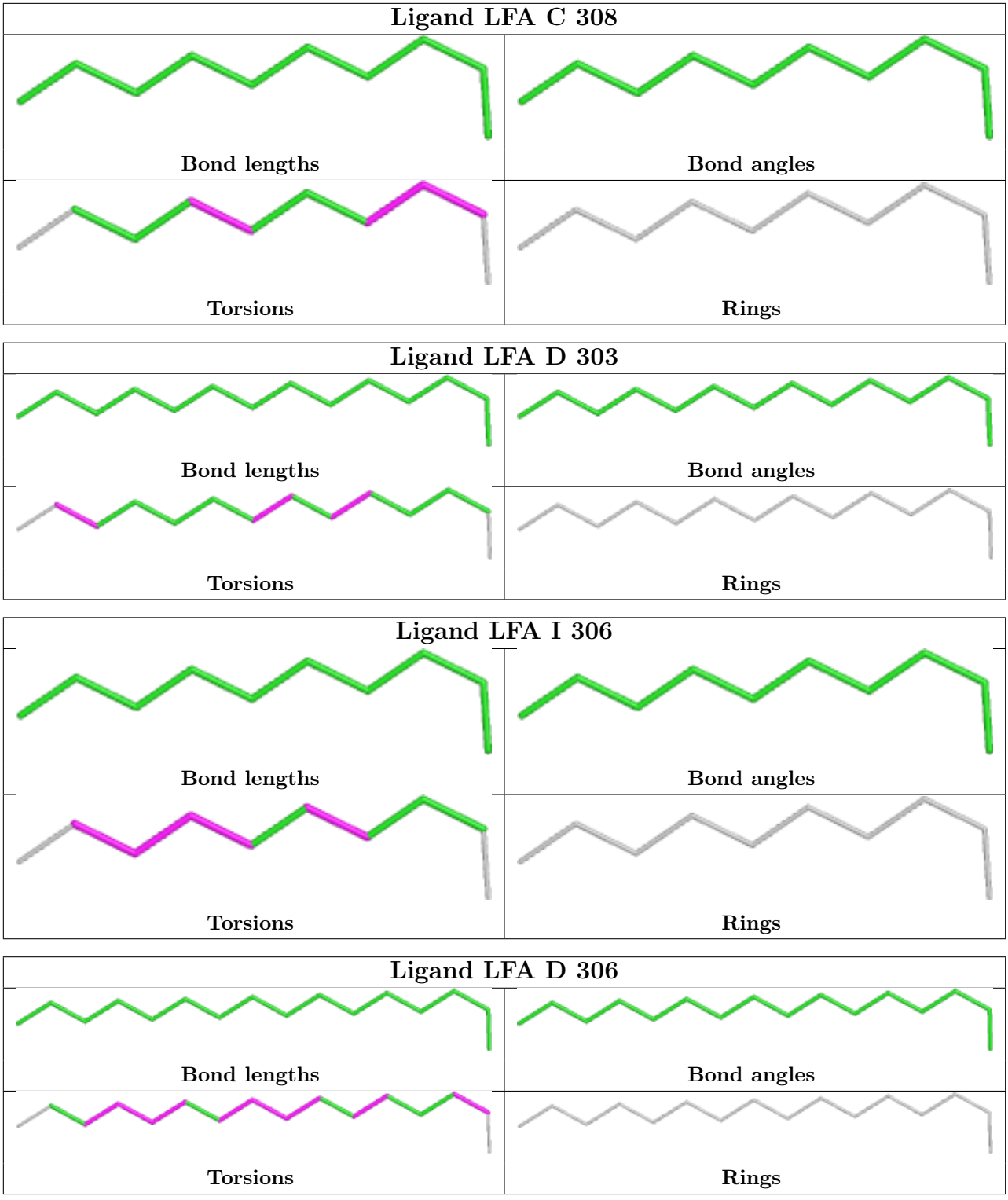


Ligand LFA D 311

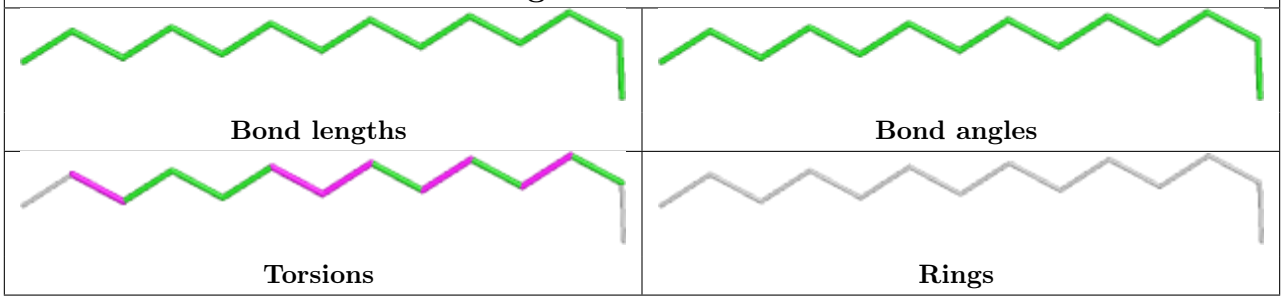


Ligand LFA C 303

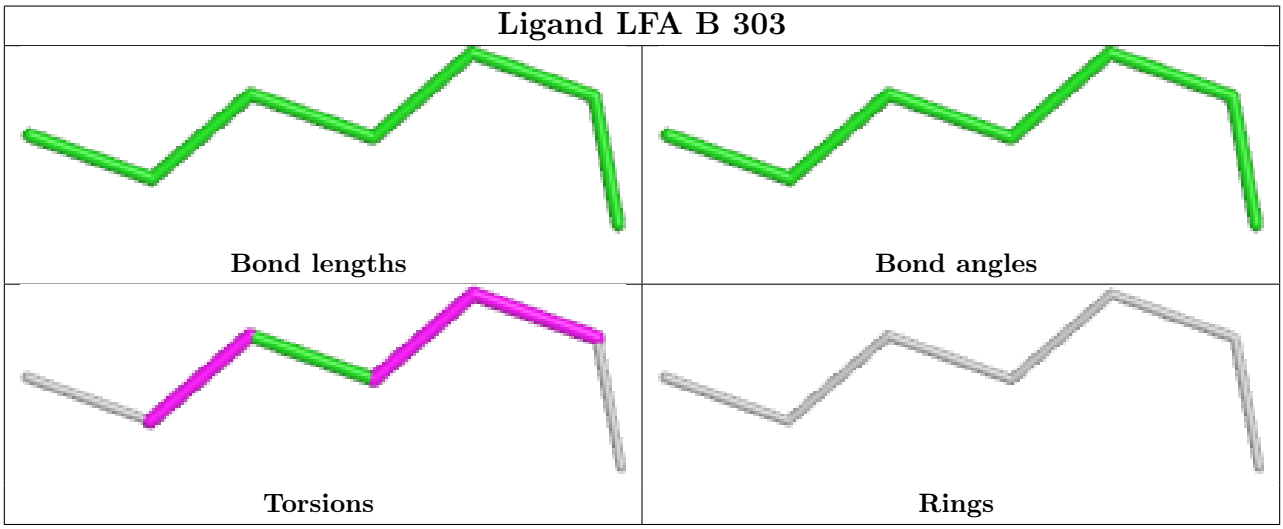



Ligand LFA C 308
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA D 303
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA I 306
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA D 306
Bond lengths
Bond angles
Torsions
Rings

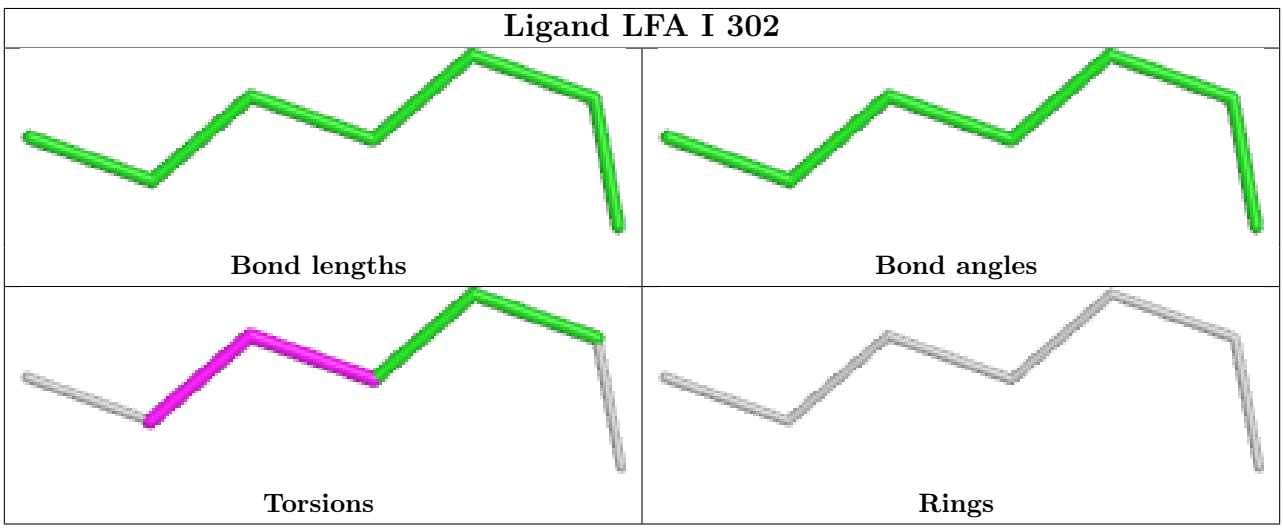
Ligand LFA G 304



Ligand LFA B 303



Ligand LFA I 302



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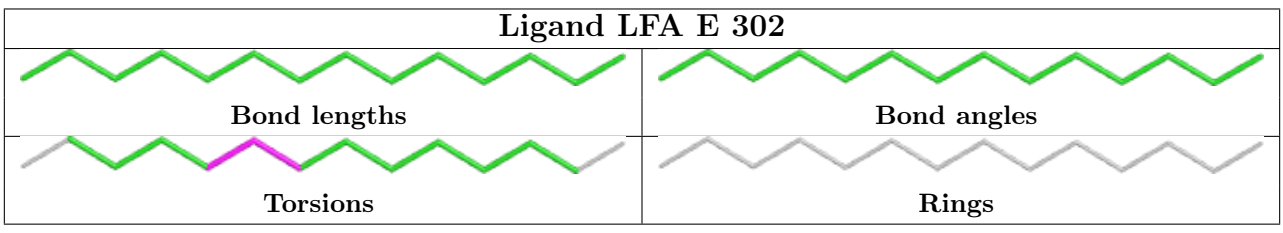
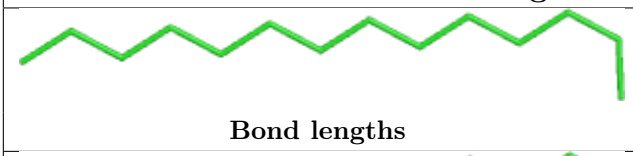
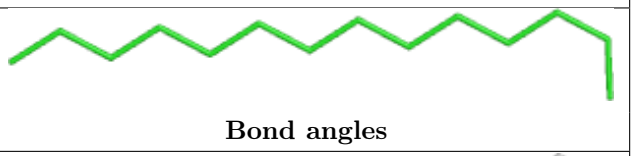


Ligand LFA F 313

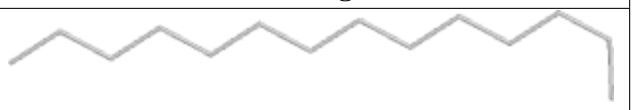


Bond lengths



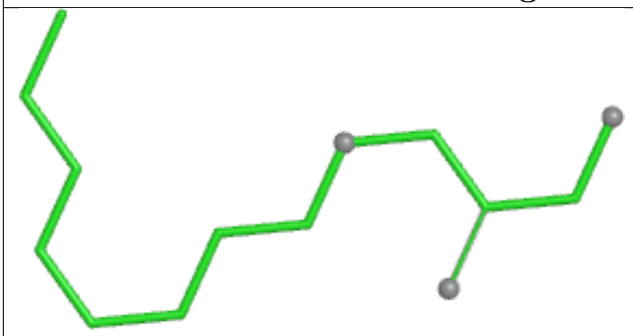
Bond angles

Torsions



Rings

Ligand MPG E 313



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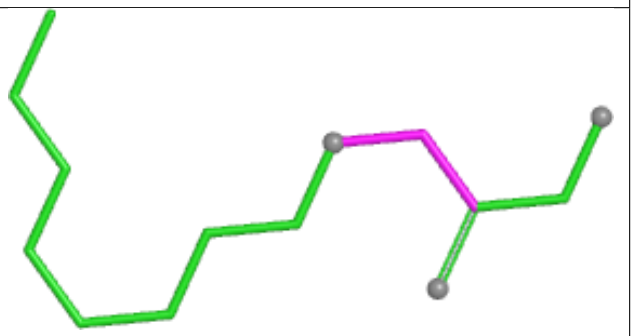
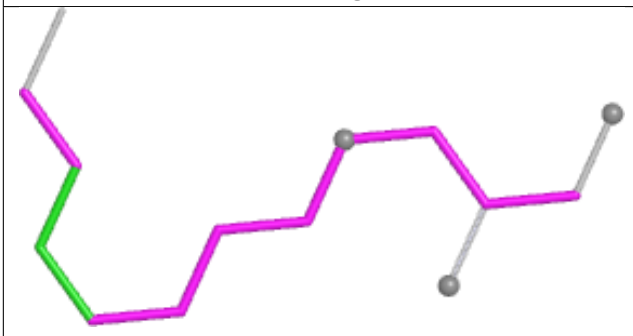


Bond angles



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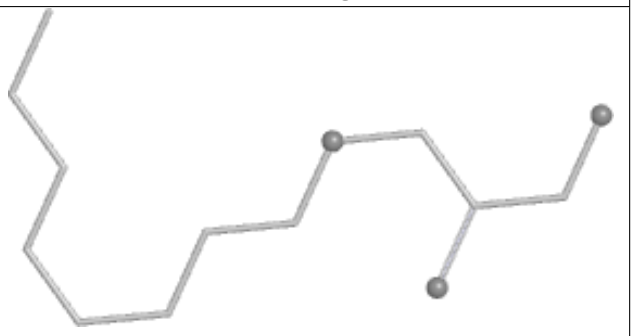
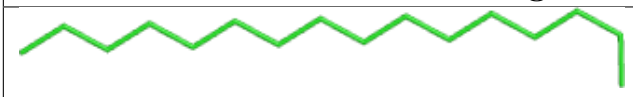
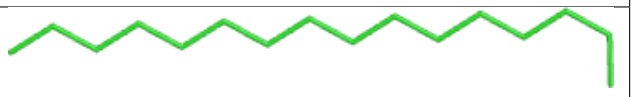


Rings

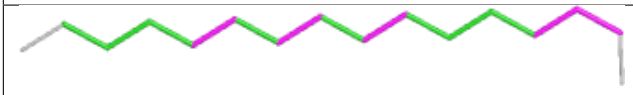
Ligand LFA C 306



Bond lengths



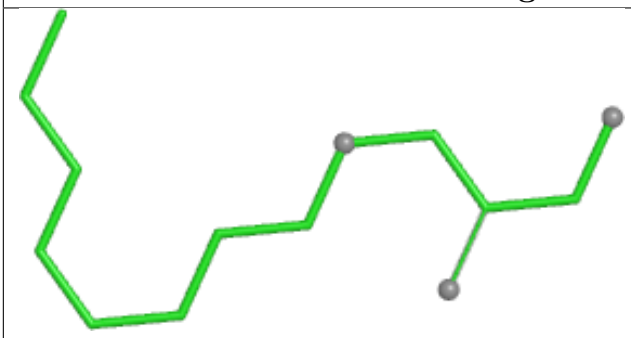
Bond angles



Torsions

Rings

Ligand MPG B 312



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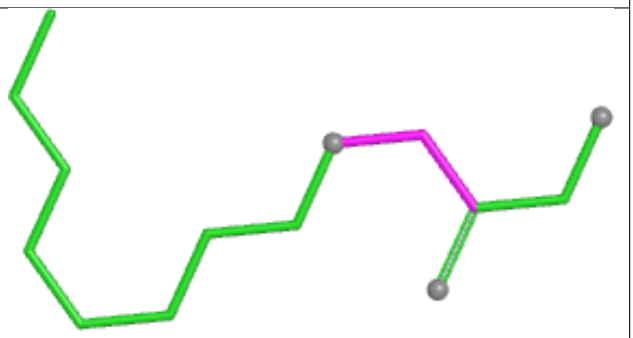
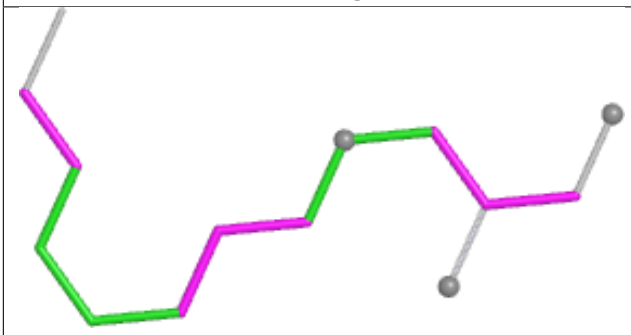
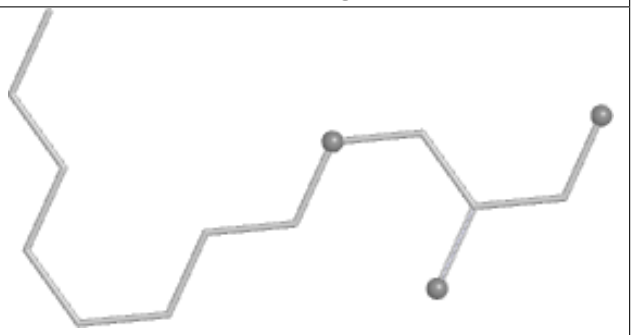


Bond angles

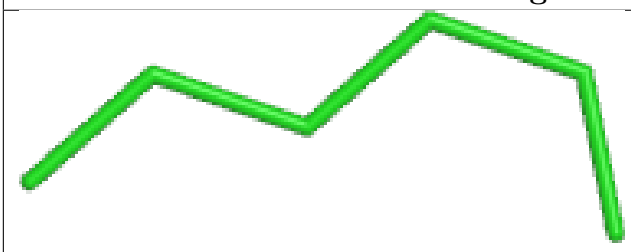


Torsions



Rings

Ligand LFA F 305



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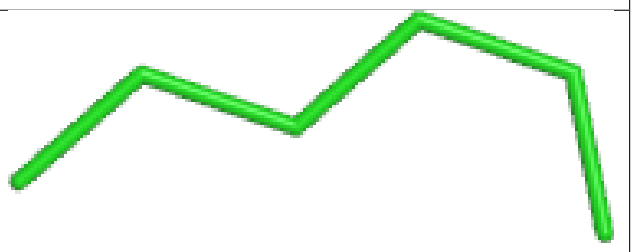
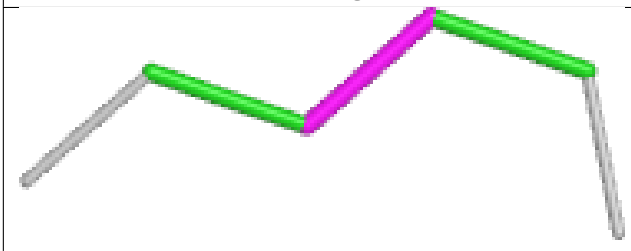


Bond angles



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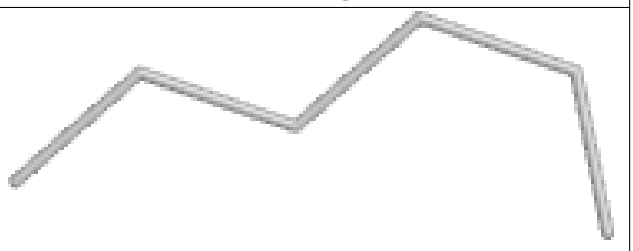
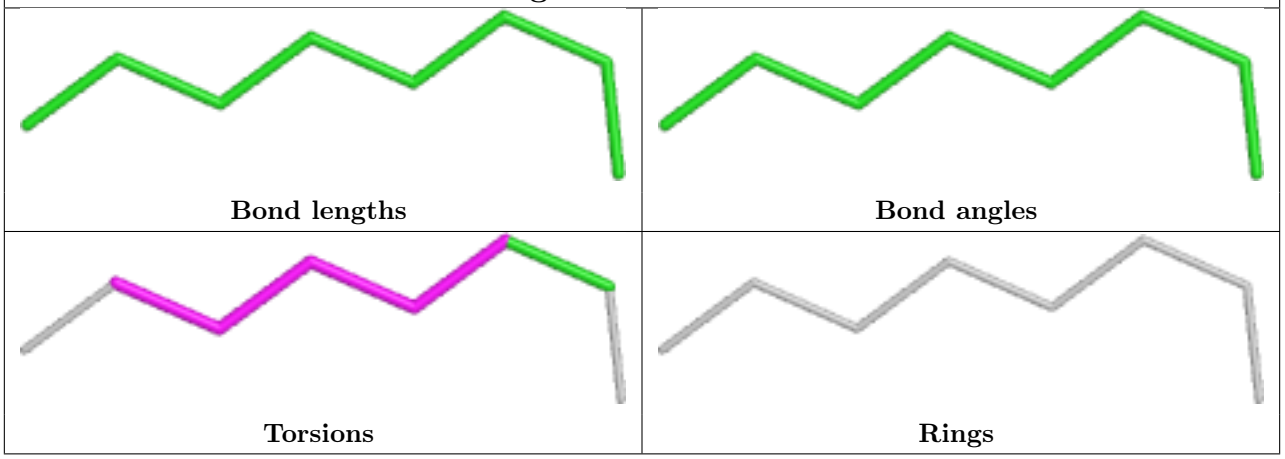
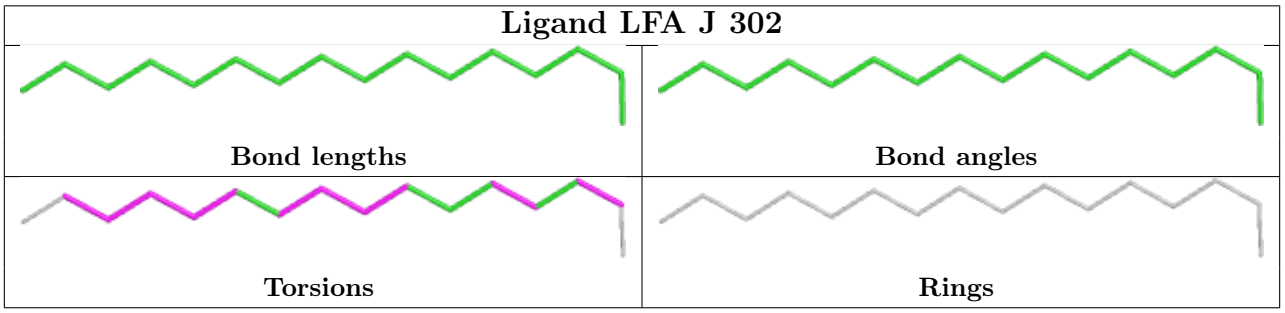


Rings

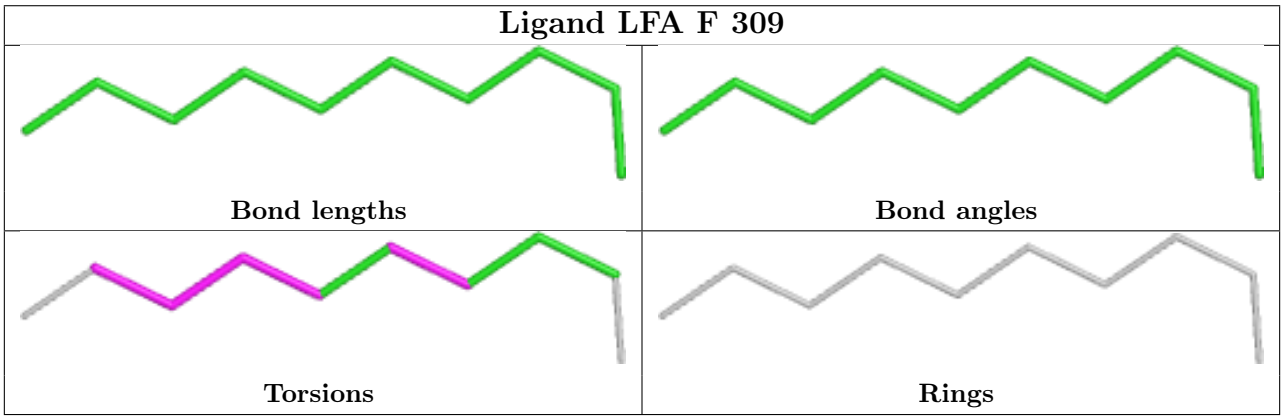
Ligand LFA E 312



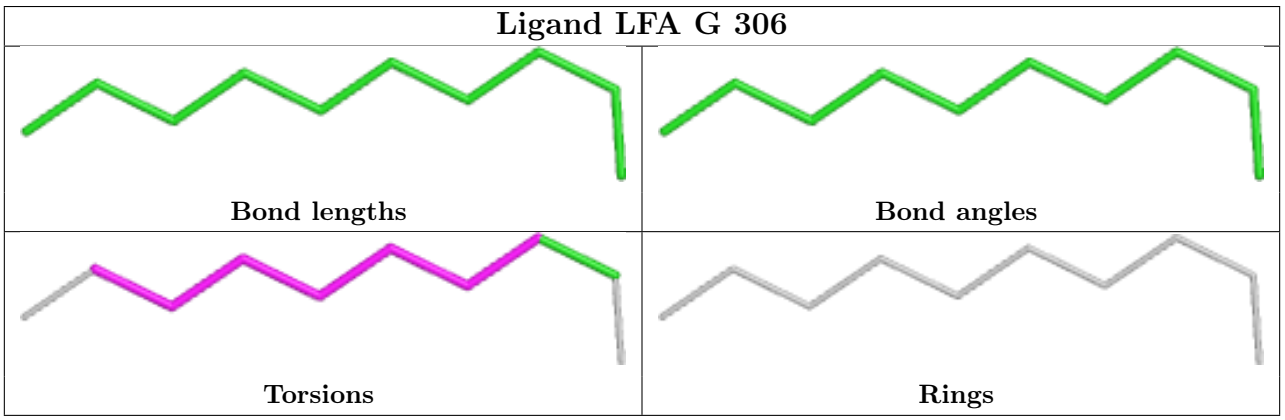
Ligand LFA J 302



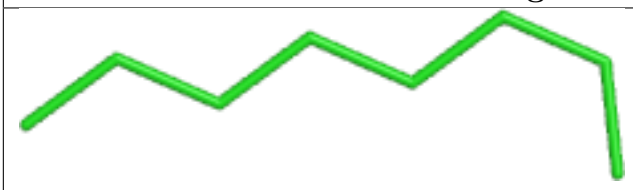
Ligand LFA F 309



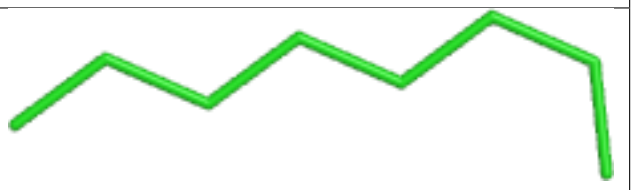
Ligand LFA G 306



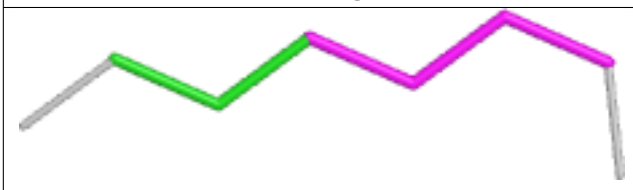
Ligand LFA D 309



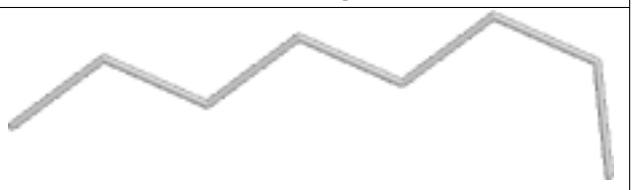
Bond lengths



Bond angles

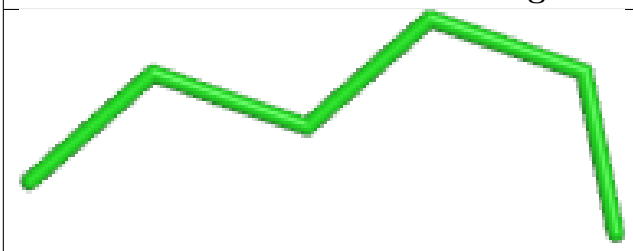


Torsions



Rings

Ligand LFA B 305



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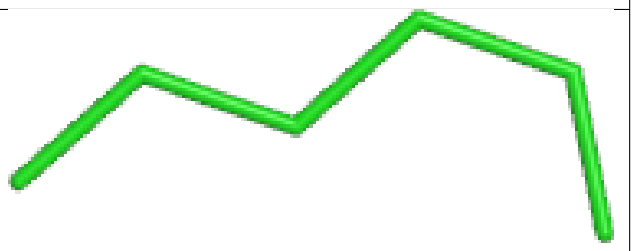
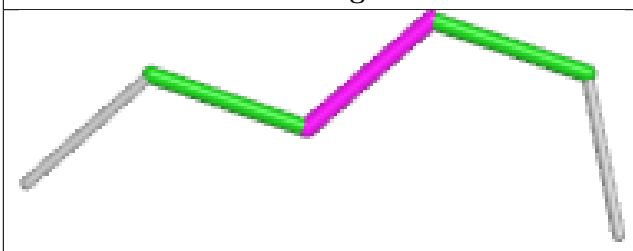


Bond angles



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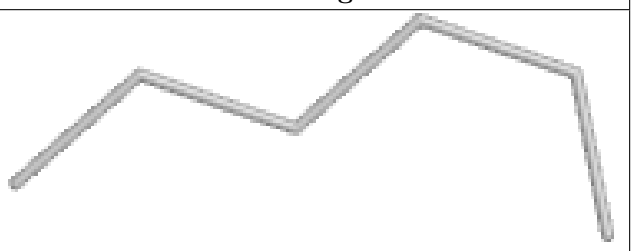
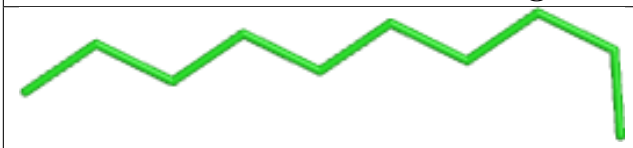
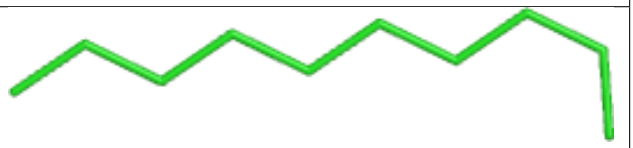


Rings

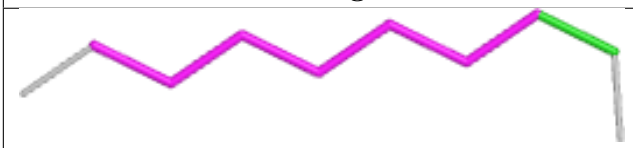
Ligand LFA C 305



Bond lengths



Bond angles



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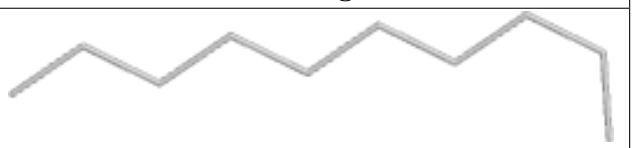
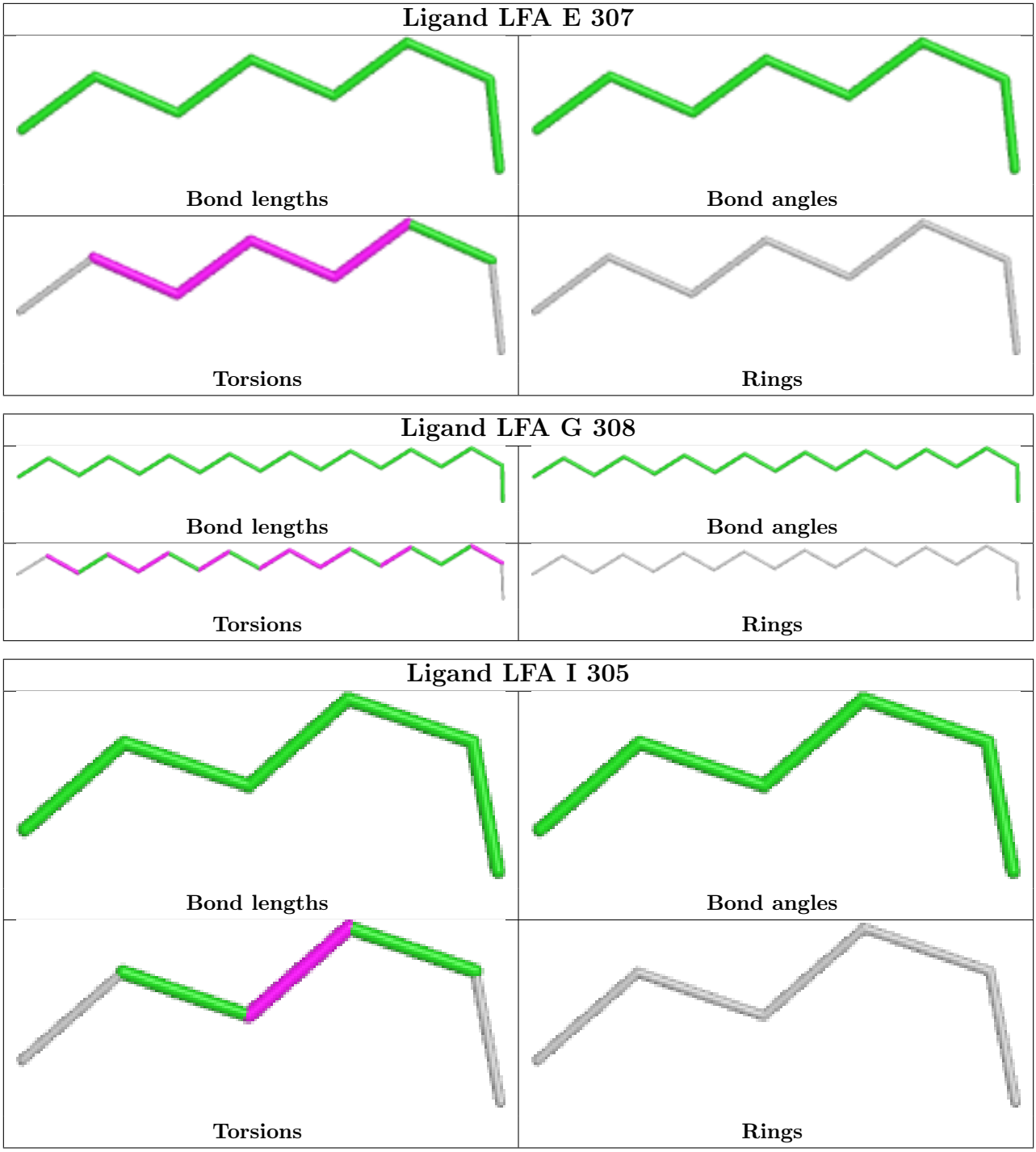
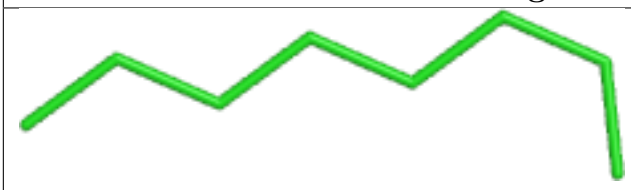


Rings


Ligand LFA E 307
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA G 308
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA I 305
Bond lengths
Bond angles
Torsions
Rings

Ligand LFA B 311



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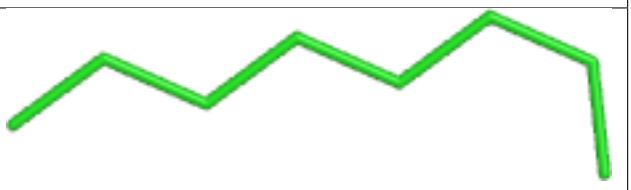
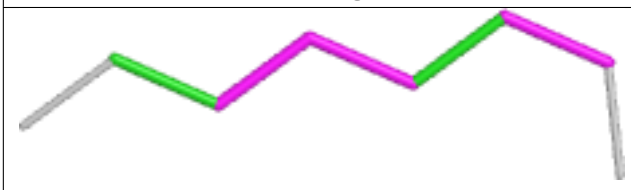


Bond angles



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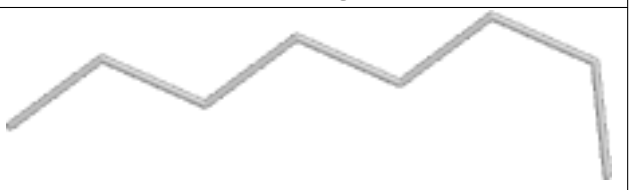
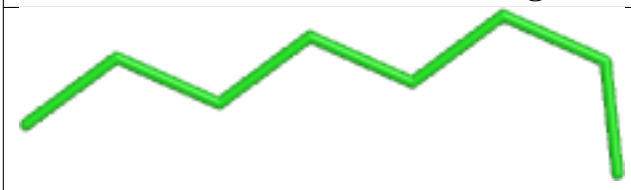


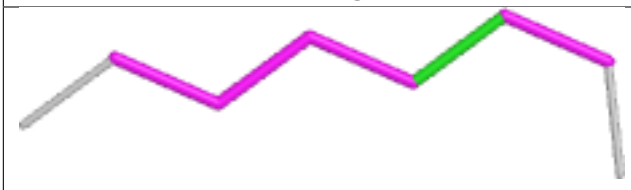
Rings

Ligand LFA G 313



Bond lengths

Bond angles



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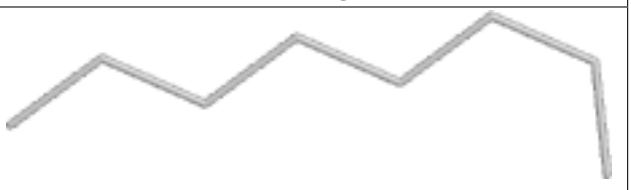
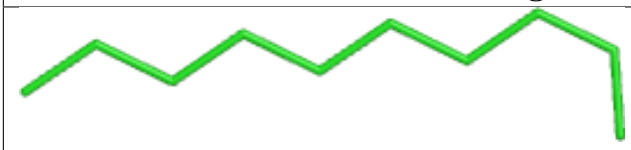


Rings

Ligand LFA A 305



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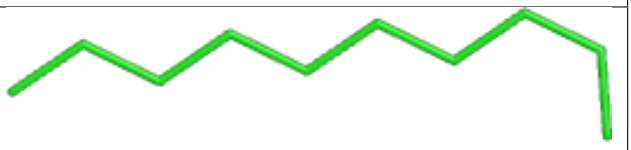
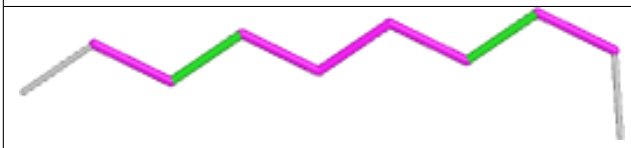
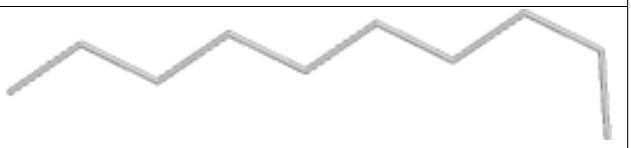


