



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2026 – 12:16 PM JST

PDB ID : 9VFC / pdb\_00009vfc  
Title : Crystal structure of eukaryotic heliorhodopsin Cv06 from Chromera velia strain CCMP2878  
Authors : Shevtsov, M.; Bukhdruker, S.; Kornilov, D.; Borshchevskiy, V.; Gordeliy, V.  
Deposited on : 2025-06-10  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

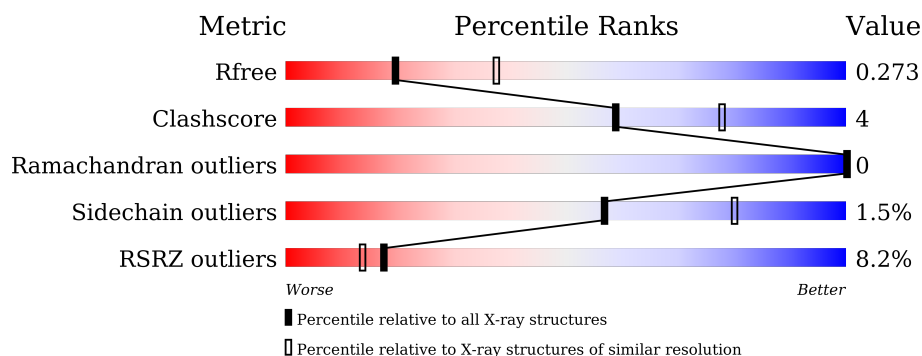
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	317	<div> <div>4%</div> <div>77% 12% 12%</div> </div>
1	B	317	<div> <div>10%</div> <div>78% 10% 12%</div> </div>
1	C	317	<div> <div>5%</div> <div>77% 10% 12%</div> </div>
1	D	317	<div> <div>6%</div> <div>77% 10% 13%</div> </div>
1	E	317	<div> <div>9%</div> <div>77% 10% 13%</div> </div>
1	F	317	<div> <div>7%</div> <div>78% 8% 13%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	317	<div><div></div><div>8%</div><div>78%</div><div>9%</div><div>13%</div></div>
1	H	317	<div><div></div><div>6%</div><div>82%</div><div>6%</div><div>12%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18544 atoms, of which 0 are hydrogens and 0 are deuteriums.

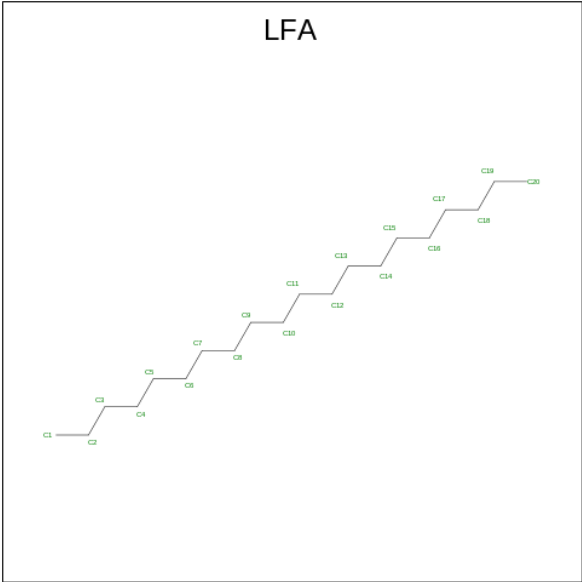
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called heliorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2130	1420	335	364	11			
1	B	278	Total	C	N	O	S	0	0	0
			2111	1412	328	360	11			
1	C	278	Total	C	N	O	S	0	0	0
			2104	1403	330	361	10			
1	D	276	Total	C	N	O	S	0	0	0
			2104	1409	327	357	11			
1	E	277	Total	C	N	O	S	0	0	0
			2098	1398	330	359	11			
1	F	275	Total	C	N	O	S	0	0	0
			2073	1384	325	353	11			
1	G	277	Total	C	N	O	S	0	0	0
			2110	1405	335	359	11			
1	H	278	Total	C	N	O	S	0	0	0
			2095	1394	327	363	11			

- Molecule 2 is EICOSANE (CCD ID: LFA) (formula: C<sub>20</sub>H<sub>42</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 9 9	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 12 12	0	0
2	A	1	Total C 13 13	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 16 16	0	0
2	A	1	Total C 13 13	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 6 6	0	0
2	A	1	Total C 14 14	0	0
2	A	1	Total C 8 8	0	0
2	B	1	Total C 11 11	0	0
2	B	1	Total C 13 13	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 16 16	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 13 13	0	0
2	B	1	Total C 12 12	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 10 10	0	0
2	B	1	Total C 17 17	0	0
2	B	1	Total C 12 12	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 10 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C 7 7	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 19 19	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 8 8	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 12 12	0	0
2	D	1	Total C 12 12	0	0
2	D	1	Total C 10 10	0	0
2	D	1	Total C 12 12	0	0
2	D	1	Total C 8 8	0	0
2	D	1	Total C 20 20	0	0
2	D	1	Total C 10 10	0	0
2	D	1	Total C 8 8	0	0
2	D	1	Total C 5 5	0	0
2	D	1	Total C 9 9	0	0
2	D	1	Total C 9 9	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C 10 10	0	0
2	D	1	Total C 10 10	0	0
2	D	1	Total C 10 10	0	0
2	D	1	Total C 11 11	0	0
2	D	1	Total C 15 15	0	0
2	D	1	Total C 20 20	0	0
2	E	1	Total C 8 8	0	0
2	E	1	Total C 8 8	0	0
2	E	1	Total C 10 10	0	0
2	E	1	Total C 10 10	0	0
2	E	1	Total C 12 12	0	0
2	E	1	Total C 7 7	0	0
2	E	1	Total C 10 10	0	0
2	E	1	Total C 7 7	0	0
2	E	1	Total C 9 9	0	0
2	E	1	Total C 6 6	0	0
2	E	1	Total C 14 14	0	0
2	E	1	Total C 15 15	0	0
2	E	1	Total C 11 11	0	0
2	E	1	Total C 7 7	0	0
2	E	1	Total C 11 11	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C 7 7	0	0
2	E	1	Total C 20 20	0	0
2	F	1	Total C 8 8	0	0
2	F	1	Total C 9 9	0	0
2	F	1	Total C 7 7	0	0
2	F	1	Total C 9 9	0	0
2	F	1	Total C 11 11	0	0
2	F	1	Total C 12 12	0	0
2	F	1	Total C 9 9	0	0
2	F	1	Total C 7 7	0	0
2	F	1	Total C 11 11	0	0
2	F	1	Total C 10 10	0	0
2	F	1	Total C 6 6	0	0
2	F	1	Total C 15 15	0	0
2	F	1	Total C 12 12	0	0
2	F	1	Total C 7 7	0	0
2	F	1	Total C 8 8	0	0
2	G	1	Total C 10 10	0	0
2	G	1	Total C 14 14	0	0
2	G	1	Total C 9 9	0	0
2	G	1	Total C 10 10	0	0

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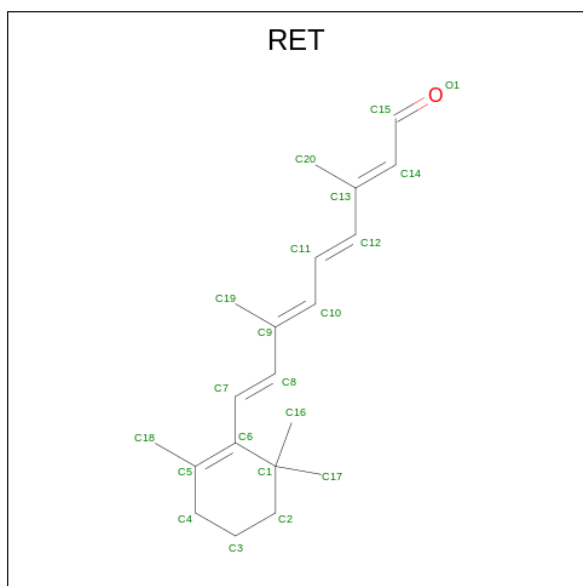
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C 8 8	0	0
2	G	1	Total C 11 11	0	0
2	G	1	Total C 10 10	0	0
2	G	1	Total C 10 10	0	0
2	G	1	Total C 14 14	0	0
2	G	1	Total C 20 20	0	0
2	G	1	Total C 14 14	0	0
2	G	1	Total C 9 9	0	0
2	G	1	Total C 12 12	0	0
2	G	1	Total C 15 15	0	0
2	G	1	Total C 11 11	0	0
2	G	1	Total C 11 11	0	0
2	G	1	Total C 6 6	0	0
2	G	1	Total C 10 10	0	0
2	H	1	Total C 7 7	0	0
2	H	1	Total C 7 7	0	0
2	H	1	Total C 9 9	0	0
2	H	1	Total C 13 13	0	0
2	H	1	Total C 11 11	0	0
2	H	1	Total C 7 7	0	0
2	H	1	Total C 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total C 6 6	0	0
2	H	1	Total C 12 12	0	0
2	H	1	Total C 10 10	0	0
2	H	1	Total C 9 9	0	0
2	H	1	Total C 8 8	0	0

- Molecule 3 is RETINAL (CCD ID: RET) (formula:  $C_{20}H_{28}O$ ) (labeled as "Ligand of Interest" by depositor).



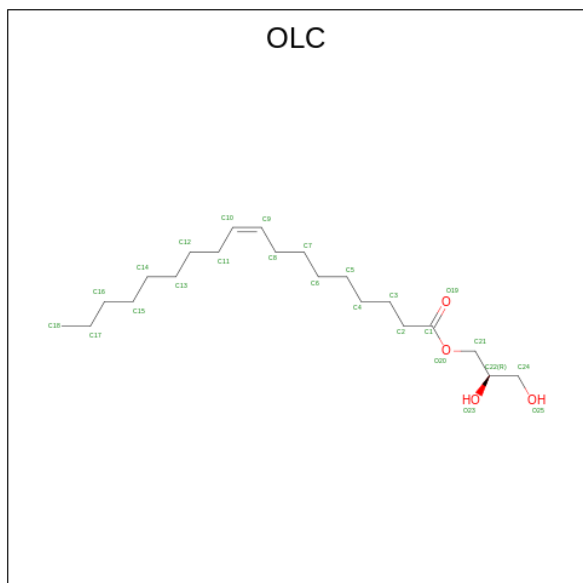
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 20 20	0	0
3	B	1	Total C 20 20	0	0
3	C	1	Total C 20 20	0	0
3	D	1	Total C 20 20	0	0
3	E	1	Total C 20 20	0	0
3	F	1	Total C 20 20	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C 20 20	0	0
3	H	1	Total C 20 20	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 25 21 4	0	0
4	C	1	Total C O 20 16 4	0	0
4	E	1	Total C O 25 21 4	0	0
4	F	1	Total C O 25 21 4	0	0
4	H	1	Total C O 25 21 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	27	Total O 27 27	0	0
5	B	16	Total O 16 16	0	0

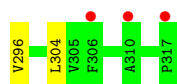
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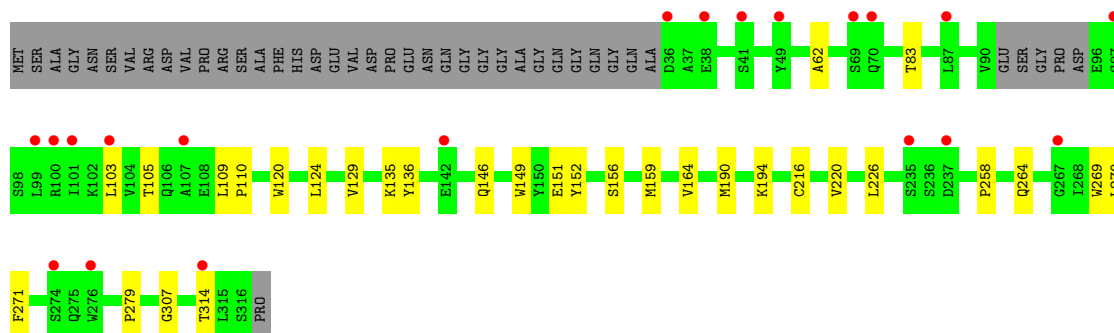
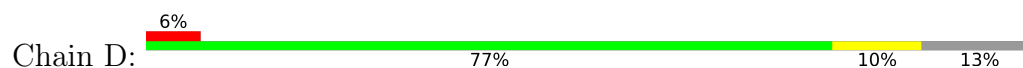
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	20	Total 20	O 20	0	0
5	D	16	Total 16	O 16	0	0
5	E	20	Total 20	O 20	0	0
5	F	21	Total 21	O 21	0	0
5	G	16	Total 16	O 16	0	0
5	H	17	Total 17	O 17	0	0

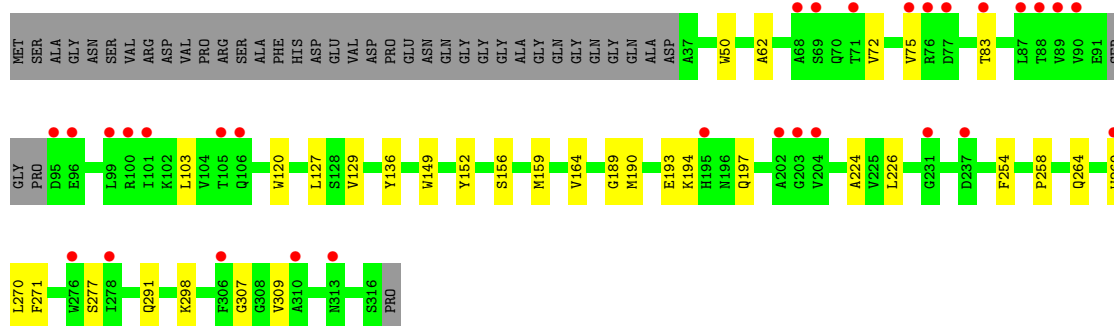
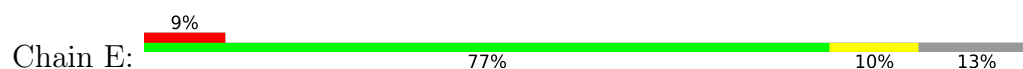




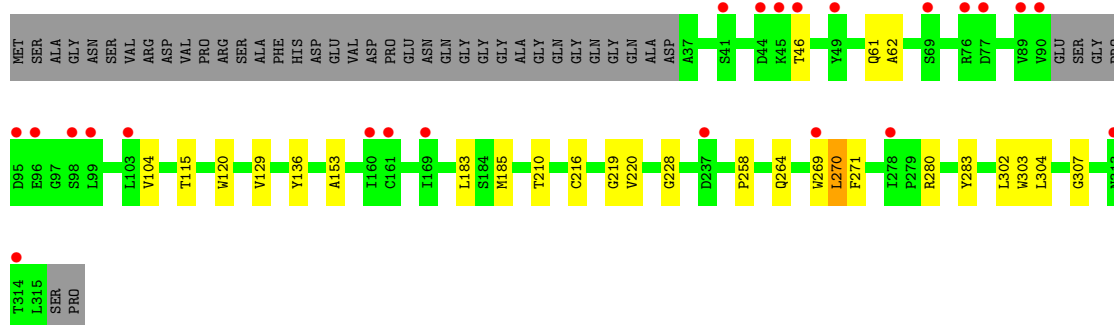
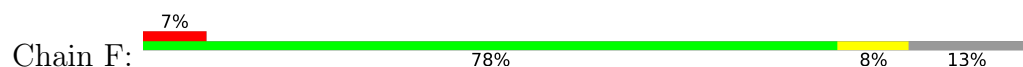
• Molecule 1: heliorhodopsin



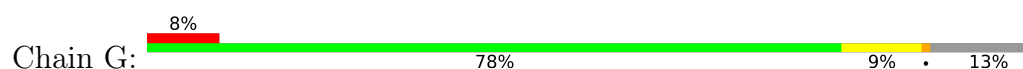
• Molecule 1: heliorhodopsin

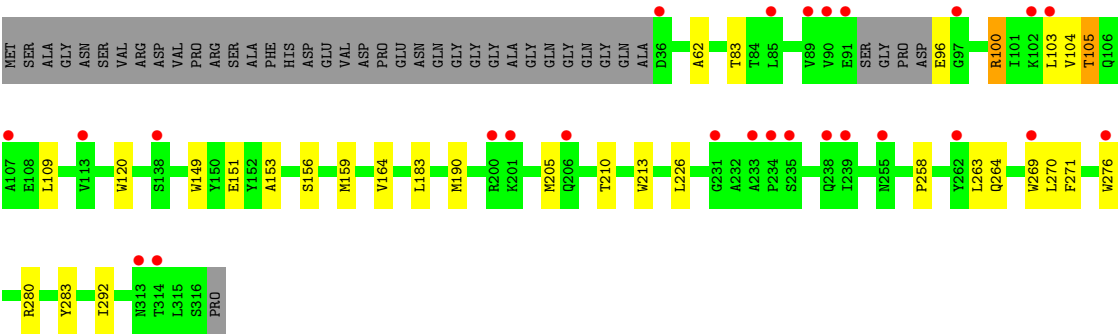


• Molecule 1: heliorhodopsin

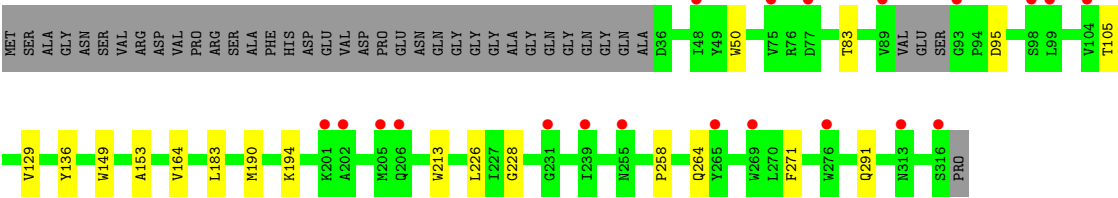
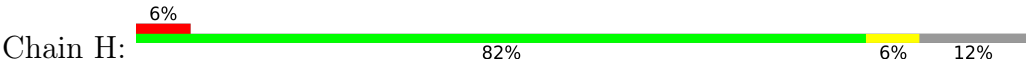


• Molecule 1: heliorhodopsin





● Molecule 1: heliorhodopsin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.89Å 77.89Å 135.99Å 105.67° 101.16° 90.02°	Depositor
Resolution (Å)	42.98 – 2.60 42.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	85.4 (42.98-2.60) 85.4 (42.98-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.230 , 0.271 0.231 , 0.273	Depositor DCC
$R_{free}$ test set	2004 reflections (2.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.4	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 87.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.119 for -h,k,-k-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	18544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OLC, LFA, RET

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	0.09	0/2190	0.24	0/2986
1	B	0.08	0/2170	0.23	0/2961
1	C	0.09	0/2164	0.23	0/2952
1	D	0.08	0/2163	0.23	0/2948
1	E	0.09	0/2157	0.22	0/2941
1	F	0.10	0/2132	0.24	0/2910
1	G	0.09	0/2168	0.23	0/2952
1	H	0.09	0/2154	0.23	0/2935
All	All	0.09	0/17298	0.23	0/23585

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 [i](#)

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	2130	0	2051	25	0
1	B	2111	0	2014	19	0
1	C	2104	0	1980	20	0
1	D	2104	0	2019	19	0
1	E	2098	0	1996	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2073	0	1958	19	0
1	G	2110	0	2015	17	0
1	H	2095	0	1978	11	0
2	A	175	0	333	10	0
2	B	186	0	356	7	0
2	C	123	0	233	7	0
2	D	179	0	348	7	0
2	E	172	0	330	4	0
2	F	141	0	267	9	0
2	G	204	0	393	5	0
2	H	106	0	197	0	0
3	A	20	0	27	4	0
3	B	20	0	27	2	0
3	C	20	0	27	3	0
3	D	20	0	27	3	0
3	E	20	0	27	5	0
3	F	20	0	27	1	0
3	G	20	0	27	1	0
3	H	20	0	27	2	0
4	B	25	0	40	2	0
4	C	20	0	27	1	0
4	E	25	0	40	0	0
4	F	25	0	40	0	0
4	H	25	0	40	1	0
5	A	27	0	0	0	0
5	B	16	0	0	0	0
5	C	20	0	0	0	0
5	D	16	0	0	0	0
5	E	20	0	0	0	0
5	F	21	0	0	0	0
5	G	16	0	0	0	0
5	H	17	0	0	0	0
All	All	18544	0	18871	162	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 4.

The worst 5 of 162 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:PHE:H	4:B:501:OLC:H24A	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:THR:HB	1:E:103:LEU:HD11	1.68	0.76
1:B:83:THR:HB	1:B:103:LEU:HD11	1.72	0.71
1:D:83:THR:HB	1:D:103:LEU:HD11	1.70	0.71
1:B:156:SER:HA	1:B:159:MET:HE3	1.73	0.70

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	276/317 (87%)	270 (98%)	6 (2%)	0	100	100
1	B	274/317 (86%)	268 (98%)	6 (2%)	0	100	100
1	C	274/317 (86%)	269 (98%)	5 (2%)	0	100	100
1	D	272/317 (86%)	266 (98%)	6 (2%)	0	100	100
1	E	273/317 (86%)	267 (98%)	6 (2%)	0	100	100
1	F	271/317 (86%)	263 (97%)	8 (3%)	0	100	100
1	G	273/317 (86%)	266 (97%)	7 (3%)	0	100	100
1	H	274/317 (86%)	268 (98%)	6 (2%)	0	100	100
All	All	2187/2536 (86%)	2137 (98%)	50 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was



analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/260 (79%)	201 (98%)	5 (2%)	43	70
1	B	198/260 (76%)	195 (98%)	3 (2%)	57	80
1	C	194/260 (75%)	193 (100%)	1 (0%)	81	92
1	D	199/260 (76%)	195 (98%)	4 (2%)	48	74
1	E	198/260 (76%)	197 (100%)	1 (0%)	81	92
1	F	191/260 (74%)	189 (99%)	2 (1%)	68	86
1	G	197/260 (76%)	190 (96%)	7 (4%)	31	58
1	H	198/260 (76%)	197 (100%)	1 (0%)	81	92
All	All	1581/2080 (76%)	1557 (98%)	24 (2%)	57	80

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	104	VAL
1	G	100	ARG
1	G	96	GLU
1	G	104	VAL
1	B	104	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	106	GLN
1	G	106	GLN
1	G	275	GLN
1	D	255	ASN
1	D	275	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

