



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2024 – 01:45 am GMT

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

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

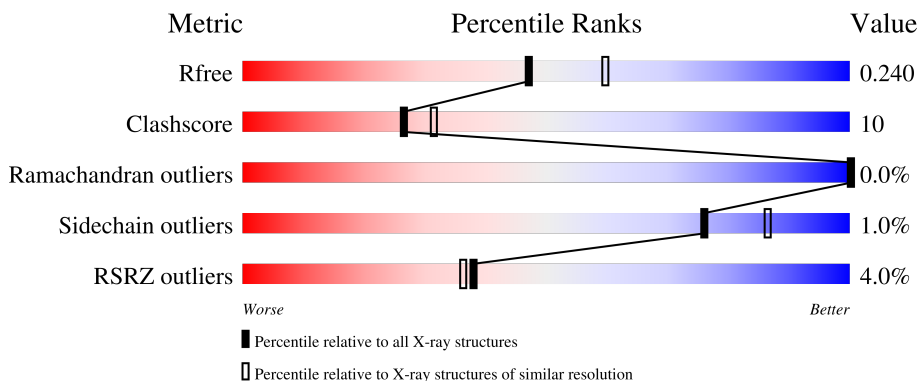
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	288	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2%      81%      14%      • 5%</p>
1	B	288	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">6%      74%      19%      • 6%</p>
1	C	288	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2%      80%      14%      6%</p>
1	D	288	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3%      82%      11%      • 6%</p>
1	E	288	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3%      78%      16%      • 6%</p>

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Mol	Chain	Length	Quality of chain
1	F	288	
1	G	288	
1	H	288	
1	I	288	
1	J	288	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LFA	A	311	-	-	-	X
3	LFA	C	306	-	-	-	X
3	LFA	D	302	-	-	-	X
3	LFA	F	302	-	-	-	X
3	LFA	G	302	-	-	-	X
3	LFA	G	307	-	-	-	X
3	LFA	J	302	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23361 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Sodium pumping rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	273	Total 2174	C 1458	N 329	O 378	S 9	0	0	0
1	B	270	Total 2158	C 1449	N 324	O 376	S 9	0	1	0
1	C	271	Total 2170	C 1457	N 326	O 378	S 9	0	2	0
1	D	271	Total 2161	C 1449	N 326	O 377	S 9	0	0	0
1	E	272	Total 2166	C 1451	N 326	O 380	S 9	0	0	0
1	F	271	Total 2166	C 1454	N 326	O 377	S 9	0	1	0
1	G	271	Total 2178	C 1462	N 328	O 379	S 9	0	3	0
1	H	273	Total 2186	C 1464	N 331	O 382	S 9	0	1	0
1	I	271	Total 2152	C 1444	N 322	O 377	S 9	0	0	0
1	J	272	Total 2175	C 1458	N 328	O 380	S 9	0	2	0

There are 80 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

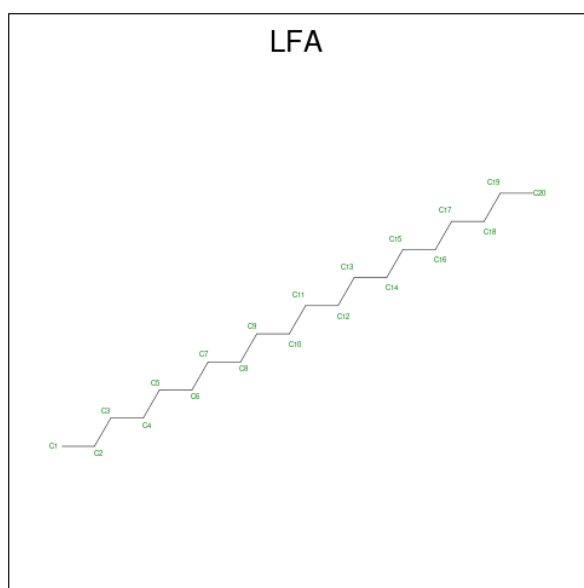
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0

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

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



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

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

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

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

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

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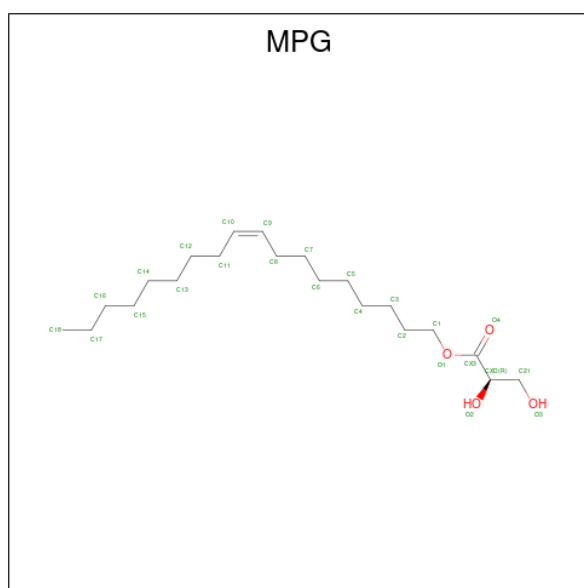
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C 14 14	0	0
3	H	1	Total C 8 8	0	0
3	H	1	Total C 5 5	0	0
3	H	1	Total C 8 8	0	0
3	H	1	Total C 7 7	0	0
3	H	1	Total C 6 6	0	0
3	I	1	Total C 7 7	0	0
3	I	1	Total C 7 7	0	0
3	I	1	Total C 14 14	0	0
3	I	1	Total C 6 6	0	0
3	I	1	Total C 10 10	0	0
3	I	1	Total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

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

- Molecule 4 is [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (three-letter code: MPG) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



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

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

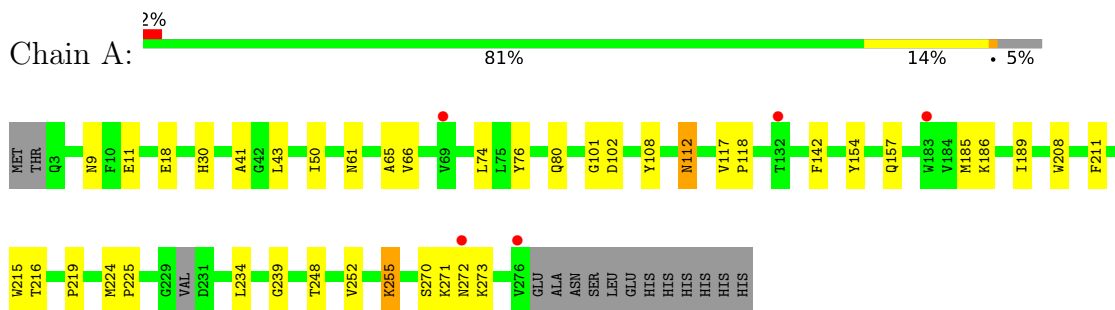
- Molecule 5 is water.

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

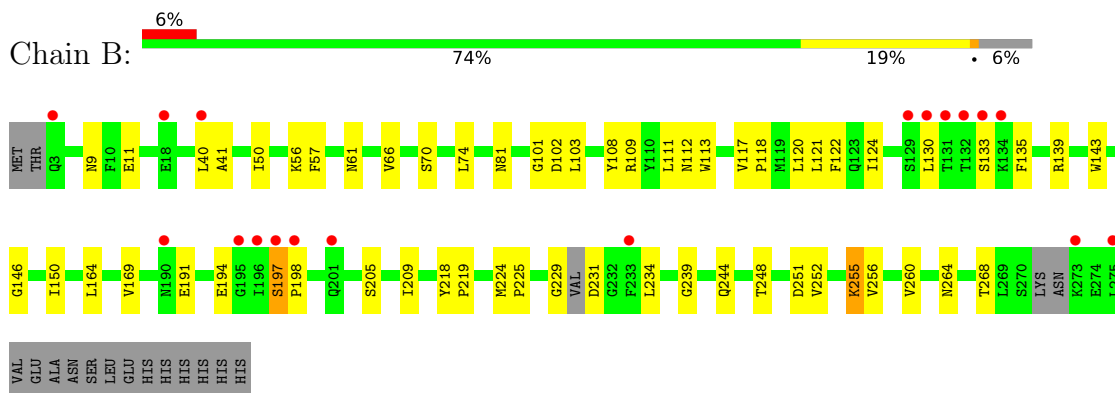
### 3 Residue-property plots [i](#)

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

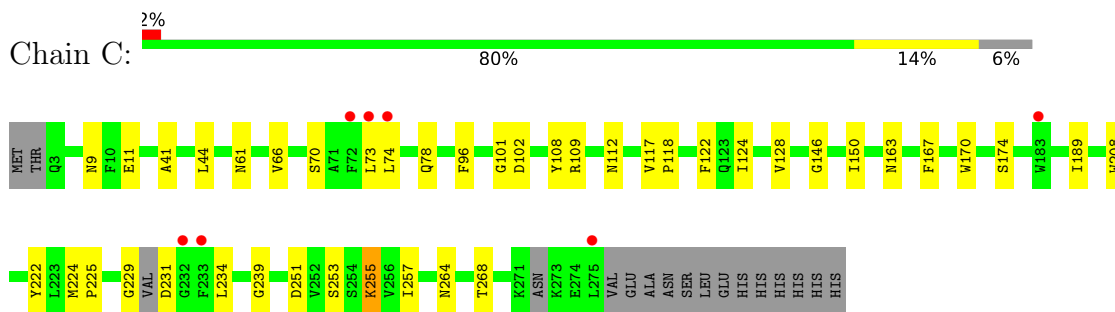
- Molecule 1: Sodium pumping rhodopsin



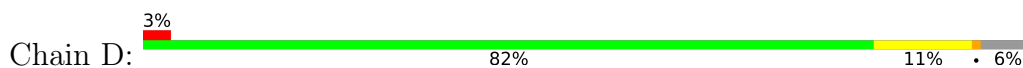
- Molecule 1: Sodium pumping rhodopsin

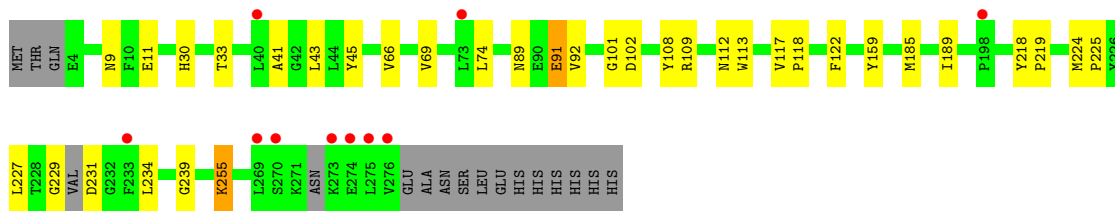


- Molecule 1: Sodium pumping rhodopsin

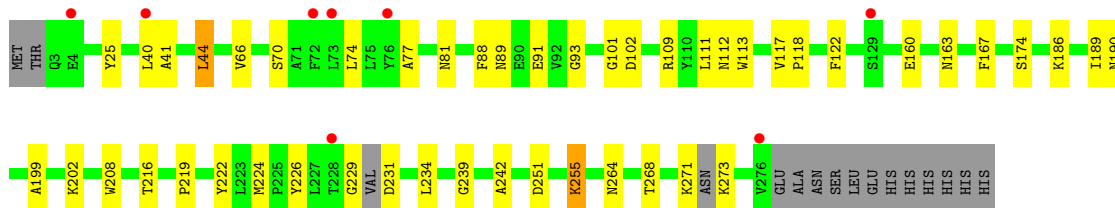
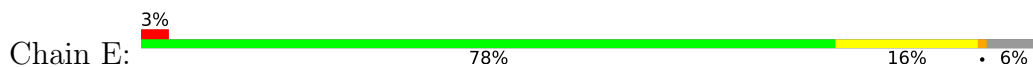


- Molecule 1: Sodium pumping rhodopsin

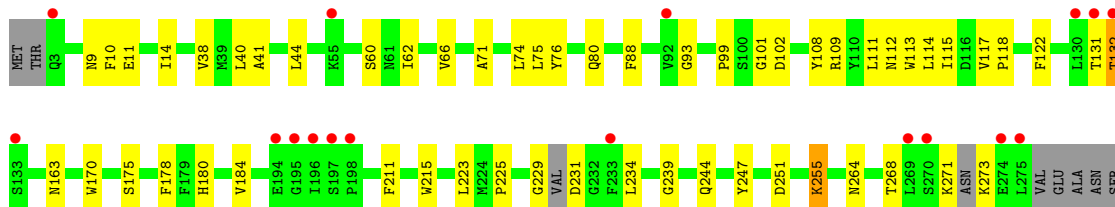
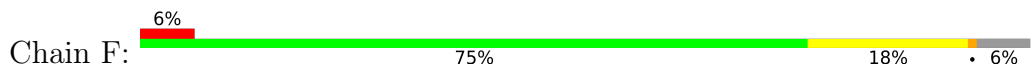




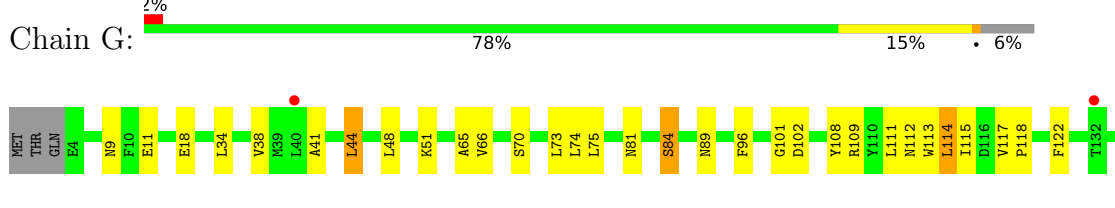
• Molecule 1: Sodium pumping rhodopsin



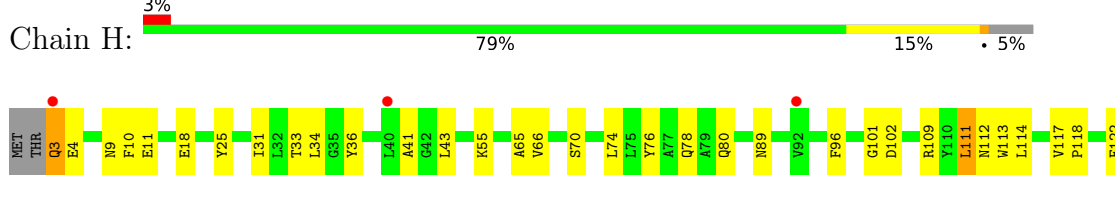
• Molecule 1: Sodium pumping rhodopsin



• Molecule 1: Sodium pumping rhodopsin



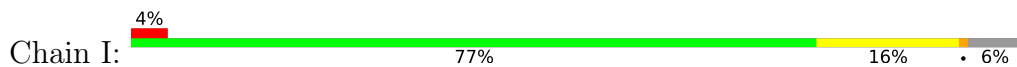
• Molecule 1: Sodium pumping rhodopsin



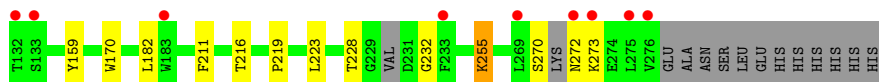
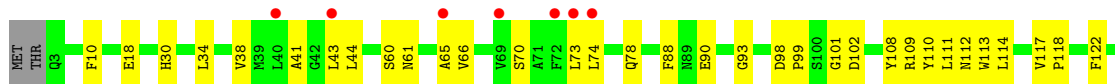
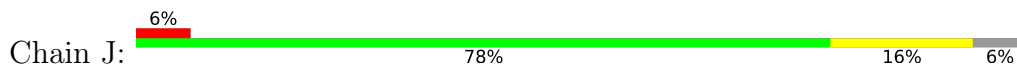




• Molecule 1: Sodium pumping rhodopsin



• Molecule 1: Sodium pumping rhodopsin



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.69Å 107.00Å 240.80Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	48.90 – 2.20 48.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.90-2.20) 96.2 (48.89-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.195 , 0.236 0.203 , 0.240	Depositor DCC
$R_{free}$ test set	9797 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtrriage
Anisotropy	0.359	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 61.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	23361	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LYR, MPG, LFA, NA

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	0.29	0/2201	0.43	0/2990
1	B	0.28	0/2187	0.42	0/2972
1	C	0.29	0/2202	0.43	0/2992
1	D	0.30	0/2187	0.42	0/2970
1	E	0.29	0/2191	0.44	0/2976
1	F	0.29	0/2195	0.42	0/2982
1	G	0.29	0/2213	0.43	0/3007
1	H	0.30	0/2215	0.43	0/3008
1	I	0.30	0/2178	0.43	0/2963
1	J	0.29	0/2207	0.44	0/3000
All	All	0.29	0/21976	0.43	0/29860

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2174	0	2164	32	0
1	B	2158	0	2144	53	0
1	C	2170	0	2156	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2161	0	2145	34	0
1	E	2166	0	2140	67	0
1	F	2166	0	2155	60	0
1	G	2178	0	2174	58	0
1	H	2186	0	2177	51	0
1	I	2152	0	2117	52	0
1	J	2175	0	2156	49	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	108	0	199	3	0
3	B	108	0	200	3	0
3	C	110	0	206	6	0
3	D	138	0	260	10	0
3	E	112	0	204	9	0
3	F	129	0	245	7	0
3	G	133	0	250	5	0
3	H	111	0	208	2	0
3	I	117	0	219	7	0
3	J	109	0	205	5	0
4	A	14	0	19	0	0
4	B	14	0	19	0	0
4	C	13	0	17	1	0
4	D	14	0	19	1	0
4	E	14	0	19	3	0
4	F	14	0	19	1	0
4	G	14	0	19	2	0
4	H	14	0	19	0	0
4	I	14	0	19	0	0
4	J	14	0	19	2	0
5	A	39	0	0	3	0
5	B	30	0	0	2	0
5	C	31	0	0	1	0
5	D	34	0	0	0	0
5	E	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	30	0	0	3	0
5	G	35	0	0	3	0
5	H	45	0	0	6	0
5	I	40	0	0	3	0
5	J	37	0	0	6	0
All	All	23361	0	23912	482	0

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

All (482) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74[B]:LEU:CD2	1:C:112[B]:ASN:CB	1.81	1.56
1:C:74[B]:LEU:CD2	1:C:112[B]:ASN:HB2	1.03	1.48
1:F:74[B]:LEU:CD2	1:F:112:ASN:HB2	1.41	1.48
1:C:74[B]:LEU:HD22	1:C:112[B]:ASN:CG	1.32	1.43
1:G:74[B]:LEU:CD1	1:G:112[B]:ASN:ND2	1.78	1.28
1:H:271:LYS:C	1:H:272:ASN:CA	2.10	1.20
1:C:74[B]:LEU:HD22	1:C:112[B]:ASN:CB	1.54	1.20
1:B:74[A]:LEU:HD11	1:B:108:TYR:O	1.43	1.17
1:G:74[B]:LEU:HD13	1:G:112[B]:ASN:ND2	1.39	1.17
1:G:74[B]:LEU:CD1	1:G:112[B]:ASN:HD21	1.48	1.15
1:F:74[B]:LEU:HD21	1:F:108:TYR:O	1.47	1.13
1:C:74[B]:LEU:HD21	1:C:112[B]:ASN:HB2	1.25	1.12
1:H:271:LYS:O	1:H:272:ASN:CA	1.98	1.12
1:B:74[A]:LEU:HD13	1:B:112:ASN:HB2	1.14	1.11
1:F:74[B]:LEU:HD23	1:F:112:ASN:CB	1.81	1.09
1:F:74[B]:LEU:HD11	1:F:108:TYR:HB3	1.29	1.08
1:F:74[B]:LEU:CD2	1:F:112:ASN:CB	2.32	1.08
1:F:74[B]:LEU:HD22	1:F:112:ASN:HB2	1.19	1.07
1:F:74[B]:LEU:HD23	1:F:112:ASN:HB2	1.16	1.06
1:B:74[A]:LEU:HD11	1:B:108:TYR:C	1.75	1.06
1:E:74:LEU:HD13	1:E:112:ASN:HB2	1.35	1.06
1:B:74[B]:LEU:HD23	1:B:112:ASN:HB2	1.37	1.05
1:G:74[B]:LEU:HD11	1:G:112[B]:ASN:ND2	1.69	1.03
3:C:306:LFA:C16	3:D:302:LFA:H11	1.89	1.01
1:B:219:PRO:HG3	1:B:255:LYR:H132	1.43	1.01
1:E:163:ASN:ND2	4:E:313:MPG:O3	1.93	0.99
1:B:74[A]:LEU:CD1	1:B:108:TYR:O	2.10	0.98
1:J:112[B]:ASN:ND2	5:J:429:HOH:O	1.97	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:81[B]:ASN:ND2	5:G:415:HOH:O	1.97	0.96
1:C:44:LEU:HD12	1:D:69:VAL:HG21	1.48	0.96
1:H:271:LYS:C	1:H:272:ASN:CB	2.34	0.95
1:H:271:LYS:C	1:H:272:ASN:HB2	1.87	0.95
1:C:74[B]:LEU:CD2	1:C:112[B]:ASN:CG	2.22	0.93
1:C:74[B]:LEU:HD22	1:C:112[B]:ASN:ND2	1.85	0.91
3:C:306:LFA:C16	3:D:302:LFA:C1	2.49	0.90
1:H:18:GLU:OE2	5:H:432:HOH:O	1.90	0.89
1:C:74[B]:LEU:HD23	1:C:112[B]:ASN:HB2	0.89	0.89
1:B:74[A]:LEU:HD13	1:B:112:ASN:CB	2.01	0.88
1:E:163:ASN:HD22	4:E:313:MPG:H3	1.16	0.88
1:B:255:LYR:H9	1:B:255:LYR:H183	1.53	0.88
1:F:74[B]:LEU:CD2	1:F:108:TYR:O	2.23	0.87
1:C:74[B]:LEU:HD23	1:C:112[B]:ASN:CB	1.72	0.87
1:B:74[B]:LEU:CD2	1:B:112:ASN:HB2	2.05	0.86
1:B:197:SER:HB2	1:B:198:PRO:HD2	1.58	0.86
1:E:74:LEU:CD1	1:E:112:ASN:HB2	2.05	0.86
1:G:74[B]:LEU:HD11	1:G:112[B]:ASN:HD21	1.28	0.85
3:D:316:LFA:H12	3:D:317:LFA:H12	1.60	0.83
1:E:74:LEU:HD13	1:E:112:ASN:CB	2.09	0.83
1:B:74[A]:LEU:CD1	1:B:112:ASN:HB2	2.05	0.82
1:C:44:LEU:HD12	1:D:69:VAL:CG2	2.09	0.82
3:E:304:LFA:C3	3:E:305:LFA:C3	2.59	0.81
1:F:255:LYR:H9	1:F:255:LYR:H183	1.62	0.81
1:E:255:LYR:H9	1:E:255:LYR:H183	1.62	0.80
1:G:255:LYR:H9	1:G:255:LYR:H183	1.64	0.80
1:H:74:LEU:HD22	5:H:431:HOH:O	1.82	0.80
1:C:255:LYR:H9	1:C:255:LYR:H183	1.65	0.79
1:I:255:LYR:H9	1:I:255:LYR:H183	1.65	0.79
1:J:18:GLU:OE2	5:J:428:HOH:O	2.02	0.78
1:B:197:SER:HB2	1:B:198:PRO:CD	2.15	0.77
1:G:74[B]:LEU:HD11	1:G:112[B]:ASN:OD1	1.84	0.77
1:J:74[A]:LEU:HD13	1:J:112[A]:ASN:HB2	1.67	0.77
1:C:74[A]:LEU:HD21	1:C:109:ARG:HA	1.66	0.76
1:J:255:LYR:H9	1:J:255:LYR:H183	1.68	0.76
1:D:74:LEU:HD13	1:D:112:ASN:HB2	1.68	0.76
1:I:271:LYS:O	1:I:273:LYS:N	2.18	0.75
1:G:18:GLU:OE2	5:G:426:HOH:O	2.03	0.75
1:F:74[B]:LEU:HD21	1:F:108:TYR:C	2.06	0.75
1:J:270:SER:C	1:J:272:ASN:HB3	2.07	0.74
1:G:74[A]:LEU:HD11	1:G:108:TYR:C	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:302:LFA:H11	3:J:302:LFA:C16	2.18	0.74
1:A:255:LYR:H9	1:A:255:LYR:H183	1.70	0.74
3:D:302:LFA:C7	3:E:311:LFA:C8	2.65	0.73
1:G:273:LYS:O	5:G:433:HOH:O	2.07	0.73
1:A:101:GLY:O	1:A:102:ASP:HB2	1.90	0.72
1:F:74[B]:LEU:CD1	1:F:108:TYR:HB3	2.15	0.71
1:E:224:MET:HE3	1:E:234:LEU:HD22	1.72	0.71
1:I:224:MET:CE	1:I:234:LEU:HD13	2.21	0.71
1:J:18:GLU:OE1	5:J:427:HOH:O	2.08	0.70
1:D:255:LYR:H9	1:D:255:LYR:H183	1.72	0.70
5:H:433:HOH:O	1:I:108:TYR:CE2	2.43	0.70
1:D:101:GLY:O	1:D:102:ASP:HB2	1.90	0.70
1:E:74:LEU:CD1	1:E:112:ASN:CB	2.70	0.70
1:B:101:GLY:O	1:B:102:ASP:HB2	1.92	0.70
1:H:255:LYR:H183	1:H:255:LYR:H9	1.71	0.70
1:F:271:LYS:O	1:F:273:LYS:N	2.25	0.70
3:F:311:LFA:H61	3:F:312:LFA:C2	2.22	0.69
1:J:101:GLY:O	1:J:102:ASP:HB2	1.92	0.69
1:H:70:SER:OG	1:H:112[B]:ASN:OD1	2.09	0.69
1:E:89:ASN:HD21	1:G:89:ASN:HD21	1.41	0.69
1:G:74[A]:LEU:HD11	1:G:109:ARG:HA	1.74	0.69
1:H:101:GLY:O	1:H:102:ASP:HB2	1.91	0.69
1:B:70:SER:OG	1:B:112:ASN:ND2	2.26	0.69
1:G:74[A]:LEU:HD13	1:G:112[A]:ASN:HB2	1.74	0.69
1:B:255:LYR:H183	1:B:255:LYR:C9	2.23	0.69
1:F:113:TRP:CD1	1:F:255:LYR:HC2	2.28	0.69
1:H:74:LEU:CD2	5:H:431:HOH:O	2.37	0.68
1:D:41:ALA:HB1	1:E:66:VAL:HG13	1.76	0.68
1:B:74[B]:LEU:HD23	1:B:112:ASN:CB	2.21	0.68
1:C:74[B]:LEU:HD21	1:C:112[B]:ASN:CB	1.98	0.68
1:E:109:ARG:NH2	1:E:251:ASP:OD2	2.26	0.68
1:G:74[A]:LEU:HD13	1:G:112[A]:ASN:CB	2.24	0.68
1:I:101:GLY:O	5:I:416:HOH:O	2.10	0.68
1:J:74[A]:LEU:HD11	1:J:108:TYR:C	2.14	0.68
1:B:244:GLN:HG2	5:B:414:HOH:O	1.94	0.68
1:C:74[A]:LEU:HD13	1:C:112[A]:ASN:HB2	1.75	0.68
1:F:74[B]:LEU:HD11	1:F:108:TYR:CB	2.16	0.68
1:F:74[B]:LEU:HD22	1:F:112:ASN:CB	2.12	0.66
1:I:224:MET:HE1	1:I:234:LEU:HD13	1.77	0.66
1:G:74[A]:LEU:CD1	1:G:108:TYR:O	2.44	0.66
5:H:424:HOH:O	1:I:111:LEU:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:LEU:HD12	1:E:112:ASN:ND2	2.11	0.66
1:F:255:LYR:H183	1:F:255:LYR:C9	2.26	0.66
3:F:304:LFA:H61	3:J:304:LFA:H11	1.76	0.65
1:A:273:LYS:O	5:A:432:HOH:O	2.15	0.65
1:I:229:GLY:O	1:I:231:ASP:N	2.30	0.65
1:D:30:HIS:HB3	1:E:111:LEU:HD22	1.79	0.65
3:F:302:LFA:C1	3:J:302:LFA:C16	2.75	0.64
1:E:77:ALA:O	3:E:311:LFA:H21	1.98	0.64
1:B:50:ILE:HD13	1:B:61:ASN:HB3	1.79	0.64
1:G:9:ASN:HB3	1:G:11:GLU:OE1	1.97	0.64
1:D:89:ASN:HD21	1:H:89:ASN:HD21	1.45	0.64
1:F:264:ASN:O	1:F:268:THR:HG23	1.97	0.63
1:H:34:LEU:HD12	1:I:115:ILE:HD11	1.80	0.63
1:E:255:LYR:H183	1:E:255:LYR:C9	2.27	0.63
1:E:101:GLY:O	1:E:102:ASP:HB2	1.98	0.63
1:G:74[A]:LEU:HD11	1:G:109:ARG:N	2.13	0.63
1:I:267:ILE:HG21	1:I:275:LEU:HD23	1.81	0.62
1:E:224:MET:CE	1:E:234:LEU:HD13	2.29	0.62
1:G:44:LEU:HD11	1:H:43:LEU:HD11	1.82	0.62
1:I:163:ASN:HD21	3:I:306:LFA:H92	1.64	0.62
1:F:229:GLY:O	1:F:231:ASP:N	2.33	0.62
1:I:267:ILE:CG2	1:I:275:LEU:HD23	2.28	0.62
1:G:74[A]:LEU:HD11	1:G:109:ARG:CA	2.29	0.62
3:G:302:LFA:C16	3:G:303:LFA:H11	2.30	0.61
3:B:307:LFA:C16	3:C:302:LFA:H11	2.30	0.61
1:F:109:ARG:NH2	1:F:251:ASP:OD2	2.32	0.61
1:I:224:MET:HE3	1:I:234:LEU:HD22	1.82	0.61
1:J:255:LYR:H183	1:J:255:LYR:C9	2.30	0.61
1:I:255:LYR:H183	1:I:255:LYR:C9	2.30	0.61
1:A:65:ALA:HB1	1:E:44:LEU:CD1	2.31	0.61
1:B:229:GLY:O	1:B:231:ASP:N	2.33	0.61
1:C:255:LYR:H183	1:C:255:LYR:C9	2.31	0.61
3:C:306:LFA:C16	3:D:302:LFA:H12	2.31	0.60
1:B:74[B]:LEU:CD2	1:B:112:ASN:CB	2.78	0.60
1:G:101:GLY:O	1:G:102:ASP:HB2	2.02	0.60
1:E:113:TRP:CD1	1:E:255:LYR:HC2	2.36	0.60
1:A:41:ALA:HB1	1:B:66:VAL:HG13	1.82	0.60
1:B:219:PRO:HG3	1:B:255:LYR:C13	2.26	0.60
1:I:41:ALA:HB1	1:J:66:VAL:HG13	1.83	0.60
1:I:44:LEU:CD1	1:J:65:ALA:HB1	2.32	0.60
1:E:70:SER:OG	1:E:112:ASN:ND2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:VAL:HB	1:F:118:PRO:HD3	1.84	0.60
1:F:247:TYR:OH	5:F:407:HOH:O	2.16	0.60
1:C:101:GLY:O	1:C:102:ASP:HB2	2.02	0.59
1:C:44:LEU:HD11	1:D:43:LEU:HD11	1.84	0.59
1:B:117:VAL:HB	1:B:118:PRO:HD3	1.83	0.59
1:F:74[B]:LEU:HD21	1:F:109:ARG:HA	1.85	0.59
3:A:311:LFA:C1	3:D:306:LFA:C16	2.81	0.58
1:C:170:TRP:HE1	4:C:313:MPG:HX31	1.67	0.58
1:H:9:ASN:HB3	1:H:11:GLU:OE1	2.03	0.58
1:I:74:LEU:HD12	1:I:112:ASN:HA	1.84	0.58
1:E:264:ASN:O	1:E:268:THR:HG23	2.04	0.58
1:F:44:LEU:HD21	1:G:65:ALA:HB1	1.86	0.58
1:J:74[A]:LEU:CD1	1:J:108:TYR:O	2.52	0.57
1:E:271:LYS:O	1:E:273:LYS:N	2.38	0.57
1:E:224:MET:HE1	1:E:234:LEU:HD13	1.87	0.57
1:H:74:LEU:HD21	1:H:109:ARG:HA	1.86	0.57
1:A:255:LYR:H183	1:A:255:LYR:C9	2.35	0.57
1:C:74[A]:LEU:CD2	1:C:109:ARG:HA	2.33	0.57
1:G:74[A]:LEU:CD1	1:G:109:ARG:HA	2.33	0.57
1:G:74[B]:LEU:HD13	1:G:112[B]:ASN:HD21	1.14	0.57
1:C:9:ASN:HB3	1:C:11:GLU:OE1	2.05	0.56
1:F:74[A]:LEU:HD13	1:F:112:ASN:HB2	1.86	0.56
1:H:255:LYR:H183	1:H:255:LYR:C9	2.34	0.56
1:H:255:LYR:H9	1:H:255:LYR:H192	1.88	0.56
1:A:185:MET:O	1:A:189:ILE:HG12	2.06	0.56
1:D:255:LYR:H9	1:D:255:LYR:H192	1.88	0.56
1:G:109:ARG:NH2	1:G:251:ASP:OD2	2.38	0.56
1:E:189:ILE:HD13	1:E:208:TRP:HB2	1.88	0.56
1:E:229:GLY:O	1:E:231:ASP:N	2.39	0.56
1:E:224:MET:HE1	1:E:234:LEU:CD1	2.35	0.56
1:A:50:ILE:HD13	1:A:61:ASN:HB3	1.87	0.56
1:F:41:ALA:HB1	1:G:66:VAL:HG13	1.88	0.56
1:G:255:LYR:H183	1:G:255:LYR:C9	2.32	0.55
1:G:117:VAL:HB	1:G:118:PRO:HD3	1.87	0.55
1:C:234:LEU:O	1:C:239:GLY:HA3	2.07	0.55
1:C:189:ILE:HD13	1:C:208:TRP:HB2	1.87	0.55
1:C:41:ALA:HB1	1:D:66:VAL:HG13	1.89	0.55
1:H:109:ARG:NH1	1:H:251:ASP:OD2	2.39	0.55
1:D:255:LYR:H183	1:D:255:LYR:C9	2.36	0.54
1:B:218:TYR:HB2	1:B:219:PRO:HD3	1.89	0.54
1:F:115:ILE:HD11	1:J:34:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:MET:HE1	1:I:234:LEU:CD1	2.38	0.54
1:F:74[A]:LEU:HD13	1:F:112:ASN:CB	2.37	0.54
1:A:255:LYR:H9	1:A:255:LYR:H192	1.87	0.54
1:F:62:ILE:O	1:F:66:VAL:HG23	2.07	0.54
1:F:66:VAL:HG13	1:J:41:ALA:HB1	1.90	0.54
1:A:9:ASN:HB3	1:A:11:GLU:OE1	2.08	0.54
1:B:133:SER:OG	1:B:191:GLU:OE2	2.26	0.53
1:C:255:LYR:H9	1:C:255:LYR:H192	1.90	0.53
1:H:272:ASN:C	1:H:273:LYS:HG3	2.29	0.53
1:J:70:SER:OG	1:J:112[B]:ASN:OD1	2.24	0.53
1:D:74:LEU:HD11	1:D:108:TYR:C	2.28	0.53
1:C:163:ASN:HD21	3:C:305:LFA:H92	1.73	0.53
1:B:234:LEU:O	1:B:239:GLY:HA3	2.09	0.53
1:F:234:LEU:O	1:F:239:GLY:HA3	2.08	0.53
1:J:255:LYR:H9	1:J:255:LYR:H192	1.91	0.53
3:F:311:LFA:H61	3:F:312:LFA:H22	1.90	0.53
1:G:111:LEU:O	1:G:114:LEU:HB2	2.09	0.53
1:D:159:TYR:CE1	4:D:315:MPG:H212	2.44	0.52
1:E:81:ASN:HA	3:E:311:LFA:H11	1.91	0.52
1:G:170:TRP:HE1	4:G:312:MPG:HX31	1.74	0.52
1:I:88:PHE:CZ	1:I:93:GLY:HA2	2.44	0.52
1:J:74[A]:LEU:HD11	1:J:108:TYR:O	2.08	0.52
1:C:70:SER:O	1:C:74[B]:LEU:HD13	2.09	0.52
1:F:76:TYR:O	1:F:80:GLN:HG2	2.09	0.52
1:F:109:ARG:O	1:F:112:ASN:HB3	2.09	0.52
1:A:66:VAL:HG13	1:E:41:ALA:HB1	1.92	0.52
3:G:302:LFA:C16	3:G:303:LFA:C1	2.87	0.52
1:A:65:ALA:HB1	1:E:44:LEU:HD11	1.90	0.52
1:A:117:VAL:HB	1:A:118:PRO:HD3	1.91	0.52
1:A:234:LEU:O	1:A:239:GLY:HA3	2.10	0.52
1:D:117:VAL:HB	1:D:118:PRO:HD3	1.92	0.52
1:C:167:PHE:CE1	1:C:222:TYR:CE2	2.97	0.51
1:J:182:LEU:HD23	1:J:211:PHE:HE1	1.74	0.51
1:D:234:LEU:O	1:D:239:GLY:HA3	2.11	0.51
1:E:88:PHE:CZ	1:E:93:GLY:HA2	2.46	0.51
1:E:199:ALA:O	1:E:202:LYS:HE2	2.10	0.51
1:H:271:LYS:N	1:H:272:ASN:HB2	2.26	0.51
1:H:41:ALA:HB1	1:I:66:VAL:HG13	1.93	0.51
1:I:101:GLY:O	1:I:102:ASP:HB2	2.11	0.51
1:J:74[A]:LEU:HD11	1:J:109:ARG:HA	1.92	0.51
1:J:270:SER:O	1:J:272:ASN:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:311:LFA:H11	3:D:306:LFA:C16	2.41	0.50
1:F:111:LEU:HD12	1:J:30:HIS:HB3	1.93	0.50
3:F:311:LFA:H61	3:F:312:LFA:H21	1.93	0.50
1:G:44:LEU:HD22	1:G:48:LEU:CD1	2.40	0.50
1:I:224:MET:N	1:I:225:PRO:HD2	2.26	0.50
1:B:121:LEU:O	1:B:124:ILE:HG22	2.12	0.50
1:F:74[B]:LEU:HD21	1:F:109:ARG:CA	2.42	0.50
1:I:9:ASN:HB3	1:I:11:GLU:OE1	2.11	0.50
1:H:174:SER:HB3	1:H:255:LYR:H142	1.94	0.50
1:E:234:LEU:O	1:E:239:GLY:HA3	2.10	0.50
1:B:146:GLY:O	1:B:150:ILE:HG12	2.11	0.50
1:D:74:LEU:HD13	1:D:112:ASN:CB	2.39	0.50
1:H:101:GLY:O	1:H:102:ASP:CB	2.59	0.50
1:D:229:GLY:O	1:D:231:ASP:N	2.45	0.50
1:I:44:LEU:HD11	1:J:65:ALA:HB1	1.94	0.50
1:F:244:GLN:HG2	5:F:413:HOH:O	2.12	0.50
1:I:244:GLN:HG2	5:I:415:HOH:O	2.11	0.50
1:B:169:VAL:HG11	3:B:306:LFA:H32	1.94	0.50
3:D:316:LFA:H12	3:D:317:LFA:C1	2.39	0.49
3:H:305:LFA:C16	3:I:303:LFA:H11	2.42	0.49
1:I:110:TYR:O	1:I:113:TRP:HB2	2.12	0.49
1:J:216:THR:O	1:J:219:PRO:HG2	2.11	0.49
1:D:224:MET:N	1:D:225:PRO:HD2	2.27	0.49
1:E:163:ASN:ND2	4:E:313:MPG:H3	1.93	0.49
3:G:307:LFA:C16	3:I:302:LFA:H11	2.43	0.49
1:H:224:MET:HB3	1:H:225:PRO:CD	2.43	0.49
1:F:101:GLY:O	1:F:102:ASP:HB2	2.12	0.49
1:J:101:GLY:O	1:J:102:ASP:CB	2.60	0.49
1:B:40:LEU:HD23	1:C:73:LEU:HD11	1.94	0.49
1:C:117:VAL:HB	1:C:118:PRO:HD3	1.94	0.49
1:G:118:PRO:O	1:G:122:PHE:HB2	2.12	0.49
1:H:117:VAL:HB	1:H:118:PRO:HD3	1.95	0.49
1:I:74:LEU:CD1	1:I:112:ASN:HA	2.42	0.49
1:C:109:ARG:NH1	1:C:251:ASP:OD2	2.46	0.49
3:C:302:LFA:C7	3:D:302:LFA:H42	2.42	0.49
1:B:197:SER:CB	1:B:198:PRO:CD	2.86	0.49
1:F:60:SER:OG	5:F:422:HOH:O	2.20	0.48
1:A:30:HIS:HB3	1:B:111:LEU:HD22	1.96	0.48
1:D:74:LEU:CD1	1:D:112:ASN:HB2	2.41	0.48
1:F:131:THR:OG1	1:F:132:THR:N	2.45	0.48
1:A:102:ASP:OD2	1:E:25:TYR:OH	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:LEU:HD11	1:D:109:ARG:HA	1.94	0.48
1:F:170:TRP:HE1	4:F:315:MPG:HX31	1.78	0.48
1:C:70:SER:OG	1:C:112[B]:ASN:ND2	2.45	0.48
1:F:38:VAL:CG2	1:G:115:ILE:HD11	2.44	0.48
1:G:51:LYS:HE2	3:G:302:LFA:H11	1.96	0.48
1:I:228:THR:O	1:I:232:GLY:HA3	2.13	0.48
1:J:88:PHE:CZ	1:J:93:GLY:HA2	2.49	0.48
1:C:74[A]:LEU:HD11	1:C:108:TYR:C	2.33	0.48
1:G:74[A]:LEU:HD23	1:G:75:LEU:HD23	1.96	0.48
1:H:33:THR:HG22	1:I:74:LEU:CD2	2.44	0.48
1:B:9:ASN:HB3	1:B:11:GLU:OE1	2.14	0.48
1:E:117:VAL:HB	1:E:118:PRO:HD3	1.96	0.47
1:A:101:GLY:O	1:A:102:ASP:CB	2.62	0.47
1:E:74:LEU:HD13	1:E:112:ASN:CA	2.43	0.47
1:H:34:LEU:CD1	1:I:115:ILE:HD11	2.44	0.47
1:E:81:ASN:HB2	3:E:311:LFA:C1	2.44	0.47
1:F:10:PHE:CE2	1:F:14:ILE:CD1	2.97	0.47
1:F:74[B]:LEU:CD2	1:F:109:ARG:HA	2.44	0.47
1:E:81:ASN:CB	3:E:311:LFA:H11	2.45	0.47
1:E:216:THR:O	1:E:219:PRO:HG2	2.14	0.47
1:E:224:MET:CE	1:E:234:LEU:HD22	2.42	0.47
1:G:44:LEU:HD22	1:G:48:LEU:HD11	1.96	0.47
1:G:70:SER:OG	1:G:112[A]:ASN:OD1	2.32	0.47
1:I:109:ARG:NH1	1:I:251:ASP:OD2	2.46	0.47
1:C:255:LYR:C9	1:C:255:LYR:H192	2.44	0.47
1:E:251:ASP:O	1:E:255:LYR:HB3	2.15	0.47
1:A:271:LYS:HA	1:A:272:ASN:HA	1.60	0.47
1:G:234:LEU:O	1:G:239:GLY:HA3	2.14	0.47
1:A:74:LEU:HD22	5:A:429:HOH:O	2.14	0.47
1:E:81:ASN:CA	3:E:311:LFA:H11	2.44	0.46
1:C:264:ASN:O	1:C:268:THR:HG23	2.15	0.46
1:D:113:TRP:CD1	1:D:255:LYR:HC2	2.49	0.46
1:H:74:LEU:HD21	1:H:109:ARG:HG3	1.96	0.46
1:J:78:GLN:OE1	1:J:78:GLN:HA	2.15	0.46
1:E:160:GLU:O	1:E:226:TYR:OH	2.25	0.46
1:E:255:LYR:H9	1:E:255:LYR:H192	1.98	0.46
1:G:44:LEU:CD1	1:H:65:ALA:HB1	2.45	0.46
1:J:61:ASN:ND2	5:J:431:HOH:O	2.47	0.46
1:J:74[A]:LEU:CD1	1:J:109:ARG:HA	2.46	0.46
1:D:91:GLU:HG2	1:H:96:PHE:CG	2.51	0.46
1:I:224:MET:HE3	1:I:234:LEU:HD13	1.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:45:TYR:CE1	3:I:309:LFA:H72	2.50	0.46
1:C:74[B]:LEU:CD2	1:C:112[B]:ASN:ND2	2.69	0.46
1:D:255:LYR:H192	1:D:255:LYR:C9	2.45	0.46
1:E:118:PRO:O	1:E:122:PHE:HB2	2.16	0.46
1:F:99:PRO:HG3	1:J:90:GLU:CG	2.46	0.46
3:G:308:LFA:H151	3:H:302:LFA:H92	1.98	0.46
1:H:113:TRP:CD1	1:H:255:LYR:HC2	2.51	0.46
1:I:44:LEU:HD11	1:J:43:LEU:HD11	1.97	0.46
1:B:169:VAL:HG11	3:B:306:LFA:C3	2.46	0.46
1:G:114:LEU:O	1:G:118:PRO:HG2	2.15	0.46
1:I:224:MET:CE	1:I:234:LEU:HD22	2.46	0.45
1:J:111:LEU:O	1:J:114:LEU:HB2	2.16	0.45
1:A:255:LYR:C9	1:A:255:LYR:H192	2.46	0.45
1:C:61:ASN:ND2	5:C:425:HOH:O	2.49	0.45
1:C:146:GLY:O	1:C:150:ILE:HG12	2.17	0.45
1:E:89:ASN:ND2	1:G:89:ASN:HD21	2.11	0.45
5:H:433:HOH:O	1:I:108:TYR:HE2	1.93	0.45
1:E:163:ASN:HD21	3:E:310:LFA:H92	1.81	0.45
1:E:186:LYS:CD	1:E:190:ASN:HD21	2.29	0.45
1:G:74[A]:LEU:CD1	1:G:108:TYR:C	2.79	0.45
1:H:114:LEU:O	1:H:118:PRO:HG2	2.17	0.45
1:H:255:LYR:H192	1:H:255:LYR:C9	2.46	0.45
1:B:81:ASN:ND2	5:B:415:HOH:O	2.40	0.45
1:H:271:LYS:CA	1:H:272:ASN:HB2	2.47	0.45
1:I:118:PRO:O	1:I:122:PHE:HB2	2.17	0.45
1:F:38:VAL:HG23	1:G:115:ILE:HD11	1.99	0.45
1:G:74[A]:LEU:HD11	1:G:108:TYR:O	2.09	0.45
1:B:109:ARG:NH2	1:B:251:ASP:OD2	2.50	0.45
1:D:33:THR:HG22	1:E:74:LEU:HD21	1.99	0.45
1:D:185:MET:O	1:D:189:ILE:HG12	2.17	0.45
1:F:9:ASN:HB3	1:F:11:GLU:OE1	2.16	0.45
1:F:251:ASP:O	1:F:255:LYR:HB3	2.16	0.45
1:B:255:LYR:H10	1:B:255:LYR:H81	1.79	0.45
1:D:45:TYR:CE1	3:D:307:LFA:H72	2.51	0.45
1:H:118:PRO:O	1:H:122:PHE:HB2	2.17	0.45
1:A:74:LEU:HD11	1:A:108:TYR:C	2.38	0.44
1:G:218:TYR:N	1:G:219:PRO:HD2	2.33	0.44
1:B:56:LYS:HE3	1:B:57:PHE:CZ	2.52	0.44
1:C:124:ILE:O	1:C:128:VAL:HG22	2.17	0.44
1:F:88:PHE:CZ	1:F:93:GLY:HA2	2.52	0.44
1:G:34:LEU:O	1:G:38:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:159:TYR:CE1	4:J:312:MPG:H212	2.52	0.44
1:A:154:TYR:O	1:A:157:GLN:HG3	2.18	0.44
1:F:163:ASN:HD21	3:F:306:LFA:H92	1.82	0.44
1:G:41:ALA:HB1	1:H:66:VAL:HG13	1.99	0.44
1:J:113:TRP:CD1	1:J:255:LYR:HC2	2.52	0.44
1:H:3:GLN:HG2	1:H:4:GLU:N	2.31	0.44
3:A:307:LFA:H51	1:B:122:PHE:HE2	1.81	0.44
1:D:255:LYR:H10	1:D:255:LYR:H81	1.79	0.44
1:E:224:MET:HE3	1:E:234:LEU:HD13	2.00	0.44
1:H:255:LYR:H81	1:H:255:LYR:H10	1.72	0.44
1:J:255:LYR:H10	1:J:255:LYR:H81	1.81	0.44
1:C:224:MET:N	1:C:225:PRO:HD2	2.32	0.44
1:D:118:PRO:O	1:D:122:PHE:HB2	2.16	0.44
1:E:202:LYS:HE2	1:E:202:LYS:HB3	1.75	0.44
1:I:224:MET:HE2	1:I:242:ALA:CB	2.48	0.44
1:B:224:MET:N	1:B:225:PRO:HD2	2.33	0.44
1:I:117:VAL:HB	1:I:118:PRO:HD3	2.00	0.44
1:I:234:LEU:O	1:I:239:GLY:HA3	2.18	0.44
1:E:224:MET:HE2	1:E:242:ALA:CB	2.48	0.43
1:B:205:SER:O	1:B:209:ILE:HG12	2.18	0.43
1:G:159:TYR:CE1	4:G:312:MPG:H212	2.53	0.43
1:I:218:TYR:N	1:I:219:PRO:HD2	2.33	0.43
1:C:96:PHE:CG	1:I:91:GLU:HG2	2.53	0.43
1:D:74:LEU:HD11	1:D:108:TYR:O	2.18	0.43
1:F:255:LYR:H10	1:F:255:LYR:H81	1.80	0.43
1:J:223:LEU:HD21	3:J:311:LFA:H32	2.00	0.43
1:A:248:THR:O	1:A:252:VAL:HG23	2.19	0.43
1:F:255:LYR:H9	1:F:255:LYR:H192	2.00	0.43
1:H:224:MET:HB3	1:H:225:PRO:HD3	2.01	0.43
1:J:110:TYR:HA	1:J:113:TRP:CE3	2.53	0.43
1:D:218:TYR:N	1:D:219:PRO:HD2	2.34	0.43
1:A:43:LEU:HD11	1:E:44:LEU:HD11	2.01	0.43
1:B:248:THR:O	1:B:252:VAL:HG23	2.19	0.43
1:C:253:SER:HA	1:C:257:ILE:HD12	2.00	0.43
1:H:74:LEU:CD2	1:H:109:ARG:HA	2.48	0.43
1:E:89:ASN:HD21	1:G:89:ASN:ND2	2.13	0.43
1:G:84:SER:O	1:G:101:GLY:HA3	2.19	0.43
1:G:216:THR:O	1:G:219:PRO:HG2	2.18	0.43
1:H:78:GLN:HA	1:H:78:GLN:OE1	2.18	0.43
1:A:76:TYR:O	1:A:80:GLN:HG2	2.19	0.43
1:A:255:LYR:H81	1:A:255:LYR:H10	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:SER:O	5:A:432:HOH:O	2.21	0.43
1:F:180:HIS:O	1:F:184:VAL:HG23	2.19	0.43
1:J:117:VAL:HB	1:J:118:PRO:HD3	2.00	0.43
1:F:115:ILE:HD11	1:J:38:VAL:HG23	2.01	0.42
1:G:113:TRP:CD1	1:G:255:LYR:HC2	2.54	0.42
1:A:224:MET:N	1:A:225:PRO:HD2	2.34	0.42
1:E:44:LEU:HD23	1:E:44:LEU:HA	1.88	0.42
1:E:74:LEU:HD12	1:E:112:ASN:CB	2.48	0.42
1:B:139:ARG:HD2	1:B:143:TRP:CH2	2.53	0.42
1:D:33:THR:HG22	1:E:74:LEU:CD2	2.49	0.42
1:I:255:LYR:H9	1:I:255:LYR:H192	2.00	0.42
1:J:255:LYR:C9	1:J:255:LYR:H192	2.48	0.42
1:E:109:ARG:O	1:E:112:ASN:HB3	2.19	0.42
1:H:234:LEU:O	1:H:239:GLY:HA3	2.18	0.42
1:J:118:PRO:O	1:J:122:PHE:HB2	2.19	0.42
1:B:113:TRP:CD1	1:B:255:LYR:HC2	2.54	0.42
1:E:224:MET:CE	1:E:234:LEU:CD1	2.94	0.42
1:I:40:LEU:HD23	1:J:73:LEU:HD11	2.02	0.42
1:J:170:TRP:HE1	4:J:312:MPG:HX31	1.85	0.42
1:J:272:ASN:OD1	1:J:273:LYS:HG3	2.20	0.42
1:F:211:PHE:CE1	1:F:215:TRP:CE2	3.08	0.42
1:H:111:LEU:HD12	1:H:111:LEU:HA	1.85	0.42
1:B:120:LEU:HD11	1:B:255:LYR:HG3	2.02	0.42
1:C:174:SER:HB3	1:C:255:LYR:H142	2.01	0.42
1:E:255:LYR:H10	1:E:255:LYR:H81	1.74	0.42
1:E:91:GLU:HG2	1:G:96:PHE:CD2	2.55	0.42
1:G:142:PHE:CZ	1:G:184:VAL:HG12	2.55	0.42
1:J:74[A]:LEU:CD1	1:J:112[A]:ASN:HB2	2.45	0.42
1:E:74:LEU:HD12	1:E:112:ASN:CG	2.39	0.41
1:E:174:SER:HB3	1:E:255:LYR:H142	2.02	0.41
1:G:70:SER:O	1:G:74[B]:LEU:HD13	2.21	0.41
1:H:74:LEU:HD22	1:H:112[B]:ASN:HD22	1.84	0.41
1:H:251:ASP:O	1:H:255:LYR:HB3	2.20	0.41
1:J:74[A]:LEU:HD11	1:J:109:ARG:N	2.34	0.41
1:A:186:LYS:HD3	1:A:208:TRP:CZ2	2.55	0.41
1:F:71:ALA:O	1:F:75:LEU:HG	2.19	0.41
1:I:223:LEU:HD21	3:I:312:LFA:H61	2.01	0.41
3:I:308:LFA:C16	3:J:307:LFA:C1	2.98	0.41
1:J:60:SER:CB	5:J:425:HOH:O	2.67	0.41
1:B:255:LYR:H9	1:B:255:LYR:H192	2.03	0.41
1:B:256:VAL:O	1:B:260:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:268:THR:CG2	1:G:275:LEU:HD11	2.50	0.41
1:I:139:ARG:HD2	1:I:143:TRP:CH2	2.56	0.41
1:B:101:GLY:O	1:B:102:ASP:CB	2.64	0.41
1:C:229:GLY:O	1:C:231:ASP:N	2.53	0.41
1:E:167:PHE:CE1	1:E:222:TYR:CE2	3.09	0.41
1:F:114:LEU:HD12	1:F:114:LEU:HA	1.95	0.41
1:G:74[A]:LEU:HD13	1:G:112[A]:ASN:HB3	2.01	0.41
1:I:44:LEU:HD23	1:I:44:LEU:HA	1.89	0.41
1:I:146:GLY:O	1:I:150:ILE:HG12	2.20	0.41
1:C:118:PRO:O	1:C:122:PHE:HB2	2.20	0.41
1:J:60:SER:HB3	5:J:425:HOH:O	2.20	0.41
1:A:74:LEU:HD13	1:A:112:ASN:HB2	2.02	0.41
1:C:251:ASP:O	1:C:255:LYR:HB3	2.20	0.41
1:H:3:GLN:HE21	1:H:3:GLN:HB3	1.69	0.41
1:H:25:TYR:OH	1:I:102:ASP:OD2	2.37	0.41
1:H:31:ILE:HD12	1:H:31:ILE:HA	1.94	0.41
1:J:98:ASP:HA	1:J:99:PRO:HD2	1.89	0.41
1:B:41:ALA:HB1	1:C:66:VAL:HG13	2.01	0.41
1:F:118:PRO:O	1:F:122:PHE:HB2	2.20	0.41
1:C:78:GLN:OE1	1:C:78:GLN:HA	2.19	0.41
1:F:10:PHE:CE2	1:F:14:ILE:HD11	2.54	0.41
1:A:216:THR:O	1:A:219:PRO:HG2	2.20	0.41
1:B:130:LEU:CD1	1:B:135:PHE:HA	2.51	0.41
1:C:255:LYR:H81	1:C:255:LYR:H10	1.71	0.41
1:D:9:ASN:HB3	1:D:11:GLU:OE1	2.21	0.41
1:E:40:LEU:HD12	1:E:40:LEU:HA	1.94	0.41
1:F:175:SER:O	1:F:178:PHE:HB3	2.20	0.41
1:H:76:TYR:O	1:H:80:GLN:HG2	2.21	0.41
1:C:74[B]:LEU:HD21	1:C:112[B]:ASN:CA	2.49	0.41
1:I:45:TYR:CD1	3:I:309:LFA:H91	2.55	0.41
1:I:100:SER:O	5:I:440:HOH:O	2.22	0.40
1:I:255:LYR:H10	1:I:255:LYR:H81	1.77	0.40
1:J:228:THR:O	1:J:232:GLY:HA3	2.21	0.40
1:D:227:LEU:HD23	1:D:227:LEU:HA	1.85	0.40
1:B:264:ASN:O	1:B:268:THR:HG23	2.21	0.40
1:F:40:LEU:HD23	1:G:73:LEU:HD11	2.04	0.40
1:F:223:LEU:C	1:F:225:PRO:HD2	2.42	0.40
1:H:160:GLU:O	1:H:226:TYR:OH	2.28	0.40
1:E:189:ILE:CD1	1:E:208:TRP:HB2	2.49	0.40
1:H:33:THR:HA	1:H:36:TYR:CE2	2.57	0.40
1:A:211:PHE:CE1	1:A:215:TRP:CE2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ALA:HB1	3:E:311:LFA:H32	2.01	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	268/288 (93%)	261 (97%)	7 (3%)	0	100	100
1	B	264/288 (92%)	252 (96%)	11 (4%)	1 (0%)	34	37
1	C	266/288 (92%)	261 (98%)	5 (2%)	0	100	100
1	D	264/288 (92%)	258 (98%)	6 (2%)	0	100	100
1	E	265/288 (92%)	259 (98%)	6 (2%)	0	100	100
1	F	265/288 (92%)	259 (98%)	6 (2%)	0	100	100
1	G	267/288 (93%)	260 (97%)	7 (3%)	0	100	100
1	H	267/288 (93%)	262 (98%)	5 (2%)	0	100	100
1	I	264/288 (92%)	259 (98%)	5 (2%)	0	100	100
1	J	267/288 (93%)	262 (98%)	5 (2%)	0	100	100
All	All	2657/2880 (92%)	2593 (98%)	63 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	197	SER

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

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/247 (92%)	223 (99%)	3 (1%)	69	81
1	B	224/247 (91%)	221 (99%)	3 (1%)	69	81
1	C	225/247 (91%)	225 (100%)	0	100	100
1	D	224/247 (91%)	222 (99%)	2 (1%)	78	88
1	E	224/247 (91%)	223 (100%)	1 (0%)	91	96
1	F	225/247 (91%)	224 (100%)	1 (0%)	91	96
1	G	228/247 (92%)	224 (98%)	4 (2%)	59	72
1	H	228/247 (92%)	224 (98%)	4 (2%)	59	72
1	I	221/247 (90%)	219 (99%)	2 (1%)	78	88
1	J	226/247 (92%)	224 (99%)	2 (1%)	78	88
All	All	2251/2470 (91%)	2229 (99%)	22 (1%)	76	86

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

Mol	Chain	Res	Type
1	A	18	GLU
1	A	112	ASN
1	A	142	PHE
1	B	103	LEU
1	B	164	LEU
1	B	194	GLU
1	D	91	GLU
1	D	92	VAL
1	E	44	LEU
1	F	132	THR
1	G	44	LEU
1	G	84	SER
1	G	114	LEU
1	G	141	GLN
1	H	3	GLN
1	H	10	PHE
1	H	55	LYS
1	H	111	LEU
1	I	10	PHE
1	I	44	LEU

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Mol	Chain	Res	Type
1	J	10	PHE
1	J	44	LEU

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

Mol	Chain	Res	Type
1	A	112	ASN
1	B	112	ASN
1	C	61	ASN
1	C	89	ASN
1	C	141	GLN
1	C	180	HIS
1	E	112	ASN
1	E	163	ASN
1	E	180	HIS
1	E	190	ASN
1	F	81	ASN
1	F	112	ASN
1	G	89	ASN
1	H	3	GLN
1	H	89	ASN
1	I	112	ASN
1	J	180	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LYR	G	255	1	27,29,30	1.20	3 (11%)	30,37,39	2.03	8 (26%)
1	LYR	J	255	1	27,29,30	1.19	3 (11%)	30,37,39	2.04	8 (26%)
1	LYR	B	255	1	27,29,30	1.21	2 (7%)	30,37,39	1.99	7 (23%)
1	LYR	I	255	1	27,29,30	1.12	4 (14%)	30,37,39	2.11	6 (20%)
1	LYR	D	255	1	27,29,30	1.24	2 (7%)	30,37,39	1.90	7 (23%)
1	LYR	C	255	1	27,29,30	1.19	2 (7%)	30,37,39	2.07	6 (20%)
1	LYR	A	255	1	27,29,30	1.31	2 (7%)	30,37,39	1.86	6 (20%)
1	LYR	E	255	1	27,29,30	1.22	3 (11%)	30,37,39	1.95	6 (20%)
1	LYR	H	255	1	27,29,30	1.25	2 (7%)	30,37,39	1.97	6 (20%)
1	LYR	F	255	1	27,29,30	1.26	3 (11%)	30,37,39	1.99	6 (20%)

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

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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	LYR	C7-C80	3.15	1.40	1.35
1	F	255	LYR	C7-C80	2.99	1.39	1.35
1	D	255	LYR	C7-C80	2.96	1.39	1.35
1	B	255	LYR	C7-C80	2.84	1.39	1.35
1	E	255	LYR	C7-C80	2.78	1.39	1.35
1	G	255	LYR	C7-C80	2.72	1.39	1.35
1	H	255	LYR	C7-C80	2.72	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	255	LYR	C7-C80	2.67	1.39	1.35
1	C	255	LYR	C7-C80	2.63	1.39	1.35
1	C	255	LYR	C2-C3	2.61	1.41	1.33
1	I	255	LYR	C7-C80	2.56	1.39	1.35
1	B	255	LYR	C2-C3	2.53	1.40	1.33
1	A	255	LYR	C2-C3	2.53	1.40	1.33
1	F	255	LYR	C2-C3	2.51	1.40	1.33
1	D	255	LYR	C2-C3	2.51	1.40	1.33
1	H	255	LYR	C2-C3	2.51	1.40	1.33
1	E	255	LYR	C2-C3	2.46	1.40	1.33
1	J	255	LYR	C2-C3	2.35	1.40	1.33
1	G	255	LYR	C2-C3	2.31	1.40	1.33
1	I	255	LYR	C2-C3	2.26	1.40	1.33
1	G	255	LYR	C5-C3	-2.21	1.41	1.45
1	F	255	LYR	C5-C3	-2.15	1.41	1.45
1	I	255	LYR	C5-C3	-2.10	1.41	1.45
1	J	255	LYR	C5-C3	-2.09	1.41	1.45
1	E	255	LYR	C1-C2	-2.05	1.38	1.48
1	I	255	LYR	C1-C2	-2.02	1.39	1.48

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	255	LYR	C13-C12-C11	-5.15	118.74	124.53
1	B	255	LYR	C13-C12-C11	-5.02	118.89	124.53
1	J	255	LYR	C13-C12-C11	-4.93	119.00	124.53
1	C	255	LYR	C13-C12-C11	-4.82	119.11	124.53
1	I	255	LYR	C13-C12-C11	-4.79	119.15	124.53
1	E	255	LYR	C13-C12-C11	-4.73	119.22	124.53
1	C	255	LYR	C10-C9-C80	-4.70	119.13	126.23
1	A	255	LYR	C13-C12-C11	-4.69	119.26	124.53
1	H	255	LYR	C10-C9-C80	-4.63	119.24	126.23
1	H	255	LYR	C1-NZ-CE	4.62	120.66	113.33
1	F	255	LYR	C13-C12-C11	-4.61	119.35	124.53
1	D	255	LYR	C1-NZ-CE	4.61	120.63	113.33
1	J	255	LYR	C1-NZ-CE	4.59	120.60	113.33
1	I	255	LYR	C1-NZ-CE	4.44	120.37	113.33
1	A	255	LYR	C1-NZ-CE	4.43	120.34	113.33
1	G	255	LYR	C1-NZ-CE	4.42	120.34	113.33
1	F	255	LYR	C1-NZ-CE	4.32	120.17	113.33
1	E	255	LYR	C10-C9-C80	-4.27	119.79	126.23
1	B	255	LYR	C7-C6-C5	-4.25	109.94	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	255	LYR	C10-C9-C80	-4.19	119.91	126.23
1	F	255	LYR	C10-C9-C80	-4.15	119.97	126.23
1	H	255	LYR	C13-C12-C11	-4.13	119.89	124.53
1	F	255	LYR	C7-C6-C5	-4.07	110.51	123.22
1	H	255	LYR	C7-C6-C5	-4.05	110.59	123.22
1	C	255	LYR	C1-NZ-CE	4.03	119.72	113.33
1	E	255	LYR	C7-C6-C5	-4.01	110.71	123.22
1	B	255	LYR	C10-C9-C80	-4.00	120.19	126.23
1	E	255	LYR	C1-NZ-CE	3.96	119.61	113.33
1	I	255	LYR	C7-C6-C5	-3.96	110.87	123.22
1	C	255	LYR	C7-C6-C5	-3.92	110.98	123.22
1	G	255	LYR	C7-C6-C5	-3.91	111.00	123.22
1	J	255	LYR	C7-C6-C5	-3.78	111.43	123.22
1	A	255	LYR	C7-C6-C5	-3.70	111.66	123.22
1	D	255	LYR	C13-C12-C11	-3.64	120.44	124.53
1	D	255	LYR	C10-C9-C80	-3.64	120.73	126.23
1	J	255	LYR	C10-C9-C80	-3.61	120.78	126.23
1	D	255	LYR	C7-C6-C5	-3.54	112.16	123.22
1	B	255	LYR	C1-NZ-CE	3.52	118.90	113.33
1	G	255	LYR	C10-C9-C80	-3.41	121.08	126.23
1	H	255	LYR	C15-C14-C12	-3.40	108.01	114.08
1	C	255	LYR	C15-C14-C12	-3.38	108.04	114.08
1	F	255	LYR	C15-C14-C12	-3.29	108.21	114.08
1	J	255	LYR	C15-C14-C12	-3.20	108.36	114.08
1	I	255	LYR	C15-C14-C12	-3.14	108.47	114.08
1	D	255	LYR	C15-C14-C12	-3.04	108.65	114.08
1	I	255	LYR	C8-C80-C7	-3.00	118.72	122.92
1	A	255	LYR	C15-C14-C12	-2.90	108.90	114.08
1	B	255	LYR	C15-C14-C12	-2.89	108.92	114.08
1	J	255	LYR	C8-C80-C7	-2.88	118.89	122.92
1	D	255	LYR	C8-C80-C7	-2.87	118.91	122.92
1	A	255	LYR	C10-C9-C80	-2.86	121.91	126.23
1	G	255	LYR	C15-C14-C12	-2.85	108.98	114.08
1	E	255	LYR	C15-C14-C12	-2.80	109.08	114.08
1	C	255	LYR	C8-C80-C7	-2.61	119.27	122.92
1	F	255	LYR	C8-C80-C7	-2.59	119.29	122.92
1	G	255	LYR	C8-C80-C7	-2.49	119.44	122.92
1	B	255	LYR	C19-C17-C11	-2.44	106.35	110.30
1	B	255	LYR	C8-C80-C7	-2.34	119.64	122.92
1	A	255	LYR	C8-C80-C7	-2.31	119.68	122.92
1	G	255	LYR	C8-C80-C9	2.30	121.70	118.08
1	H	255	LYR	C8-C80-C7	-2.24	119.78	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	255	LYR	C17-C11-C10	2.18	121.96	115.78
1	D	255	LYR	C6-C7-C80	-2.16	124.23	127.31
1	J	255	LYR	C6-C7-C80	-2.14	124.26	127.31
1	E	255	LYR	C8-C80-C7	-2.07	120.02	122.92
1	J	255	LYR	C18-C17-C11	-2.05	106.97	110.30

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	255	LYR	C2-C1-NZ-CE
1	D	255	LYR	C2-C1-NZ-CE
1	E	255	LYR	C2-C1-NZ-CE
1	G	255	LYR	C2-C1-NZ-CE
1	I	255	LYR	C2-C1-NZ-CE
1	C	255	LYR	C2-C1-NZ-CE
1	F	255	LYR	C2-C1-NZ-CE
1	H	255	LYR	C2-C1-NZ-CE
1	J	255	LYR	C2-C1-NZ-CE
1	A	255	LYR	C2-C1-NZ-CE
1	E	255	LYR	CE-CD-CG-CB
1	F	255	LYR	CE-CD-CG-CB
1	C	255	LYR	CE-CD-CG-CB
1	B	255	LYR	CE-CD-CG-CB
1	G	255	LYR	CE-CD-CG-CB
1	H	255	LYR	CE-CD-CG-CB
1	A	255	LYR	CE-CD-CG-CB
1	J	255	LYR	CE-CD-CG-CB
1	D	255	LYR	CE-CD-CG-CB
1	F	255	LYR	CG-CD-CE-NZ
1	I	255	LYR	CE-CD-CG-CB
1	A	255	LYR	CG-CD-CE-NZ
1	B	255	LYR	CD-CE-NZ-C1
1	I	255	LYR	CD-CE-NZ-C1
1	A	255	LYR	CD-CE-NZ-C1
1	G	255	LYR	CD-CE-NZ-C1
1	F	255	LYR	CD-CE-NZ-C1
1	J	255	LYR	CD-CE-NZ-C1
1	D	255	LYR	CD-CE-NZ-C1
1	C	255	LYR	CD-CE-NZ-C1
1	E	255	LYR	CD-CE-NZ-C1
1	H	255	LYR	CD-CE-NZ-C1

There are no ring outliers.