Bond angles

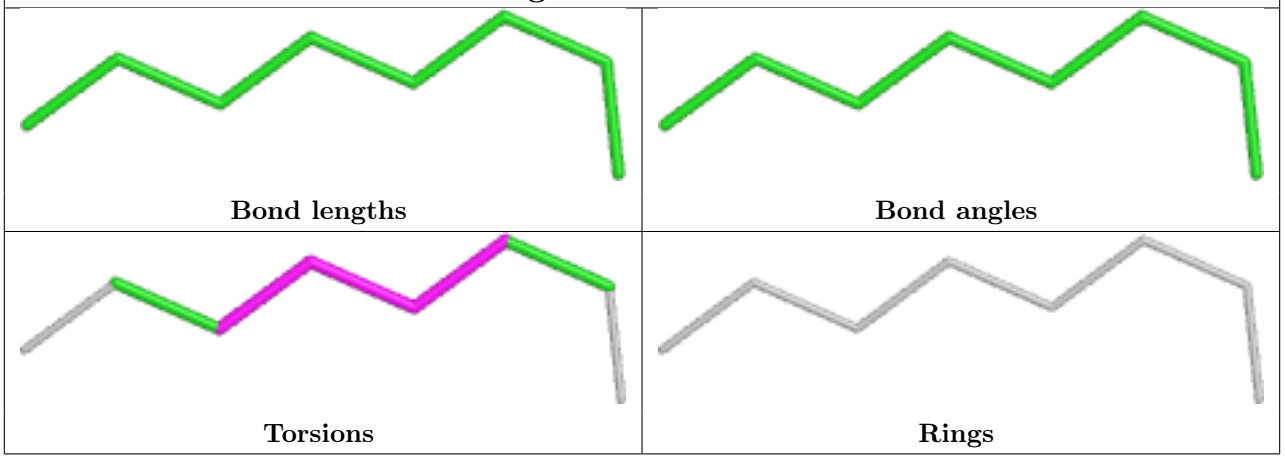


Torsions

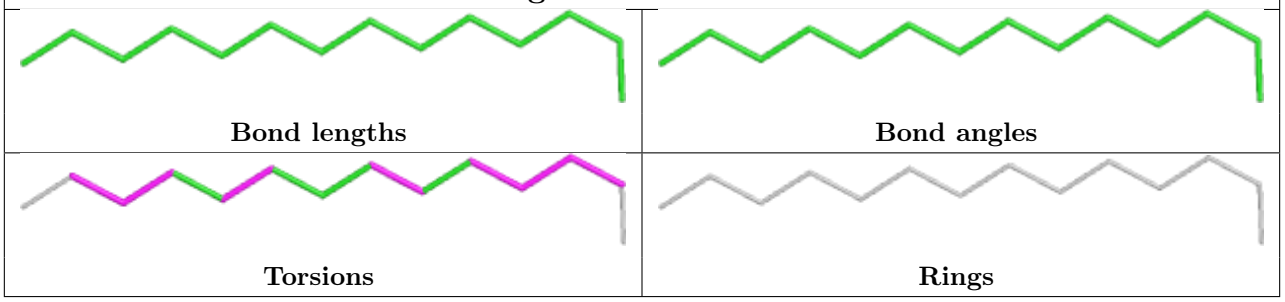


Rings

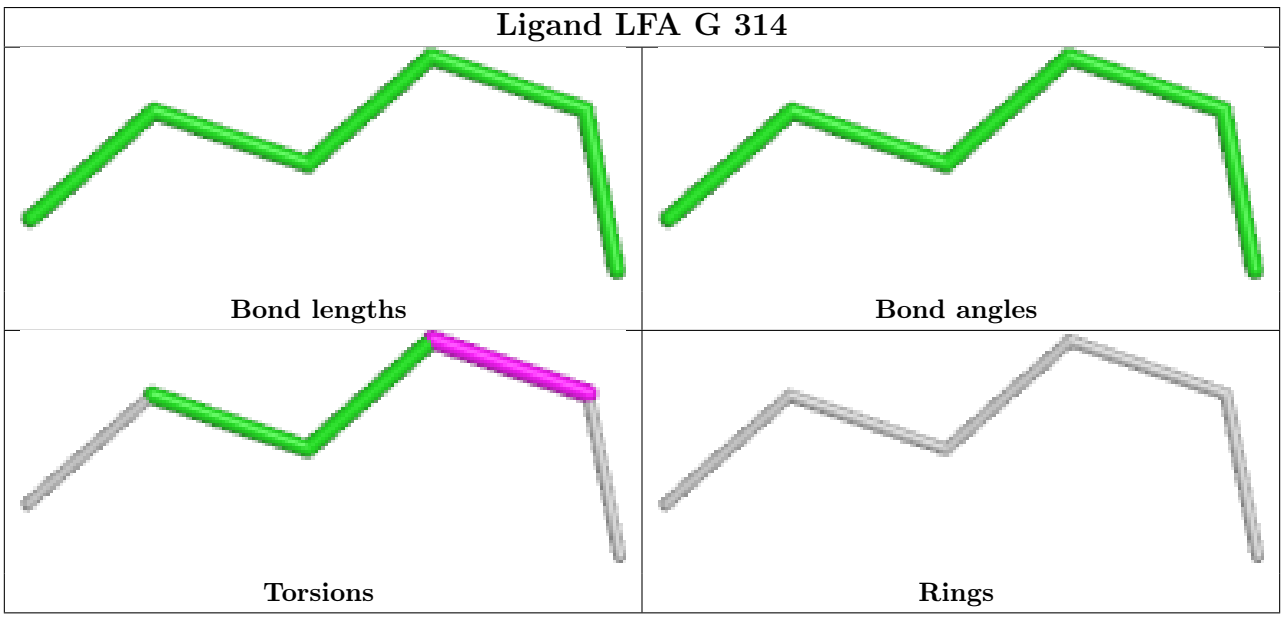
Ligand LFA H 310



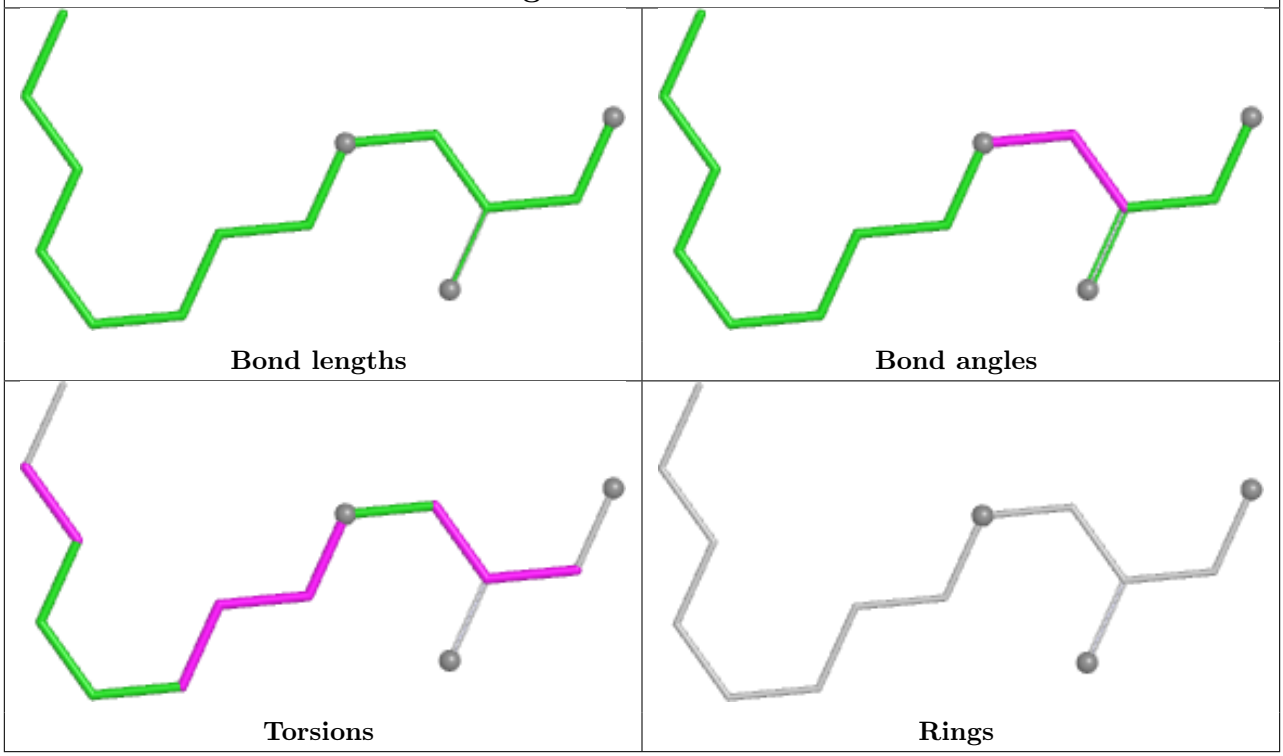
Ligand LFA H 307



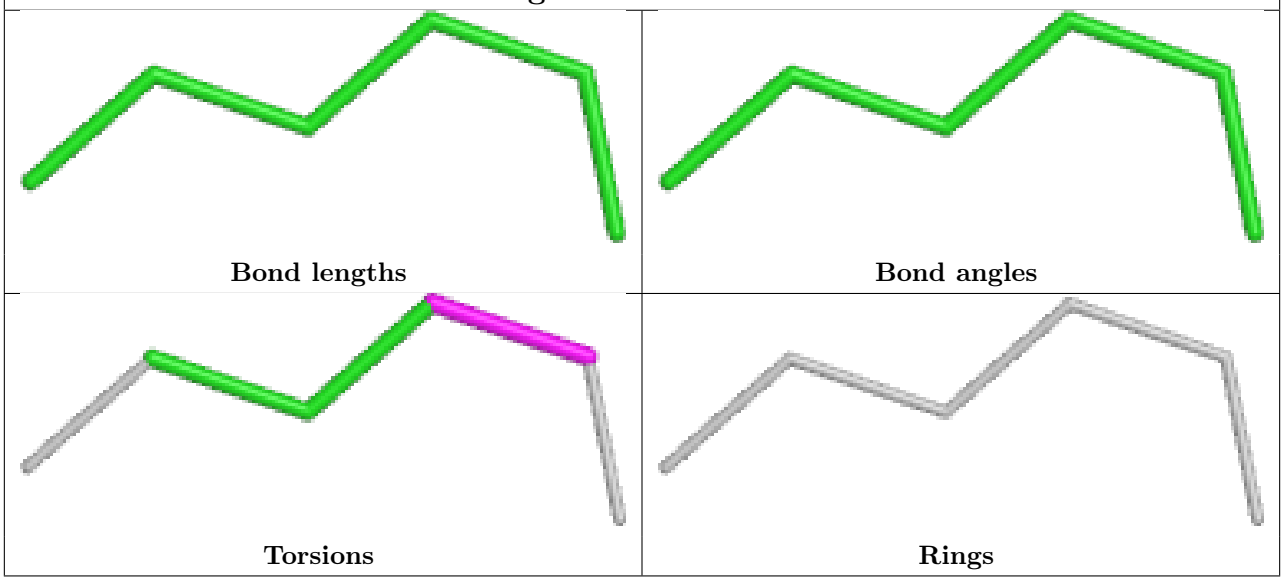
Ligand LFA G 314



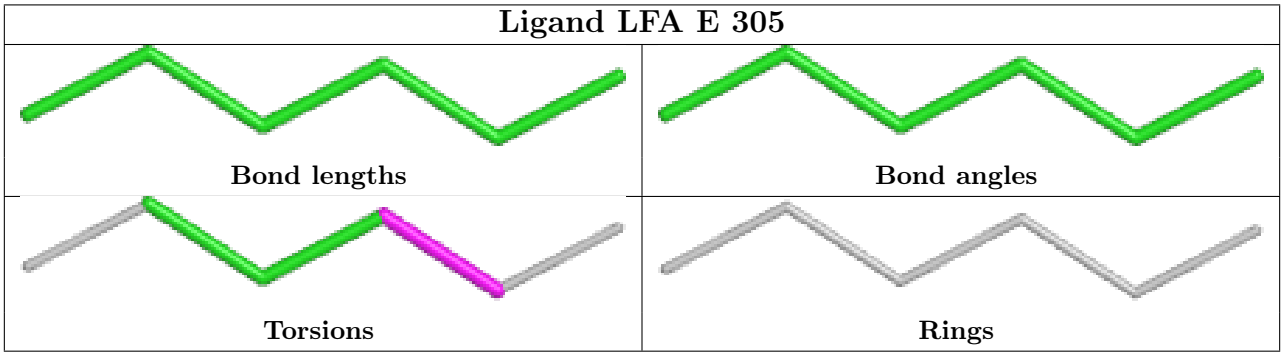
Ligand MPG J 312



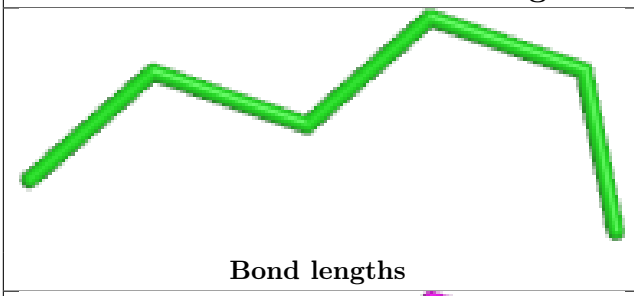
Ligand LFA H 312



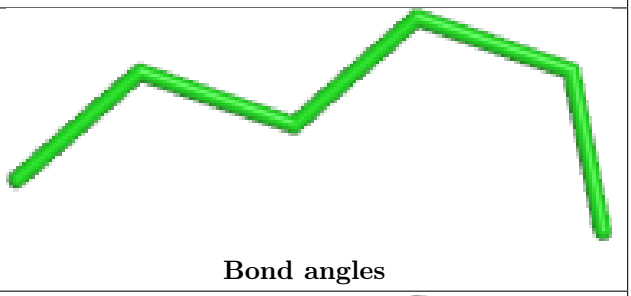
Ligand LFA E 305



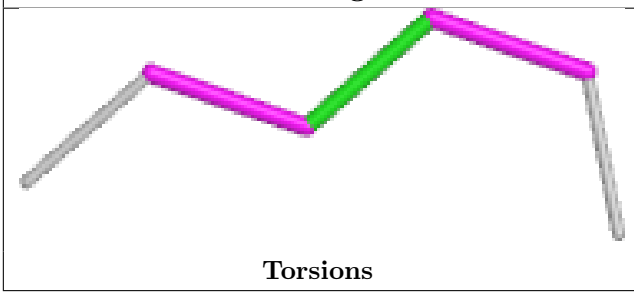
Ligand LFA E 309



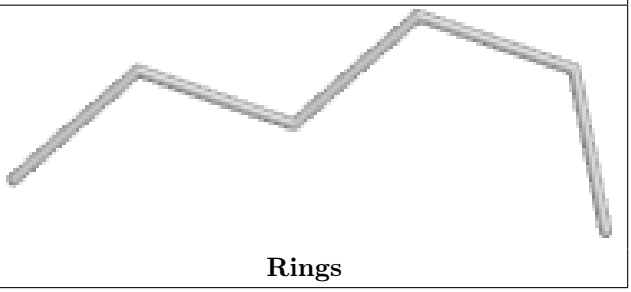
Bond lengths



Bond angles

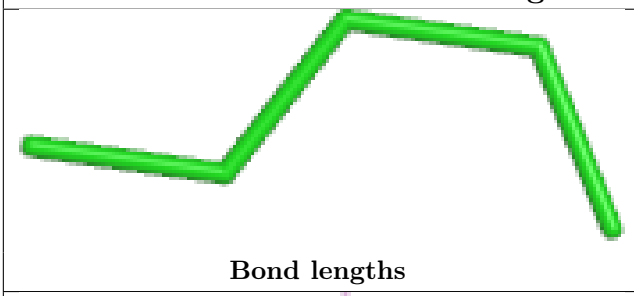


Torsions

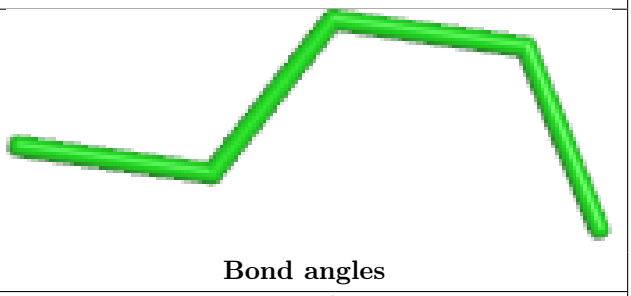


Rings

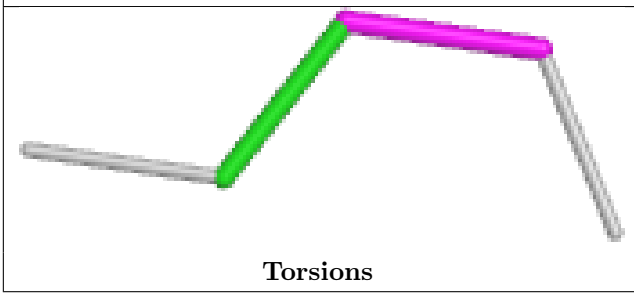
Ligand LFA D 316



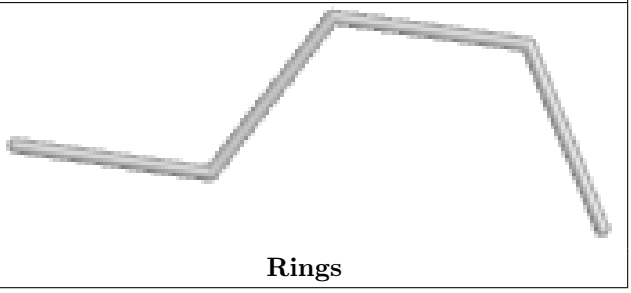
Bond lengths



Bond angles

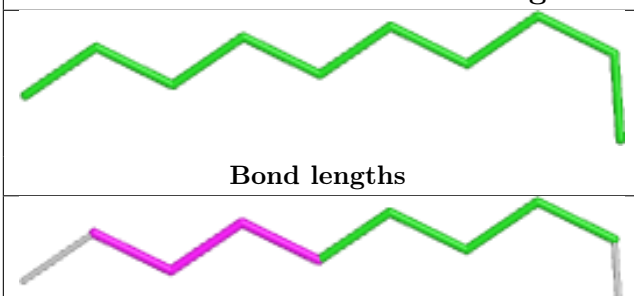


Torsions

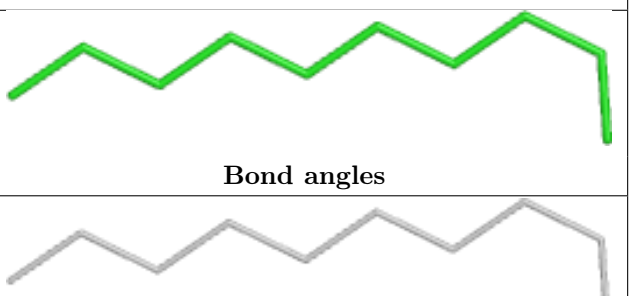


Rings

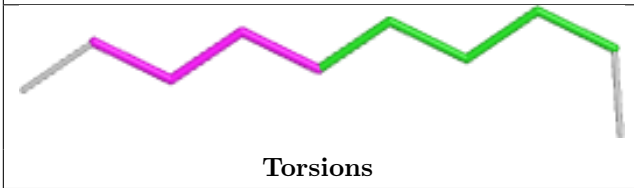
Ligand LFA E 310



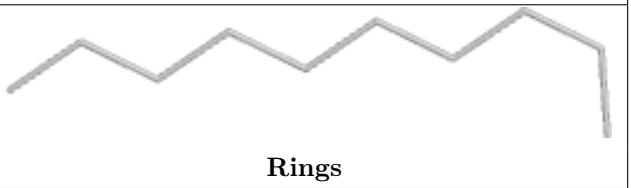
Bond lengths



Bond angles

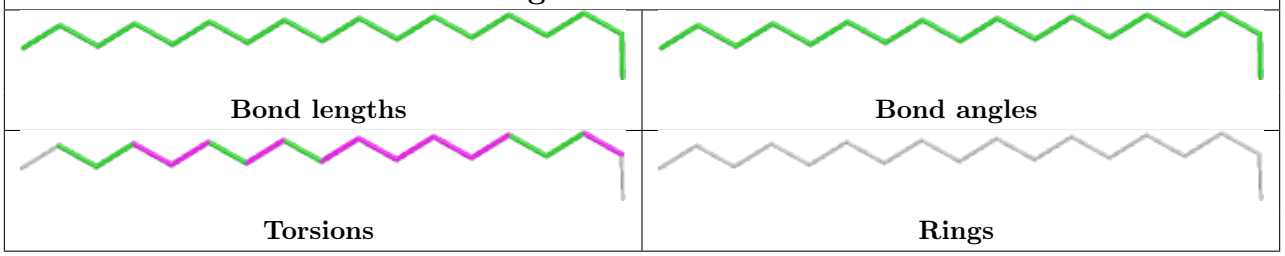


Torsions

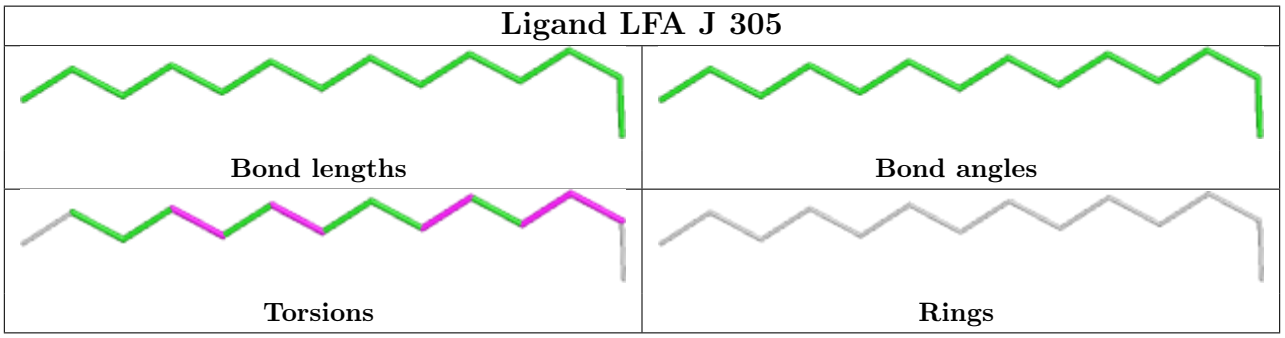


Rings

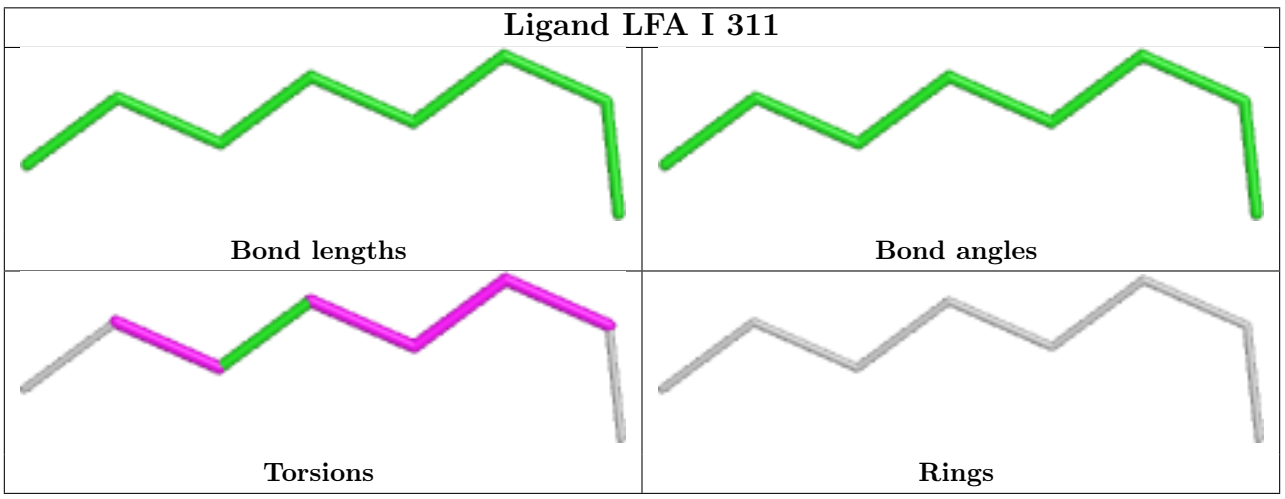
Ligand LFA H 306



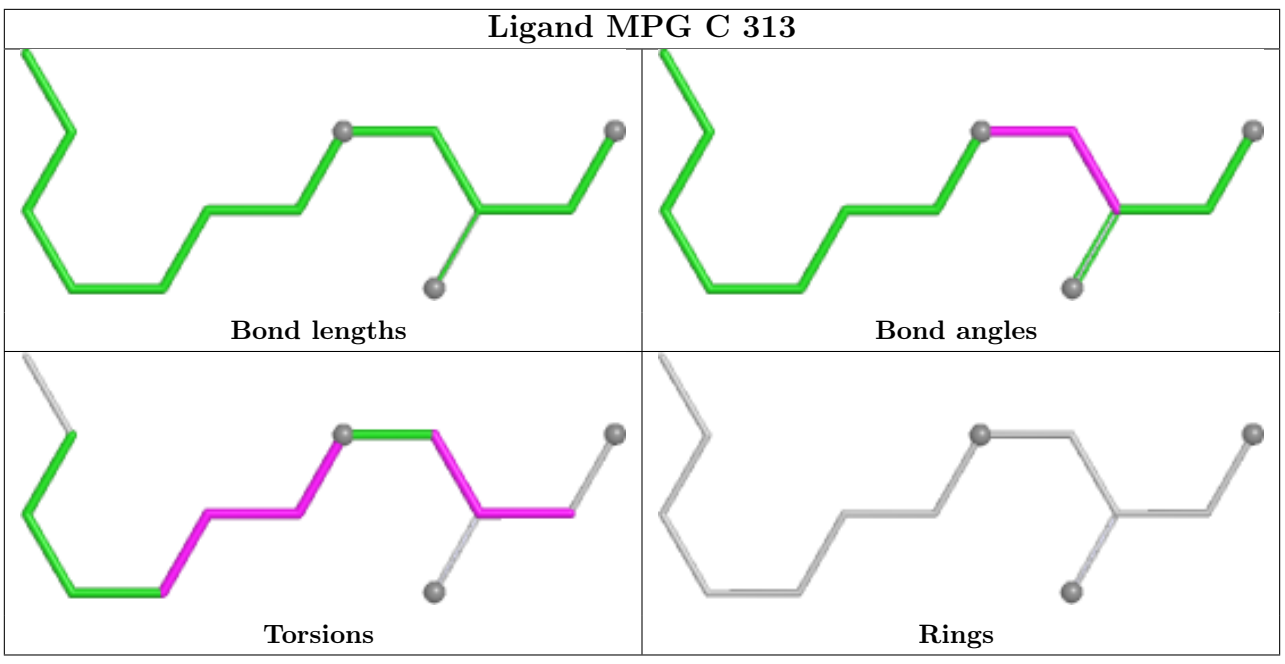
Ligand LFA J 305



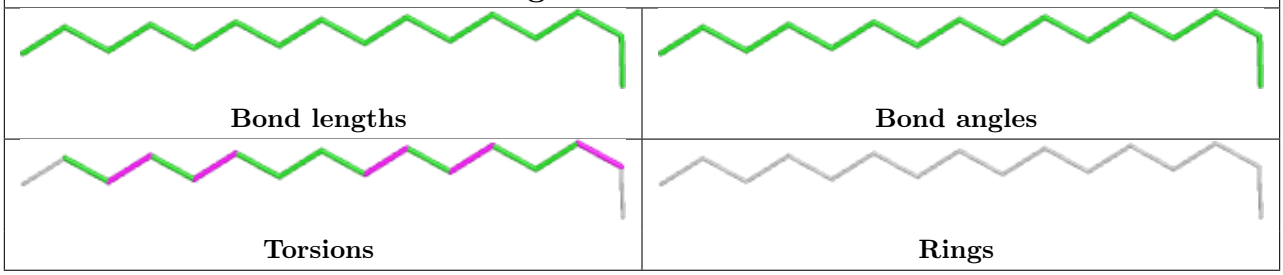
Ligand LFA I 311



Ligand MPG C 313



Ligand LFA G 302



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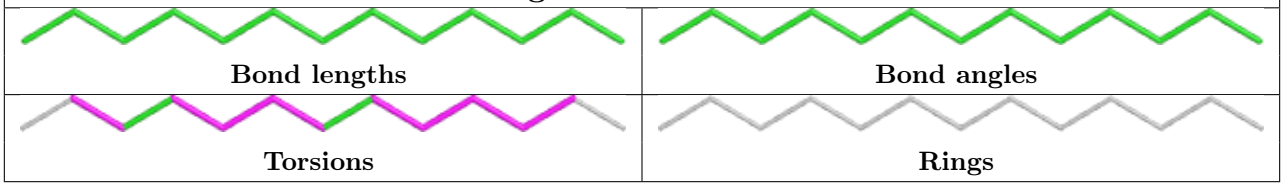

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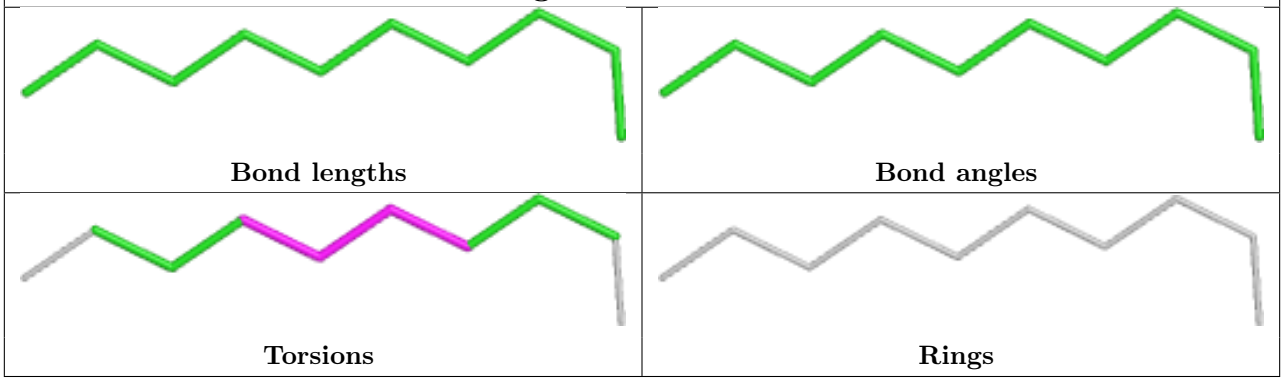
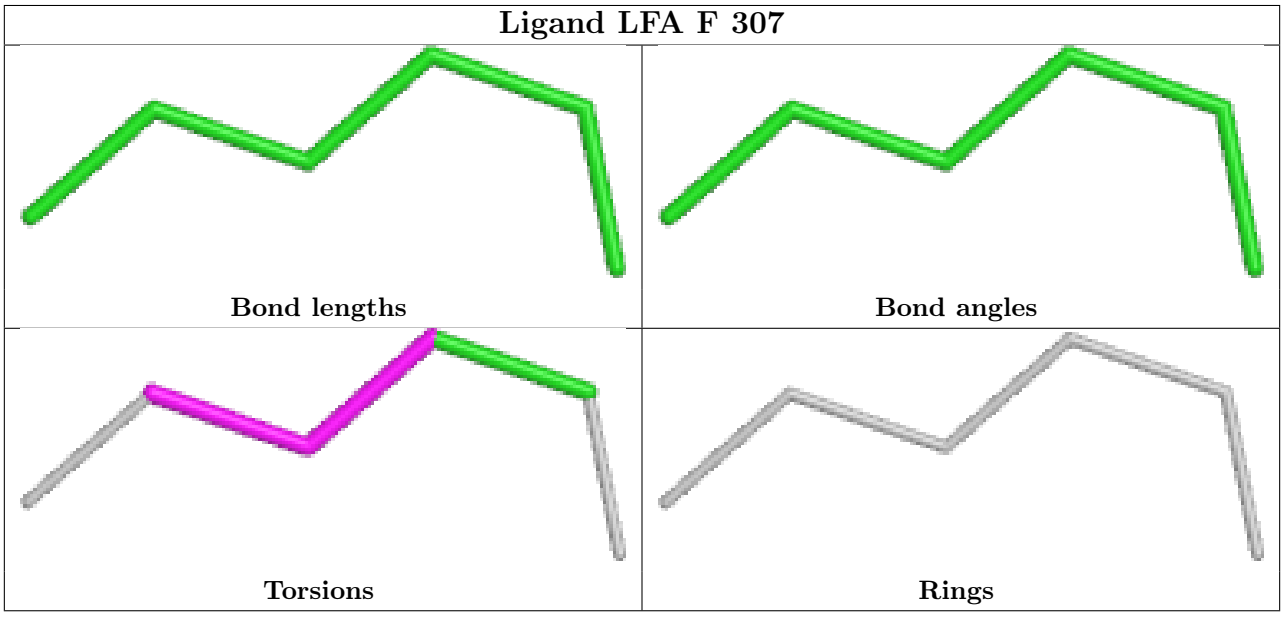
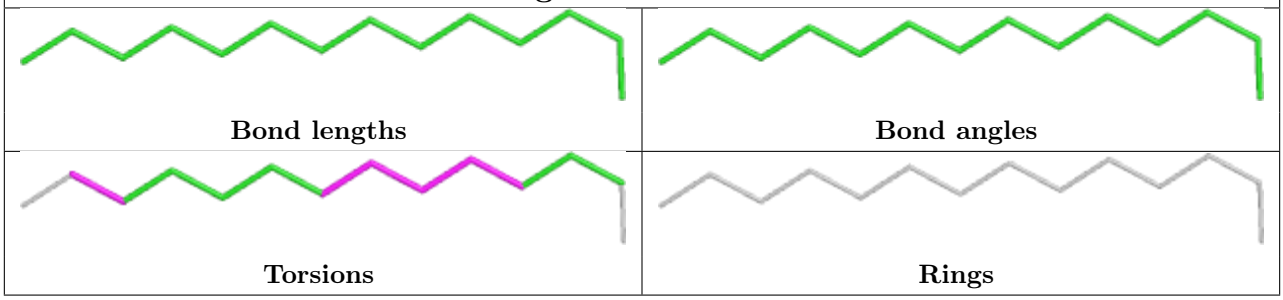


Ligand LFA F 307



Ligand LFA I 304



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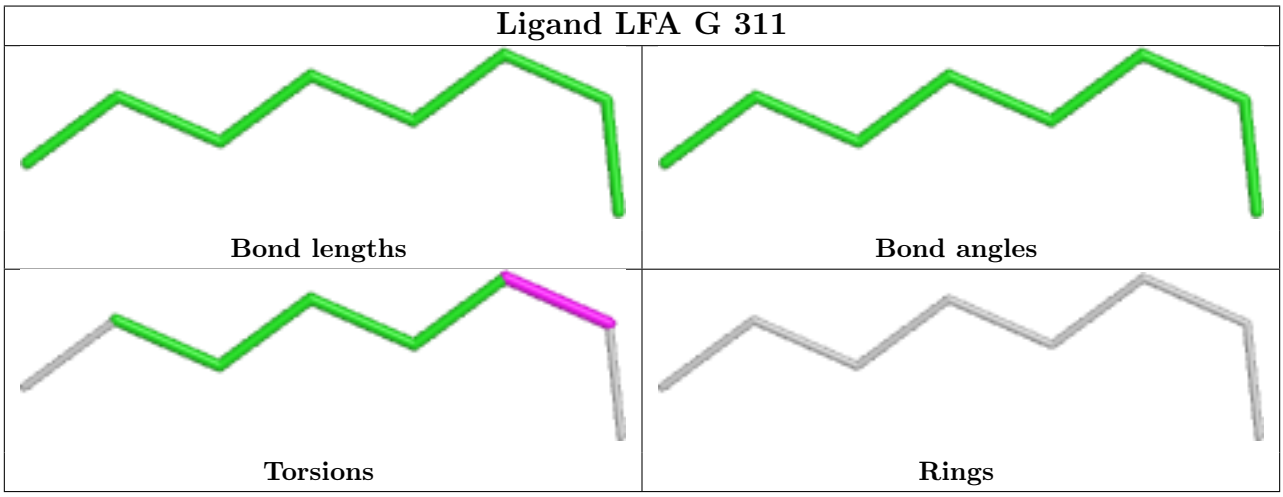
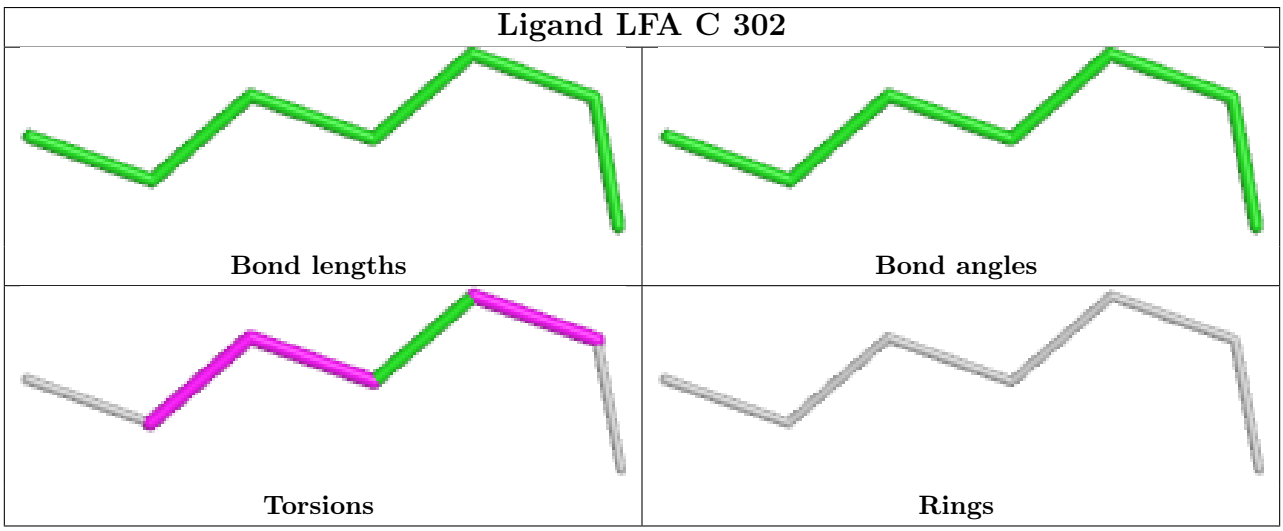
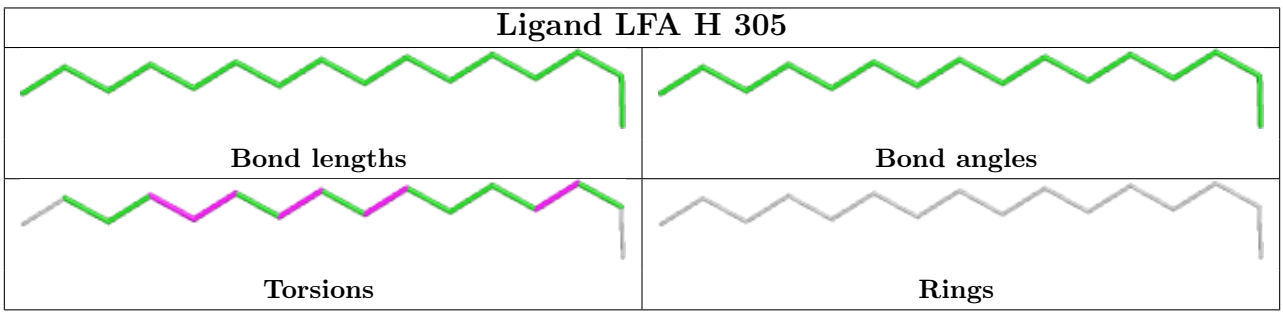