137 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	LFA	G	409	-	13,13,19	0.26	0	12,12,18	0.20	0
2	LFA	F	513	-	14,14,19	0.24	0	13,13,18	0.22	0
4	OLC	C	501	-	19,19,24	0.36	0	20,20,25	0.46	0
2	LFA	C	507	-	6,6,19	0.28	0	5,5,18	0.12	0
3	RET	F	516	1	20,20,21	0.43	0	27,27,28	0.72	0
2	LFA	D	410	-	8,8,19	0.28	0	7,7,18	0.13	0
2	LFA	A	516	-	13,13,19	0.25	0	12,12,18	0.18	0
2	LFA	F	514	-	11,11,19	0.26	0	10,10,18	0.19	0
2	LFA	G	411	-	13,13,19	0.25	0	12,12,18	0.20	0
2	LFA	H	505	-	12,12,19	0.26	0	11,11,18	0.18	0
2	LFA	B	506	-	9,9,19	0.28	0	8,8,18	0.13	0
3	RET	A	518	1	20,20,21	0.48	0	27,27,28	0.68	0
2	LFA	D	411	-	9,9,19	0.26	0	8,8,18	0.17	0
2	LFA	A	503	-	11,11,19	0.26	0	10,10,18	0.17	0
2	LFA	A	502	-	7,7,19	0.29	0	6,6,18	0.13	0
2	LFA	D	412	-	9,9,19	0.26	0	8,8,18	0.16	0
2	LFA	C	509	-	18,18,19	0.25	0	17,17,18	0.18	0
2	LFA	A	506	-	10,10,19	0.27	0	9,9,18	0.16	0
2	LFA	G	402	-	13,13,19	0.25	0	12,12,18	0.25	0
2	LFA	H	508	-	6,6,19	0.29	0	5,5,18	0.11	0
2	LFA	G	417	-	5,5,19	0.29	0	4,4,18	0.14	0
2	LFA	H	504	-	8,8,19	0.27	0	7,7,18	0.15	0
2	LFA	H	503	-	6,6,19	0.29	0	5,5,18	0.12	0
2	LFA	B	504	-	11,11,19	0.26	0	10,10,18	0.19	0
2	LFA	D	402	-	9,9,19	0.26	0	8,8,18	0.18	0
3	RET	G	419	1	20,20,21	0.41	0	27,27,28	0.66	0
2	LFA	E	514	-	6,6,19	0.29	0	5,5,18	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LFA	D	409	-	8,8,19	0.28	0	7,7,18	0.15	0
2	LFA	B	505	-	11,11,19	0.25	0	10,10,18	0.21	0
2	LFA	E	502	-	7,7,19	0.28	0	6,6,18	0.13	0
2	LFA	E	512	-	14,14,19	0.25	0	13,13,18	0.21	0
2	LFA	H	507	-	6,6,19	0.30	0	5,5,18	0.12	0
2	LFA	A	514	-	6,6,19	0.28	0	5,5,18	0.09	0
2	LFA	C	508	-	8,8,19	0.26	0	7,7,18	0.19	0
2	LFA	A	504	-	12,12,19	0.27	0	11,11,18	0.14	0
2	LFA	E	503	-	9,9,19	0.27	0	8,8,18	0.15	0
4	OLC	H	501	-	24,24,24	0.35	0	25,25,25	0.43	0
2	LFA	H	510	-	11,11,19	0.25	0	10,10,18	0.19	0
2	LFA	C	511	-	9,9,19	0.27	0	8,8,18	0.15	0
2	LFA	A	512	-	6,6,19	0.29	0	5,5,18	0.13	0
2	LFA	E	507	-	9,9,19	0.27	0	8,8,18	0.15	0
2	LFA	C	512	-	7,7,19	0.28	0	6,6,18	0.14	0
2	LFA	H	502	-	6,6,19	0.29	0	5,5,18	0.11	0
2	LFA	H	512	-	8,8,19	0.27	0	7,7,18	0.17	0
2	LFA	B	516	-	16,16,19	0.23	0	15,15,18	0.25	0
2	LFA	G	408	-	9,9,19	0.25	0	8,8,18	0.23	0
2	LFA	A	505	-	10,10,19	0.26	0	9,9,18	0.19	0
2	LFA	G	413	-	11,11,19	0.26	0	10,10,18	0.18	0
2	LFA	A	511	-	12,12,19	0.25	0	11,11,18	0.21	0
2	LFA	G	414	-	14,14,19	0.25	0	13,13,18	0.20	0
2	LFA	A	509	-	10,10,19	0.26	0	9,9,18	0.18	0
3	RET	B	518	1	20,20,21	0.42	0	27,27,28	0.69	0
2	LFA	B	503	-	12,12,19	0.25	0	11,11,18	0.19	0
2	LFA	F	503	-	8,8,19	0.28	0	7,7,18	0.16	0
2	LFA	G	405	-	7,7,19	0.29	0	6,6,18	0.13	0
2	LFA	G	407	-	9,9,19	0.25	0	8,8,18	0.19	0
2	LFA	F	515	-	6,6,19	0.29	0	5,5,18	0.13	0
2	LFA	F	510	-	10,10,19	0.25	0	9,9,18	0.19	0
2	LFA	E	506	-	6,6,19	0.27	0	5,5,18	0.15	0
2	LFA	B	507	-	9,9,19	0.26	0	8,8,18	0.19	0
2	LFA	F	507	-	11,11,19	0.26	0	10,10,18	0.16	0
2	LFA	B	502	-	10,10,19	0.26	0	9,9,18	0.19	0
2	LFA	E	505	-	11,11,19	0.25	0	10,10,18	0.20	0
2	LFA	E	513	-	10,10,19	0.25	0	9,9,18	0.18	0
2	LFA	G	416	-	10,10,19	0.26	0	9,9,18	0.16	0
2	LFA	D	403	-	11,11,19	0.25	0	10,10,18	0.19	0
2	LFA	E	501	-	7,7,19	0.28	0	6,6,18	0.13	0
2	LFA	E	515	-	10,10,19	0.26	0	9,9,18	0.18	0
2	LFA	E	510	-	5,5,19	0.29	0	4,4,18	0.14	0
2	LFA	F	505	-	8,8,19	0.28	0	7,7,18	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LFA	G	410	-	19,19,19	0.25	0	18,18,18	0.21	0
2	LFA	H	506	-	10,10,19	0.25	0	9,9,18	0.19	0
2	LFA	A	515	-	5,5,19	0.29	0	4,4,18	0.14	0
2	LFA	G	403	-	8,8,19	0.27	0	7,7,18	0.15	0
3	RET	C	515	1	20,20,21	0.39	0	27,27,28	0.70	0
2	LFA	H	511	-	9,9,19	0.27	0	8,8,18	0.17	0
2	LFA	G	415	-	10,10,19	0.26	0	9,9,18	0.18	0
2	LFA	E	519	-	19,19,19	0.24	0	18,18,18	0.21	0
2	LFA	G	412	-	8,8,19	0.27	0	7,7,18	0.14	0
2	LFA	C	510	-	6,6,19	0.28	0	5,5,18	0.13	0
2	LFA	B	511	-	6,6,19	0.27	0	5,5,18	0.16	0
2	LFA	F	511	-	9,9,19	0.25	0	8,8,18	0.19	0
2	LFA	E	511	-	13,13,19	0.25	0	12,12,18	0.19	0
2	LFA	A	507	-	6,6,19	0.30	0	5,5,18	0.10	0
2	LFA	F	504	-	6,6,19	0.28	0	5,5,18	0.12	0
2	LFA	B	509	-	8,8,19	0.28	0	7,7,18	0.15	0
2	LFA	D	404	-	7,7,19	0.28	0	6,6,18	0.11	0
2	LFA	B	508	-	15,15,19	0.25	0	14,14,18	0.20	0
2	LFA	A	501	-	8,8,19	0.27	0	7,7,18	0.17	0
2	LFA	F	508	-	8,8,19	0.26	0	7,7,18	0.17	0
4	OLC	E	518	-	24,24,24	0.35	0	25,25,25	0.41	0
3	RET	E	517	1	20,20,21	0.42	0	27,27,28	0.65	0
2	LFA	E	504	-	9,9,19	0.26	0	8,8,18	0.18	0
4	OLC	F	501	-	24,24,24	0.35	0	25,25,25	0.36	0
2	LFA	C	502	-	7,7,19	0.29	0	6,6,18	0.12	0
2	LFA	C	506	-	6,6,19	0.29	0	5,5,18	0.12	0
2	LFA	D	406	-	9,9,19	0.27	0	8,8,18	0.13	0
2	LFA	G	404	-	9,9,19	0.27	0	8,8,18	0.18	0
2	LFA	E	508	-	6,6,19	0.29	0	5,5,18	0.11	0
2	LFA	A	513	-	10,10,19	0.26	0	9,9,18	0.18	0
2	LFA	D	413	-	9,9,19	0.26	0	8,8,18	0.16	0
2	LFA	A	508	-	10,10,19	0.26	0	9,9,18	0.22	0
2	LFA	C	514	-	11,11,19	0.25	0	10,10,18	0.20	0
2	LFA	B	517	-	11,11,19	0.26	0	10,10,18	0.16	0
2	LFA	B	512	-	12,12,19	0.24	0	11,11,18	0.21	0
2	LFA	F	509	-	6,6,19	0.29	0	5,5,18	0.12	0
2	LFA	C	504	-	6,6,19	0.29	0	5,5,18	0.13	0
2	LFA	C	513	-	8,8,19	0.28	0	7,7,18	0.15	0
2	LFA	A	510	-	15,15,19	0.25	0	14,14,18	0.19	0
2	LFA	D	405	-	19,19,19	0.26	0	18,18,18	0.19	0
2	LFA	H	513	-	7,7,19	0.29	0	6,6,18	0.12	0
2	LFA	F	517	-	7,7,19	0.29	0	6,6,18	0.12	0
2	LFA	E	516	-	6,6,19	0.28	0	5,5,18	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	LFA	D	416	-	19,19,19	0.25	0	18,18,18	0.18	0
2	LFA	H	509	-	5,5,19	0.28	0	4,4,18	0.14	0
2	LFA	D	401	-	11,11,19	0.26	0	10,10,18	0.18	0
2	LFA	F	506	-	10,10,19	0.26	0	9,9,18	0.18	0
2	LFA	F	502	-	7,7,19	0.29	0	6,6,18	0.11	0
2	LFA	C	505	-	9,9,19	0.25	0	8,8,18	0.21	0
2	LFA	B	510	-	11,11,19	0.26	0	10,10,18	0.18	0
2	LFA	D	408	-	4,4,19	0.29	0	3,3,18	0.24	0
2	LFA	D	414	-	10,10,19	0.28	0	9,9,18	0.12	0
2	LFA	A	517	-	7,7,19	0.28	0	6,6,18	0.12	0
2	LFA	D	407	-	7,7,19	0.28	0	6,6,18	0.14	0
2	LFA	B	513	-	11,11,19	0.25	0	10,10,18	0.21	0
2	LFA	D	415	-	14,14,19	0.25	0	13,13,18	0.18	0
2	LFA	G	418	-	9,9,19	0.27	0	8,8,18	0.16	0
3	RET	D	417	1	20,20,21	0.41	0	27,27,28	0.63	0
2	LFA	B	515	-	9,9,19	0.26	0	8,8,18	0.18	0
2	LFA	F	512	-	5,5,19	0.28	0	4,4,18	0.15	0
3	RET	H	514	1	20,20,21	0.41	0	27,27,28	0.70	0
4	OLC	B	501	-	24,24,24	0.35	0	25,25,25	0.42	0
2	LFA	G	406	-	10,10,19	0.25	0	9,9,18	0.22	0
2	LFA	C	503	-	9,9,19	0.26	0	8,8,18	0.18	0
2	LFA	G	401	-	9,9,19	0.27	0	8,8,18	0.17	0
2	LFA	B	514	-	9,9,19	0.26	0	8,8,18	0.16	0
2	LFA	E	509	-	8,8,19	0.27	0	7,7,18	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	G	409	-	-	0/11/11/17	-
2	LFA	F	513	-	-	0/12/12/17	-
4	OLC	C	501	-	-	9/19/19/24	-
2	LFA	C	507	-	-	1/4/4/17	-
3	RET	F	516	1	-	4/13/30/31	0/1/1/1
2	LFA	D	410	-	-	1/6/6/17	-
2	LFA	A	516	-	-	0/11/11/17	-
2	LFA	F	514	-	-	1/9/9/17	-
2	LFA	G	411	-	-	1/11/11/17	-
2	LFA	H	505	-	-	2/10/10/17	-
2	LFA	B	506	-	-	0/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RET	A	518	1	-	4/13/30/31	0/1/1/1
2	LFA	D	411	-	-	4/7/7/17	-
2	LFA	A	503	-	-	4/9/9/17	-
2	LFA	A	502	-	-	0/5/5/17	-
2	LFA	D	412	-	-	2/7/7/17	-
2	LFA	C	509	-	-	8/16/16/17	-
2	LFA	A	506	-	-	2/8/8/17	-
2	LFA	G	402	-	-	1/11/11/17	-
2	LFA	H	508	-	-	2/4/4/17	-
2	LFA	G	417	-	-	0/3/3/17	-
2	LFA	H	504	-	-	0/6/6/17	-
2	LFA	H	503	-	-	0/4/4/17	-
2	LFA	B	504	-	-	1/9/9/17	-
2	LFA	D	402	-	-	0/7/7/17	-
3	RET	G	419	1	-	4/13/30/31	0/1/1/1
2	LFA	E	514	-	-	0/4/4/17	-
2	LFA	D	409	-	-	1/6/6/17	-
2	LFA	B	505	-	-	0/9/9/17	-
2	LFA	E	502	-	-	0/5/5/17	-
2	LFA	E	512	-	-	8/12/12/17	-
2	LFA	H	507	-	-	0/4/4/17	-
2	LFA	A	514	-	-	0/4/4/17	-
2	LFA	C	508	-	-	0/6/6/17	-
2	LFA	A	504	-	-	3/10/10/17	-
2	LFA	E	503	-	-	1/7/7/17	-
4	OLC	H	501	-	-	9/24/24/24	-
2	LFA	H	510	-	-	2/9/9/17	-
2	LFA	C	511	-	-	3/7/7/17	-
2	LFA	A	512	-	-	1/4/4/17	-
2	LFA	E	507	-	-	1/7/7/17	-
2	LFA	C	512	-	-	1/5/5/17	-
2	LFA	H	502	-	-	0/4/4/17	-
2	LFA	H	512	-	-	0/6/6/17	-
2	LFA	B	516	-	-	5/14/14/17	-
2	LFA	G	408	-	-	0/7/7/17	-
2	LFA	A	505	-	-	0/8/8/17	-
2	LFA	G	413	-	-	1/9/9/17	-
2	LFA	A	511	-	-	0/10/10/17	-
2	LFA	G	414	-	-	2/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	A	509	-	-	3/8/8/17	-
3	RET	B	518	1	-	4/13/30/31	0/1/1/1
2	LFA	B	503	-	-	2/10/10/17	-
2	LFA	F	503	-	-	0/6/6/17	-
2	LFA	G	405	-	-	1/5/5/17	-
2	LFA	G	407	-	-	0/7/7/17	-
2	LFA	F	515	-	-	0/4/4/17	-
2	LFA	F	510	-	-	0/8/8/17	-
2	LFA	E	506	-	-	2/4/4/17	-
2	LFA	B	507	-	-	0/7/7/17	-
2	LFA	F	507	-	-	0/9/9/17	-
2	LFA	B	502	-	-	1/8/8/17	-
2	LFA	E	505	-	-	0/9/9/17	-
2	LFA	E	513	-	-	1/8/8/17	-
2	LFA	G	416	-	-	2/8/8/17	-
2	LFA	D	403	-	-	1/9/9/17	-
2	LFA	E	501	-	-	0/5/5/17	-
2	LFA	E	515	-	-	0/8/8/17	-
2	LFA	E	510	-	-	0/3/3/17	-
2	LFA	F	505	-	-	0/6/6/17	-
2	LFA	G	410	-	-	3/17/17/17	-
2	LFA	H	506	-	-	0/8/8/17	-
2	LFA	A	515	-	-	0/3/3/17	-
2	LFA	G	403	-	-	0/6/6/17	-
3	RET	C	515	1	-	4/13/30/31	0/1/1/1
2	LFA	H	511	-	-	1/7/7/17	-
2	LFA	G	415	-	-	2/8/8/17	-
2	LFA	E	519	-	-	0/17/17/17	-
2	LFA	G	412	-	-	0/6/6/17	-
2	LFA	C	510	-	-	0/4/4/17	-
2	LFA	B	511	-	-	0/4/4/17	-
2	LFA	F	511	-	-	1/7/7/17	-
2	LFA	E	511	-	-	2/11/11/17	-
2	LFA	A	507	-	-	0/4/4/17	-
2	LFA	F	504	-	-	0/4/4/17	-
2	LFA	B	509	-	-	1/6/6/17	-
2	LFA	D	404	-	-	0/5/5/17	-
2	LFA	B	508	-	-	1/13/13/17	-
2	LFA	A	501	-	-	0/6/6/17	-
2	LFA	F	508	-	-	1/6/6/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OLC	E	518	-	-	3/24/24/24	-
3	RET	E	517	1	-	4/13/30/31	0/1/1/1
2	LFA	E	504	-	-	2/7/7/17	-
4	OLC	F	501	-	-	5/24/24/24	-
2	LFA	C	502	-	-	0/5/5/17	-
2	LFA	C	506	-	-	0/4/4/17	-
2	LFA	D	406	-	-	1/7/7/17	-
2	LFA	G	404	-	-	0/7/7/17	-
2	LFA	E	508	-	-	0/4/4/17	-
2	LFA	A	513	-	-	3/8/8/17	-
2	LFA	D	413	-	-	3/7/7/17	-
2	LFA	A	508	-	-	0/8/8/17	-
2	LFA	C	514	-	-	0/9/9/17	-
2	LFA	B	517	-	-	3/9/9/17	-
2	LFA	B	512	-	-	0/10/10/17	-
2	LFA	F	509	-	-	1/4/4/17	-
2	LFA	C	504	-	-	0/4/4/17	-
2	LFA	C	513	-	-	1/6/6/17	-
2	LFA	A	510	-	-	4/13/13/17	-
2	LFA	D	405	-	-	4/17/17/17	-
2	LFA	H	513	-	-	0/5/5/17	-
2	LFA	F	517	-	-	0/5/5/17	-
2	LFA	E	516	-	-	0/4/4/17	-
2	LFA	D	416	-	-	3/17/17/17	-
2	LFA	H	509	-	-	1/3/3/17	-
2	LFA	D	401	-	-	0/9/9/17	-
2	LFA	F	506	-	-	2/8/8/17	-
2	LFA	F	502	-	-	0/5/5/17	-
2	LFA	C	505	-	-	0/7/7/17	-
2	LFA	B	510	-	-	2/9/9/17	-
2	LFA	D	408	-	-	0/2/2/17	-
2	LFA	D	414	-	-	1/8/8/17	-
2	LFA	A	517	-	-	0/5/5/17	-
2	LFA	D	407	-	-	0/5/5/17	-
2	LFA	B	513	-	-	4/9/9/17	-
2	LFA	D	415	-	-	1/12/12/17	-
2	LFA	G	418	-	-	0/7/7/17	-
3	RET	D	417	1	-	4/13/30/31	0/1/1/1
2	LFA	B	515	-	-	0/7/7/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LFA	F	512	-	-	0/3/3/17	-
3	RET	H	514	1	-	4/13/30/31	0/1/1/1
4	OLC	B	501	-	-	10/24/24/24	-
2	LFA	G	406	-	-	0/8/8/17	-
2	LFA	C	503	-	-	0/7/7/17	-
2	LFA	G	401	-	-	0/7/7/17	-
2	LFA	B	514	-	-	0/7/7/17	-
2	LFA	E	509	-	-	0/6/6/17	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 188 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	518	RET	C5-C6-C7-C8
3	A	518	RET	C7-C8-C9-C10
3	A	518	RET	C7-C8-C9-C19
3	B	518	RET	C5-C6-C7-C8
3	B	518	RET	C7-C8-C9-C10

There are no ring outliers.

49 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	501	OLC	1	0
3	F	516	RET	1	0
2	A	516	LFA	1	0
2	F	514	LFA	2	0
2	G	411	LFA	1	0
3	A	518	RET	4	0
2	D	411	LFA	1	0
2	C	509	LFA	1	0
3	G	419	RET	1	0
2	B	505	LFA	1	0
2	A	514	LFA	1	0
2	C	508	LFA	3	0
2	E	503	LFA	1	0
4	H	501	OLC	1	0
2	C	511	LFA	1	0

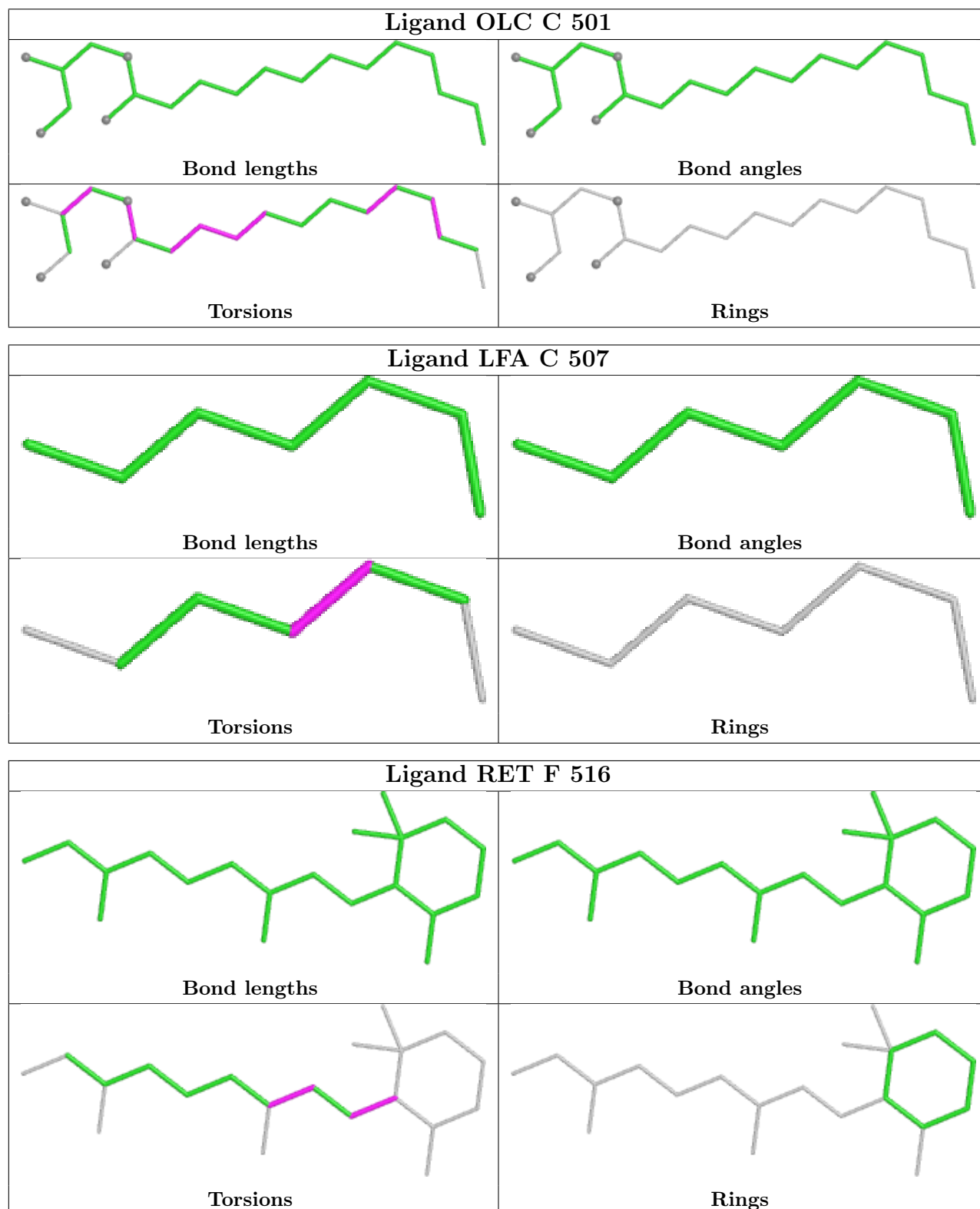
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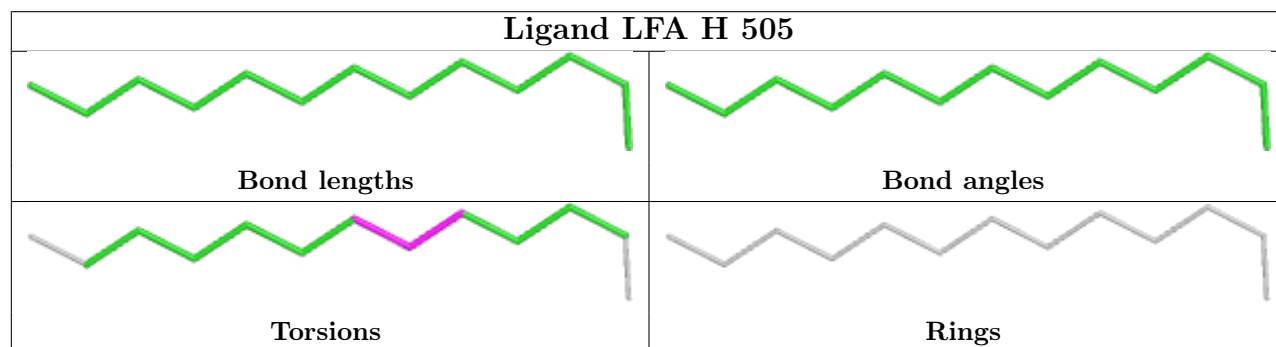
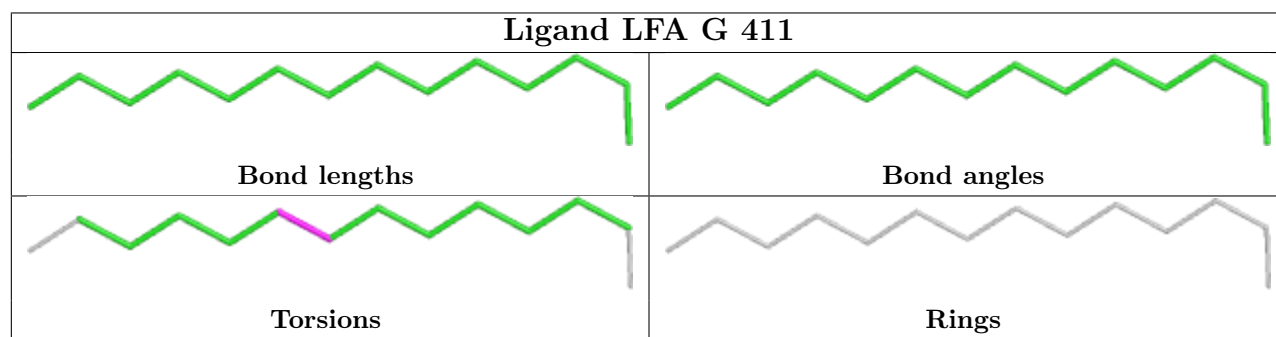
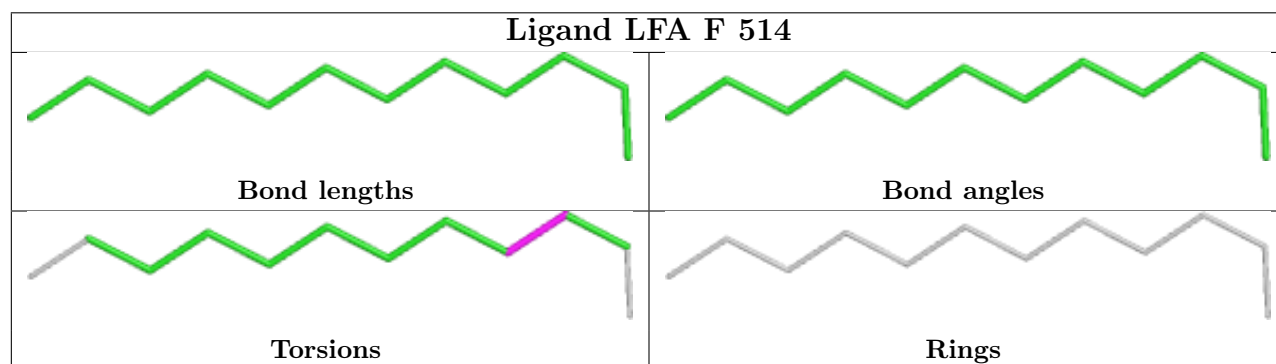
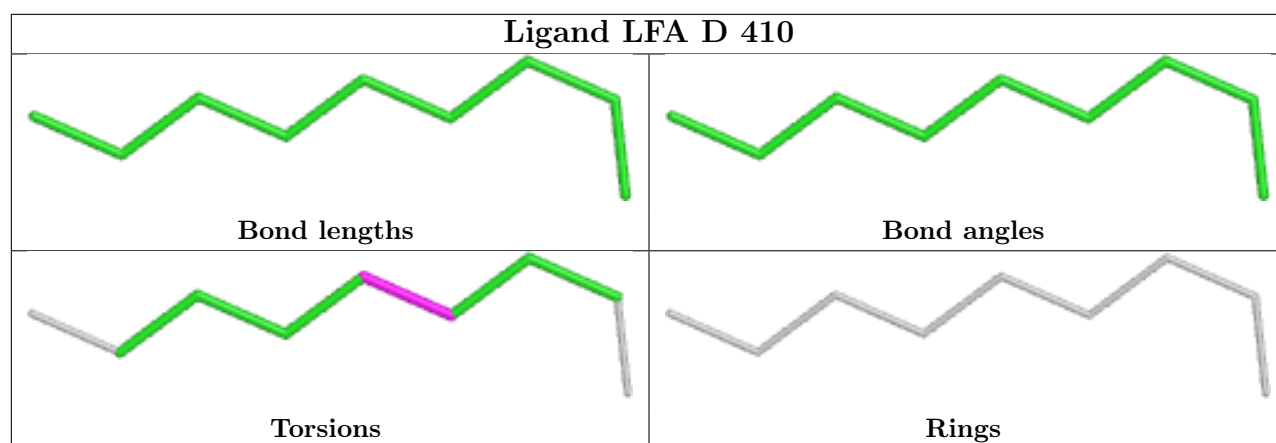
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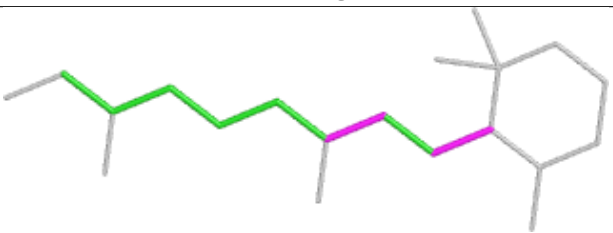
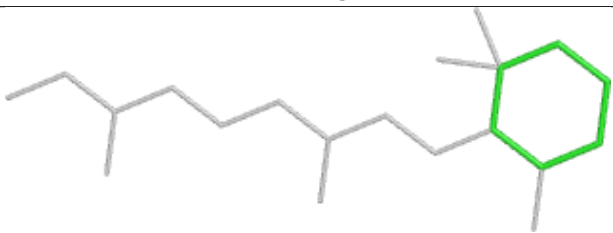
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	512	LFA	1	0
2	A	505	LFA	1	0
2	G	413	LFA	1	0
2	A	511	LFA	1	0
2	G	414	LFA	1	0
2	A	509	LFA	2	0
3	B	518	RET	2	0
2	F	510	LFA	3	0
2	B	507	LFA	1	0
2	F	507	LFA	1	0
2	E	505	LFA	1	0
2	E	515	LFA	1	0
2	G	410	LFA	1	0
2	G	403	LFA	1	0
3	C	515	RET	3	0
2	E	519	LFA	1	0
2	B	511	LFA	2	0
2	F	511	LFA	2	0
2	B	509	LFA	1	0
2	B	508	LFA	1	0
3	E	517	RET	5	0
2	G	404	LFA	1	0
2	C	514	LFA	4	0
2	A	510	LFA	3	0
2	D	405	LFA	2	0
2	D	416	LFA	1	0
2	F	506	LFA	2	0
2	A	517	LFA	1	0
2	B	513	LFA	1	0
2	D	415	LFA	3	0
3	D	417	RET	3	0
2	B	515	LFA	1	0
3	H	514	RET	2	0
4	B	501	OLC	2	0


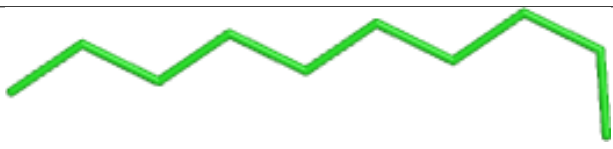

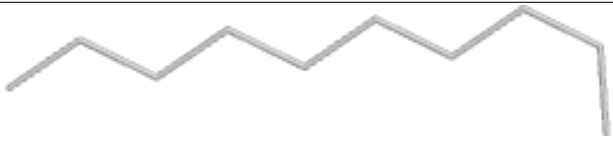
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

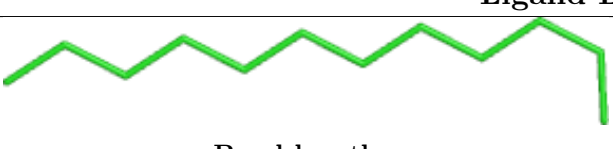
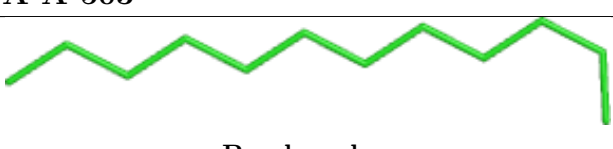
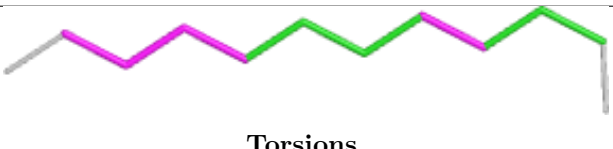