10 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	255	LYR	3	0
1	J	255	LYR	6	0
1	B	255	LYR	8	0
1	I	255	LYR	4	0
1	D	255	LYR	6	0
1	C	255	LYR	7	0
1	A	255	LYR	5	0
1	E	255	LYR	7	0
1	H	255	LYR	8	0
1	F	255	LYR	6	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 138 ligands modelled in this entry, 10 are monoatomic - leaving 128 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	LFA	H	307	-	13,13,19	0.26	0	12,12,18	0.52	0
3	LFA	H	312	-	5,5,19	0.27	0	4,4,18	0.38	0
3	LFA	E	311	-	7,7,19	0.27	0	6,6,18	0.46	0
3	LFA	E	304	-	7,7,19	0.31	0	6,6,18	0.44	0
3	LFA	J	302	-	15,15,19	0.26	0	14,14,18	0.54	0
3	LFA	B	307	-	15,15,19	0.27	0	14,14,18	0.56	0
3	LFA	I	311	-	7,7,19	0.27	0	6,6,18	0.47	0
3	LFA	A	304	-	9,9,19	0.27	0	8,8,18	0.48	0
3	LFA	C	312	-	3,3,19	0.37	0	2,2,18	0.59	0
3	LFA	E	306	-	11,11,19	0.28	0	10,10,18	0.49	0
3	LFA	I	308	-	15,15,19	0.24	0	14,14,18	0.59	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LFA	C	304	-	5,5,19	0.28	0	4,4,18	0.34	0
3	LFA	G	306	-	9,9,19	0.28	0	8,8,18	0.43	0
3	LFA	E	308	-	13,13,19	0.27	0	12,12,18	0.50	0
3	LFA	E	307	-	7,7,19	0.25	0	6,6,18	0.48	0
3	LFA	E	312	-	7,7,19	0.26	0	6,6,18	0.44	0
3	LFA	G	315	-	5,5,19	0.27	0	4,4,18	0.36	0
3	LFA	G	307	-	15,15,19	0.26	0	14,14,18	0.58	0
3	LFA	J	307	-	6,6,19	0.26	0	5,5,18	0.41	0
3	LFA	J	311	-	3,3,19	0.38	0	2,2,18	0.61	0
3	LFA	D	304	-	5,5,19	0.25	0	4,4,18	0.41	0
3	LFA	I	306	-	9,9,19	0.25	0	8,8,18	0.51	0
3	LFA	C	303	-	9,9,19	0.29	0	8,8,18	0.42	0
3	LFA	E	305	-	5,5,19	0.30	0	4,4,18	0.35	0
3	LFA	F	303	-	13,13,19	0.27	0	12,12,18	0.50	0
3	LFA	I	312	-	6,6,19	0.24	0	5,5,18	0.46	0
3	LFA	D	311	-	6,6,19	0.25	0	5,5,18	0.44	0
3	LFA	D	307	-	17,17,19	0.26	0	16,16,18	0.48	0
3	LFA	J	308	-	13,13,19	0.32	0	12,12,18	0.42	0
3	LFA	E	302	-	13,13,19	0.28	0	12,12,18	0.56	0
3	LFA	G	309	-	7,7,19	0.27	0	6,6,18	0.46	0
3	LFA	C	311	-	7,7,19	0.27	0	6,6,18	0.45	0
3	LFA	H	304	-	9,9,19	0.28	0	8,8,18	0.51	0
3	LFA	G	302	-	15,15,19	0.25	0	14,14,18	0.57	0
3	LFA	G	314	-	5,5,19	0.26	0	4,4,18	0.37	0
3	LFA	D	308	-	9,9,19	0.28	0	8,8,18	0.47	0
3	LFA	B	306	-	7,7,19	0.31	0	6,6,18	0.42	0
3	LFA	D	318	-	4,4,19	0.29	0	3,3,18	0.35	0
4	MPG	D	315	-	13,13,24	0.44	0	13,13,25	1.01	1 (7%)
3	LFA	I	307	-	5,5,19	0.27	0	4,4,18	0.33	0
3	LFA	D	302	-	6,6,19	0.24	0	5,5,18	0.47	0
3	LFA	H	306	-	17,17,19	0.29	0	16,16,18	0.47	0
3	LFA	C	310	-	12,12,19	0.29	0	11,11,18	0.51	0
3	LFA	I	302	-	6,6,19	0.27	0	5,5,18	0.42	0
3	LFA	A	309	-	7,7,19	0.27	0	6,6,18	0.48	0
4	MPG	C	313	-	12,12,24	0.44	0	12,12,25	0.96	1 (8%)
3	LFA	D	314	-	6,6,19	0.27	0	5,5,18	0.41	0
3	LFA	A	308	-	7,7,19	0.29	0	6,6,18	0.42	0
4	MPG	J	312	-	13,13,24	0.44	0	13,13,25	1.03	1 (7%)
3	LFA	D	313	-	5,5,19	0.27	0	4,4,18	0.36	0
3	LFA	G	305	-	5,5,19	0.28	0	4,4,18	0.35	0
3	LFA	D	305	-	9,9,19	0.27	0	8,8,18	0.51	0
3	LFA	A	305	-	9,9,19	0.28	0	8,8,18	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LFA	F	308	-	7,7,19	0.29	0	6,6,18	0.40	0
3	LFA	I	309	-	17,17,19	0.30	0	16,16,18	0.45	0
3	LFA	B	308	-	17,17,19	0.28	0	16,16,18	0.50	0
3	LFA	J	309	-	9,9,19	0.25	0	8,8,18	0.50	0
3	LFA	B	302	-	6,6,19	0.26	0	5,5,18	0.41	0
3	LFA	C	307	-	17,17,19	0.27	0	16,16,18	0.48	0
4	MPG	G	312	-	13,13,24	0.45	0	13,13,25	1.03	1 (7%)
4	MPG	B	312	-	13,13,24	0.46	0	13,13,25	0.97	1 (7%)
3	LFA	F	314	-	7,7,19	0.28	0	6,6,18	0.44	0
3	LFA	J	306	-	7,7,19	0.26	0	6,6,18	0.48	0
3	LFA	I	313	-	3,3,19	0.39	0	2,2,18	0.63	0
3	LFA	C	302	-	6,6,19	0.28	0	5,5,18	0.40	0
3	LFA	F	306	-	9,9,19	0.27	0	8,8,18	0.49	0
3	LFA	I	305	-	5,5,19	0.29	0	4,4,18	0.32	0
3	LFA	B	305	-	5,5,19	0.30	0	4,4,18	0.30	0
3	LFA	H	305	-	15,15,19	0.26	0	14,14,18	0.52	0
3	LFA	J	310	-	9,9,19	0.27	0	8,8,18	0.47	0
3	LFA	H	308	-	7,7,19	0.26	0	6,6,18	0.47	0
3	LFA	B	309	-	12,12,19	0.32	0	11,11,18	0.45	0
3	LFA	J	305	-	13,13,19	0.30	0	12,12,18	0.46	0
3	LFA	J	304	-	7,7,19	0.28	0	6,6,18	0.44	0
3	LFA	A	312	-	4,4,19	0.33	0	3,3,18	0.34	0
3	LFA	B	303	-	6,6,19	0.26	0	5,5,18	0.46	0
3	LFA	H	303	-	5,5,19	0.25	0	4,4,18	0.41	0
3	LFA	D	317	-	4,4,19	0.27	0	3,3,18	0.37	0
4	MPG	I	314	-	13,13,24	0.34	0	13,13,25	0.96	1 (7%)
3	LFA	C	308	-	9,9,19	0.29	0	8,8,18	0.45	0
3	LFA	E	303	-	17,17,19	0.26	0	16,16,18	0.50	0
3	LFA	D	309	-	7,7,19	0.26	0	6,6,18	0.45	0
3	LFA	J	303	-	17,17,19	0.27	0	16,16,18	0.50	0
3	LFA	D	310	-	7,7,19	0.27	0	6,6,18	0.46	0
3	LFA	C	309	-	7,7,19	0.27	0	6,6,18	0.45	0
3	LFA	A	306	-	13,13,19	0.28	0	12,12,18	0.51	0
3	LFA	B	311	-	7,7,19	0.28	0	6,6,18	0.44	0
3	LFA	F	312	-	7,7,19	0.25	0	6,6,18	0.48	0
3	LFA	F	302	-	6,6,19	0.24	0	5,5,18	0.47	0
3	LFA	F	304	-	9,9,19	0.28	0	8,8,18	0.46	0
3	LFA	E	309	-	5,5,19	0.29	0	4,4,18	0.34	0
3	LFA	G	310	-	9,9,19	0.30	0	8,8,18	0.43	0
3	LFA	H	311	-	6,6,19	0.21	0	5,5,18	0.53	0
3	LFA	B	304	-	13,13,19	0.29	0	12,12,18	0.49	0
3	LFA	G	308	-	17,17,19	0.28	0	16,16,18	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LFA	H	302	-	12,12,19	0.28	0	11,11,18	0.50	0
3	LFA	D	306	-	15,15,19	0.28	0	14,14,18	0.51	0
3	LFA	A	310	-	7,7,19	0.26	0	6,6,18	0.45	0
4	MPG	H	313	-	13,13,24	0.42	0	13,13,25	0.96	1 (7%)
3	LFA	D	303	-	13,13,19	0.27	0	12,12,18	0.53	0
3	LFA	C	306	-	15,15,19	0.28	0	14,14,18	0.54	0
3	LFA	F	310	-	17,17,19	0.27	0	16,16,18	0.48	0
3	LFA	F	305	-	5,5,19	0.27	0	4,4,18	0.35	0
3	LFA	D	312	-	5,5,19	0.27	0	4,4,18	0.37	0
3	LFA	I	310	-	13,13,19	0.26	0	12,12,18	0.54	0
3	LFA	A	303	-	5,5,19	0.27	0	4,4,18	0.38	0
3	LFA	B	310	-	10,10,19	0.27	0	9,9,18	0.49	0
3	LFA	E	310	-	9,9,19	0.29	0	8,8,18	0.44	0
3	LFA	D	316	-	4,4,19	0.26	0	3,3,18	0.36	0
3	LFA	H	309	-	4,4,19	0.27	0	3,3,18	0.37	0
3	LFA	H	310	-	7,7,19	0.28	0	6,6,18	0.43	0
3	LFA	I	304	-	13,13,19	0.28	0	12,12,18	0.50	0
3	LFA	C	305	-	9,9,19	0.26	0	8,8,18	0.48	0
3	LFA	F	309	-	9,9,19	0.31	0	8,8,18	0.41	0
3	LFA	G	311	-	7,7,19	0.25	0	6,6,18	0.48	0
3	LFA	A	311	-	6,6,19	0.24	0	5,5,18	0.45	0
4	MPG	E	313	-	13,13,24	0.44	0	13,13,25	0.96	1 (7%)
3	LFA	A	307	-	17,17,19	0.23	0	16,16,18	0.56	0
3	LFA	A	302	-	13,13,19	0.26	0	12,12,18	0.51	0
3	LFA	I	303	-	6,6,19	0.27	0	5,5,18	0.42	0
4	MPG	F	315	-	13,13,24	0.41	0	13,13,25	1.02	1 (7%)
3	LFA	F	313	-	13,13,19	0.29	0	12,12,18	0.49	0
3	LFA	G	303	-	6,6,19	0.26	0	5,5,18	0.41	0
4	MPG	A	313	-	13,13,24	0.47	0	13,13,25	1.01	1 (7%)
3	LFA	F	307	-	5,5,19	0.30	0	4,4,18	0.32	0
3	LFA	G	304	-	13,13,19	0.30	0	12,12,18	0.47	0
3	LFA	F	311	-	9,9,19	0.30	0	8,8,18	0.43	0
3	LFA	G	313	-	7,7,19	0.28	0	6,6,18	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	H	307	-	-	7/11/11/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	H	312	-	-	1/3/3/17	-
3	LFA	E	311	-	-	1/5/5/17	-
3	LFA	E	304	-	-	2/5/5/17	-
3	LFA	J	302	-	-	9/13/13/17	-
3	LFA	B	307	-	-	7/13/13/17	-
3	LFA	I	311	-	-	4/5/5/17	-
3	LFA	A	304	-	-	5/7/7/17	-
3	LFA	C	312	-	-	0/1/1/17	-
3	LFA	E	306	-	-	4/9/9/17	-
3	LFA	I	308	-	-	5/13/13/17	-
3	LFA	C	304	-	-	1/3/3/17	-
3	LFA	G	306	-	-	6/7/7/17	-
3	LFA	E	308	-	-	6/11/11/17	-
3	LFA	E	307	-	-	4/5/5/17	-
3	LFA	E	312	-	-	4/5/5/17	-
3	LFA	G	315	-	-	0/3/3/17	-
3	LFA	G	307	-	-	6/13/13/17	-
3	LFA	J	307	-	-	3/4/4/17	-
3	LFA	J	311	-	-	0/1/1/17	-
3	LFA	D	304	-	-	0/3/3/17	-
3	LFA	I	306	-	-	4/7/7/17	-
3	LFA	C	303	-	-	3/7/7/17	-
3	LFA	E	305	-	-	1/3/3/17	-
3	LFA	F	303	-	-	6/11/11/17	-
3	LFA	I	312	-	-	1/4/4/17	-
3	LFA	D	311	-	-	2/4/4/17	-
3	LFA	D	307	-	-	9/15/15/17	-
3	LFA	J	308	-	-	6/11/11/17	-
3	LFA	E	302	-	-	2/11/11/17	-
3	LFA	G	309	-	-	2/5/5/17	-
3	LFA	C	311	-	-	1/5/5/17	-
3	LFA	H	304	-	-	4/7/7/17	-
3	LFA	G	302	-	-	5/13/13/17	-
3	LFA	G	314	-	-	1/3/3/17	-
3	LFA	D	308	-	-	4/7/7/17	-
3	LFA	B	306	-	-	1/5/5/17	-
3	LFA	D	318	-	-	0/2/2/17	-

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	A	312	-	-	0/2/2/17	-
3	LFA	B	303	-	-	3/4/4/17	-
3	LFA	H	303	-	-	0/3/3/17	-
3	LFA	D	317	-	-	0/2/2/17	-
4	MPG	I	314	-	-	9/12/12/25	-
3	LFA	C	308	-	-	3/7/7/17	-
3	LFA	E	303	-	-	11/15/15/17	-
3	LFA	D	309	-	-	3/5/5/17	-
3	LFA	J	303	-	-	8/15/15/17	-
3	LFA	D	310	-	-	1/5/5/17	-
3	LFA	C	309	-	-	3/5/5/17	-
3	LFA	A	306	-	-	8/11/11/17	-
3	LFA	B	311	-	-	3/5/5/17	-
3	LFA	F	312	-	-	3/5/5/17	-
3	LFA	F	302	-	-	2/4/4/17	-
3	LFA	F	304	-	-	2/7/7/17	-
3	LFA	E	309	-	-	2/3/3/17	-
3	LFA	G	310	-	-	3/7/7/17	-
3	LFA	H	311	-	-	1/4/4/17	-
3	LFA	B	304	-	-	6/11/11/17	-
3	LFA	G	308	-	-	9/15/15/17	-
3	LFA	H	302	-	-	8/10/10/17	-
3	LFA	D	306	-	-	8/13/13/17	-
3	LFA	A	310	-	-	0/5/5/17	-
4	MPG	H	313	-	-	8/12/12/25	-
3	LFA	D	303	-	-	3/11/11/17	-
3	LFA	C	306	-	-	5/13/13/17	-
3	LFA	F	310	-	-	10/15/15/17	-
3	LFA	F	305	-	-	1/3/3/17	-
3	LFA	D	312	-	-	0/3/3/17	-
3	LFA	I	310	-	-	4/11/11/17	-
3	LFA	A	303	-	-	1/3/3/17	-
3	LFA	B	310	-	-	7/8/8/17	-
3	LFA	E	310	-	-	3/7/7/17	-
3	LFA	D	316	-	-	1/2/2/17	-
3	LFA	H	309	-	-	1/2/2/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LFA	H	310	-	-	3/5/5/17	-
3	LFA	I	304	-	-	5/11/11/17	-
3	LFA	C	305	-	-	6/7/7/17	-
3	LFA	F	309	-	-	4/7/7/17	-
3	LFA	G	311	-	-	1/5/5/17	-
3	LFA	A	311	-	-	3/4/4/17	-
4	MPG	E	313	-	-	10/12/12/25	-
3	LFA	A	307	-	-	13/15/15/17	-
3	LFA	A	302	-	-	7/11/11/17	-
3	LFA	I	303	-	-	3/4/4/17	-
4	MPG	F	315	-	-	9/12/12/25	-
3	LFA	F	313	-	-	4/11/11/17	-
3	LFA	G	303	-	-	3/4/4/17	-
4	MPG	A	313	-	-	7/12/12/25	-
3	LFA	F	307	-	-	2/3/3/17	-
3	LFA	G	304	-	-	5/11/11/17	-
3	LFA	F	311	-	-	3/7/7/17	-
3	LFA	G	313	-	-	4/5/5/17	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	312	MPG	O1-CX3-CXD	3.11	120.03	109.52
4	A	313	MPG	O1-CX3-CXD	3.07	119.91	109.52
4	J	312	MPG	O1-CX3-CXD	3.07	119.89	109.52
4	D	315	MPG	O1-CX3-CXD	2.97	119.56	109.52
4	B	312	MPG	O1-CX3-CXD	2.92	119.39	109.52
4	F	315	MPG	O1-CX3-CXD	2.87	119.23	109.52
4	I	314	MPG	O1-CX3-CXD	2.79	118.95	109.52
4	H	313	MPG	O1-CX3-CXD	2.79	118.94	109.52
4	C	313	MPG	O1-CX3-CXD	2.67	118.54	109.52
4	E	313	MPG	O1-CX3-CXD	2.61	118.34	109.52

There are no chirality outliers.

All (503) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	313	MPG	O3-C21-CXD-CX3
4	B	312	MPG	O1-CX3-CXD-O2
4	B	312	MPG	O1-CX3-CXD-C21
4	C	313	MPG	O3-C21-CXD-O2
4	C	313	MPG	O3-C21-CXD-CX3
4	C	313	MPG	O1-CX3-CXD-C21
4	D	315	MPG	O3-C21-CXD-CX3
4	D	315	MPG	O1-CX3-CXD-C21
4	E	313	MPG	O1-CX3-CXD-O2
4	F	315	MPG	O3-C21-CXD-CX3
4	F	315	MPG	O1-CX3-CXD-C21
4	G	312	MPG	O1-CX3-CXD-C21
4	H	313	MPG	O3-C21-CXD-CX3
4	H	313	MPG	O1-CX3-CXD-C21
4	I	314	MPG	O3-C21-CXD-CX3
4	J	312	MPG	O3-C21-CXD-CX3
4	J	312	MPG	O1-CX3-CXD-C21
4	C	313	MPG	C2-C1-O1-CX3
4	D	315	MPG	C2-C1-O1-CX3
4	C	313	MPG	O1-CX3-CXD-O2
4	D	315	MPG	O1-CX3-CXD-O2
4	G	312	MPG	C2-C1-O1-CX3
4	J	312	MPG	C2-C1-O1-CX3
4	H	313	MPG	C2-C1-O1-CX3
4	G	312	MPG	O1-CX3-CXD-O2
4	H	313	MPG	O1-CX3-CXD-O2
4	I	314	MPG	O1-CX3-CXD-O2
4	J	312	MPG	O1-CX3-CXD-O2
4	I	314	MPG	C2-C1-O1-CX3
4	B	312	MPG	O3-C21-CXD-O2
4	D	315	MPG	O3-C21-CXD-O2
4	I	314	MPG	O3-C21-CXD-O2
4	A	313	MPG	O1-C1-C2-C3
4	D	315	MPG	O1-C1-C2-C3
4	F	315	MPG	O1-C1-C2-C3
4	H	313	MPG	O1-C1-C2-C3
3	C	303	LFA	C4-C5-C6-C7
4	G	312	MPG	O1-C1-C2-C3
4	E	313	MPG	O1-C1-C2-C3
4	J	312	MPG	O1-C1-C2-C3
4	F	315	MPG	O1-CX3-CXD-O2
4	B	312	MPG	O1-C1-C2-C3
4	C	313	MPG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	J	305	LFA	C9-C10-C11-C12
3	B	308	LFA	C10-C11-C12-C13
3	F	310	LFA	C10-C11-C12-C13
3	E	303	LFA	C11-C10-C9-C8
3	E	303	LFA	C10-C11-C12-C13
3	E	310	LFA	C6-C7-C8-C9
3	E	311	LFA	C4-C5-C6-C7
3	G	308	LFA	C11-C10-C9-C8
3	G	308	LFA	C10-C11-C12-C13
3	G	313	LFA	C4-C5-C6-C7
3	I	309	LFA	C2-C3-C4-C5
3	I	309	LFA	C4-C5-C6-C7
3	J	303	LFA	C7-C8-C9-C10
4	E	313	MPG	O1-CX3-CXD-C21
4	I	314	MPG	O1-CX3-CXD-C21
3	A	307	LFA	C7-C8-C9-C10
3	C	307	LFA	C9-C10-C11-C12
3	D	311	LFA	C3-C4-C5-C6
3	F	309	LFA	C5-C6-C7-C8
3	I	309	LFA	C10-C11-C12-C13
3	J	302	LFA	C11-C12-C13-C14
3	J	310	LFA	C4-C5-C6-C7
3	H	306	LFA	C7-C8-C9-C10
3	I	304	LFA	C6-C7-C8-C9
3	A	307	LFA	C6-C7-C8-C9
3	A	307	LFA	C10-C11-C12-C13
3	B	307	LFA	C2-C3-C4-C5
3	B	307	LFA	C10-C11-C12-C13
3	E	303	LFA	C7-C8-C9-C10
3	F	303	LFA	C6-C7-C8-C9
3	J	309	LFA	C5-C6-C7-C8
4	I	314	MPG	O1-C1-C2-C3
3	A	307	LFA	C11-C10-C9-C8
3	C	307	LFA	C13-C14-C15-C16
3	E	302	LFA	C10-C11-C12-C13
3	G	308	LFA	C7-C8-C9-C10
3	I	304	LFA	C3-C4-C5-C6
3	J	307	LFA	C2-C3-C4-C5
3	J	308	LFA	C2-C3-C4-C5
3	F	310	LFA	C11-C10-C9-C8
3	F	310	LFA	C13-C14-C15-C16
3	G	304	LFA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	H	306	LFA	C10-C11-C12-C13
3	I	307	LFA	C2-C3-C4-C5
3	A	306	LFA	C11-C10-C9-C8
3	C	305	LFA	C6-C7-C8-C9
3	D	309	LFA	C2-C3-C4-C5
3	E	306	LFA	C4-C5-C6-C7
3	F	306	LFA	C6-C7-C8-C9
3	H	306	LFA	C6-C7-C8-C9
3	J	308	LFA	C5-C6-C7-C8
3	B	305	LFA	C2-C3-C4-C5
3	C	302	LFA	C3-C4-C5-C6
3	C	307	LFA	C10-C11-C12-C13
3	D	307	LFA	C10-C11-C12-C13
3	E	303	LFA	C4-C5-C6-C7
3	G	302	LFA	C12-C13-C14-C15
3	H	305	LFA	C11-C10-C9-C8
3	J	306	LFA	C3-C4-C5-C6
3	J	309	LFA	C4-C5-C6-C7
3	A	302	LFA	C7-C8-C9-C10
3	D	311	LFA	C2-C3-C4-C5
3	F	310	LFA	C6-C7-C8-C9
3	J	303	LFA	C13-C14-C15-C16
4	B	312	MPG	O3-C21-CXD-CX3
4	E	313	MPG	O3-C21-CXD-CX3
3	A	302	LFA	C5-C6-C7-C8
3	A	307	LFA	C4-C5-C6-C7
3	B	310	LFA	C4-C5-C6-C7
3	C	307	LFA	C2-C3-C4-C5
3	C	307	LFA	C5-C6-C7-C8
3	C	307	LFA	C11-C10-C9-C8
3	F	310	LFA	C7-C8-C9-C10
3	H	306	LFA	C11-C10-C9-C8
3	H	307	LFA	C2-C3-C4-C5
3	J	303	LFA	C6-C7-C8-C9
3	A	311	LFA	C2-C3-C4-C5
3	B	308	LFA	C13-C14-C15-C16
3	G	302	LFA	C4-C5-C6-C7
3	G	308	LFA	C6-C7-C8-C9
3	J	302	LFA	C11-C10-C9-C8
3	A	302	LFA	C10-C11-C12-C13
3	F	308	LFA	C3-C4-C5-C6
3	F	310	LFA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	H	306	LFA	C12-C13-C14-C15
4	E	313	MPG	C1-C2-C3-C4
3	H	302	LFA	C7-C8-C9-C10
3	I	311	LFA	C2-C3-C4-C5
3	A	306	LFA	C11-C12-C13-C14
3	B	304	LFA	C3-C4-C5-C6
3	C	306	LFA	C10-C11-C12-C13
3	G	307	LFA	C11-C12-C13-C14
3	H	308	LFA	C2-C3-C4-C5
4	G	312	MPG	C1-C2-C3-C4
3	B	310	LFA	C2-C3-C4-C5
3	F	310	LFA	C12-C13-C14-C15
3	H	302	LFA	C4-C5-C6-C7
4	D	315	MPG	C1-C2-C3-C4
3	C	304	LFA	C2-C3-C4-C5
3	C	305	LFA	C5-C6-C7-C8
3	F	312	LFA	C3-C4-C5-C6
3	D	307	LFA	C4-C5-C6-C7
3	F	311	LFA	C2-C3-C4-C5
3	G	308	LFA	C4-C5-C6-C7
4	A	313	MPG	C1-C2-C3-C4
4	C	313	MPG	C1-C2-C3-C4
3	A	309	LFA	C2-C3-C4-C5
3	F	305	LFA	C2-C3-C4-C5
3	F	313	LFA	C7-C8-C9-C10
3	H	307	LFA	C10-C11-C12-C13
3	I	309	LFA	C13-C14-C15-C16
4	F	315	MPG	C2-C1-O1-CX3
4	A	313	MPG	O3-C21-CXD-O2
4	E	313	MPG	O3-C21-CXD-O2
4	H	313	MPG	O3-C21-CXD-O2
3	E	304	LFA	C5-C6-C7-C8
3	I	305	LFA	C2-C3-C4-C5
3	B	311	LFA	C4-C5-C6-C7
4	J	312	MPG	C1-C2-C3-C4
3	B	308	LFA	C11-C10-C9-C8
3	D	307	LFA	C5-C6-C7-C8
3	J	303	LFA	C10-C11-C12-C13
4	A	313	MPG	C4-C5-C6-C7
3	C	303	LFA	C2-C3-C4-C5
3	H	306	LFA	C13-C14-C15-C16
4	F	315	MPG	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	C	308	LFA	C2-C3-C4-C5
3	D	305	LFA	C6-C7-C8-C9
3	D	307	LFA	C11-C12-C13-C14
3	D	309	LFA	C3-C4-C5-C6
3	E	306	LFA	C7-C8-C9-C10
3	E	307	LFA	C4-C5-C6-C7
3	A	308	LFA	C2-C3-C4-C5
3	F	304	LFA	C5-C6-C7-C8
3	D	310	LFA	C4-C5-C6-C7
3	B	307	LFA	C12-C13-C14-C15
3	C	307	LFA	C11-C12-C13-C14
4	H	313	MPG	C1-C2-C3-C4
4	A	313	MPG	C2-C1-O1-CX3
3	D	302	LFA	C3-C4-C5-C6
3	G	304	LFA	C11-C12-C13-C14
3	J	303	LFA	C11-C10-C9-C8
3	D	303	LFA	C4-C5-C6-C7
3	G	307	LFA	C12-C13-C14-C15
3	G	310	LFA	C7-C8-C9-C10
3	D	307	LFA	C13-C14-C15-C16
3	A	307	LFA	C11-C12-C13-C14
3	B	308	LFA	C5-C6-C7-C8
3	C	307	LFA	C6-C7-C8-C9
3	F	308	LFA	C2-C3-C4-C5
3	I	309	LFA	C7-C8-C9-C10
3	B	304	LFA	C6-C7-C8-C9
3	C	306	LFA	C11-C10-C9-C8
3	D	306	LFA	C6-C7-C8-C9
3	F	312	LFA	C2-C3-C4-C5
3	I	303	LFA	C3-C4-C5-C6
3	F	307	LFA	C2-C3-C4-C5
3	D	308	LFA	C4-C5-C6-C7
3	D	308	LFA	C5-C6-C7-C8
3	B	310	LFA	C3-C4-C5-C6
3	C	311	LFA	C4-C5-C6-C7
3	B	309	LFA	C6-C7-C8-C9
3	G	302	LFA	C10-C11-C12-C13
3	B	307	LFA	C11-C12-C13-C14
3	D	307	LFA	C9-C10-C11-C12
4	I	314	MPG	C1-C2-C3-C4
3	D	306	LFA	C10-C11-C12-C13
3	D	307	LFA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
3	G	308	LFA	C13-C14-C15-C16
3	J	302	LFA	C10-C11-C12-C13
3	J	303	LFA	C4-C5-C6-C7
3	J	303	LFA	C11-C12-C13-C14
3	A	307	LFA	C14-C15-C16-C17
3	J	310	LFA	C3-C4-C5-C6
3	E	312	LFA	C4-C5-C6-C7
3	G	310	LFA	C10-C11-C12-C13
3	H	311	LFA	C2-C3-C4-C5
3	B	307	LFA	C11-C10-C9-C8
3	D	307	LFA	C11-C10-C9-C8
3	F	304	LFA	C4-C5-C6-C7
3	G	310	LFA	C11-C10-C9-C8
3	J	309	LFA	C6-C7-C8-C9
3	E	308	LFA	C1-C2-C3-C4
3	E	310	LFA	C7-C8-C9-C10
3	G	302	LFA	C6-C7-C8-C9
3	F	311	LFA	C5-C6-C7-C8
3	H	305	LFA	C6-C7-C8-C9
3	B	302	LFA	C1-C2-C3-C4
3	D	316	LFA	C1-C2-C3-C4
3	E	309	LFA	C1-C2-C3-C4
3	A	304	LFA	C6-C7-C8-C9
3	B	310	LFA	C5-C6-C7-C8
3	D	302	LFA	C2-C3-C4-C5
3	E	304	LFA	C3-C4-C5-C6
3	I	311	LFA	C1-C2-C3-C4
3	A	303	LFA	C3-C4-C5-C6
3	D	303	LFA	C6-C7-C8-C9
3	F	302	LFA	C4-C5-C6-C7
4	J	312	MPG	O3-C21-CXD-O2
3	C	302	LFA	C4-C5-C6-C7
3	D	307	LFA	C6-C7-C8-C9
3	F	308	LFA	C5-C6-C7-C8
3	H	308	LFA	C4-C5-C6-C7
3	I	309	LFA	C1-C2-C3-C4
3	B	309	LFA	C7-C8-C9-C10
3	H	302	LFA	C11-C10-C9-C8
3	E	303	LFA	C11-C12-C13-C14
3	A	308	LFA	C1-C2-C3-C4
3	A	311	LFA	C1-C2-C3-C4
3	B	309	LFA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
3	B	304	LFA	C11-C12-C13-C14
3	D	305	LFA	C7-C8-C9-C10
4	B	312	MPG	C1-C2-C3-C4
3	E	308	LFA	C11-C12-C13-C14
3	H	302	LFA	C11-C12-C13-C14
3	G	308	LFA	C1-C2-C3-C4
3	H	306	LFA	C1-C2-C3-C4
3	I	308	LFA	C10-C11-C12-C13
3	F	310	LFA	C2-C3-C4-C5
3	B	303	LFA	C2-C3-C4-C5
3	C	305	LFA	C7-C8-C9-C10
3	D	306	LFA	C1-C2-C3-C4
3	H	309	LFA	C1-C2-C3-C4
3	B	304	LFA	C1-C2-C3-C4
3	B	308	LFA	C2-C3-C4-C5
3	J	307	LFA	C1-C2-C3-C4
3	F	310	LFA	C1-C2-C3-C4
3	G	307	LFA	C1-C2-C3-C4
3	H	302	LFA	C5-C6-C7-C8
3	A	307	LFA	C1-C2-C3-C4
3	B	303	LFA	C1-C2-C3-C4
3	F	307	LFA	C3-C4-C5-C6
3	I	308	LFA	C1-C2-C3-C4
3	I	309	LFA	C5-C6-C7-C8
3	F	311	LFA	C7-C8-C9-C10
3	J	310	LFA	C5-C6-C7-C8
3	F	302	LFA	C1-C2-C3-C4
3	J	302	LFA	C1-C2-C3-C4
3	C	307	LFA	C4-C5-C6-C7
3	F	303	LFA	C11-C12-C13-C14
3	B	309	LFA	C11-C12-C13-C14
3	F	309	LFA	C6-C7-C8-C9
3	G	308	LFA	C12-C13-C14-C15
3	J	305	LFA	C7-C8-C9-C10
3	E	310	LFA	C5-C6-C7-C8
3	C	307	LFA	C1-C2-C3-C4
3	B	308	LFA	C4-C5-C6-C7
3	G	307	LFA	C10-C11-C12-C13
3	G	306	LFA	C5-C6-C7-C8
3	C	308	LFA	C5-C6-C7-C8
3	A	302	LFA	C9-C10-C11-C12
3	D	303	LFA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
3	G	303	LFA	C3-C4-C5-C6
3	H	306	LFA	C4-C5-C6-C7
3	C	310	LFA	C3-C4-C5-C6
3	C	310	LFA	C5-C6-C7-C8
3	J	302	LFA	C6-C7-C8-C9
3	J	306	LFA	C5-C6-C7-C8
3	B	308	LFA	C11-C12-C13-C14
3	H	302	LFA	C3-C4-C5-C6
4	F	315	MPG	O3-C21-CXD-O2
3	F	313	LFA	C4-C5-C6-C7
3	A	304	LFA	C2-C3-C4-C5
3	A	306	LFA	C6-C7-C8-C9
3	G	306	LFA	C7-C8-C9-C10
3	I	310	LFA	C6-C7-C8-C9
3	C	310	LFA	C10-C11-C12-C13
3	D	306	LFA	C11-C10-C9-C8
3	I	308	LFA	C6-C7-C8-C9
3	F	308	LFA	C4-C5-C6-C7
3	G	313	LFA	C5-C6-C7-C8
3	D	309	LFA	C1-C2-C3-C4
3	E	303	LFA	C13-C14-C15-C16
3	G	303	LFA	C1-C2-C3-C4
3	G	309	LFA	C2-C3-C4-C5
3	I	306	LFA	C6-C7-C8-C9
3	D	308	LFA	C1-C2-C3-C4
3	B	307	LFA	C6-C7-C8-C9
3	E	306	LFA	C3-C4-C5-C6
3	H	305	LFA	C2-C3-C4-C5
3	I	304	LFA	C11-C12-C13-C14
3	B	302	LFA	C2-C3-C4-C5
3	F	306	LFA	C3-C4-C5-C6
3	B	309	LFA	C3-C4-C5-C6
3	E	303	LFA	C6-C7-C8-C9
3	I	302	LFA	C3-C4-C5-C6
3	A	304	LFA	C5-C6-C7-C8
3	B	308	LFA	C12-C13-C14-C15
3	B	310	LFA	C7-C8-C9-C10
3	H	305	LFA	C11-C12-C13-C14
3	G	302	LFA	C1-C2-C3-C4
3	I	308	LFA	C11-C12-C13-C14
3	J	302	LFA	C7-C8-C9-C10
3	E	308	LFA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	I	304	LFA	C4-C5-C6-C7
3	A	307	LFA	C5-C6-C7-C8
3	B	308	LFA	C1-C2-C3-C4
3	C	309	LFA	C3-C4-C5-C6
3	E	312	LFA	C5-C6-C7-C8
3	E	312	LFA	C2-C3-C4-C5
3	G	305	LFA	C2-C3-C4-C5
3	B	303	LFA	C4-C5-C6-C7
3	H	305	LFA	C10-C11-C12-C13
3	A	306	LFA	C3-C4-C5-C6
3	E	308	LFA	C6-C7-C8-C9
4	E	313	MPG	CXD-CX3-O1-C1
3	J	305	LFA	C1-C2-C3-C4
3	I	309	LFA	C12-C13-C14-C15
3	F	303	LFA	C4-C5-C6-C7
3	D	305	LFA	C1-C2-C3-C4
3	I	308	LFA	C2-C3-C4-C5
3	J	302	LFA	C13-C14-C15-C16
3	C	306	LFA	C1-C2-C3-C4
3	I	302	LFA	C4-C5-C6-C7
3	D	306	LFA	C4-C5-C6-C7
3	H	306	LFA	C5-C6-C7-C8
3	A	302	LFA	C3-C4-C5-C6
3	B	311	LFA	C1-C2-C3-C4
3	C	308	LFA	C1-C2-C3-C4
3	A	302	LFA	C4-C5-C6-C7
3	A	304	LFA	C7-C8-C9-C10
3	F	309	LFA	C3-C4-C5-C6
3	H	304	LFA	C5-C6-C7-C8
4	D	315	MPG	CXD-CX3-O1-C1
3	F	303	LFA	C5-C6-C7-C8
3	A	307	LFA	C15-C16-C17-C18
3	G	314	LFA	C1-C2-C3-C4
3	A	307	LFA	C13-C14-C15-C16
3	C	306	LFA	C6-C7-C8-C9
3	C	307	LFA	C7-C8-C9-C10
3	I	306	LFA	C3-C4-C5-C6
3	C	305	LFA	C4-C5-C6-C7
3	H	307	LFA	C11-C12-C13-C14
3	B	311	LFA	C3-C4-C5-C6
3	A	305	LFA	C5-C6-C7-C8
3	D	308	LFA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	J	307	LFA	C3-C4-C5-C6
3	E	307	LFA	C5-C6-C7-C8
3	J	308	LFA	C11-C12-C13-C14
3	C	309	LFA	C4-C5-C6-C7
4	E	313	MPG	C2-C1-O1-CX3
3	H	304	LFA	C6-C7-C8-C9
3	J	308	LFA	C9-C10-C11-C12
4	B	312	MPG	C5-C6-C7-C8
3	E	303	LFA	C15-C16-C17-C18
3	G	306	LFA	C3-C4-C5-C6
3	E	303	LFA	C12-C13-C14-C15
3	I	311	LFA	C3-C4-C5-C6
3	H	312	LFA	C1-C2-C3-C4
3	H	302	LFA	C9-C10-C11-C12
3	G	311	LFA	C1-C2-C3-C4
3	H	304	LFA	C7-C8-C9-C10
3	J	303	LFA	C9-C10-C11-C12
3	I	303	LFA	C4-C5-C6-C7
3	D	306	LFA	C12-C13-C14-C15
4	I	314	MPG	C5-C6-C7-C8
3	A	306	LFA	C12-C13-C14-C15
3	D	306	LFA	C7-C8-C9-C10
3	E	302	LFA	C9-C10-C11-C12
3	H	304	LFA	C2-C3-C4-C5
3	B	304	LFA	C5-C6-C7-C8
3	E	307	LFA	C2-C3-C4-C5
3	I	304	LFA	C5-C6-C7-C8
3	G	307	LFA	C13-C14-C15-C16
3	G	304	LFA	C7-C8-C9-C10
3	H	307	LFA	C3-C4-C5-C6
3	H	307	LFA	C1-C2-C3-C4
3	A	302	LFA	C1-C2-C3-C4
3	B	304	LFA	C4-C5-C6-C7
3	E	303	LFA	C14-C15-C16-C17
3	J	308	LFA	C11-C10-C9-C8
3	G	307	LFA	C2-C3-C4-C5
3	D	314	LFA	C3-C4-C5-C6
3	J	302	LFA	C12-C13-C14-C15
3	D	302	LFA	C1-C2-C3-C4
3	E	305	LFA	C3-C4-C5-C6
3	B	310	LFA	C11-C10-C9-C8
3	I	306	LFA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
3	G	313	LFA	C1-C2-C3-C4
4	H	313	MPG	CXD-CX3-O1-C1
3	H	307	LFA	C11-C10-C9-C8
3	E	312	LFA	C3-C4-C5-C6
3	I	311	LFA	C5-C6-C7-C8
3	B	310	LFA	C6-C7-C8-C9
3	D	305	LFA	C5-C6-C7-C8
4	J	312	MPG	C5-C6-C7-C8
3	I	309	LFA	C11-C12-C13-C14
3	F	313	LFA	C11-C10-C9-C8
3	E	308	LFA	C5-C6-C7-C8
3	C	306	LFA	C2-C3-C4-C5
3	I	309	LFA	C11-C10-C9-C8
3	H	307	LFA	C5-C6-C7-C8
3	A	305	LFA	C3-C4-C5-C6
3	A	307	LFA	C9-C10-C11-C12
3	C	303	LFA	C5-C6-C7-C8
3	D	306	LFA	C11-C12-C13-C14
3	F	312	LFA	C1-C2-C3-C4
3	J	305	LFA	C2-C3-C4-C5
3	E	306	LFA	C11-C10-C9-C8
3	A	311	LFA	C3-C4-C5-C6
3	A	305	LFA	C4-C5-C6-C7
3	J	304	LFA	C3-C4-C5-C6
3	C	305	LFA	C3-C4-C5-C6
3	C	310	LFA	C7-C8-C9-C10
3	B	308	LFA	C9-C10-C11-C12
3	G	309	LFA	C1-C2-C3-C4
4	F	315	MPG	CXD-CX3-O1-C1
3	G	308	LFA	C15-C16-C17-C18
4	E	313	MPG	C5-C6-C7-C8
3	G	304	LFA	C2-C3-C4-C5
3	I	312	LFA	C1-C2-C3-C4
3	H	310	LFA	C3-C4-C5-C6
3	C	309	LFA	C2-C3-C4-C5
3	A	305	LFA	C1-C2-C3-C4
3	E	309	LFA	C3-C4-C5-C6
3	G	306	LFA	C6-C7-C8-C9
3	I	310	LFA	C10-C11-C12-C13
3	F	303	LFA	C1-C2-C3-C4
3	A	306	LFA	C5-C6-C7-C8
3	B	309	LFA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	309	LFA	C1-C2-C3-C4
3	I	310	LFA	C5-C6-C7-C8
4	D	315	MPG	C5-C6-C7-C8
3	E	307	LFA	C3-C4-C5-C6
3	G	303	LFA	C4-C5-C6-C7
3	E	303	LFA	C1-C2-C3-C4
3	J	308	LFA	C6-C7-C8-C9
3	H	310	LFA	C4-C5-C6-C7
3	J	305	LFA	C4-C5-C6-C7
3	F	313	LFA	C9-C10-C11-C12
3	A	305	LFA	C7-C8-C9-C10
3	I	306	LFA	C5-C6-C7-C8
3	I	309	LFA	C9-C10-C11-C12
3	J	302	LFA	C3-C4-C5-C6
3	G	313	LFA	C3-C4-C5-C6
3	A	306	LFA	C13-C14-C15-C16
4	I	314	MPG	C3-C4-C5-C6
3	A	304	LFA	C1-C2-C3-C4
3	F	303	LFA	C2-C3-C4-C5
3	I	303	LFA	C2-C3-C4-C5
3	G	306	LFA	C2-C3-C4-C5
3	G	306	LFA	C4-C5-C6-C7
3	I	310	LFA	C2-C3-C4-C5
4	F	315	MPG	C5-C6-C7-C8
3	I	309	LFA	C6-C7-C8-C9
3	C	302	LFA	C1-C2-C3-C4
3	C	305	LFA	C2-C3-C4-C5
3	F	309	LFA	C7-C8-C9-C10
4	A	313	MPG	C5-C6-C7-C8
3	A	307	LFA	C12-C13-C14-C15
3	H	310	LFA	C2-C3-C4-C5
4	E	313	MPG	C2-C3-C4-C5
3	B	308	LFA	C15-C16-C17-C18
3	H	302	LFA	C2-C3-C4-C5
3	G	304	LFA	C4-C5-C6-C7
3	B	307	LFA	C1-C2-C3-C4
3	F	310	LFA	C15-C16-C17-C18
3	E	308	LFA	C7-C8-C9-C10
3	A	306	LFA	C4-C5-C6-C7
3	B	306	LFA	C3-C4-C5-C6

There are no ring outliers.

43 monomers are involved in 52 short contacts:

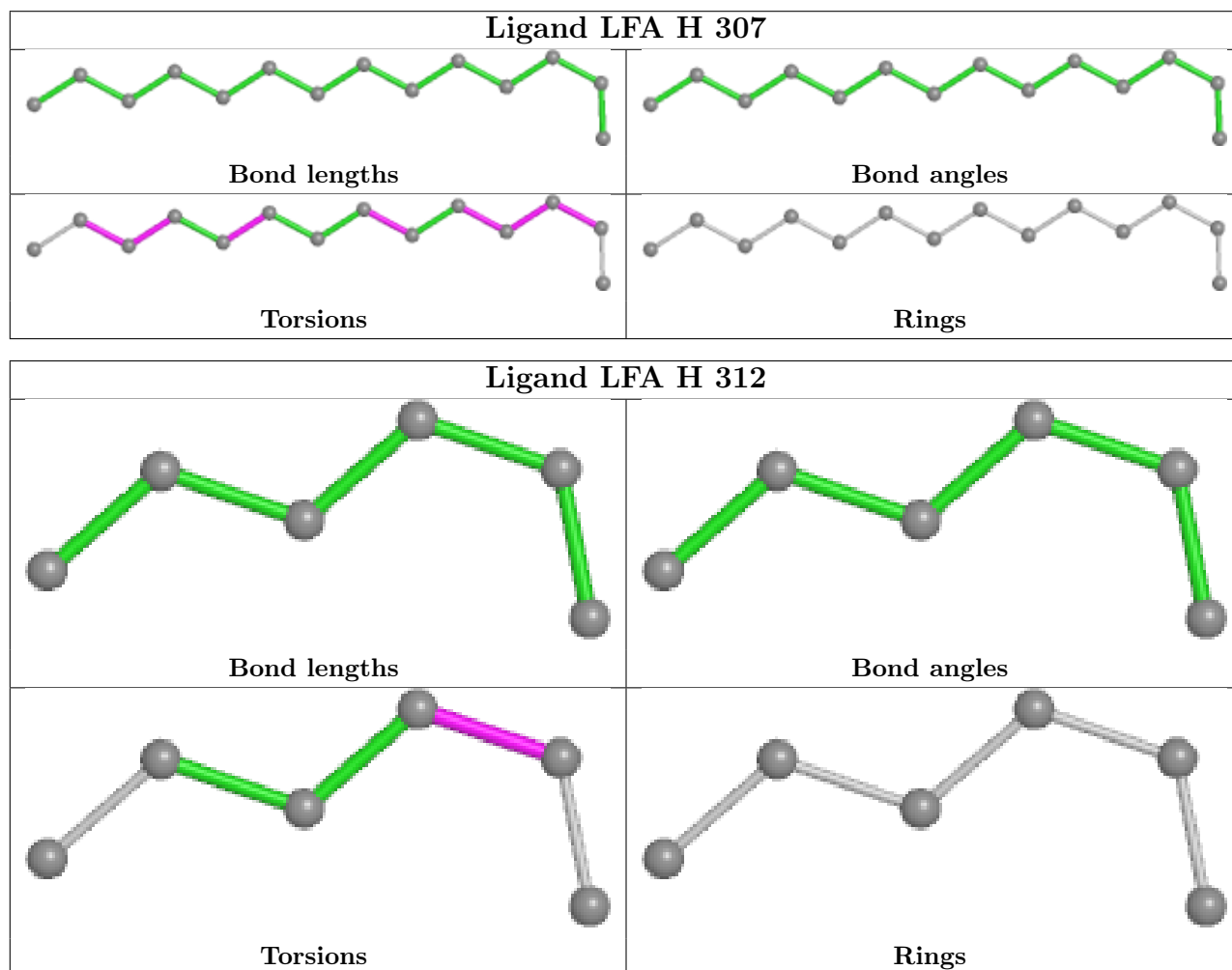
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	311	LFA	7	0
3	E	304	LFA	1	0
3	J	302	LFA	2	0
3	B	307	LFA	1	0
3	I	308	LFA	1	0
3	G	307	LFA	1	0
3	J	307	LFA	1	0
3	J	311	LFA	1	0
3	I	306	LFA	1	0
3	E	305	LFA	1	0
3	I	312	LFA	1	0
3	D	307	LFA	1	0
3	G	302	LFA	3	0
3	B	306	LFA	2	0
4	D	315	MPG	1	0
3	D	302	LFA	5	0
3	I	302	LFA	1	0
4	C	313	MPG	1	0
4	J	312	MPG	2	0
3	I	309	LFA	2	0
4	G	312	MPG	2	0
3	C	302	LFA	2	0
3	F	306	LFA	1	0
3	H	305	LFA	1	0
3	J	304	LFA	1	0
3	D	317	LFA	2	0
3	F	312	LFA	3	0
3	F	302	LFA	2	0
3	F	304	LFA	1	0
3	G	308	LFA	1	0
3	H	302	LFA	1	0
3	D	306	LFA	2	0
3	C	306	LFA	3	0
3	E	310	LFA	1	0
3	D	316	LFA	2	0
3	C	305	LFA	1	0
3	A	311	LFA	2	0
4	E	313	MPG	3	0
3	A	307	LFA	1	0
3	I	303	LFA	1	0
4	F	315	MPG	1	0
3	G	303	LFA	2	0

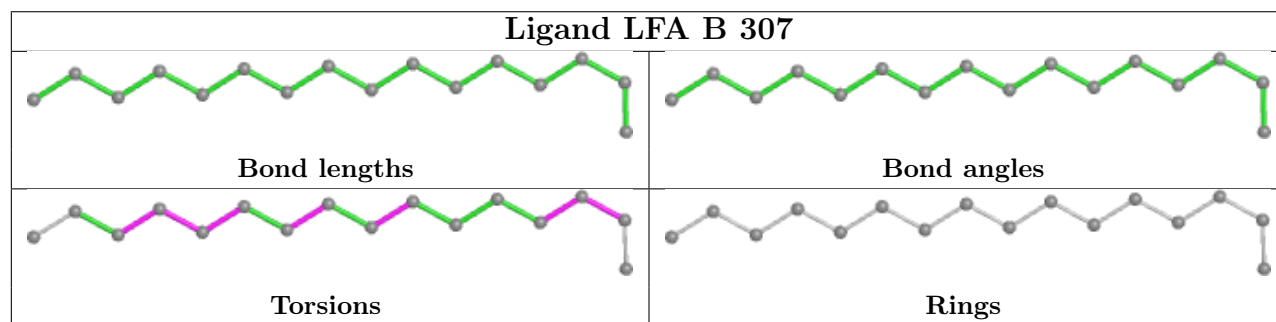
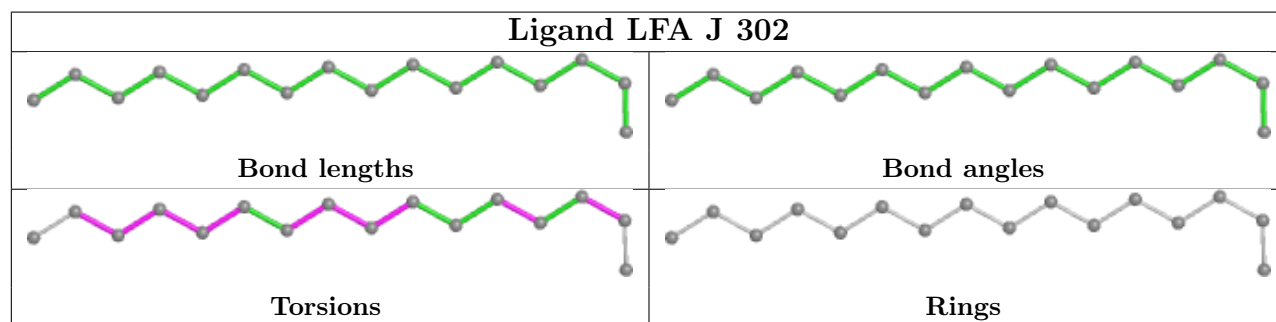
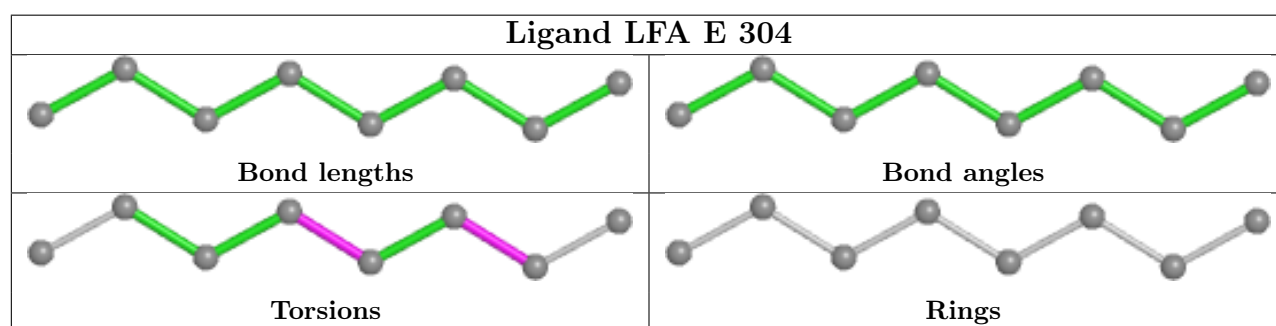
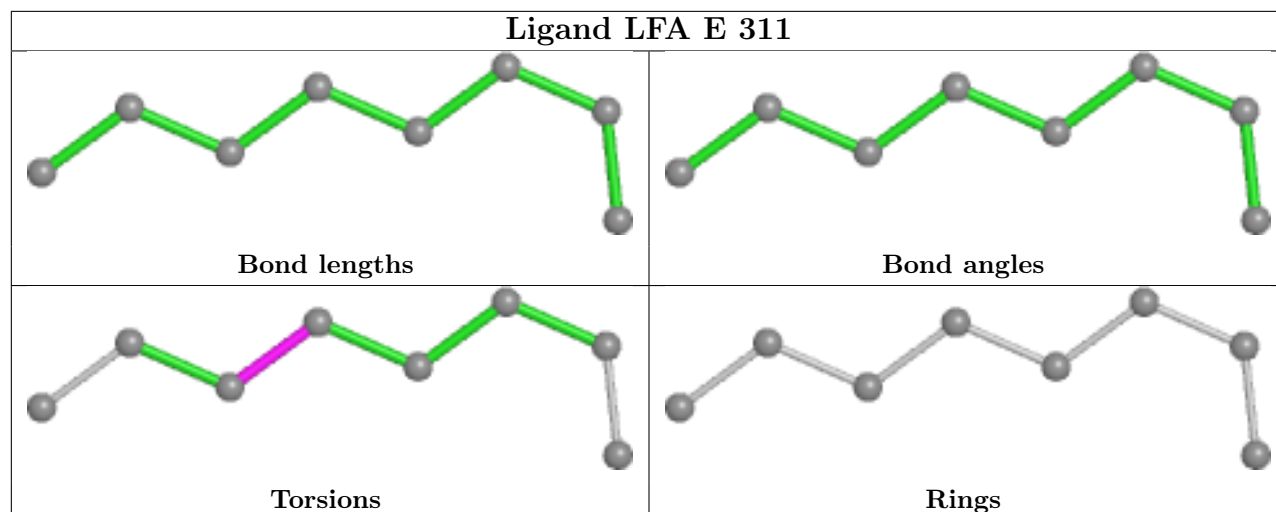
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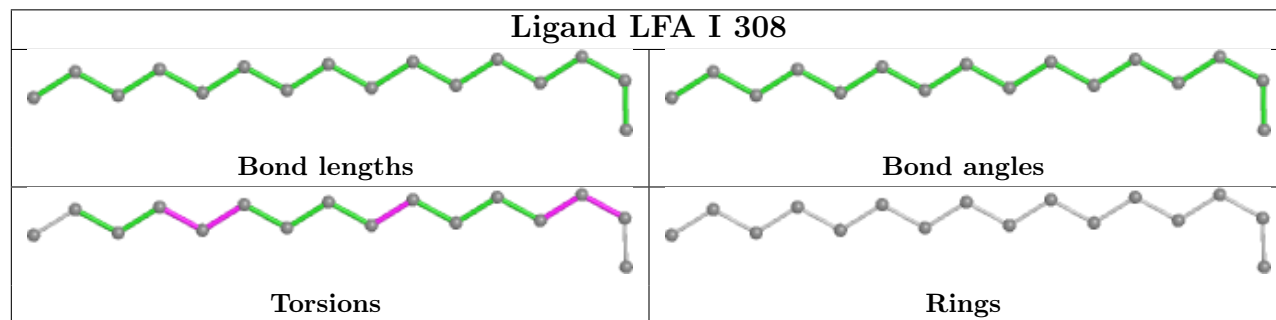
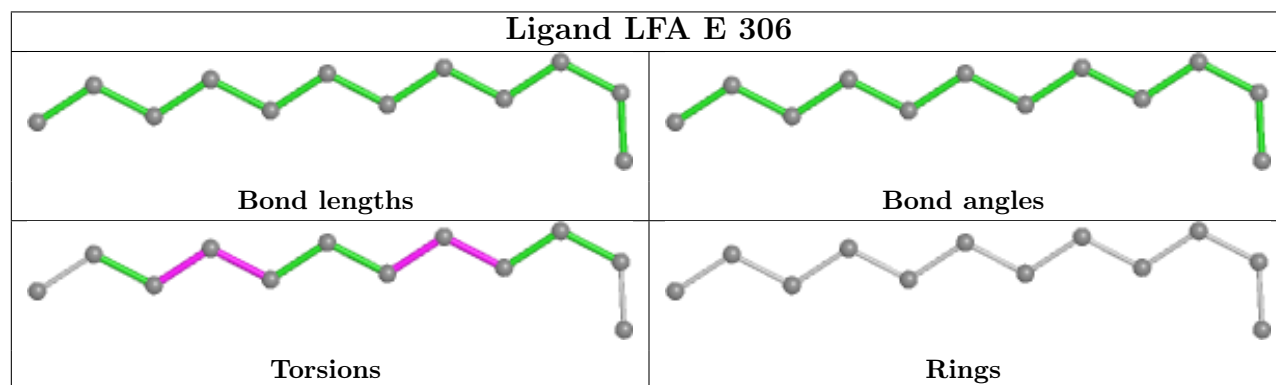
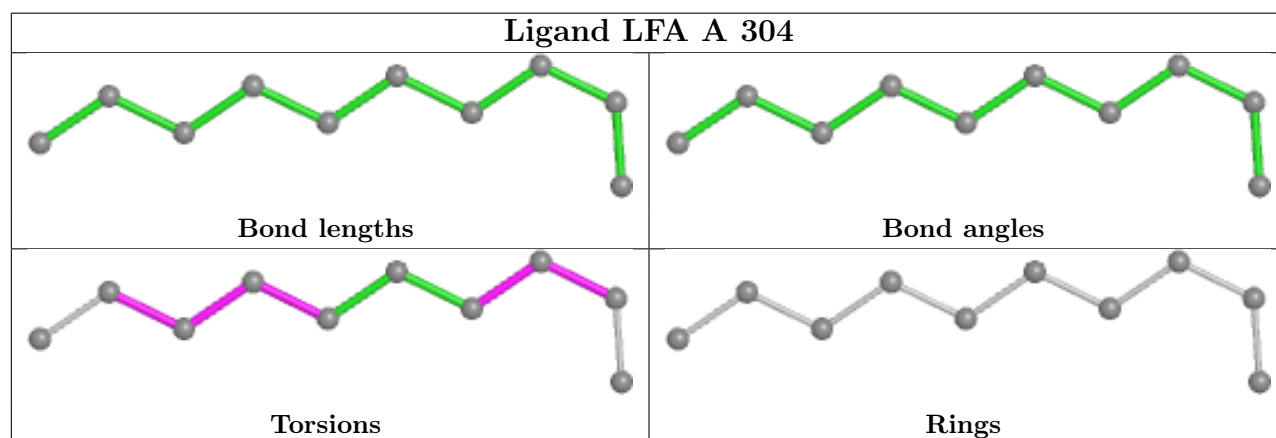
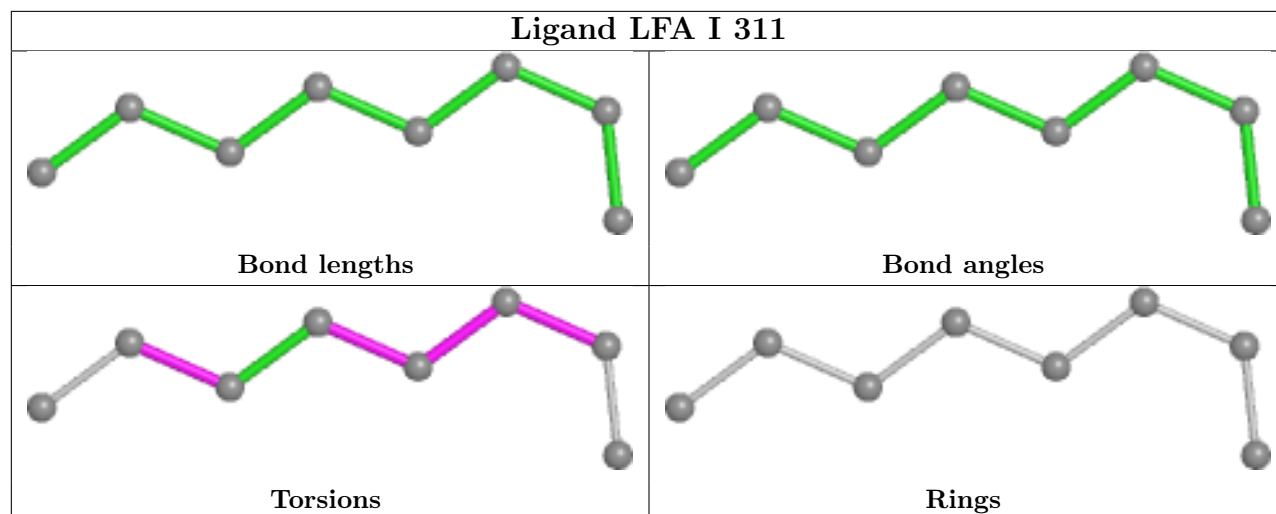
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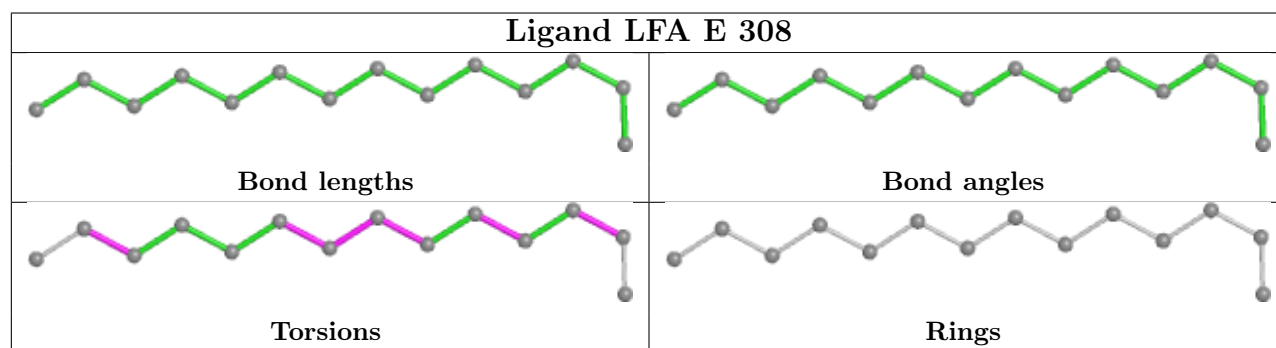
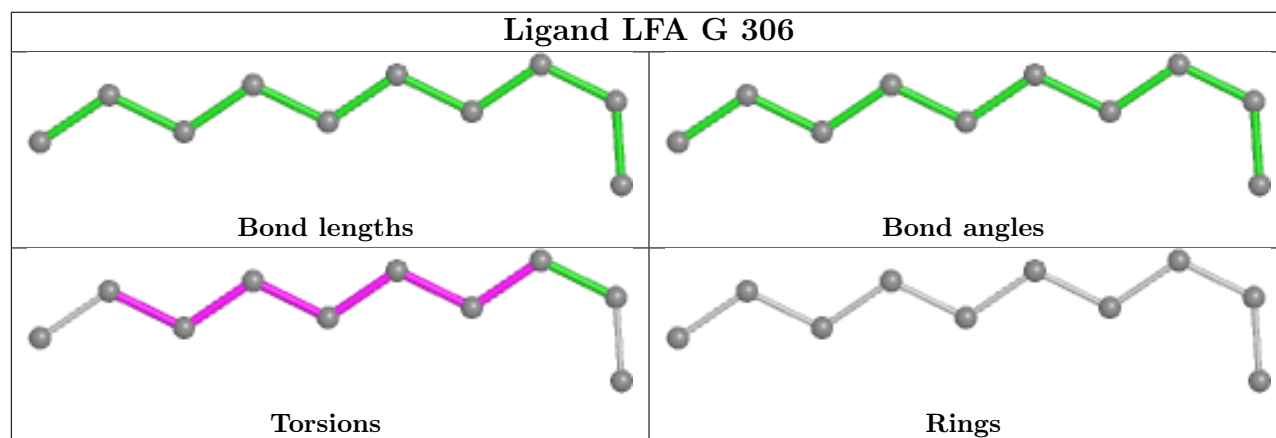
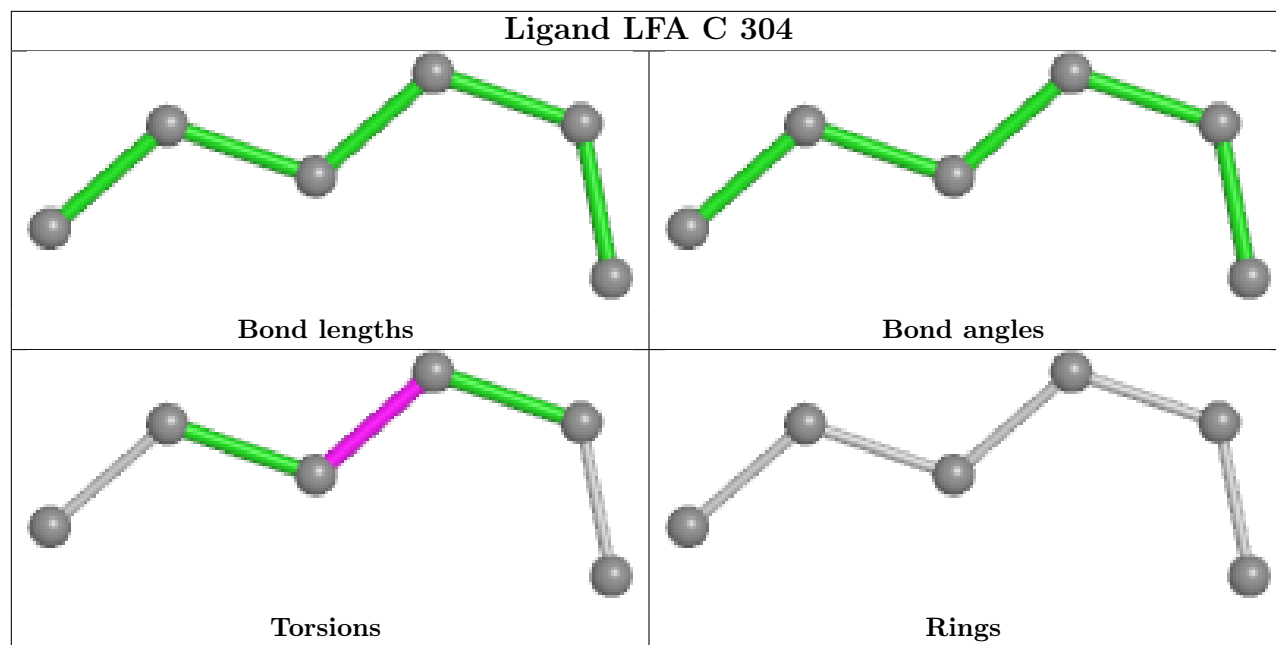
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	311	LFA	3	0

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.

