



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 06:54 PM UTC

PDB ID : 8H8R / pdb_00008h8r
Title : Bovine Heart Cytochrome c Oxidase in the Calcium-bound Fully Oxidized State
Authors : Muramoto, K.; Shinzawa-Itoh, K.
Deposited on : 2022-10-24
Resolution : 1.70 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

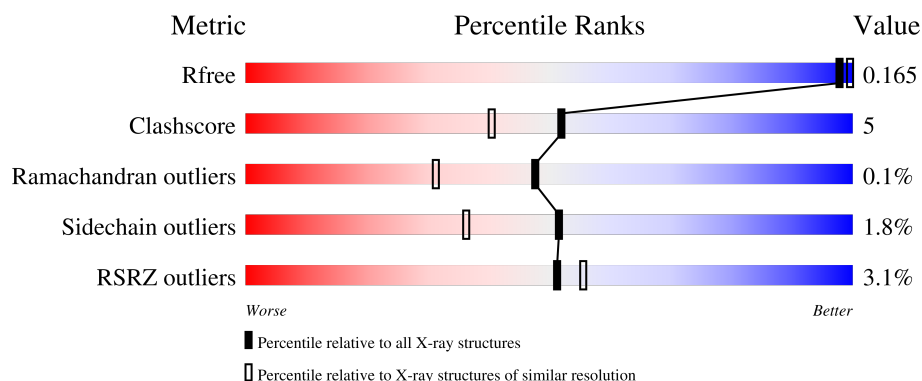
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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.



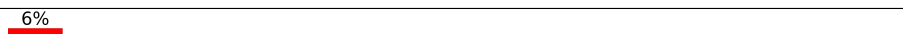
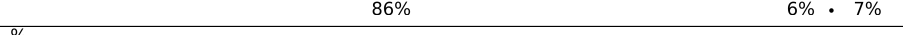
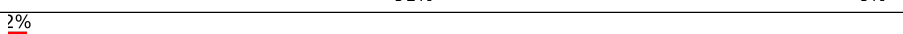
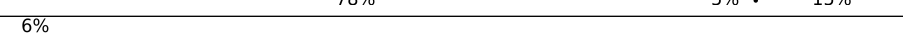
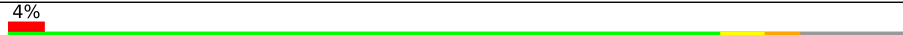
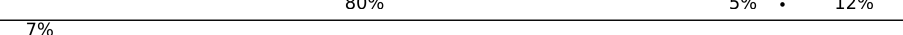
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	0% 90% 9% .
1	N	514	0% 91% 8% .
2	B	227	7% 85% 13% .
2	O	227	4% 87% 12% .
3	C	261	2% 85% 13% .

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Mol	Chain	Length	Quality of chain
3	P	261	
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
19	LFA	C	308	-	-	-	X
20	DMU	N	611	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 33049 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			

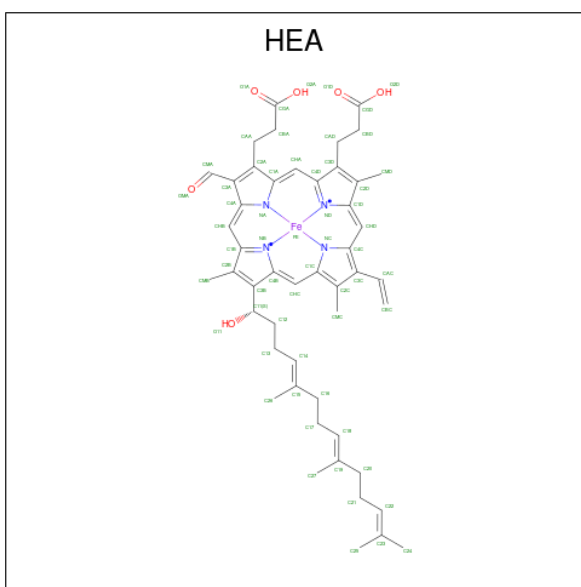
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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	C	Fe	N	O	
			69	58	1	4	6	1
14	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
14	N	1	Total	C	Fe	N	O	
			69	58	1	4	6	1
14	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	0

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

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

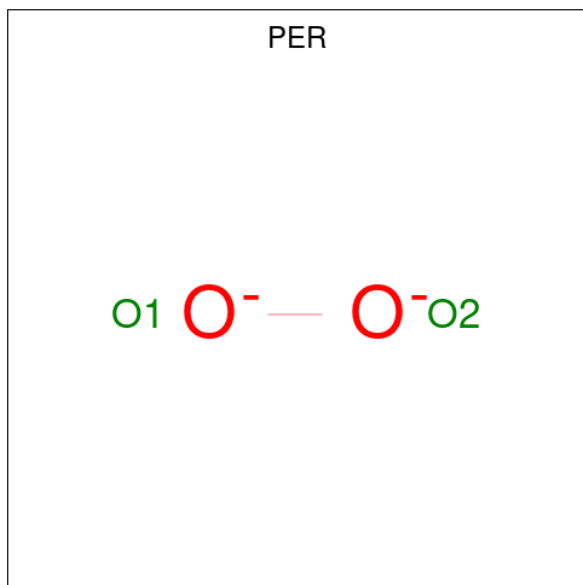
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

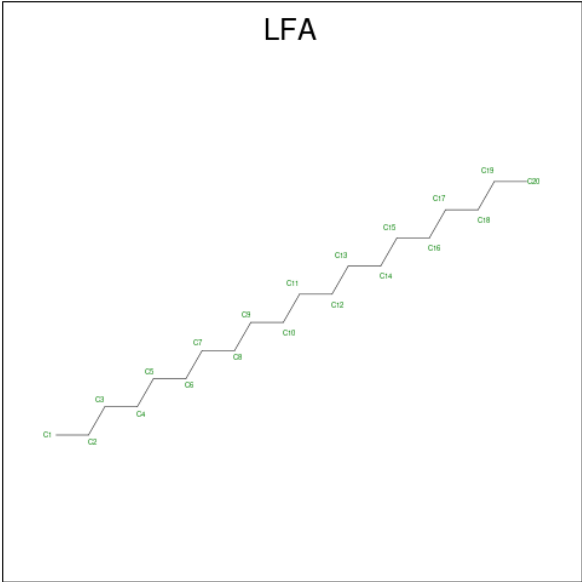
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total 1	Ca 1	0	0
17	N	1	Total 1	Ca 1	0	0

- 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 EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



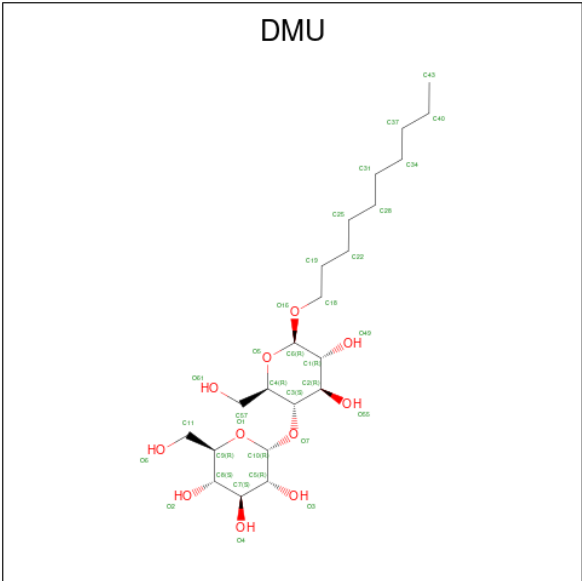
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	C	0	0
			14	14		
19	A	1	Total	C	0	0
			14	14		
19	B	1	Total	C	0	0
			17	17		
19	C	1	Total	C	0	0
			11	11		
19	C	1	Total	C	0	0
			6	6		
19	C	1	Total	C	0	0
			18	18		
19	C	1	Total	C	0	0
			11	11		
19	C	1	Total	C	0	0
			14	14		
19	C	1	Total	C	0	0
	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

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

- Molecule 20 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



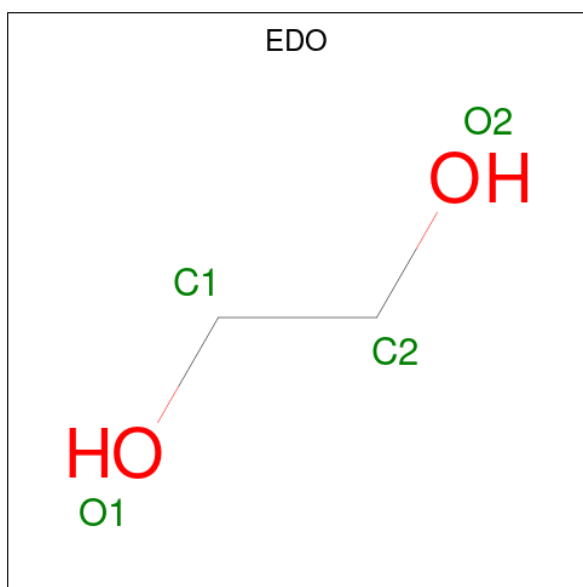
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C 7 7	0	0
20	A	1	Total C O 33 22 11	0	0
20	A	1	Total C O 11 10 1	0	0
20	A	1	Total C O 11 10 1	0	0
20	B	1	Total C O 11 10 1	0	0
20	B	1	Total C O 22 16 6	0	0
20	B	1	Total C O 22 16 6	0	0
20	C	1	Total C O 11 10 1	0	0
20	C	1	Total C O 33 22 11	0	0
20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

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

- Molecule 21 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



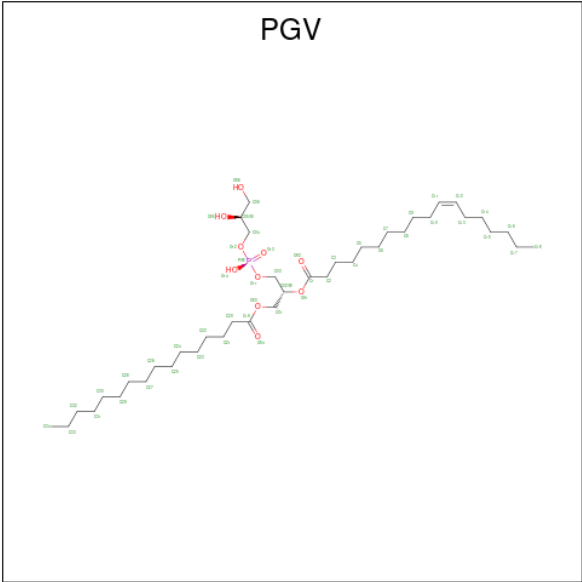
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21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

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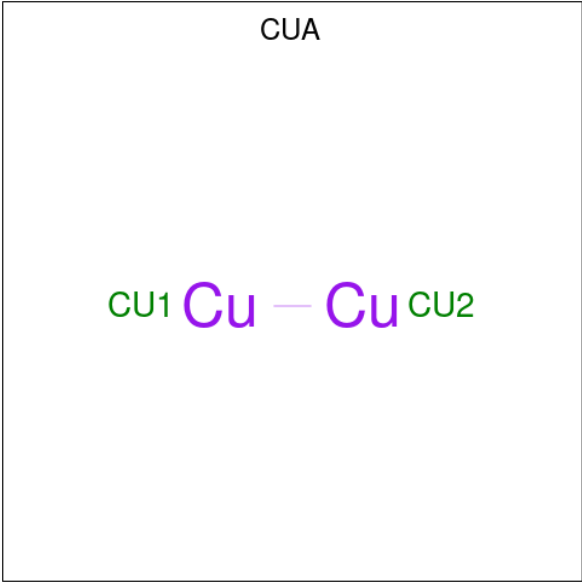
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	O	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21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

- Molecule 22 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



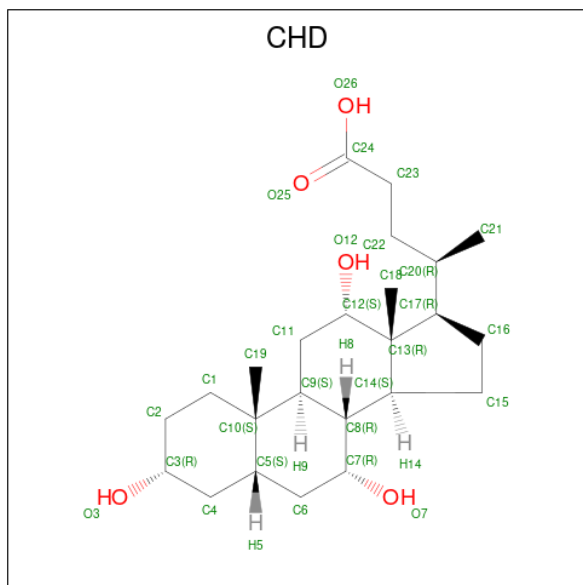
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	O	P	0	0
			51	40	10	1		
22	C	1	Total	C	O	P	0	0
			51	40	10	1		
22	N	1	Total	C	O	P	0	0
			51	40	10	1		
22	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 23 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 24 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).

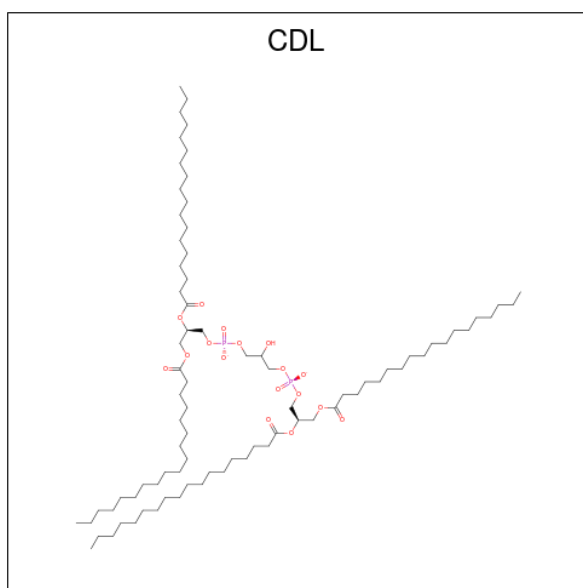


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	O	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0

- Molecule 25 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

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

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

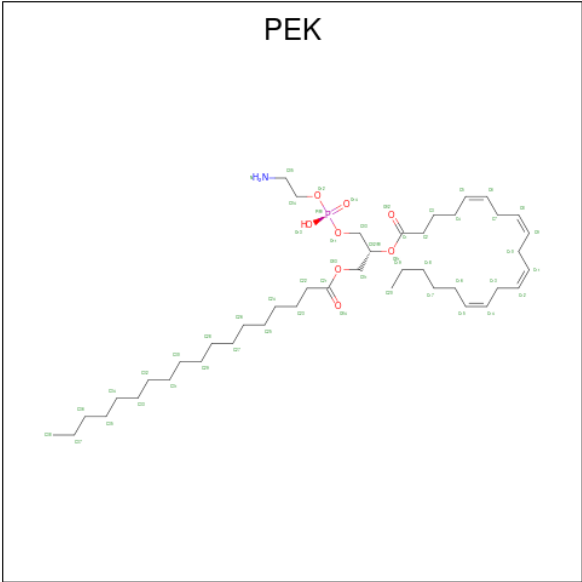


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			87	68	17	2		
26	I	1	Total	C	O	P	0	0
			64	45	17	2		
26	L	1	Total	C	O	P	0	0
			94	75	17	2		
26	O	1	Total	C	O	P	0	0
			64	45	17	2		
26	P	1	Total	C	O	P	0	0
			87	68	17	2		
26	Y	1	Total	C	O	P	0	0
			94	75	17	2		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 28 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: $C_{43}H_{78}NO_8P$).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	239	Total	O	0	11
			250	250		
29	B	175	Total	O	0	2
			177	177		
29	C	102	Total	O	0	1
			103	103		
29	D	135	Total	O	0	9
			144	144		
29	E	109	Total	O	0	7
			116	116		
29	F	104	Total	O	0	7
			111	111		
29	G	42	Total	O	0	1
			43	43		
29	H	61	Total	O	0	0
			61	61		
29	I	41	Total	O	0	0
			41	41		
29	J	20	Total	O	0	0
			20	20		

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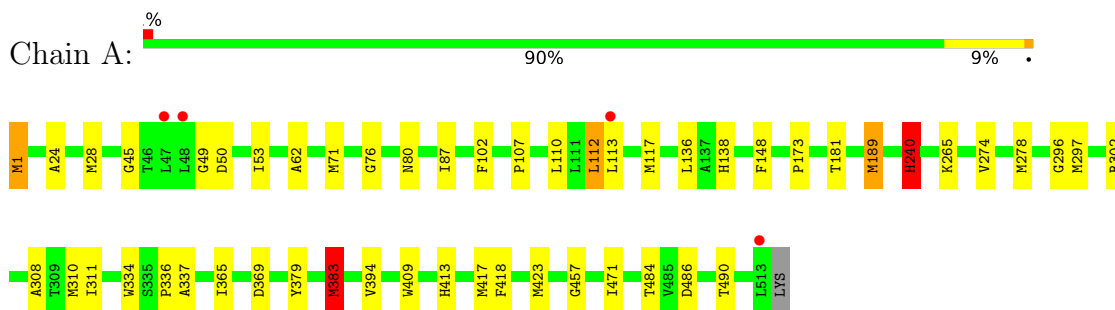
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	K	22	Total 22	O 22	0	0
29	L	25	Total 27	O 27	0	2
29	M	21	Total 21	O 21	0	0
29	N	227	Total 237	O 237	0	10
29	O	148	Total 149	O 149	0	1
29	P	101	Total 102	O 102	0	1
29	Q	81	Total 86	O 86	0	5
29	R	87	Total 94	O 94	0	7
29	S	87	Total 93	O 93	0	6
29	T	37	Total 38	O 38	0	1
29	U	46	Total 46	O 46	0	0
29	V	22	Total 22	O 22	0	0
29	W	15	Total 15	O 15	0	0
29	X	18	Total 18	O 18	0	0
29	Y	25	Total 27	O 27	0	2
29	Z	17	Total 17	O 17	0	0

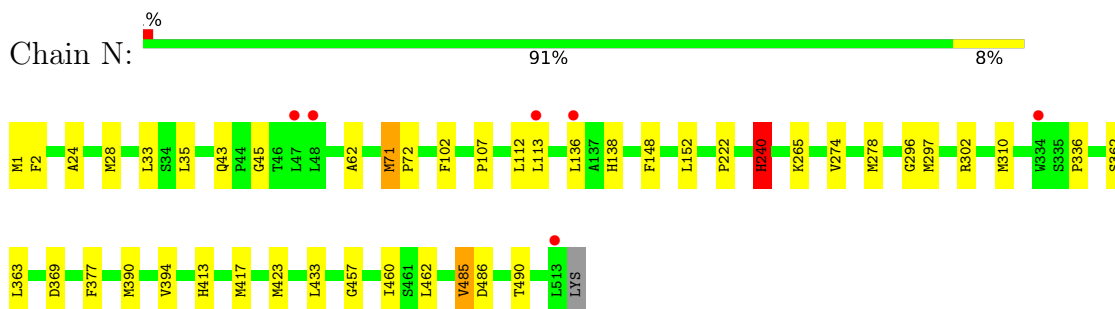
3 Residue-property plots [i](#)

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.

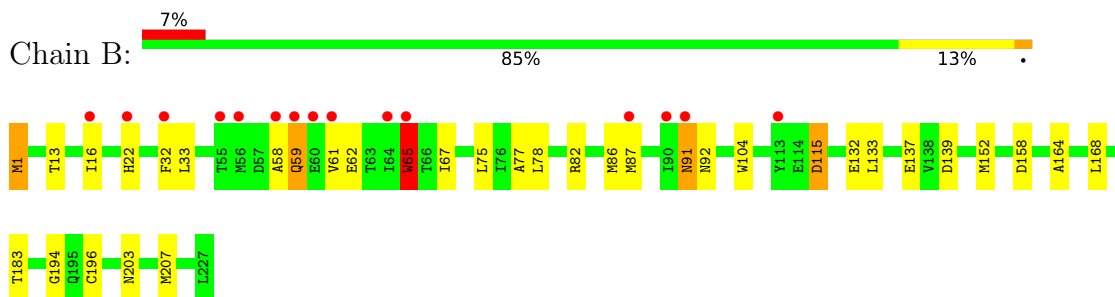
- Molecule 1: Cytochrome c oxidase subunit 1



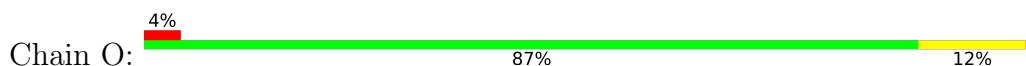
- Molecule 1: Cytochrome c oxidase subunit 1

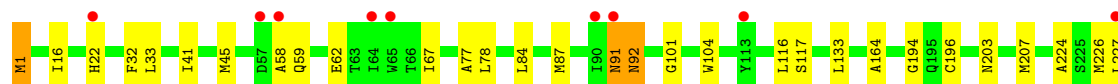


- Molecule 2: Cytochrome c oxidase subunit 2

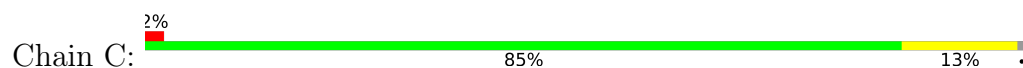


- Molecule 2: Cytochrome c oxidase subunit 2

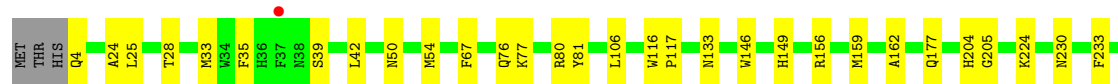




• Molecule 3: Cytochrome c oxidase subunit 3



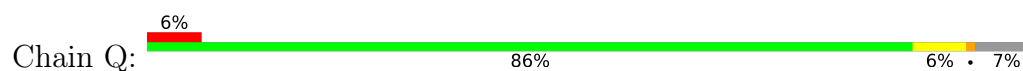
• Molecule 3: Cytochrome c oxidase subunit 3



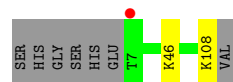
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



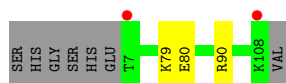
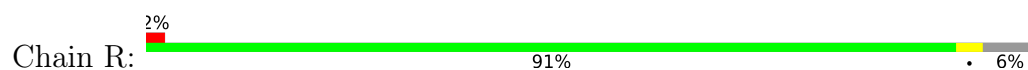
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



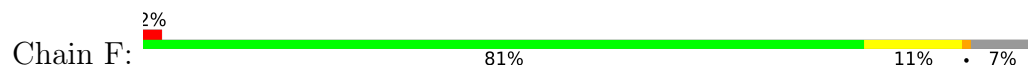
• Molecule 5: Cytochrome c oxidase subunit 5A



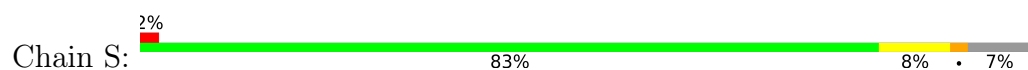
• Molecule 5: Cytochrome c oxidase subunit 5A



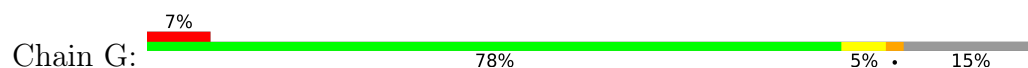
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



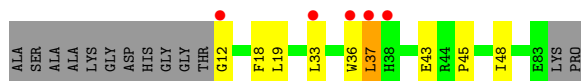
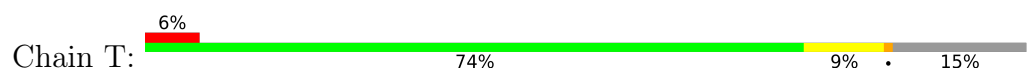
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



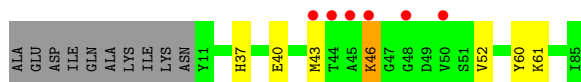
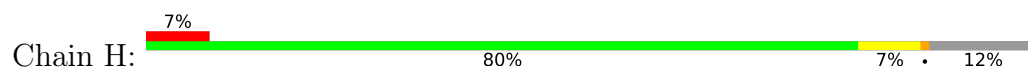
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



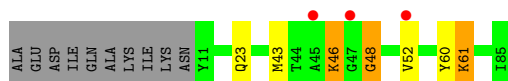
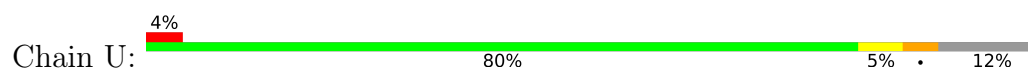
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



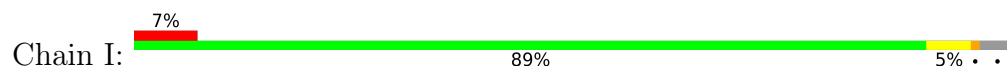
- Molecule 8: Cytochrome c oxidase subunit 6B1



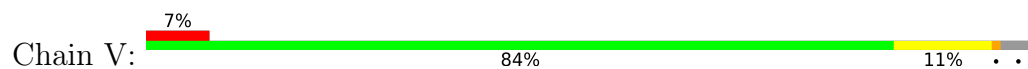
- Molecule 8: Cytochrome c oxidase subunit 6B1



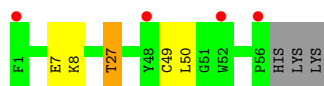
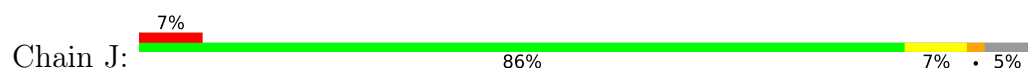
• Molecule 9: Cytochrome c oxidase subunit 6C



