



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 13, 2026 – 10:45 PM JST

PDB ID : 9KUK / pdb_00009kuk
Title : Bovine Heart Cytochrome c Oxidase in the Xenon-bound Fully Oxidized State under Aerobic Condition
Authors : Muramoto, K.; Shinzawa-Itoh, K.
Deposited on : 2024-12-04
Resolution : 1.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

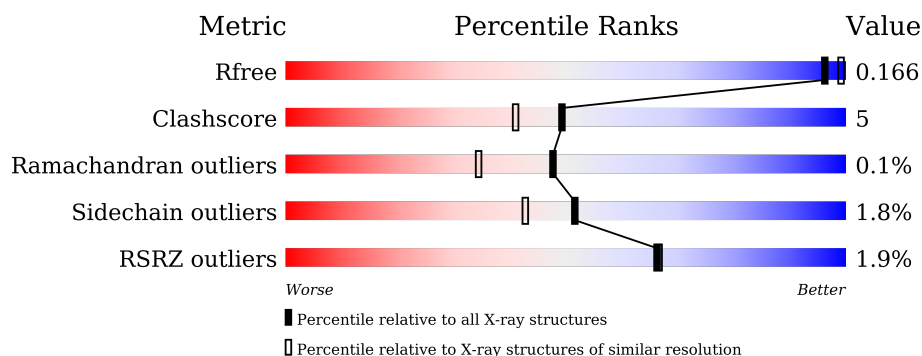
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



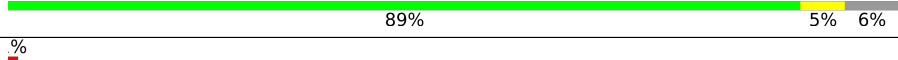
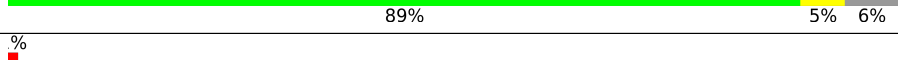
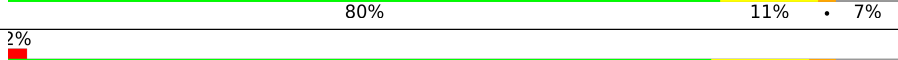
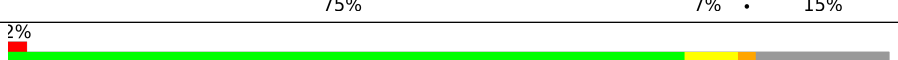
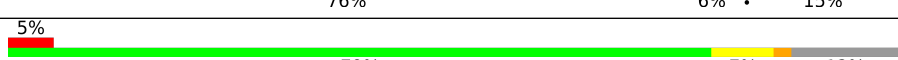
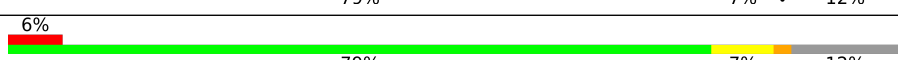
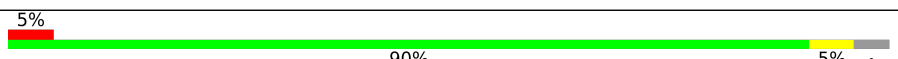
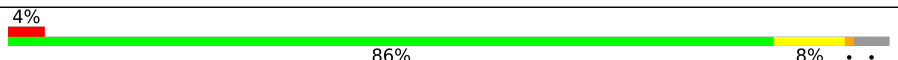
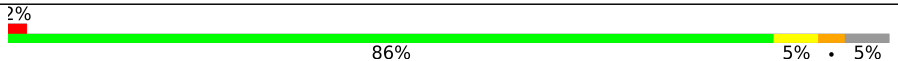
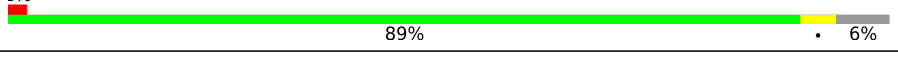
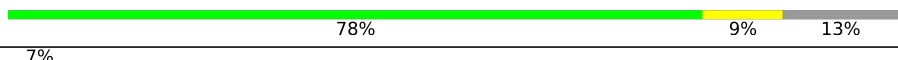
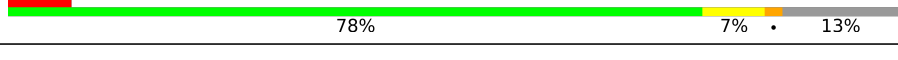
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	514	90% 9% .
1	N	514	90% 9%
2	B	227	5% 83% 15% ..
2	O	227	2% 84% 14% .
3	C	261	87% 12% .
3	P	261	87% 10% ..

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Mol	Chain	Length	Quality of chain
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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
20	LFA	P	311	-	-	-	X
23	XE	B	301	-	-	X	-
23	XE	O	303	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33061 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	15	0
			4130	2757	636	696	41			
1	N	513	Total	C	N	O	S	0	15	0
			4130	2757	636	696	41			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	5	0
			1870	1216	288	347	19			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1216	288	347	19			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	258	Total	C	N	O	S	0	9	0
			2171	1449	342	364	16			
3	P	258	Total	C	N	O	S	0	9	0
			2172	1449	343	364	16			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	143	Total	C	N	O	S	0	1	0
			1192	776	195	217	4			
4	Q	137	Total	C	N	O	S	0	1	0
			1148	749	188	207	4			

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	102	Total	C	N	O	S	0	0	0
			825	528	139	156	2			
5	R	102	Total	C	N	O	S	0	0	0
			825	528	139	156	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	91	Total	C	N	O	S	0	2	0
			709	441	124	138	6			
6	S	91	Total	C	N	O	S	0	2	0
			709	441	124	138	6			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	72	Total	C	N	O	S	0	1	0
			606	396	114	95	1			
7	T	72	Total	C	N	O	S	0	1	0
			606	396	114	95	1			

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			
8	U	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			575	375	103	93	4			
9	V	70	Total	C	N	O	S	0	0	0
			575	375	103	93	4			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	56	Total	C	N	O	S	0	0	0
			441	285	73	80	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	56	Total	C	N	O	S	0	0	0
			441	285	73	80	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

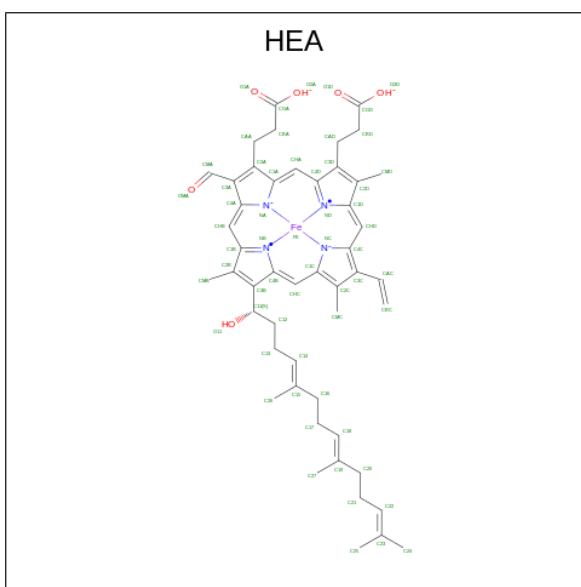
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	44	Total	C	N	O	S	0	0	0
			360	242	59	57	2			
12	Y	44	Total	C	N	O	S	0	0	0
			360	242	59	57	2			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	40	Total	C	N	O	0	0	0
			311	208	48	55			
13	Z	40	Total	C	N	O	0	0	0
			311	208	48	55			

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 69	C 58	Fe 1	N 4	O 6	0	1
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 69	C 58	Fe 1	N 4	O 6	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Cu	0	0
			1	1		
15	N	1	Total	Cu	0	0
			1	1		

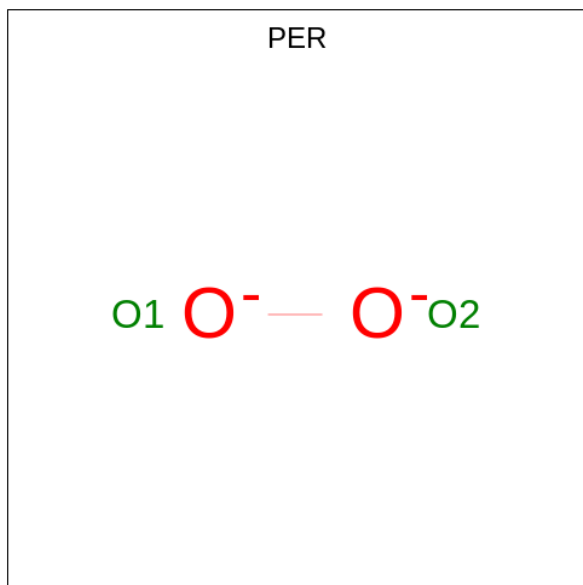
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

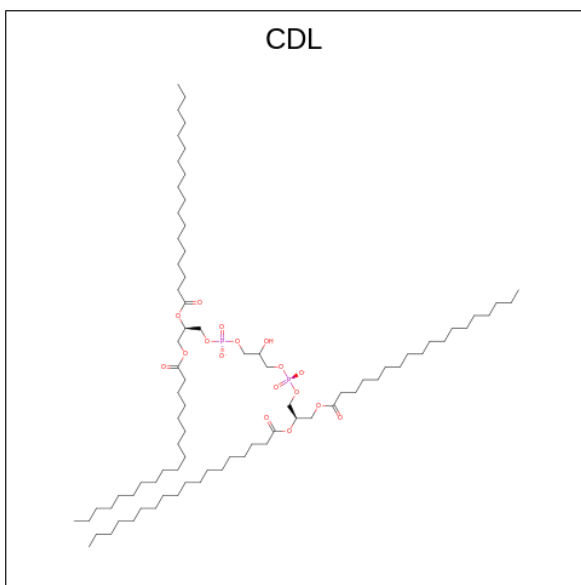
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total 1	Na 1	0	0
17	N	1	Total 1	Na 1	0	0

- Molecule 18 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



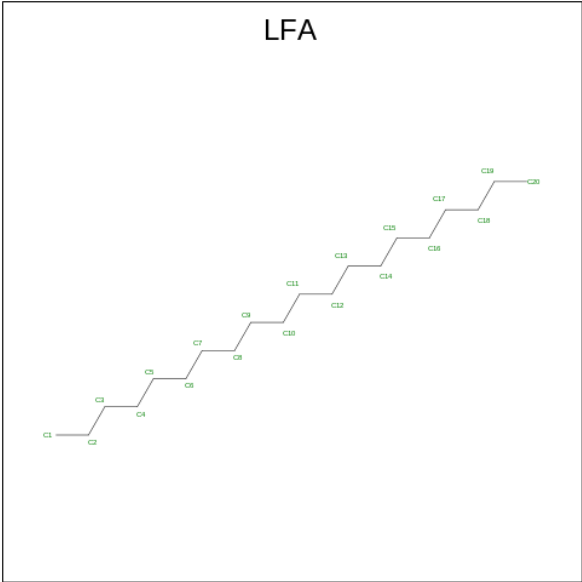
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total 2	O 2	0	0
18	N	1	Total 2	O 2	0	0

- Molecule 19 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			64	45	17	2		
19	C	1	Total	C	O	P	0	0
			87	68	17	2		
19	L	1	Total	C	O	P	0	0
			94	75	17	2		
19	P	1	Total	C	O	P	0	0
			87	68	17	2		
19	V	1	Total	C	O	P	0	0
			64	45	17	2		
19	Y	1	Total	C	O	P	0	0
			94	75	17	2		

- Molecule 20 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



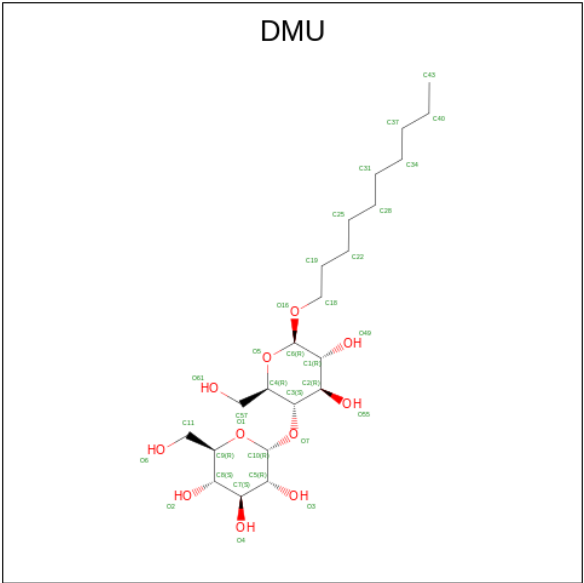
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	C	0	0
			14	14		
20	A	1	Total	C	0	0
			14	14		
20	B	1	Total	C	0	0
			17	17		
20	C	1	Total	C	0	0
			11	11		
20	C	1	Total	C	0	0
			6	6		
20	C	1	Total	C	0	0
			18	18		
20	C	1	Total	C	0	0
			11	11		
20	C	1	Total	C	0	0
			14	14		
20	C	1	Total	C	0	0
			11	11		
20	C	1	Total	C	0	0
			15	15		
20	C	1	Total	C	0	0
			13	13		
20	C	1	Total	C	0	0
			15	15		
20	G	1	Total	C	0	0
			14	14		
20	N	1	Total	C	0	0
			17	17		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	N	1	Total C 14 14	0	0
20	O	1	Total C 11 11	0	0
20	P	1	Total C 15 15	0	0
20	P	1	Total C 11 11	0	0
20	P	1	Total C 6 6	0	0
20	P	1	Total C 18 18	0	0
20	P	1	Total C 11 11	0	0
20	P	1	Total C 14 14	0	0
20	P	1	Total C 11 11	0	0
20	P	1	Total C 15 15	0	0
20	P	1	Total C 13 13	0	0
20	T	1	Total C 11 11	0	0

- Molecule 21 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



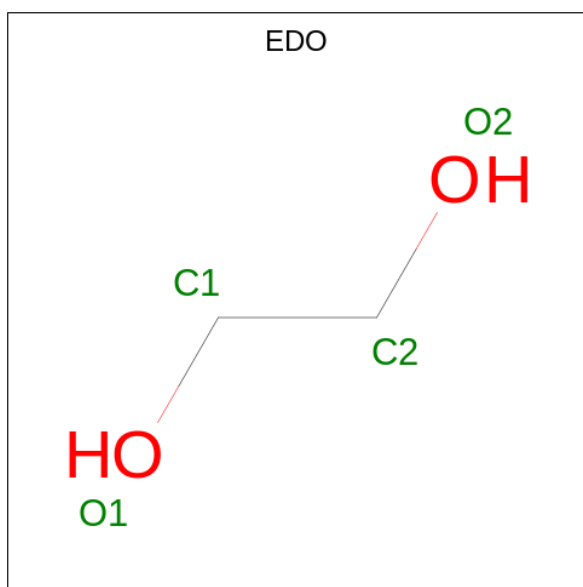
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 7 7	0	0
21	A	1	Total C O 33 22 11	0	0
21	A	1	Total C O 33 22 11	0	0
21	A	1	Total C O 11 10 1	0	0
21	B	1	Total C O 11 10 1	0	0
21	B	1	Total C O 11 10 1	0	0
21	B	1	Total C O 22 16 6	0	0
21	B	1	Total C O 22 16 6	0	0
21	C	1	Total C O 11 10 1	0	0
21	C	1	Total C O 33 22 11	0	0
21	C	1	Total C 7 7	0	0
21	C	1	Total C O 22 16 6	0	0
21	C	1	Total C O 33 22 11	0	0
21	C	1	Total C O 33 22 11	0	0
21	C	1	Total C O 33 22 11	0	0
21	D	1	Total C O 33 22 11	0	0
21	G	1	Total C O 22 16 6	0	0
21	J	1	Total C O 11 10 1	0	0
21	L	1	Total C O 22 16 6	0	0
21	M	1	Total C O 33 22 11	0	0
21	M	1	Total C 8 8	0	0
21	N	1	Total C O 11 10 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	N	1	Total C 7 7	0	0
21	N	1	Total C O 33 22 11	0	0
21	O	1	Total C O 22 16 6	0	0
21	O	1	Total C O 11 10 1	0	0
21	O	1	Total C O 11 10 1	0	0
21	O	1	Total C O 22 16 6	0	0
21	P	1	Total C O 11 10 1	0	0
21	P	1	Total C O 33 22 11	0	0
21	P	1	Total C 7 7	0	0
21	P	1	Total C O 22 16 6	0	0
21	P	1	Total C O 33 22 11	0	0
21	P	1	Total C O 33 22 11	0	0
21	P	1	Total C O 33 22 11	0	0
21	Q	1	Total C O 33 22 11	0	0
21	T	1	Total C O 22 16 6	0	0
21	U	1	Total C O 33 22 11	0	0
21	W	1	Total C O 11 10 1	0	0
21	Y	1	Total C O 22 16 6	0	0
21	Z	1	Total C O 33 22 11	0	0
21	Z	1	Total C 8 8	0	0

- Molecule 22 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			4	2	2		
22	A	1	Total	C	O	0	0
			4	2	2		
22	A	1	Total	C	O	0	0
			4	2	2		
22	A	1	Total	C	O	0	0
			4	2	2		
22	B	1	Total	C	O	0	0
			4	2	2		
22	C	1	Total	C	O	0	0
			4	2	2		
22	C	1	Total	C	O	0	0
			4	2	2		
22	C	1	Total	C	O	0	0
			4	2	2		
22	E	1	Total	C	O	0	0
			4	2	2		
22	E	1	Total	C	O	0	0
			4	2	2		
22	E	1	Total	C	O	0	0
			4	2	2		
22	F	1	Total	C	O	0	0
			4	2	2		
22	F	1	Total	C	O	0	0
			4	2	2		
22	G	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	N	1	Total C O 4 2 2	0	0
22	N	1	Total C O 4 2 2	0	0
22	N	1	Total C O 4 2 2	0	0
22	N	1	Total C O 4 2 2	0	0
22	N	1	Total C O 4 2 2	0	0
22	O	1	Total C O 4 2 2	0	0
22	P	1	Total C O 4 2 2	0	0
22	P	1	Total C O 4 2 2	0	0
22	P	1	Total C O 4 2 2	0	0
22	R	1	Total C O 4 2 2	0	0
22	R	1	Total C O 4 2 2	0	0
22	R	1	Total C O 4 2 2	0	0
22	S	1	Total C O 4 2 2	0	0
22	S	1	Total C O 4 2 2	0	0
22	T	1	Total C O 4 2 2	0	0

- Molecule 23 is XENON (CCD ID: XE) (formula: Xe) (labeled as "Ligand of Interest" by depositor).

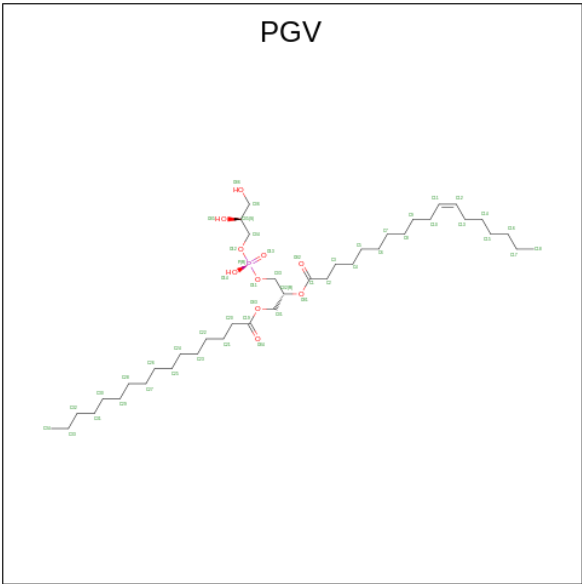
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	5	Total Xe 5 5	0	0
23	B	1	Total Xe 1 1	0	0
23	C	1	Total Xe 1 1	0	0
23	N	5	Total Xe 5 5	0	0

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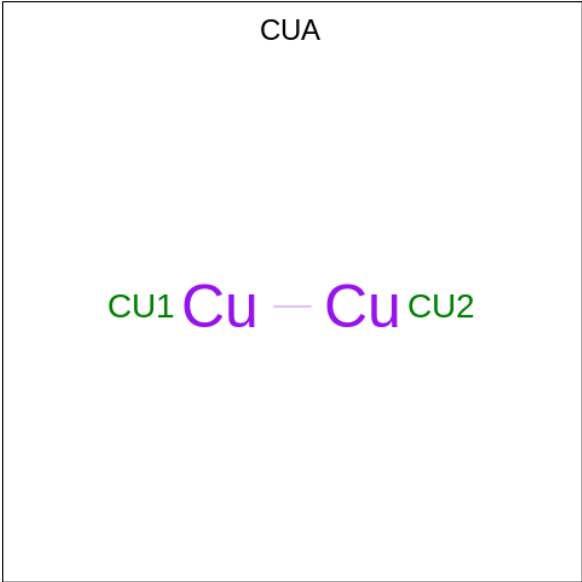
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	O	1	Total	Xe	0	0
			1	1		
23	P	1	Total	Xe	0	0
			1	1		

- Molecule 24 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



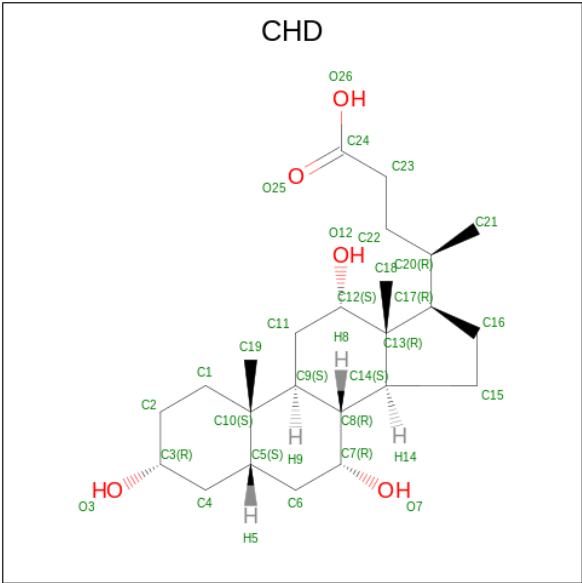
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	O	P	0	0
			51	40	10	1		
24	C	1	Total	C	O	P	0	0
			51	40	10	1		
24	N	1	Total	C	O	P	0	0
			51	40	10	1		
24	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 25 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	B	1	Total	Cu	0	0
			2	2		
25	O	1	Total	Cu	0	0
			2	2		

- Molecule 26 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	B	1	Total	C	O	0
			29	24	5	
26	C	1	Total	C	O	0
			29	24	5	

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	C	1	Total	C	O	0	0
			29	24	5		
26	G	1	Total	C	O	0	0
			29	24	5		
26	P	1	Total	C	O	0	0
			29	24	5		
26	P	1	Total	C	O	0	0
			29	24	5		

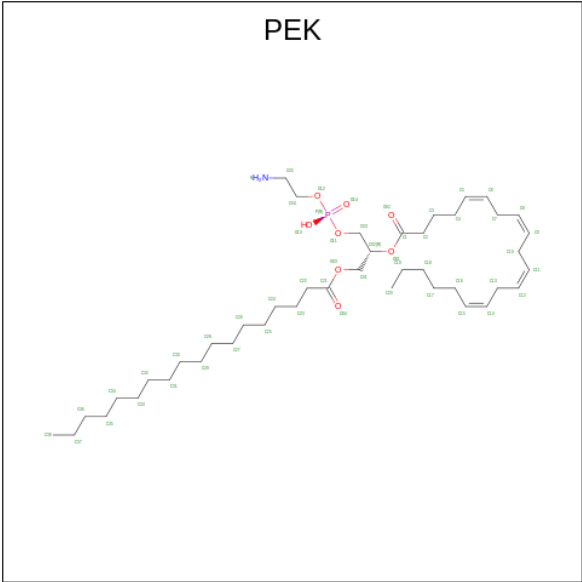
- Molecule 27 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	C	1	Total	X	0	0
			1	1		
27	P	1	Total	X	0	0
			1	1		

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	F	1	Total	Zn	0	0
			1	1		
28	S	1	Total	Zn	0	0
			1	1		

- Molecule 29 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
29	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	246	Total	O	0	11
			257	257		
30	B	177	Total	O	0	2
			179	179		
30	C	101	Total	O	0	1
			102	102		
30	D	139	Total	O	0	9
			148	148		
30	E	110	Total	O	0	7
			117	117		
30	F	97	Total	O	0	7
			104	104		
30	G	45	Total	O	0	1
			46	46		
30	H	58	Total	O	0	0
			58	58		
30	I	37	Total	O	0	0
			37	37		
30	J	21	Total	O	0	0
			21	21		

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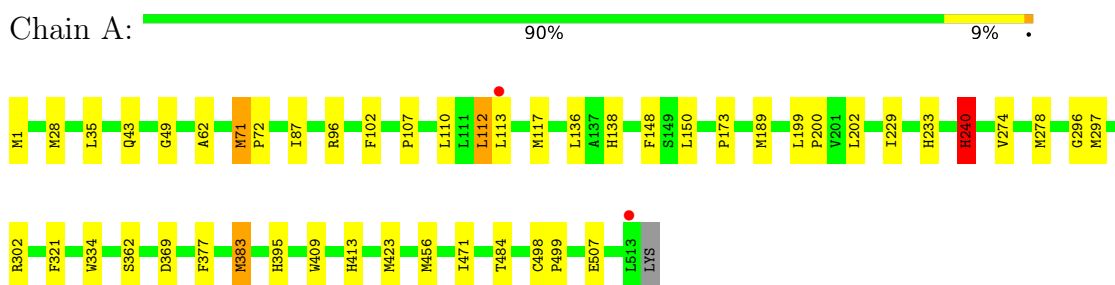
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	21	Total 21	O 21	0	0
30	L	25	Total 27	O 27	0	2
30	M	20	Total 20	O 20	0	0
30	N	226	Total 236	O 236	0	10
30	O	146	Total 147	O 147	0	1
30	P	101	Total 102	O 102	0	1
30	Q	78	Total 82	O 82	0	4
30	R	89	Total 97	O 97	0	8
30	S	86	Total 92	O 92	0	6
30	T	37	Total 38	O 38	0	1
30	U	49	Total 49	O 49	0	0
30	V	23	Total 23	O 23	0	0
30	W	15	Total 15	O 15	0	0
30	X	17	Total 17	O 17	0	0
30	Y	24	Total 26	O 26	0	2
30	Z	17	Total 17	O 17	0	0

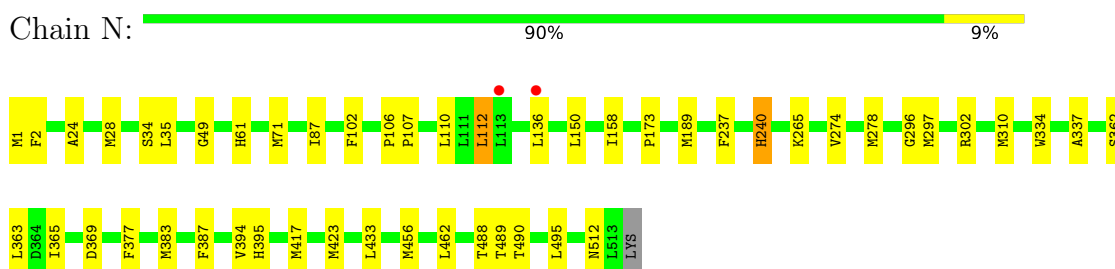
3 Residue-property plots [i](#)

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

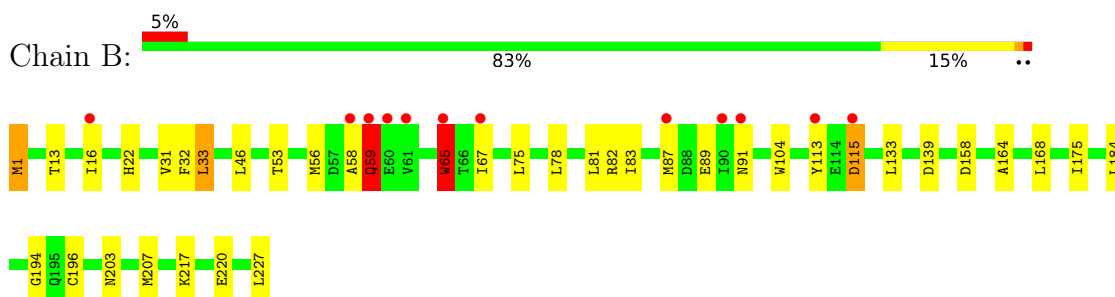
- Molecule 1: Cytochrome c oxidase subunit 1



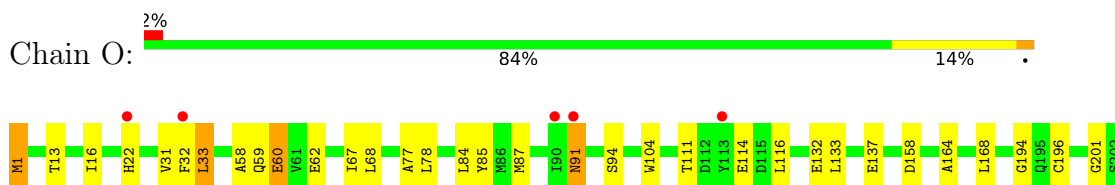
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2





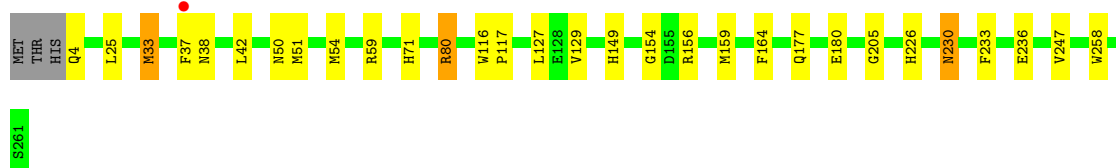
- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 87% 12% .



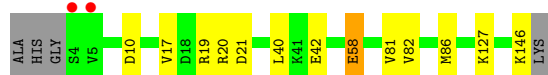
- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 87% 10% ..



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 88% 8% ..



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q: 88% 7% ..



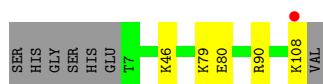
- Molecule 5: Cytochrome c oxidase subunit 5A

Chain E: 89% 5% 6%

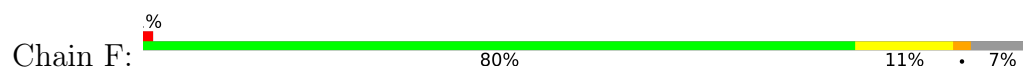


- Molecule 5: Cytochrome c oxidase subunit 5A

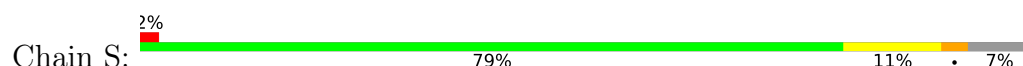
Chain R: 89% 5% 6%



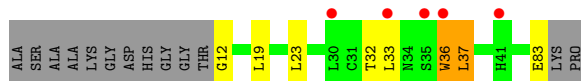
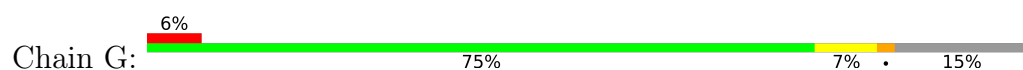
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



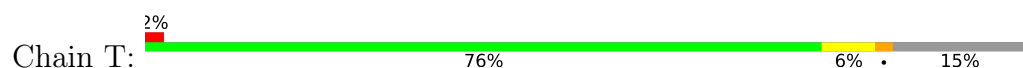
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



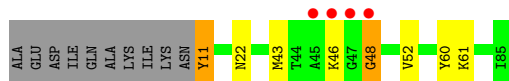
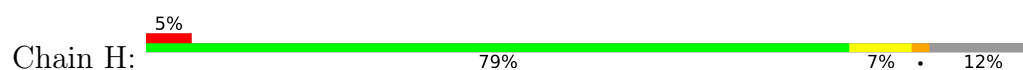
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



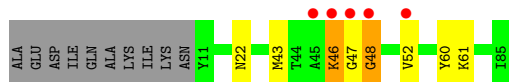
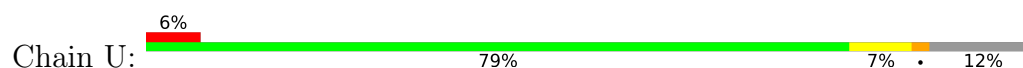
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



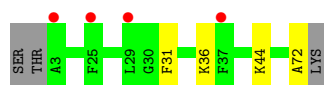
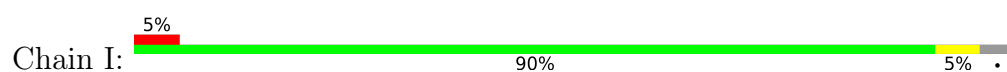
- Molecule 8: Cytochrome c oxidase subunit 6B1



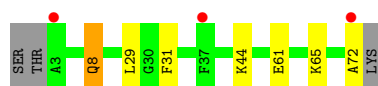
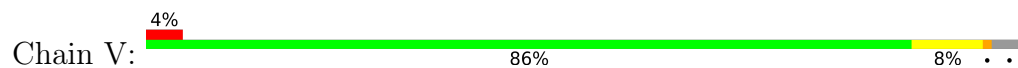
- Molecule 8: Cytochrome c oxidase subunit 6B1



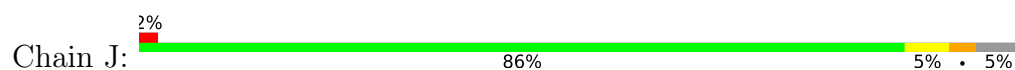
- Molecule 9: Cytochrome c oxidase subunit 6C



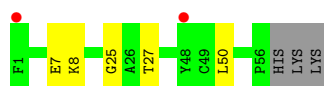
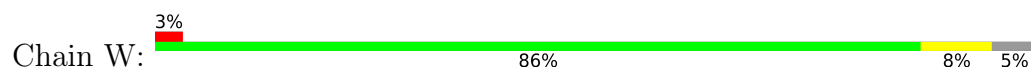
- Molecule 9: Cytochrome c oxidase subunit 6C



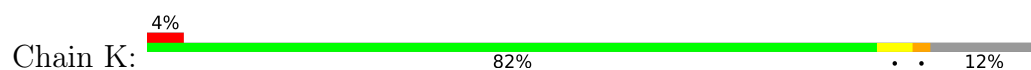
- Molecule 10: Cytochrome c oxidase subunit 7A1



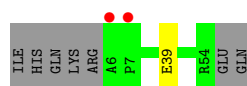
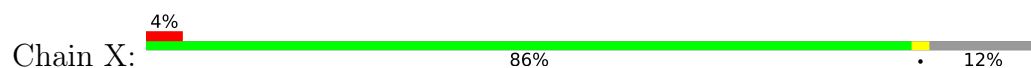
- Molecule 10: Cytochrome c oxidase subunit 7A1



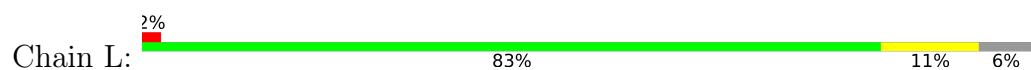
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



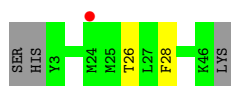
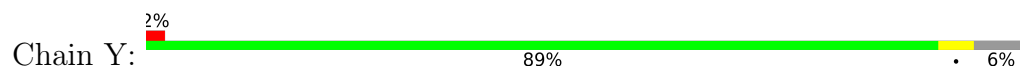
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



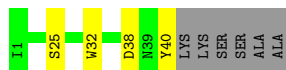
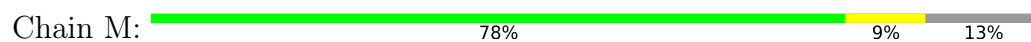
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



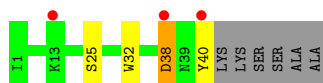
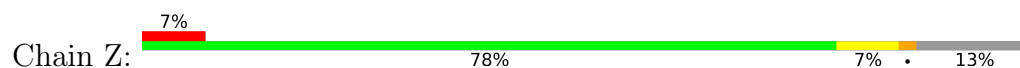
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.90Å 204.00Å 178.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 40.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.80) 100.0 (40.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.120 , 0.156 0.137 , 0.166	Depositor DCC
R_{free} test set	30185 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33061	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PER, ZN, DMU, MG, EDO, CHD, UNX, CDL, PGV, HEA, LFA, CU, XE, PEK, FME, NA, CUA

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	1.06	7/4259 (0.2%)	1.17	8/5816 (0.1%)
1	N	1.05	4/4259 (0.1%)	1.17	6/5816 (0.1%)
2	B	1.12	2/1908 (0.1%)	1.27	15/2598 (0.6%)
2	O	1.09	0/1908	1.25	4/2598 (0.2%)
3	C	1.03	1/2258 (0.0%)	1.14	3/3084 (0.1%)
3	P	1.03	1/2258 (0.0%)	1.15	3/3084 (0.1%)
4	D	1.10	2/1226 (0.2%)	1.17	5/1657 (0.3%)
4	Q	1.07	0/1182	1.29	0/1598
5	E	1.06	2/843 (0.2%)	1.17	2/1145 (0.2%)
5	R	1.01	0/843	1.26	1/1145 (0.1%)
6	F	1.08	1/724 (0.1%)	1.20	0/983
6	S	1.15	3/724 (0.4%)	1.20	1/983 (0.1%)
7	G	1.08	1/633 (0.2%)	1.19	1/864 (0.1%)
7	T	1.11	0/633	1.22	0/864
8	H	1.06	1/648 (0.2%)	1.32	0/877
8	U	1.07	0/648	1.25	0/877
9	I	1.13	0/588	1.39	1/781 (0.1%)
9	V	1.08	0/588	1.41	1/781 (0.1%)
10	J	1.08	0/451	1.30	2/610 (0.3%)
10	W	1.05	0/451	1.31	2/610 (0.3%)
11	K	1.19	1/398 (0.3%)	1.36	1/546 (0.2%)
11	X	1.12	0/398	1.27	0/546
12	L	1.11	1/372 (0.3%)	1.23	3/500 (0.6%)
12	Y	1.12	0/372	1.20	0/500
13	M	1.07	0/321	1.11	0/440
13	Z	1.05	0/321	1.43	0/440
All	All	1.07	27/29214 (0.1%)	1.22	59/39743 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	N	0	1
All	All	0	4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	MET	C-O	8.40	1.34	1.24
11	K	10	HIS	CE1-NE2	8.05	1.40	1.32
3	P	71	HIS	CE1-NE2	7.20	1.39	1.32
1	A	233	HIS	CE1-NE2	7.13	1.39	1.32
1	A	49	GLY	C-O	7.13	1.33	1.23

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	65	TRP	CB-CG-CD1	-12.57	108.04	126.90
1	N	240	HIS	CA-CB-CG	-11.25	102.55	113.80
1	A	240	HIS	CA-CB-CG	-11.06	102.74	113.80
2	B	65	TRP	CA-CB-CG	10.19	132.95	113.60
9	V	72	ALA	CA-C-O	-9.72	104.28	120.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
1	A	383	MET	Mainchain
1	N	296	GLY	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4102	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4130	0	4102	49	0
2	B	1870	0	1870	32	0
2	O	1870	0	1870	33	0
3	C	2171	0	2080	29	0
3	P	2172	0	2081	27	0
4	D	1192	0	1178	8	0
4	Q	1148	0	1131	5	0
5	E	825	0	823	1	0
5	R	825	0	823	3	0
6	F	709	0	691	11	0
6	S	709	0	691	9	0
7	G	606	0	577	4	0
7	T	606	0	577	7	0
8	H	628	0	580	13	0
8	U	628	0	580	14	0
9	I	575	0	584	4	0
9	V	575	0	584	7	0
10	J	441	0	439	5	0
10	W	441	0	439	4	0
11	K	384	0	366	1	0
11	X	384	0	366	1	0
12	L	360	0	360	4	0
12	Y	360	0	360	5	0
13	M	311	0	321	3	0
13	Z	311	0	321	5	0
14	A	129	0	88	4	0
14	N	129	0	88	7	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	1	0
19	A	64	0	72	0	0
19	C	87	0	124	18	0
19	L	94	0	141	4	0
19	P	87	0	124	14	0
19	V	64	0	72	1	0
19	Y	94	0	141	4	0
20	A	28	0	54	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	17	0	33	1	0
20	C	114	0	202	6	0
20	G	14	0	27	6	0
20	N	31	0	60	5	0
20	O	11	0	21	2	0
20	P	114	0	202	8	0
20	T	11	0	21	0	0
21	A	84	0	106	3	0
21	B	66	0	104	2	0
21	C	172	0	228	6	0
21	D	33	0	42	3	0
21	G	22	0	31	0	0
21	J	11	0	21	0	0
21	L	22	0	31	1	0
21	M	41	0	56	0	0
21	N	51	0	76	1	0
21	O	66	0	104	0	0
21	P	172	0	228	6	0
21	Q	33	0	42	1	0
21	T	22	0	31	1	0
21	U	33	0	27	1	0
21	W	11	0	21	0	0
21	Y	22	0	31	1	0
21	Z	41	0	56	0	0
22	A	16	0	24	1	0
22	B	4	0	6	0	0
22	C	12	0	17	0	0
22	E	12	0	18	0	0
22	F	8	0	12	0	0
22	G	4	0	6	0	0
22	N	20	0	30	0	0
22	O	4	0	6	0	0
22	P	12	0	18	0	0
22	R	12	0	18	0	0
22	S	8	0	12	0	0
22	T	4	0	6	0	0
23	A	5	0	0	2	0
23	B	1	0	0	3	0
23	C	1	0	0	0	0
23	N	5	0	0	1	0
23	O	1	0	0	3	0
23	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	A	51	0	76	0	0
24	C	51	0	76	1	0
24	N	51	0	76	2	0
24	P	51	0	76	0	0
25	B	2	0	0	0	0
25	O	2	0	0	0	0
26	B	29	0	39	1	0
26	C	58	0	78	1	0
26	G	29	0	39	1	0
26	P	58	0	78	3	0
27	C	1	0	0	1	0
27	P	1	0	0	0	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	G	53	0	77	0	0
29	T	53	0	77	4	0
30	A	257	0	0	9	0
30	B	179	0	0	5	0
30	C	102	0	0	3	0
30	D	148	0	0	2	0
30	E	117	0	0	0	0
30	F	104	0	0	1	0
30	G	46	0	0	0	0
30	H	58	0	0	1	0
30	I	37	0	0	1	0
30	J	21	0	0	0	0
30	K	21	0	0	0	0
30	L	27	0	0	0	0
30	M	20	0	0	0	0
30	N	236	0	0	7	0
30	O	147	0	0	1	0
30	P	102	0	0	3	0
30	Q	82	0	0	2	0
30	R	97	0	0	2	0
30	S	92	0	0	0	0
30	T	38	0	0	1	0
30	U	49	0	0	2	0
30	V	23	0	0	2	0
30	W	15	0	0	0	0
30	X	17	0	0	0	0
30	Y	26	0	0	0	0
30	Z	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	33061	0	31466	336	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 5.

The worst 5 of 336 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)
18:N:608:PER:O2	18:N:608:PER:O1	1.58	1.18
1:A:112:LEU:HG	30:A:2035:HOH:O	1.38	1.18
18:A:606:PER:O2	18:A:606:PER:O1	1.60	1.16
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.19	1.13
8:H:52:VAL:HG12	8:U:46:LYS:CG	1.80	1.11

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	526/514 (102%)	513 (98%)	13 (2%)	0	100	100
1	N	526/514 (102%)	512 (97%)	14 (3%)	0	100	100
2	B	230/227 (101%)	224 (97%)	6 (3%)	0	100	100
2	O	230/227 (101%)	225 (98%)	5 (2%)	0	100	100
3	C	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
3	P	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	136/147 (92%)	132 (97%)	4 (3%)	0	100	100
5	E	100/109 (92%)	100 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	100/109 (92%)	100 (100%)	0	0	100	100
6	F	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
6	S	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
7	G	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
7	T	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
8	H	73/85 (86%)	71 (97%)	1 (1%)	1 (1%)	9	2
8	U	73/85 (86%)	70 (96%)	2 (3%)	1 (1%)	9	2
9	I	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
9	V	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
10	J	54/59 (92%)	54 (100%)	0	0	100	100
10	W	54/59 (92%)	54 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
12	Y	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
13	M	38/46 (83%)	38 (100%)	0	0	100	100
13	Z	38/46 (83%)	38 (100%)	0	0	100	100
All	All	3488/3614 (96%)	3417 (98%)	69 (2%)	2 (0%)	48	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	48	GLY
8	U	48	GLY

5.3.2 Protein sidechains ⓘ

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	440/426 (103%)	438 (100%)	2 (0%)	81	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	440/426 (103%)	437 (99%)	3 (1%)	76	73
2	B	215/210 (102%)	208 (97%)	7 (3%)	33	21
2	O	215/210 (102%)	208 (97%)	7 (3%)	33	21
3	C	232/226 (103%)	230 (99%)	2 (1%)	70	67
3	P	232/226 (103%)	228 (98%)	4 (2%)	53	45
4	D	128/129 (99%)	128 (100%)	0	100	100
4	Q	122/129 (95%)	120 (98%)	2 (2%)	55	47
5	E	89/95 (94%)	89 (100%)	0	100	100
5	R	89/95 (94%)	88 (99%)	1 (1%)	65	60
6	F	78/81 (96%)	75 (96%)	3 (4%)	29	17
6	S	78/81 (96%)	75 (96%)	3 (4%)	29	17
7	G	63/69 (91%)	60 (95%)	3 (5%)	23	11
7	T	63/69 (91%)	60 (95%)	3 (5%)	23	11
8	H	67/75 (89%)	65 (97%)	2 (3%)	36	24
8	U	67/75 (89%)	64 (96%)	3 (4%)	24	12
9	I	55/58 (95%)	54 (98%)	1 (2%)	51	43
9	V	55/58 (95%)	51 (93%)	4 (7%)	13	4
10	J	47/50 (94%)	46 (98%)	1 (2%)	47	36
10	W	47/50 (94%)	45 (96%)	2 (4%)	26	13
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	28
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	37/40 (92%)	37 (100%)	0	100	100
12	Y	37/40 (92%)	37 (100%)	0	100	100
13	M	34/38 (90%)	33 (97%)	1 (3%)	37	25
13	Z	34/38 (90%)	33 (97%)	1 (3%)	37	25
All	All	3042/3086 (99%)	2986 (98%)	56 (2%)	51	43

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	68	LEU
13	Z	38	ASP
3	P	159	MET