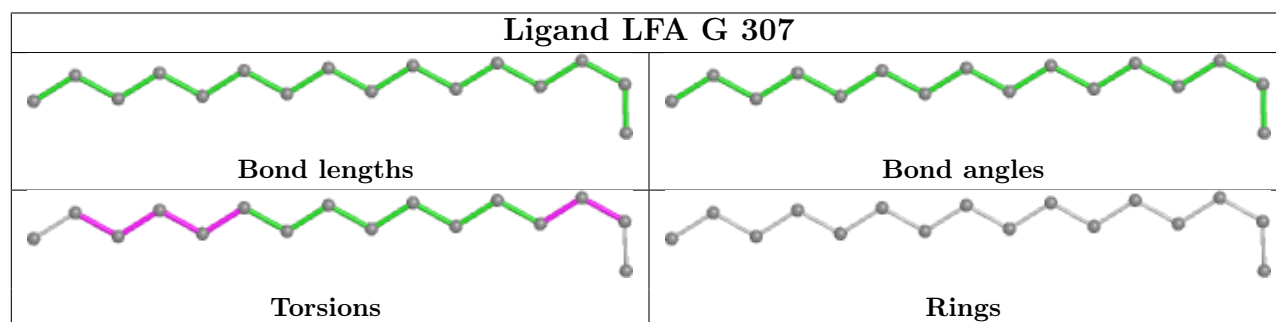
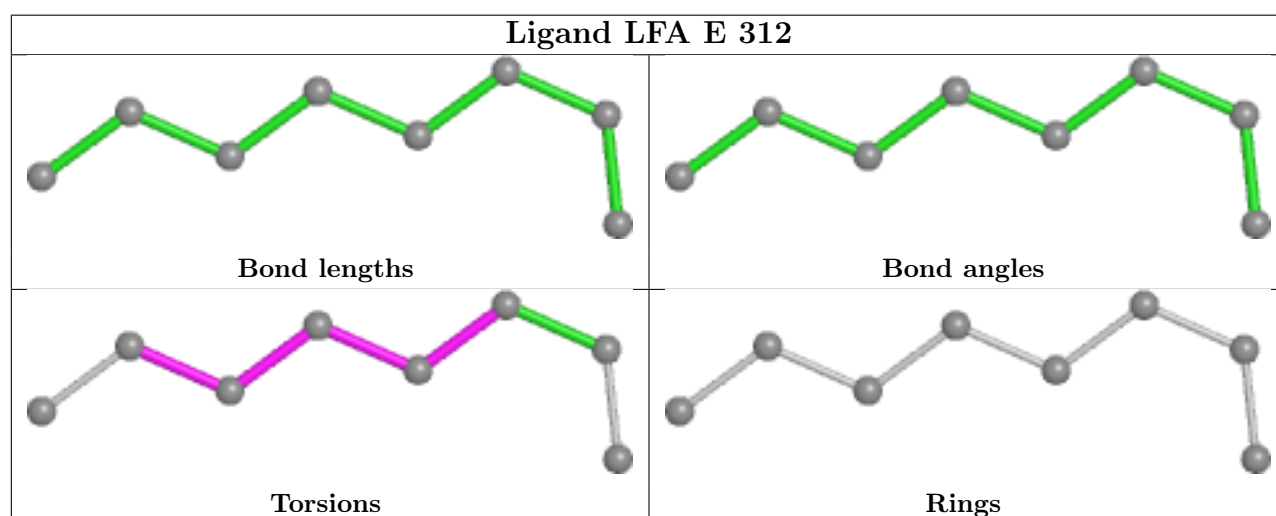
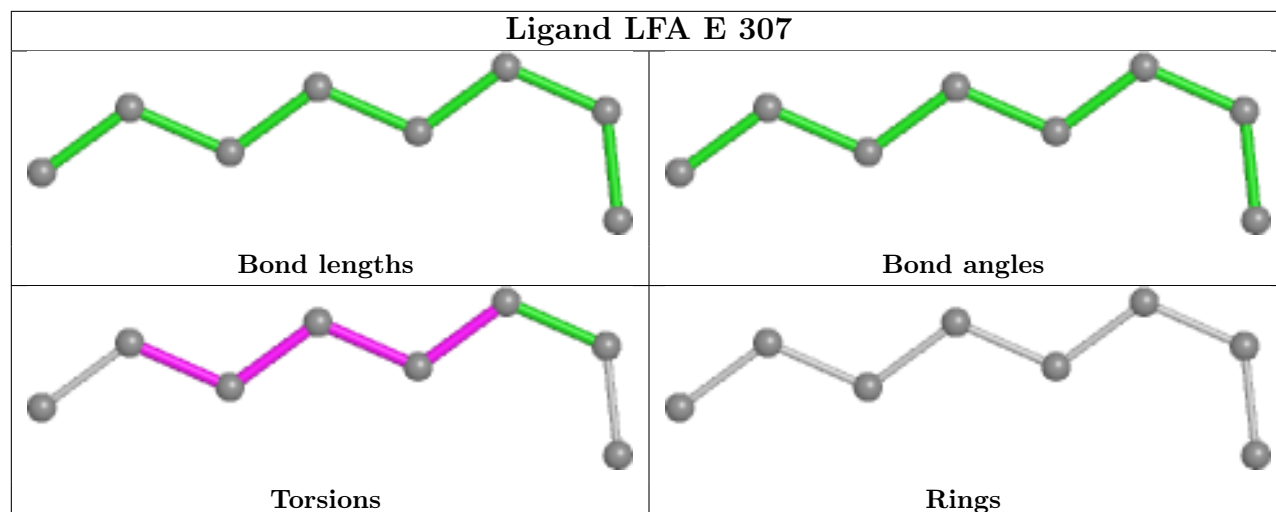


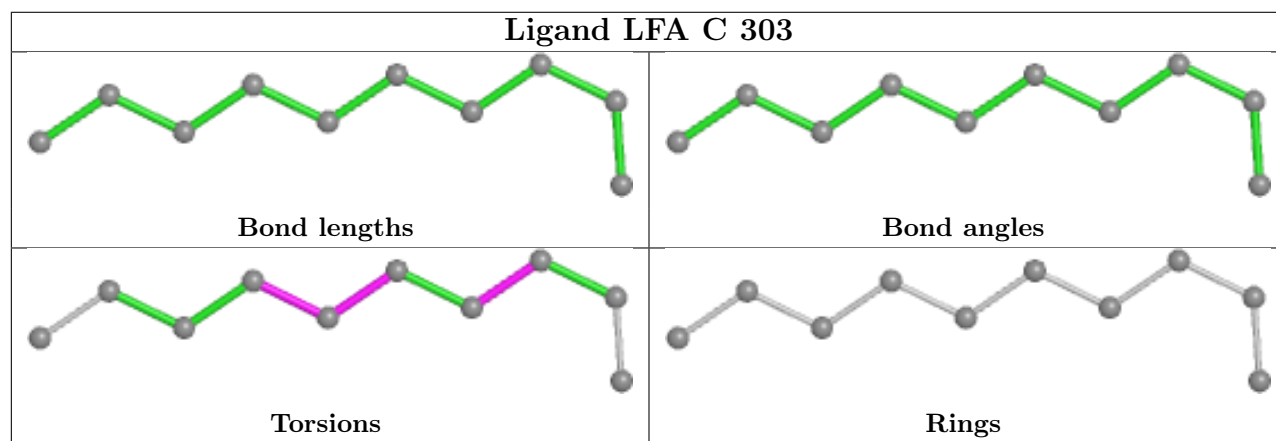
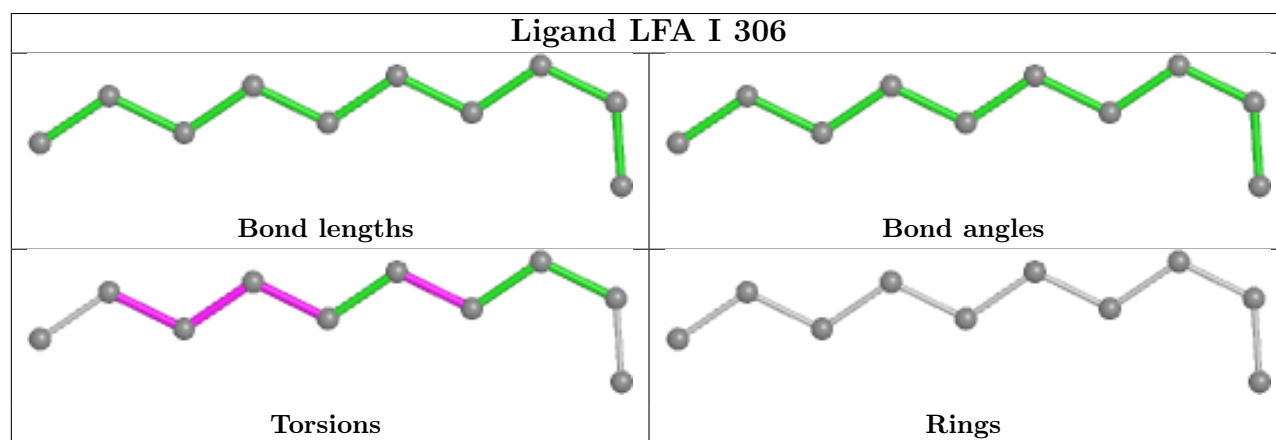
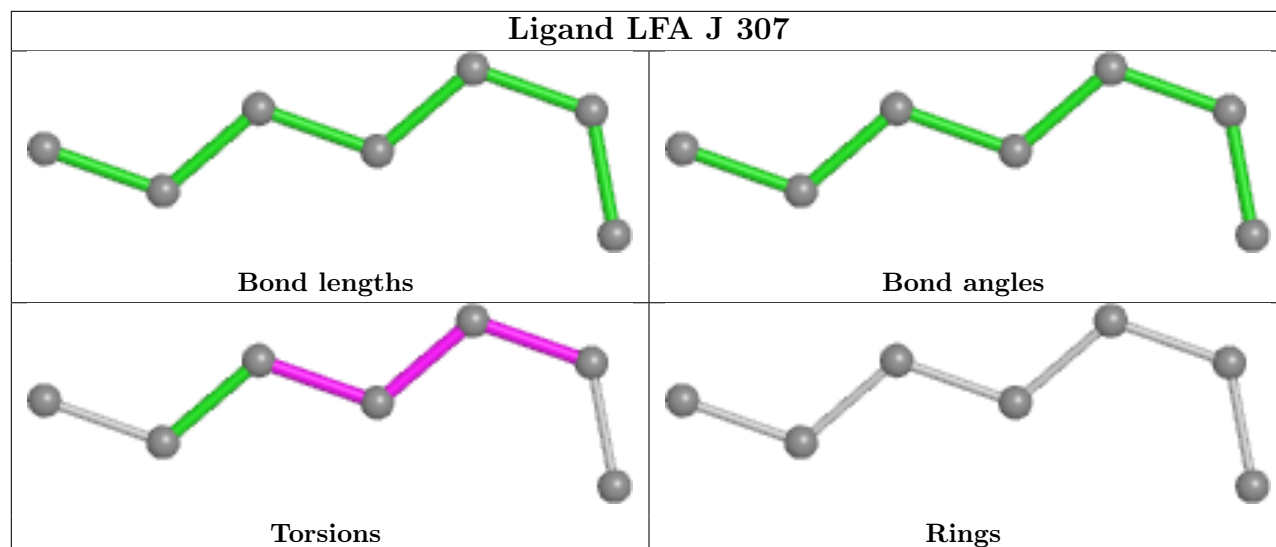


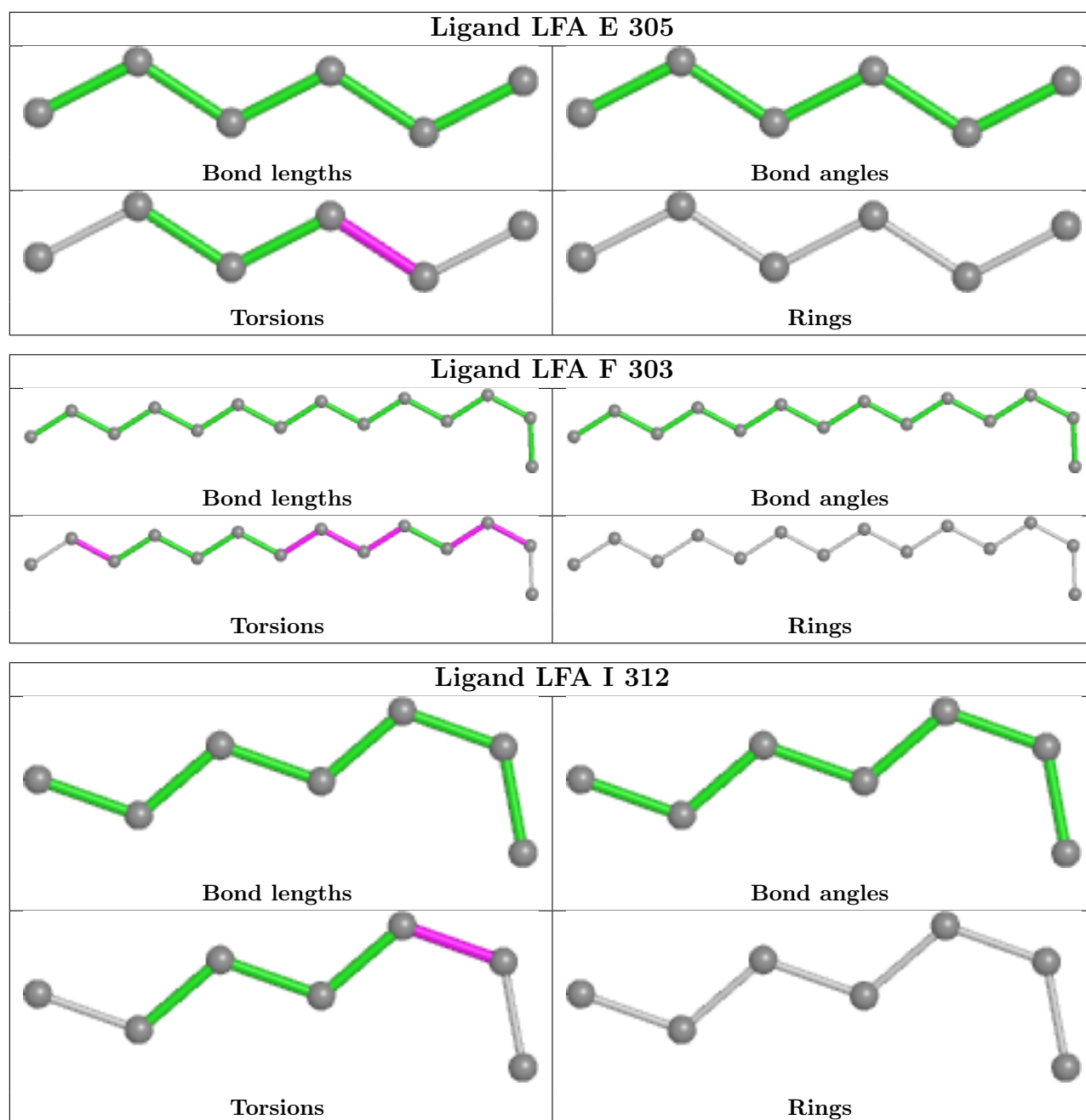


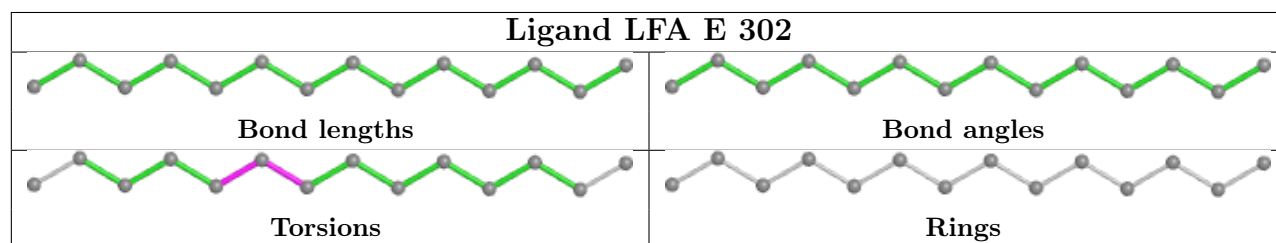
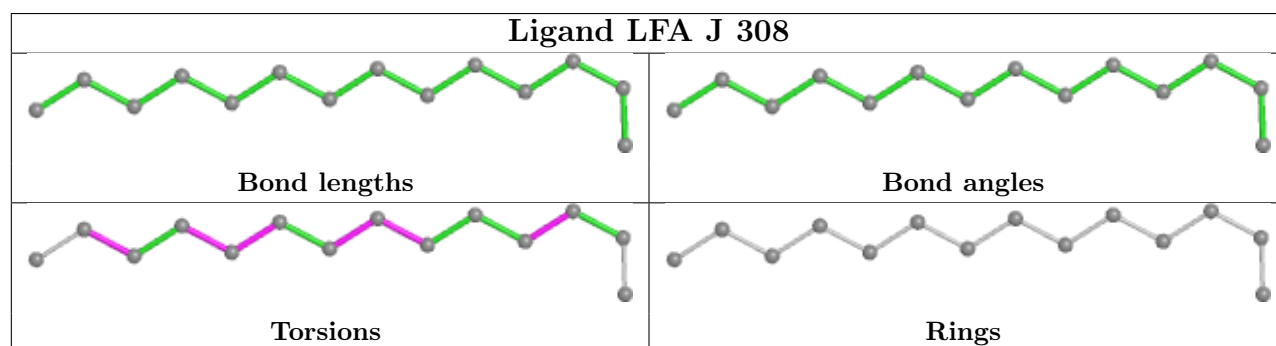
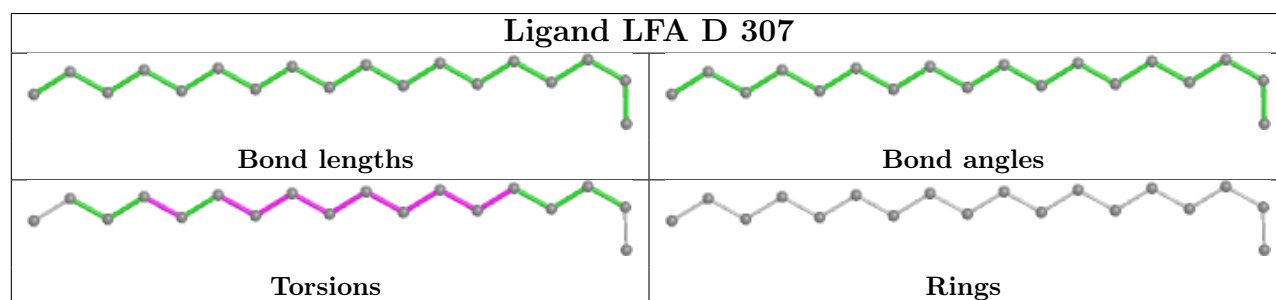
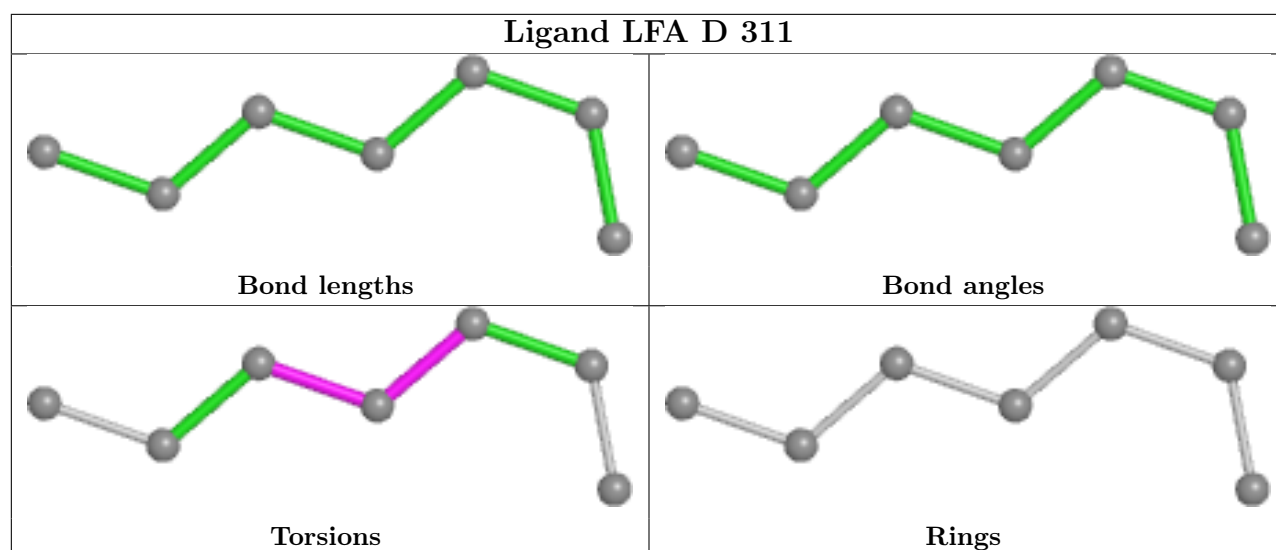


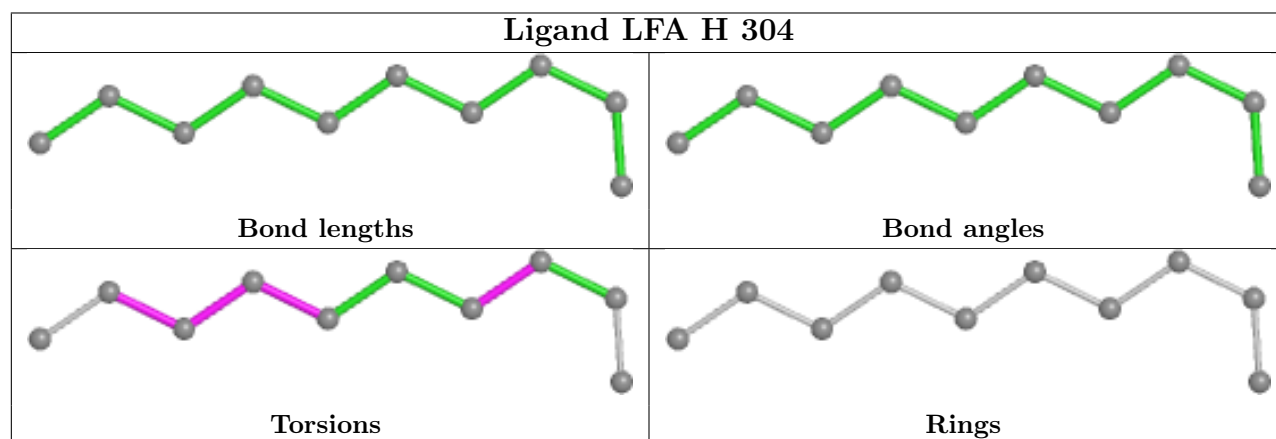
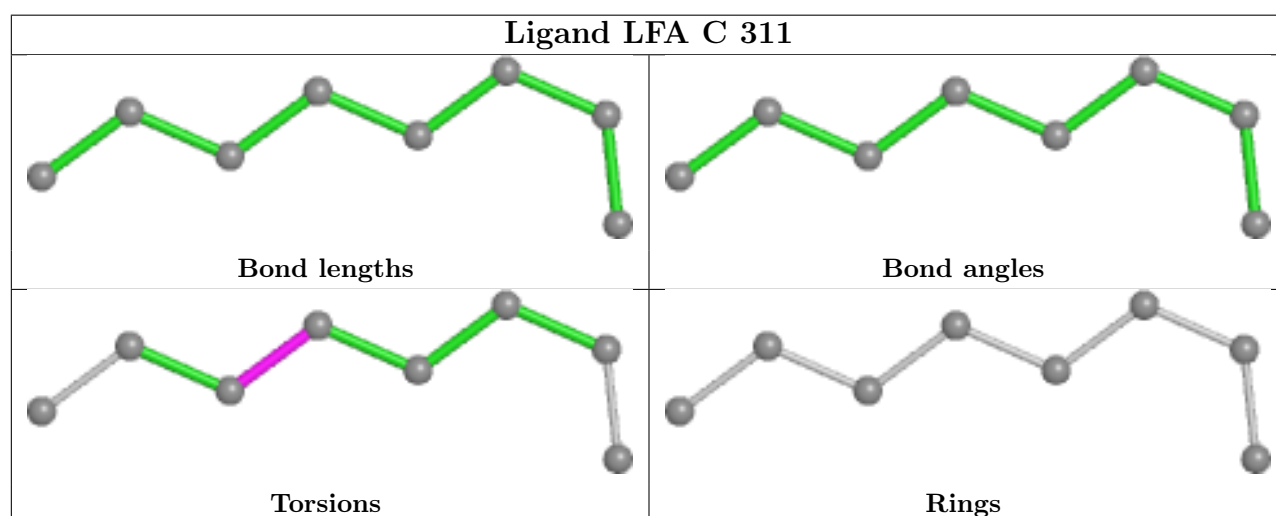
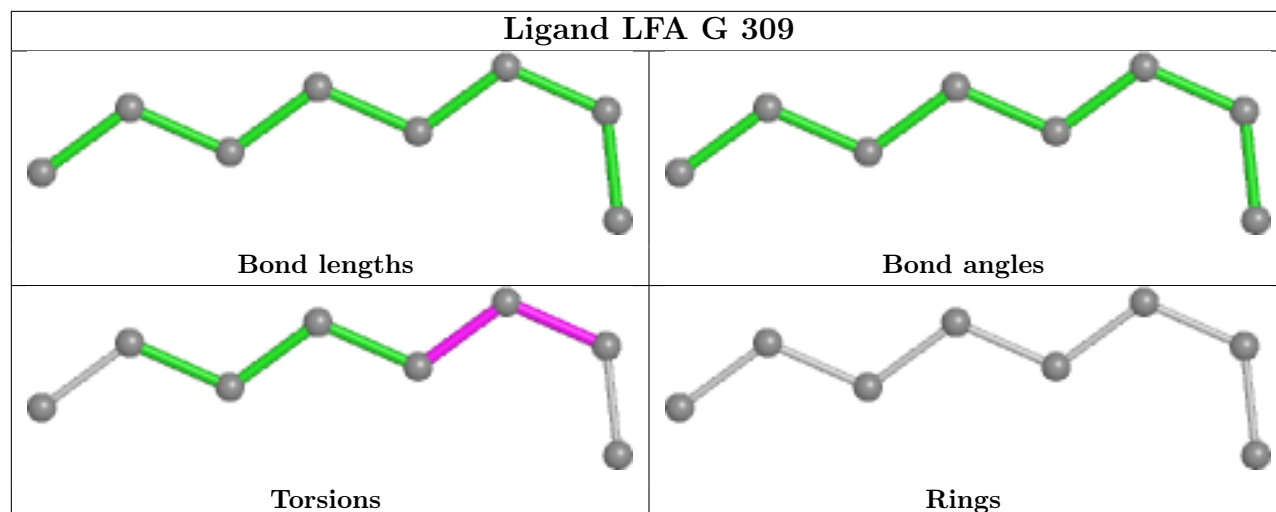


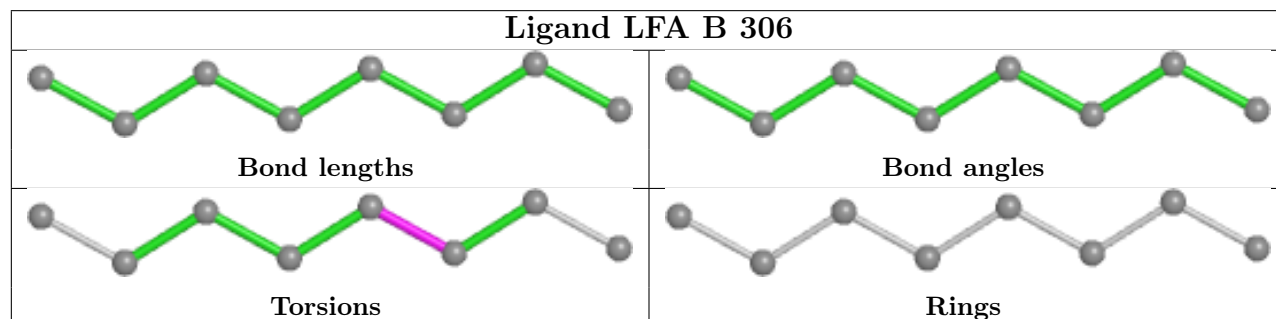
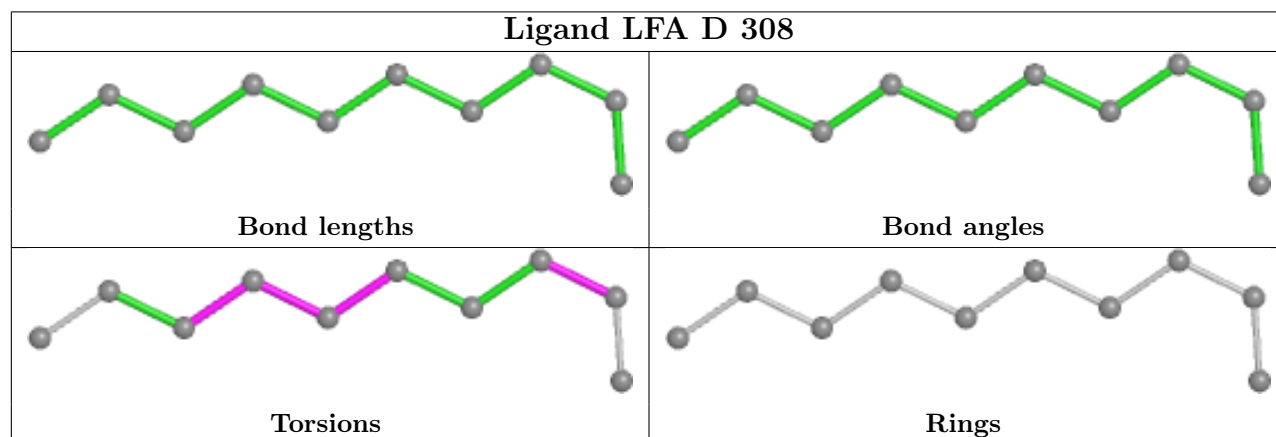
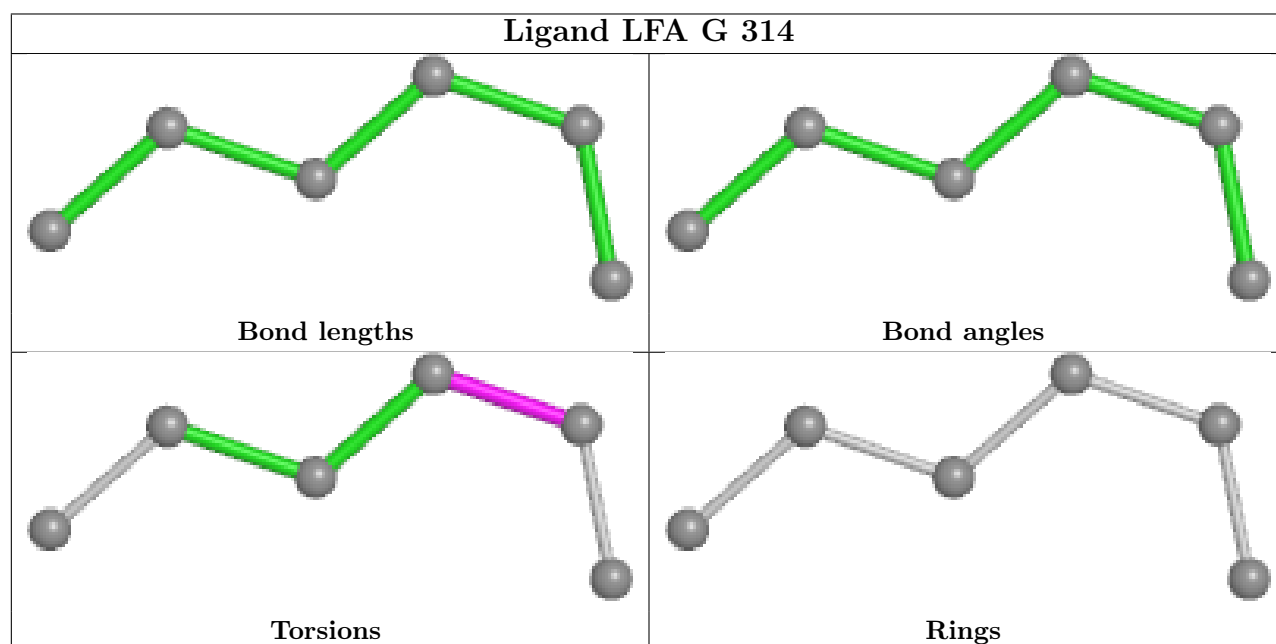
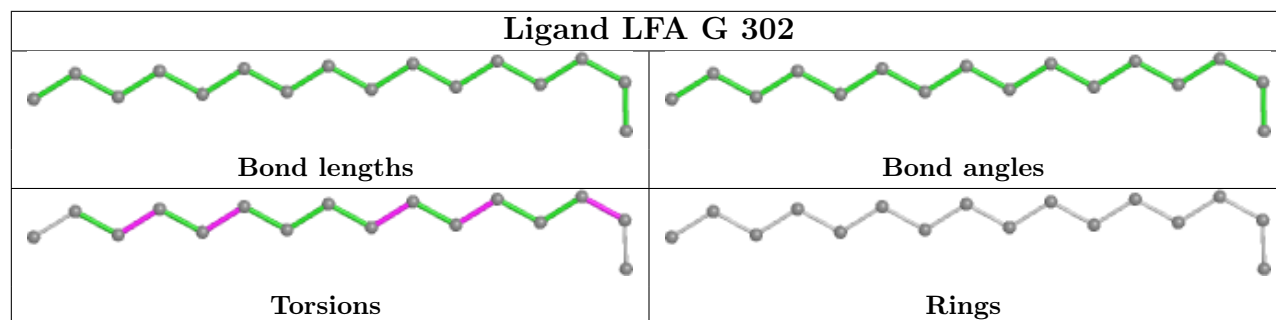


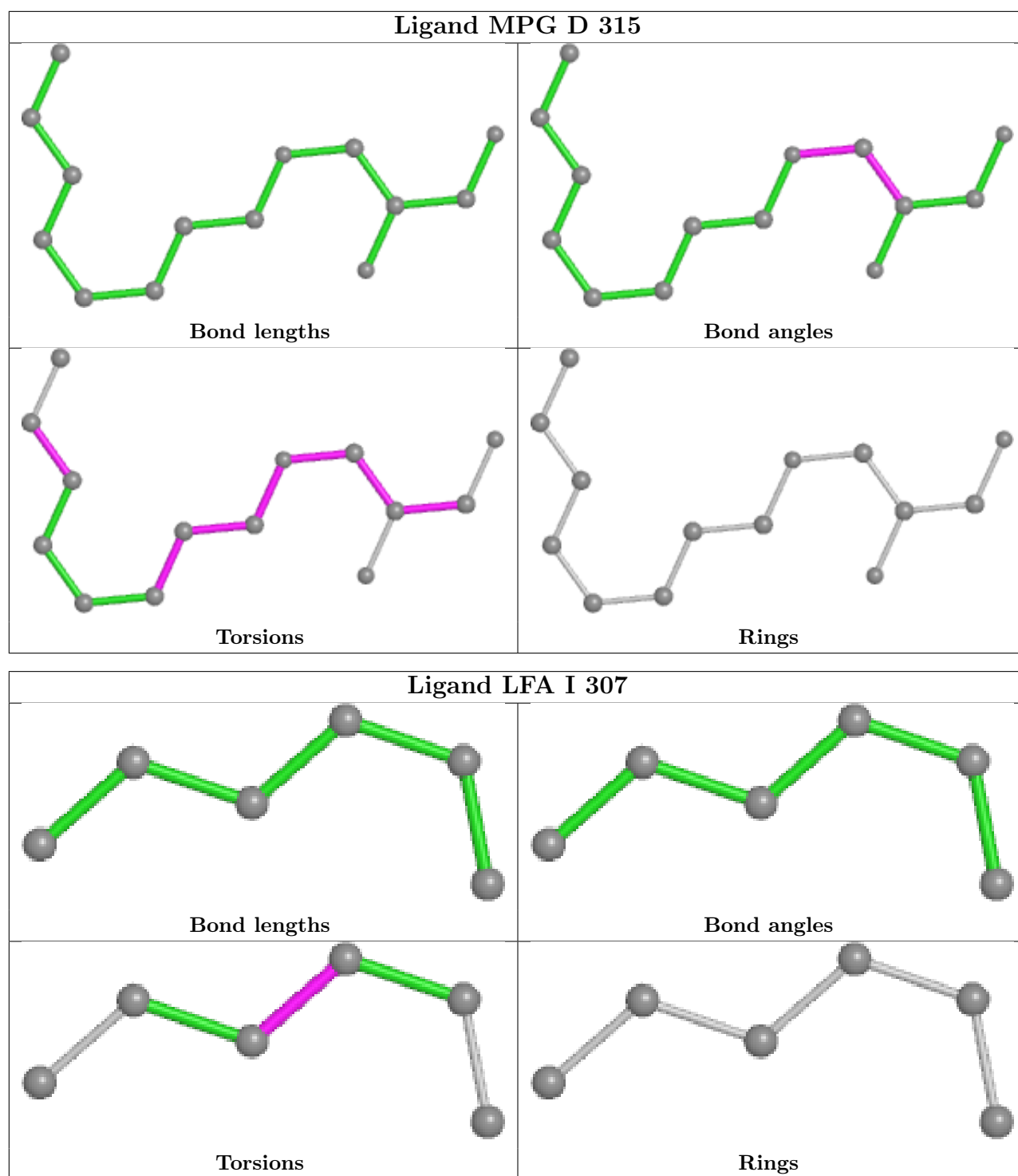


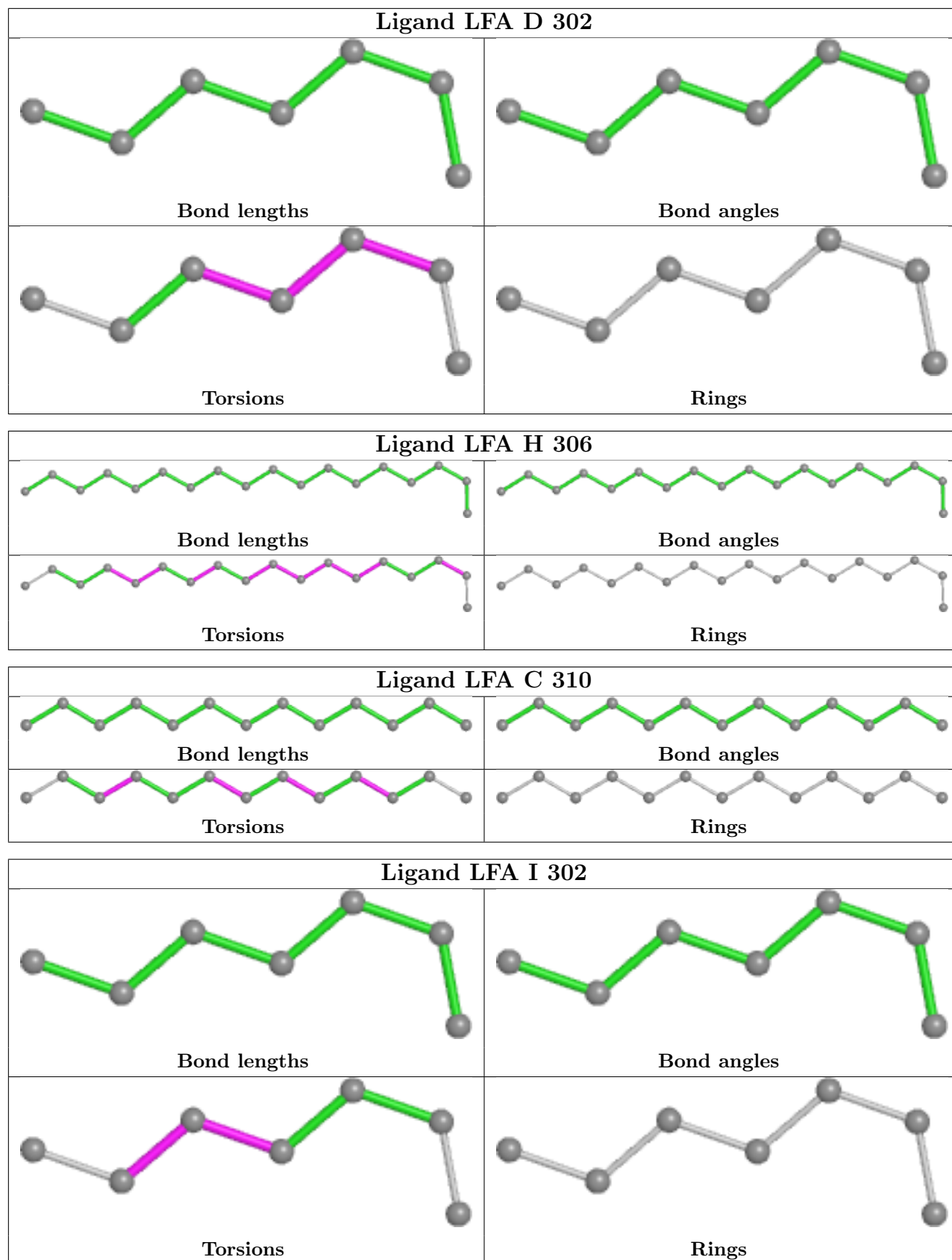




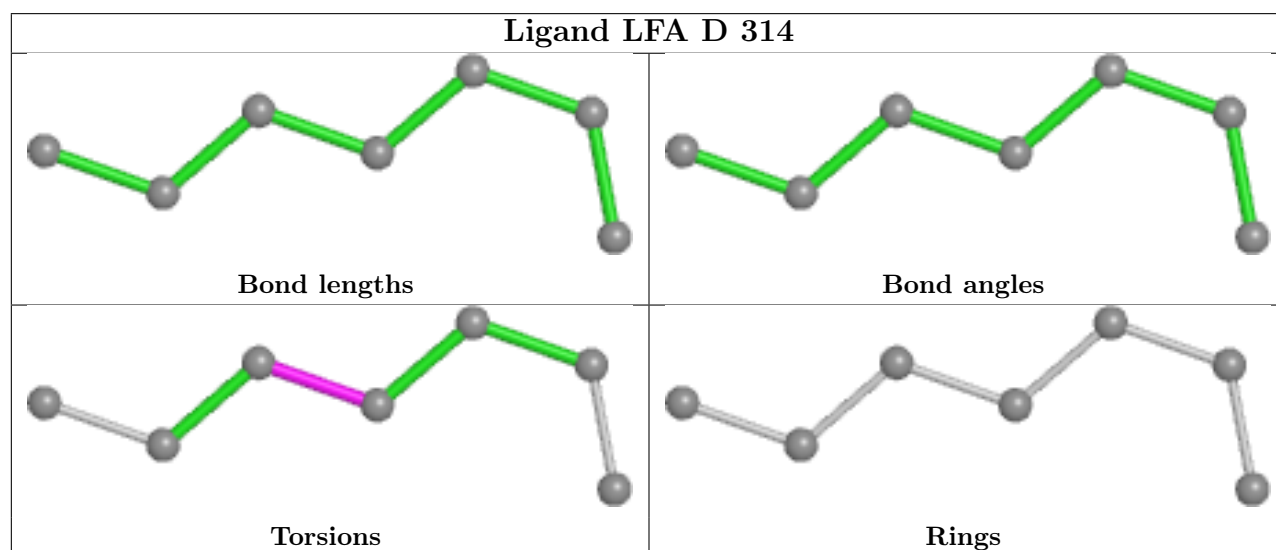
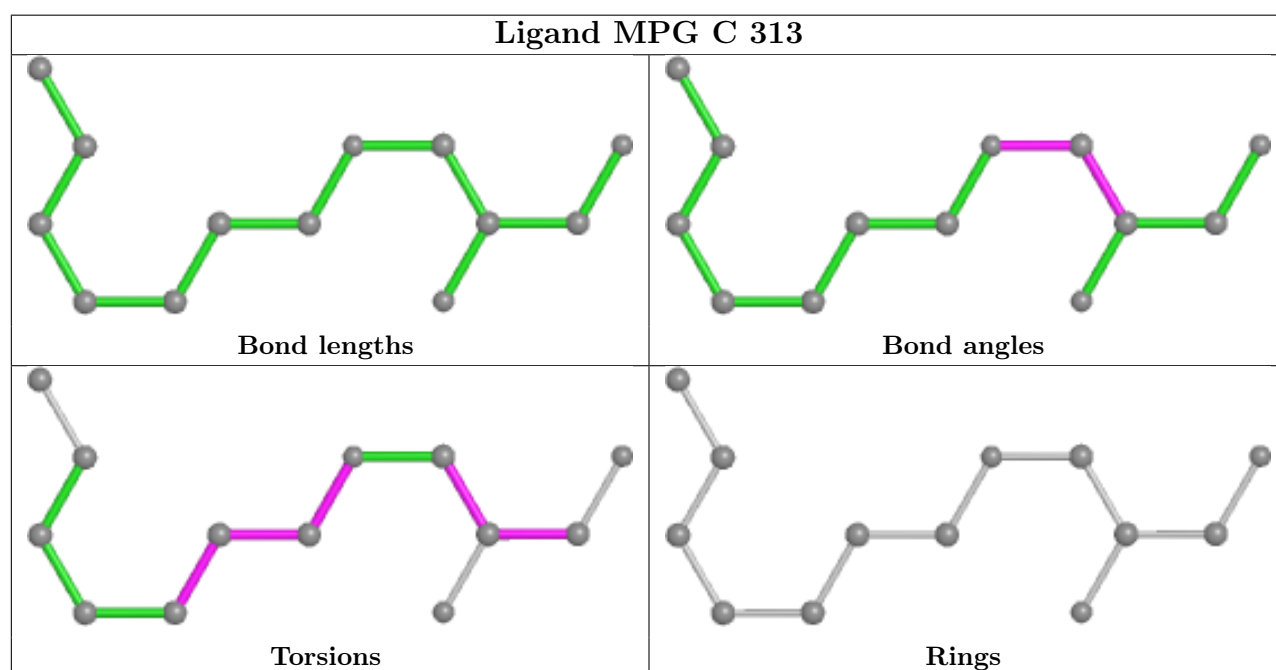
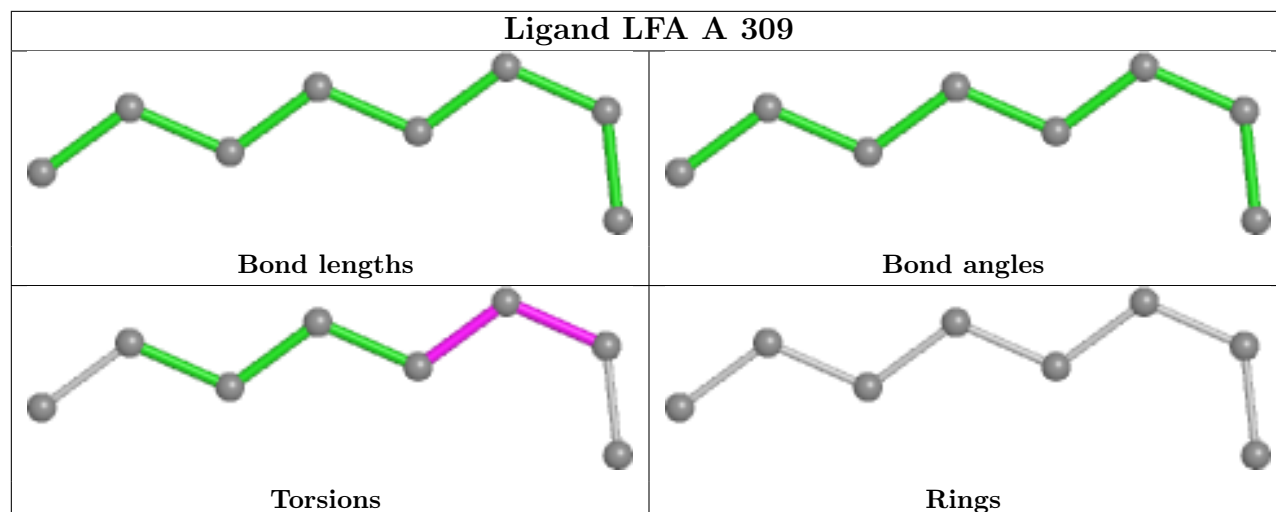


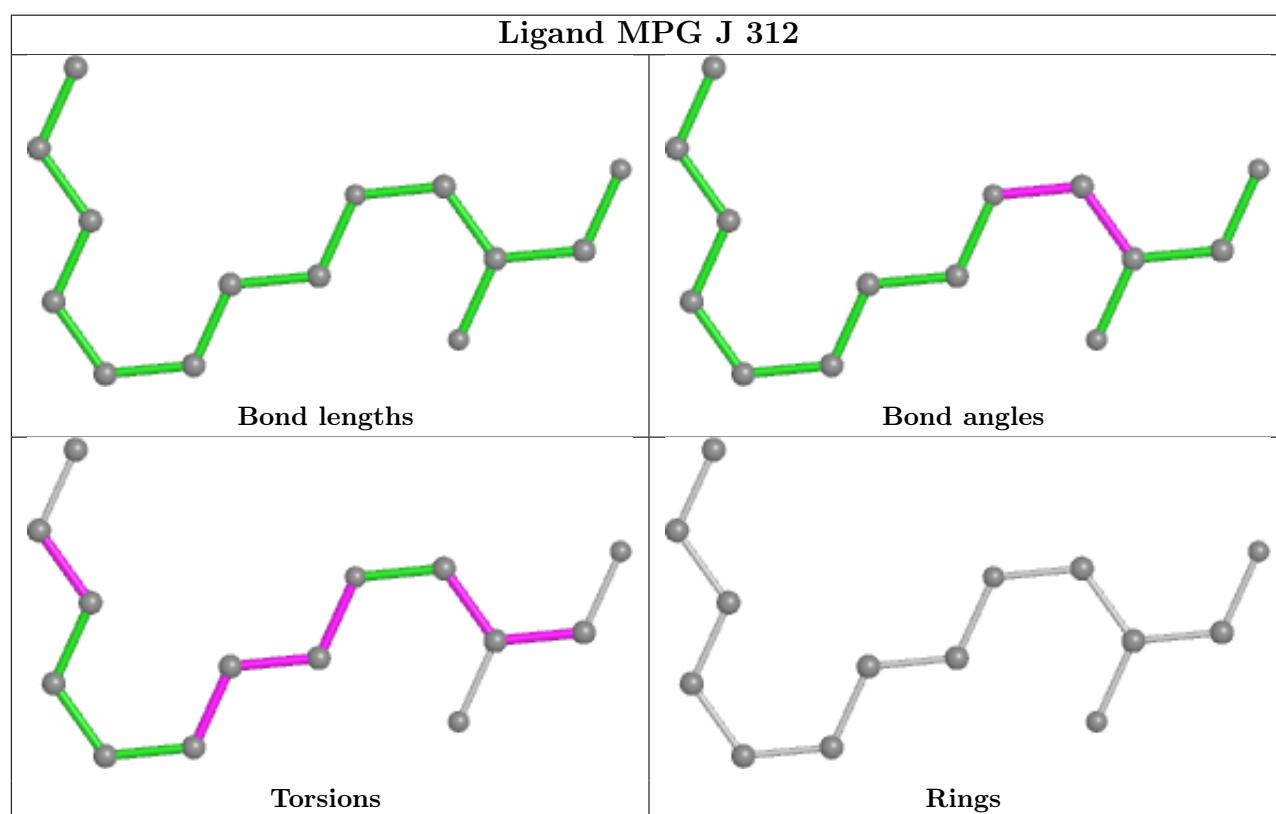
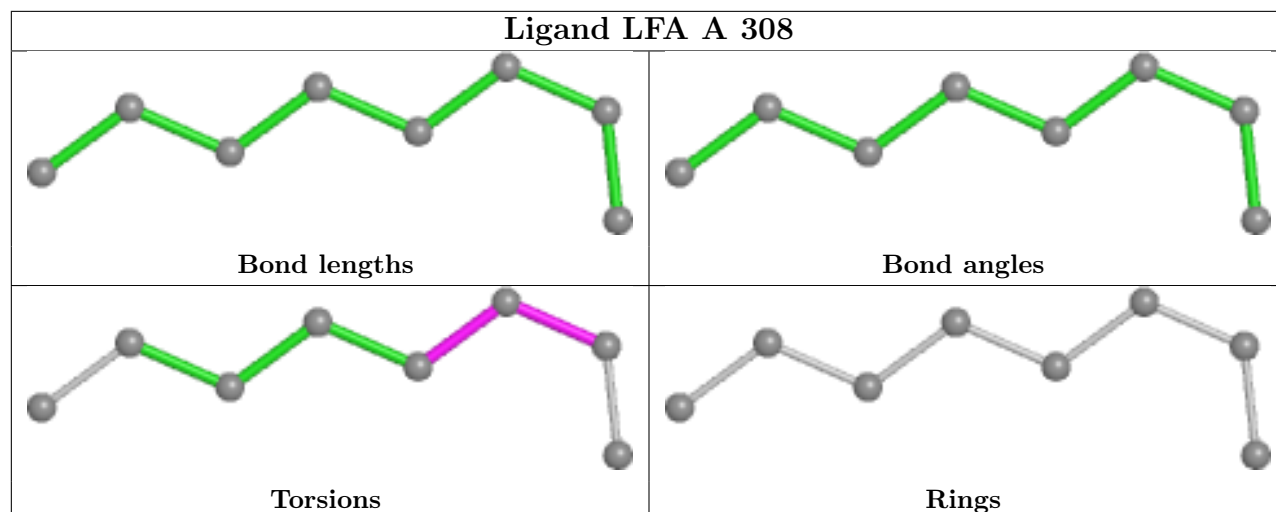


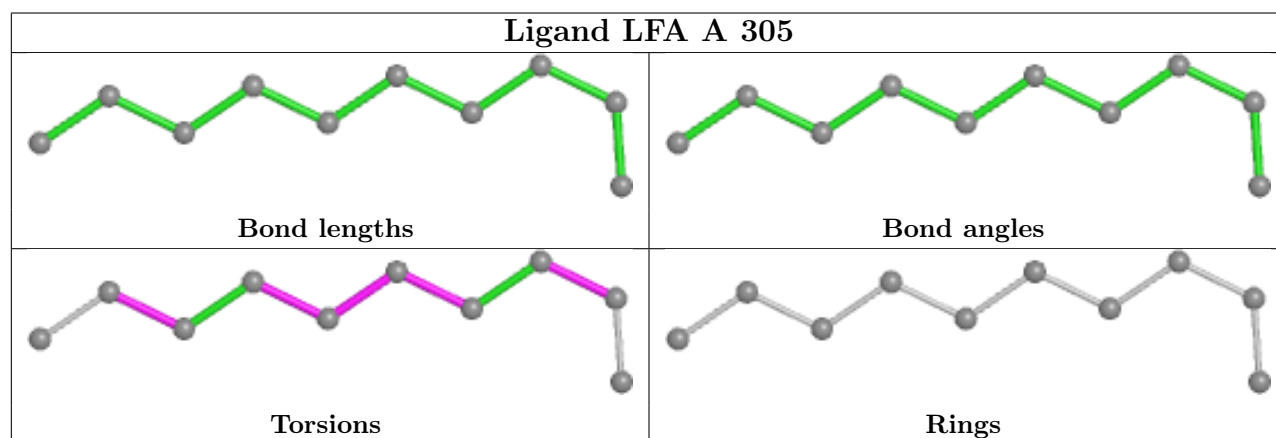
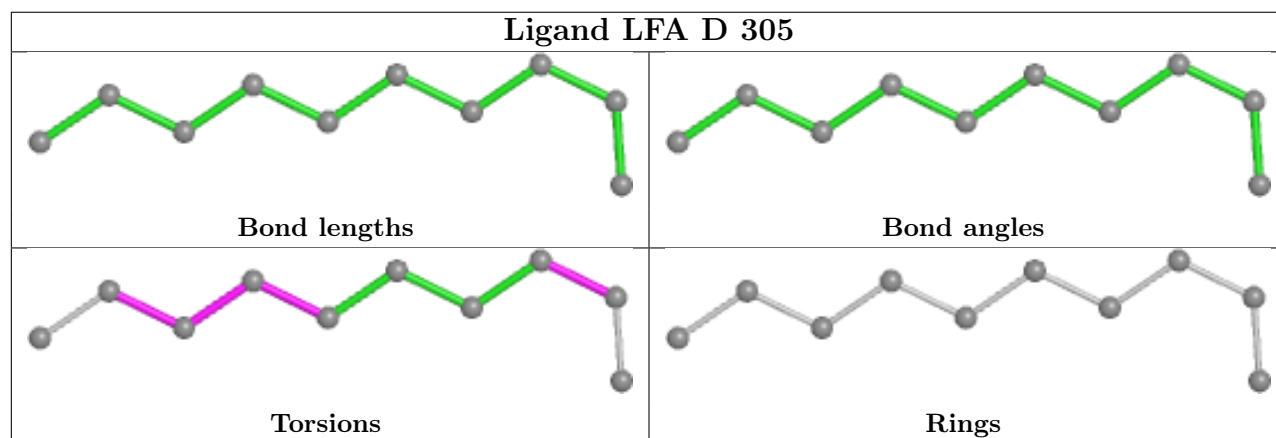
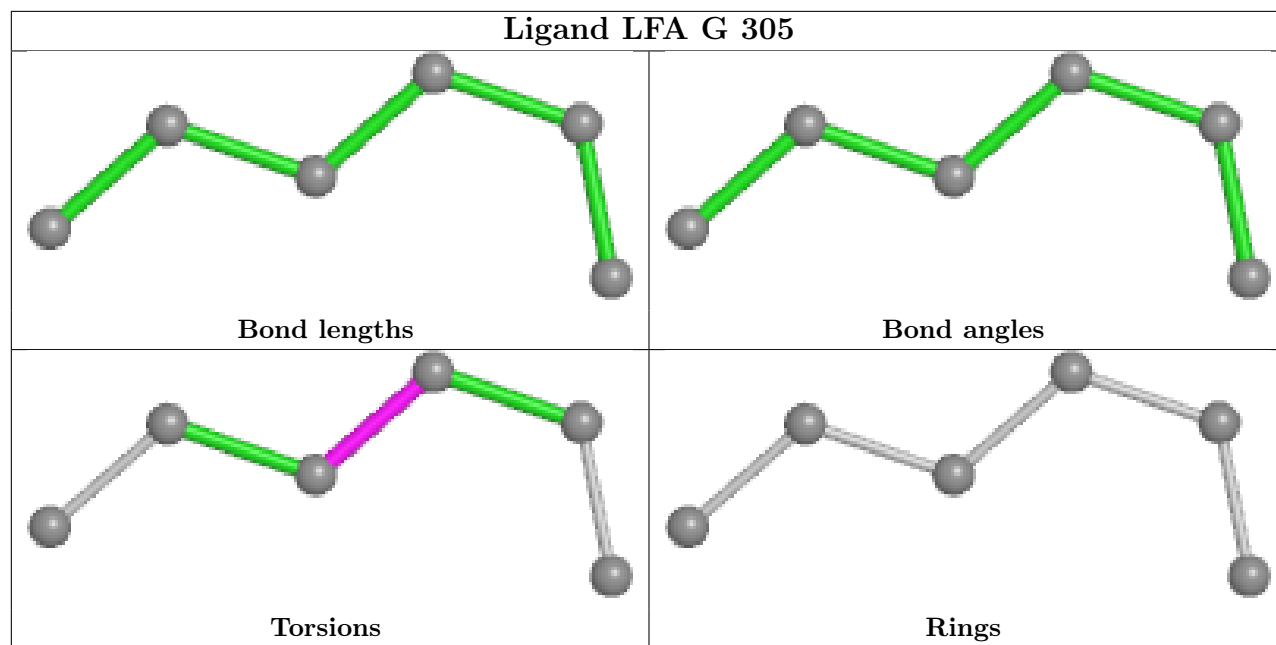