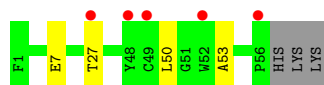
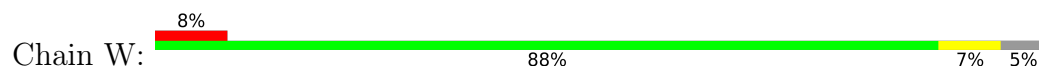
• Molecule 9: Cytochrome c oxidase subunit 6C



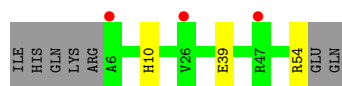
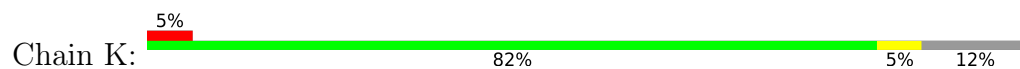
• Molecule 10: Cytochrome c oxidase subunit 7A1



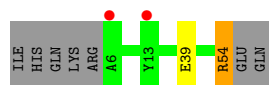
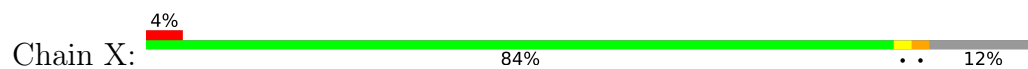
• Molecule 10: Cytochrome c oxidase subunit 7A1



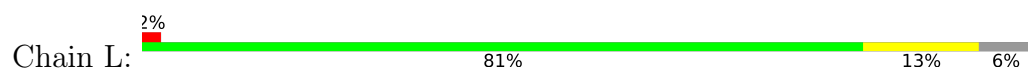
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

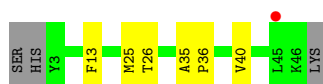


• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

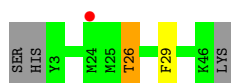
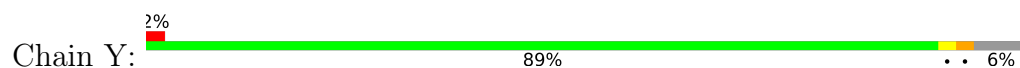


• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

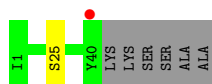
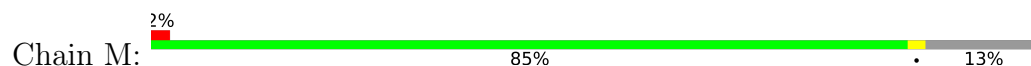




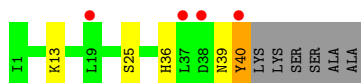
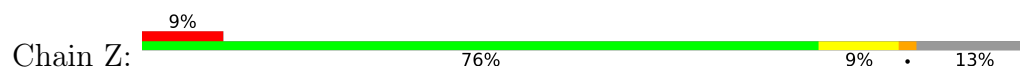
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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	182.80Å 205.70Å 177.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.70 40.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.70) 100.0 (40.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.123 , 0.153 0.139 , 0.165	Depositor DCC
R_{free} test set	36325 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for l,k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33049	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.07	5/4259 (0.1%)	1.21	6/5816 (0.1%)
1	N	1.05	0/4259	1.21	9/5816 (0.2%)
2	B	1.11	1/1908 (0.1%)	1.28	11/2598 (0.4%)
2	O	1.05	1/1908 (0.1%)	1.26	1/2598 (0.0%)
3	C	1.07	3/2258 (0.1%)	1.18	3/3084 (0.1%)
3	P	1.05	1/2258 (0.0%)	1.20	4/3084 (0.1%)
4	D	1.09	1/1226 (0.1%)	1.19	1/1657 (0.1%)
4	Q	1.04	1/1182 (0.1%)	1.34	3/1598 (0.2%)
5	E	1.04	1/843 (0.1%)	1.20	1/1145 (0.1%)
5	R	1.06	1/843 (0.1%)	1.26	0/1145
6	F	1.08	0/724	1.16	0/983
6	S	1.13	1/724 (0.1%)	1.16	2/983 (0.2%)
7	G	1.11	2/633 (0.3%)	1.18	0/864
7	T	1.09	1/633 (0.2%)	1.23	1/864 (0.1%)
8	H	1.01	0/648	1.34	0/877
8	U	1.03	1/648 (0.2%)	1.32	2/877 (0.2%)
9	I	1.15	1/588 (0.2%)	1.41	3/781 (0.4%)
9	V	1.05	0/588	1.40	2/781 (0.3%)
10	J	1.03	0/451	1.30	2/610 (0.3%)
10	W	1.04	0/451	1.31	0/610
11	K	1.16	1/398 (0.3%)	1.27	0/546
11	X	1.13	0/398	1.31	1/546 (0.2%)
12	L	1.03	0/372	1.20	2/500 (0.4%)
12	Y	1.07	0/372	1.26	1/500 (0.2%)
13	M	1.09	0/321	1.10	0/440
13	Z	1.06	0/321	1.34	0/440
All	All	1.07	22/29214 (0.1%)	1.24	55/39743 (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
6	S	0	1
All	All	0	5

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	MET	C-O	8.51	1.35	1.24
4	D	58	GLU	CD-OE1	7.96	1.40	1.25
3	C	243	HIS	CE1-NE2	6.99	1.39	1.32
4	Q	142	LYS	C-O	6.96	1.33	1.23
5	R	80	GLU	CD-OE1	6.88	1.38	1.25

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	65	TRP	CA-CB-CG	10.79	134.10	113.60
1	N	240	HIS	CA-CB-CG	-10.66	103.14	113.80
1	A	240	HIS	CA-CB-CG	-10.30	103.50	113.80
4	D	58	GLU	CB-CG-CD	9.77	129.21	112.60
2	B	65	TRP	CB-CA-C	-9.51	93.03	110.63

There are no chirality outliers.

All (5) 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	240	HIS	Sidechain
6	S	92	VAL	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4102	48	0
1	N	4130	0	4102	44	0
2	B	1870	0	1870	24	0
2	O	1870	0	1870	28	0
3	C	2171	0	2080	38	0
3	P	2172	0	2081	25	0
4	D	1192	0	1178	7	0
4	Q	1148	0	1131	9	0
5	E	825	0	823	1	0
5	R	825	0	823	1	0
6	F	709	0	691	9	0
6	S	709	0	691	5	0
7	G	606	0	577	4	0
7	T	606	0	577	5	0
8	H	628	0	580	9	0
8	U	628	0	580	11	0
9	I	575	0	584	1	0
9	V	575	0	584	4	0
10	J	441	0	439	4	0
10	W	441	0	439	5	0
11	K	384	0	366	1	0
11	X	384	0	366	1	0
12	L	360	0	360	7	0
12	Y	360	0	360	5	0
13	M	311	0	321	2	0
13	Z	311	0	321	4	0
14	A	129	0	88	4	0
14	N	129	0	88	3	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	28	0	54	15	0
19	B	17	0	33	3	0
19	C	114	0	203	4	0
19	N	45	0	87	7	0
19	O	11	0	21	4	0
19	P	100	0	174	6	0
19	T	25	0	48	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	62	0	96	2	0
20	B	55	0	83	0	0
20	C	194	0	262	10	0
20	D	33	0	41	4	0
20	H	33	0	26	1	0
20	J	11	0	21	0	0
20	L	22	0	31	2	0
20	M	41	0	57	1	0
20	N	84	0	100	0	0
20	O	66	0	104	0	0
20	P	194	0	262	2	0
20	Q	33	0	41	2	0
20	W	11	0	21	0	0
20	Y	22	0	31	2	0
20	Z	41	0	56	0	0
21	A	16	0	24	0	0
21	B	4	0	6	0	0
21	C	12	0	17	0	0
21	E	12	0	18	0	0
21	F	8	0	12	0	0
21	G	4	0	6	0	0
21	N	20	0	30	2	0
21	O	4	0	6	0	0
21	P	12	0	18	1	0
21	R	12	0	18	0	0
21	S	8	0	12	0	0
21	T	4	0	6	0	0
22	A	51	0	76	1	0
22	C	51	0	76	2	0
22	N	51	0	76	1	0
22	P	51	0	76	0	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	29	0	39	0	0
24	C	58	0	78	1	0
24	O	29	0	39	1	0
24	P	58	0	78	4	0
25	C	1	0	0	1	0
25	P	1	0	0	1	0
26	C	87	0	124	17	0
26	I	64	0	72	0	0
26	L	94	0	141	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	O	64	0	72	1	0
26	P	87	0	124	10	0
26	Y	94	0	141	4	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	53	0	77	2	0
28	T	53	0	77	4	0
29	A	250	0	0	6	0
29	B	177	0	0	3	0
29	C	103	0	0	4	0
29	D	144	0	0	2	0
29	E	116	0	0	1	0
29	F	111	0	0	1	0
29	G	43	0	0	2	0
29	H	61	0	0	0	0
29	I	41	0	0	1	0
29	J	20	0	0	0	0
29	K	22	0	0	0	0
29	L	27	0	0	1	0
29	M	21	0	0	0	0
29	N	237	0	0	7	0
29	O	149	0	0	2	0
29	P	102	0	0	5	0
29	Q	86	0	0	3	0
29	R	94	0	0	1	0
29	S	93	0	0	0	0
29	T	38	0	0	2	0
29	U	46	0	0	0	0
29	V	22	0	0	0	0
29	W	15	0	0	0	0
29	X	18	0	0	0	0
29	Y	27	0	0	1	0
29	Z	17	0	0	0	0
All	All	33049	0	31463	315	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 315 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)
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.23	1.14
18:N:608:PER:O2	18:N:608:PER:O1	1.64	1.14
18:A:606:PER:O2	18:A:606:PER:O1	1.68	1.10
3:P:4:GLN:N	29:P:402:HOH:O	1.88	1.07
19:A:607:LFA:H12	19:A:608:LFA:H11	1.45	0.99

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%)	512 (97%)	14 (3%)	0	100	100
1	N	526/514 (102%)	514 (98%)	12 (2%)	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%)	261 (98%)	4 (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%)	3 (2%)	1 (1%)	18	7
5	E	100/109 (92%)	100 (100%)	0	0	100	100
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%)	67 (94%)	4 (6%)	0	100	100
7	T	71/85 (84%)	68 (96%)	3 (4%)	0	100	100
8	H	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
8	U	73/85 (86%)	71 (97%)	1 (1%)	1 (1%)	9	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	37 (97%)	1 (3%)	0	100	100
All	All	3488/3614 (96%)	3415 (98%)	71 (2%)	2 (0%)	48	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	U	48	GLY
4	Q	11	TYR

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%)	437 (99%)	3 (1%)	76	69
1	N	440/426 (103%)	436 (99%)	4 (1%)	70	62
2	B	215/210 (102%)	208 (97%)	7 (3%)	33	17
2	O	215/210 (102%)	212 (99%)	3 (1%)	59	46
3	C	232/226 (103%)	230 (99%)	2 (1%)	70	62
3	P	232/226 (103%)	230 (99%)	2 (1%)	70	62
4	D	128/129 (99%)	128 (100%)	0	100	100
4	Q	122/129 (95%)	121 (99%)	1 (1%)	73	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	89/95 (94%)	89 (100%)	0	100	100
5	R	89/95 (94%)	88 (99%)	1 (1%)	65	54
6	F	78/81 (96%)	75 (96%)	3 (4%)	29	13
6	S	78/81 (96%)	75 (96%)	3 (4%)	29	13
7	G	63/69 (91%)	60 (95%)	3 (5%)	23	8
7	T	63/69 (91%)	59 (94%)	4 (6%)	16	5
8	H	67/75 (89%)	64 (96%)	3 (4%)	24	9
8	U	67/75 (89%)	64 (96%)	3 (4%)	24	9
9	I	55/58 (95%)	53 (96%)	2 (4%)	31	14
9	V	55/58 (95%)	50 (91%)	5 (9%)	9	2
10	J	47/50 (94%)	47 (100%)	0	100	100
10	W	47/50 (94%)	45 (96%)	2 (4%)	26	10
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	23
11	X	39/46 (85%)	38 (97%)	1 (3%)	40	23
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%)	34 (100%)	0	100	100
13	Z	34/38 (90%)	32 (94%)	2 (6%)	18	5
All	All	3042/3086 (99%)	2987 (98%)	55 (2%)	51	36

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	33	LEU
6	S	37	LYS
13	Z	40	TYR
9	V	70	GLN
2	O	78	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
5	R	94	ASN
6	S	54	ASN
8	U	32	ASN

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Mol	Chain	Res	Type
6	F	54	ASN
5	E	94	ASN

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	N	1	1	8,9,10	0.49	0	8,9,11	0.95	1 (12%)
2	FME	B	1	2	8,9,10	1.14	1 (12%)	8,9,11	1.36	1 (12%)
1	FME	A	1	1	8,9,10	0.45	0	8,9,11	1.03	1 (12%)
2	FME	O	1	2	8,9,10	0.61	0	8,9,11	0.98	1 (12%)

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	N	1	1	-	3/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-2.83	1.66	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-2.59	104.95	112.87
1	N	1	FME	O-C-CA	-2.27	118.92	124.77
2	O	1	FME	O-C-CA	-2.19	119.14	124.77
1	A	1	FME	O-C-CA	-2.02	119.58	124.77

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	A	1	FME	C-CA-CB-CG
1	N	1	FME	CA-CB-CG-SD

There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 135 ligands modelled in this entry, 8 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
20	DMU	B	307	-	22,22,34	0.50	0	27,27,45	1.25	2 (7%)
19	LFA	N	601	-	16,16,19	0.33	0	15,15,18	0.21	0
22	PGV	P	304	-	50,50,50	0.78	1 (2%)	53,56,56	0.94	3 (5%)
26	CDL	P	305	-	86,86,99	0.50	0	92,98,111	0.84	5 (5%)
21	EDO	C	322	-	3,3,3	0.82	0	2,2,2	0.70	0
14	HEA	N	603[A]	-	67,67,67	1.77	20 (29%)	81,103,103	2.35	28 (34%)
21	EDO	A	614	-	3,3,3	0.30	0	2,2,2	0.10	0
21	EDO	R	201	-	3,3,3	0.17	0	2,2,2	0.18	0
19	LFA	P	313	-	14,14,19	0.32	0	13,13,18	0.22	0
19	LFA	P	309	-	5,5,19	0.17	0	4,4,18	0.08	0
20	DMU	Z	101	-	34,34,34	0.99	3 (8%)	45,45,45	0.98	3 (6%)
21	EDO	A	612	-	3,3,3	0.06	0	2,2,2	0.06	0
21	EDO	A	613	-	3,3,3	0.38	0	2,2,2	0.12	0
21	EDO	R	203	-	3,3,3	0.25	0	2,2,2	0.51	0
28	PEK	G	101	-	52,52,52	0.58	1 (1%)	55,57,57	0.61	0
20	DMU	C	317	-	22,22,34	0.57	0	27,27,45	1.26	4 (14%)
19	LFA	C	312	-	10,10,19	0.25	0	9,9,18	0.18	0
19	LFA	N	610	-	13,13,19	0.62	0	12,12,18	0.39	0
20	DMU	A	617	-	10,10,34	0.24	0	9,9,45	0.56	0
14	HEA	A	601[B]	-	67,67,67	1.80	15 (22%)	81,103,103	2.41	28 (34%)
19	LFA	P	301	-	14,14,19	0.27	0	13,13,18	0.17	0
20	DMU	C	315	-	34,34,34	0.98	1 (2%)	45,45,45	1.65	10 (22%)
23	CUA	O	305	2	0,1,1	-	-	-	-	-
19	LFA	C	311	-	13,13,19	0.24	0	12,12,18	0.13	0
18	PER	N	608	15,14	1,1,1	1.54	0	-	-	-
21	EDO	N	615	-	3,3,3	0.46	0	2,2,2	0.33	0
21	EDO	N	613	-	3,3,3	0.17	0	2,2,2	0.18	0
24	CHD	B	305	-	32,32,32	0.67	0	51,51,51	0.90	1 (1%)
21	EDO	P	320	-	3,3,3	0.19	0	2,2,2	0.12	0
20	DMU	N	619	19	34,34,34	0.82	1 (2%)	45,45,45	1.32	6 (13%)
20	DMU	P	315	-	34,34,34	0.81	2 (5%)	45,45,45	1.35	4 (8%)
20	DMU	Q	201	-	34,34,34	1.29	6 (17%)	45,45,45	1.49	4 (8%)
20	DMU	B	303	-	22,22,34	0.90	1 (4%)	27,27,45	0.87	1 (3%)
19	LFA	O	302	-	10,10,19	0.23	0	9,9,18	0.16	0
21	EDO	P	321	-	3,3,3	0.19	0	2,2,2	0.15	0
22	PGV	A	616	-	50,50,50	0.70	0	53,56,56	1.21	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	DMU	A	615	-	10,10,34	0.30	0	9,9,45	0.52	0
21	EDO	A	611	-	3,3,3	0.32	0	2,2,2	0.52	0
20	DMU	A	609	-	6,6,34	0.65	0	5,5,45	0.31	0
21	EDO	S	102	-	3,3,3	0.39	0	2,2,2	0.35	0
14	HEA	A	602	1,18	67,67,67	1.72	18 (26%)	81,103,103	2.25	27 (33%)
20	DMU	D	201	-	34,34,34	1.46	8 (23%)	45,45,45	1.54	5 (11%)
23	CUA	B	301	2	0,1,1	-	-	-	-	-
20	DMU	M	102	-	7,7,34	0.27	0	6,6,45	0.56	0
21	EDO	C	320	-	3,3,3	0.06	0	2,2,2	0.08	0
20	DMU	A	610	-	34,34,34	1.25	6 (17%)	45,45,45	1.19	5 (11%)
24	CHD	C	301	-	32,32,32	0.87	1 (3%)	51,51,51	0.72	0
14	HEA	A	601[A]	-	67,67,67	1.79	15 (22%)	81,103,103	2.42	26 (32%)
19	LFA	C	313	-	14,14,19	0.31	0	13,13,18	0.41	0
20	DMU	C	316	-	6,6,34	0.28	0	5,5,45	0.49	0
20	DMU	P	318	-	34,34,34	0.92	3 (8%)	45,45,45	1.17	4 (8%)
20	DMU	J	101	-	10,10,34	0.20	0	9,9,45	0.58	0
26	CDL	O	304	-	63,63,99	0.41	0	69,75,111	0.71	1 (1%)
21	EDO	S	103	-	3,3,3	0.14	0	2,2,2	0.09	0
19	LFA	C	310	-	10,10,19	0.12	0	9,9,18	0.11	0
20	DMU	P	323	-	22,22,34	0.76	0	27,27,45	1.48	1 (3%)
19	LFA	A	607	-	13,13,19	0.41	0	12,12,18	0.26	0
19	LFA	P	311	-	10,10,19	0.15	0	9,9,18	0.11	0
21	EDO	N	614	-	3,3,3	0.19	0	2,2,2	0.37	0
22	PGV	N	618	-	50,50,50	0.78	1 (2%)	53,56,56	1.23	3 (5%)
24	CHD	O	301	-	32,32,32	0.73	0	51,51,51	0.77	0
19	LFA	A	608	-	13,13,19	0.74	1 (7%)	12,12,18	0.55	0
21	EDO	E	202	-	3,3,3	0.17	0	2,2,2	0.10	0
19	LFA	P	308	-	10,10,19	0.27	0	9,9,18	0.28	0
21	EDO	F	103	-	3,3,3	0.20	0	2,2,2	0.28	0
20	DMU	W	101	-	10,10,34	0.29	0	9,9,45	0.56	0
20	DMU	P	319	-	34,34,34	0.78	2 (5%)	45,45,45	1.21	3 (6%)
20	DMU	P	317	-	22,22,34	0.93	1 (4%)	27,27,45	1.32	2 (7%)
26	CDL	Y	101	-	93,93,99	0.35	0	99,105,111	0.44	1 (1%)
20	DMU	Y	102	-	22,22,34	0.56	0	27,27,45	1.00	1 (3%)
21	EDO	G	102	-	3,3,3	0.27	0	2,2,2	0.17	0
20	DMU	H	101	19	34,34,34	0.90	2 (5%)	45,45,45	1.11	4 (8%)
20	DMU	O	307	-	10,10,34	0.53	0	9,9,45	0.44	0
21	EDO	T	104	-	3,3,3	0.18	0	2,2,2	0.16	0
21	EDO	E	203	-	3,3,3	0.42	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	DMU	N	612	-	34,34,34	1.32	4 (11%)	45,45,45	1.00	3 (6%)
20	DMU	M	101	-	34,34,34	0.86	1 (2%)	45,45,45	1.13	3 (6%)
24	CHD	P	306	-	32,32,32	0.81	1 (3%)	51,51,51	1.30	5 (9%)
21	EDO	P	322	-	3,3,3	0.39	0	2,2,2	0.76	0
19	LFA	C	309	20	17,17,19	0.25	0	16,16,18	0.19	0
20	DMU	N	602	-	10,10,34	0.28	0	9,9,45	0.52	0
21	EDO	E	201	-	3,3,3	0.07	0	2,2,2	0.16	0
21	EDO	N	616	-	3,3,3	0.21	0	2,2,2	0.05	0
21	EDO	O	309	-	3,3,3	0.45	0	2,2,2	0.22	0
19	LFA	C	308	-	5,5,19	0.19	0	4,4,18	0.05	0
20	DMU	C	324	-	34,34,34	0.85	1 (2%)	45,45,45	1.17	4 (8%)
19	LFA	C	307	-	10,10,19	0.16	0	9,9,18	0.19	0
20	DMU	C	323	-	22,22,34	0.66	1 (4%)	27,27,45	1.03	1 (3%)
22	PGV	C	303	-	50,50,50	0.79	2 (4%)	53,56,56	1.08	3 (5%)
20	DMU	B	302	-	10,10,34	0.21	0	9,9,45	0.58	0
26	CDL	L	101	-	93,93,99	0.44	0	99,105,111	0.63	2 (2%)
20	DMU	C	306	-	10,10,34	0.43	0	9,9,45	0.58	0
20	DMU	O	306	-	10,10,34	0.13	0	9,9,45	0.63	0
20	DMU	C	319	-	34,34,34	0.83	1 (2%)	45,45,45	1.30	5 (11%)
26	CDL	C	304	-	86,86,99	0.56	0	92,98,111	1.12	8 (8%)
19	LFA	C	325	-	14,14,19	0.14	0	13,13,18	0.10	0
19	LFA	P	310	20	17,17,19	0.20	0	16,16,18	0.17	0
19	LFA	P	312	-	10,10,19	0.20	0	9,9,18	0.32	0
20	DMU	P	307	-	10,10,34	0.33	0	9,9,45	0.56	0
24	CHD	P	302	-	32,32,32	0.77	2 (6%)	51,51,51	0.85	0
19	LFA	N	609	-	13,13,19	0.36	0	12,12,18	0.41	0
20	DMU	P	316	-	6,6,34	0.30	0	5,5,45	0.49	0
26	CDL	I	101	-	63,63,99	0.47	0	69,75,111	1.04	4 (5%)
19	LFA	T	102	-	13,13,19	0.23	0	12,12,18	0.15	0
14	HEA	N	603[B]	-	67,67,67	1.78	20 (29%)	81,103,103	2.29	27 (33%)
20	DMU	O	303	-	22,22,34	0.74	0	27,27,45	1.46	3 (11%)
19	LFA	T	103	-	10,10,19	0.27	0	9,9,18	0.13	0
20	DMU	O	308	-	22,22,34	0.69	0	27,27,45	1.07	2 (7%)
21	EDO	C	321	-	3,3,3	0.30	0	2,2,2	0.35	0
19	LFA	C	314	-	12,12,19	0.31	0	11,11,18	0.27	0
21	EDO	B	304	-	3,3,3	0.40	0	2,2,2	0.14	0
21	EDO	R	202	-	3,3,3	0.20	0	2,2,2	0.28	0
19	LFA	B	306	-	16,16,19	0.39	0	15,15,18	0.18	0
21	EDO	N	617	-	3,3,3	0.38	0	2,2,2	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	PEK	T	101	-	52,52,52	0.62	2 (3%)	55,57,57	0.99	3 (5%)
18	PER	A	606	15,14	1,1,1	1.85	0	-		
20	DMU	C	318	-	34,34,34	0.88	2 (5%)	45,45,45	1.26	2 (4%)
19	LFA	P	314	-	12,12,19	0.34	0	11,11,18	0.25	0
24	CHD	C	305	-	32,32,32	0.70	1 (3%)	51,51,51	1.57	9 (17%)
21	EDO	F	102	-	3,3,3	0.19	0	2,2,2	0.09	0
20	DMU	Z	102	-	7,7,34	0.28	0	6,6,45	0.45	0
14	HEA	N	604	1,18	67,67,67	1.77	16 (23%)	81,103,103	2.30	28 (34%)
20	DMU	N	611	-	6,6,34	0.37	0	5,5,45	0.37	0
20	DMU	L	102	-	22,22,34	0.73	1 (4%)	27,27,45	1.20	4 (14%)
20	DMU	P	324	-	34,34,34	0.69	0	45,45,45	1.55	4 (8%)