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Mol	Chain	Res	Type
10	W	50	LEU
9	V	8	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
4	Q	119	GLN
8	U	32	ASN
4	Q	143	ASN
8	U	22	ASN
7	G	38	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	FME	A	1	1	8,9,10	0.43	0	7,9,11	0.92	0
1	FME	N	1	1	8,9,10	0.68	0	7,9,11	1.14	1 (14%)
2	FME	B	1	2	8,9,10	1.41	1 (12%)	7,9,11	1.41	1 (14%)
2	FME	O	1	2	8,9,10	0.87	1 (12%)	7,9,11	1.12	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
1	FME	A	1	1	-	2/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-3.43	1.63	1.81
2	O	1	FME	CG-SD	-2.09	1.70	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-3.30	103.78	112.95
1	N	1	FME	O-C-CA	-2.23	118.94	124.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
1	N	1	FME	CA-CB-CG-SD
1	A	1	FME	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
2	B	1	FME	1	0
2	O	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 149 ligands modelled in this entry, 22 are monoatomic and 2 are unknown - leaving 125 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
21	DMU	Y	102	-	22,22,34	0.66	1 (4%)	27,27,45	0.89	1 (3%)
21	DMU	O	305	-	10,10,34	0.25	0	9,9,45	0.51	0
21	DMU	N	611	-	34,34,34	1.39	6 (17%)	45,45,45	1.16	3 (6%)
21	DMU	C	323	-	34,34,34	0.77	0	45,45,45	1.22	3 (6%)
21	DMU	L	102	-	22,22,34	0.69	0	27,27,45	1.02	1 (3%)
21	DMU	P	320	-	34,34,34	0.93	1 (2%)	45,45,45	1.31	4 (8%)
22	EDO	R	202	-	3,3,3	0.09	0	2,2,2	0.20	0
21	DMU	C	316	-	6,6,34	0.21	0	5,5,45	0.62	0
22	EDO	S	102	-	3,3,3	0.54	0	2,2,2	0.34	0
14	HEA	A	601[B]	-	66,67,67	1.99	20 (30%)	78,103,103	2.43	27 (34%)
19	CDL	P	305	-	86,86,99	0.52	0	92,98,111	0.99	6 (6%)
20	LFA	C	310	-	10,10,19	0.23	0	9,9,18	0.15	0
29	PEK	T	101	-	52,52,52	0.73	2 (3%)	55,57,57	1.05	3 (5%)
14	HEA	A	602	18,1	66,67,67	1.91	19 (28%)	78,103,103	2.45	28 (35%)
26	CHD	P	302	-	32,32,32	0.91	2 (6%)	51,51,51	0.65	0
21	DMU	N	602	-	10,10,34	0.37	0	9,9,45	0.53	0
19	CDL	V	101	-	63,63,99	0.50	0	69,75,111	0.96	5 (7%)
21	DMU	P	307	-	10,10,34	0.31	0	9,9,45	0.64	0
22	EDO	A	612	-	3,3,3	0.34	0	2,2,2	0.23	0
22	EDO	O	308	-	3,3,3	0.08	0	2,2,2	0.31	0
20	LFA	P	313	-	10,10,19	0.25	0	9,9,18	0.23	0
18	PER	N	608	14,15	1,1,1	1.51	0	-		
20	LFA	C	313	-	14,14,19	0.28	0	13,13,18	0.41	0
22	EDO	R	203	-	3,3,3	0.37	0	2,2,2	0.46	0
20	LFA	P	311	-	10,10,19	0.13	0	9,9,18	0.09	0
24	PGV	A	621	-	50,50,50	0.70	0	53,56,56	1.16	3 (5%)
22	EDO	P	322	-	3,3,3	0.20	0	2,2,2	0.11	0
26	CHD	P	306	-	32,32,32	0.82	1 (3%)	51,51,51	1.18	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	DMU	P	324	-	34,34,34	0.72	0	45,45,45	1.47	4 (8%)
20	LFA	P	315	-	12,12,19	0.21	0	11,11,18	0.27	0
20	LFA	C	325	-	14,14,19	0.16	0	13,13,18	0.08	0
22	EDO	R	201	-	3,3,3	0.14	0	2,2,2	0.06	0
14	HEA	N	604	18,1	66,67,67	1.70	17 (25%)	78,103,103	2.47	34 (43%)
19	CDL	C	304	-	86,86,99	0.56	0	92,98,111	1.21	10 (10%)
22	EDO	N	613	-	3,3,3	0.09	0	2,2,2	0.23	0
19	CDL	A	607	-	63,63,99	0.52	0	69,75,111	0.99	4 (5%)
21	DMU	P	316	-	34,34,34	0.83	0	45,45,45	1.41	5 (11%)
21	DMU	B	309	-	22,22,34	0.79	0	27,27,45	1.42	3 (11%)
25	CUA	B	302	2	0,1,1	-	-	-	-	-
14	HEA	N	603[A]	-	66,67,67	1.92	18 (27%)	78,103,103	2.56	27 (34%)
22	EDO	E	203	-	3,3,3	0.10	0	2,2,2	0.20	0
22	EDO	N	614	-	3,3,3	0.38	0	2,2,2	0.27	0
20	LFA	P	309	-	5,5,19	0.29	0	4,4,18	0.08	0
29	PEK	G	101	-	52,52,52	0.54	1 (1%)	55,57,57	0.63	0
21	DMU	M	101	-	34,34,34	1.14	3 (8%)	45,45,45	1.07	3 (6%)
22	EDO	E	201	-	3,3,3	0.09	0	2,2,2	0.20	0
22	EDO	E	202	-	3,3,3	0.21	0	2,2,2	0.14	0
26	CHD	G	102	-	32,32,32	0.68	0	51,51,51	0.82	0
22	EDO	C	320	-	3,3,3	0.13	0	2,2,2	0.16	0
20	LFA	T	102	-	10,10,19	0.22	0	9,9,18	0.16	0
20	LFA	N	601	-	16,16,19	0.32	0	15,15,18	0.28	0
22	EDO	N	616	-	3,3,3	0.50	0	2,2,2	0.45	0
25	CUA	O	304	2	0,1,1	-	-	-	-	-
20	LFA	A	609	-	13,13,19	0.77	0	12,12,18	0.56	0
21	DMU	C	319	-	34,34,34	0.76	1 (2%)	45,45,45	1.35	7 (15%)
20	LFA	P	312	-	13,13,19	0.15	0	12,12,18	0.12	0
21	DMU	Z	102	-	7,7,34	0.41	0	6,6,45	0.39	0
21	DMU	B	303	-	10,10,34	0.19	0	9,9,45	0.58	0
21	DMU	T	103	-	22,22,34	0.56	0	27,27,45	1.51	2 (7%)
20	LFA	O	301	-	10,10,19	0.28	0	9,9,18	0.18	0
21	DMU	C	318	-	34,34,34	0.96	2 (5%)	45,45,45	1.24	4 (8%)
20	LFA	P	301	-	14,14,19	0.14	0	13,13,18	0.13	0
21	DMU	C	317	-	22,22,34	0.54	0	27,27,45	1.50	4 (14%)
22	EDO	S	103	-	3,3,3	0.10	0	2,2,2	0.14	0
21	DMU	A	623	-	10,10,34	0.24	0	9,9,45	0.59	0
22	EDO	N	615	-	3,3,3	0.30	0	2,2,2	0.13	0
26	CHD	B	307	-	32,32,32	0.68	0	51,51,51	0.70	0
18	PER	A	606	14,15	1,1,1	1.75	0	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	N	603[B]	-	66,67,67	1.91	18 (27%)	78,103,103	2.54	30 (38%)
22	EDO	N	612	-	3,3,3	0.39	0	2,2,2	0.20	0
22	EDO	P	321	-	3,3,3	0.26	0	2,2,2	0.09	0
21	DMU	C	315	-	34,34,34	0.80	1 (2%)	45,45,45	1.49	7 (15%)
21	DMU	O	307	-	22,22,34	0.70	1 (4%)	27,27,45	1.32	4 (14%)
24	PGV	P	304	-	50,50,50	0.90	3 (6%)	53,56,56	0.98	5 (9%)
26	CHD	C	301	-	32,32,32	1.00	2 (6%)	51,51,51	0.73	1 (1%)
20	LFA	C	312	-	10,10,19	0.25	0	9,9,18	0.26	0
21	DMU	J	101	-	10,10,34	0.18	0	9,9,45	0.67	0
22	EDO	A	615	-	3,3,3	0.26	0	2,2,2	0.28	0
24	PGV	N	622	-	50,50,50	0.72	2 (4%)	53,56,56	1.14	3 (5%)
22	EDO	F	103	-	3,3,3	0.20	0	2,2,2	0.24	0
21	DMU	A	610	-	6,6,34	0.61	0	5,5,45	0.35	0
22	EDO	G	104	-	3,3,3	0.35	0	2,2,2	0.13	0
21	DMU	D	201	-	34,34,34	1.35	5 (14%)	45,45,45	1.46	5 (11%)
20	LFA	C	307	-	10,10,19	0.24	0	9,9,18	0.18	0
22	EDO	C	321	-	3,3,3	0.19	0	2,2,2	0.29	0
20	LFA	P	310	21	17,17,19	0.23	0	16,16,18	0.20	0
21	DMU	U	101	20	34,34,34	0.94	2 (5%)	45,45,45	1.29	5 (11%)
24	PGV	C	303	-	50,50,50	0.60	0	53,56,56	1.11	3 (5%)
21	DMU	Q	201	-	34,34,34	1.30	6 (17%)	45,45,45	1.57	7 (15%)
22	EDO	A	614	-	3,3,3	0.61	0	2,2,2	0.26	0
21	DMU	O	306	-	10,10,34	0.49	0	9,9,45	0.48	0
21	DMU	O	302	-	22,22,34	0.82	1 (4%)	27,27,45	1.28	3 (11%)
20	LFA	N	609	-	13,13,19	0.23	0	12,12,18	0.39	0
21	DMU	A	622	20	34,34,34	0.98	2 (5%)	45,45,45	1.26	5 (11%)
21	DMU	P	317	-	6,6,34	0.21	0	5,5,45	0.55	0
21	DMU	P	319	-	34,34,34	0.96	3 (8%)	45,45,45	1.09	2 (4%)
21	DMU	Z	101	-	34,34,34	0.92	2 (5%)	45,45,45	1.03	3 (6%)
20	LFA	B	308	-	16,16,19	0.40	0	15,15,18	0.18	0
21	DMU	P	318	-	22,22,34	0.90	1 (4%)	27,27,45	1.32	4 (14%)
20	LFA	C	314	-	12,12,19	0.22	0	11,11,18	0.22	0
20	LFA	C	308	-	5,5,19	0.21	0	4,4,18	0.07	0
26	CHD	C	305	-	32,32,32	0.68	0	51,51,51	1.57	8 (15%)
20	LFA	G	105	-	13,13,19	0.73	0	12,12,18	0.41	0
21	DMU	G	103	-	22,22,34	0.58	0	27,27,45	1.14	2 (7%)
20	LFA	C	309	21	17,17,19	0.22	0	16,16,18	0.27	0
21	DMU	M	102	-	7,7,34	0.30	0	6,6,45	0.75	0
21	DMU	B	304	-	10,10,34	0.41	0	9,9,45	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	DMU	C	306	-	10,10,34	0.39	0	9,9,45	0.46	0
20	LFA	P	314	-	14,14,19	0.46	0	13,13,18	0.26	0
19	CDL	L	101	-	93,93,99	0.40	0	99,105,111	0.60	2 (2%)
22	EDO	C	322	-	3,3,3	0.98	0	2,2,2	0.92	0
20	LFA	A	608	-	13,13,19	0.46	0	12,12,18	0.20	0
22	EDO	B	306	-	3,3,3	0.19	0	2,2,2	0.29	0
21	DMU	W	101	-	10,10,34	0.17	0	9,9,45	0.61	0
21	DMU	B	305	-	22,22,34	1.00	1 (4%)	27,27,45	1.20	4 (14%)
21	DMU	N	610	-	6,6,34	0.38	0	5,5,45	0.35	0
19	CDL	Y	101	-	93,93,99	0.36	0	99,105,111	0.49	1 (1%)
22	EDO	P	323	-	3,3,3	0.36	0	2,2,2	0.95	0
14	HEA	A	601[A]	-	66,67,67	2.00	20 (30%)	78,103,103	2.43	25 (32%)
22	EDO	T	104	-	3,3,3	0.27	0	2,2,2	0.08	0
20	LFA	C	311	-	13,13,19	0.19	0	12,12,18	0.15	0
22	EDO	A	613	-	3,3,3	0.28	0	2,2,2	0.30	0
21	DMU	A	611	-	34,34,34	1.12	2 (5%)	45,45,45	1.22	5 (11%)
22	EDO	F	102	-	3,3,3	0.29	0	2,2,2	0.17	0
20	LFA	P	308	-	10,10,19	0.18	0	9,9,18	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	DMU	Y	102	-	-	10/13/33/59	0/1/1/2
21	DMU	O	305	-	-	5/8/8/59	-
21	DMU	N	611	-	-	7/19/59/59	0/2/2/2
21	DMU	C	323	-	-	7/19/59/59	0/2/2/2
21	DMU	L	102	-	-	8/13/33/59	0/1/1/2
21	DMU	P	320	-	-	10/19/59/59	0/2/2/2
22	EDO	R	202	-	-	0/1/1/1	-
21	DMU	C	316	-	-	3/4/4/59	-
22	EDO	S	102	-	-	0/1/1/1	-
14	HEA	A	601[B]	-	-	5/36/76/76	-
19	CDL	P	305	-	-	53/97/97/110	-
20	LFA	C	310	-	-	7/8/8/17	-
29	PEK	T	101	-	-	20/56/56/56	-
14	HEA	A	602	18,1	-	4/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHD	P	302	-	-	2/9/74/74	0/4/4/4
21	DMU	N	602	-	-	3/8/8/59	-
19	CDL	V	101	-	-	43/74/74/110	-
21	DMU	P	307	-	-	2/8/8/59	-
22	EDO	A	612	-	-	0/1/1/1	-
22	EDO	O	308	-	-	0/1/1/1	-
20	LFA	P	313	-	-	2/8/8/17	-
22	EDO	R	203	-	-	1/1/1/1	-
20	LFA	C	313	-	-	4/12/12/17	-
24	PGV	A	621	-	-	12/55/55/55	-
20	LFA	P	311	-	-	5/8/8/17	-
22	EDO	P	322	-	-	0/1/1/1	-
26	CHD	P	306	-	-	5/9/74/74	0/4/4/4
21	DMU	P	324	-	-	6/19/59/59	0/2/2/2
20	LFA	P	315	-	-	5/10/10/17	-
20	LFA	C	325	-	-	6/12/12/17	-
22	EDO	R	201	-	-	1/1/1/1	-
14	HEA	N	604	18,1	-	4/36/76/76	-
19	CDL	C	304	-	-	49/97/97/110	-
22	EDO	N	613	-	-	0/1/1/1	-
19	CDL	A	607	-	-	33/74/74/110	-
21	DMU	P	316	-	-	10/19/59/59	0/2/2/2
21	DMU	B	309	-	-	9/13/33/59	0/1/1/2
14	HEA	N	603[A]	-	-	6/36/76/76	-
22	EDO	E	203	-	-	0/1/1/1	-
22	EDO	N	614	-	-	0/1/1/1	-
20	LFA	P	309	-	-	1/3/3/17	-
29	PEK	G	101	-	-	9/56/56/56	-
21	DMU	M	101	-	-	3/19/59/59	0/2/2/2
22	EDO	E	201	-	-	0/1/1/1	-
22	EDO	E	202	-	-	0/1/1/1	-
26	CHD	G	102	-	-	2/9/74/74	0/4/4/4
22	EDO	C	320	-	-	1/1/1/1	-
20	LFA	T	102	-	-	5/8/8/17	-
20	LFA	N	601	-	-	11/14/14/17	-
22	EDO	N	616	-	-	0/1/1/1	-
20	LFA	A	609	-	-	5/11/11/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	DMU	C	319	-	-	10/19/59/59	0/2/2/2
20	LFA	P	312	-	-	6/11/11/17	-
21	DMU	Z	102	-	-	3/5/5/59	-
21	DMU	B	303	-	-	3/8/8/59	-
21	DMU	T	103	-	-	8/13/33/59	0/1/1/2
20	LFA	O	301	-	-	4/8/8/17	-
21	DMU	C	318	-	-	12/19/59/59	0/2/2/2
20	LFA	P	301	-	-	8/12/12/17	-
21	DMU	C	317	-	-	8/13/33/59	0/1/1/2
22	EDO	S	103	-	-	0/1/1/1	-
21	DMU	A	623	-	-	3/8/8/59	-
22	EDO	N	615	-	-	0/1/1/1	-
26	CHD	B	307	-	-	2/9/74/74	0/4/4/4
22	EDO	N	612	-	-	0/1/1/1	-
14	HEA	N	603[B]	-	-	2/36/76/76	-
22	EDO	P	321	-	-	1/1/1/1	-
21	DMU	C	315	-	-	12/19/59/59	0/2/2/2
21	DMU	O	307	-	-	6/13/33/59	0/1/1/2
24	PGV	P	304	-	-	9/55/55/55	-
26	CHD	C	301	-	-	2/9/74/74	0/4/4/4
20	LFA	C	312	-	-	3/8/8/17	-
21	DMU	J	101	-	-	5/8/8/59	-
22	EDO	A	615	-	-	0/1/1/1	-
24	PGV	N	622	-	-	9/55/55/55	-
22	EDO	F	103	-	-	0/1/1/1	-
21	DMU	A	610	-	-	3/4/4/59	-
22	EDO	G	104	-	-	0/1/1/1	-
21	DMU	D	201	-	-	7/19/59/59	0/2/2/2
20	LFA	C	307	-	-	4/8/8/17	-
22	EDO	C	321	-	-	0/1/1/1	-
20	LFA	P	310	21	-	8/15/15/17	-
21	DMU	U	101	20	-	4/19/59/59	0/2/2/2
24	PGV	C	303	-	-	11/55/55/55	-
21	DMU	Q	201	-	-	8/19/59/59	0/2/2/2
22	EDO	A	614	-	-	0/1/1/1	-
21	DMU	O	306	-	-	5/8/8/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	DMU	O	302	-	-	7/13/33/59	0/1/1/2
20	LFA	N	609	-	-	3/11/11/17	-
21	DMU	A	622	20	-	4/19/59/59	0/2/2/2
21	DMU	P	317	-	-	1/4/4/59	-
21	DMU	P	319	-	-	13/19/59/59	0/2/2/2
21	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
20	LFA	B	308	-	-	9/14/14/17	-
21	DMU	P	318	-	-	6/13/33/59	0/1/1/2
20	LFA	C	314	-	-	4/10/10/17	-
20	LFA	C	308	-	-	1/3/3/17	-
26	CHD	C	305	-	-	8/9/74/74	0/4/4/4
20	LFA	G	105	-	-	5/11/11/17	-
21	DMU	G	103	-	-	7/13/33/59	0/1/1/2
20	LFA	C	309	21	-	7/15/15/17	-
21	DMU	M	102	-	-	4/5/5/59	-
21	DMU	B	304	-	-	5/8/8/59	-
21	DMU	C	306	-	-	3/8/8/59	-
20	LFA	P	314	-	-	5/12/12/17	-
19	CDL	L	101	-	-	52/104/104/110	-
22	EDO	C	322	-	-	0/1/1/1	-
20	LFA	A	608	-	-	3/11/11/17	-
22	EDO	B	306	-	-	0/1/1/1	-
21	DMU	W	101	-	-	7/8/8/59	-
21	DMU	B	305	-	-	10/13/33/59	0/1/1/2
21	DMU	N	610	-	-	4/4/4/59	-
19	CDL	Y	101	-	-	55/104/104/110	-
22	EDO	P	323	-	-	0/1/1/1	-
14	HEA	A	601[A]	-	-	6/36/76/76	-
22	EDO	T	104	-	-	0/1/1/1	-
20	LFA	C	311	-	-	5/11/11/17	-
22	EDO	A	613	-	-	1/1/1/1	-
21	DMU	A	611	-	-	7/19/59/59	0/2/2/2
22	EDO	F	102	-	-	0/1/1/1	-
20	LFA	P	308	-	-	7/8/8/17	-

The worst 5 of 166 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	603[A]	HEA	C1D-ND	-4.99	1.31	1.40
14	N	603[B]	HEA	C1D-ND	-4.99	1.31	1.40
14	A	601[A]	HEA	C3A-C2A	4.88	1.47	1.36
14	A	601[B]	HEA	C3A-C2A	4.88	1.47	1.36
14	A	601[A]	HEA	C1D-ND	-4.84	1.32	1.40

The worst 5 of 330 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601[A]	HEA	C3C-C4C-NC	9.48	116.08	110.25
14	A	601[B]	HEA	C3C-C4C-NC	9.48	116.08	110.25
14	N	603[A]	HEA	C3D-C4D-ND	7.40	117.52	110.36
14	N	603[B]	HEA	C3D-C4D-ND	7.40	117.52	110.36
14	N	603[A]	HEA	C3C-C4C-NC	7.07	114.60	110.25

There are no chirality outliers.

5 of 804 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C18-C19-C20-C21
14	A	601[B]	HEA	C18-C19-C20-C21
14	A	601[B]	HEA	C27-C19-C20-C21
19	A	607	CDL	C1-CA2-OA2-PA1
19	A	607	CDL	CA3-OA5-PA1-OA2

There are no ring outliers.

52 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	Y	102	DMU	1	0
21	C	323	DMU	3	0
21	L	102	DMU	1	0
19	P	305	CDL	14	0
29	T	101	PEK	4	0
26	P	302	CHD	1	0
19	V	101	CDL	1	0
20	P	313	LFA	1	0
18	N	608	PER	1	0
20	C	313	LFA	1	0
26	P	306	CHD	2	0
21	P	324	DMU	5	0
20	P	315	LFA	1	0

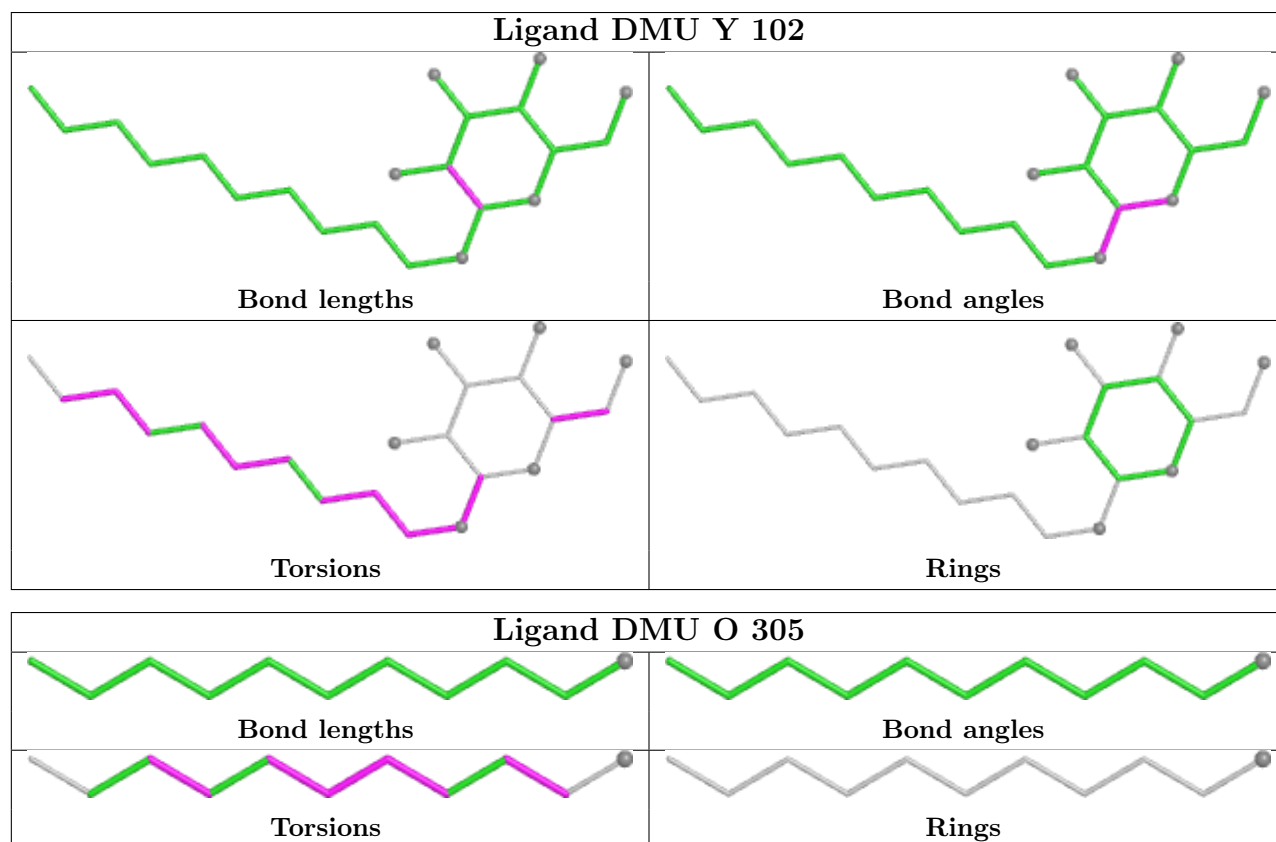
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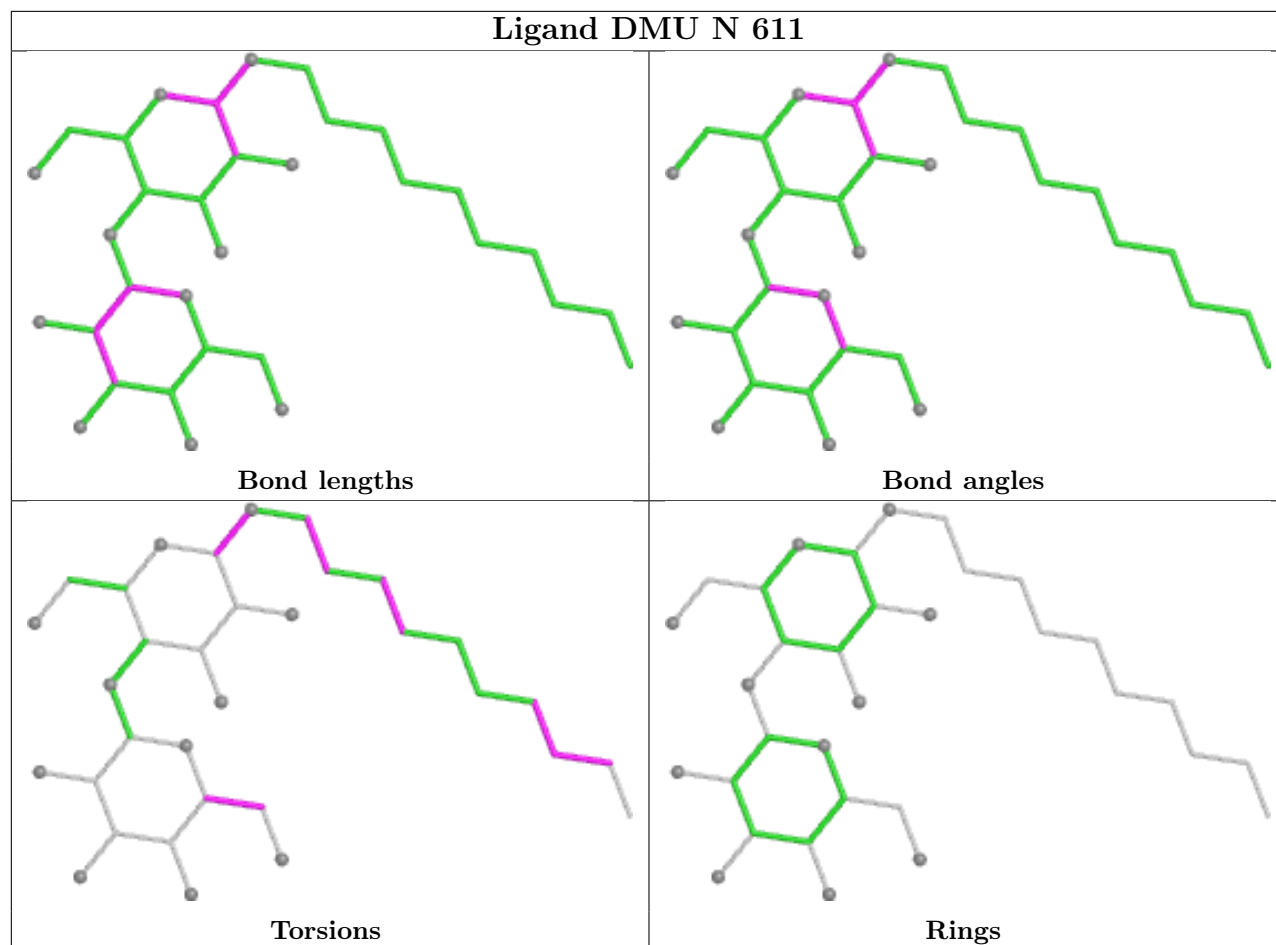
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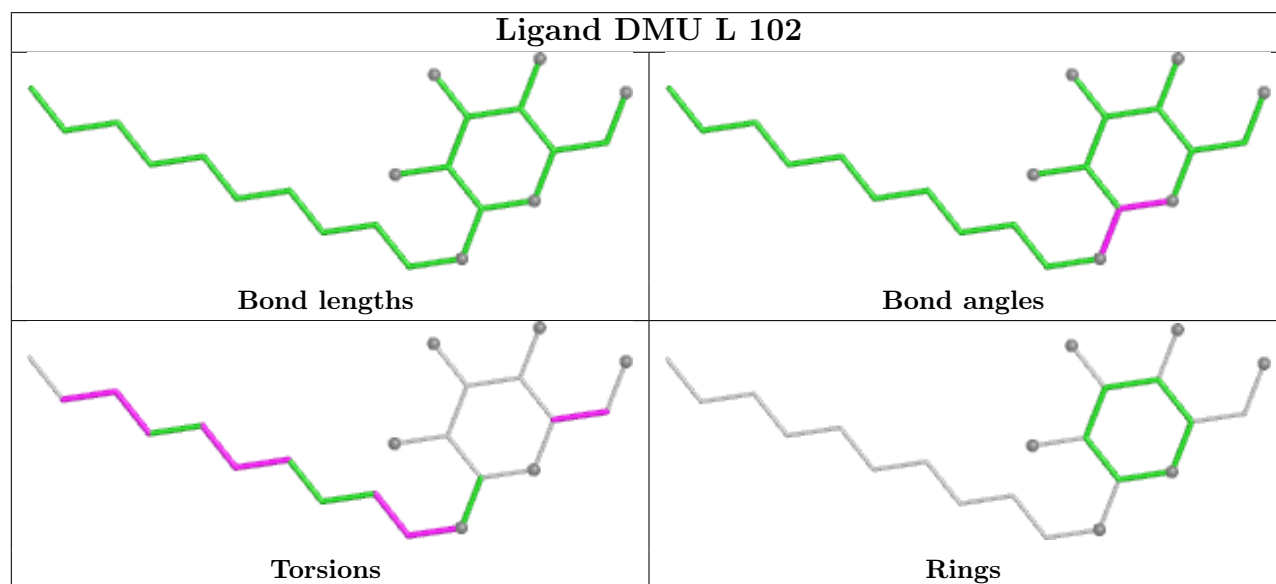
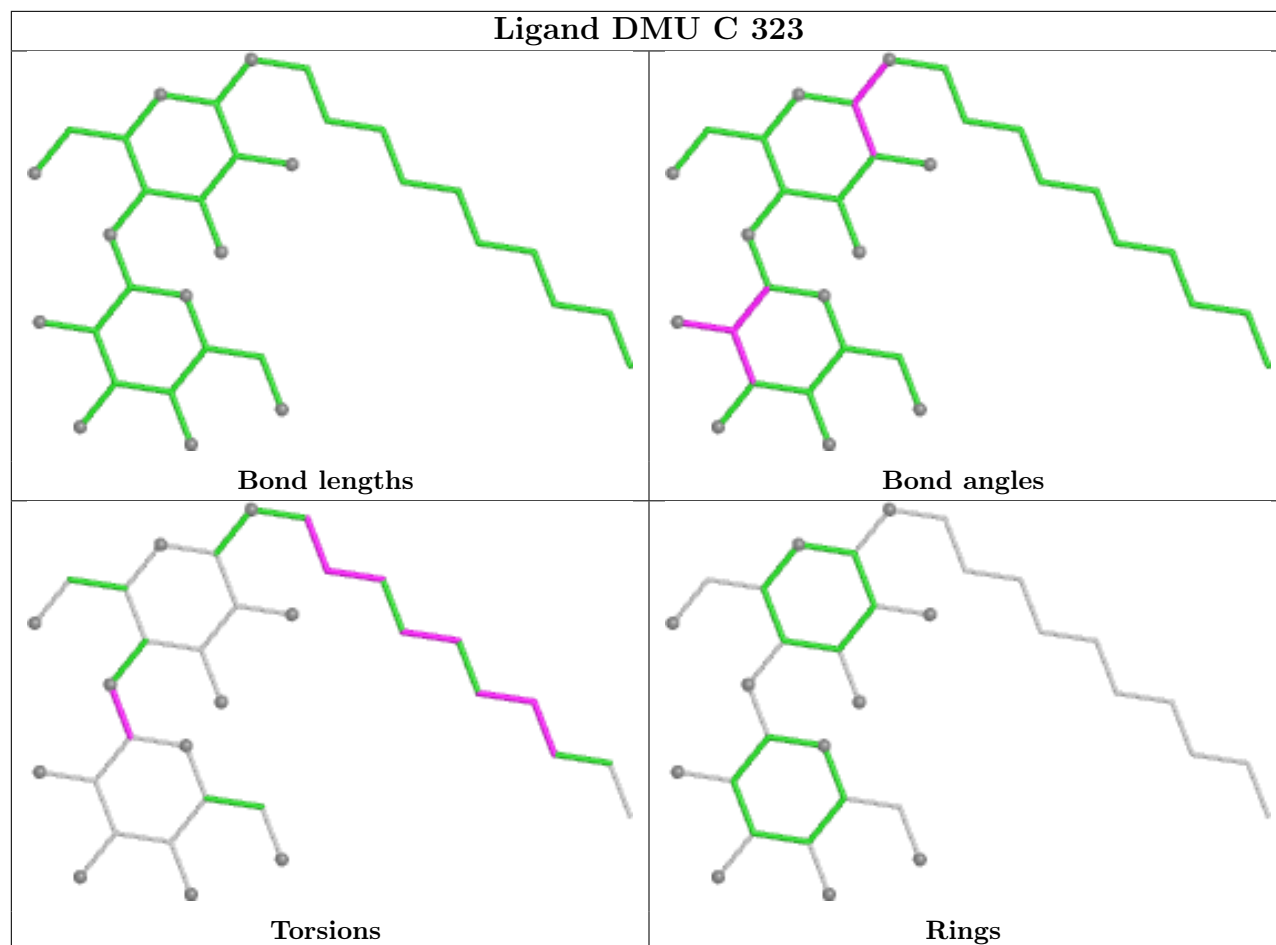
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	604	HEA	2	0
19	C	304	CDL	18	0
21	B	309	DMU	1	0
14	N	603[A]	HEA	4	0
26	G	102	CHD	1	0
20	N	601	LFA	1	0
20	A	609	LFA	6	0
21	T	103	DMU	1	0
20	O	301	LFA	2	0
21	C	318	DMU	3	0
26	B	307	CHD	1	0
18	A	606	PER	1	0
14	N	603[B]	HEA	1	0
20	C	312	LFA	2	0
24	N	622	PGV	2	0
21	A	610	DMU	1	0
21	D	201	DMU	3	0
20	C	307	LFA	3	0
20	P	310	LFA	3	0
21	U	101	DMU	1	0
24	C	303	PGV	1	0
21	Q	201	DMU	1	0
20	N	609	LFA	4	0
21	A	622	DMU	1	0
21	P	319	DMU	1	0
20	B	308	LFA	1	0
20	C	314	LFA	1	0
26	C	305	CHD	1	0
20	G	105	LFA	6	0
20	P	314	LFA	3	0
19	L	101	CDL	4	0
20	A	608	LFA	3	0
21	B	305	DMU	1	0
21	N	610	DMU	1	0
19	Y	101	CDL	4	0
14	A	601[A]	HEA	4	0
22	A	613	EDO	1	0
21	A	611	DMU	1	0
20	P	308	LFA	1	0

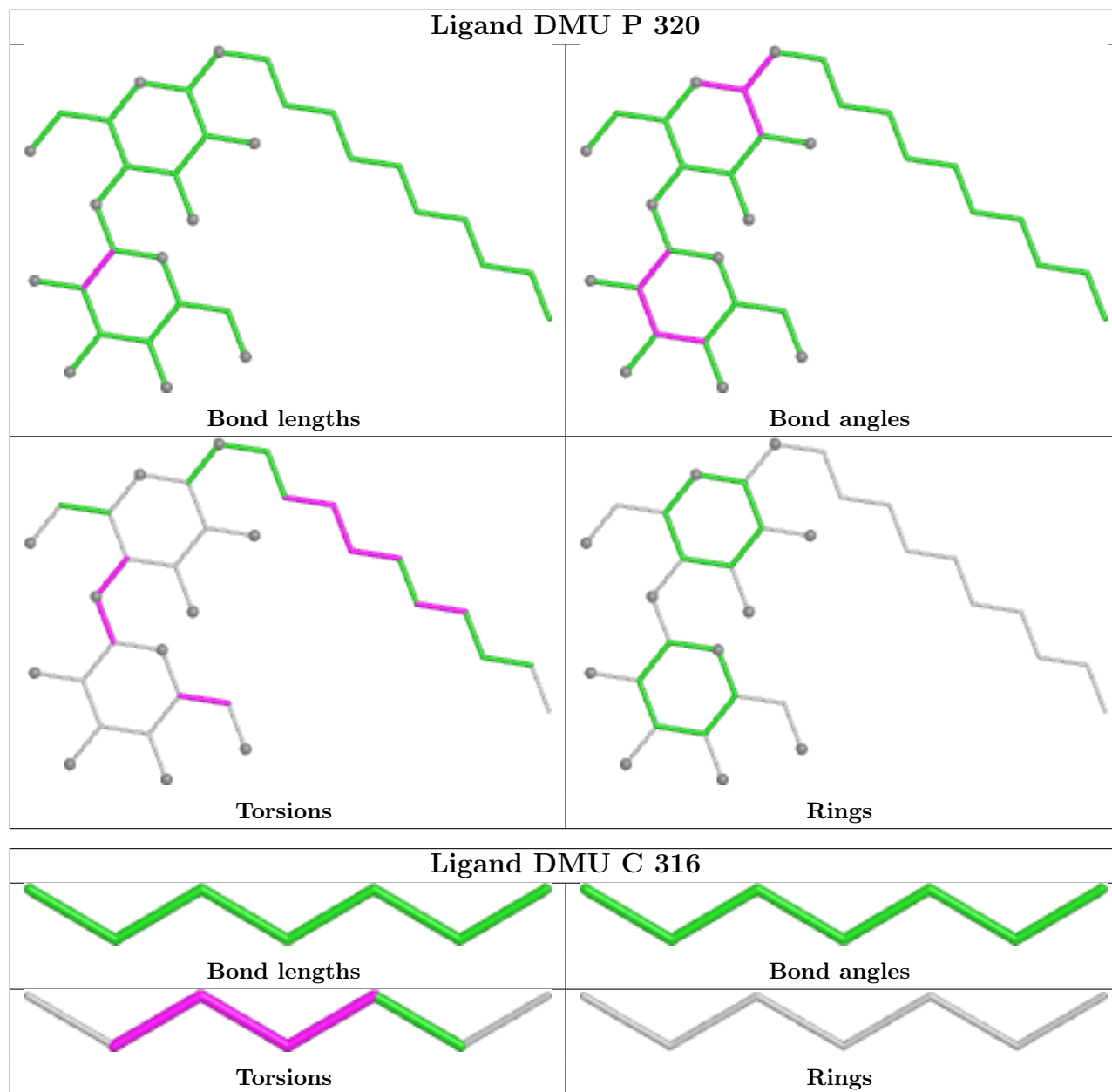
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

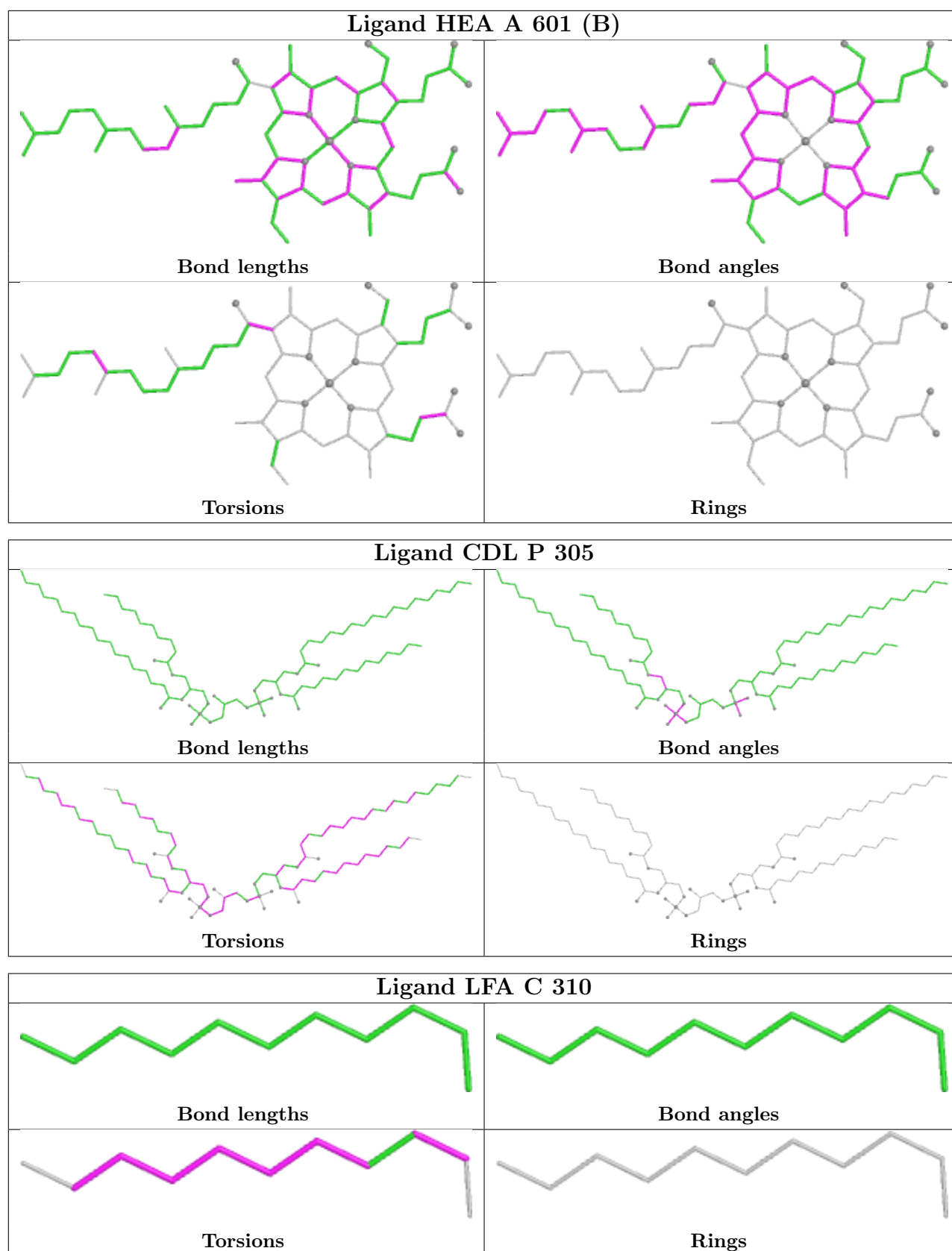
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

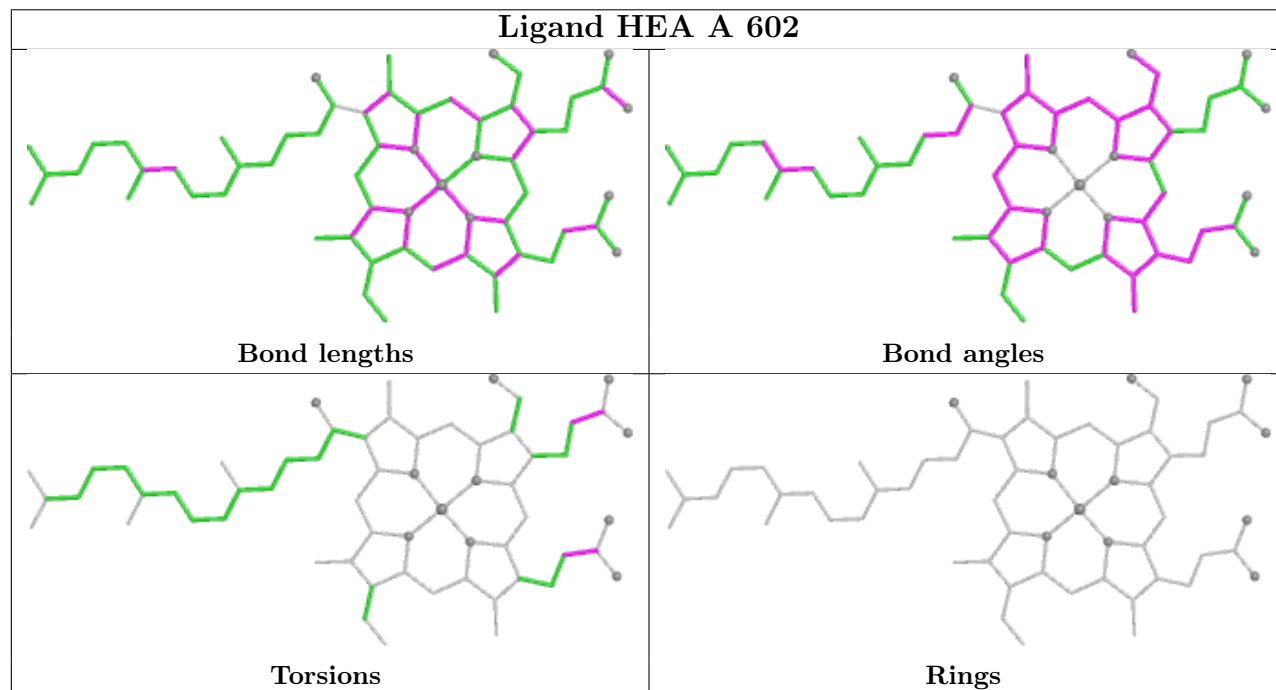
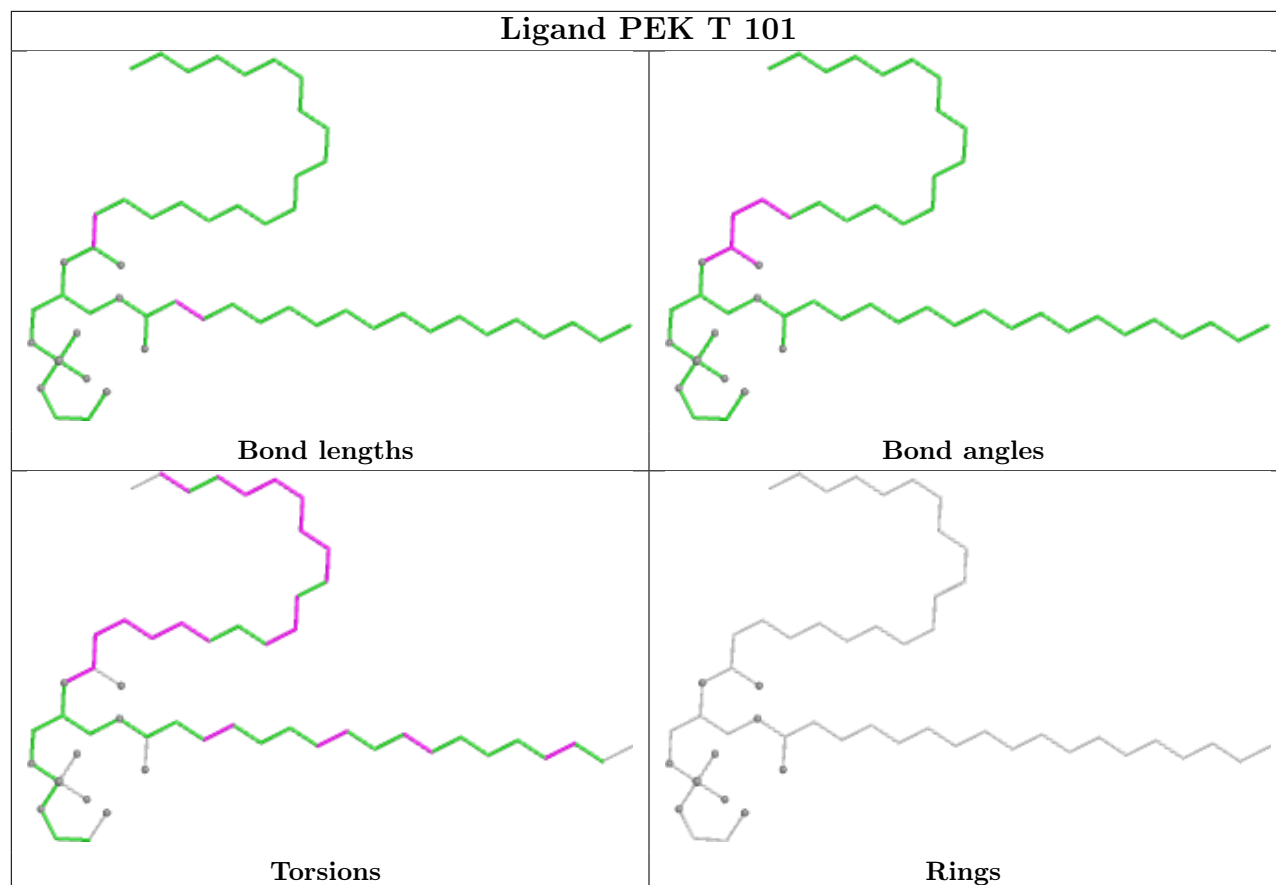


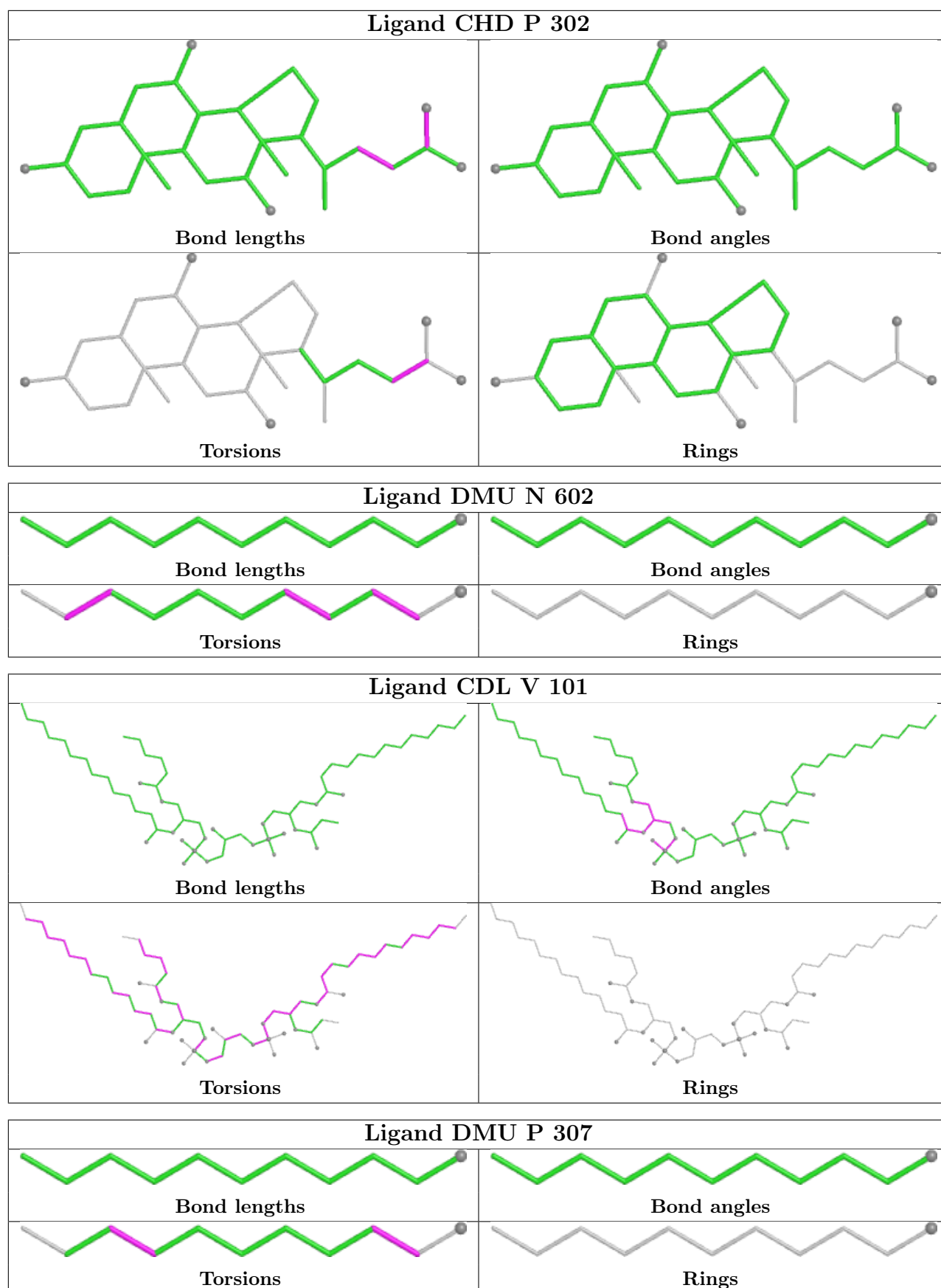


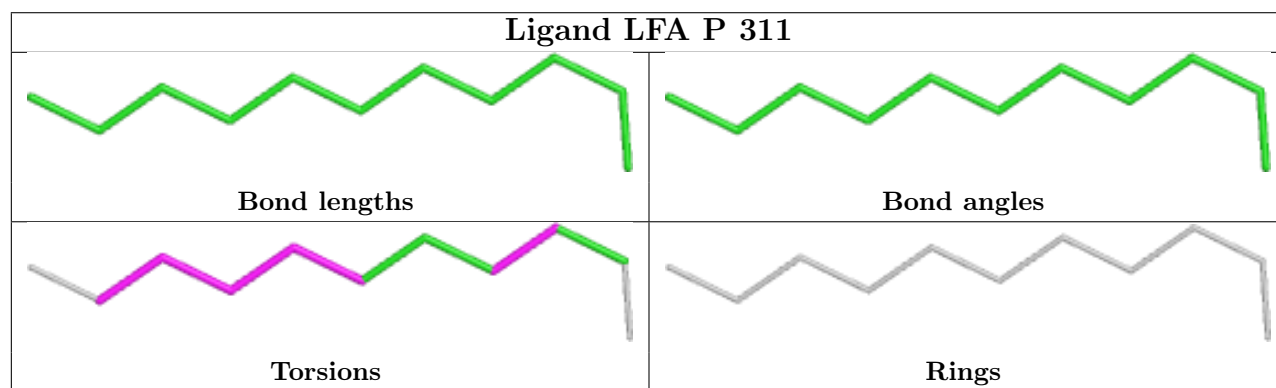
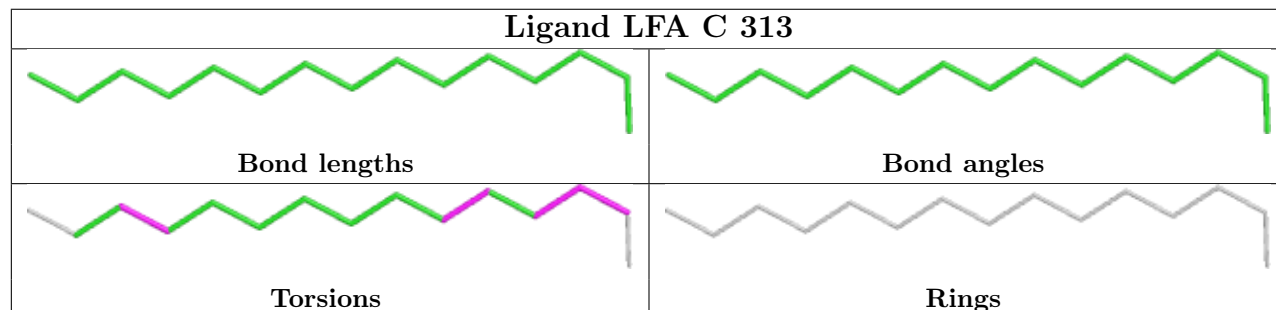
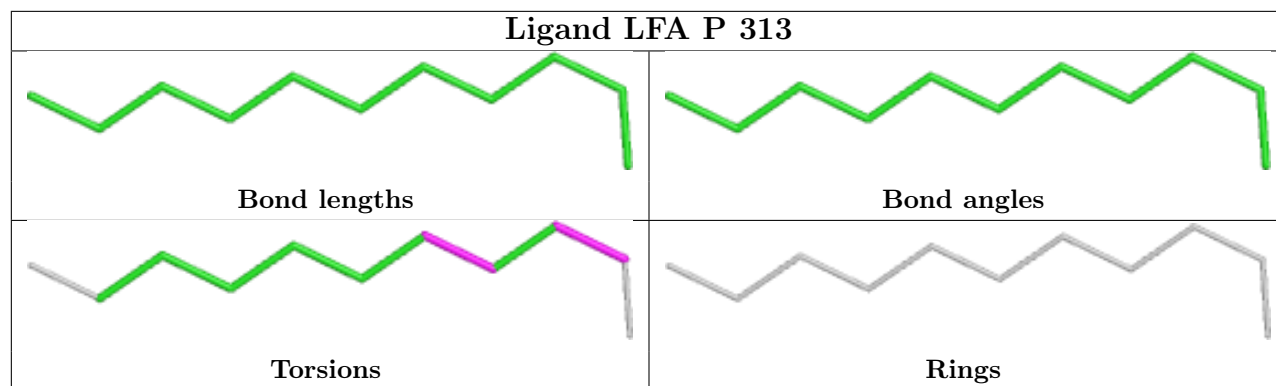