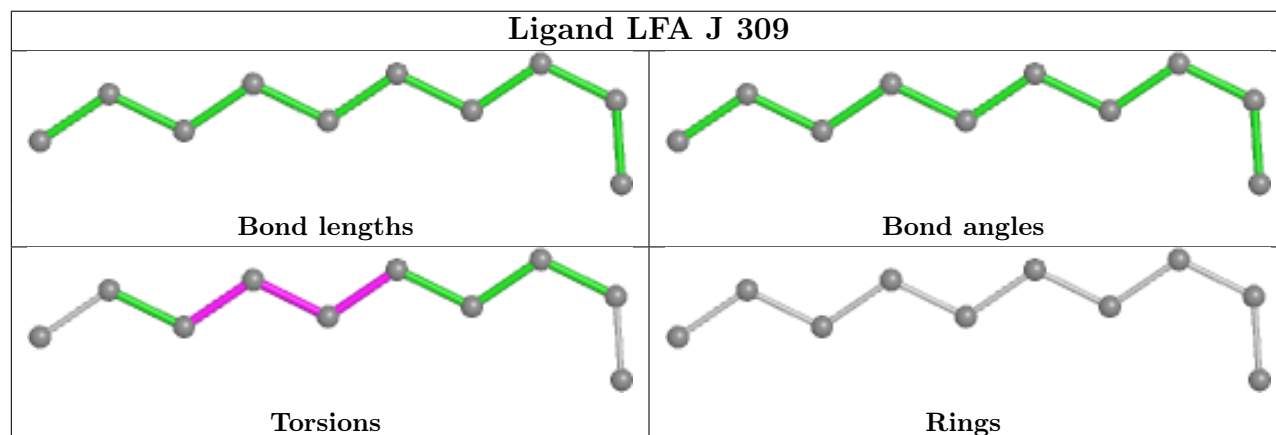
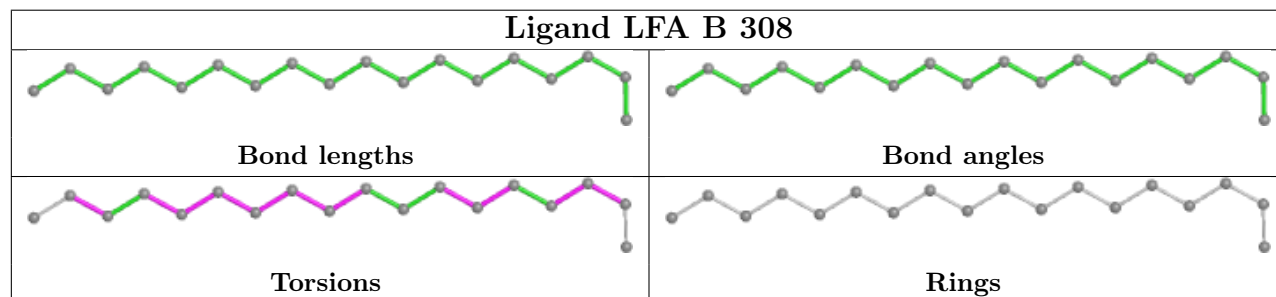
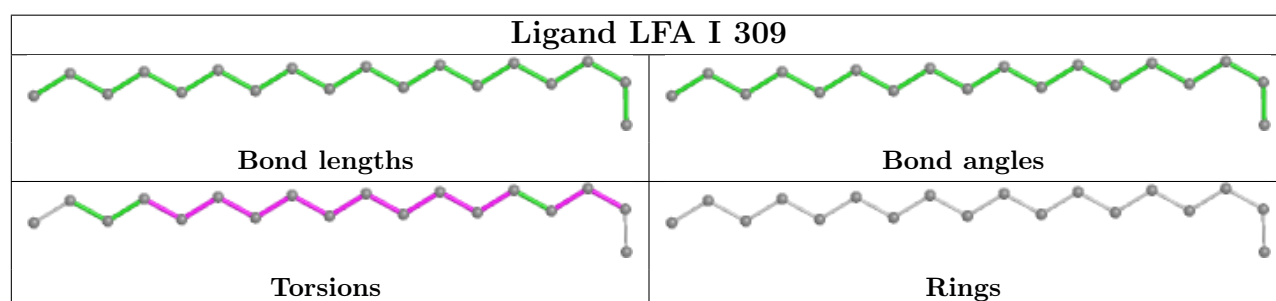
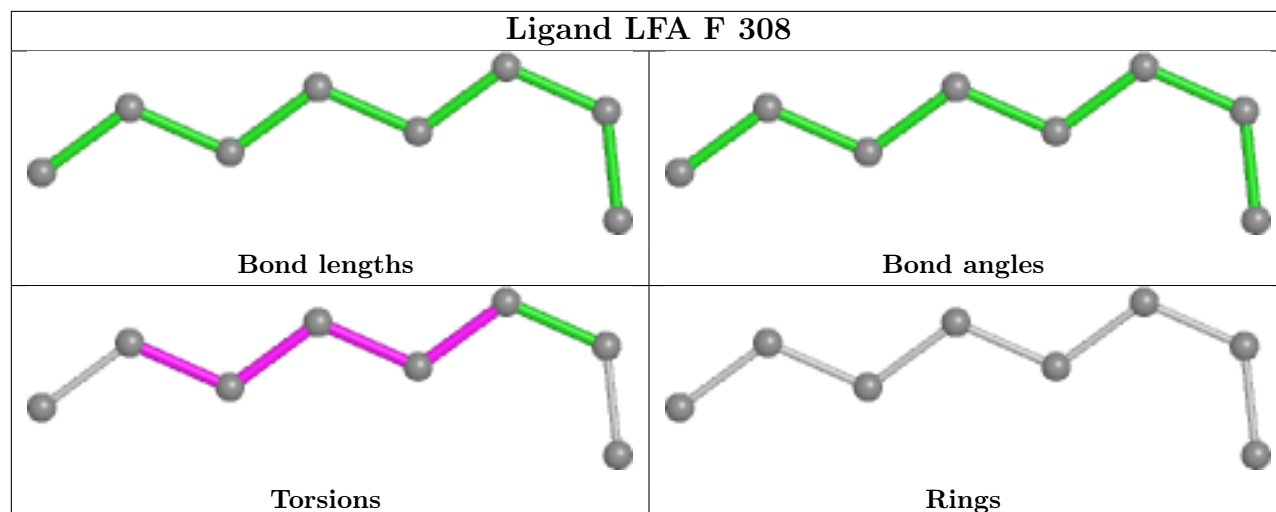


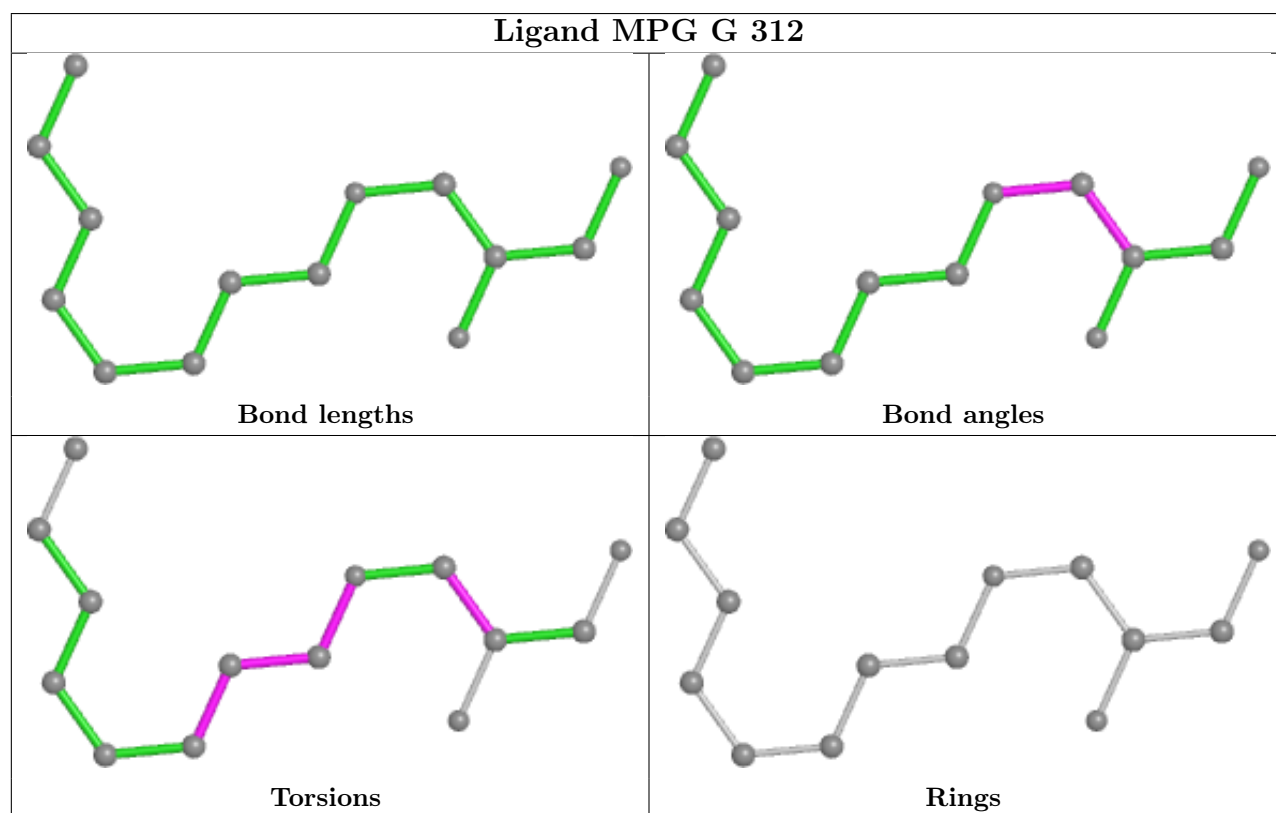
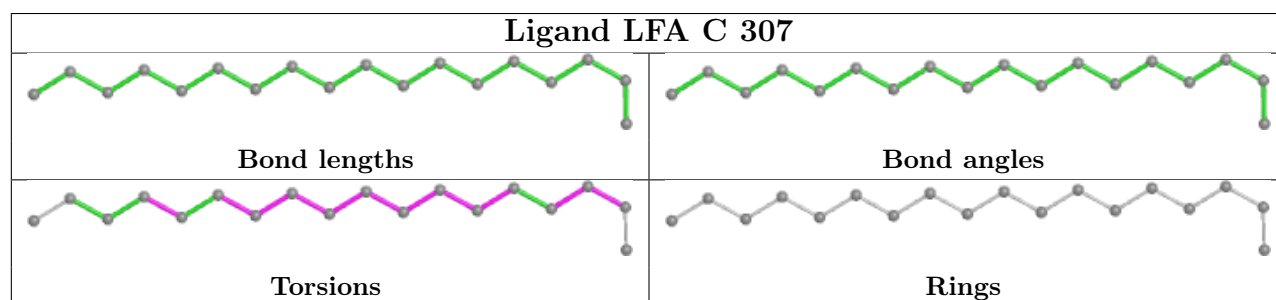
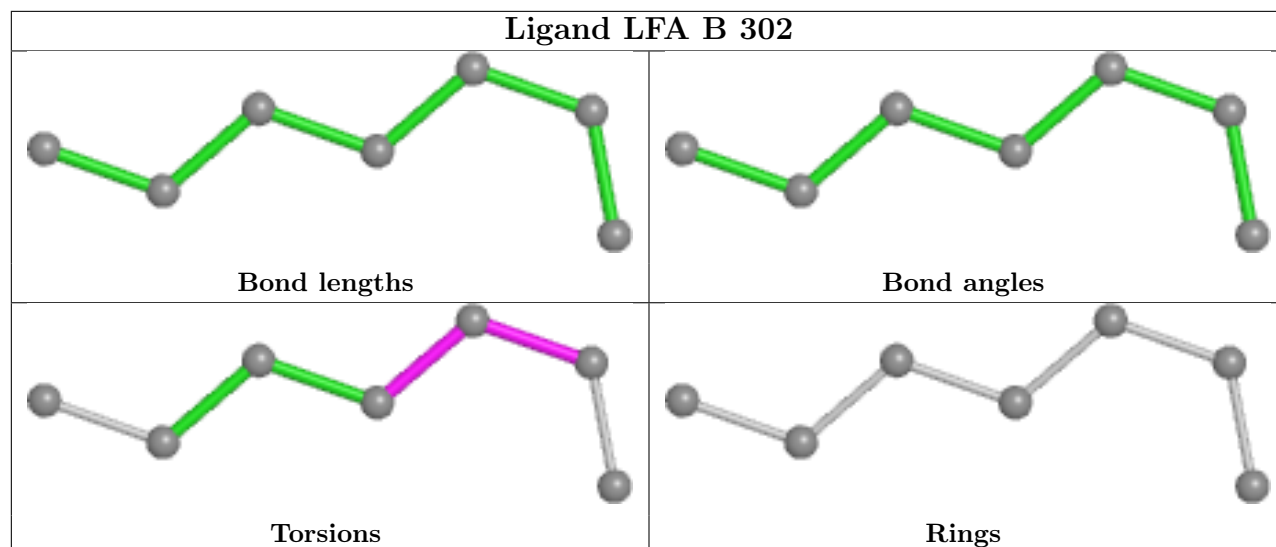


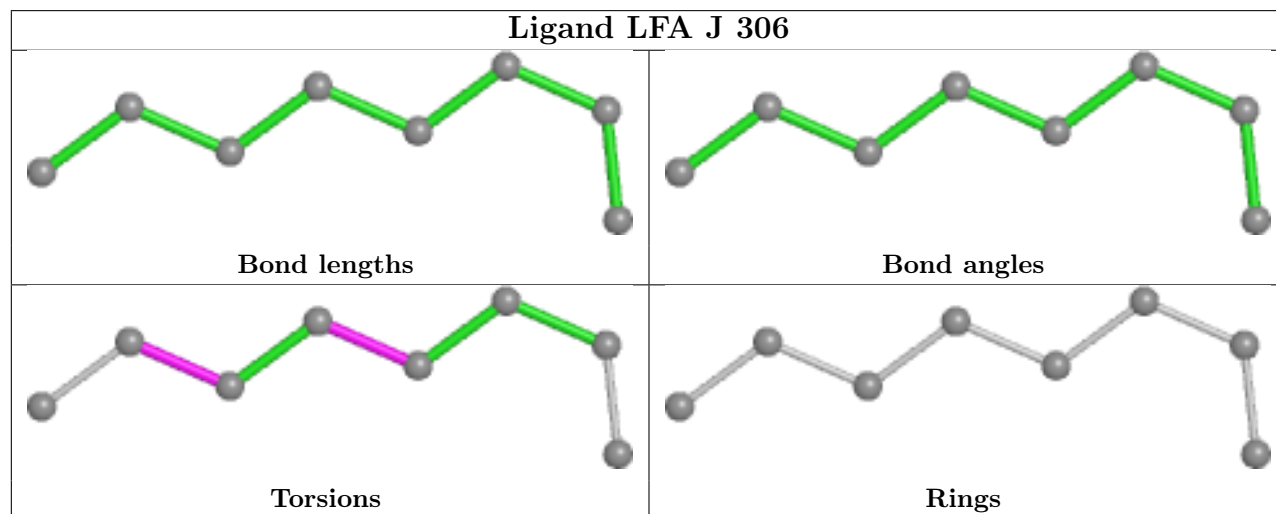
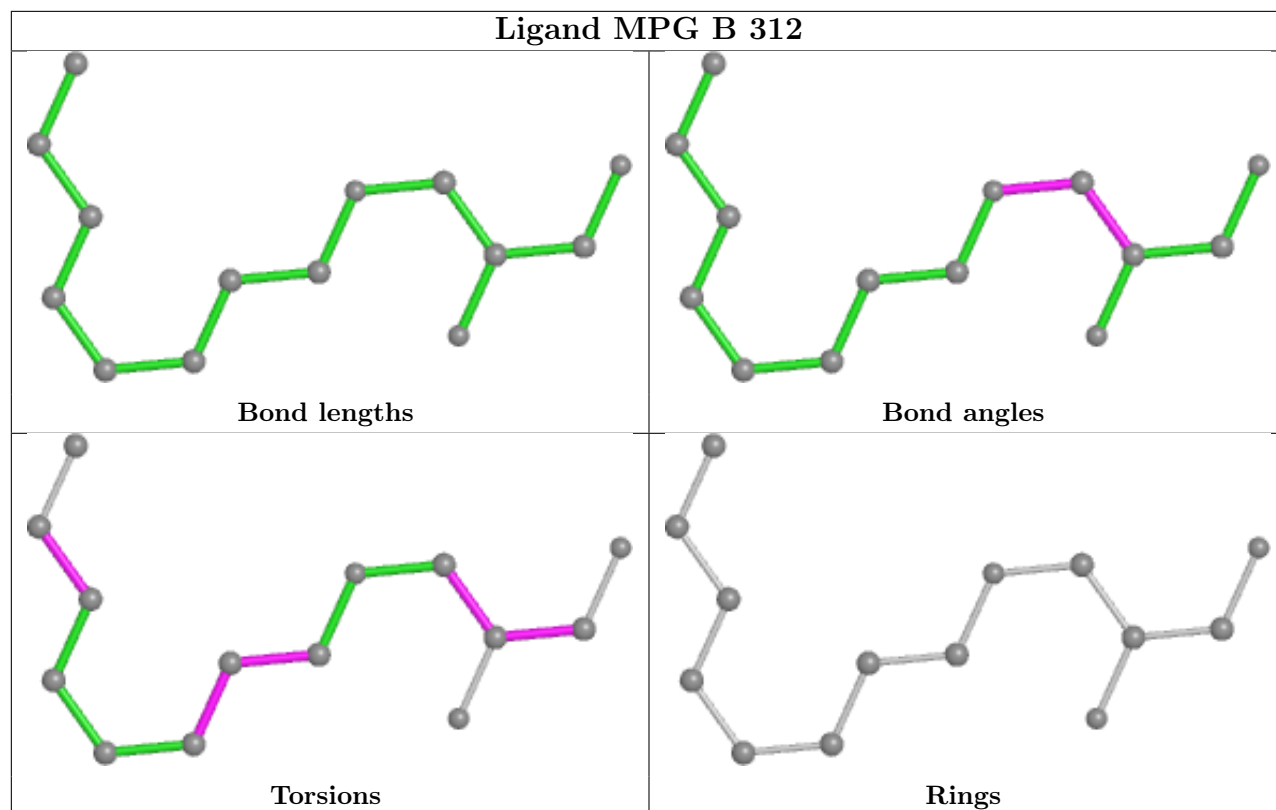


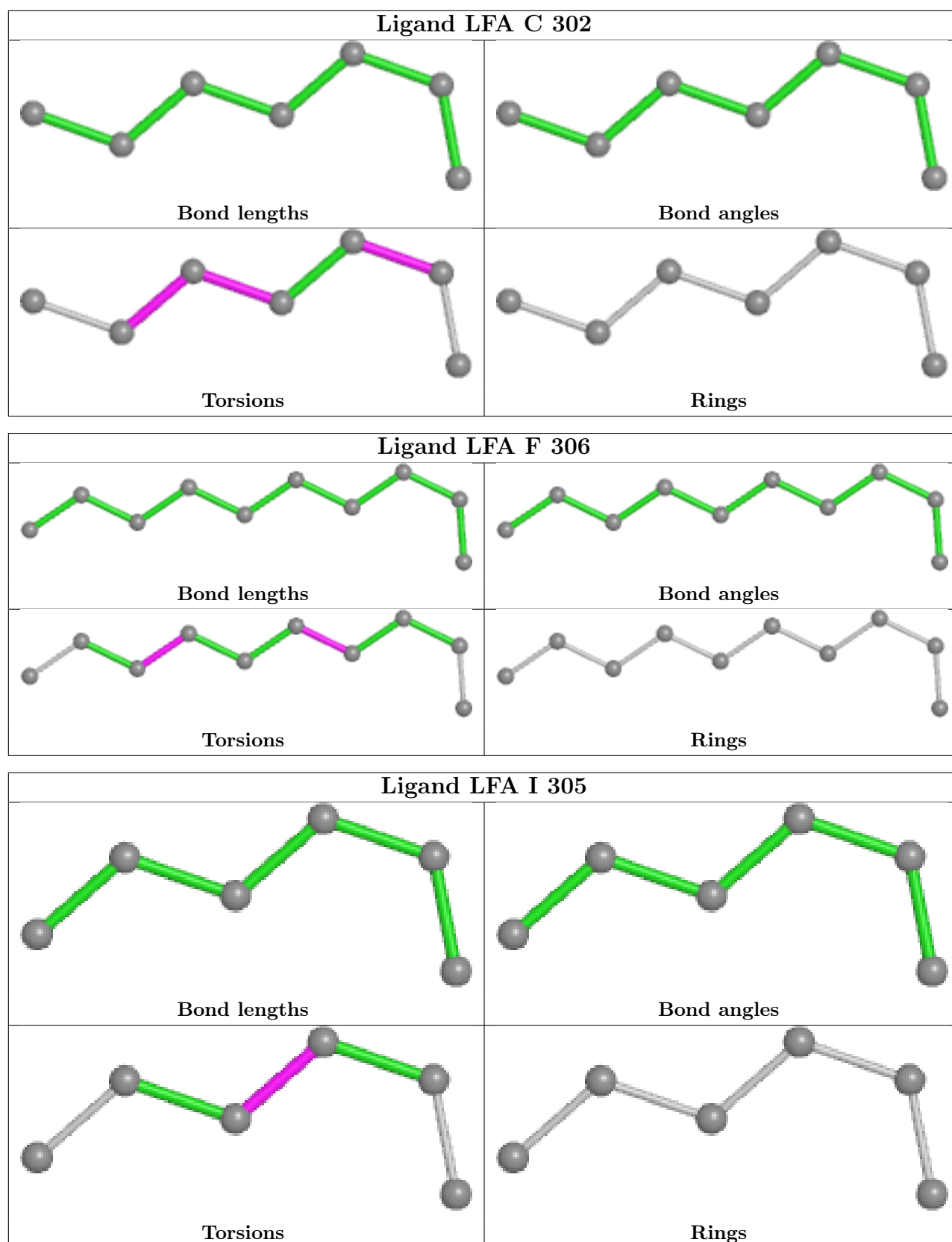


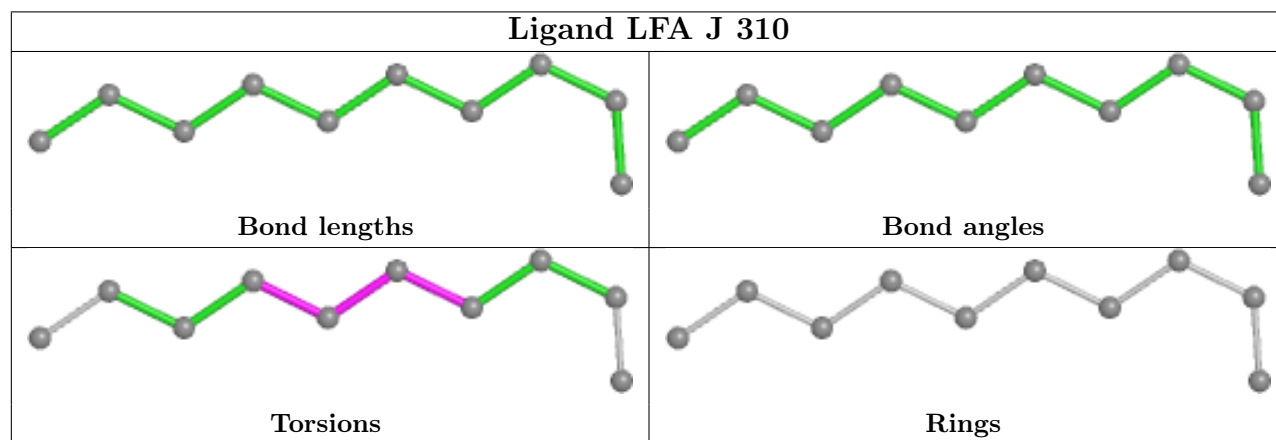
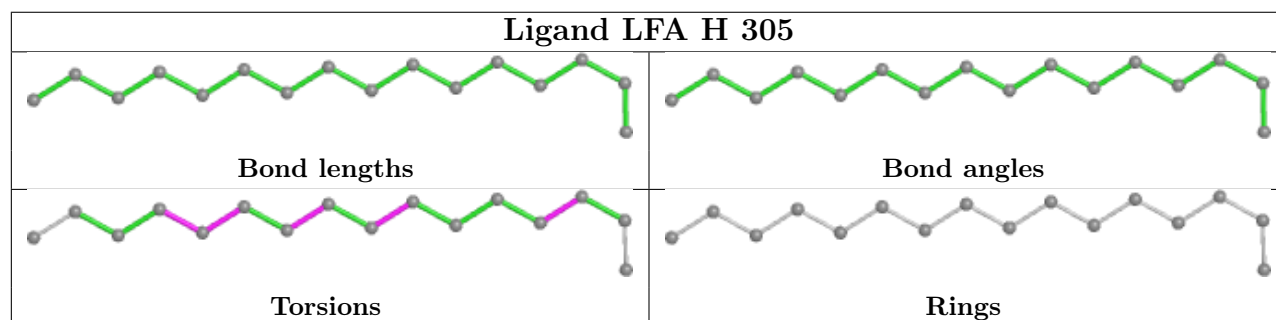
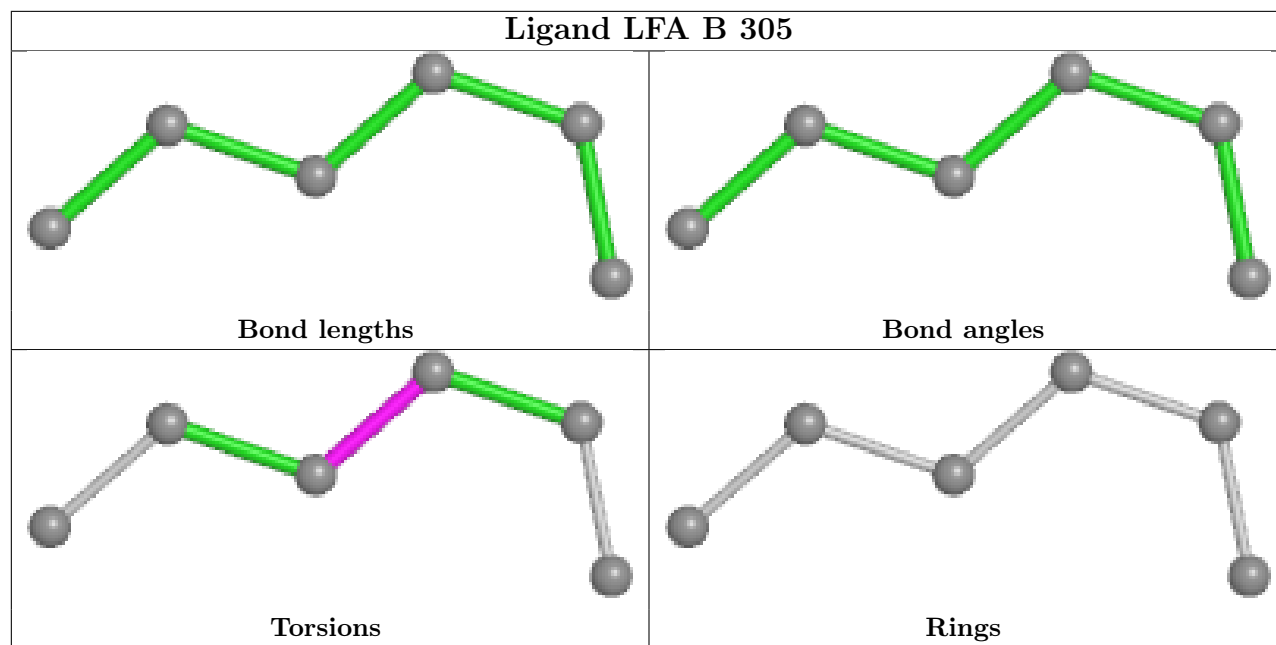




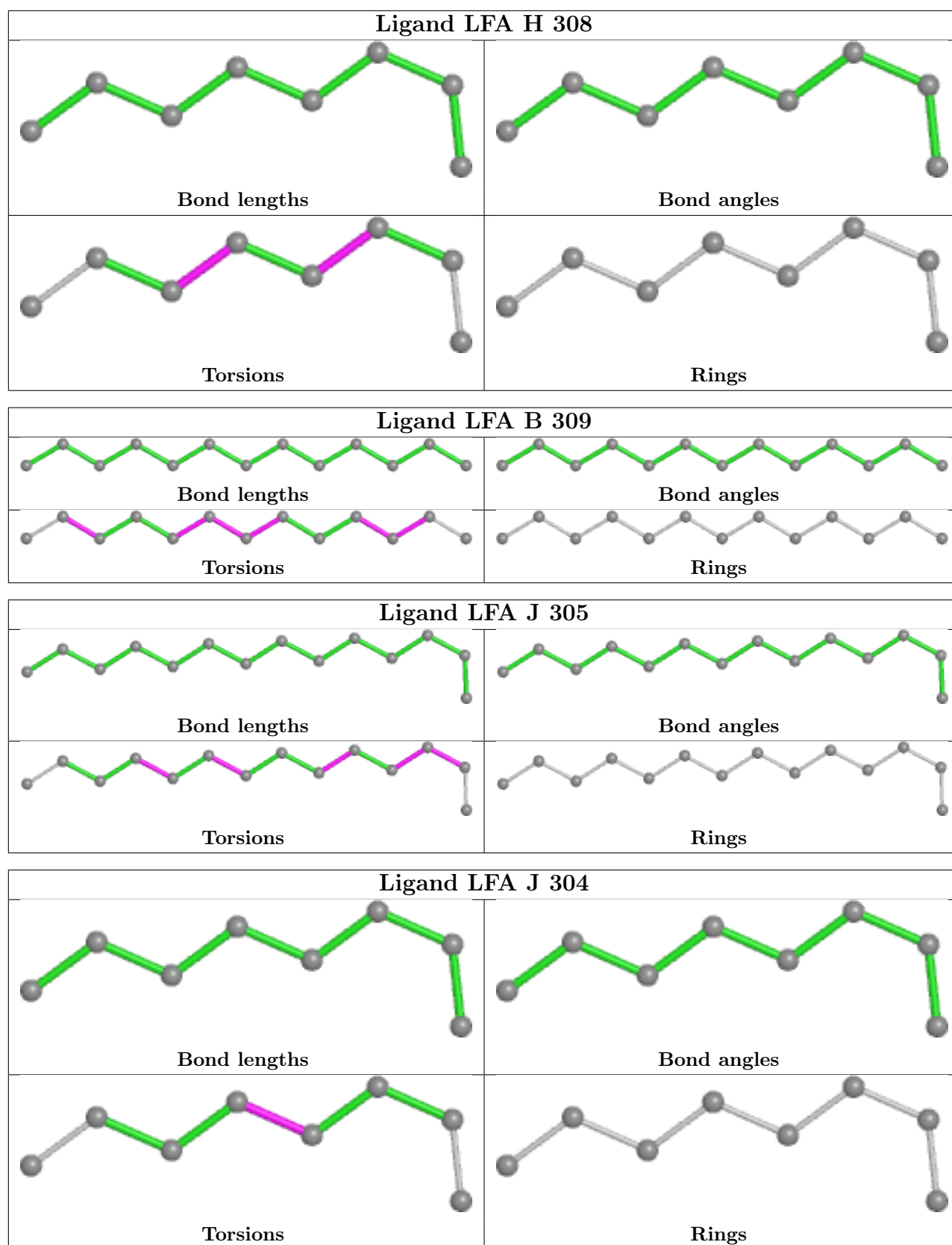


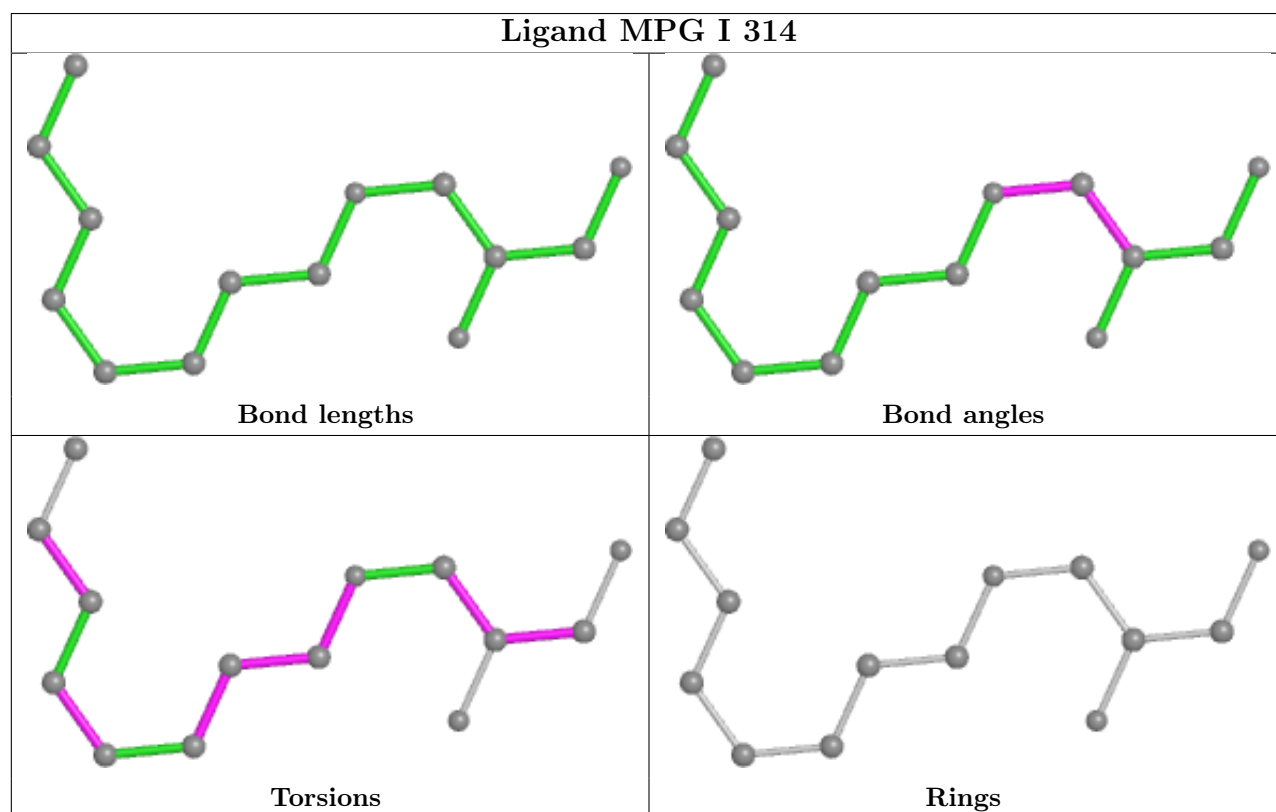
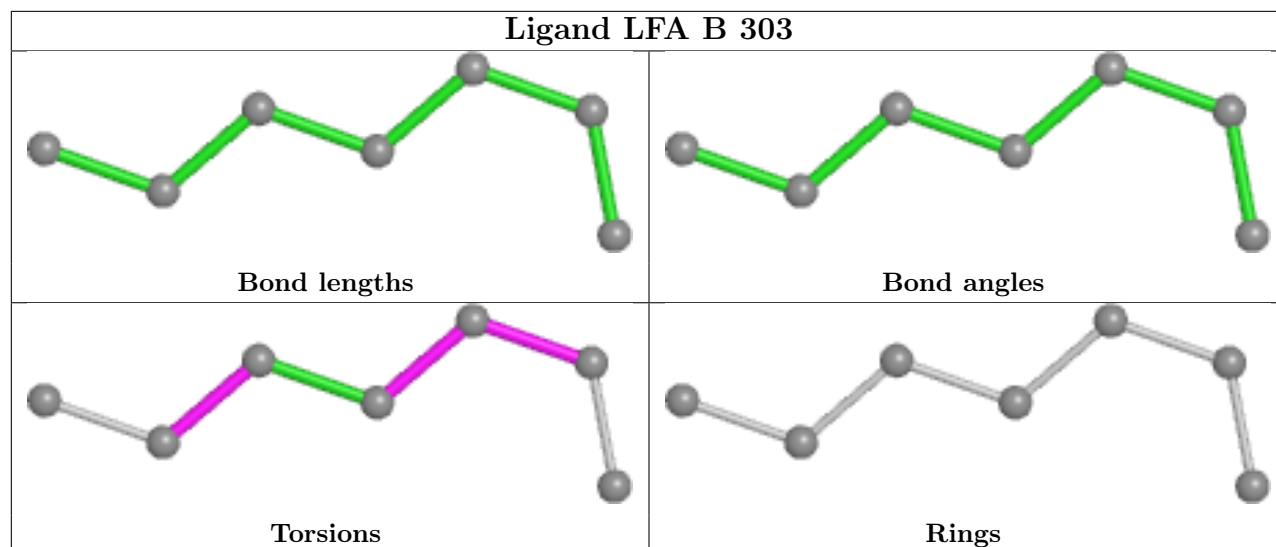


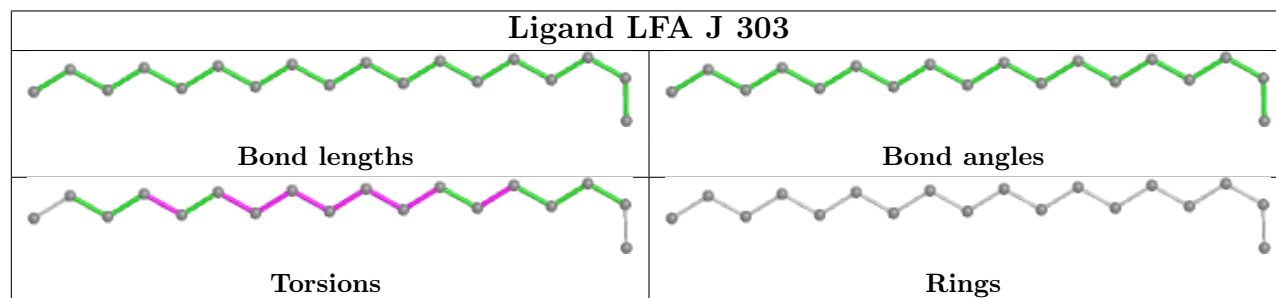
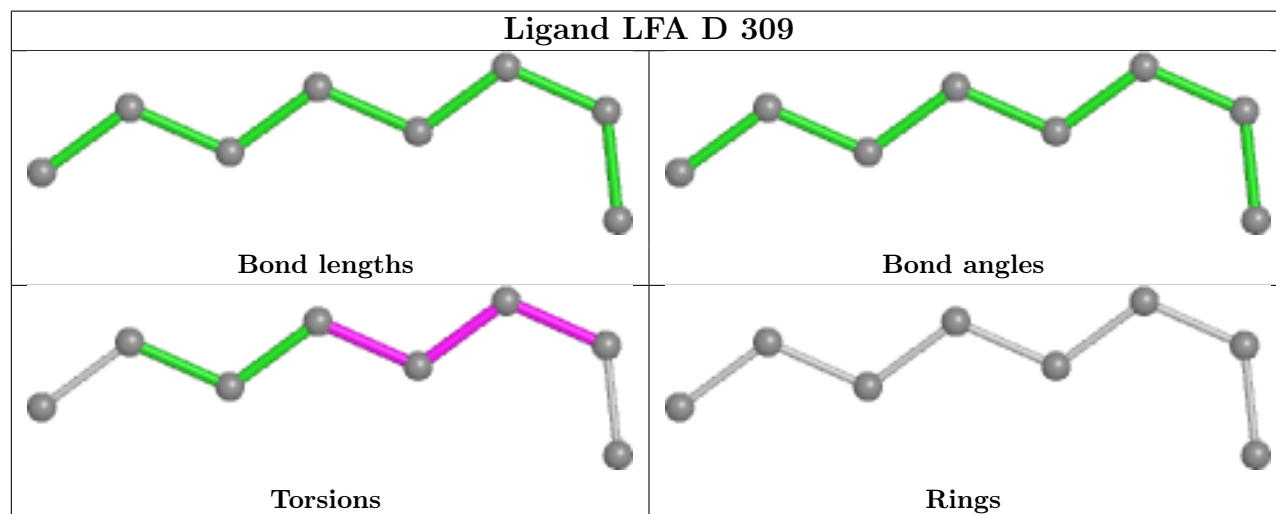
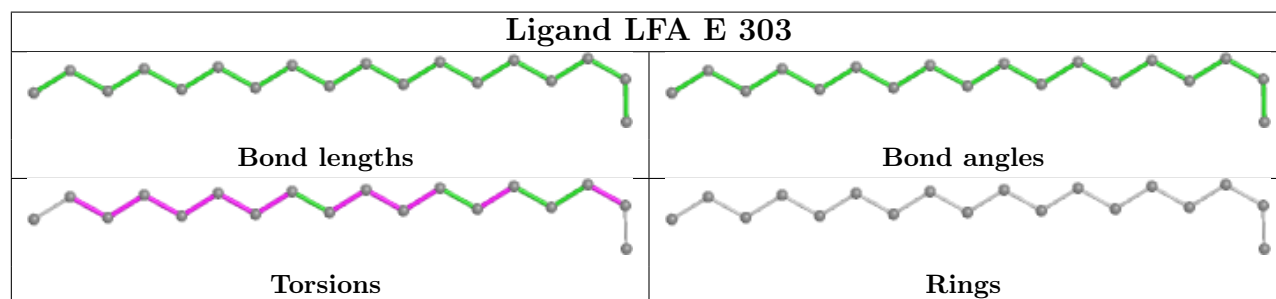
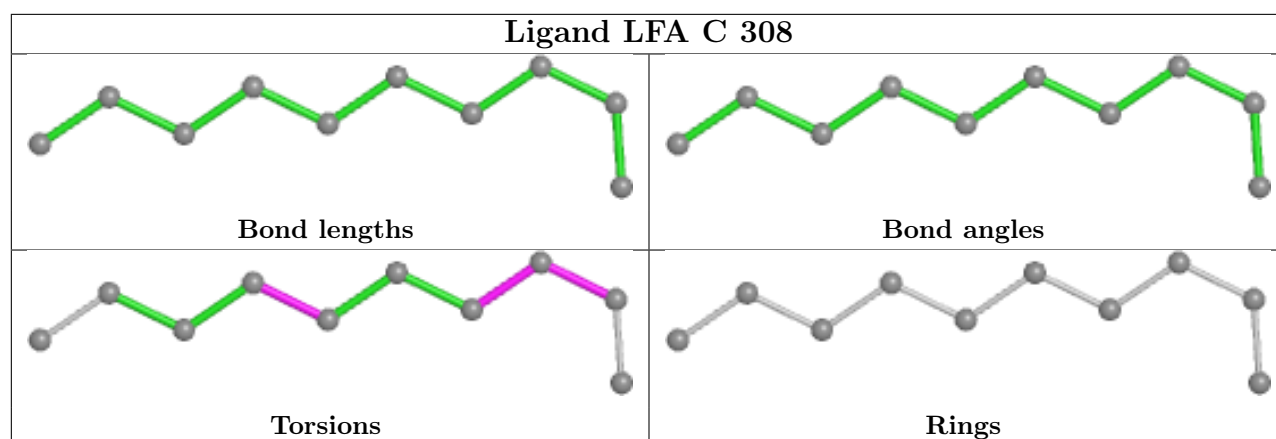


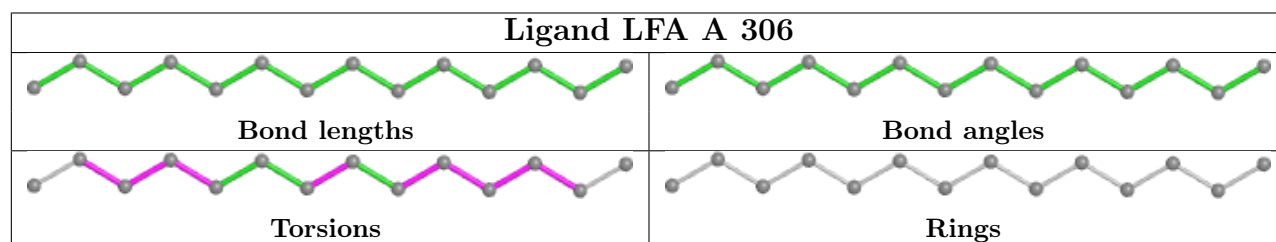
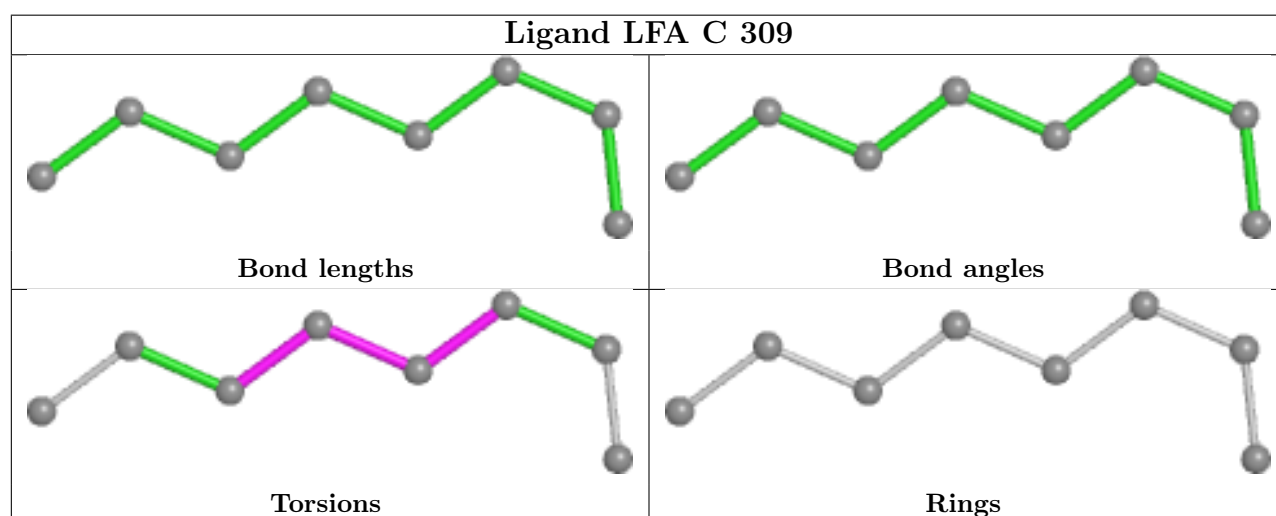
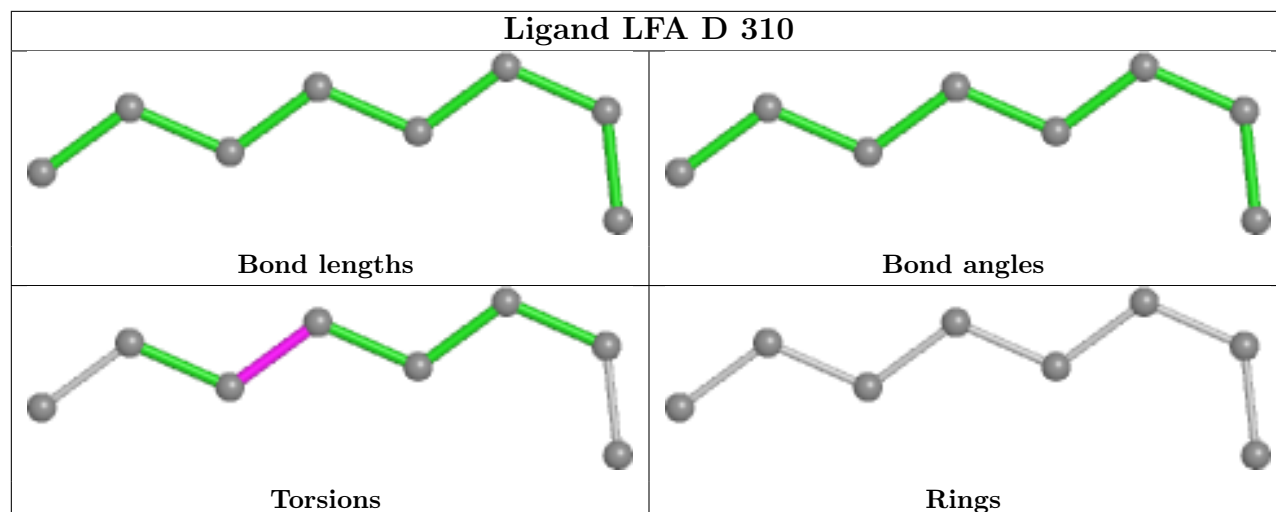


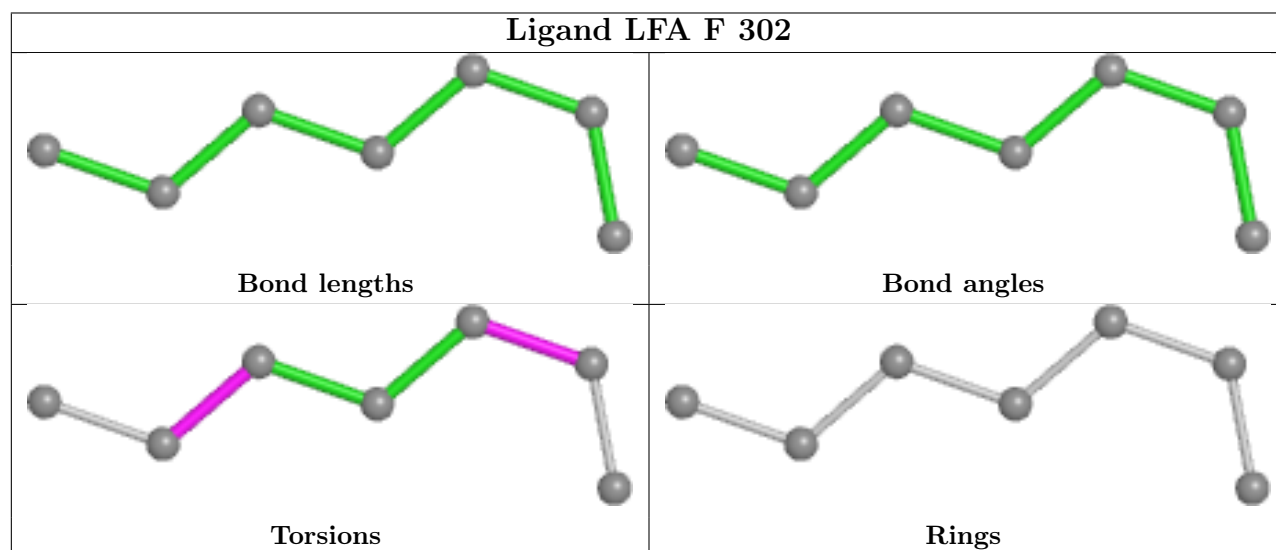
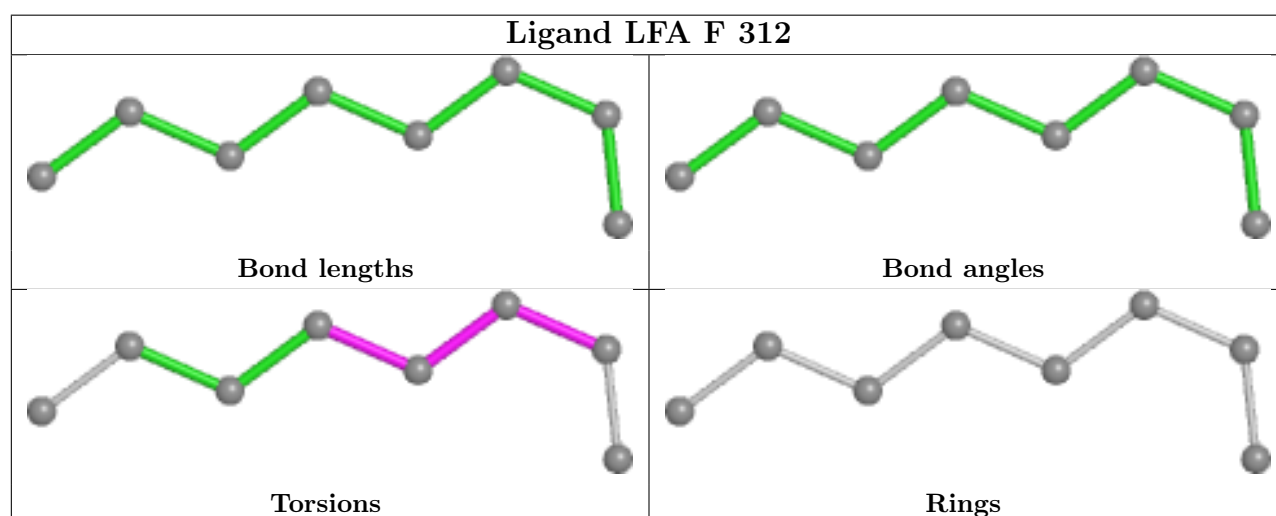
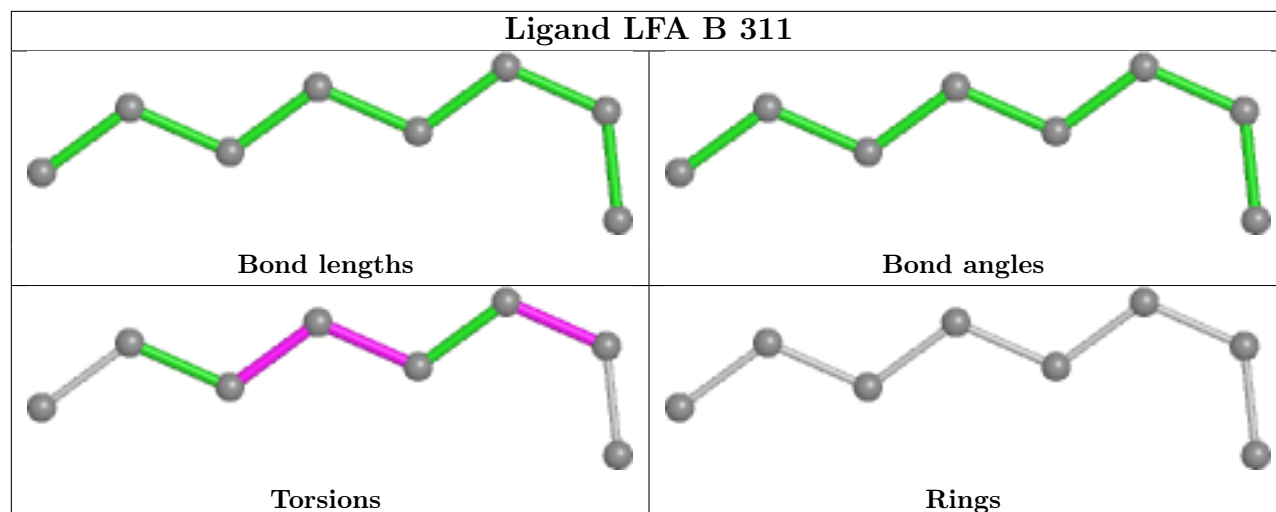


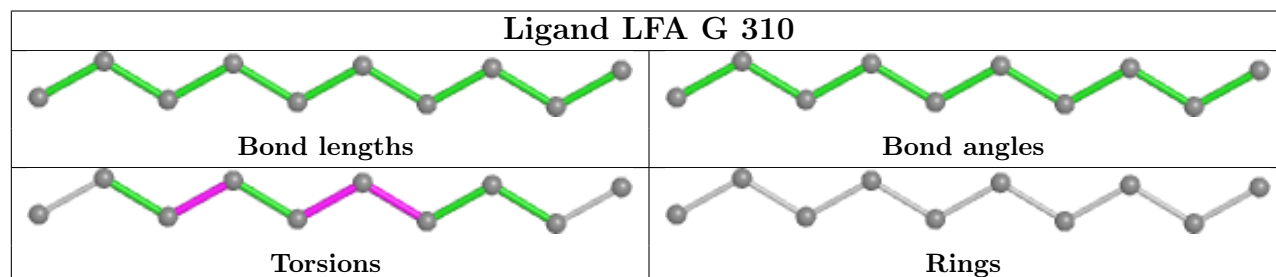
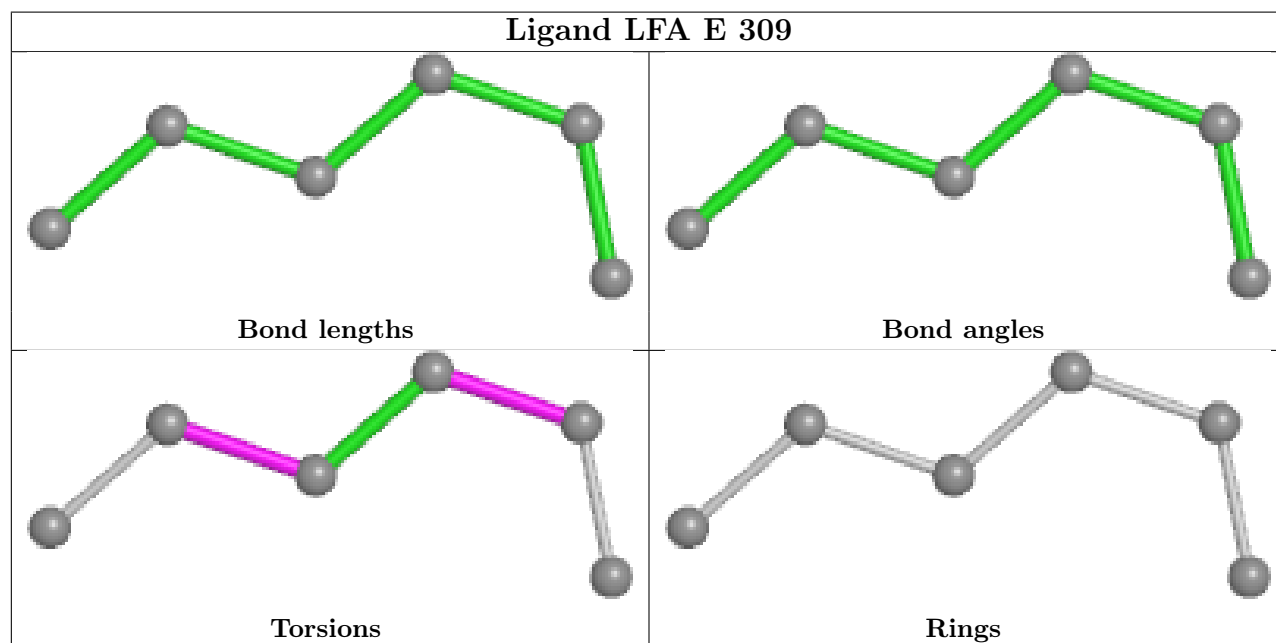
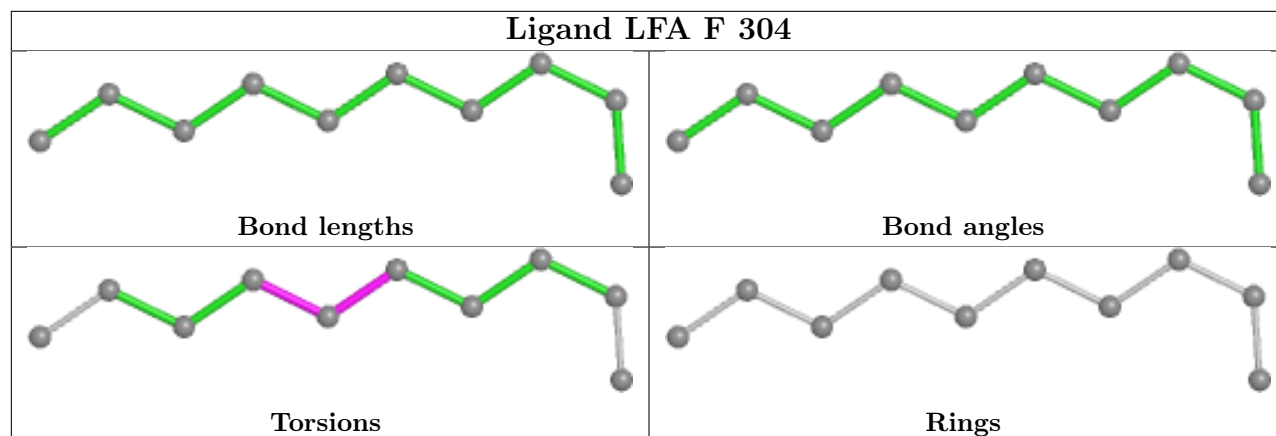


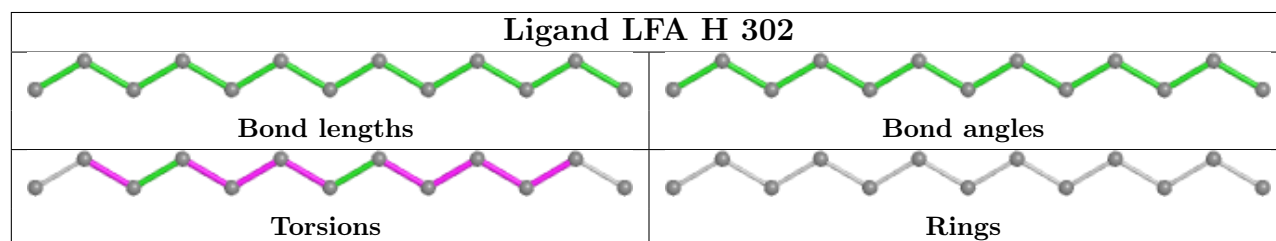
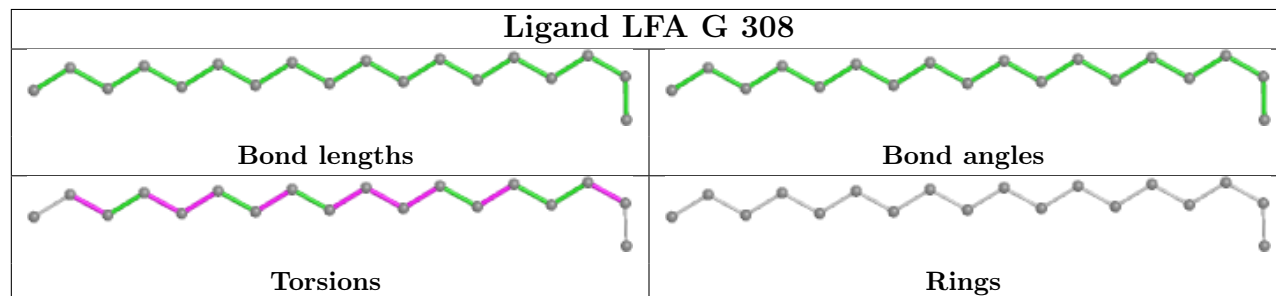
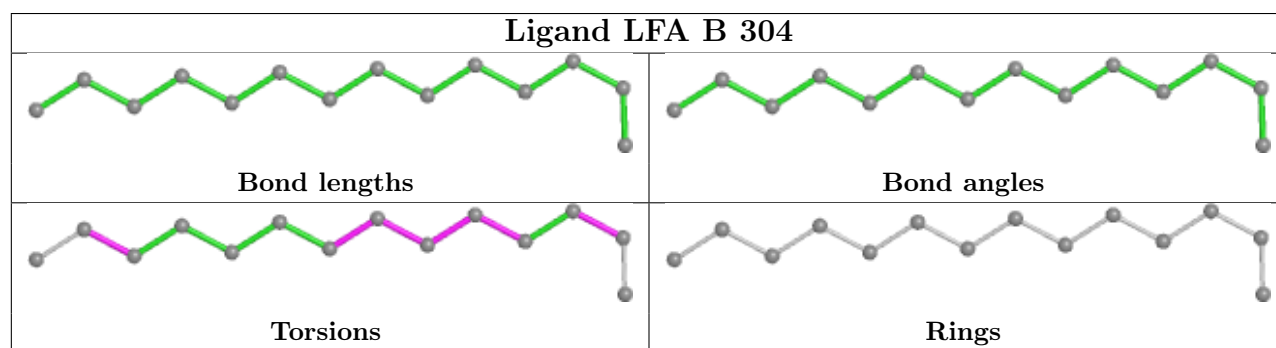
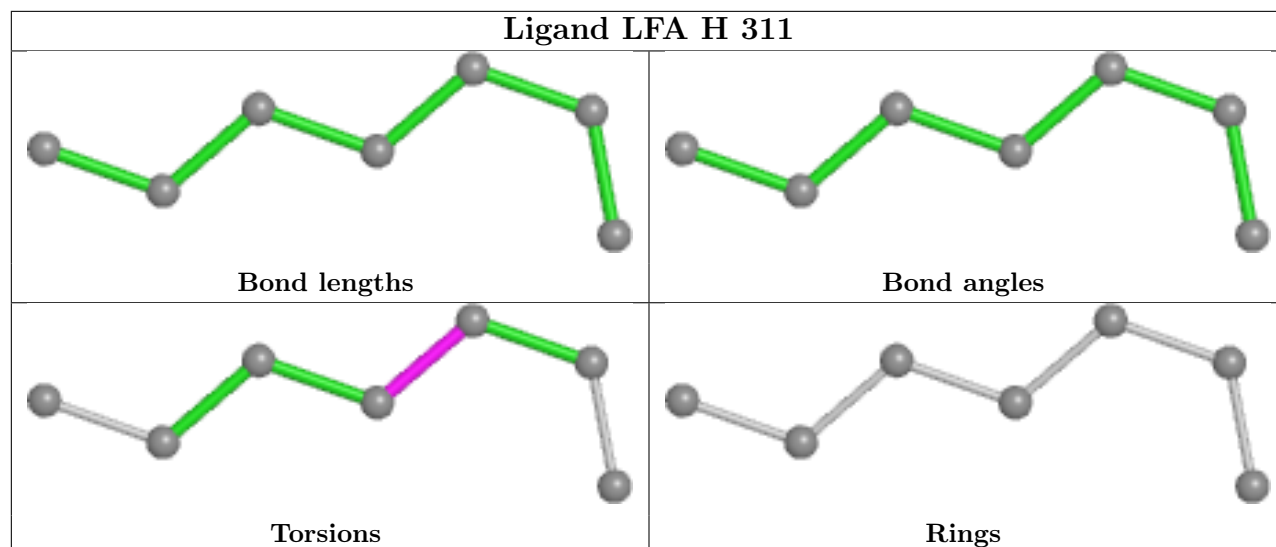