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
20	DMU	B	307	-	-	9/13/33/59	0/1/1/2
19	LFA	N	601	-	-	10/14/14/17	-
22	PGV	P	304	-	-	11/55/55/55	-
26	CDL	P	305	-	-	45/97/97/110	-
21	EDO	C	322	-	-	0/1/1/1	-
14	HEA	N	603[A]	-	-	7/36/76/76	-
21	EDO	A	614	-	-	1/1/1/1	-
21	EDO	R	201	-	-	1/1/1/1	-
19	LFA	P	313	-	-	5/12/12/17	-
19	LFA	P	309	-	-	1/3/3/17	-
20	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
21	EDO	A	612	-	-	1/1/1/1	-
21	EDO	A	613	-	-	0/1/1/1	-
21	EDO	R	203	-	-	1/1/1/1	-
28	PEK	G	101	-	-	15/56/56/56	-
20	DMU	C	317	-	-	8/13/33/59	0/1/1/2
19	LFA	C	312	-	-	4/8/8/17	-
19	LFA	N	610	-	-	7/11/11/17	-
20	DMU	A	617	-	-	6/8/8/59	-
14	HEA	A	601[B]	-	-	2/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LFA	P	301	-	-	7/12/12/17	-
20	DMU	C	315	-	-	12/19/59/59	0/2/2/2
19	LFA	C	311	-	-	5/11/11/17	-
21	EDO	N	615	-	-	0/1/1/1	-
21	EDO	N	613	-	-	0/1/1/1	-
24	CHD	B	305	-	-	2/9/74/74	0/4/4/4
21	EDO	P	320	-	-	1/1/1/1	-
20	DMU	N	619	19	-	5/19/59/59	0/2/2/2
20	DMU	P	315	-	-	6/19/59/59	0/2/2/2
20	DMU	Q	201	-	-	8/19/59/59	0/2/2/2
20	DMU	B	303	-	-	7/13/33/59	0/1/1/2
19	LFA	O	302	-	-	3/8/8/17	-
21	EDO	P	321	-	-	1/1/1/1	-
22	PGV	A	616	-	-	10/55/55/55	-
20	DMU	A	615	-	-	6/8/8/59	-
21	EDO	A	611	-	-	0/1/1/1	-
20	DMU	A	609	-	-	3/4/4/59	-
21	EDO	S	102	-	-	0/1/1/1	-
14	HEA	A	602	1,18	-	4/36/76/76	-
20	DMU	D	201	-	-	7/19/59/59	0/2/2/2
20	DMU	M	102	-	-	5/5/5/59	-
21	EDO	C	320	-	-	0/1/1/1	-
20	DMU	A	610	-	-	7/19/59/59	0/2/2/2
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
14	HEA	A	601[A]	-	-	6/36/76/76	-
19	LFA	C	313	-	-	3/12/12/17	-
20	DMU	C	316	-	-	3/4/4/59	-
20	DMU	P	318	-	-	15/19/59/59	0/2/2/2
20	DMU	J	101	-	-	6/8/8/59	-
26	CDL	O	304	-	-	40/74/74/110	-
21	EDO	S	103	-	-	0/1/1/1	-
19	LFA	C	310	-	-	8/8/8/17	-
20	DMU	P	323	-	-	6/13/33/59	0/1/1/2
19	LFA	A	607	-	-	3/11/11/17	-
19	LFA	P	311	-	-	5/8/8/17	-
21	EDO	N	614	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PGV	N	618	-	-	8/55/55/55	-
24	CHD	O	301	-	-	2/9/74/74	0/4/4/4
19	LFA	A	608	-	-	5/11/11/17	-
21	EDO	E	202	-	-	0/1/1/1	-
19	LFA	P	308	-	-	4/8/8/17	-
21	EDO	F	103	-	-	1/1/1/1	-
20	DMU	W	101	-	-	5/8/8/59	-
20	DMU	P	319	-	-	8/19/59/59	0/2/2/2
20	DMU	P	317	-	-	8/13/33/59	0/1/1/2
26	CDL	Y	101	-	-	52/104/104/110	-
20	DMU	Y	102	-	-	9/13/33/59	0/1/1/2
21	EDO	G	102	-	-	0/1/1/1	-
20	DMU	H	101	19	-	5/19/59/59	0/2/2/2
20	DMU	O	307	-	-	5/8/8/59	-
21	EDO	T	104	-	-	0/1/1/1	-
21	EDO	E	203	-	-	1/1/1/1	-
20	DMU	N	612	-	-	5/19/59/59	0/2/2/2
20	DMU	M	101	-	-	3/19/59/59	0/2/2/2
24	CHD	P	306	-	-	9/9/74/74	0/4/4/4
21	EDO	P	322	-	-	0/1/1/1	-
19	LFA	C	309	20	-	9/15/15/17	-
20	DMU	N	602	-	-	4/8/8/59	-
21	EDO	E	201	-	-	0/1/1/1	-
21	EDO	N	616	-	-	0/1/1/1	-
21	EDO	O	309	-	-	0/1/1/1	-
19	LFA	C	308	-	-	1/3/3/17	-
20	DMU	C	324	-	-	5/19/59/59	0/2/2/2
19	LFA	C	307	-	-	7/8/8/17	-
20	DMU	C	323	-	-	10/13/33/59	0/1/1/2
22	PGV	C	303	-	-	14/55/55/55	-
20	DMU	B	302	-	-	5/8/8/59	-
26	CDL	L	101	-	-	54/104/104/110	-
20	DMU	C	306	-	-	3/8/8/59	-
20	DMU	O	306	-	-	5/8/8/59	-
20	DMU	C	319	-	-	10/19/59/59	0/2/2/2
26	CDL	C	304	-	-	40/97/97/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LFA	C	325	-	-	8/12/12/17	-
19	LFA	P	310	20	-	6/15/15/17	-
19	LFA	P	312	-	-	5/8/8/17	-
20	DMU	P	307	-	-	2/8/8/59	-
24	CHD	P	302	-	-	2/9/74/74	0/4/4/4
19	LFA	N	609	-	-	4/11/11/17	-
20	DMU	P	316	-	-	3/4/4/59	-
26	CDL	I	101	-	-	43/74/74/110	-
19	LFA	T	102	-	-	6/11/11/17	-
14	HEA	N	603[B]	-	-	3/36/76/76	-
20	DMU	O	303	-	-	7/13/33/59	0/1/1/2
19	LFA	T	103	-	-	3/8/8/17	-
20	DMU	O	308	-	-	4/13/33/59	0/1/1/2
21	EDO	C	321	-	-	0/1/1/1	-
19	LFA	C	314	-	-	5/10/10/17	-
21	EDO	B	304	-	-	0/1/1/1	-
21	EDO	R	202	-	-	0/1/1/1	-
19	LFA	B	306	-	-	11/14/14/17	-
21	EDO	N	617	-	-	0/1/1/1	-
28	PEK	T	101	-	-	19/56/56/56	-
20	DMU	C	318	-	-	13/19/59/59	0/2/2/2
19	LFA	P	314	-	-	3/10/10/17	-
24	CHD	C	305	-	-	8/9/74/74	0/4/4/4
21	EDO	F	102	-	-	0/1/1/1	-
20	DMU	Z	102	-	-	2/5/5/59	-
14	HEA	N	604	1,18	-	4/36/76/76	-
20	DMU	N	611	-	-	2/4/4/59	-
20	DMU	L	102	-	-	11/13/33/59	0/1/1/2
20	DMU	P	324	-	-	7/19/59/59	0/2/2/2

The worst 5 of 164 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	603[A]	HEA	C1D-ND	-5.06	1.31	1.40
14	N	603[B]	HEA	C1D-ND	-5.06	1.31	1.40
20	N	612	DMU	O16-C6	-4.88	1.32	1.40
14	N	603[A]	HEA	C3B-C2B	4.54	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	603[B]	HEA	C3B-C2B	4.54	1.45	1.34

The worst 5 of 306 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601[A]	HEA	C3D-C4D-ND	8.05	118.13	110.35
14	A	601[B]	HEA	C3D-C4D-ND	8.05	118.13	110.35
14	N	603[A]	HEA	C3D-C4D-ND	7.34	117.44	110.35
14	N	603[B]	HEA	C3D-C4D-ND	7.34	117.44	110.35
14	A	601[A]	HEA	C3C-C4C-NC	6.96	115.66	109.80

There are no chirality outliers.

5 of 815 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	N	603[A]	HEA	C27-C19-C20-C21
20	C	318	DMU	C19-C18-O16-C6
20	C	323	DMU	C19-C18-O16-C6
20	L	102	DMU	C19-C18-O16-C6
20	O	303	DMU	C19-C18-O16-C6

There are no ring outliers.

49 monomers are involved in 126 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	N	601	LFA	1	0
26	P	305	CDL	10	0
14	N	603[A]	HEA	1	0
28	G	101	PEK	2	0
19	C	312	LFA	1	0
19	N	610	LFA	3	0
14	A	601[B]	HEA	1	0
18	N	608	PER	1	0
20	Q	201	DMU	2	0
19	O	302	LFA	4	0
21	P	321	EDO	1	0
22	A	616	PGV	1	0
20	A	609	DMU	1	0
20	D	201	DMU	4	0
20	A	610	DMU	1	0
14	A	601[A]	HEA	3	0

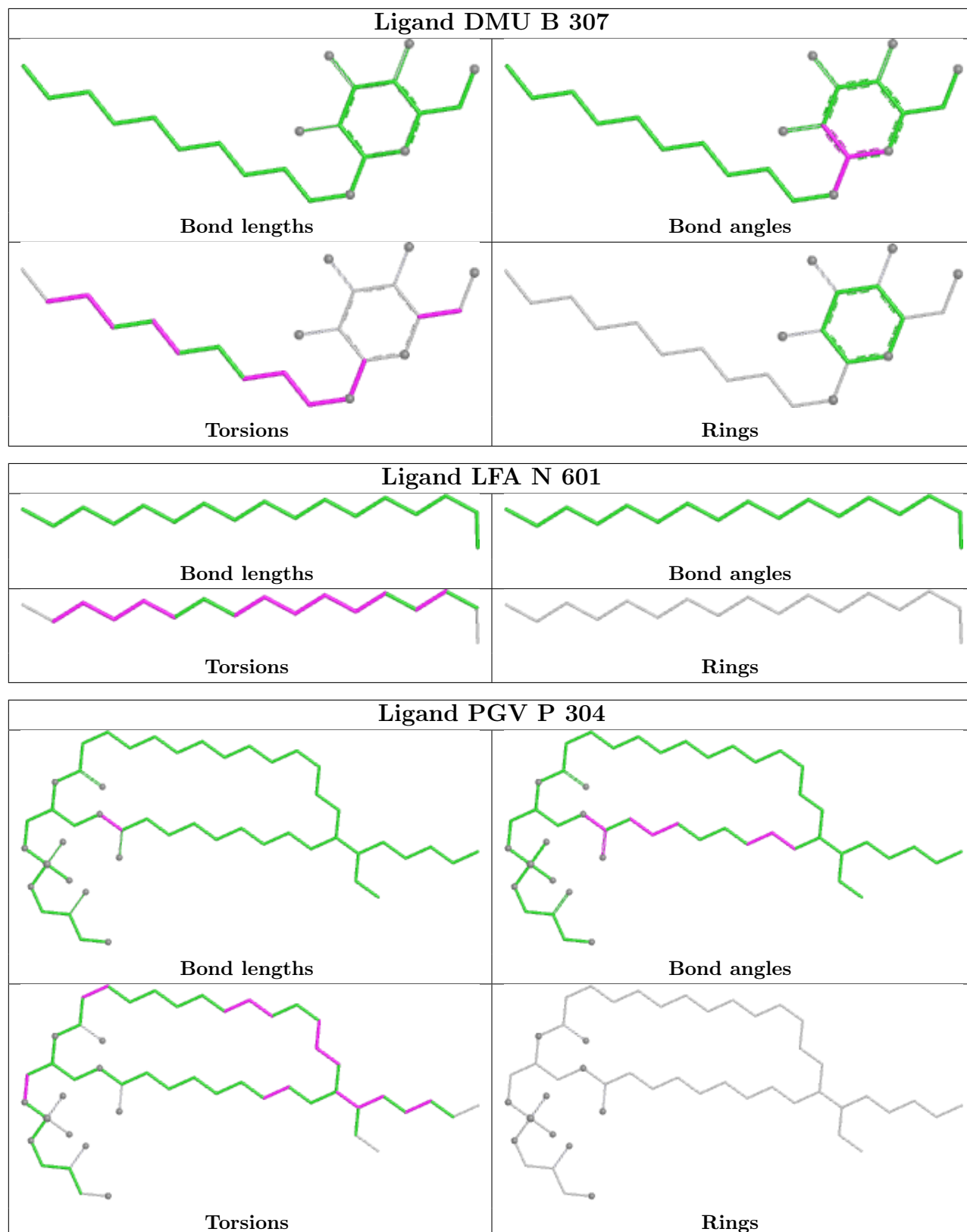
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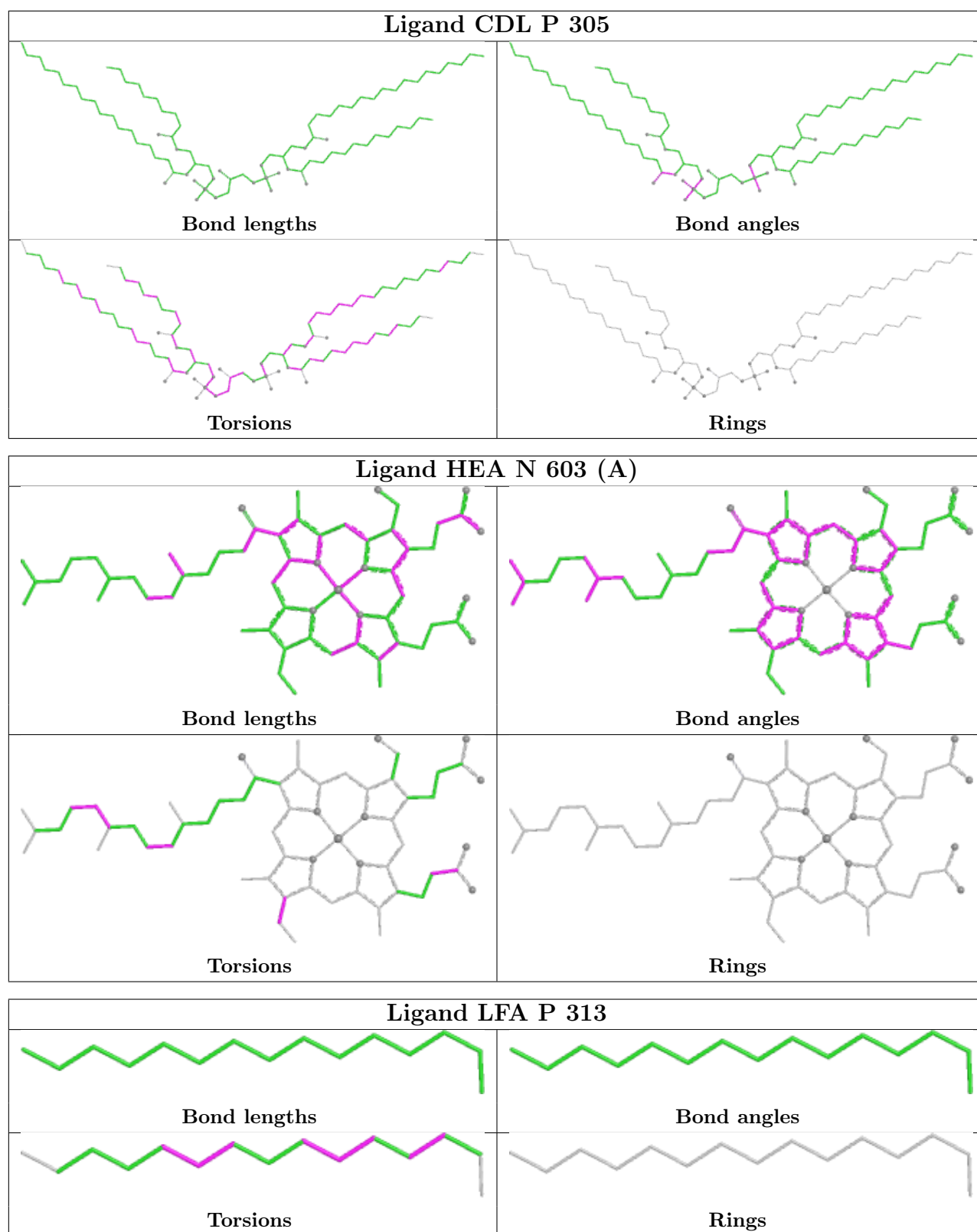
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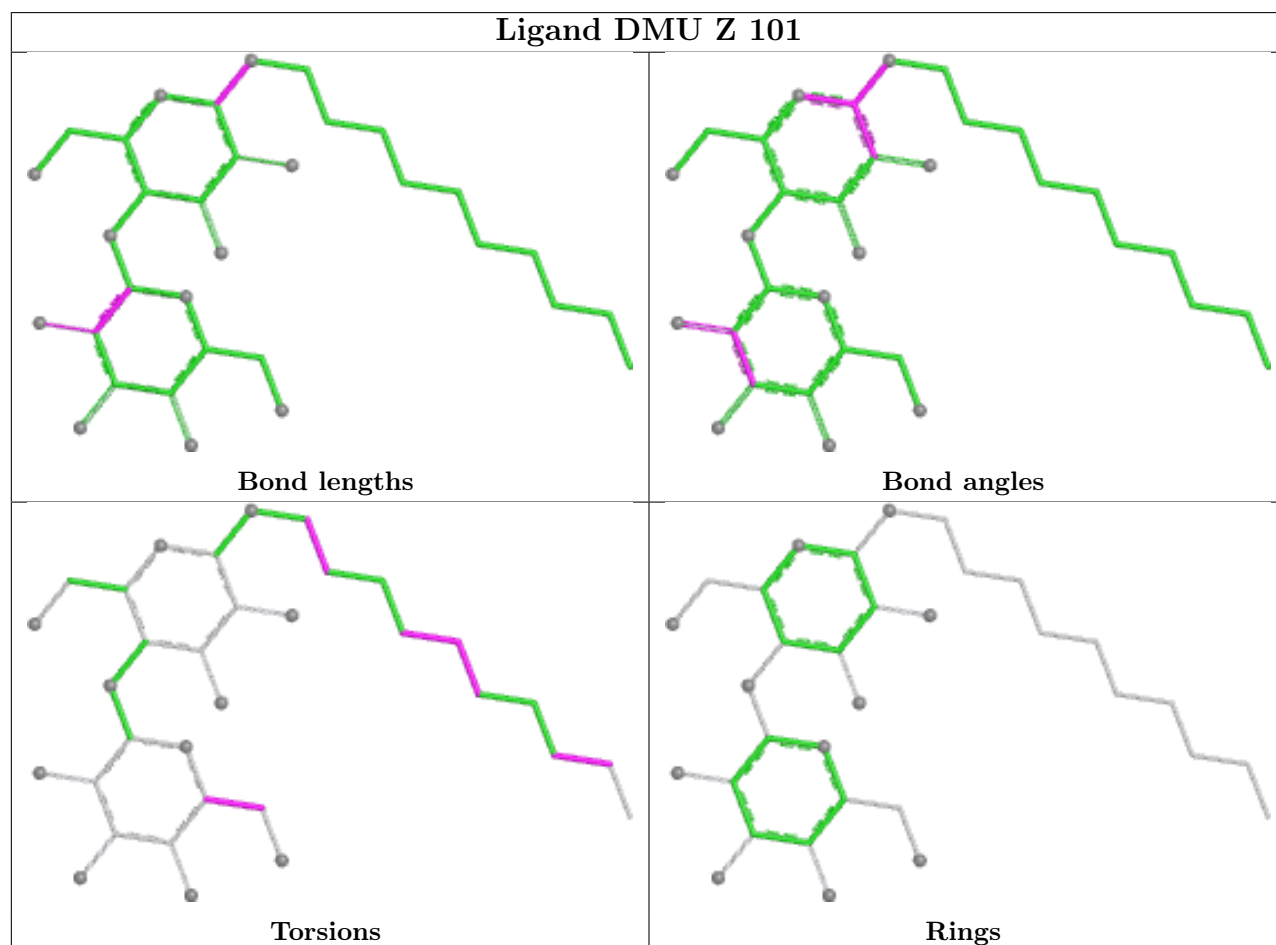
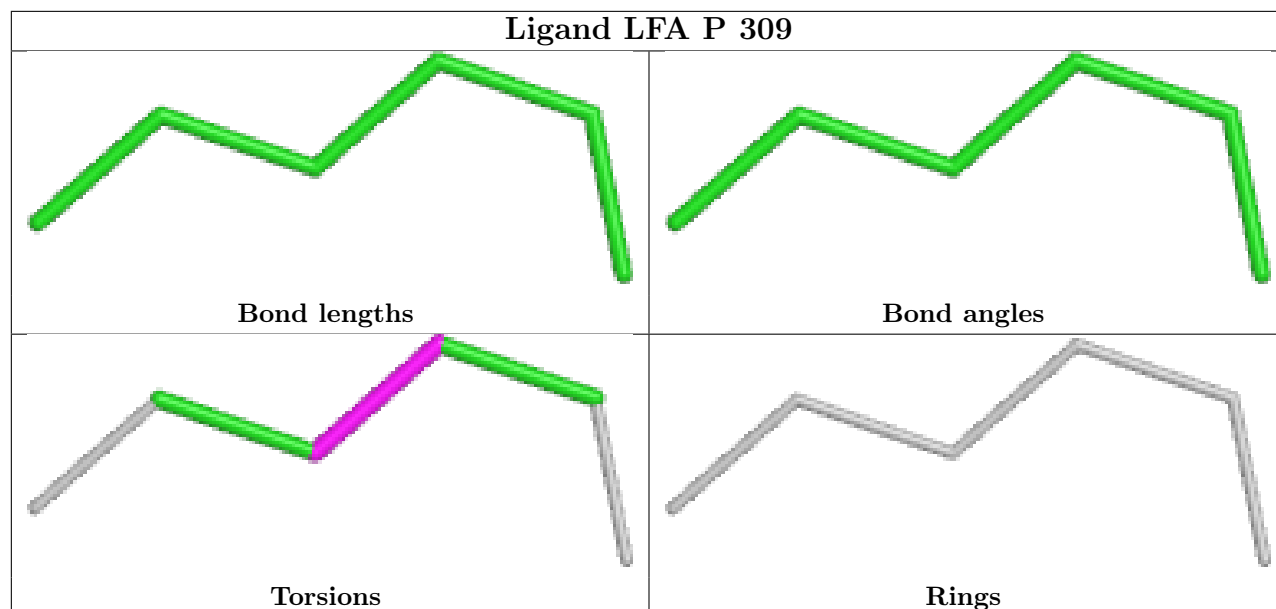
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	313	LFA	1	0
26	O	304	CDL	1	0
19	A	607	LFA	5	0
19	P	311	LFA	1	0
22	N	618	PGV	1	0
24	O	301	CHD	1	0
19	A	608	LFA	12	0
19	P	308	LFA	2	0
26	Y	101	CDL	4	0
20	Y	102	DMU	2	0
20	H	101	DMU	1	0
20	M	101	DMU	1	0
24	P	306	CHD	4	0
20	C	324	DMU	8	0
19	C	307	LFA	2	0
20	C	323	DMU	1	0
22	C	303	PGV	2	0
26	L	101	CDL	3	0
26	C	304	CDL	17	0
19	P	310	LFA	2	0
19	P	312	LFA	1	0
19	N	609	LFA	3	0
14	N	603[B]	HEA	1	0
19	C	314	LFA	1	0
19	B	306	LFA	3	0
21	N	617	EDO	2	0
28	T	101	PEK	4	0
18	A	606	PER	1	0
20	C	318	DMU	1	0
24	C	305	CHD	1	0
14	N	604	HEA	1	0
20	L	102	DMU	2	0
20	P	324	DMU	2	0