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

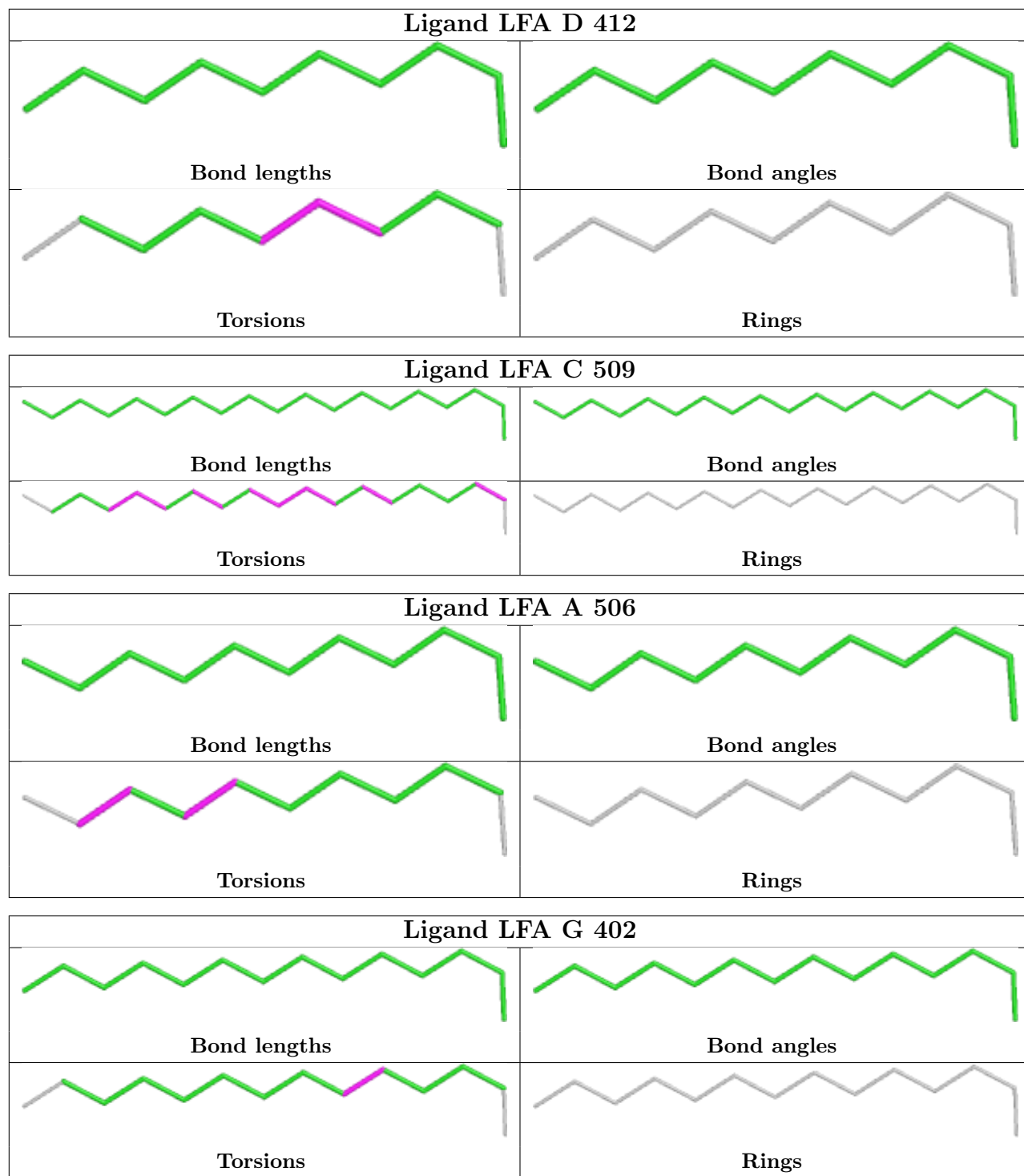


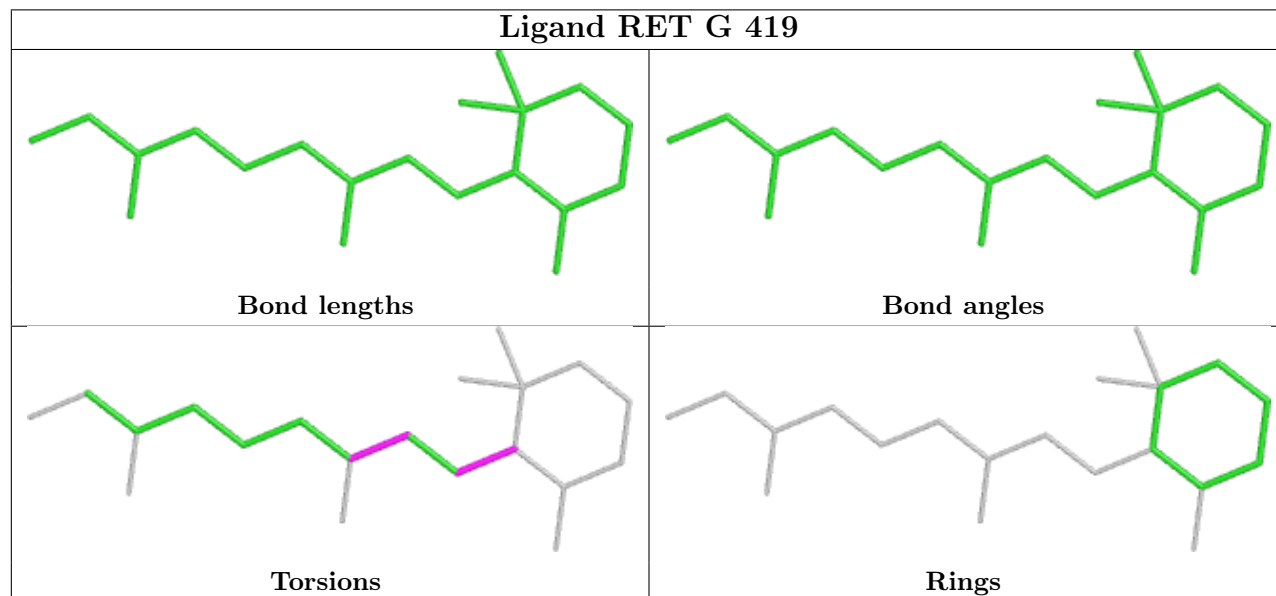
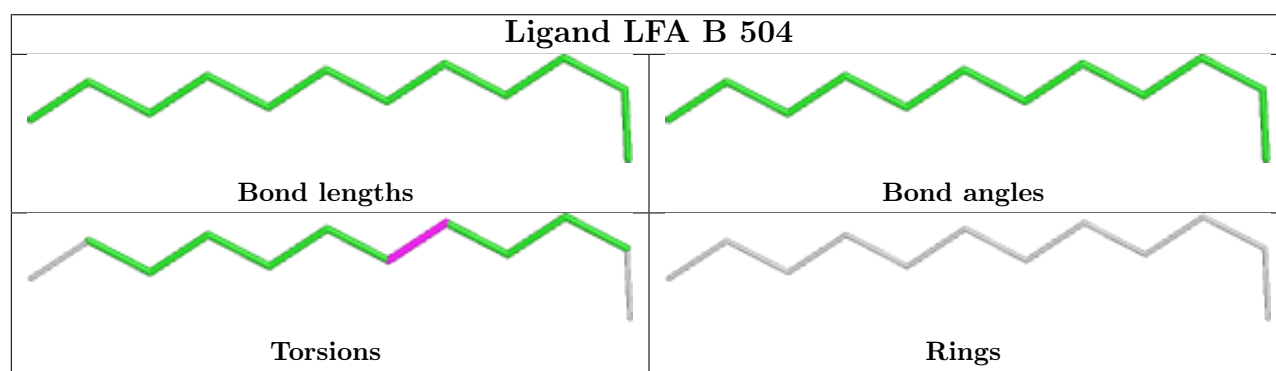
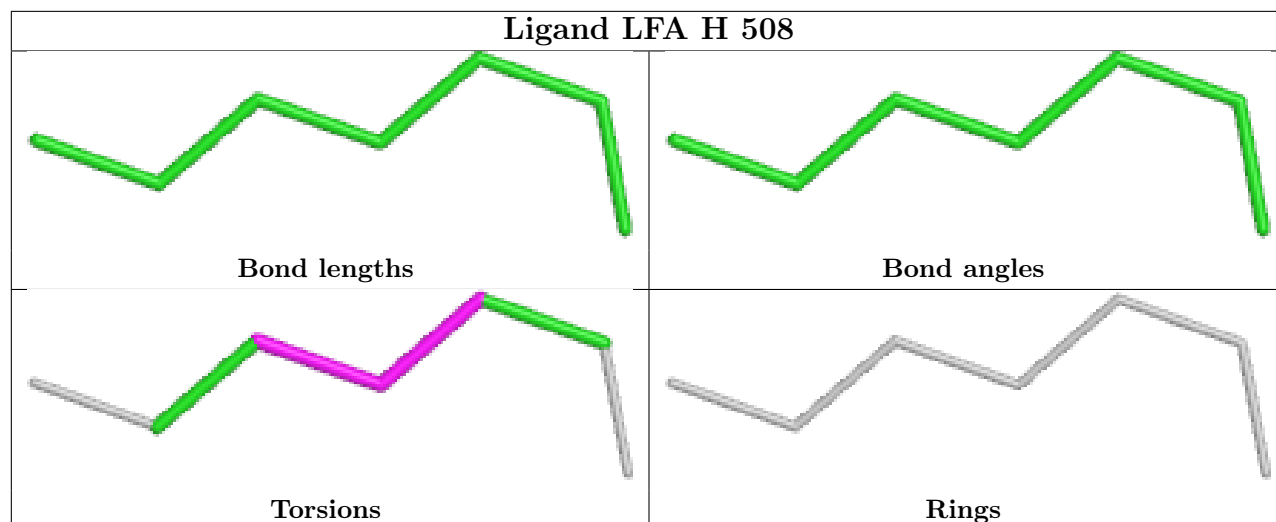


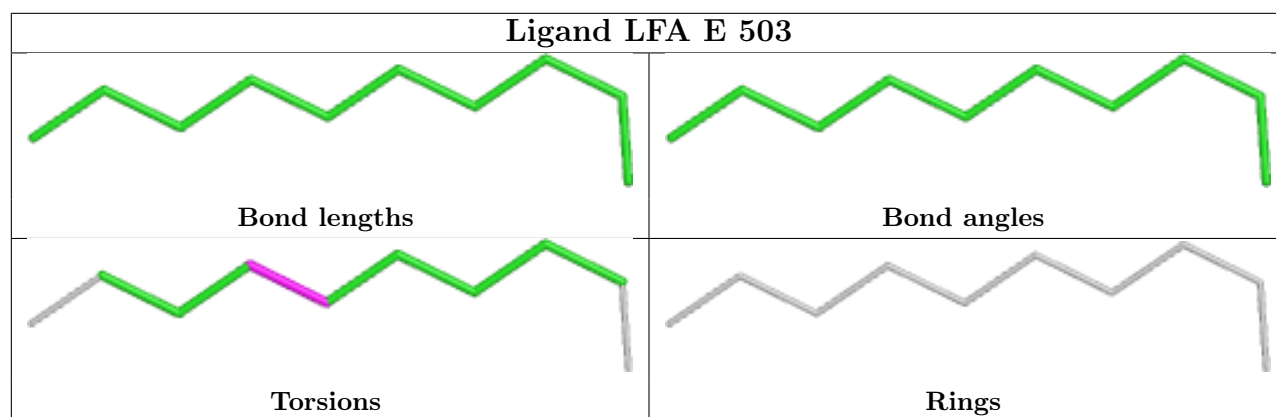
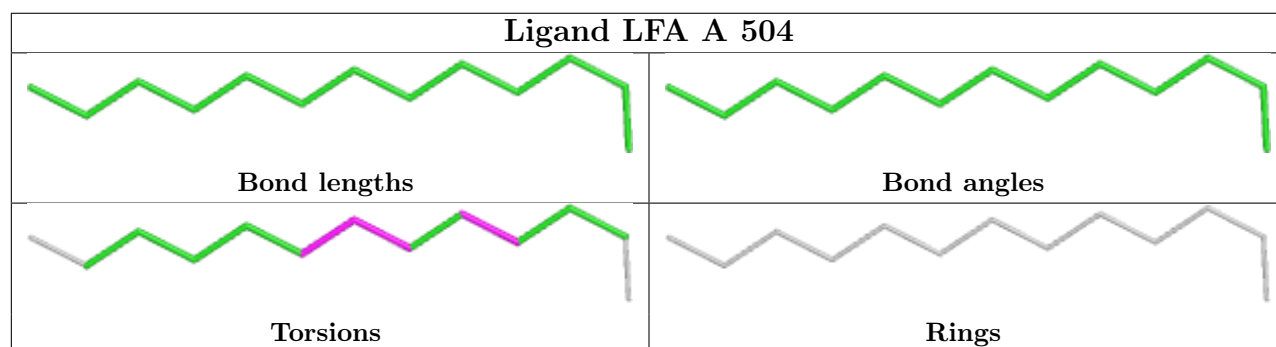
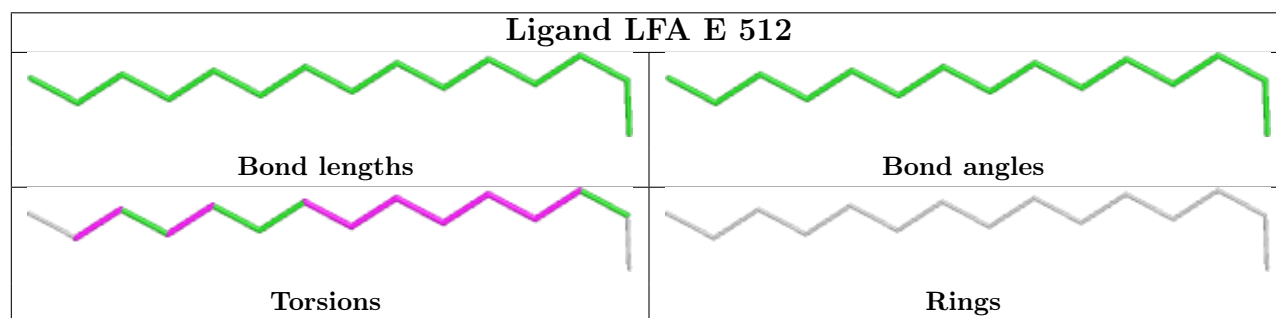
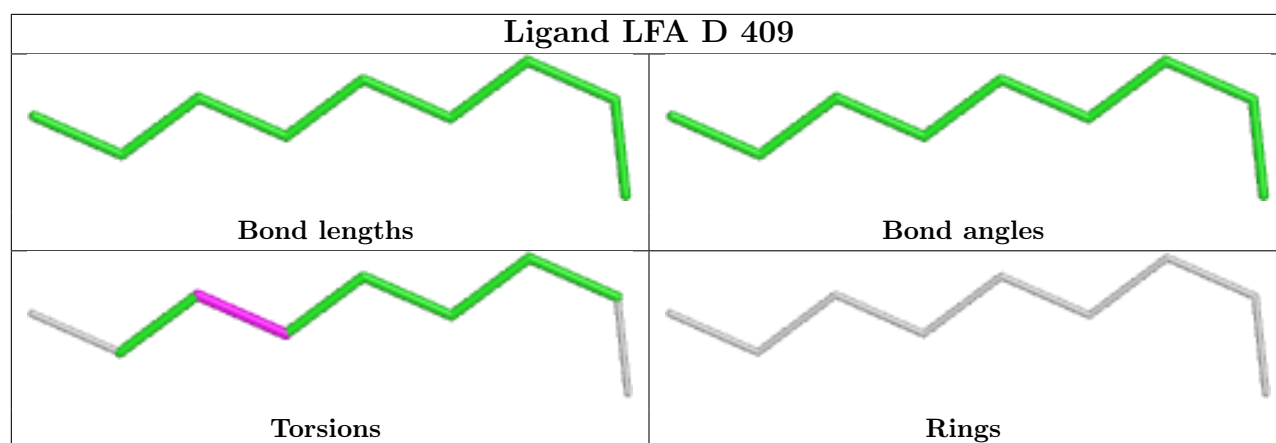
Ligand RET A 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LFA D 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

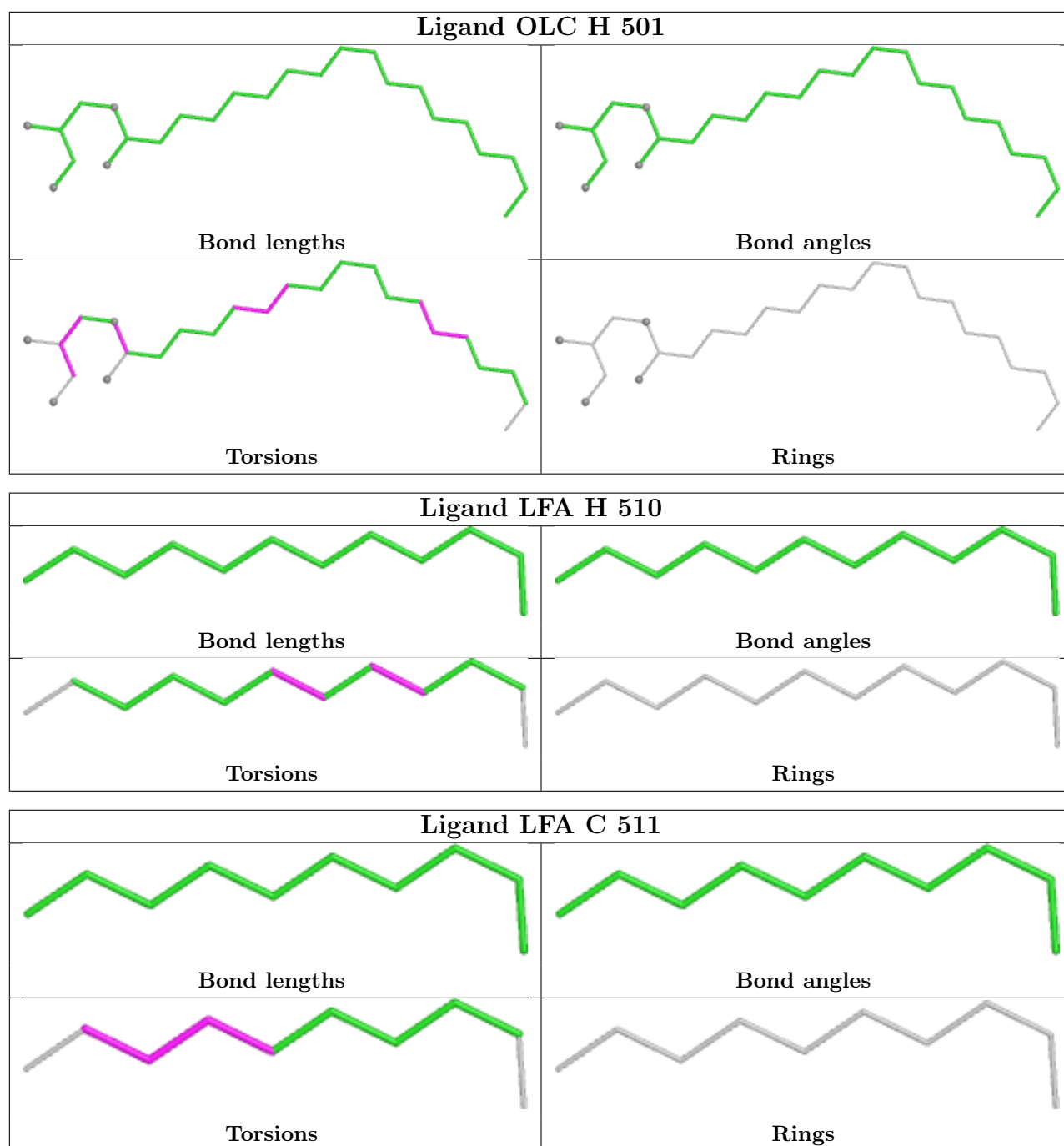
Ligand LFA A 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

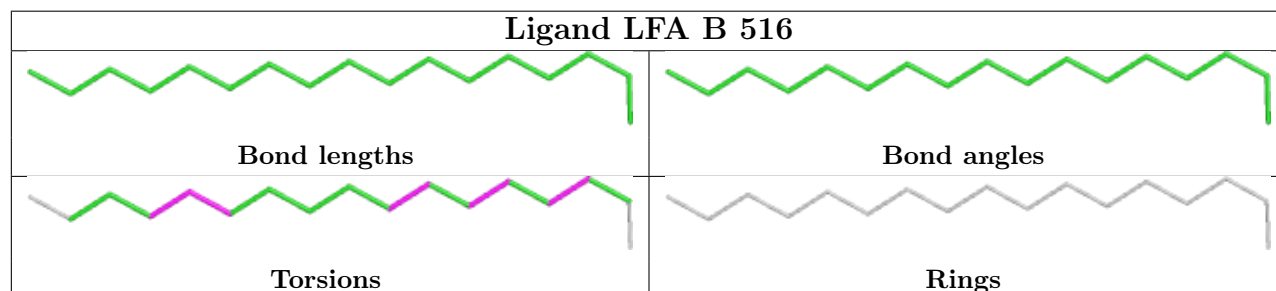
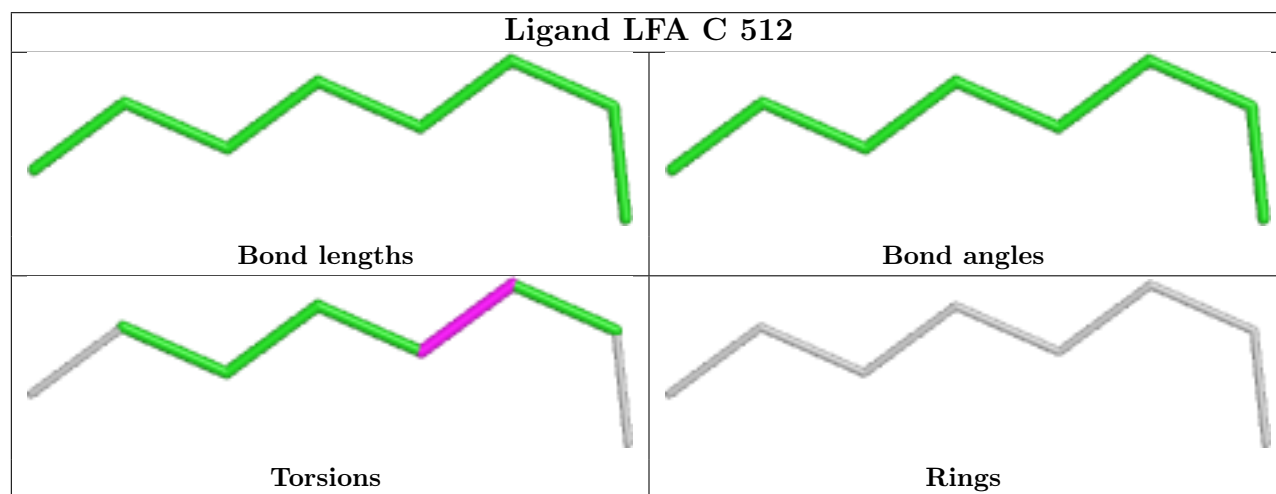
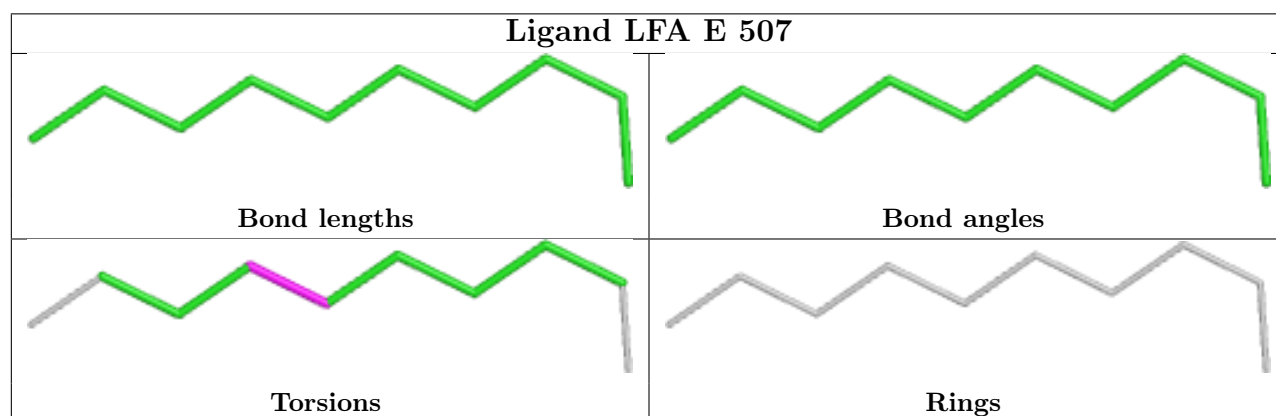
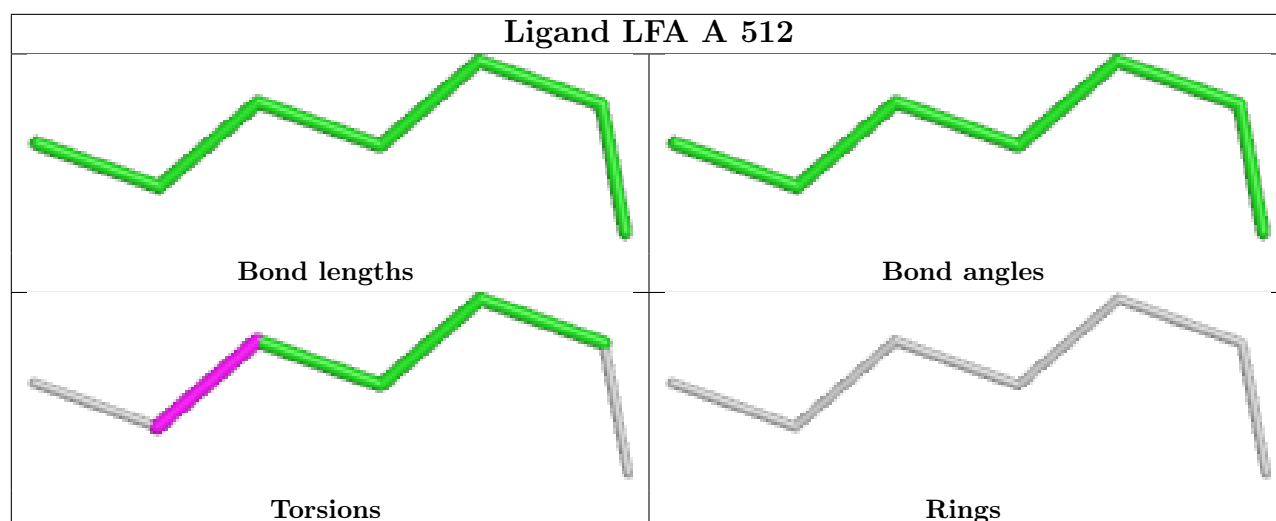