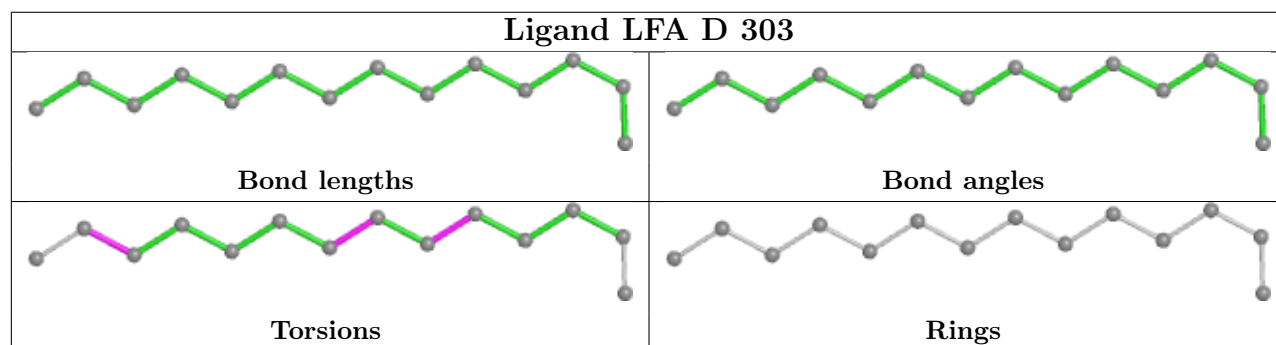
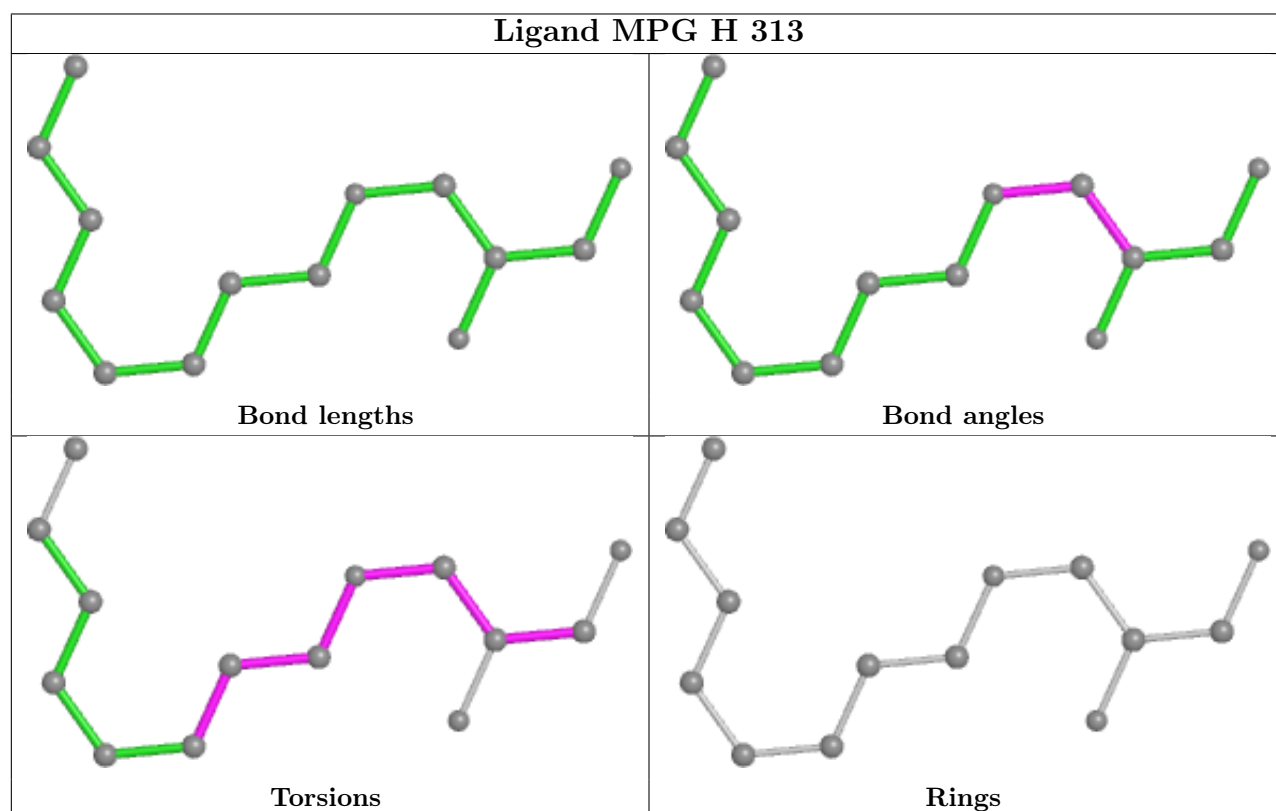
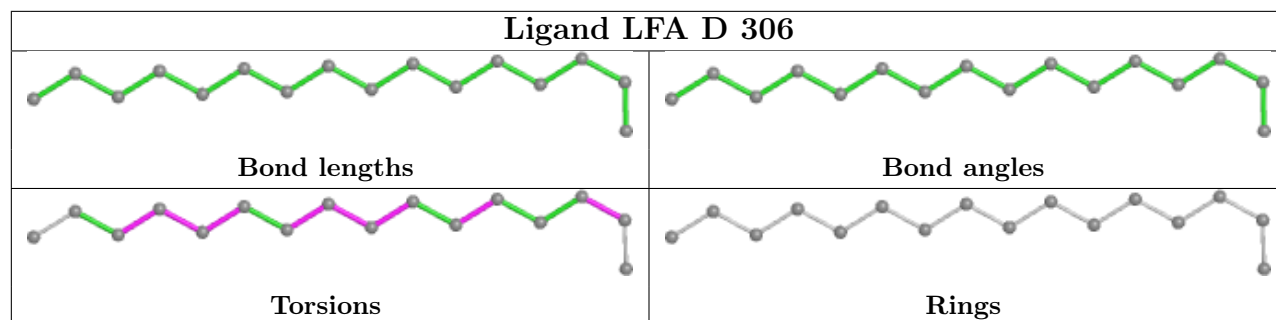




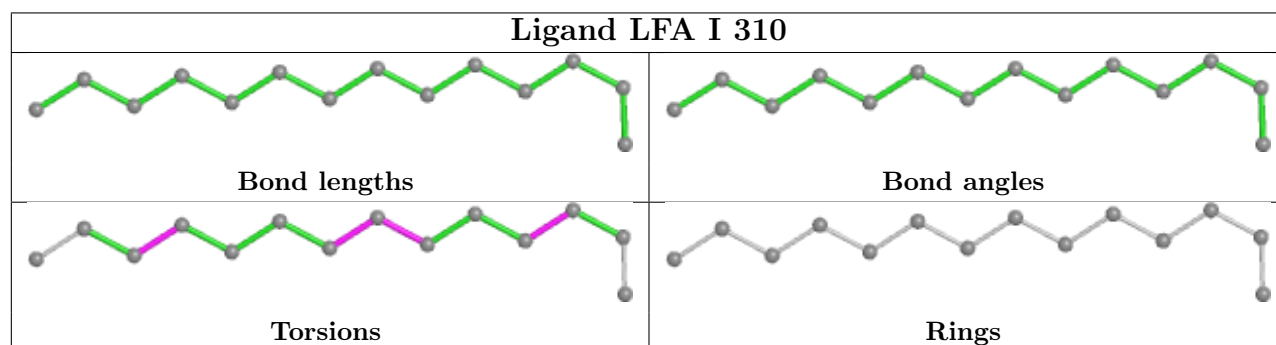
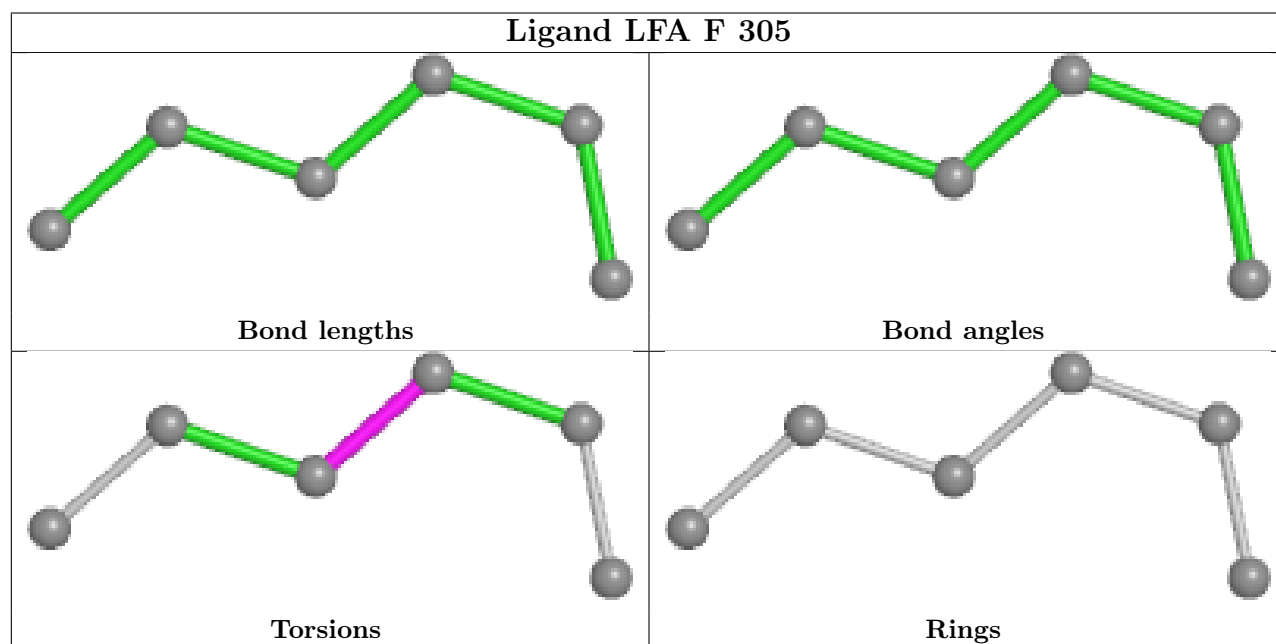
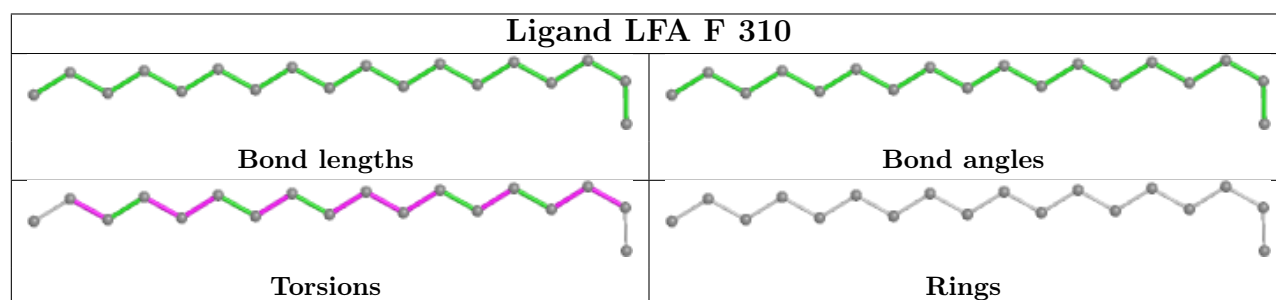
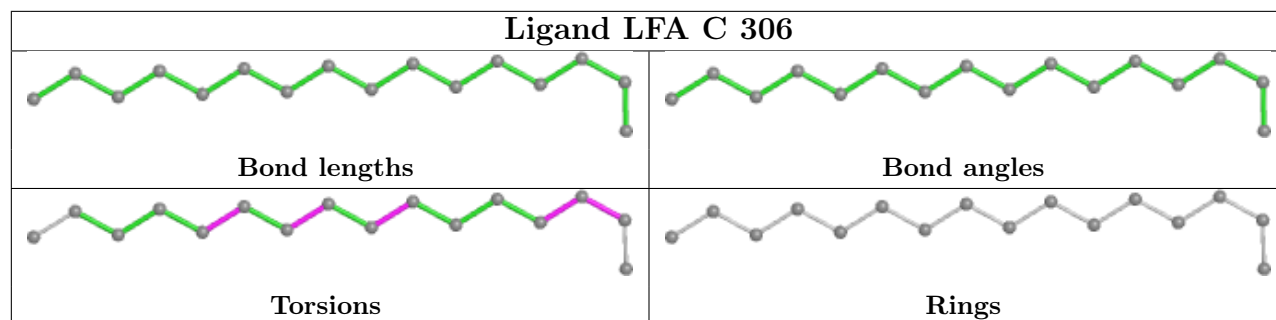


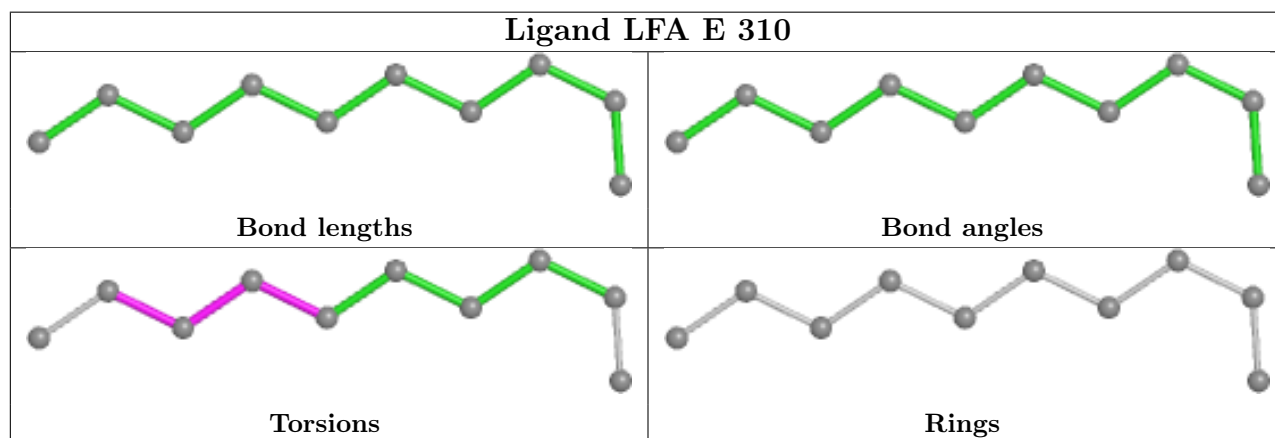
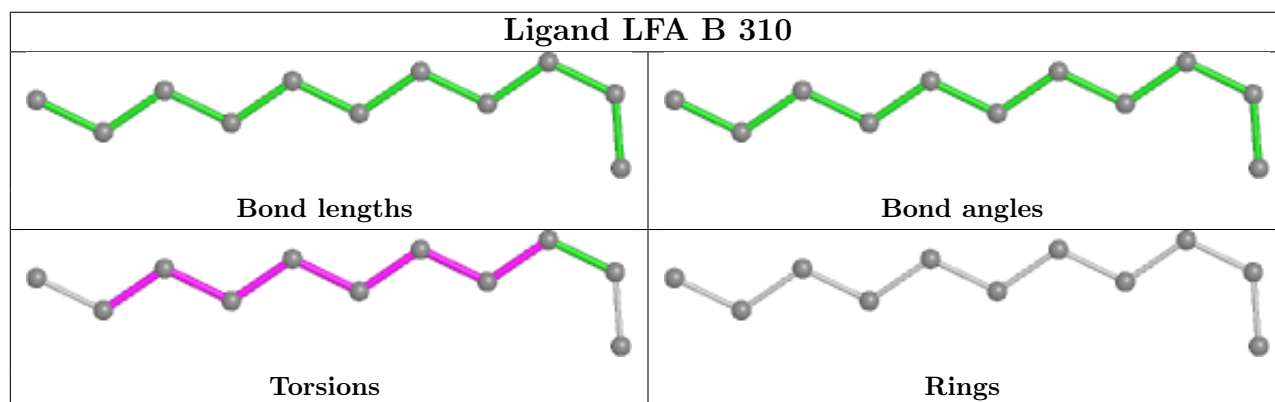
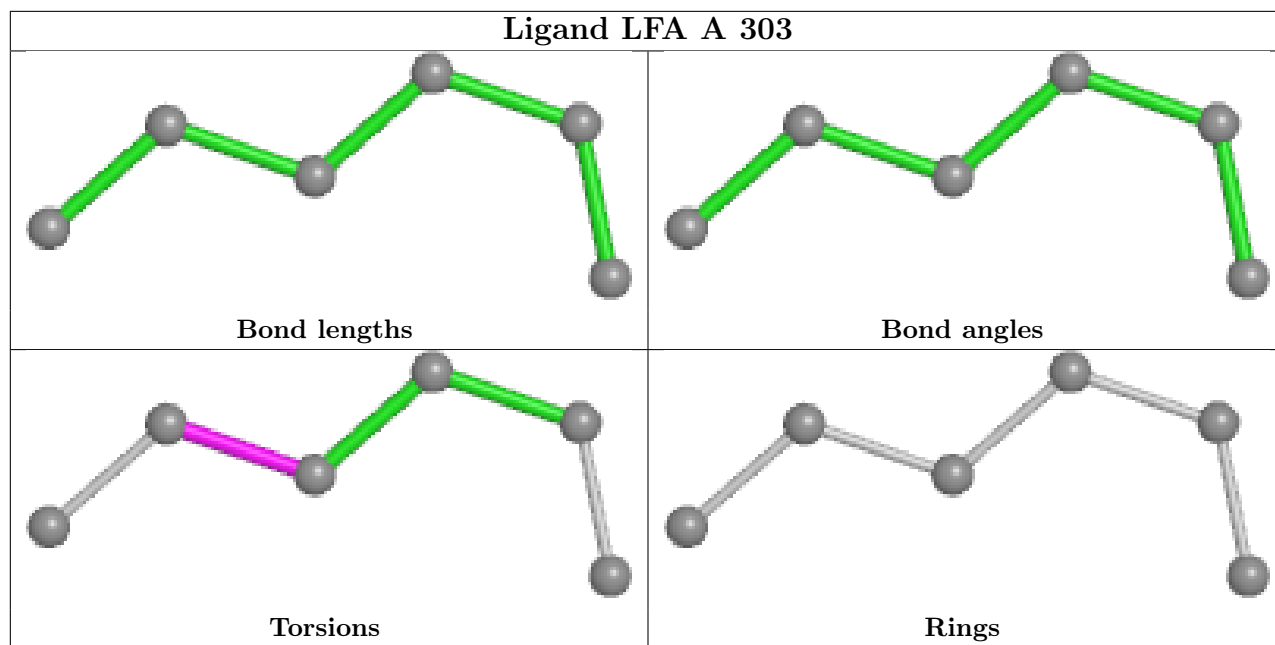


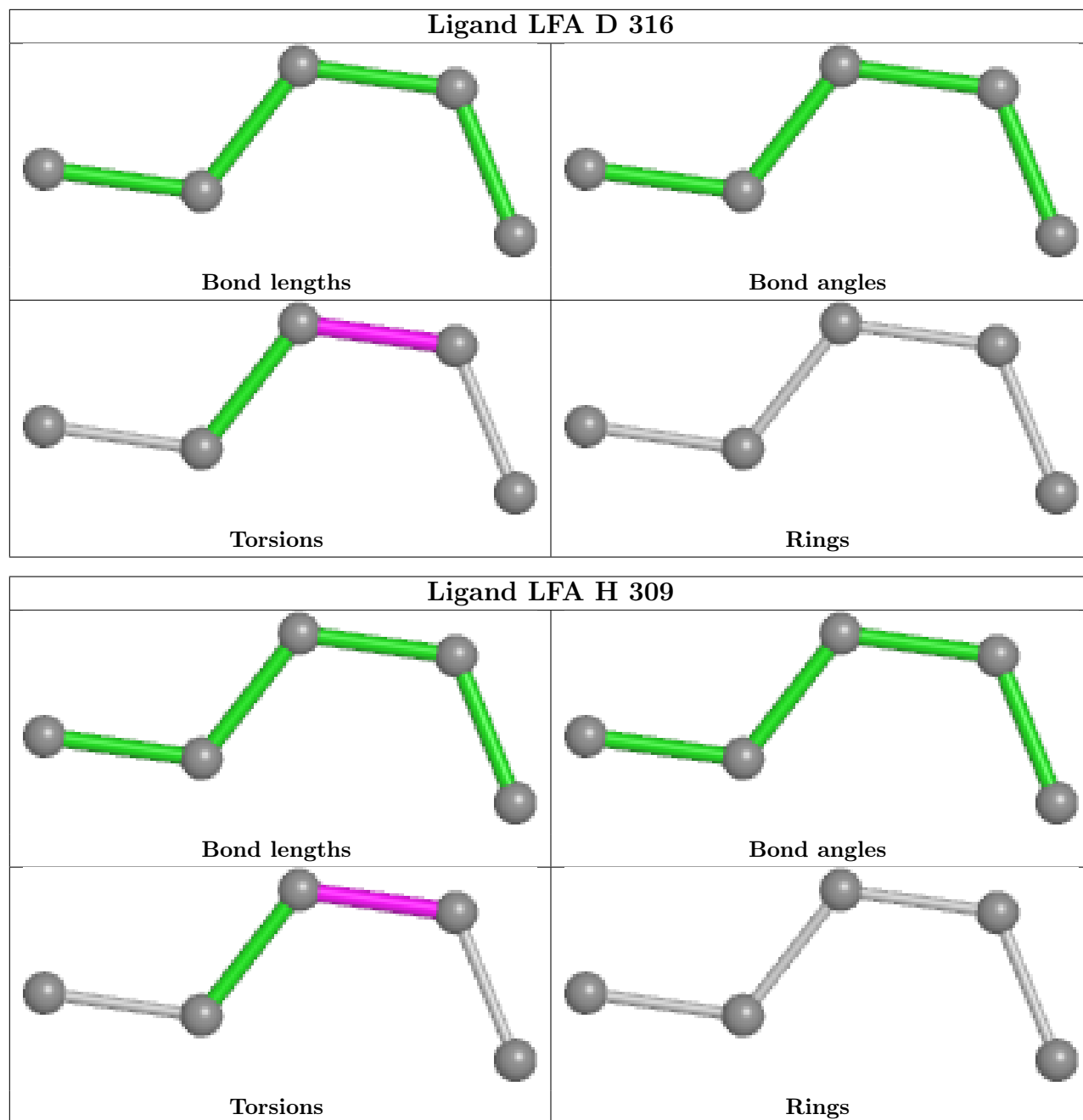


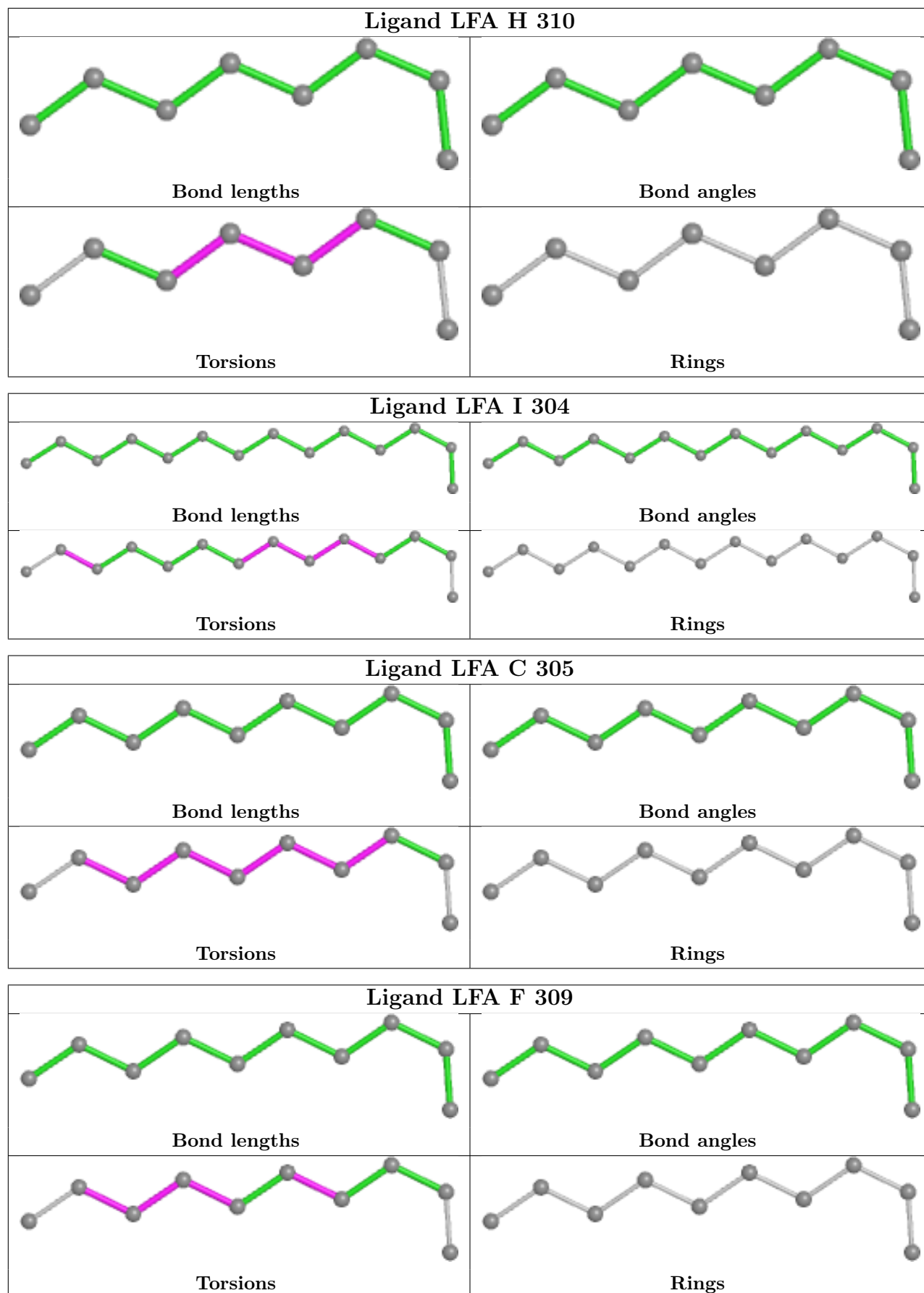


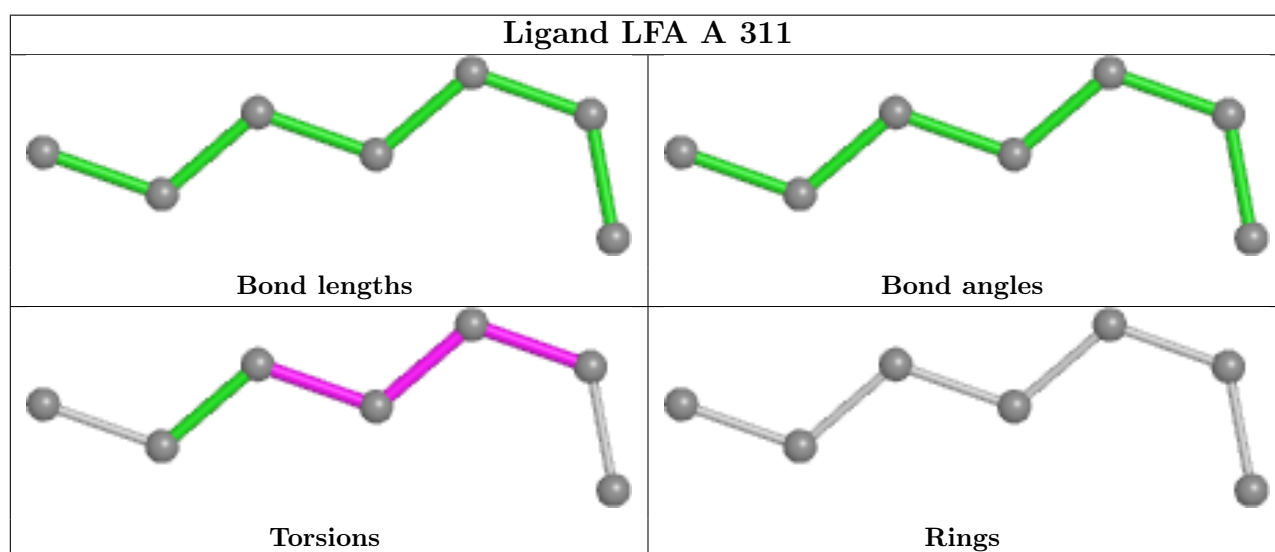
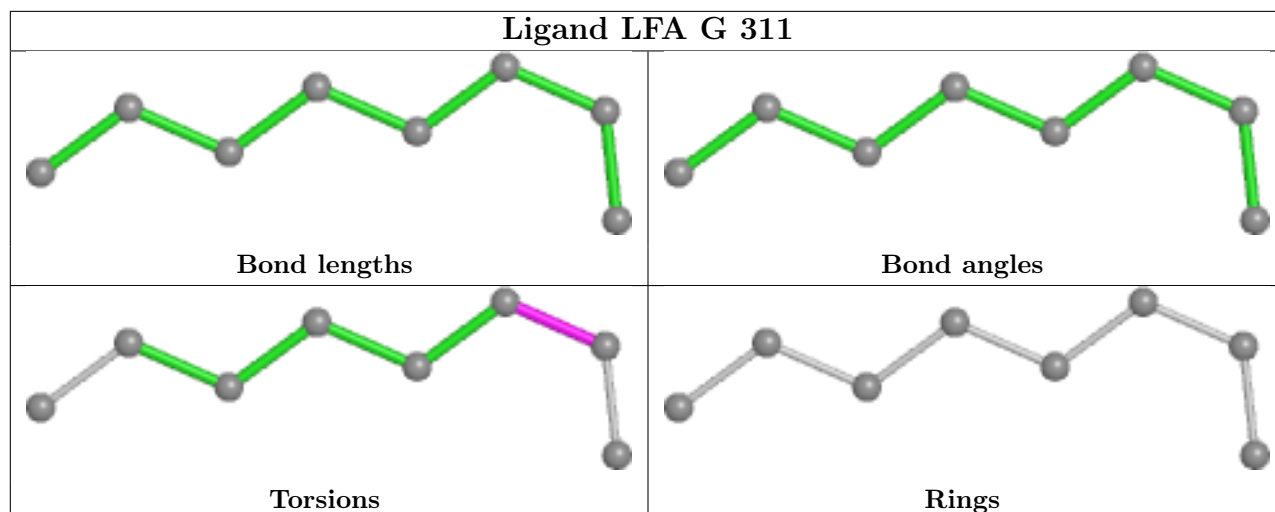


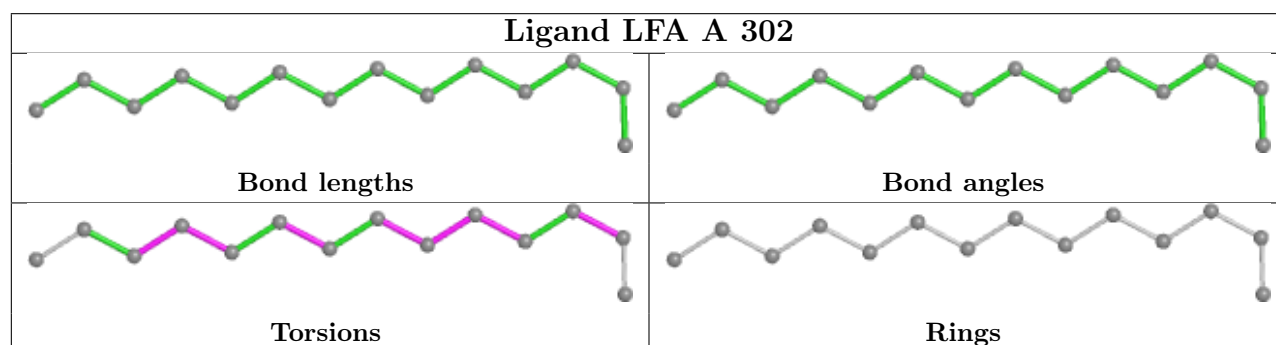
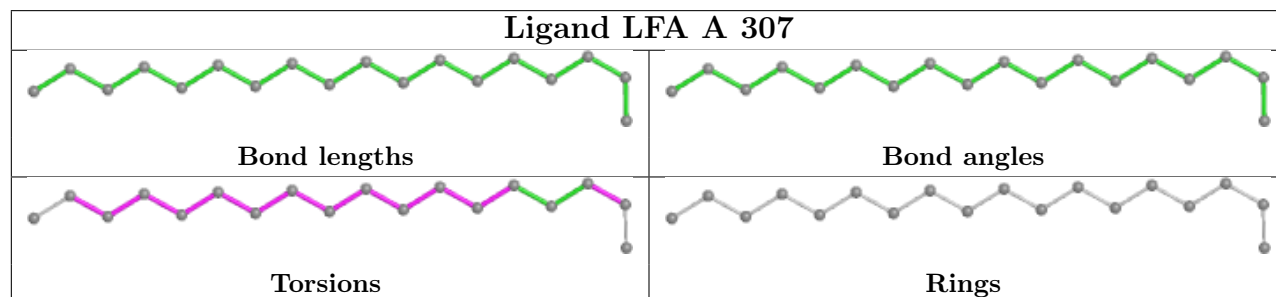
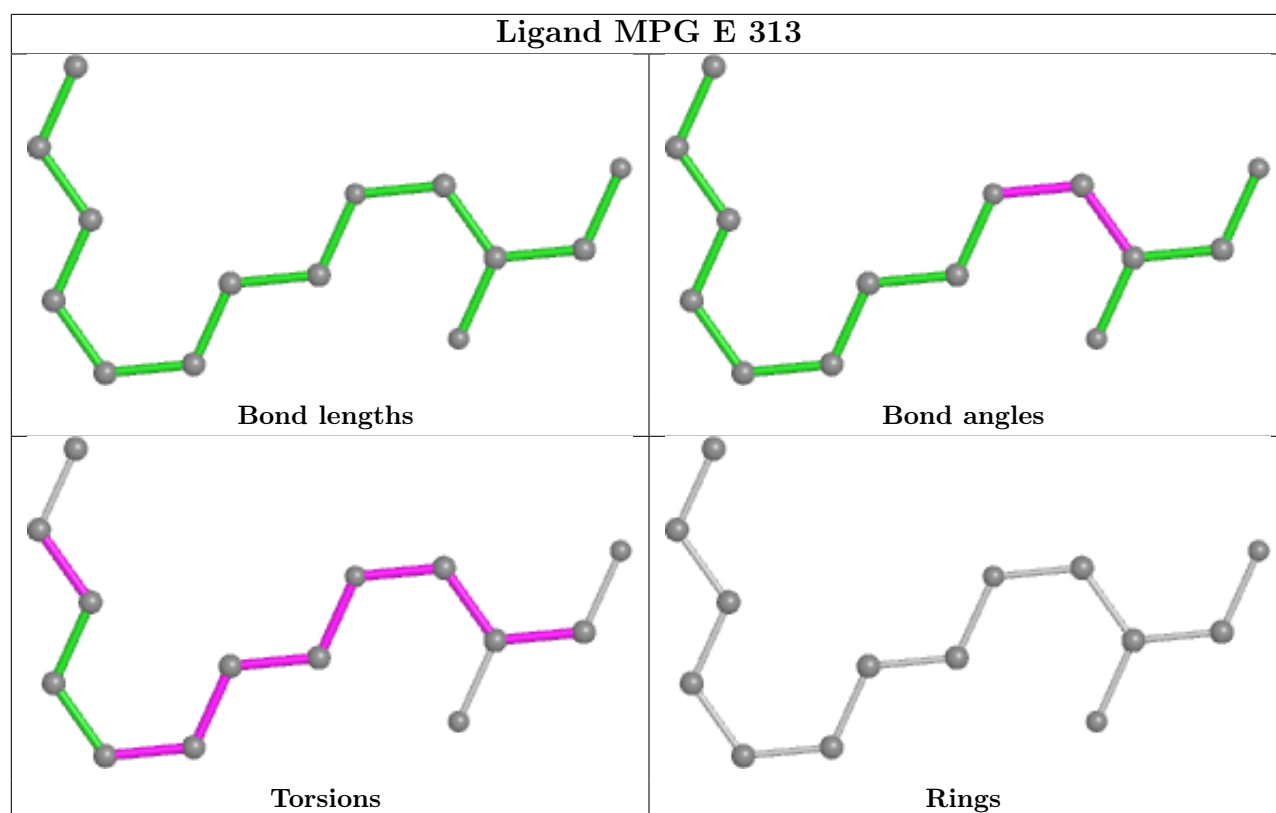


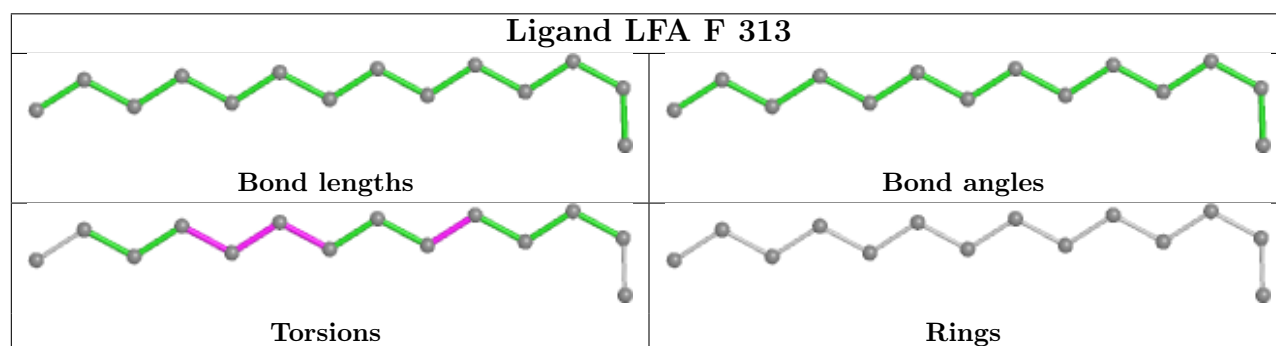
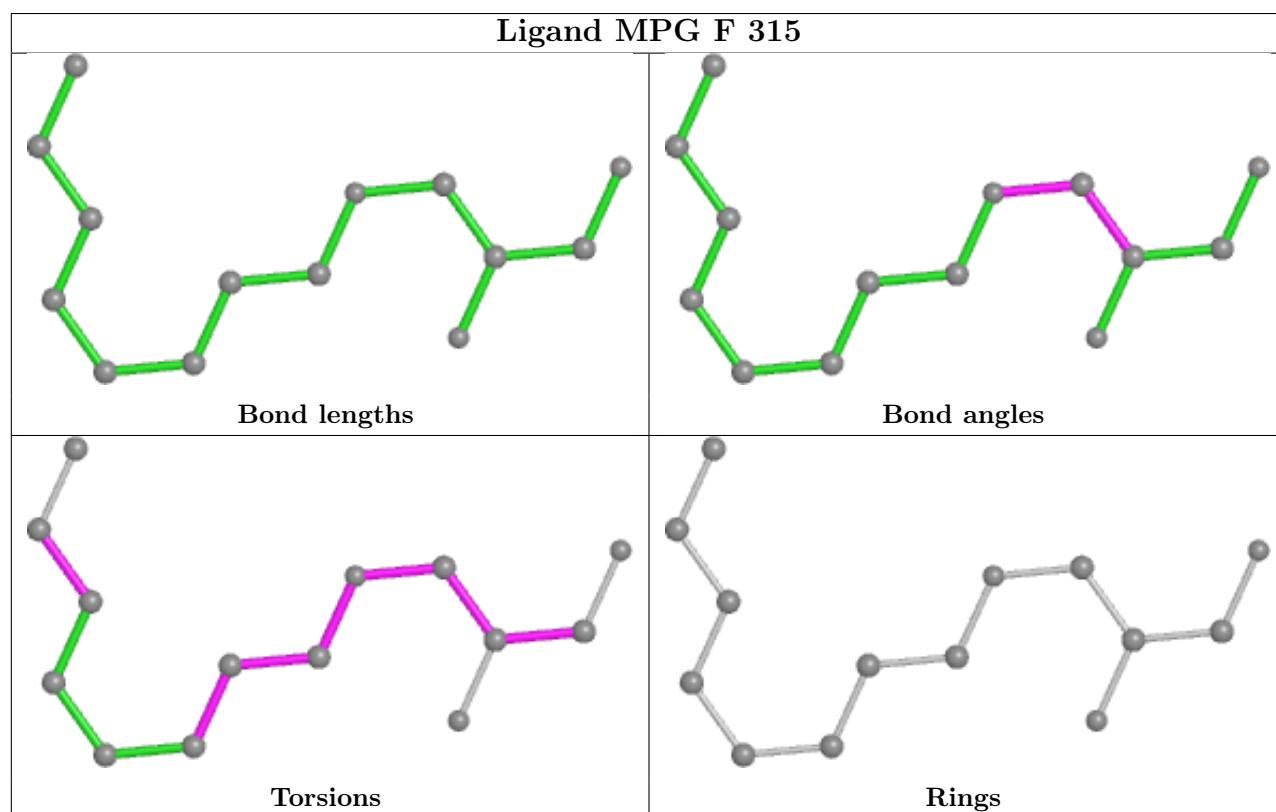
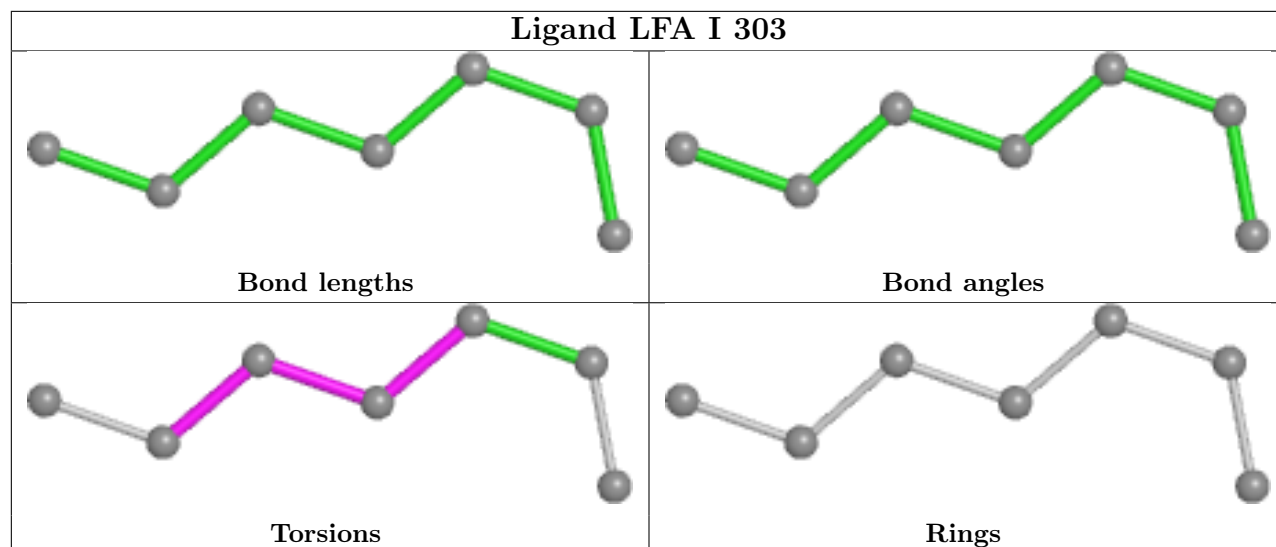


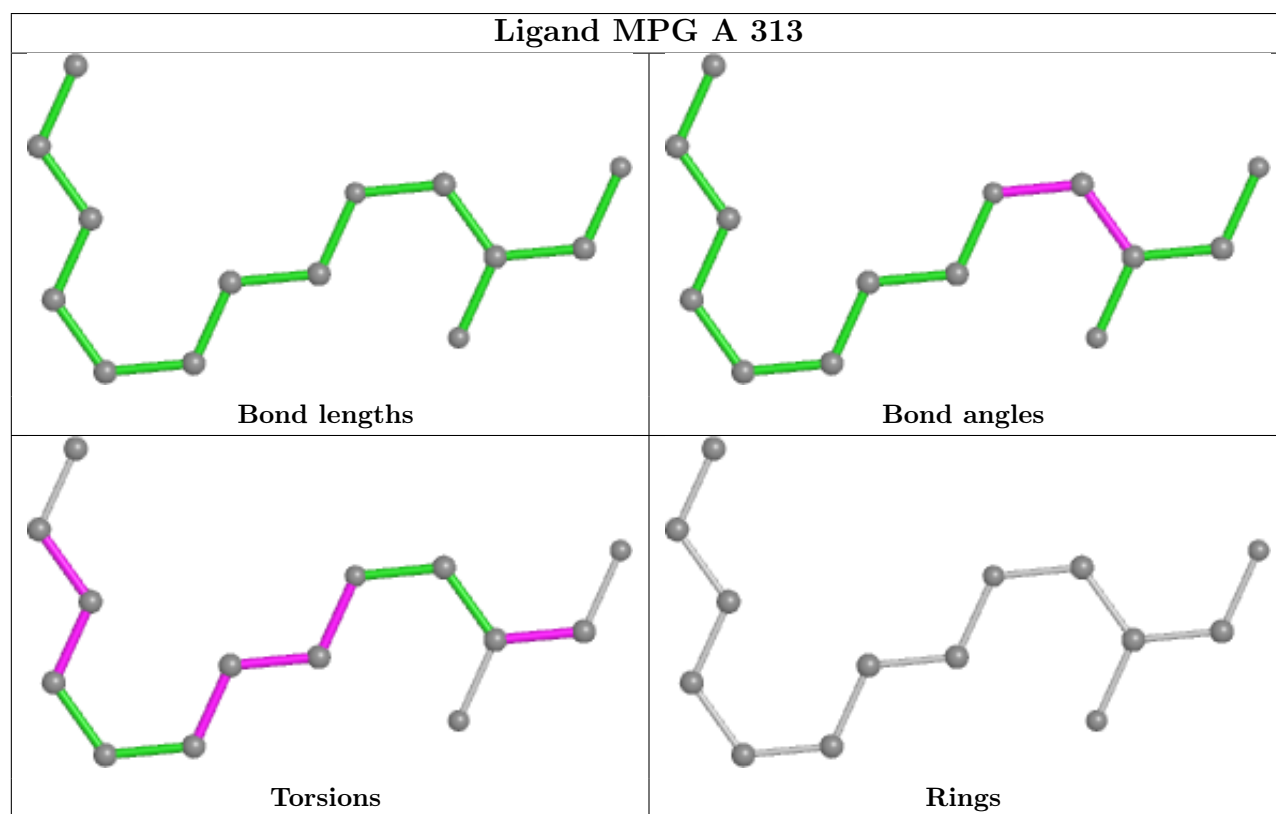
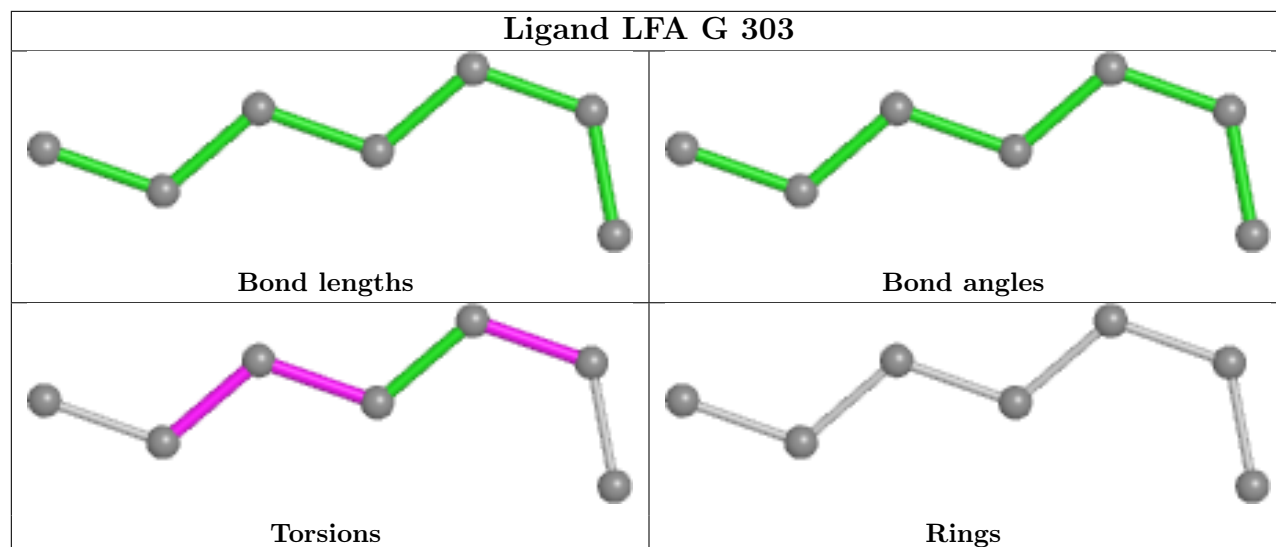




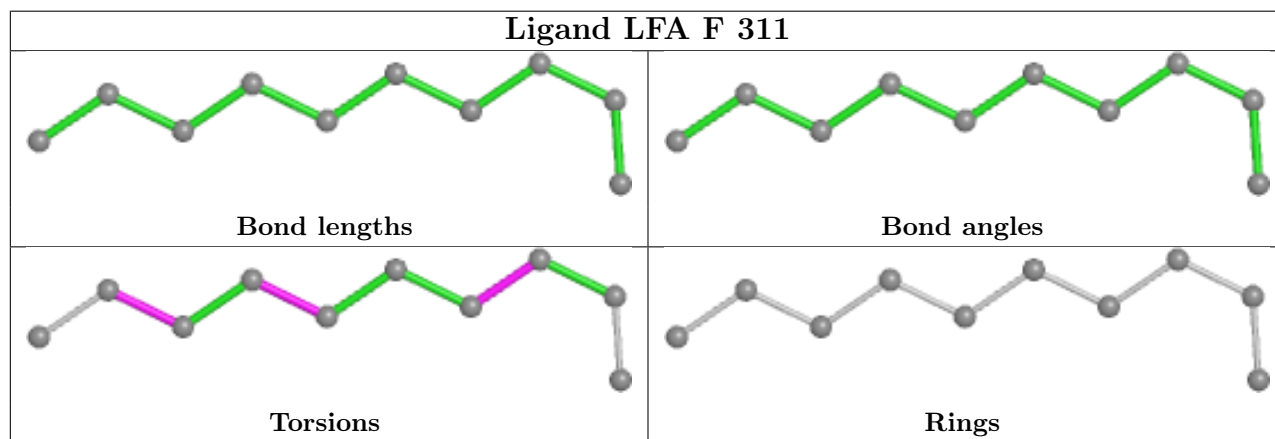
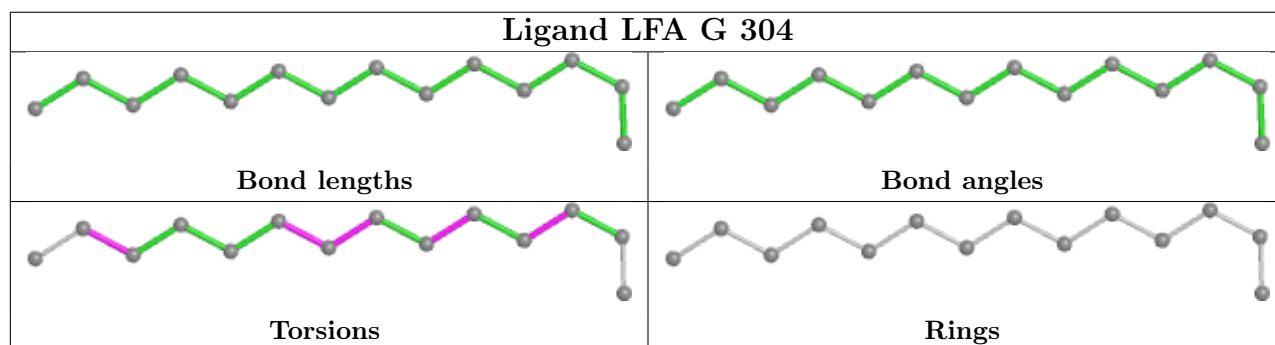
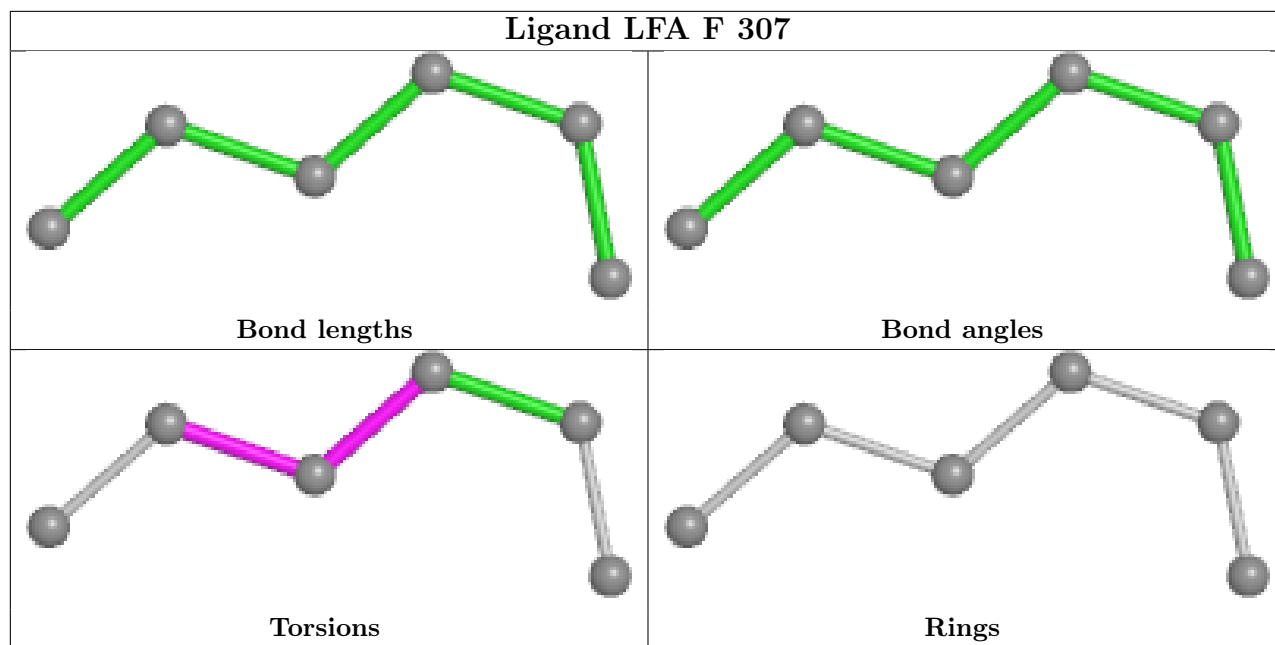


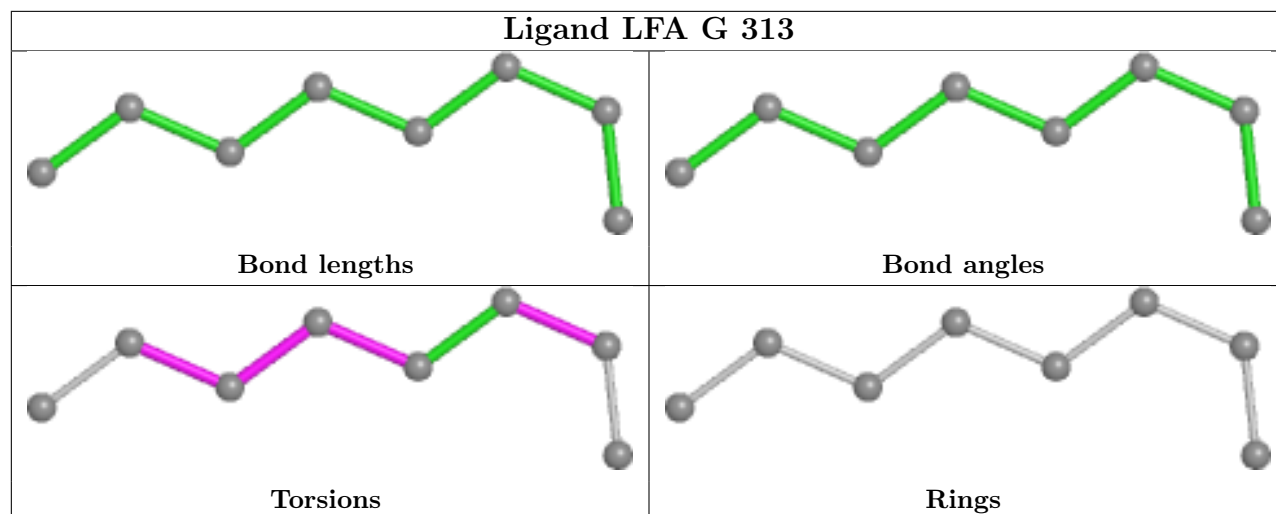












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	272/288 (94%)	-0.07	5 (1%) 68 66	24, 34, 52, 81	0
1	B	269/288 (93%)	0.15	18 (6%) 17 16	26, 39, 67, 90	0
1	C	270/288 (93%)	-0.04	7 (2%) 56 53	24, 34, 51, 74	0
1	D	270/288 (93%)	0.01	10 (3%) 41 39	22, 32, 49, 73	0
1	E	271/288 (94%)	0.02	8 (2%) 50 48	23, 34, 54, 69	0
1	F	270/288 (93%)	0.08	17 (6%) 20 19	25, 35, 56, 76	0
1	G	270/288 (93%)	-0.09	7 (2%) 56 53	23, 34, 51, 82	0
1	H	272/288 (94%)	-0.06	9 (3%) 46 44	23, 32, 51, 91	0
1	I	270/288 (93%)	-0.09	11 (4%) 37 35	21, 30, 49, 76	0
1	J	271/288 (94%)	0.11	16 (5%) 22 21	23, 32, 49, 76	0
All	All	2705/2880 (93%)	0.00	108 (3%) 38 36	21, 33, 54, 91	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	275	LEU	8.4
1	I	275	LEU	7.1
1	I	276	VAL	6.1
1	H	276	VAL	5.9
1	H	272	ASN	5.7
1	J	276	VAL	5.6
1	F	132	THR	5.1
1	B	195	GLY	5.1
1	B	3	GLN	5.1
1	G	276	VAL	4.9
1	A	132	THR	4.8
1	J	275	LEU	4.6
1	B	198	PRO	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	132	THR	4.3
1	H	3	GLN	4.3
1	F	195	GLY	4.2
1	J	233	PHE	4.2
1	F	196	ILE	4.1
1	B	196	ILE	4.1
1	D	276	VAL	3.9
1	B	129	SER	3.8
1	E	276	VAL	3.7
1	B	273	LYS	3.7
1	J	272	ASN	3.6
1	B	133	SER	3.5
1	C	233	PHE	3.4
1	A	276	VAL	3.4
1	B	197	SER	3.4
1	F	130	LEU	3.4
1	J	183	TRP	3.3
1	C	183	TRP	3.2
1	B	131	THR	3.2
1	A	183	TRP	3.1
1	C	275	LEU	3.1
1	B	275	LEU	3.1
1	F	3	GLN	3.0
1	D	270	SER	3.0
1	D	198	PRO	3.0
1	F	233	PHE	3.0
1	B	134	LYS	2.9
1	B	233	PHE	2.9
1	J	69	VAL	2.9
1	G	233	PHE	2.9
1	F	274	GLU	2.9
1	A	272	ASN	2.9
1	C	232	GLY	2.9
1	B	190	ASN	2.8
1	H	195	GLY	2.8
1	B	130	LEU	2.8
1	F	198	PRO	2.8
1	J	133	SER	2.8
1	D	275	LEU	2.7
1	J	40	LEU	2.7
1	F	194	GLU	2.7
1	J	74[A]	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	274	GLU	2.6
1	F	197	SER	2.6
1	I	40	LEU	2.6
1	J	43	LEU	2.6
1	D	233	PHE	2.6
1	G	40	LEU	2.6
1	J	73	LEU	2.6
1	B	18	GLU	2.6
1	D	273	LYS	2.5
1	F	270	SER	2.5
1	C	73	LEU	2.5
1	I	274	GLU	2.5
1	E	76	TYR	2.5
1	D	73	LEU	2.4
1	J	72	PHE	2.4
1	F	275	LEU	2.4
1	D	269	LEU	2.4
1	I	92	VAL	2.4
1	F	131	THR	2.3
1	G	132	THR	2.3
1	H	92	VAL	2.3
1	I	73	LEU	2.3
1	E	73	LEU	2.3
1	E	129	SER	2.3
1	J	65	ALA	2.3
1	D	274	GLU	2.3
1	C	74[A]	LEU	2.3
1	E	40	LEU	2.3
1	I	75	LEU	2.2
1	H	233	PHE	2.2
1	G	183	TRP	2.2
1	H	40	LEU	2.2
1	F	92	VAL	2.2
1	B	40	LEU	2.2
1	F	269	LEU	2.2
1	C	72	PHE	2.2
1	D	40	LEU	2.2
1	G	195	GLY	2.2
1	J	269	LEU	2.1
1	I	74	LEU	2.1
1	J	132	THR	2.1
1	I	76	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	43	LEU	2.1
1	B	201	GLN	2.1
1	G	164	LEU	2.1
1	E	4	GLU	2.1
1	F	55	LYS	2.1
1	I	132	THR	2.1
1	F	133	SER	2.1
1	E	72	PHE	2.0
1	E	228	THR	2.0
1	A	69	VAL	2.0
1	J	273	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
1	LYR	B	255	29/30	0.91	0.14	31,38,44,49	0
1	LYR	A	255	29/30	0.92	0.14	26,29,34,36	0
1	LYR	E	255	29/30	0.92	0.14	28,34,43,47	0
1	LYR	C	255	29/30	0.93	0.15	29,33,39,43	0
1	LYR	G	255	29/30	0.93	0.14	25,31,38,43	0
1	LYR	H	255	29/30	0.93	0.14	25,30,37,40	0
1	LYR	J	255	29/30	0.93	0.15	22,27,32,35	0
1	LYR	F	255	29/30	0.94	0.14	27,33,37,44	0
1	LYR	I	255	29/30	0.94	0.15	22,26,33,38	0
1	LYR	D	255	29/30	0.94	0.14	25,27,35,36	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
3	LFA	C	303	10/20	0.49	0.24	61,77,88,94	0
3	LFA	F	313	14/20	0.61	0.27	65,74,78,82	0
3	LFA	E	304	8/20	0.62	0.22	60,64,68,72	0
3	LFA	C	309	8/20	0.62	0.30	66,78,84,92	0
3	LFA	J	305	14/20	0.62	0.25	60,72,80,81	0
3	LFA	C	308	10/20	0.65	0.25	67,74,85,88	0
3	LFA	G	310	10/20	0.65	0.20	53,66,73,74	0
3	LFA	E	306	12/20	0.65	0.27	66,78,86,89	0
3	LFA	D	318	5/20	0.66	0.23	63,66,66,68	0
3	LFA	F	308	8/20	0.68	0.20	47,59,64,65	0
3	LFA	H	304	10/20	0.68	0.18	56,62,64,65	0
3	LFA	B	311	8/20	0.68	0.21	57,70,73,82	0
3	LFA	B	305	6/20	0.69	0.20	50,58,59,64	0
3	LFA	C	310	13/20	0.69	0.27	58,69,79,81	0
3	LFA	E	309	6/20	0.70	0.27	60,66,70,70	0
3	LFA	J	304	8/20	0.71	0.20	46,54,63,63	0
3	LFA	F	311	10/20	0.71	0.20	64,77,86,87	0
3	LFA	A	311	7/20	0.72	1.10	59,61,67,69	0
3	LFA	A	308	8/20	0.73	0.18	55,61,65,72	0
3	LFA	D	310	8/20	0.73	0.22	56,69,70,74	0
3	LFA	F	304	10/20	0.73	0.21	58,61,73,73	0
3	LFA	F	314	8/20	0.73	0.17	61,71,76,76	0
3	LFA	C	304	6/20	0.74	0.22	60,63,65,68	0
3	LFA	D	302	7/20	0.74	1.00	57,62,68,69	0
3	LFA	E	310	10/20	0.75	0.16	42,48,60,60	0
3	LFA	G	309	8/20	0.75	0.18	53,59,62,62	0
3	LFA	B	304	14/20	0.75	0.24	50,61,77,78	0
3	LFA	A	310	8/20	0.75	0.25	54,62,70,72	0
3	LFA	B	309	13/20	0.75	0.26	50,69,76,80	0
3	LFA	B	310	11/20	0.75	0.22	50,60,67,69	0
3	LFA	G	302	16/20	0.76	0.46	46,51,57,58	0
3	LFA	D	317	5/20	0.77	0.18	56,64,69,70	0
3	LFA	D	308	10/20	0.77	0.29	56,61,70,70	0
3	LFA	I	304	14/20	0.77	0.22	41,54,62,65	0
3	LFA	F	309	10/20	0.77	0.17	37,42,45,46	0
3	LFA	A	305	10/20	0.77	0.14	45,52,58,58	0
3	LFA	J	306	8/20	0.77	0.20	60,73,81,81	0
3	LFA	B	308	18/20	0.78	0.29	44,58,74,77	0
3	LFA	C	306	16/20	0.79	0.54	49,54,71,77	0
3	LFA	E	305	6/20	0.79	0.18	54,59,67,68	0
3	LFA	J	302	16/20	0.79	0.52	45,53,60,61	0
3	LFA	G	307	16/20	0.79	0.43	48,54,59,59	0
3	LFA	F	302	7/20	0.79	1.31	76,83,88,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LFA	D	313	6/20	0.79	0.12	44,51,57,57	0
3	LFA	I	303	7/20	0.80	1.05	52,62,74,80	0
3	LFA	I	310	14/20	0.80	0.19	47,55,63,64	0
3	LFA	B	306	8/20	0.81	0.14	53,63,65,66	0
3	LFA	I	305	6/20	0.81	0.22	48,57,60,61	0
3	LFA	F	312	8/20	0.81	0.17	48,64,82,84	0
3	LFA	D	306	16/20	0.81	0.51	44,56,67,67	0
3	LFA	G	313	8/20	0.81	0.20	48,55,59,65	0
3	LFA	B	307	16/20	0.81	0.53	46,57,66,66	0
3	LFA	C	312	4/20	0.81	0.15	44,46,47,47	0
4	MPG	E	313	14/25	0.81	0.18	48,53,68,72	0
3	LFA	H	307	14/20	0.82	0.20	56,65,71,71	0
3	LFA	F	306	10/20	0.82	0.12	48,54,59,63	0
3	LFA	D	305	10/20	0.82	0.19	51,54,63,64	0
3	LFA	G	304	14/20	0.82	0.25	39,54,62,62	0
4	MPG	A	313	14/25	0.82	0.25	54,60,66,70	0
3	LFA	A	303	6/20	0.82	0.18	52,54,59,63	0
3	LFA	F	307	6/20	0.83	0.19	43,43,46,48	0
3	LFA	F	305	6/20	0.83	0.24	54,56,58,58	0
3	LFA	D	309	8/20	0.83	0.26	56,70,81,82	0
3	LFA	G	311	8/20	0.83	0.20	51,62,68,69	0
3	LFA	J	307	7/20	0.83	0.90	56,61,78,83	0
3	LFA	G	305	6/20	0.83	0.21	55,56,58,64	0
4	MPG	D	315	14/25	0.83	0.20	49,54,63,68	0
3	LFA	H	302	13/20	0.83	0.20	41,52,61,61	0
3	LFA	C	302	7/20	0.84	0.93	45,57,66,69	0
3	LFA	J	309	10/20	0.84	0.15	49,52,58,58	0
3	LFA	D	303	14/20	0.84	0.25	40,67,73,73	0
3	LFA	E	302	14/20	0.84	0.56	44,56,65,66	0
3	LFA	H	308	8/20	0.84	0.20	64,70,71,72	0
3	LFA	G	315	6/20	0.85	0.20	45,53,58,59	0
3	LFA	I	302	7/20	0.85	1.29	59,70,82,84	0
3	LFA	B	302	7/20	0.85	1.06	60,62,73,76	0
3	LFA	B	303	7/20	0.85	1.07	54,62,93,97	0
3	LFA	E	307	8/20	0.85	0.19	61,68,70,73	0
4	MPG	J	312	14/25	0.85	0.22	51,59,67,68	0
3	LFA	D	304	6/20	0.86	0.19	47,51,52,57	0
3	LFA	A	302	14/20	0.86	0.24	49,55,63,65	0
3	LFA	G	306	10/20	0.86	0.14	45,54,57,57	0
3	LFA	E	311	8/20	0.86	0.37	40,45,48,50	0
3	LFA	A	304	10/20	0.87	0.16	47,50,55,57	0
3	LFA	J	308	14/20	0.87	0.23	39,52,59,60	0