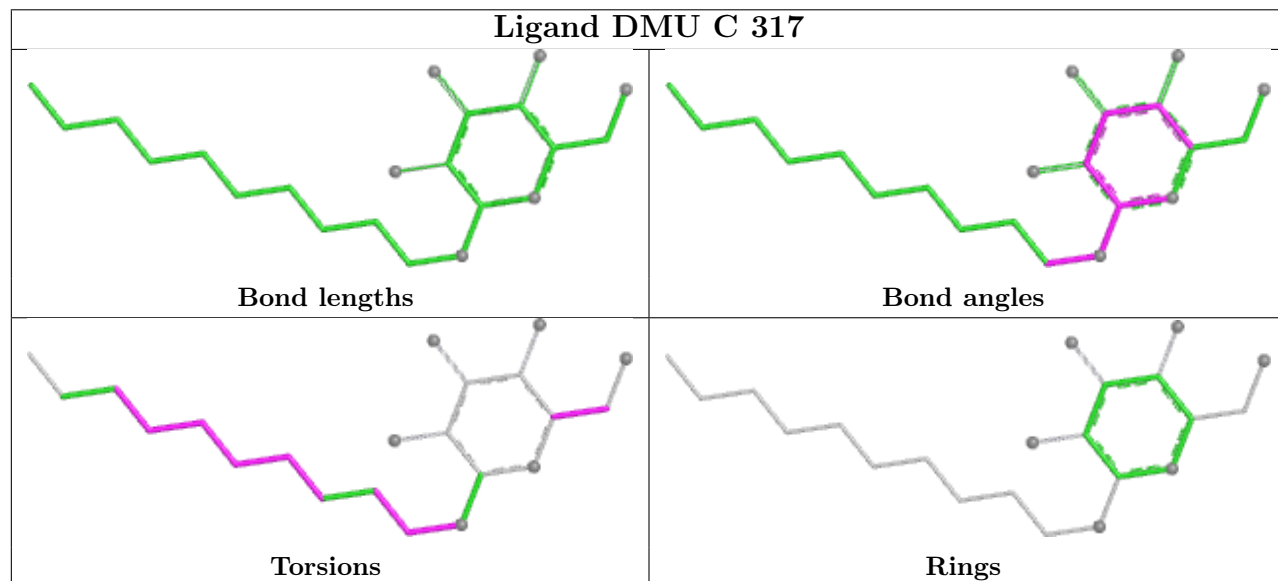
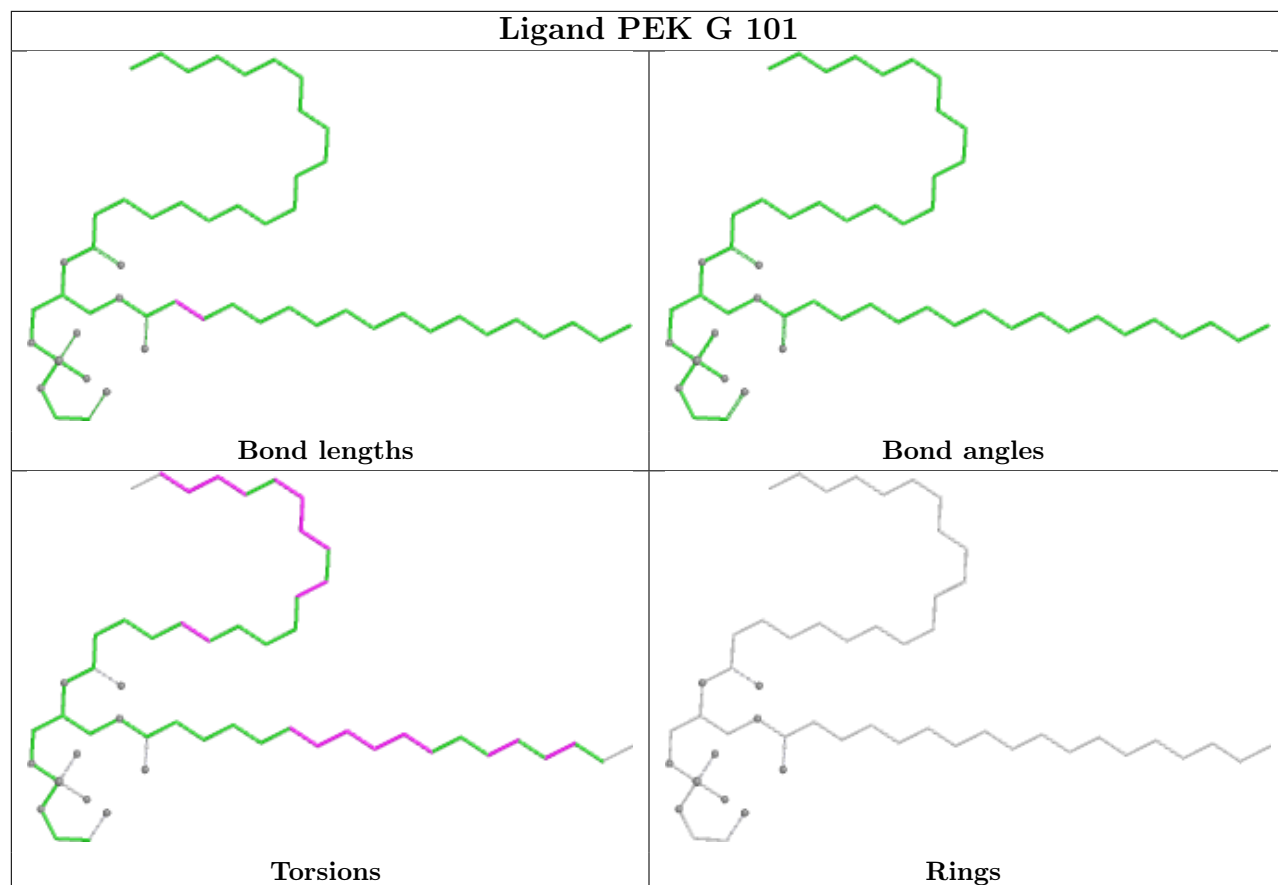
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

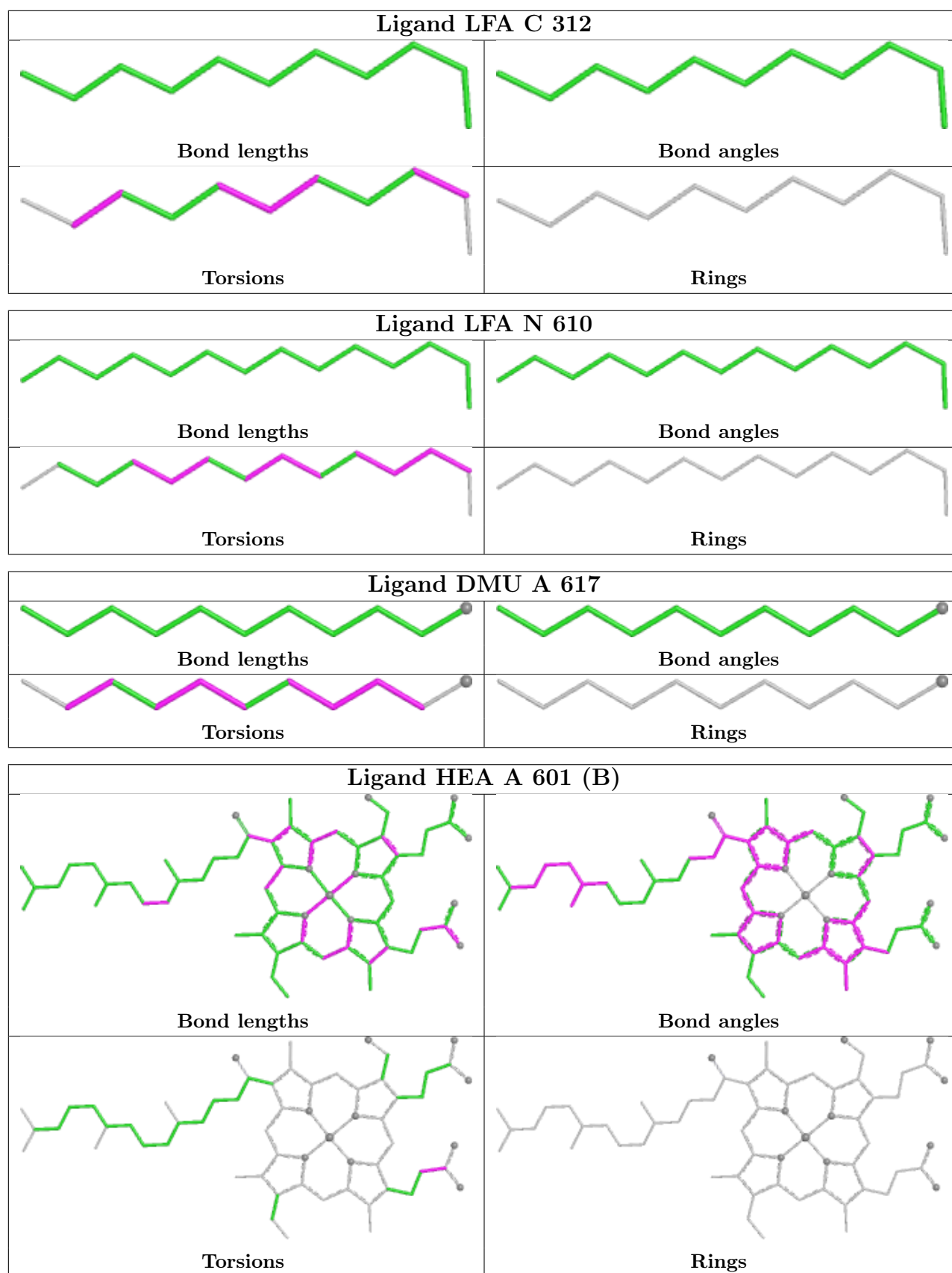
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

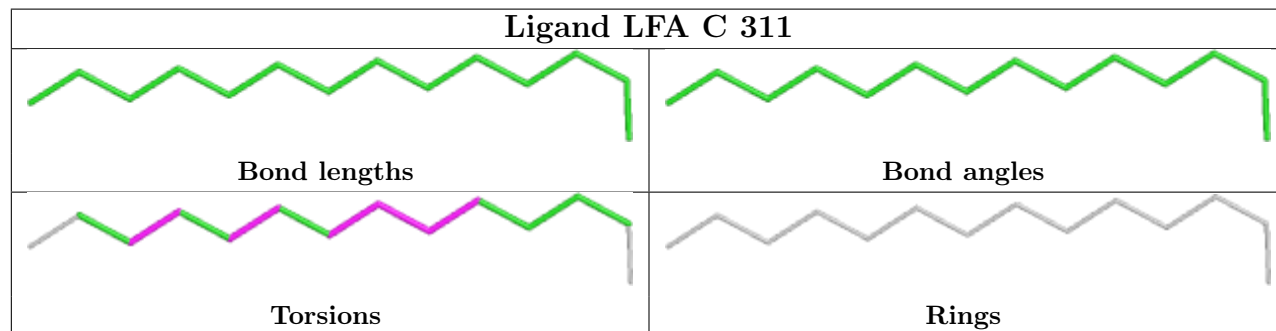
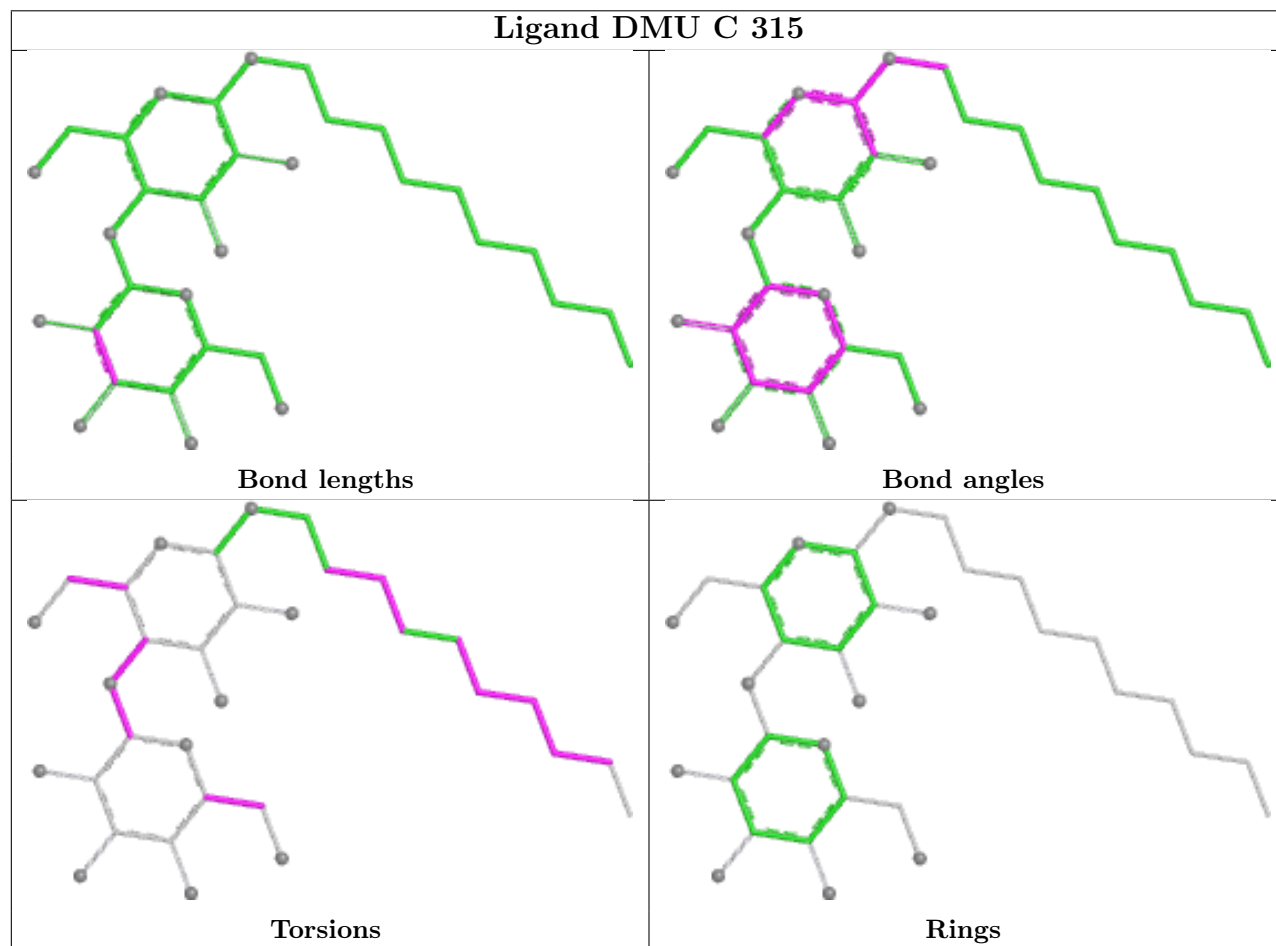
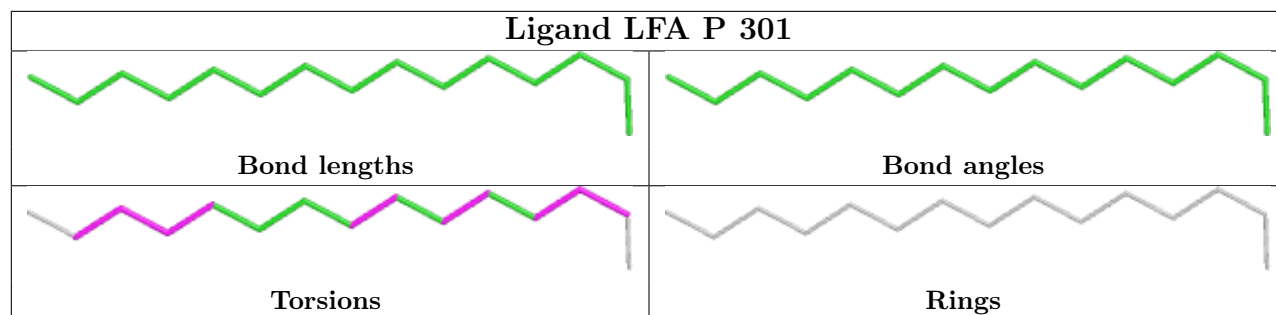


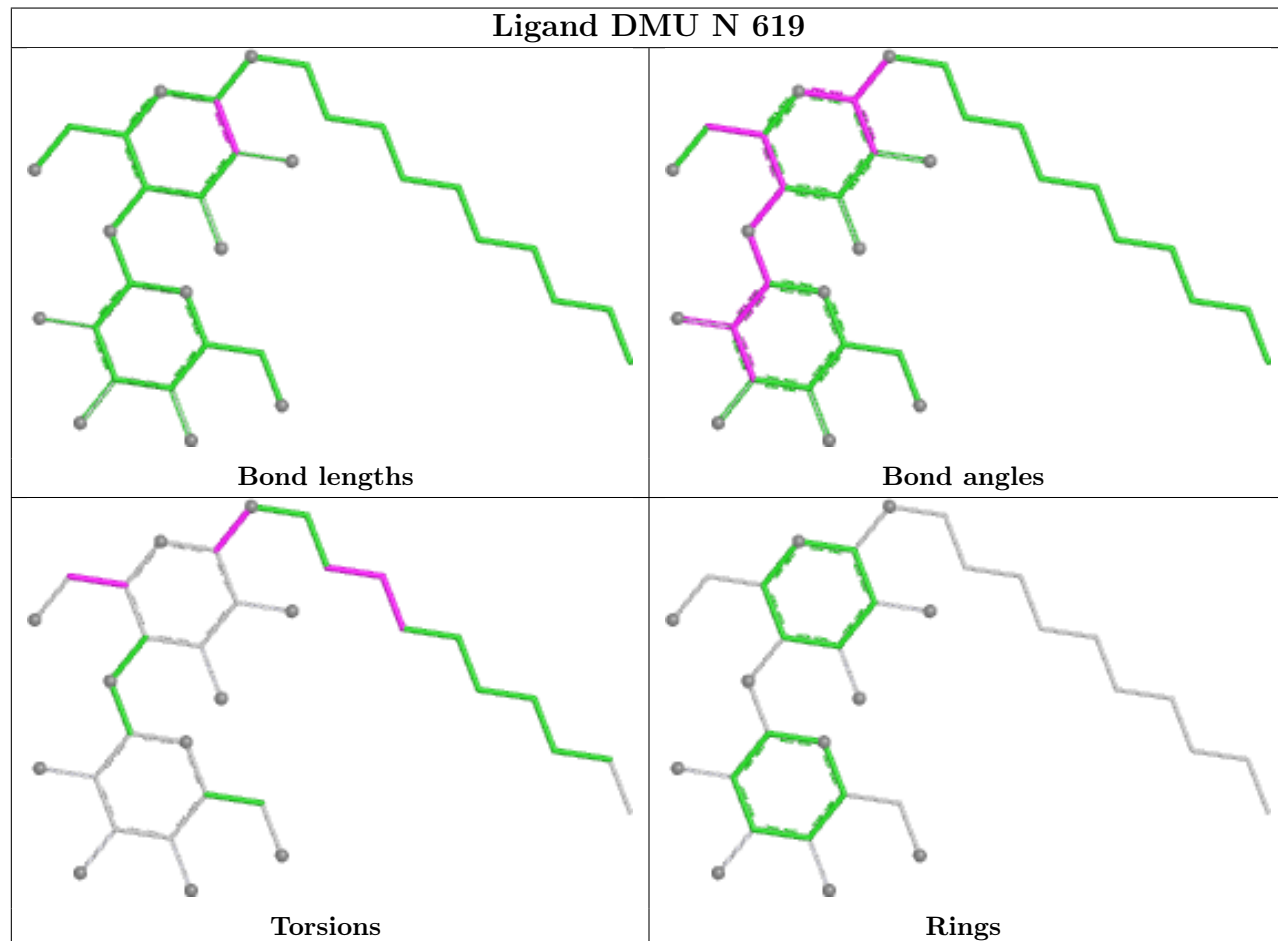
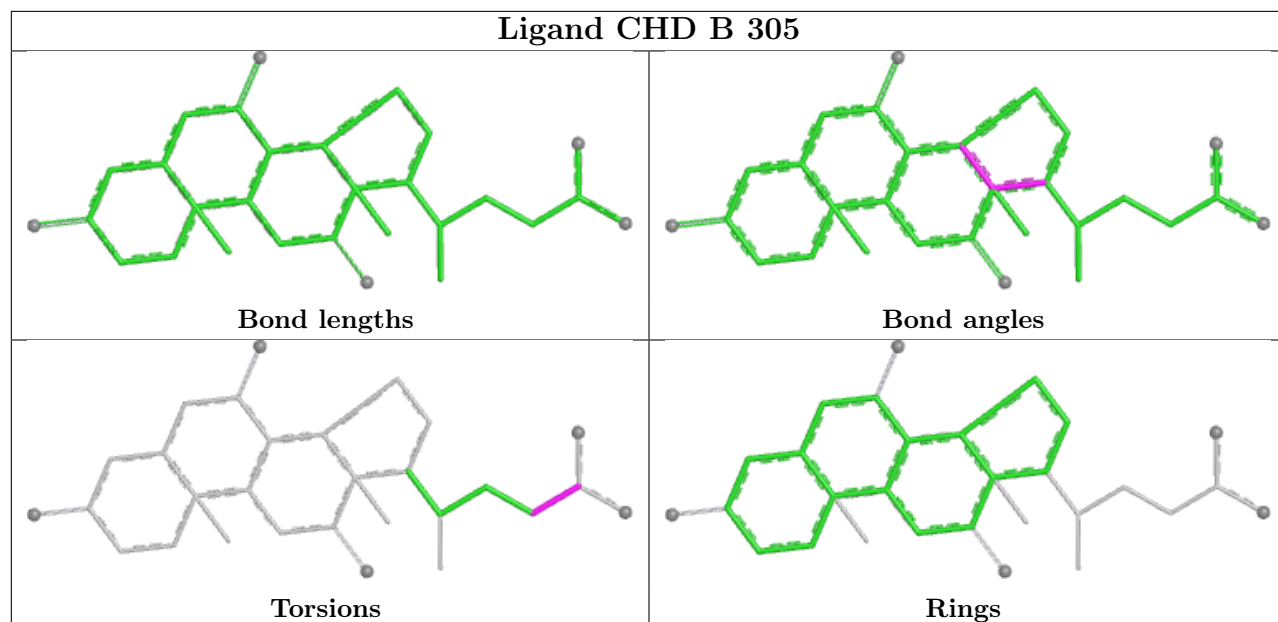