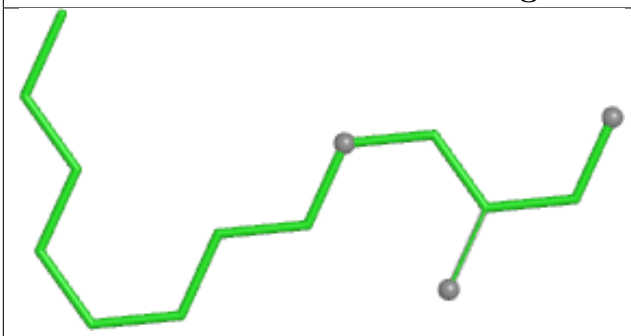
Ligand LFA C 302



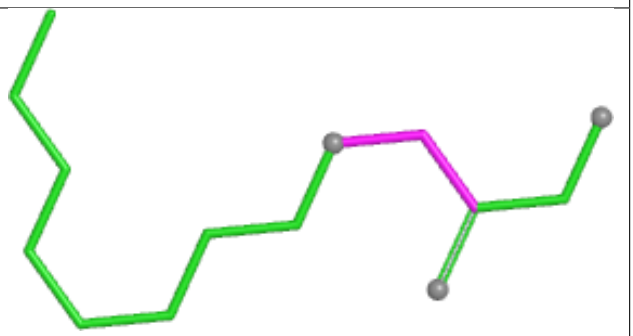
Ligand LFA H 305



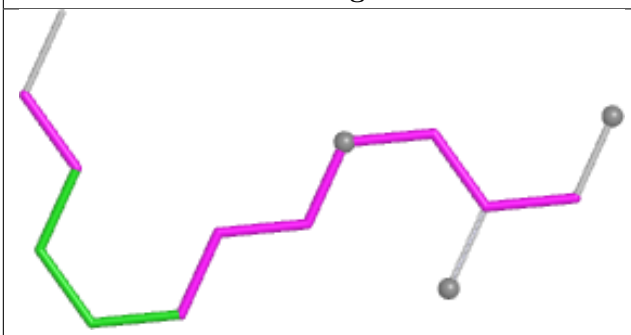
Ligand MPG F 315



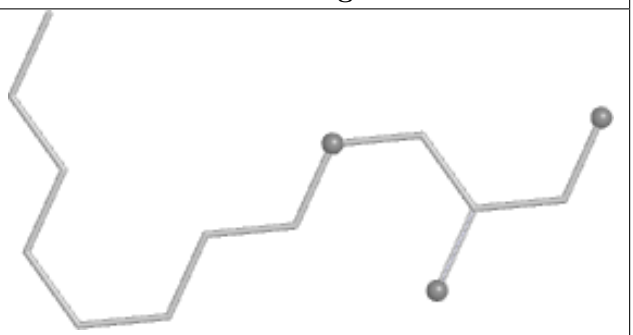
Bond lengths



Bond angles

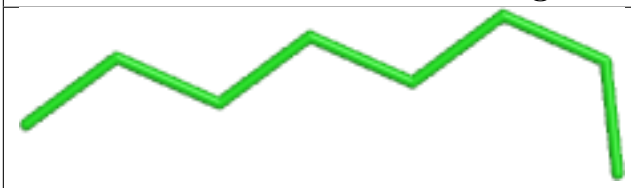


Torsions



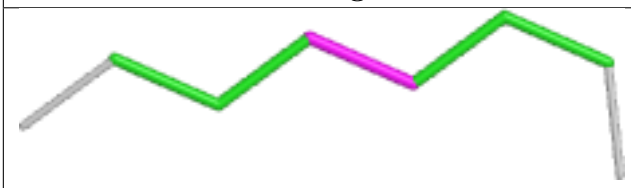
Rings

Ligand LFA J 304

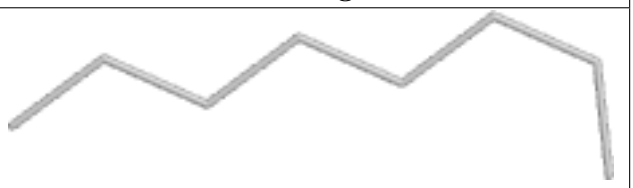


Bond lengths

Bond angles

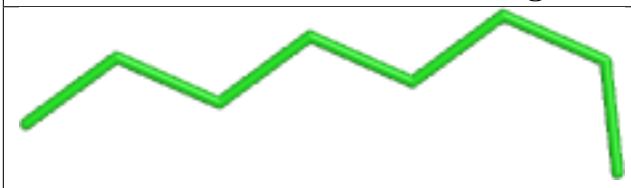


Torsions

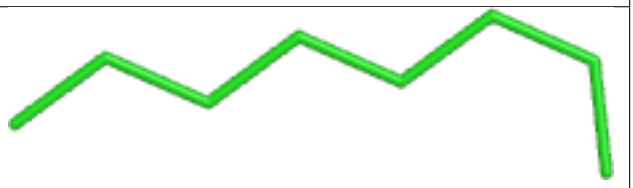


Rings

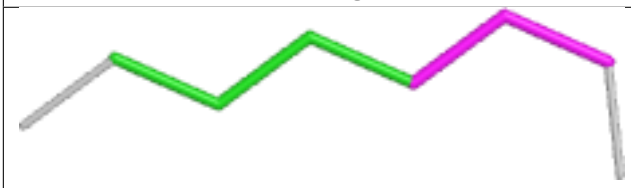
Ligand LFA G 309



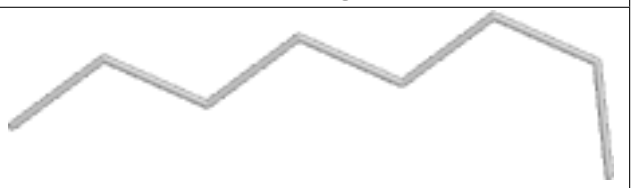
Bond lengths



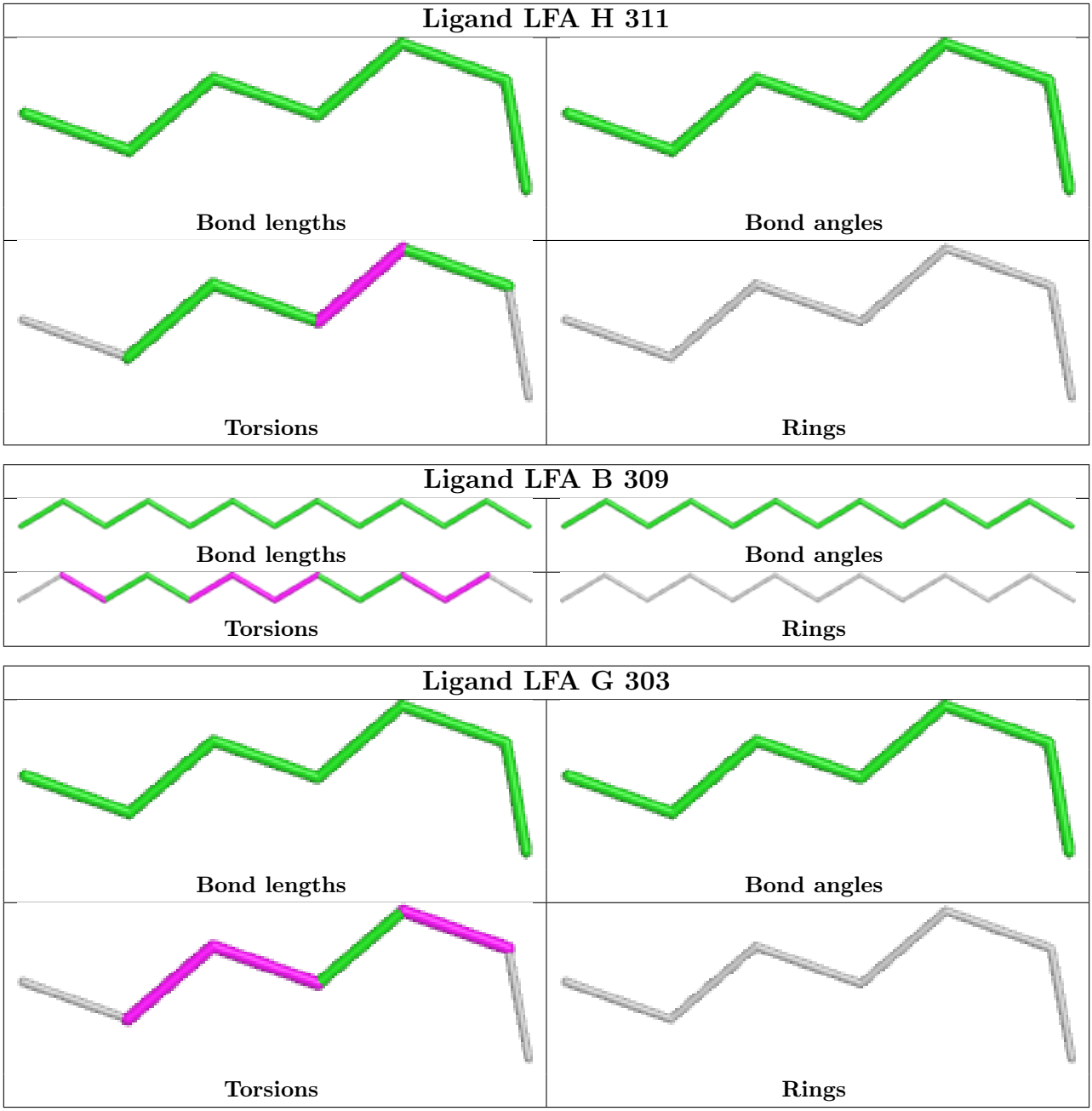
Bond angles



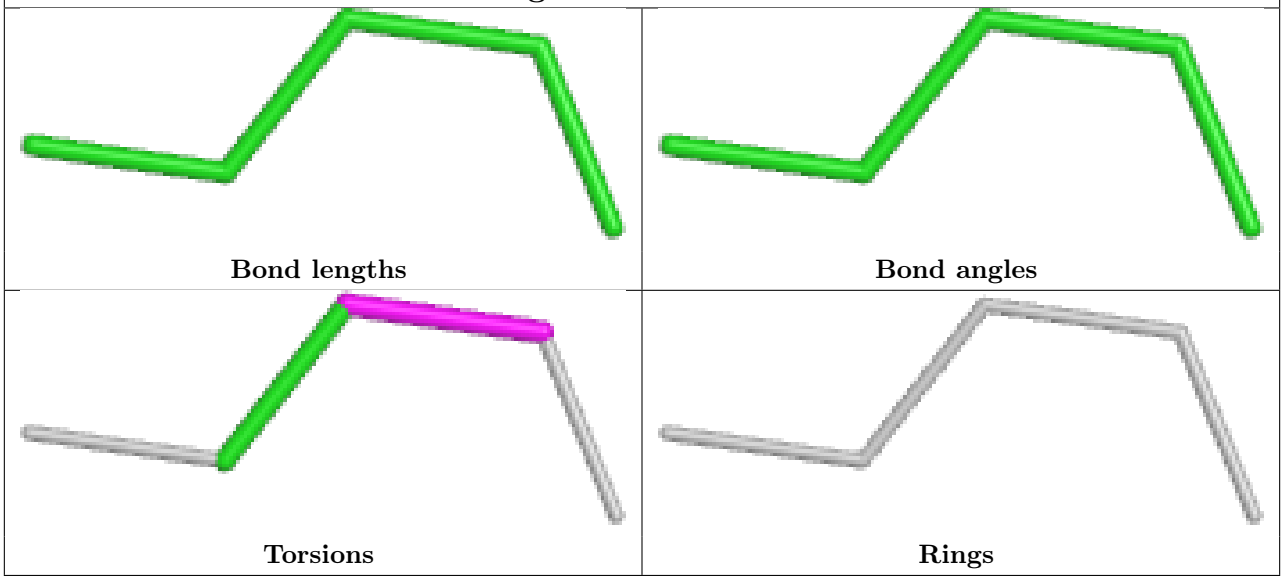
Torsions



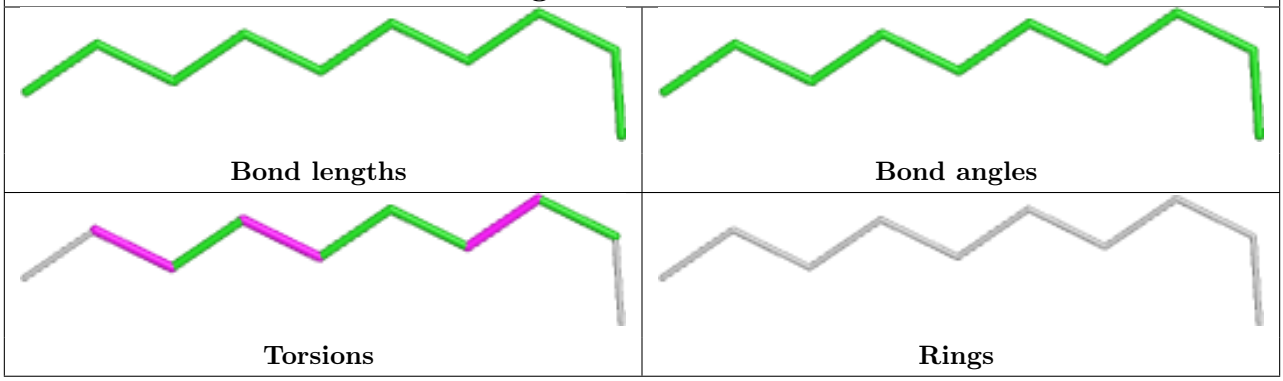
Rings


Ligand LFA H 311
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA B 309
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA G 303
Bond lengths
Bond angles
Torsions
Rings

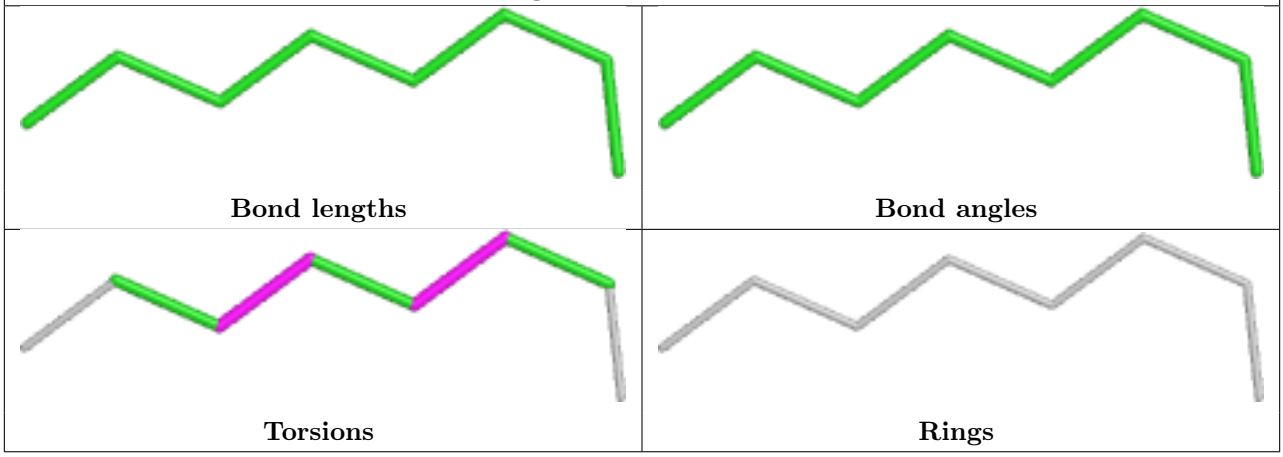
Ligand LFA H 309



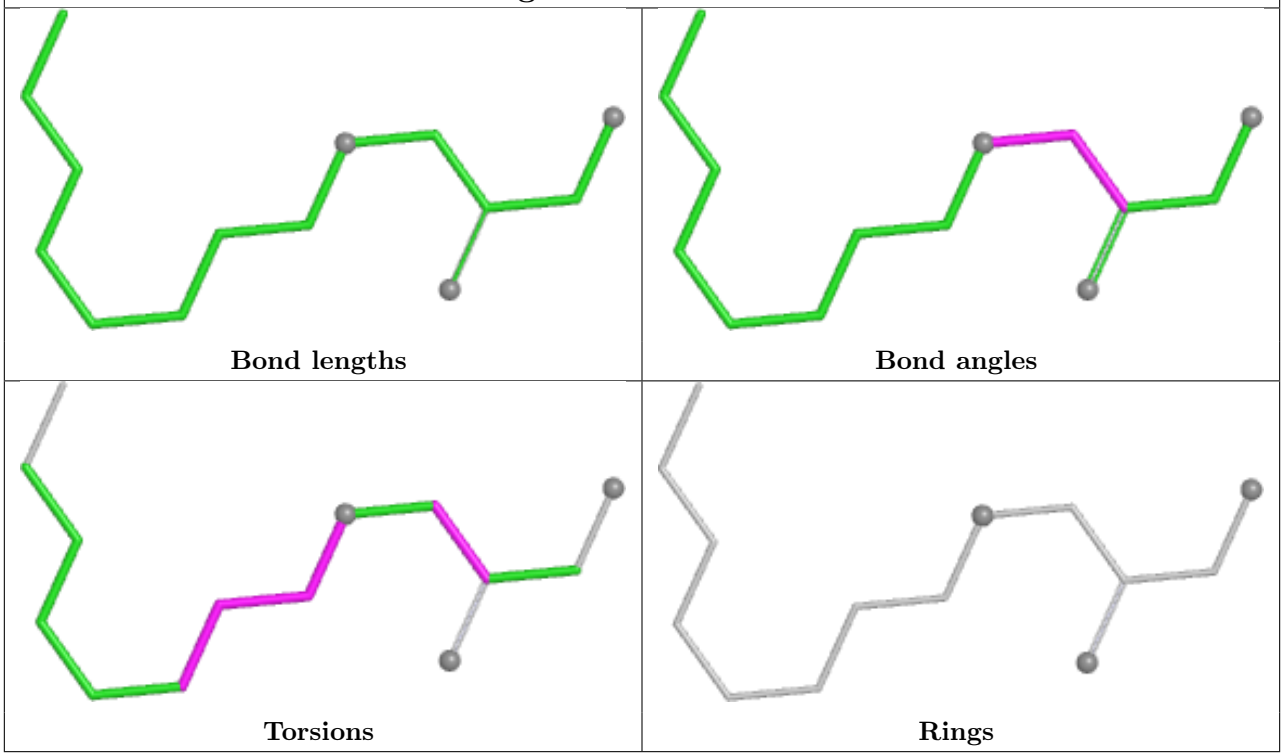
Ligand LFA F 311



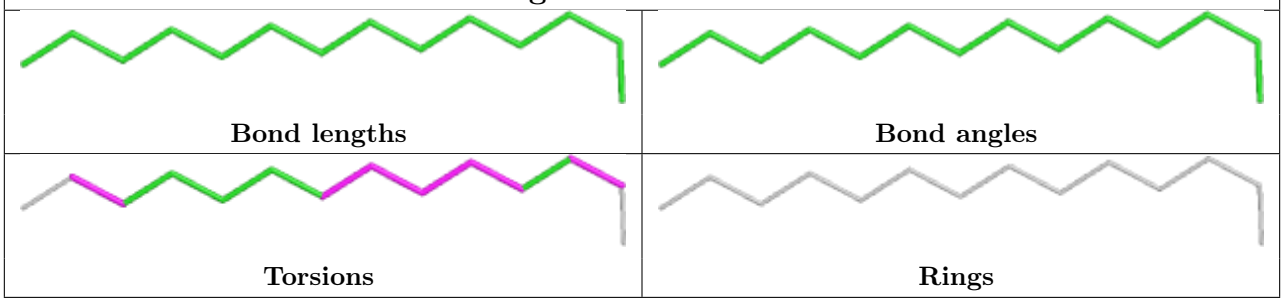
Ligand LFA H 308



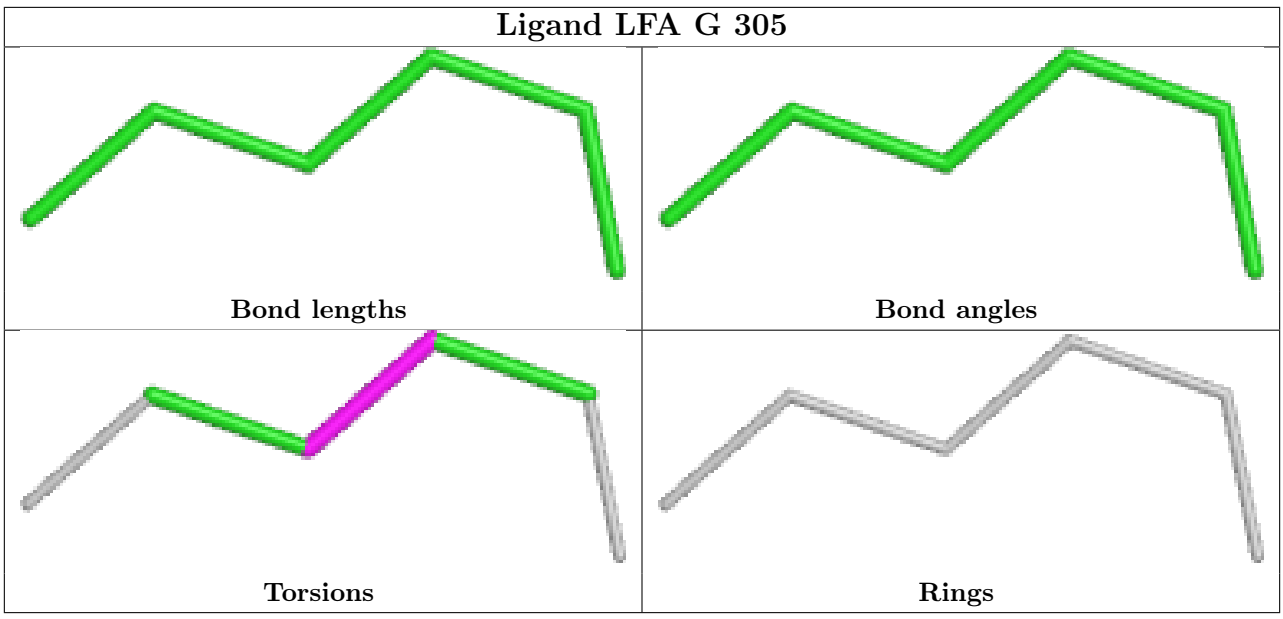
Ligand MPG G 312



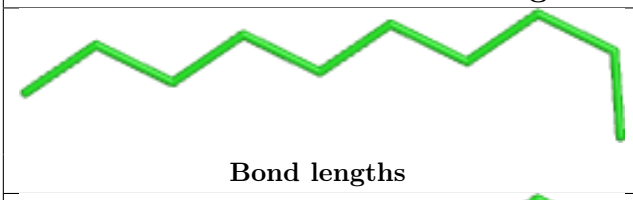
Ligand LFA B 304



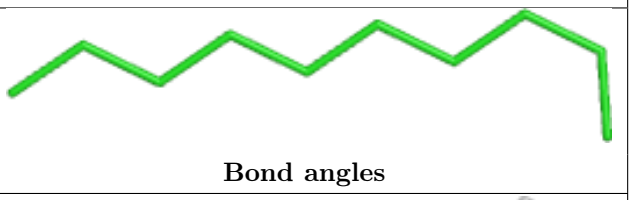
Ligand LFA G 305



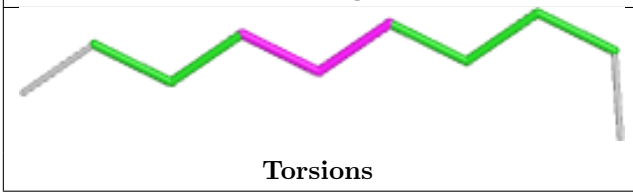
Ligand LFA F 304



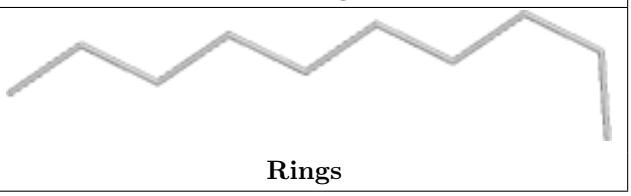
Bond lengths



Bond angles



Torsions

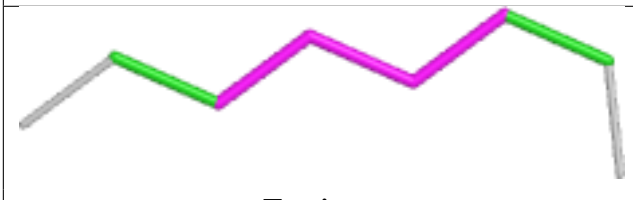


Rings

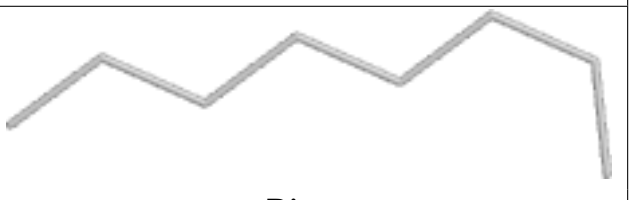
Ligand LFA C 309

Bond lengths

Bond angles

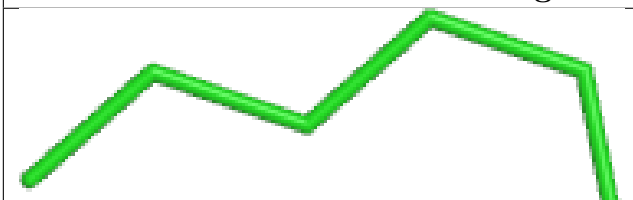


Torsions

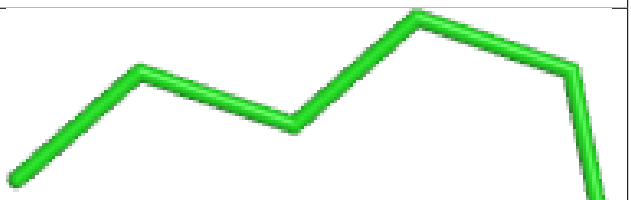


Rings

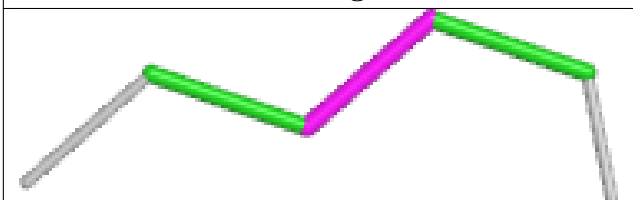
Ligand LFA I 307



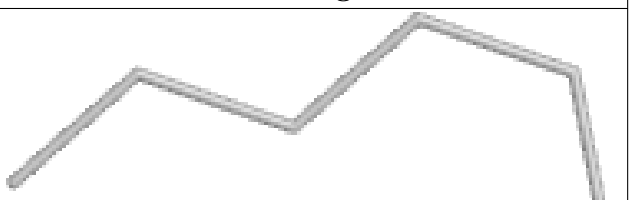
Bond lengths



Bond angles

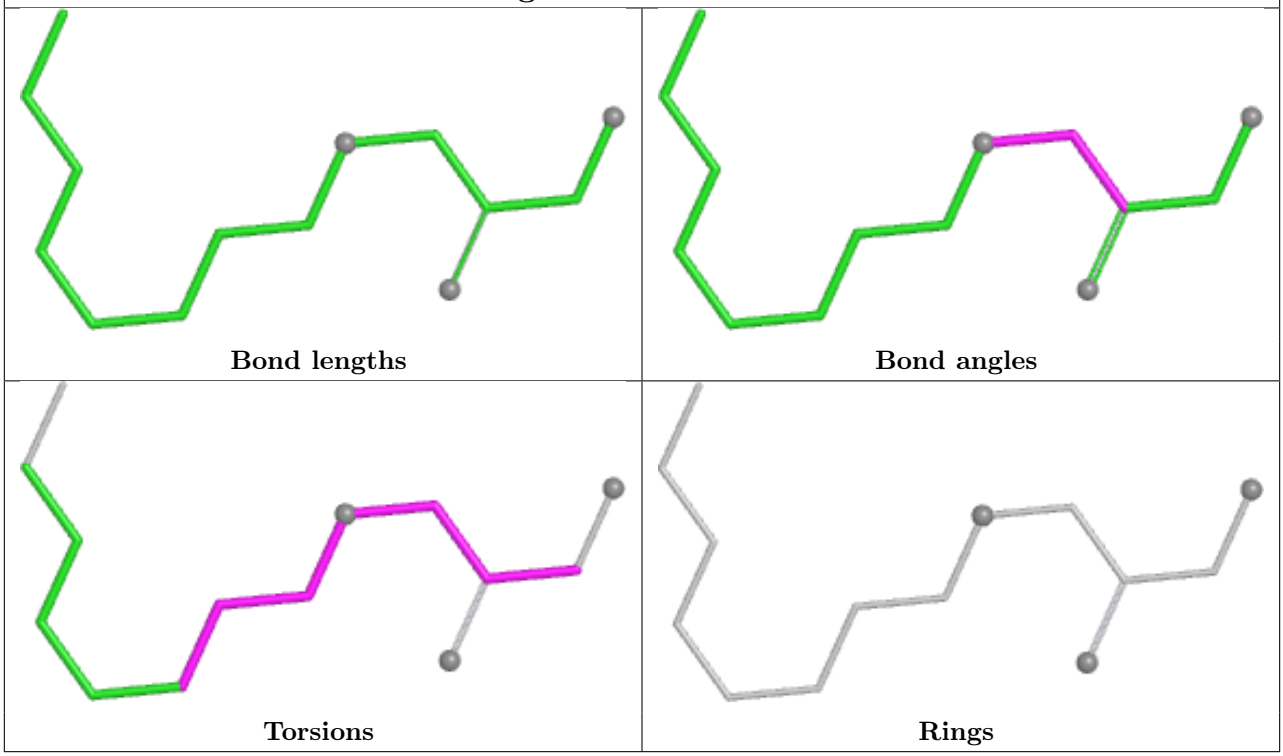


Torsions

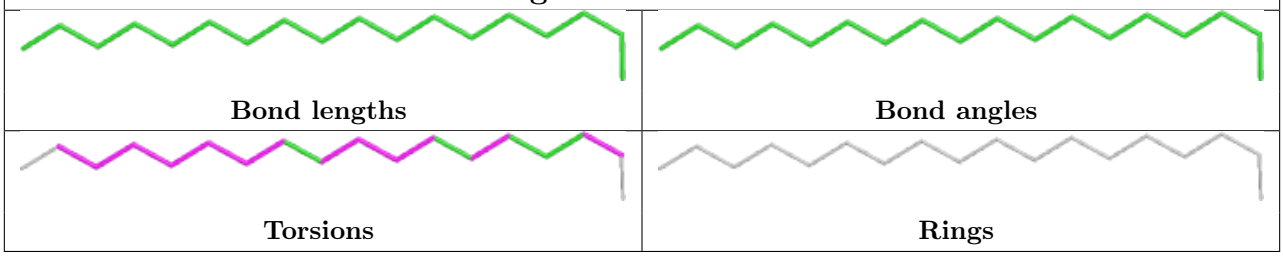


Rings

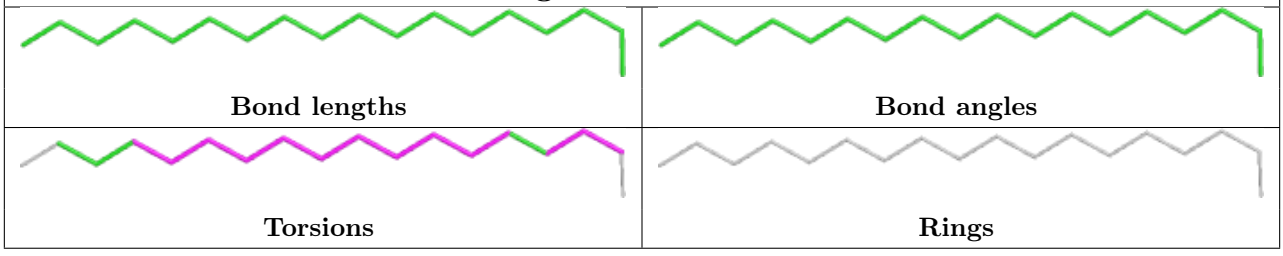
Ligand MPG H 313



Ligand LFA E 303



Ligand LFA I 309



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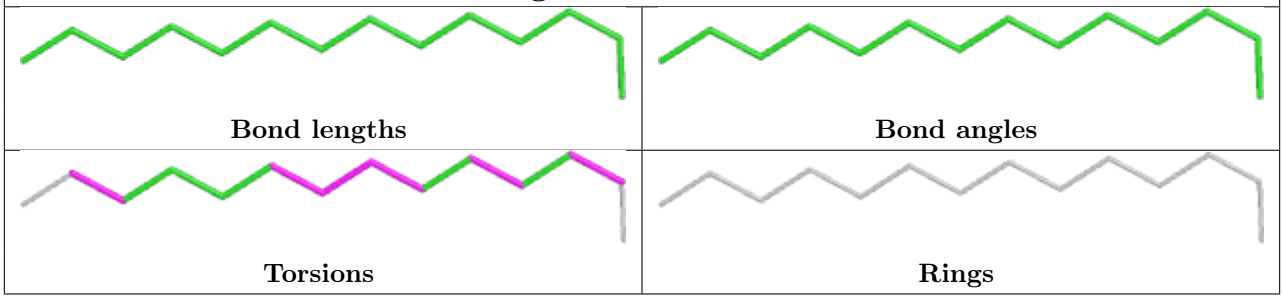

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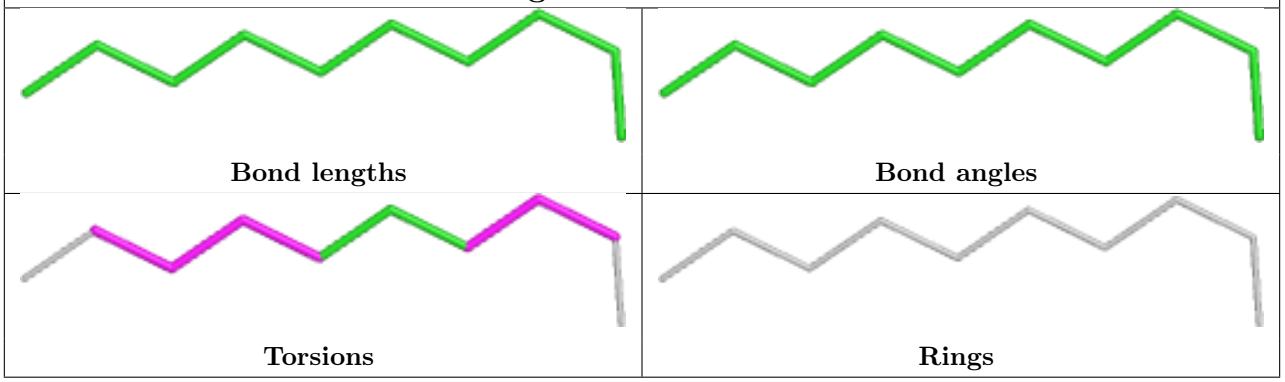
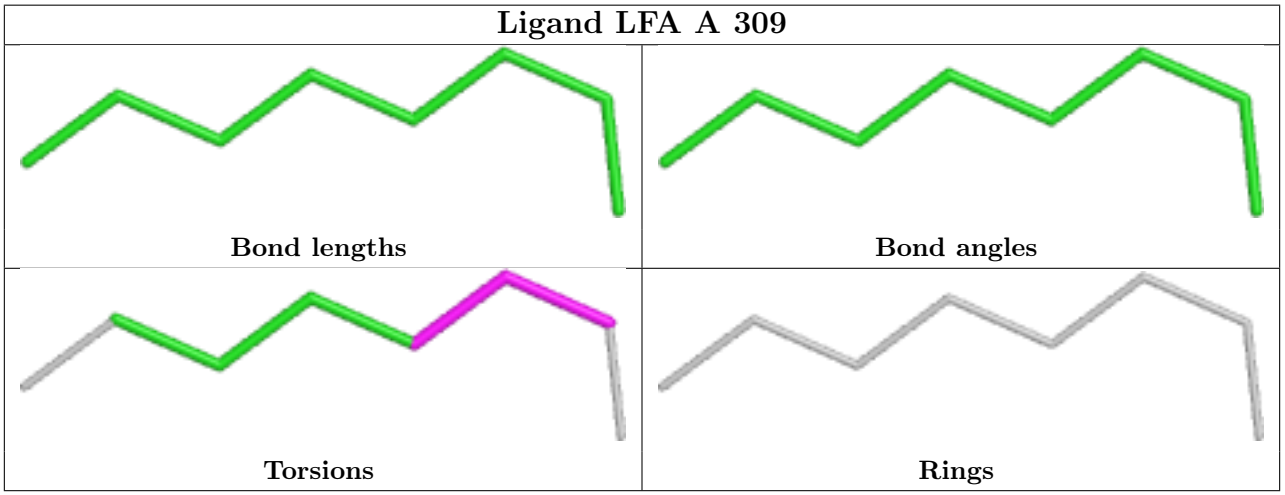
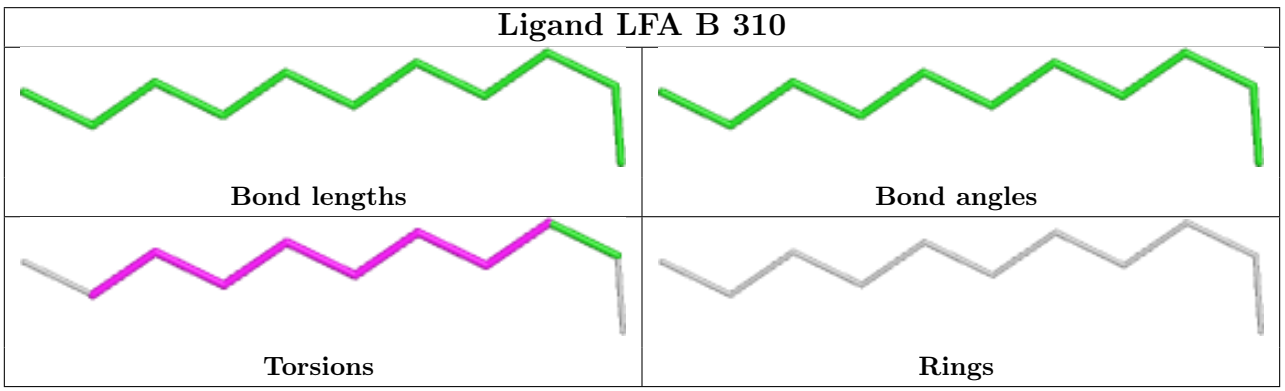


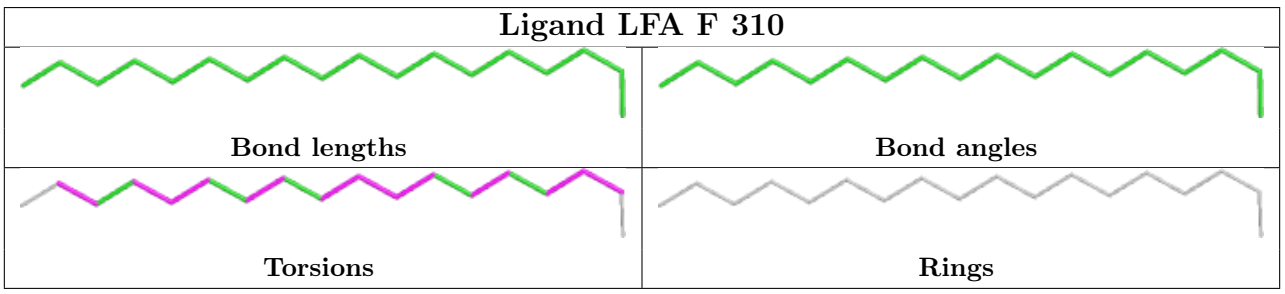
Ligand LFA A 309



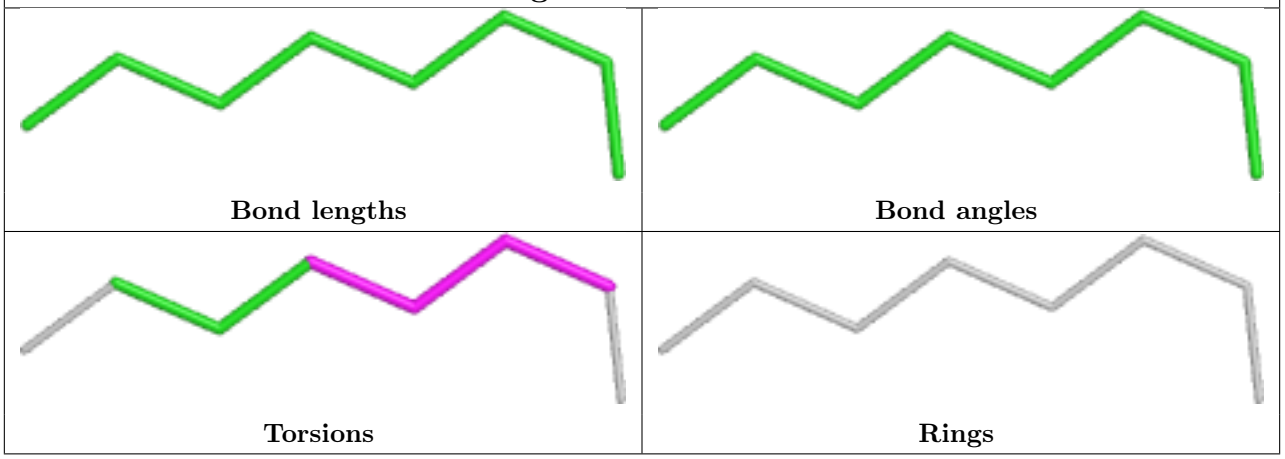
Ligand LFA B 310



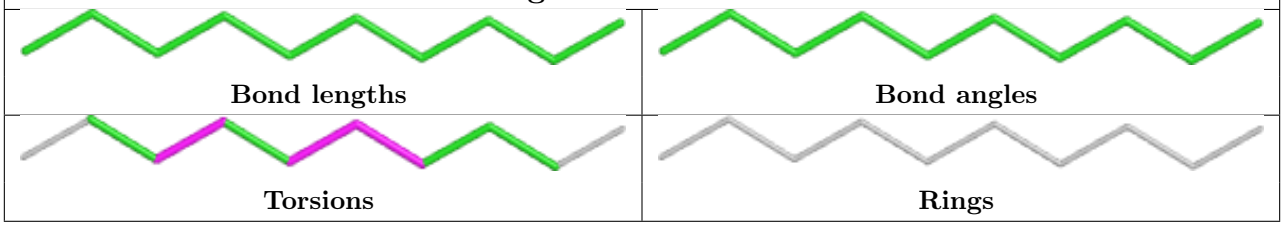
Ligand LFA F 310



Ligand LFA F 312



Ligand LFA G 310



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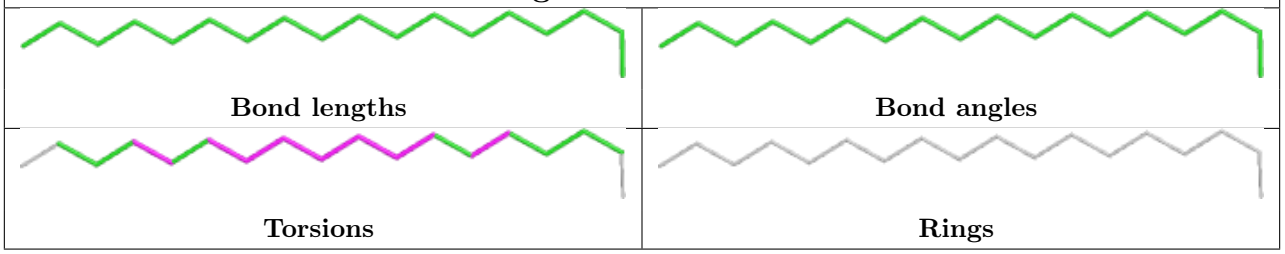

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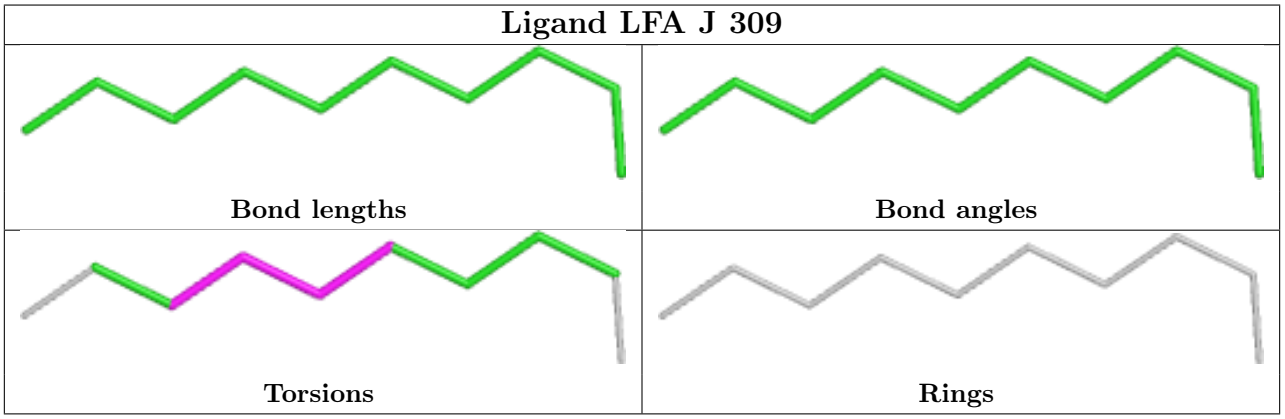
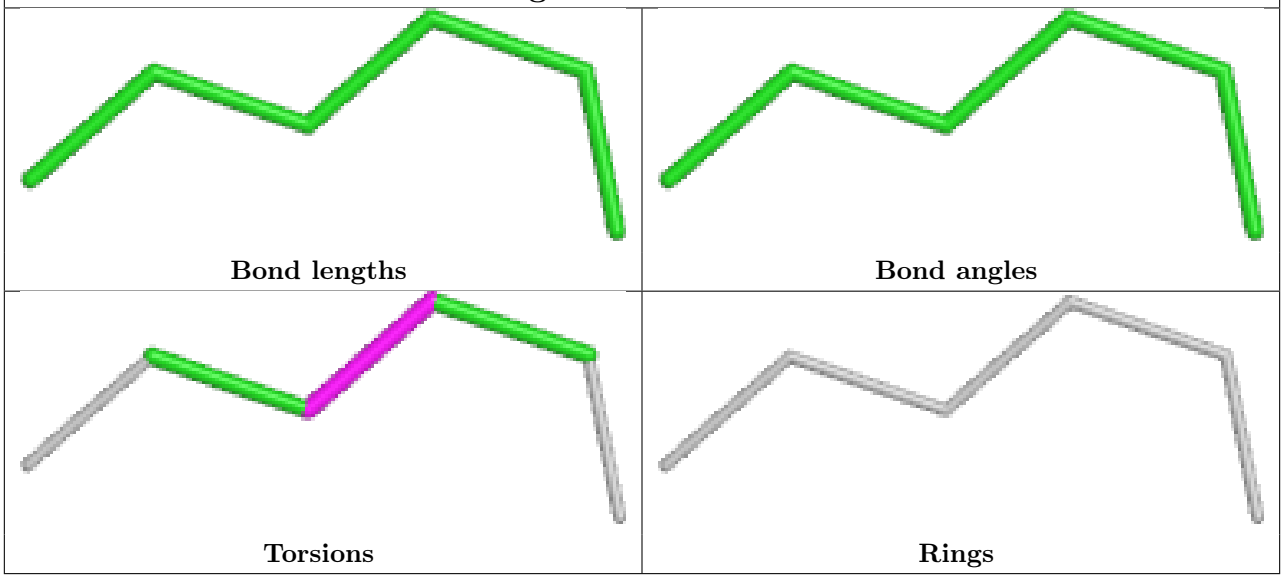