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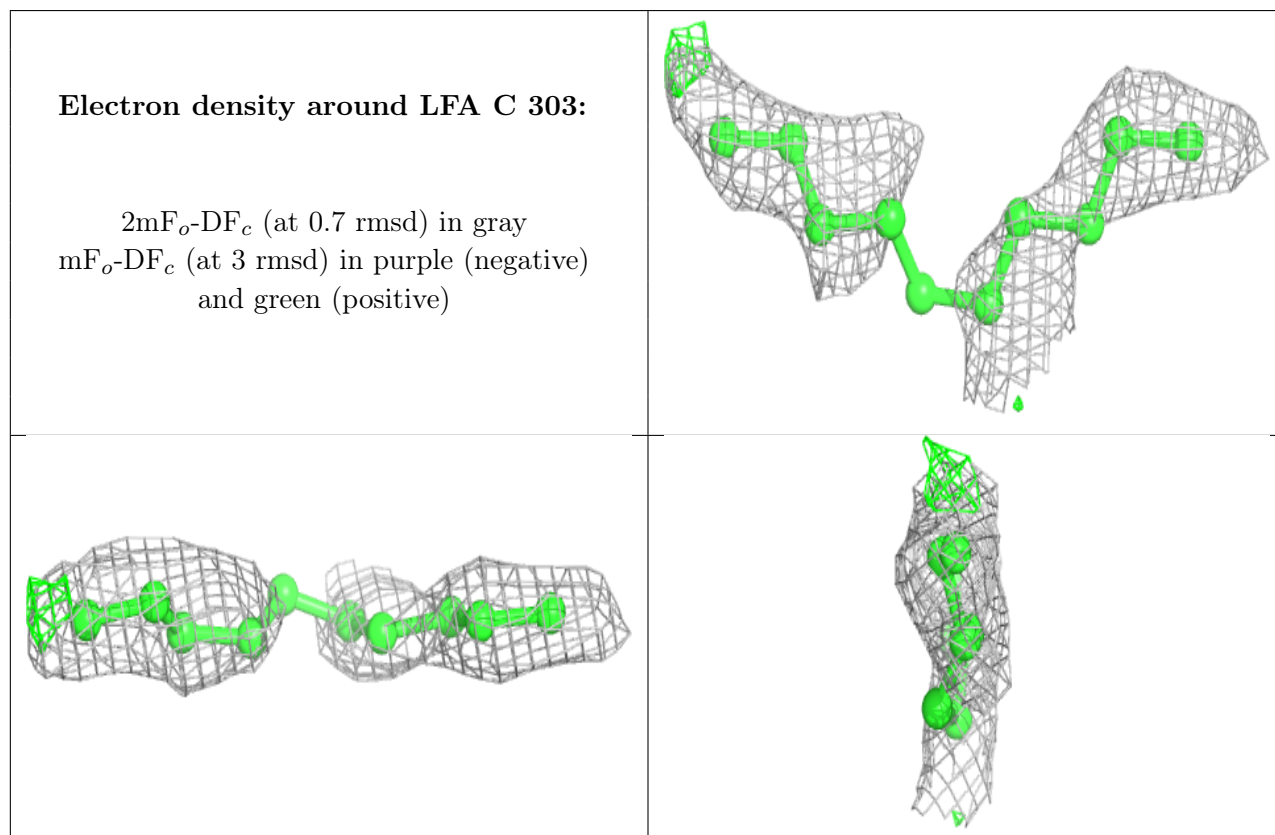
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LFA	E	312	8/20	0.87	0.15	47,52,55,57	0
3	LFA	J	310	10/20	0.87	0.12	51,56,58,60	0
3	LFA	D	311	7/20	0.88	0.14	51,53,55,57	0
3	LFA	H	303	6/20	0.88	0.18	54,55,57,63	0
3	LFA	C	311	8/20	0.88	0.24	59,64,67,71	0
3	LFA	I	308	16/20	0.88	0.49	42,53,68,72	0
3	LFA	I	309	18/20	0.88	0.29	32,42,64,75	0
3	LFA	D	314	7/20	0.88	0.12	50,55,59,60	0
3	LFA	D	316	5/20	0.88	0.11	50,52,53,54	0
3	LFA	H	312	6/20	0.88	0.12	51,53,54,56	0
3	LFA	F	303	14/20	0.88	0.27	54,61,66,70	0
3	LFA	C	307	18/20	0.89	0.31	42,48,57,57	0
3	LFA	E	308	14/20	0.89	0.20	51,56,64,65	0
3	LFA	J	303	18/20	0.89	0.30	37,45,57,62	0
3	LFA	H	305	16/20	0.89	0.44	40,51,56,59	0
4	MPG	C	313	13/25	0.89	0.12	46,53,64,74	0
3	LFA	G	303	7/20	0.89	1.08	57,59,75,79	0
3	LFA	G	308	18/20	0.89	0.28	43,48,60,64	0
3	LFA	F	310	18/20	0.89	0.29	39,51,65,66	0
3	LFA	I	307	6/20	0.90	0.15	38,41,44,47	0
3	LFA	A	309	8/20	0.90	0.17	55,61,70,73	0
4	MPG	B	312	14/25	0.90	0.23	50,62,71,72	0
3	LFA	H	306	18/20	0.90	0.25	42,46,52,53	0
3	LFA	G	314	6/20	0.90	0.22	50,54,54,55	0
3	LFA	A	306	14/20	0.90	0.49	47,51,56,56	0
4	MPG	F	315	14/25	0.90	0.18	41,51,57,62	0
4	MPG	G	312	14/25	0.90	0.20	48,54,62,64	0
3	LFA	H	309	5/20	0.90	0.17	41,42,45,47	0
3	LFA	C	305	10/20	0.91	0.12	41,47,51,52	0
3	LFA	E	303	18/20	0.91	0.29	35,46,62,66	0
3	LFA	I	306	10/20	0.91	0.12	37,39,41,42	0
4	MPG	H	313	14/25	0.91	0.21	49,62,72,75	0
3	LFA	A	312	5/20	0.91	0.11	43,45,50,54	0
3	LFA	A	307	18/20	0.92	0.25	37,45,63,71	0
3	LFA	H	310	8/20	0.92	0.12	39,46,48,50	0
4	MPG	I	314	14/25	0.92	0.16	35,42,60,72	0
3	LFA	I	311	8/20	0.92	0.12	45,54,56,59	0
3	LFA	D	307	18/20	0.93	0.26	34,39,50,60	0
3	LFA	I	313	4/20	0.93	0.09	38,42,43,44	0
3	LFA	H	311	7/20	0.93	0.18	44,44,53,57	0
3	LFA	D	312	6/20	0.94	0.14	40,45,49,52	0
3	LFA	I	312	7/20	0.95	0.12	30,34,45,48	0

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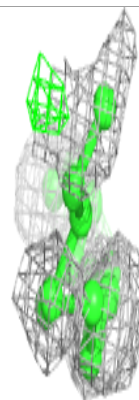
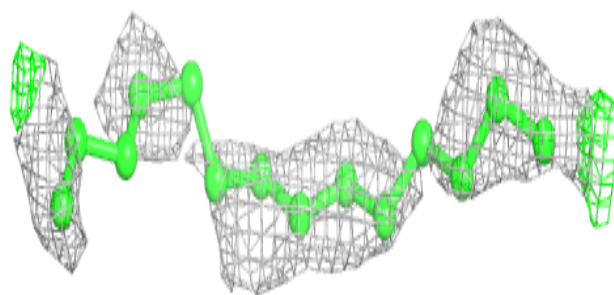
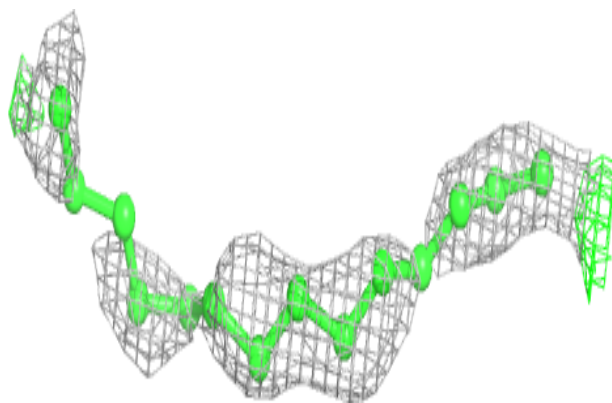
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LFA	J	311	4/20	0.96	0.09	33,35,36,37	0
2	NA	B	301	1/1	0.97	0.06	29,29,29,29	0
2	NA	H	301	1/1	0.97	0.08	30,30,30,30	0
2	NA	E	301	1/1	0.98	0.10	27,27,27,27	0
2	NA	F	301	1/1	0.98	0.12	29,29,29,29	0
2	NA	D	301	1/1	0.98	0.09	29,29,29,29	0
2	NA	I	301	1/1	0.98	0.07	23,23,23,23	0
2	NA	G	301	1/1	0.99	0.17	26,26,26,26	0
2	NA	C	301	1/1	0.99	0.14	28,28,28,28	0
2	NA	A	301	1/1	0.99	0.15	34,34,34,34	0
2	NA	J	301	1/1	0.99	0.09	28,28,28,28	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.

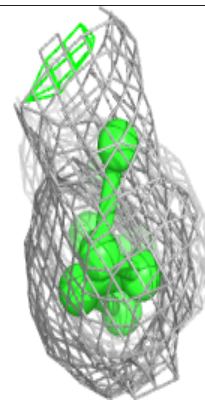
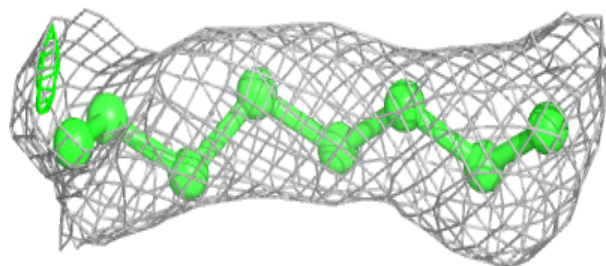
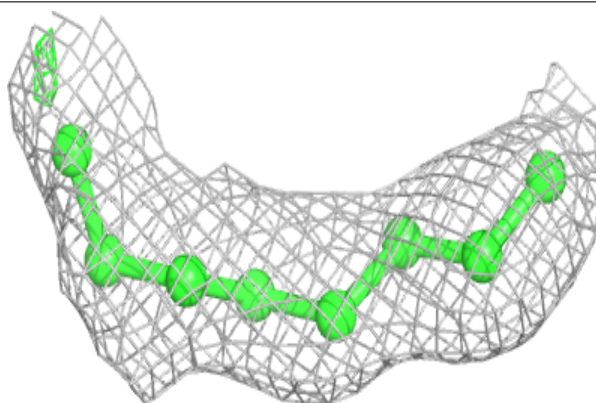


**Electron density around LFA F 313:**

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

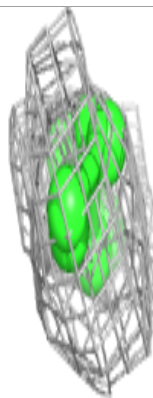
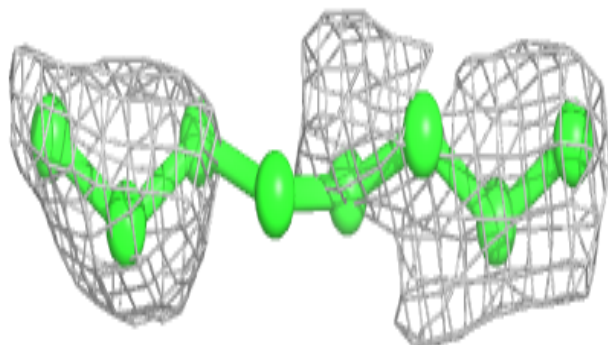
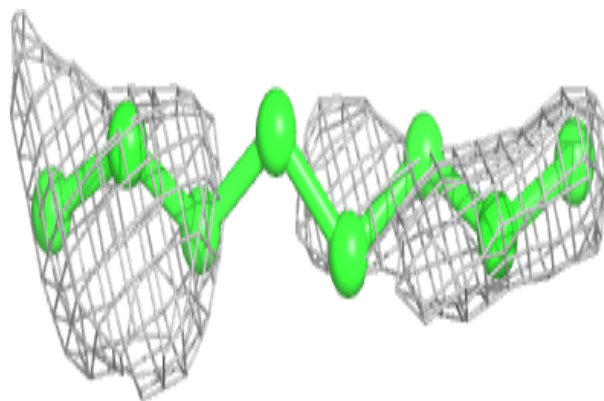
**Electron density around LFA E 304:**

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

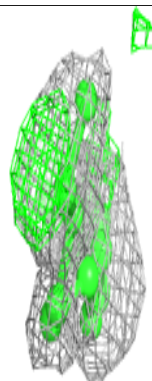
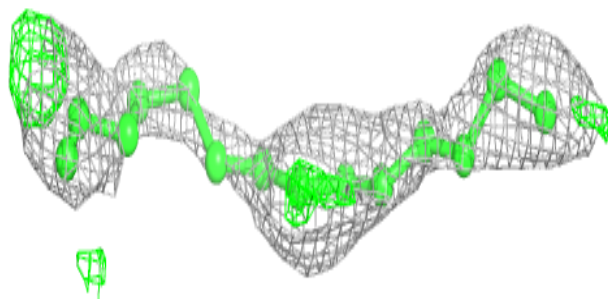
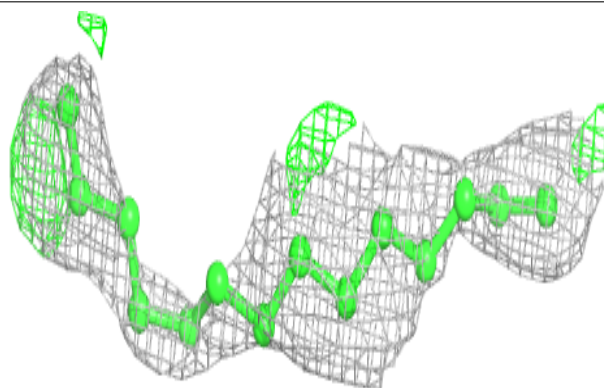


**Electron density around LFA C 309:**

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

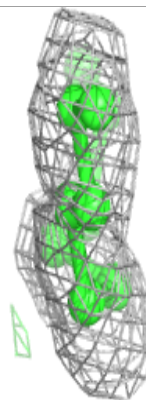
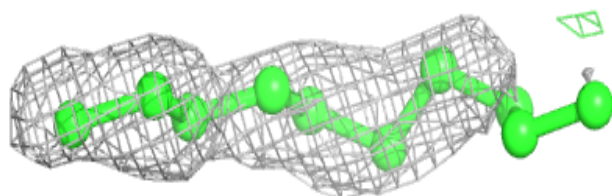
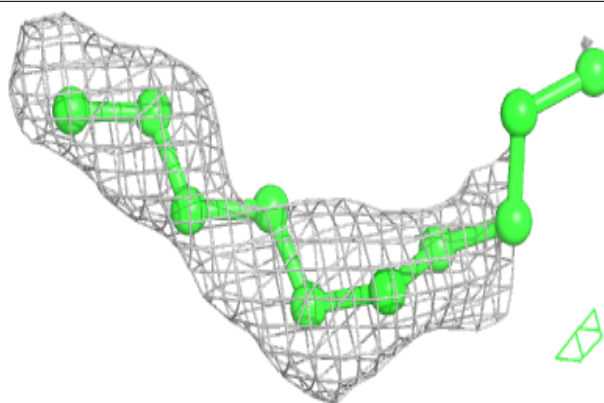
**Electron density around LFA J 305:**

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

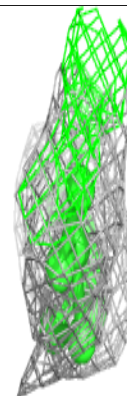
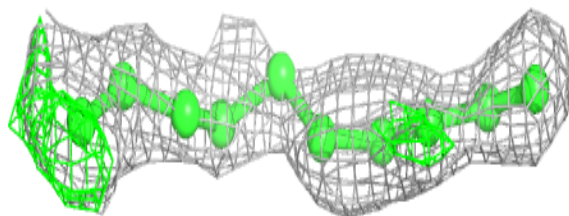
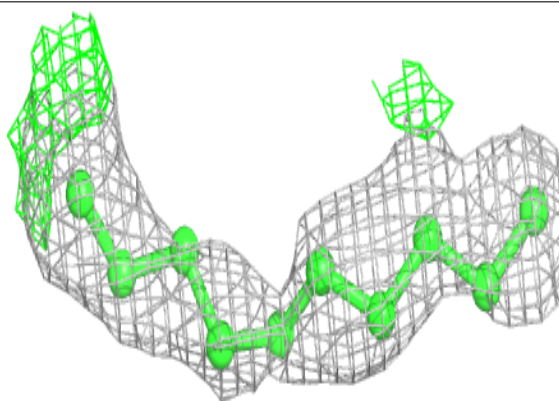


**Electron density around LFA C 308:**

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

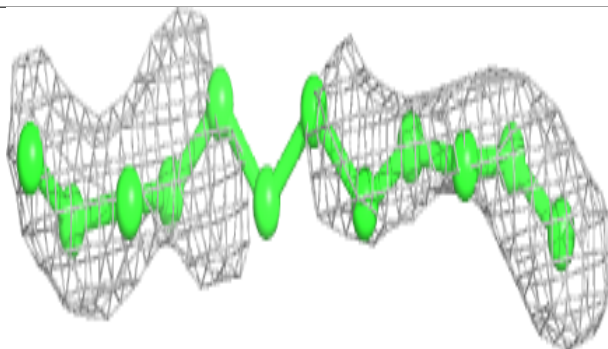
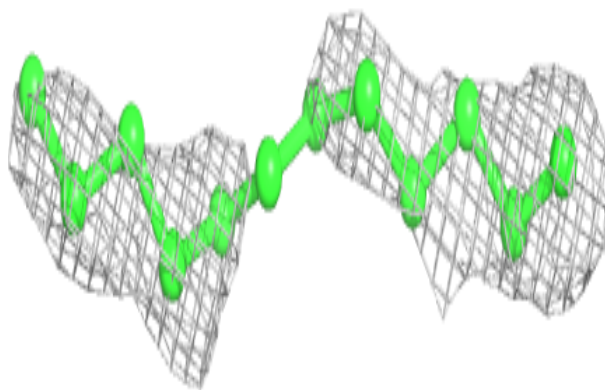
**Electron density around LFA G 310:**

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

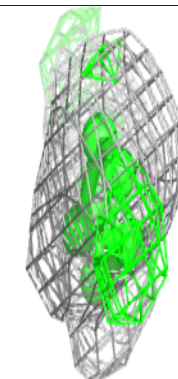
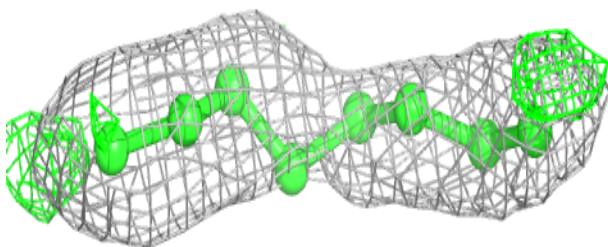
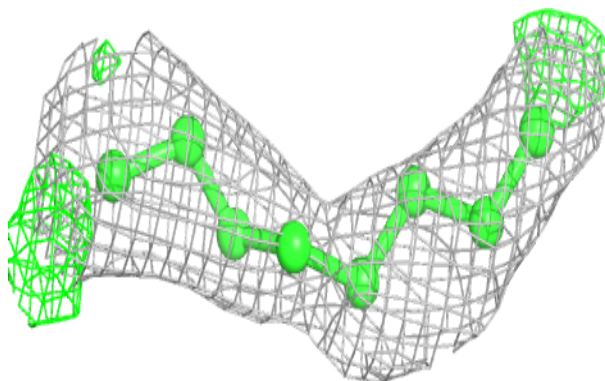


**Electron density around LFA E 306:**

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

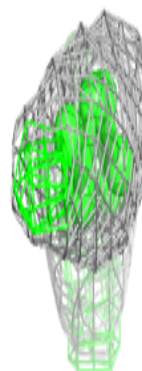
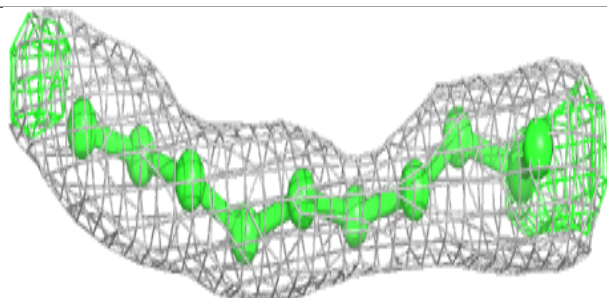
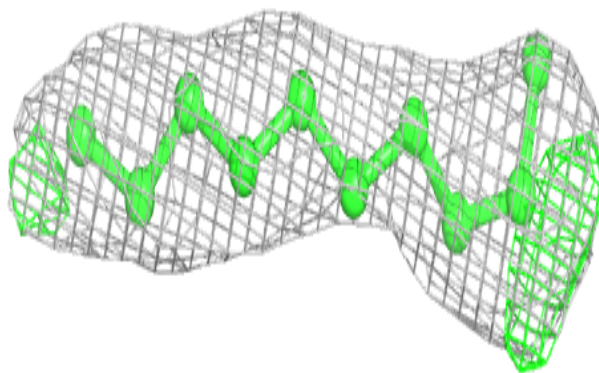
**Electron density around LFA F 308:**

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

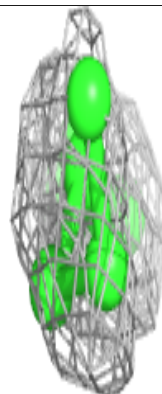
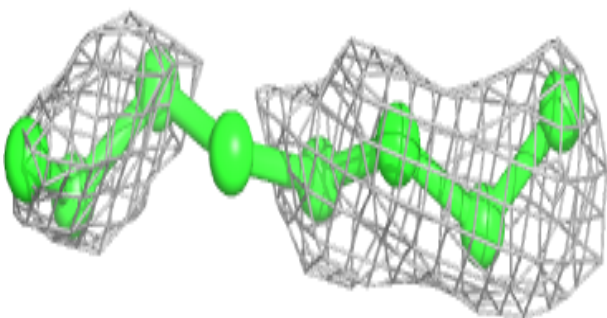
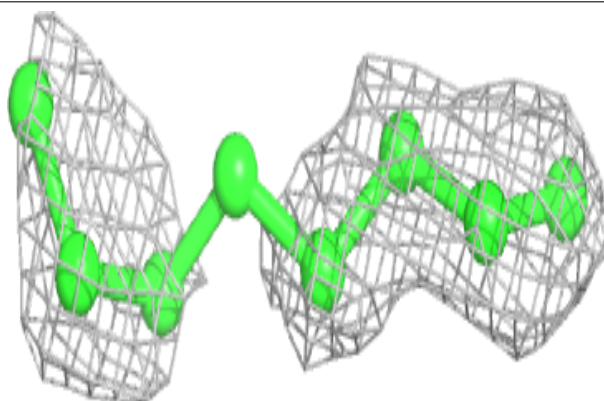


**Electron density around LFA H 304:**

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

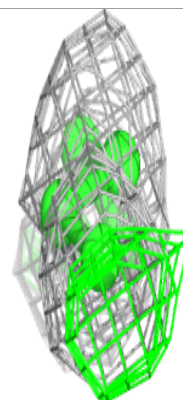
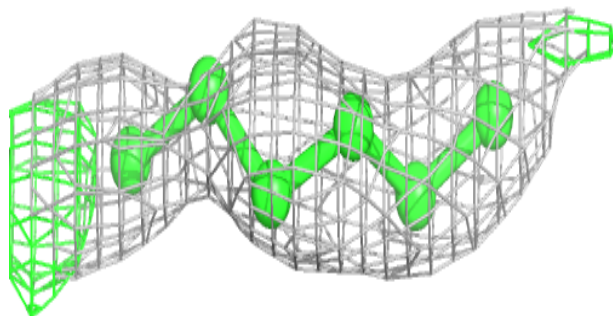
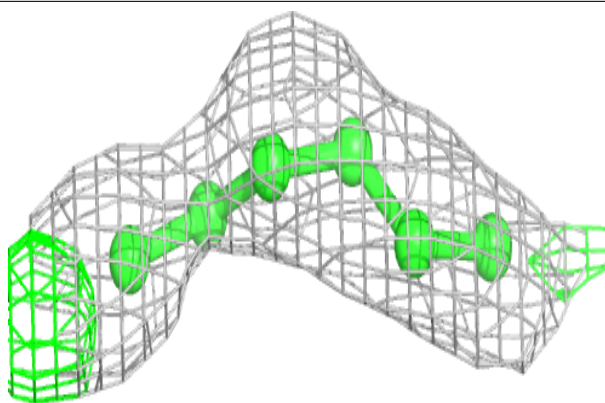
**Electron density around LFA B 311:**

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

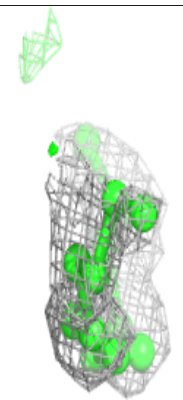
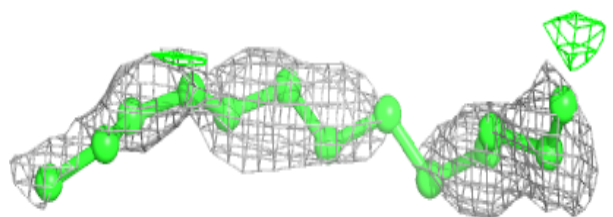
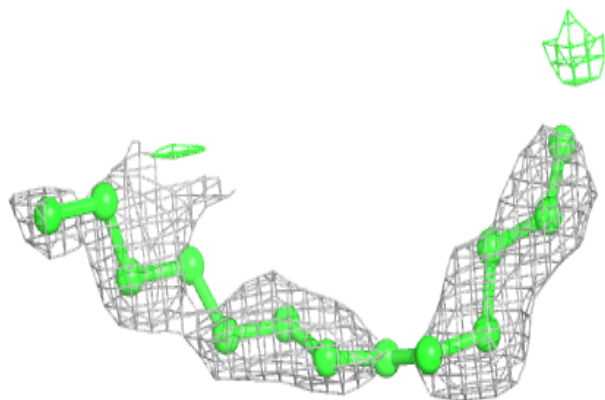


**Electron density around LFA B 305:**

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

**Electron density around LFA C 310:**

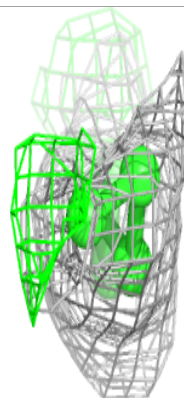
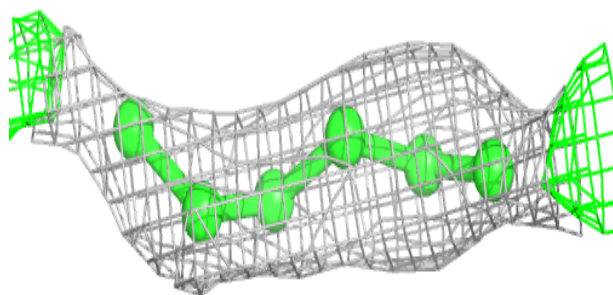
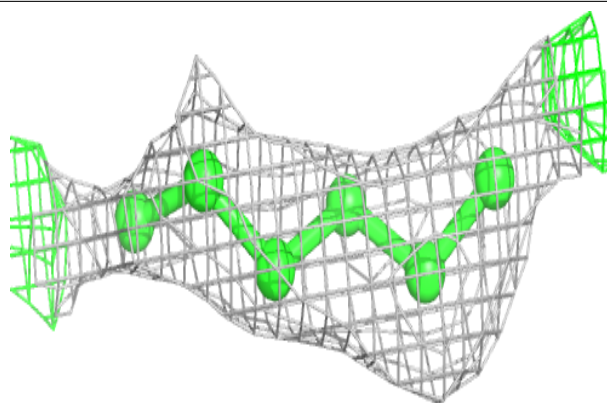
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



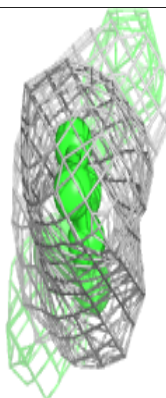
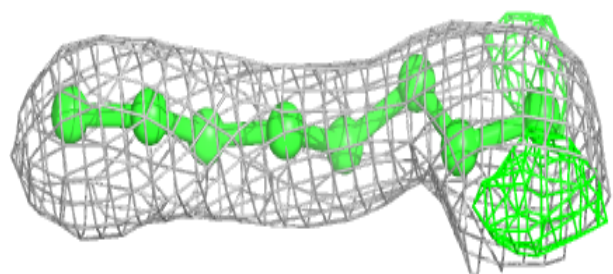
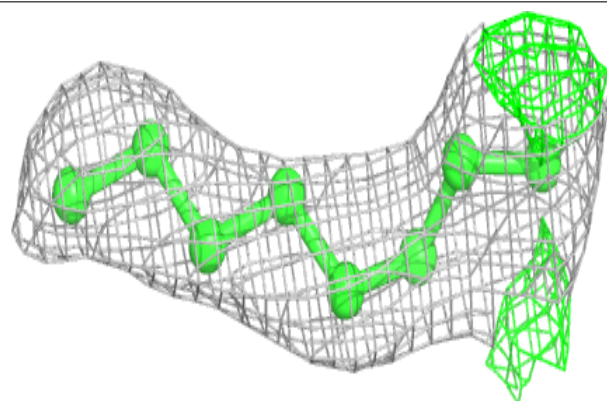


**Electron density around LFA E 309:**

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

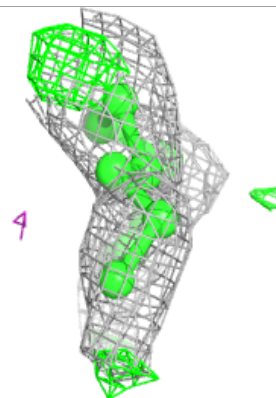
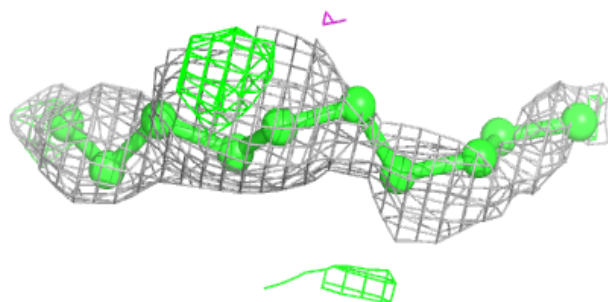
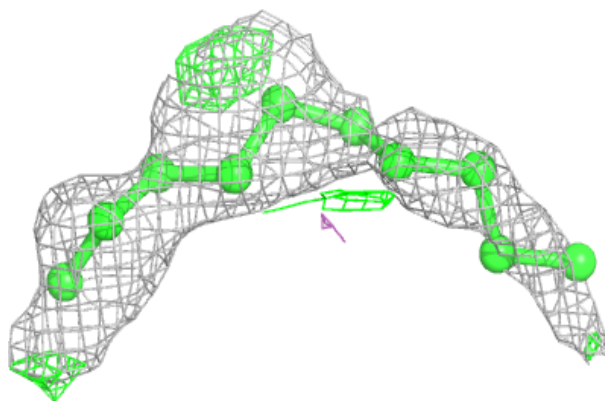
**Electron density around LFA J 304:**

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

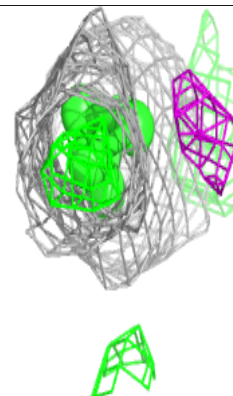
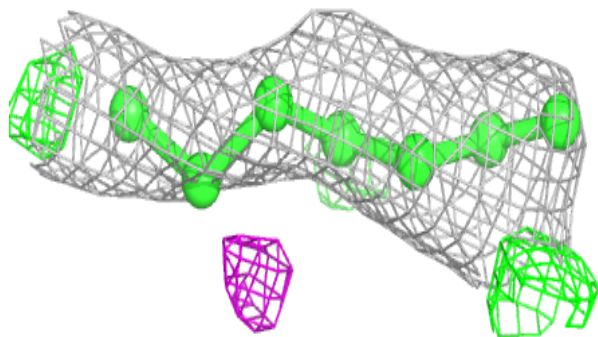
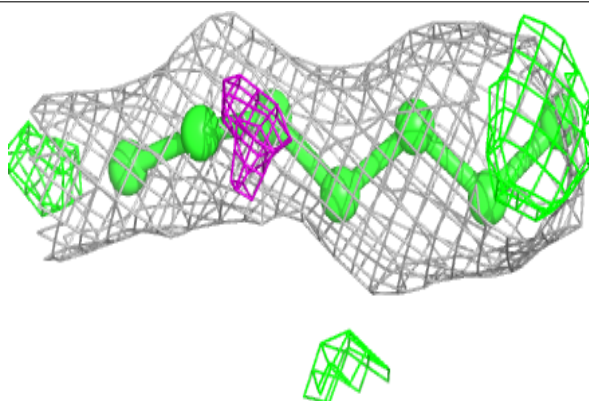


**Electron density around LFA F 311:**

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

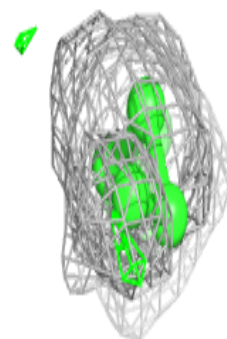
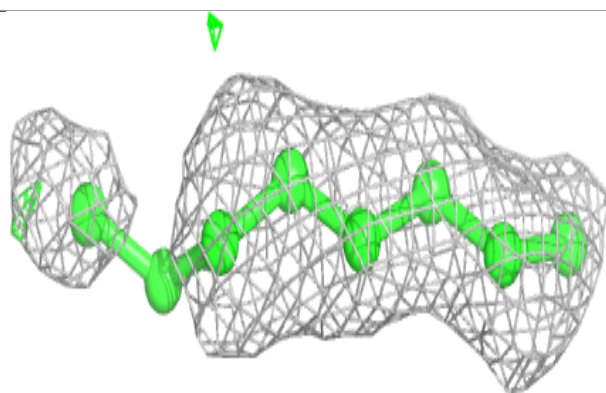
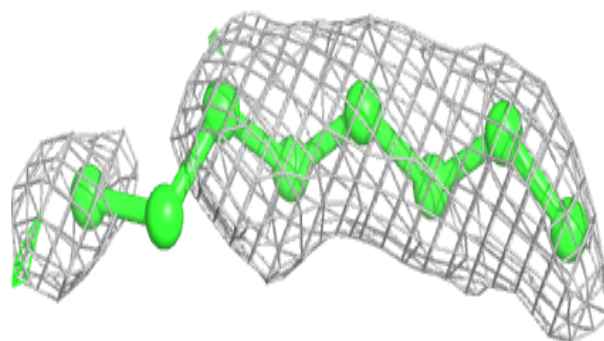
**Electron density around LFA A 311:**

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

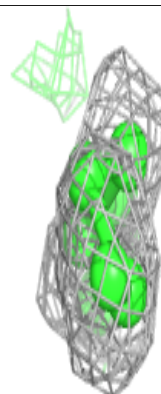
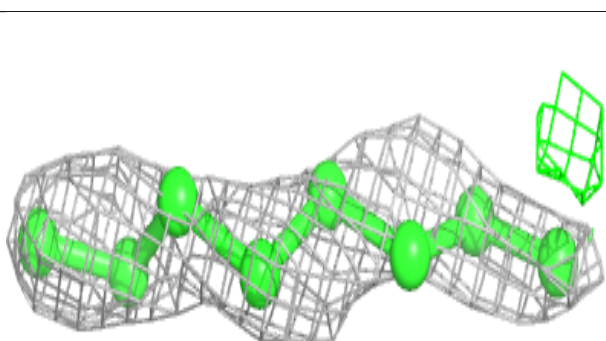
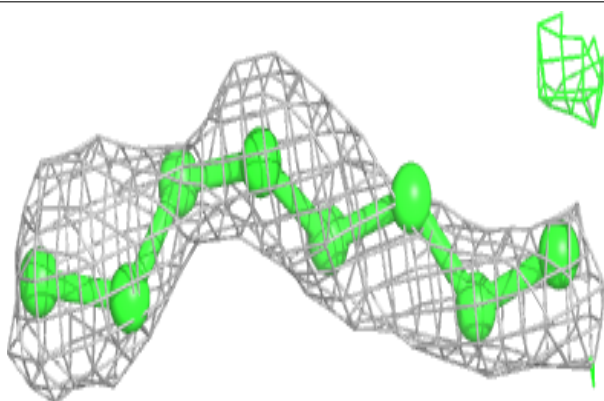


**Electron density around LFA A 308:**

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

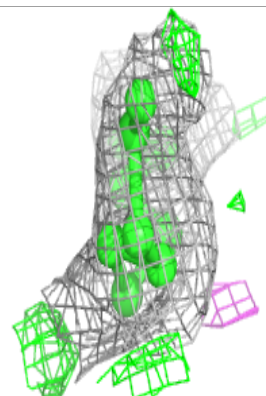
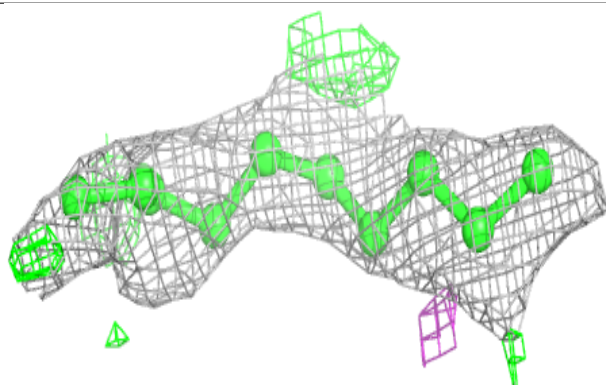
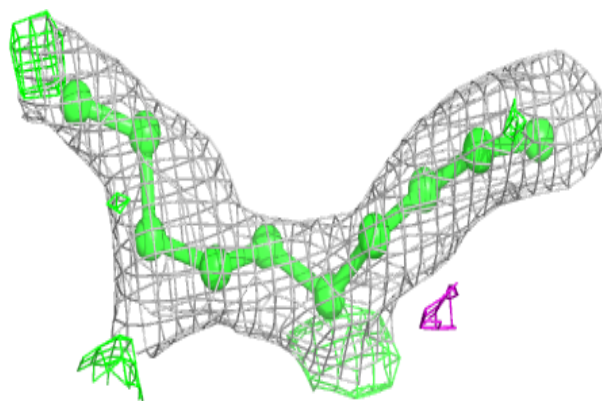
**Electron density around LFA D 310:**

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

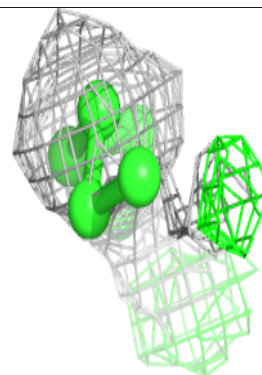
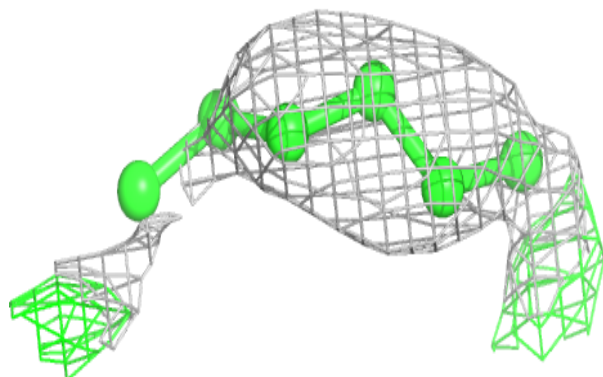
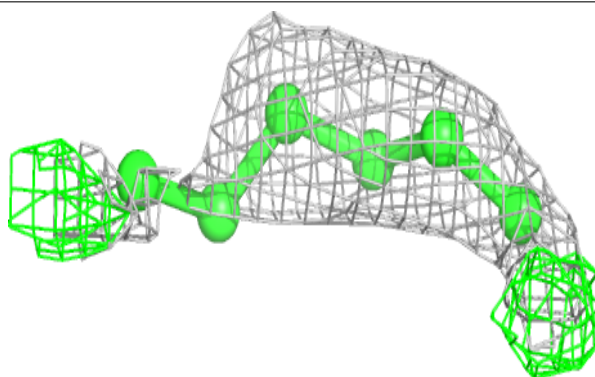


**Electron density around LFA F 304:**

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

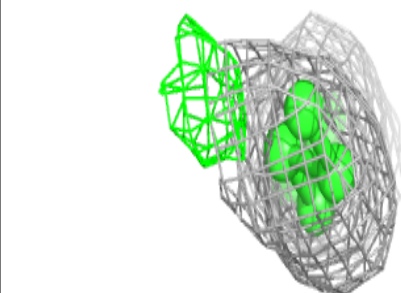
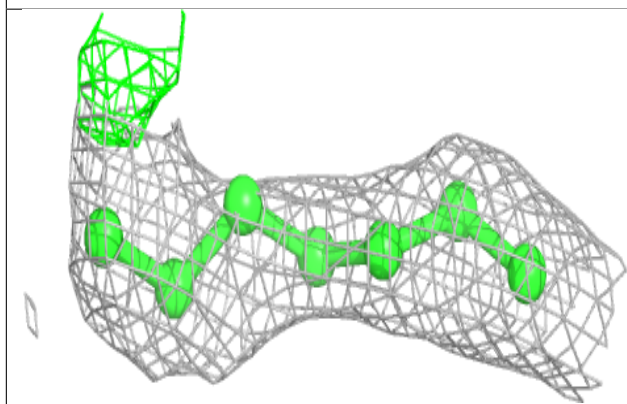
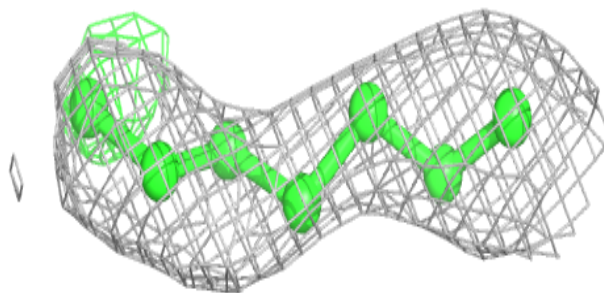
**Electron density around LFA C 304:**

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

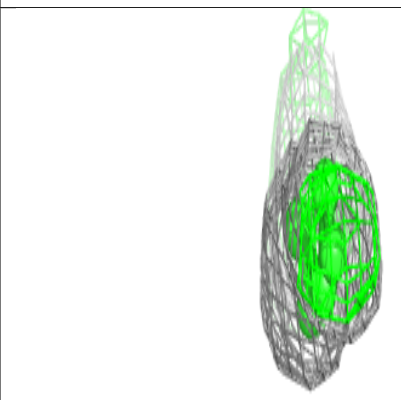
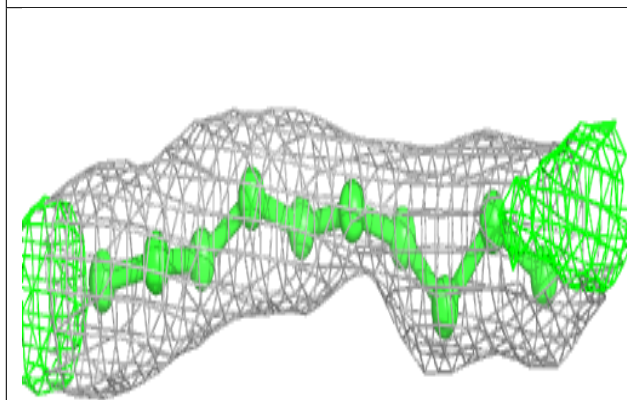
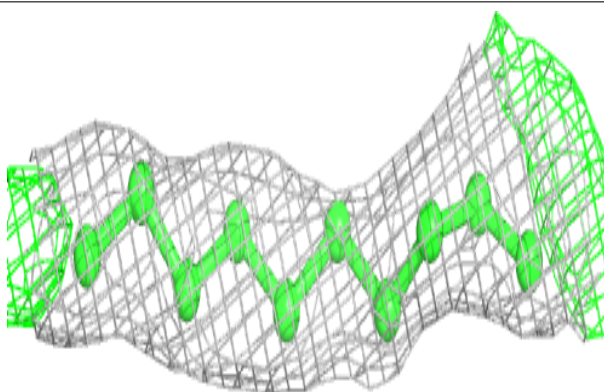


**Electron density around LFA D 302:**

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

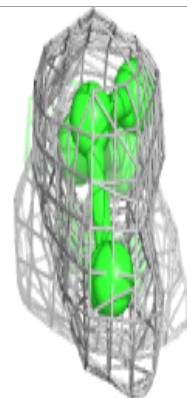
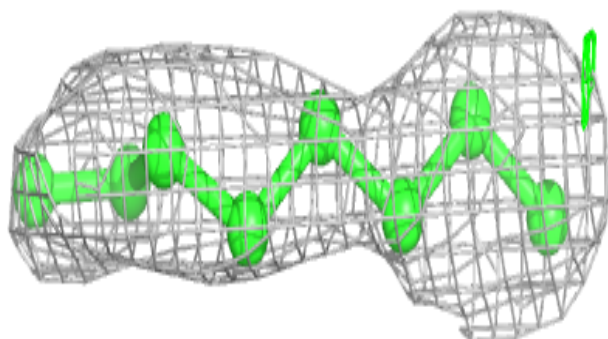
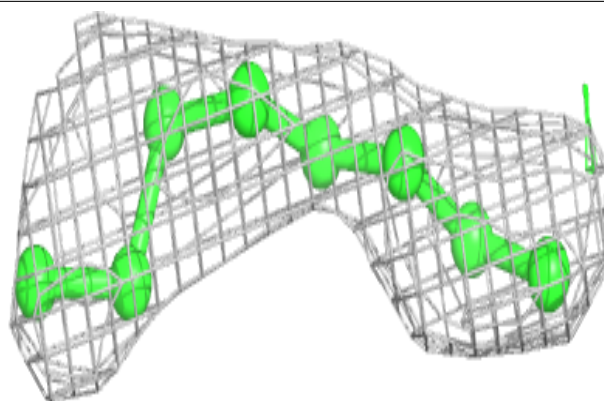
**Electron density around LFA E 310:**

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

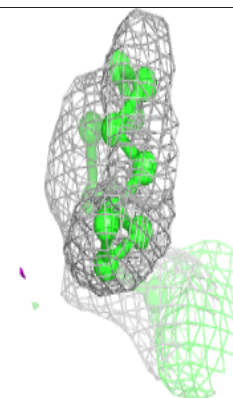
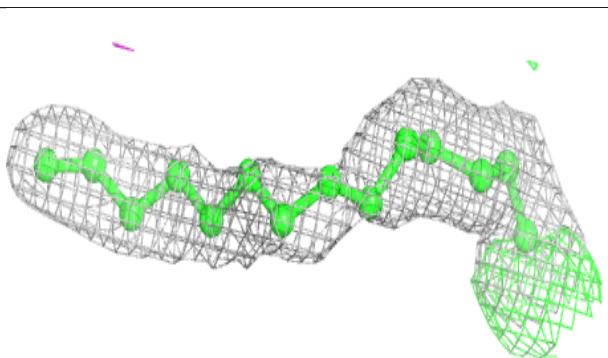
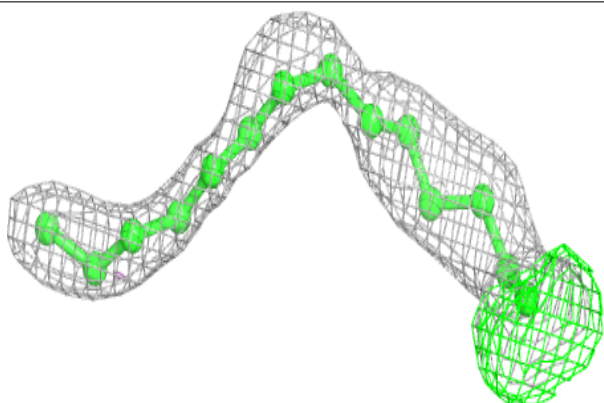


**Electron density around LFA G 309:**

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

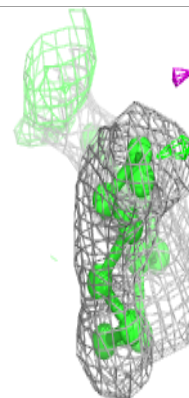
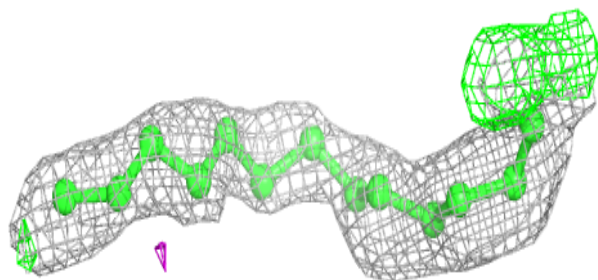
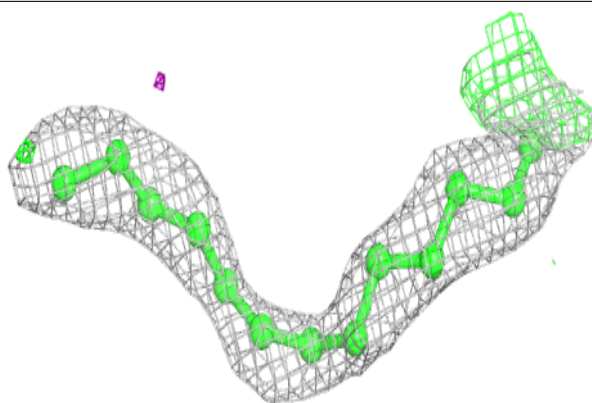
**Electron density around LFA B 304:**

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

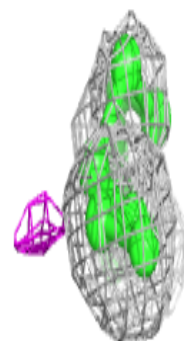
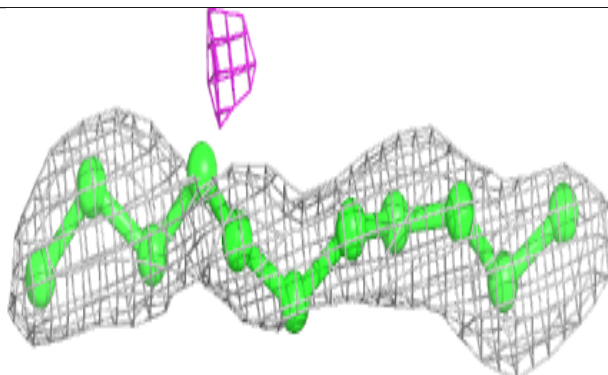
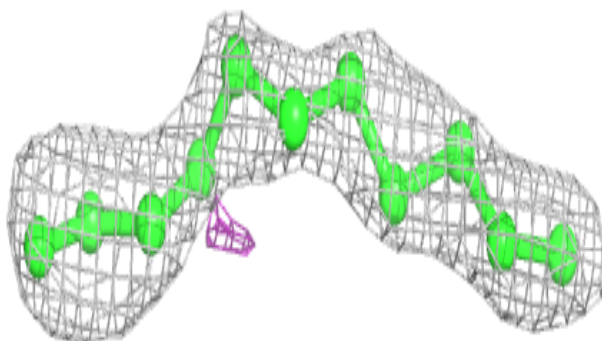


**Electron density around LFA B 309:**

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

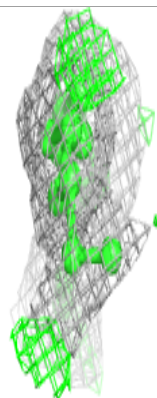
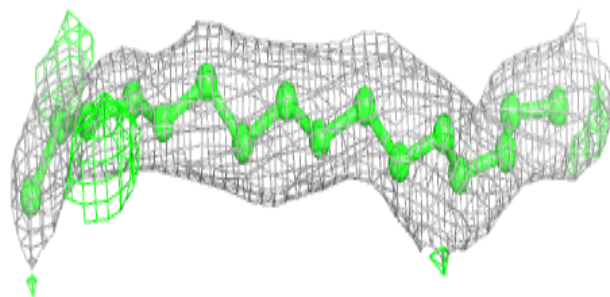
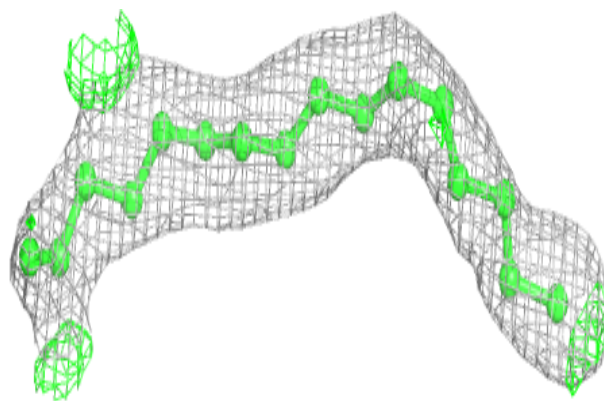
**Electron density around LFA B 310:**

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

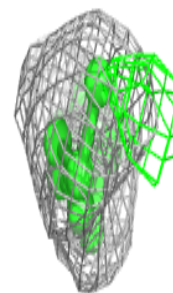
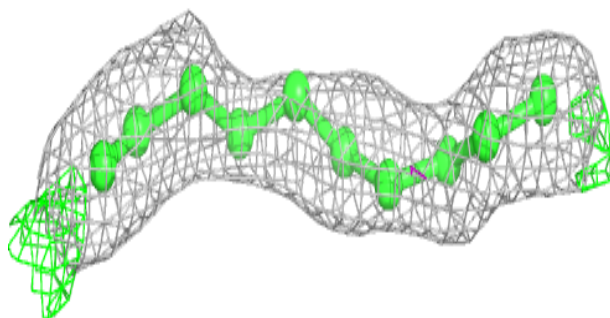
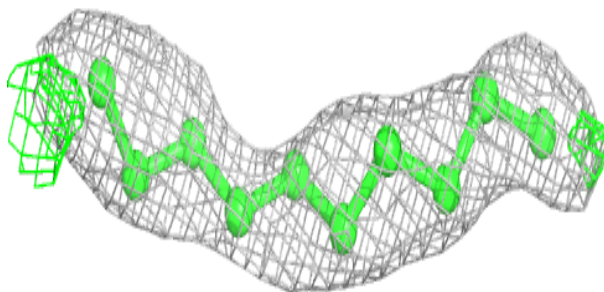


**Electron density around LFA G 302:**

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

**Electron density around LFA D 308:**

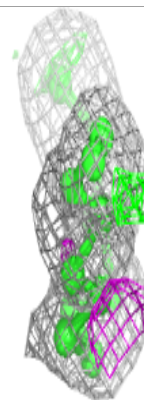
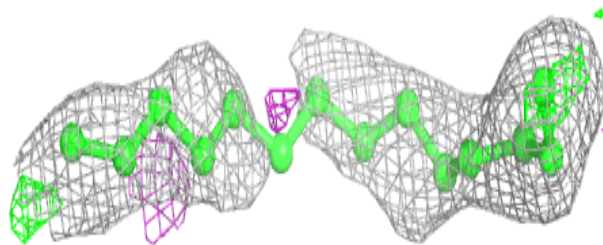
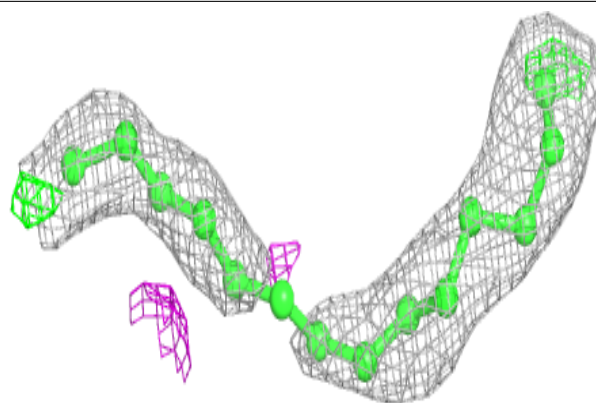
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



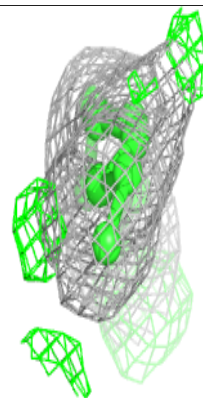
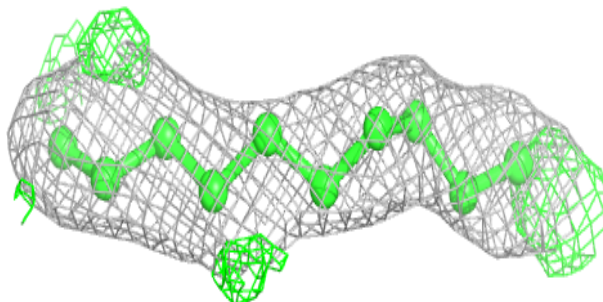
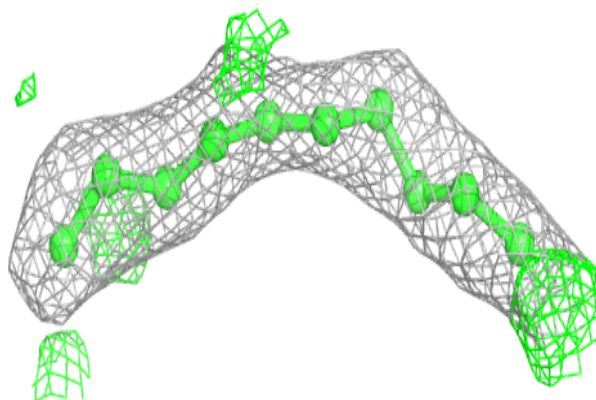


**Electron density around LFA I 304:**

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

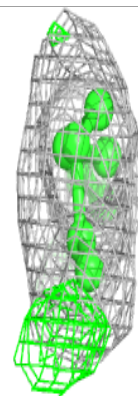
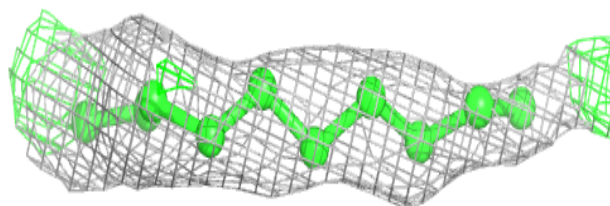
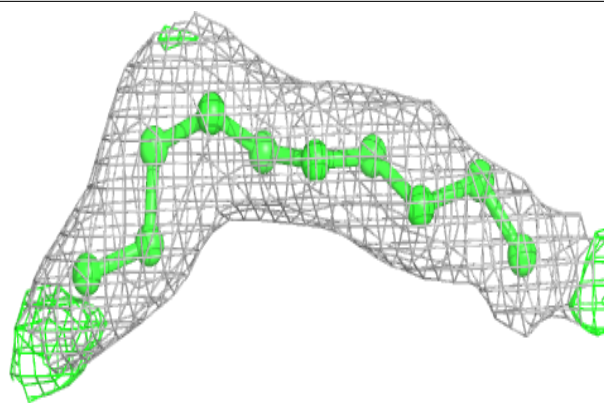
**Electron density around LFA F 309:**

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

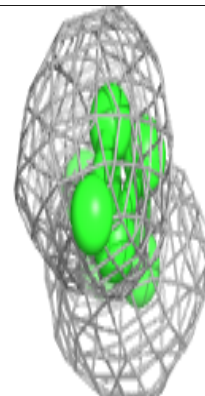
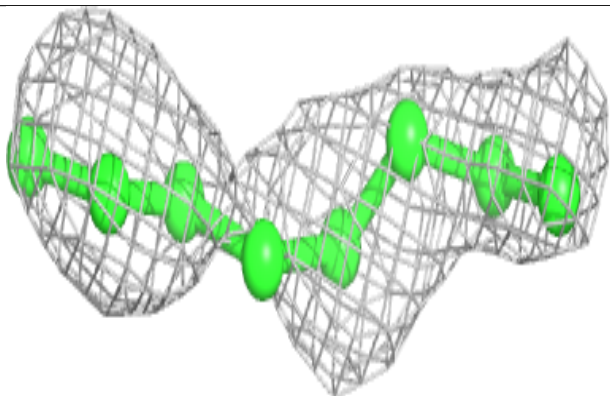
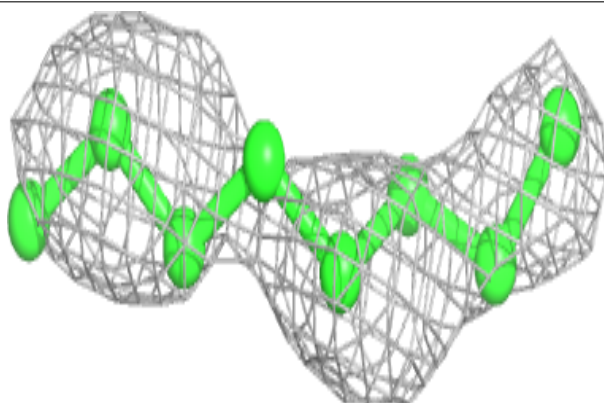


**Electron density around LFA A 305:**

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

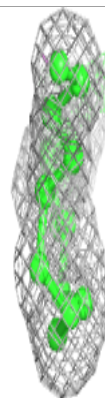
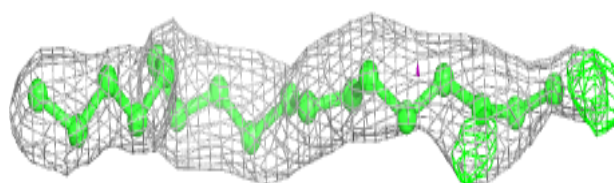
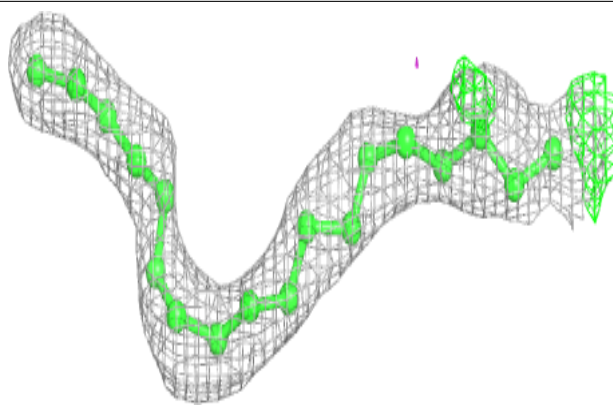
**Electron density around LFA J 306:**