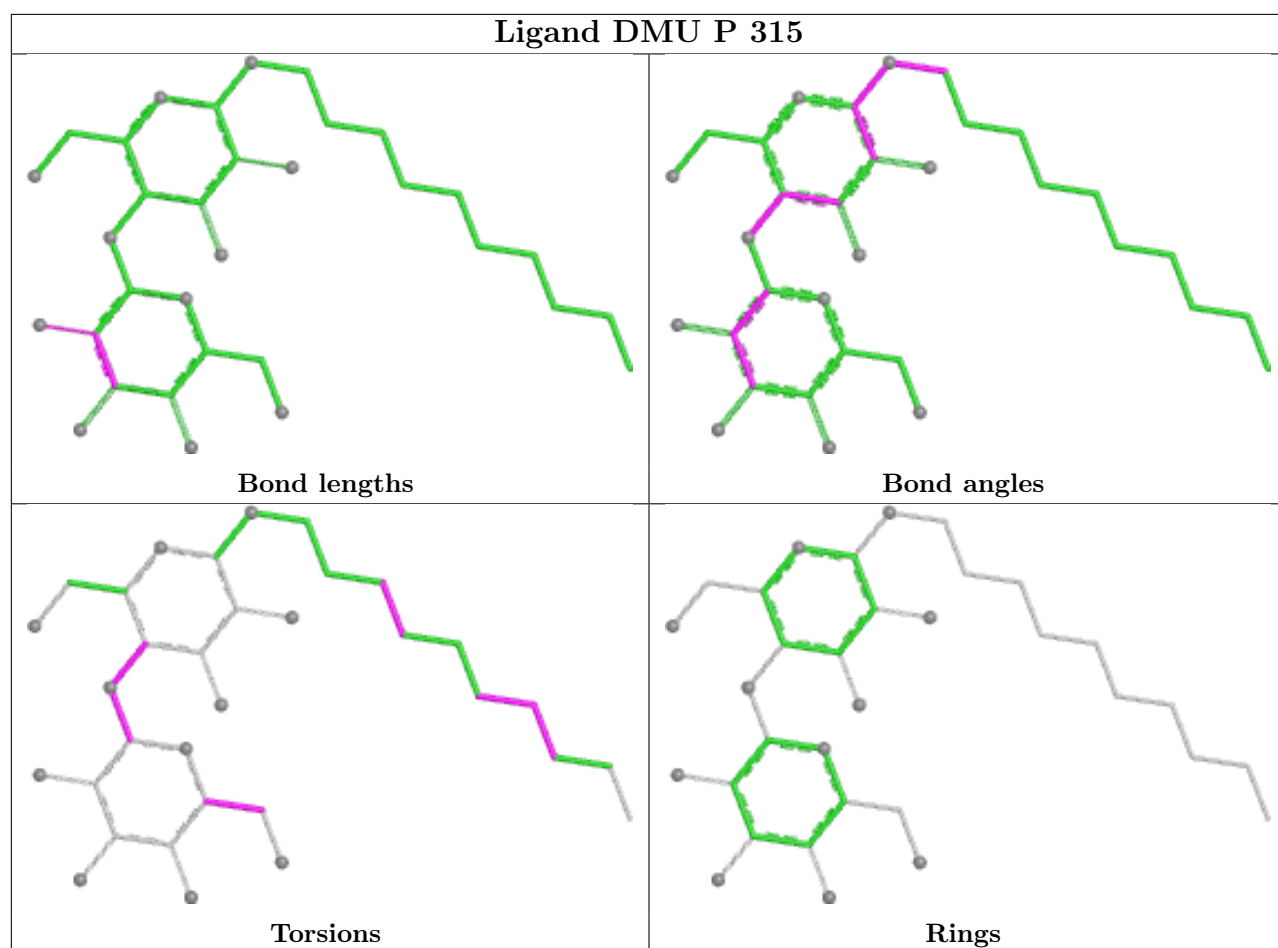


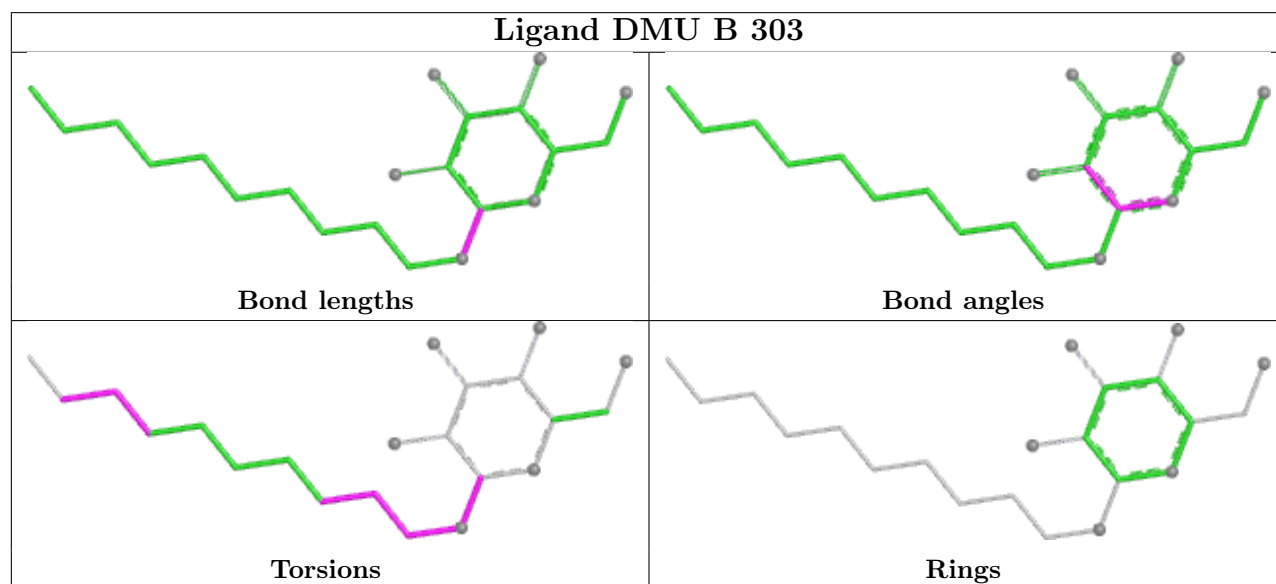
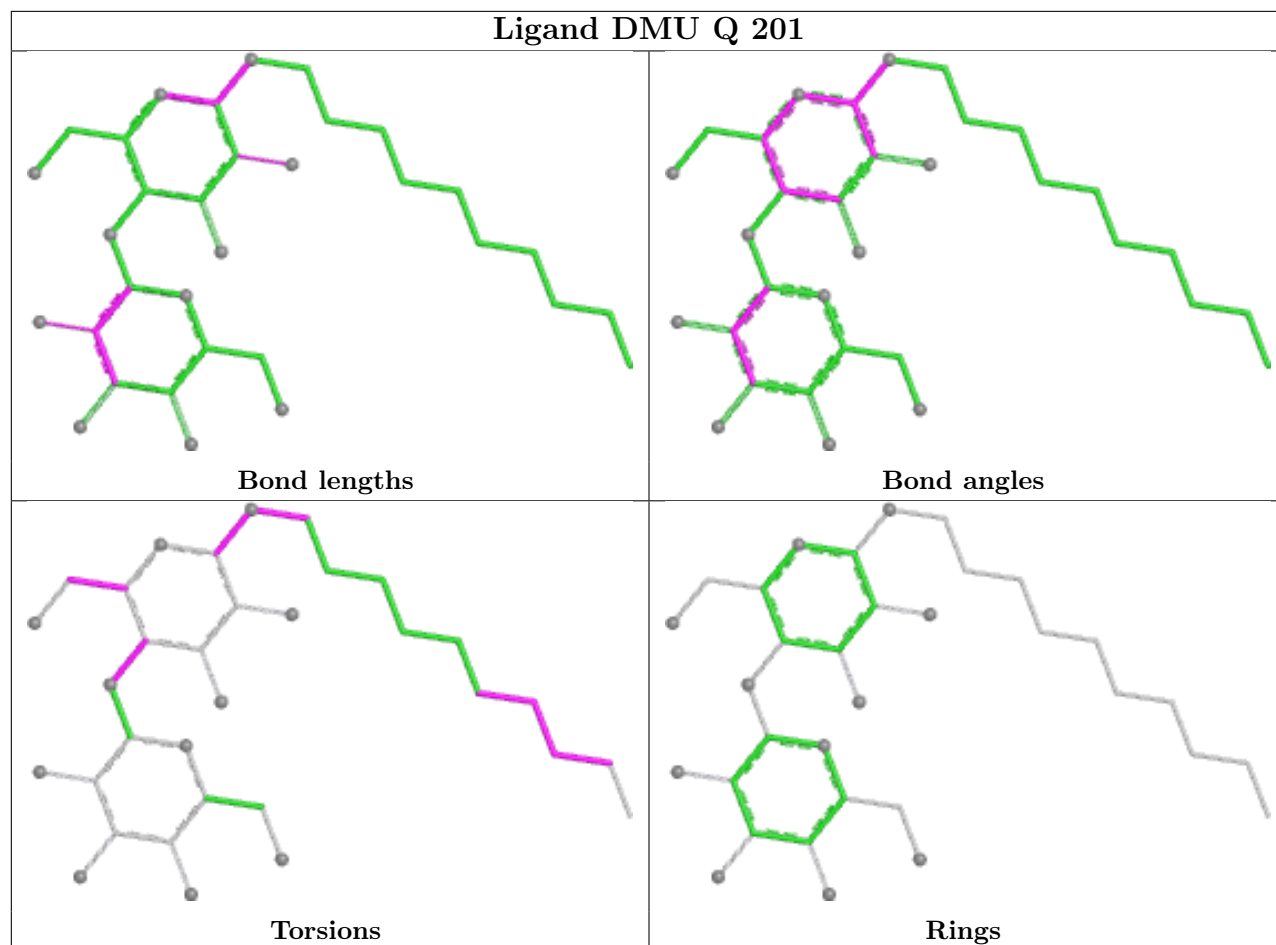


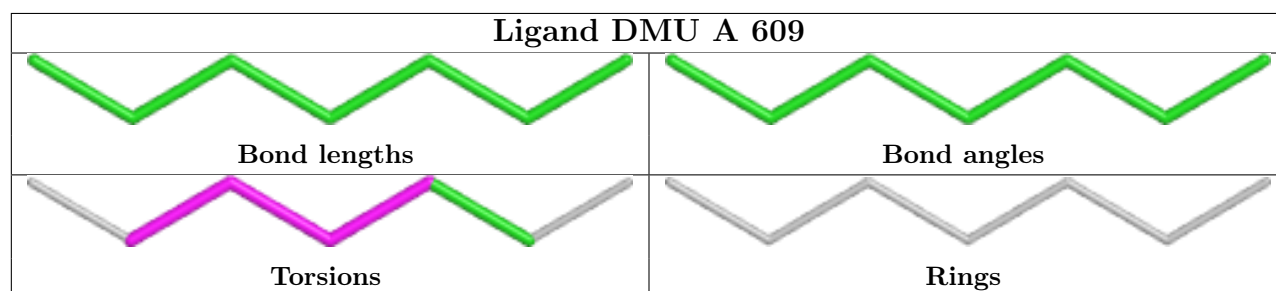
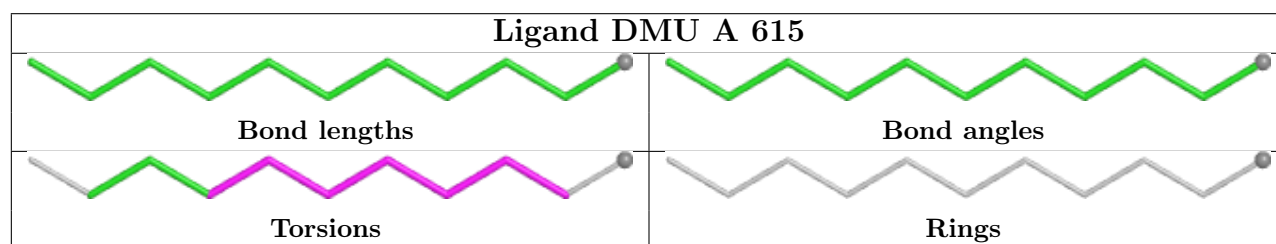
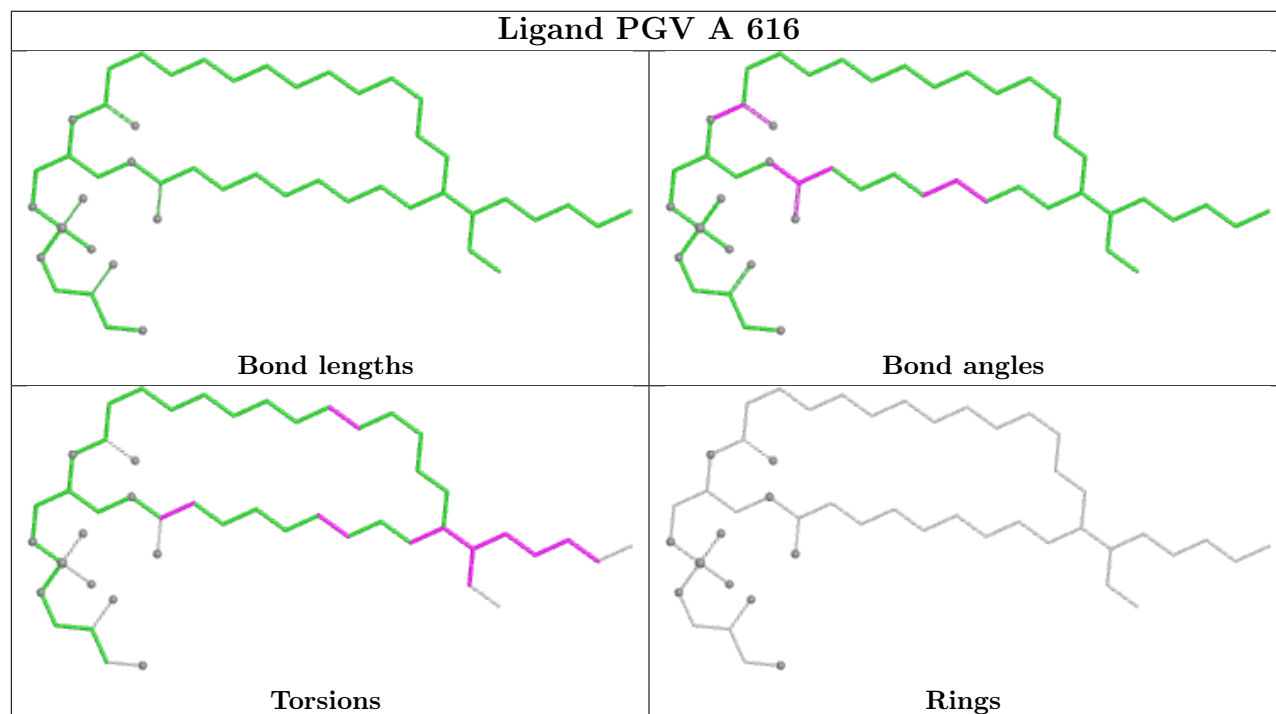
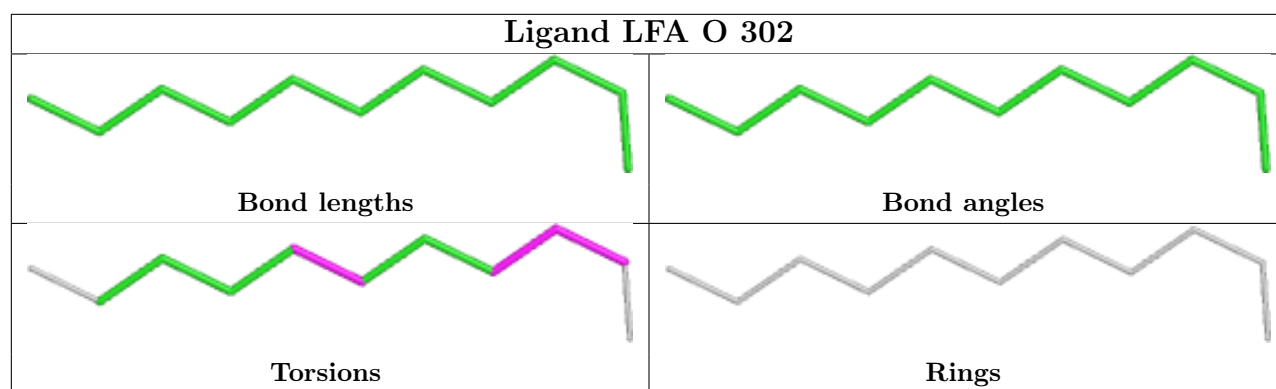


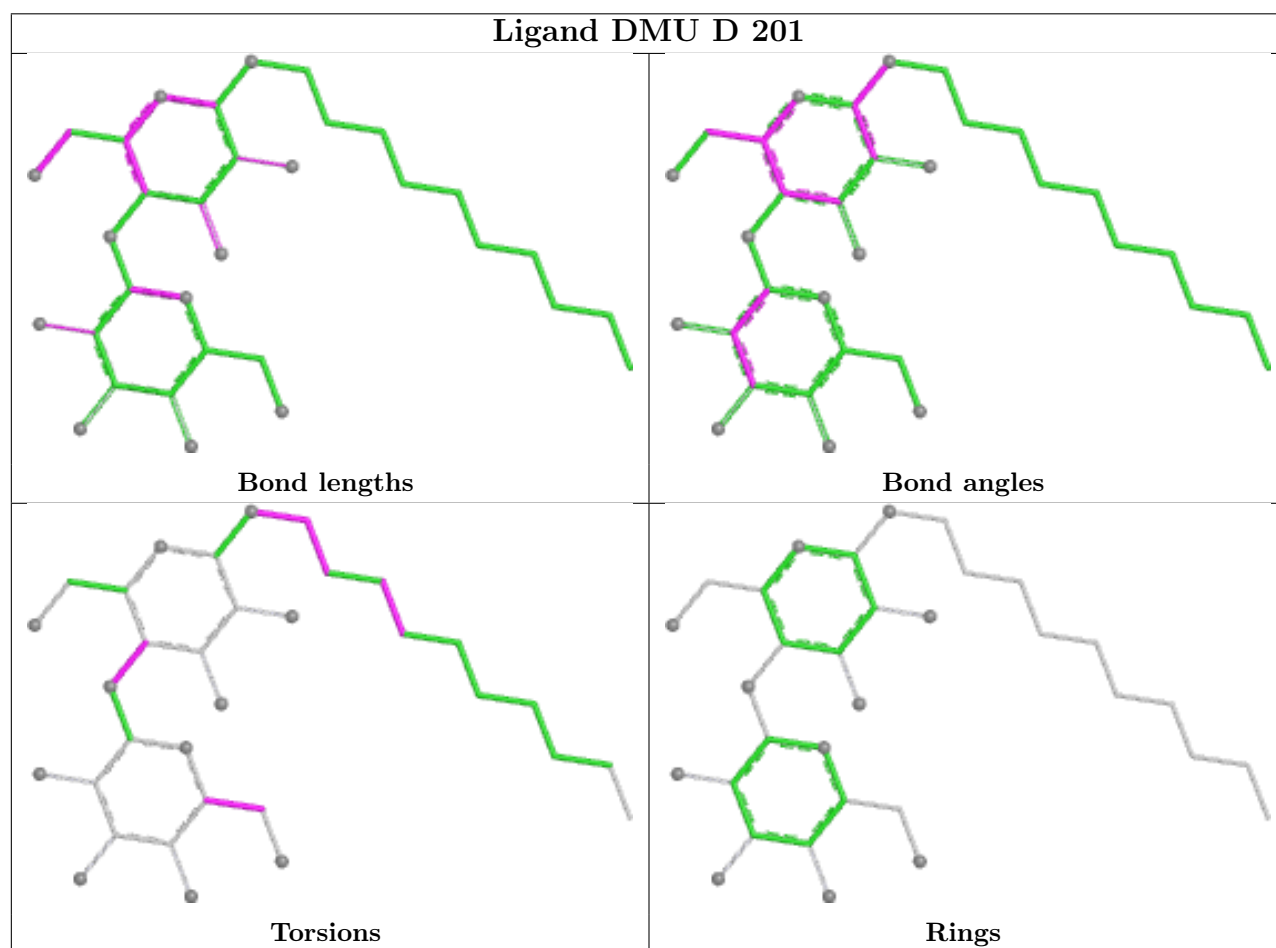
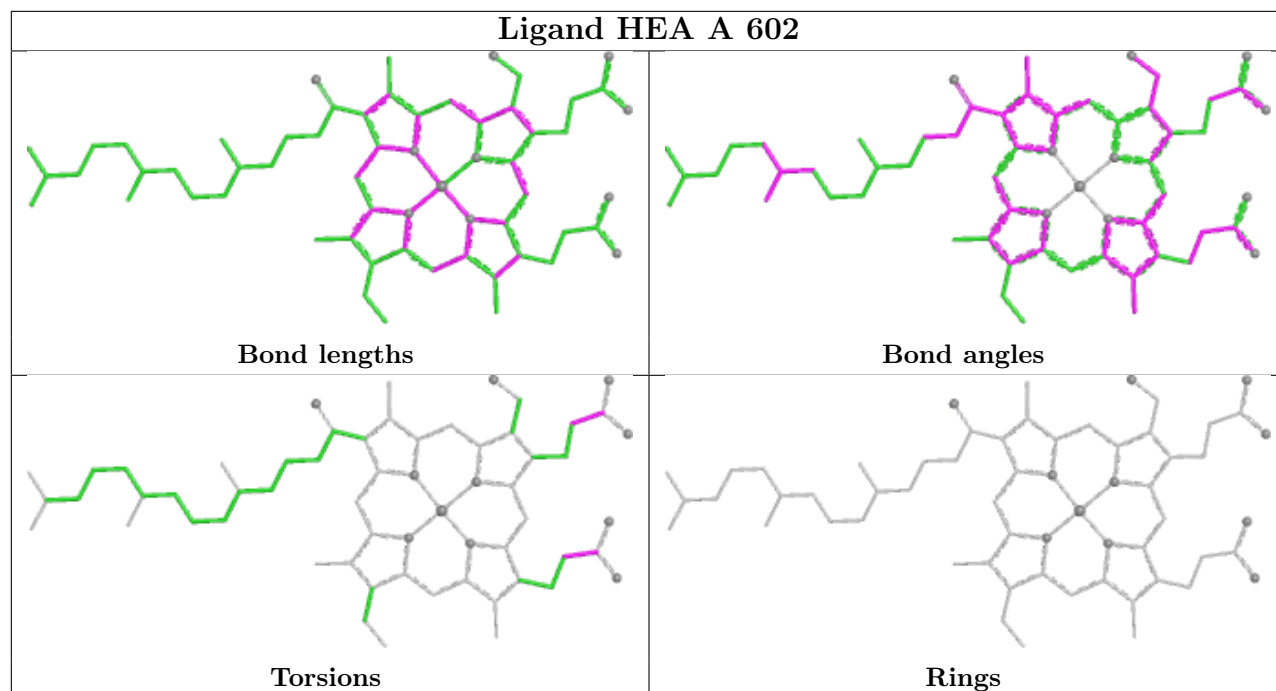


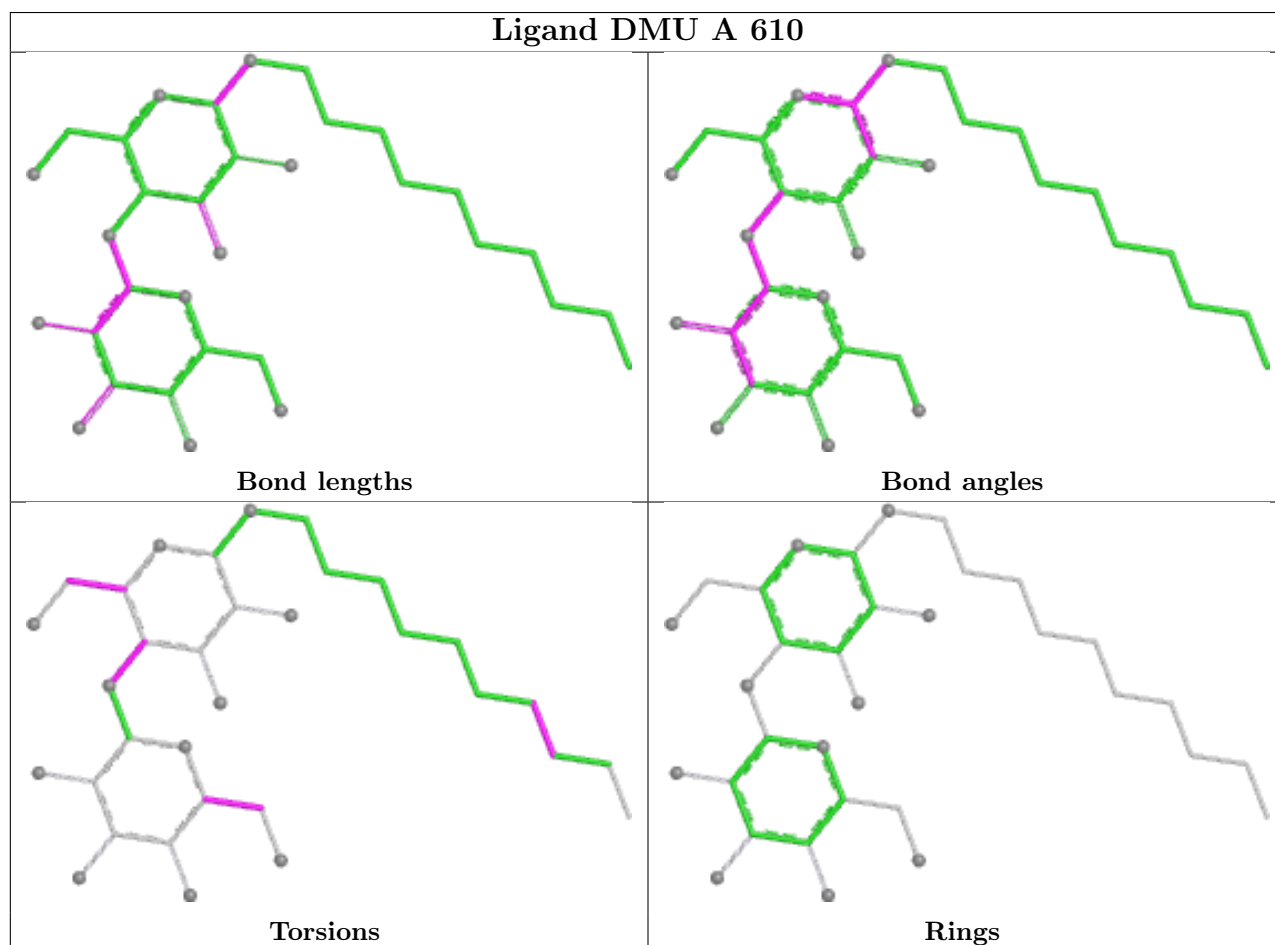
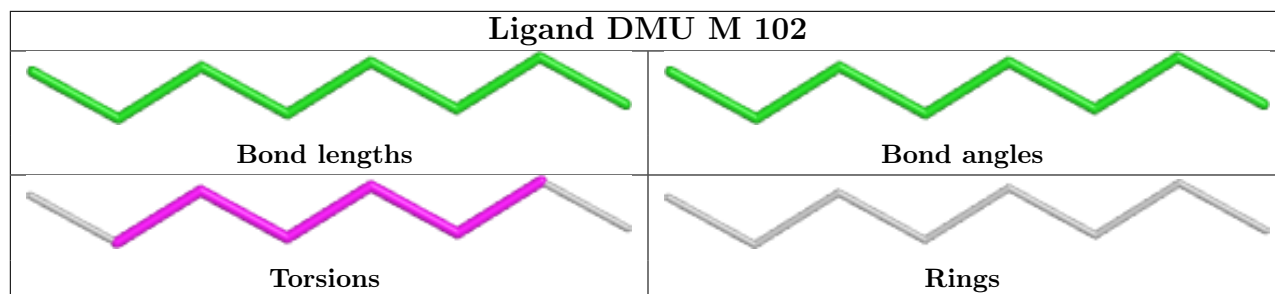