Ligand LFA C 304



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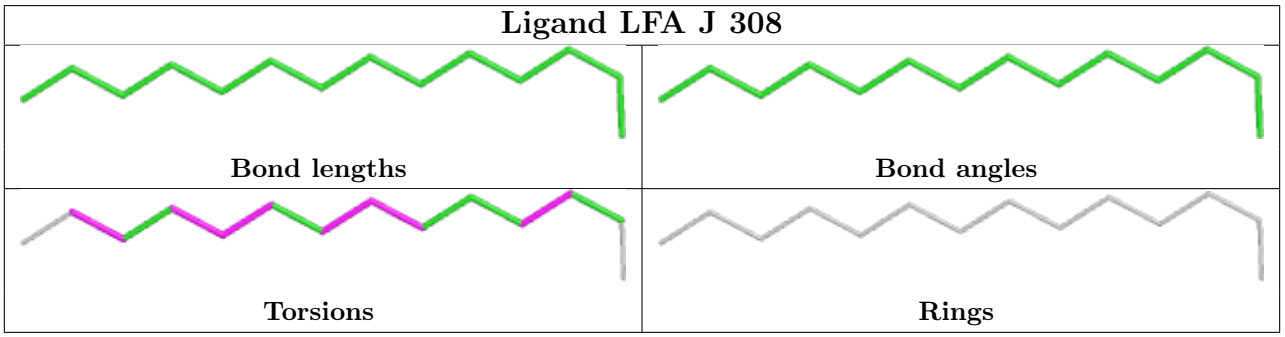
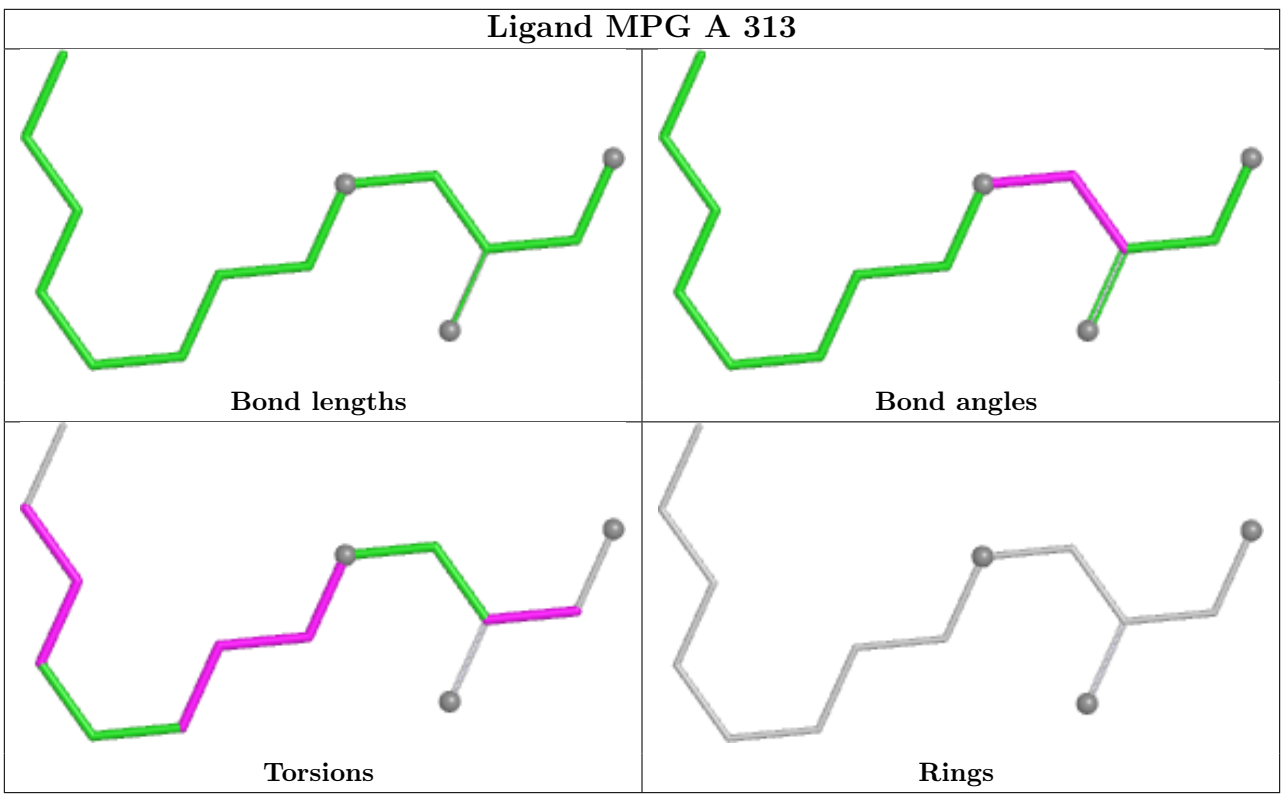
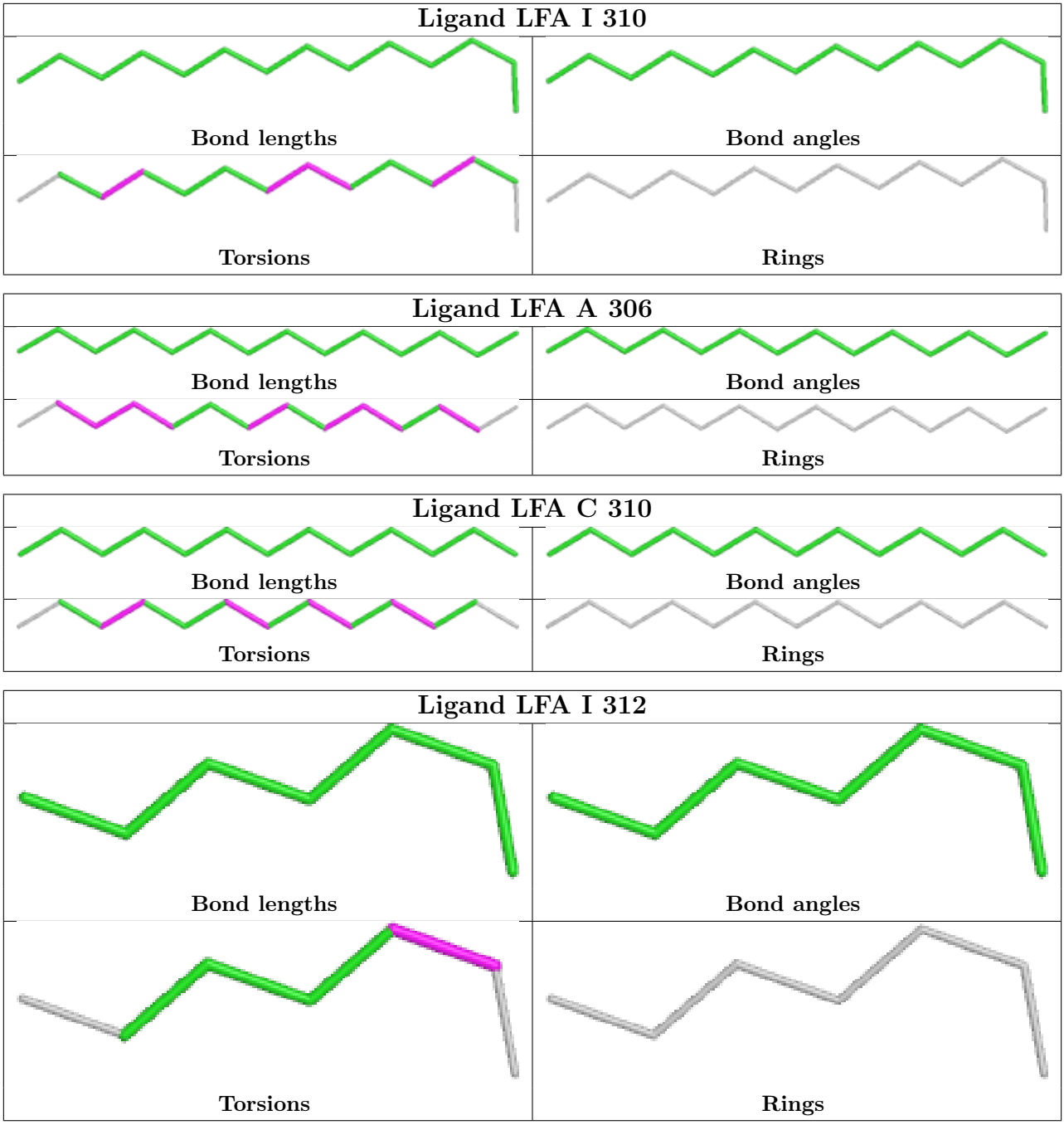
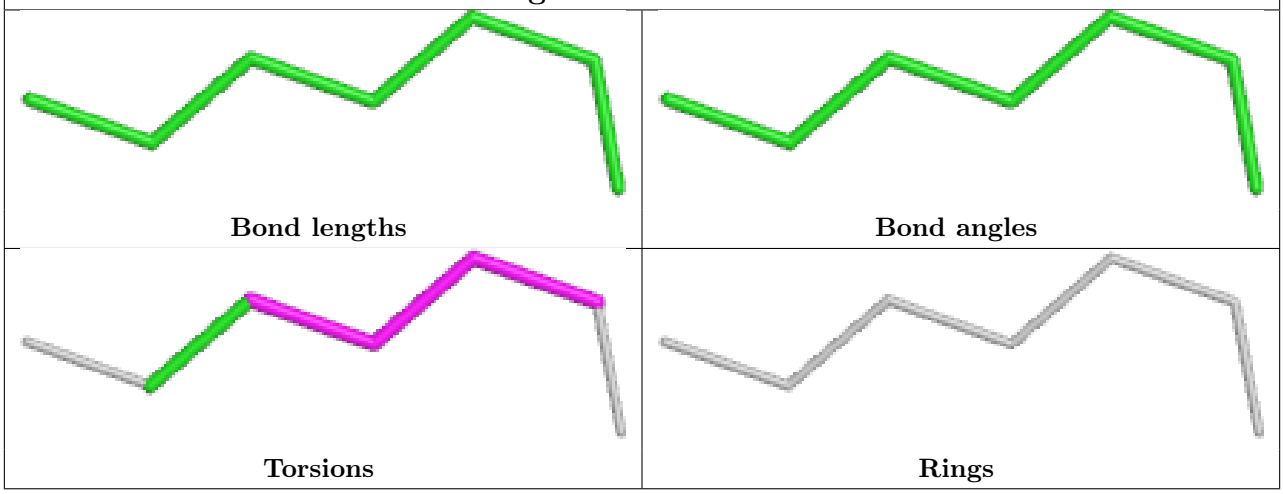


Ligand MPG A 313




Ligand LFA I 310
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA A 306
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA C 310
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA I 312
Bond lengths
Bond angles
Torsions
Rings

Ligand LFA A 311



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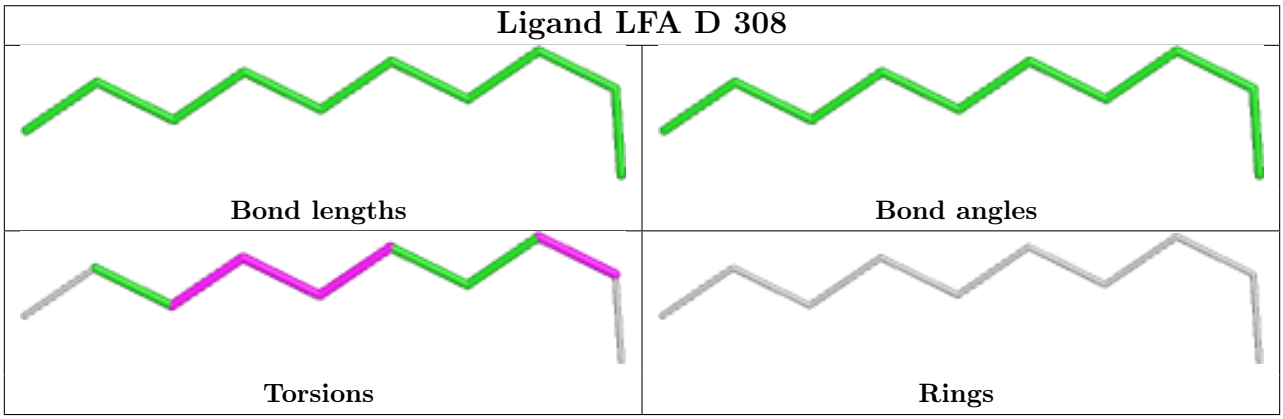

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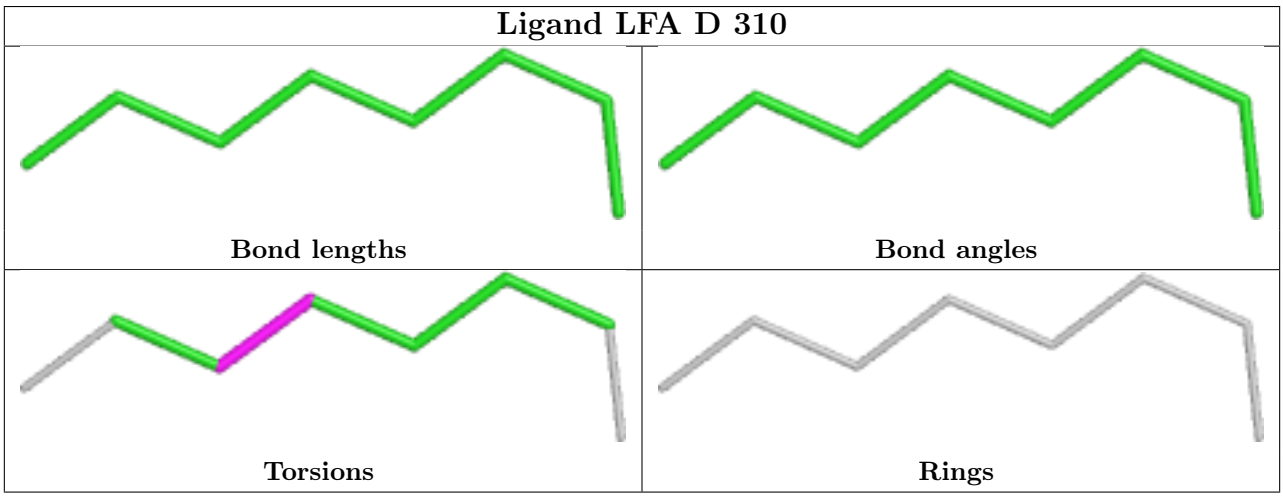
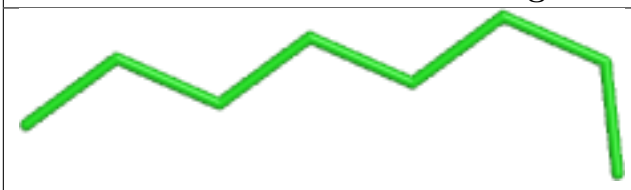
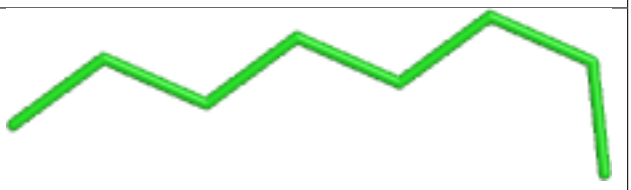


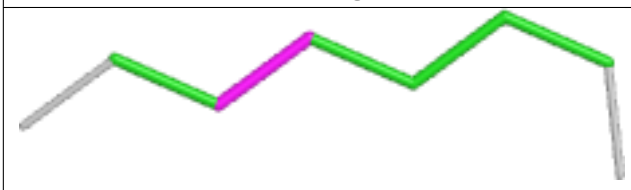
Ligand LFA C 311



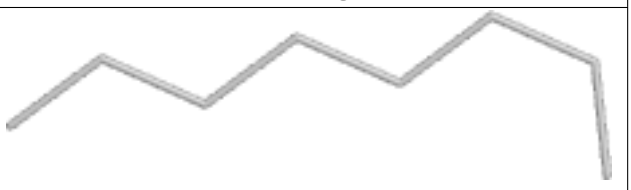
Bond lengths



Bond angles



Torsions

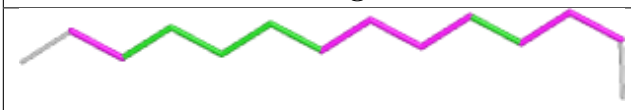


Rings

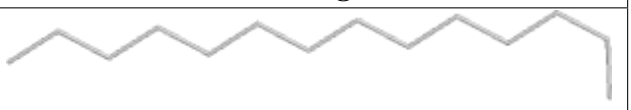
Ligand LFA F 303

Bond lengths

Bond angles

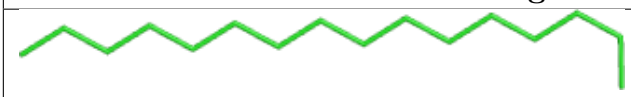


Torsions

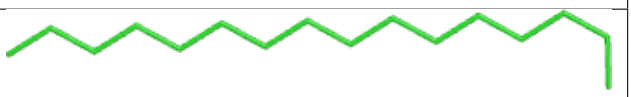


Rings

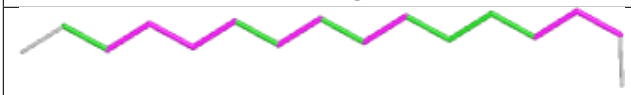
Ligand LFA B 307



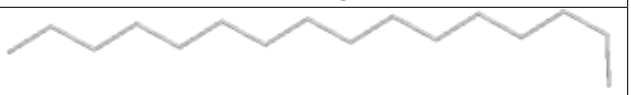
Bond lengths



Bond angles

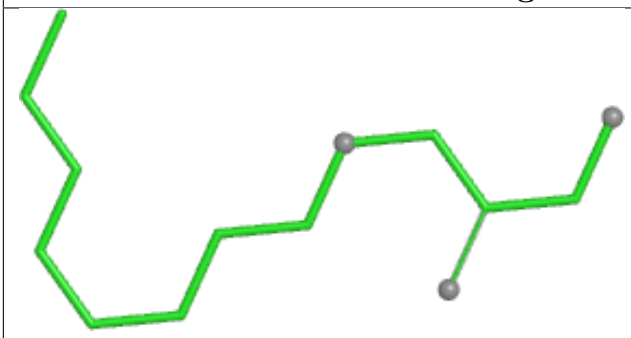


Torsions

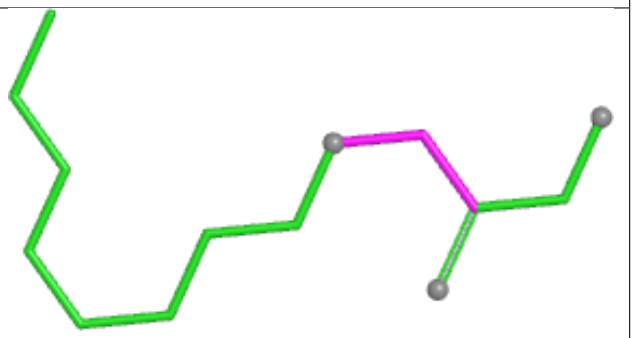


Rings

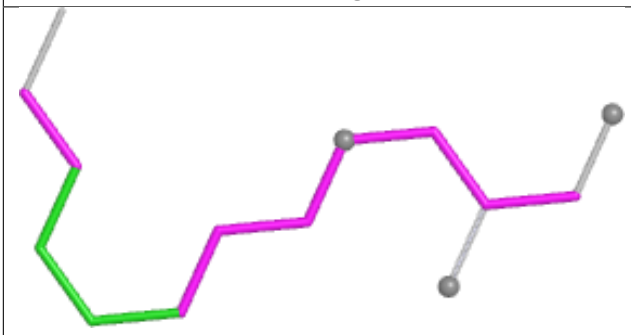
Ligand MPG D 315



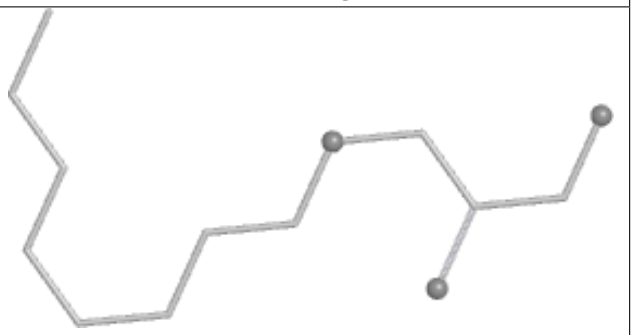
Bond lengths



Bond angles

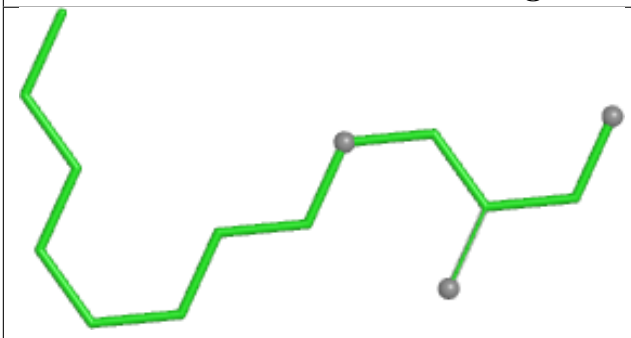


Torsions

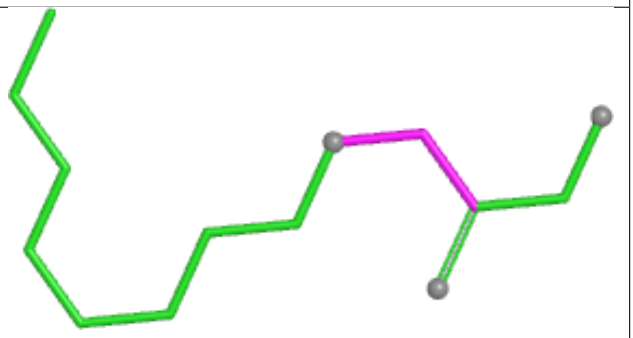


Rings

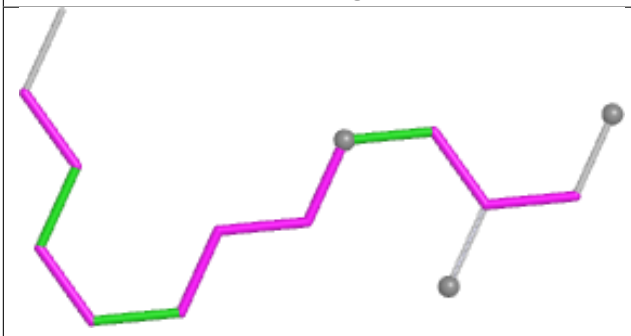
Ligand MPG I 314



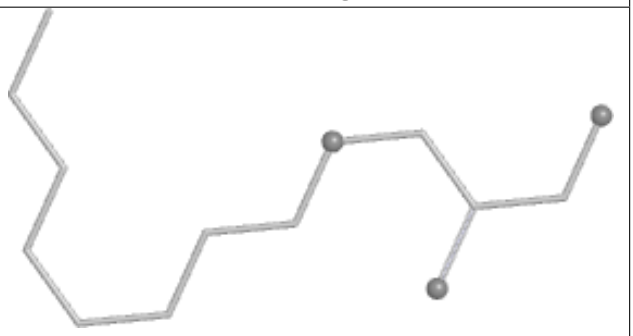
Bond lengths



Bond angles

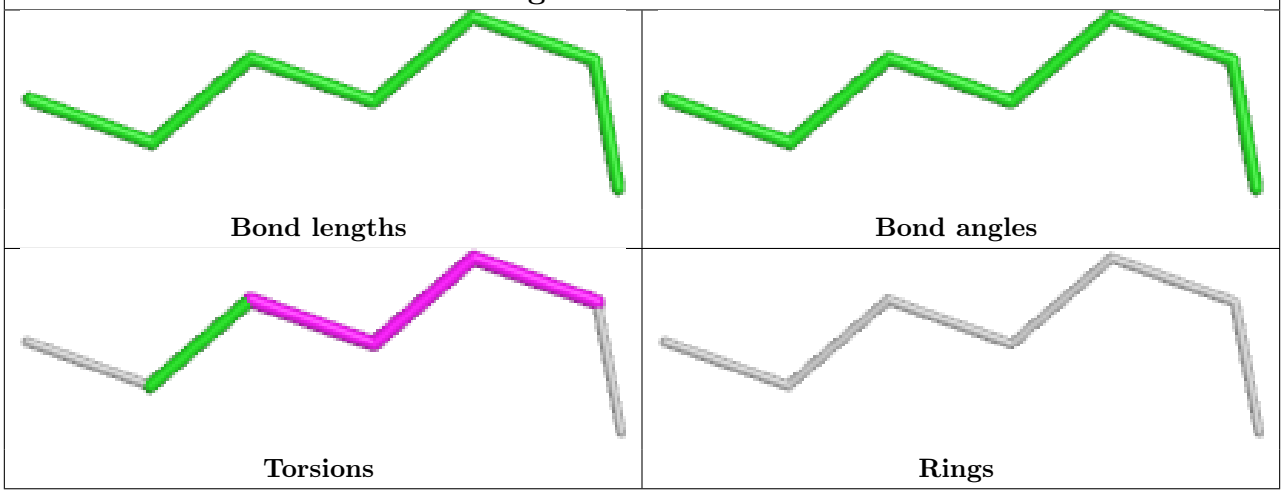


Torsions

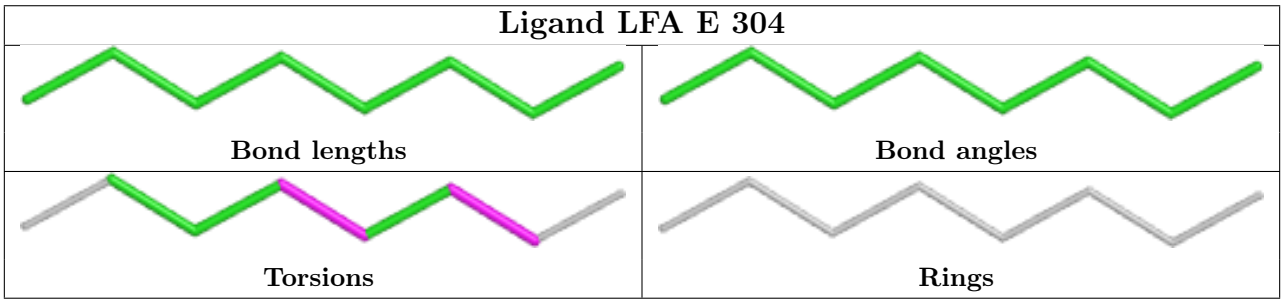


Rings

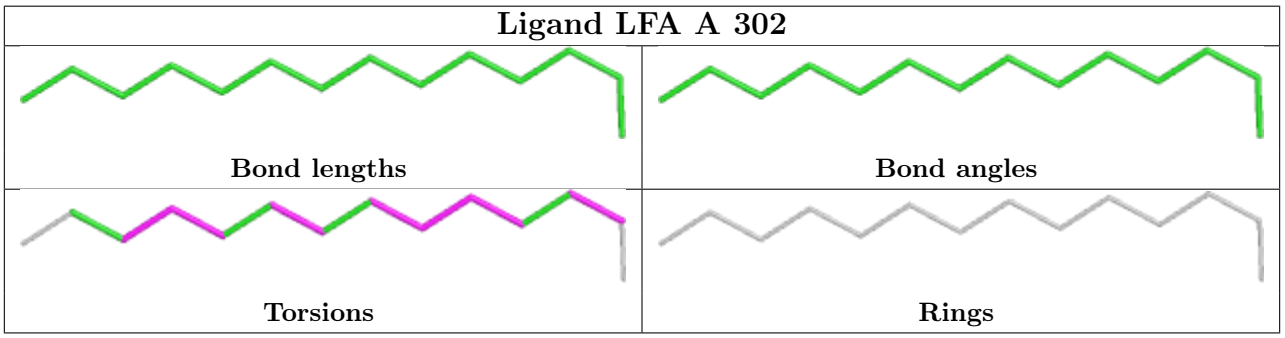
Ligand LFA D 302



Ligand LFA E 304



Ligand LFA A 302



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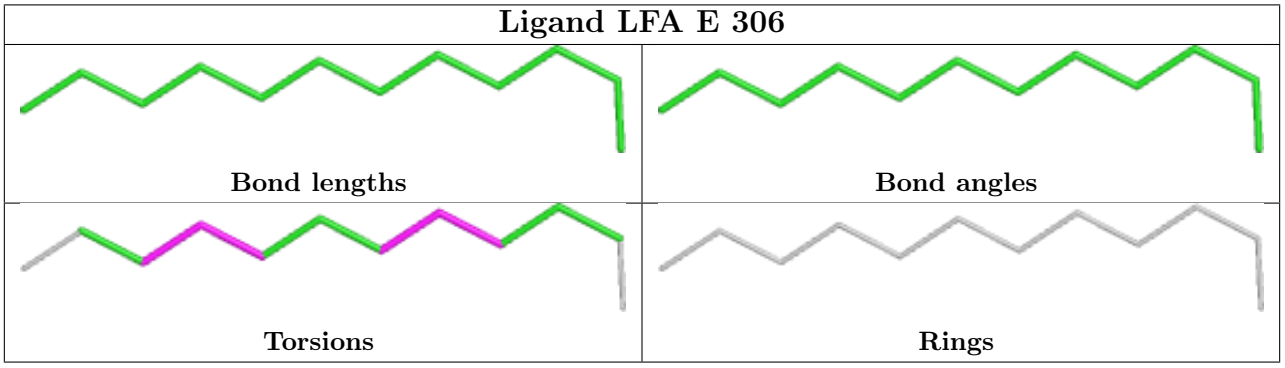
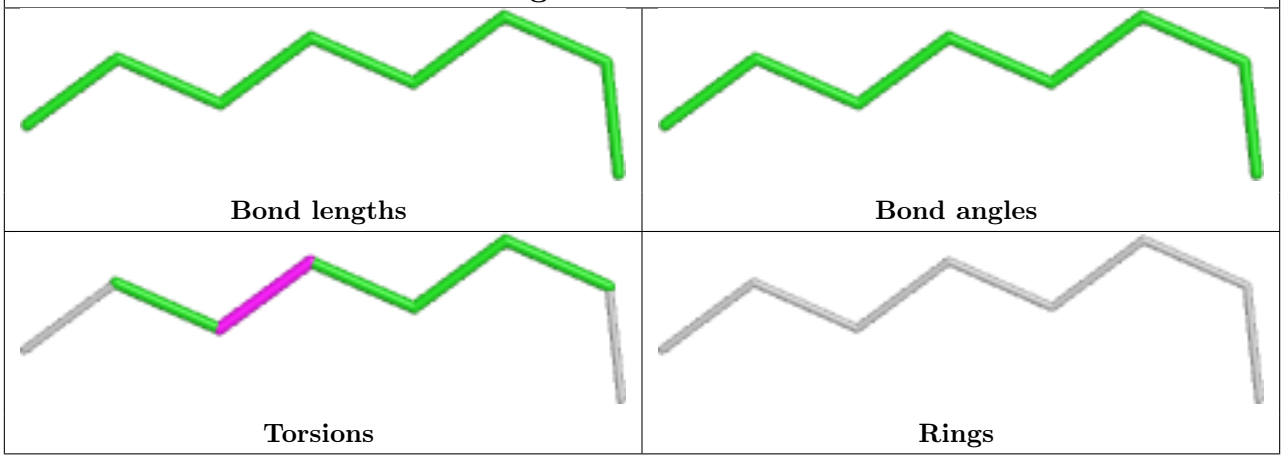
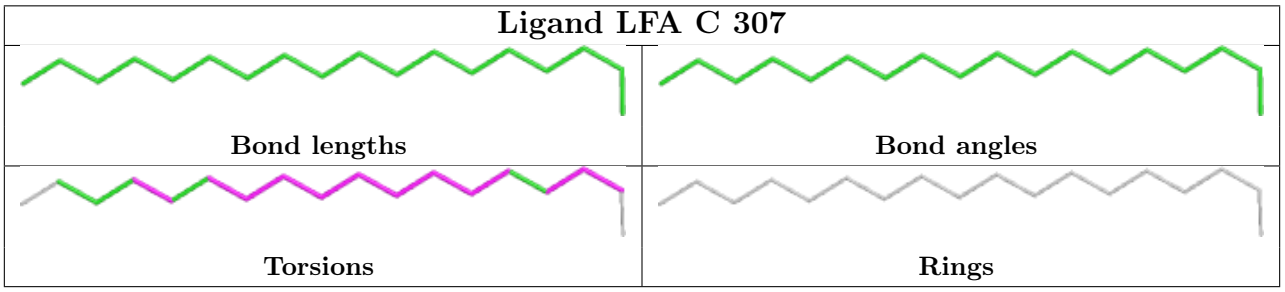


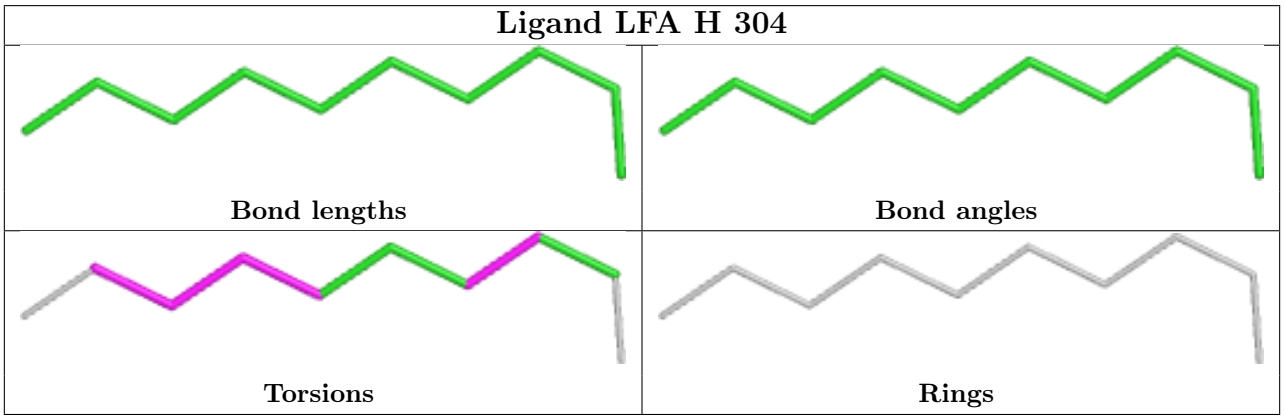
Ligand LFA E 311



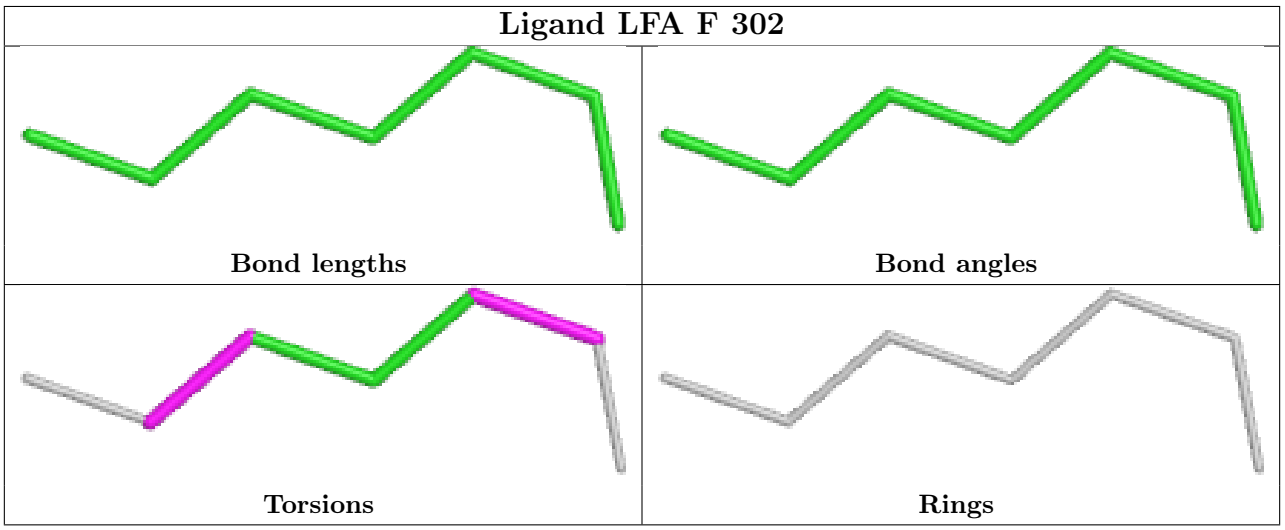
Ligand LFA C 307

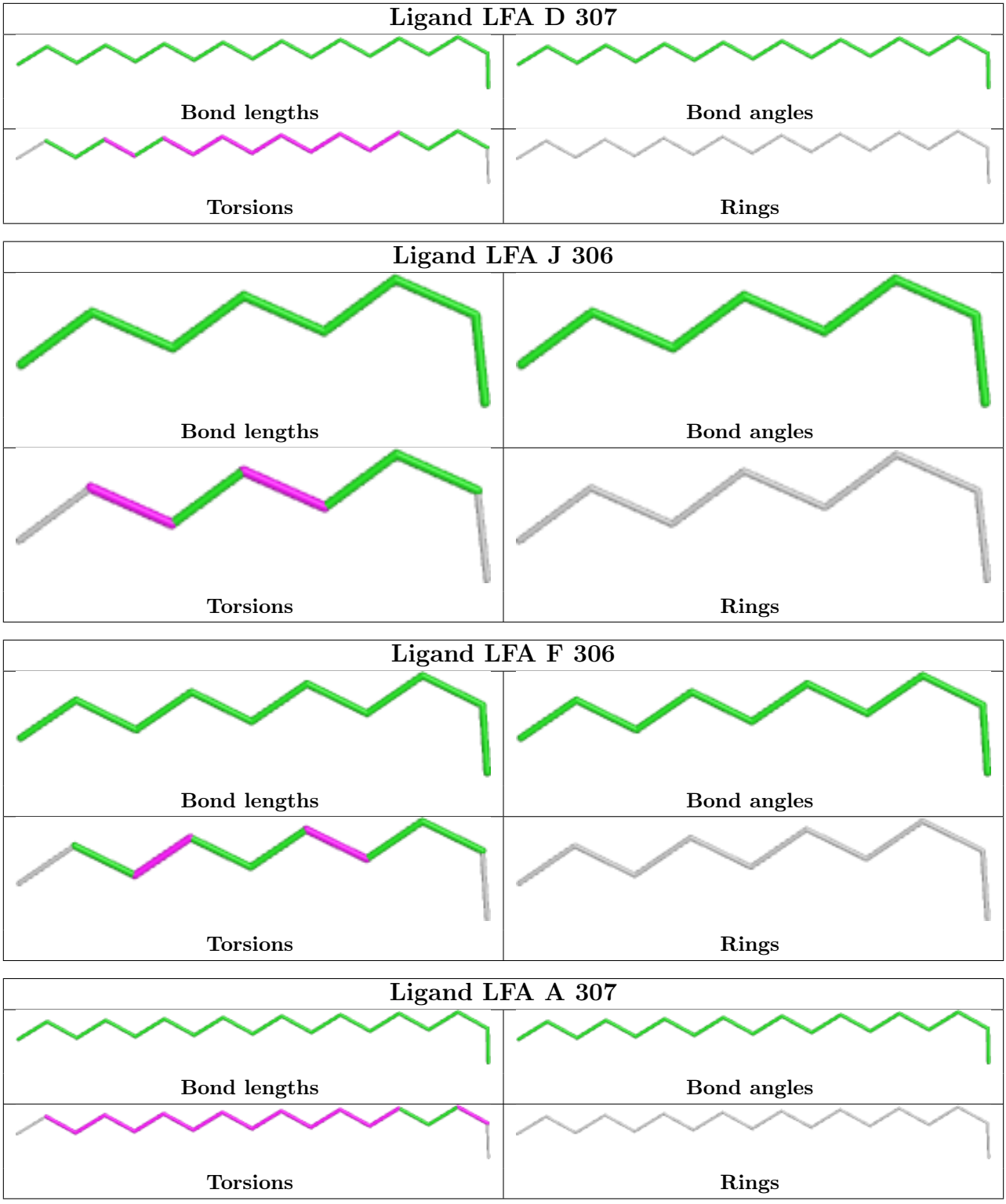


Ligand LFA H 304

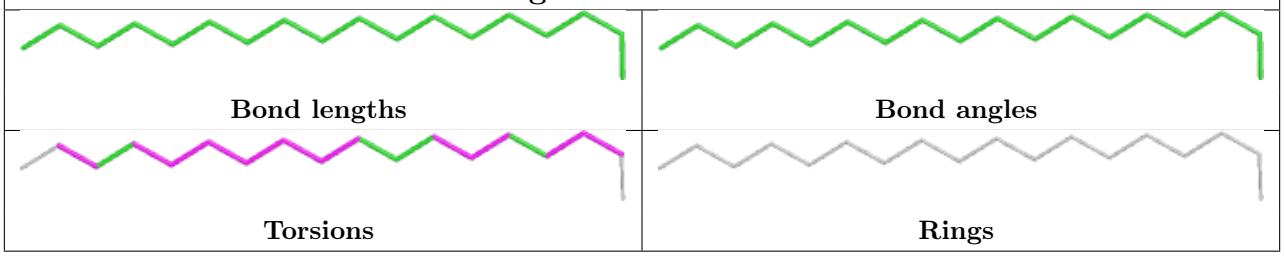


Ligand LFA F 302

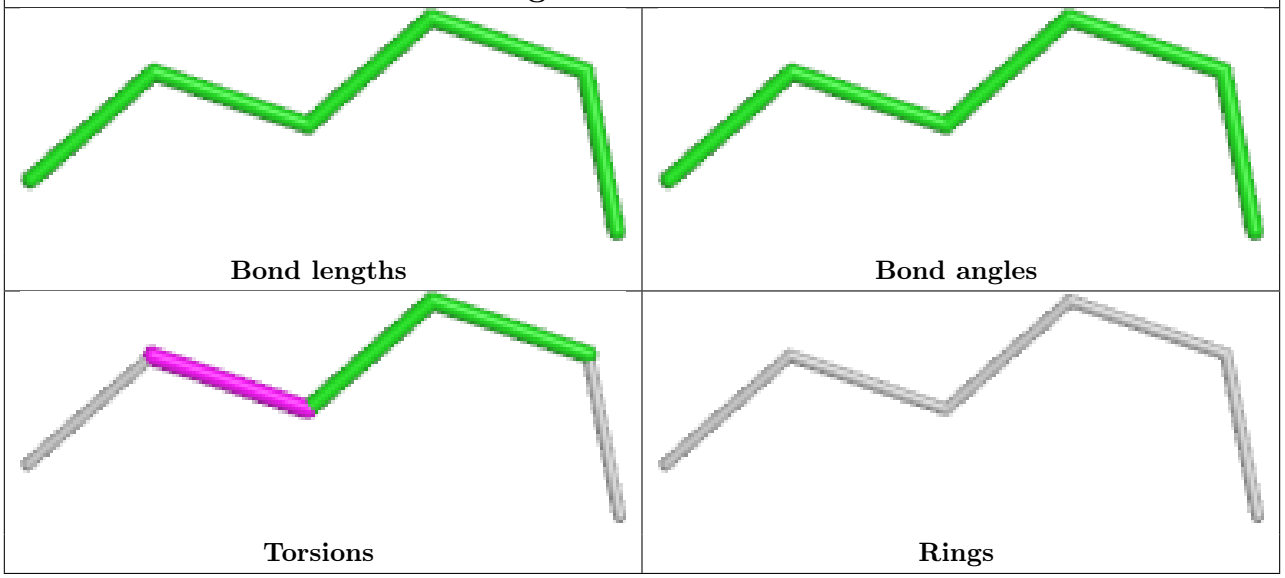



Ligand LFA D 307
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA J 306
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA F 306
Bond lengths
Bond angles
Torsions
Rings
Ligand LFA A 307
Bond lengths
Bond angles
Torsions
Rings