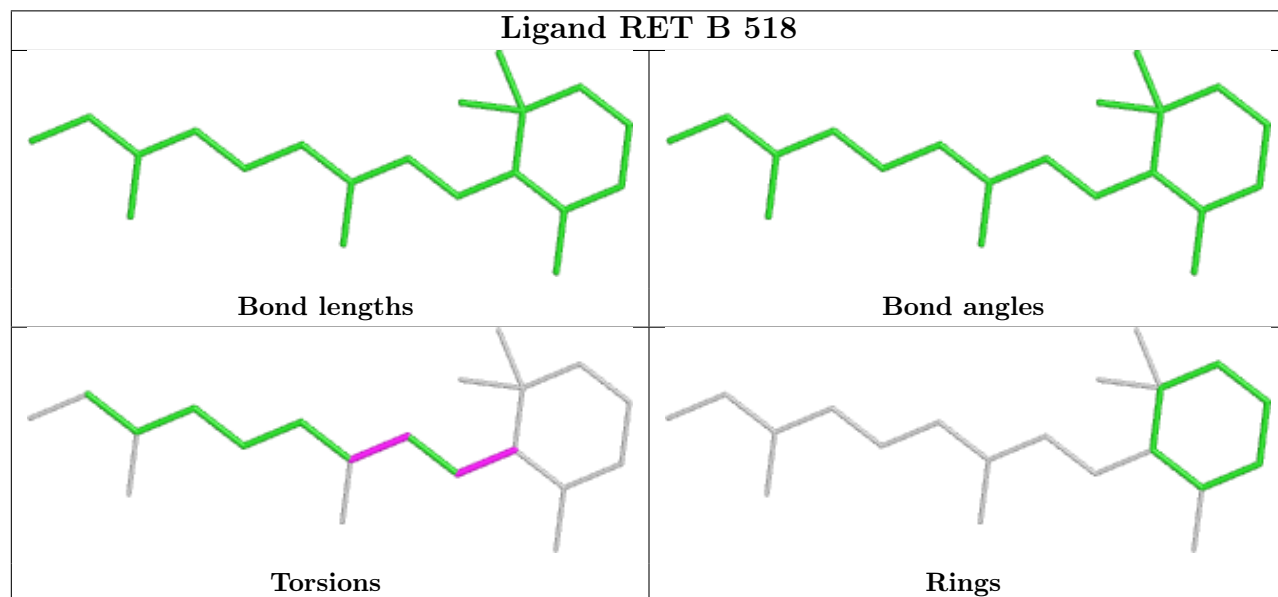
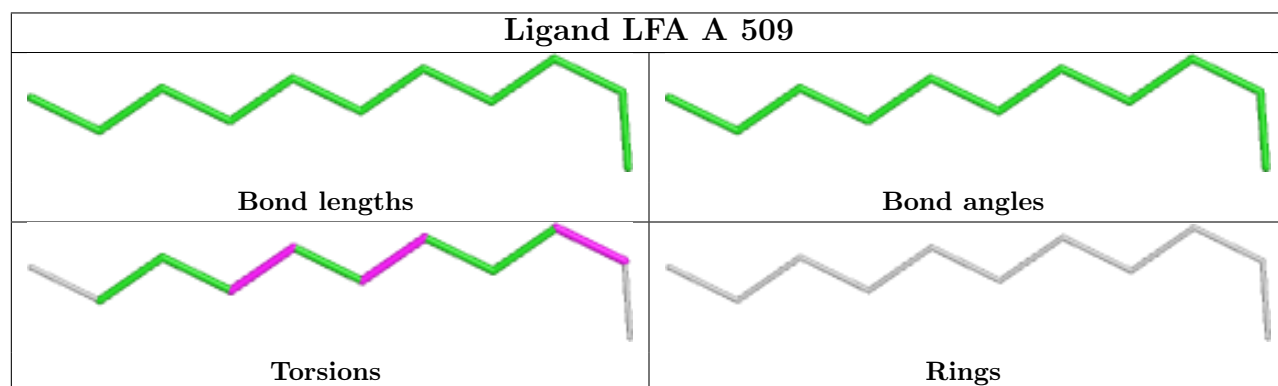
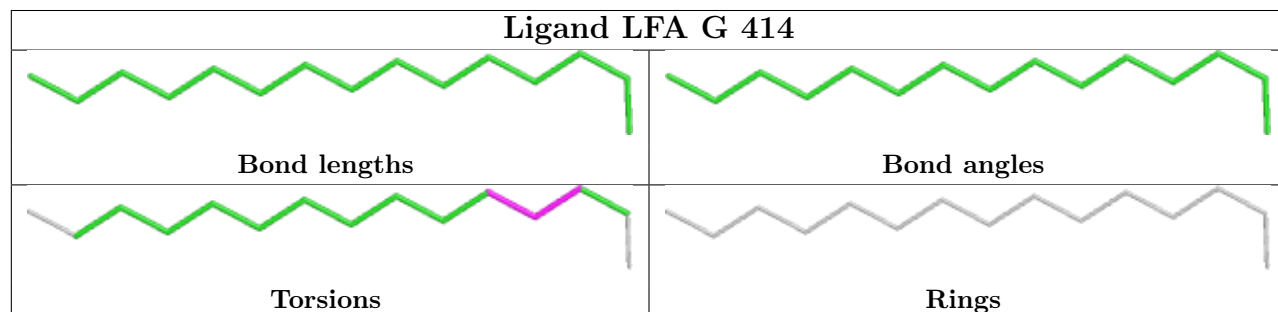
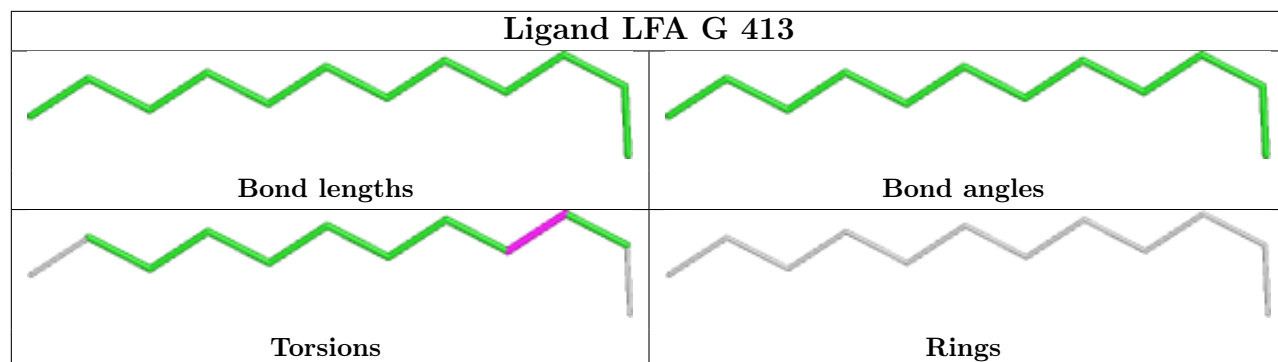


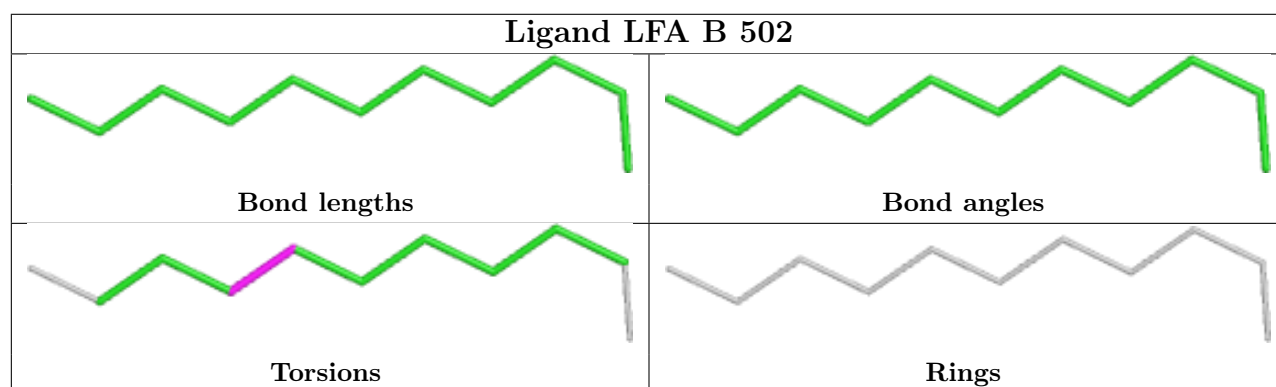
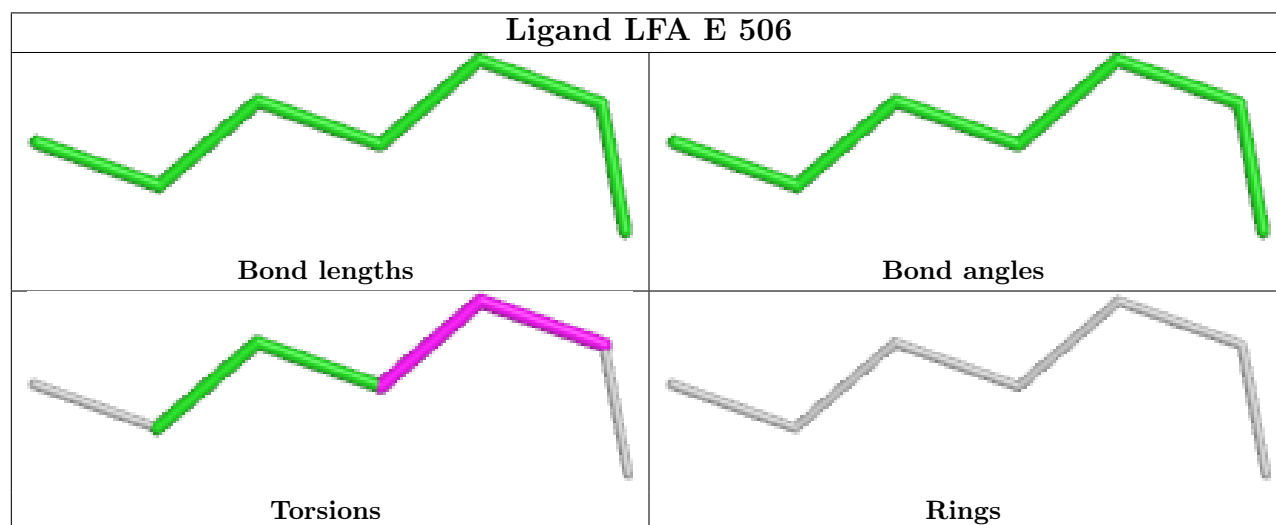
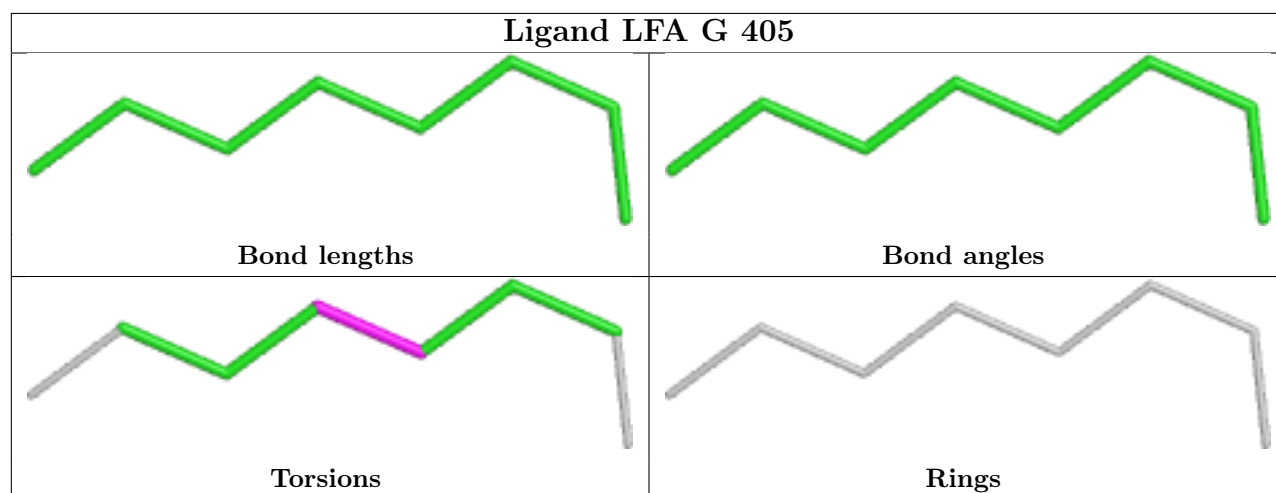
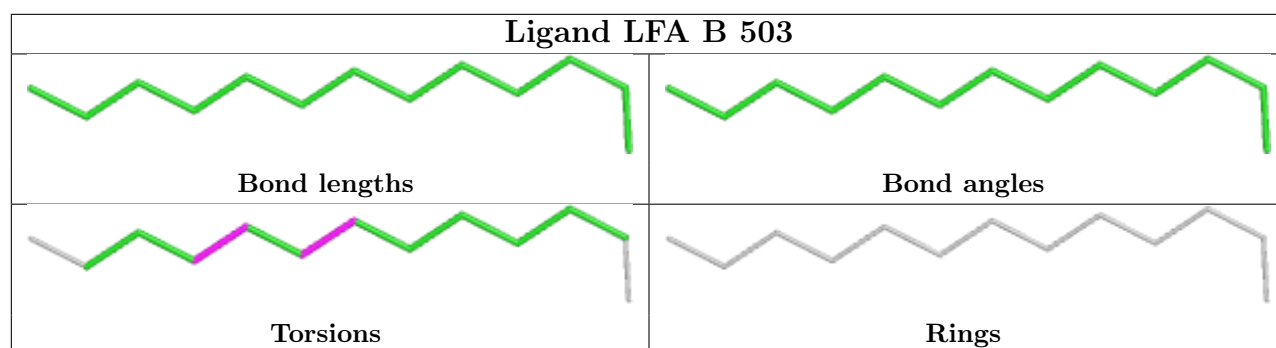


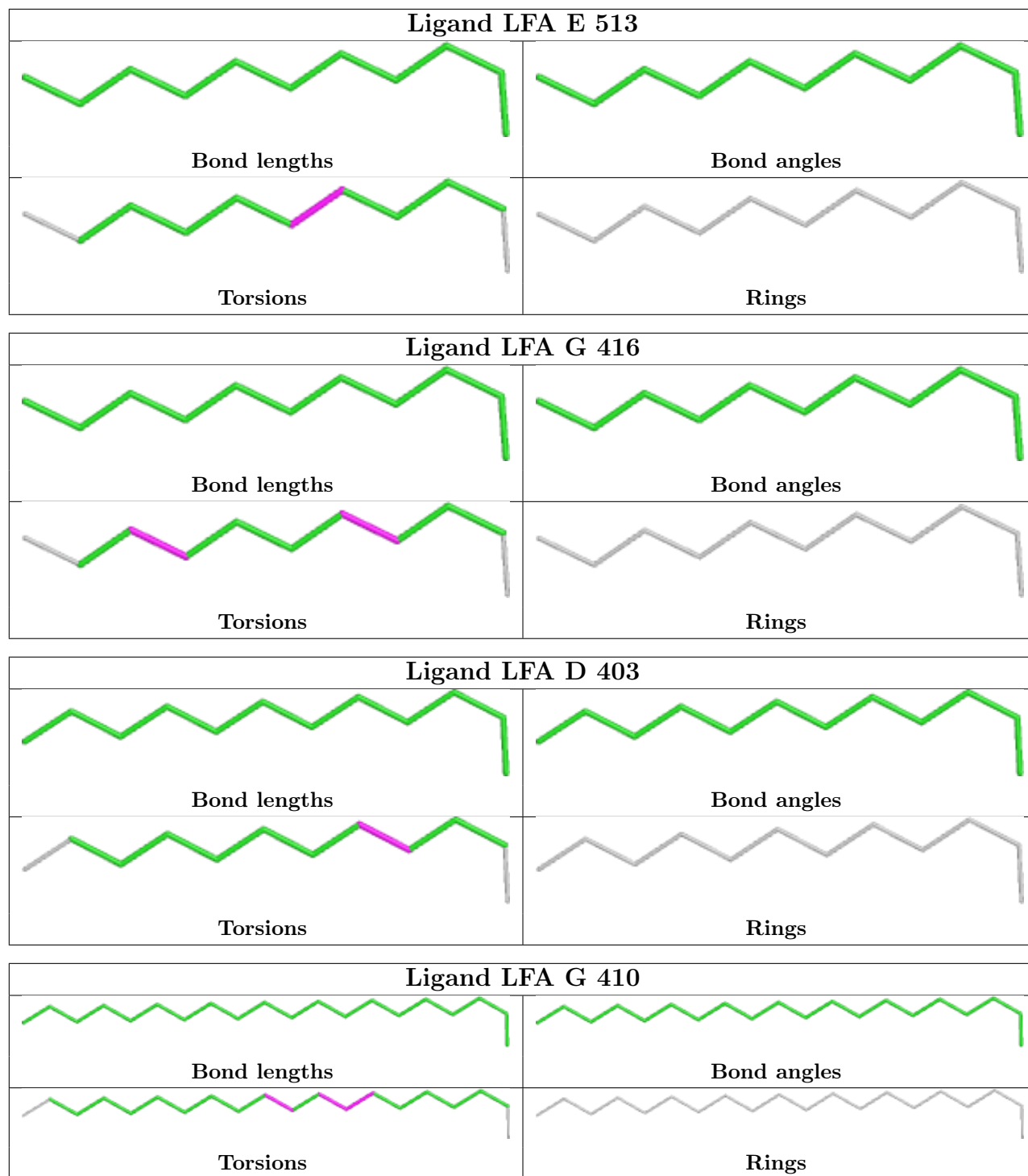


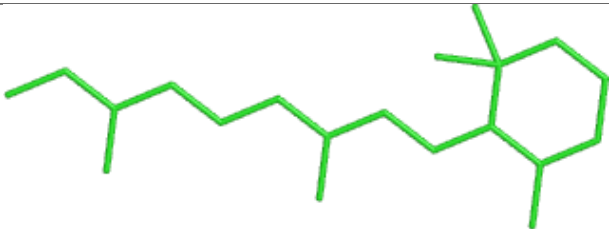
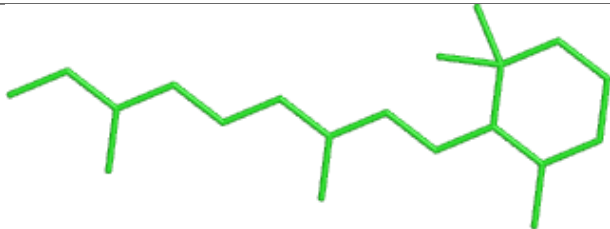
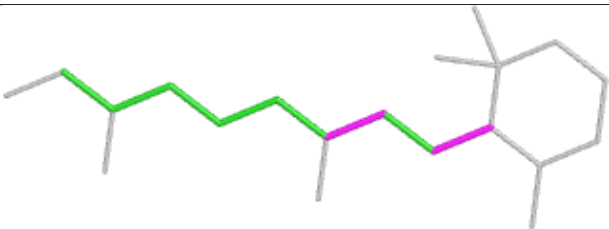
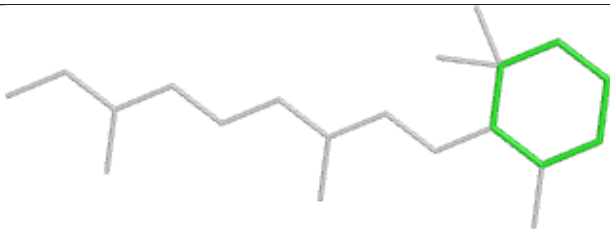








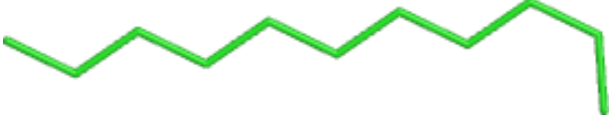
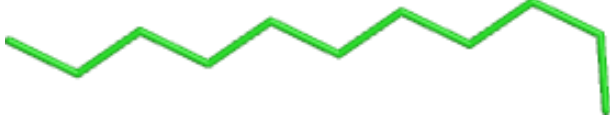
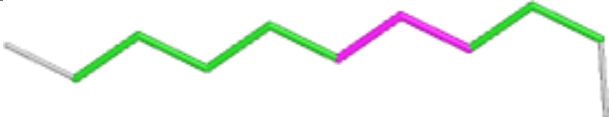
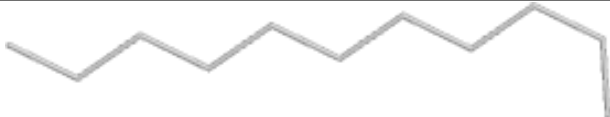


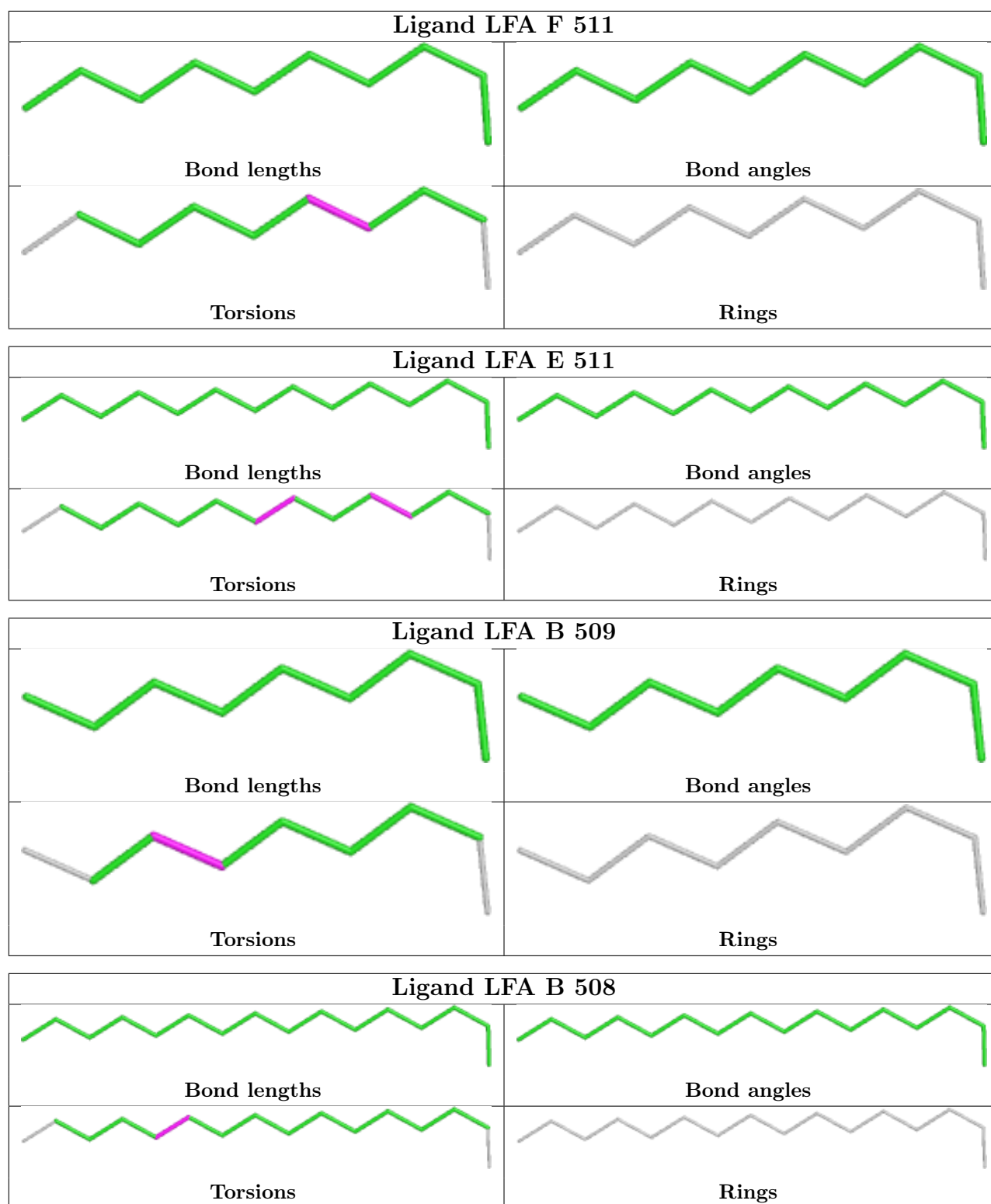


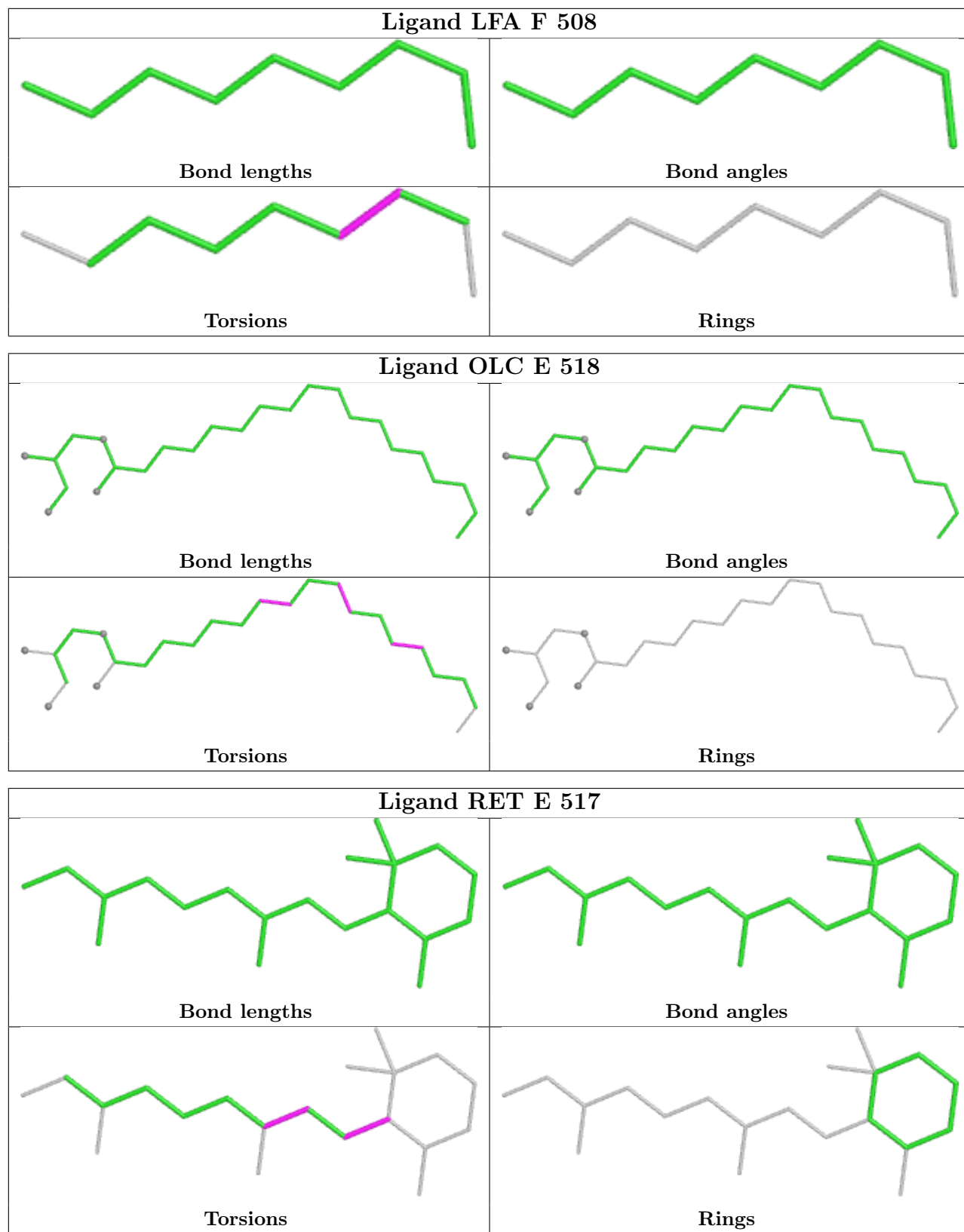


Ligand RET C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

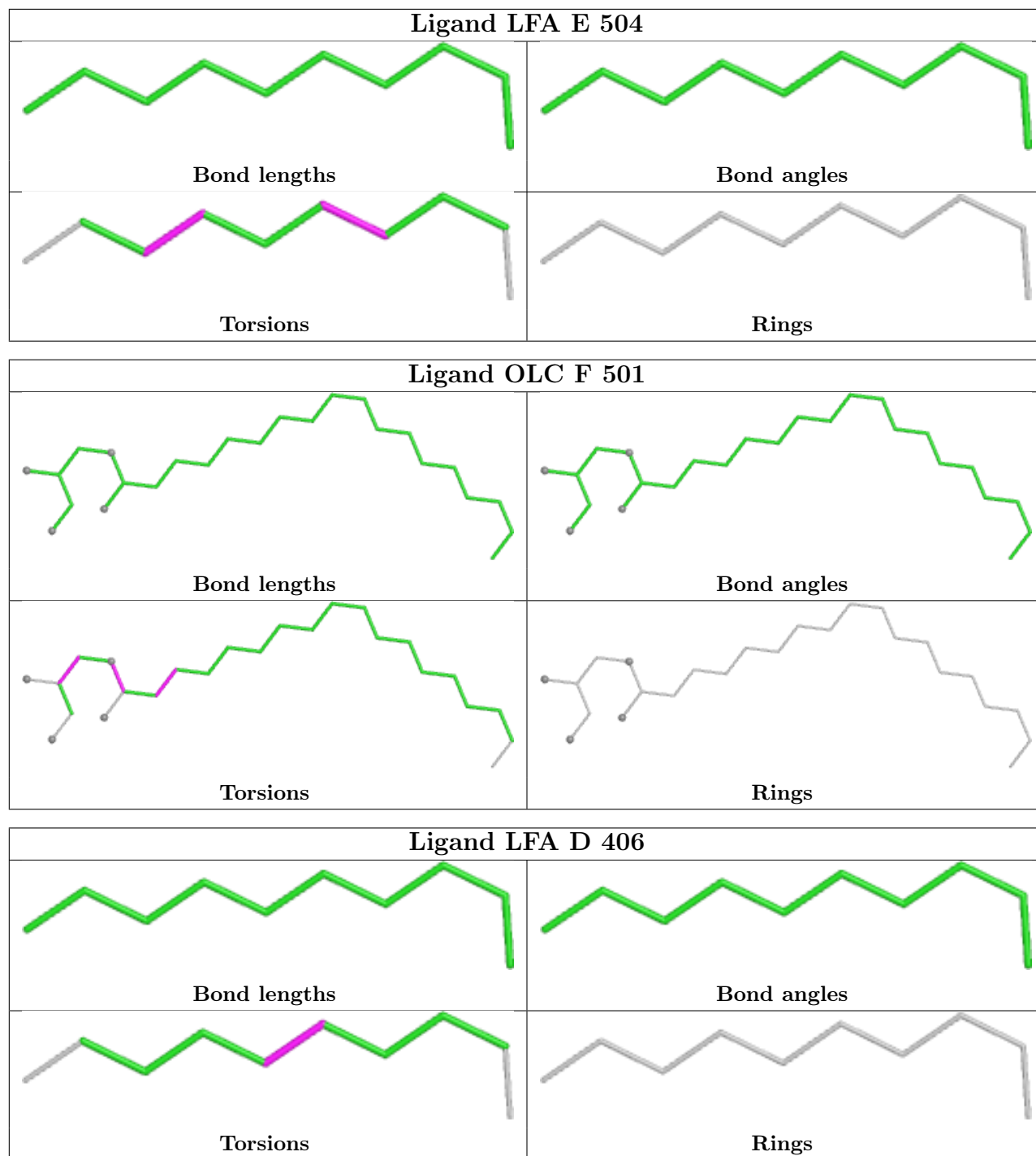
Ligand LFA H 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