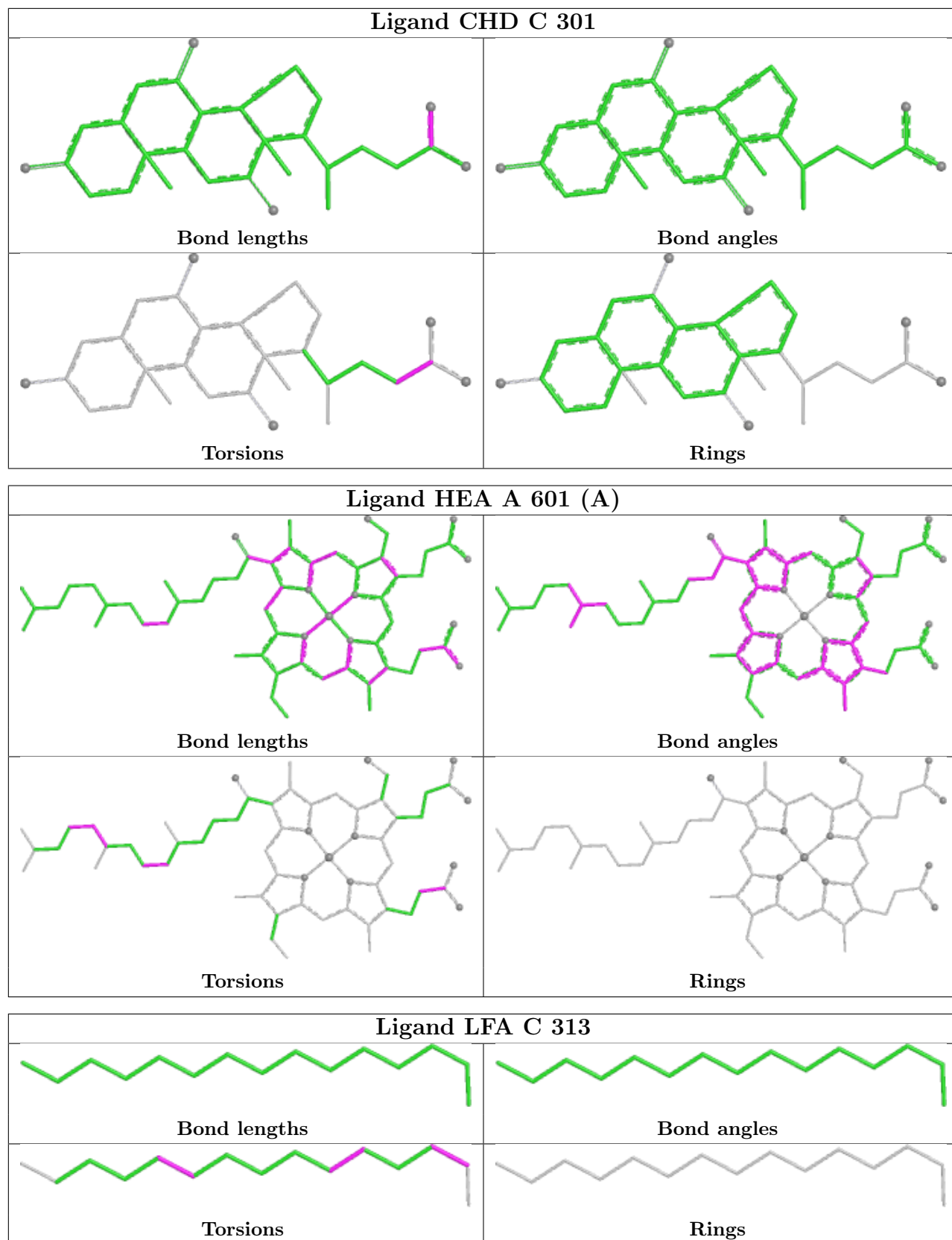


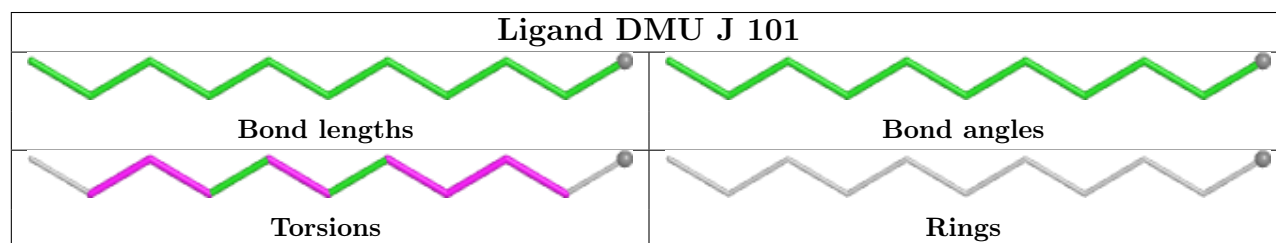
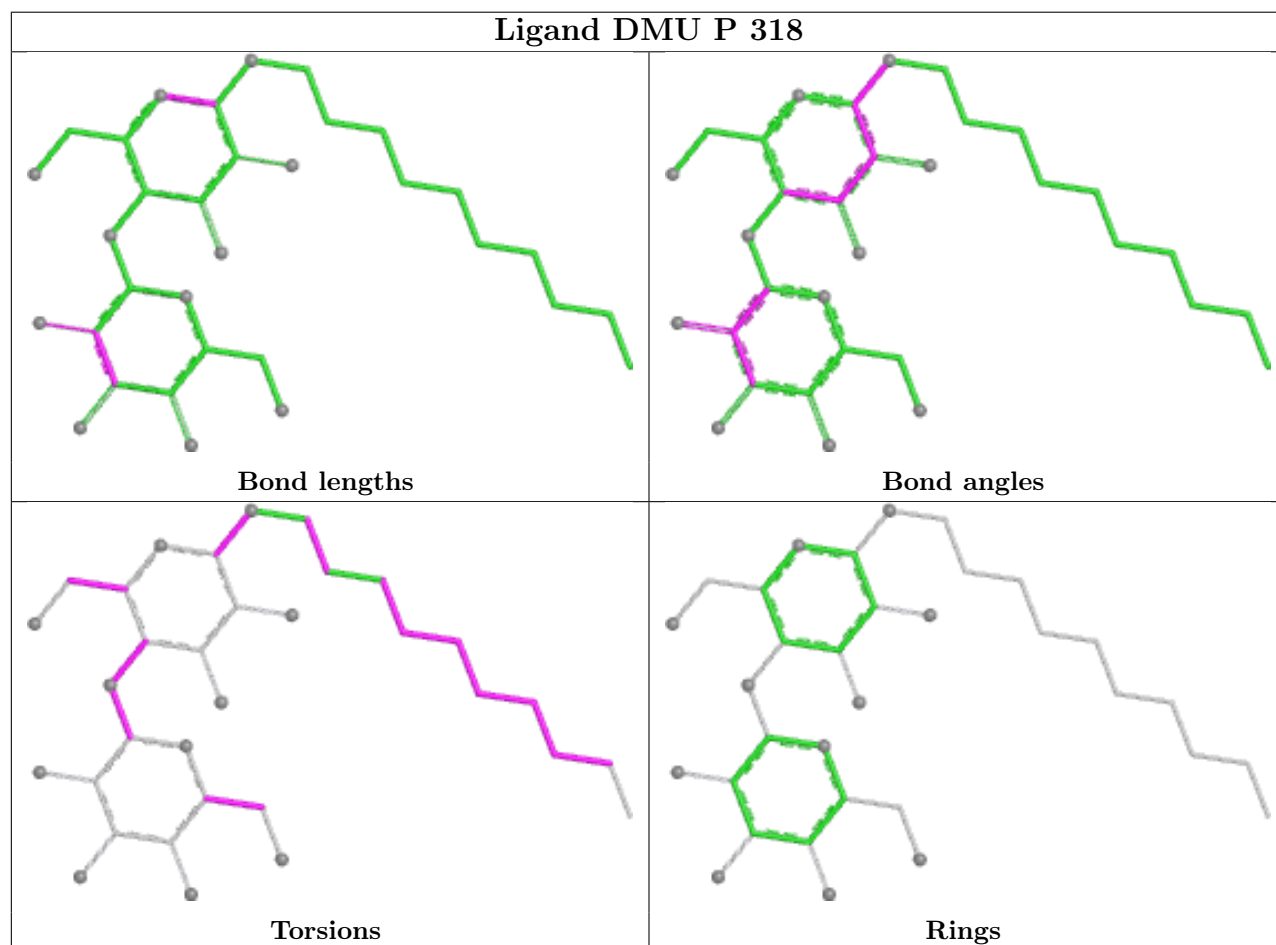
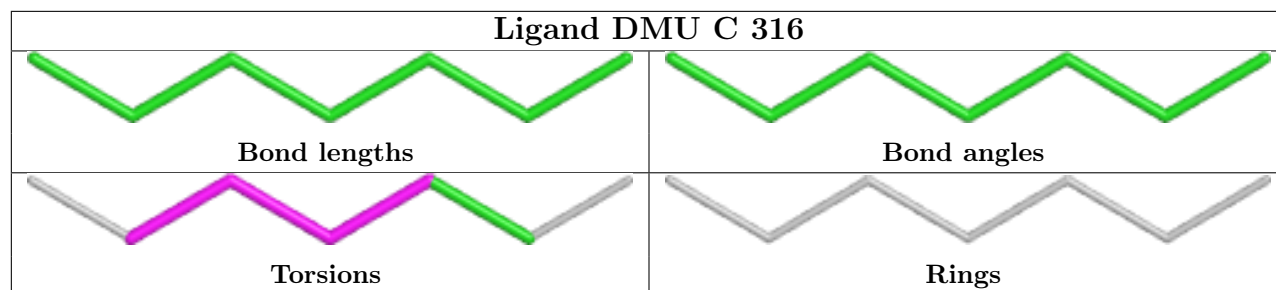


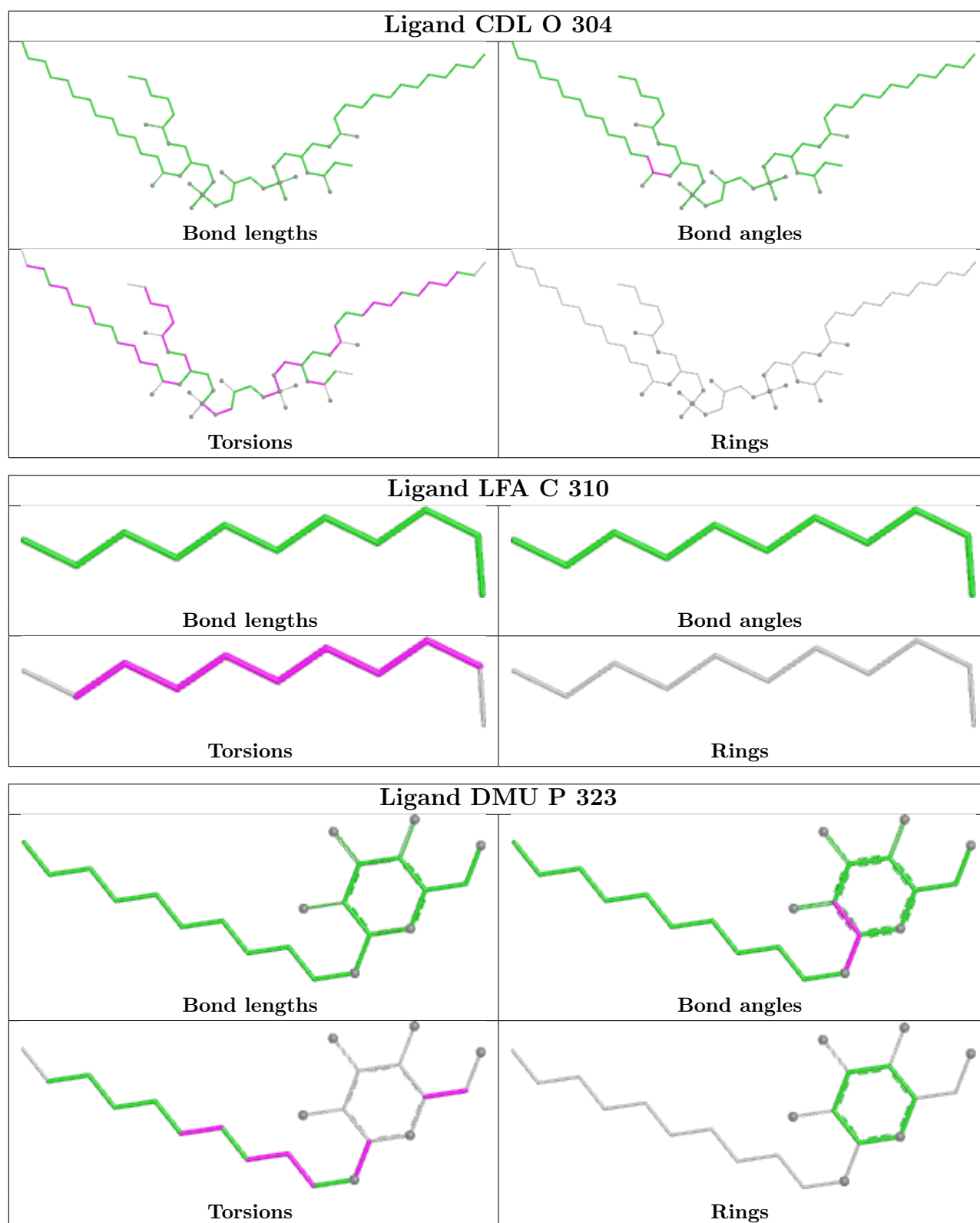


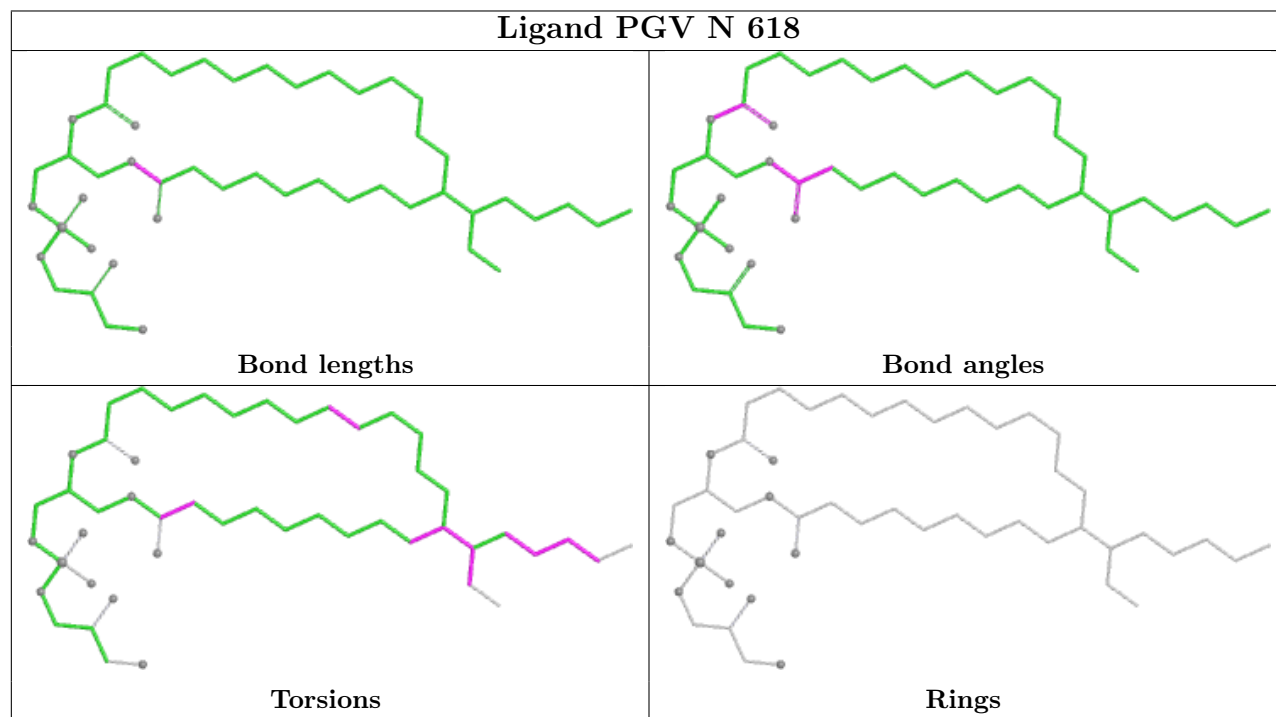
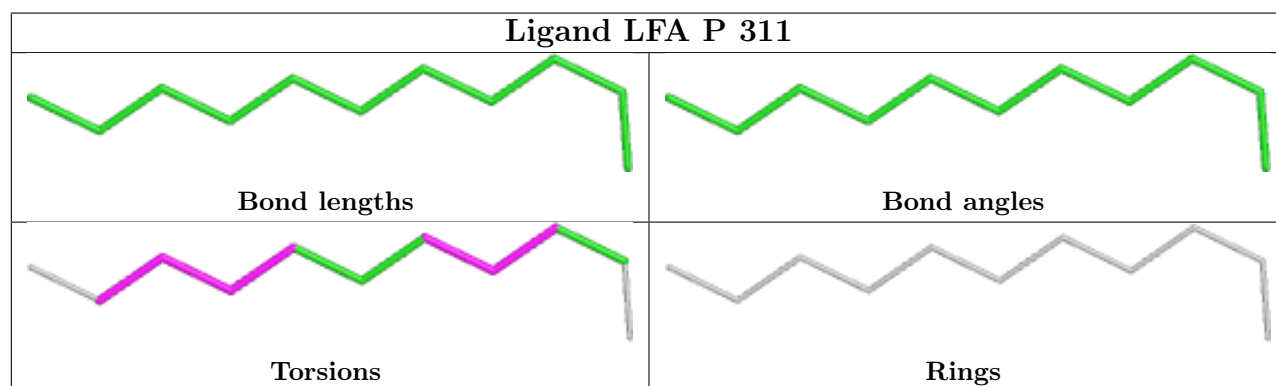
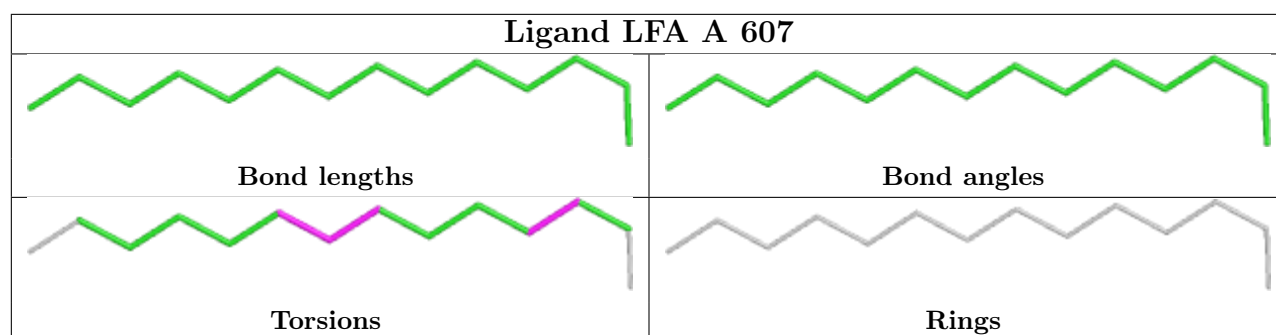


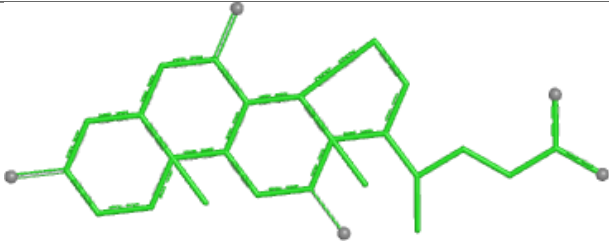
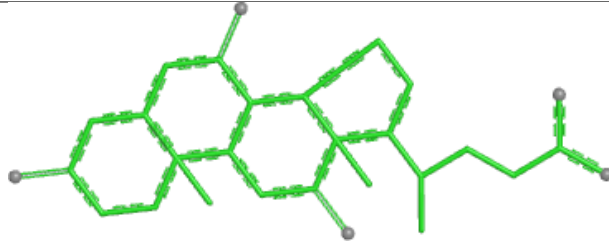
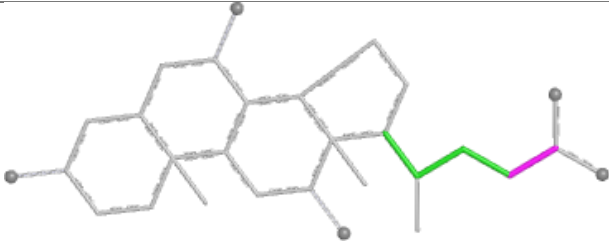
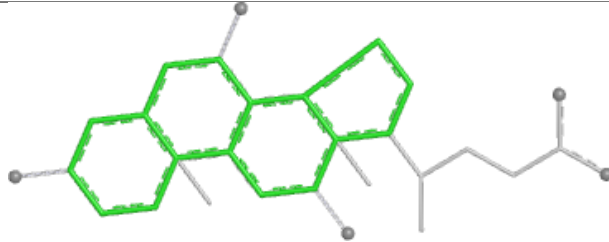




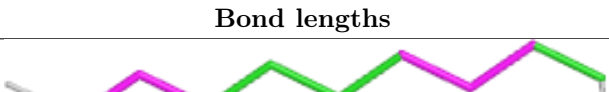
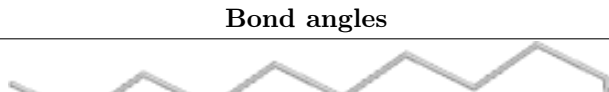




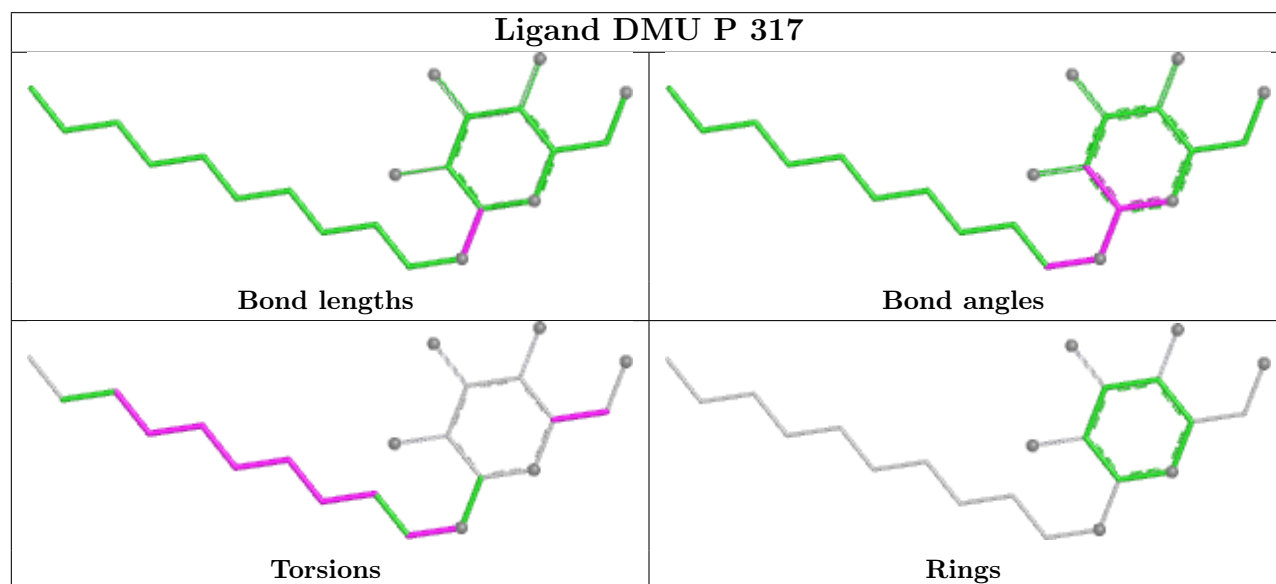
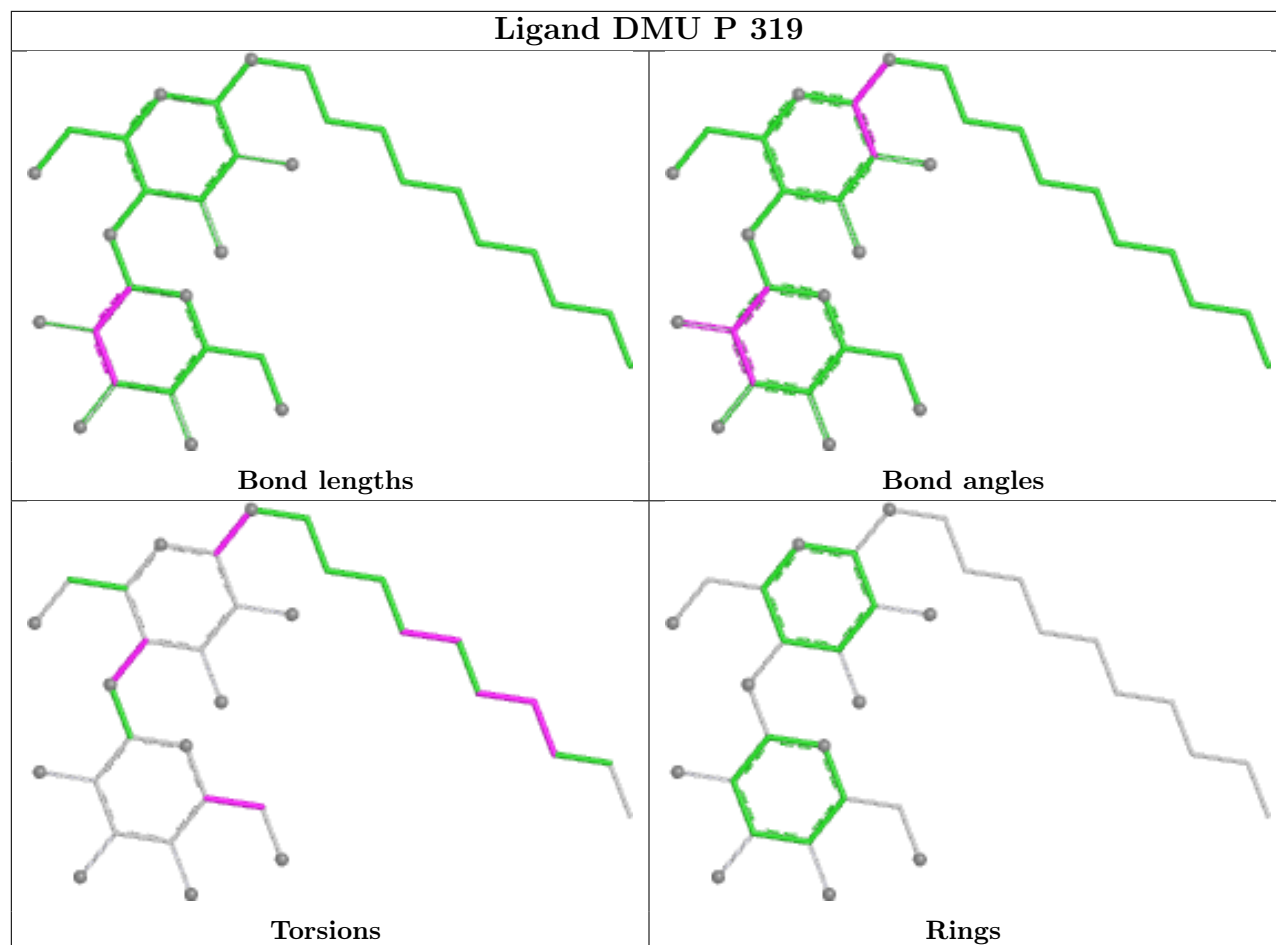