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

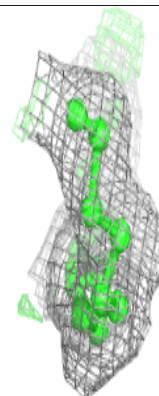
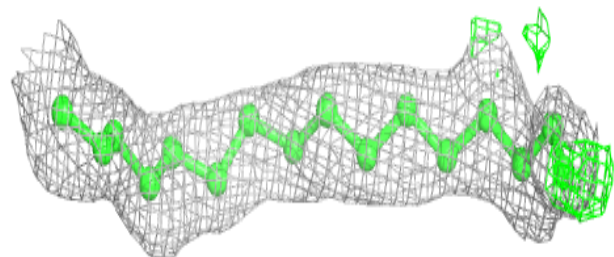
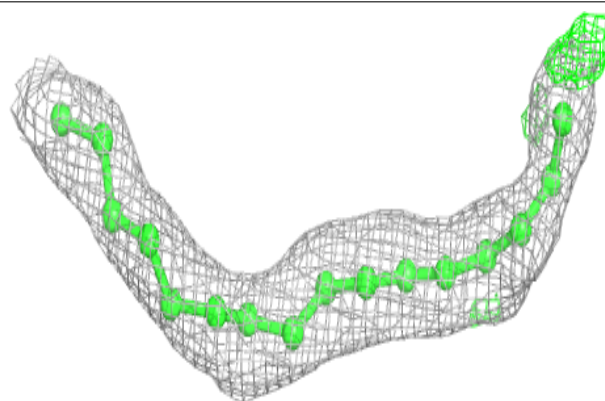


**Electron density around LFA B 308:**

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

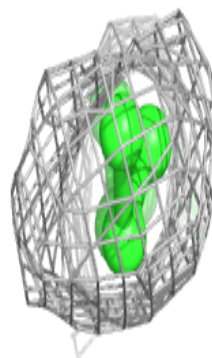
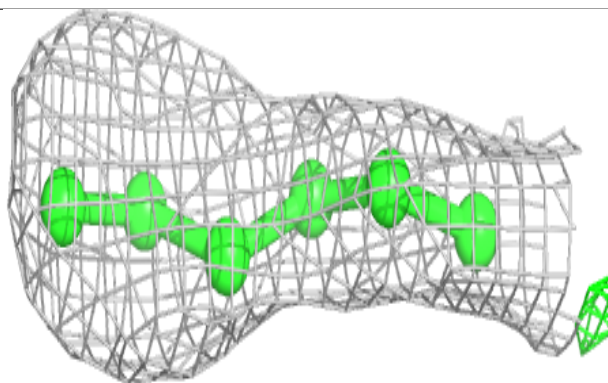
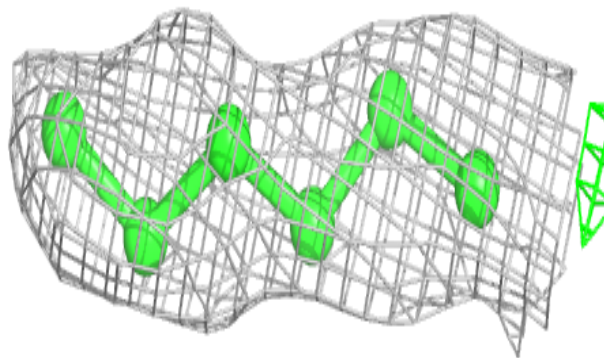
**Electron density around LFA C 306:**

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

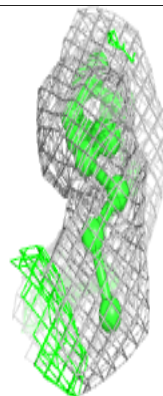
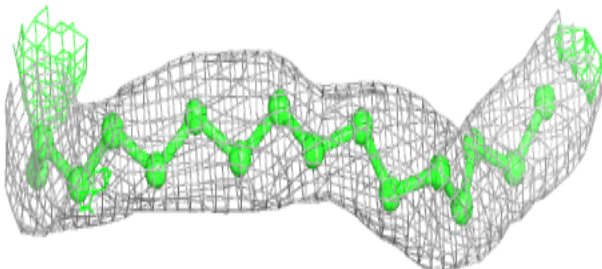
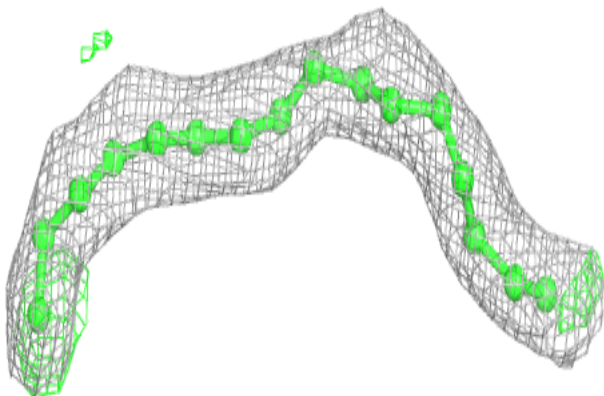


**Electron density around LFA E 305:**

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

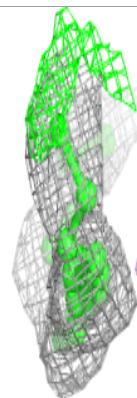
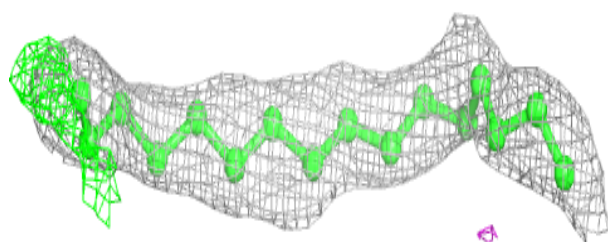
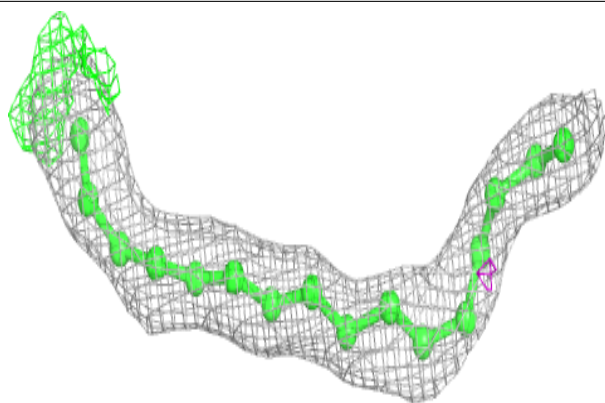
**Electron density around LFA J 302:**

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

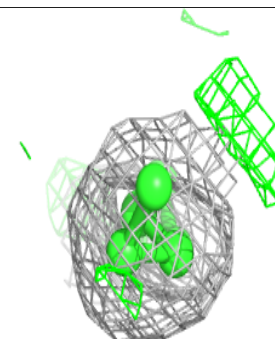
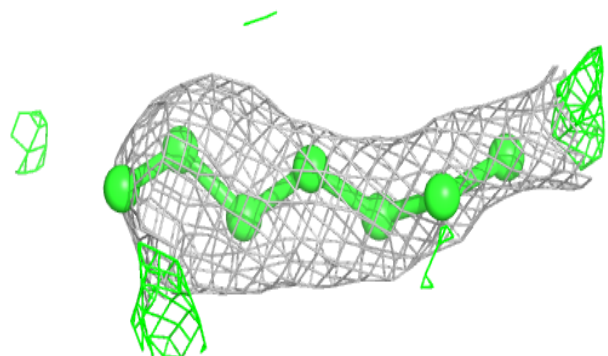
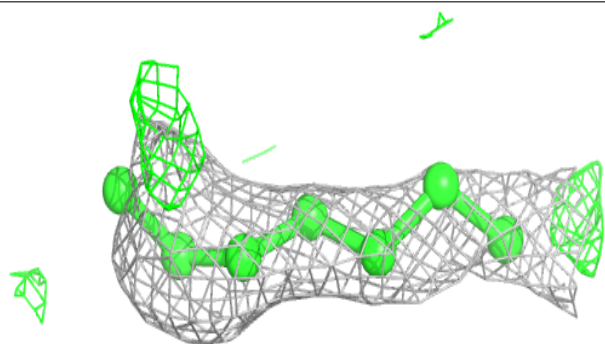


**Electron density around LFA G 307:**

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

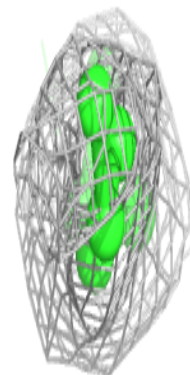
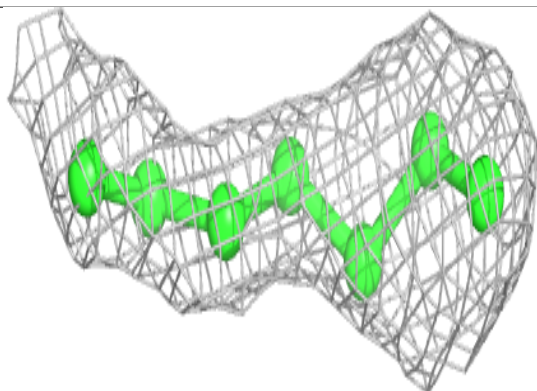
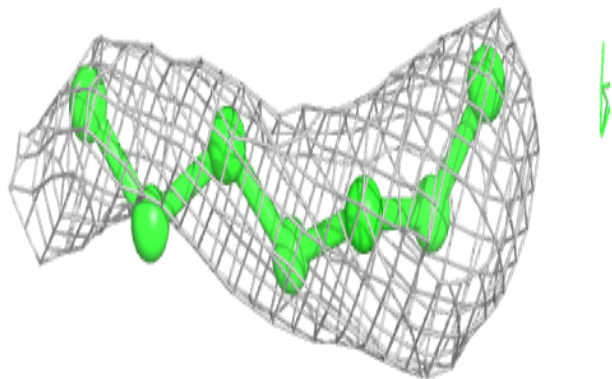
**Electron density around LFA F 302:**

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

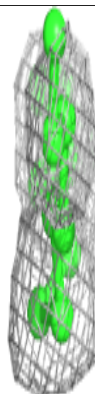
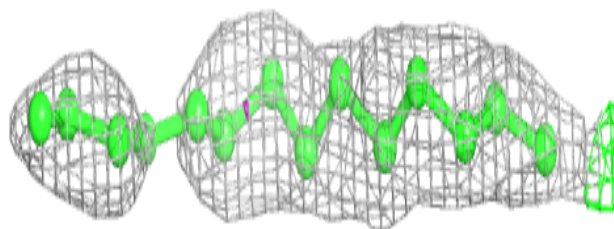
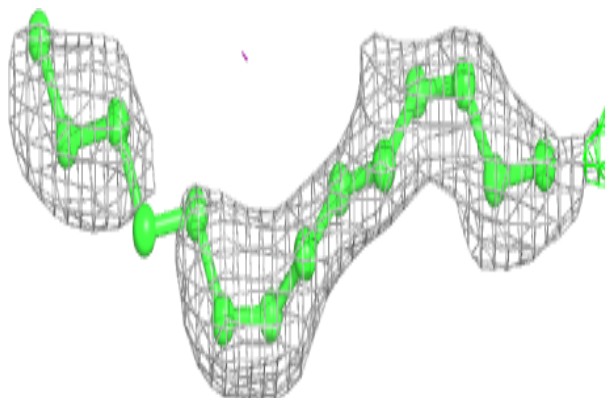


**Electron density around LFA I 303:**

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

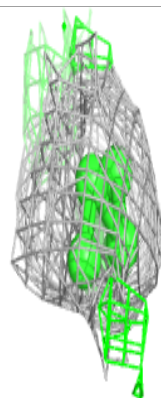
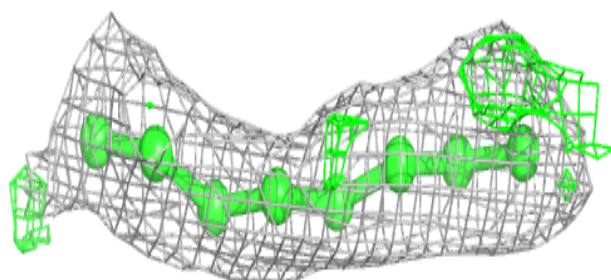
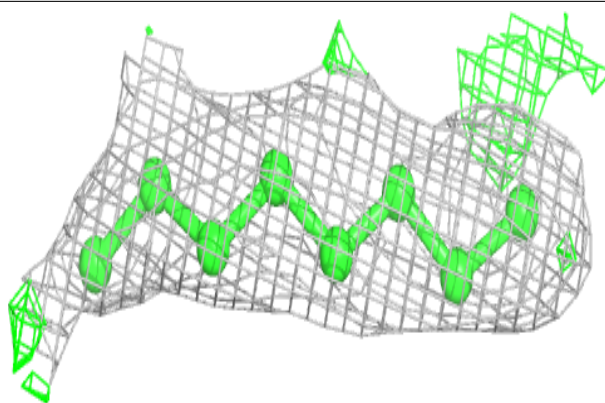
**Electron density around LFA I 310:**

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

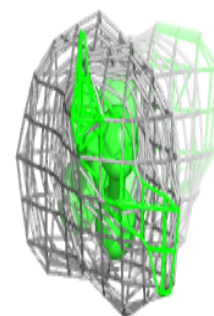
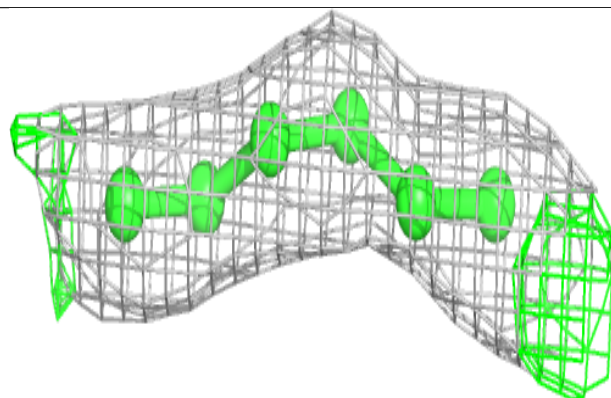
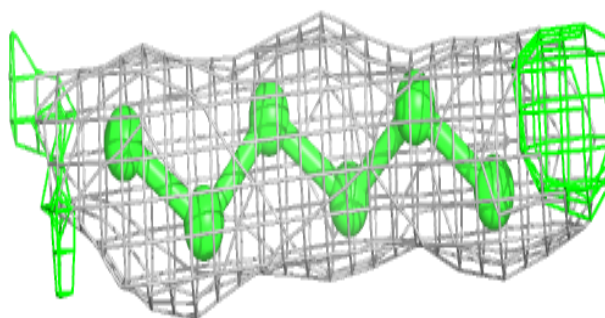


**Electron density around LFA B 306:**

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

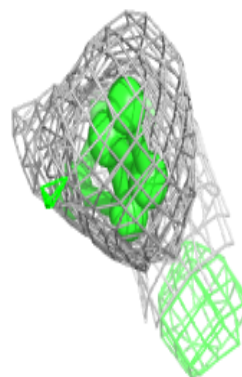
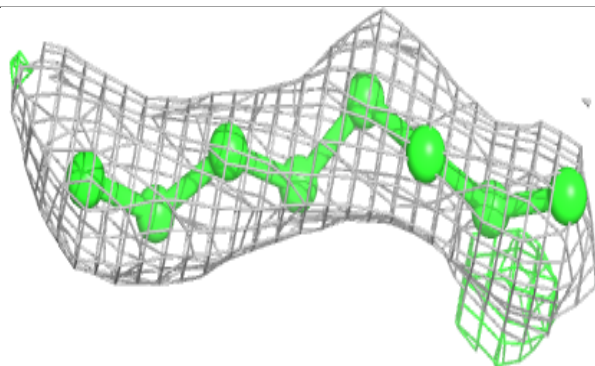
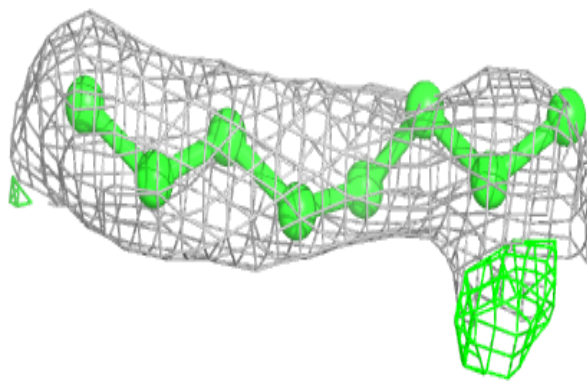
**Electron density around LFA I 305:**

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

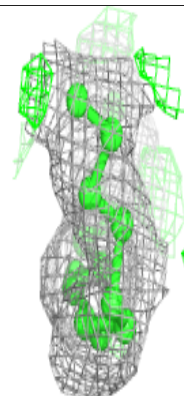
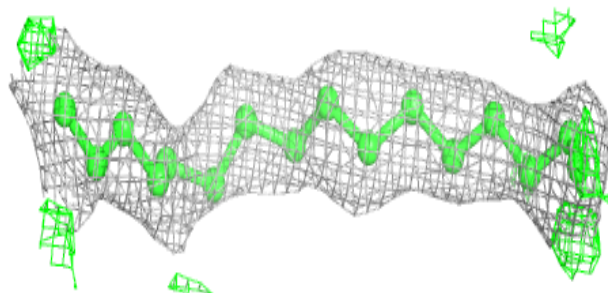
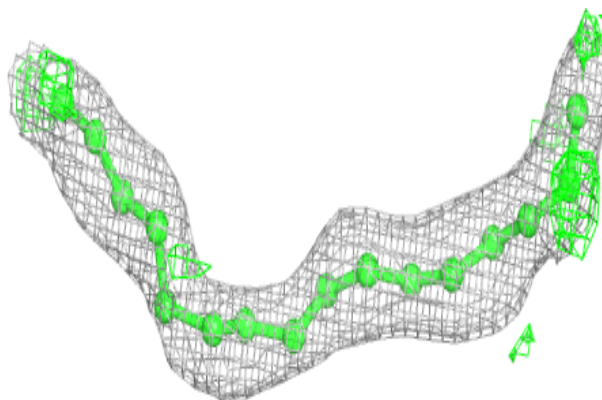


**Electron density around LFA F 312:**

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

**Electron density around LFA D 306:**

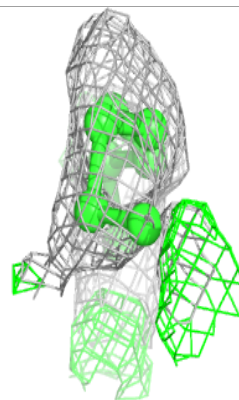
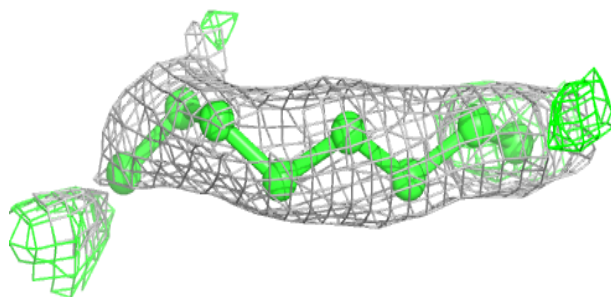
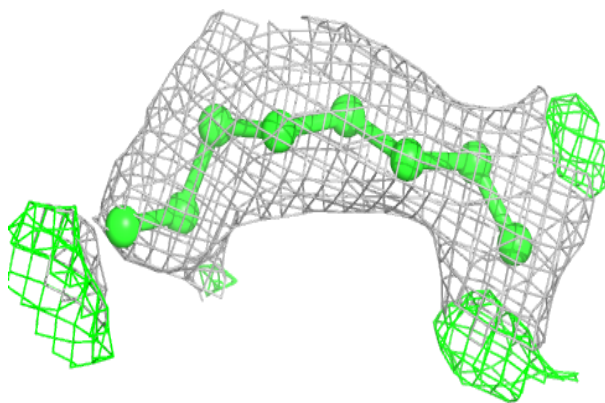
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



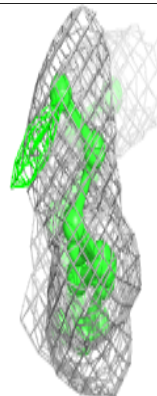
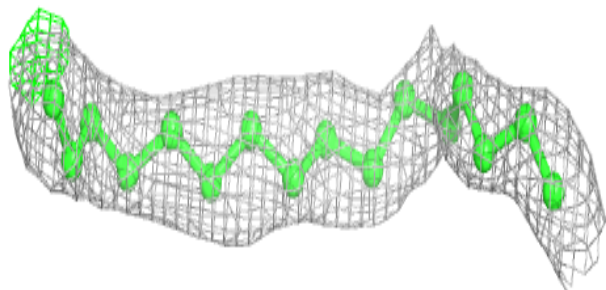
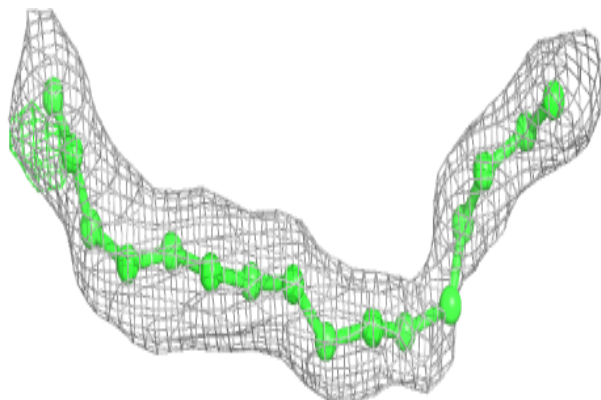


**Electron density around LFA G 313:**

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

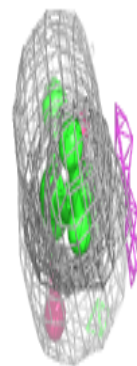
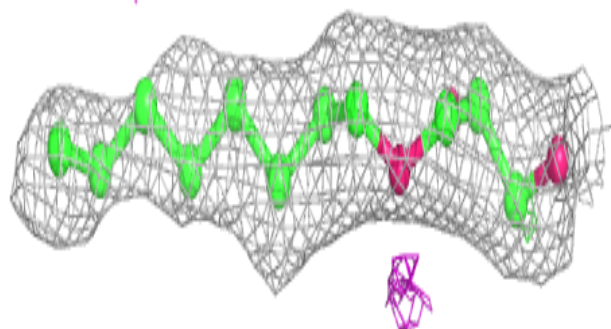
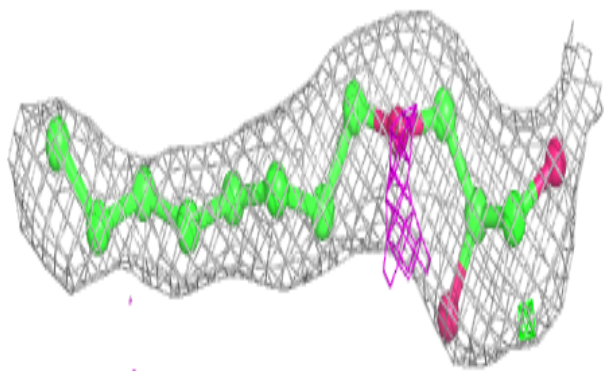
**Electron density around LFA B 307:**

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

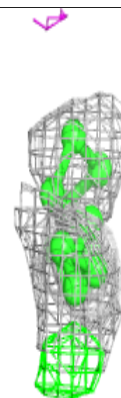
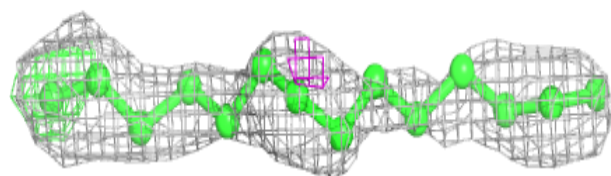
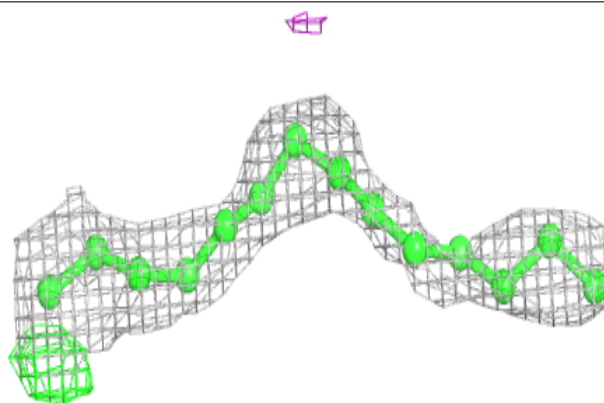


**Electron density around MPG E 313:**

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

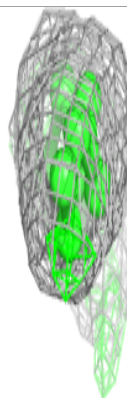
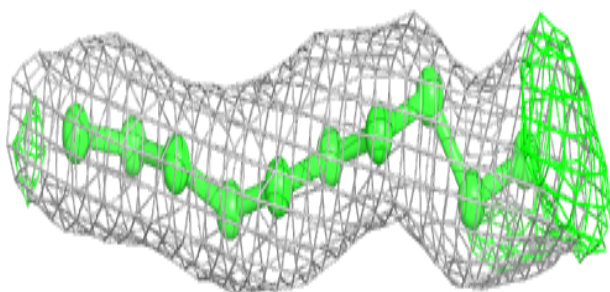
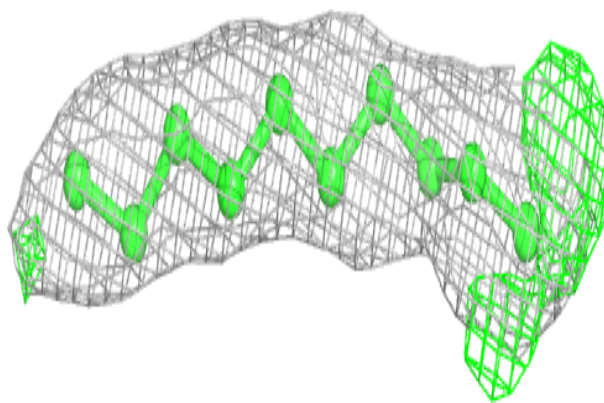
**Electron density around LFA H 307:**

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

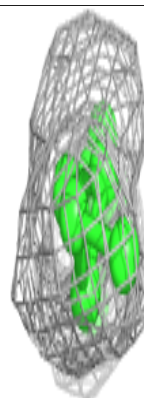
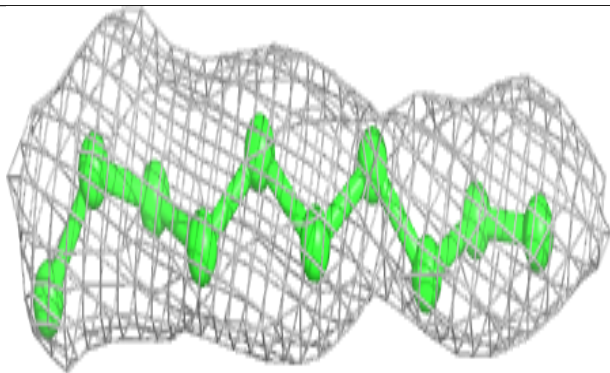
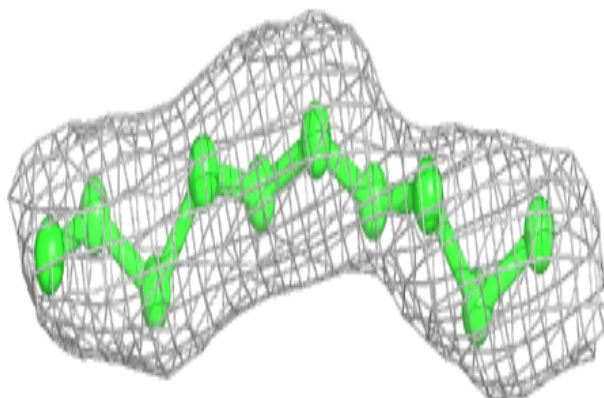


**Electron density around LFA F 306:**

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

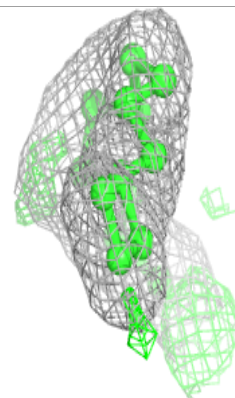
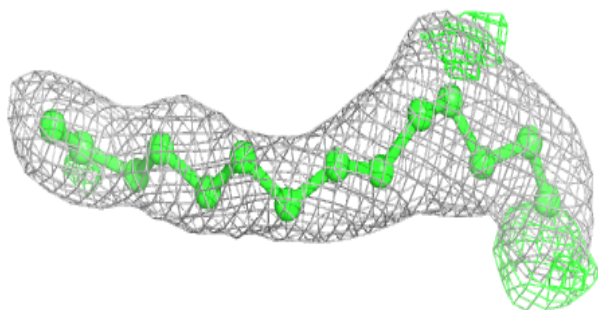
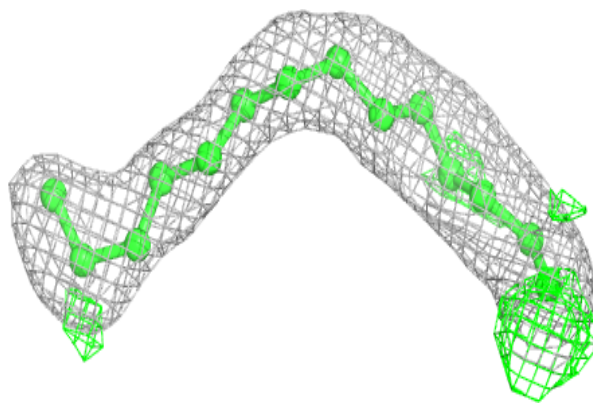
**Electron density around LFA D 305:**

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

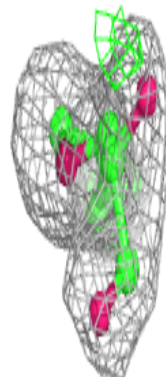
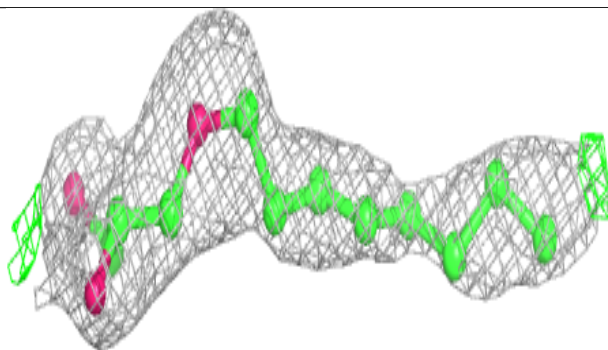
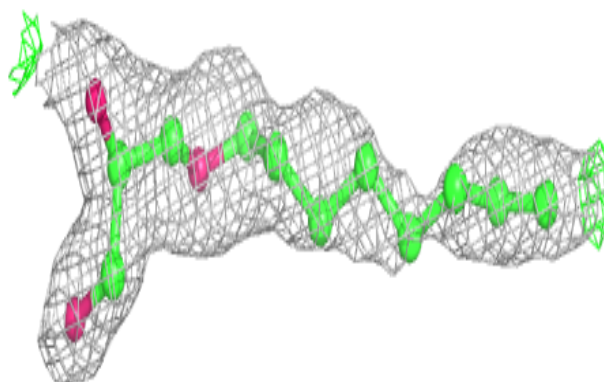


**Electron density around LFA G 304:**

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

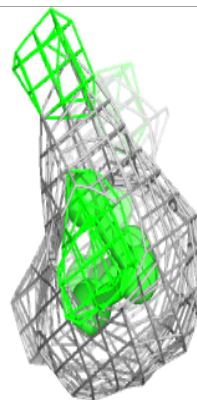
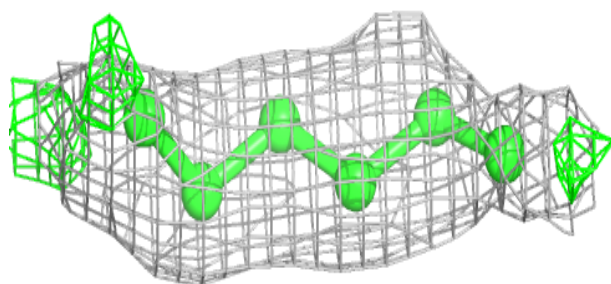
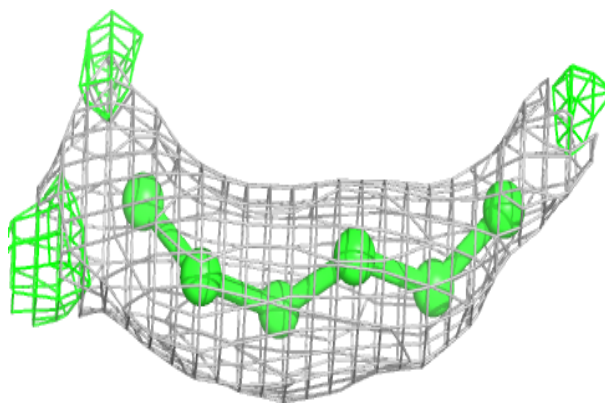
**Electron density around MPG A 313:**

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

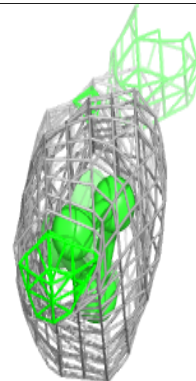
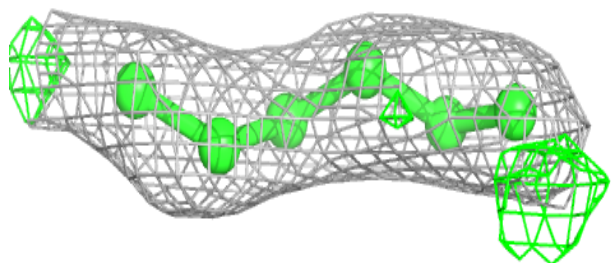
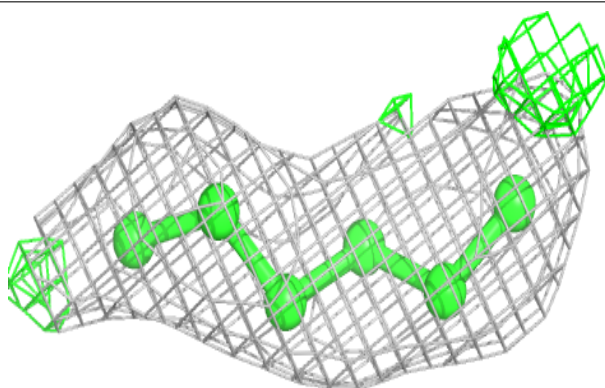


**Electron density around LFA A 303:**

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

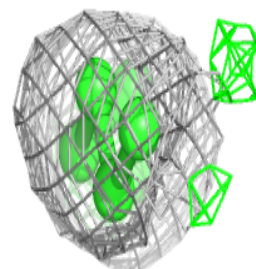
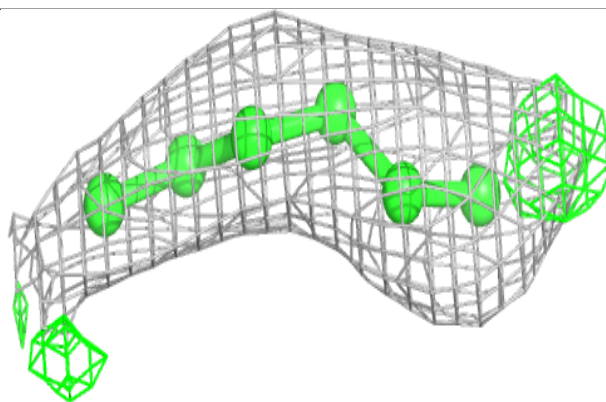
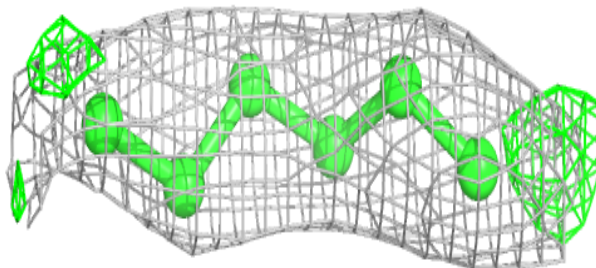
**Electron density around LFA F 307:**

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

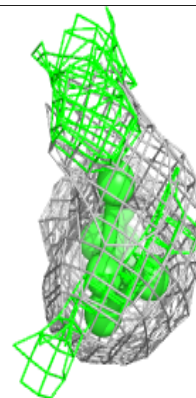
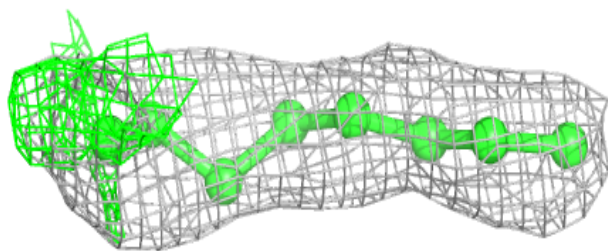
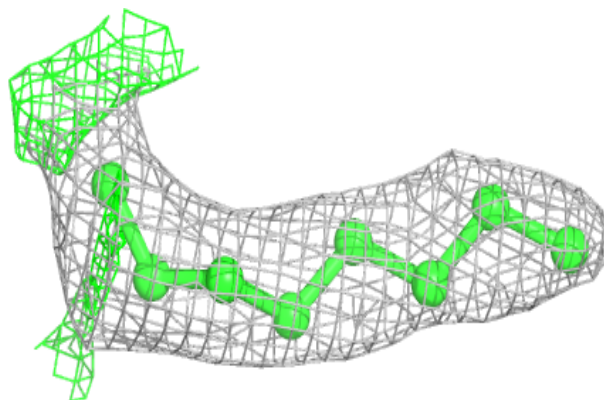


**Electron density around LFA F 305:**

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

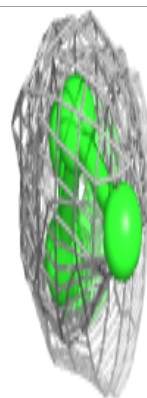
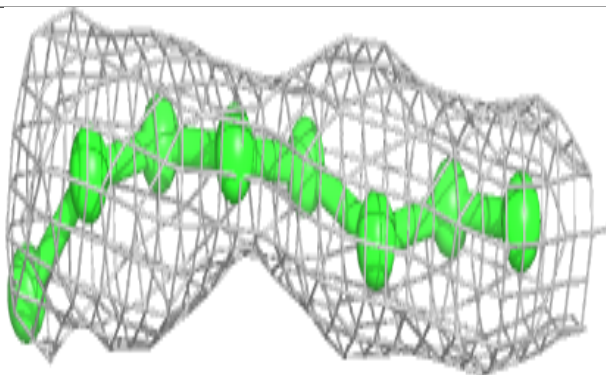
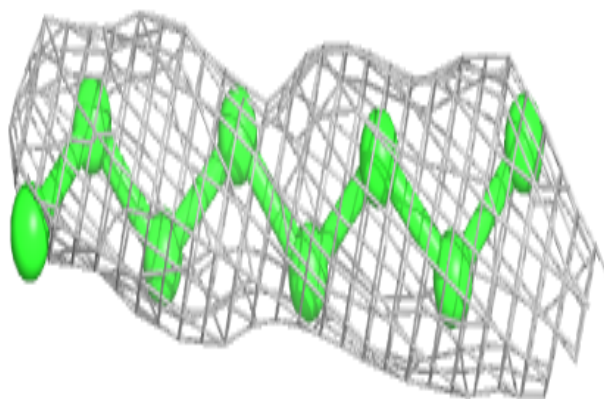
**Electron density around LFA D 309:**

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

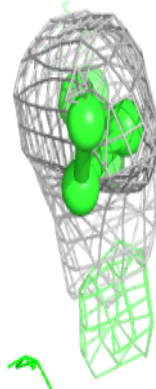
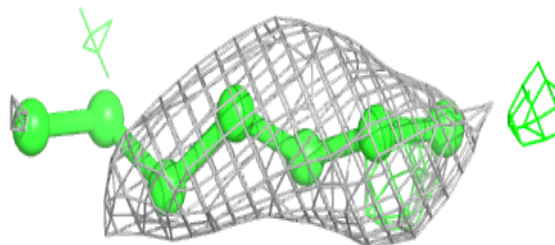
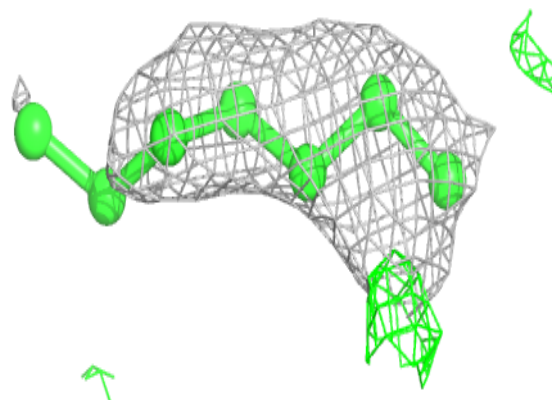


**Electron density around LFA G 311:**

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

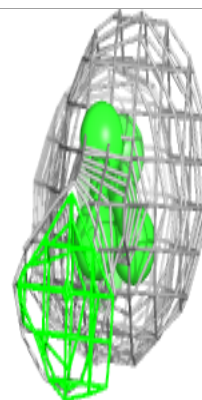
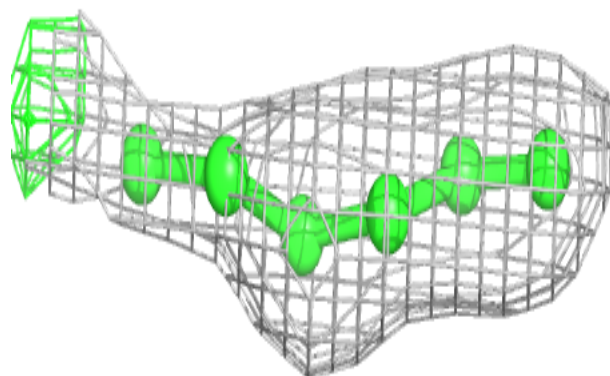
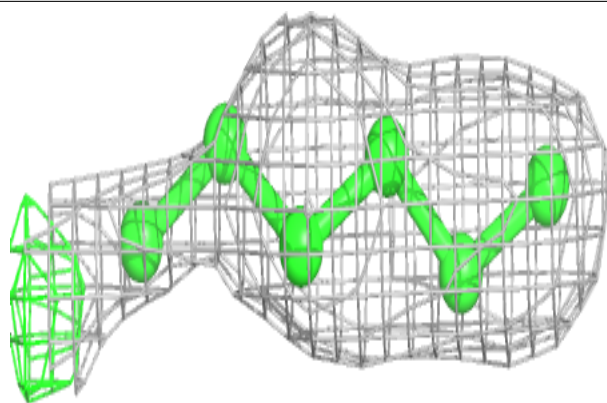
**Electron density around LFA J 307:**

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

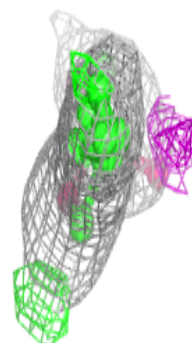
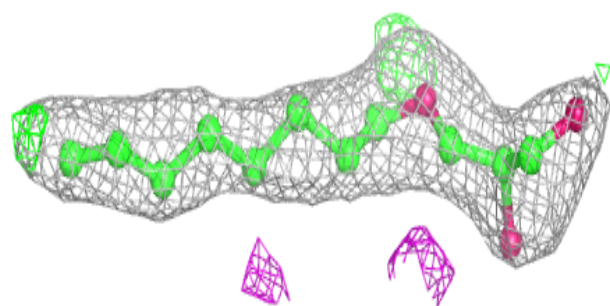
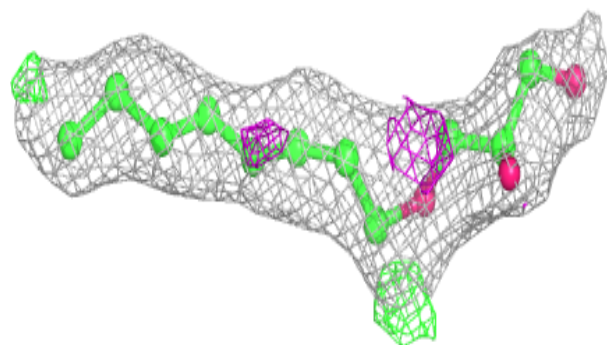


**Electron density around LFA G 305:**

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

**Electron density around MPG D 315:**

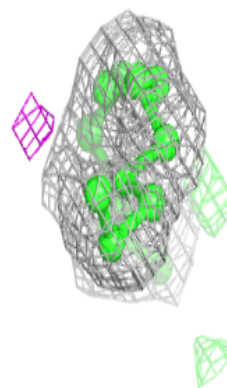
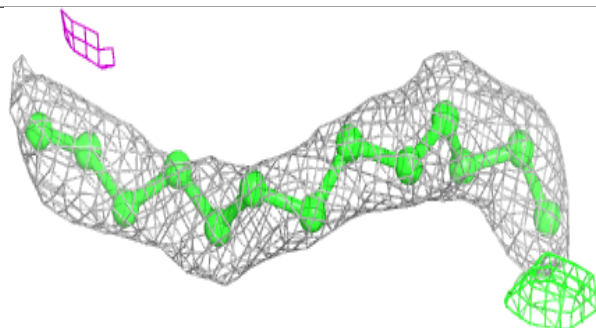
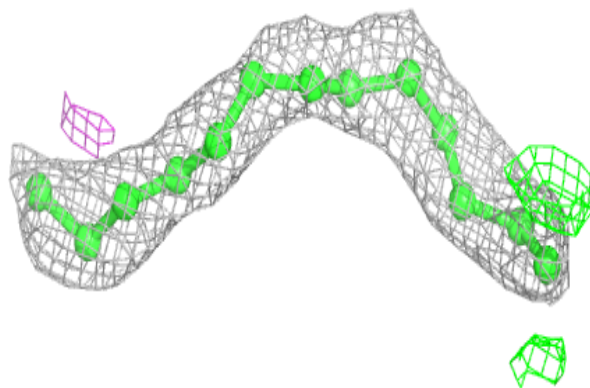
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



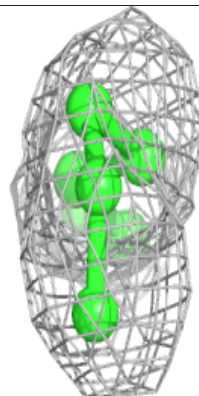
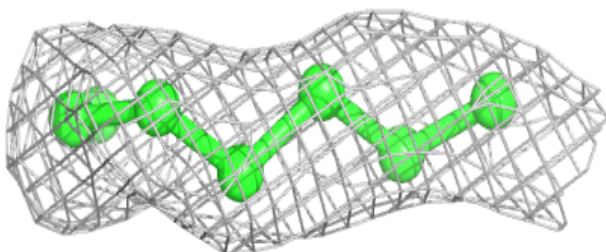
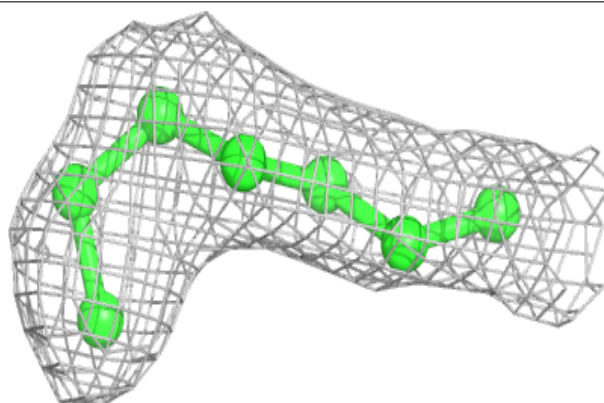


**Electron density around LFA H 302:**

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

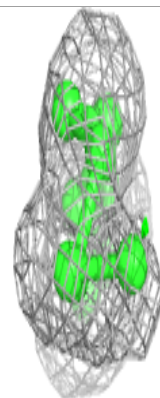
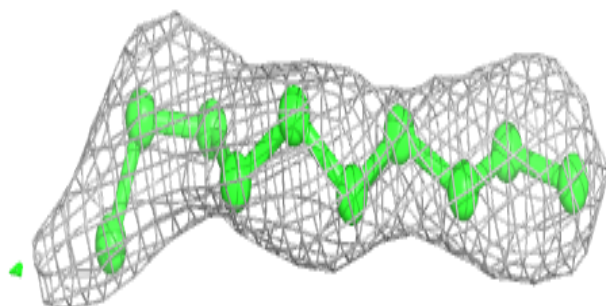
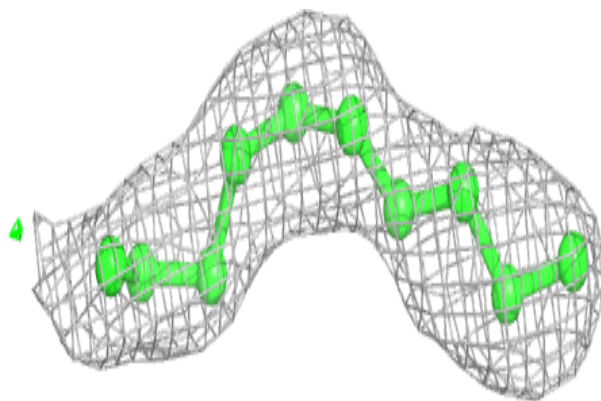
**Electron density around LFA C 302:**

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

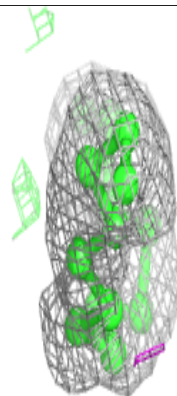
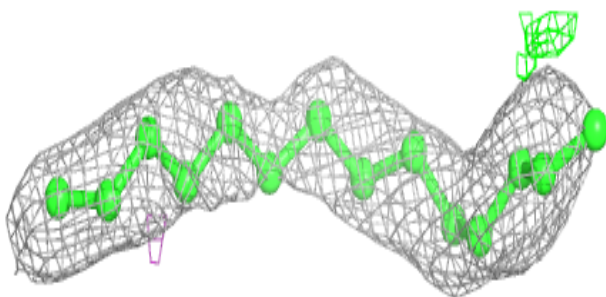
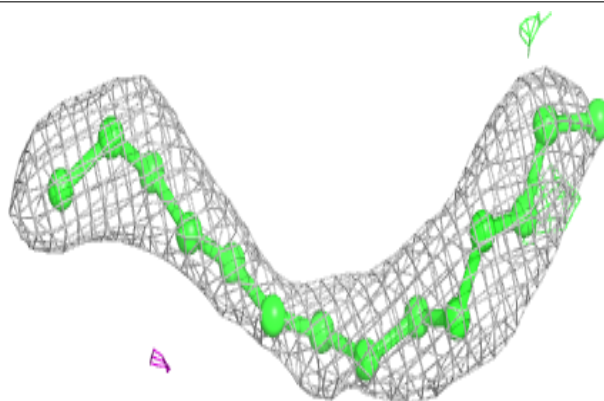


**Electron density around LFA J 309:**

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

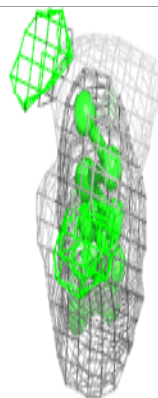
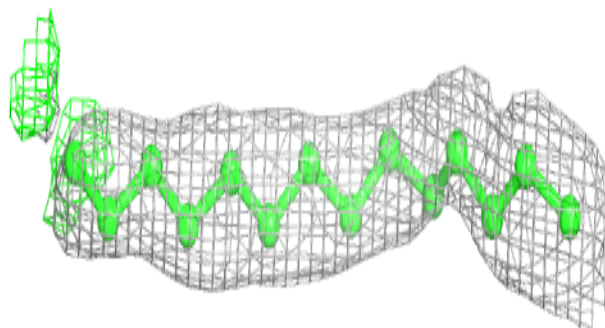
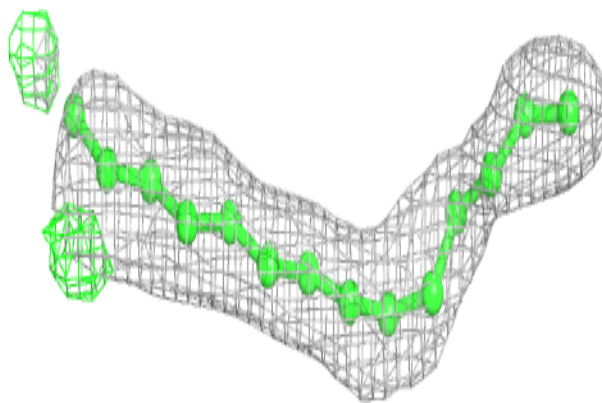
**Electron density around LFA D 303:**

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

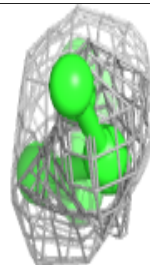
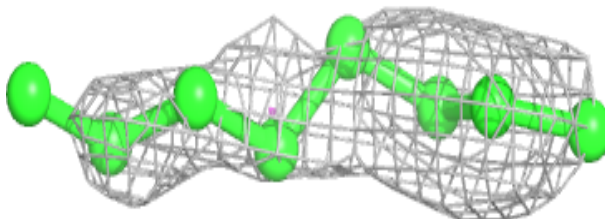
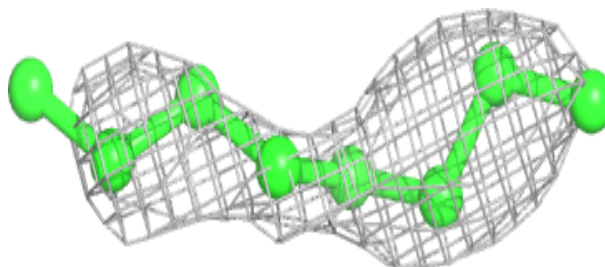


**Electron density around LFA E 302:**

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

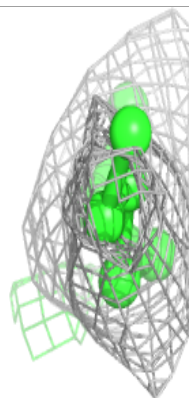
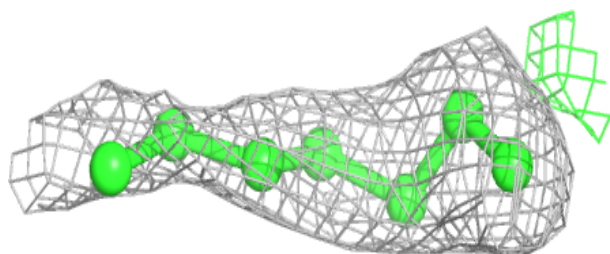
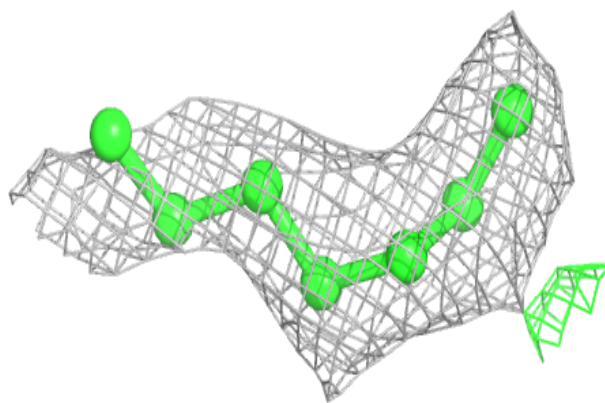
**Electron density around LFA H 308:**

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

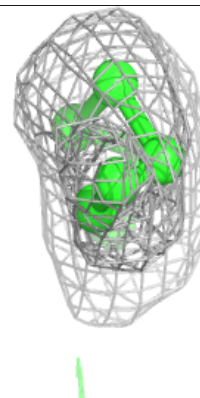
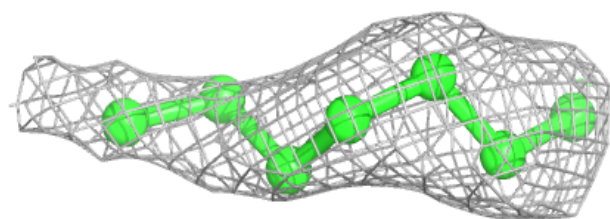
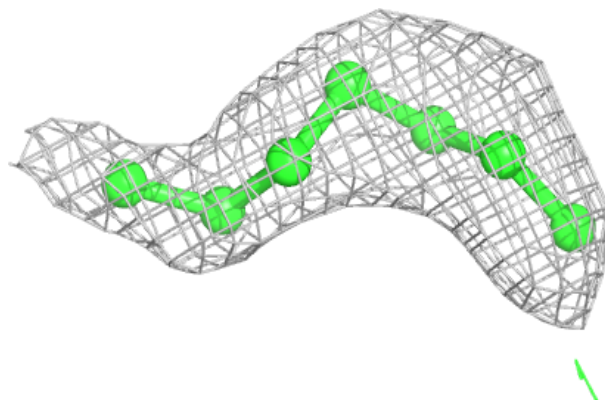


**Electron density around LFA I 302:**

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

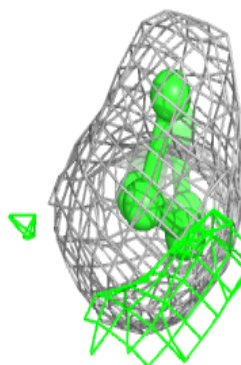
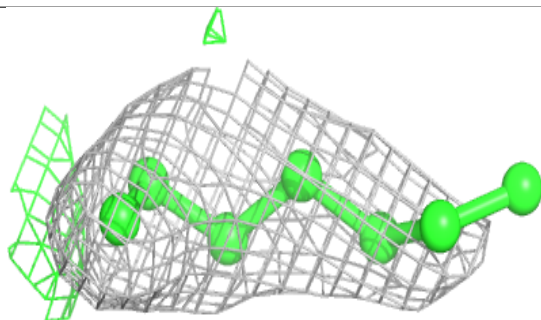
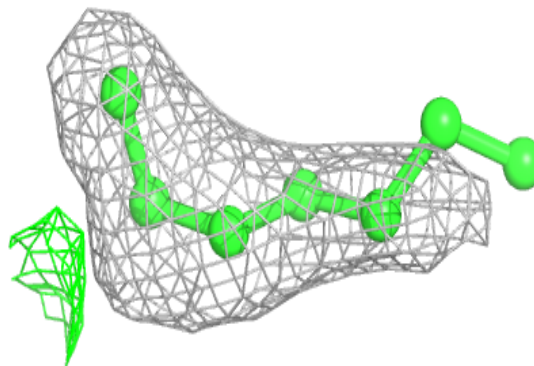
**Electron density around LFA B 302:**

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

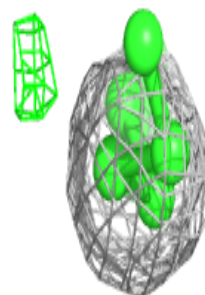
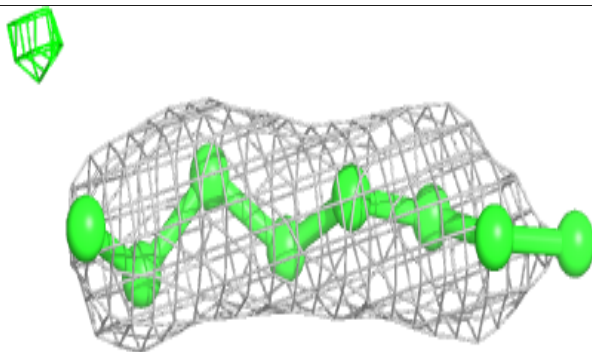
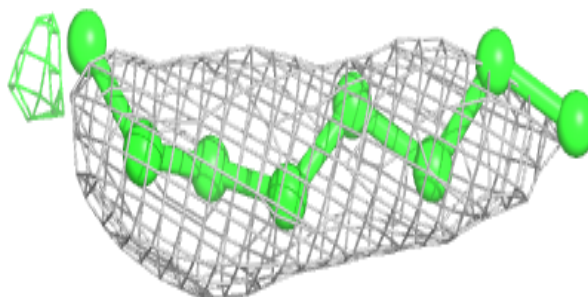


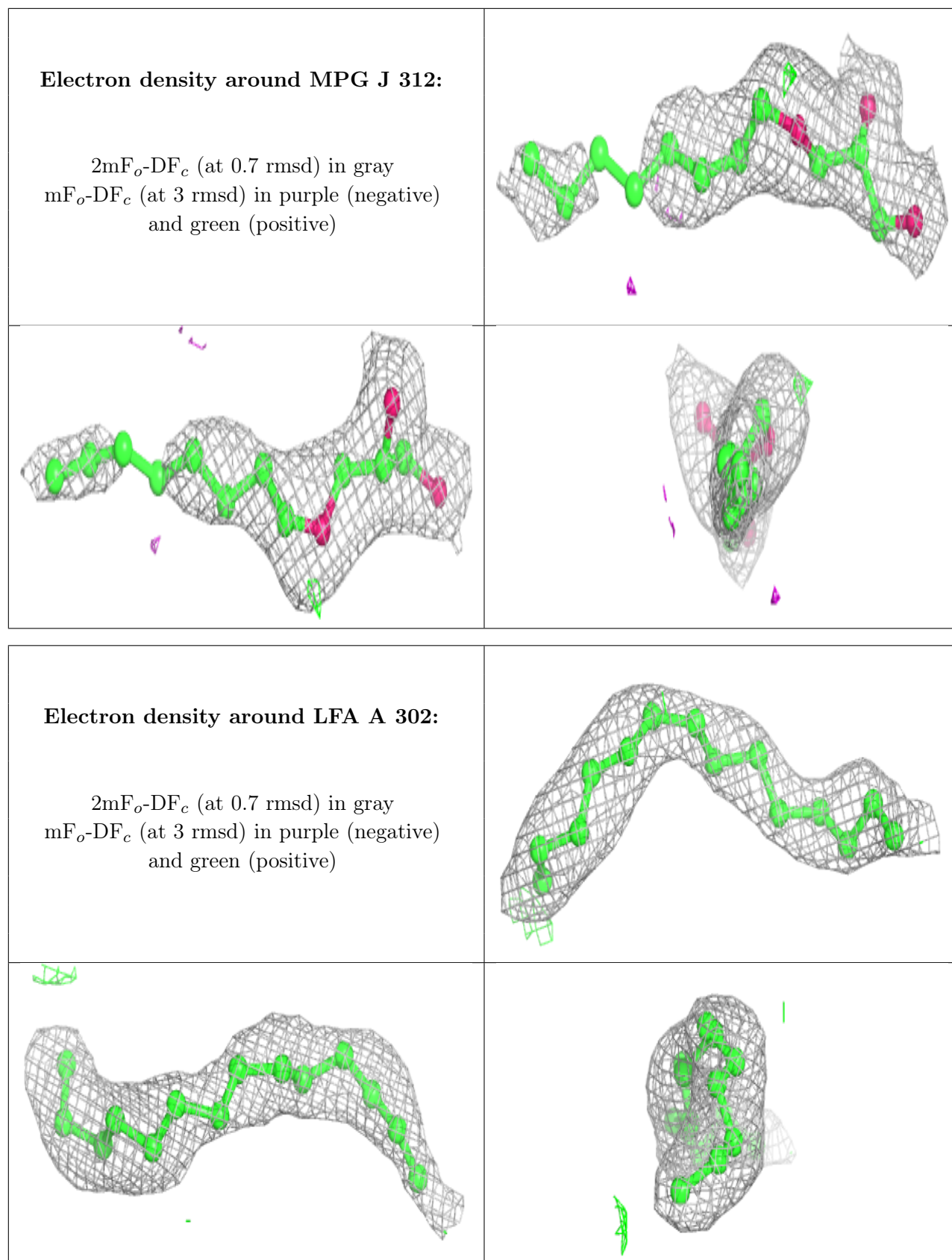
**Electron density around LFA B 303:**

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

**Electron density around LFA E 307:**

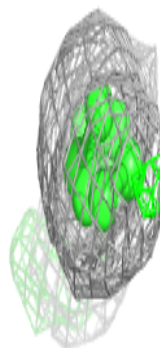
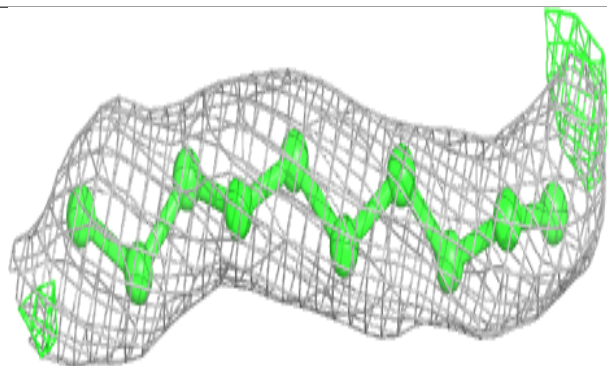
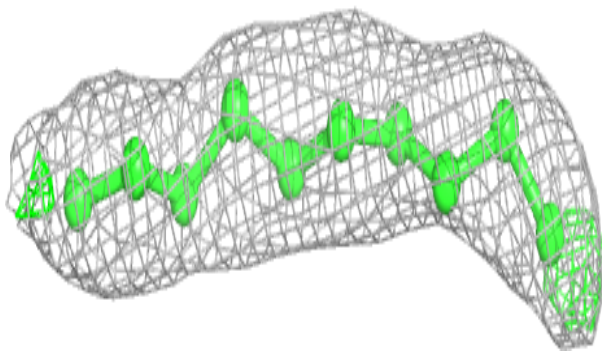
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