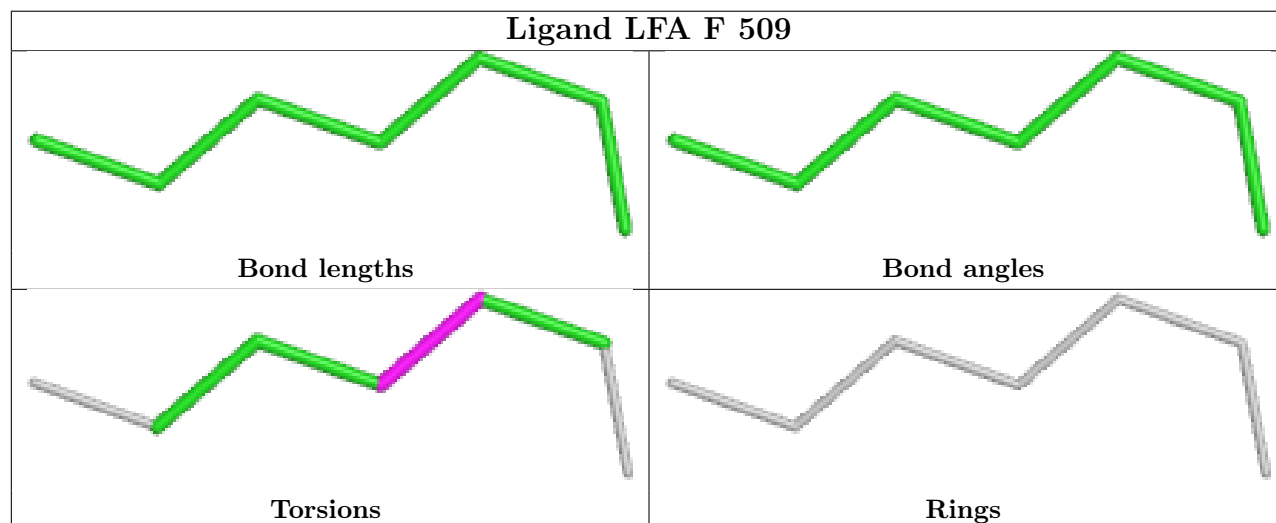
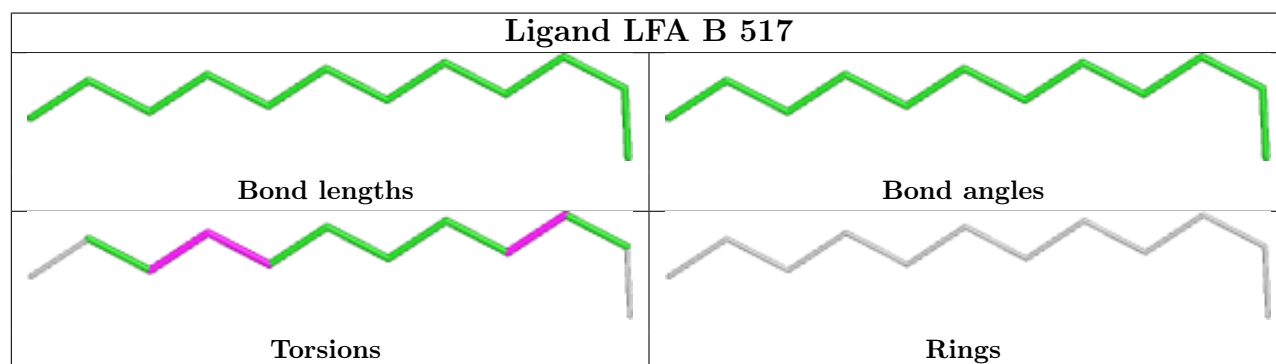
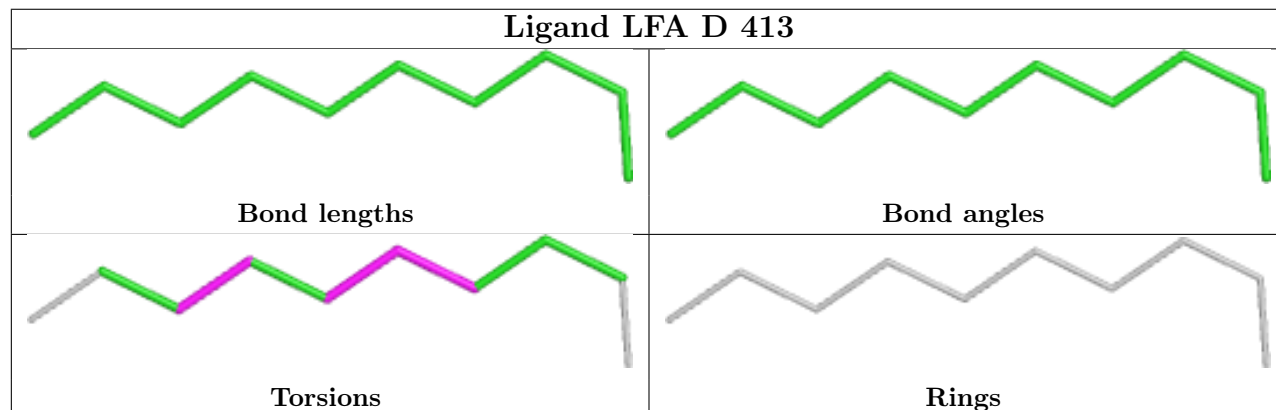
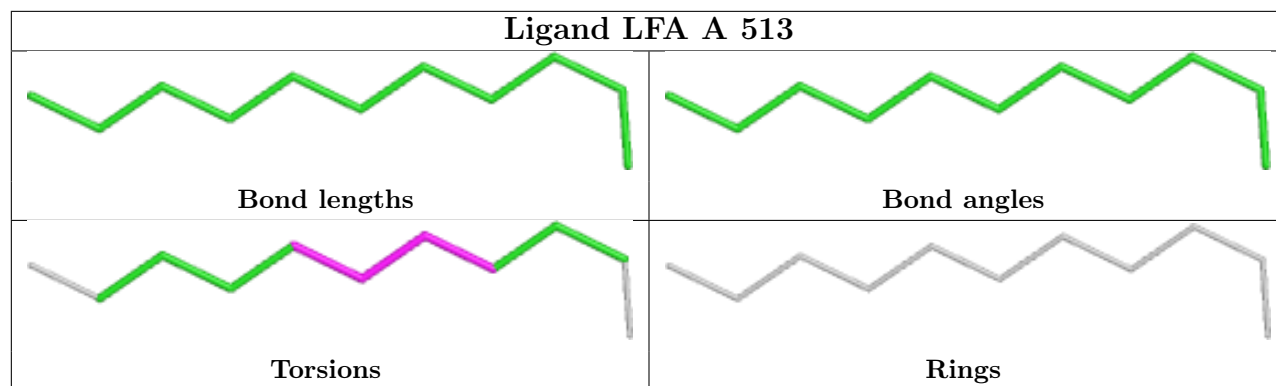
Ligand LFA G 415	
	
Bond lengths	Bond angles
	
Torsions	Rings

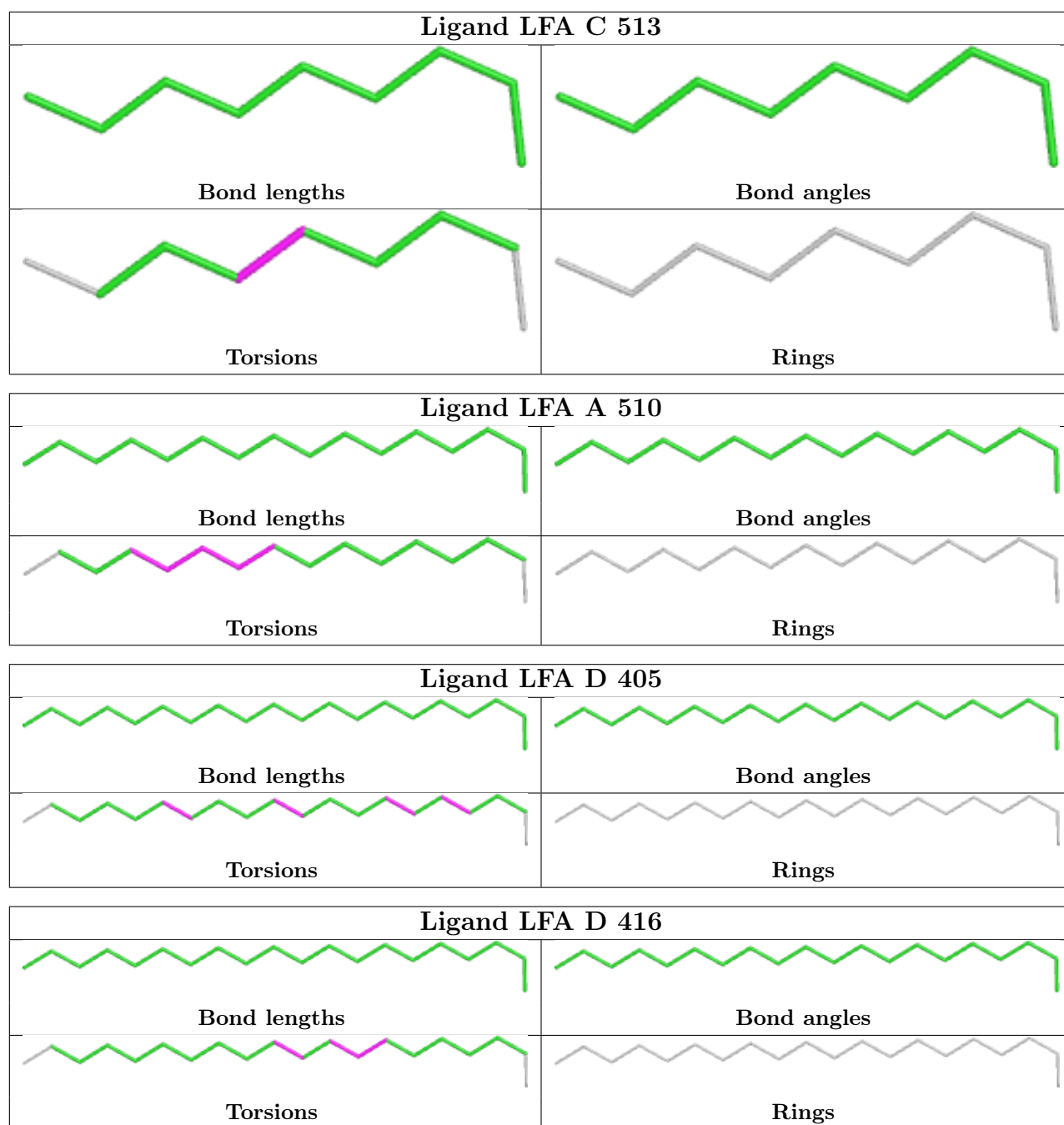


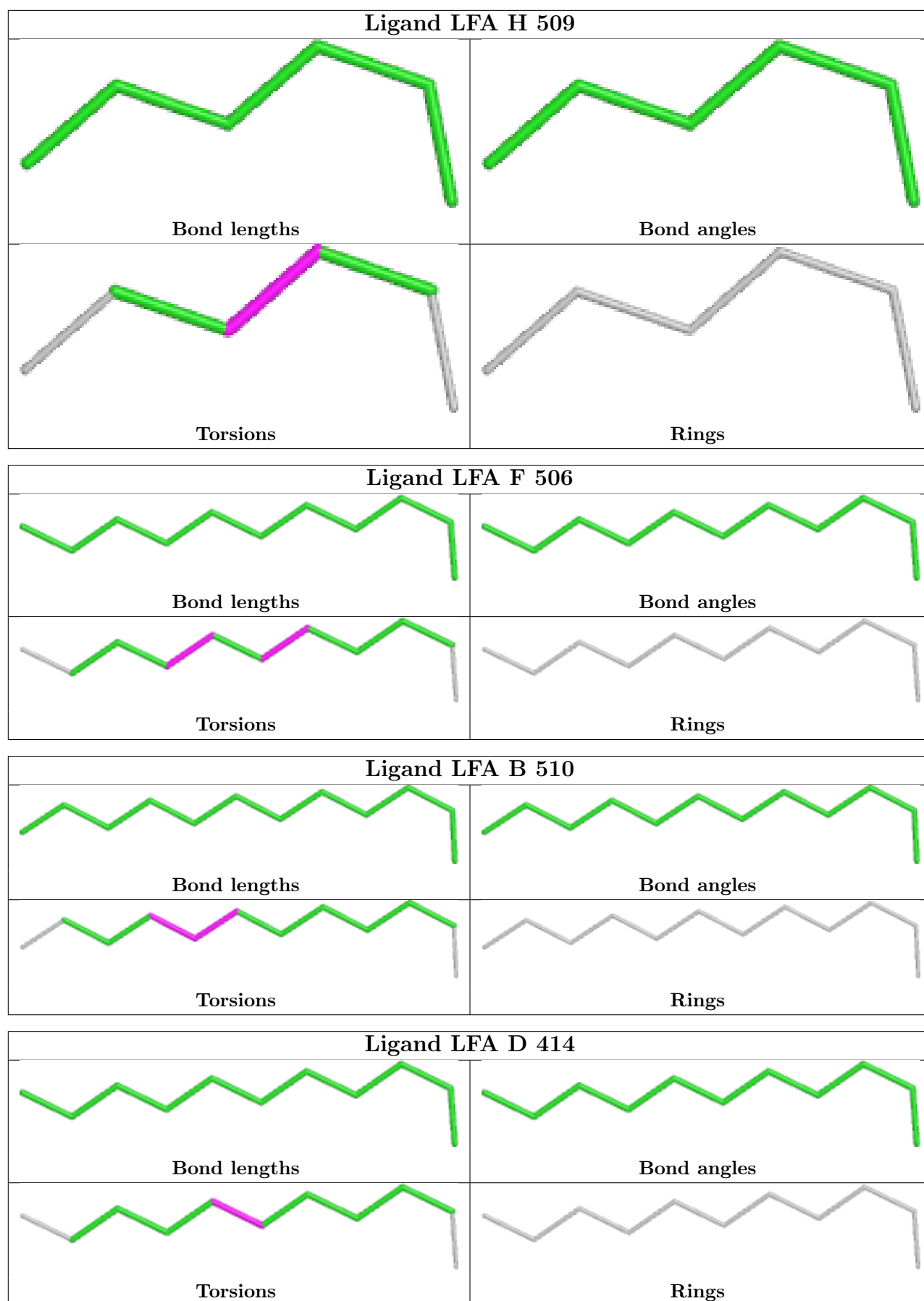


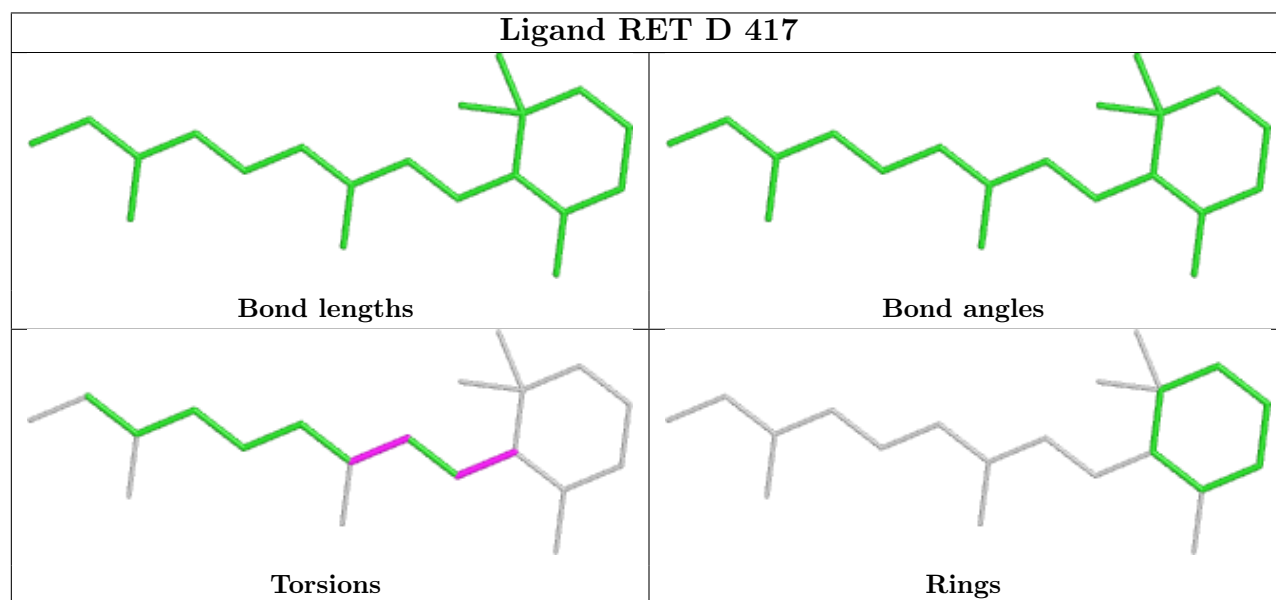
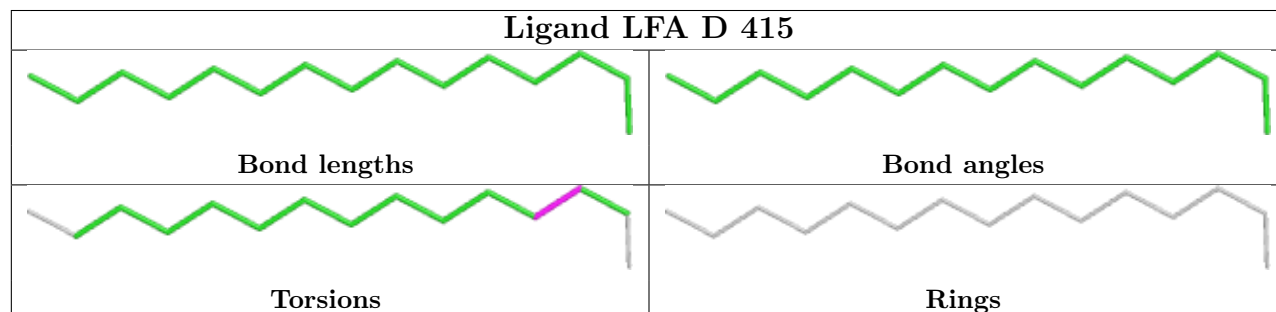
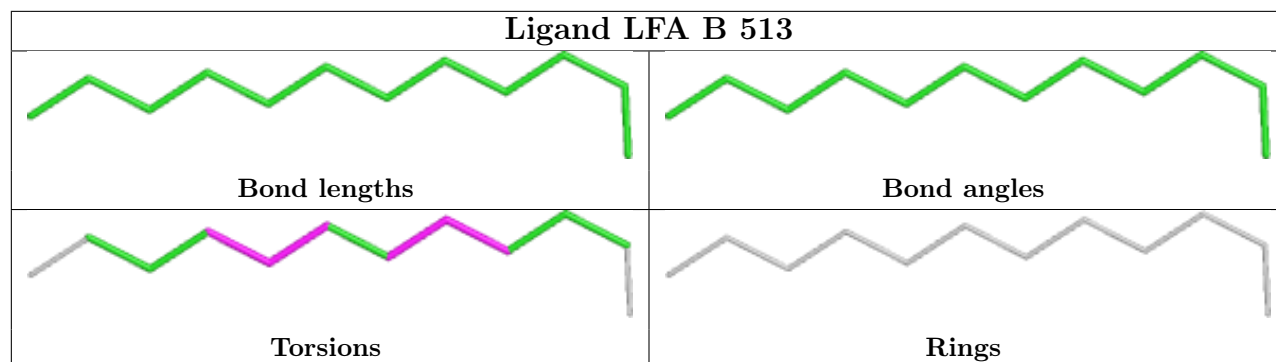


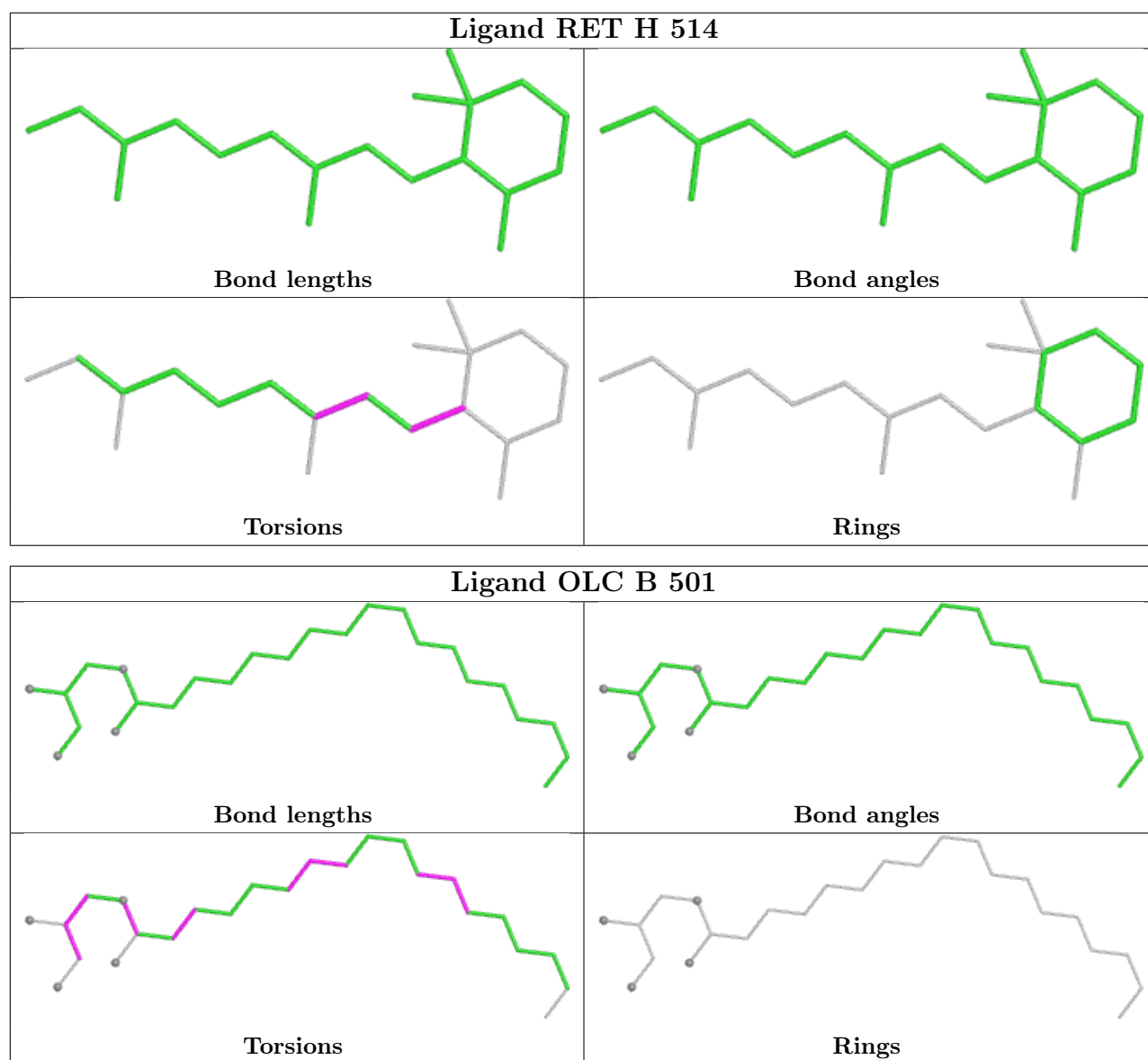












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	280/317 (88%)	0.63	14 (5%) 34 28	42, 56, 98, 156	0
1	B	278/317 (87%)	0.73	32 (11%) 9 7	42, 58, 96, 127	0
1	C	278/317 (87%)	0.68	17 (6%) 27 22	42, 58, 96, 124	0
1	D	276/317 (87%)	0.67	20 (7%) 21 17	39, 55, 96, 137	0
1	E	277/317 (87%)	0.77	30 (10%) 11 8	46, 61, 101, 132	0
1	F	275/317 (86%)	0.77	23 (8%) 17 13	43, 60, 98, 136	0
1	G	277/317 (87%)	0.72	26 (9%) 14 11	42, 58, 102, 138	0
1	H	278/317 (87%)	0.71	20 (7%) 21 17	43, 59, 104, 139	0
All	All	2219/2536 (87%)	0.71	182 (8%) 17 14	39, 58, 100, 156	0

The worst 5 of 182 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	SER	6.4
1	B	77	ASP	6.3
1	E	77	ASP	5.4
1	H	77	ASP	5.3
1	H	93	GLY	5.2