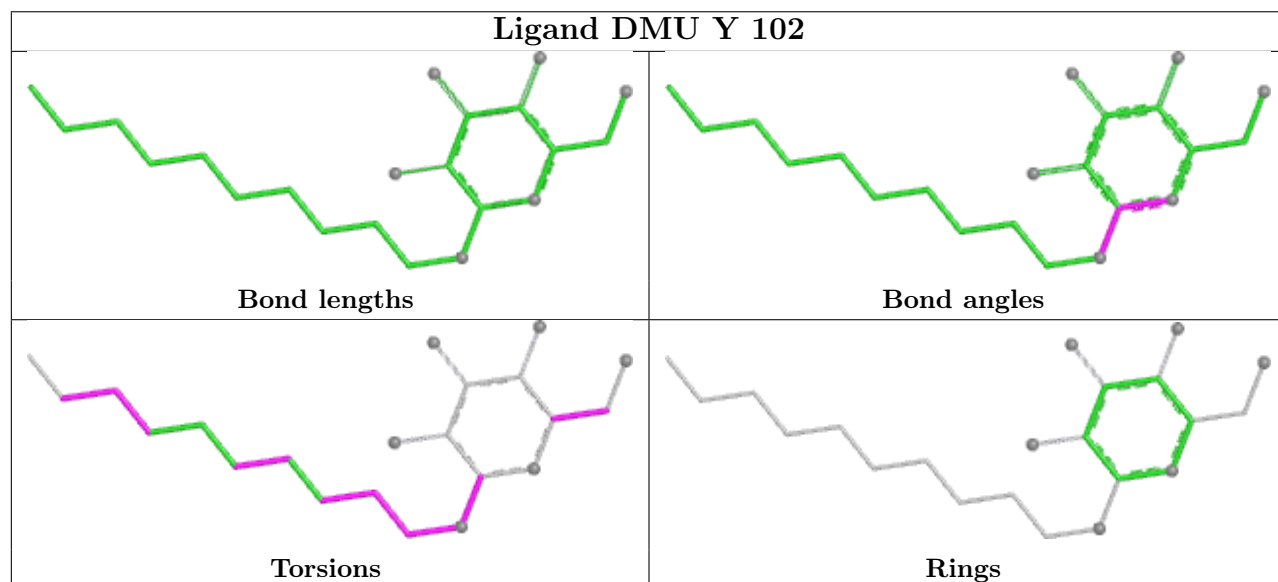
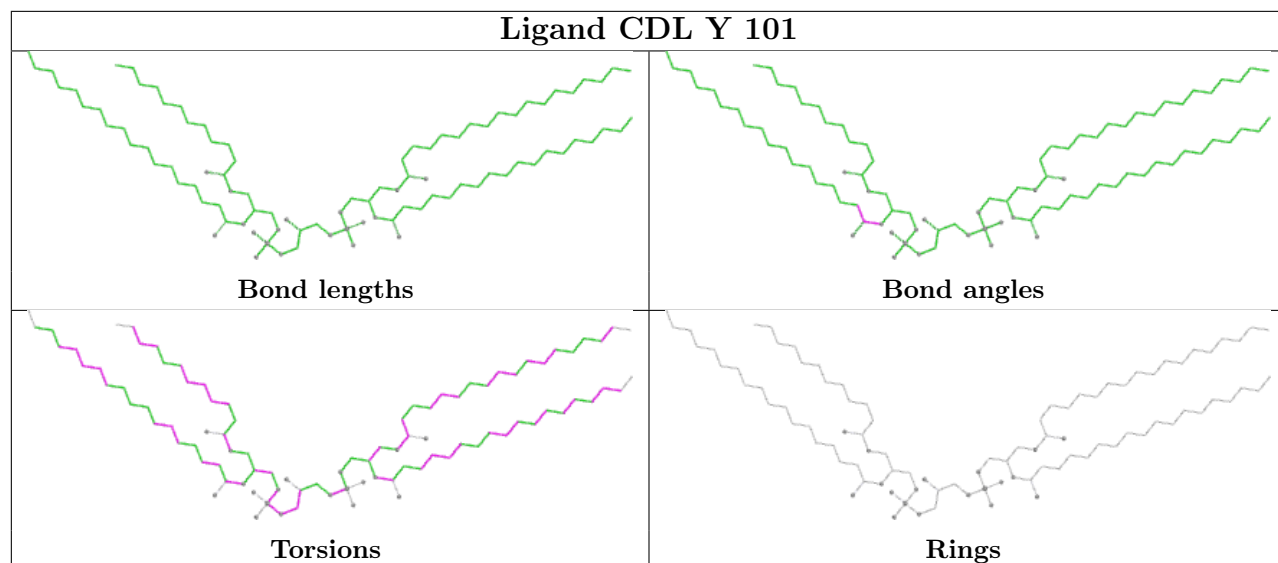
Ligand CHD O 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

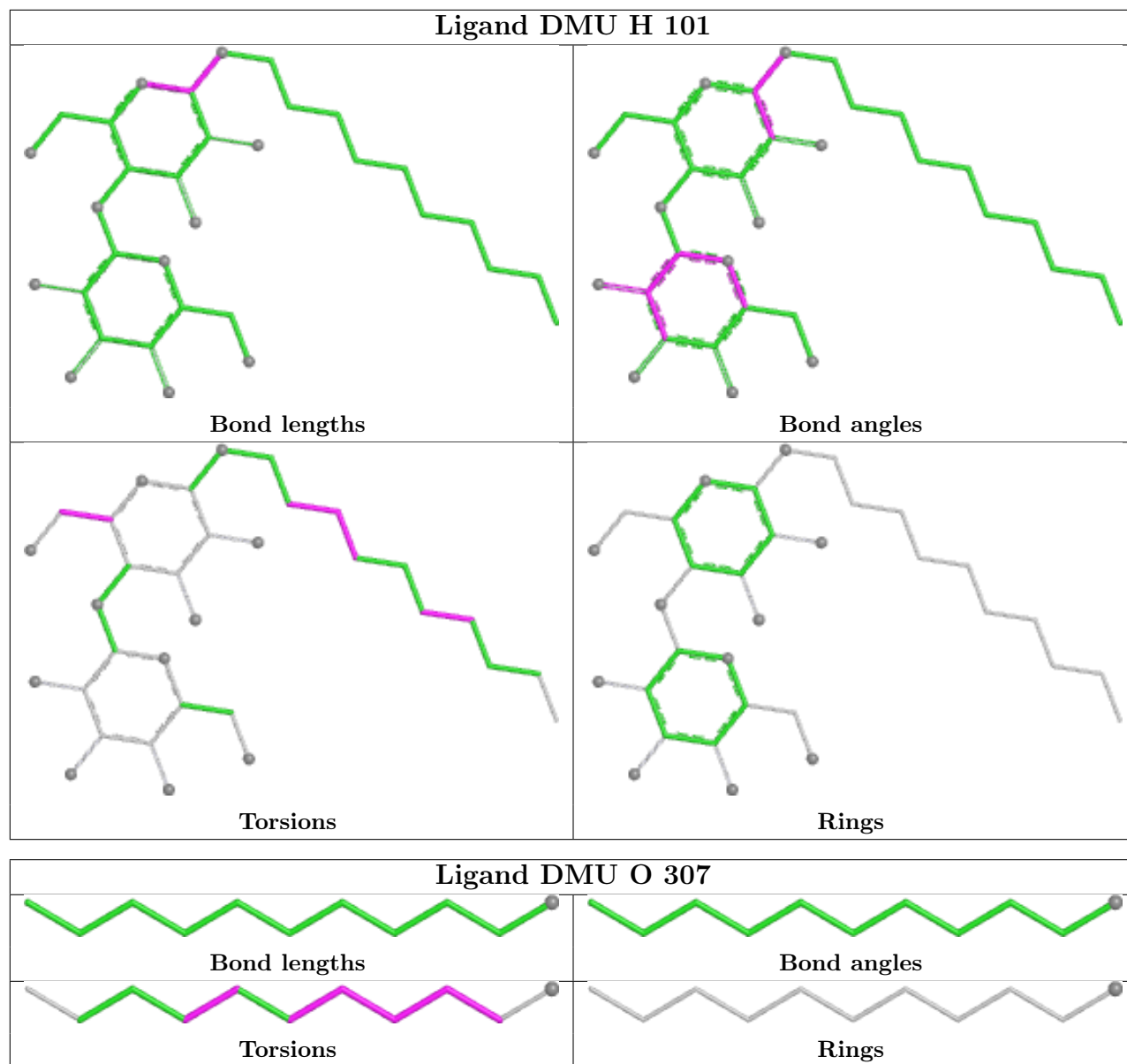
Ligand LFA A 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

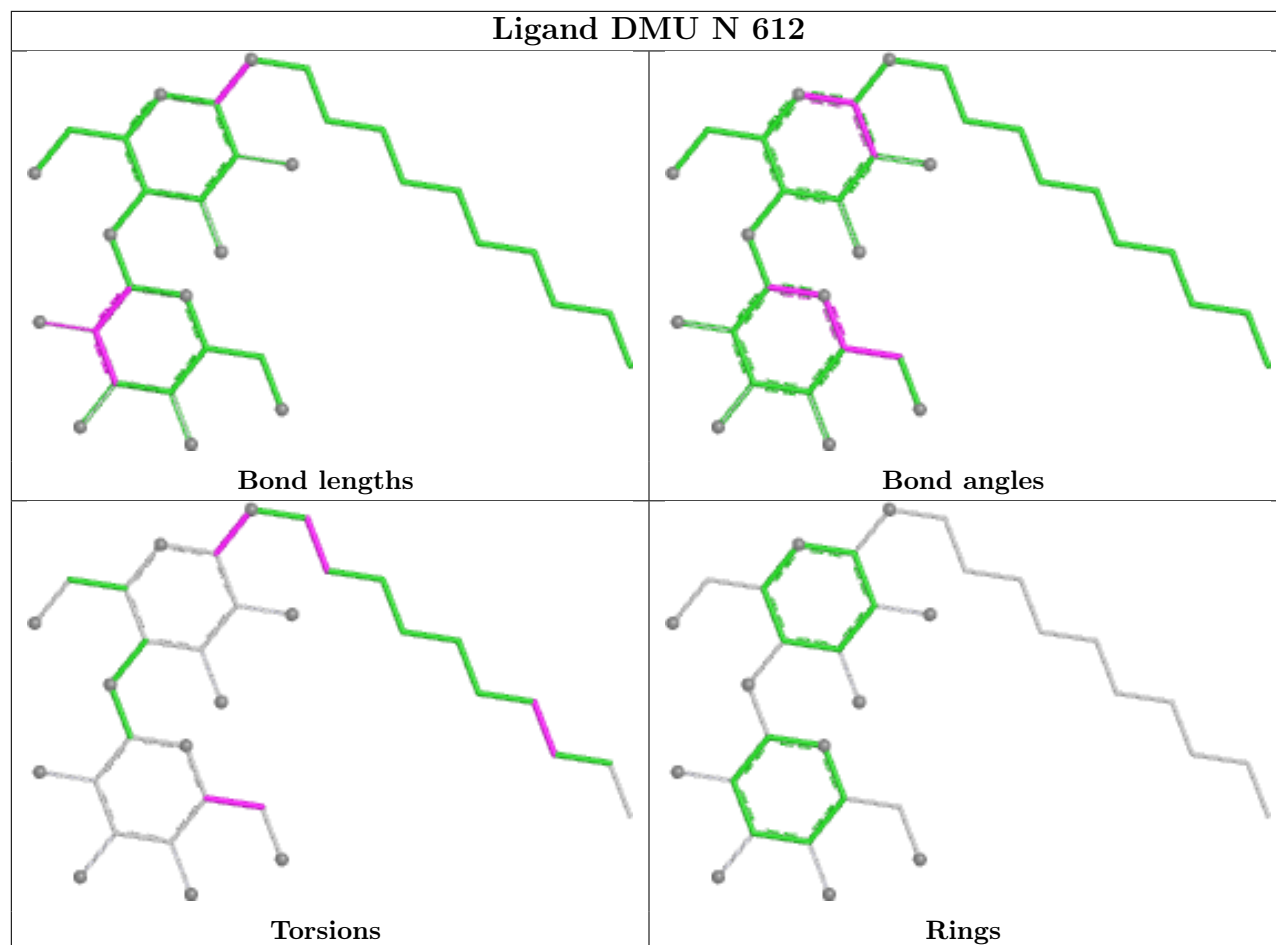
Ligand LFA P 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DMU W 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