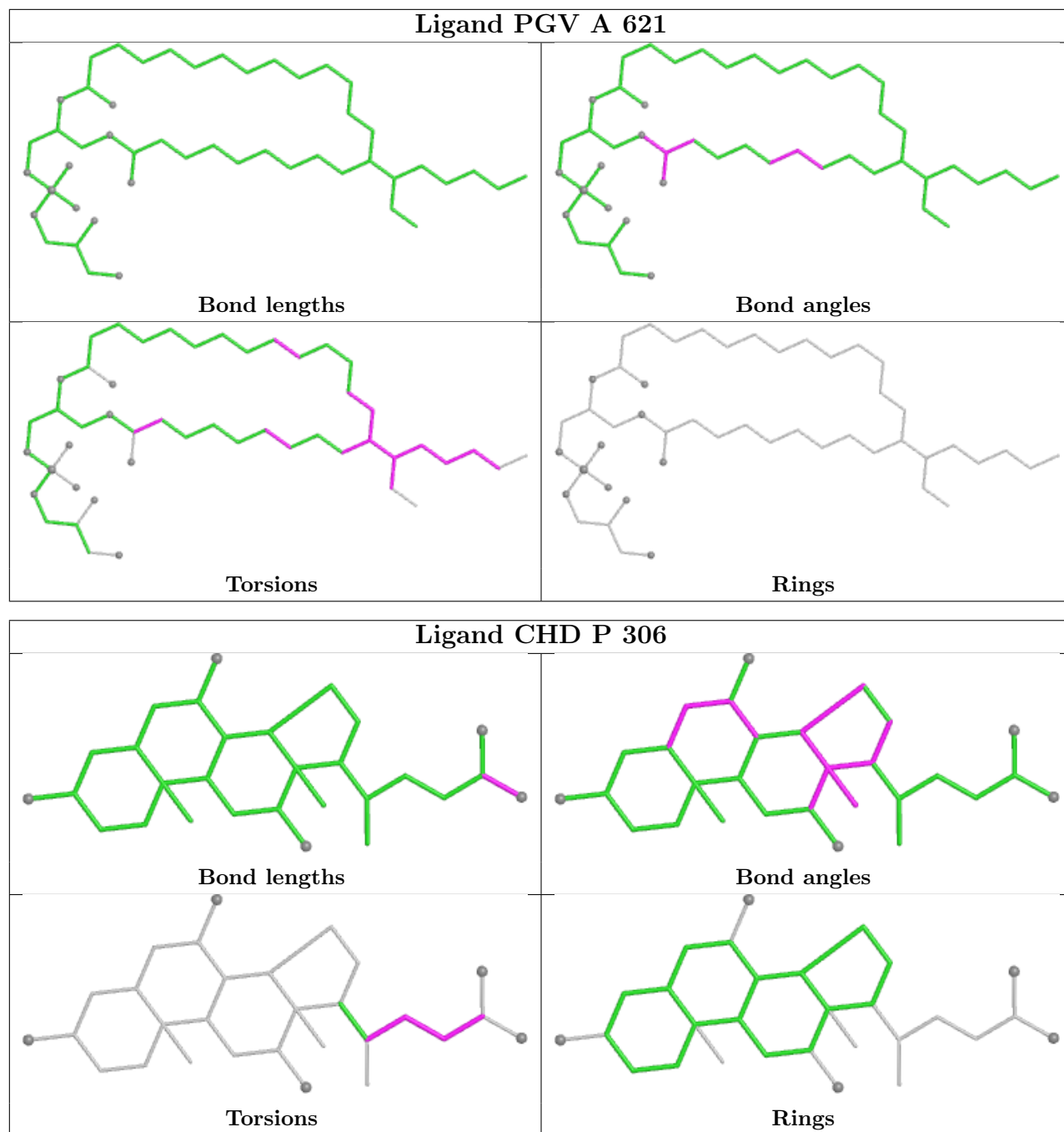


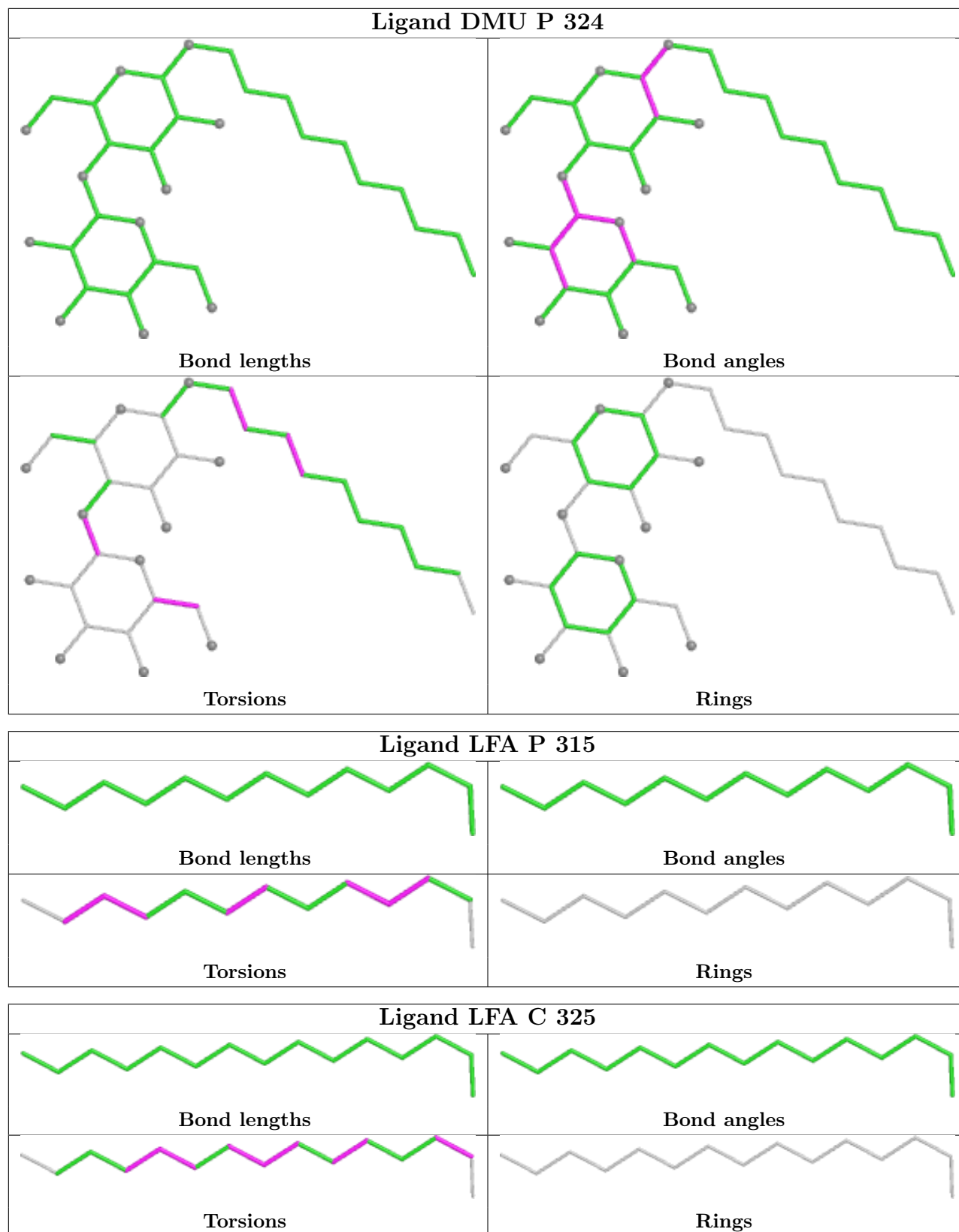


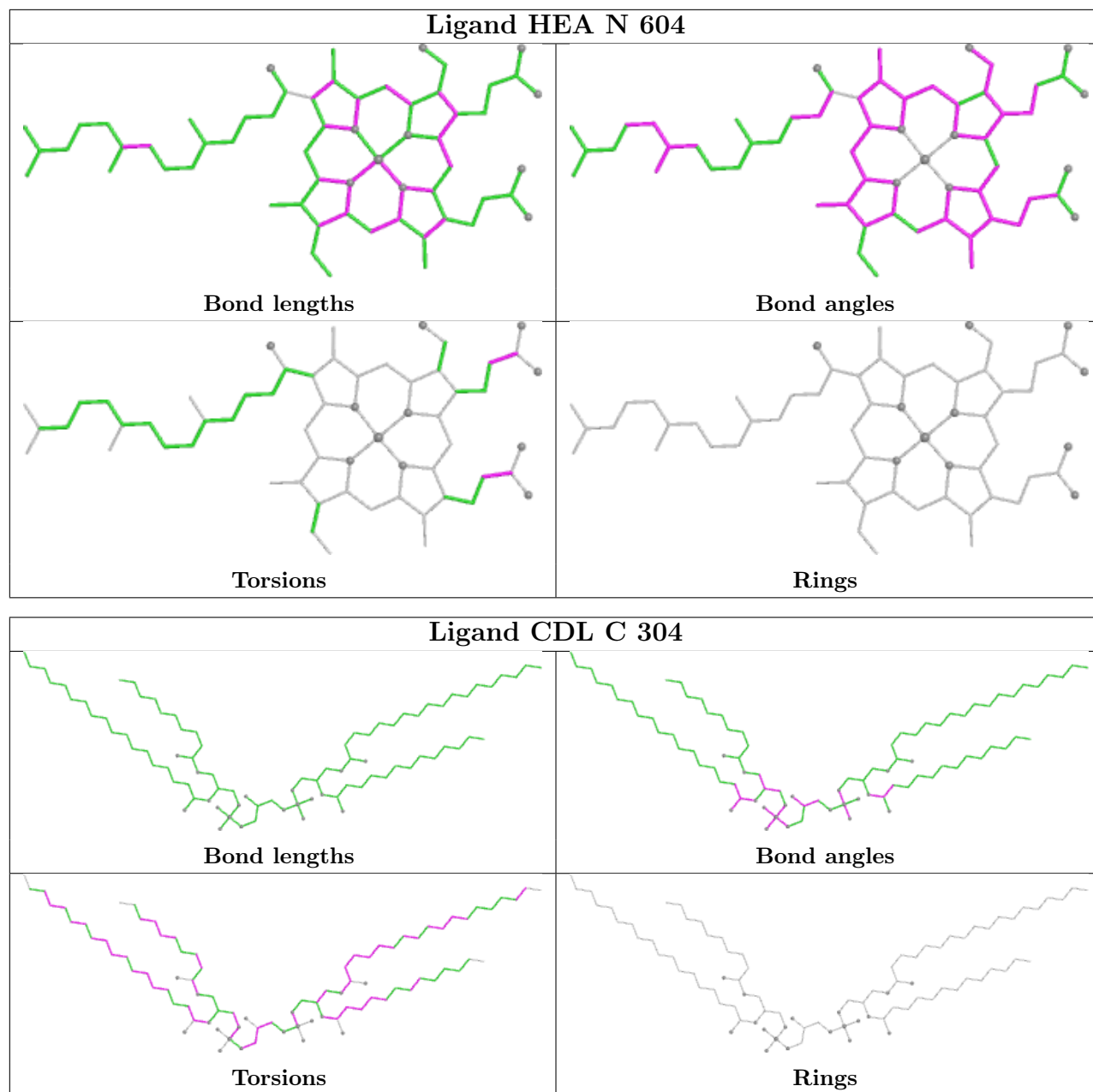


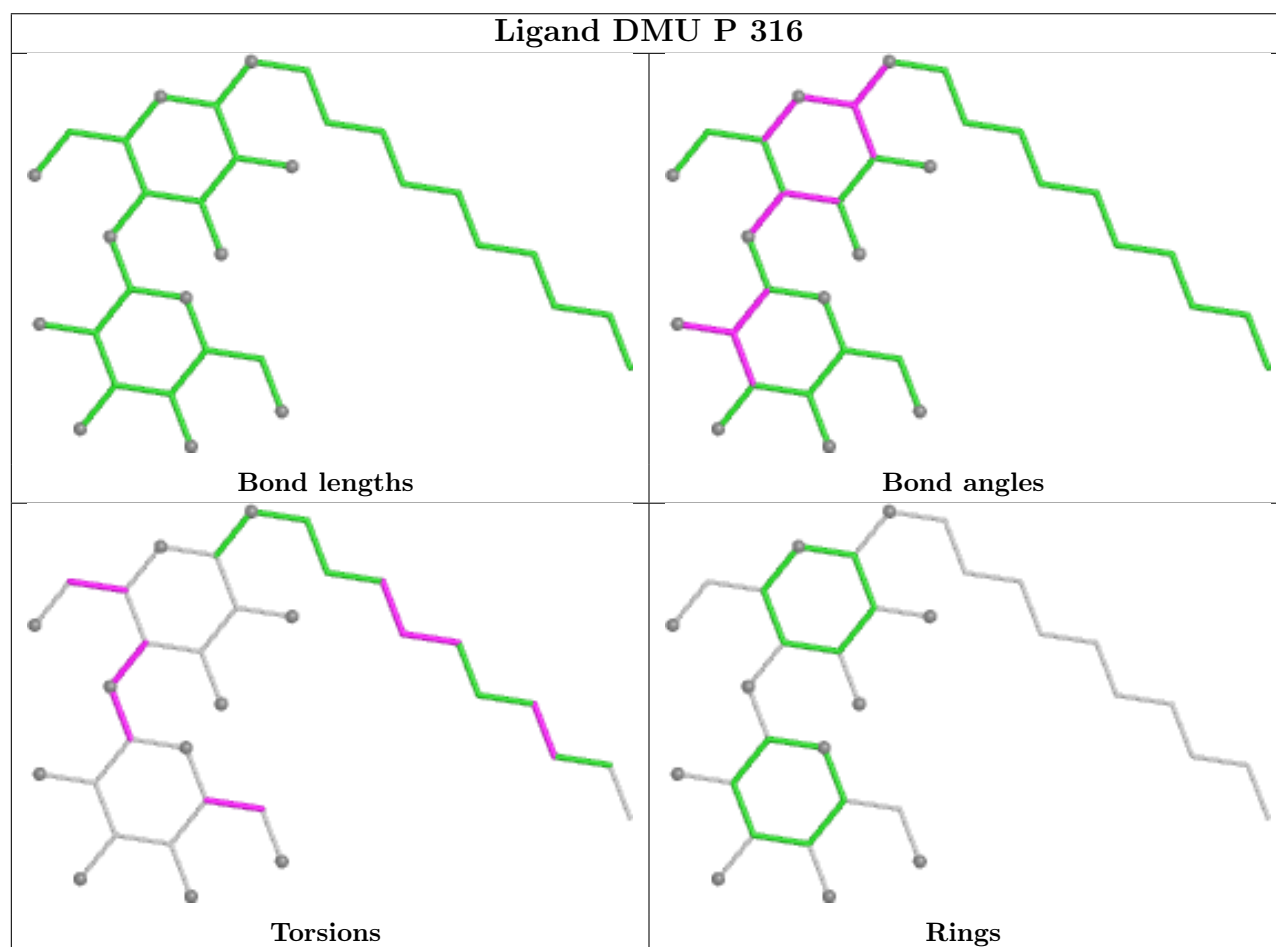
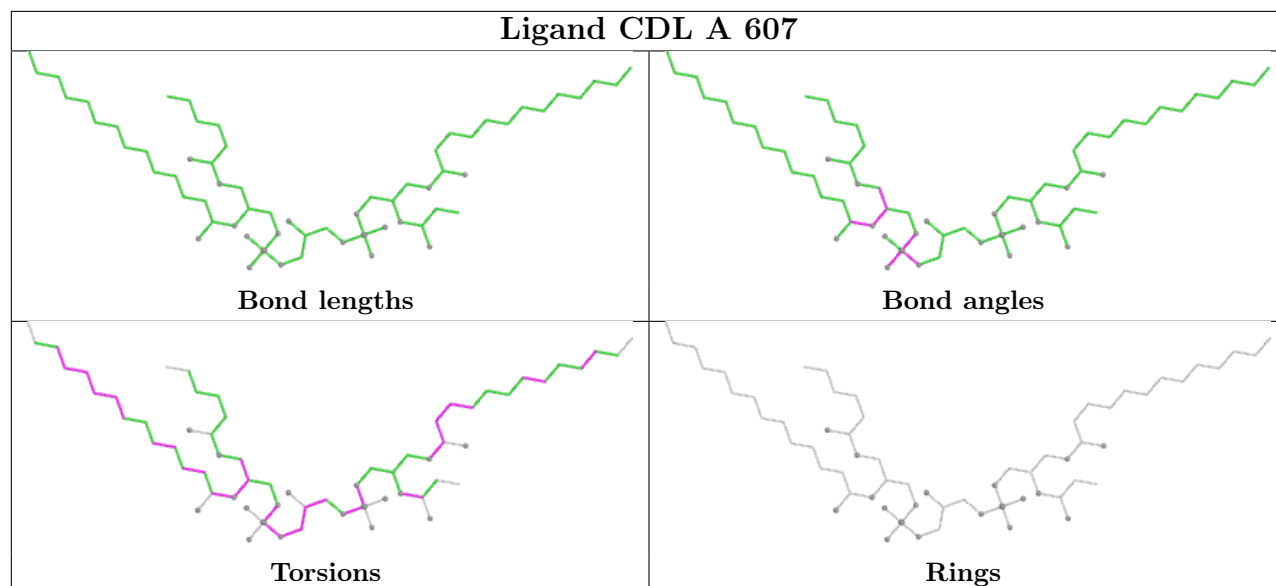


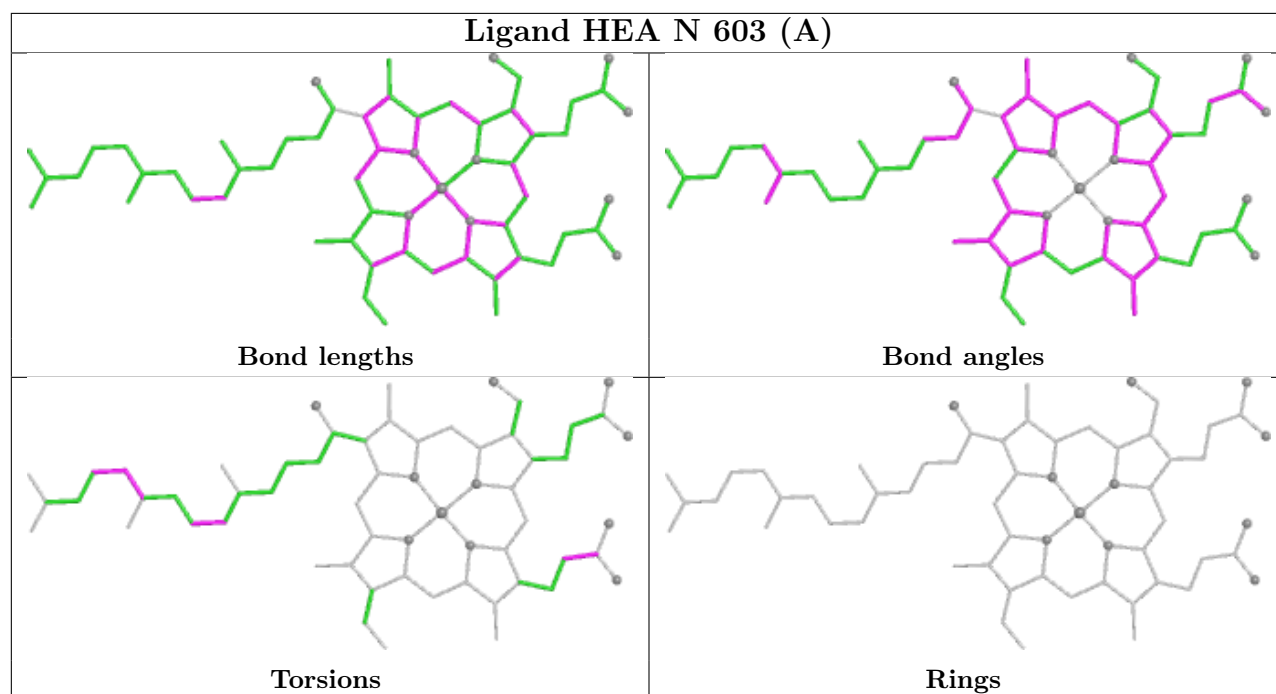
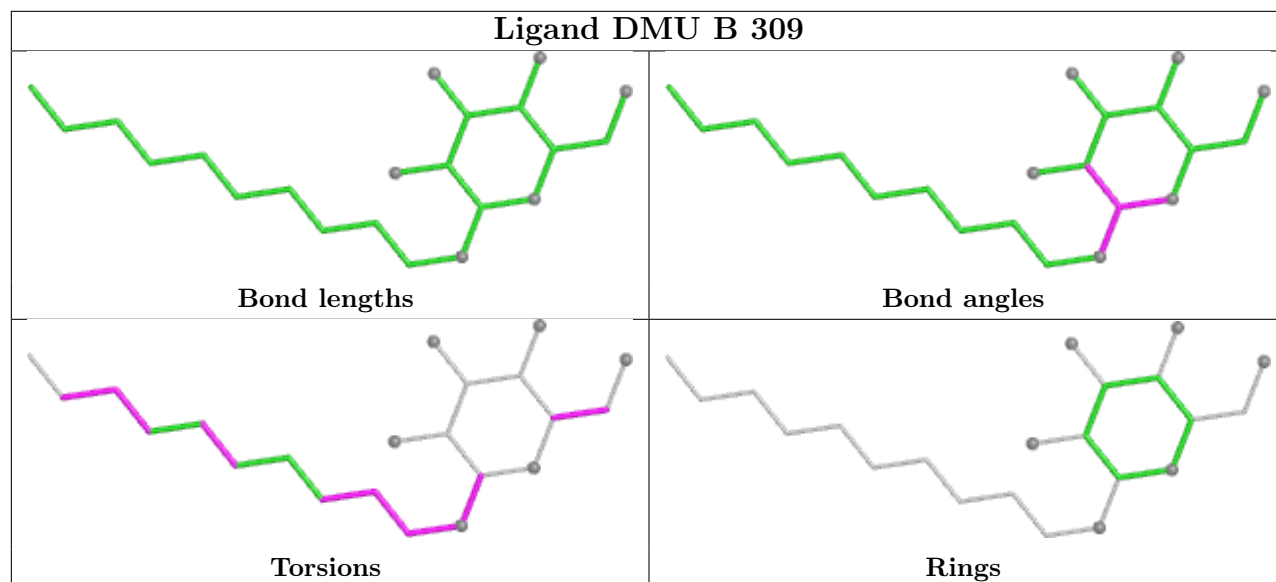


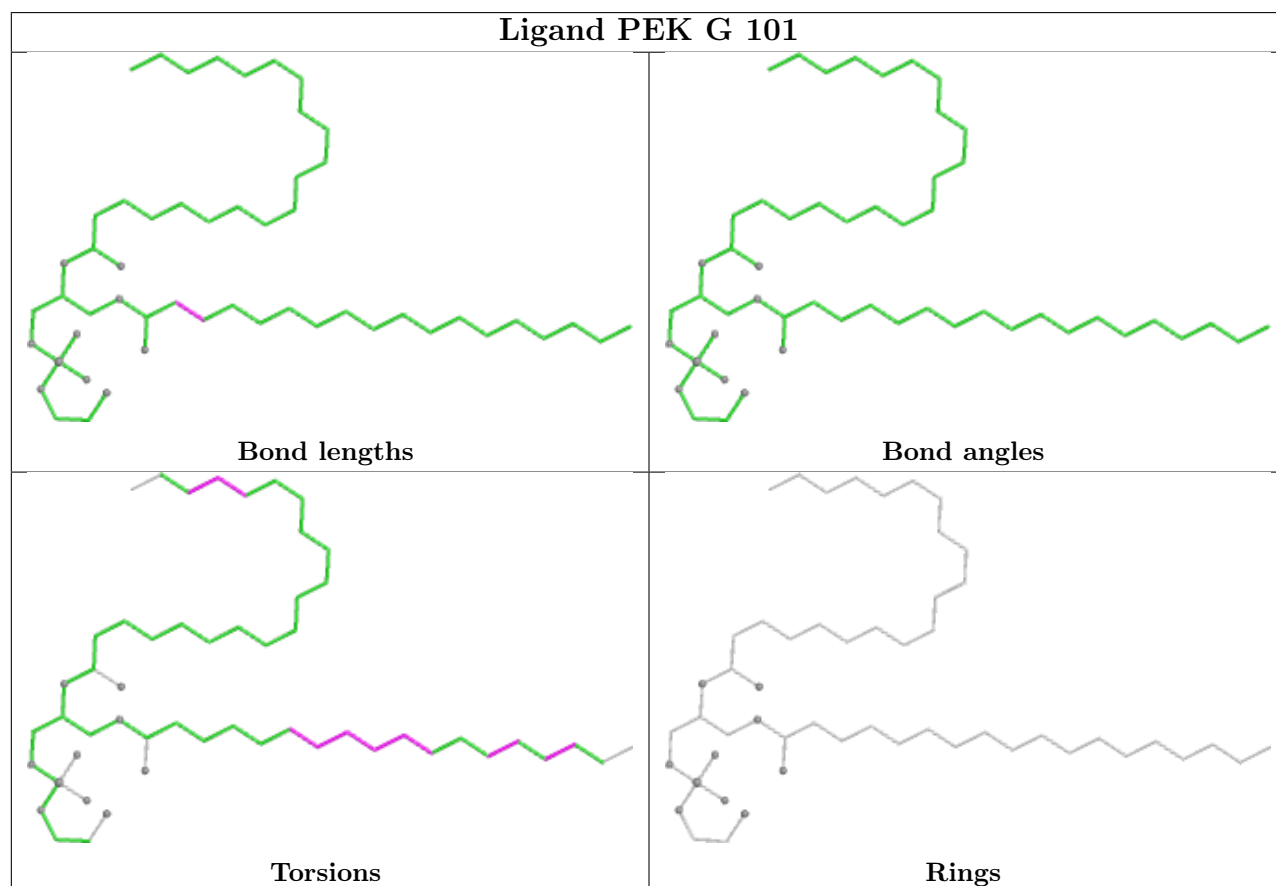
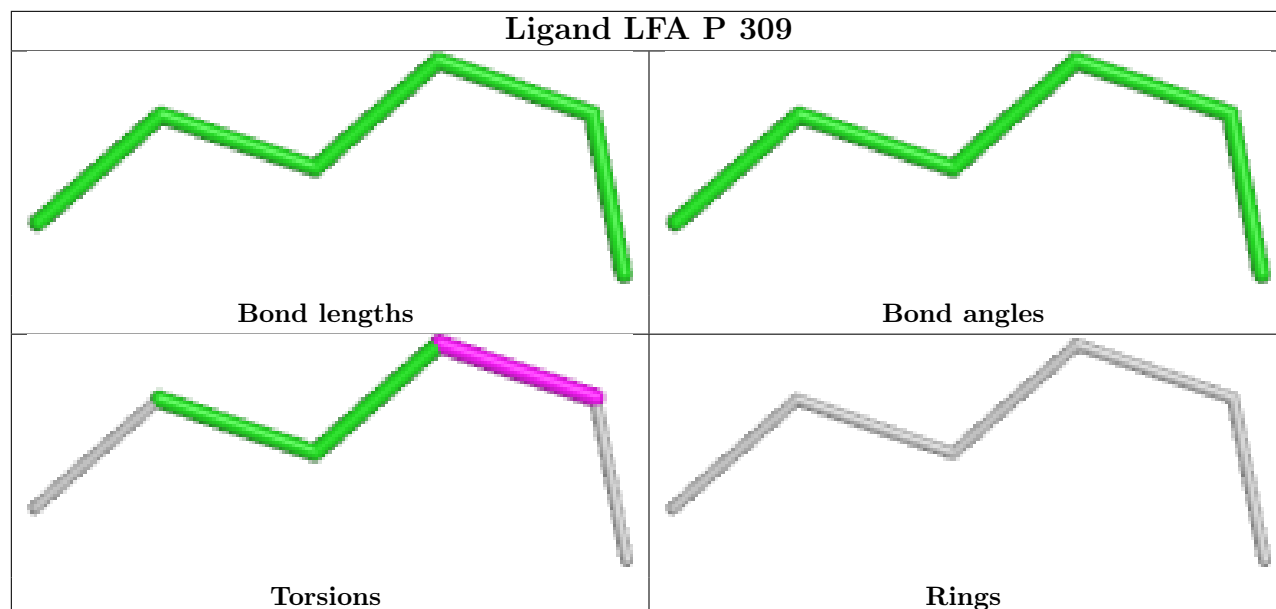


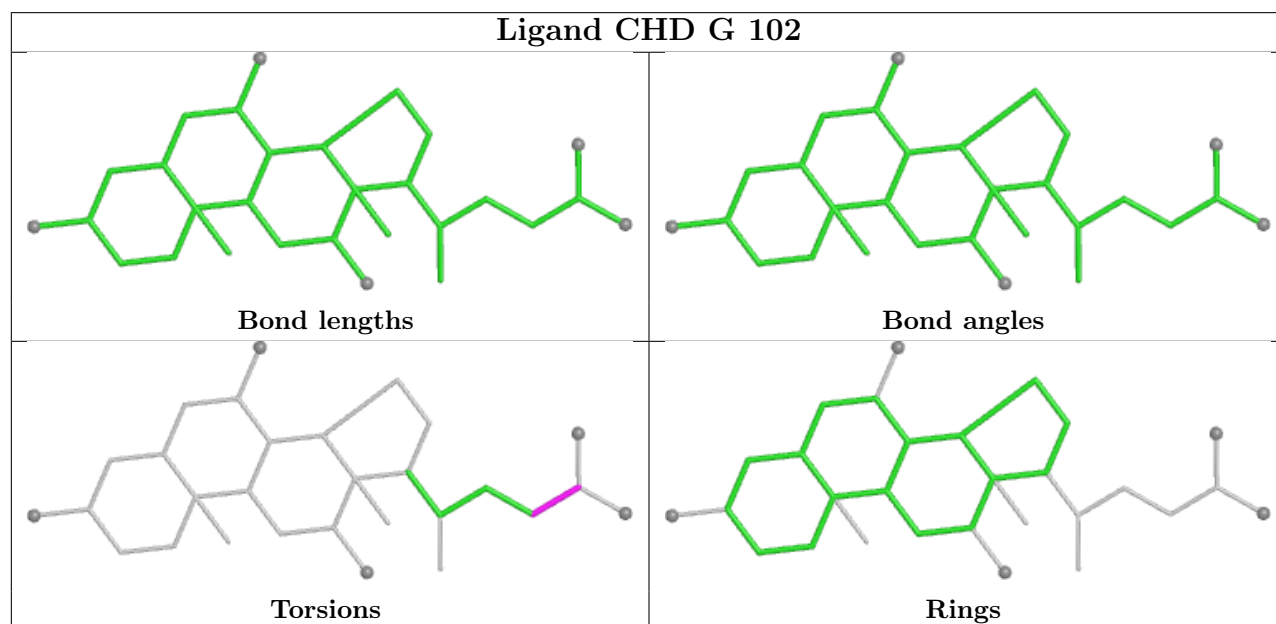
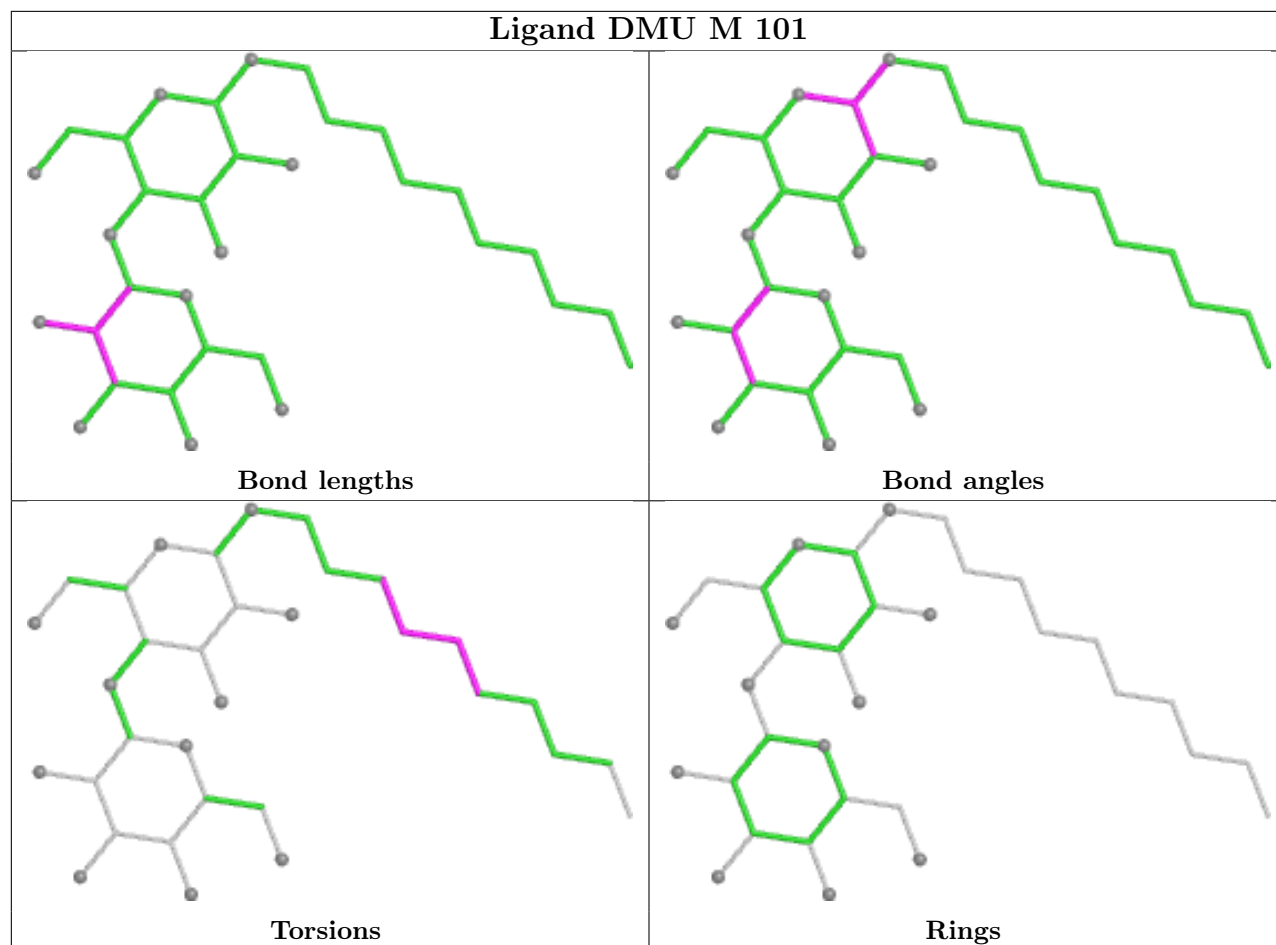