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	LFA	E	509	9/20	0.69	0.25	68,70,77,79	0
2	LFA	C	511	10/20	0.71	0.22	56,71,77,79	0
2	LFA	H	509	6/20	0.71	0.20	63,68,71,76	0
2	LFA	C	512	8/20	0.74	0.21	54,62,66,70	0
2	LFA	C	513	9/20	0.74	0.23	40,68,76,81	0
2	LFA	H	511	10/20	0.74	0.19	65,83,90,93	0
2	LFA	F	515	7/20	0.75	0.18	60,69,72,75	0
2	LFA	A	503	12/20	0.76	0.17	58,66,72,73	0
2	LFA	E	506	7/20	0.76	0.18	58,64,68,75	0
2	LFA	B	502	11/20	0.76	0.19	61,66,72,72	0
2	LFA	E	508	7/20	0.77	0.23	63,70,79,85	0
2	LFA	G	418	10/20	0.77	0.19	51,65,71,76	0
2	LFA	G	416	11/20	0.78	0.22	76,79,86,87	0
2	LFA	E	510	6/20	0.78	0.17	62,63,65,72	0
2	LFA	H	505	13/20	0.78	0.16	43,53,58,60	0
2	LFA	A	516	14/20	0.78	0.18	64,72,75,76	0
2	LFA	G	415	11/20	0.78	0.20	48,57,68,70	0
2	LFA	D	413	10/20	0.79	0.19	60,64,70,73	0
2	LFA	D	405	20/20	0.80	0.22	56,67,77,80	0
2	LFA	G	417	6/20	0.80	0.19	58,61,62,62	0
2	LFA	H	512	9/20	0.80	0.22	50,60,66,67	0
2	LFA	D	410	9/20	0.81	0.17	39,57,64,67	0
2	LFA	G	407	10/20	0.81	0.18	43,51,63,70	0
2	LFA	G	410	20/20	0.81	0.19	50,59,68,69	0
2	LFA	C	506	7/20	0.81	0.19	50,62,70,70	0
2	LFA	C	509	19/20	0.81	0.20	53,68,78,79	0
2	LFA	D	404	8/20	0.81	0.20	47,50,64,71	0
2	LFA	A	513	11/20	0.81	0.19	46,53,62,63	0
2	LFA	D	407	8/20	0.81	0.17	54,59,62,63	0
2	LFA	E	512	15/20	0.81	0.20	58,67,80,84	0
2	LFA	F	508	9/20	0.81	0.19	53,64,73,78	0
2	LFA	F	509	7/20	0.81	0.20	54,56,61,61	0
2	LFA	C	510	7/20	0.82	0.15	52,54,63,63	0
2	LFA	E	519	20/20	0.82	0.18	51,68,81,82	0
2	LFA	D	415	15/20	0.82	0.21	48,55,71,73	0
2	LFA	B	507	10/20	0.82	0.18	61,66,74,74	0
2	LFA	H	504	9/20	0.82	0.17	55,59,61,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LFA	F	512	6/20	0.82	0.17	51,58,70,72	0
2	LFA	H	507	7/20	0.82	0.19	51,55,60,62	0
2	LFA	D	406	10/20	0.82	0.20	50,59,68,70	0
2	LFA	A	501	9/20	0.82	0.13	55,60,64,67	0
2	LFA	A	515	6/20	0.82	0.17	47,57,59,62	0
2	LFA	E	515	11/20	0.83	0.20	45,63,66,66	0
2	LFA	D	414	11/20	0.83	0.20	35,52,62,64	0
2	LFA	F	507	12/20	0.83	0.18	46,54,66,67	0
2	LFA	A	511	13/20	0.83	0.16	51,63,72,76	0
2	LFA	D	403	12/20	0.83	0.19	47,53,61,70	0
2	LFA	F	510	11/20	0.83	0.17	57,64,69,71	0
2	LFA	H	506	11/20	0.83	0.17	53,63,74,82	0
2	LFA	D	408	5/20	0.83	0.15	53,56,58,63	0
2	LFA	D	409	9/20	0.83	0.22	38,48,53,60	0
2	LFA	C	508	9/20	0.83	0.20	54,59,67,78	0
2	LFA	A	505	11/20	0.83	0.17	51,54,62,67	0
4	OLC	C	501	20/25	0.83	0.15	39,48,75,78	0
2	LFA	E	514	7/20	0.84	0.18	60,64,69,74	0
2	LFA	E	507	10/20	0.84	0.17	51,56,59,61	0
2	LFA	H	502	7/20	0.84	0.18	39,52,60,63	0
2	LFA	F	513	15/20	0.84	0.18	52,62,68,71	0
2	LFA	C	504	7/20	0.84	0.16	49,50,54,58	0
2	LFA	G	404	10/20	0.84	0.18	47,53,67,67	0
2	LFA	F	503	9/20	0.84	0.17	39,50,64,64	0
2	LFA	G	409	14/20	0.84	0.15	52,62,69,72	0
2	LFA	A	507	7/20	0.84	0.16	43,53,57,61	0
2	LFA	B	510	12/20	0.84	0.17	47,56,67,72	0
2	LFA	B	513	12/20	0.84	0.16	51,56,62,65	0
2	LFA	B	512	13/20	0.85	0.16	41,54,66,70	0
2	LFA	D	416	20/20	0.85	0.15	46,64,75,79	0
2	LFA	G	405	8/20	0.85	0.18	48,54,60,63	0
2	LFA	E	503	10/20	0.85	0.19	48,53,66,68	0
2	LFA	C	514	12/20	0.85	0.16	63,71,75,77	0
2	LFA	B	508	16/20	0.85	0.15	50,65,73,78	0
2	LFA	G	411	14/20	0.85	0.16	49,61,71,71	0
2	LFA	A	504	13/20	0.85	0.19	43,56,67,71	0
2	LFA	F	502	8/20	0.85	0.14	40,51,53,61	0
2	LFA	H	513	8/20	0.85	0.22	53,57,65,68	0
2	LFA	F	514	12/20	0.85	0.16	55,65,79,79	0
4	OLC	H	501	25/25	0.85	0.17	40,56,73,78	0
2	LFA	B	515	10/20	0.86	0.16	45,59,61,66	0
2	LFA	F	517	8/20	0.86	0.17	52,56,64,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LFA	G	402	14/20	0.86	0.18	39,55,62,63	0
2	LFA	B	504	12/20	0.86	0.15	52,59,67,69	0
2	LFA	F	506	11/20	0.86	0.16	55,59,65,68	0
2	LFA	D	401	12/20	0.86	0.15	44,50,59,62	0
2	LFA	D	402	10/20	0.86	0.15	43,55,61,61	0
2	LFA	E	511	14/20	0.86	0.16	46,57,62,65	0
2	LFA	E	501	8/20	0.86	0.20	49,53,60,65	0
2	LFA	A	506	11/20	0.86	0.18	50,56,62,69	0
4	OLC	B	501	25/25	0.86	0.16	46,57,68,82	0
2	LFA	E	504	10/20	0.86	0.17	49,62,65,71	0
4	OLC	E	518	25/25	0.86	0.15	42,56,66,71	0
4	OLC	F	501	25/25	0.86	0.14	43,58,65,72	0
2	LFA	B	503	13/20	0.86	0.14	43,50,63,71	0
2	LFA	G	413	12/20	0.87	0.15	52,63,70,74	0
2	LFA	G	406	11/20	0.87	0.16	38,49,61,65	0
2	LFA	A	502	8/20	0.87	0.15	46,56,57,64	0
2	LFA	B	516	17/20	0.87	0.19	48,61,84,84	0
2	LFA	A	510	16/20	0.87	0.15	46,53,61,61	0
2	LFA	H	510	12/20	0.87	0.15	47,56,74,74	0
2	LFA	F	511	10/20	0.87	0.19	38,57,71,77	0
2	LFA	A	508	11/20	0.88	0.12	44,51,55,56	0
2	LFA	G	401	10/20	0.88	0.19	45,52,60,60	0
2	LFA	H	503	7/20	0.88	0.15	47,47,61,62	0
2	LFA	A	509	11/20	0.88	0.16	47,54,59,67	0
2	LFA	B	517	12/20	0.88	0.14	46,56,60,65	0
2	LFA	C	502	8/20	0.88	0.16	43,48,54,56	0
2	LFA	E	516	7/20	0.88	0.14	59,71,71,74	0
2	LFA	H	508	7/20	0.88	0.18	50,54,59,59	0
2	LFA	B	509	9/20	0.88	0.14	43,50,57,58	0
2	LFA	E	502	8/20	0.89	0.13	49,53,57,62	0
2	LFA	F	504	7/20	0.89	0.16	39,47,56,66	0
2	LFA	A	517	8/20	0.89	0.14	46,53,57,61	0
2	LFA	C	507	7/20	0.89	0.17	47,50,53,54	0
2	LFA	B	506	10/20	0.90	0.15	44,54,60,67	0
2	LFA	B	511	7/20	0.90	0.13	35,45,56,57	0
2	LFA	G	414	15/20	0.90	0.16	45,54,64,71	0
2	LFA	B	514	10/20	0.90	0.16	52,61,67,71	0
2	LFA	G	403	9/20	0.90	0.13	44,50,57,58	0
2	LFA	D	412	10/20	0.90	0.14	43,54,67,70	0
2	LFA	E	513	11/20	0.91	0.15	48,61,64,68	0
2	LFA	B	505	12/20	0.91	0.13	50,56,70,71	0
2	LFA	A	512	7/20	0.91	0.15	47,53,54,54	0

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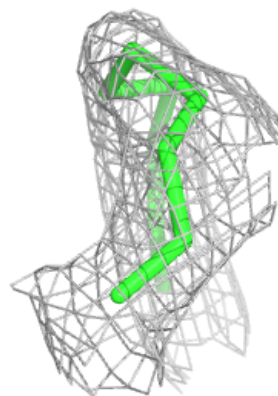
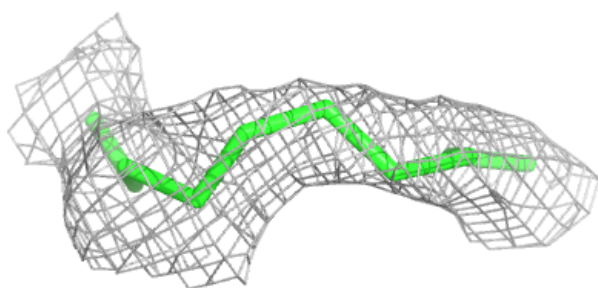
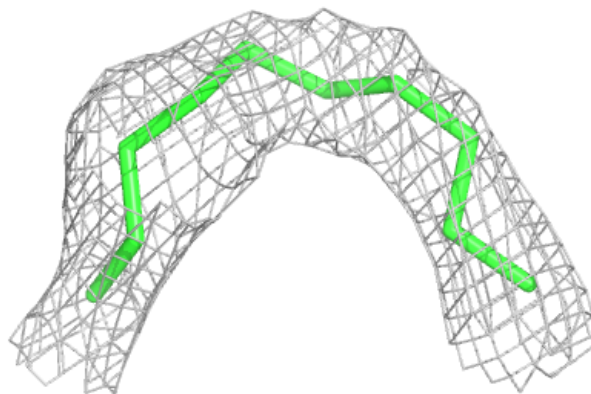
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LFA	C	503	10/20	0.91	0.10	39,46,54,55	0
2	LFA	D	411	10/20	0.92	0.12	39,53,60,63	0
2	LFA	G	412	9/20	0.92	0.13	55,61,64,74	0
2	LFA	C	505	10/20	0.92	0.14	42,53,60,61	0
2	LFA	E	505	12/20	0.92	0.15	47,52,63,64	0
2	LFA	F	505	9/20	0.92	0.13	45,52,60,65	0
3	RET	H	514	20/21	0.93	0.11	45,50,54,57	0
2	LFA	A	514	7/20	0.93	0.12	35,40,51,54	0
2	LFA	G	408	10/20	0.93	0.12	40,51,61,64	0
3	RET	C	515	20/21	0.93	0.12	41,47,53,53	0
3	RET	D	417	20/21	0.93	0.13	39,46,53,53	0
3	RET	F	516	20/21	0.93	0.13	44,51,60,60	0
3	RET	E	517	20/21	0.94	0.12	44,46,57,57	0
3	RET	A	518	20/21	0.94	0.12	38,46,53,54	0
3	RET	G	419	20/21	0.94	0.12	40,47,54,56	0
3	RET	B	518	20/21	0.95	0.11	43,46,53,54	0

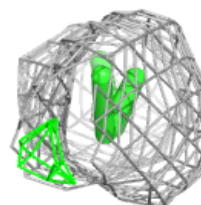
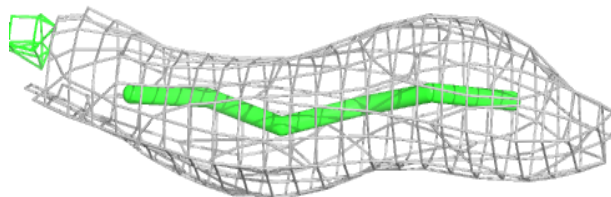
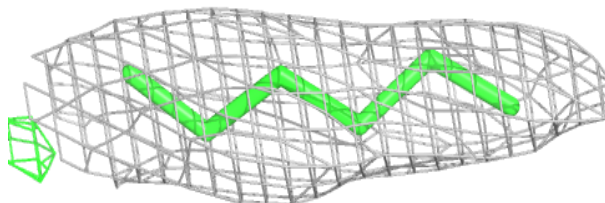
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LFA C 511:**

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

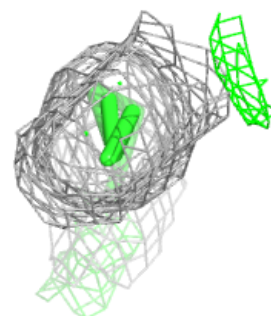
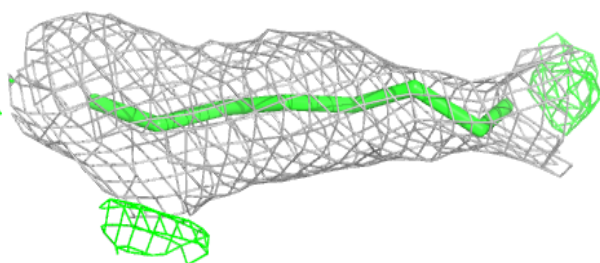
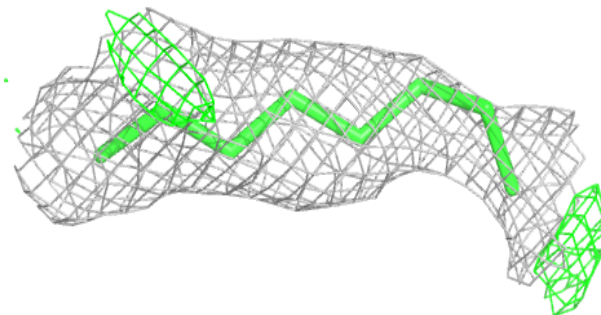
**Electron density around LFA H 509:**

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

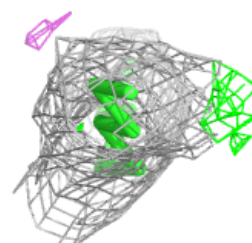
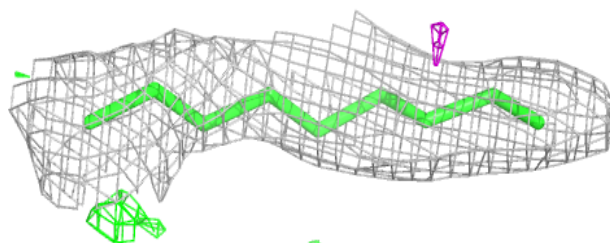
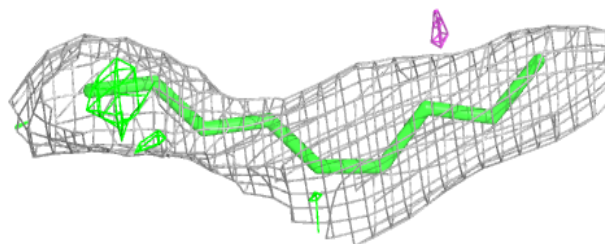


**Electron density around LFA C 512:**

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

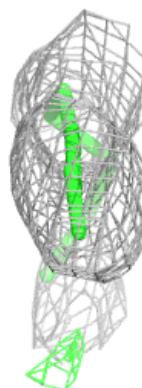
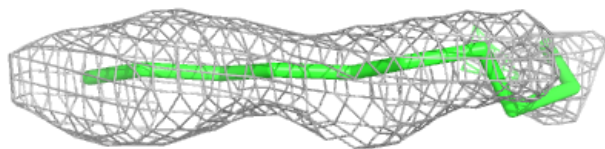
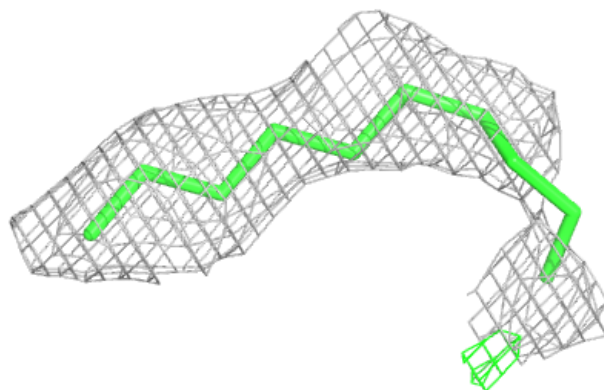
**Electron density around LFA C 513:**

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

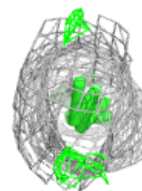
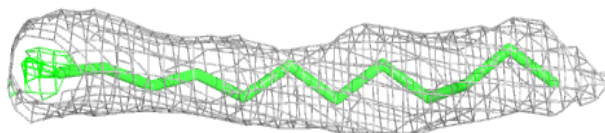
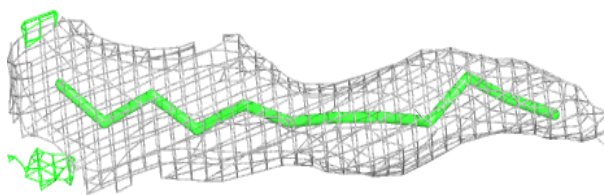


**Electron density around LFA H 511:**

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

**Electron density around LFA A 503:**

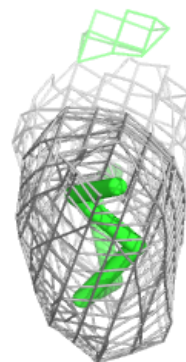
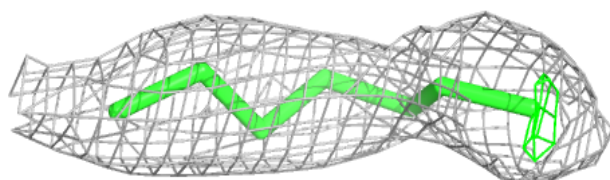
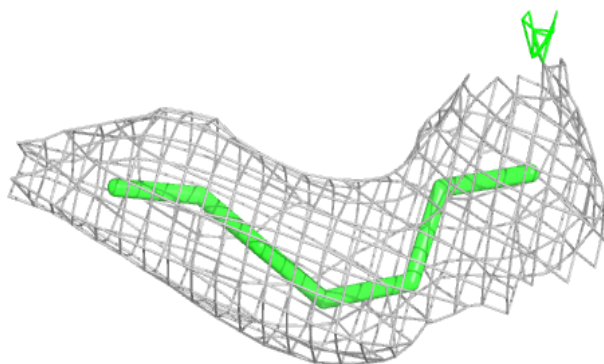
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



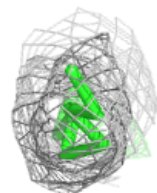
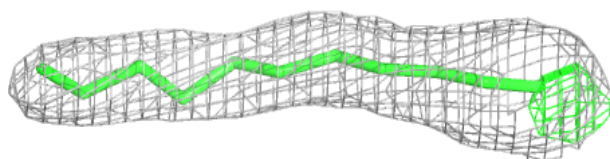
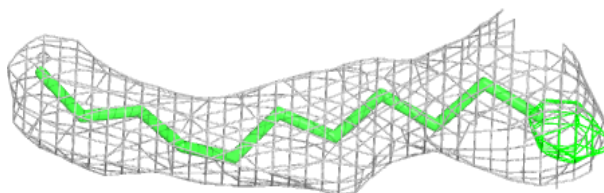


**Electron density around LFA E 506:**

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

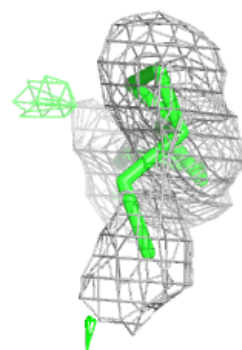
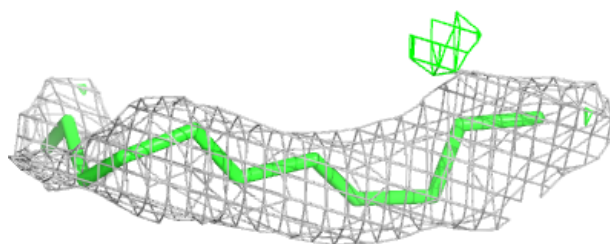
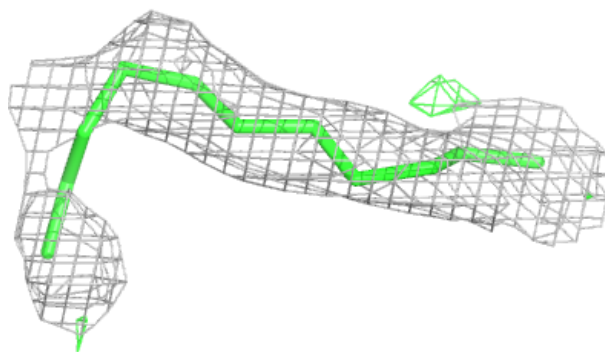
**Electron density around LFA B 502:**

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

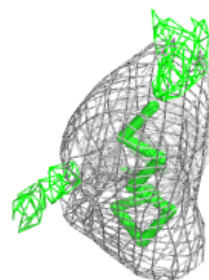
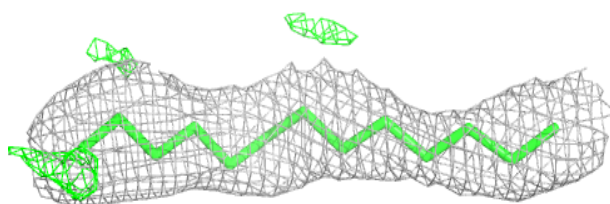
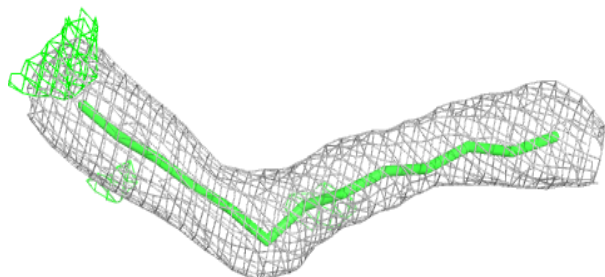


**Electron density around LFA G 416:**

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

**Electron density around LFA H 505:**

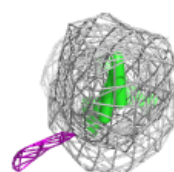
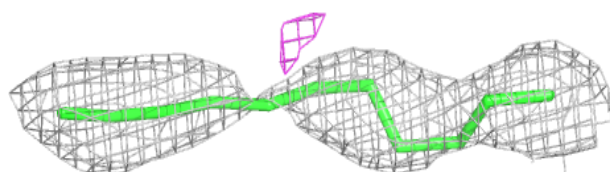
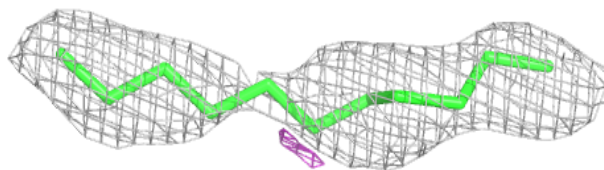
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



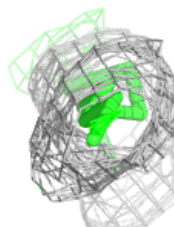
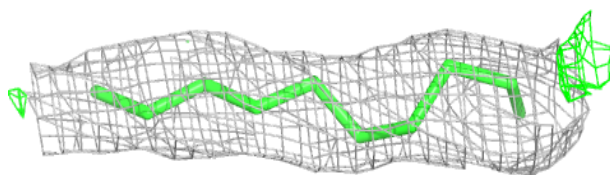
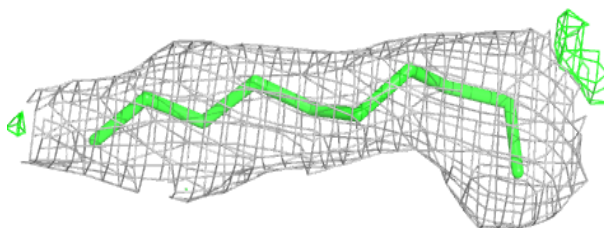


**Electron density around LFA G 415:**

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

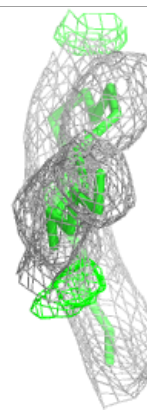
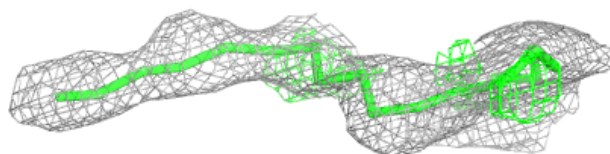
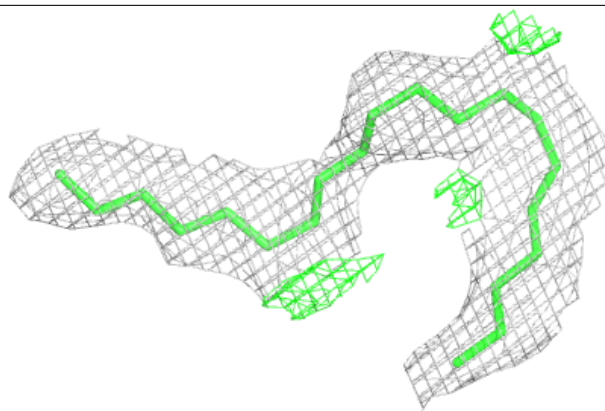
**Electron density around LFA D 413:**

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

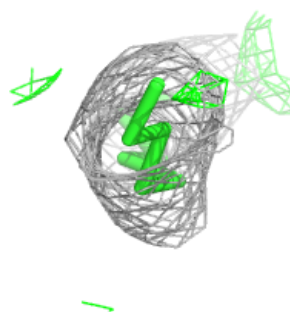
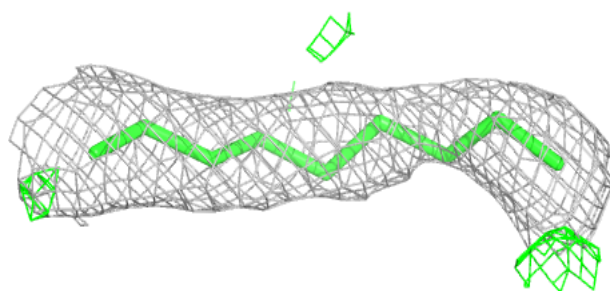
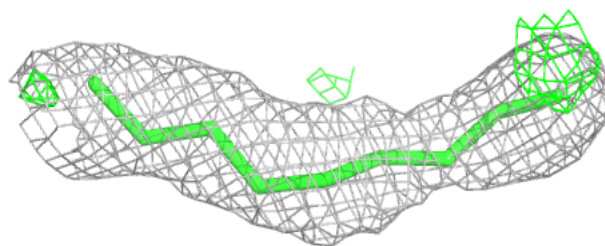


**Electron density around LFA D 405:**

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

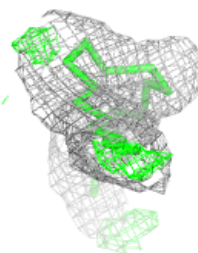
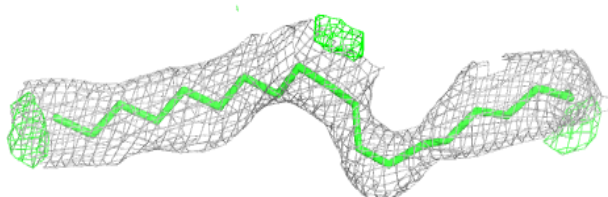
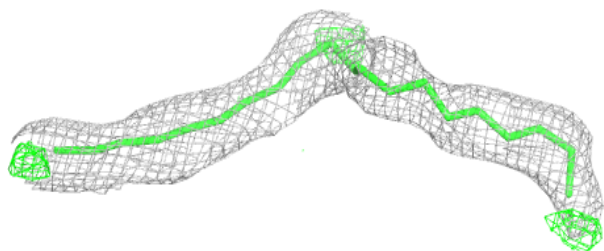
**Electron density around LFA D 410:**

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

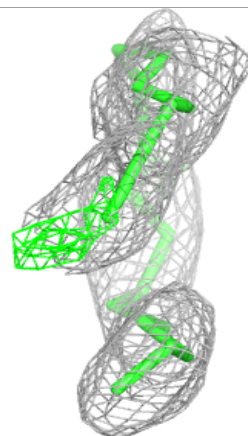
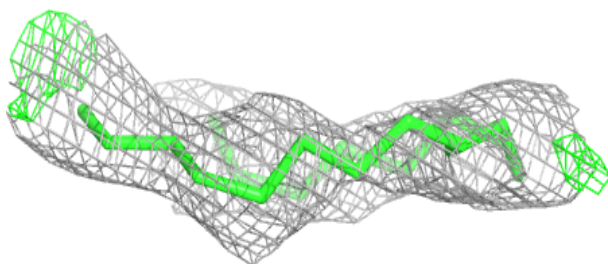
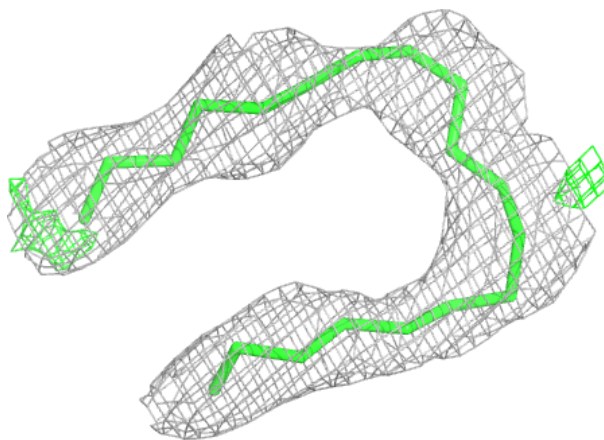


**Electron density around LFA G 410:**

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

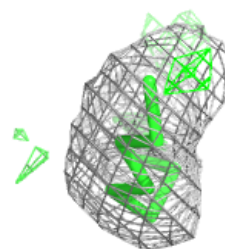
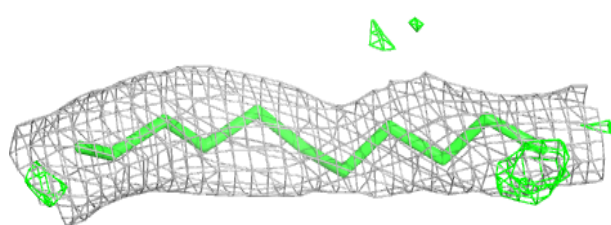
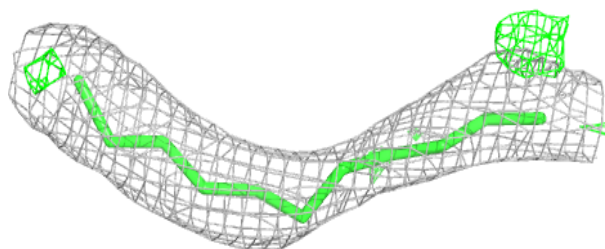
**Electron density around LFA C 509:**