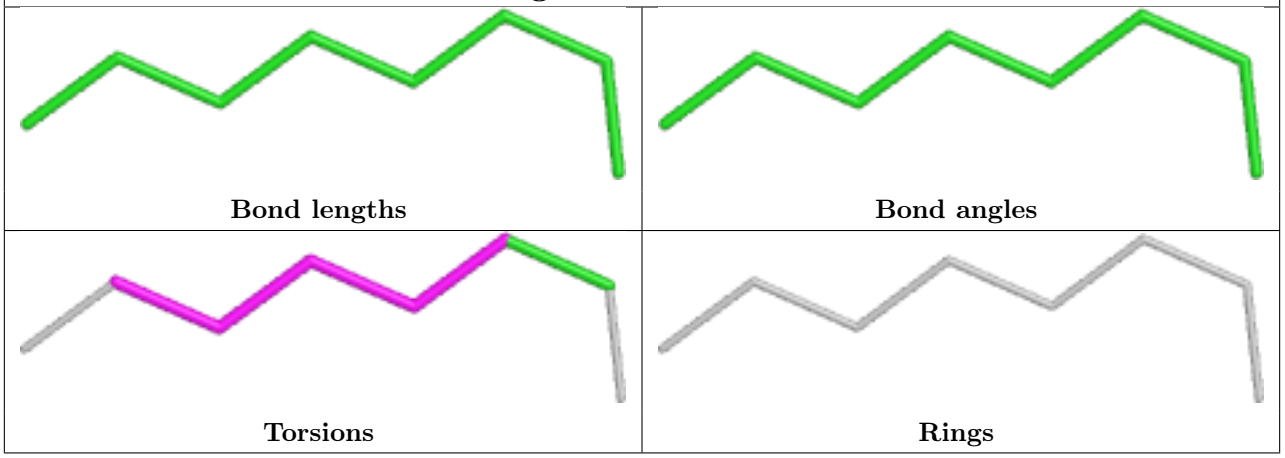
Ligand LFA B 308

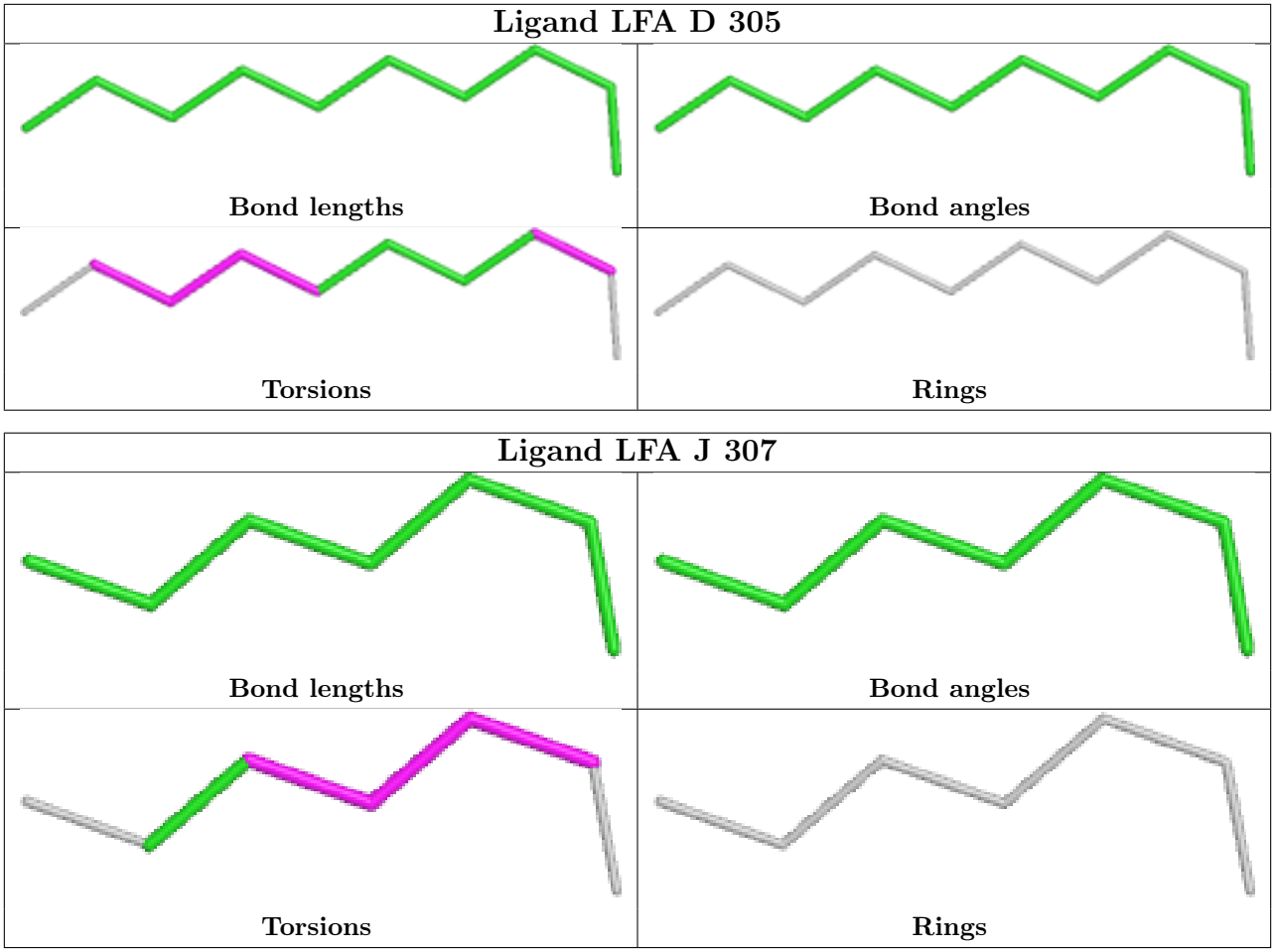


Ligand LFA A 303



Ligand LFA F 308





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	272/288 (94%)	0.01	6 (2%)	62	59	24, 34, 52, 81	0
1	B	269/288 (93%)	0.32	15 (5%)	30	27	20, 39, 67, 90	1 (0%)
1	C	270/288 (93%)	-0.00	5 (1%)	66	63	22, 34, 51, 74	2 (0%)
1	D	270/288 (93%)	-0.07	7 (2%)	57	54	22, 32, 49, 73	0
1	E	271/288 (94%)	0.10	4 (1%)	72	69	23, 34, 54, 69	0
1	F	270/288 (93%)	0.14	7 (2%)	57	54	22, 35, 56, 76	1 (0%)
1	G	270/288 (93%)	-0.01	3 (1%)	78	76	18, 34, 51, 82	3 (1%)
1	H	272/288 (94%)	-0.11	6 (2%)	62	59	21, 32, 51, 91	1 (0%)
1	I	270/288 (93%)	-0.11	5 (1%)	66	63	21, 30, 49, 76	0
1	J	271/288 (94%)	-0.03	8 (2%)	52	49	17, 32, 49, 76	2 (0%)
All	All	2705/2880 (93%)	0.02	66 (2%)	59	56	17, 33, 54, 91	10 (0%)

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	198	PRO	4.2
1	C	3	GLN	4.1
1	I	275	LEU	3.8
1	A	276	VAL	3.6
1	J	3	GLN	3.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LYR	B	255	29/30	0.92	0.11	31,38,44,49	0
1	LYR	F	255	29/30	0.93	0.10	27,33,37,44	0
1	LYR	G	255	29/30	0.93	0.09	25,31,38,43	0
1	LYR	A	255	29/30	0.94	0.09	26,29,34,36	0
1	LYR	E	255	29/30	0.94	0.09	28,34,43,47	0
1	LYR	H	255	29/30	0.94	0.09	25,30,37,40	0
1	LYR	C	255	29/30	0.95	0.08	29,33,39,43	0
1	LYR	D	255	29/30	0.95	0.07	25,27,35,36	0
1	LYR	J	255	29/30	0.95	0.08	22,27,32,35	0
1	LYR	I	255	29/30	0.96	0.07	22,26,33,38	0

6.3 Carbohydrates (i)

There are no oligosaccharides 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
3	LFA	C	303	10/20	0.73	0.28	61,77,88,94	0
3	LFA	C	308	10/20	0.73	0.24	67,74,85,88	0
3	LFA	D	317	5/20	0.73	0.26	56,64,69,70	0
3	LFA	G	310	10/20	0.74	0.24	53,66,73,74	0
3	LFA	F	313	14/20	0.75	0.23	65,74,78,82	0
3	LFA	J	305	14/20	0.75	0.27	60,72,80,81	0
3	LFA	D	310	8/20	0.76	0.23	56,69,70,74	0
3	LFA	F	314	8/20	0.76	0.20	61,71,76,76	0
3	LFA	F	304	10/20	0.76	0.25	58,61,73,73	0
3	LFA	F	311	10/20	0.76	0.26	64,77,86,87	0
3	LFA	D	316	5/20	0.77	0.23	50,52,53,54	0
3	LFA	G	313	8/20	0.77	0.20	48,55,59,65	0
3	LFA	E	309	6/20	0.77	0.24	60,66,70,70	0
3	LFA	C	312	4/20	0.78	0.18	44,46,47,47	0
3	LFA	E	306	12/20	0.78	0.24	66,78,86,89	0
3	LFA	B	304	14/20	0.79	0.19	50,61,77,78	0
3	LFA	B	309	13/20	0.79	0.23	50,69,76,80	0
3	LFA	H	304	10/20	0.79	0.22	56,62,64,65	0
3	LFA	H	308	8/20	0.79	0.21	64,70,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LFA	B	311	8/20	0.79	0.18	57,70,73,82	0
3	LFA	J	307	7/20	0.79	0.22	56,61,78,83	0
4	MPG	D	315	14/25	0.79	0.21	49,54,63,68	0
3	LFA	F	302	7/20	0.80	0.30	76,83,88,92	0
3	LFA	G	311	8/20	0.80	0.20	51,62,68,69	0
3	LFA	D	318	5/20	0.80	0.23	63,66,66,68	0
3	LFA	F	306	10/20	0.80	0.18	48,54,59,63	0
3	LFA	F	307	6/20	0.80	0.20	43,43,46,48	0
3	LFA	C	304	6/20	0.80	0.23	60,63,65,68	0
3	LFA	C	310	13/20	0.80	0.23	58,69,79,81	0
3	LFA	E	310	10/20	0.80	0.18	42,48,60,60	0
3	LFA	H	302	13/20	0.81	0.18	41,52,61,61	0
3	LFA	D	308	10/20	0.81	0.20	56,61,70,70	0
3	LFA	E	304	8/20	0.81	0.21	60,64,68,72	0
3	LFA	I	302	7/20	0.81	0.24	59,70,82,84	0
3	LFA	I	304	14/20	0.81	0.19	41,54,62,65	0
3	LFA	J	304	8/20	0.81	0.20	46,54,63,63	0
3	LFA	C	311	8/20	0.81	0.18	59,64,67,71	0
3	LFA	A	308	8/20	0.81	0.23	55,61,65,72	0
3	LFA	D	302	7/20	0.81	0.22	57,62,68,69	0
3	LFA	B	302	7/20	0.82	0.22	60,62,73,76	0
3	LFA	G	307	16/20	0.82	0.18	48,54,59,59	0
3	LFA	I	305	6/20	0.82	0.19	48,57,60,61	0
3	LFA	C	309	8/20	0.82	0.27	66,78,84,92	0
3	LFA	H	307	14/20	0.82	0.21	56,65,71,71	0
3	LFA	B	306	8/20	0.82	0.24	53,63,65,66	0
3	LFA	H	310	8/20	0.82	0.14	39,46,48,50	0
3	LFA	A	311	7/20	0.83	0.21	59,61,67,69	0
3	LFA	G	304	14/20	0.83	0.19	39,54,62,62	0
3	LFA	I	307	6/20	0.83	0.16	38,41,44,47	0
3	LFA	F	308	8/20	0.83	0.22	47,59,64,65	0
3	LFA	A	312	5/20	0.83	0.19	43,45,50,54	0
3	LFA	F	312	8/20	0.83	0.23	48,64,82,84	0
3	LFA	J	308	14/20	0.83	0.17	39,52,59,60	0
3	LFA	A	310	8/20	0.83	0.21	54,62,70,72	0
3	LFA	B	305	6/20	0.84	0.17	50,58,59,64	0
3	LFA	B	310	11/20	0.84	0.19	50,60,67,69	0
3	LFA	E	311	8/20	0.84	0.19	40,45,48,50	0
3	LFA	D	305	10/20	0.84	0.19	51,54,63,64	0
3	LFA	F	303	14/20	0.84	0.18	54,61,66,70	0
3	LFA	D	306	16/20	0.84	0.18	44,56,67,67	0
3	LFA	B	308	18/20	0.84	0.20	44,58,74,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LFA	D	309	8/20	0.84	0.23	56,70,81,82	0
3	LFA	B	303	7/20	0.85	0.23	54,62,93,97	0
3	LFA	A	305	10/20	0.85	0.16	45,52,58,58	0
3	LFA	G	308	18/20	0.85	0.17	43,48,60,64	0
4	MPG	A	313	14/25	0.85	0.15	54,60,66,70	0
3	LFA	E	302	14/20	0.85	0.17	44,56,65,66	0
4	MPG	E	313	14/25	0.85	0.17	48,53,68,72	0
3	LFA	A	304	10/20	0.86	0.16	47,50,55,57	0
3	LFA	F	305	6/20	0.86	0.18	54,56,58,58	0
3	LFA	G	314	6/20	0.86	0.17	50,54,54,55	0
3	LFA	I	308	16/20	0.86	0.18	42,53,68,72	0
3	LFA	I	310	14/20	0.86	0.15	47,55,63,64	0
3	LFA	I	313	4/20	0.86	0.17	38,42,43,44	0
3	LFA	J	302	16/20	0.86	0.15	45,53,60,61	0
3	LFA	D	313	6/20	0.86	0.16	44,51,57,57	0
3	LFA	C	306	16/20	0.86	0.17	49,54,71,77	0
3	LFA	E	305	6/20	0.86	0.18	54,59,67,68	0
3	LFA	F	309	10/20	0.86	0.16	37,42,45,46	0
3	LFA	G	309	8/20	0.86	0.21	53,59,62,62	0
4	MPG	B	312	14/25	0.86	0.17	50,62,71,72	0
3	LFA	A	303	6/20	0.86	0.20	52,54,59,63	0
3	LFA	I	303	7/20	0.86	0.22	52,62,74,80	0
3	LFA	A	307	18/20	0.87	0.17	37,45,63,71	0
3	LFA	G	302	16/20	0.87	0.16	46,51,57,58	0
3	LFA	C	302	7/20	0.87	0.17	45,57,66,69	0
3	LFA	G	305	6/20	0.87	0.18	55,56,58,64	0
3	LFA	I	306	10/20	0.87	0.16	37,39,41,42	0
3	LFA	J	309	10/20	0.87	0.17	49,52,58,58	0
3	LFA	A	302	14/20	0.87	0.16	49,55,63,65	0
3	LFA	E	308	14/20	0.87	0.15	51,56,64,65	0
4	MPG	C	313	13/25	0.87	0.14	46,53,64,74	0
3	LFA	B	307	16/20	0.87	0.18	46,57,66,66	0
3	LFA	D	311	7/20	0.87	0.16	51,53,55,57	0
4	MPG	G	312	14/25	0.87	0.17	48,54,62,64	0
4	MPG	J	312	14/25	0.87	0.16	51,59,67,68	0
3	LFA	C	305	10/20	0.88	0.15	41,47,51,52	0
3	LFA	H	312	6/20	0.88	0.17	51,53,54,56	0
3	LFA	J	306	8/20	0.88	0.20	60,73,81,81	0
3	LFA	H	306	18/20	0.88	0.14	42,46,52,53	0
3	LFA	H	309	5/20	0.88	0.14	41,42,45,47	0
4	MPG	F	315	14/25	0.88	0.13	41,51,57,62	0
3	LFA	J	303	18/20	0.88	0.17	37,45,57,62	0

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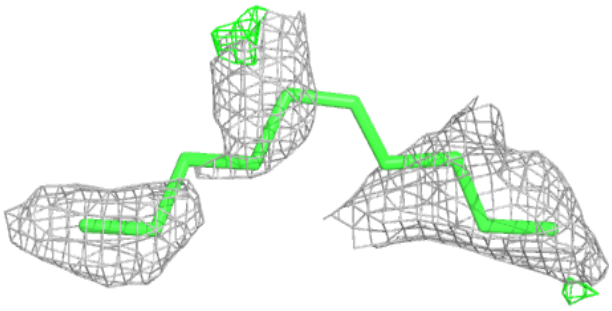
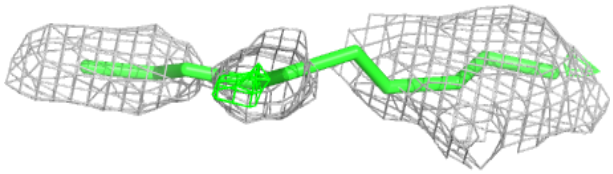
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LFA	J	310	10/20	0.88	0.16	51,56,58,60	0
3	LFA	I	309	18/20	0.89	0.15	32,42,64,75	0
3	LFA	G	306	10/20	0.89	0.15	45,54,57,57	0
3	LFA	I	311	8/20	0.89	0.15	45,54,56,59	0
3	LFA	H	305	16/20	0.89	0.14	40,51,56,59	0
3	LFA	E	312	8/20	0.89	0.14	47,52,55,57	0
3	LFA	G	315	6/20	0.89	0.15	45,53,58,59	0
3	LFA	G	303	7/20	0.89	0.18	57,59,75,79	0
3	LFA	A	309	8/20	0.90	0.17	55,61,70,73	0
3	LFA	F	310	18/20	0.90	0.17	39,51,65,66	0
3	LFA	D	312	6/20	0.90	0.12	40,45,49,52	0
3	LFA	E	303	18/20	0.90	0.15	35,46,62,66	0
3	LFA	D	303	14/20	0.90	0.17	40,67,73,73	0
3	LFA	D	304	6/20	0.90	0.13	47,51,52,57	0
4	MPG	I	314	14/25	0.90	0.15	35,42,60,72	0
3	LFA	A	306	14/20	0.90	0.13	47,51,56,56	0
3	LFA	D	307	18/20	0.91	0.12	34,39,50,60	0
4	MPG	H	313	14/25	0.91	0.14	49,62,72,75	0
3	LFA	D	314	7/20	0.91	0.13	50,55,59,60	0
3	LFA	E	307	8/20	0.91	0.15	61,68,70,73	0
3	LFA	H	303	6/20	0.92	0.16	54,55,57,63	0
3	LFA	J	311	4/20	0.92	0.15	33,35,36,37	0
3	LFA	H	311	7/20	0.92	0.14	44,44,53,57	0
3	LFA	C	307	18/20	0.93	0.12	42,48,57,57	0
3	LFA	I	312	7/20	0.94	0.09	30,34,45,48	0
2	NA	A	301	1/1	0.96	0.09	34,34,34,34	0
2	NA	E	301	1/1	0.98	0.08	27,27,27,27	0
2	NA	B	301	1/1	0.98	0.07	29,29,29,29	0
2	NA	D	301	1/1	0.98	0.08	29,29,29,29	0
2	NA	G	301	1/1	0.99	0.15	26,26,26,26	0
2	NA	H	301	1/1	0.99	0.07	30,30,30,30	0
2	NA	I	301	1/1	0.99	0.05	23,23,23,23	0
2	NA	J	301	1/1	0.99	0.09	28,28,28,28	0
2	NA	C	301	1/1	0.99	0.09	28,28,28,28	0
2	NA	F	301	1/1	0.99	0.07	29,29,29,29	0

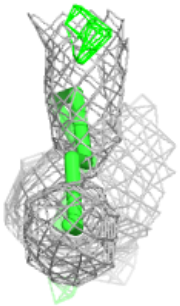
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LFA C 303:

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

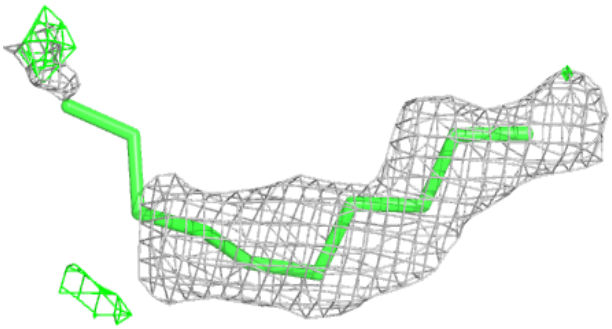


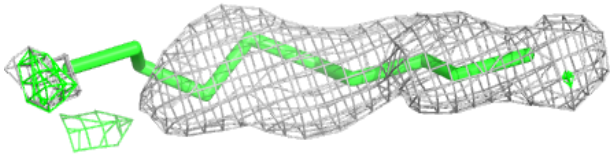


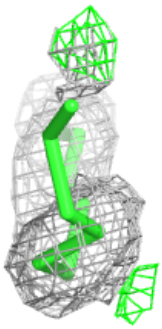


Electron density around LFA C 308:

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

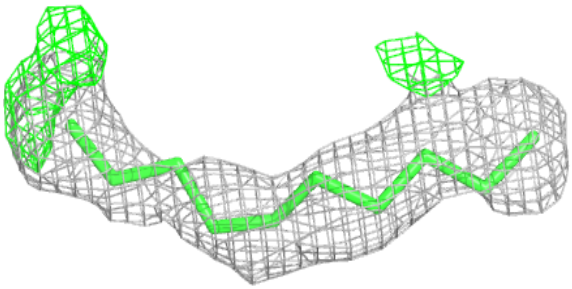


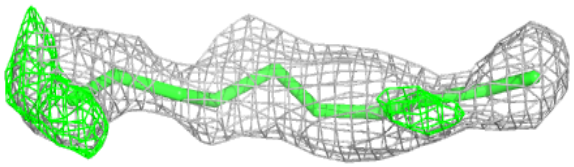


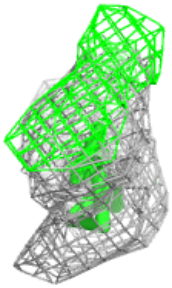


Electron density around LFA G 310:

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

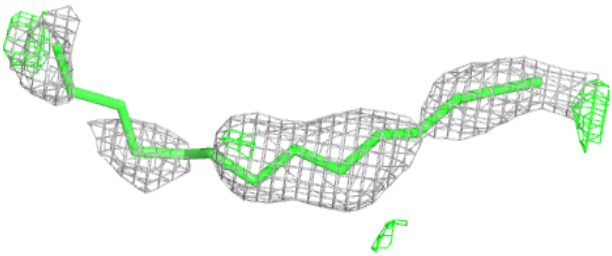


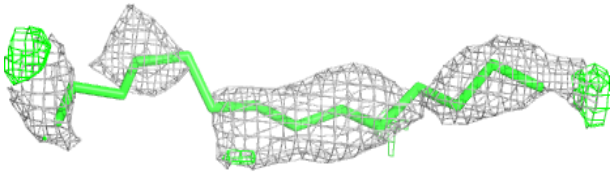


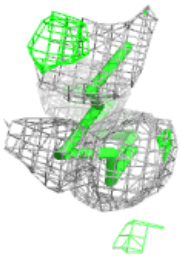


Electron density around LFA F 313:

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

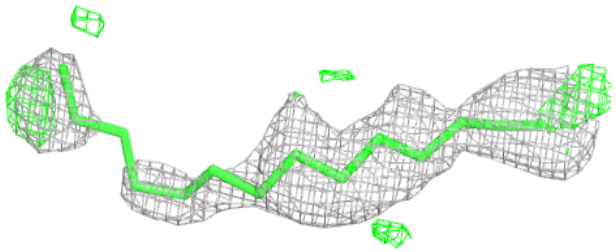


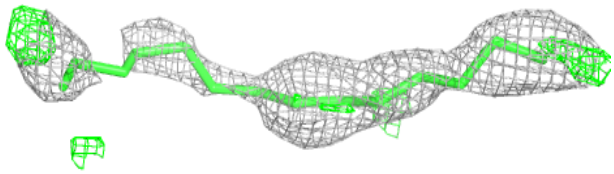


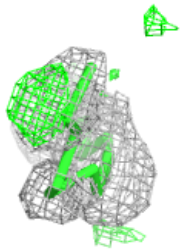


Electron density around LFA J 305:

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

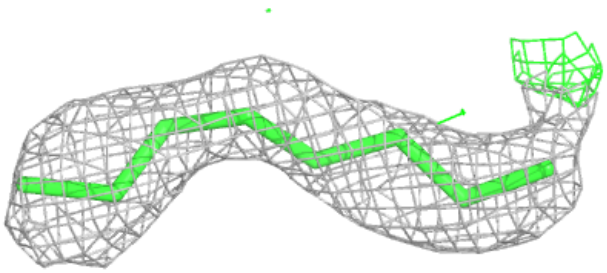


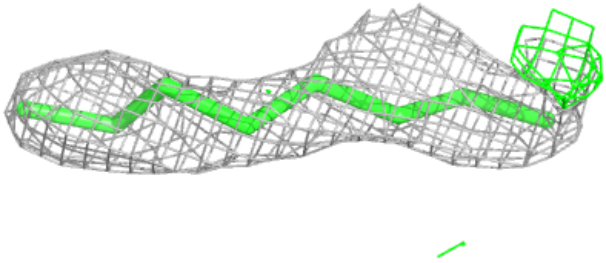


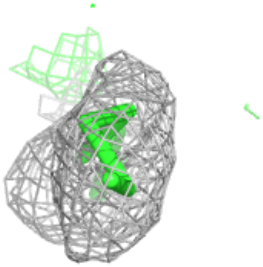


Electron density around LFA D 310:

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

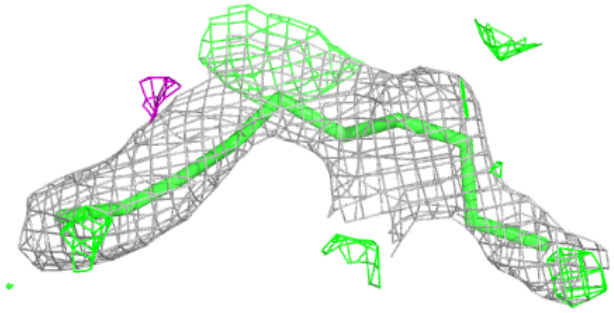


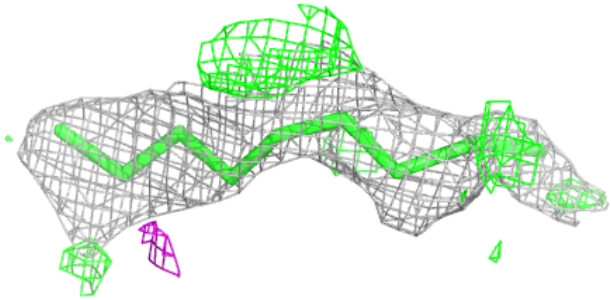


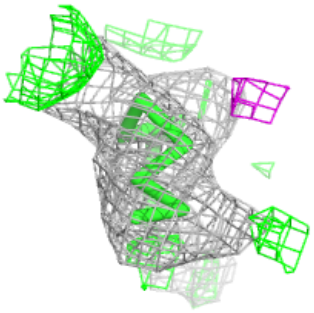


Electron density around LFA F 304:

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

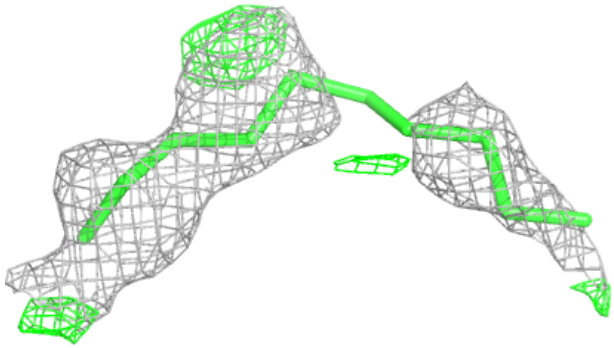


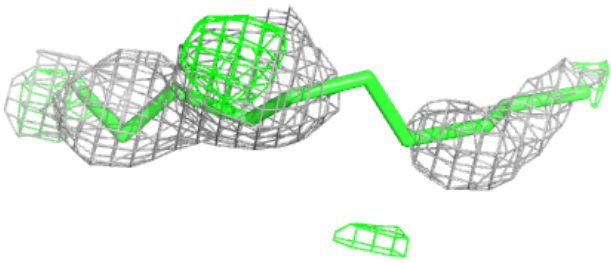


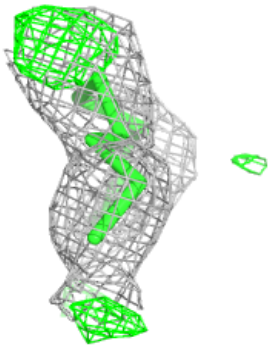


Electron density around LFA F 311:

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

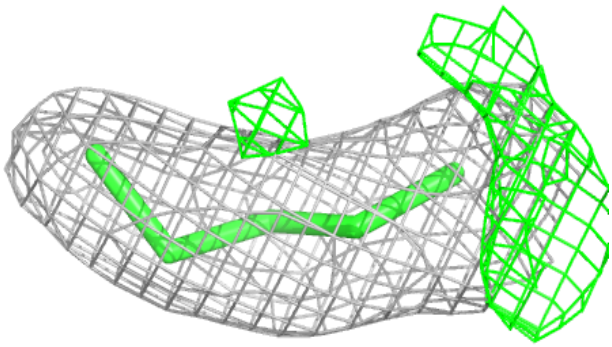


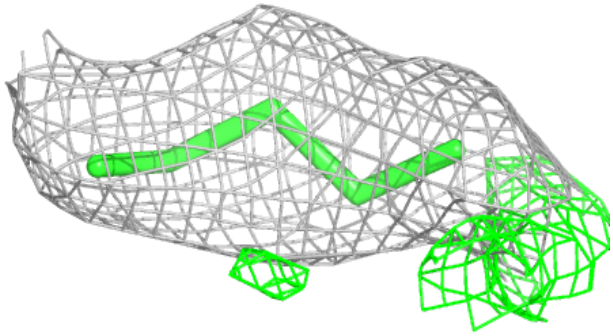


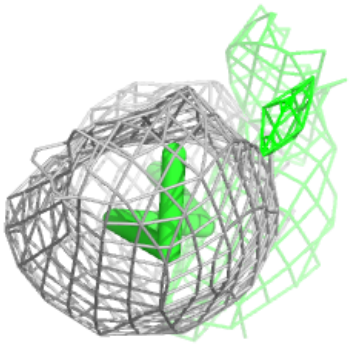


Electron density around LFA D 316:

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

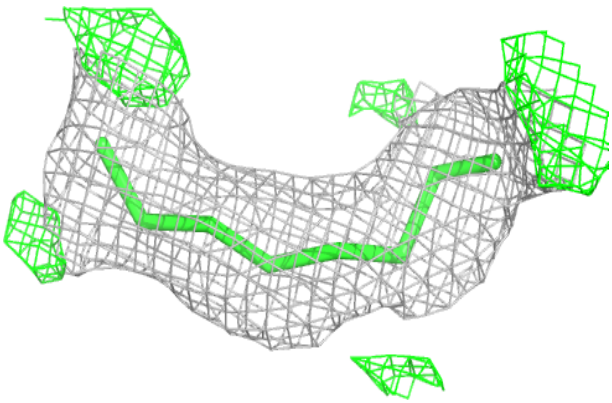


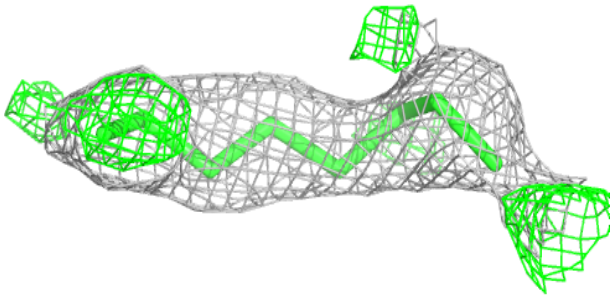


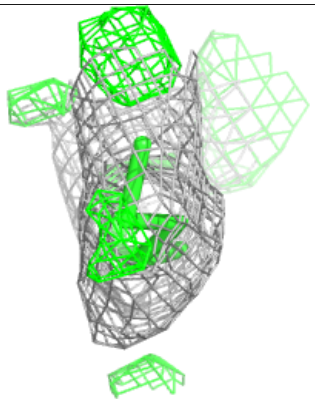


Electron density around LFA G 313:

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

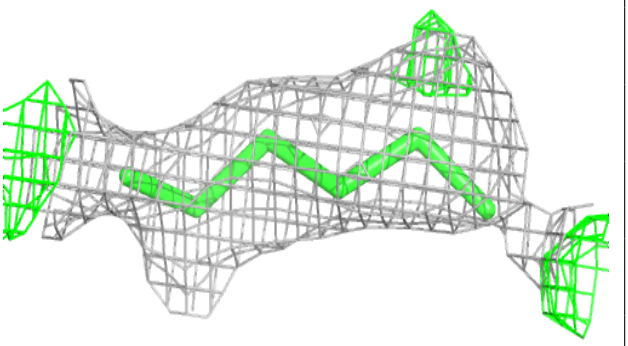


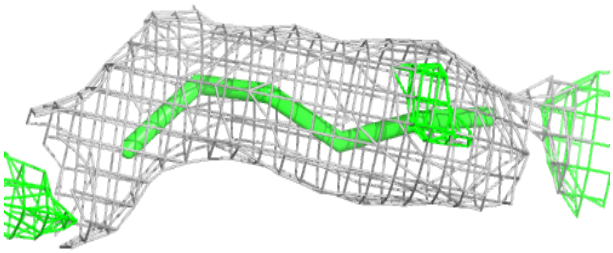


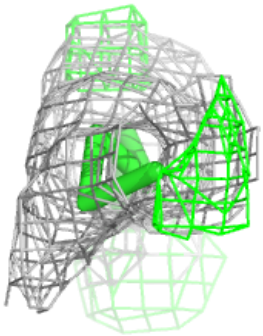


Electron density around LFA E 309:

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

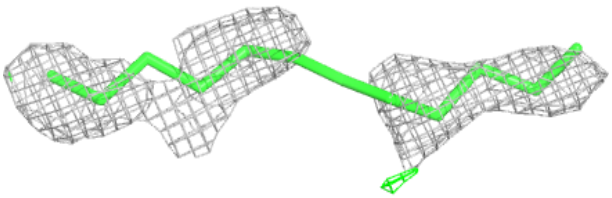


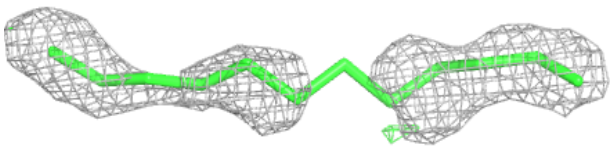


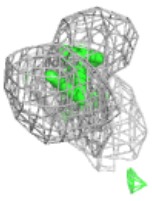


Electron density around LFA E 306:

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

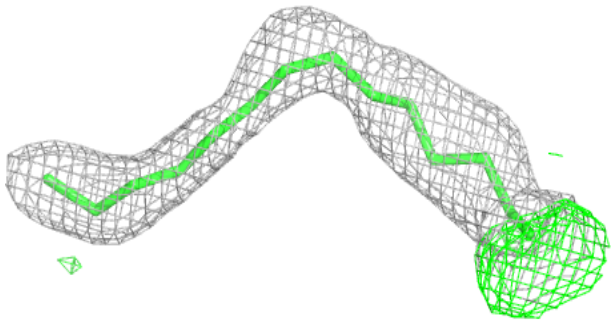


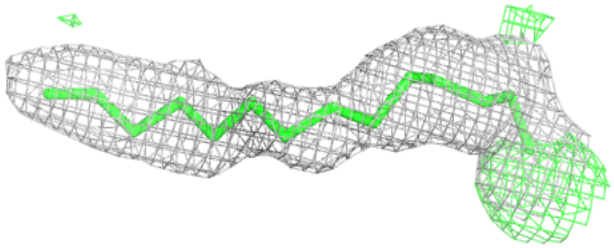


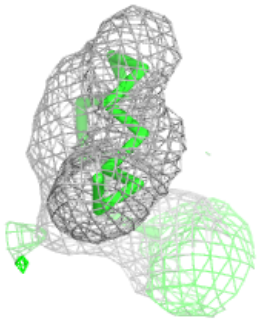


Electron density around LFA B 304:

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

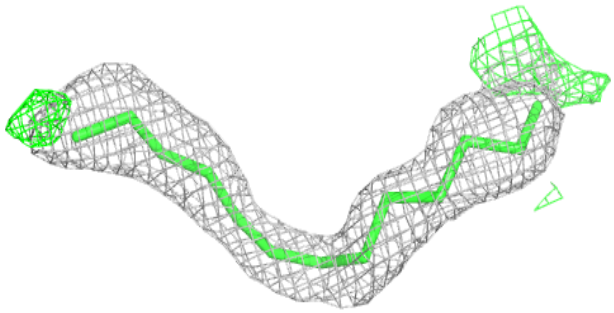


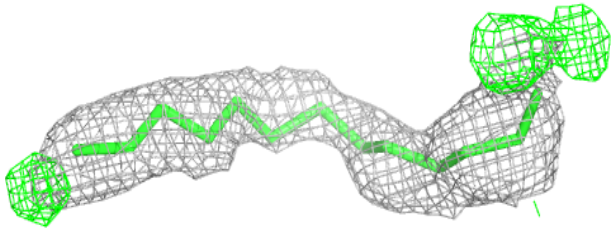


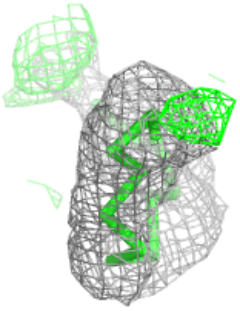


Electron density around LFA B 309:

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

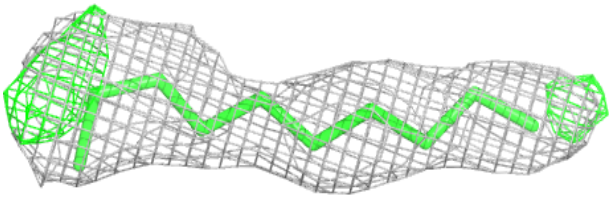


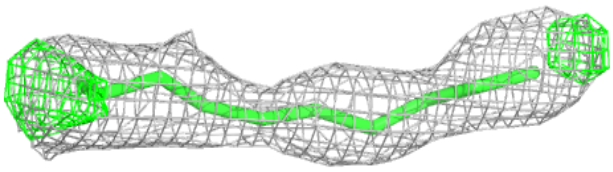


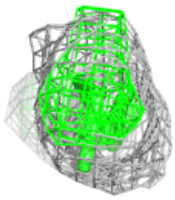


Electron density around LFA H 304:

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

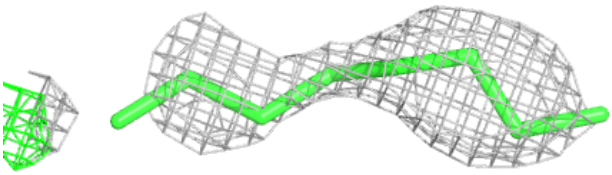


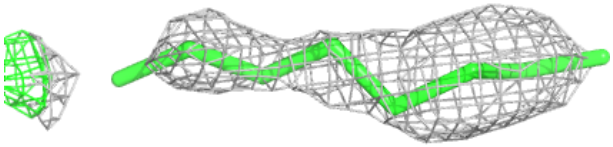


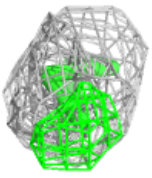


Electron density around LFA H 308:

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

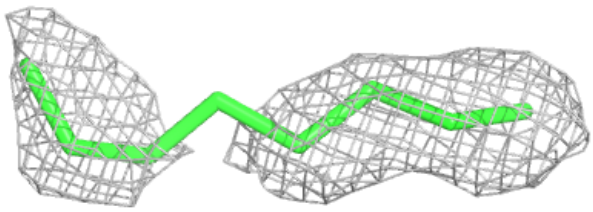


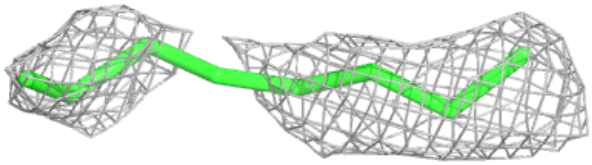


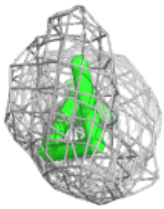


Electron density around LFA B 311:

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

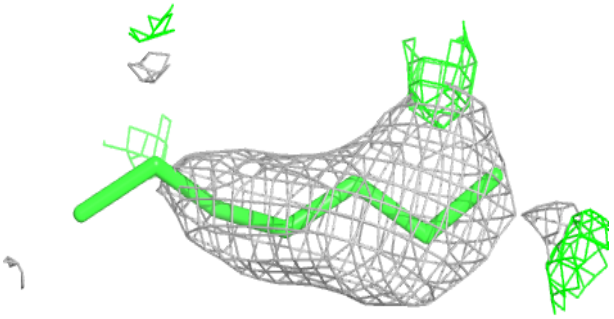


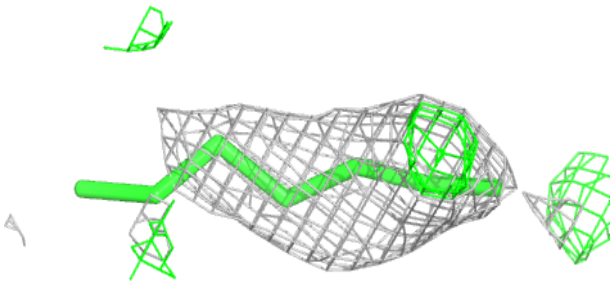


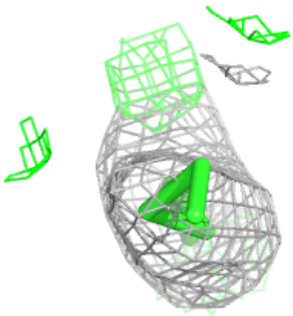


Electron density around LFA J 307:

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

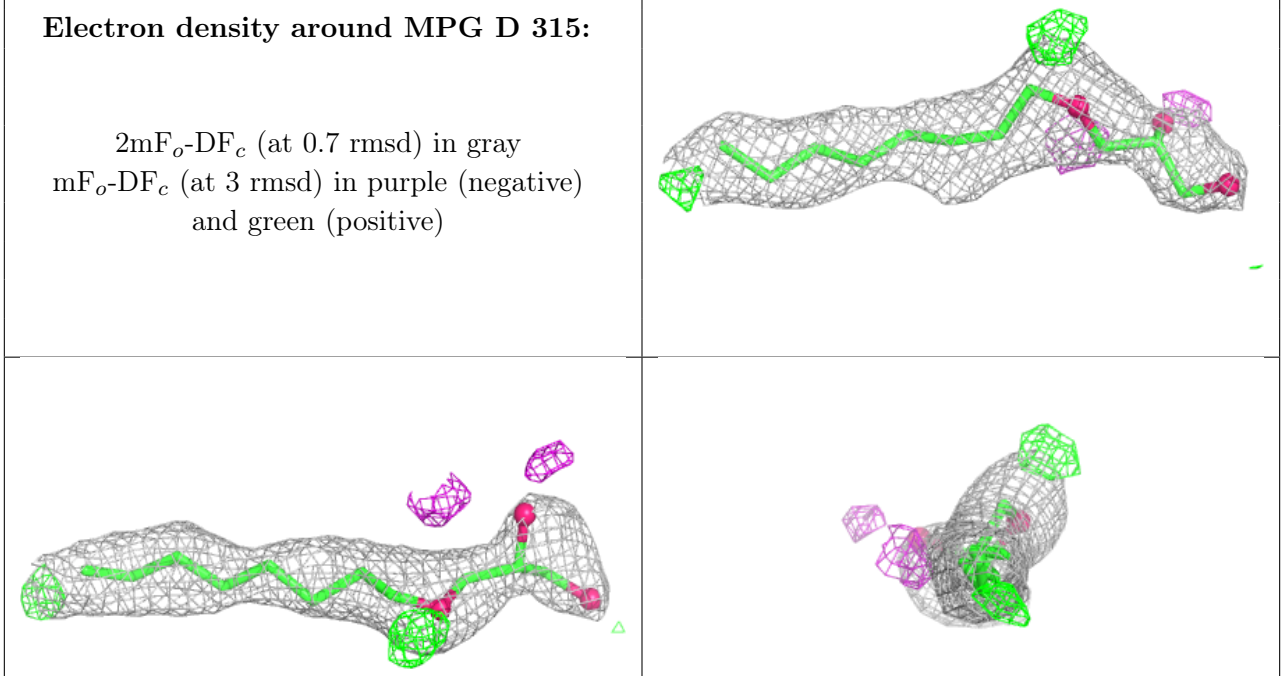






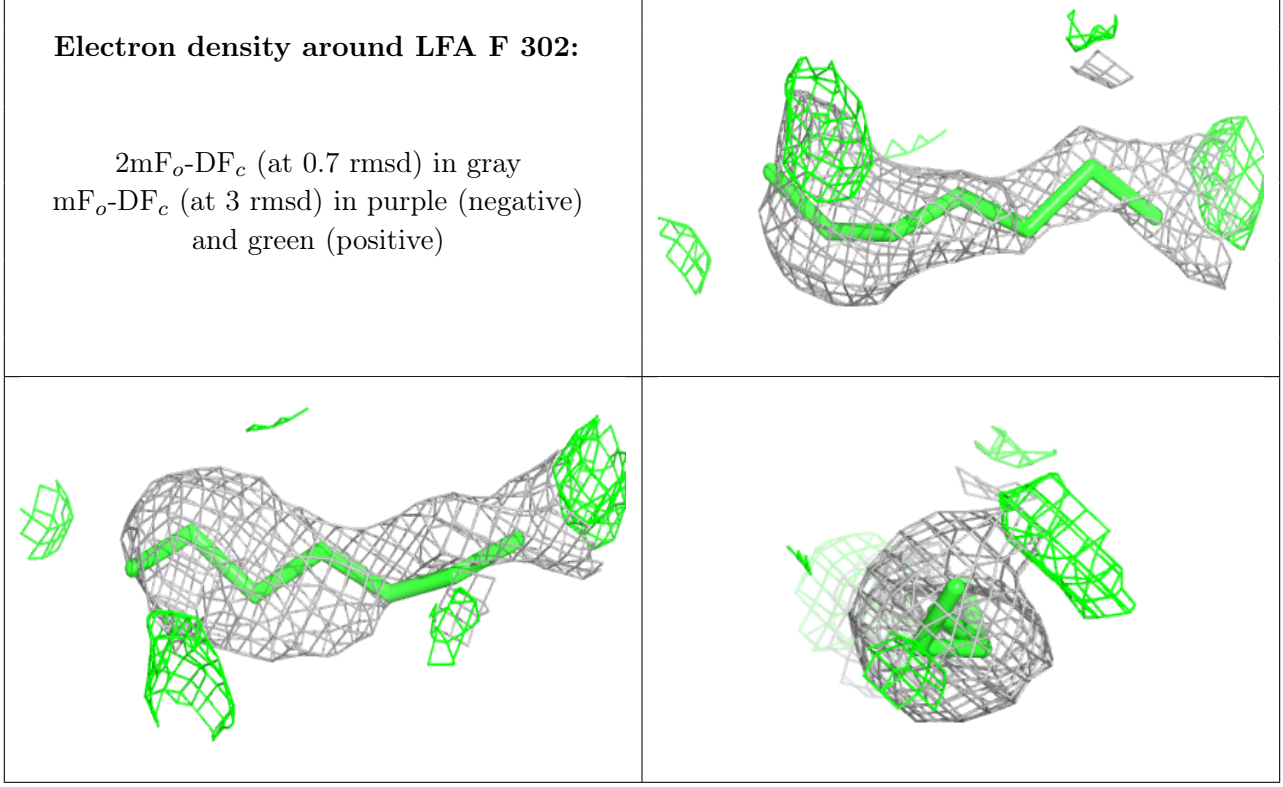
Electron density around MPG D 315:

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



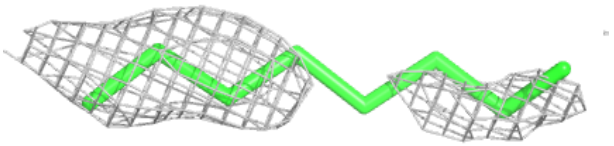
Electron density around LFA F 302:

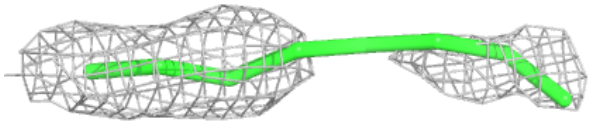
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

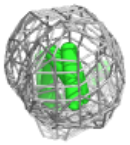


Electron density around LFA G 311:

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

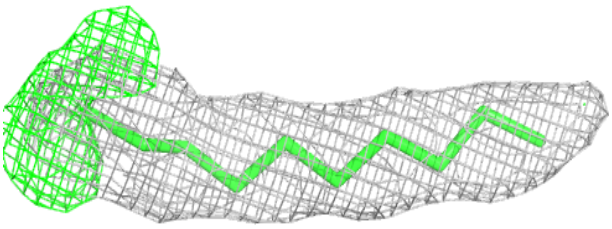


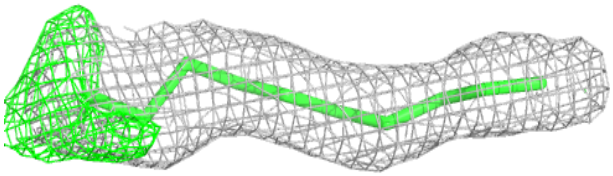


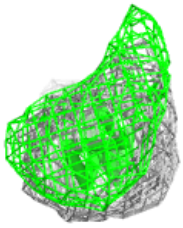


Electron density around LFA F 306:

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

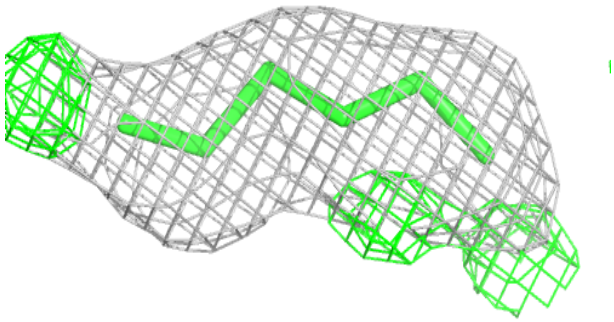


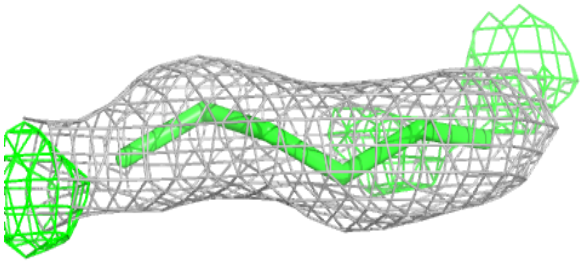


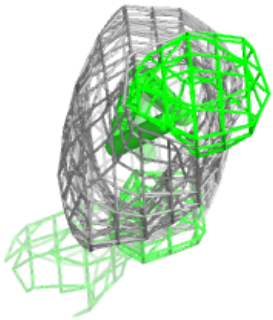


Electron density around LFA F 307:

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

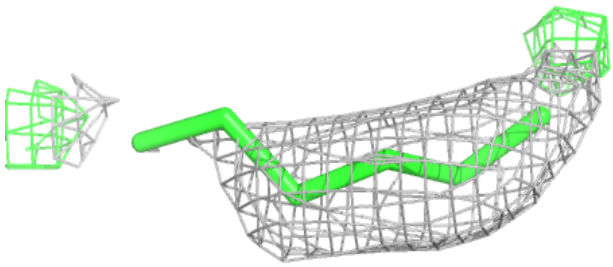


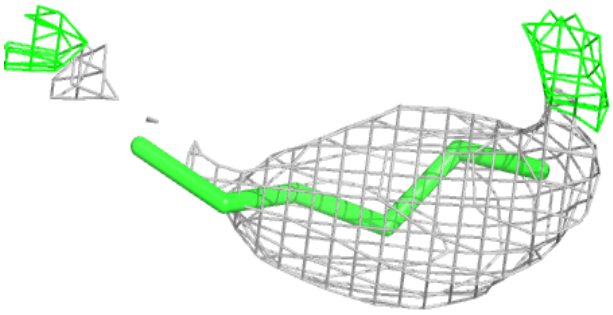


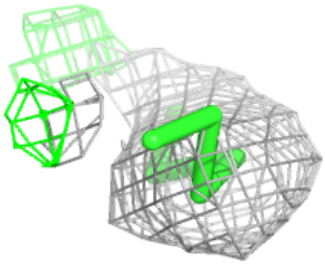


Electron density around LFA C 304:

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

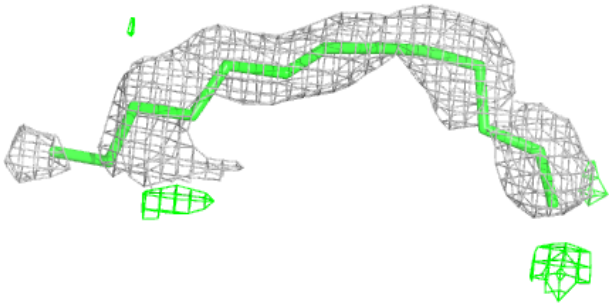


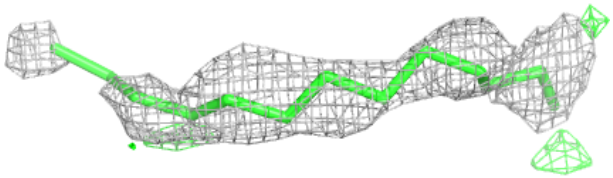


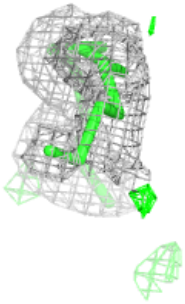


Electron density around LFA C 310:

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

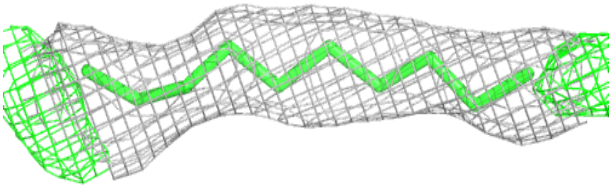


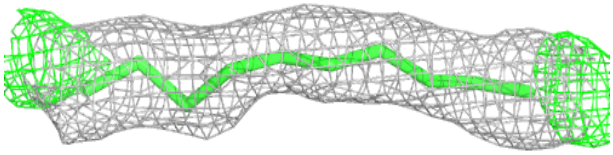


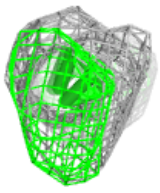


Electron density around LFA E 310:

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

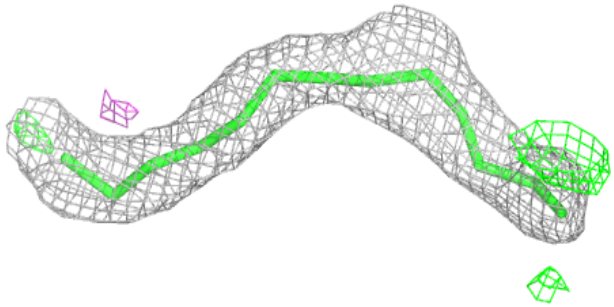


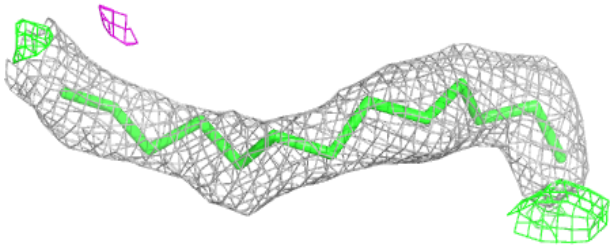


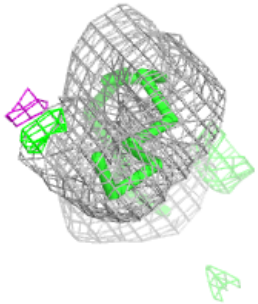


Electron density around LFA H 302:

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

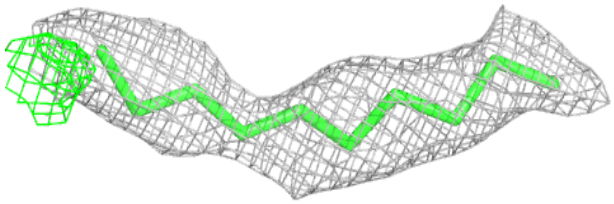


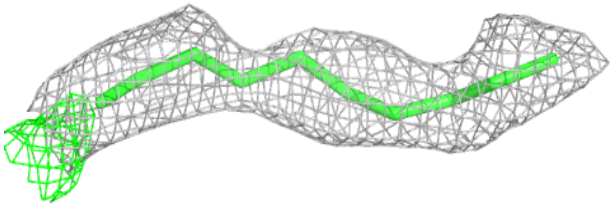


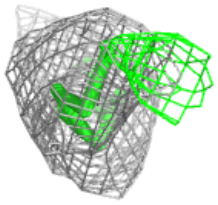


Electron density around LFA D 308:

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

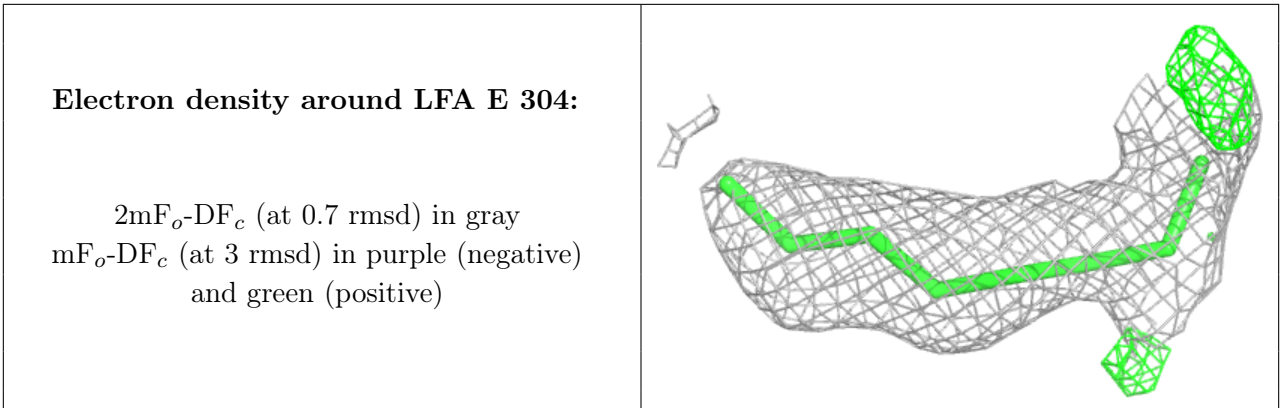


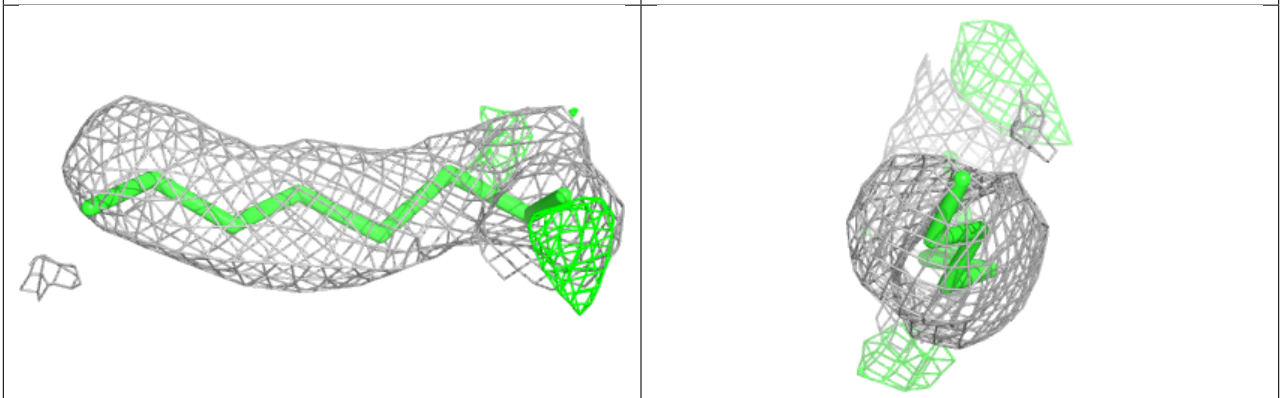




Electron density around LFA E 304:

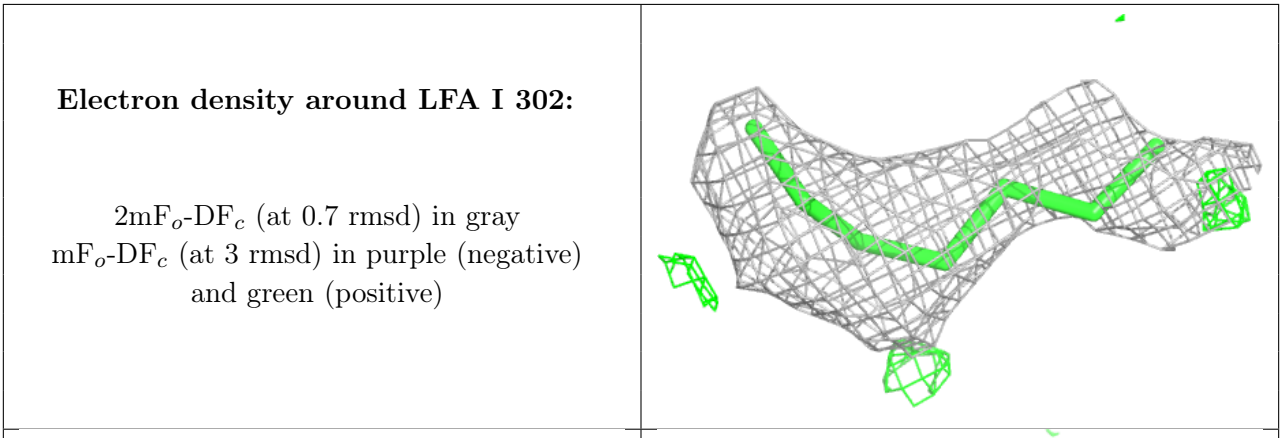
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

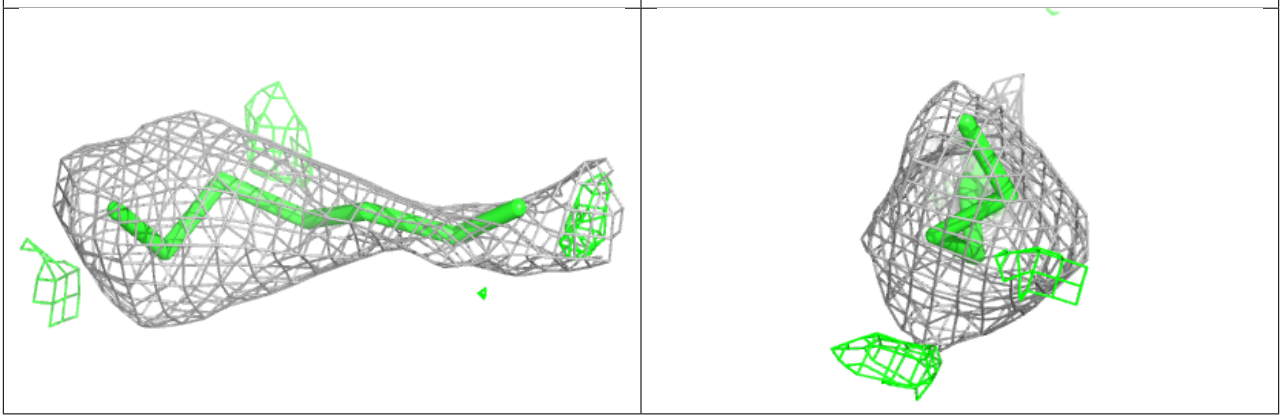




Electron density around LFA I 302:

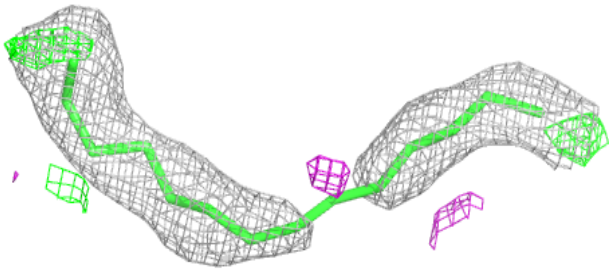
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

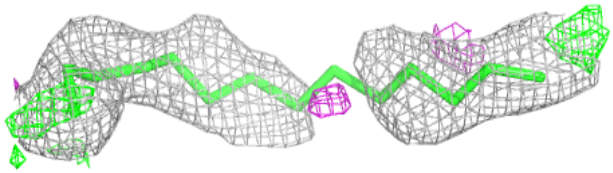


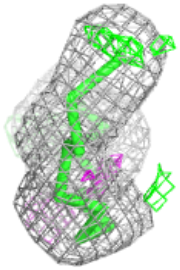


Electron density around LFA I 304:

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

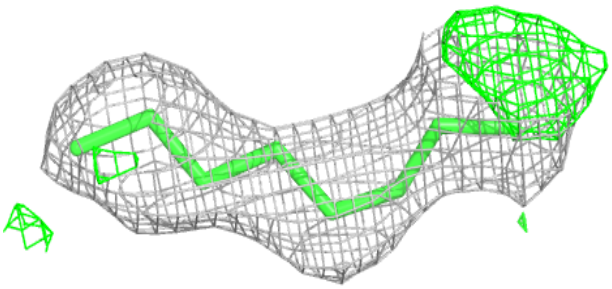


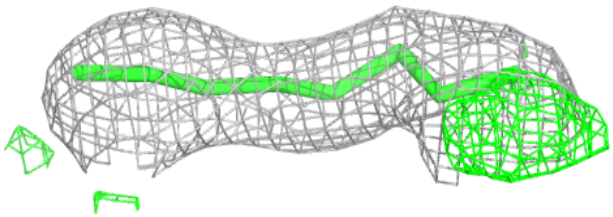


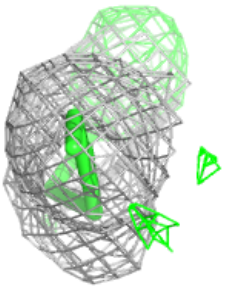


Electron density around LFA J 304:

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

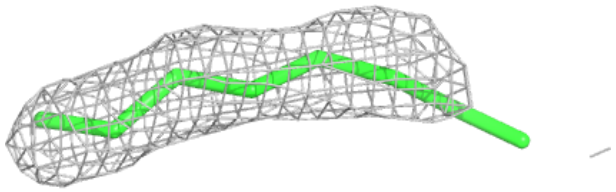


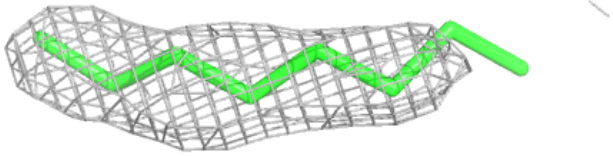


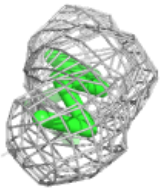


Electron density around LFA C 311:

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

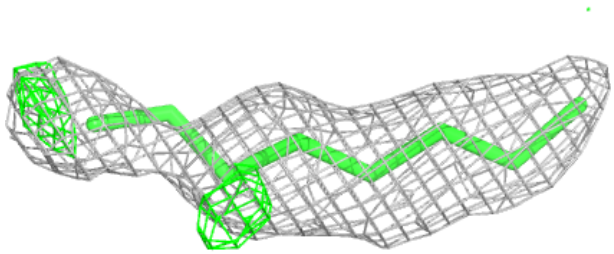


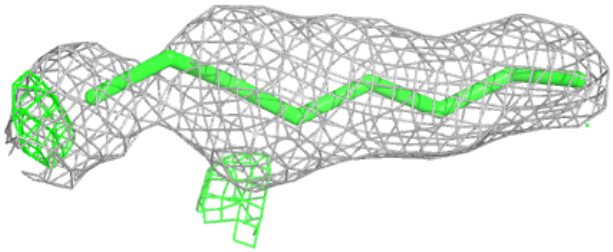


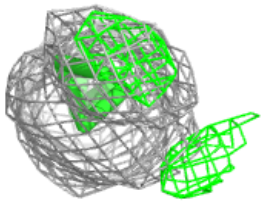


Electron density around LFA A 308:

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

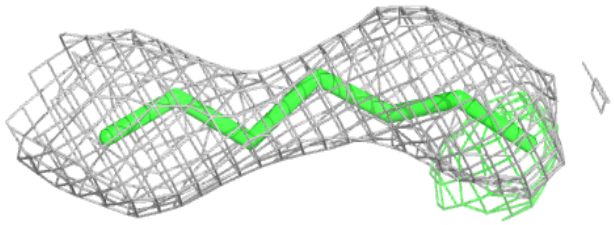


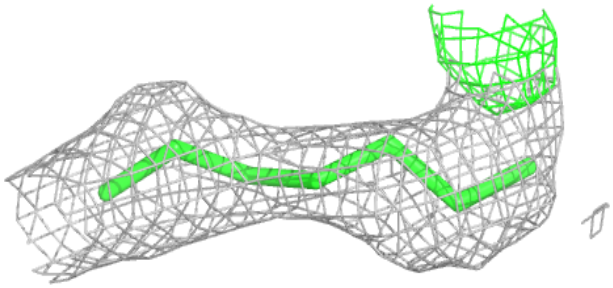


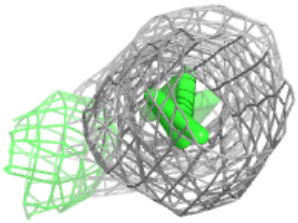


Electron density around LFA D 302:

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

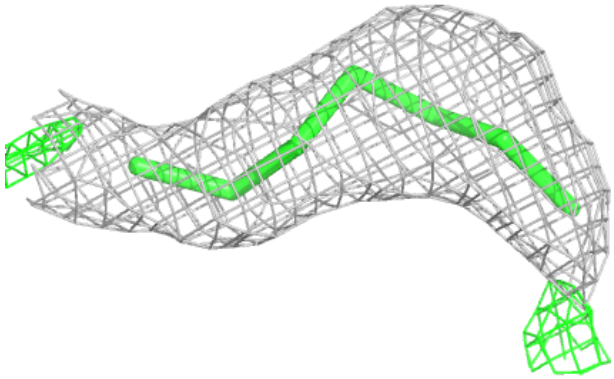


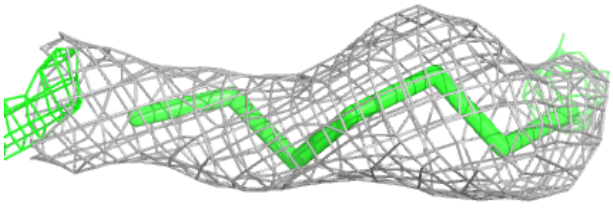


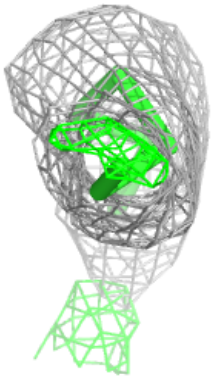


Electron density around LFA B 302:

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

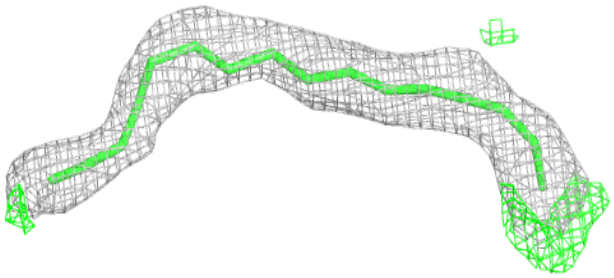


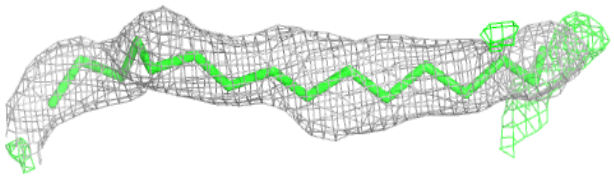


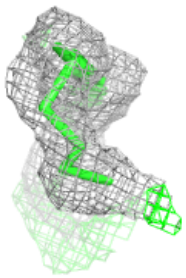


Electron density around LFA G 307:

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

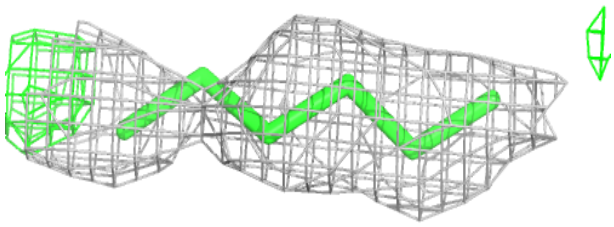


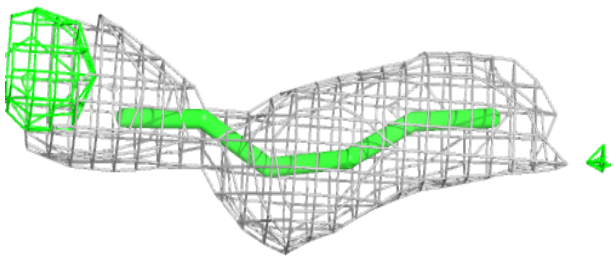


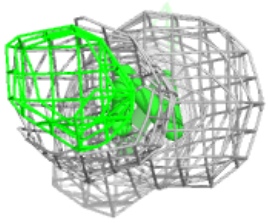


Electron density around LFA I 305:

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

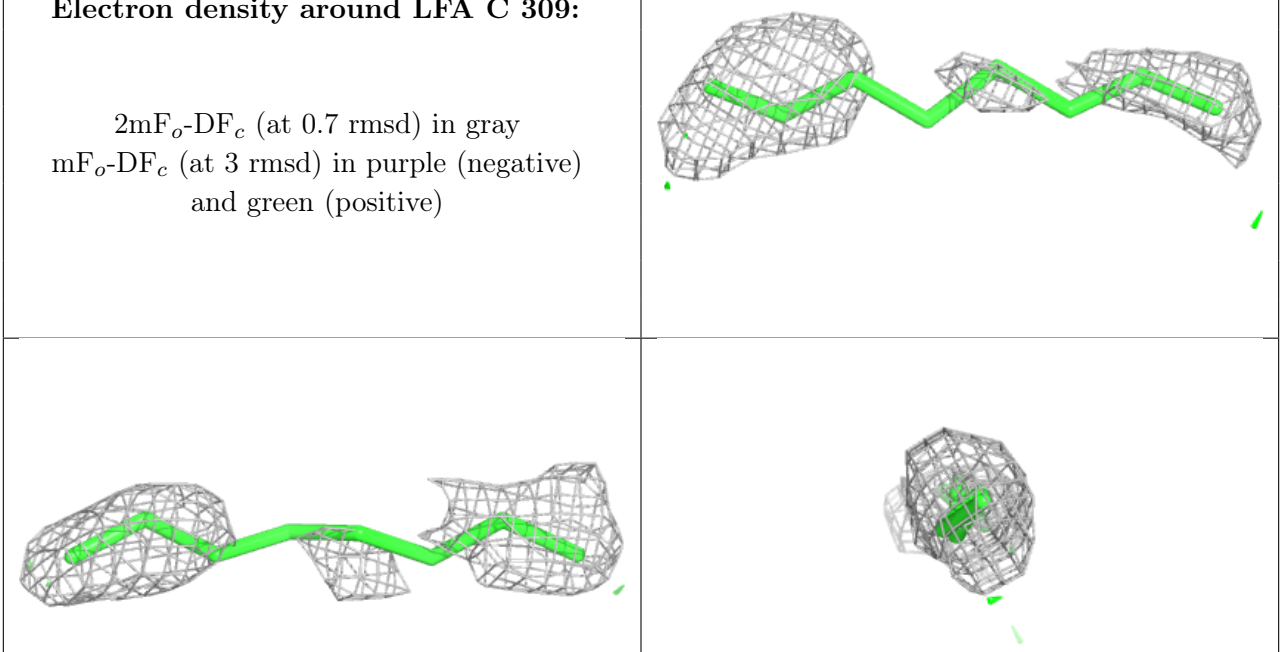






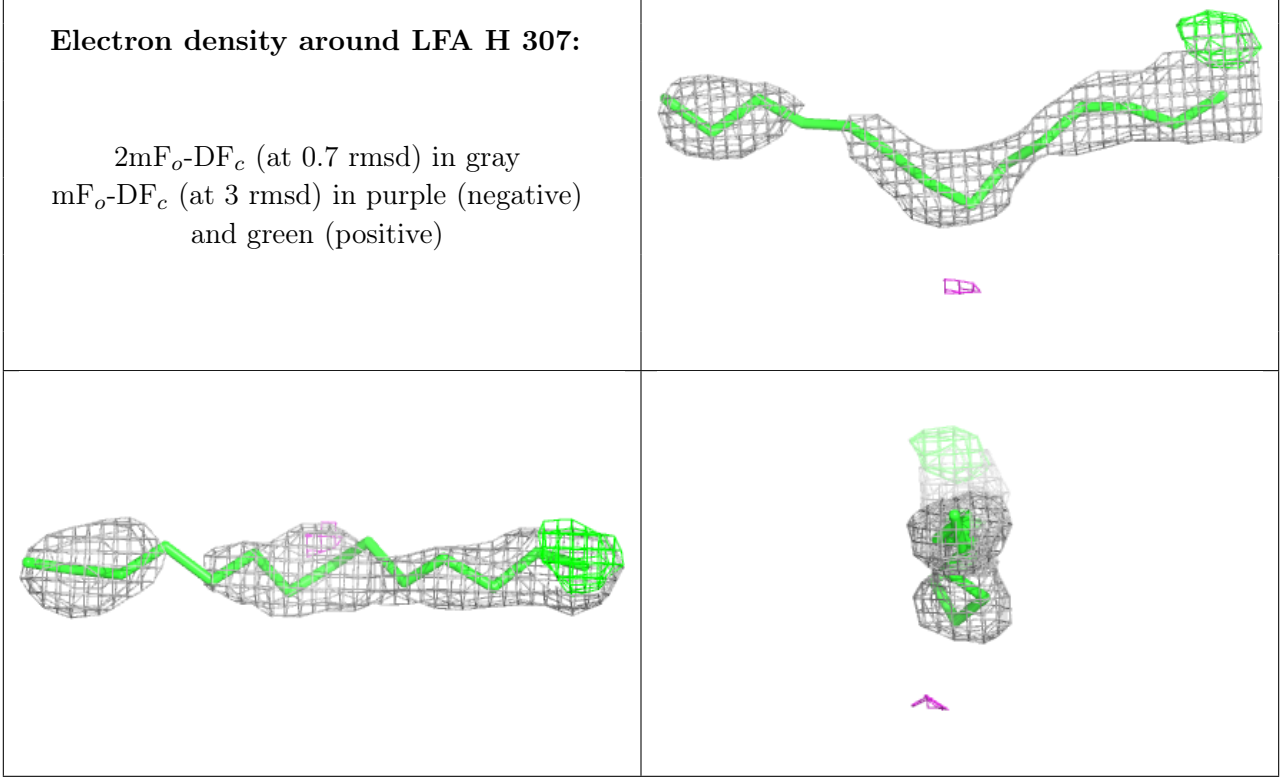
Electron density around LFA C 309:

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



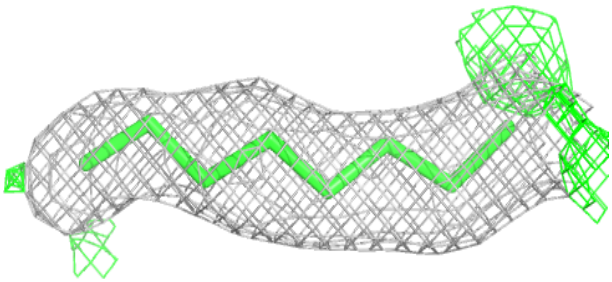
Electron density around LFA H 307:

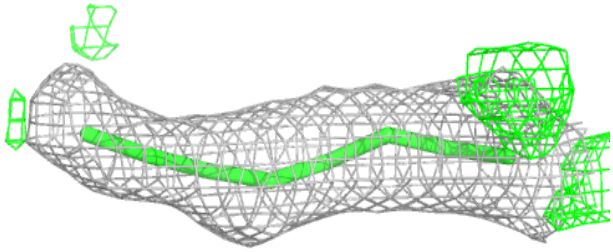
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

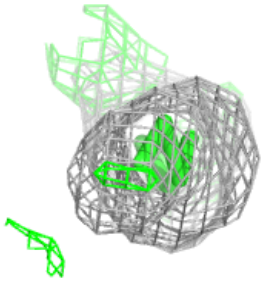


Electron density around LFA H 310:

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

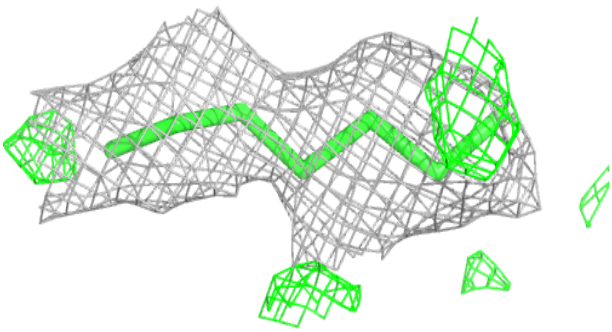


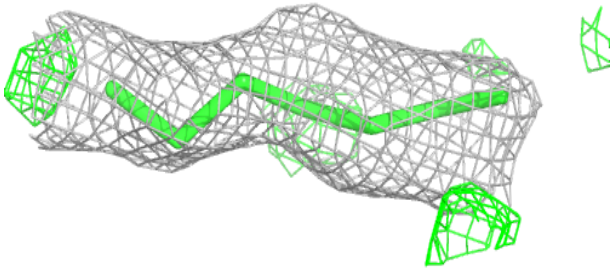


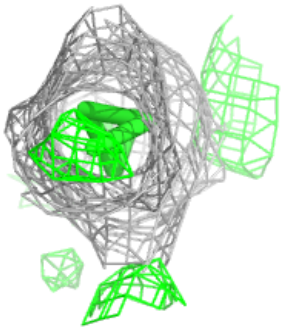


Electron density around LFA A 311:

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

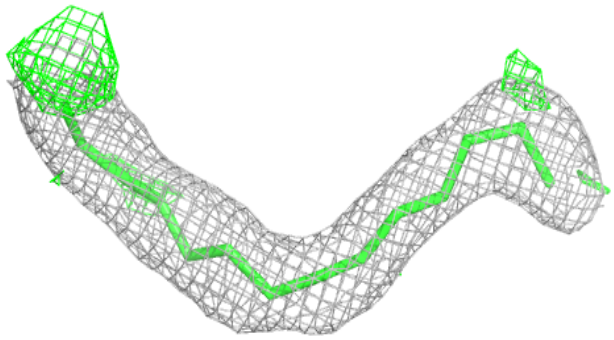


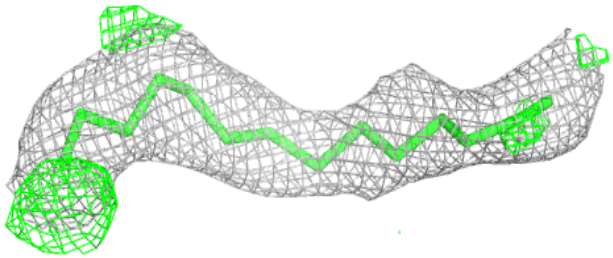


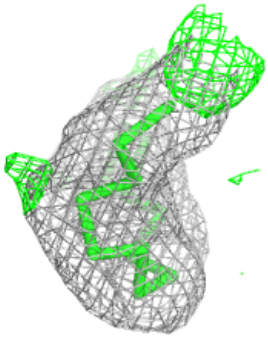


Electron density around LFA G 304:

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

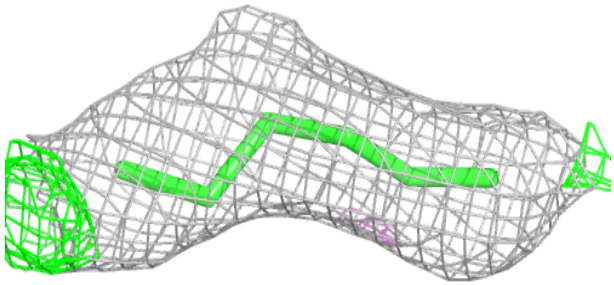


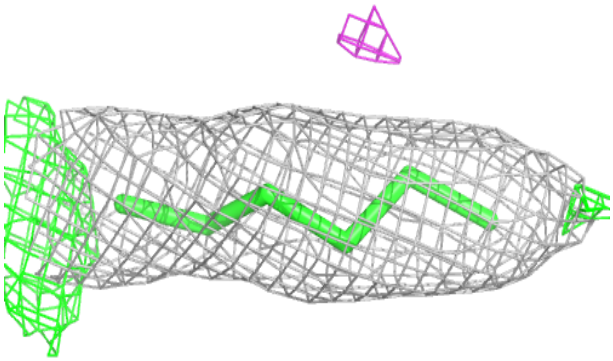


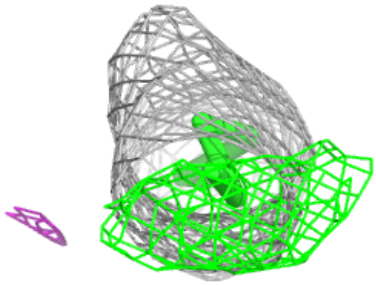


Electron density around LFA I 307:

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

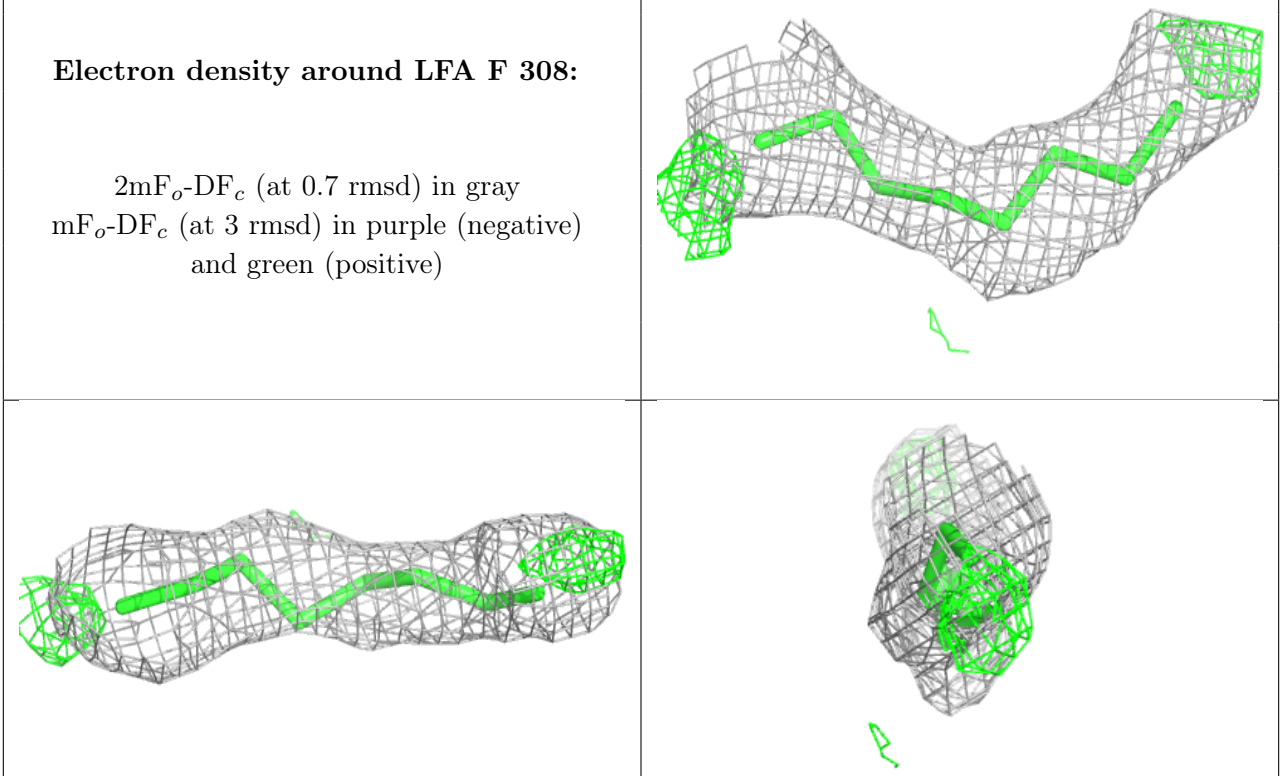






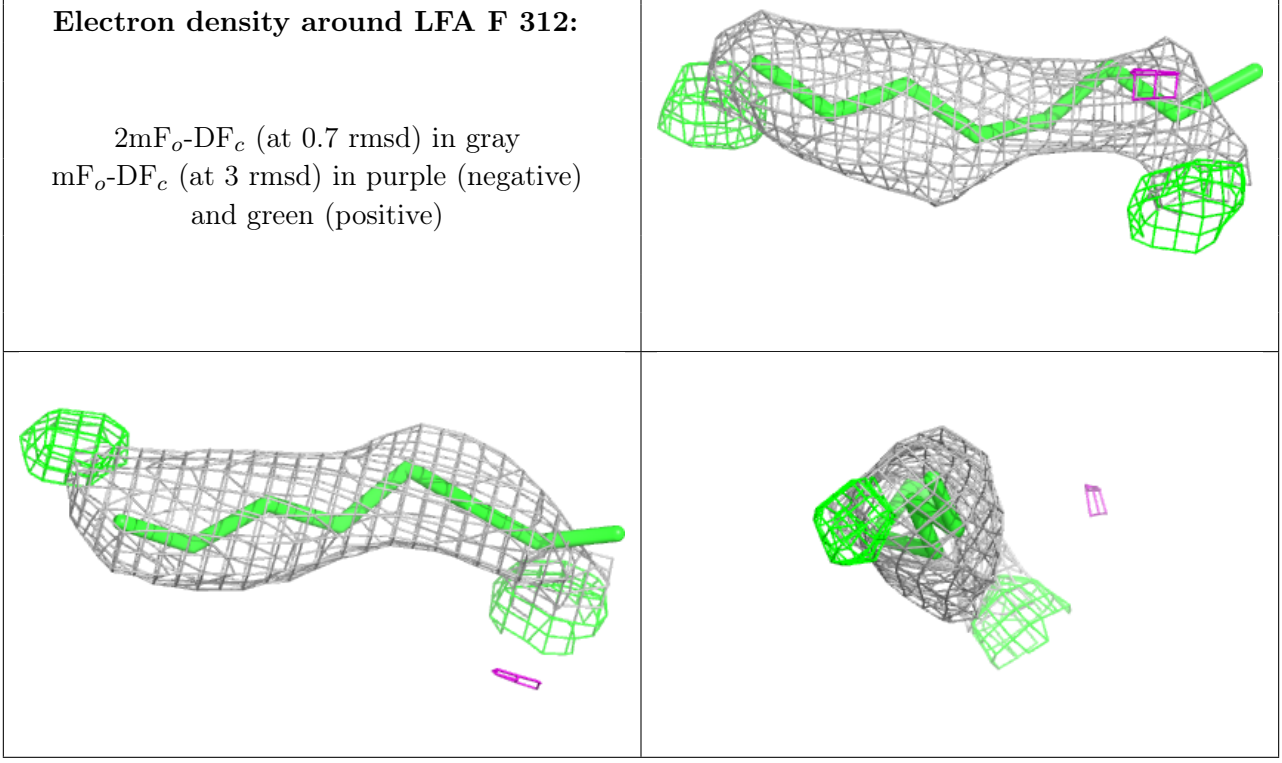
Electron density around LFA F 308:

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



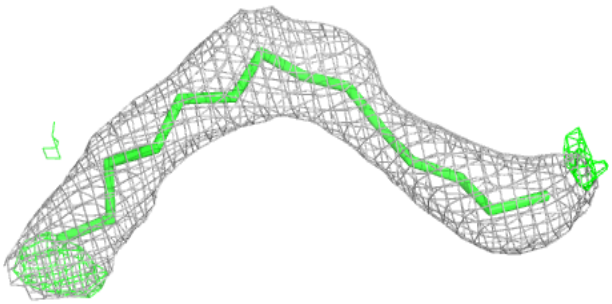
Electron density around LFA F 312:

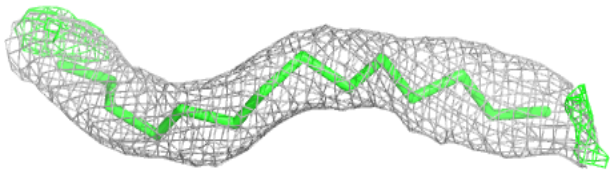
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

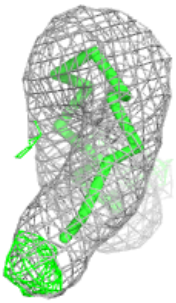


Electron density around LFA J 308:

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

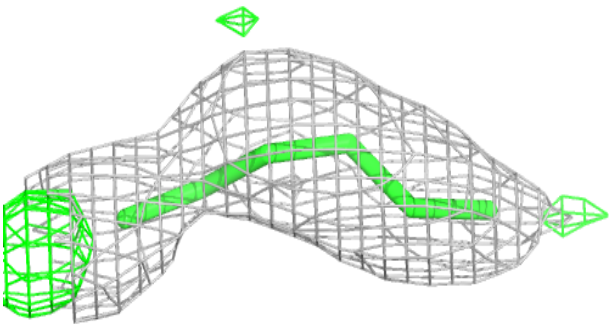


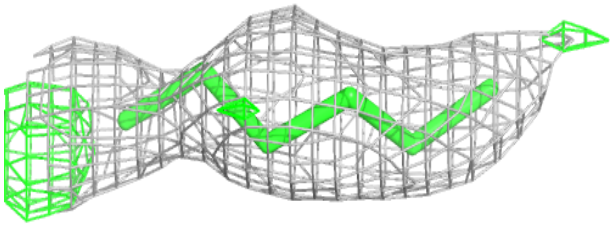


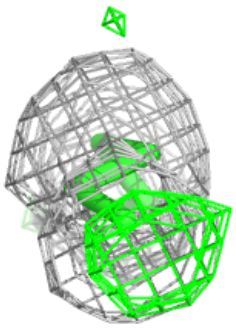


Electron density around LFA B 305:

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

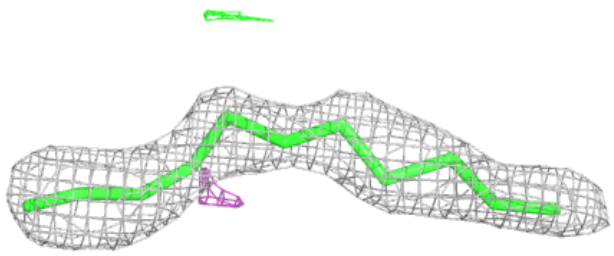


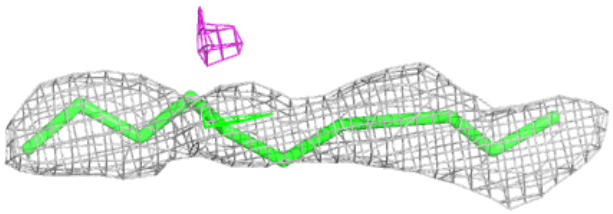


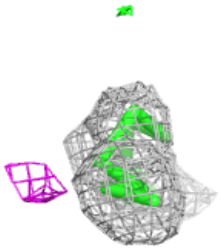


Electron density around LFA B 310:

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

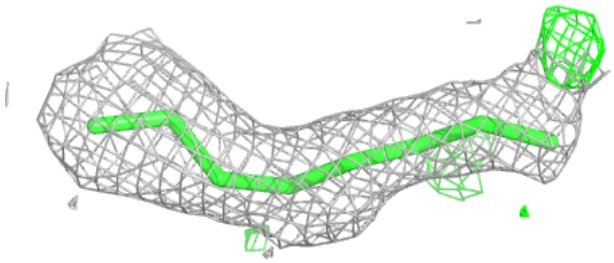


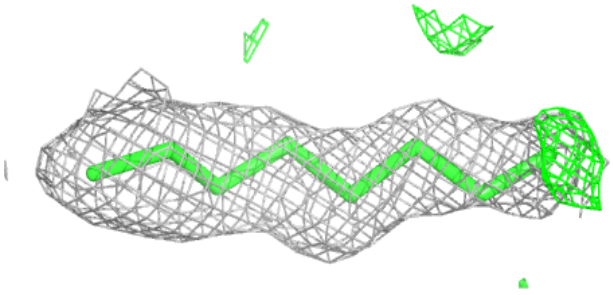


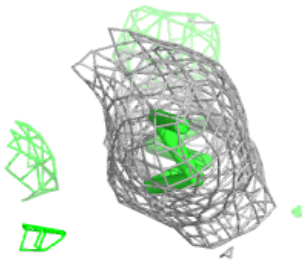


Electron density around LFA E 311:

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

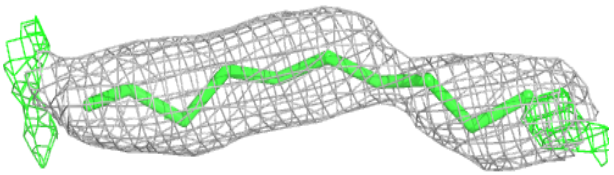


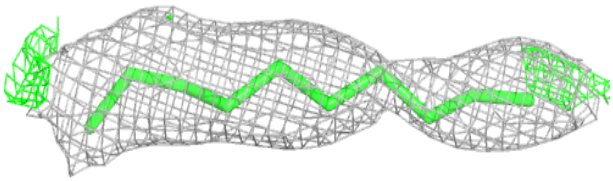


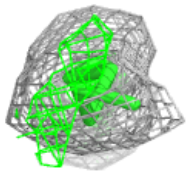


Electron density around LFA D 305:

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

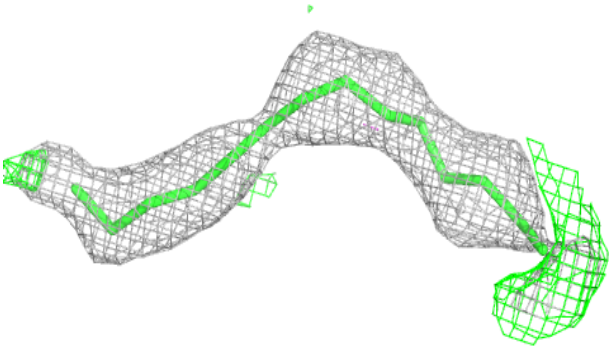


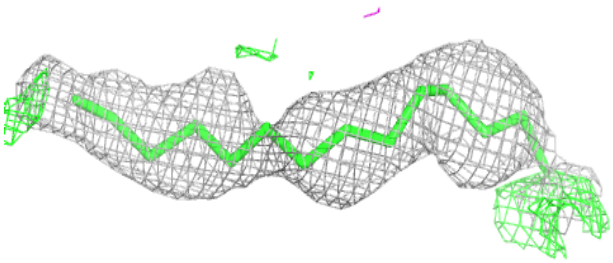


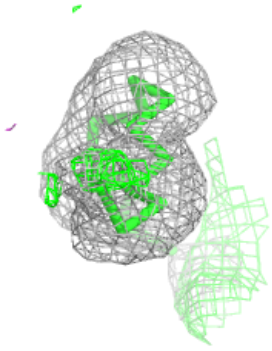


Electron density around LFA F 303:

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

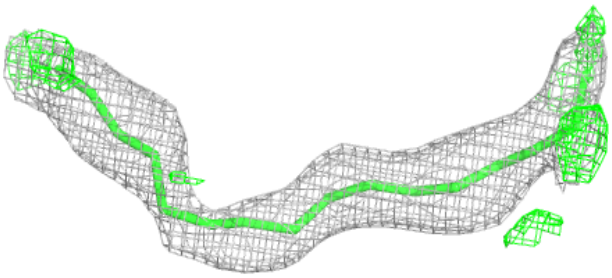


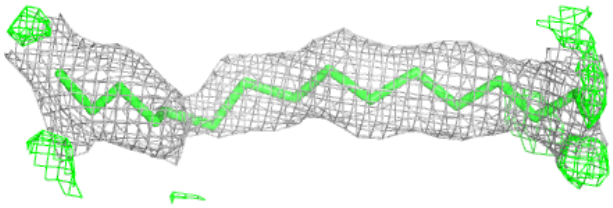


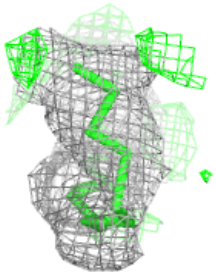


Electron density around LFA D 306:

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

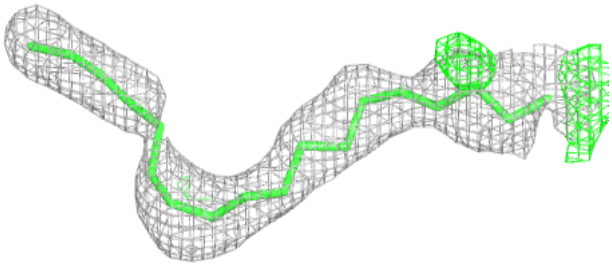


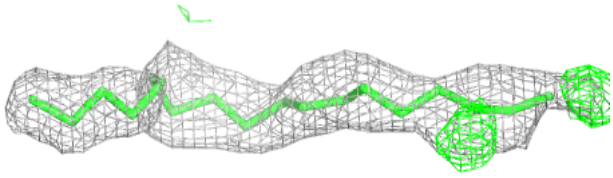


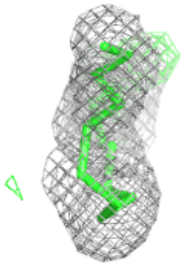


Electron density around LFA B 308:

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

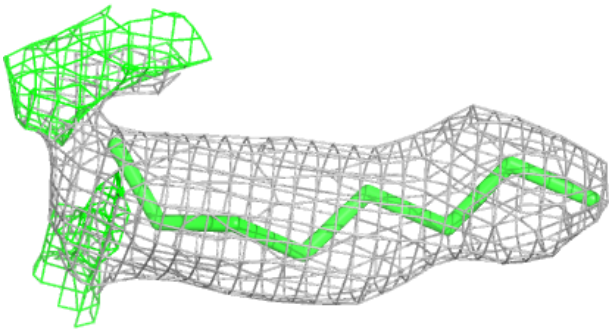


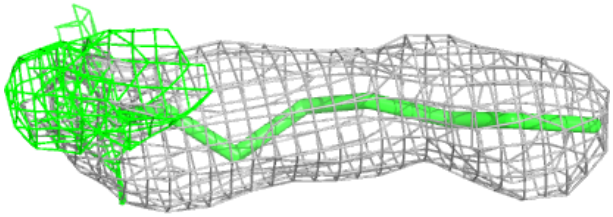


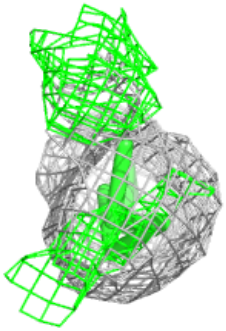


Electron density around LFA D 309:

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

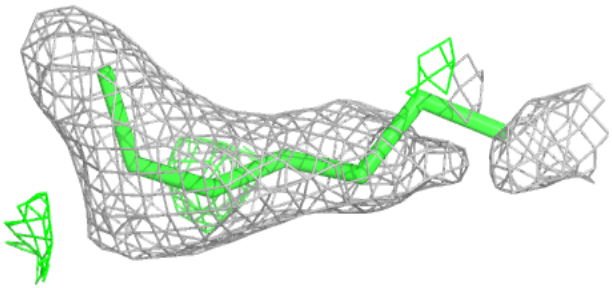


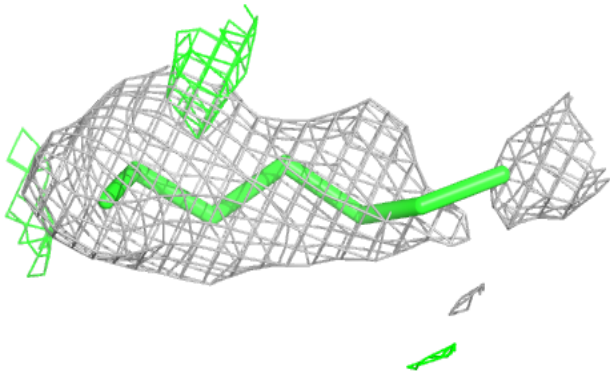


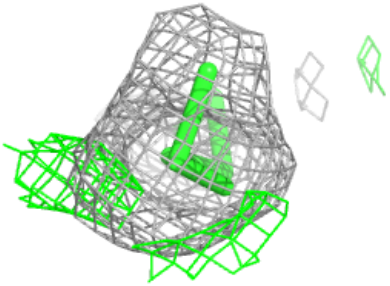


Electron density around LFA B 303:

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

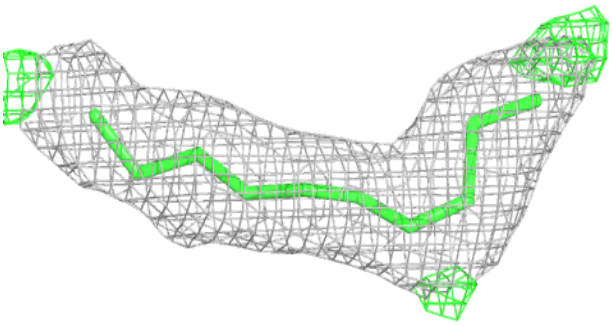


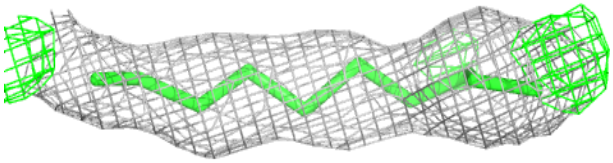


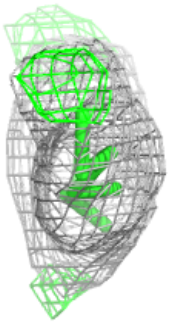


Electron density around LFA A 305:

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

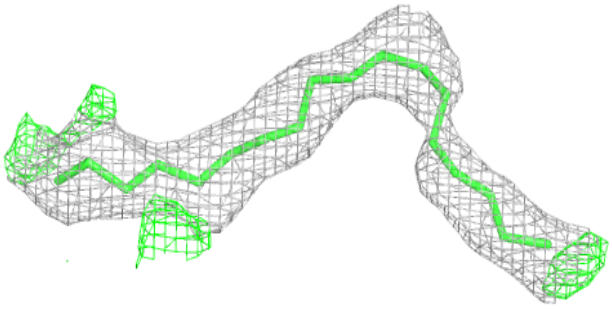


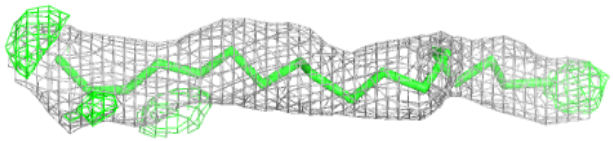


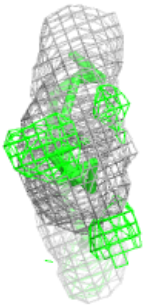


Electron density around LFA G 308:

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

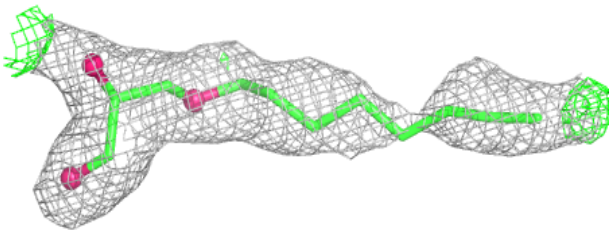


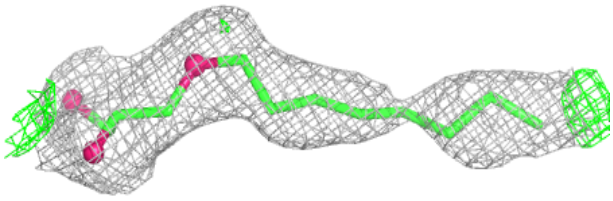


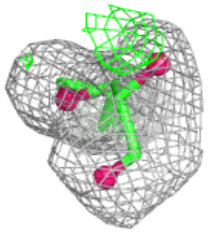


Electron density around MPG A 313:

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

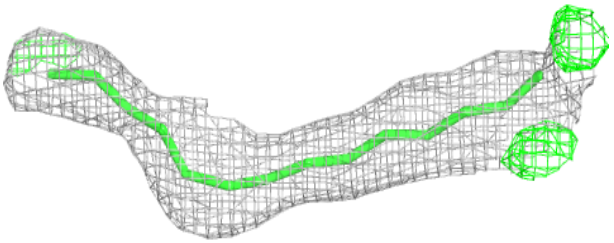


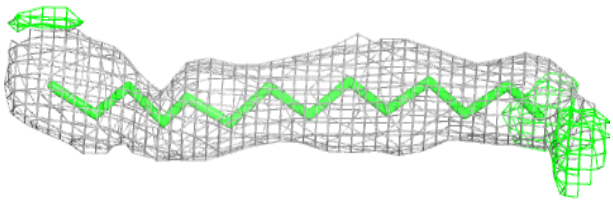


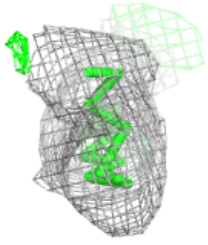


Electron density around LFA E 302:

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

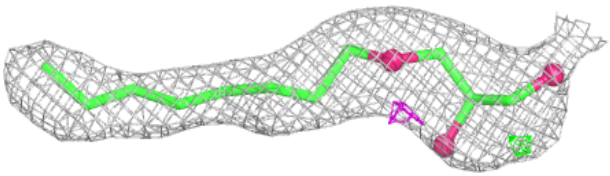


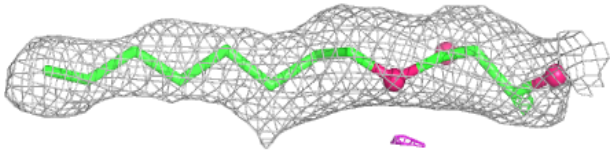


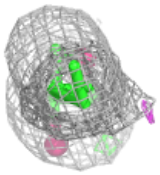


Electron density around MPG E 313:

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

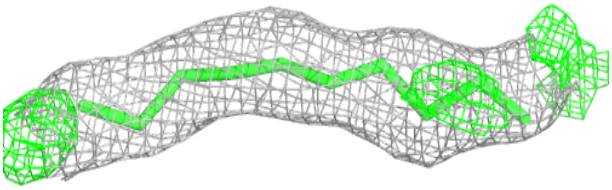


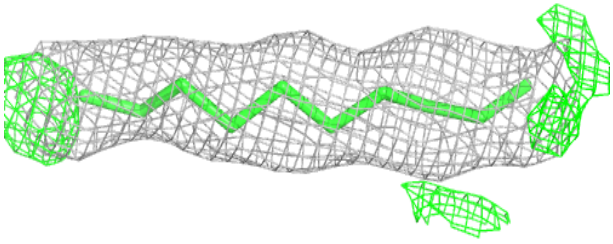


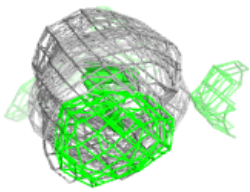


Electron density around LFA A 304:

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

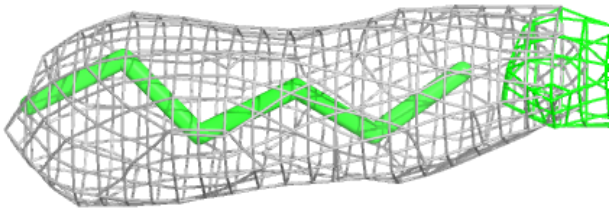


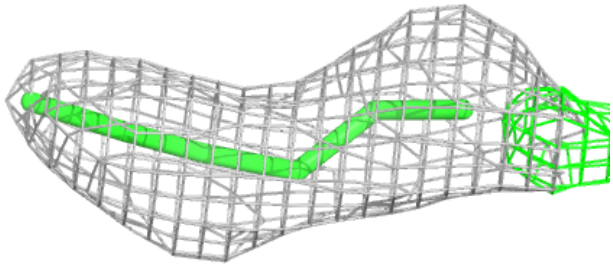


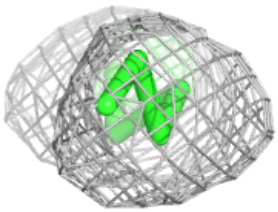


Electron density around LFA F 305:

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

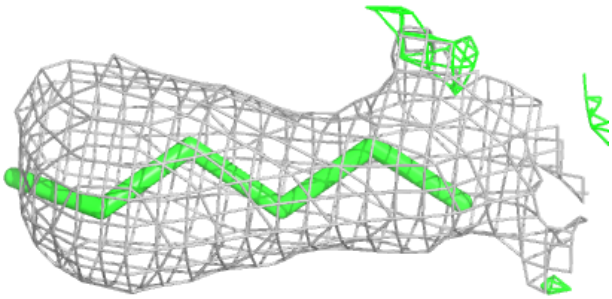


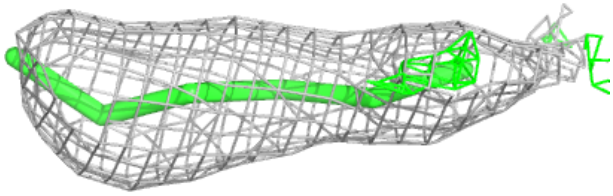


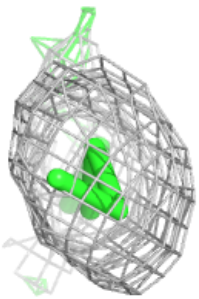


Electron density around LFA G 314:

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

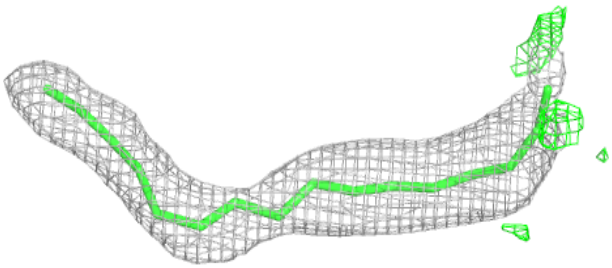


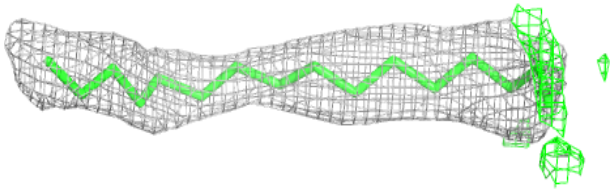


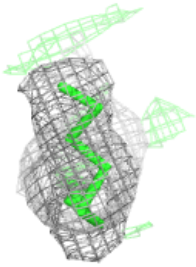


Electron density around LFA I 308:

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

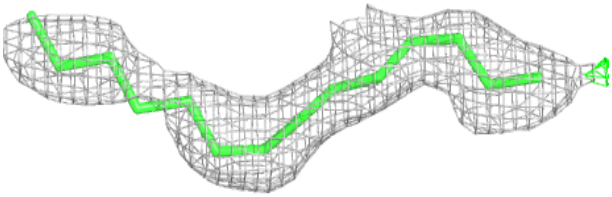


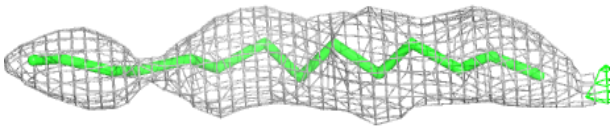


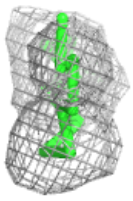


Electron density around LFA I 310:

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

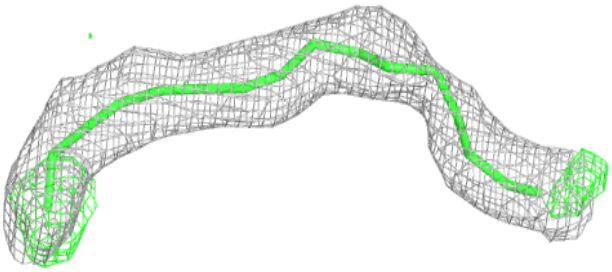


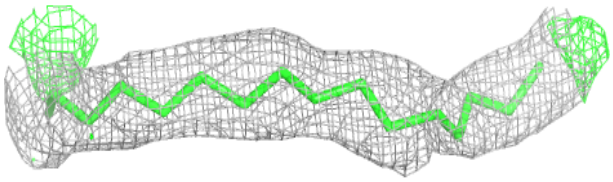


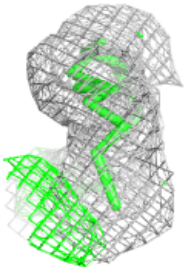


Electron density around LFA J 302:

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

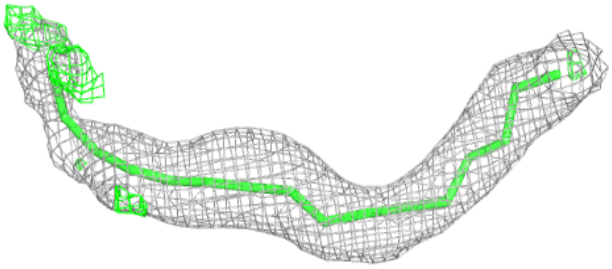


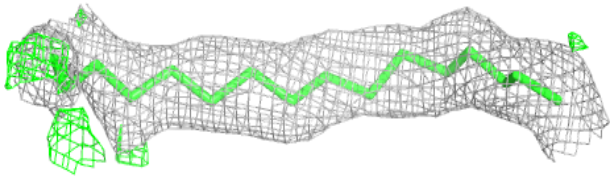


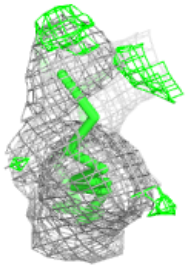


Electron density around LFA C 306:

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

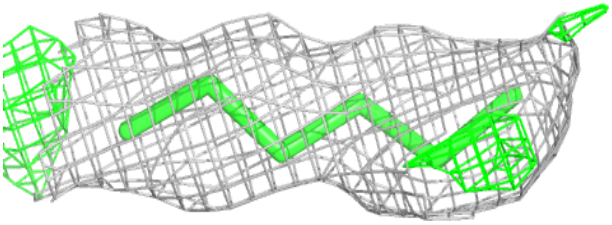


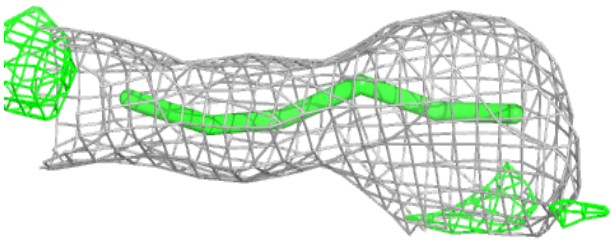


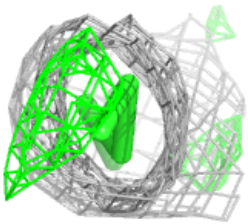


Electron density around LFA E 305:

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

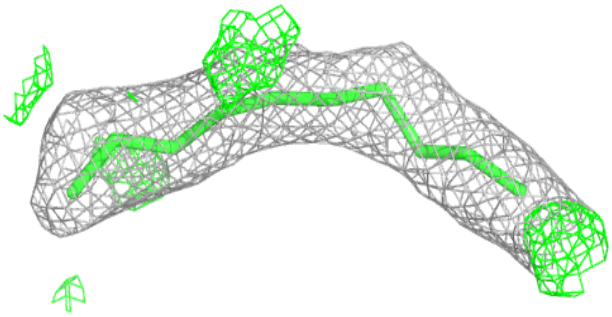


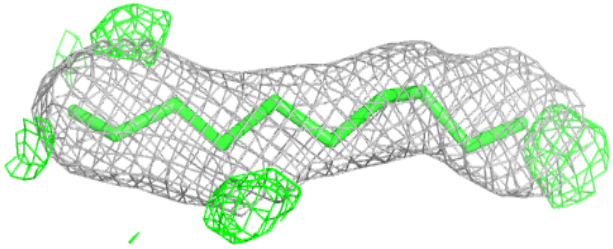


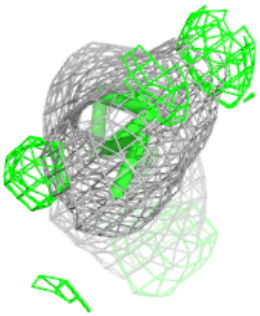


Electron density around LFA F 309:

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

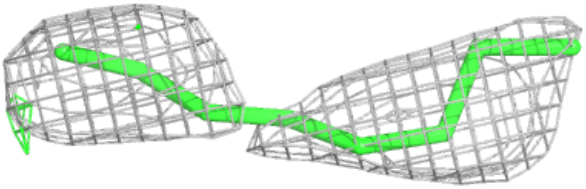


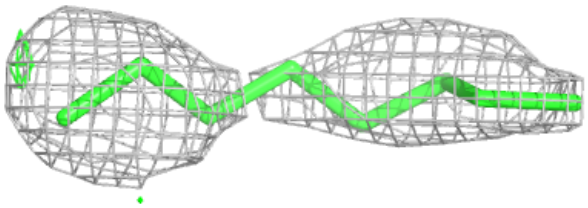


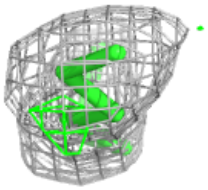


Electron density around LFA G 309:

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

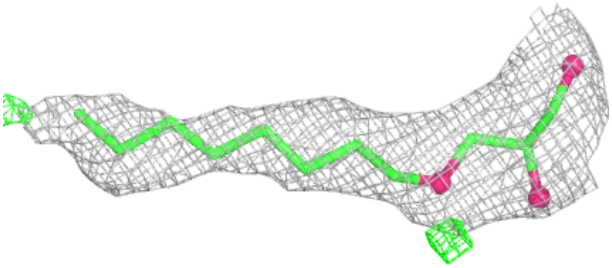


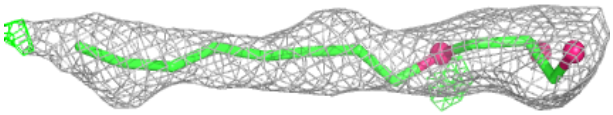


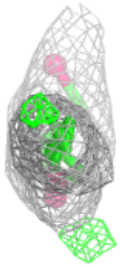


Electron density around MPG B 312:

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

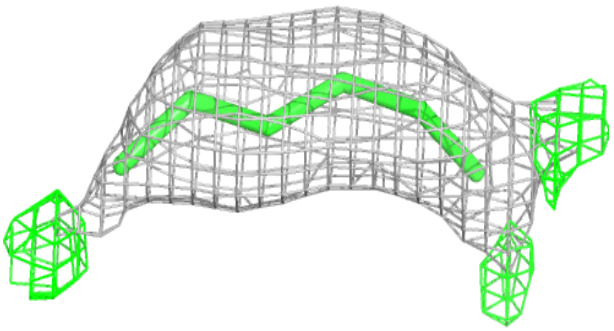


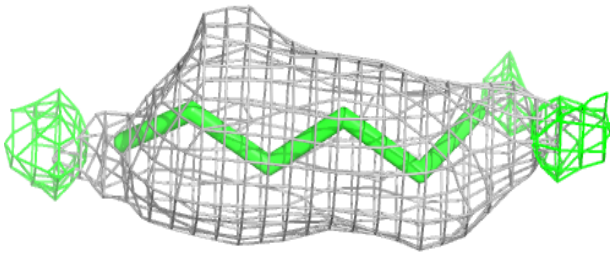


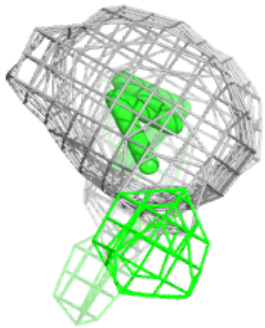


Electron density around LFA A 303:

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

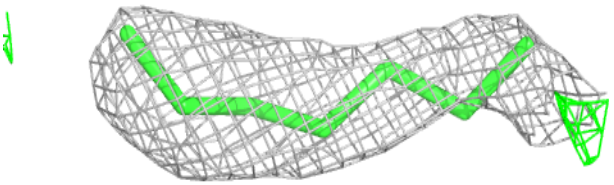


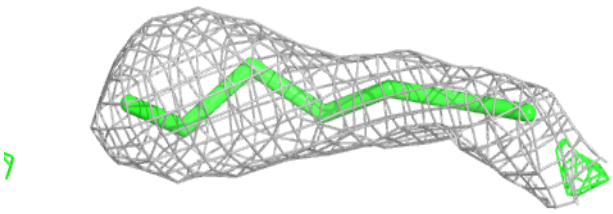


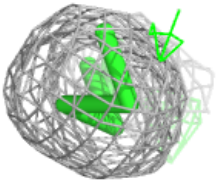


Electron density around LFA I 303:

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

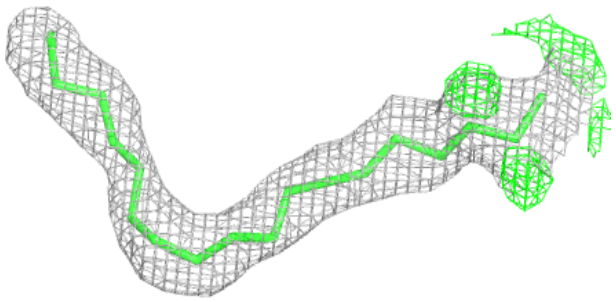


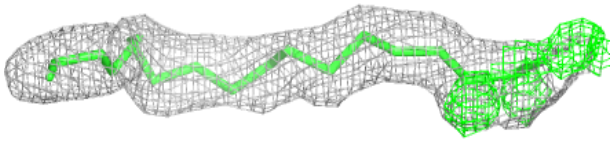




Electron density around LFA A 307:

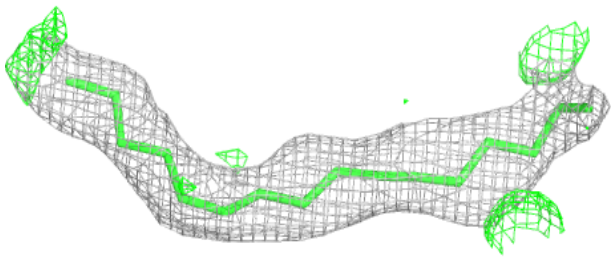
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

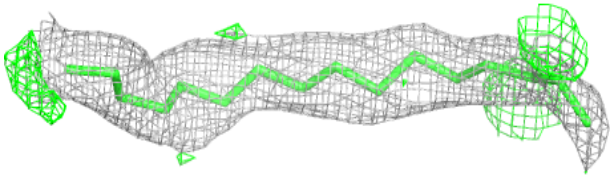


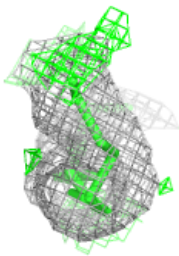


Electron density around LFA G 302:

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

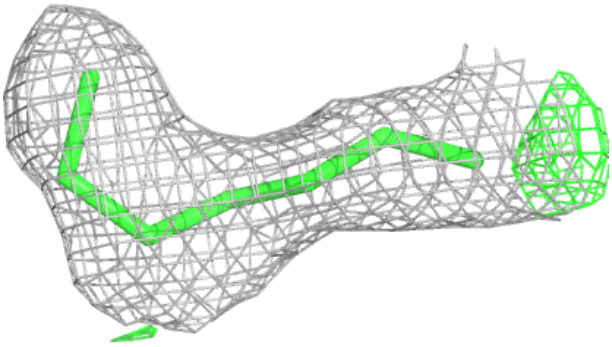


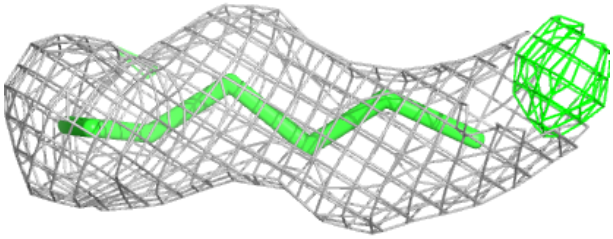


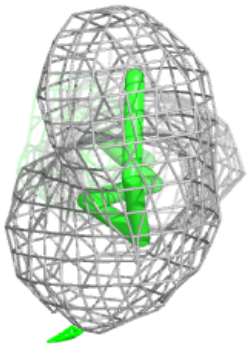


Electron density around LFA C 302:

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

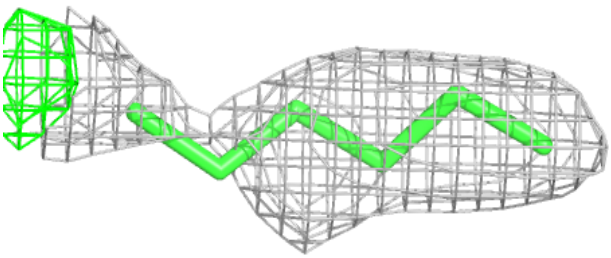


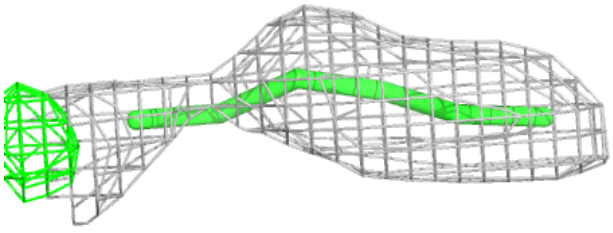


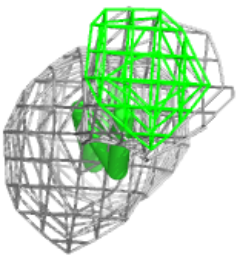


Electron density around LFA G 305:

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

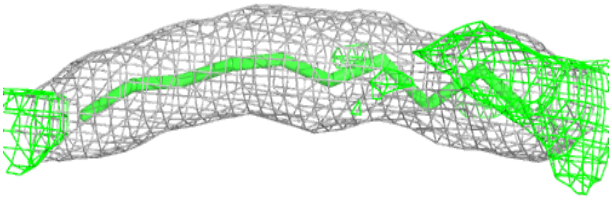


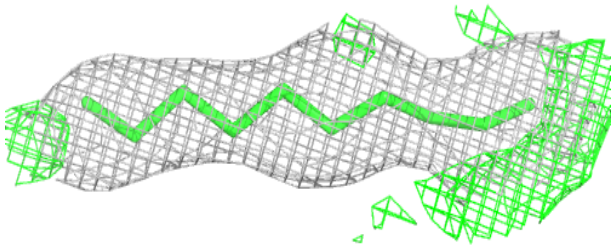


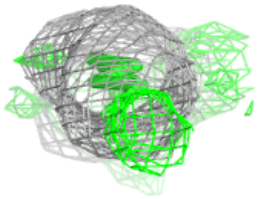


Electron density around LFA I 306:

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

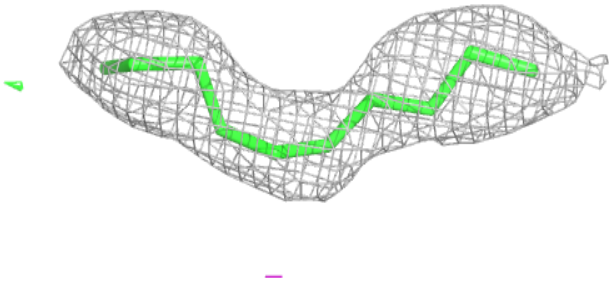


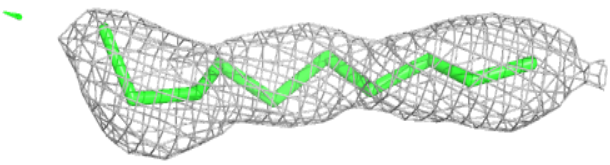


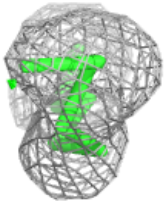


Electron density around LFA J 309:

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

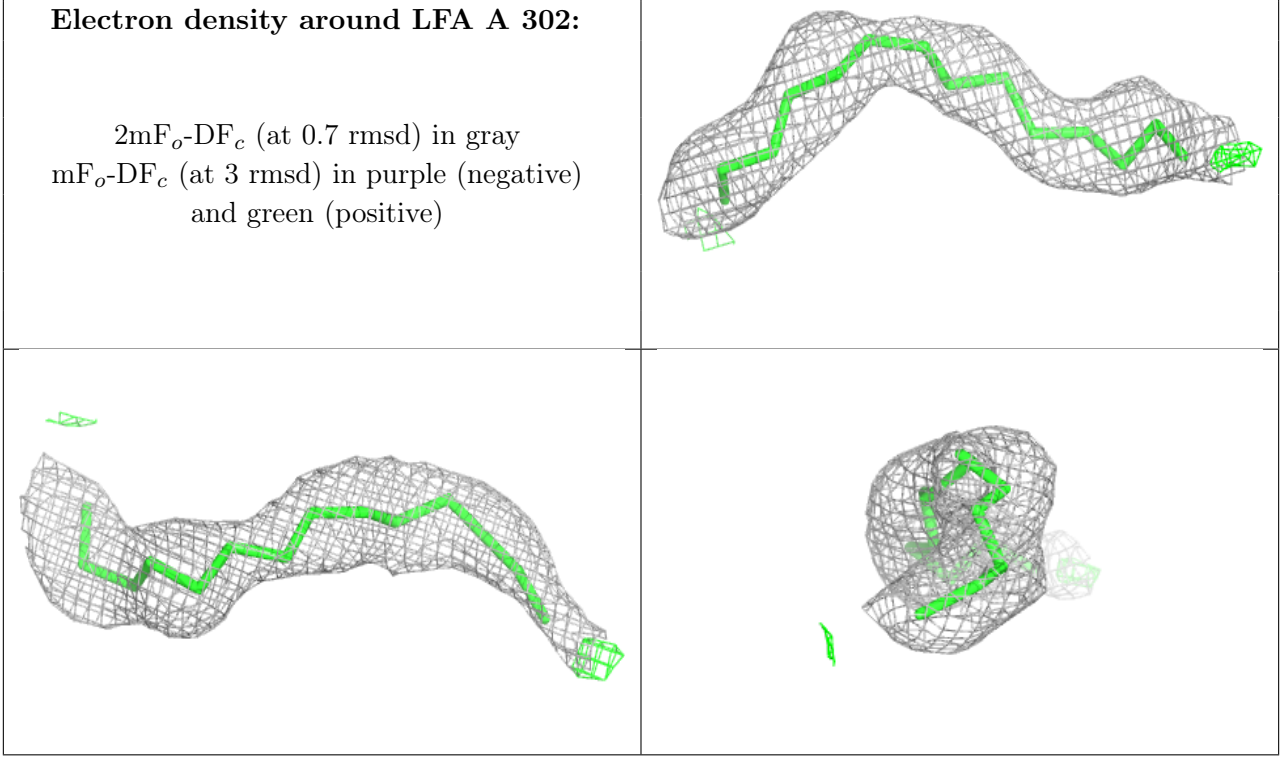






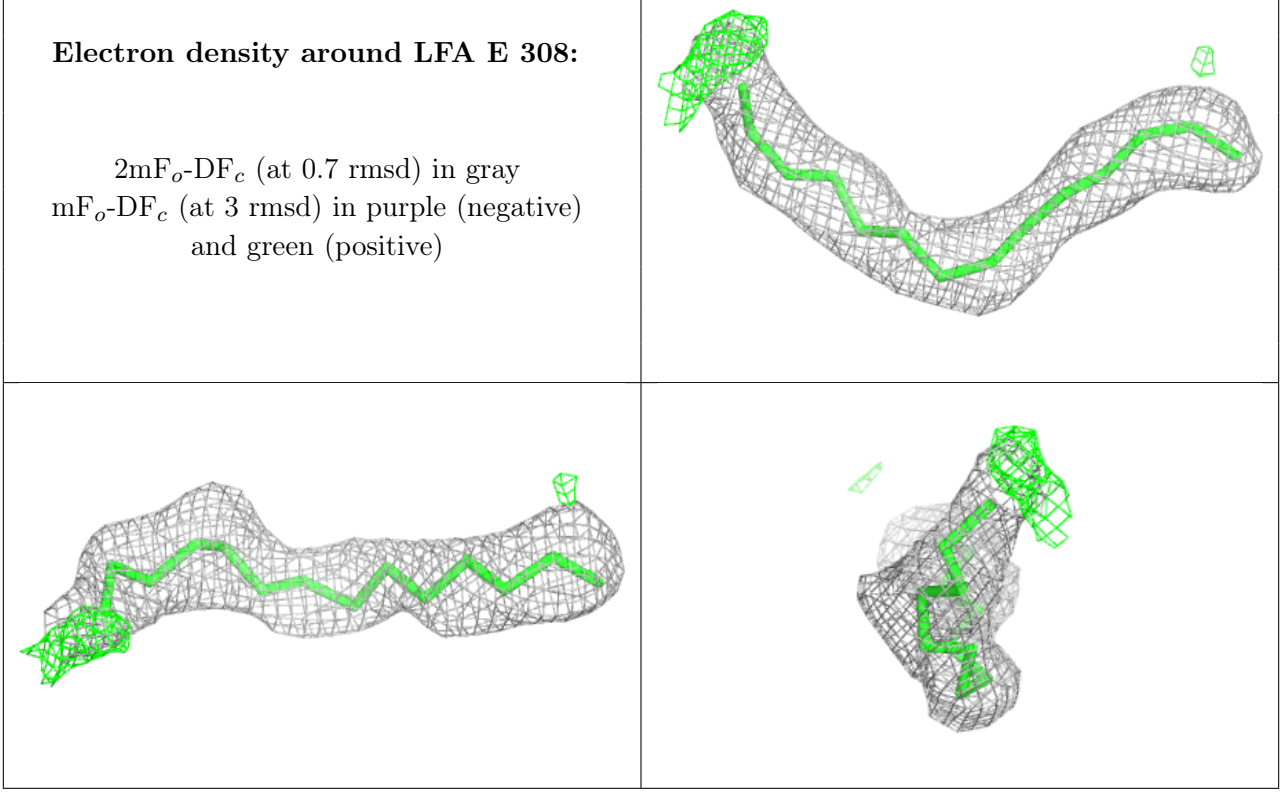
Electron density around LFA A 302:

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



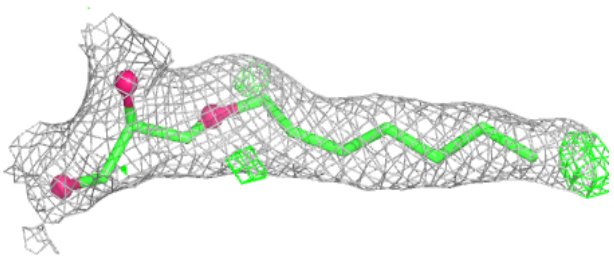
Electron density around LFA E 308:

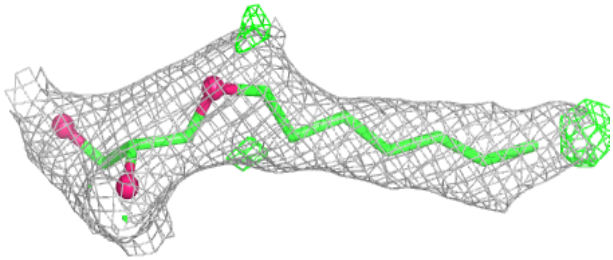
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

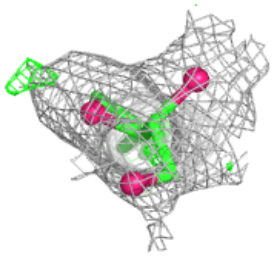


Electron density around MPG C 313:

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

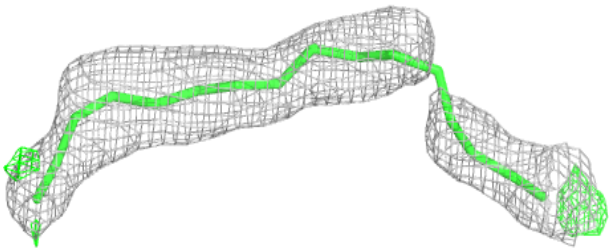


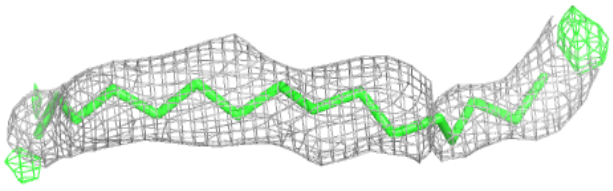


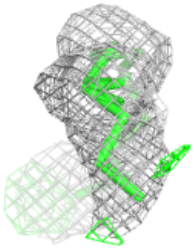


Electron density around LFA B 307:

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

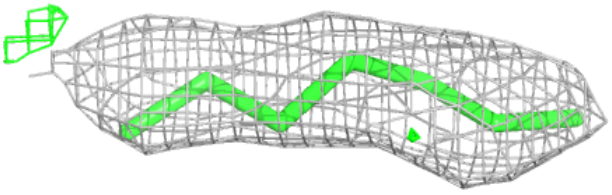


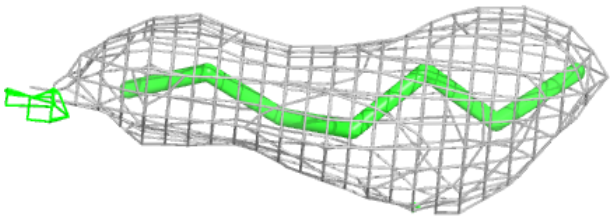


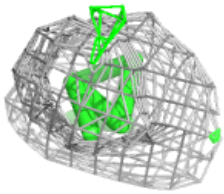


Electron density around LFA D 311:

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

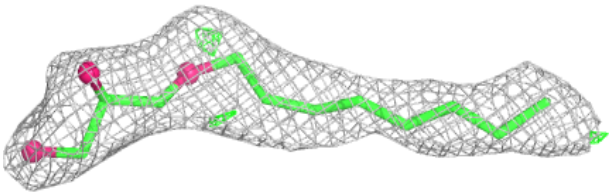


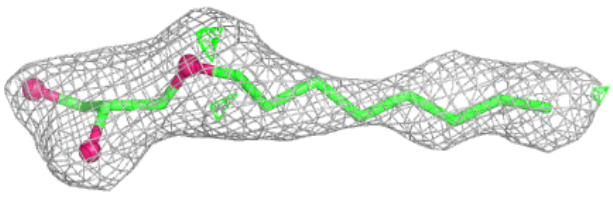


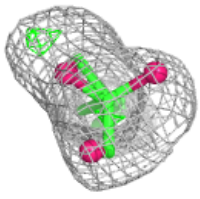


Electron density around MPG G 312:

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

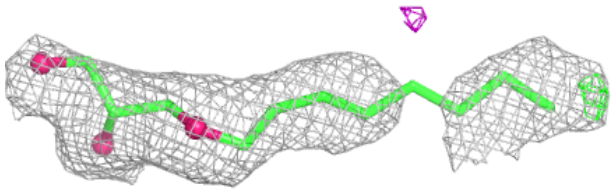


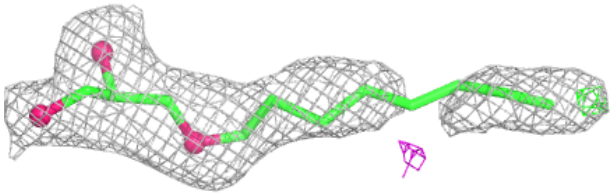


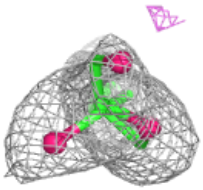


Electron density around MPG J 312:

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

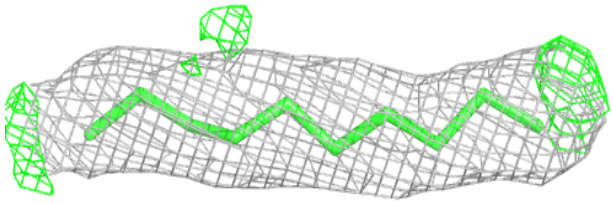


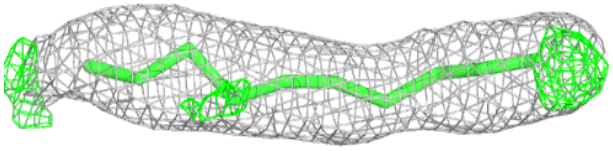


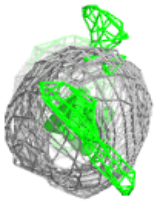


Electron density around LFA C 305:

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

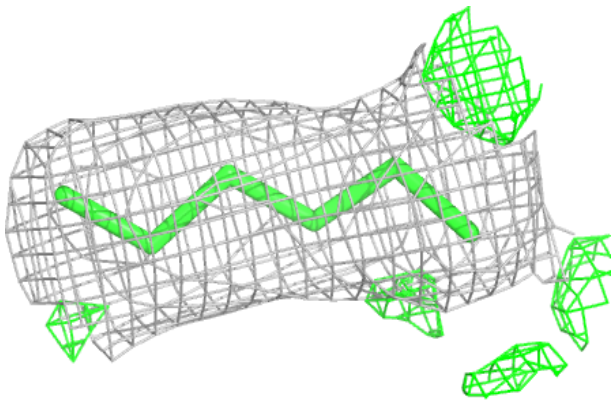


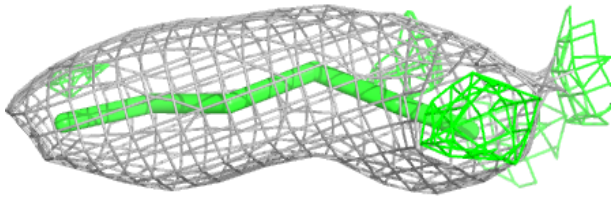


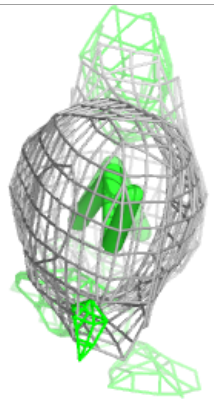


Electron density around LFA H 312:

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

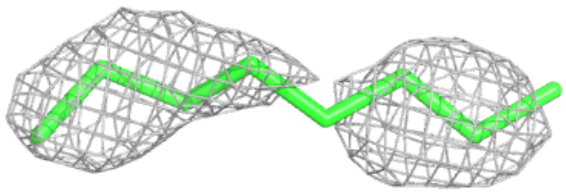


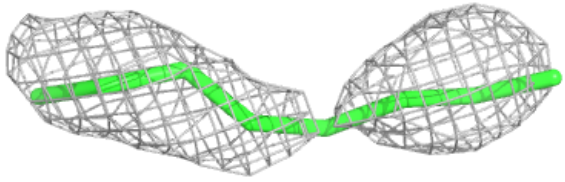


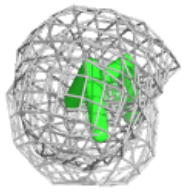


Electron density around LFA J 306:

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

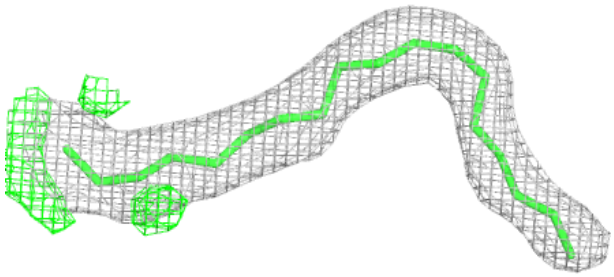


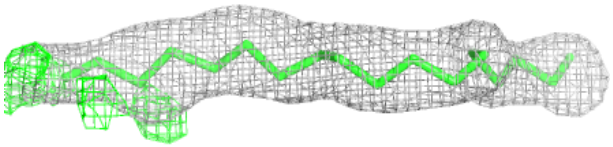


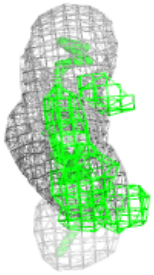


Electron density around LFA H 306:

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

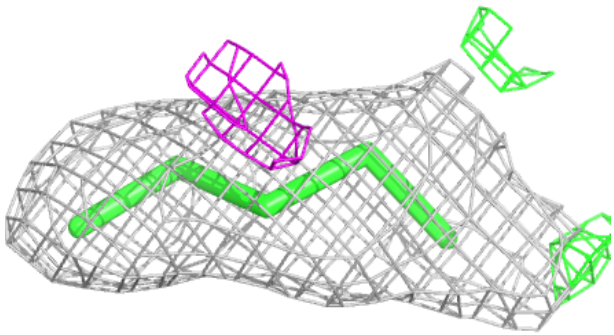


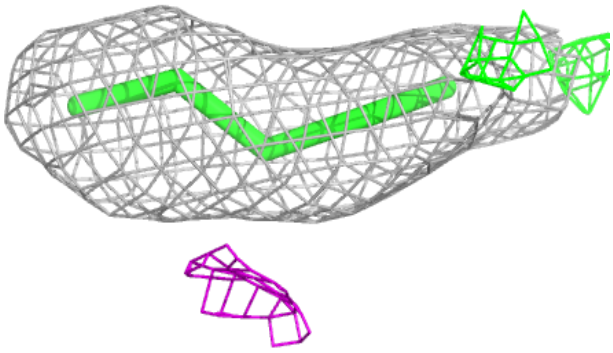


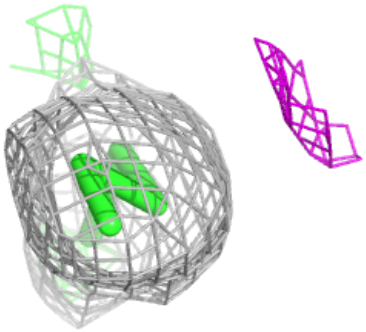


Electron density around LFA H 309:

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

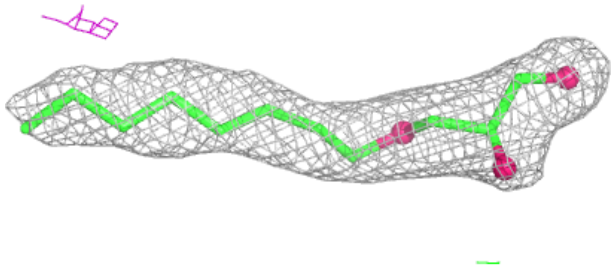


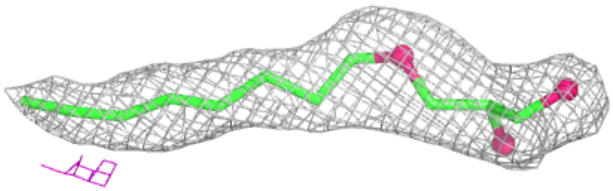


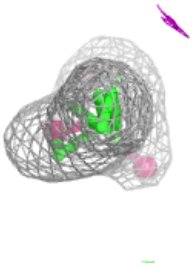


Electron density around MPG F 315:

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

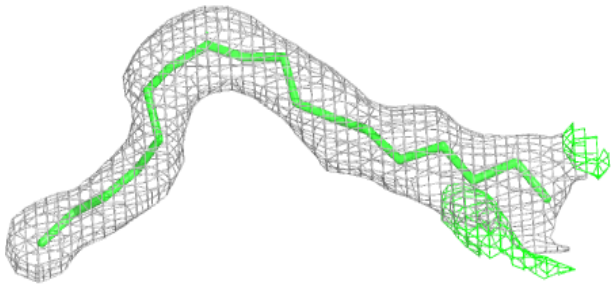


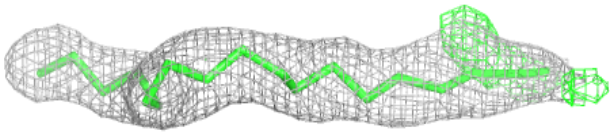


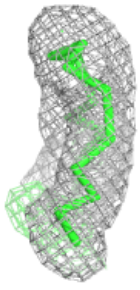


Electron density around LFA J 303:

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

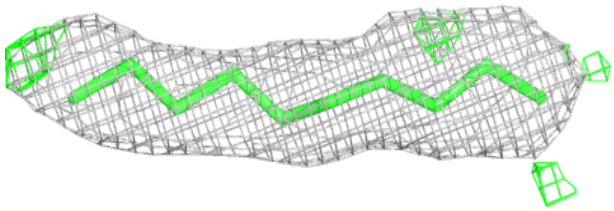


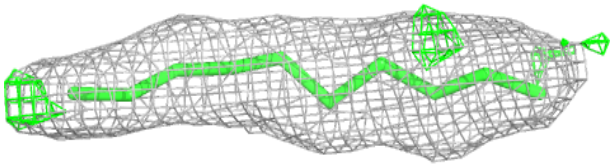


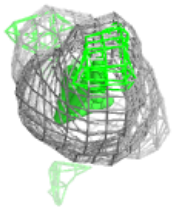


Electron density around LFA J 310:

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

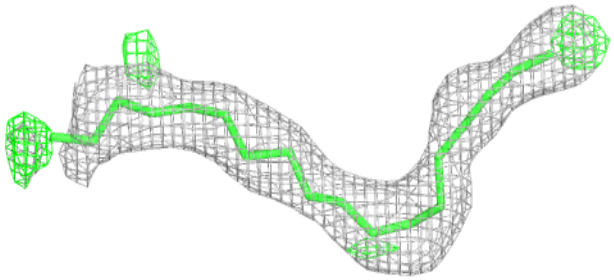


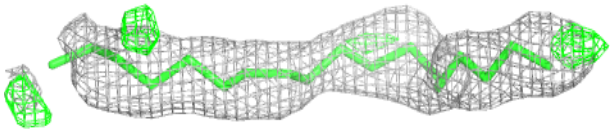


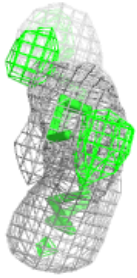


Electron density around LFA I 309:

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

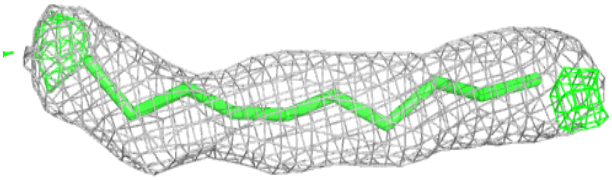


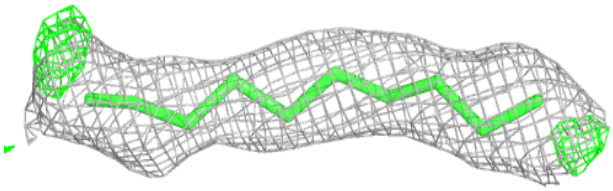


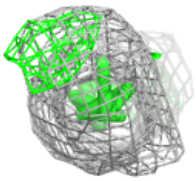


Electron density around LFA G 306:

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

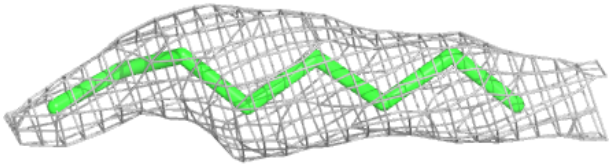


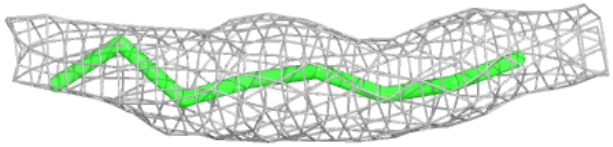


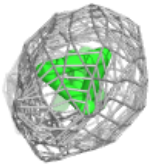


Electron density around LFA I 311:

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

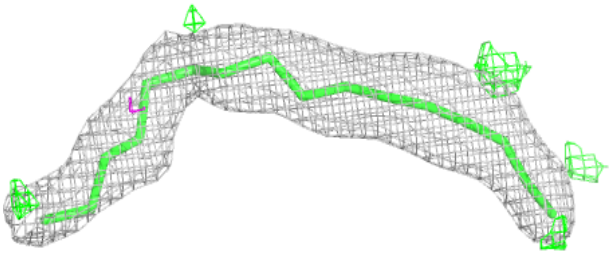


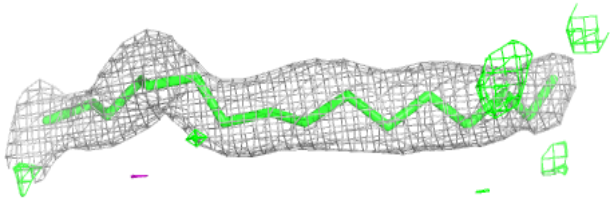


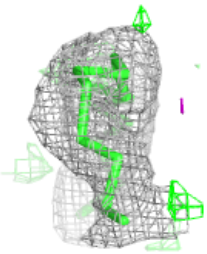


Electron density around LFA H 305:

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

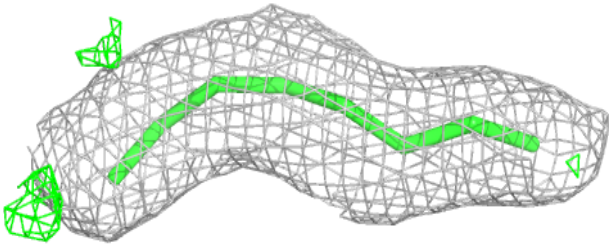


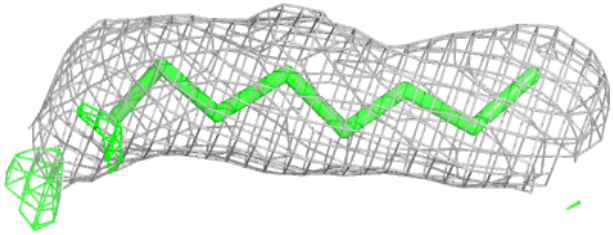


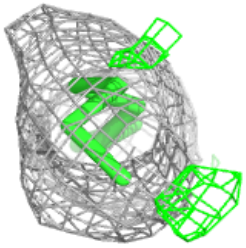


Electron density around LFA E 312:

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

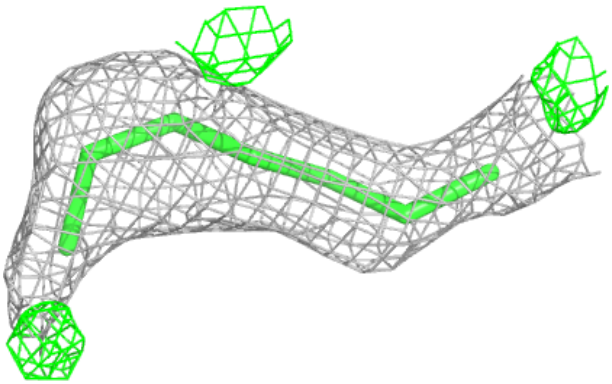


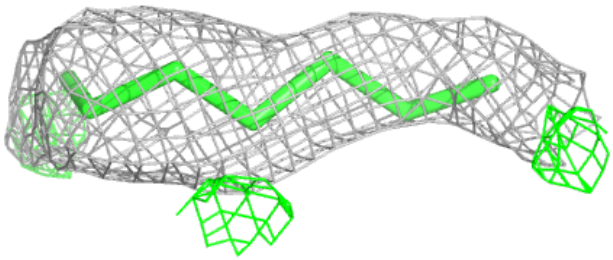


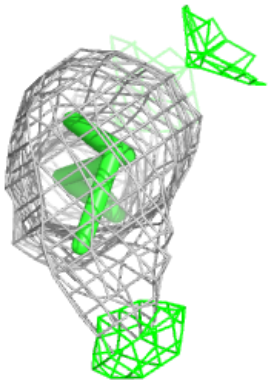


Electron density around LFA G 303:

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

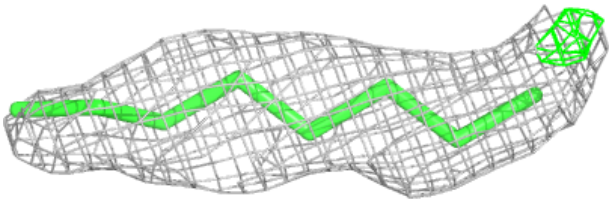


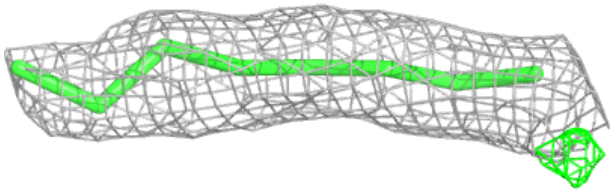


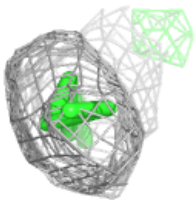


Electron density around LFA A 309:

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

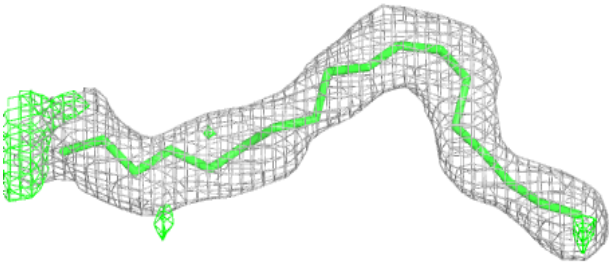


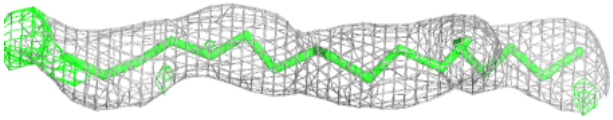


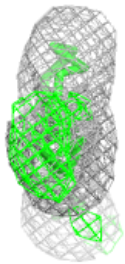


Electron density around LFA F 310:

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

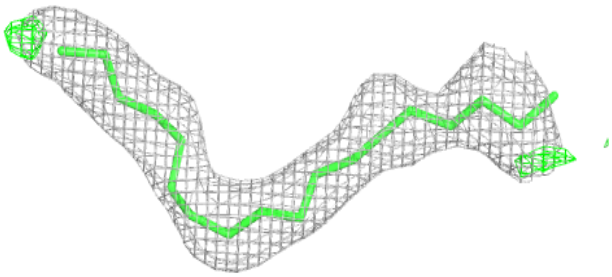


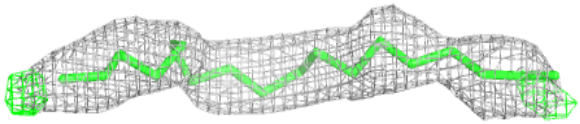


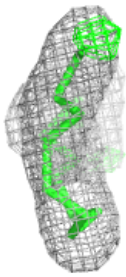


Electron density around LFA E 303:

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

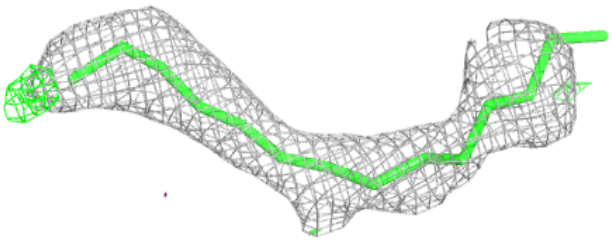


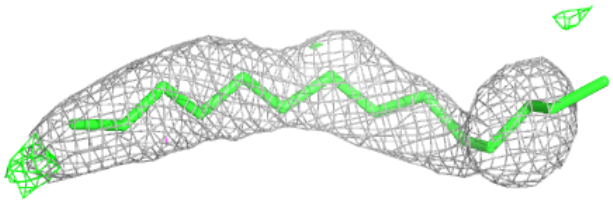


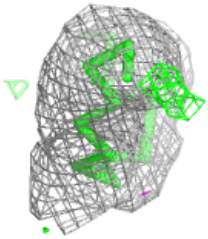


Electron density around LFA D 303:

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

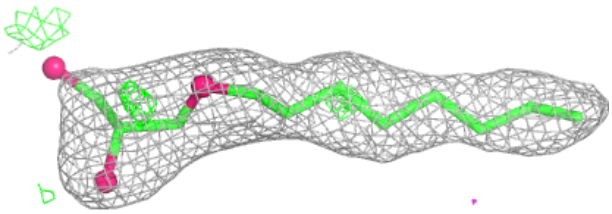


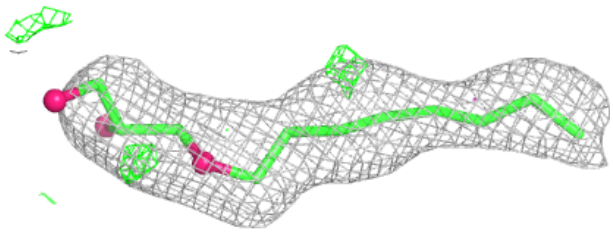


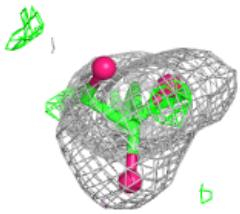


Electron density around MPG I 314:

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

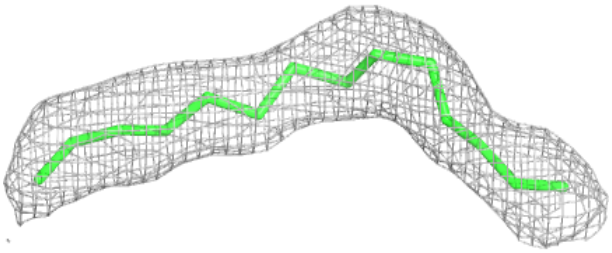


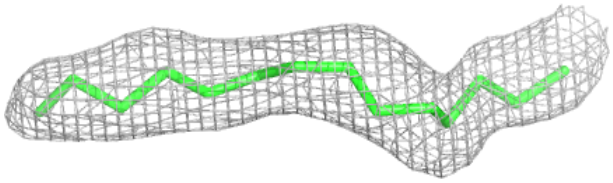




Electron density around LFA A 306:

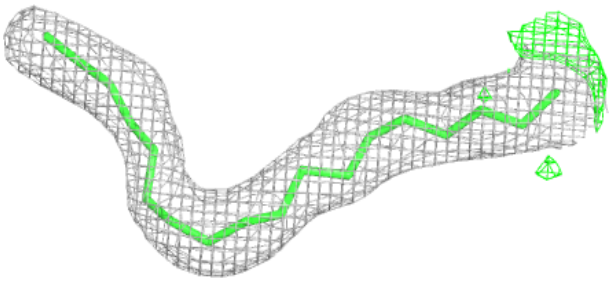
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

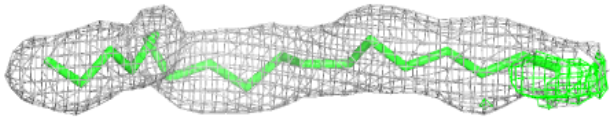




Electron density around LFA D 307:

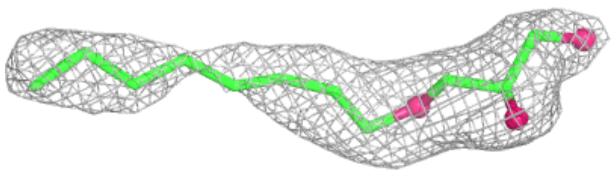
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

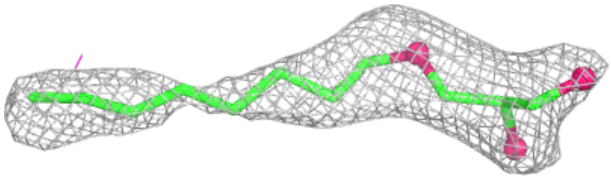


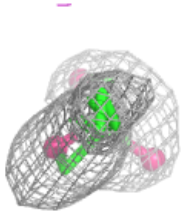


Electron density around MPG H 313:

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

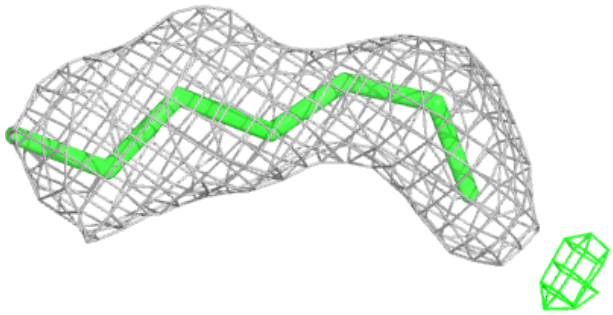


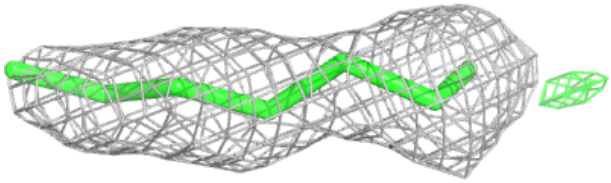


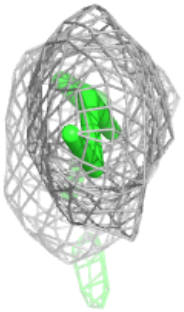


Electron density around LFA D 314:

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

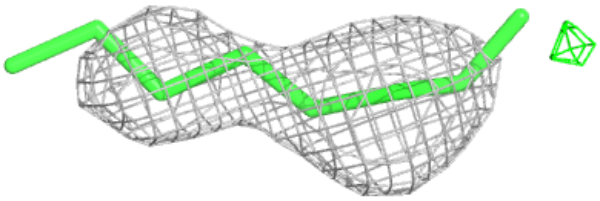


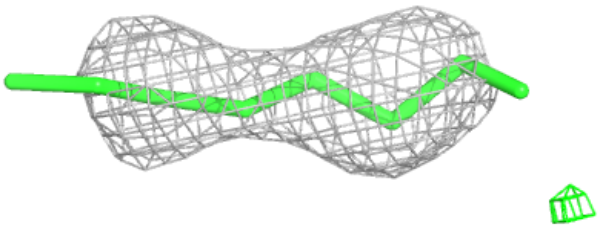


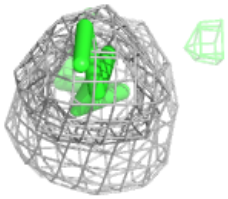


Electron density around LFA E 307:

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

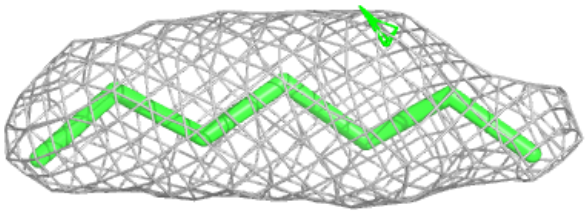


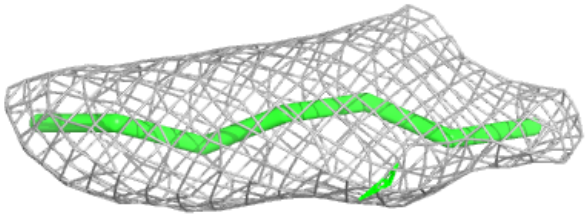


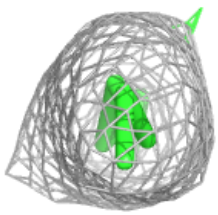


Electron density around LFA H 311:

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

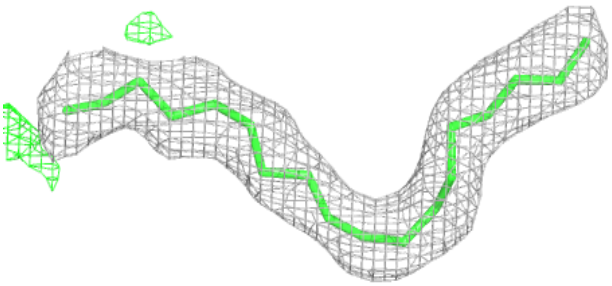


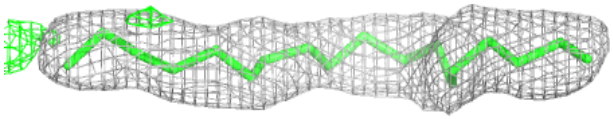


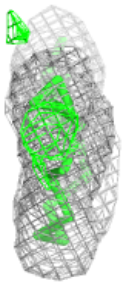


Electron density around LFA C 307:

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

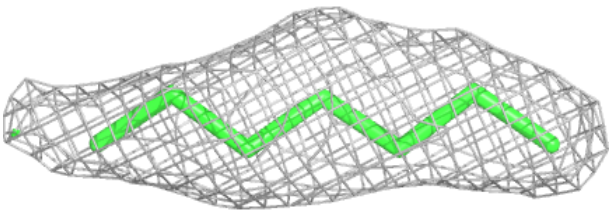


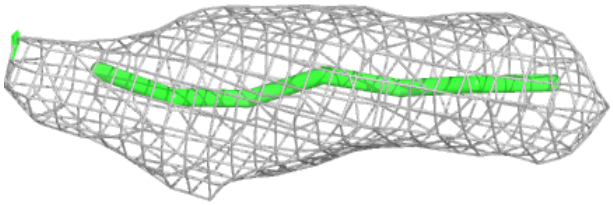


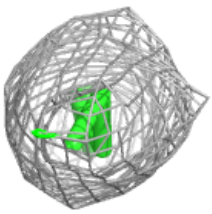


Electron density around LFA I 312:

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







6.5 Other polymers (i)

There are no such residues in this entry.