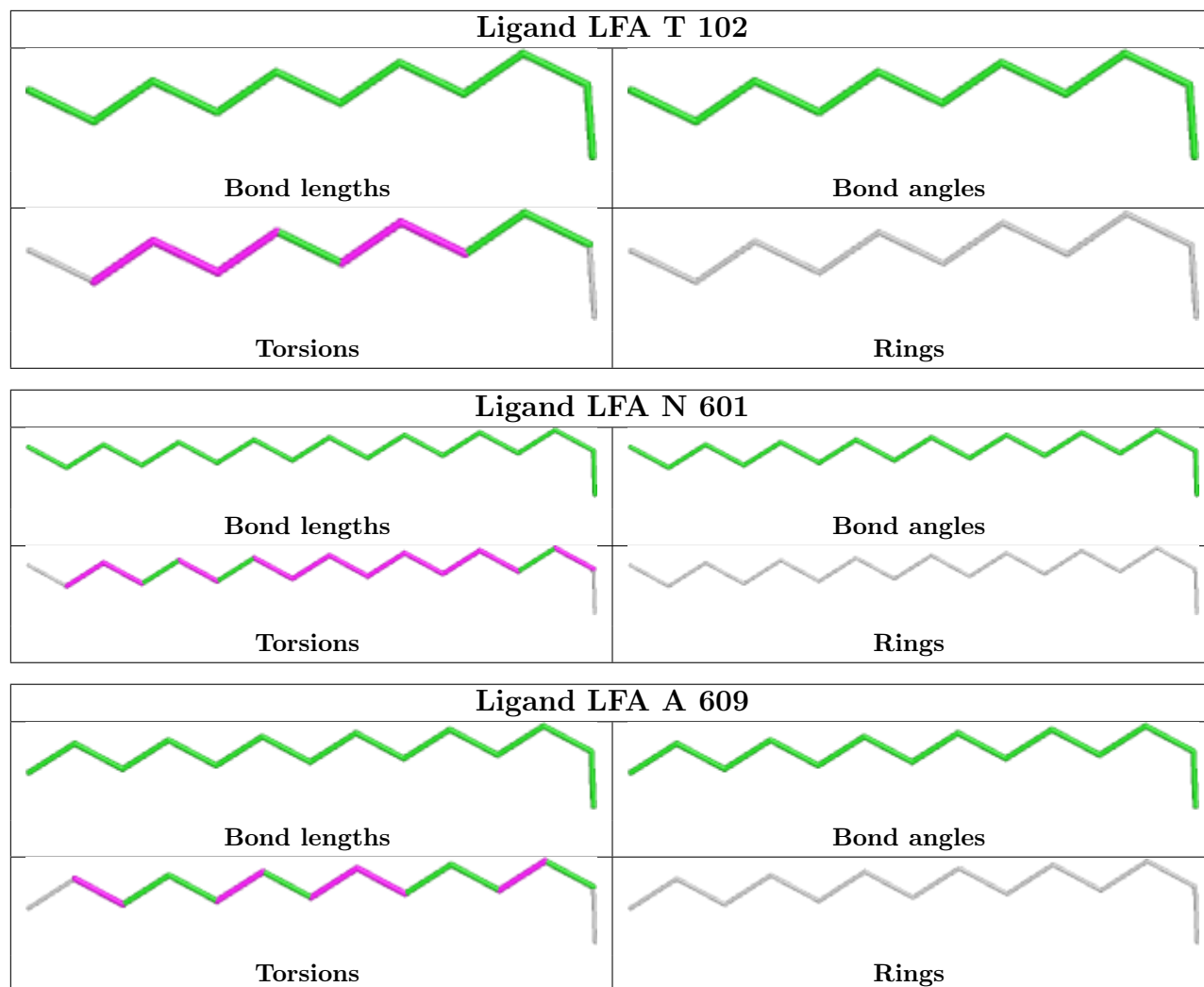


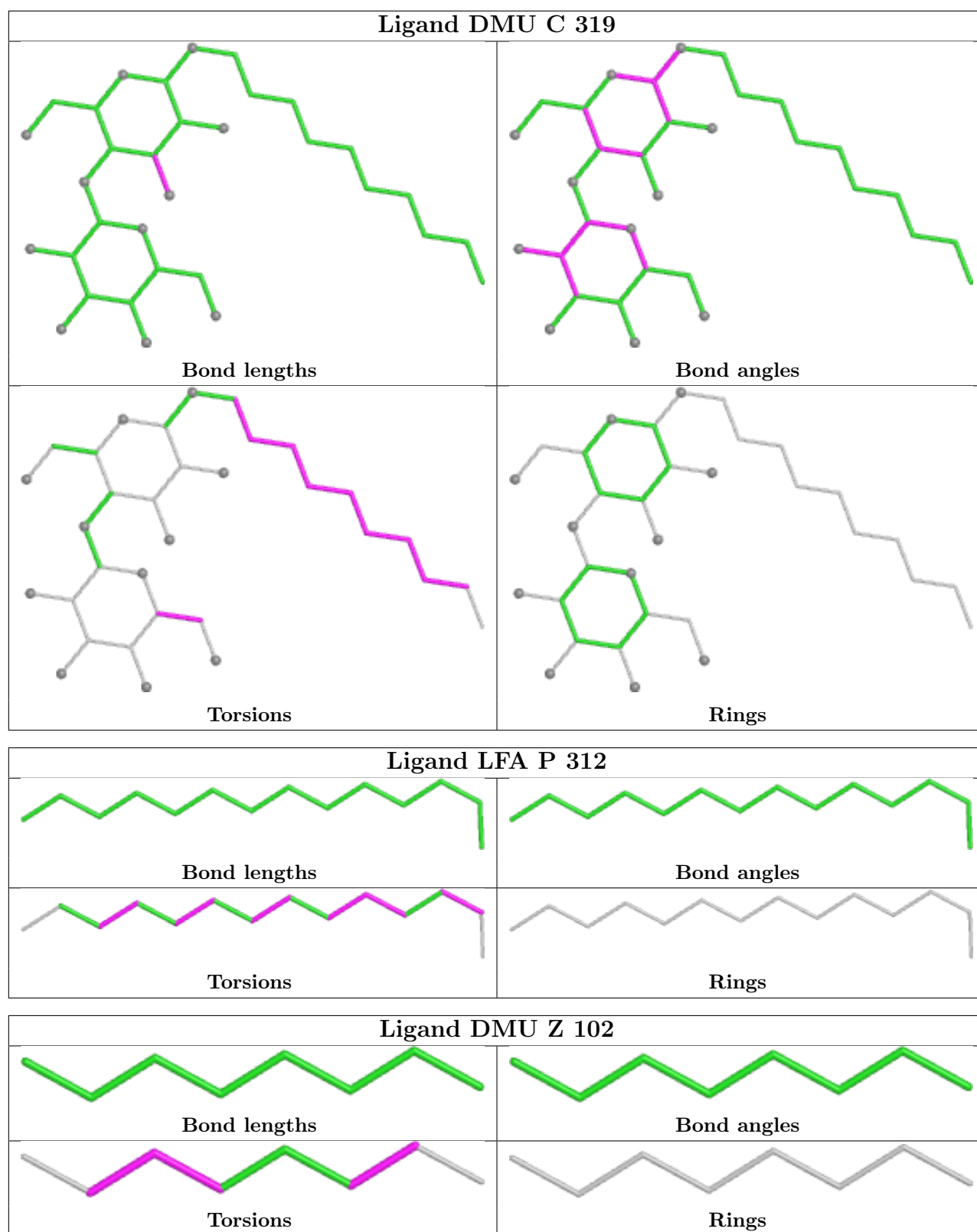


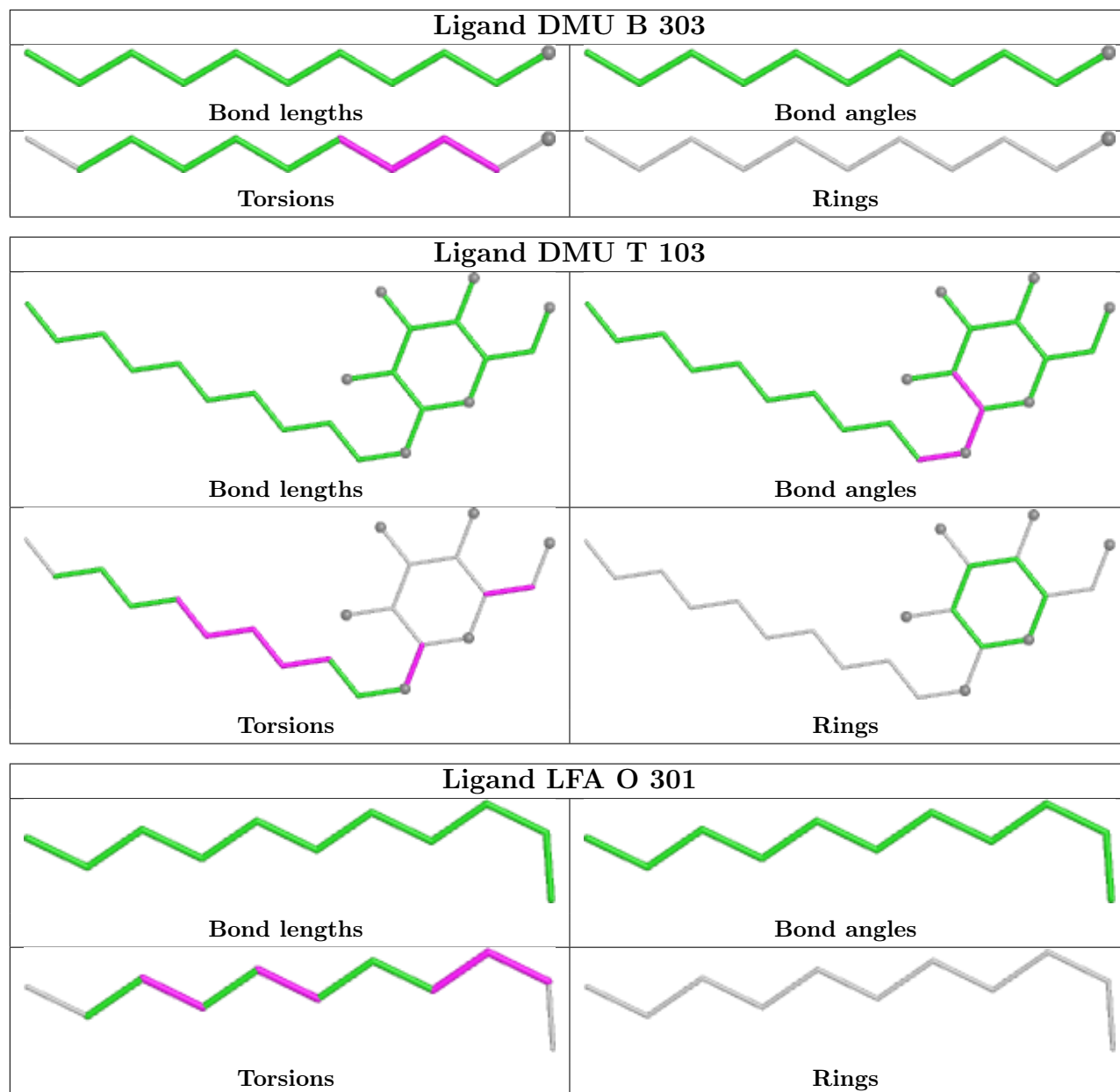


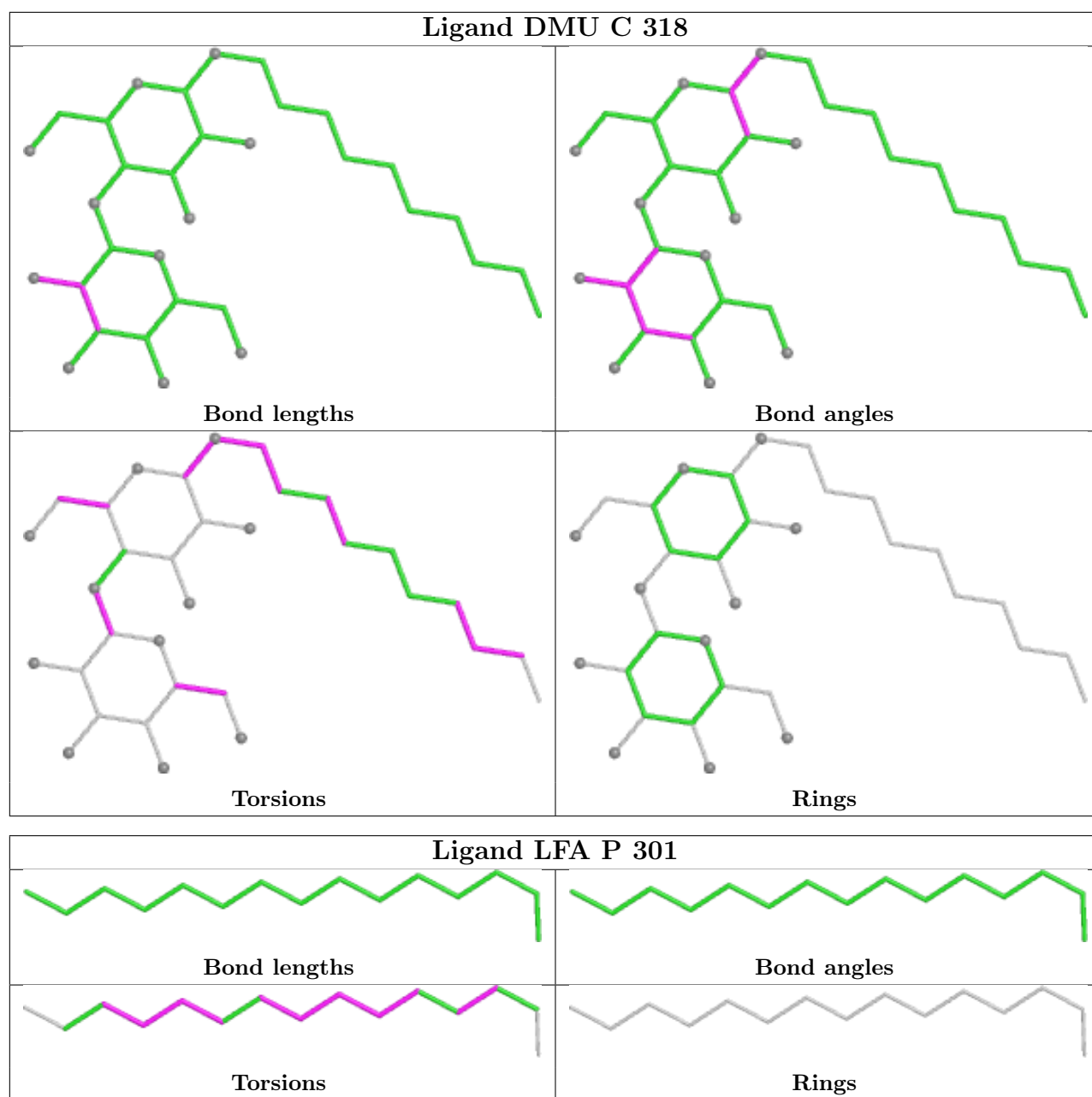


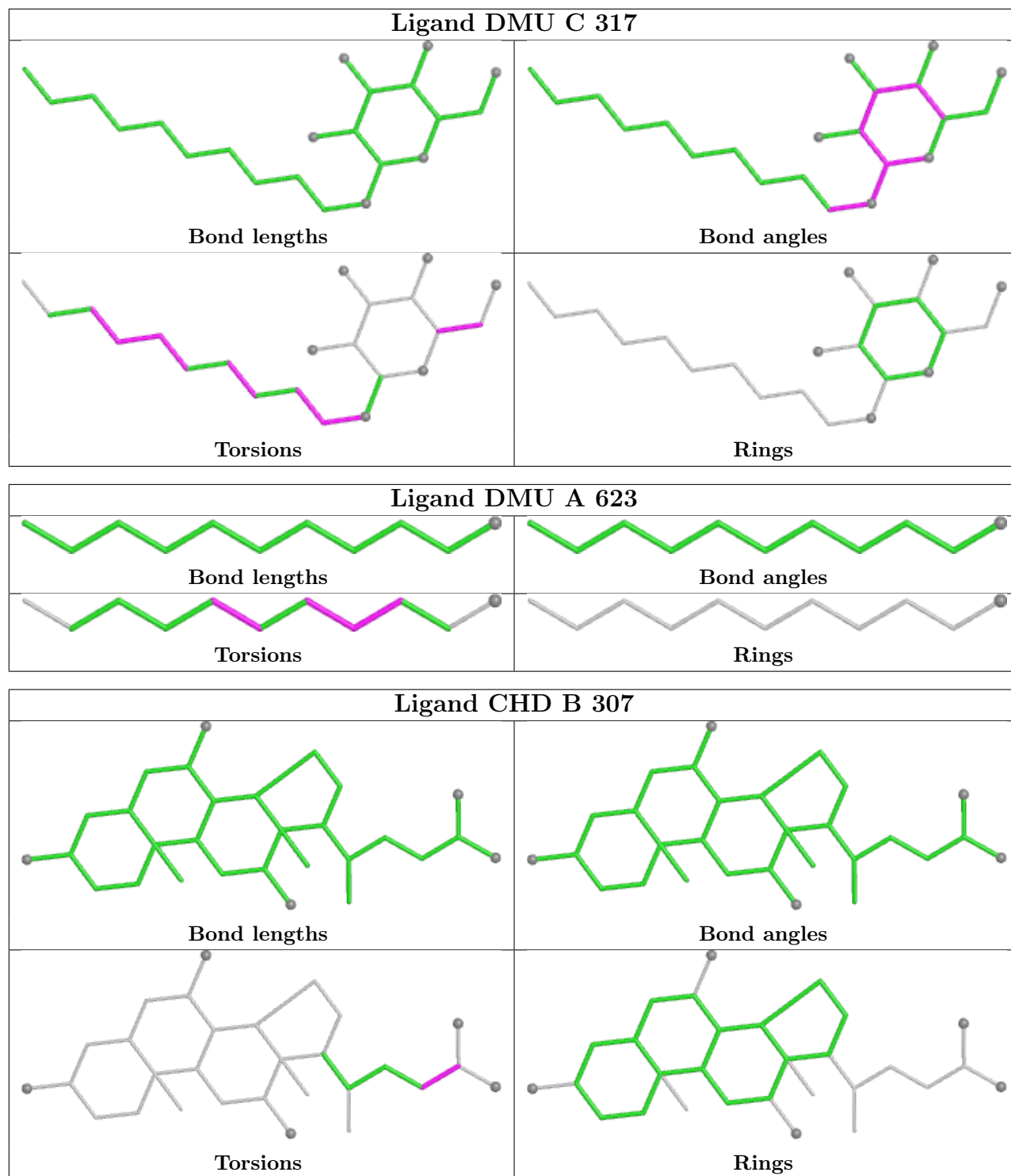


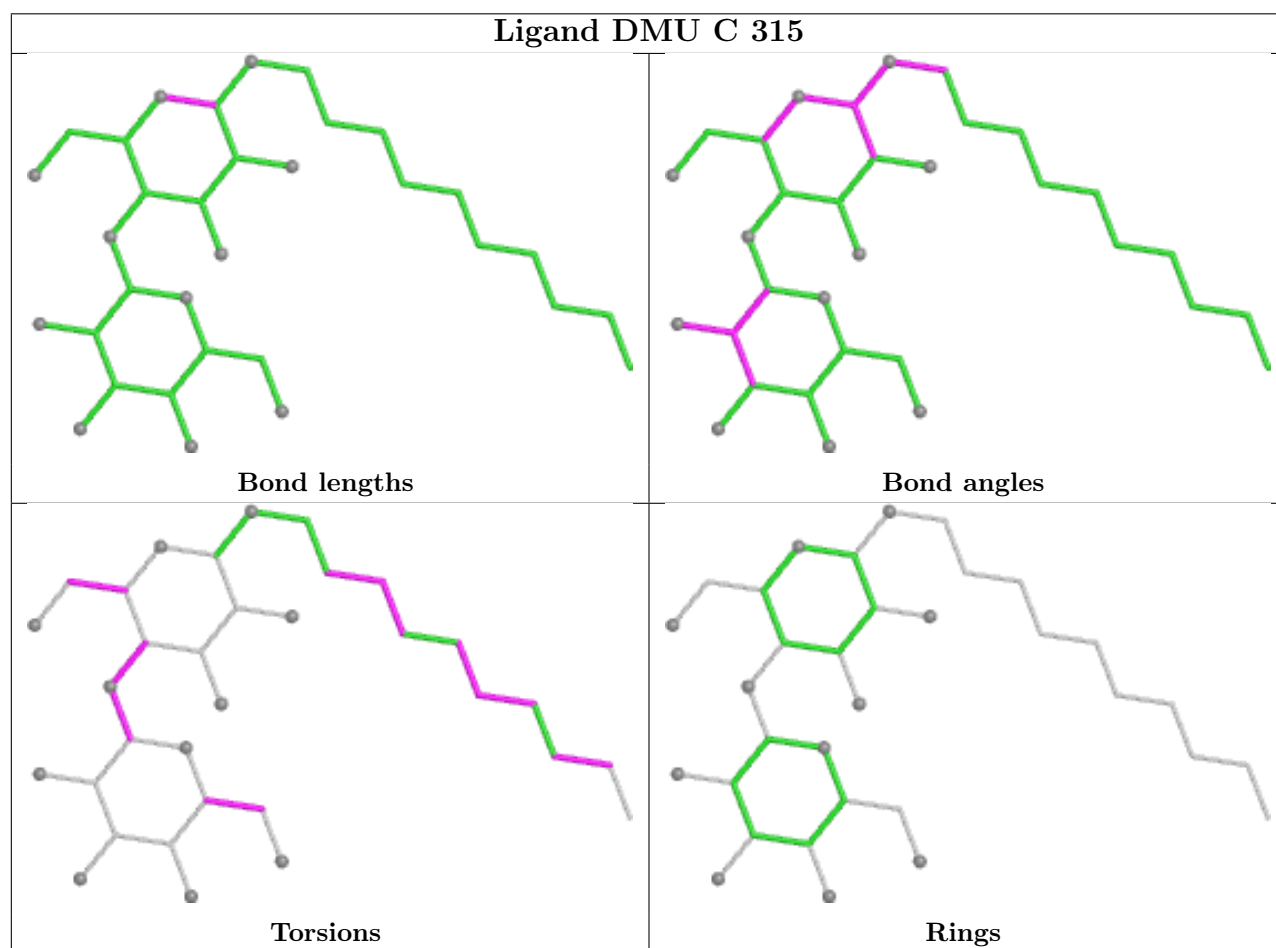
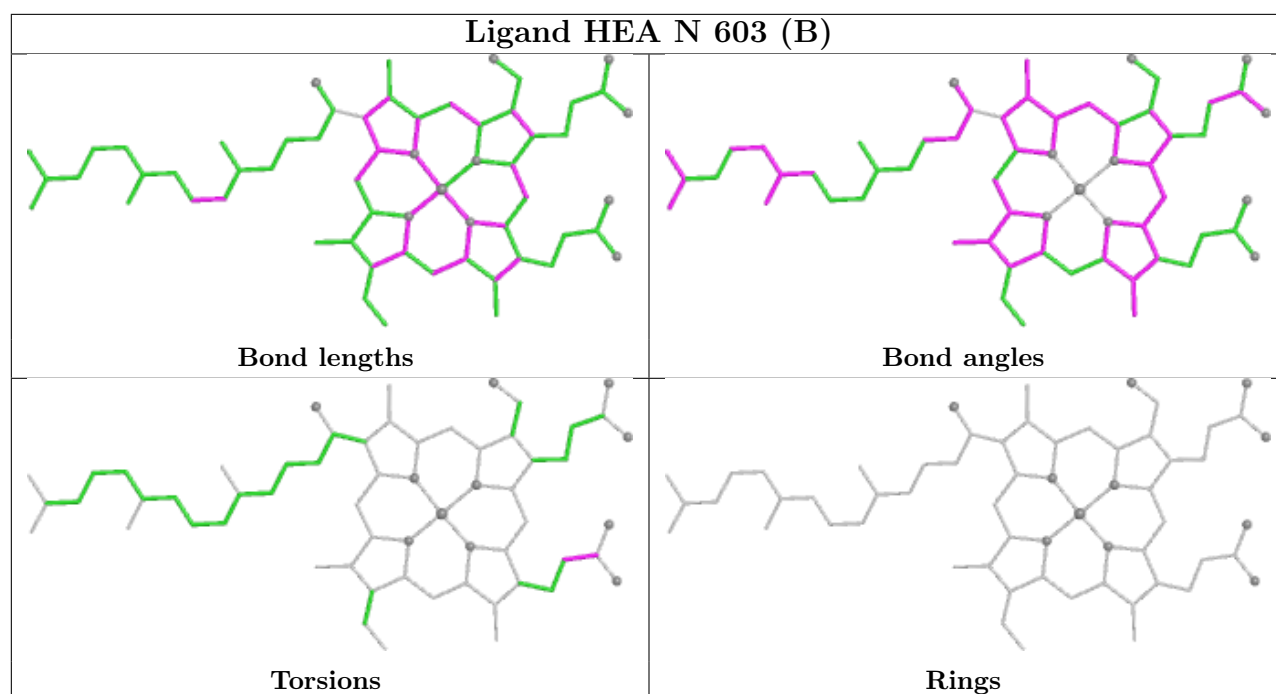


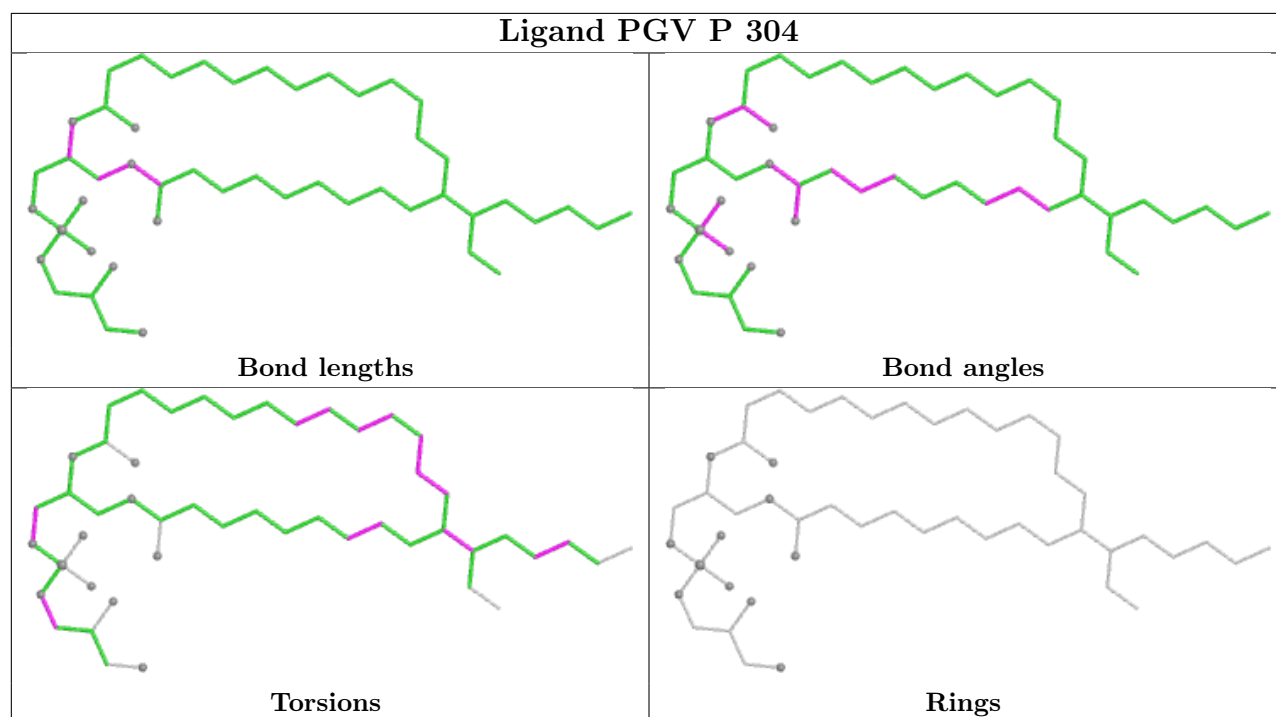
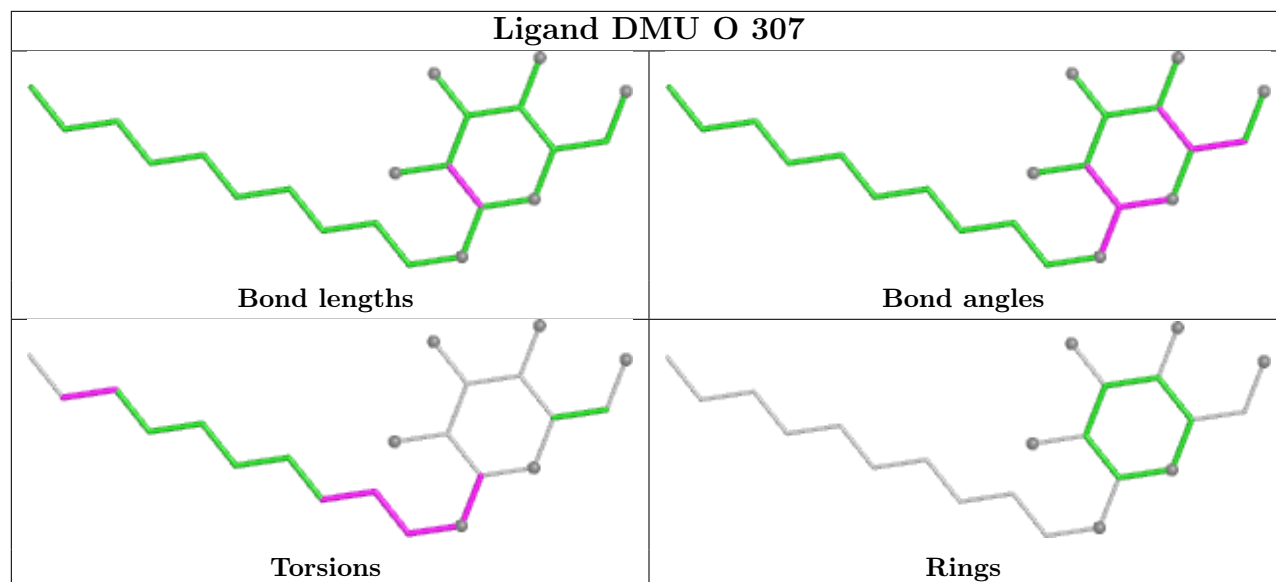


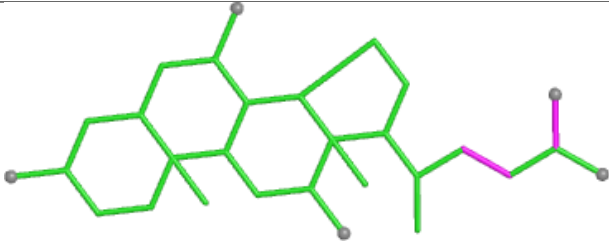
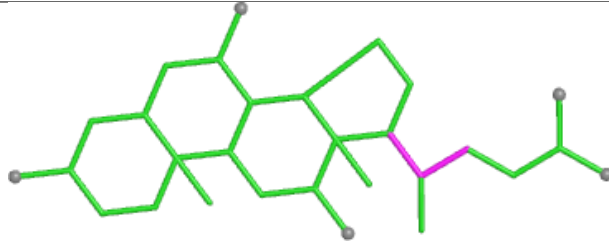
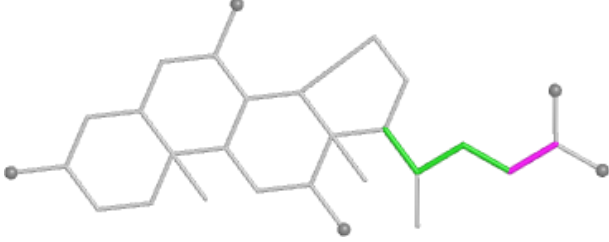
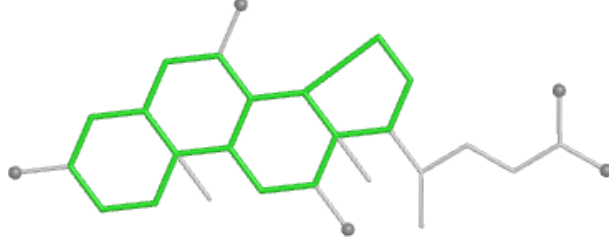


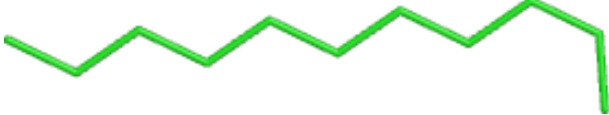
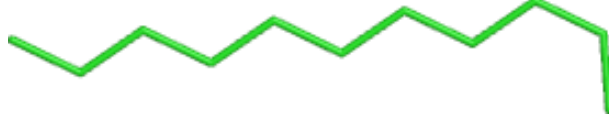
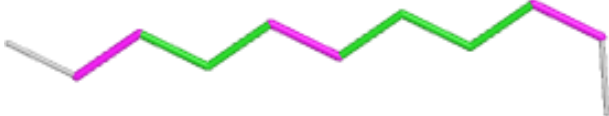
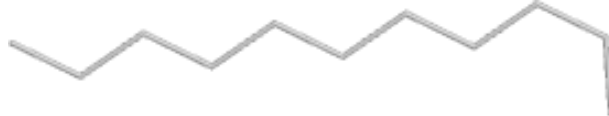


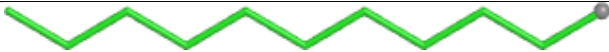
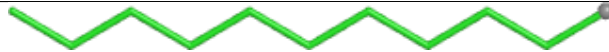


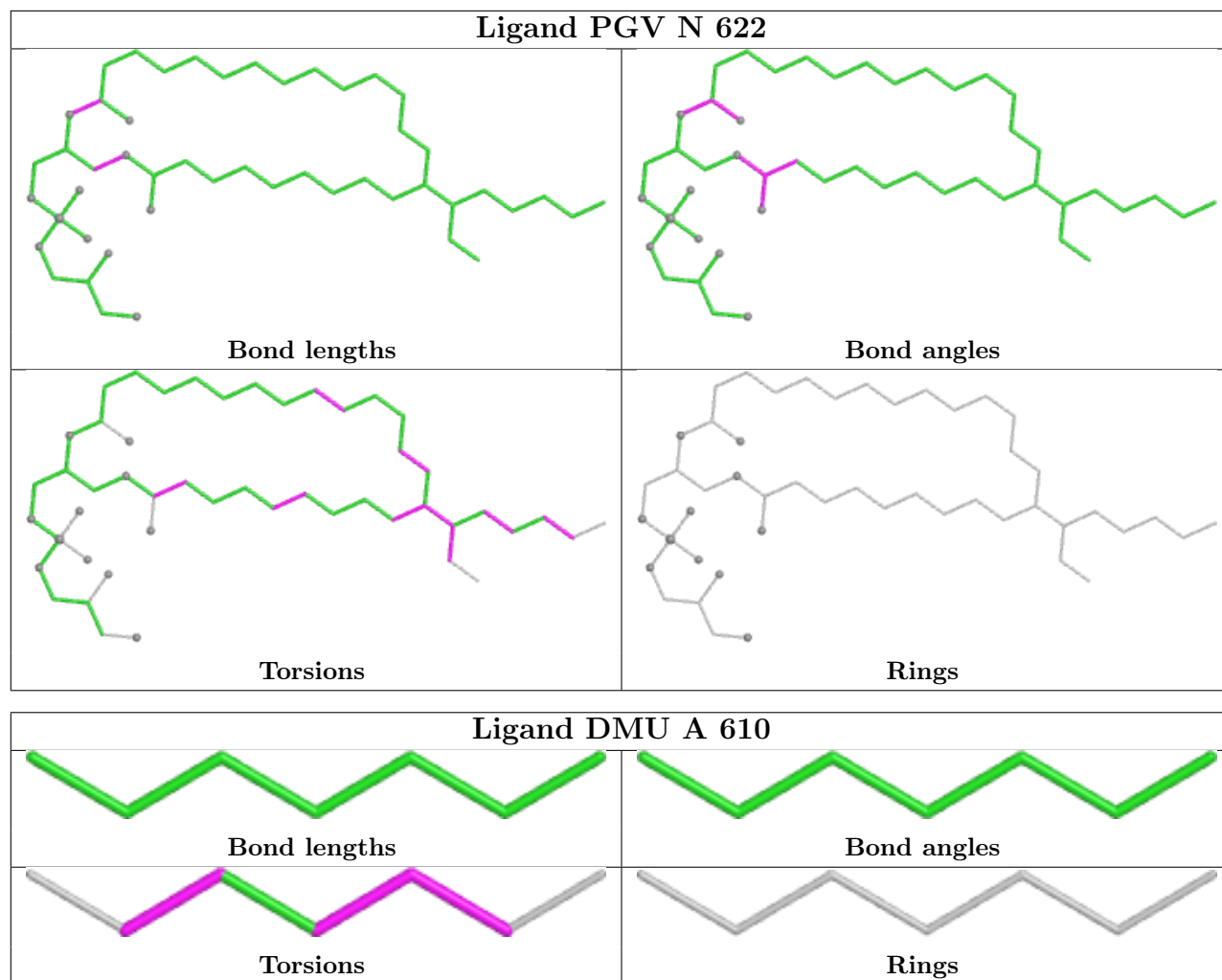


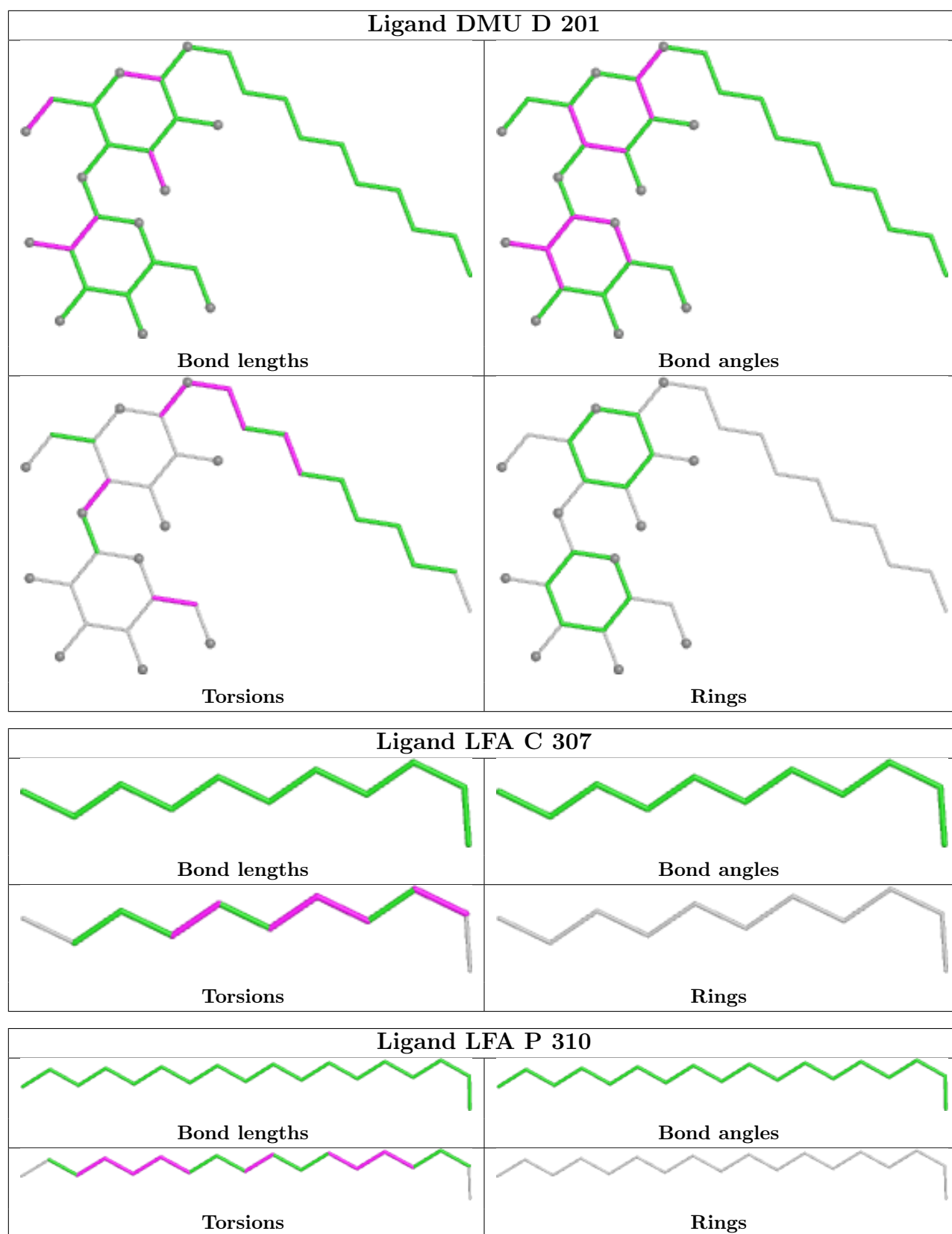


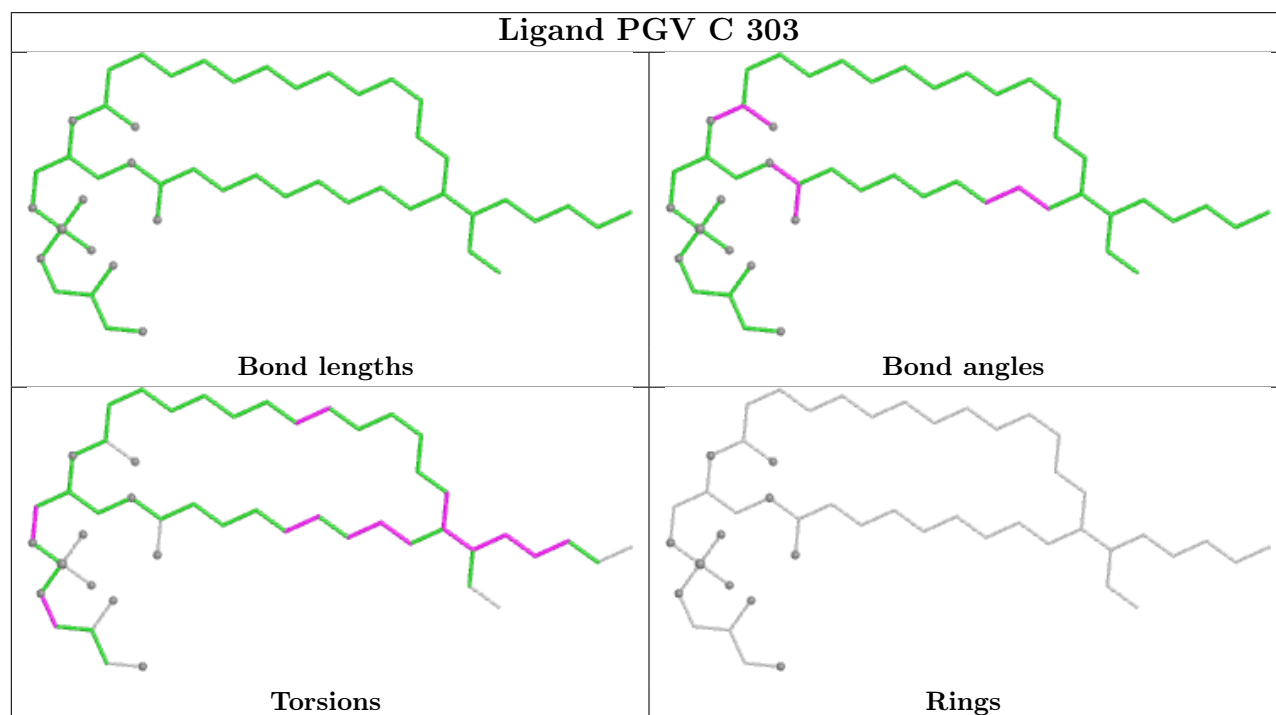
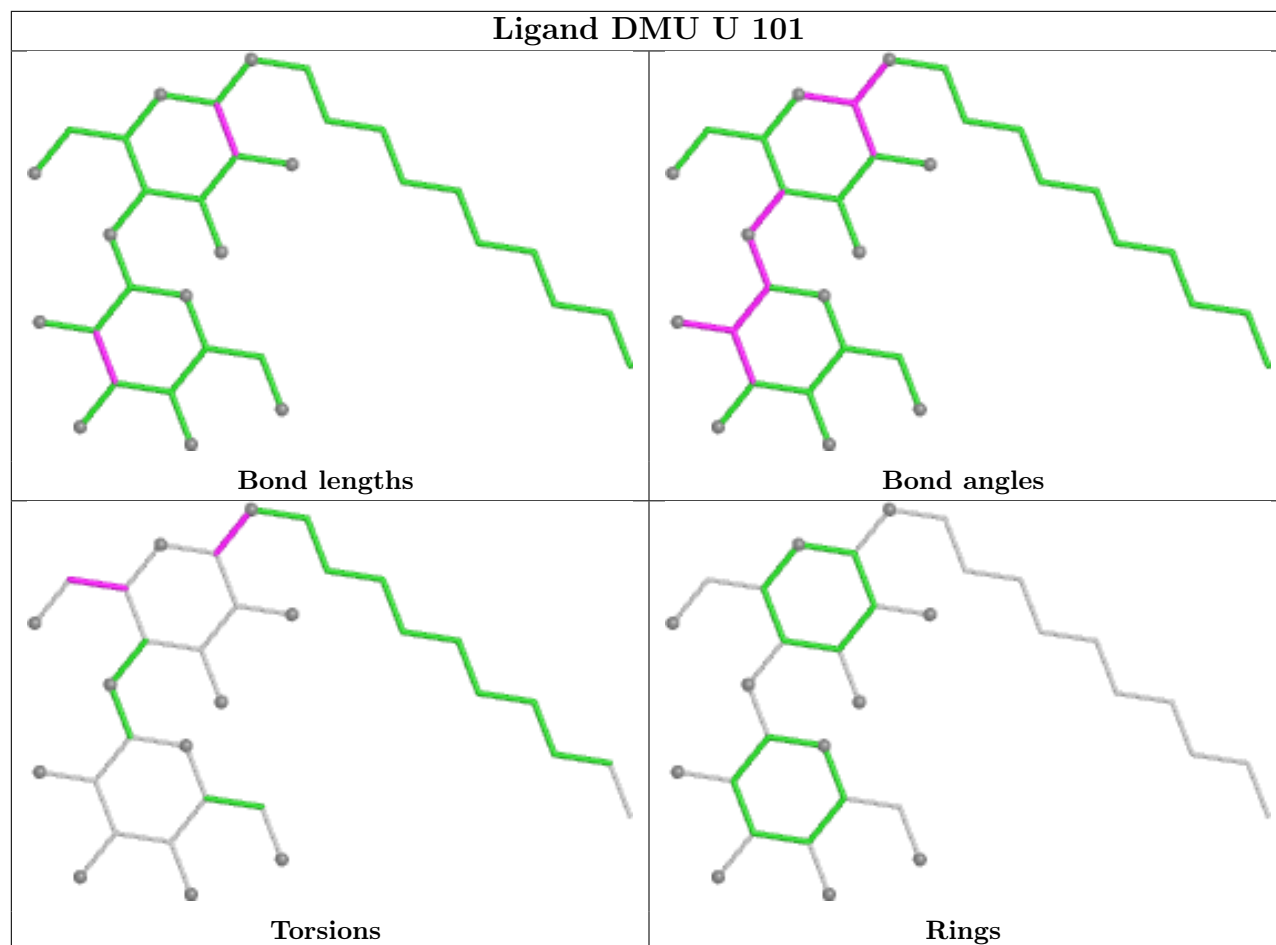
Ligand CHD C 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

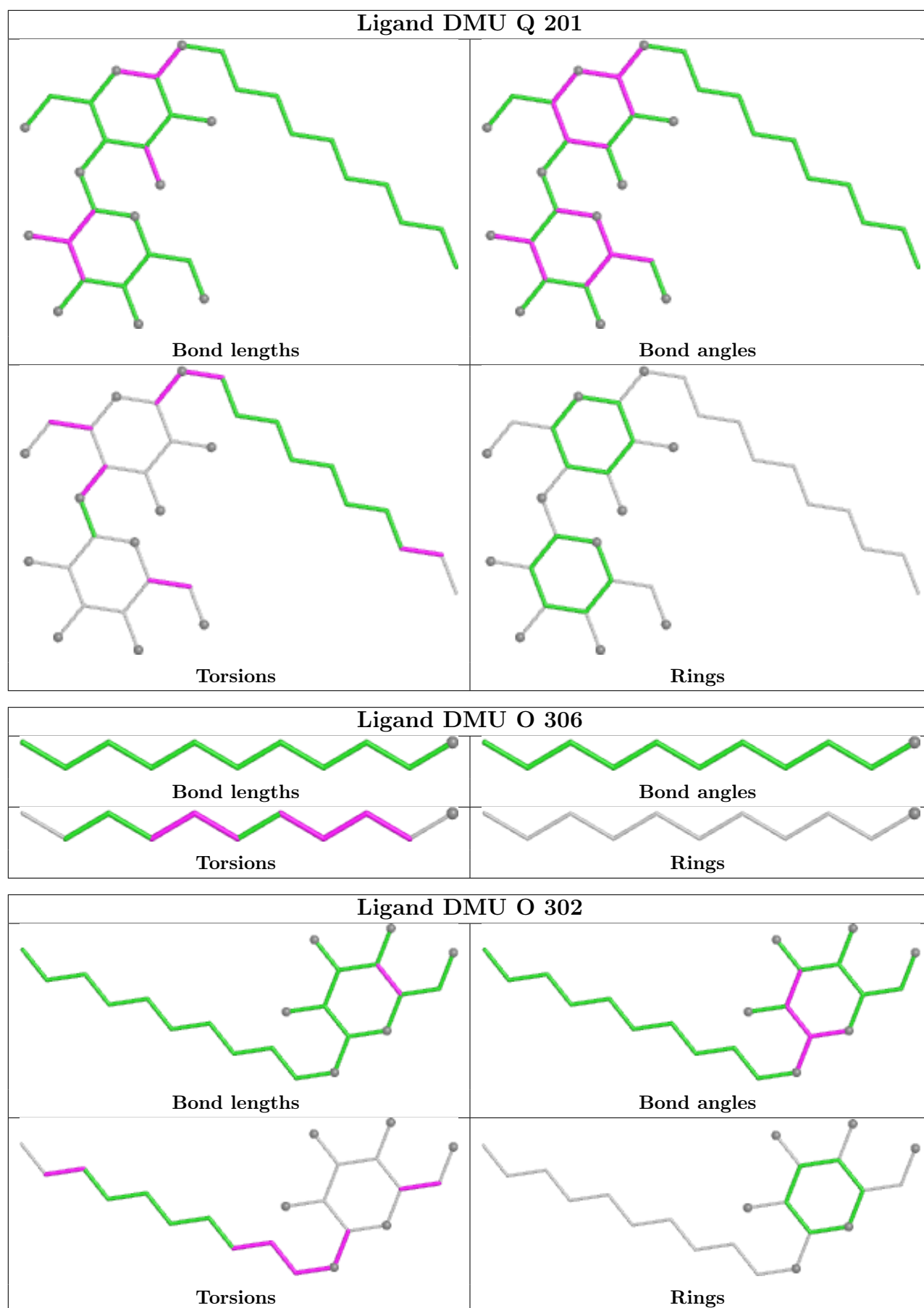
Ligand LFA C 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

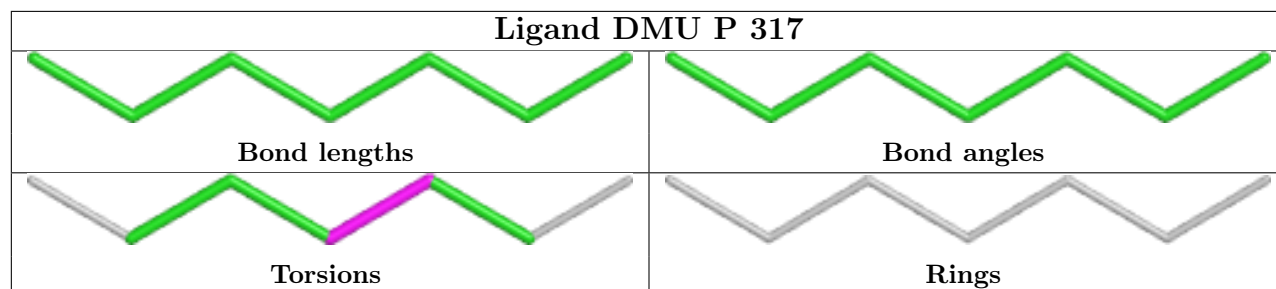
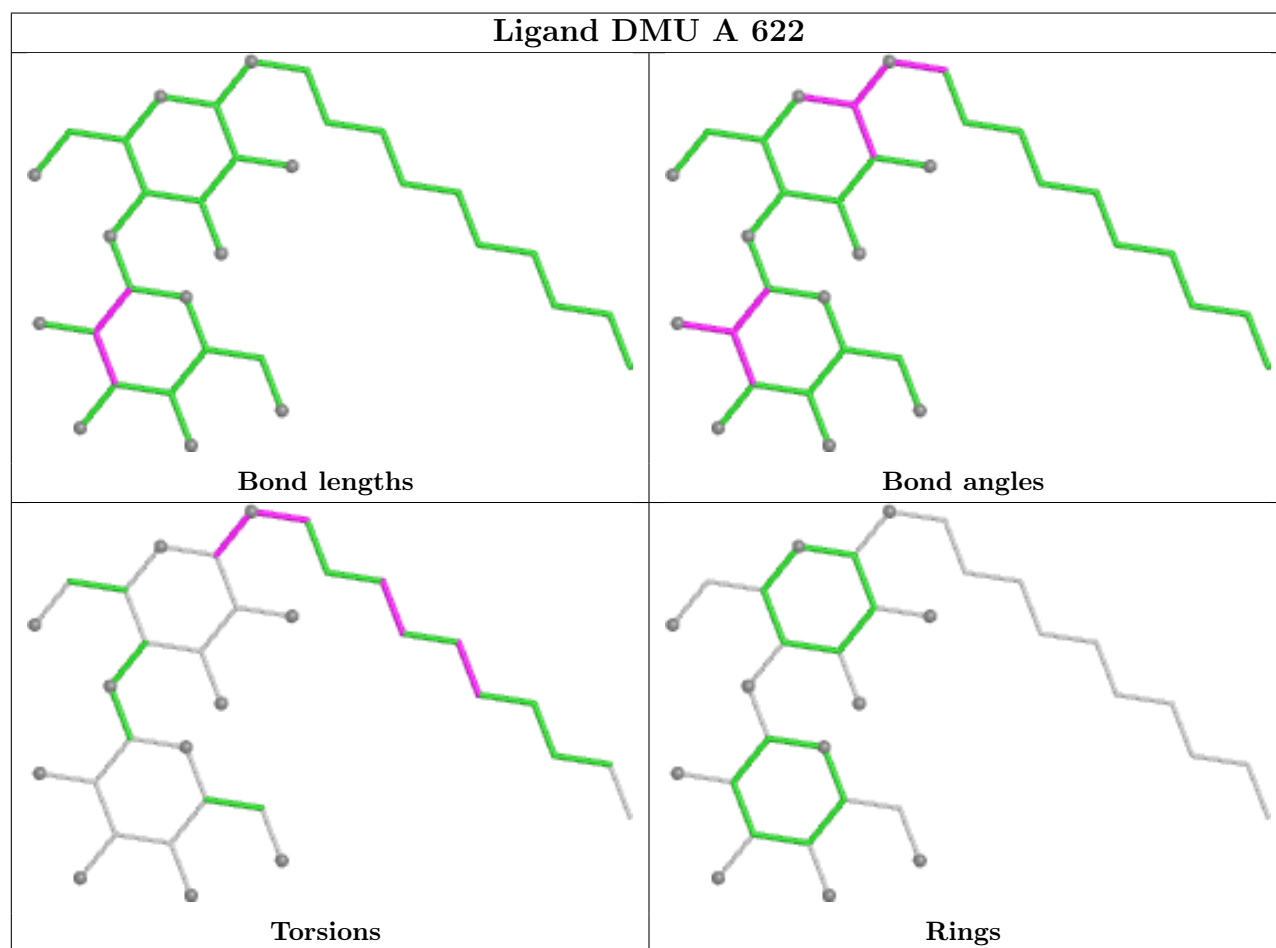
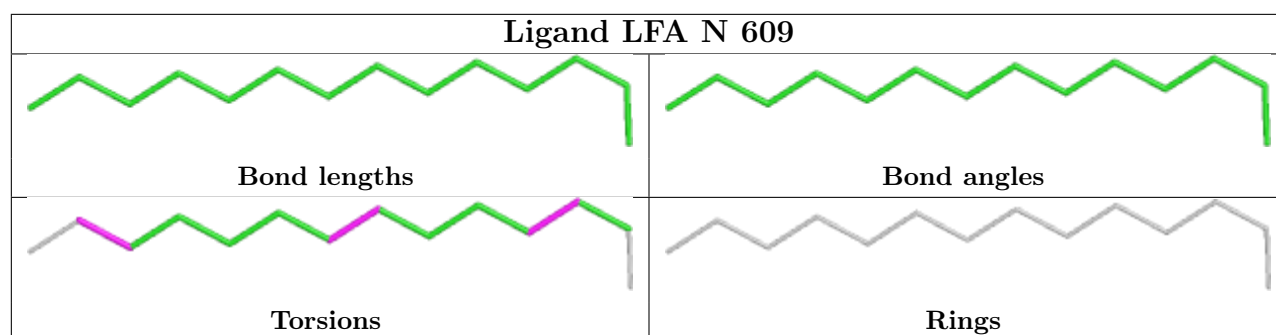
Ligand DMU J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