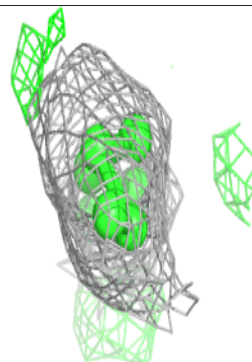
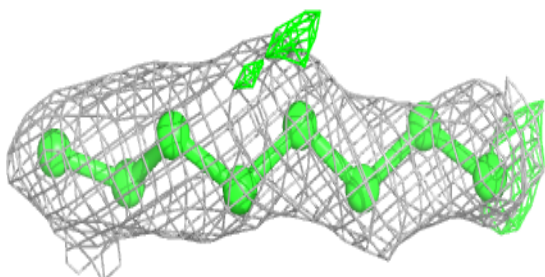
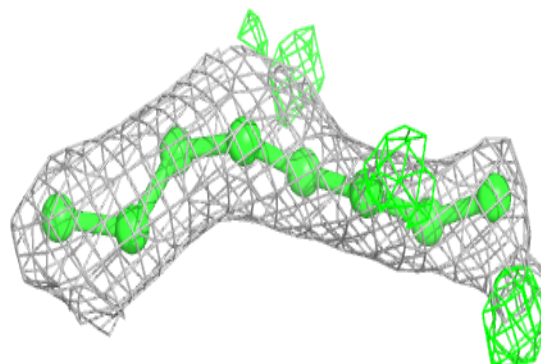


**Electron density around LFA G 306:**

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

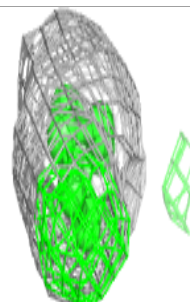
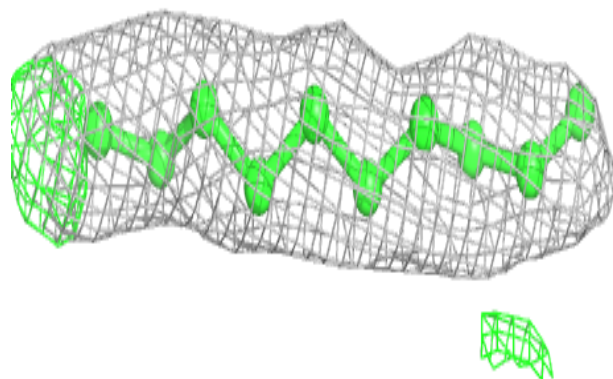
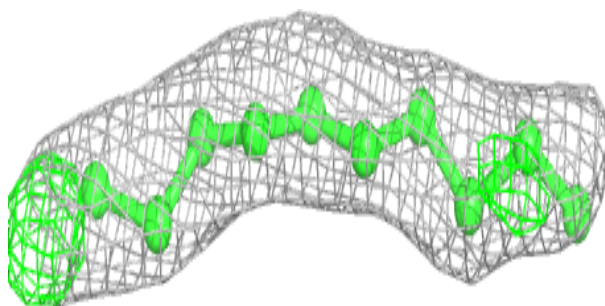
**Electron density around LFA E 311:**

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

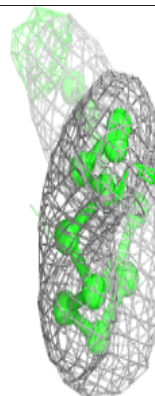
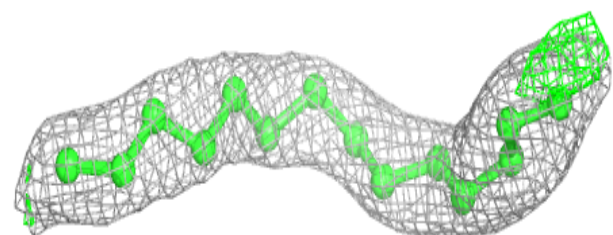
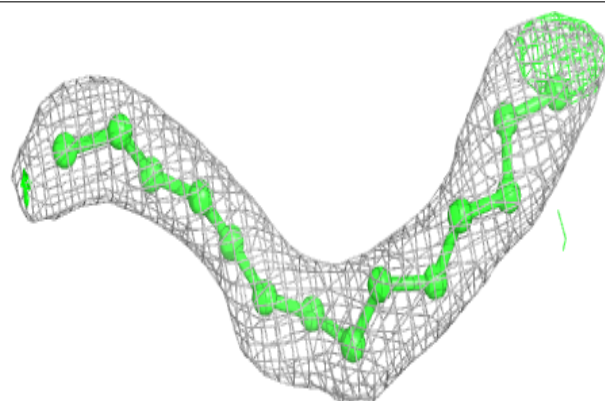


**Electron density around LFA A 304:**

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

**Electron density around LFA J 308:**

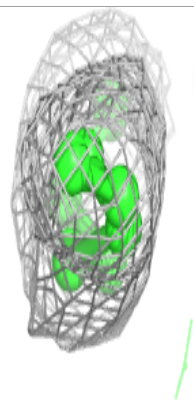
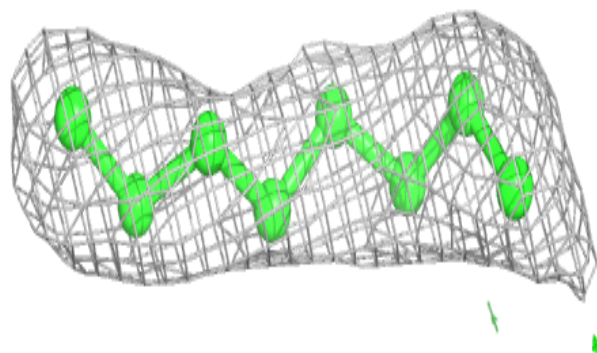
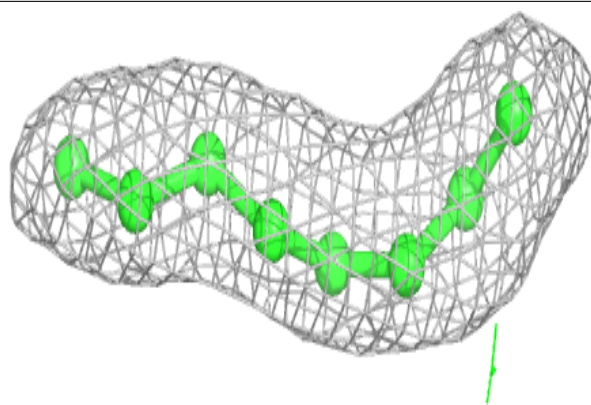
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



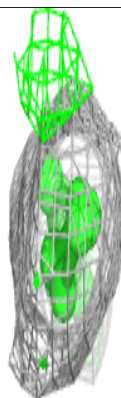
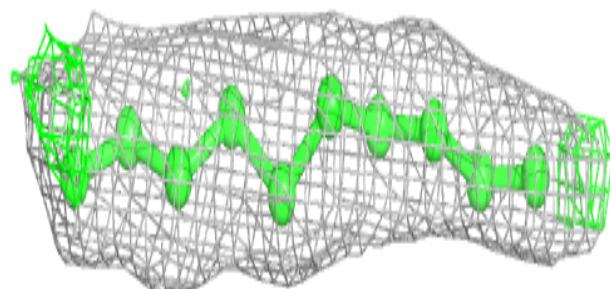
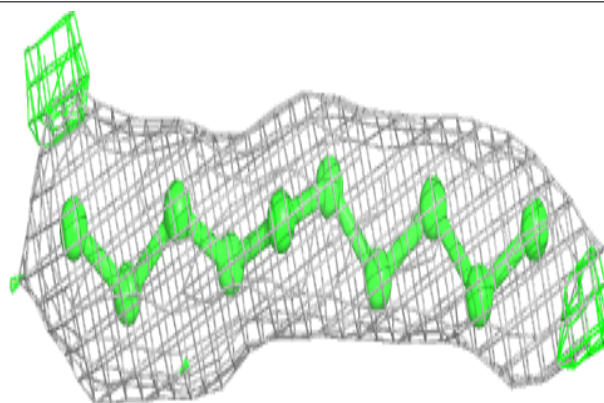


**Electron density around LFA E 312:**

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

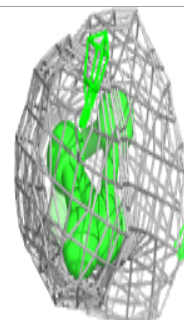
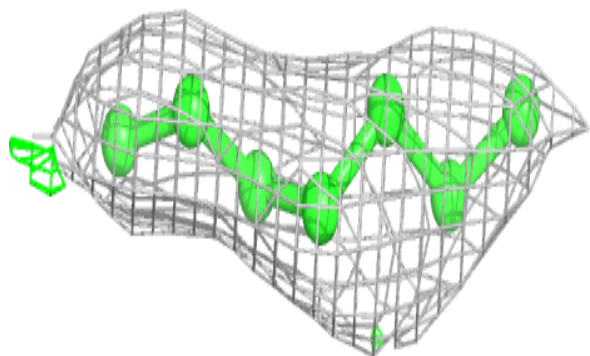
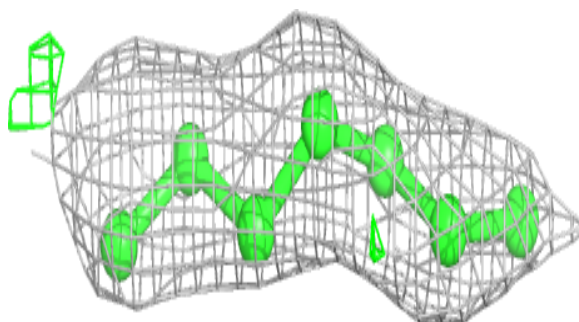
**Electron density around LFA J 310:**

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

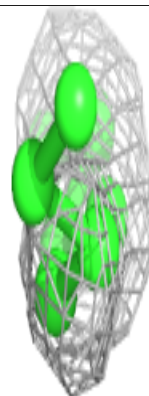
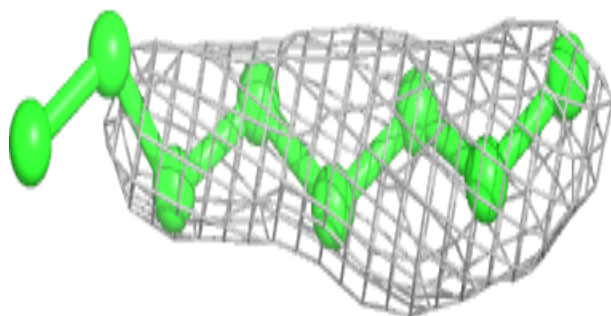
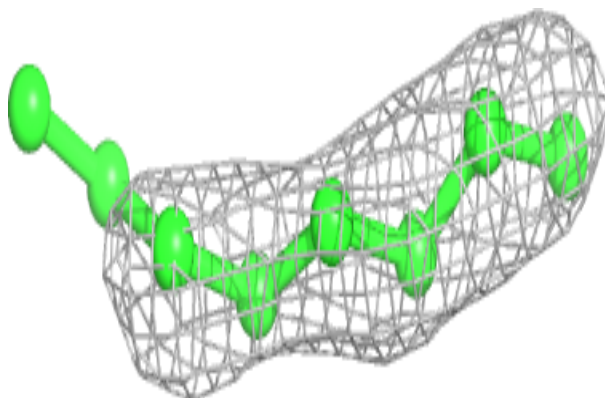


**Electron density around LFA D 311:**

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

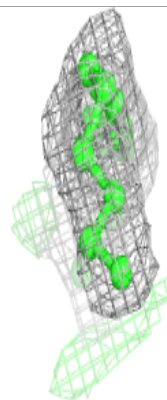
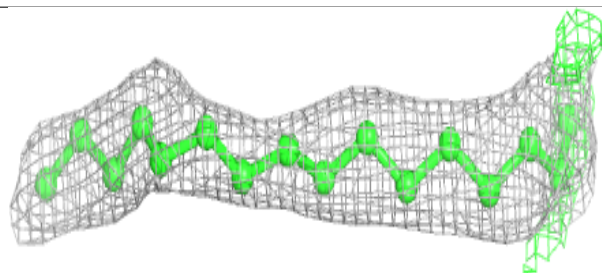
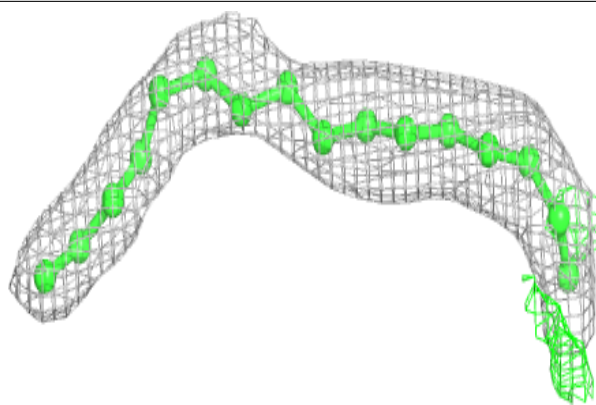
**Electron density around LFA C 311:**

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

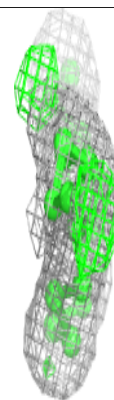
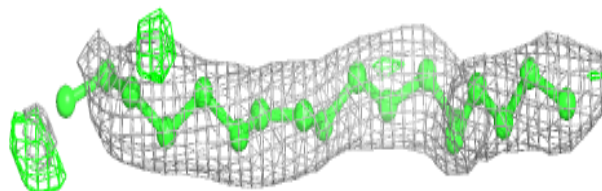
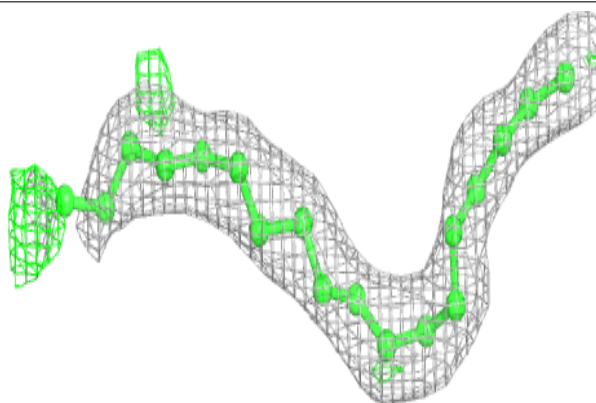


**Electron density around LFA I 308:**

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

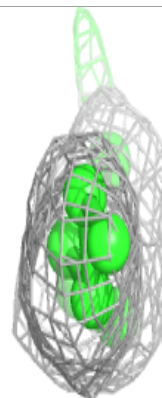
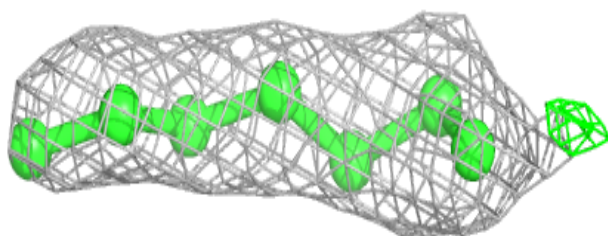
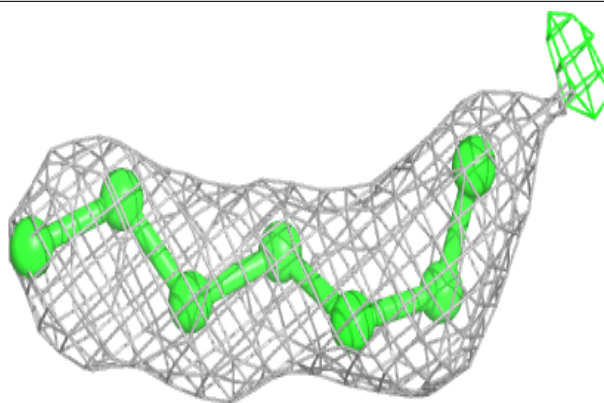
**Electron density around LFA I 309:**

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

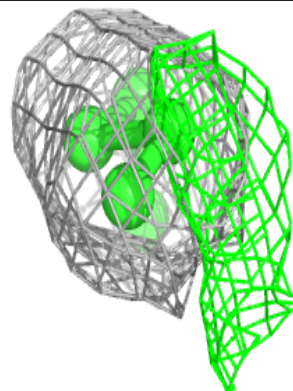
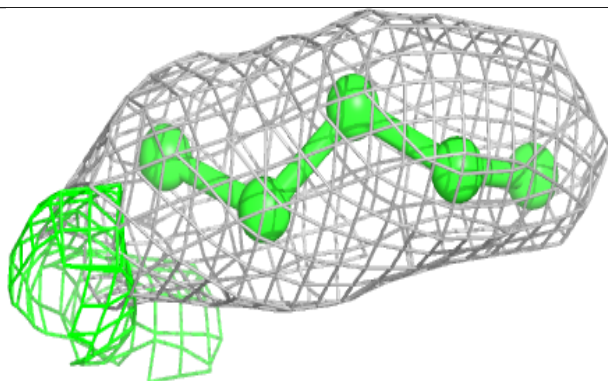
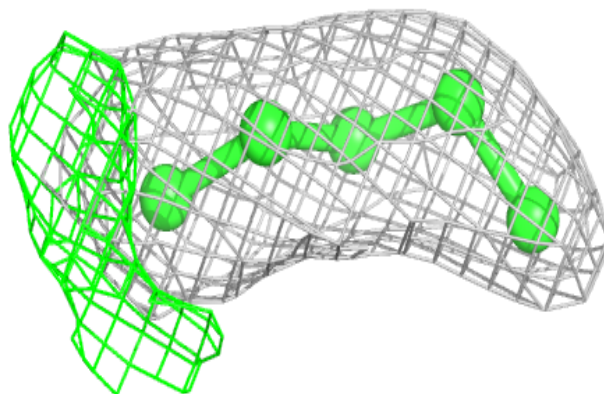


**Electron density around LFA D 314:**

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

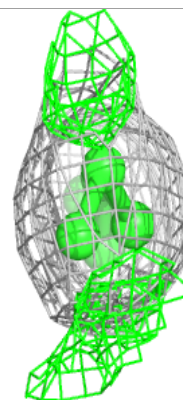
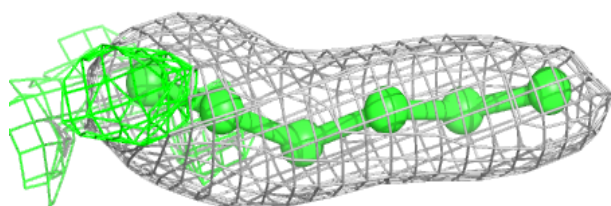
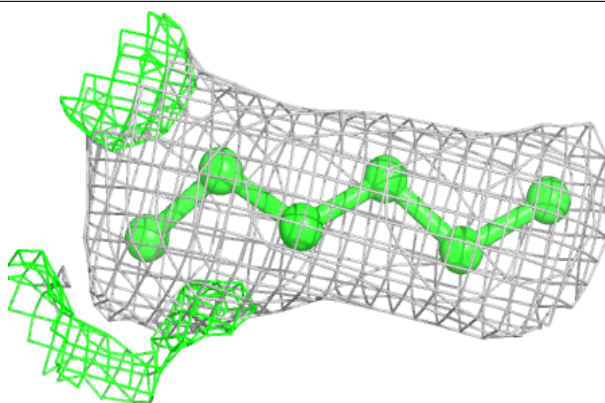
**Electron density around LFA D 316:**

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

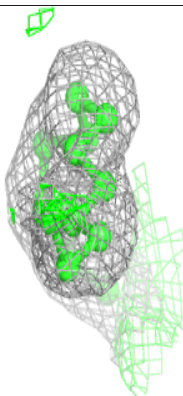
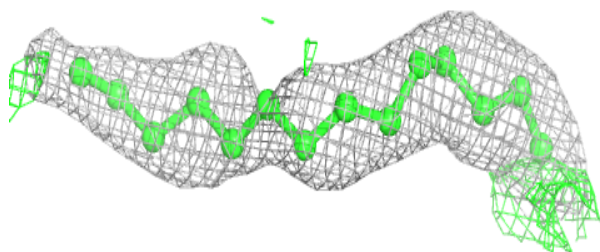
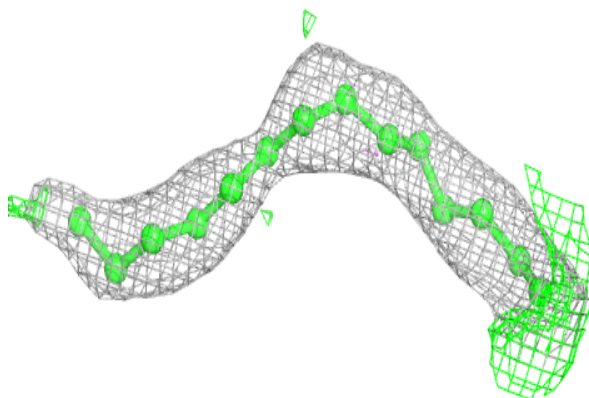


**Electron density around LFA H 312:**

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

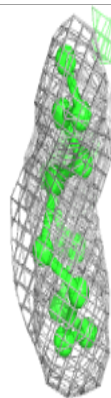
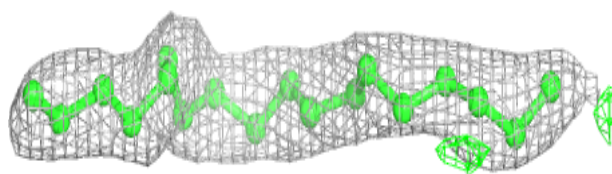
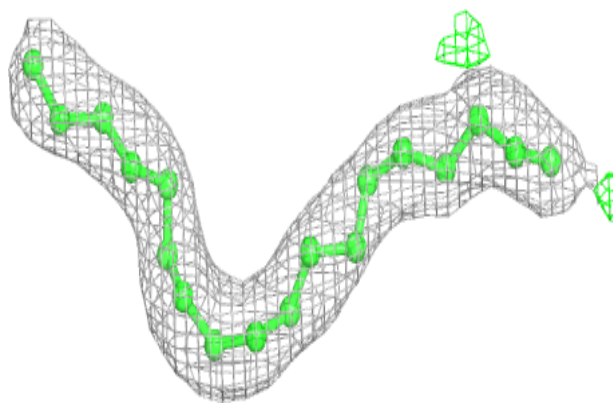
**Electron density around LFA F 303:**

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

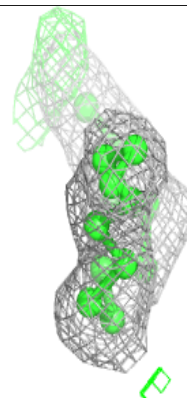
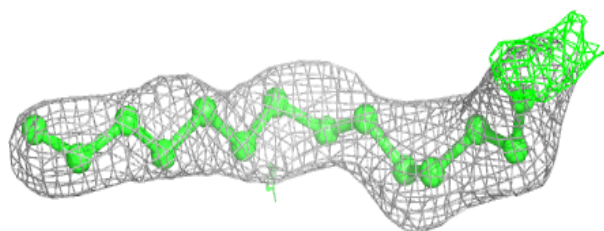
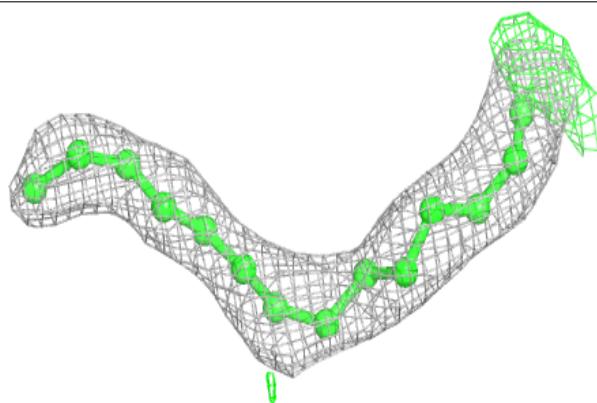


**Electron density around LFA C 307:**

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

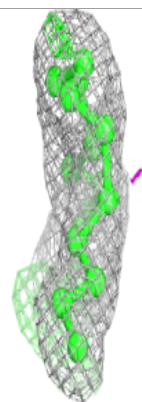
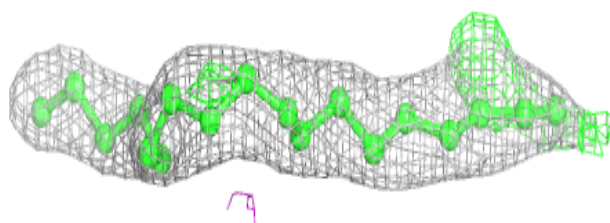
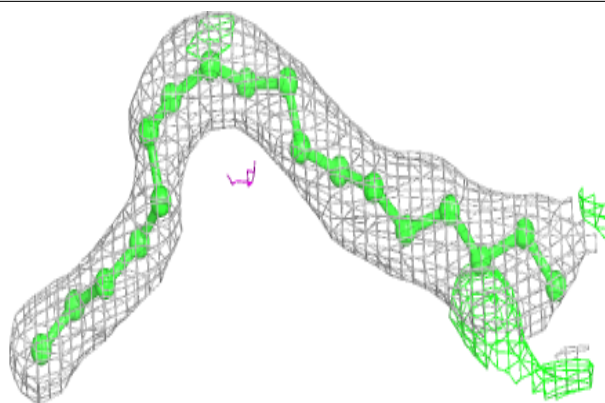
**Electron density around LFA E 308:**

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

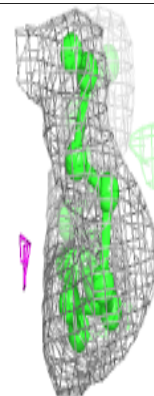
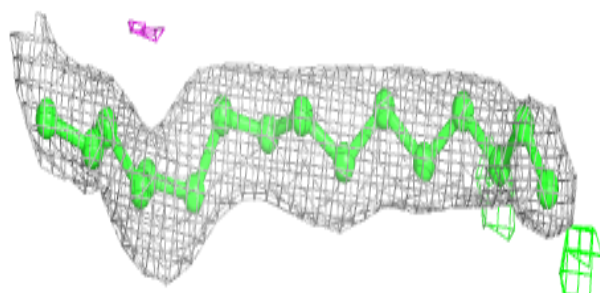
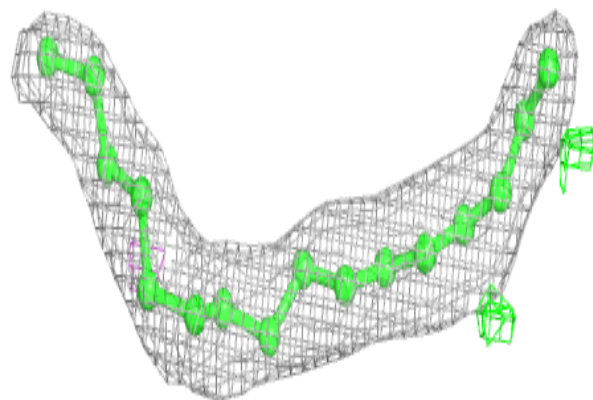


**Electron density around LFA J 303:**

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

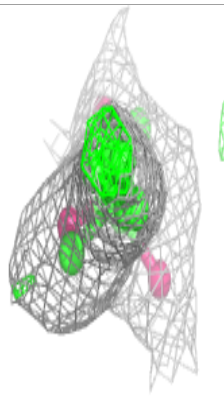
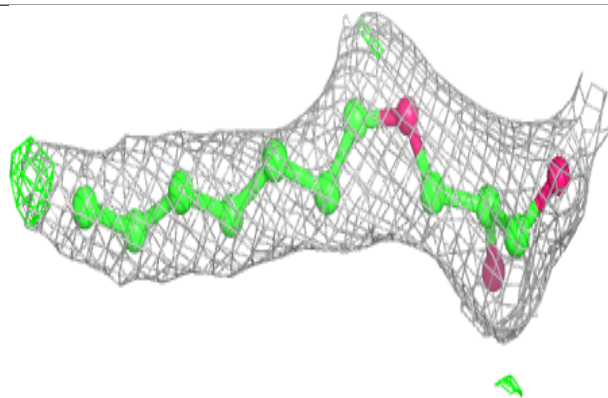
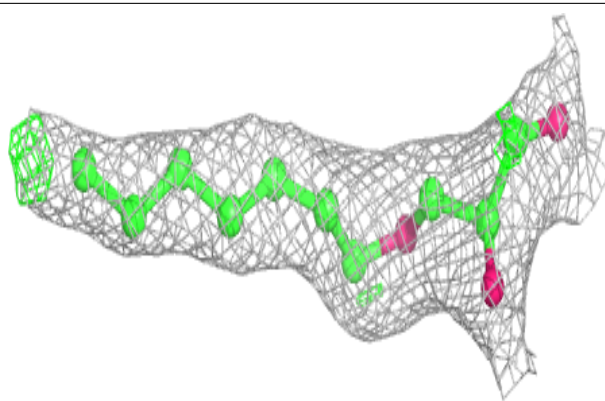
**Electron density around LFA H 305:**

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

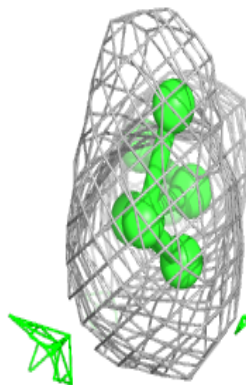
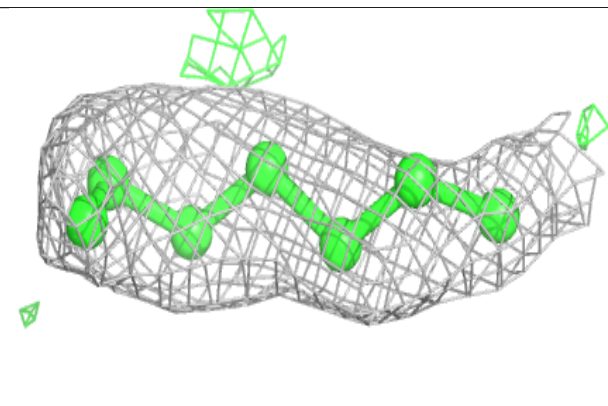
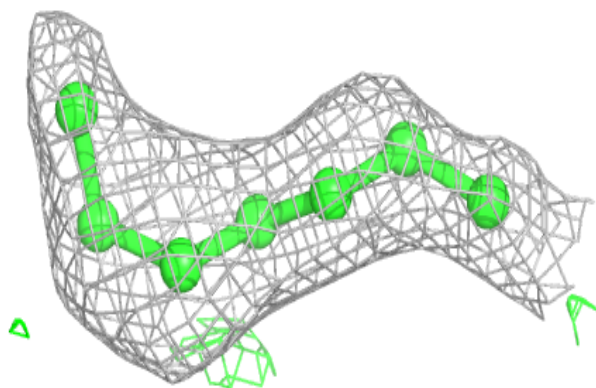


**Electron density around MPG C 313:**

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

**Electron density around LFA G 303:**

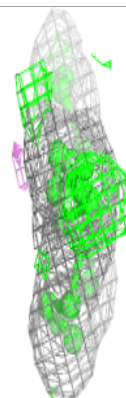
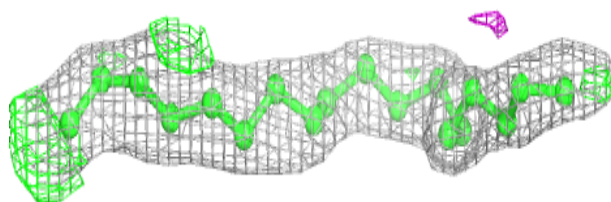
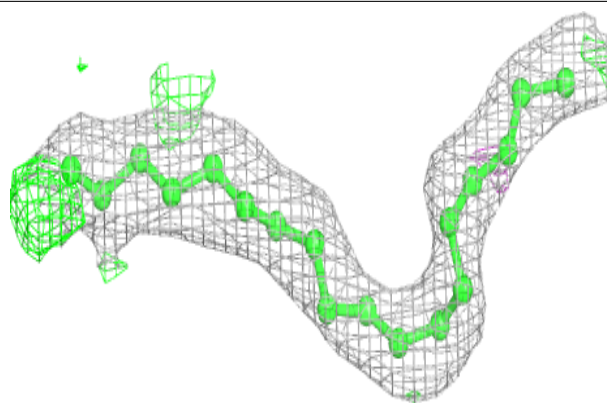
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



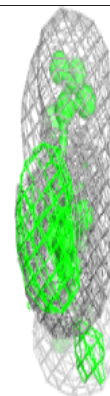
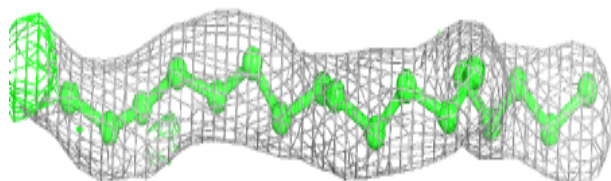
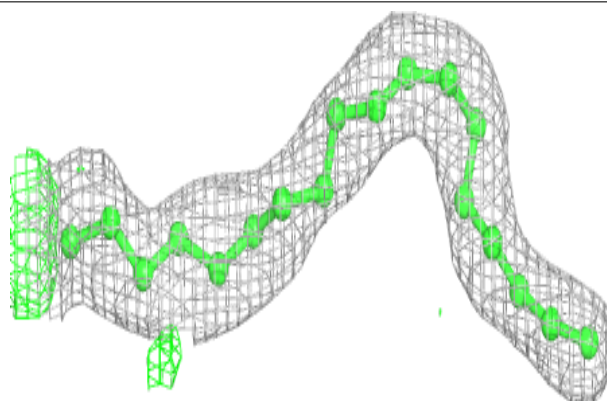


**Electron density around LFA G 308:**

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

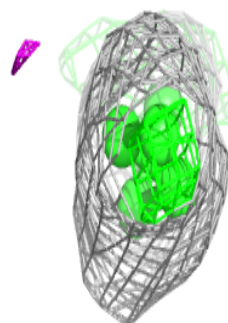
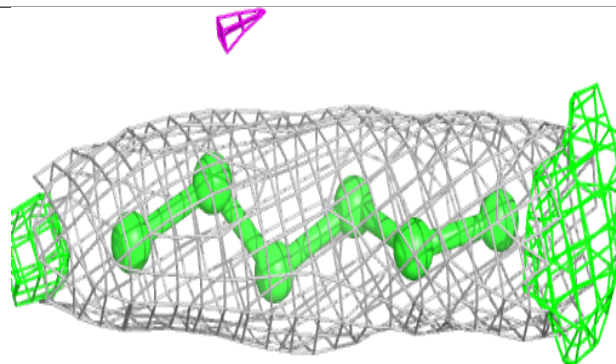
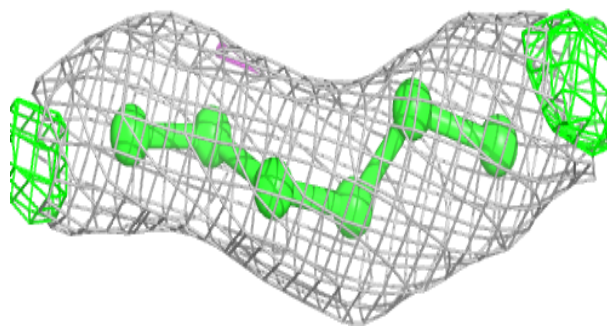
**Electron density around LFA F 310:**

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

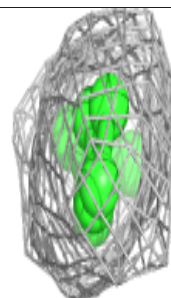
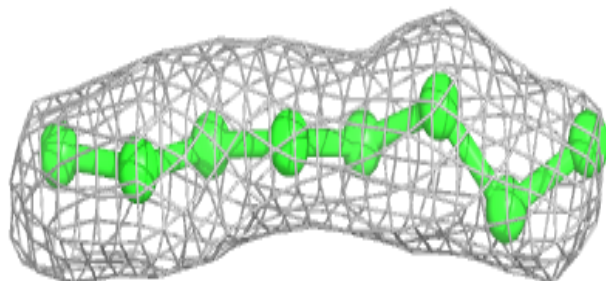
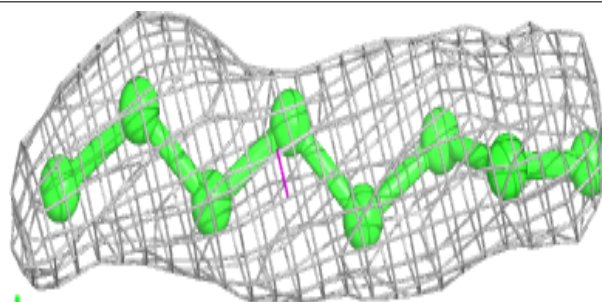


**Electron density around LFA I 307:**

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

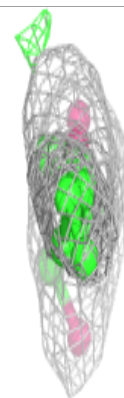
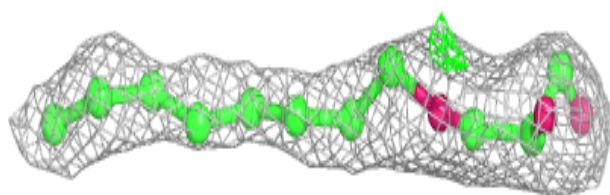
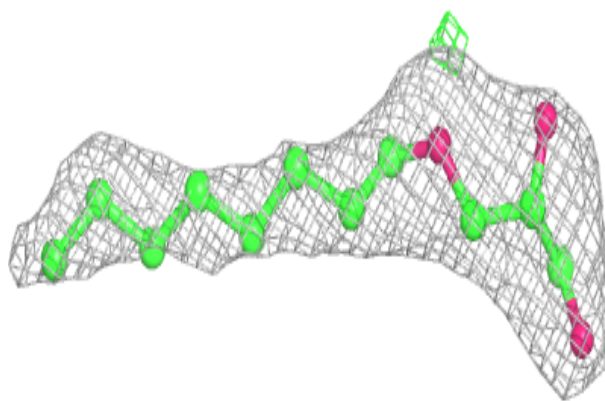
**Electron density around LFA A 309:**

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

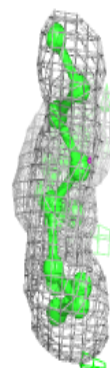
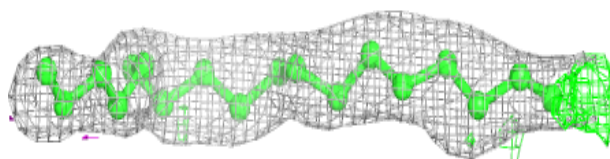
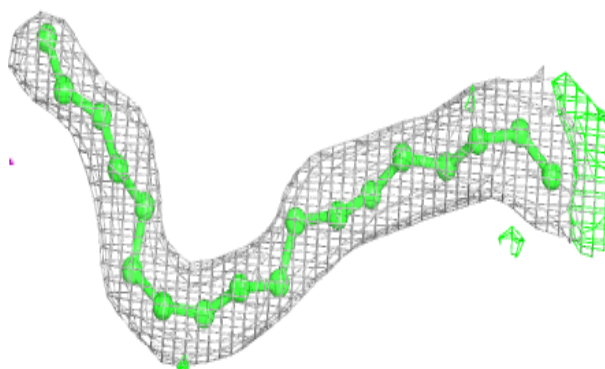


**Electron density around MPG B 312:**

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

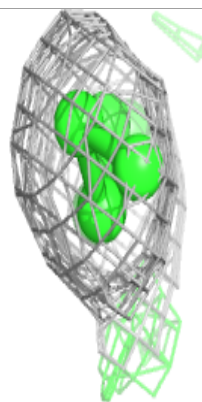
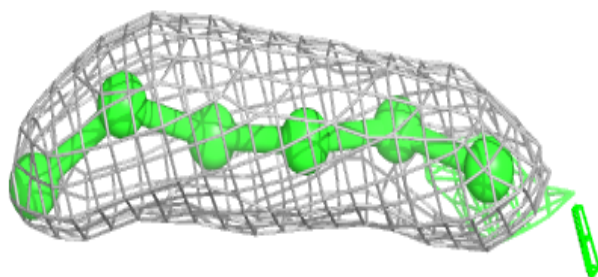
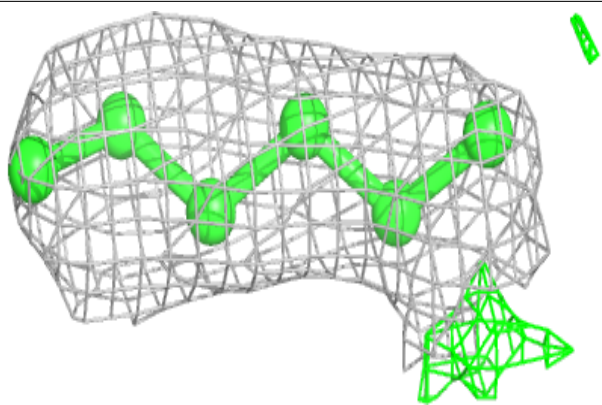
**Electron density around LFA H 306:**

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

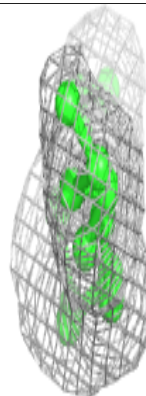
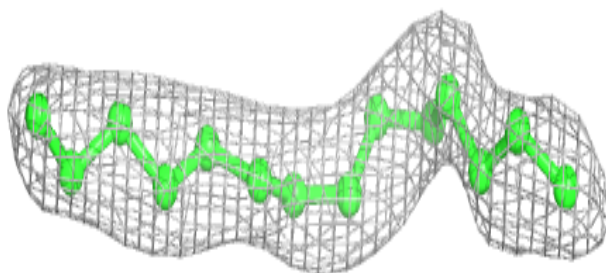
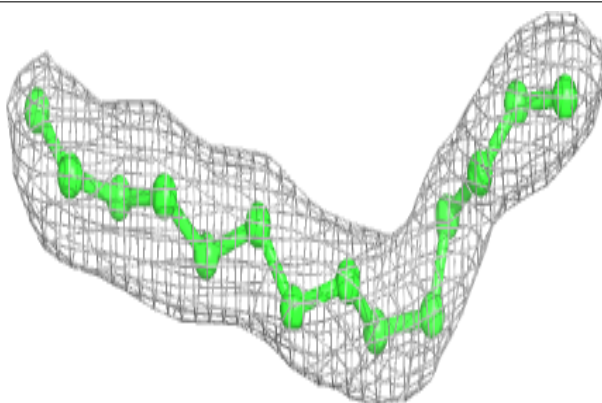


**Electron density around LFA G 314:**

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

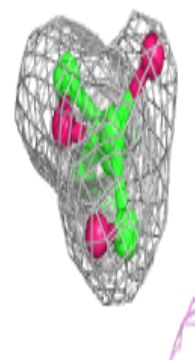
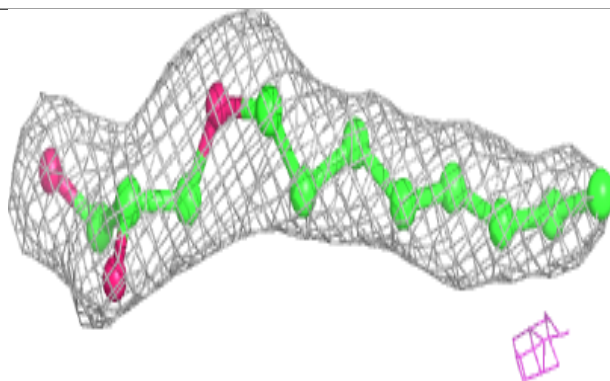
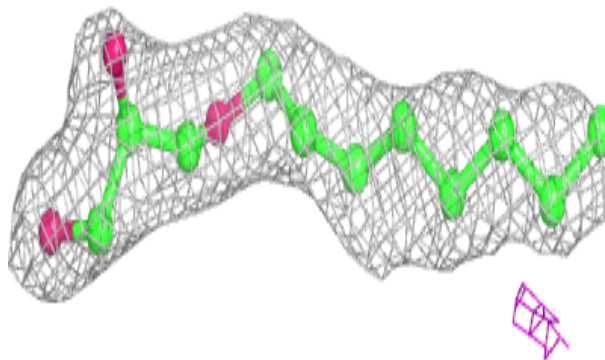
**Electron density around LFA A 306:**

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

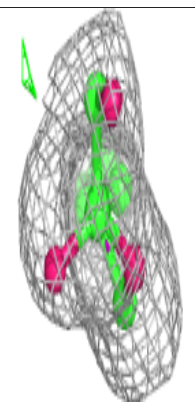
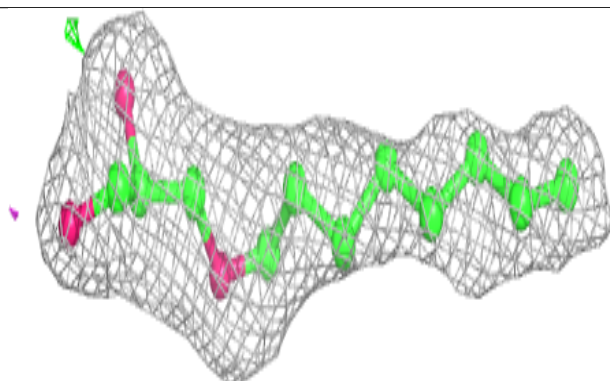
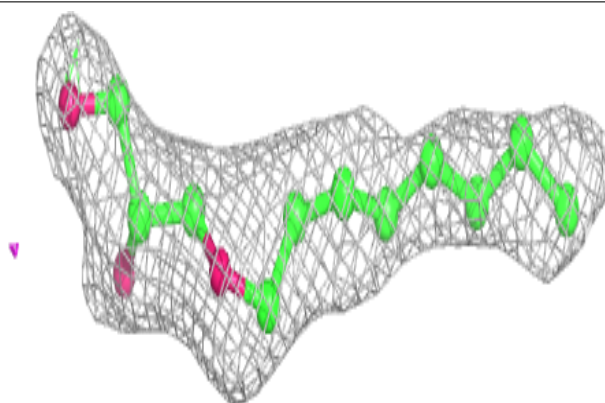


**Electron density around MPG F 315:**

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

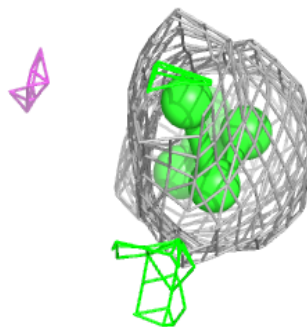
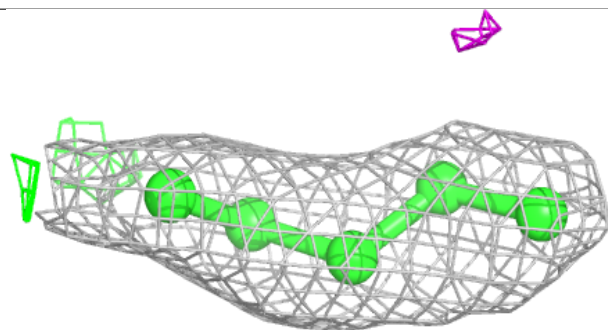
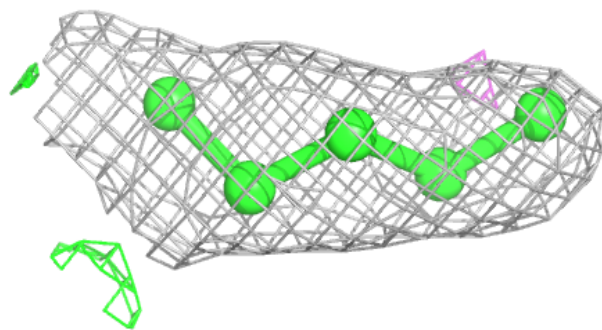
**Electron density around MPG G 312:**

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

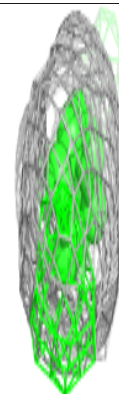
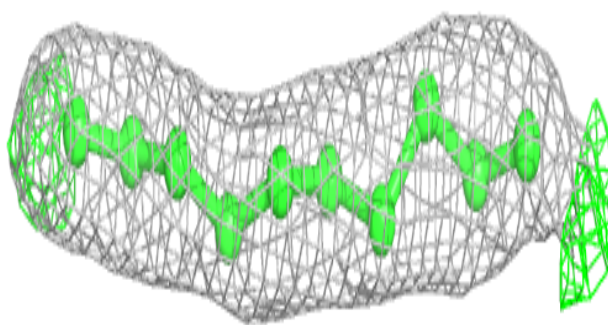
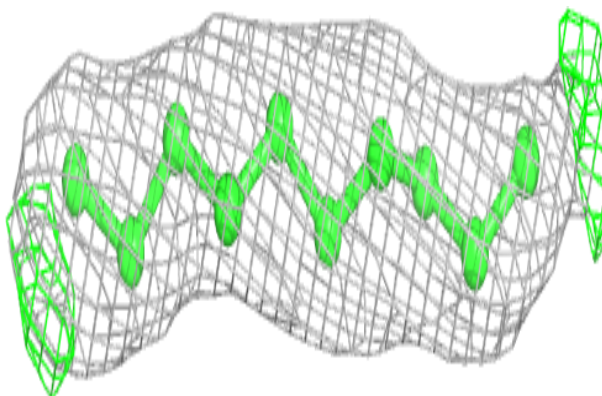


**Electron density around LFA H 309:**

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

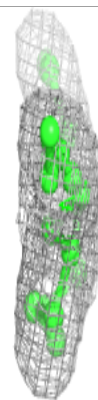
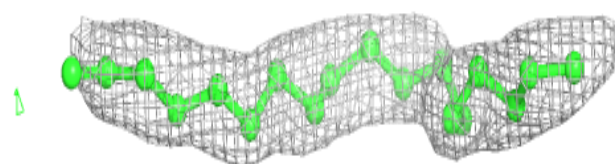
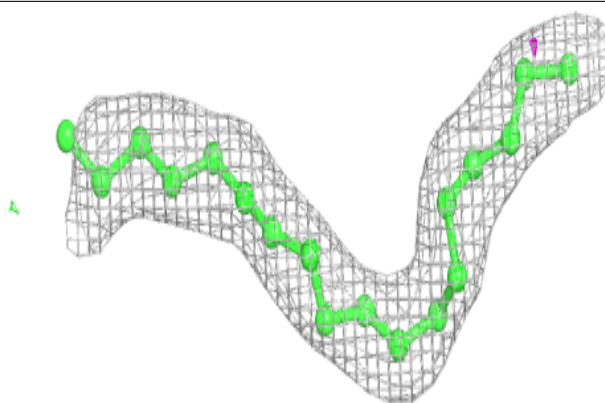
**Electron density around LFA C 305:**

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

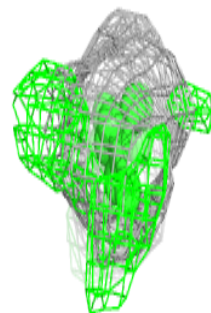
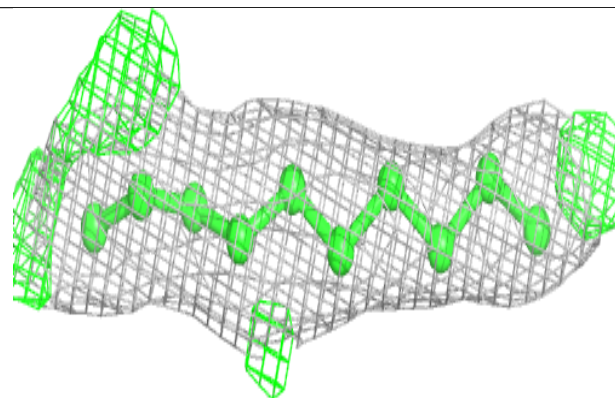
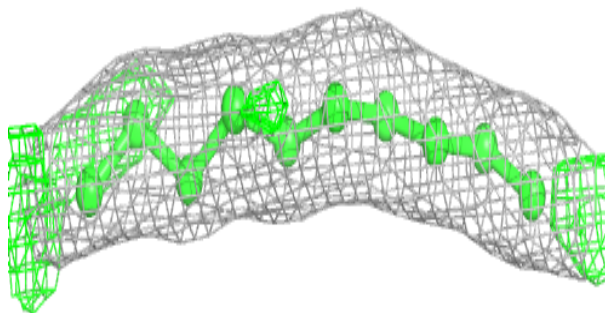


**Electron density around LFA E 303:**

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

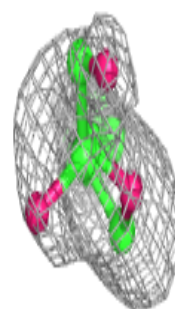
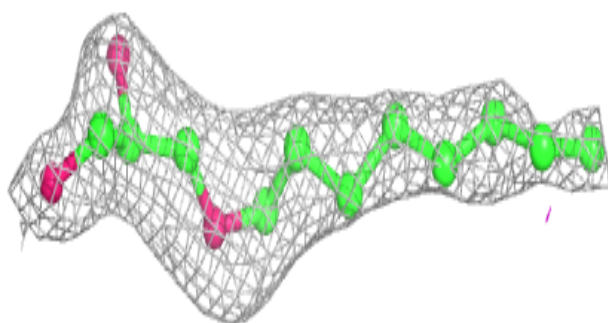
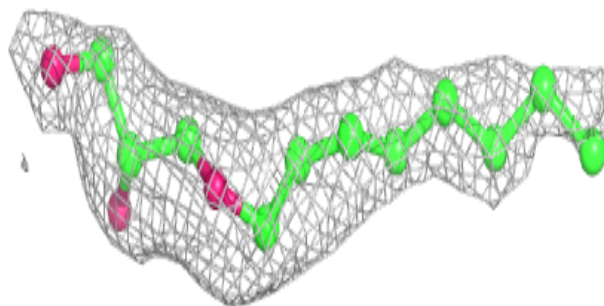
**Electron density around LFA I 306:**

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

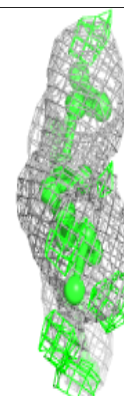
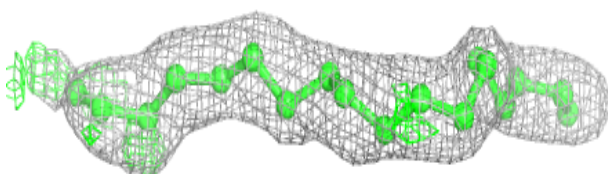
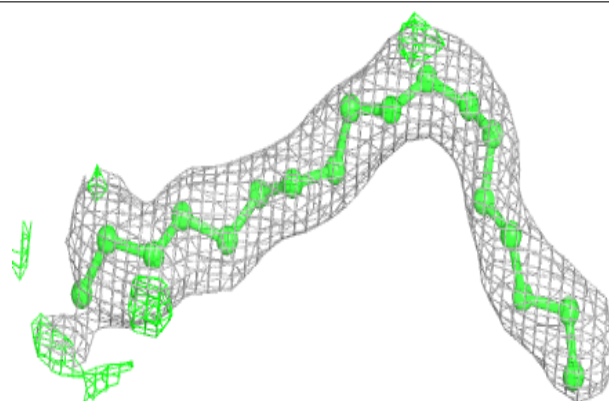


**Electron density around MPG H 313:**

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

**Electron density around LFA A 307:**

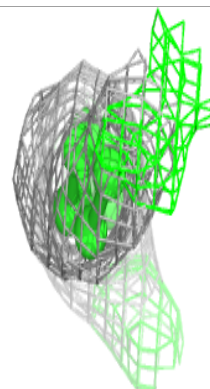
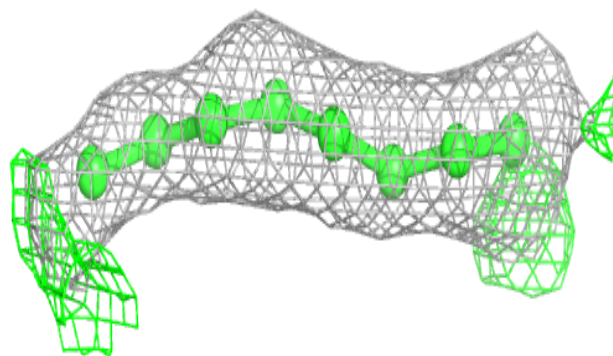
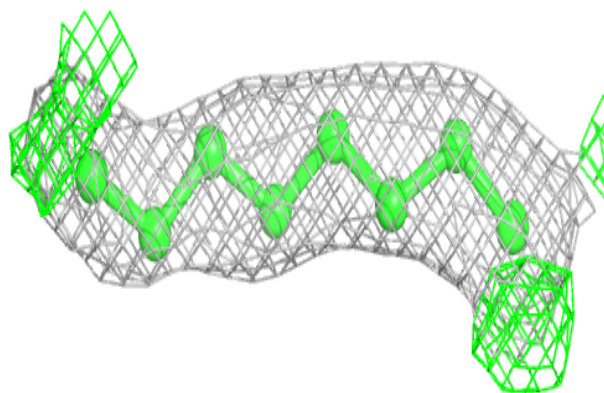
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



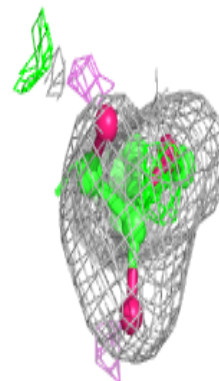
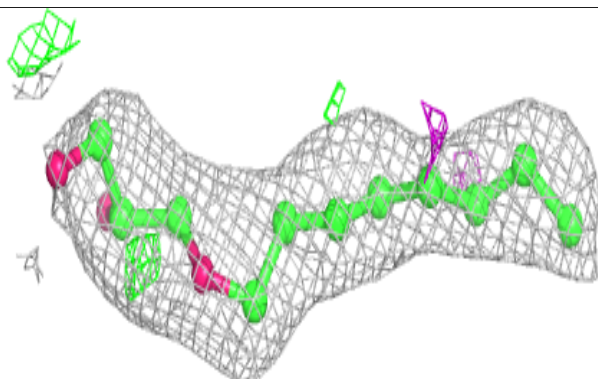
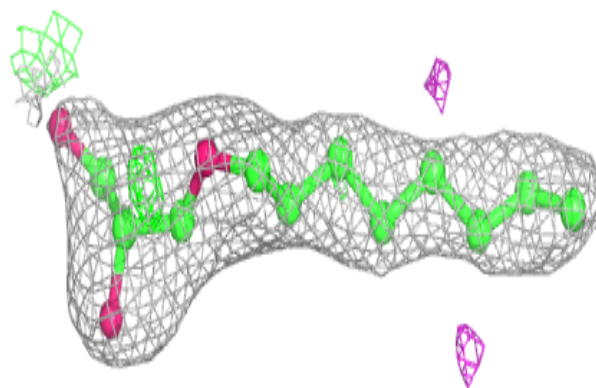


**Electron density around LFA H 310:**

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

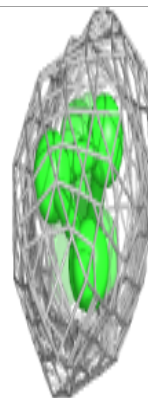
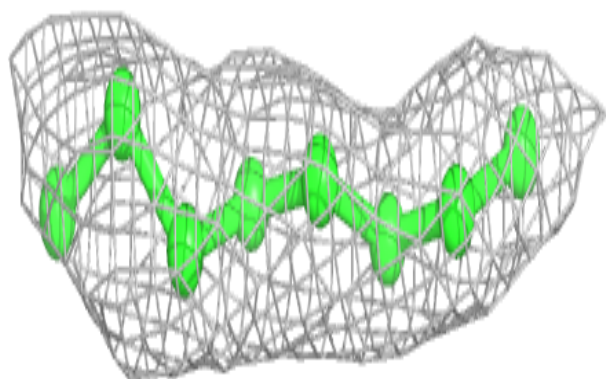
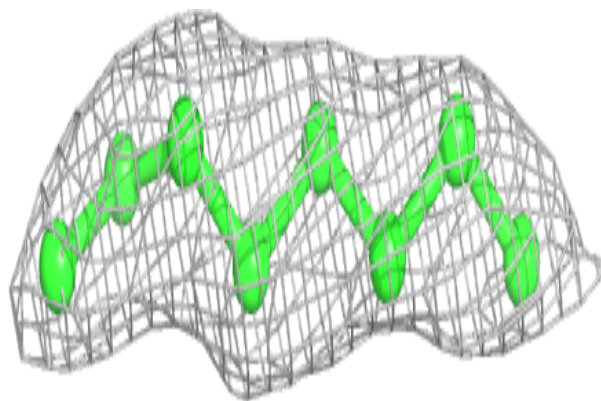
**Electron density around MPG I 314:**

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

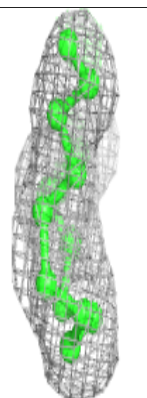
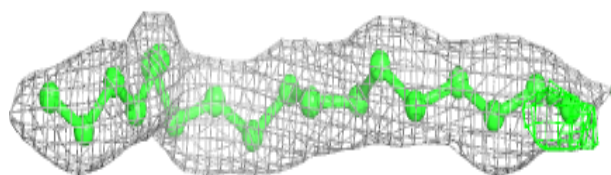
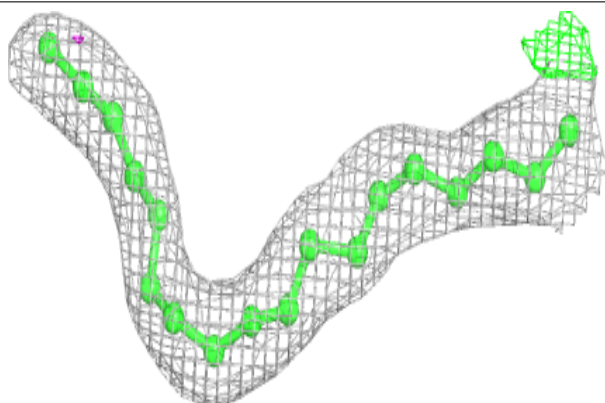


**Electron density around LFA I 311:**

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

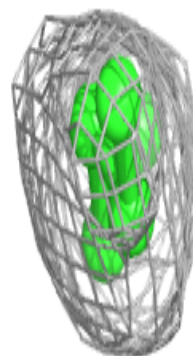
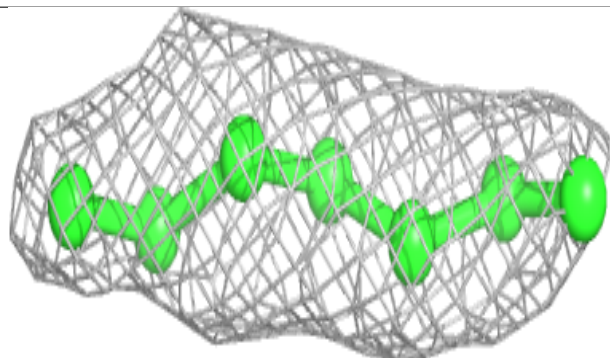
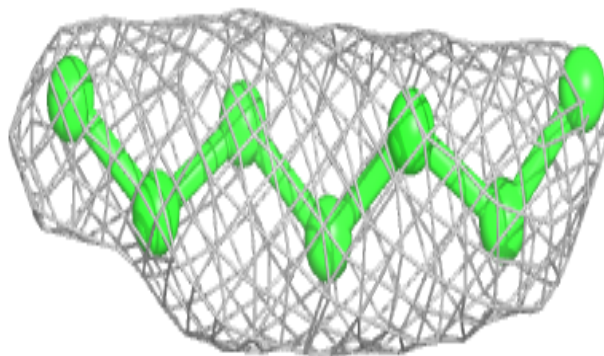
**Electron density around LFA D 307:**

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

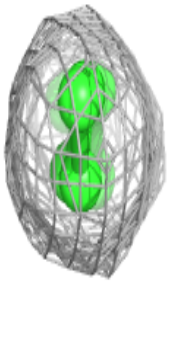
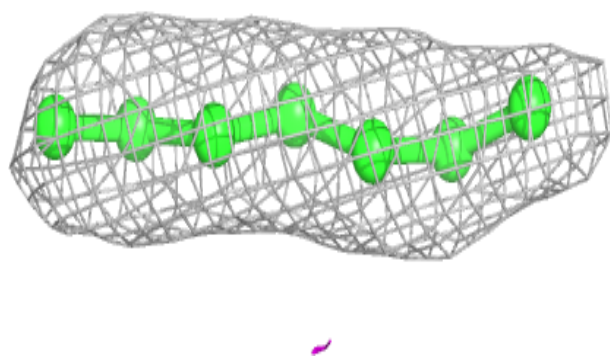
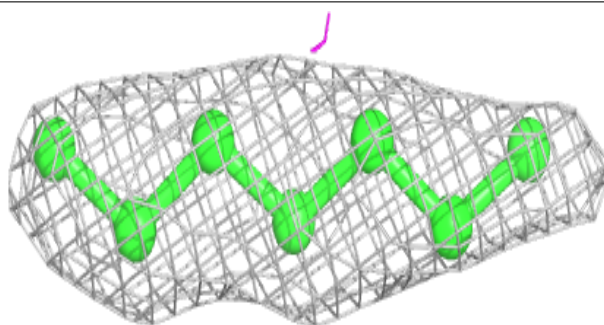


**Electron density around LFA H 311:**

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

**Electron density around LFA I 312:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.