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

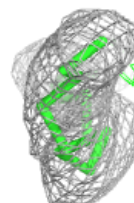
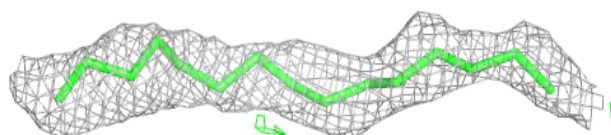
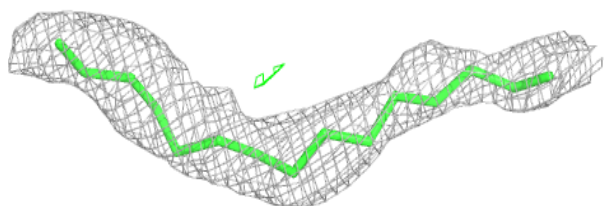


**Electron density around LFA A 513:**

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

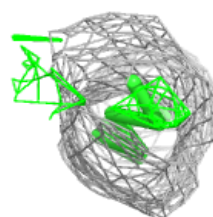
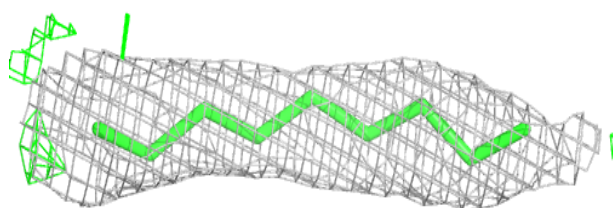
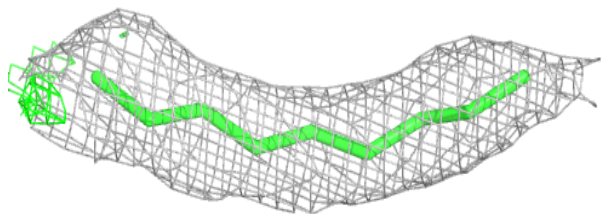
**Electron density around LFA E 512:**

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

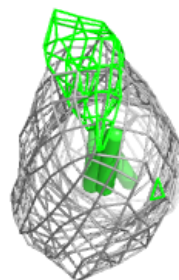
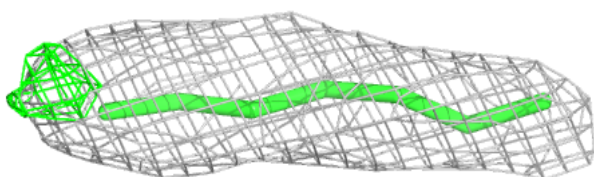
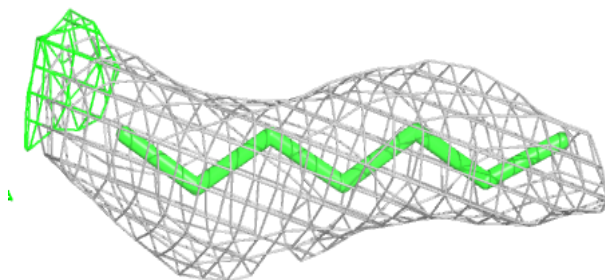


**Electron density around LFA F 508:**

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

**Electron density around LFA F 509:**

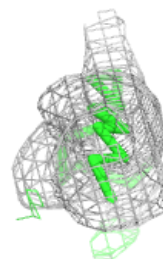
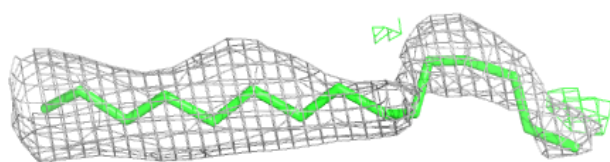
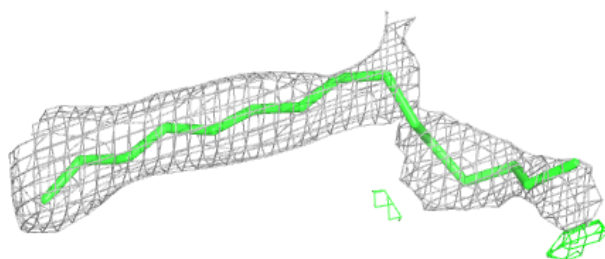
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



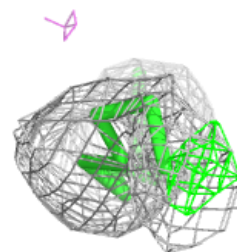
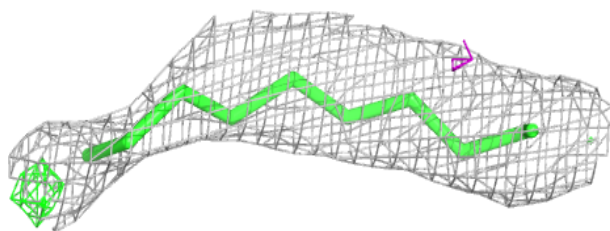
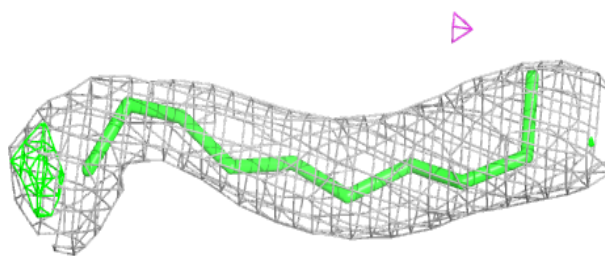


**Electron density around LFA D 415:**

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

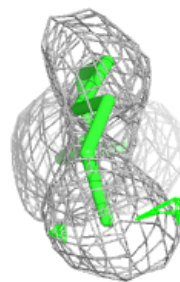
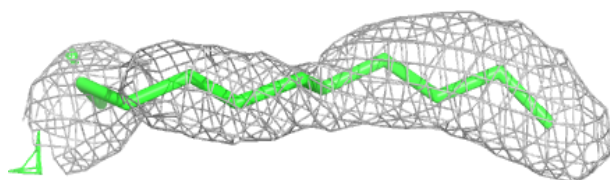
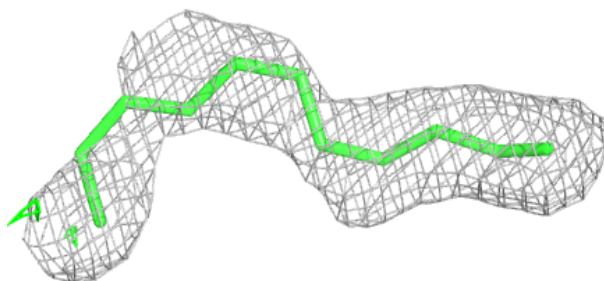
**Electron density around LFA D 406:**

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

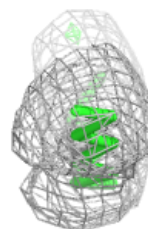
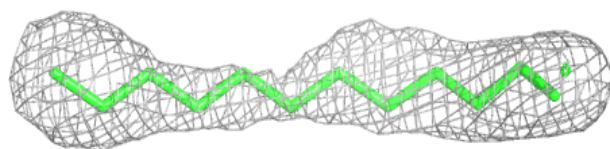
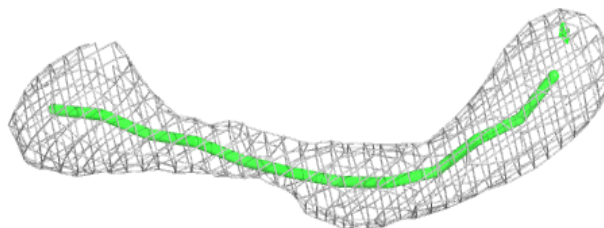


**Electron density around LFA D 414:**

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

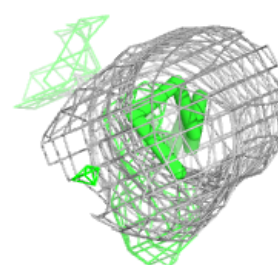
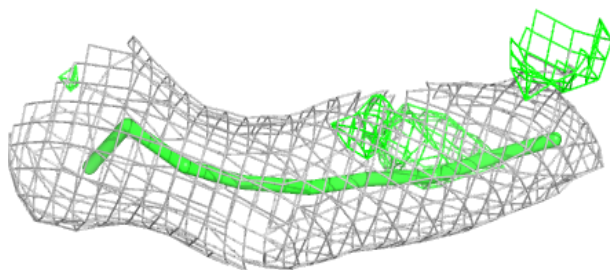
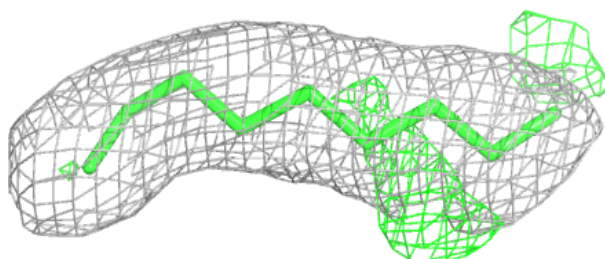
**Electron density around LFA D 403:**

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

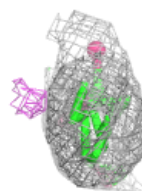
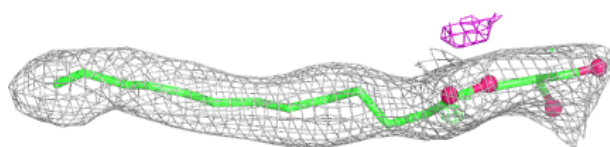
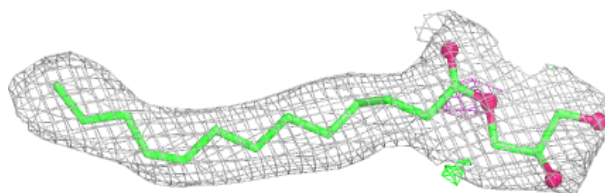


**Electron density around LFA D 409:**

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

**Electron density around OLC C 501:**

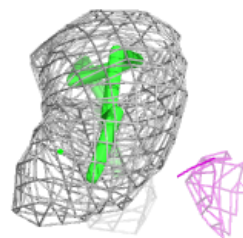
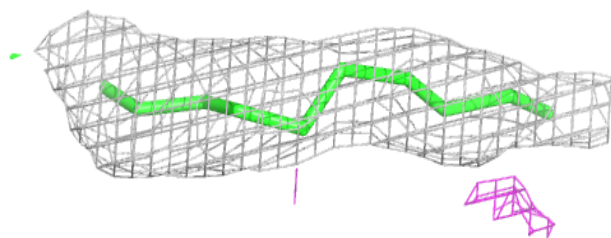
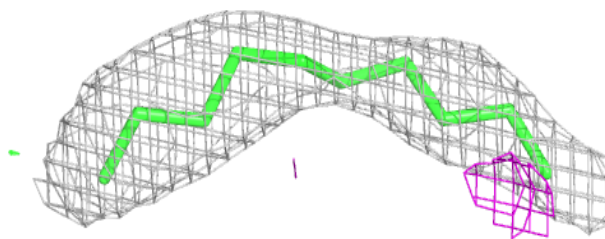
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



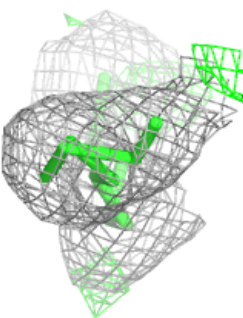
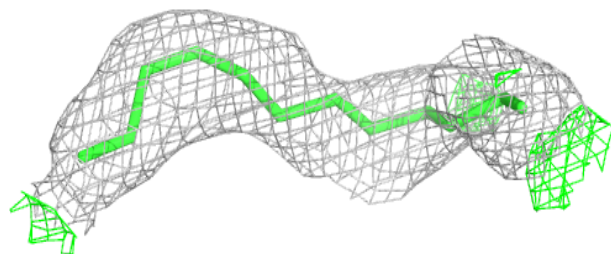
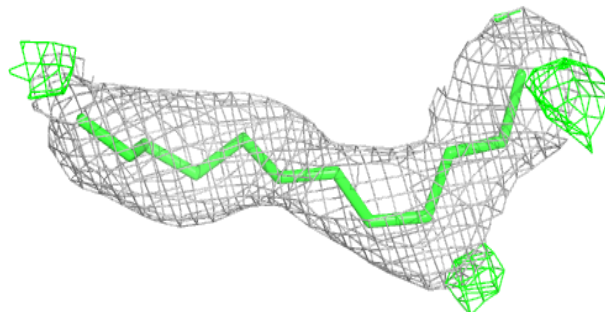


**Electron density around LFA E 507:**

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

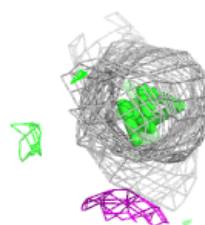
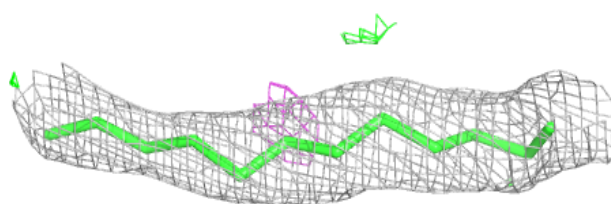
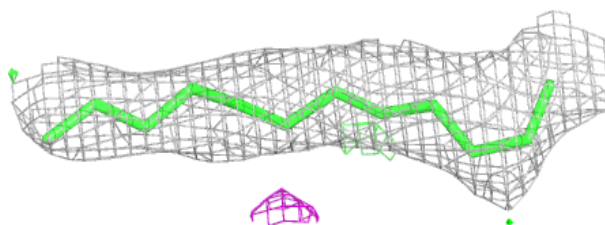
**Electron density around LFA B 510:**

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

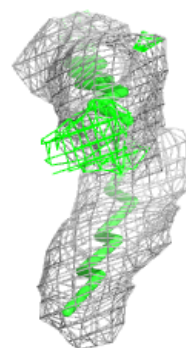
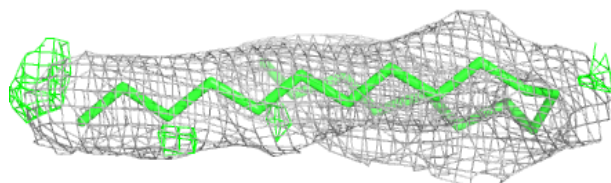
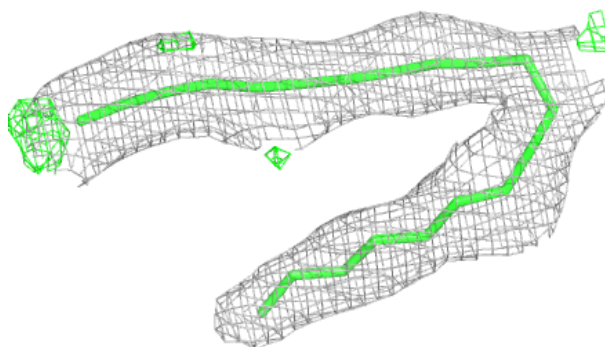


**Electron density around LFA B 513:**

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

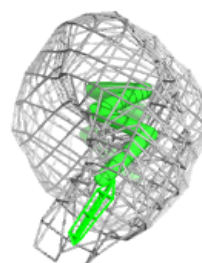
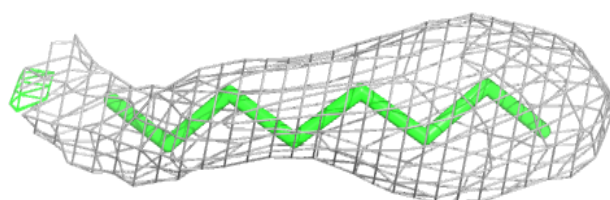
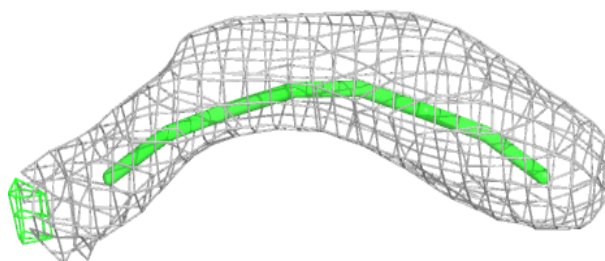
**Electron density around LFA D 416:**

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

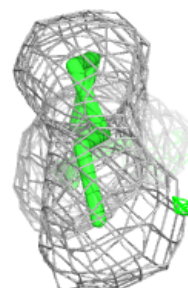
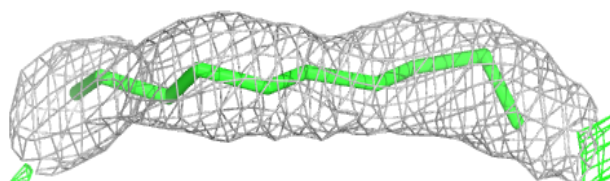
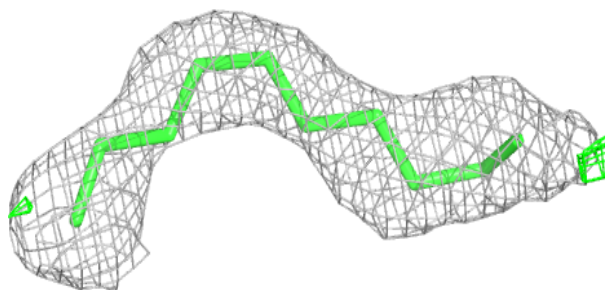


**Electron density around LFA G 405:**

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

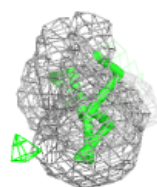
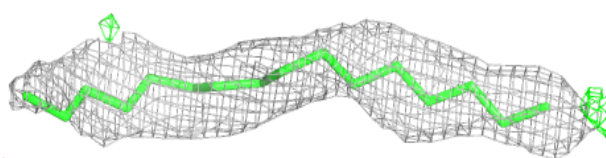
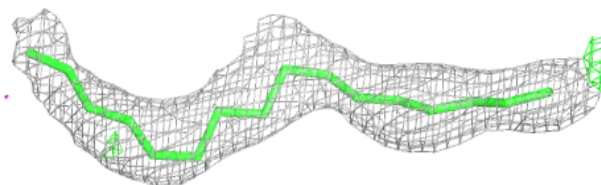
**Electron density around LFA E 503:**

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

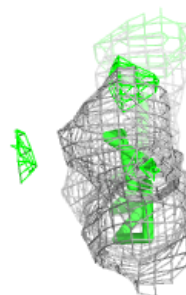
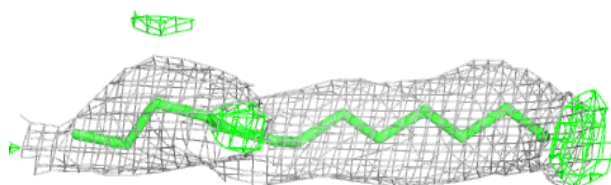
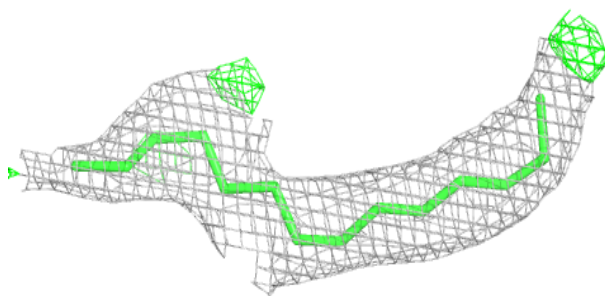


**Electron density around LFA B 508:**

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

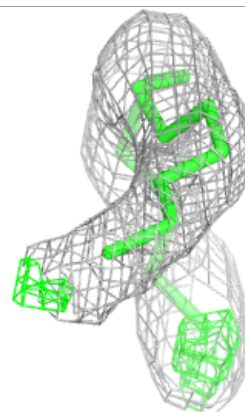
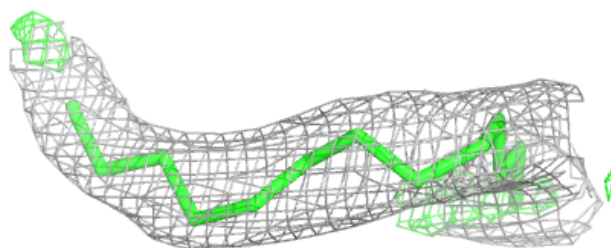
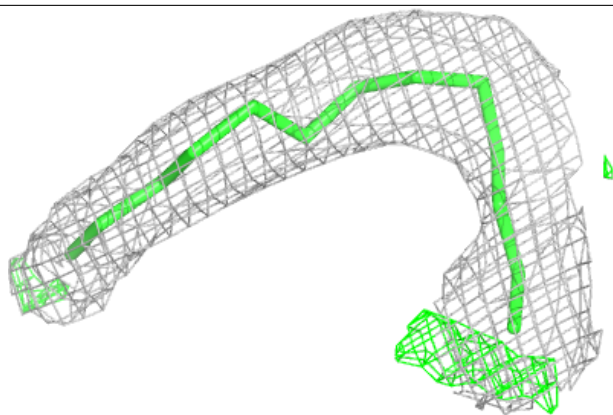
**Electron density around LFA G 411:**

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

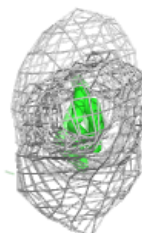
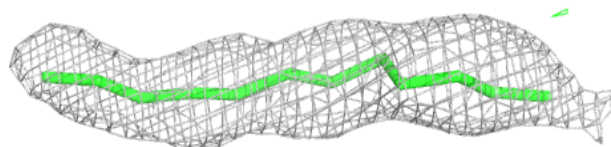
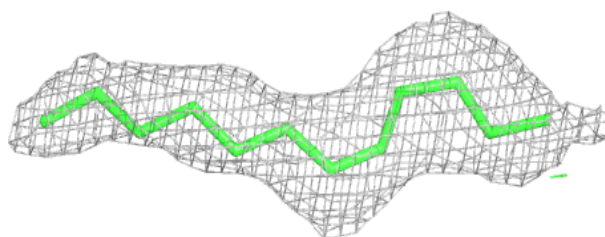


**Electron density around LFA A 504:**

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

**Electron density around LFA F 514:**

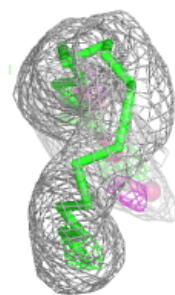
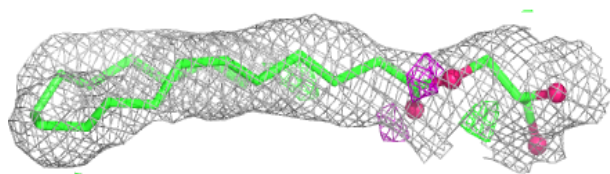
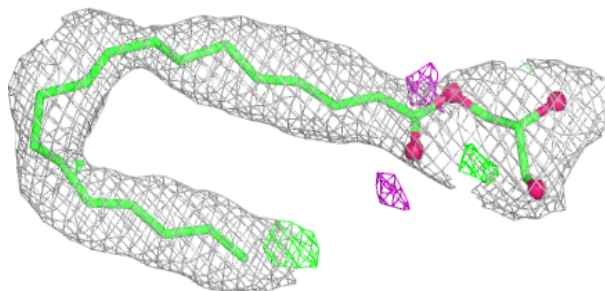
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



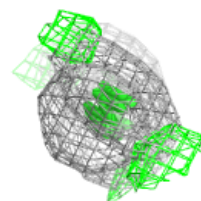
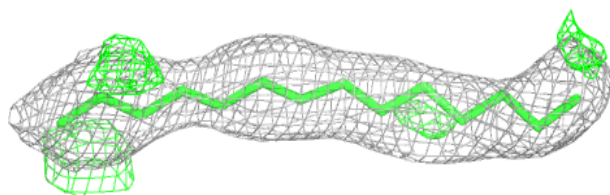
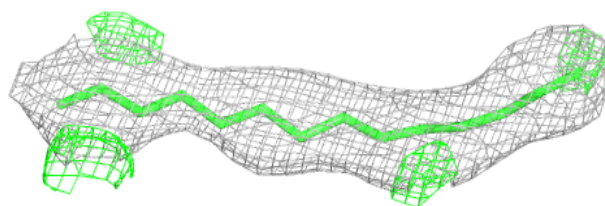


**Electron density around OLC H 501:**

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

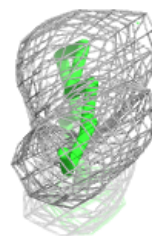
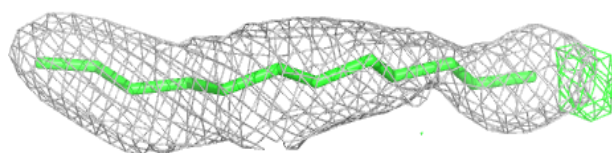
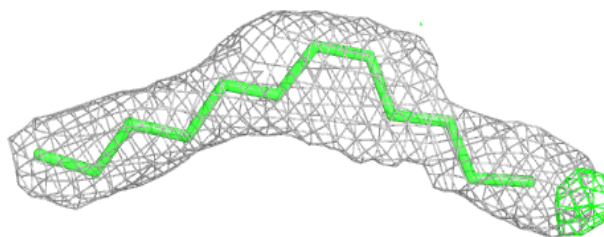
**Electron density around LFA G 402:**

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

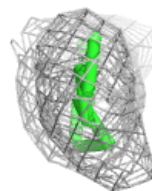
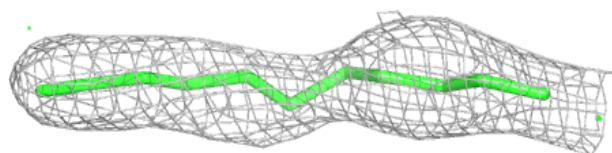
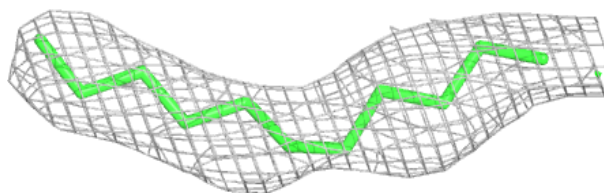


**Electron density around LFA B 504:**

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

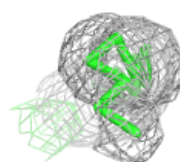
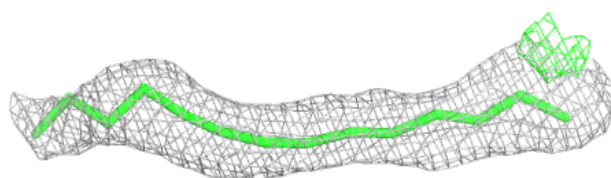
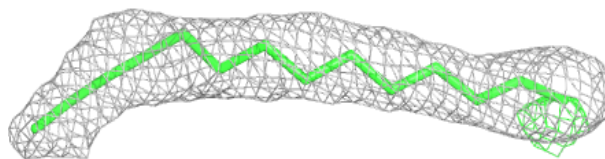
**Electron density around LFA F 506:**

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

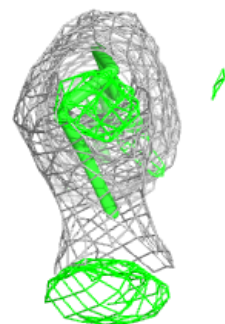
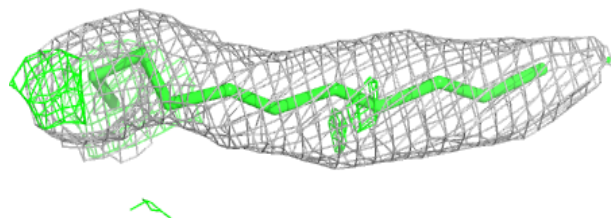
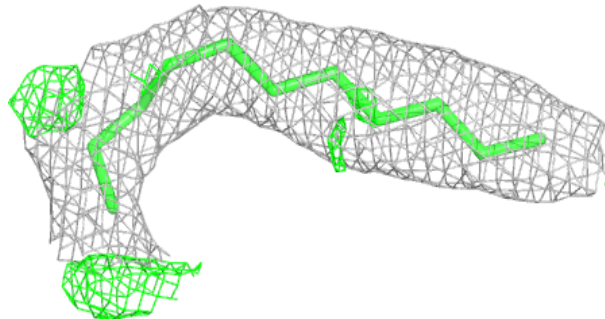