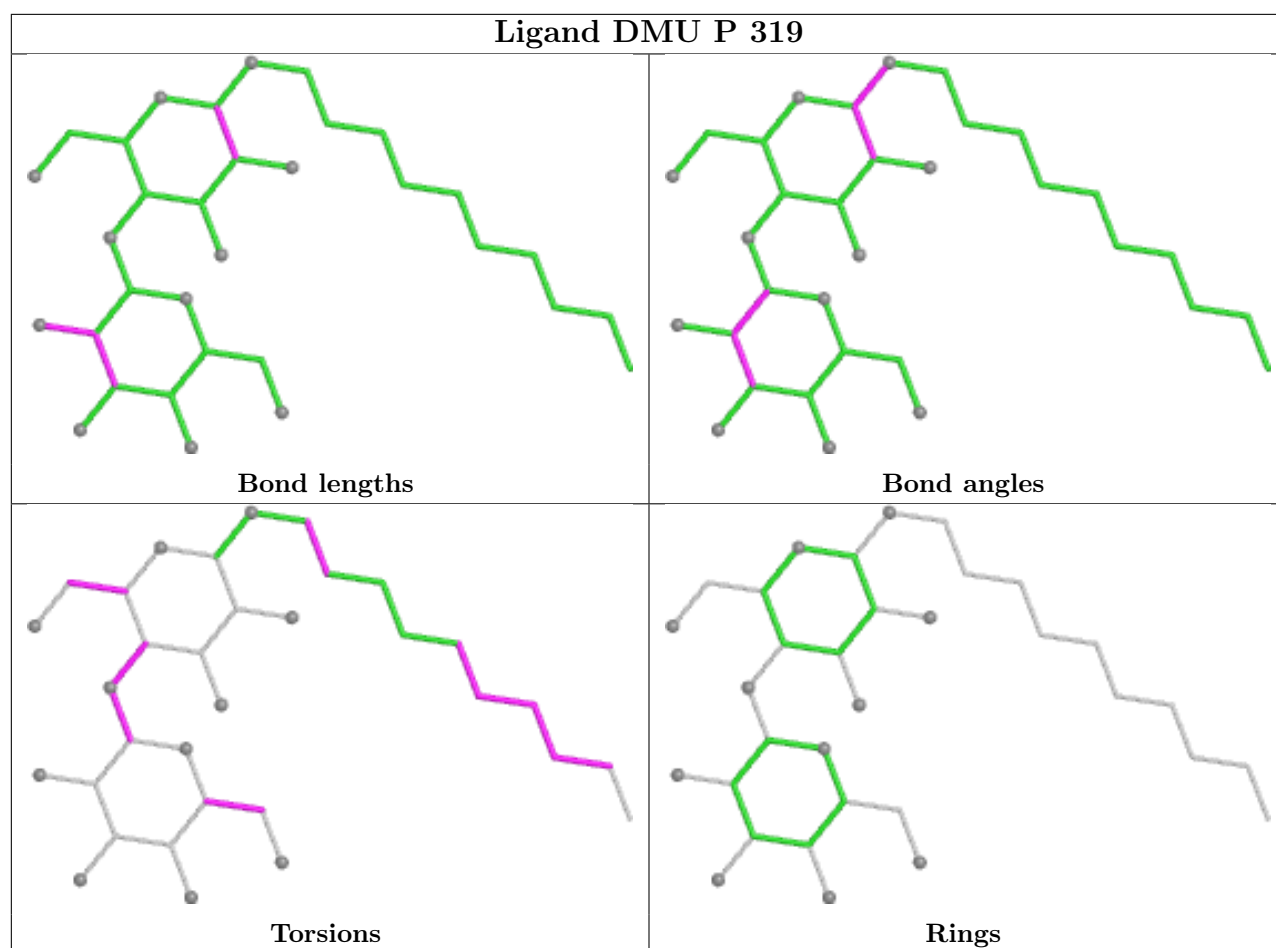


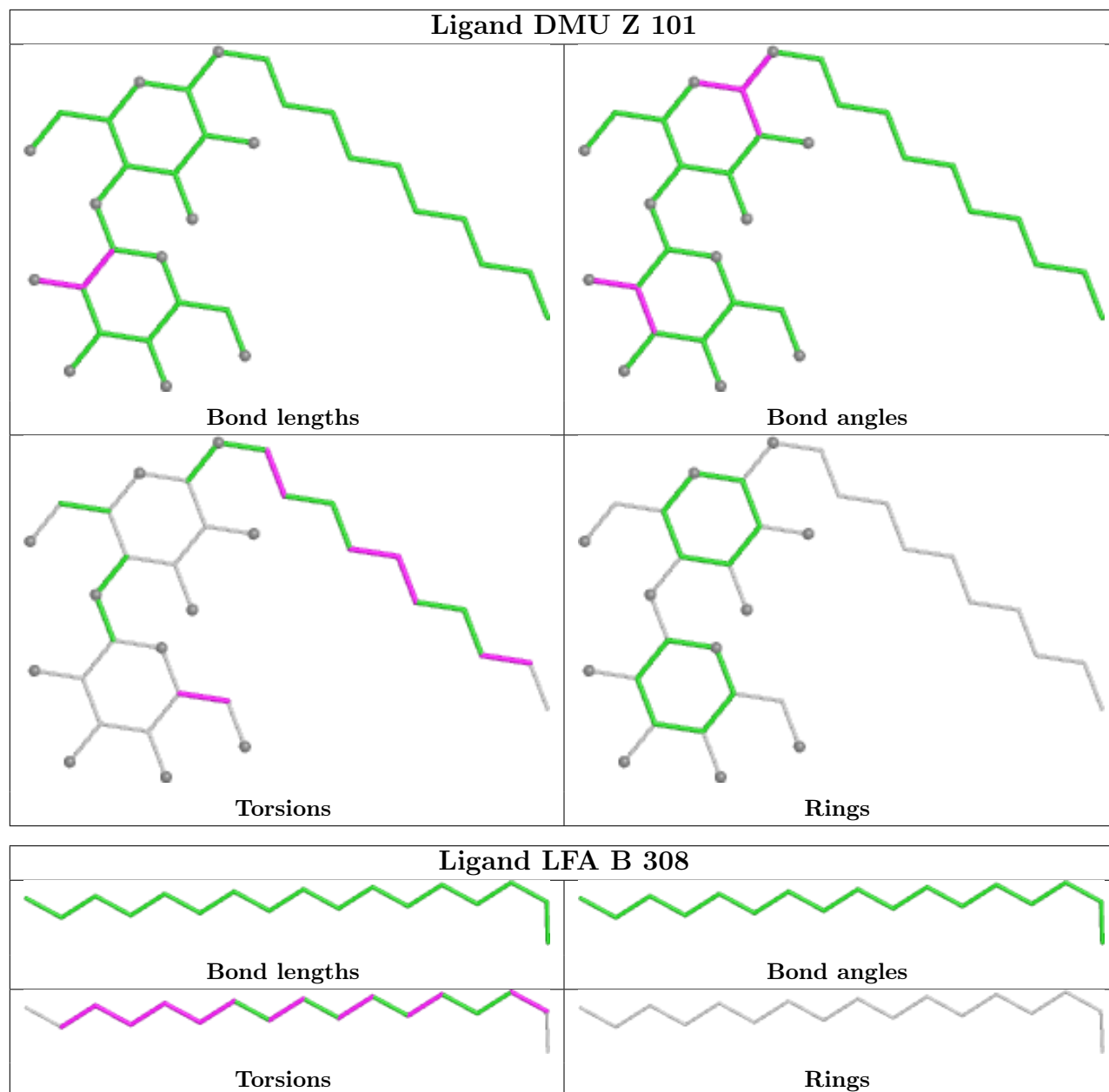


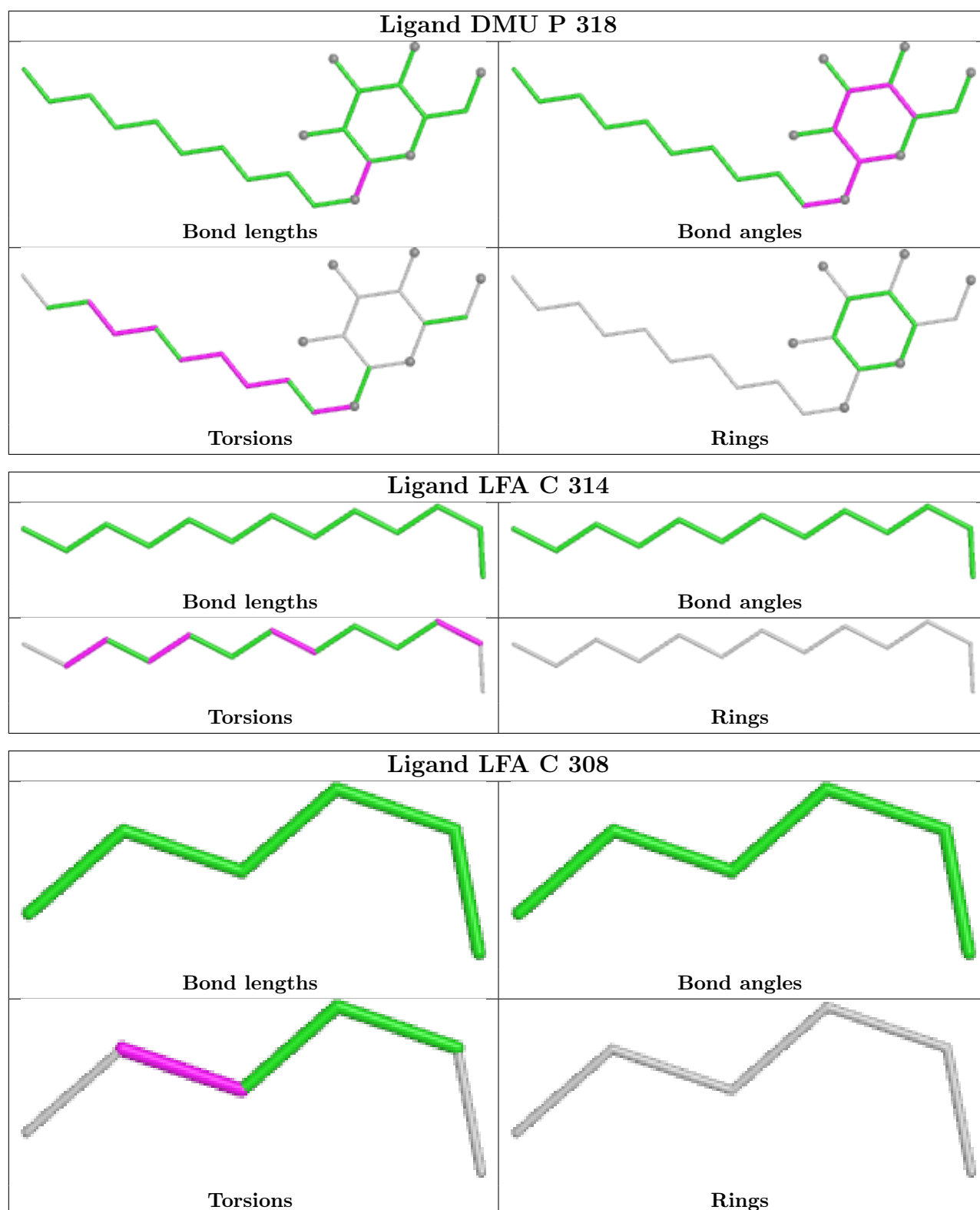


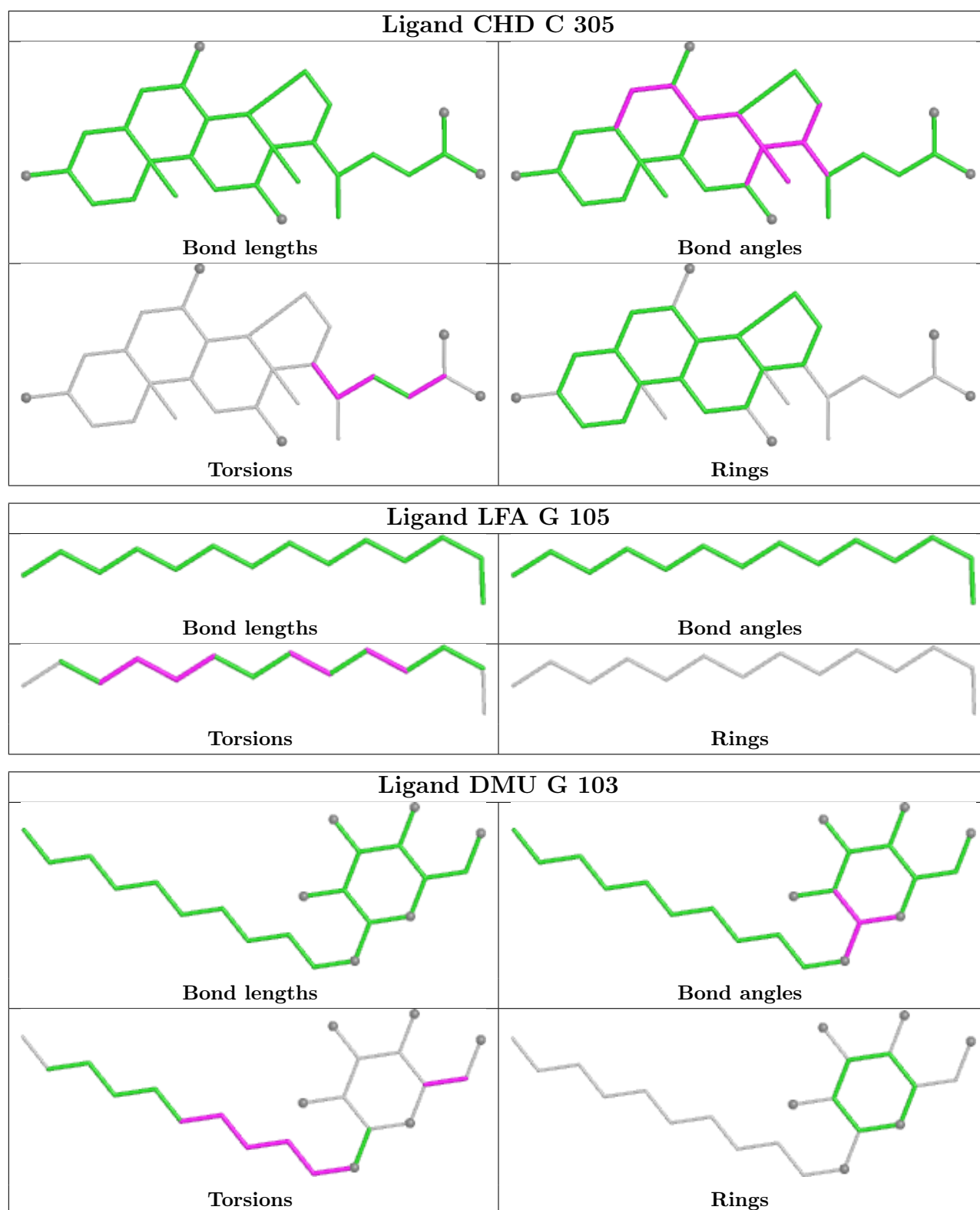


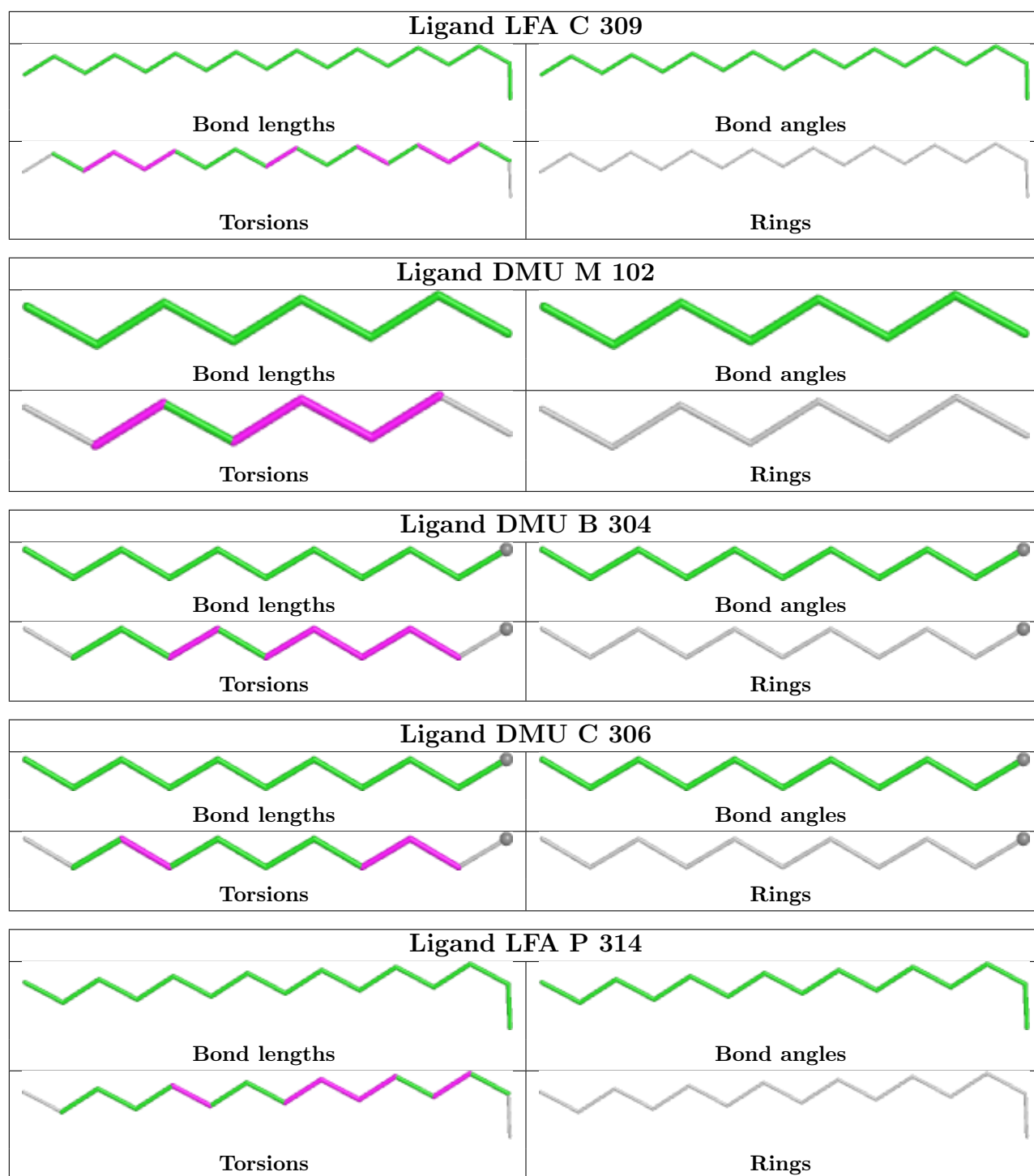


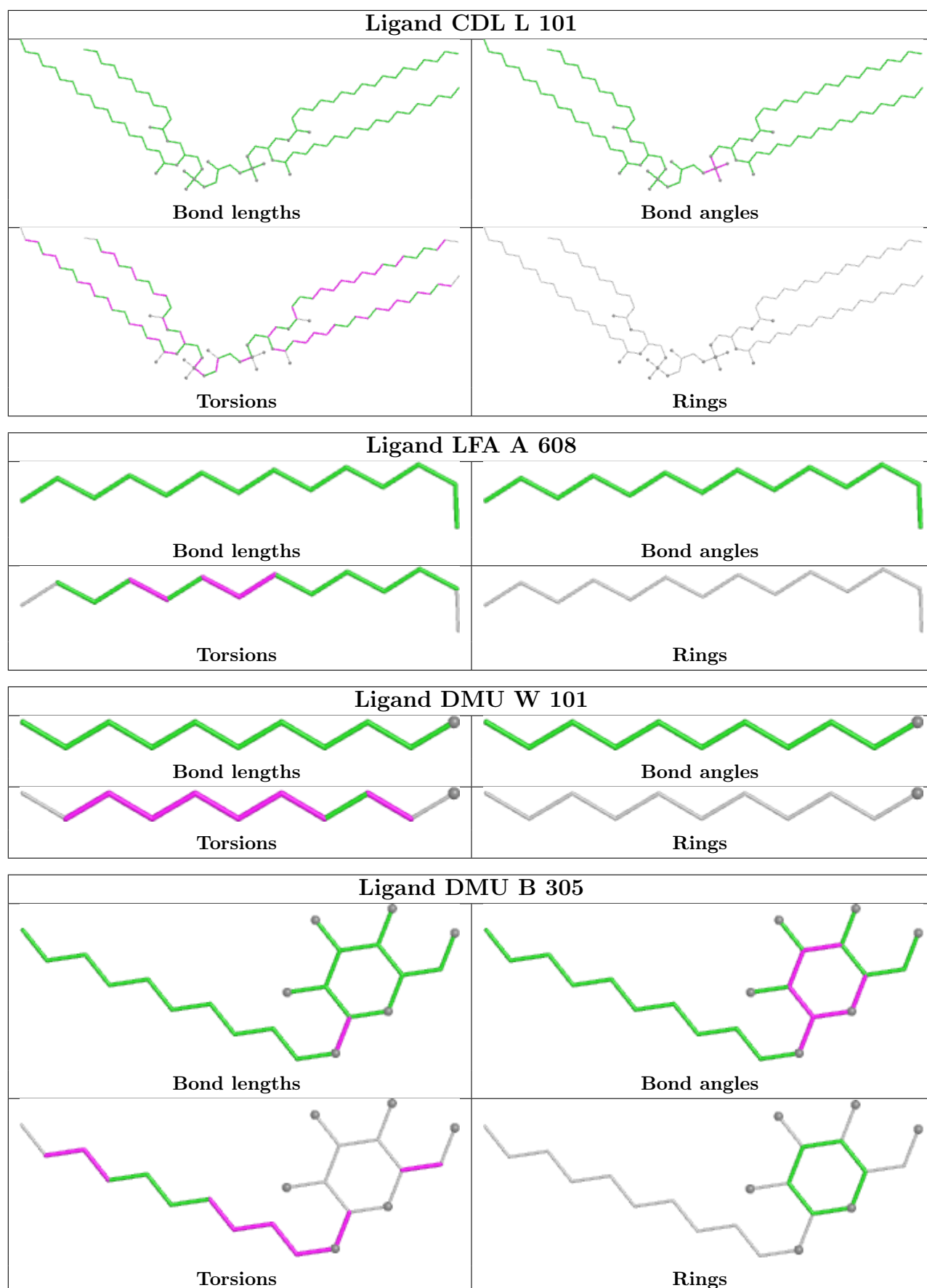


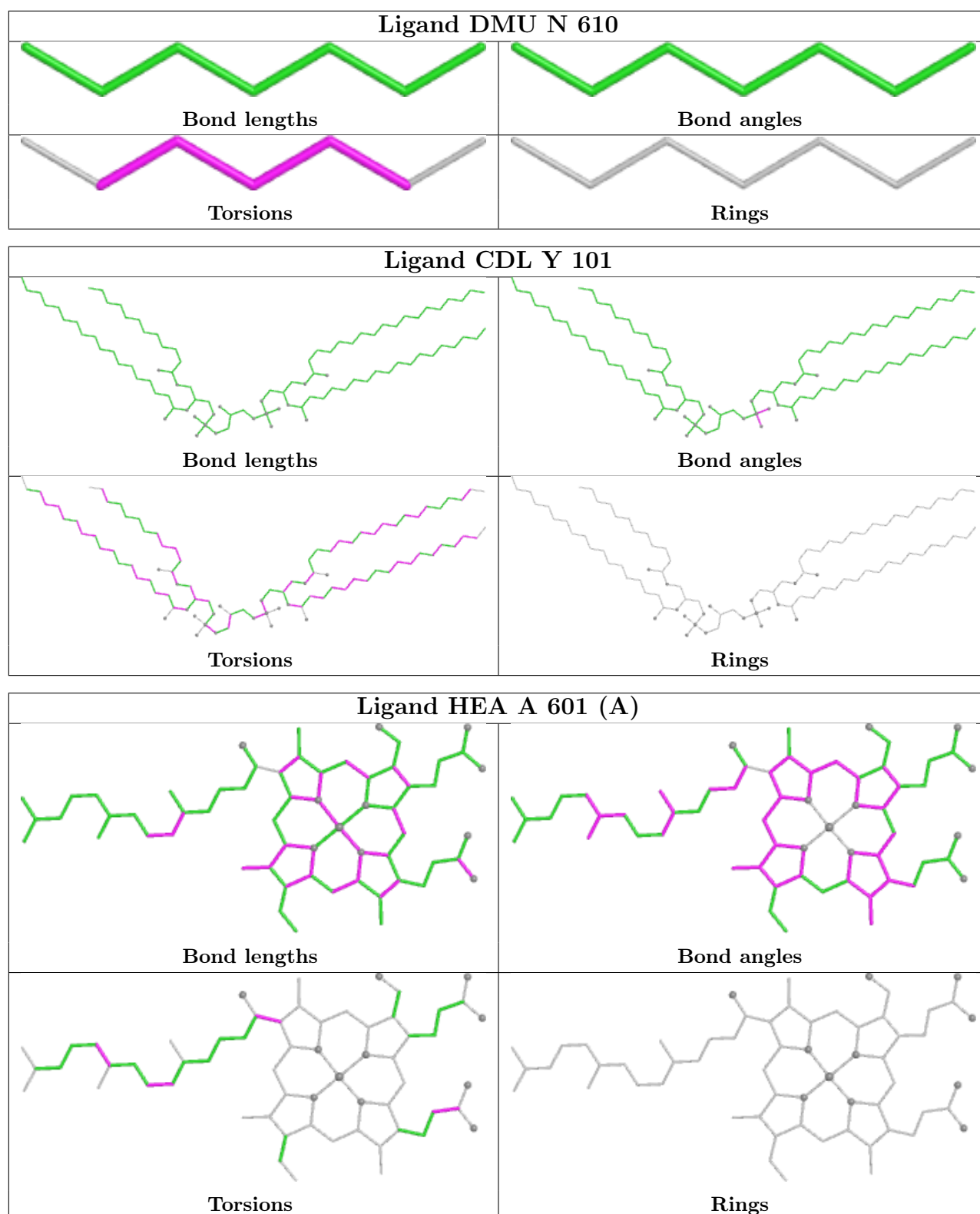


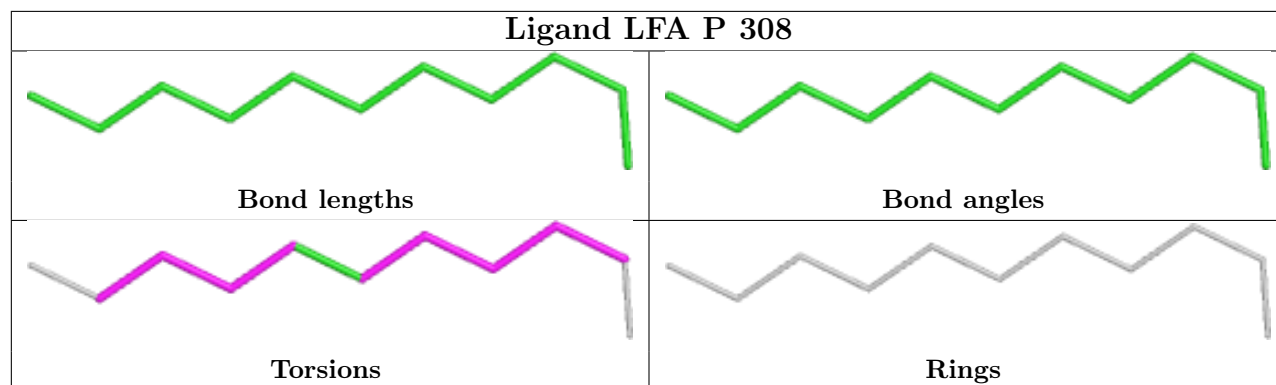
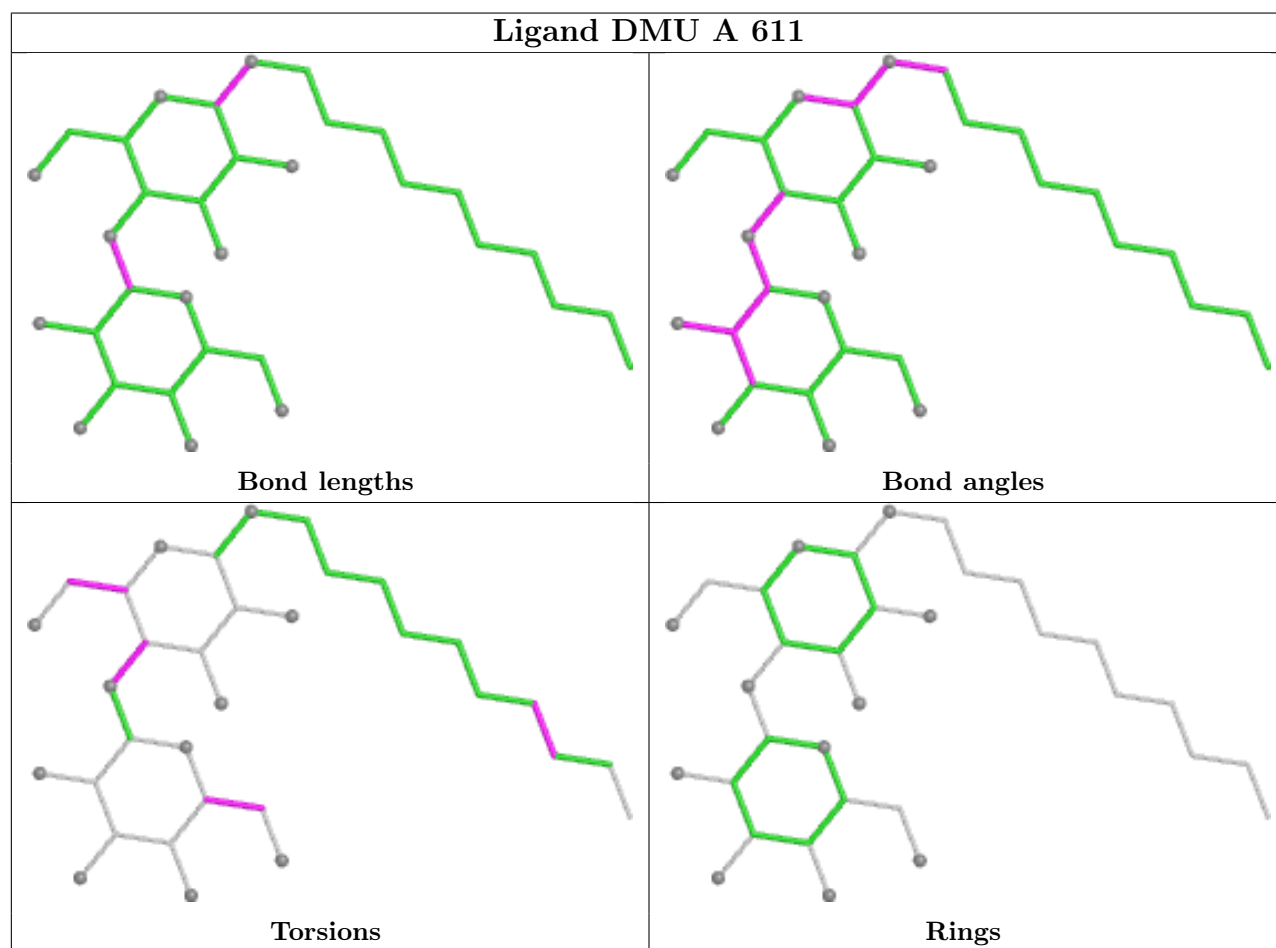
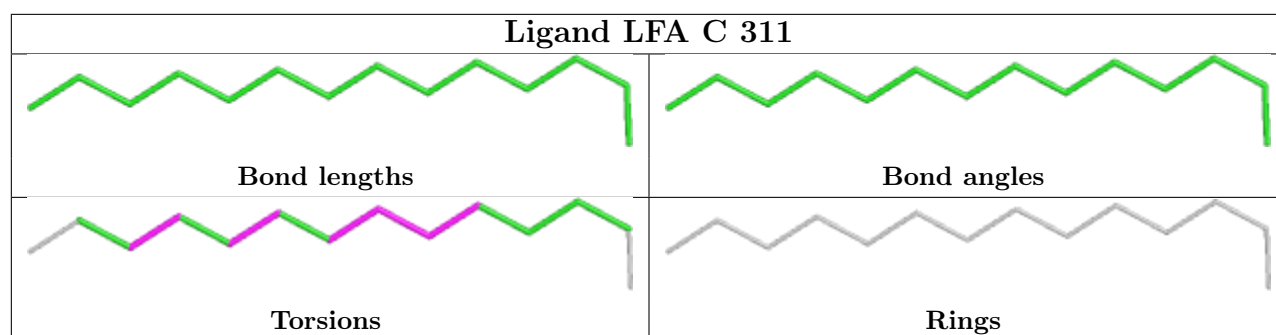












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	512/514 (99%)	-0.40	2 (0%) 88 89	15, 31, 38, 54	15 (2%)
1	N	512/514 (99%)	-0.32	2 (0%) 88 89	16, 33, 42, 54	15 (2%)
2	B	226/227 (99%)	0.05	12 (5%) 32 31	20, 37, 57, 77	5 (2%)
2	O	226/227 (99%)	0.07	5 (2%) 62 62	21, 41, 67, 92	5 (2%)
3	C	258/261 (98%)	-0.25	1 (0%) 88 89	15, 34, 44, 56	9 (3%)
3	P	258/261 (98%)	-0.25	1 (0%) 88 89	16, 35, 47, 65	9 (3%)
4	D	143/147 (97%)	-0.07	2 (1%) 73 73	19, 39, 54, 71	1 (0%)
4	Q	137/147 (93%)	0.30	3 (2%) 62 62	23, 50, 77, 89	1 (0%)
5	E	102/109 (93%)	-0.20	0 100 100	33, 40, 53, 70	0
5	R	102/109 (93%)	0.02	1 (0%) 79 80	36, 48, 65, 78	0
6	F	91/98 (92%)	-0.03	1 (1%) 78 78	19, 40, 62, 74	2 (2%)
6	S	91/98 (92%)	0.04	2 (2%) 62 62	18, 39, 60, 66	2 (2%)
7	G	72/85 (84%)	0.19	5 (6%) 23 21	20, 40, 82, 96	1 (1%)
7	T	72/85 (84%)	0.34	2 (2%) 55 55	21, 43, 76, 100	1 (1%)
8	H	75/85 (88%)	0.24	4 (5%) 32 31	34, 43, 83, 118	0
8	U	75/85 (88%)	0.32	5 (6%) 24 22	38, 46, 89, 117	0
9	I	70/73 (95%)	0.34	4 (5%) 29 28	36, 49, 73, 96	0
9	V	70/73 (95%)	0.47	3 (4%) 40 39	37, 55, 74, 104	0
10	J	56/59 (94%)	0.23	1 (1%) 67 68	35, 44, 67, 79	0
10	W	56/59 (94%)	0.30	2 (3%) 46 46	36, 47, 68, 84	0
11	K	49/56 (87%)	0.32	2 (4%) 41 41	38, 45, 60, 79	0
11	X	49/56 (87%)	0.68	2 (4%) 41 41	43, 53, 72, 101	0
12	L	44/47 (93%)	-0.09	1 (2%) 61 61	32, 36, 49, 61	0
12	Y	44/47 (93%)	0.01	1 (2%) 61 61	36, 42, 57, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	40/46 (86%)	0.07	0 100 100	34, 37, 54, 68	0
13	Z	40/46 (86%)	0.47	3 (7%) 20 18	40, 47, 70, 88	0
All	All	3470/3614 (96%)	-0.06	67 (1%) 66 66	15, 38, 63, 118	66 (1%)

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	36	TRP	6.9
11	X	6	ALA	4.7
2	O	113	TYR	4.6
2	B	59	GLN	4.5
6	S	3	GLY	4.3

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	FME	A	1	10/11	0.94	0.12	41,49,80,95	0
1	FME	N	1	10/11	0.95	0.12	43,50,80,90	0
2	FME	B	1	10/11	0.97	0.09	32,37,47,87	0
2	FME	O	1	10/11	0.98	0.09	38,40,52,75	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
21	DMU	P	318	22/33	0.70	0.33	35,60,73,85	22

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	EDO	P	323	4/4	0.70	0.35	33,34,37,42	4
20	LFA	P	311	11/20	0.73	0.41	49,65,73,78	11
21	DMU	A	610	7/33	0.76	0.38	54,60,67,69	7
21	DMU	N	610	7/33	0.78	0.40	61,64,67,74	7
21	DMU	B	309	22/33	0.78	0.32	54,74,85,98	22
22	EDO	C	322	4/4	0.78	0.31	32,36,40,42	4
21	DMU	C	317	22/33	0.78	0.26	37,65,77,87	22
23	XE	A	618	1/1	0.78	0.25	48,48,48,48	1
21	DMU	C	318	33/33	0.79	0.34	40,55,70,94	33
21	DMU	O	302	22/33	0.80	0.29	50,62,83,96	22
22	EDO	A	613	4/4	0.81	0.31	36,44,47,48	4
23	XE	N	619	1/1	0.81	0.32	57,57,57,57	1
21	DMU	C	315	33/33	0.82	0.33	43,56,64,65	33
20	LFA	C	308	6/20	0.82	0.36	41,45,52,54	6
22	EDO	E	201	4/4	0.82	0.36	39,40,41,50	4
26	CHD	P	306	29/29	0.82	0.18	68,76,97,108	0
21	DMU	N	611	33/33	0.83	0.25	41,57,79,86	33
20	LFA	P	309	6/20	0.83	0.35	44,48,48,51	6
21	DMU	C	323	33/33	0.83	0.20	38,58,75,84	33
21	DMU	P	319	33/33	0.83	0.31	47,56,71,93	33
21	DMU	P	320	33/33	0.83	0.26	50,68,80,86	33
26	CHD	C	305	29/29	0.83	0.17	57,85,103,115	0
20	LFA	C	311	14/20	0.83	0.34	40,59,66,70	14
21	DMU	C	319	33/33	0.84	0.24	41,64,73,75	33
20	LFA	P	313	11/20	0.84	0.30	33,51,60,62	11
20	LFA	C	325	15/20	0.84	0.34	50,53,65,68	15
20	LFA	P	301	15/20	0.84	0.31	47,55,62,69	15
20	LFA	C	314	13/20	0.85	0.29	52,58,75,79	13
20	LFA	C	309	18/20	0.85	0.23	38,46,63,63	18
20	LFA	O	301	11/20	0.85	0.31	42,54,68,76	11
21	DMU	P	316	33/33	0.85	0.28	43,58,69,73	33
20	LFA	P	312	14/20	0.85	0.32	38,56,70,75	14
21	DMU	B	303	11/33	0.86	0.33	49,58,65,77	11
20	LFA	C	312	11/20	0.86	0.33	45,55,64,70	11
21	DMU	M	102	8/33	0.86	0.23	42,49,56,60	8
20	LFA	N	601	17/20	0.86	0.27	37,55,70,76	17
20	LFA	A	609	14/20	0.86	0.25	40,44,59,61	14
21	DMU	A	622	33/33	0.86	0.23	35,46,53,67	33
21	DMU	A	623	11/33	0.87	0.30	42,51,69,75	11
20	LFA	C	313	15/20	0.87	0.26	43,53,74,78	15
21	DMU	P	317	7/33	0.87	0.24	51,55,60,67	7
21	DMU	B	304	11/33	0.87	0.27	38,55,67,69	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	LFA	C	310	11/20	0.87	0.29	57,63,68,71	11
20	LFA	B	308	17/20	0.87	0.28	38,60,74,80	17
20	LFA	C	307	11/20	0.87	0.29	41,48,61,61	11
21	DMU	P	324	33/33	0.88	0.18	41,60,88,95	33
19	CDL	V	101	64/100	0.88	0.17	50,82,127,147	0
21	DMU	C	316	7/33	0.88	0.30	47,53,62,69	7
21	DMU	O	305	11/33	0.88	0.33	45,50,61,73	11
22	EDO	N	613	4/4	0.88	0.28	37,43,44,51	4
21	DMU	G	103	22/33	0.88	0.26	45,54,61,64	22
21	DMU	J	101	11/33	0.88	0.34	58,63,76,86	11
20	LFA	P	308	11/20	0.88	0.30	41,50,63,68	11
21	DMU	N	602	11/33	0.88	0.29	41,53,65,71	11
20	LFA	G	105	14/20	0.88	0.25	40,46,57,60	14
21	DMU	W	101	11/33	0.89	0.35	64,72,80,83	11
21	DMU	Y	102	22/33	0.89	0.34	53,62,73,80	22
20	LFA	A	608	14/20	0.89	0.23	36,43,70,79	14
20	LFA	P	315	13/20	0.89	0.22	46,54,71,78	13
19	CDL	C	304	87/100	0.89	0.18	41,80,116,127	0
19	CDL	P	305	87/100	0.89	0.18	39,83,128,160	0
22	EDO	P	321	4/4	0.89	0.22	50,51,56,68	4
20	LFA	P	310	18/20	0.89	0.23	40,50,56,57	18
19	CDL	A	607	64/100	0.89	0.16	50,81,119,133	0
19	CDL	Y	101	94/100	0.89	0.17	52,84,134,147	0
21	DMU	Q	201	33/33	0.89	0.20	38,51,64,74	33
21	DMU	U	101	33/33	0.89	0.22	34,48,65,68	33
20	LFA	P	314	15/20	0.90	0.19	42,47,55,59	15
21	DMU	L	102	22/33	0.90	0.30	46,59,67,71	22
21	DMU	O	307	22/33	0.90	0.18	35,52,58,58	22
21	DMU	T	103	22/33	0.90	0.20	43,54,67,70	22
21	DMU	A	611	33/33	0.90	0.18	35,47,61,65	33
20	LFA	T	102	11/20	0.90	0.27	51,56,68,73	11
21	DMU	D	201	33/33	0.90	0.18	28,48,60,76	33
22	EDO	A	612	4/4	0.90	0.15	27,29,31,32	4
21	DMU	B	305	22/33	0.90	0.21	40,69,83,91	22
19	CDL	L	101	94/100	0.91	0.15	43,81,124,142	0
20	LFA	N	609	14/20	0.91	0.23	37,50,68,69	14
21	DMU	Z	102	8/33	0.92	0.22	51,54,55,56	8
22	EDO	A	615	4/4	0.92	0.13	36,43,46,49	4
22	EDO	F	102	4/4	0.92	0.16	22,23,29,32	4
22	EDO	R	203	4/4	0.92	0.24	40,41,49,56	4
21	DMU	P	307	11/33	0.93	0.24	45,50,58,71	11
22	EDO	R	202	4/4	0.93	0.19	35,36,39,40	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	EDO	G	104	4/4	0.93	0.14	29,33,35,36	4
22	EDO	N	612	4/4	0.93	0.14	30,31,32,32	4
21	DMU	C	306	11/33	0.93	0.23	50,54,60,69	11
22	EDO	N	614	4/4	0.93	0.19	30,31,32,33	4
22	EDO	E	203	4/4	0.93	0.24	34,37,43,44	4
22	EDO	C	320	4/4	0.94	0.26	46,54,57,76	4
22	EDO	C	321	4/4	0.94	0.18	35,37,38,38	4
22	EDO	S	102	4/4	0.94	0.11	21,24,28,29	4
22	EDO	N	616	4/4	0.94	0.21	30,30,33,38	4
22	EDO	O	308	4/4	0.94	0.12	30,31,33,37	4
21	DMU	O	306	11/33	0.94	0.23	38,53,61,62	11
21	DMU	Z	101	33/33	0.94	0.10	51,58,72,76	0
22	EDO	E	202	4/4	0.95	0.20	31,33,35,35	4
26	CHD	C	301	29/29	0.95	0.08	32,36,41,43	0
27	UNX	P	303	1/1	0.95	0.29	45,45,45,45	0
21	DMU	M	101	33/33	0.96	0.08	45,52,66,73	0
22	EDO	R	201	4/4	0.96	0.25	57,59,65,68	4
23	XE	N	620	1/1	0.96	0.17	52,52,52,52	1
22	EDO	A	614	4/4	0.96	0.17	26,27,28,28	4
22	EDO	N	615	4/4	0.96	0.14	36,37,38,39	4
22	EDO	P	322	4/4	0.96	0.18	36,38,40,43	4
22	EDO	T	104	4/4	0.96	0.11	34,34,36,40	4
22	EDO	B	306	4/4	0.97	0.09	25,27,28,31	4
23	XE	A	619	1/1	0.97	0.10	49,49,49,49	1
26	CHD	P	302	29/29	0.97	0.07	33,37,42,45	0
24	PGV	N	622	51/51	0.97	0.09	31,45,76,79	0
27	UNX	C	302	1/1	0.97	0.18	44,44,44,44	0
26	CHD	B	307	29/29	0.97	0.06	31,34,38,49	0
29	PEK	G	101	53/53	0.97	0.11	34,53,94,116	0
29	PEK	T	101	53/53	0.97	0.11	36,55,97,109	0
26	CHD	G	102	29/29	0.98	0.06	30,33,36,44	0
24	PGV	C	303	51/51	0.98	0.09	30,39,104,112	0
22	EDO	S	103	4/4	0.98	0.08	31,37,38,40	4
24	PGV	P	304	51/51	0.98	0.08	30,40,97,116	0
22	EDO	F	103	4/4	0.98	0.08	32,32,32,36	4
23	XE	P	325	1/1	0.98	0.06	49,49,49,49	1
24	PGV	A	621	51/51	0.98	0.09	29,44,79,87	0
14	HEA	A	601[B]	60/60	0.99	0.05	26,28,44,49	9
14	HEA	A	602	60/60	0.99	0.05	25,28,35,41	0
14	HEA	N	603[A]	60/60	0.99	0.06	28,31,44,50	9
14	HEA	N	603[B]	60/60	0.99	0.06	28,31,45,45	9
14	HEA	N	604	60/60	0.99	0.05	27,30,36,42	0

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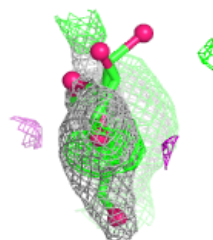
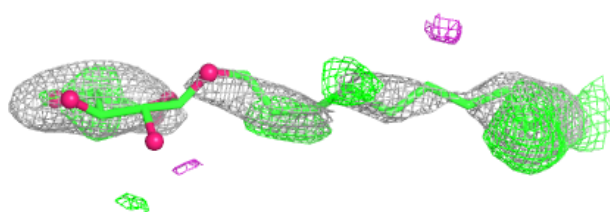
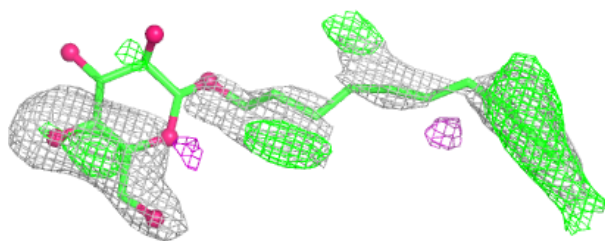
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	MG	A	604	1/1	0.99	0.03	31,31,31,31	0
16	MG	N	606	1/1	0.99	0.02	34,34,34,34	0
17	NA	A	605	1/1	0.99	0.05	34,34,34,34	0
18	PER	A	606	2/2	0.99	0.04	26,26,26,36	0
18	PER	N	608	2/2	0.99	0.07	29,29,29,38	0
14	HEA	A	601[A]	60/60	0.99	0.05	26,28,38,44	9
23	XE	A	620	1/1	1.00	0.11	52,52,52,52	1
23	XE	B	301	1/1	1.00	0.32	54,54,54,54	1
25	CUA	B	302	2/2	1.00	0.02	30,30,30,30	0
25	CUA	O	304	2/2	1.00	0.02	34,34,34,34	0
23	XE	C	324	1/1	1.00	0.06	51,51,51,51	1
23	XE	N	617	1/1	1.00	0.21	50,50,50,50	0
23	XE	N	618	1/1	1.00	0.27	49,49,49,49	1
17	NA	N	607	1/1	1.00	0.06	39,39,39,39	0
23	XE	A	616	1/1	1.00	0.23	49,49,49,49	0
23	XE	N	621	1/1	1.00	0.09	53,53,53,53	1
23	XE	O	303	1/1	1.00	0.27	51,51,51,51	1
23	XE	A	617	1/1	1.00	0.26	47,47,47,47	1
28	ZN	F	101	1/1	1.00	0.01	35,35,35,35	0
28	ZN	S	101	1/1	1.00	0.01	35,35,35,35	0
15	CU	N	605	1/1	1.00	0.02	30,30,30,30	0
15	CU	A	603	1/1	1.00	0.01	29,29,29,29	0

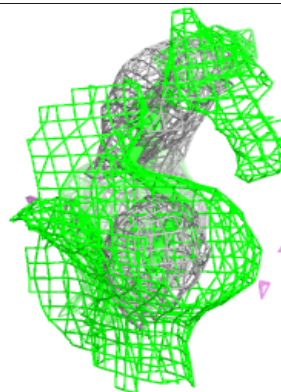
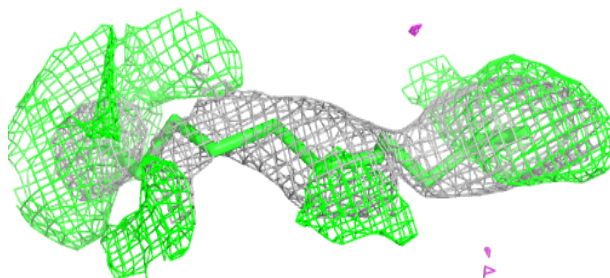
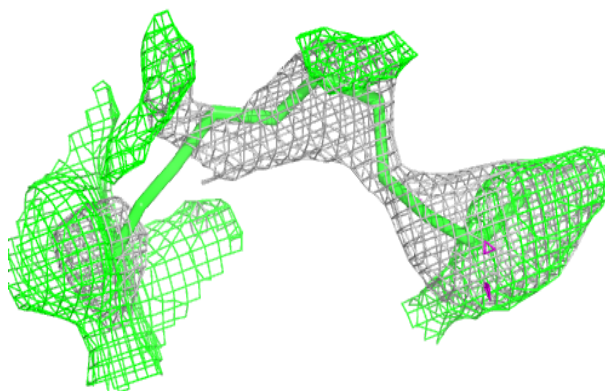
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU P 318:

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

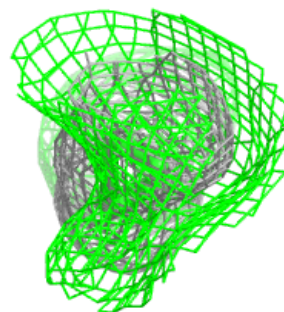
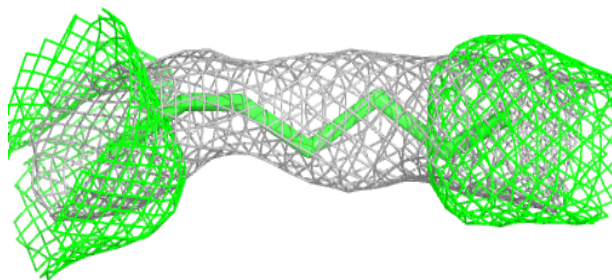
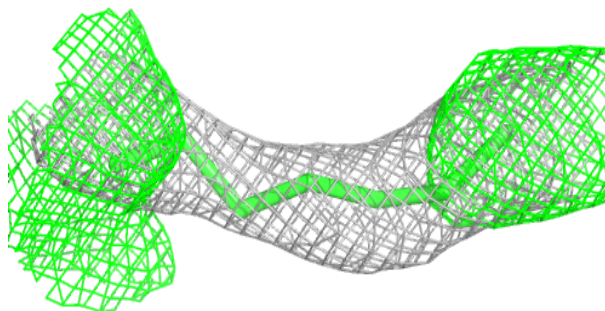
**Electron density around LFA P 311:**

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

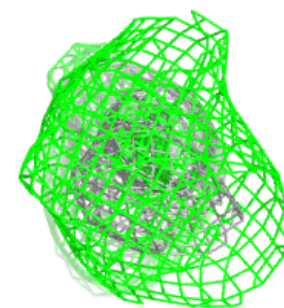
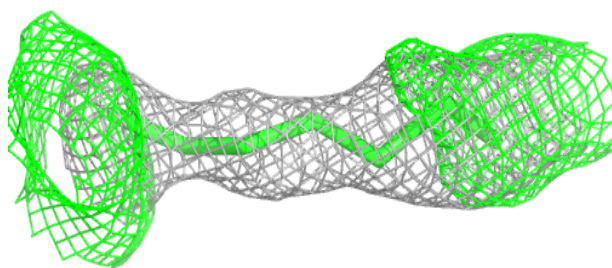
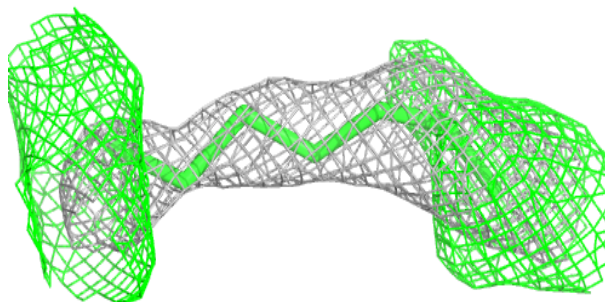


Electron density around DMU A 610:

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

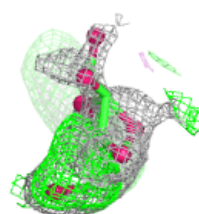
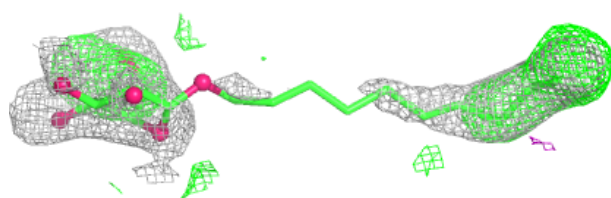
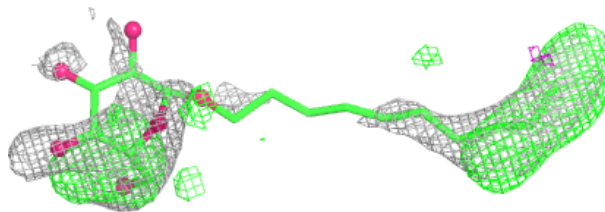
**Electron density around DMU N 610:**

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

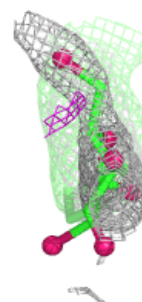
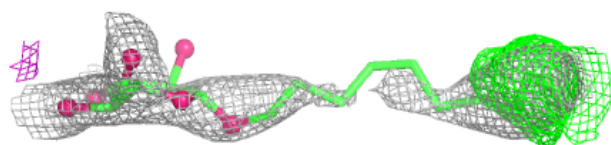
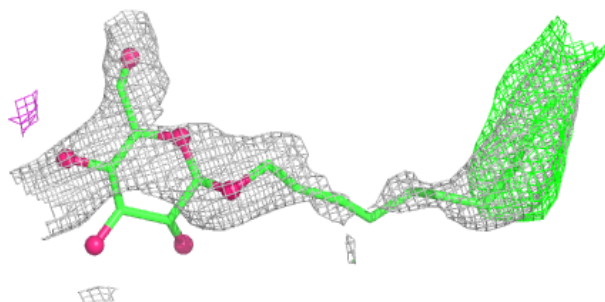


Electron density around DMU B 309:

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

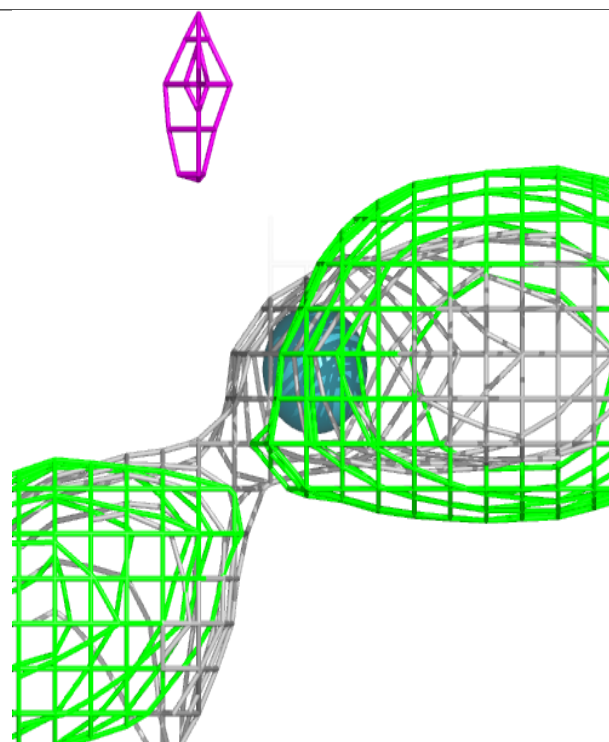
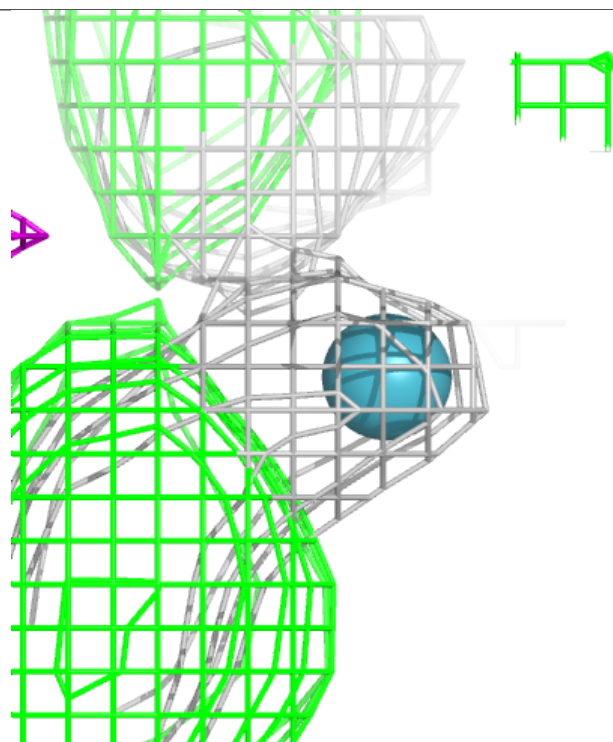
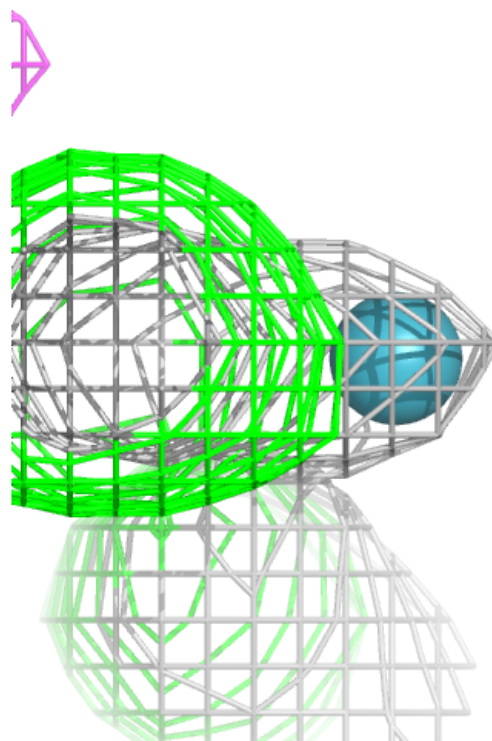
**Electron density around DMU C 317:**

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



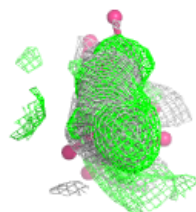
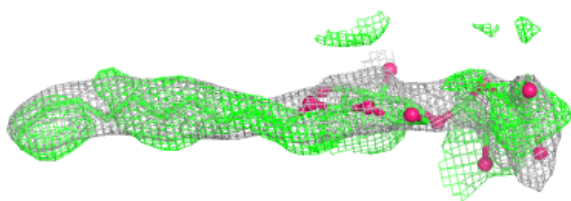
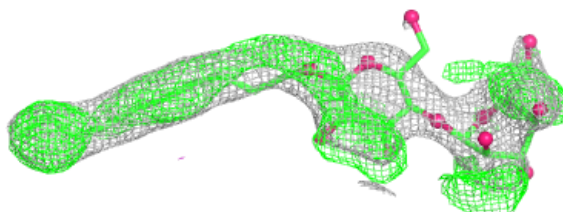
Electron density around XE A 618:

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

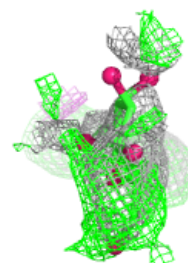
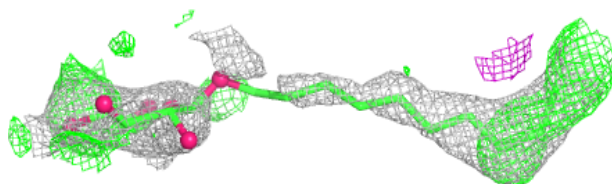
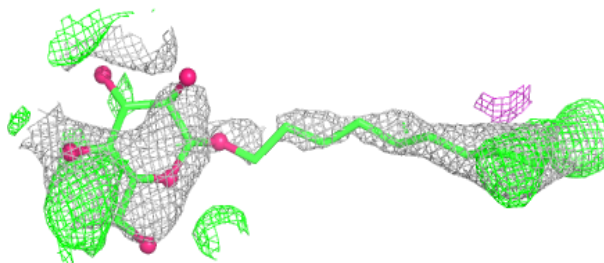


Electron density around DMU C 318:

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

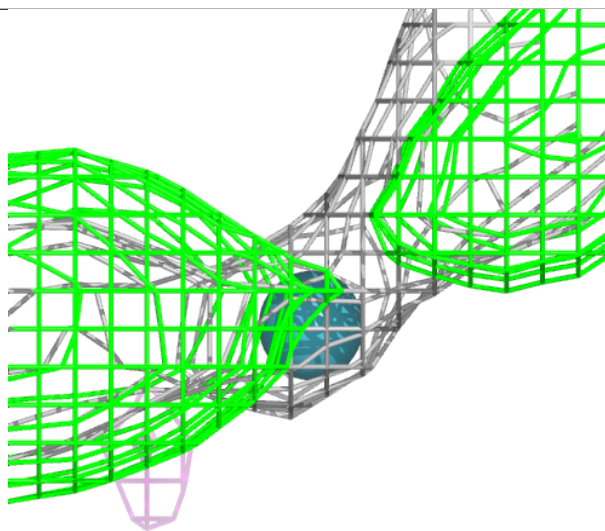
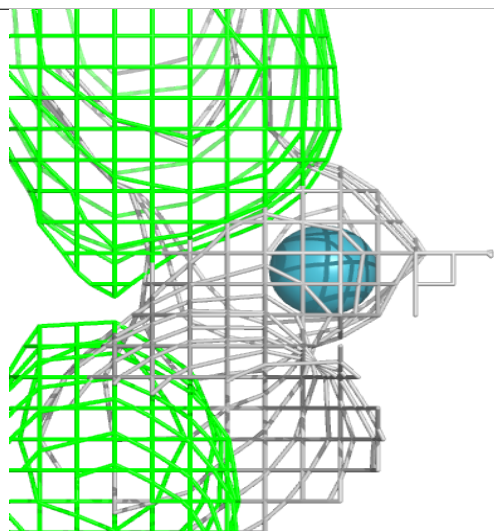
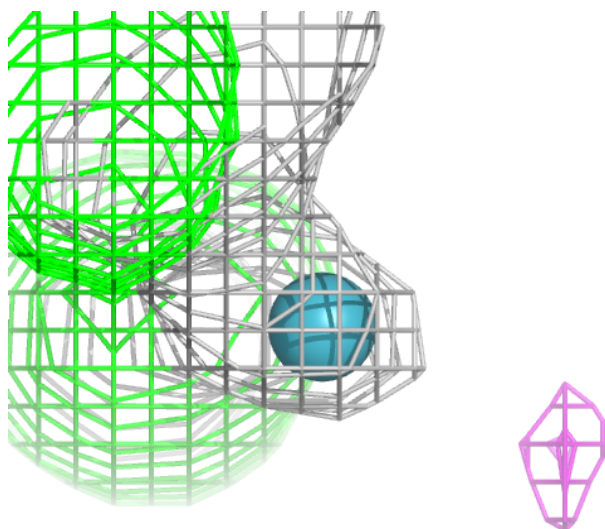
**Electron density around DMU O 302:**

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



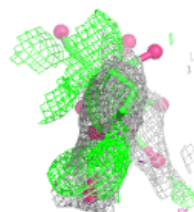
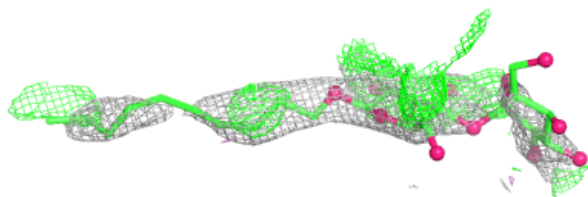
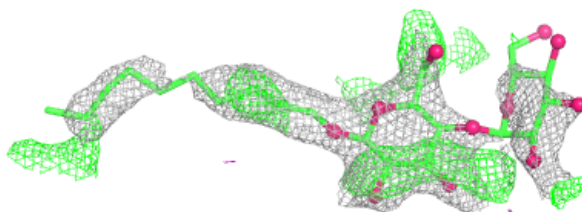
Electron density around XE N 619:

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

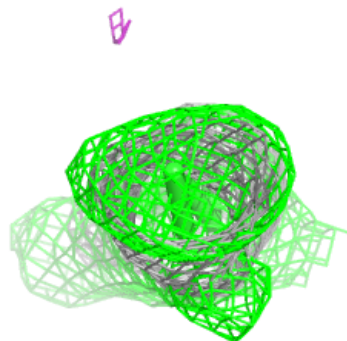
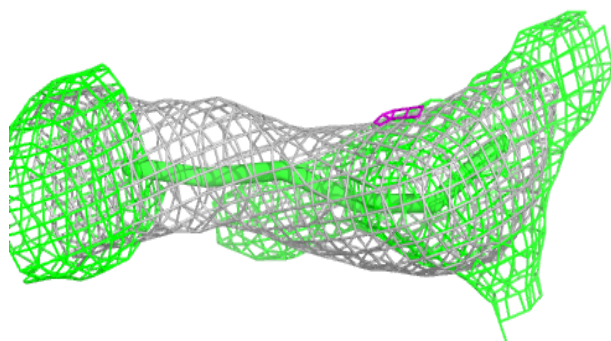
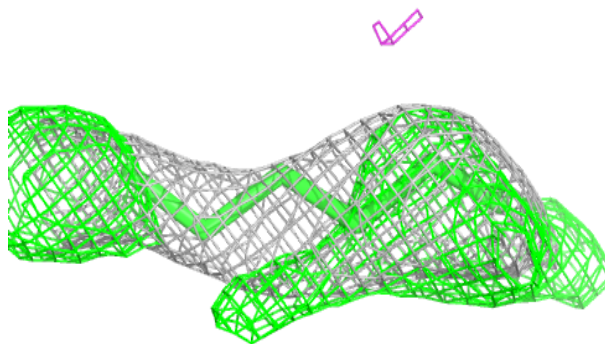


Electron density around DMU C 315:

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

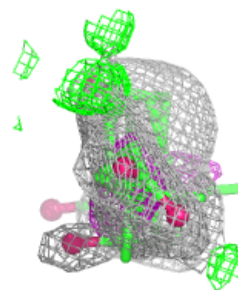
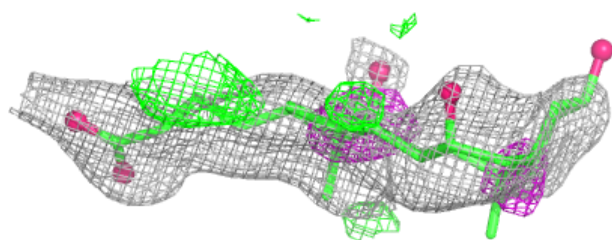
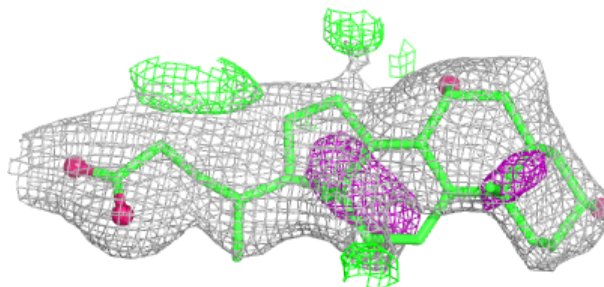
**Electron density around LFA C 308:**

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

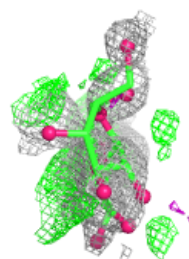
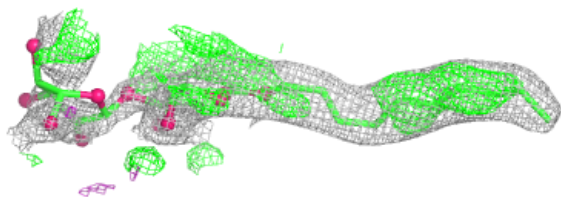
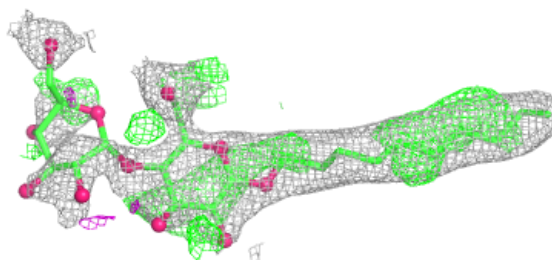


Electron density around CHD P 306:

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

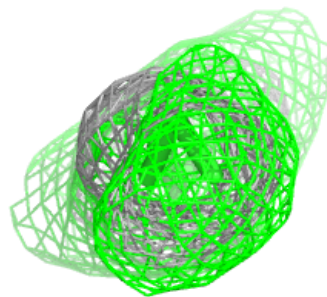
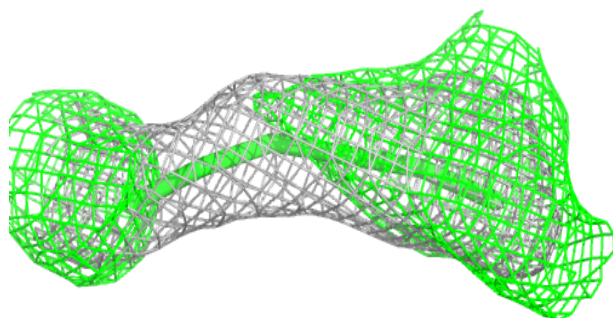
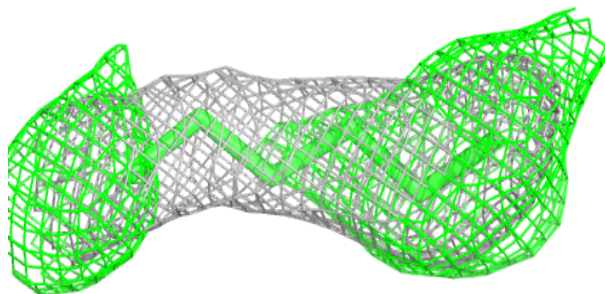
**Electron density around DMU N 611:**

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

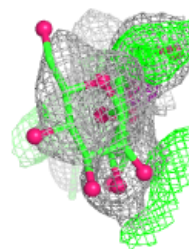
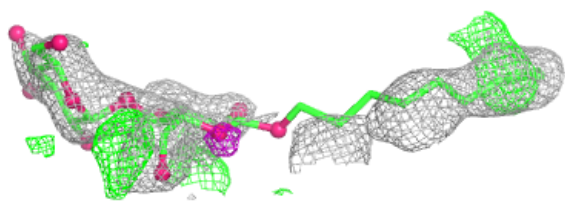
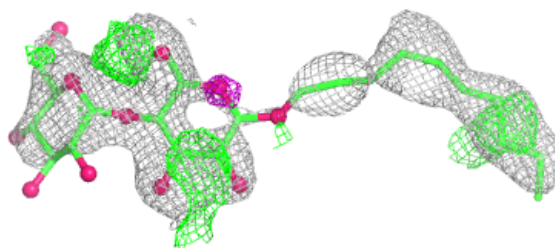


Electron density around LFA P 309:

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

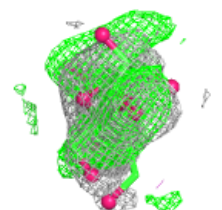
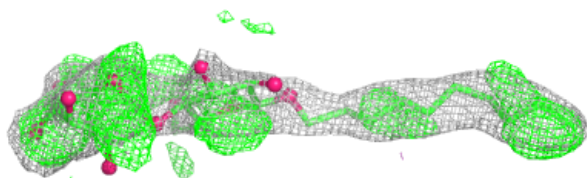
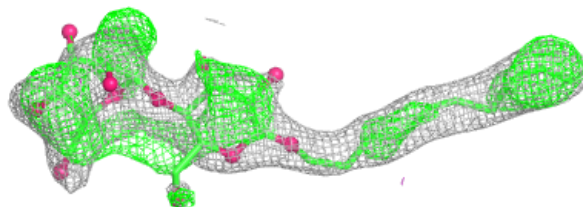
**Electron density around DMU C 323:**

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

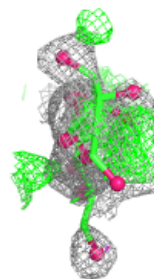
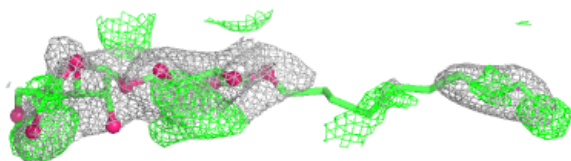
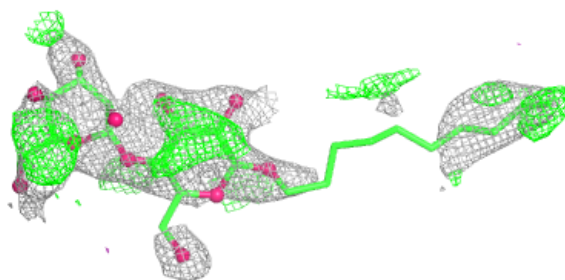


Electron density around DMU P 319:

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

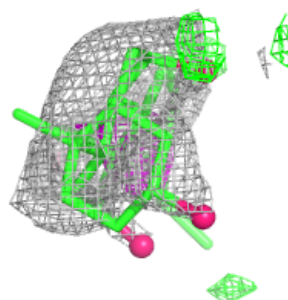
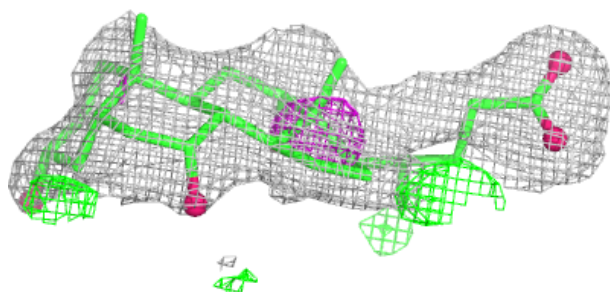
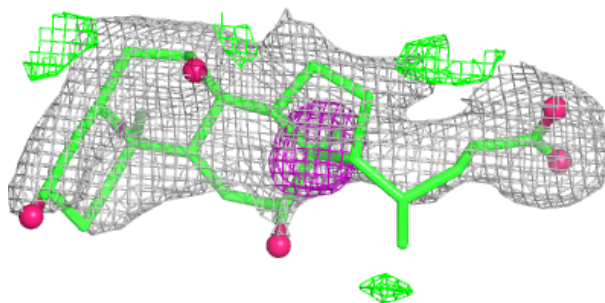
**Electron density around DMU P 320:**

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

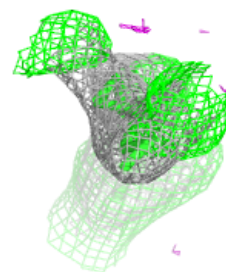
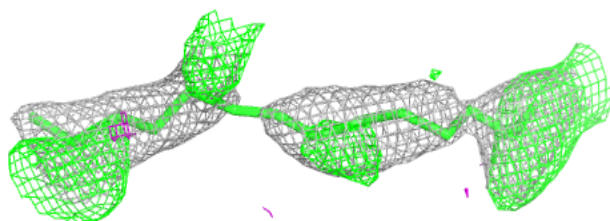
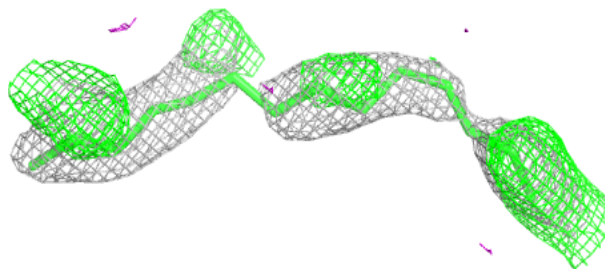


Electron density around CHD C 305:

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

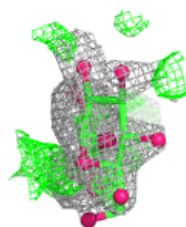
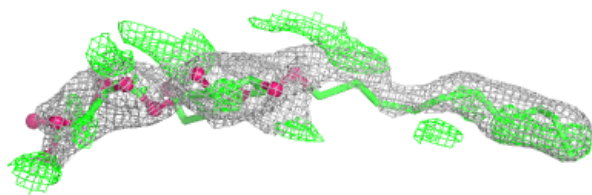
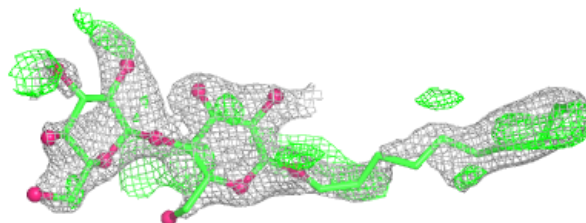
**Electron density around LFA C 311:**

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

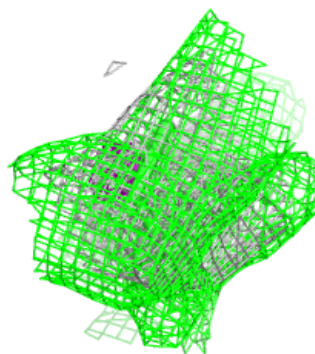
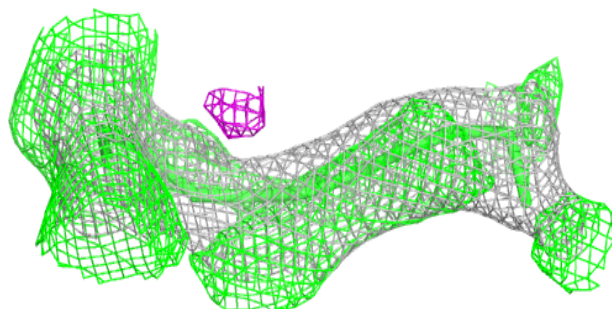
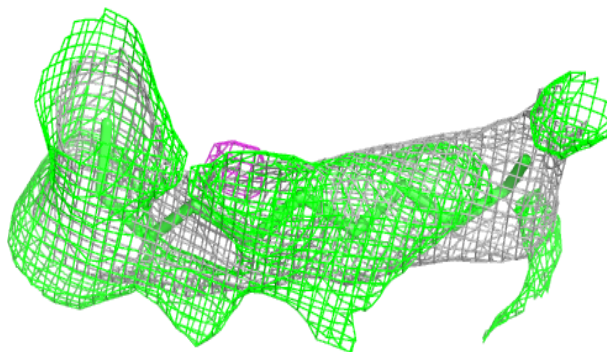


Electron density around DMU C 319:

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

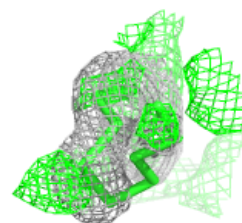
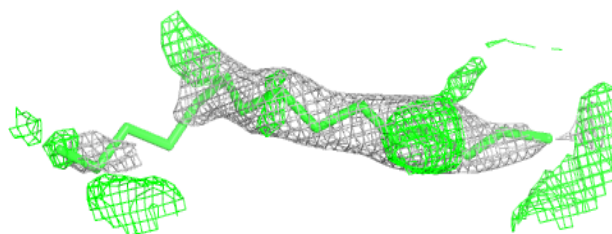
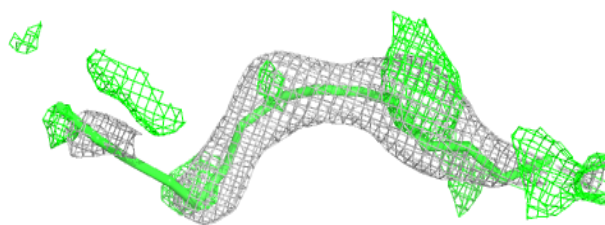
**Electron density around LFA P 313:**

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

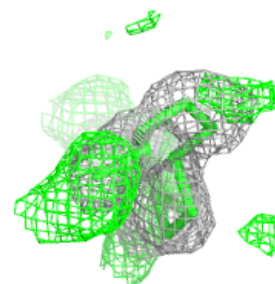
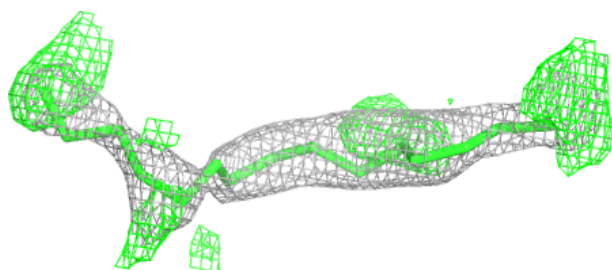
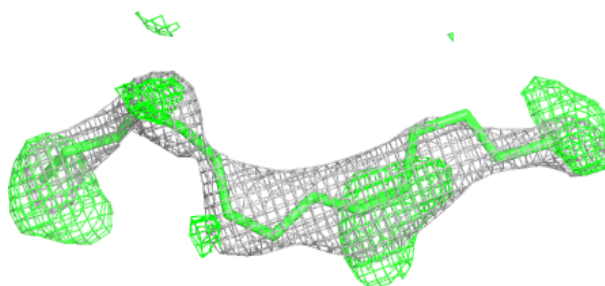


Electron density around LFA C 325:

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

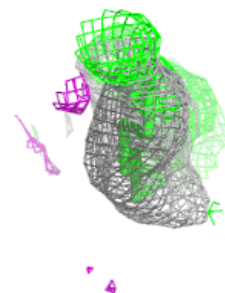
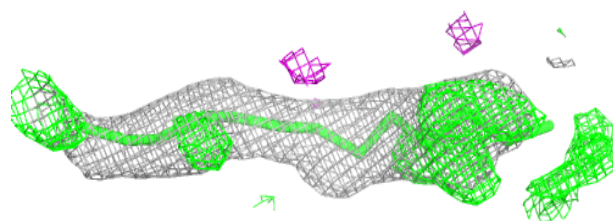
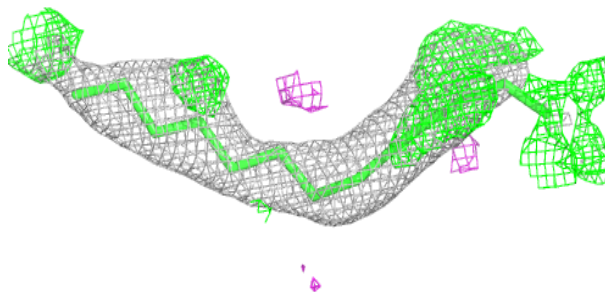
**Electron density around LFA P 301:**

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

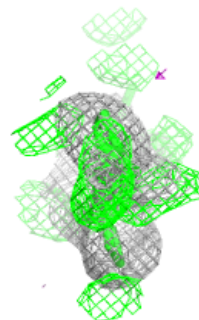
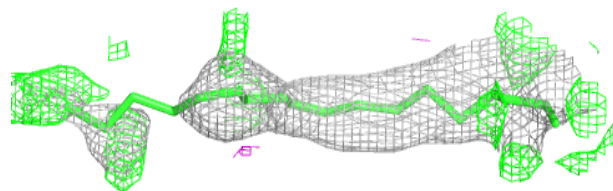
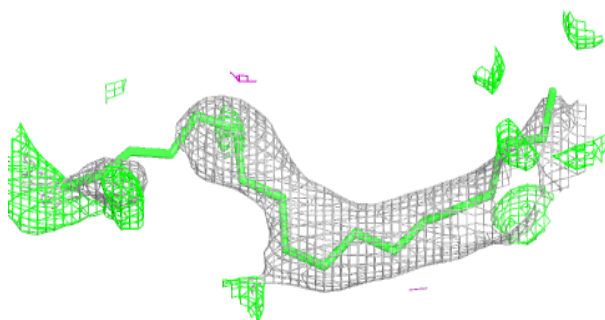


Electron density around LFA C 314:

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

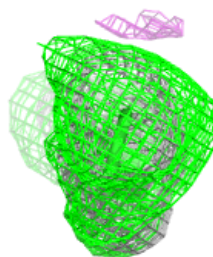
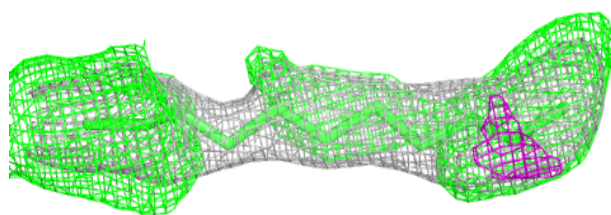
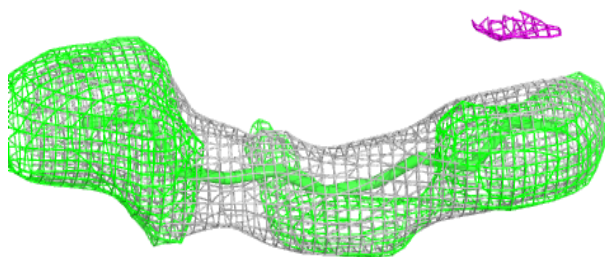
**Electron density around LFA C 309:**

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

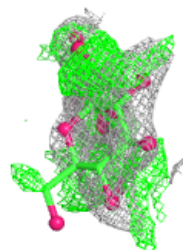
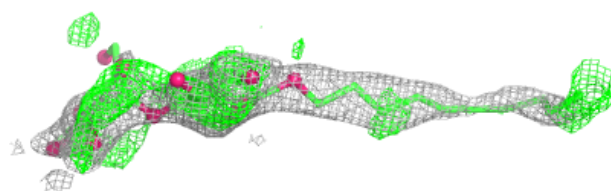
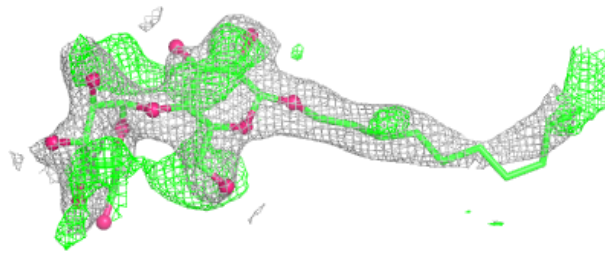


Electron density around LFA O 301:

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

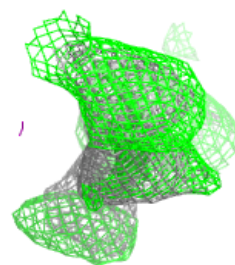
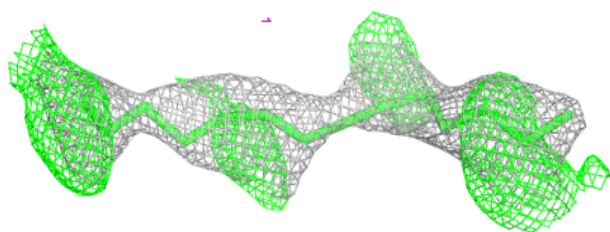
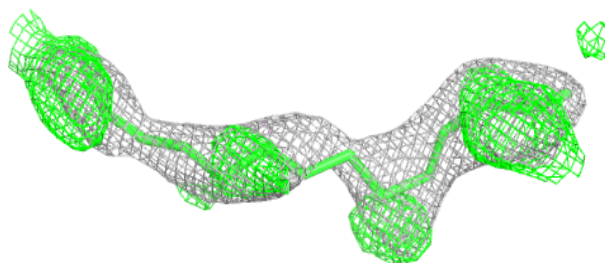
**Electron density around DMU P 316:**

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

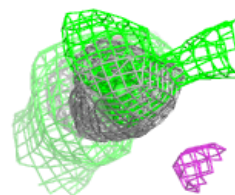
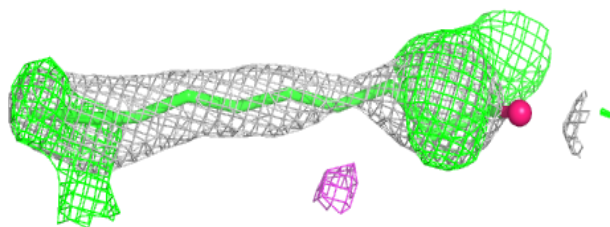
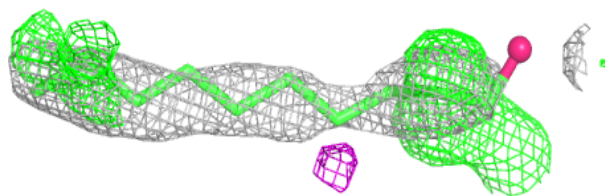


Electron density around LFA P 312:

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

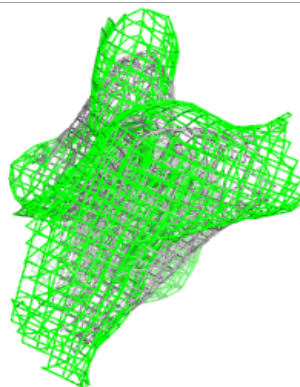
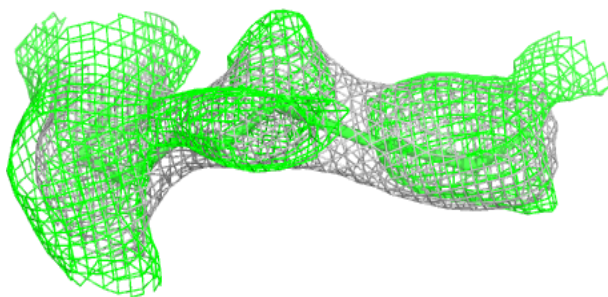
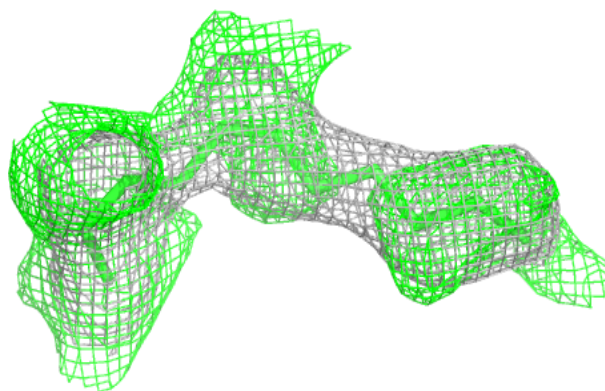
**Electron density around DMU B 303:**

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

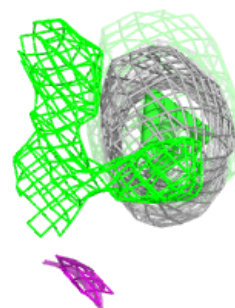
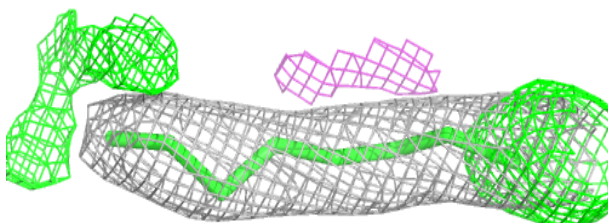
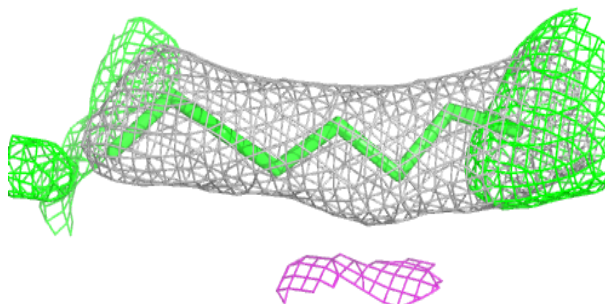


Electron density around LFA C 312:

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

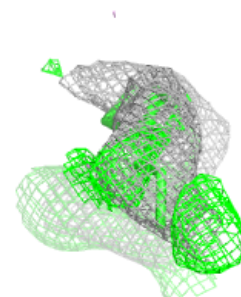
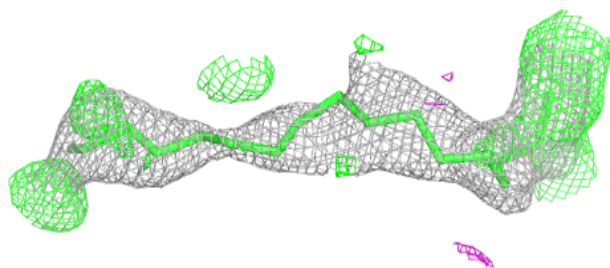
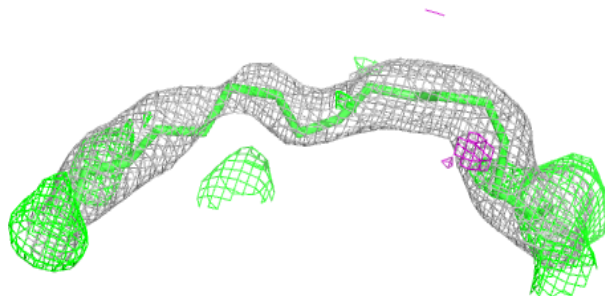
**Electron density around DMU M 102:**

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

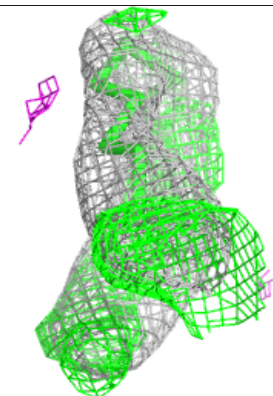
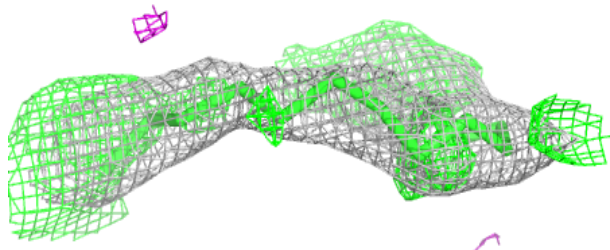
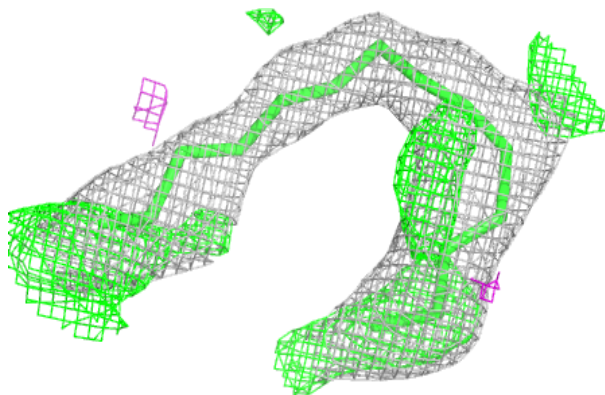


Electron density around LFA N 601:

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

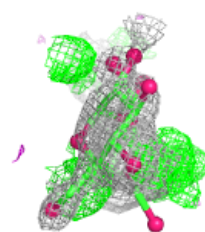
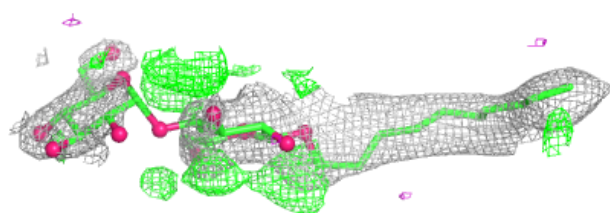
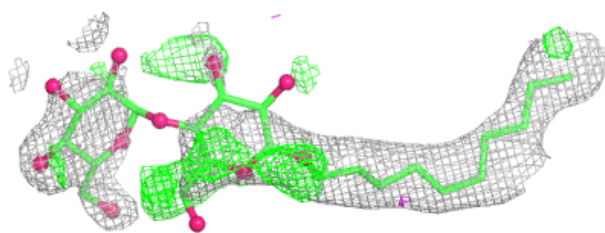
**Electron density around LFA A 609:**

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

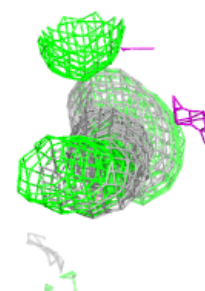
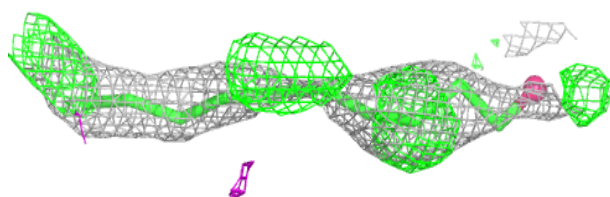
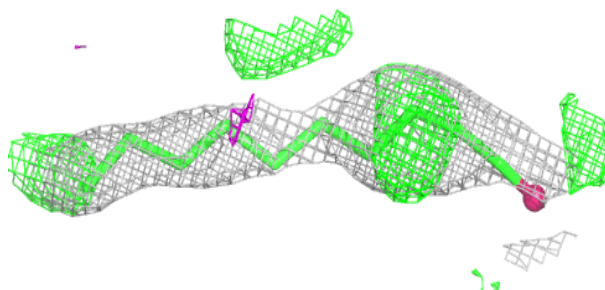


Electron density around DMU A 622:

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

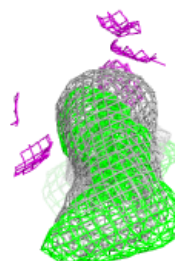
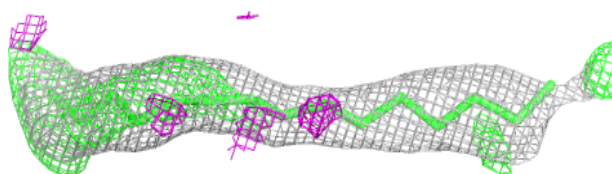
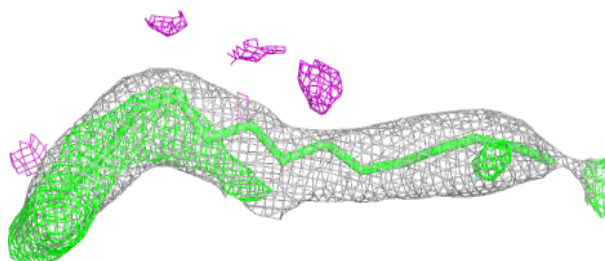
**Electron density around DMU A 623:**

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

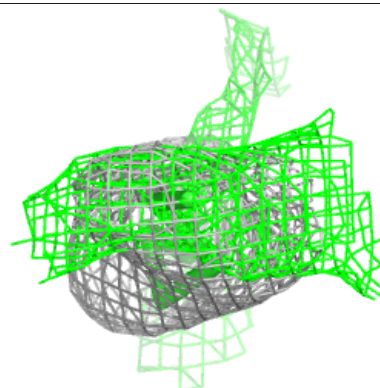
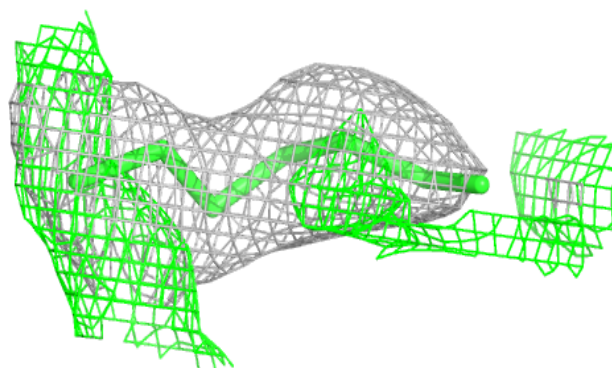
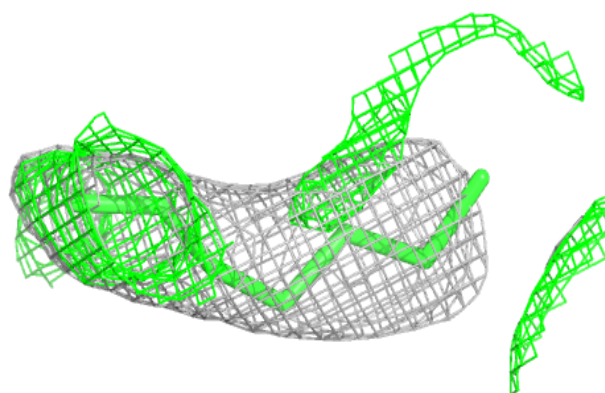


Electron density around LFA C 313:

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

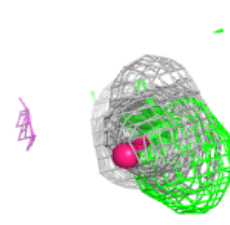
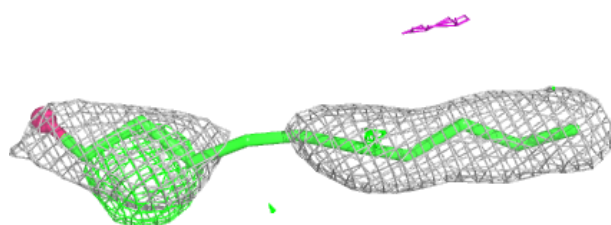
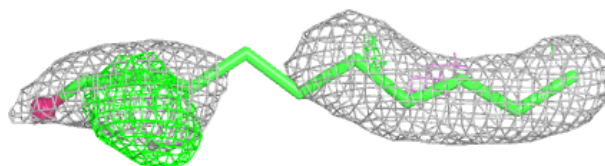
**Electron density around DMU P 317:**

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

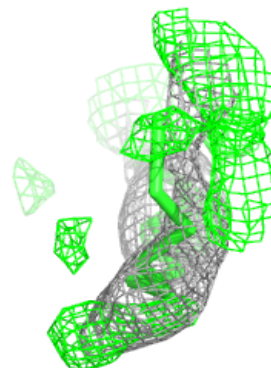
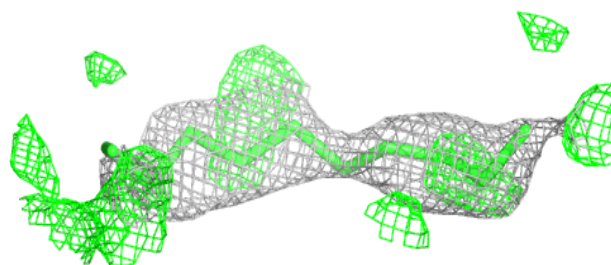
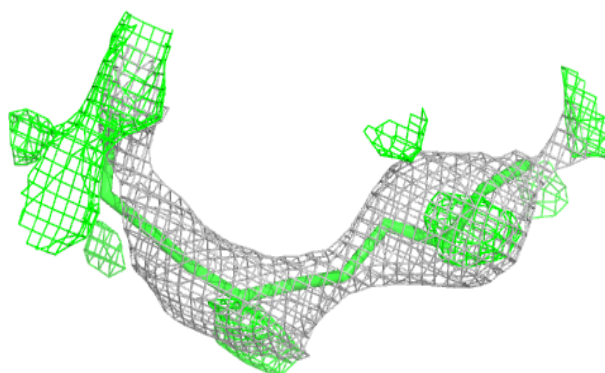


Electron density around DMU B 304:

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

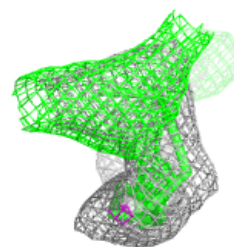
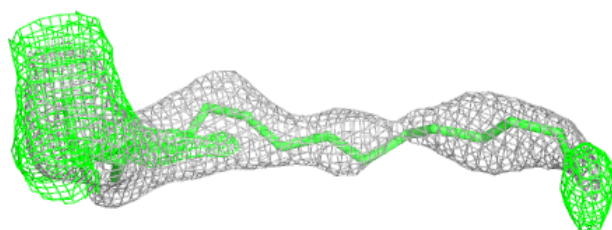
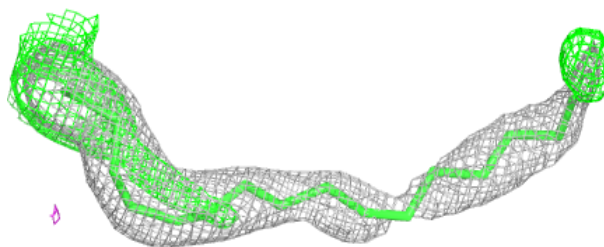
**Electron density around LFA C 310:**

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

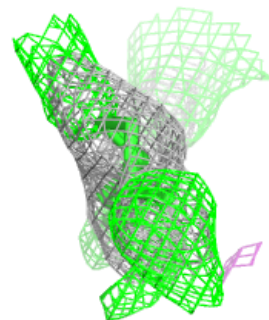
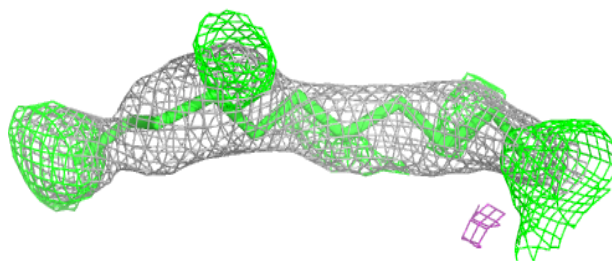
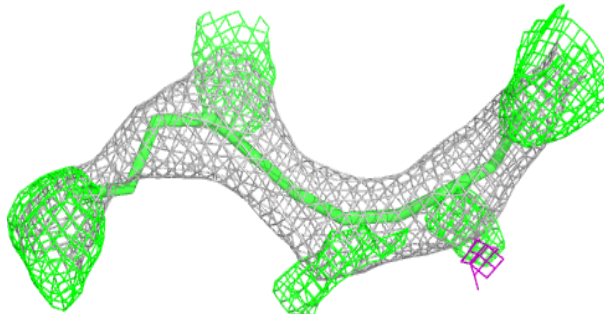


Electron density around LFA B 308:

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

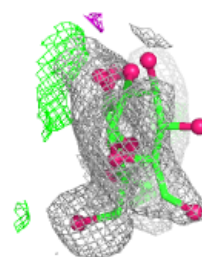
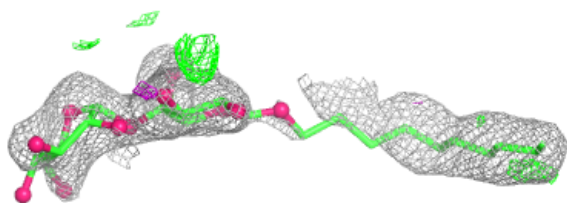
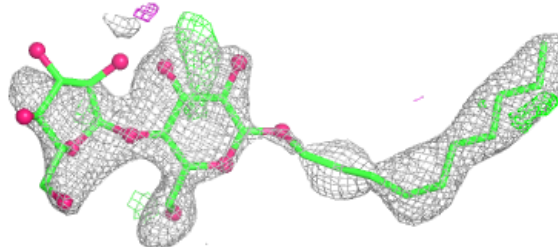
**Electron density around LFA C 307:**

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

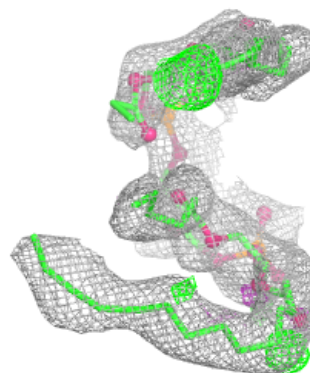
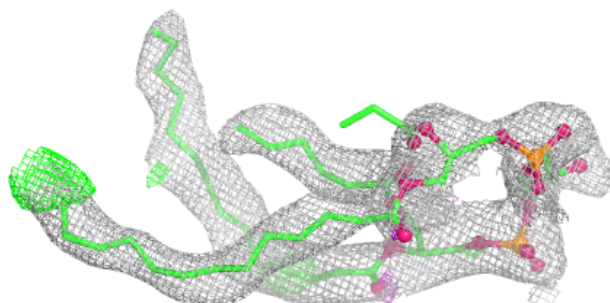
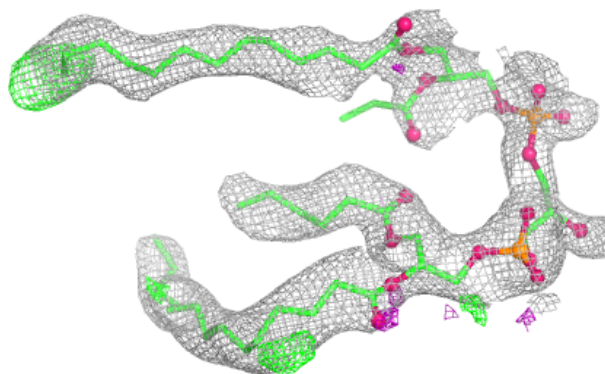


Electron density around DMU P 324:

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

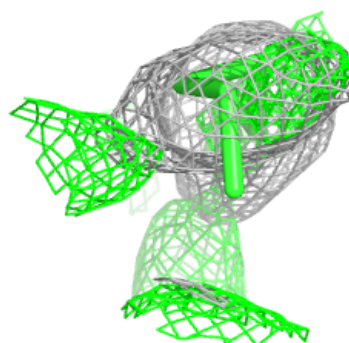
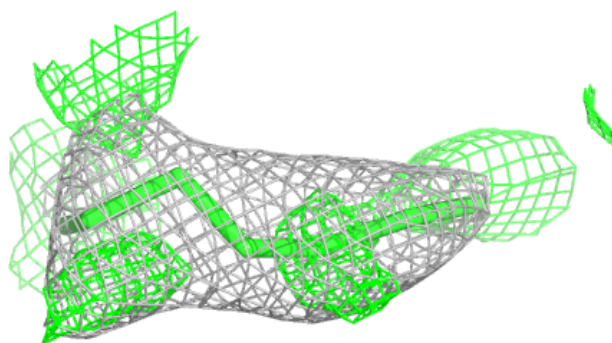
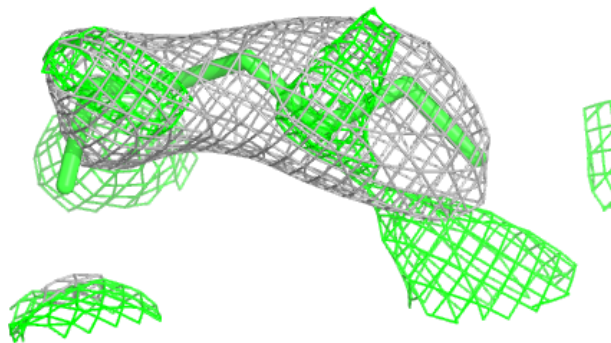
**Electron density around CDL V 101:**

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

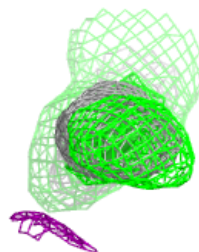
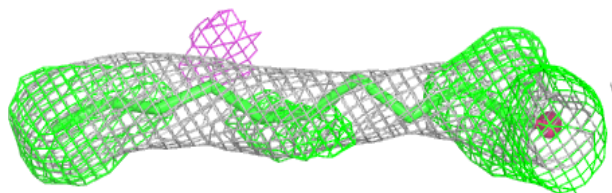
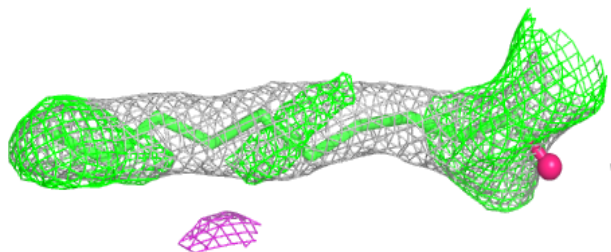


Electron density around DMU C 316:

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

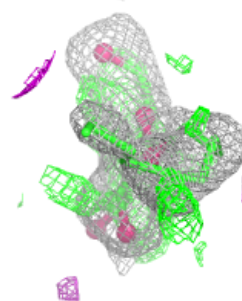
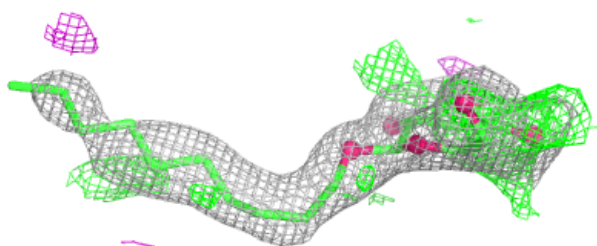
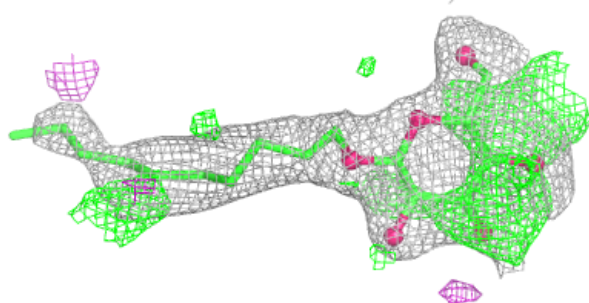
**Electron density around DMU O 305:**

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

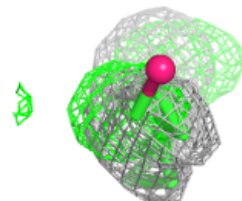
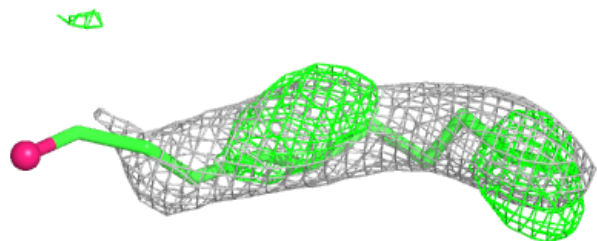
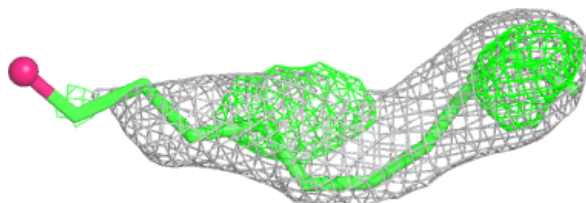


Electron density around DMU G 103:

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

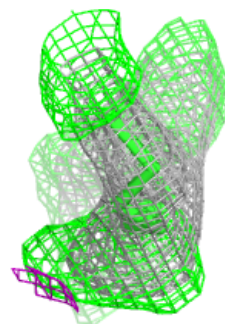
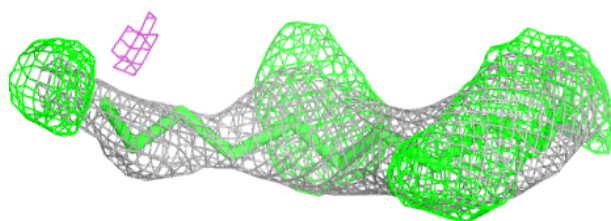
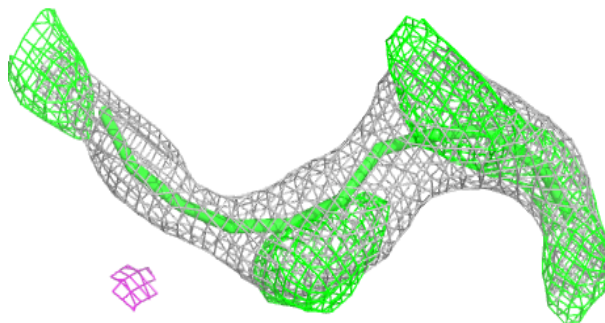
**Electron density around DMU J 101:**

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

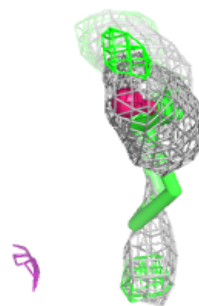
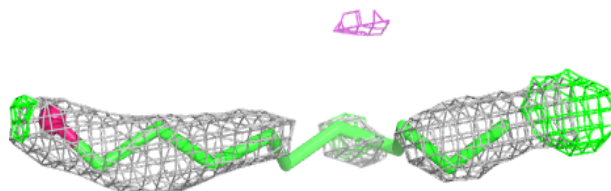
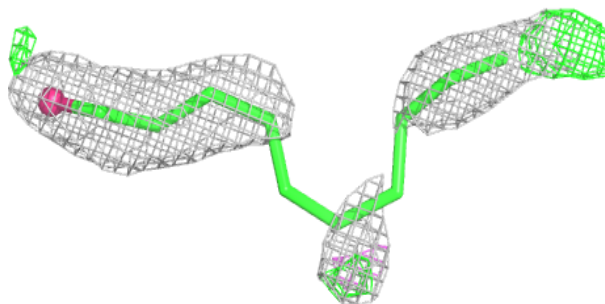


Electron density around LFA P 308:

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

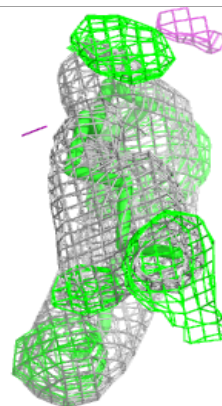
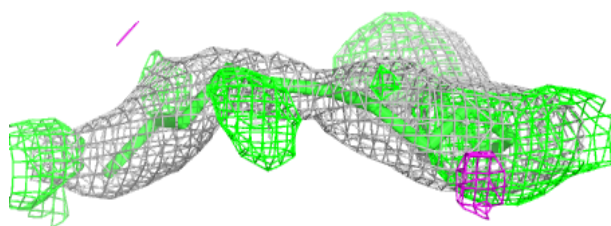
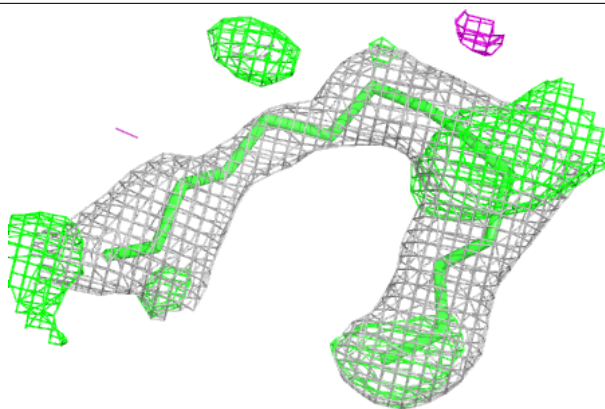
**Electron density around DMU N 602:**

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

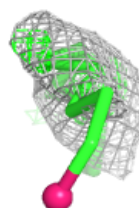
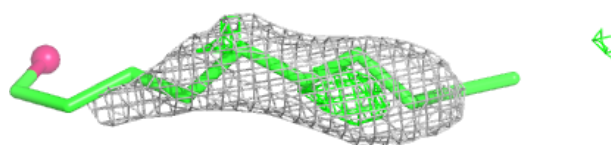
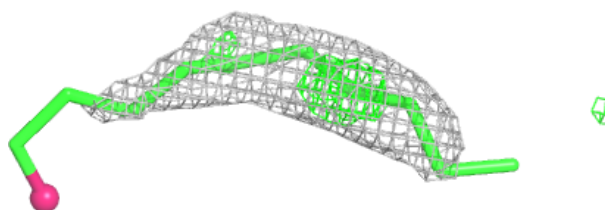


Electron density around LFA G 105:

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

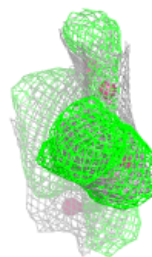
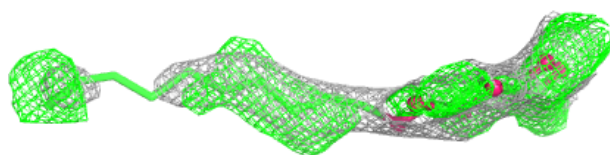
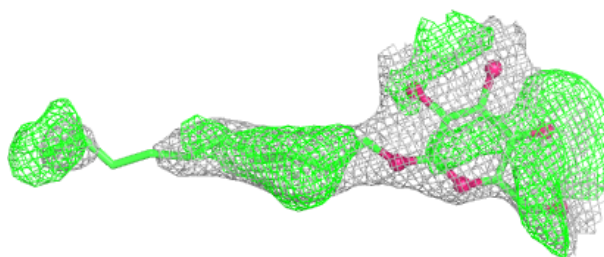
**Electron density around DMU W 101:**

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

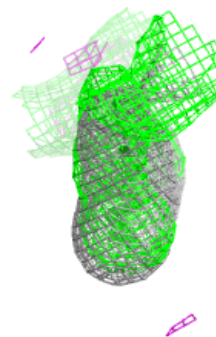
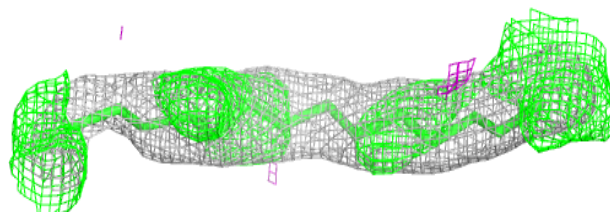
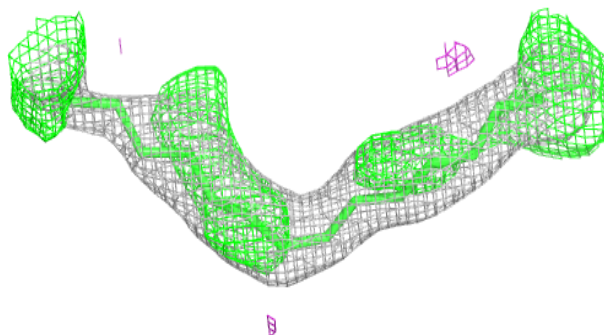


Electron density around DMU Y 102:

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

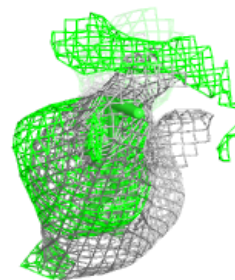
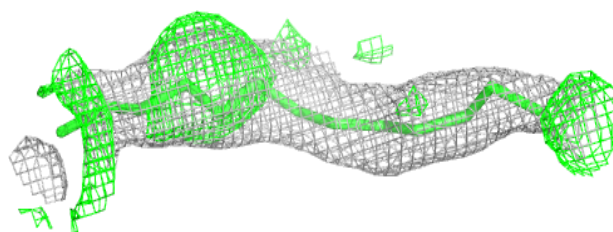
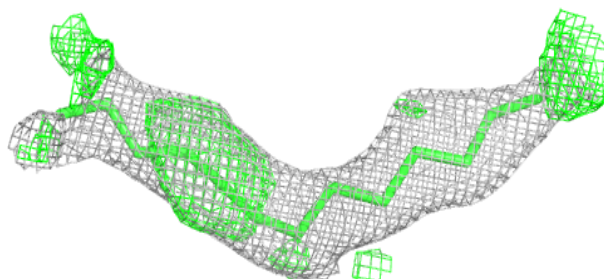
**Electron density around LFA A 608:**

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

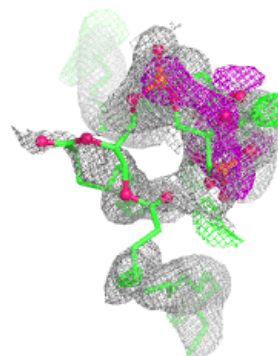
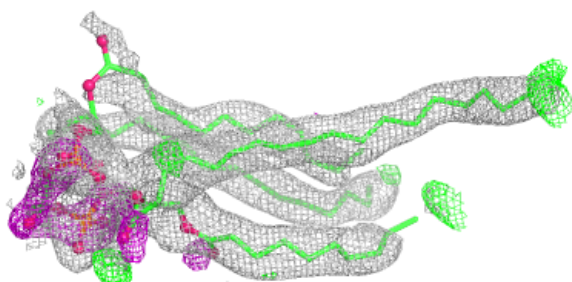
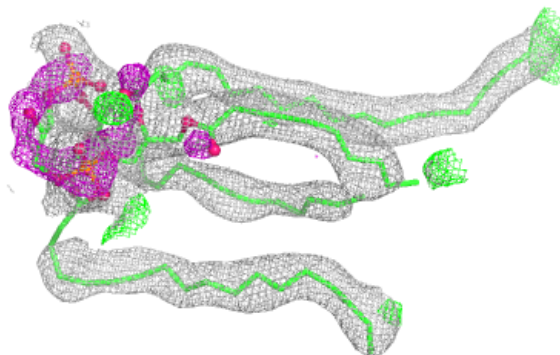


Electron density around LFA P 315:

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

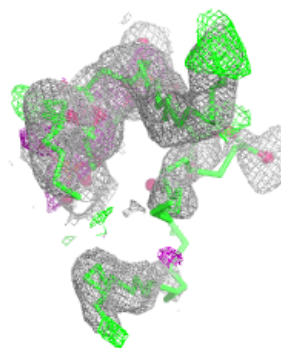
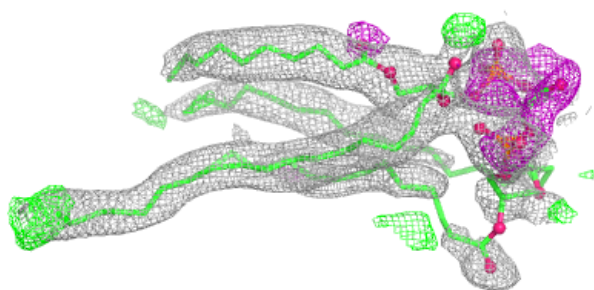
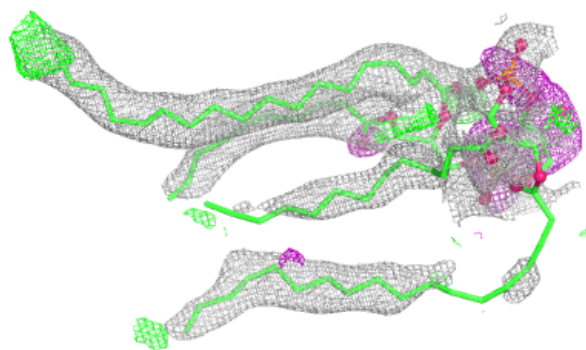
**Electron density around CDL C 304:**

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

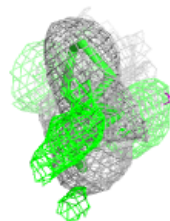
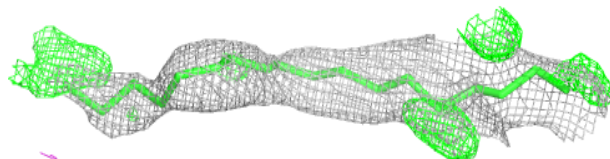
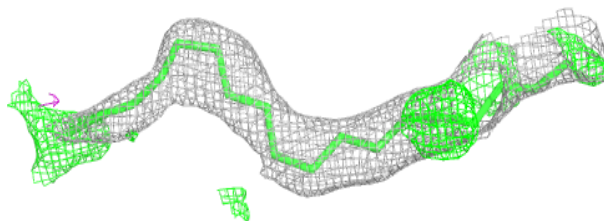


Electron density around CDL P 305:

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

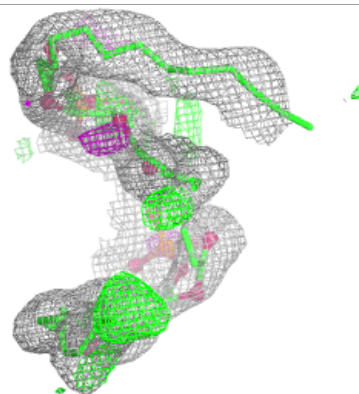
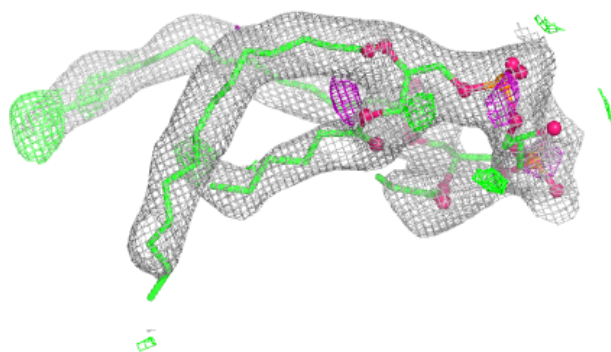
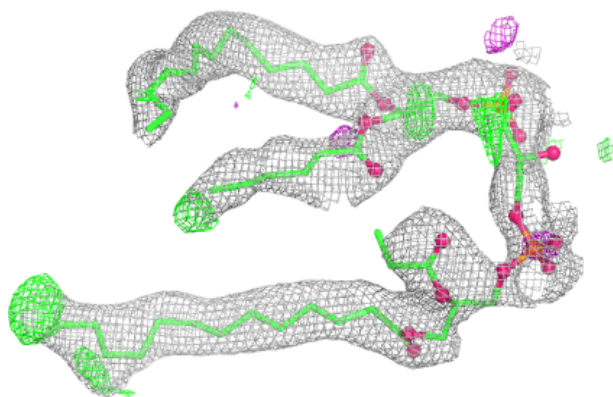
**Electron density around LFA P 310:**

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



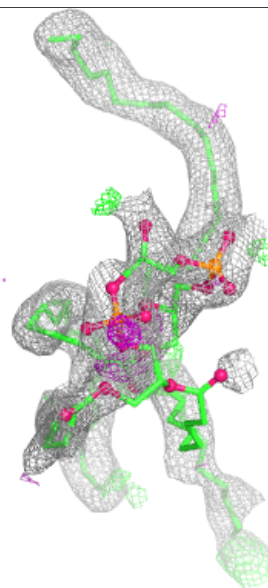
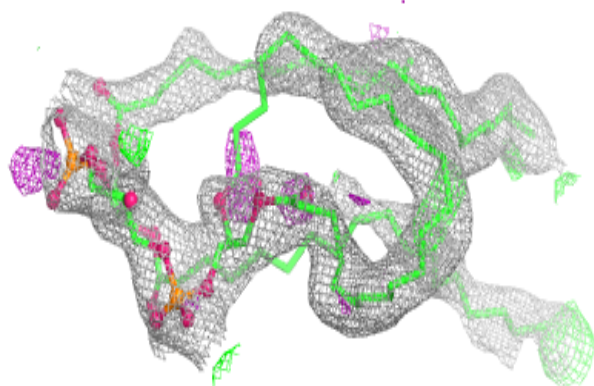
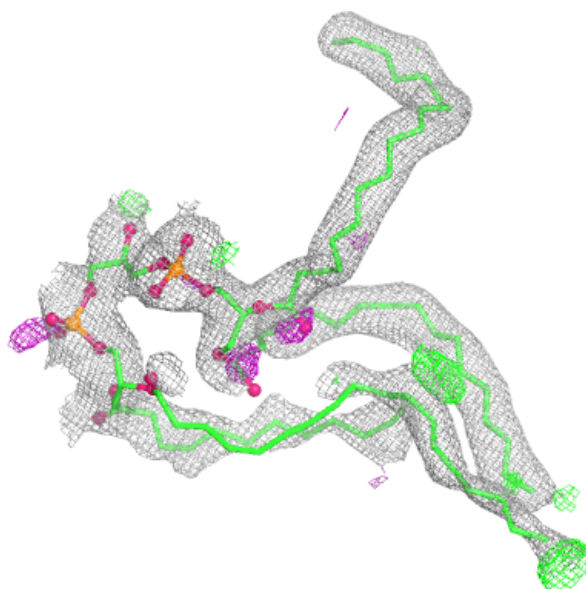
Electron density around CDL A 607:

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



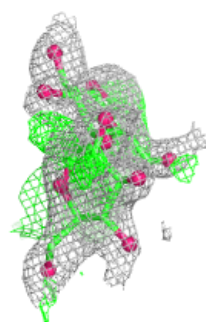
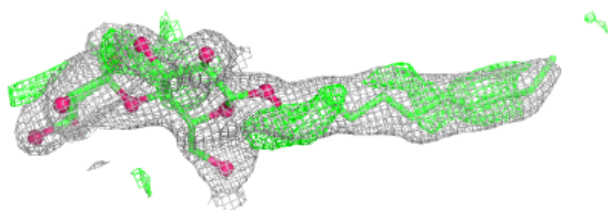
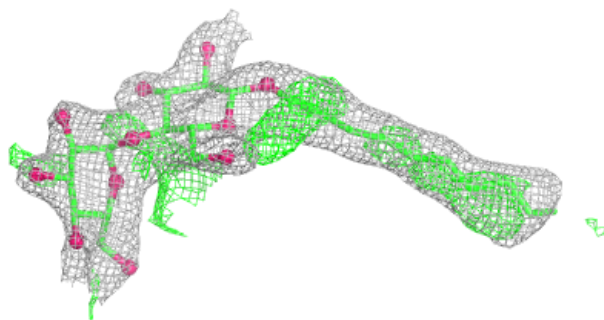
Electron density around CDL Y 101:

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

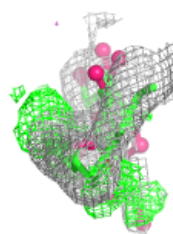
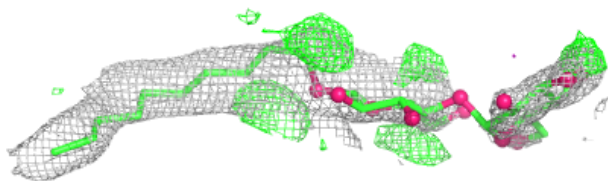
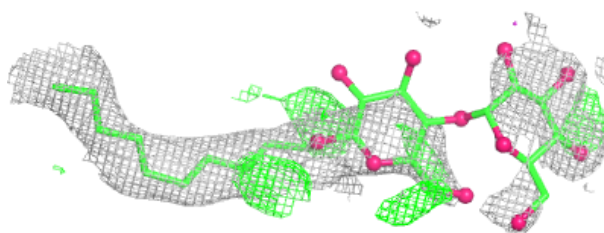


Electron density around DMU Q 201:

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

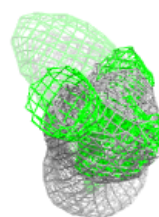
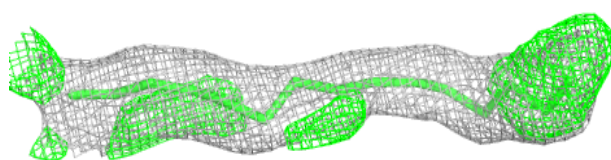
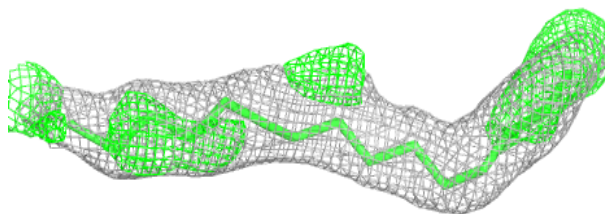
**Electron density around DMU U 101:**

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

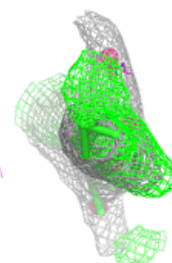
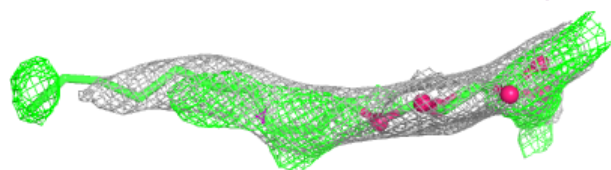
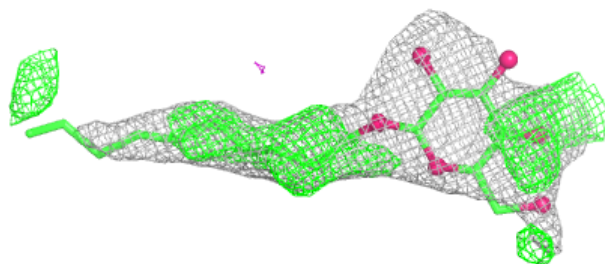


Electron density around LFA P 314:

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

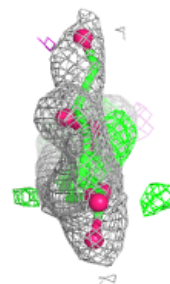
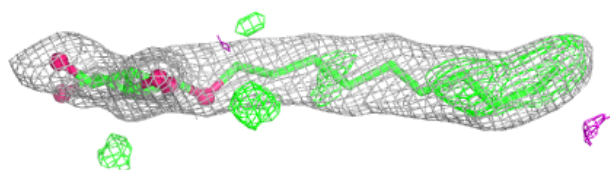
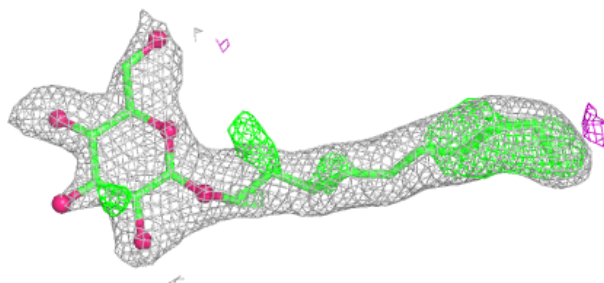
**Electron density around DMU L 102:**

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

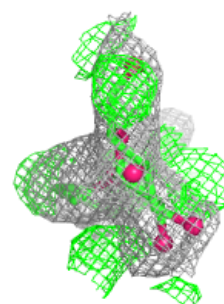
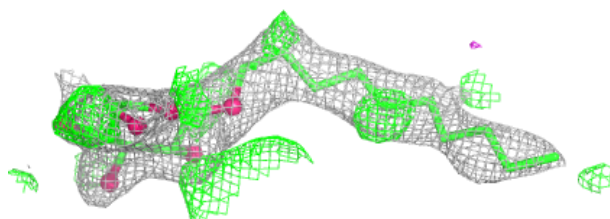
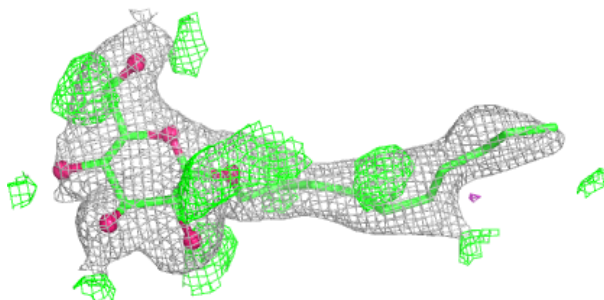


Electron density around DMU O 307:

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

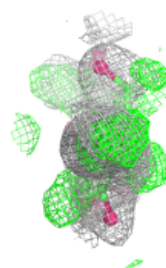
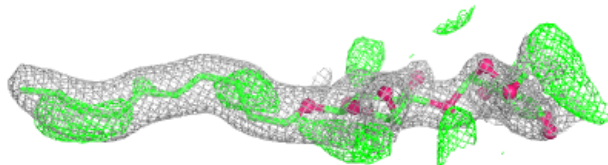
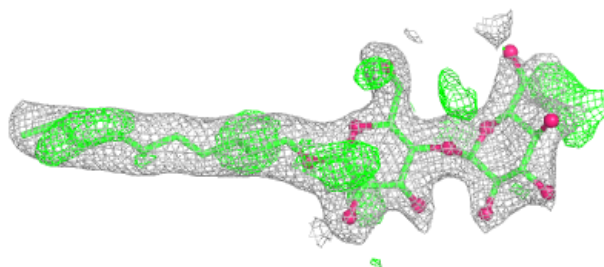
**Electron density around DMU T 103:**

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

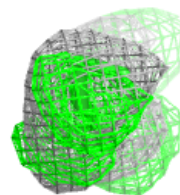
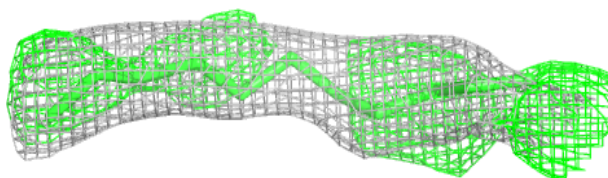
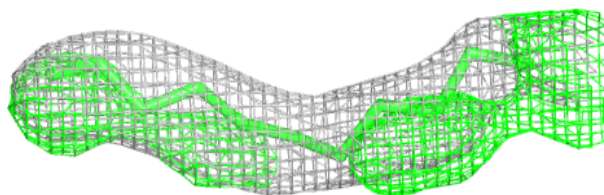


Electron density around DMU A 611:

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

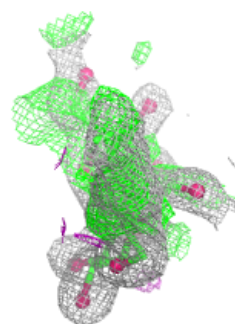
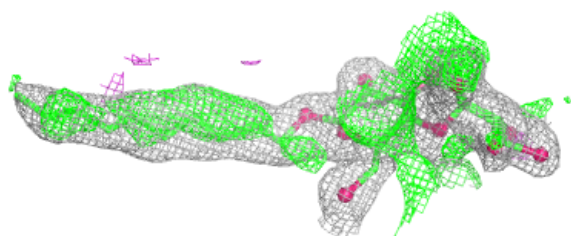
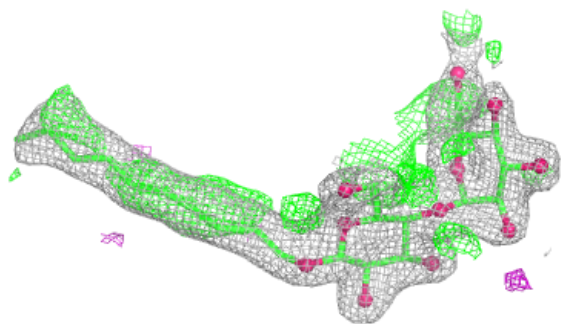
**Electron density around LFA T 102:**

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

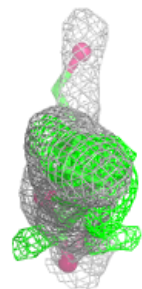
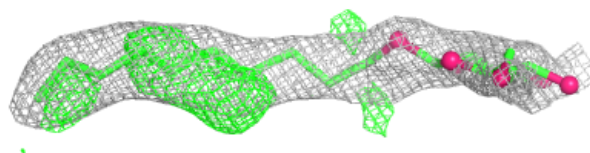
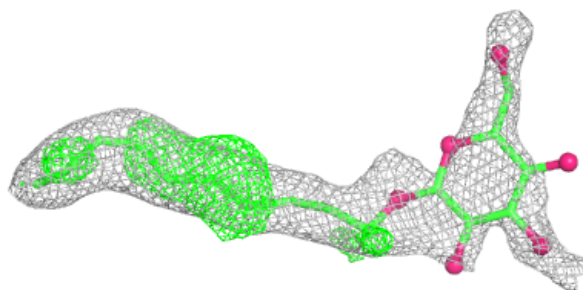


Electron density around DMU D 201:

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

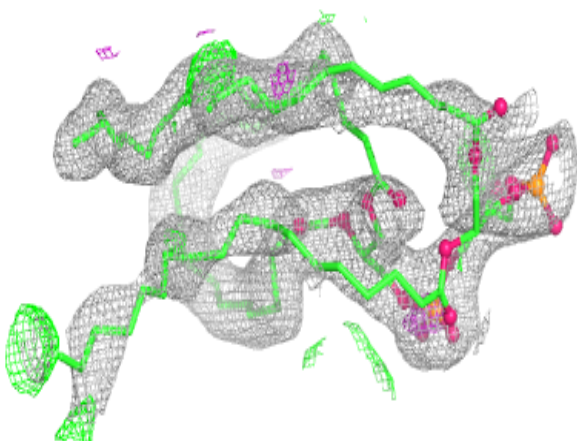
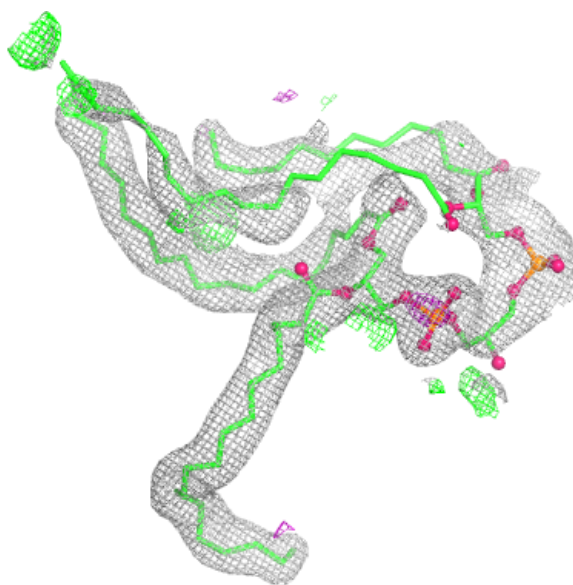
**Electron density around DMU B 305:**

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



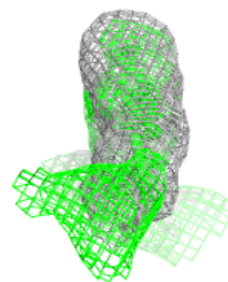
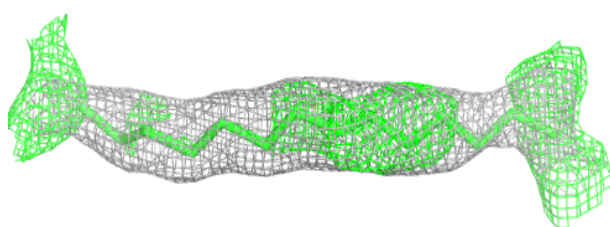
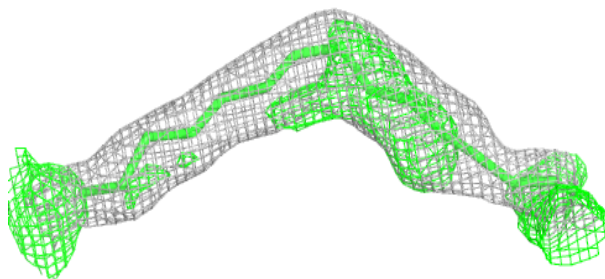
Electron density around CDL L 101:

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

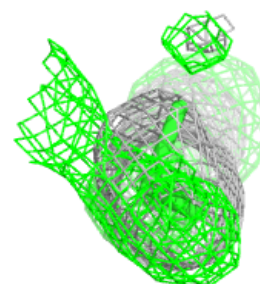
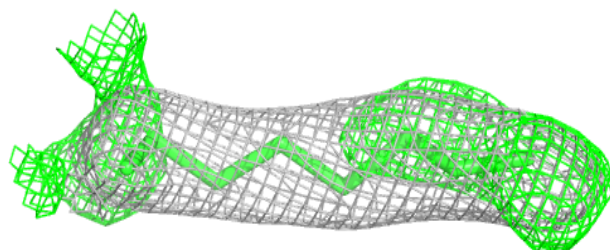
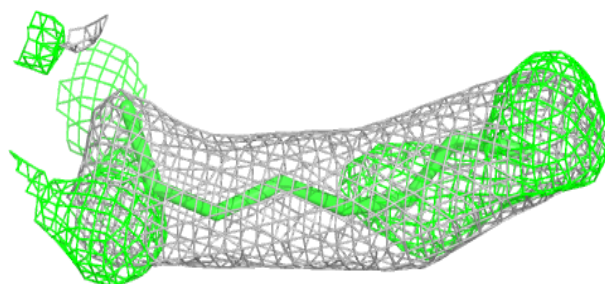


Electron density around LFA N 609:

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

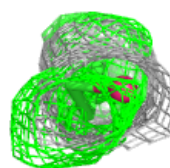
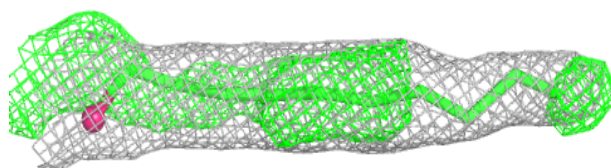
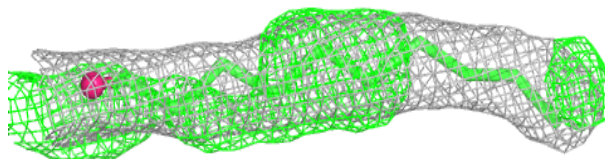
**Electron density around DMU Z 102:**

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

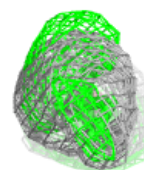
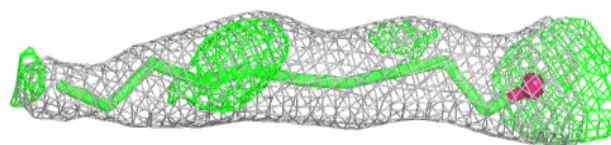
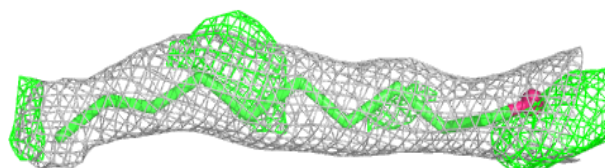


Electron density around DMU P 307:

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

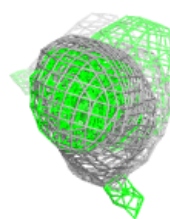
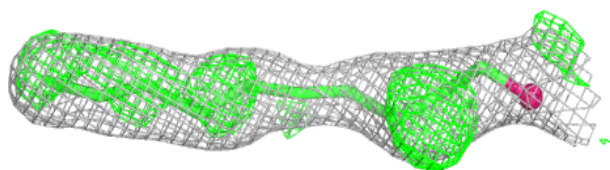
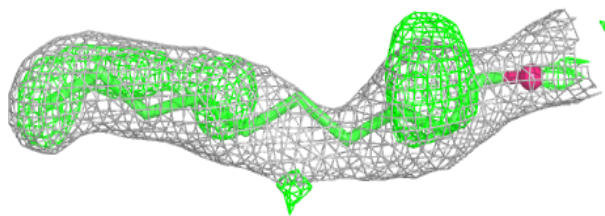
**Electron density around DMU C 306:**

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

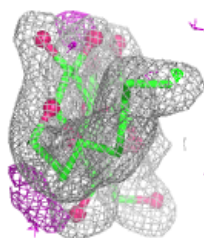
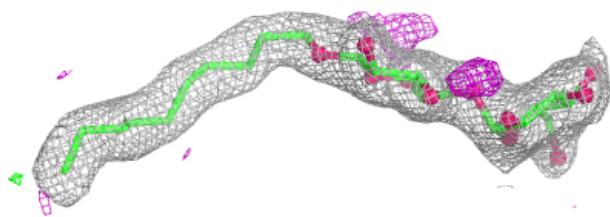
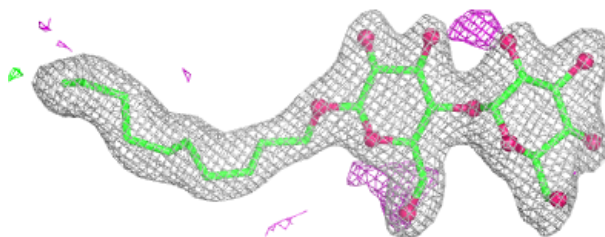


Electron density around DMU O 306:

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

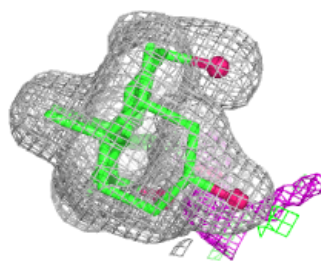
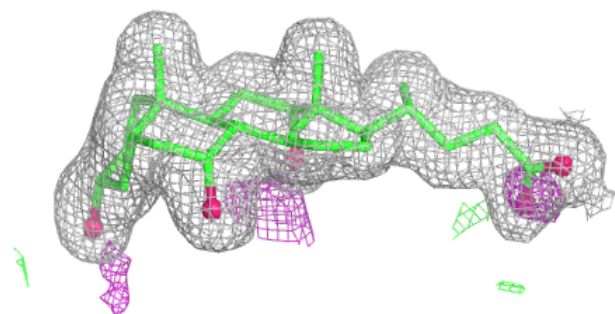
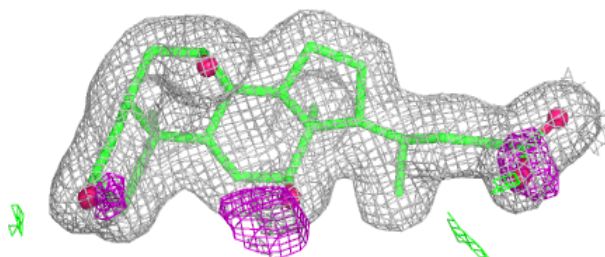
**Electron density around DMU Z 101:**

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

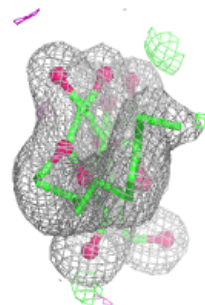
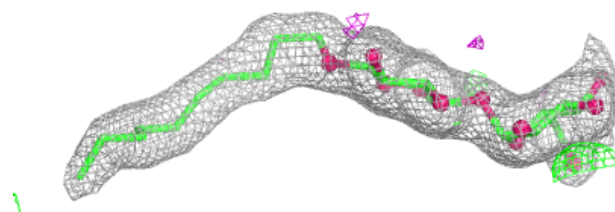
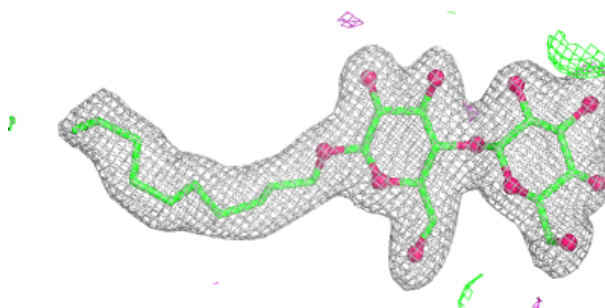


Electron density around CHD C 301:

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

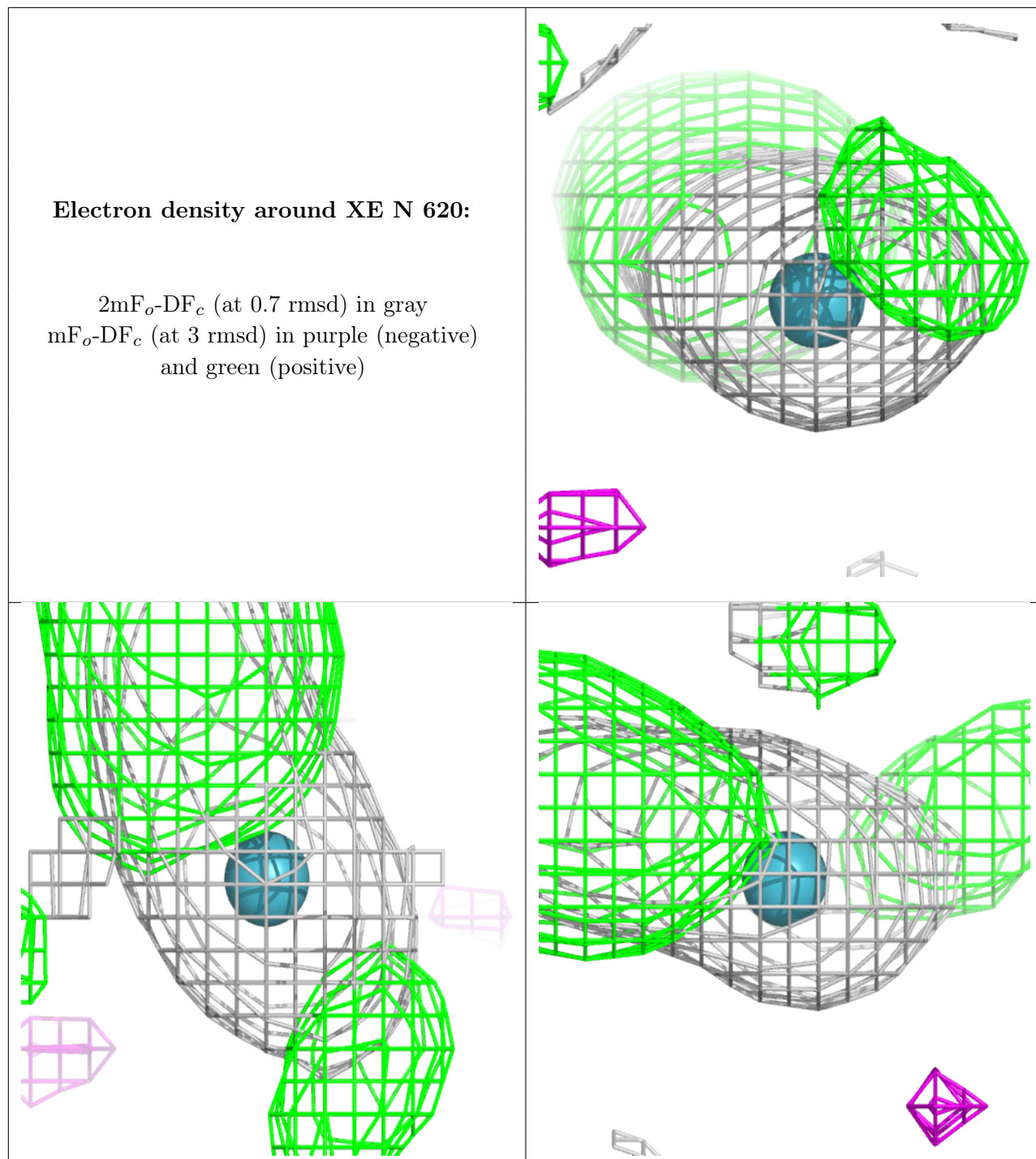
**Electron density around DMU M 101:**

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



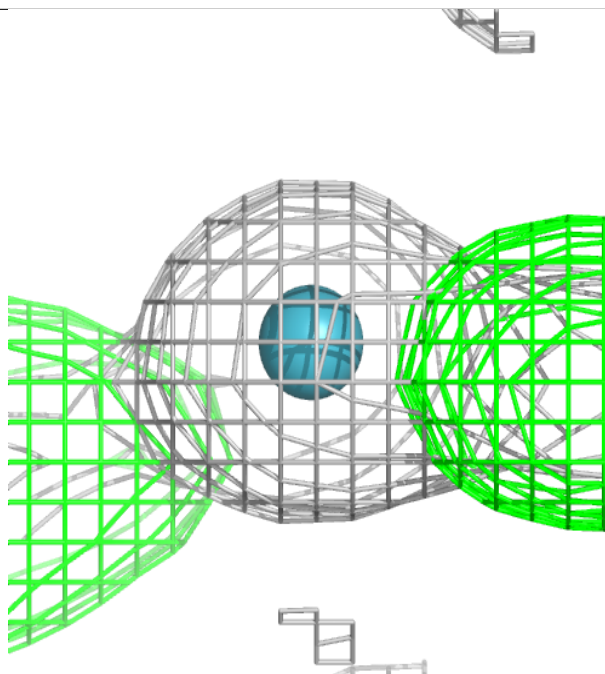
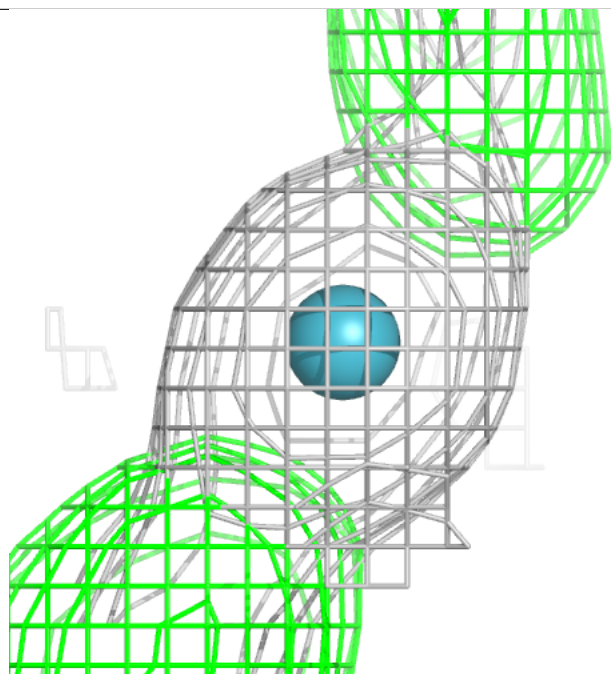
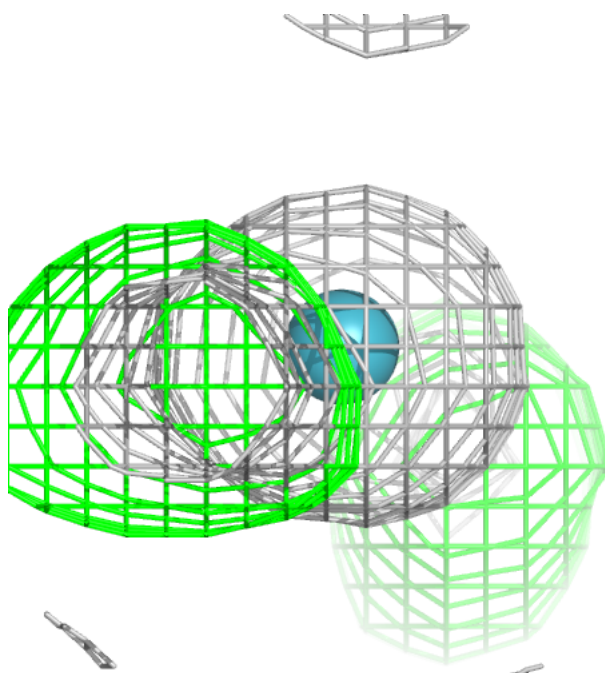
Electron density around XE N 620:

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



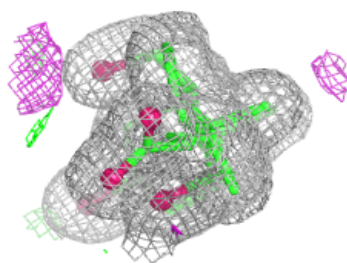
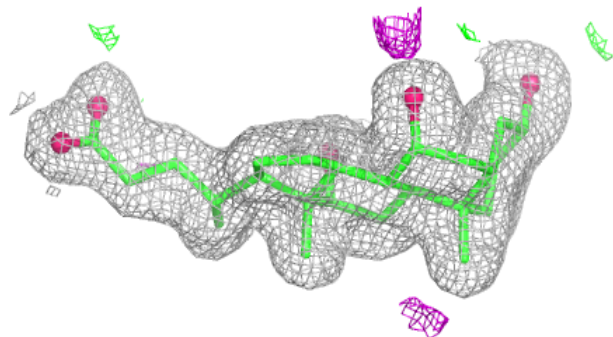
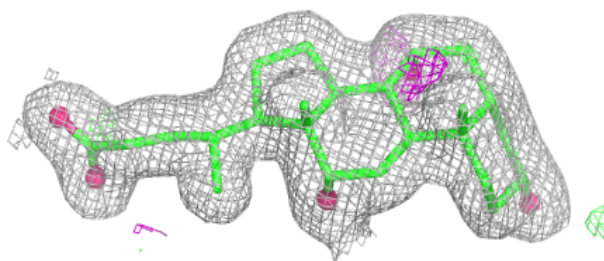
Electron density around XE A 619:

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

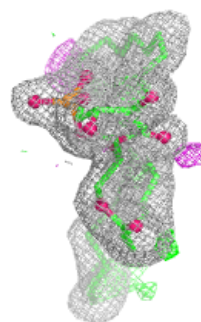
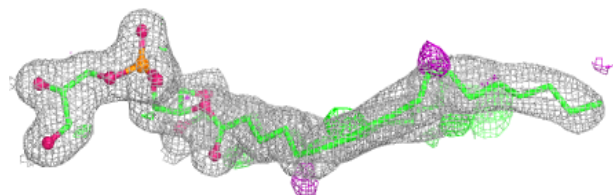
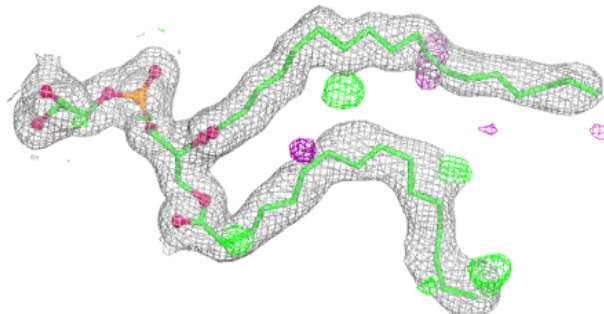


Electron density around CHD P 302:

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

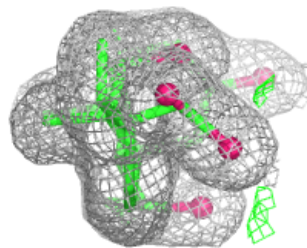
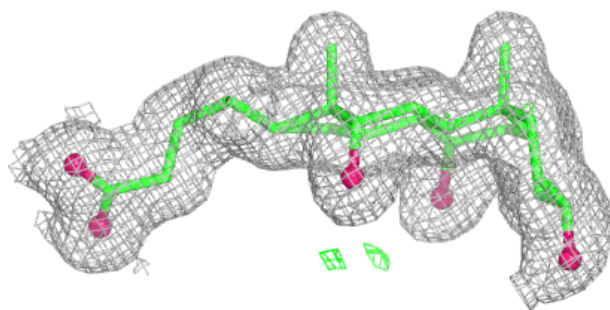
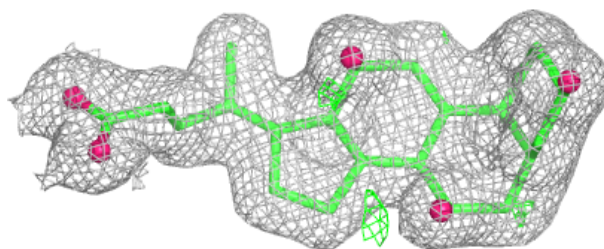
**Electron density around PGV N 622:**