**Electron density around LFA E 511:**

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

**Electron density around LFA A 506:**

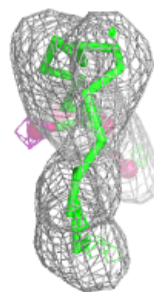
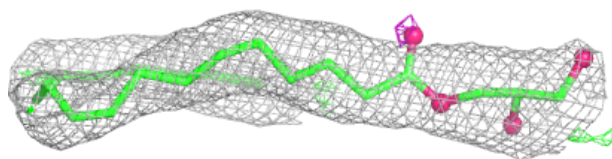
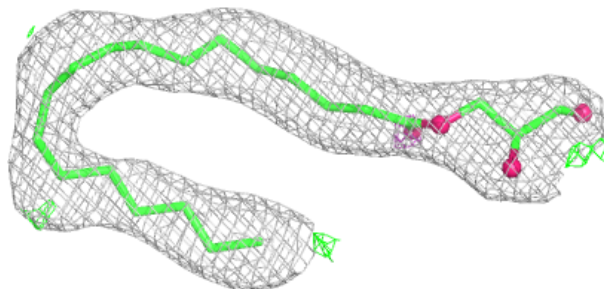
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



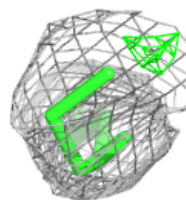
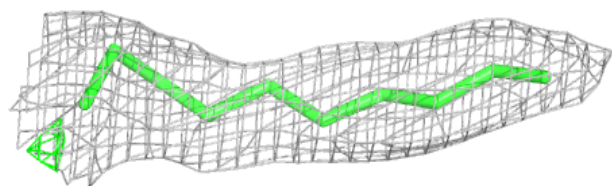
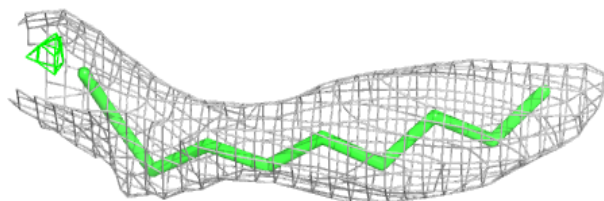


**Electron density around OLC B 501:**

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

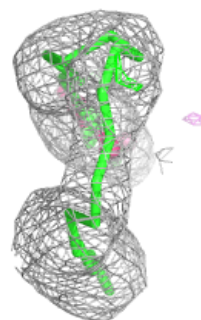
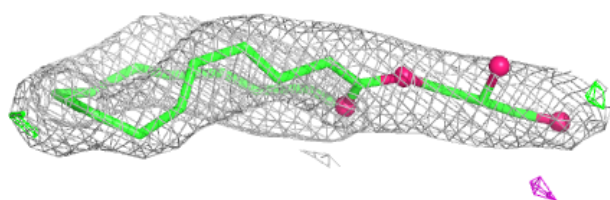
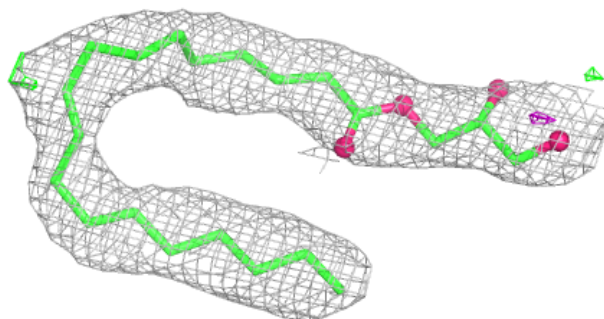
**Electron density around LFA E 504:**

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

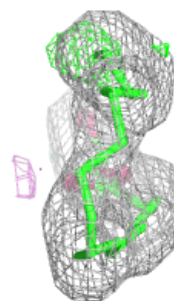
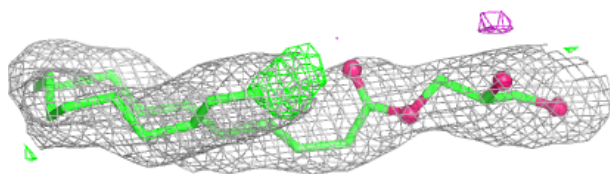
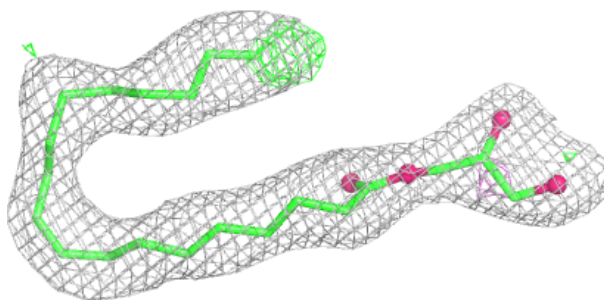


**Electron density around OLC E 518:**

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

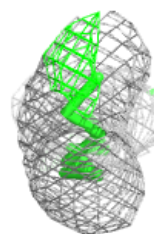
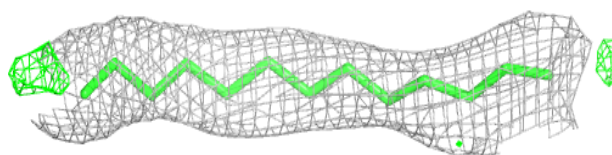
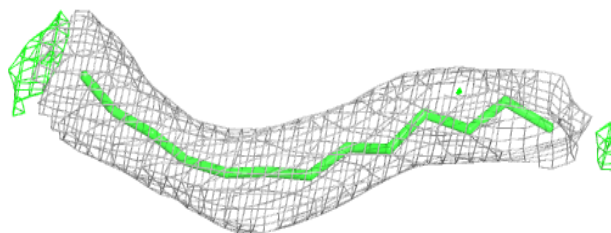
**Electron density around OLC F 501:**

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

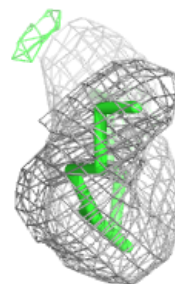
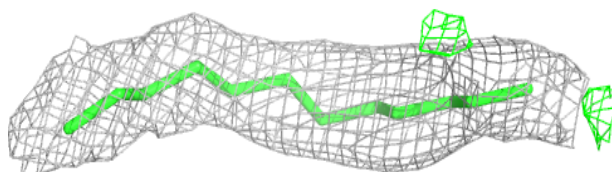
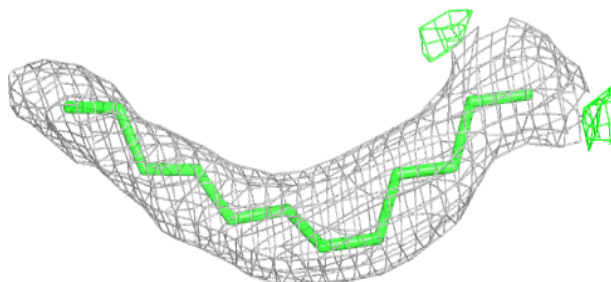


**Electron density around LFA B 503:**

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

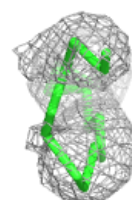
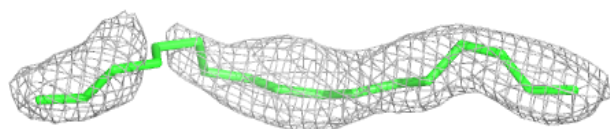
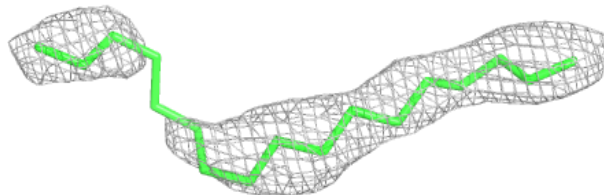
**Electron density around LFA G 413:**

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

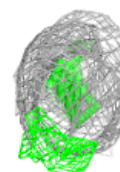
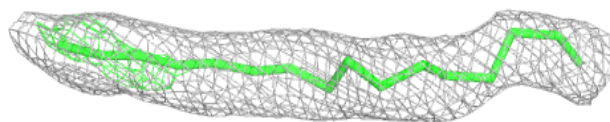
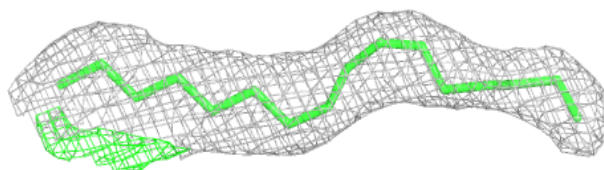


**Electron density around LFA B 516:**

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

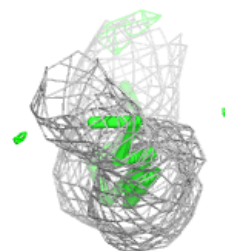
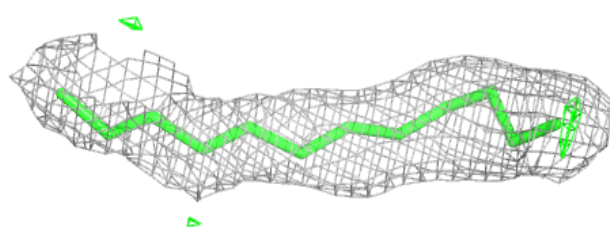
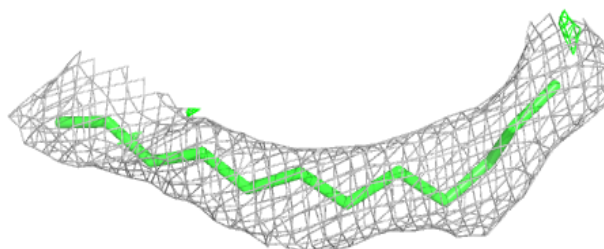
**Electron density around LFA A 510:**

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

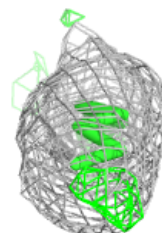
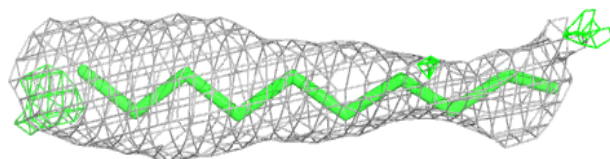
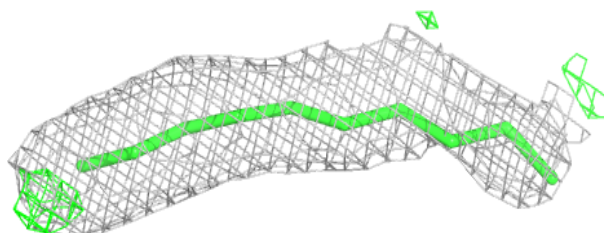


**Electron density around LFA H 510:**

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

**Electron density around LFA F 511:**

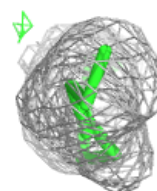
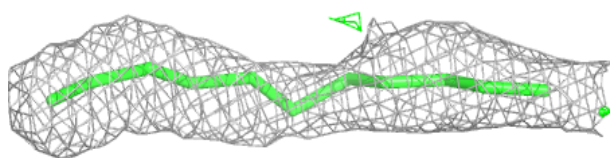
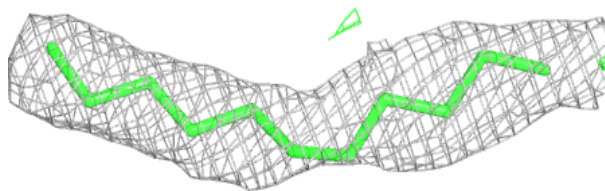
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



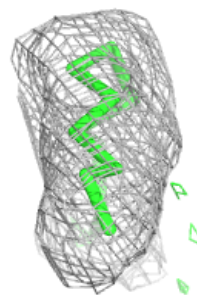
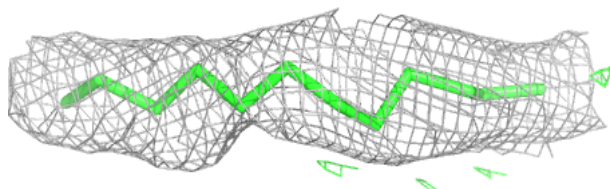
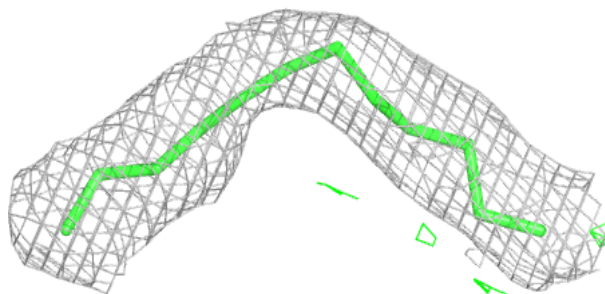


**Electron density around LFA A 509:**

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

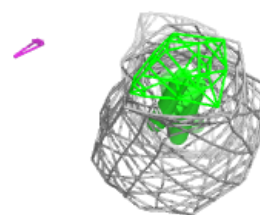
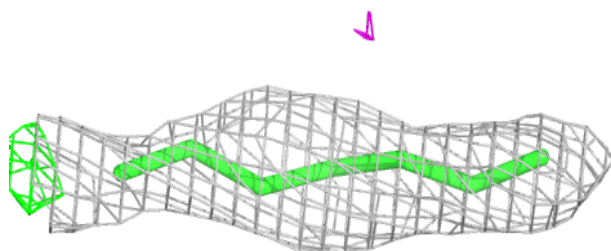
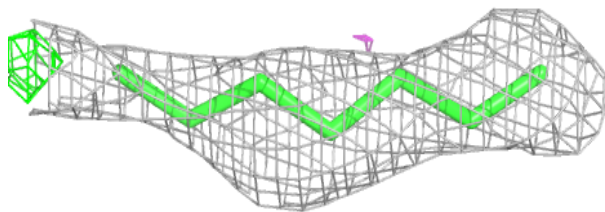
**Electron density around LFA B 517:**

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

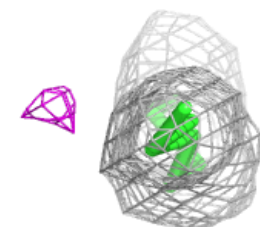
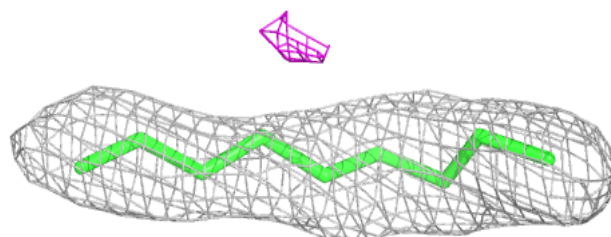
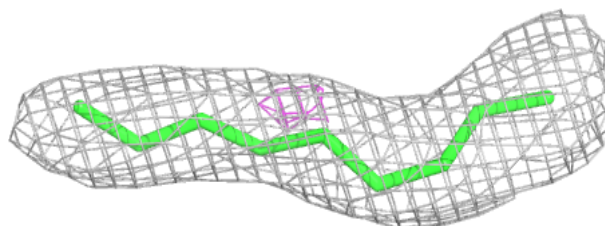


**Electron density around LFA H 508:**

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

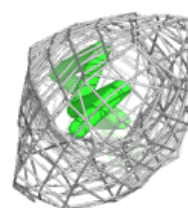
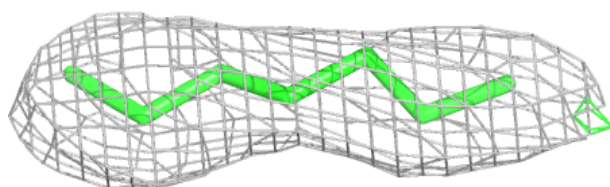
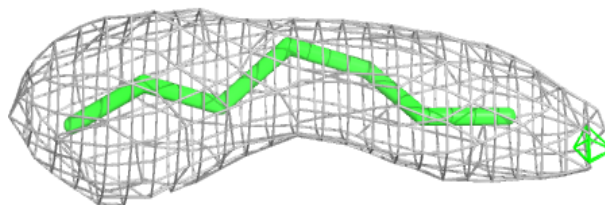
**Electron density around LFA B 509:**

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

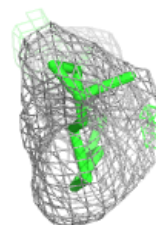
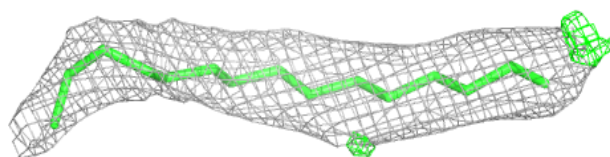
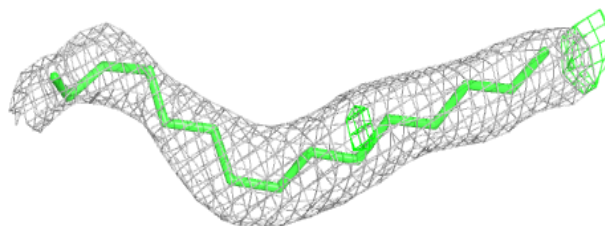


**Electron density around LFA C 507:**

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

**Electron density around LFA G 414:**

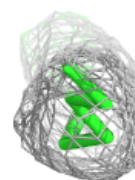
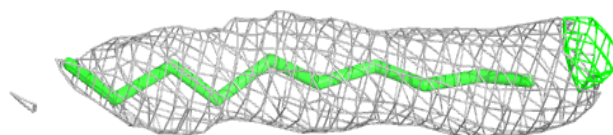
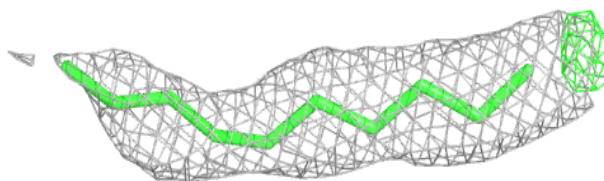
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



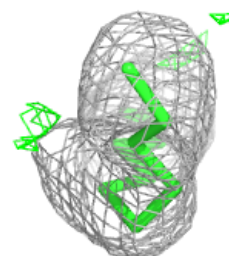
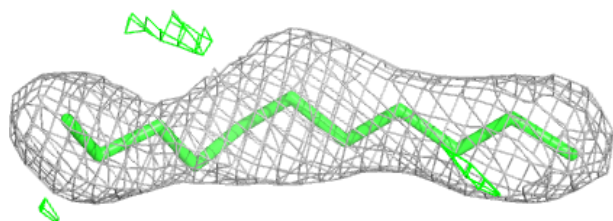
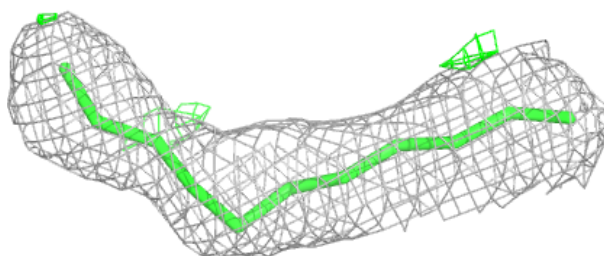


**Electron density around LFA D 412:**

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

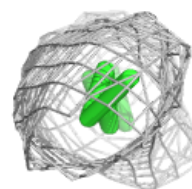
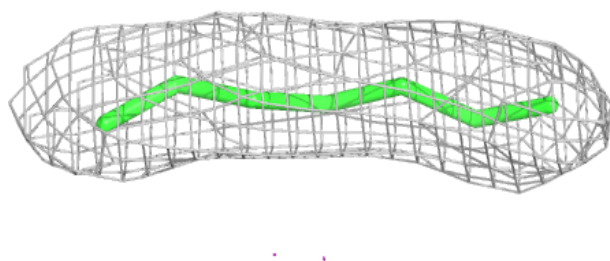
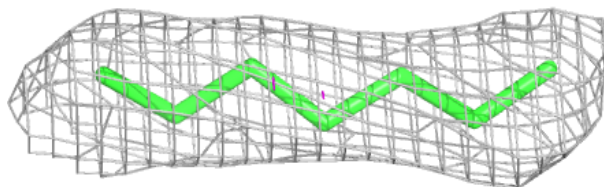
**Electron density around LFA E 513:**

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

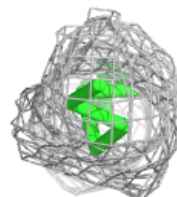
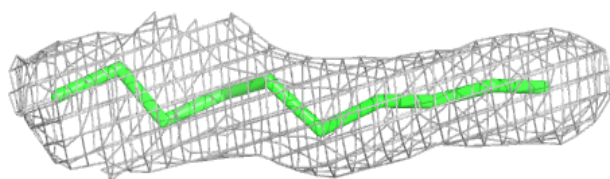
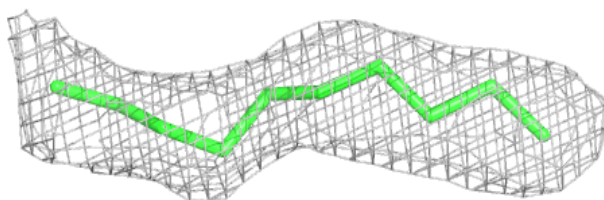


**Electron density around LFA A 512:**

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

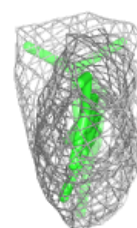
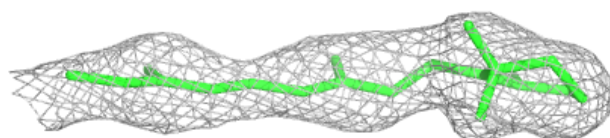
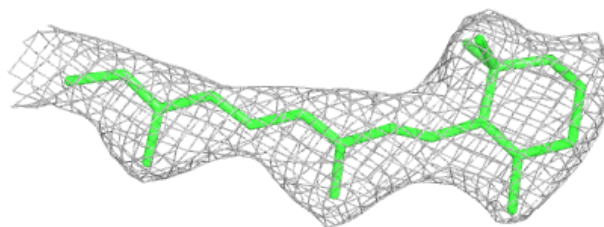
**Electron density around LFA D 411:**

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

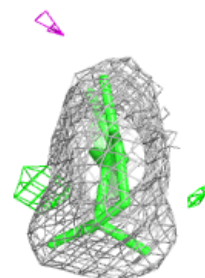
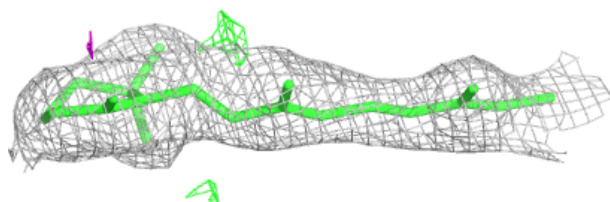
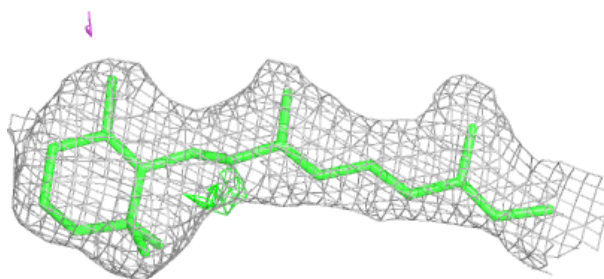


**Electron density around RET H 514:**

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

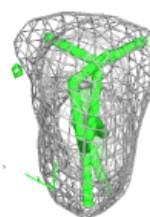
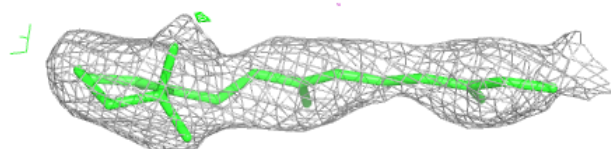
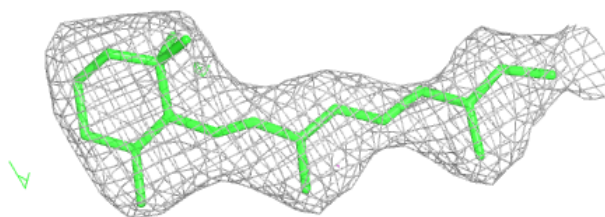
**Electron density around RET C 515:**

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

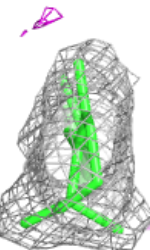
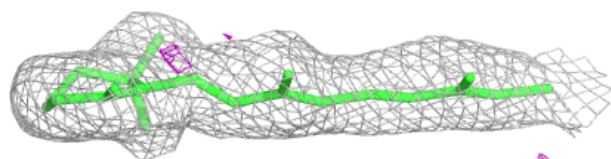
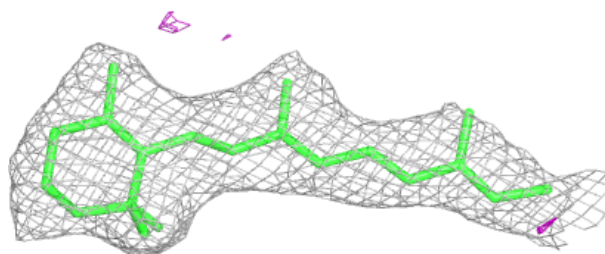


**Electron density around RET D 417:**

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

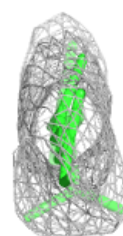
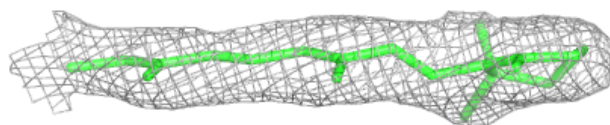
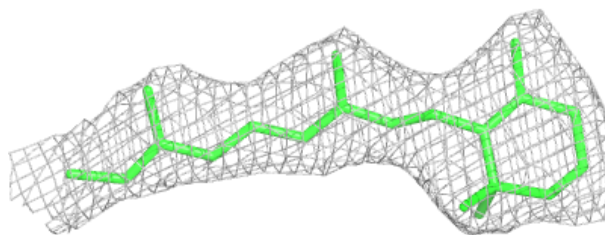
**Electron density around RET F 516:**

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

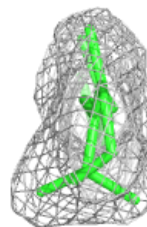
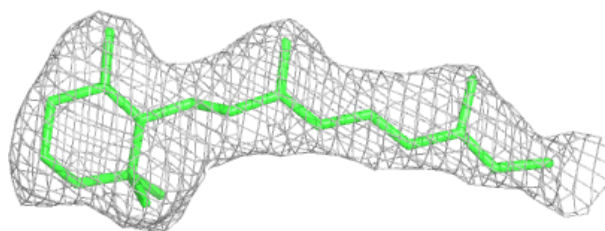


**Electron density around RET E 517:**

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

**Electron density around RET A 518:**

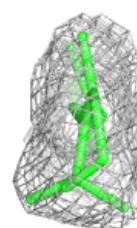
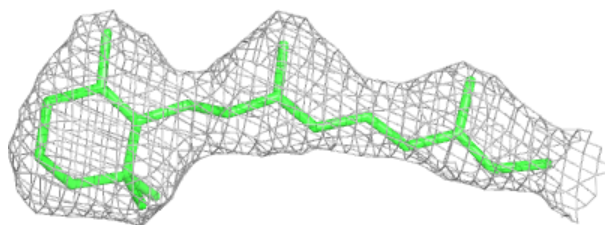
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



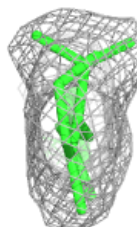
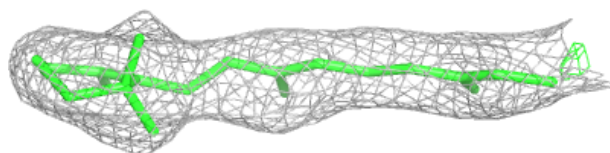
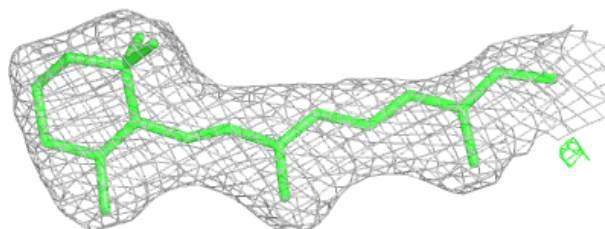


**Electron density around RET G 419:**

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

**Electron density around RET B 518:**

$2mF_o-DF_c$  (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.