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

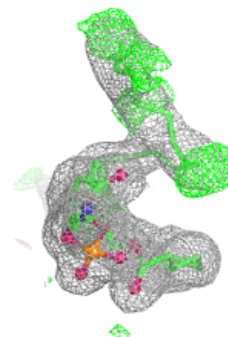
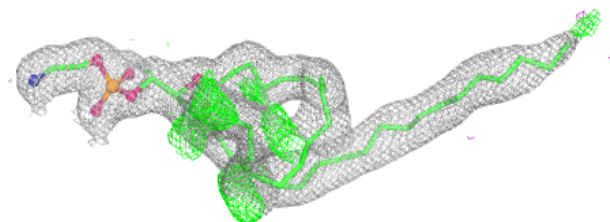
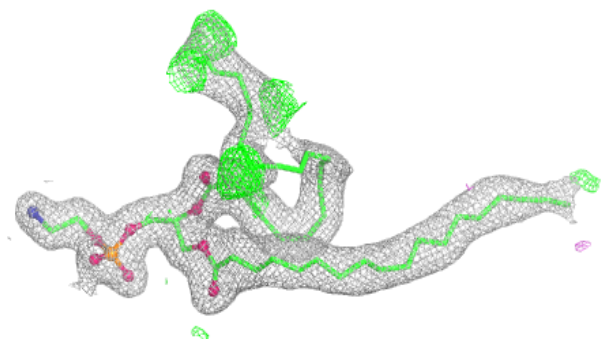


Electron density around CHD B 307:

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

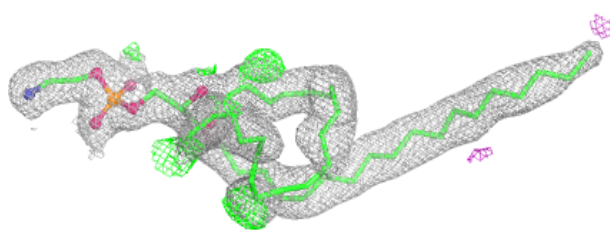
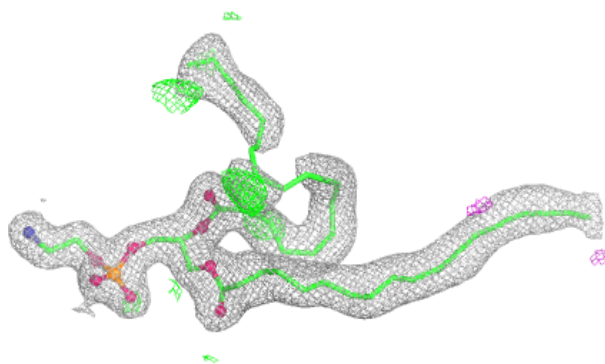
**Electron density around PEK G 101:**

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

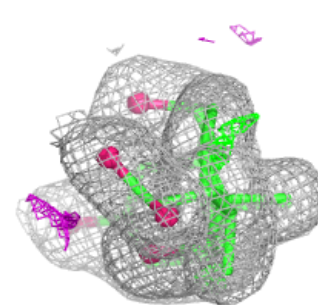
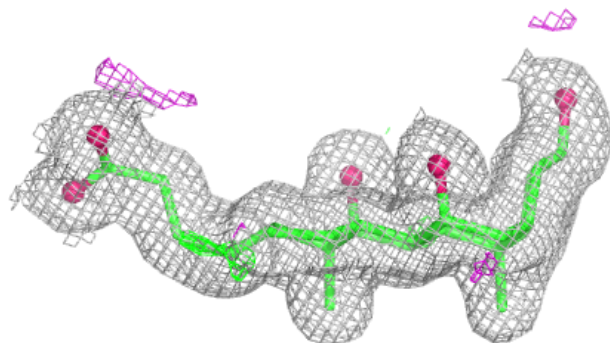
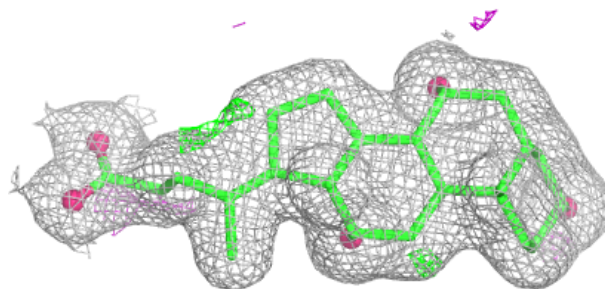


Electron density around PEK T 101:

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

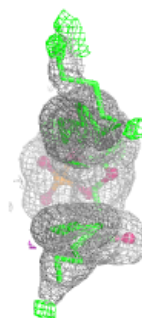
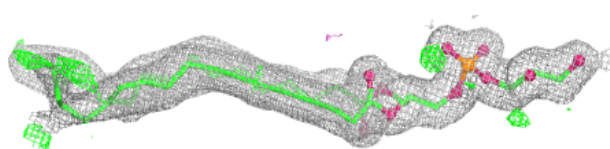
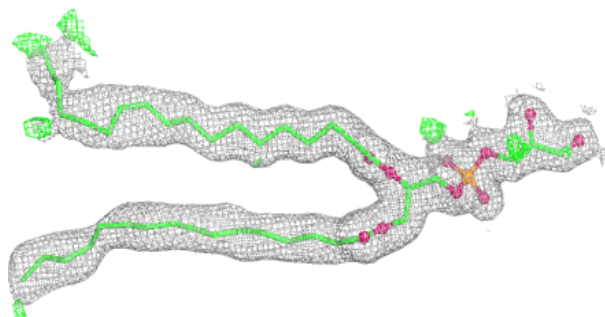
**Electron density around CHD G 102:**

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

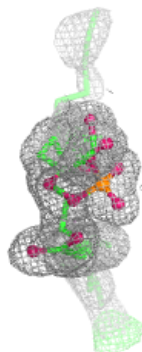
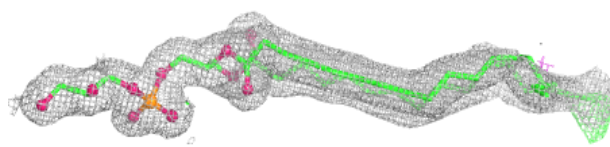
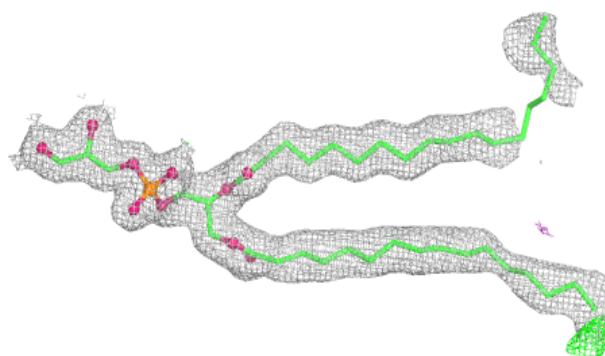


Electron density around PGV C 303:

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

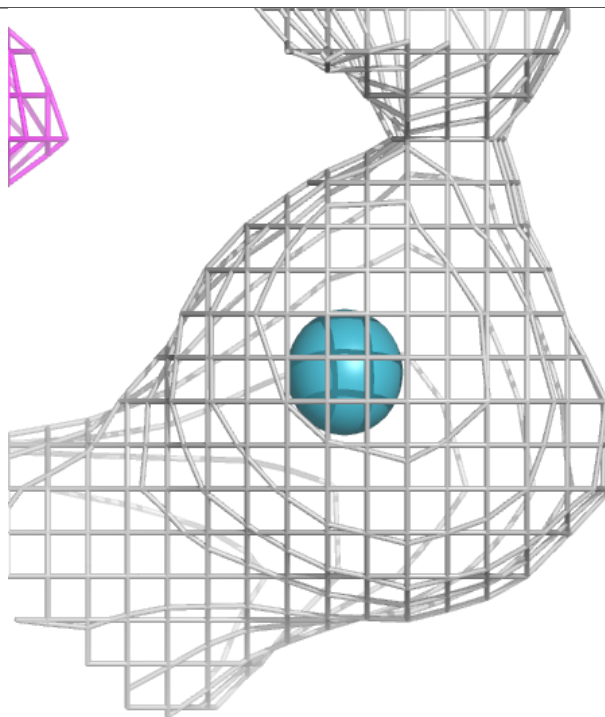
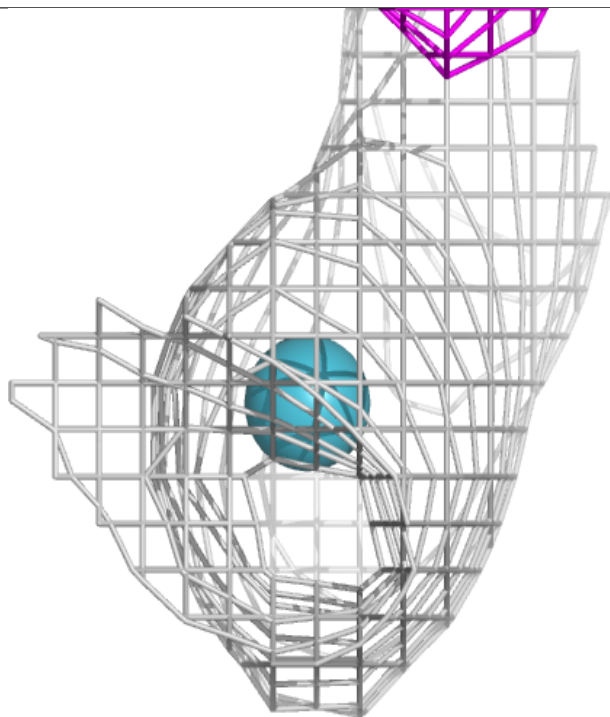
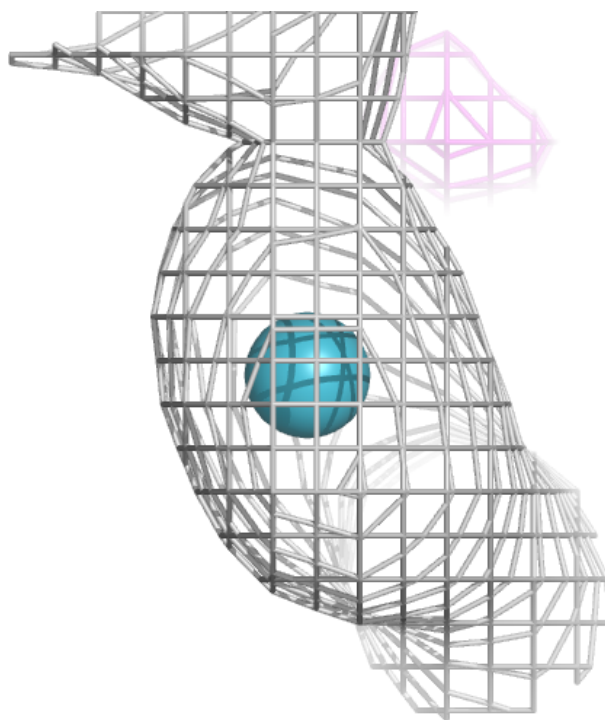
**Electron density around PGV P 304:**

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



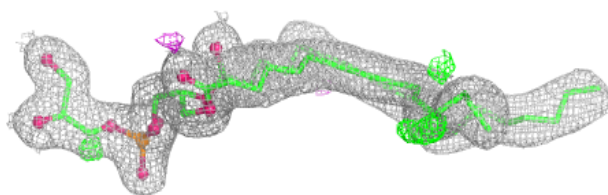
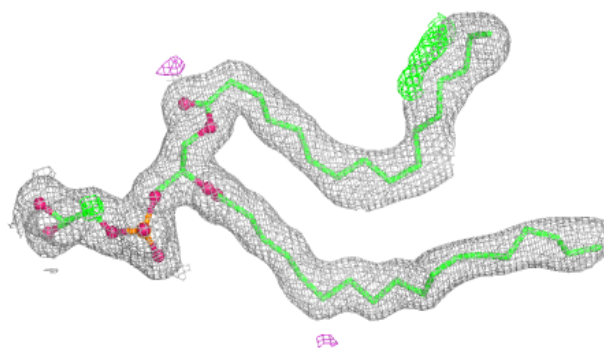
Electron density around XE P 325:

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

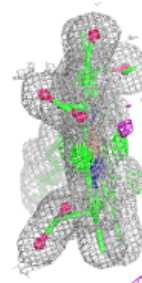
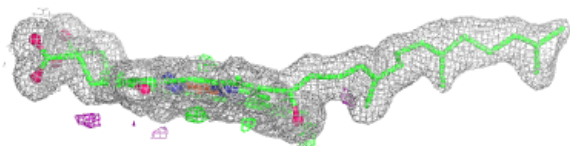
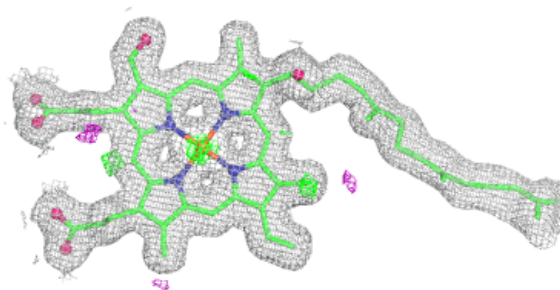


Electron density around PGV A 621:

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

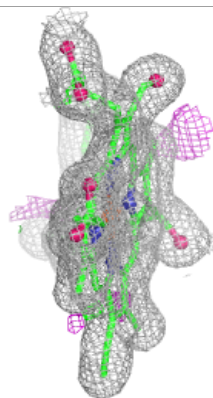
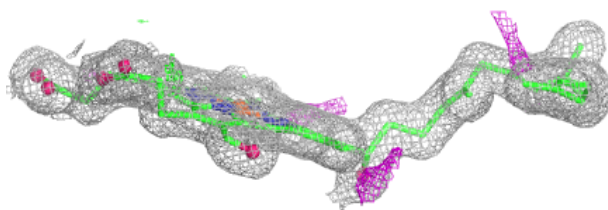
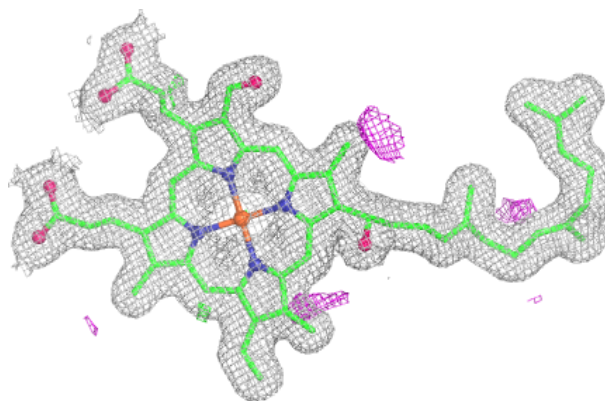
**Electron density around HEA A 601 (B):**

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

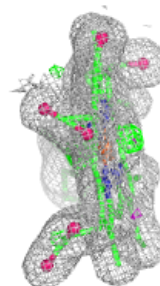
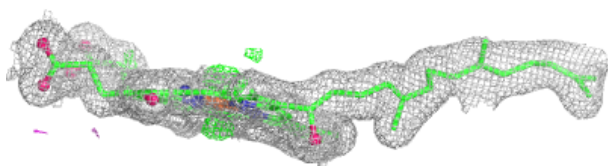
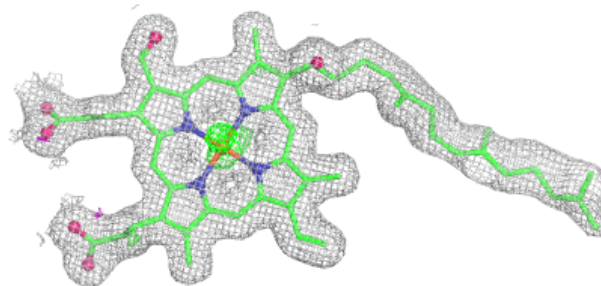


Electron density around HEA A 602:

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

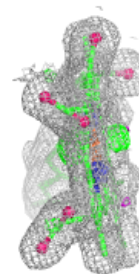
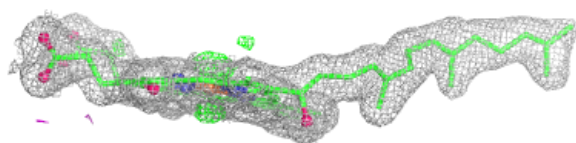
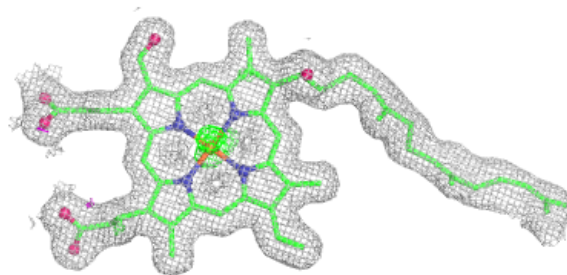
**Electron density around HEA N 603 (A):**

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

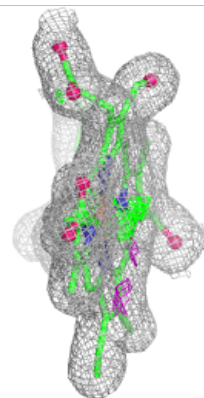
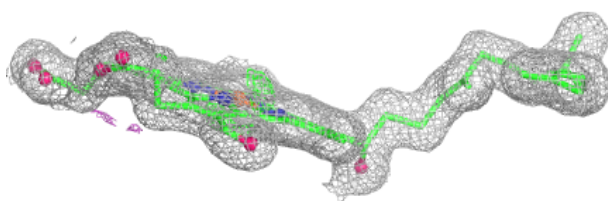
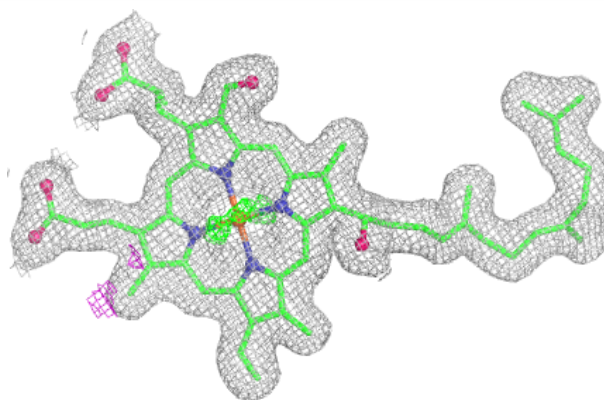


Electron density around HEA N 603 (B):

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

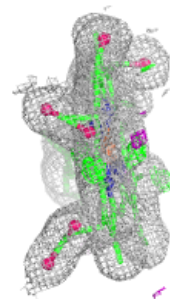
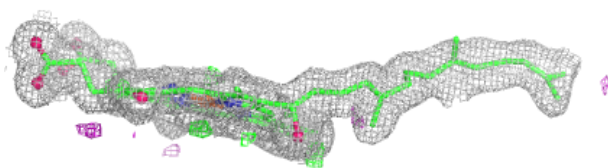
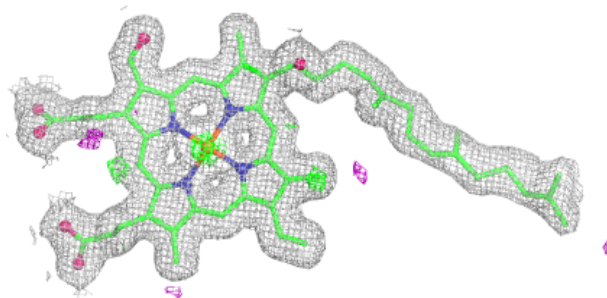
**Electron density around HEA N 604:**

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



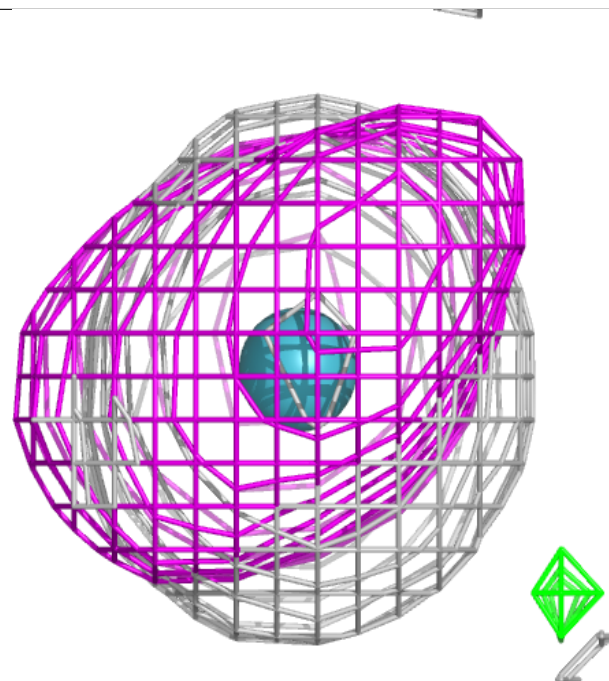
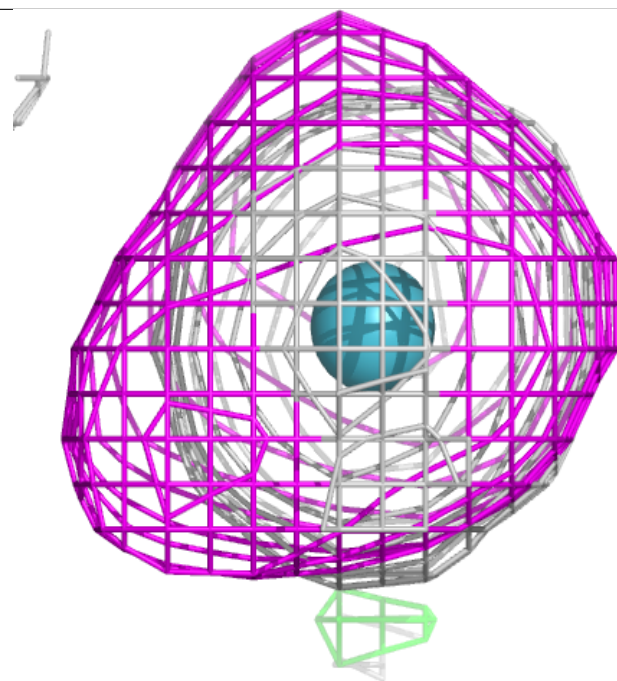
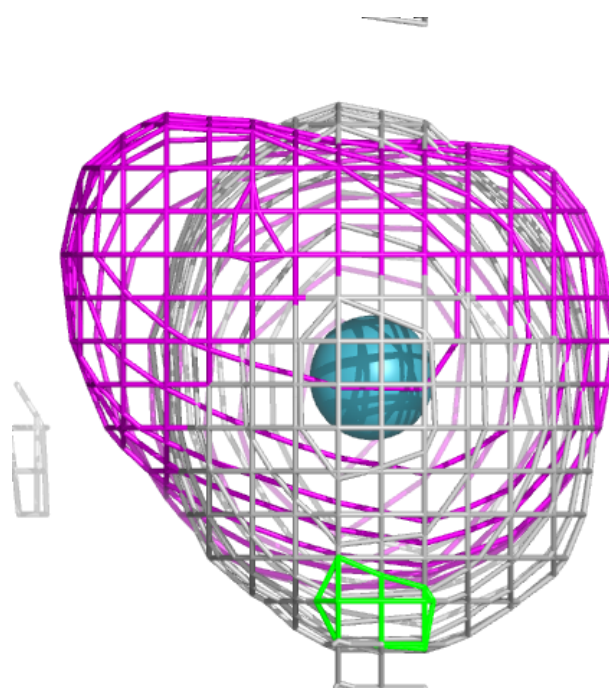
Electron density around HEA A 601 (A):

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



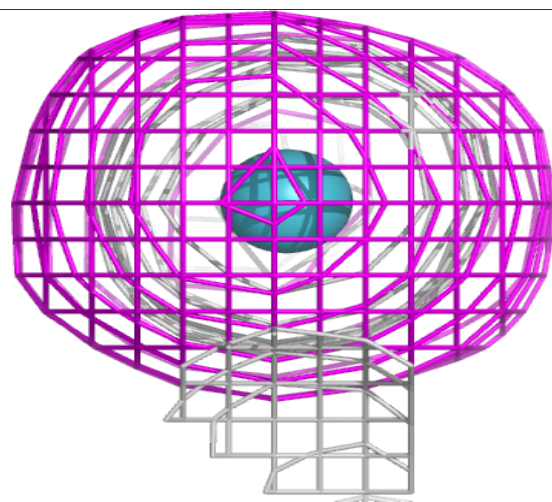
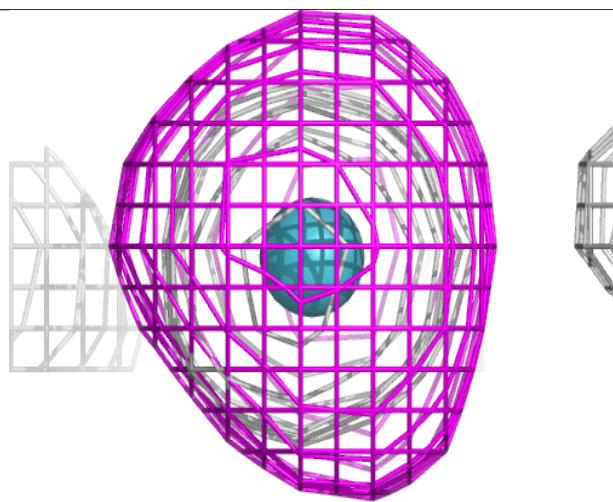
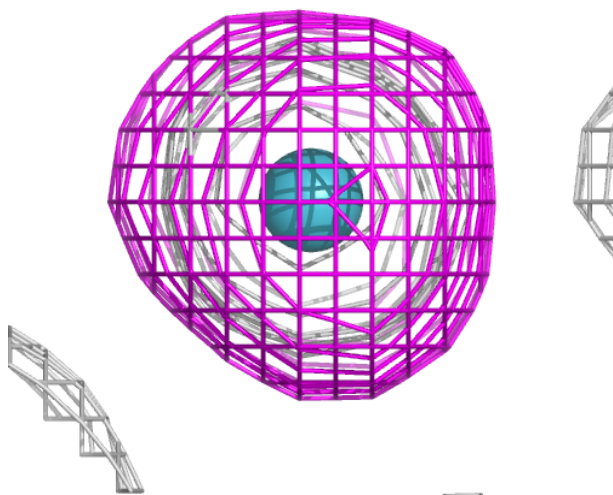
Electron density around XE A 620:

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



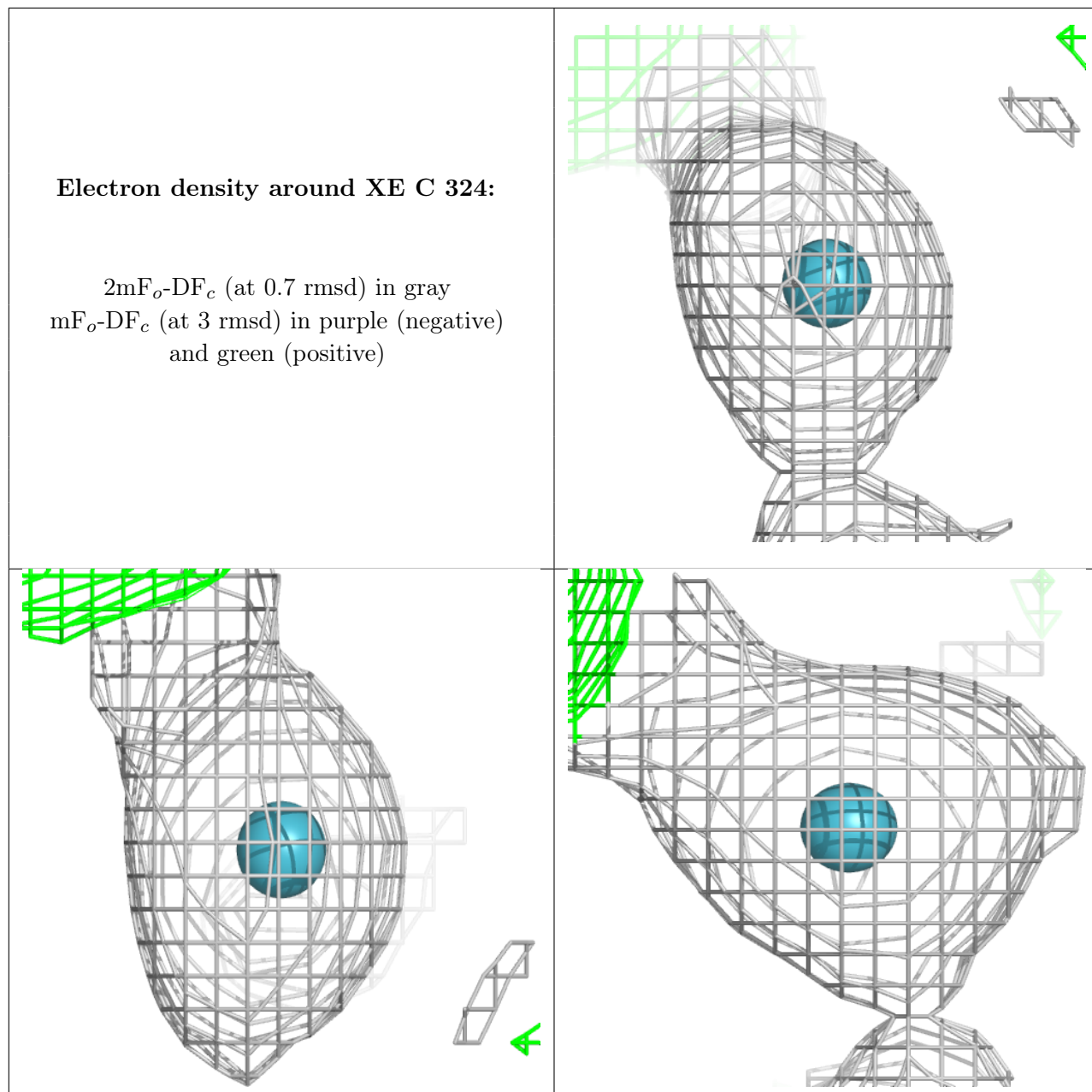
Electron density around XE B 301:

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



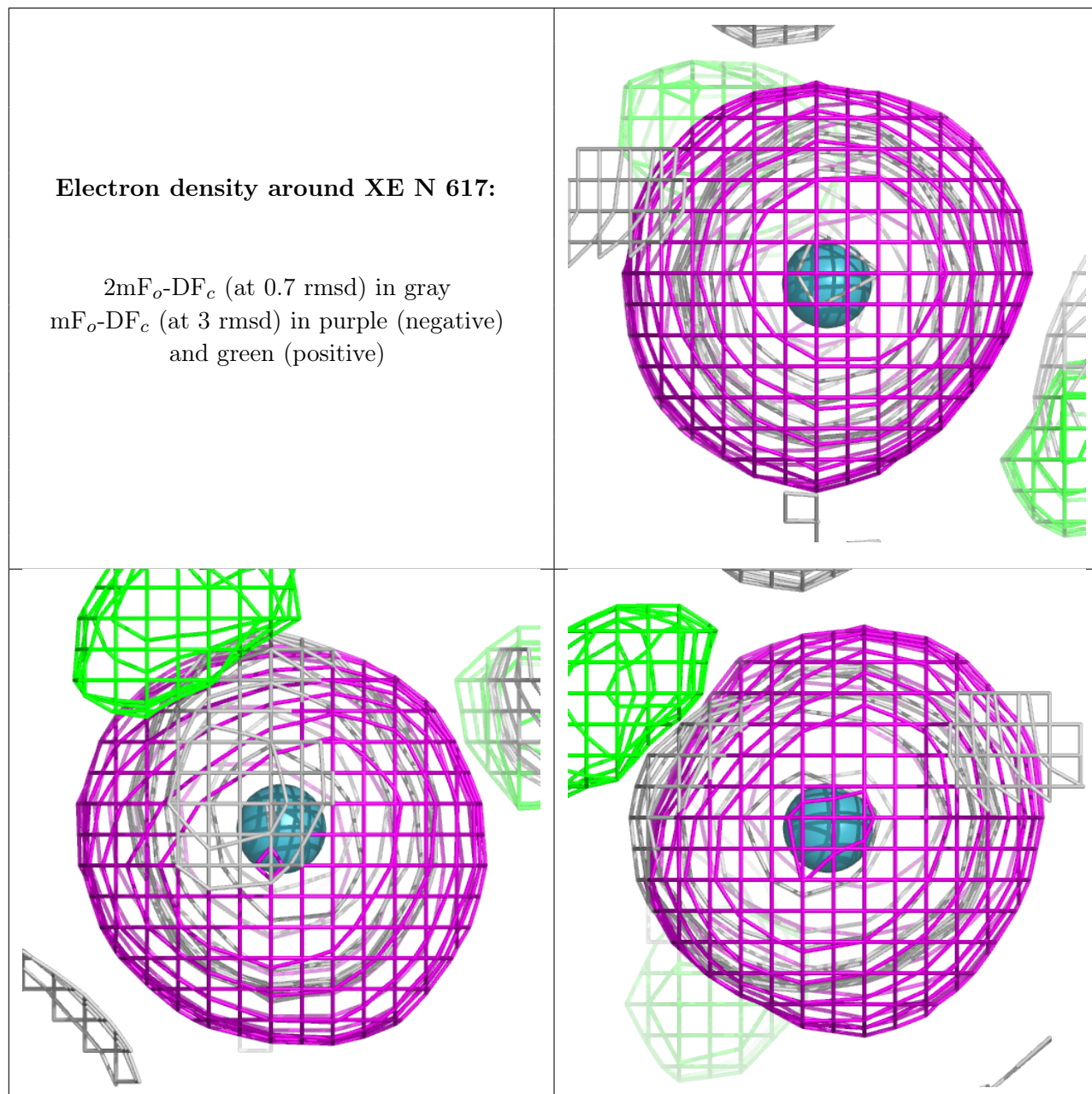
Electron density around XE C 324:

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



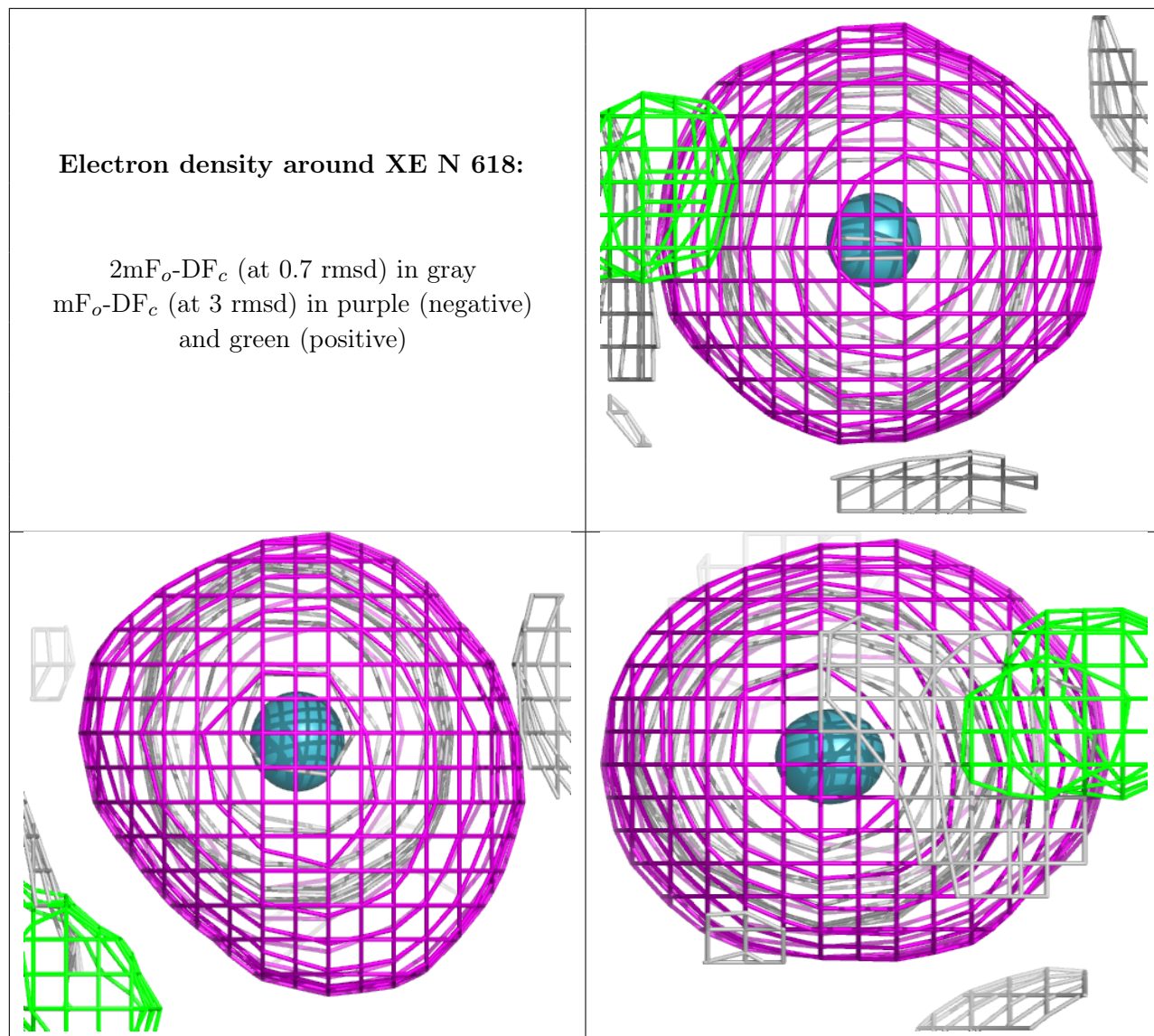
Electron density around XE N 617:

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



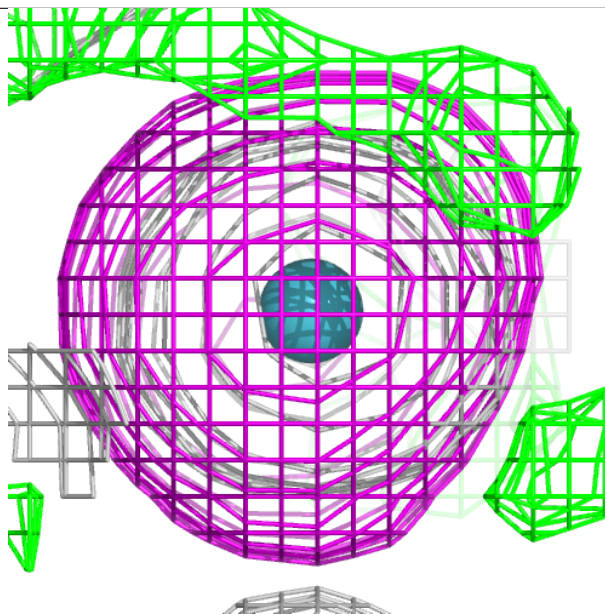
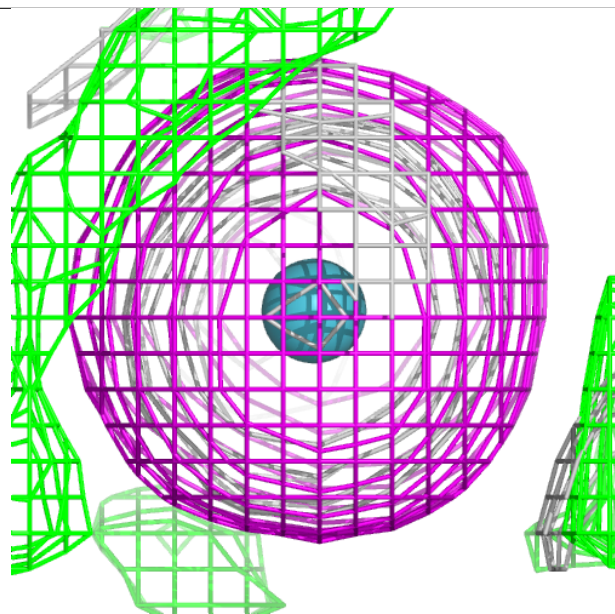
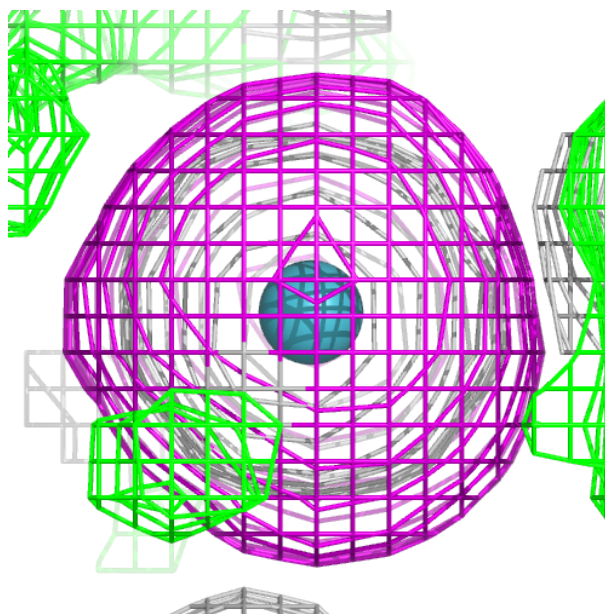
Electron density around XE N 618:

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



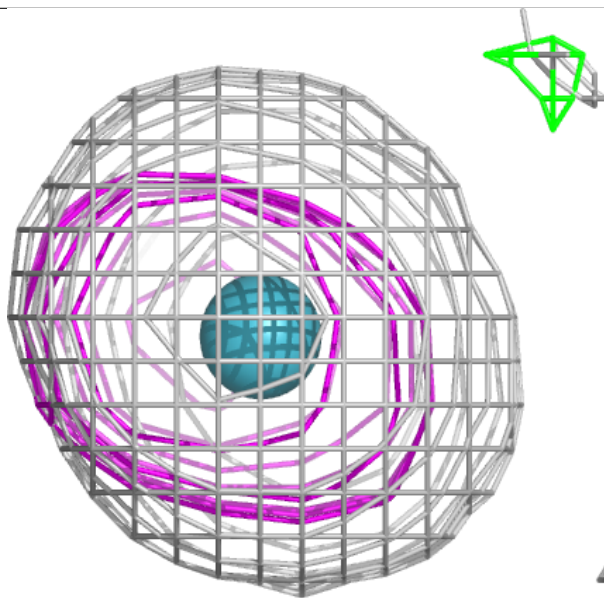
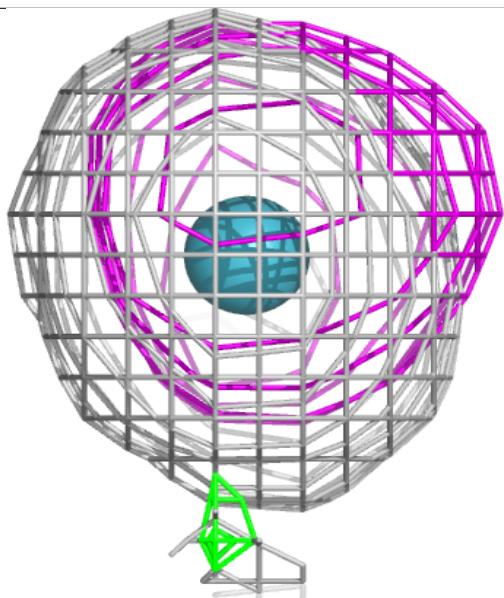
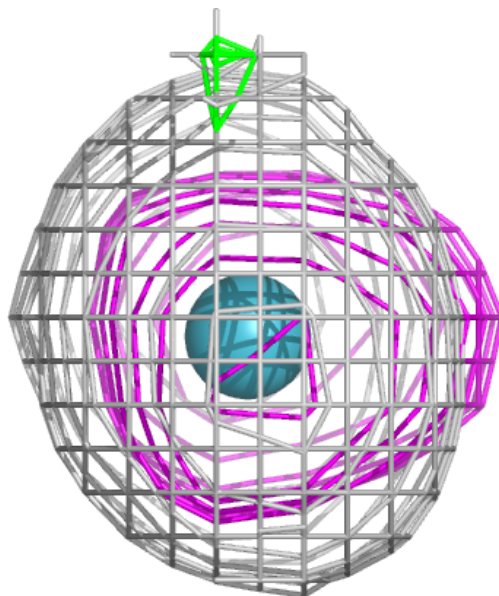
Electron density around XE A 616:

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



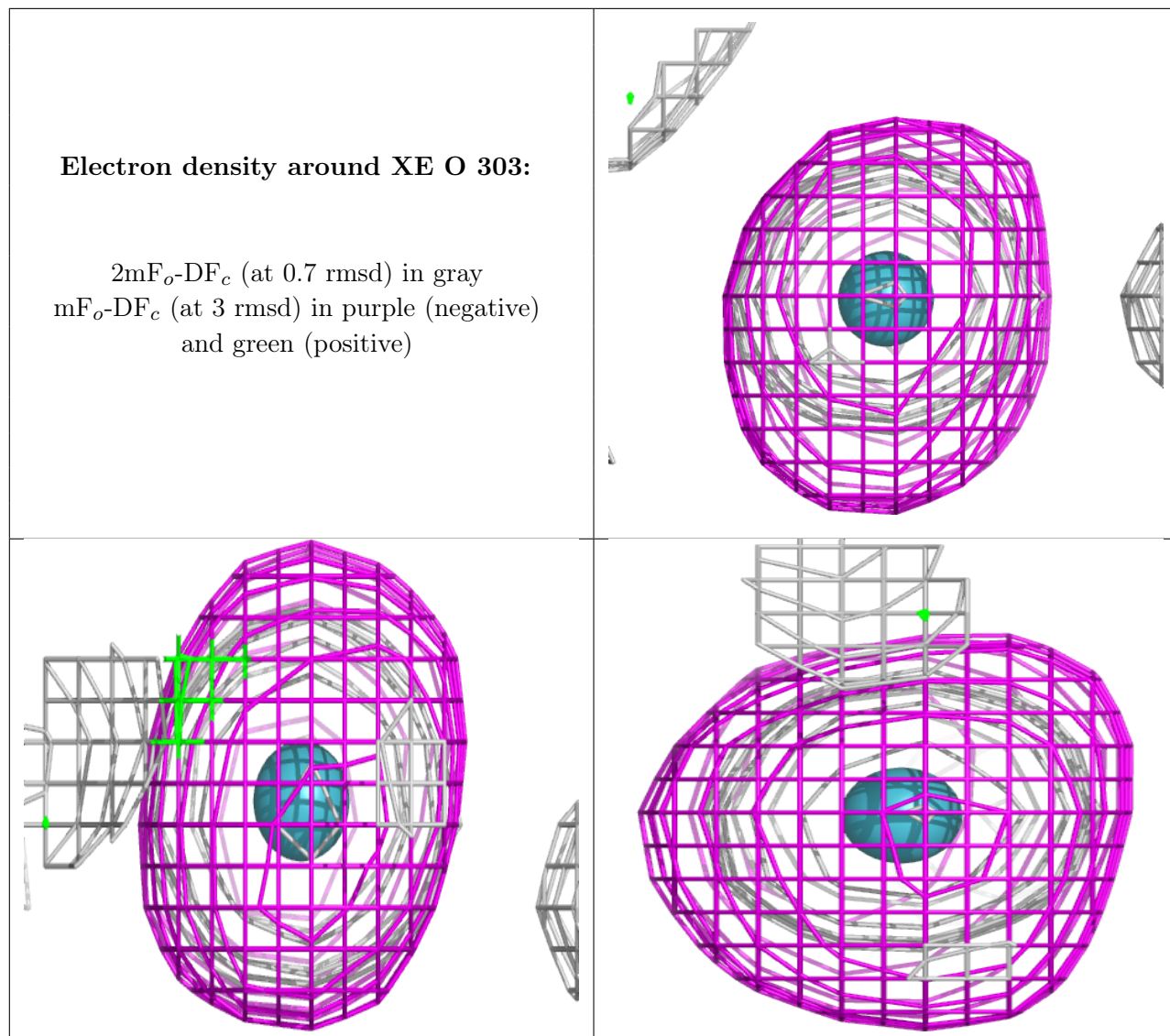
Electron density around XE N 621:

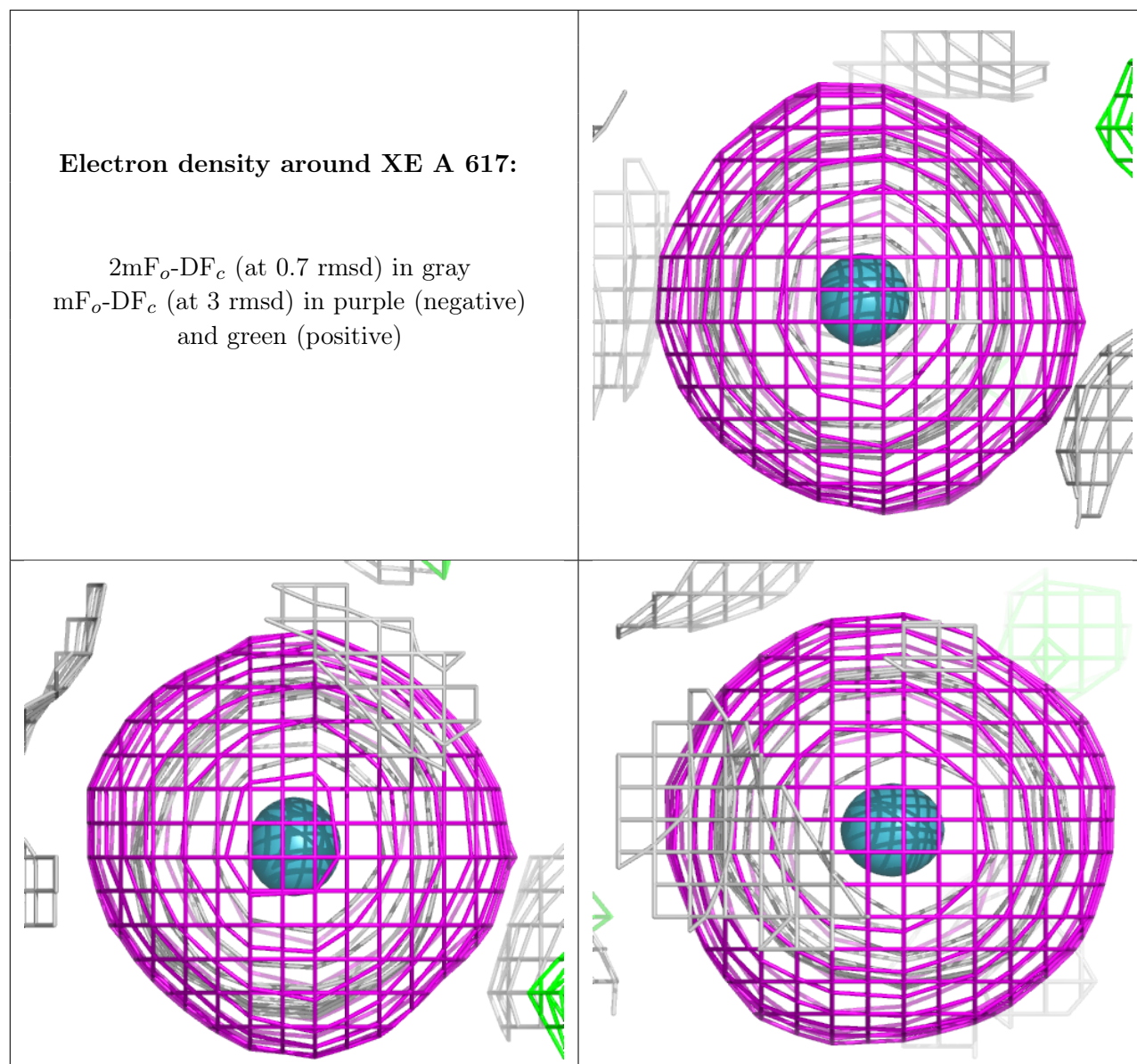
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around XE O 303:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.