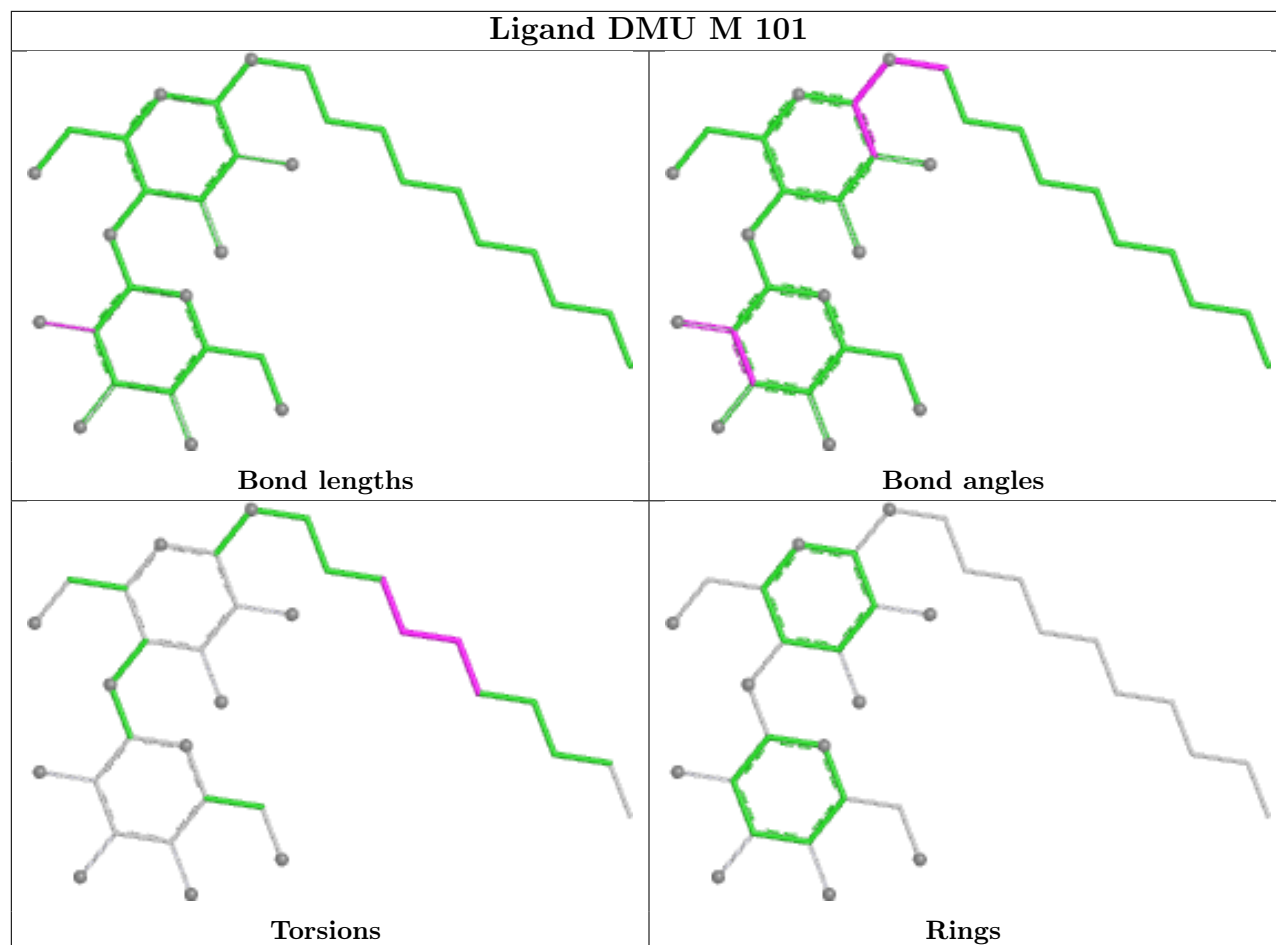




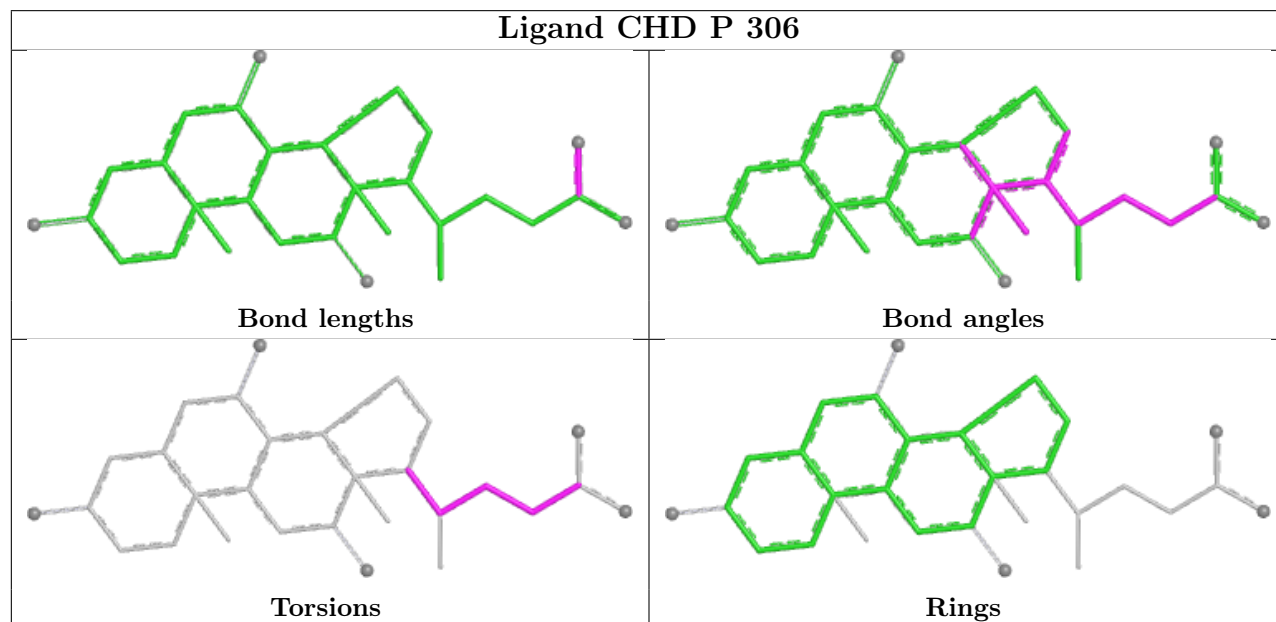


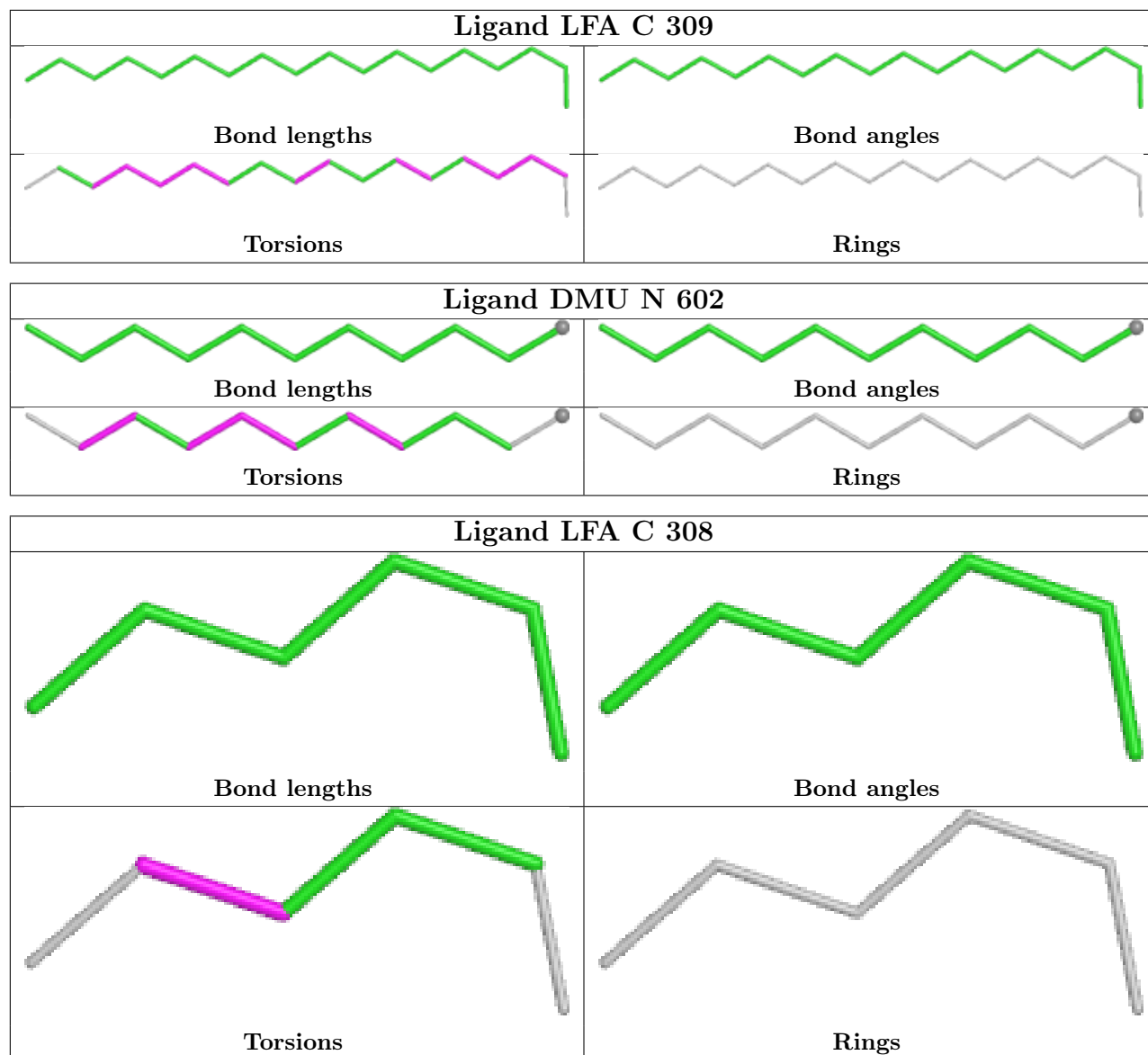


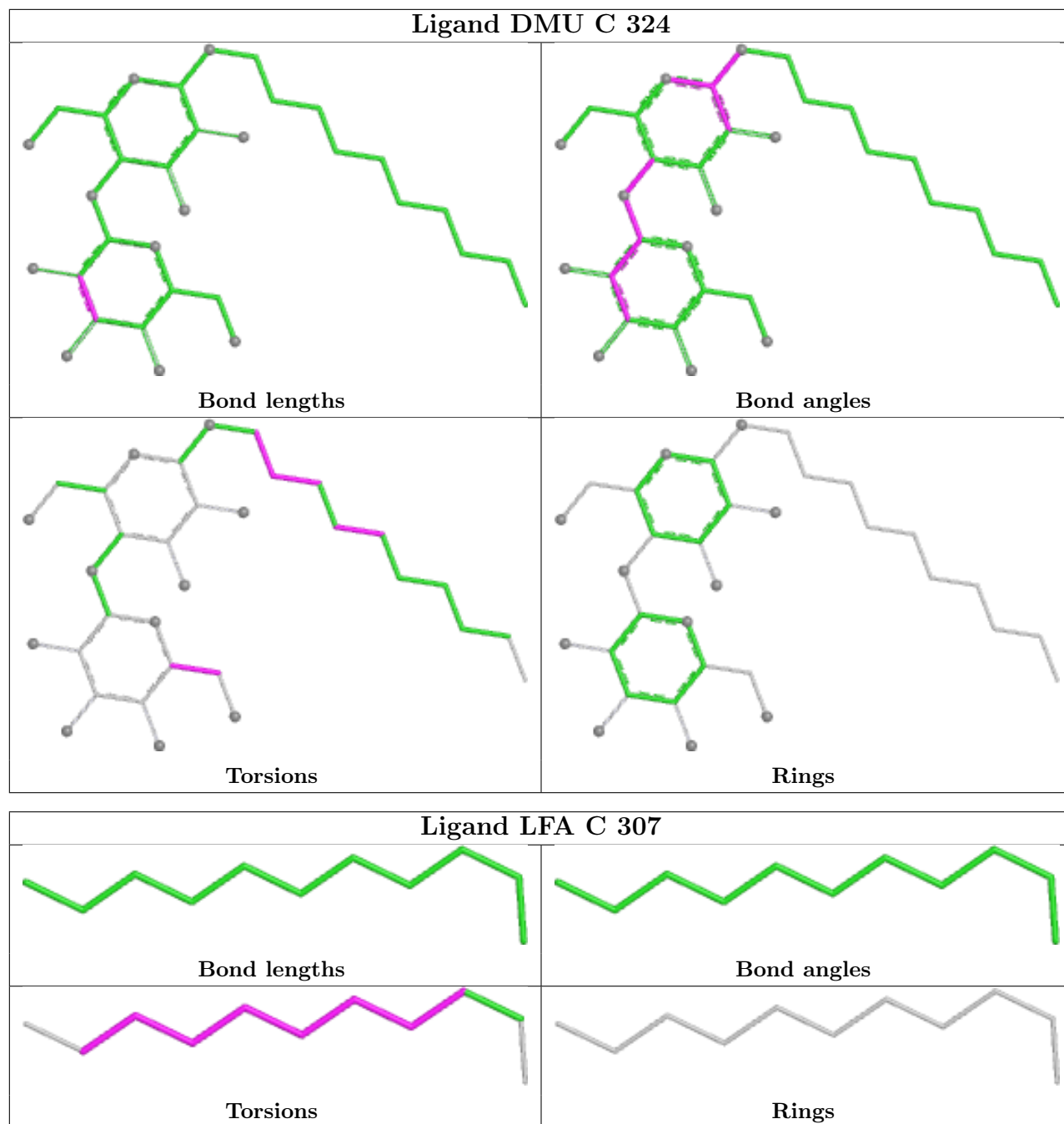
Ligand DMU M 101

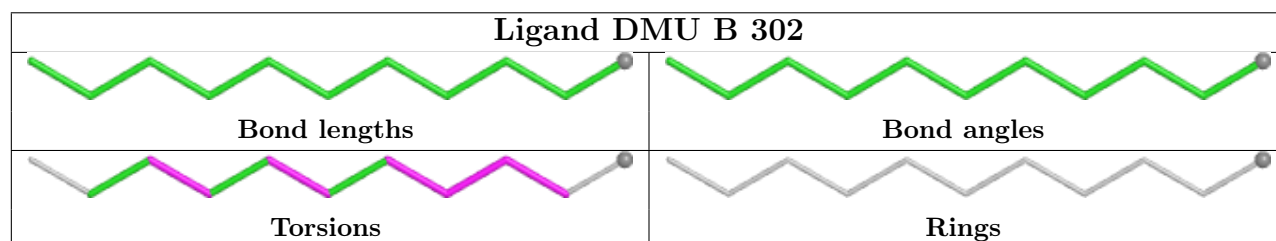
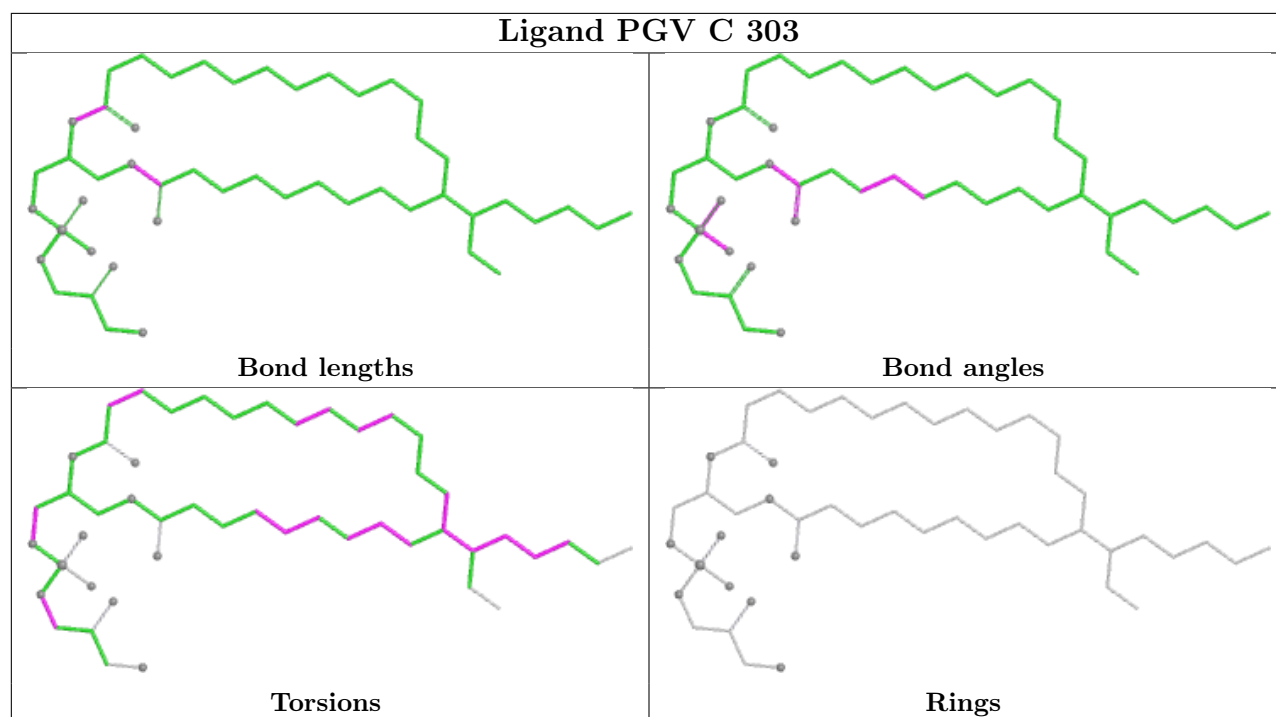
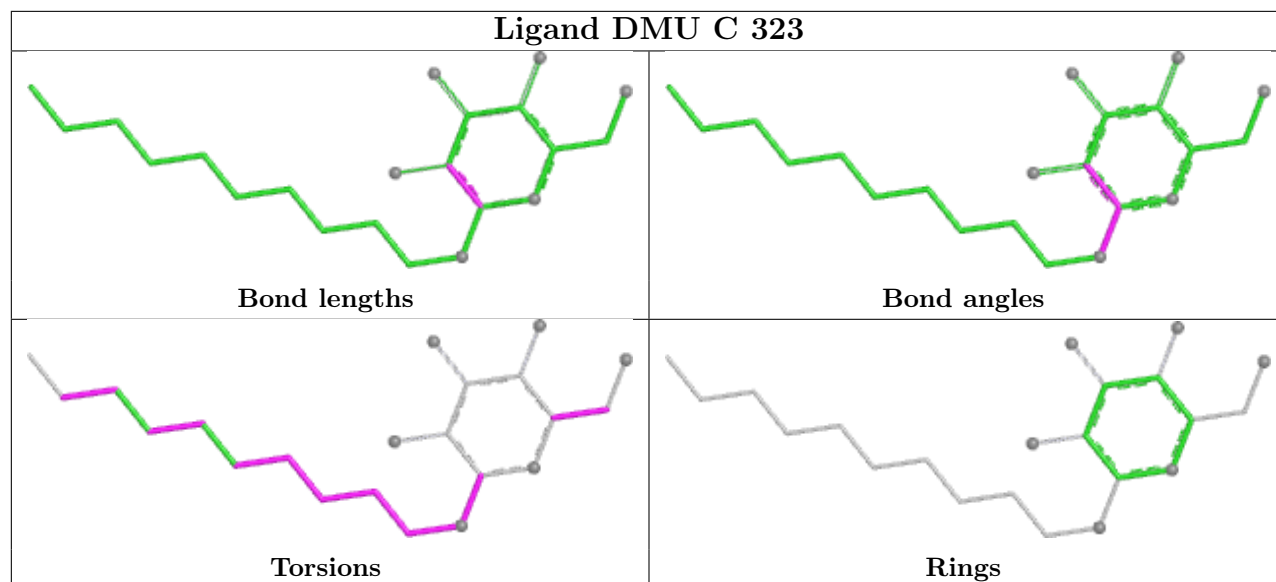


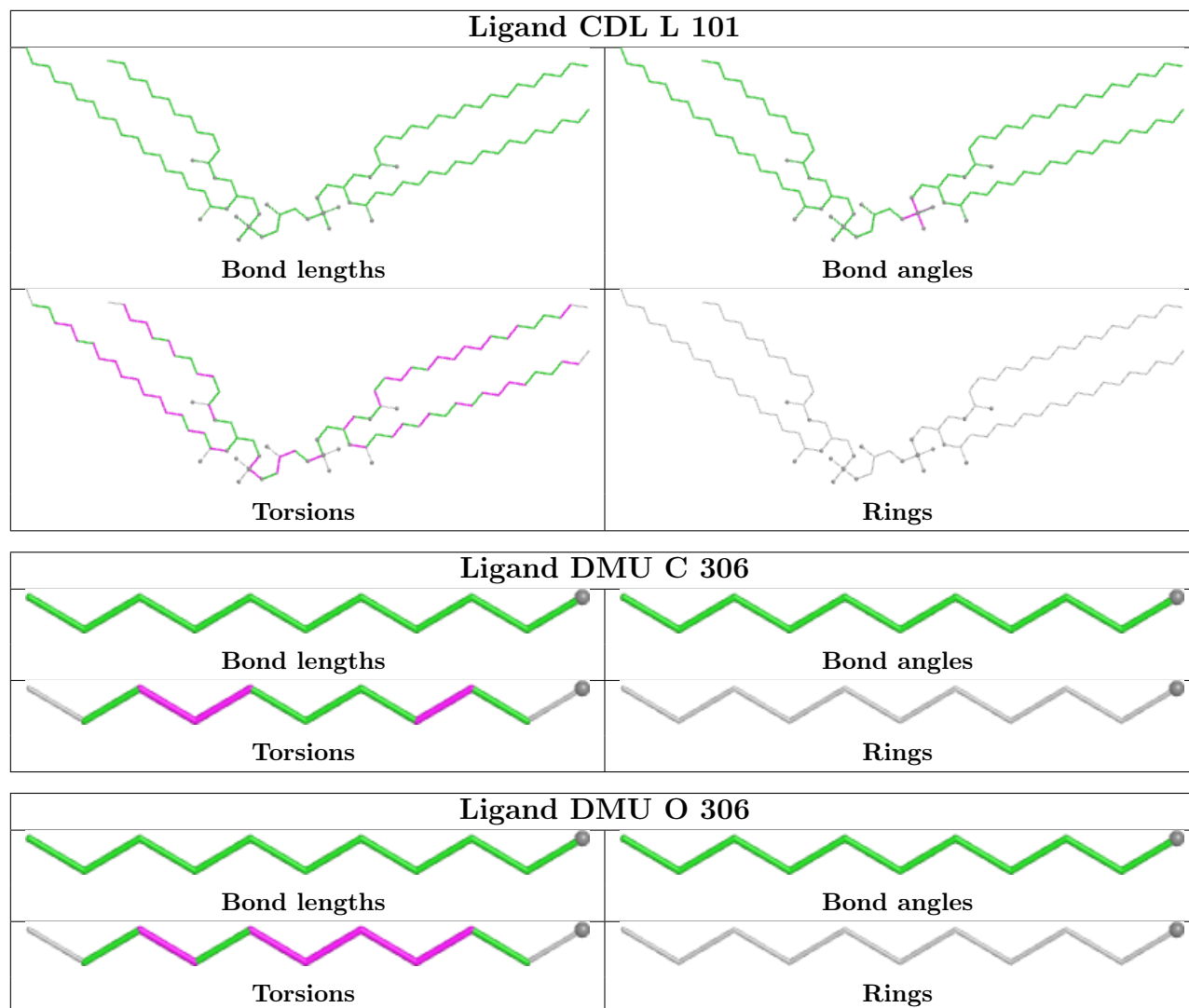
Ligand CHD P 306

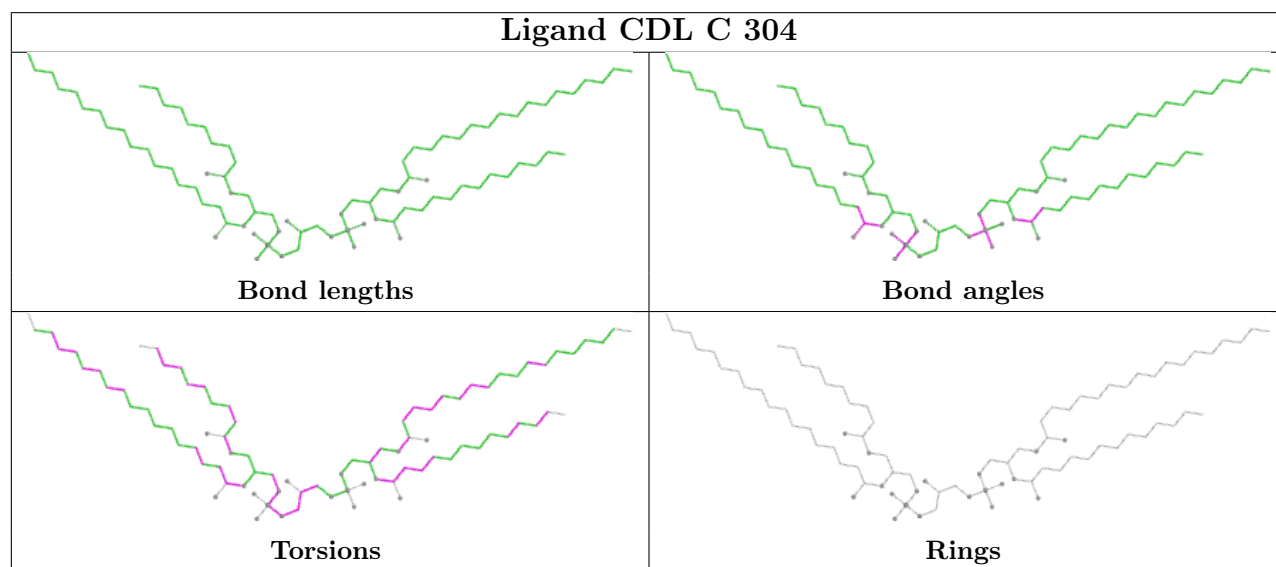
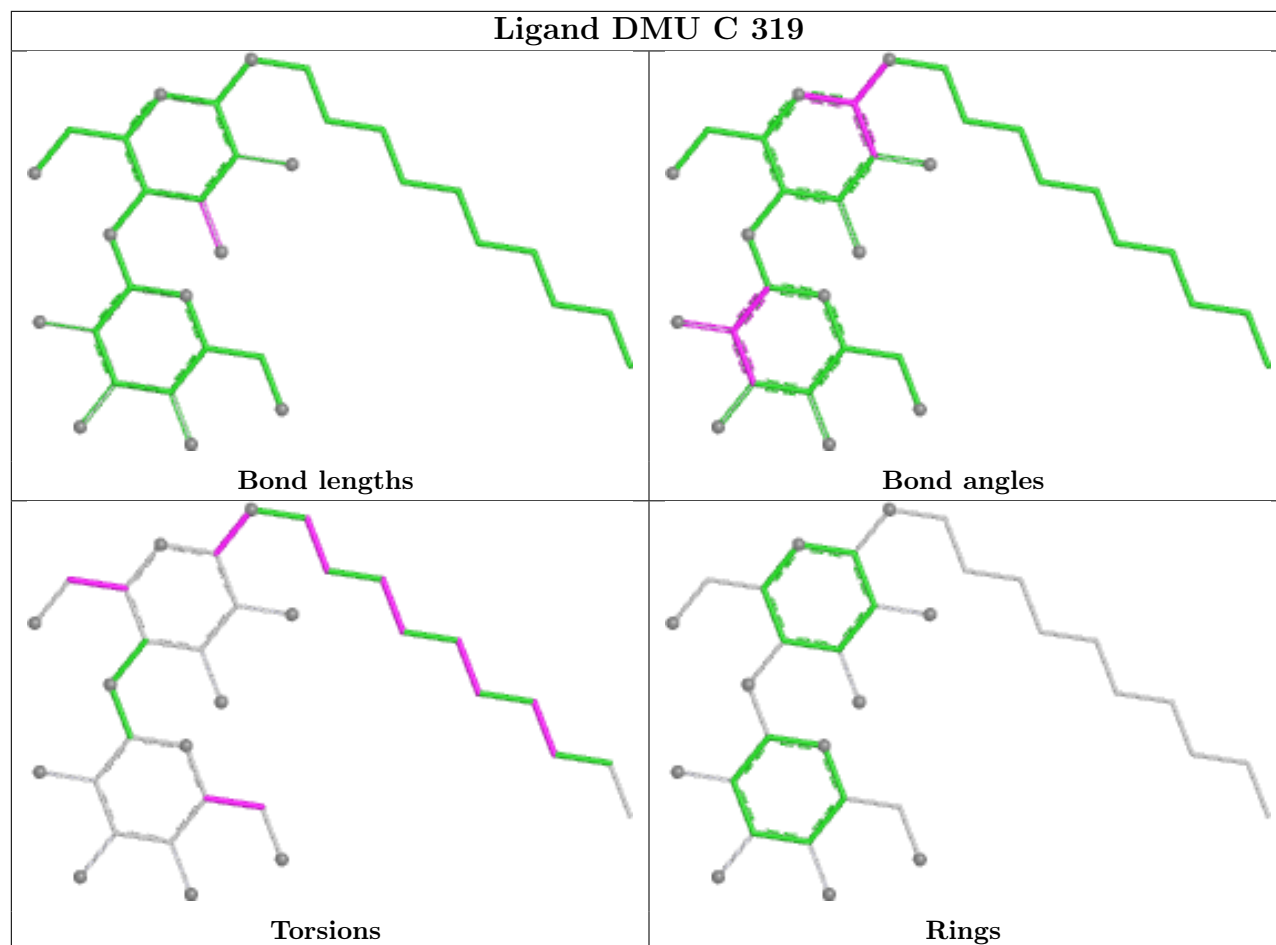


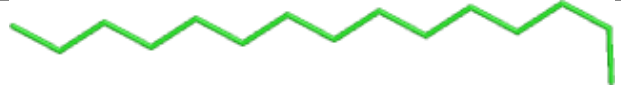
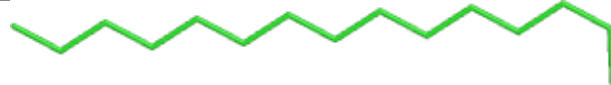
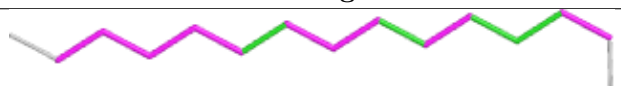
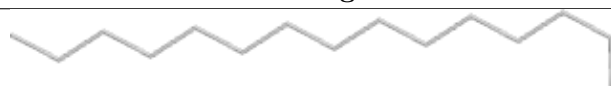
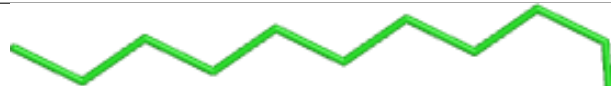
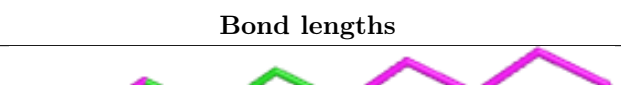
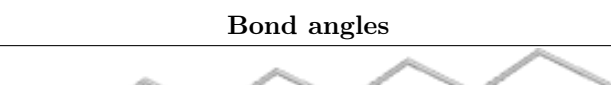


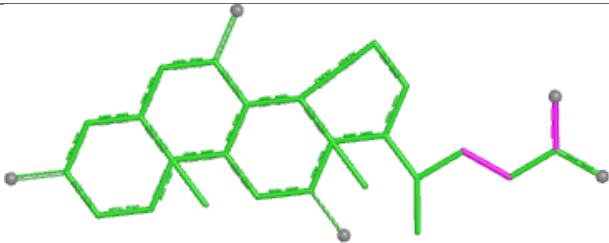
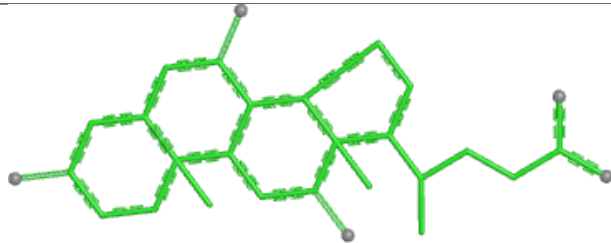
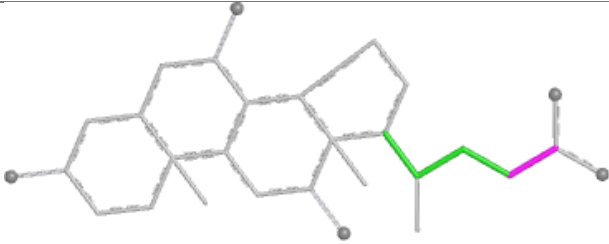
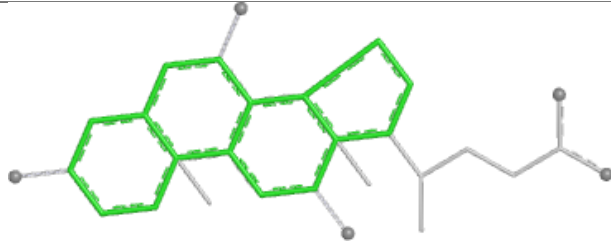


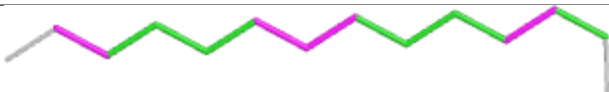




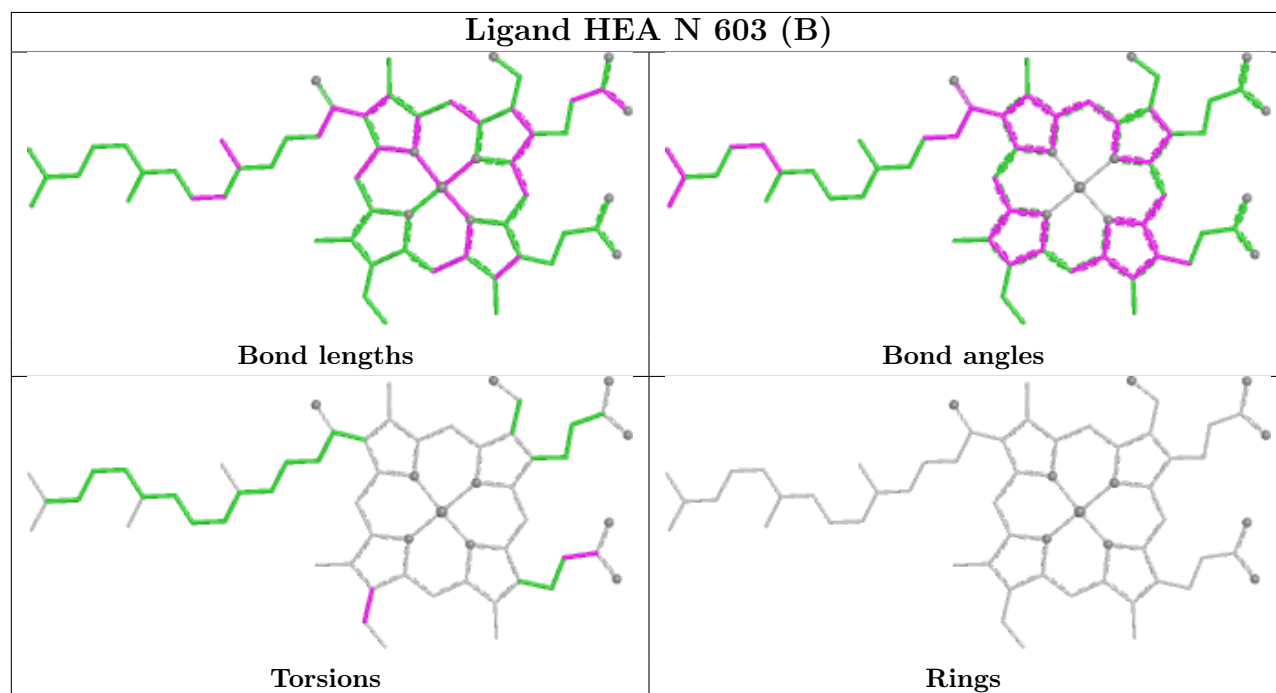
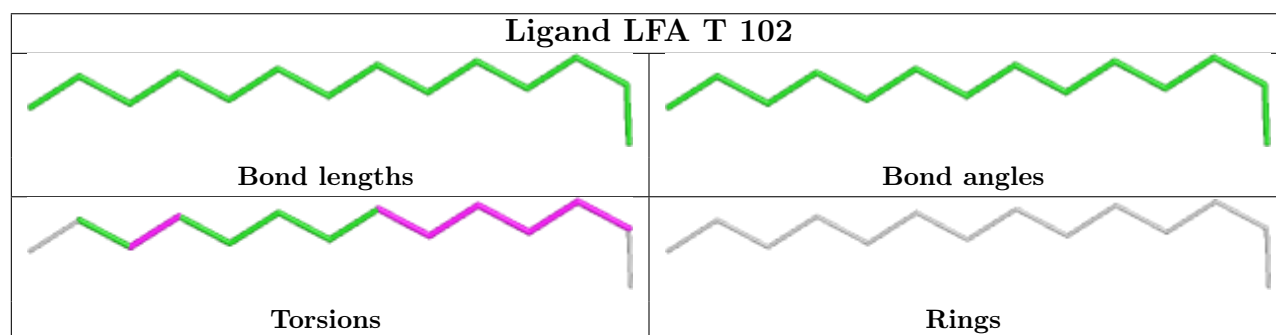
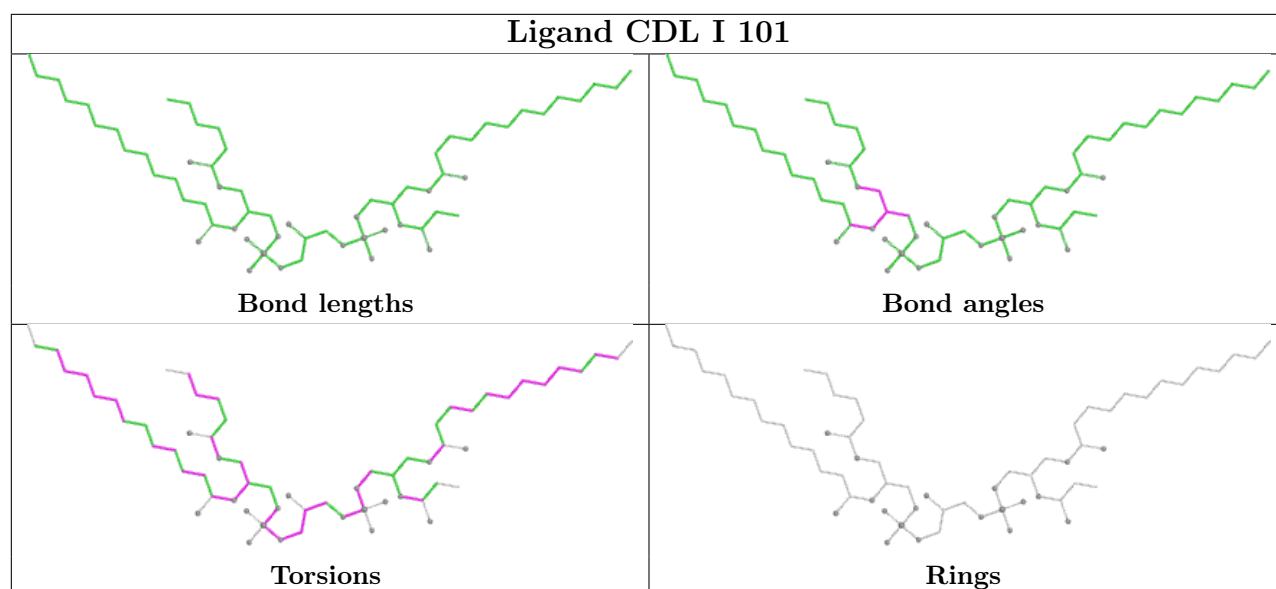


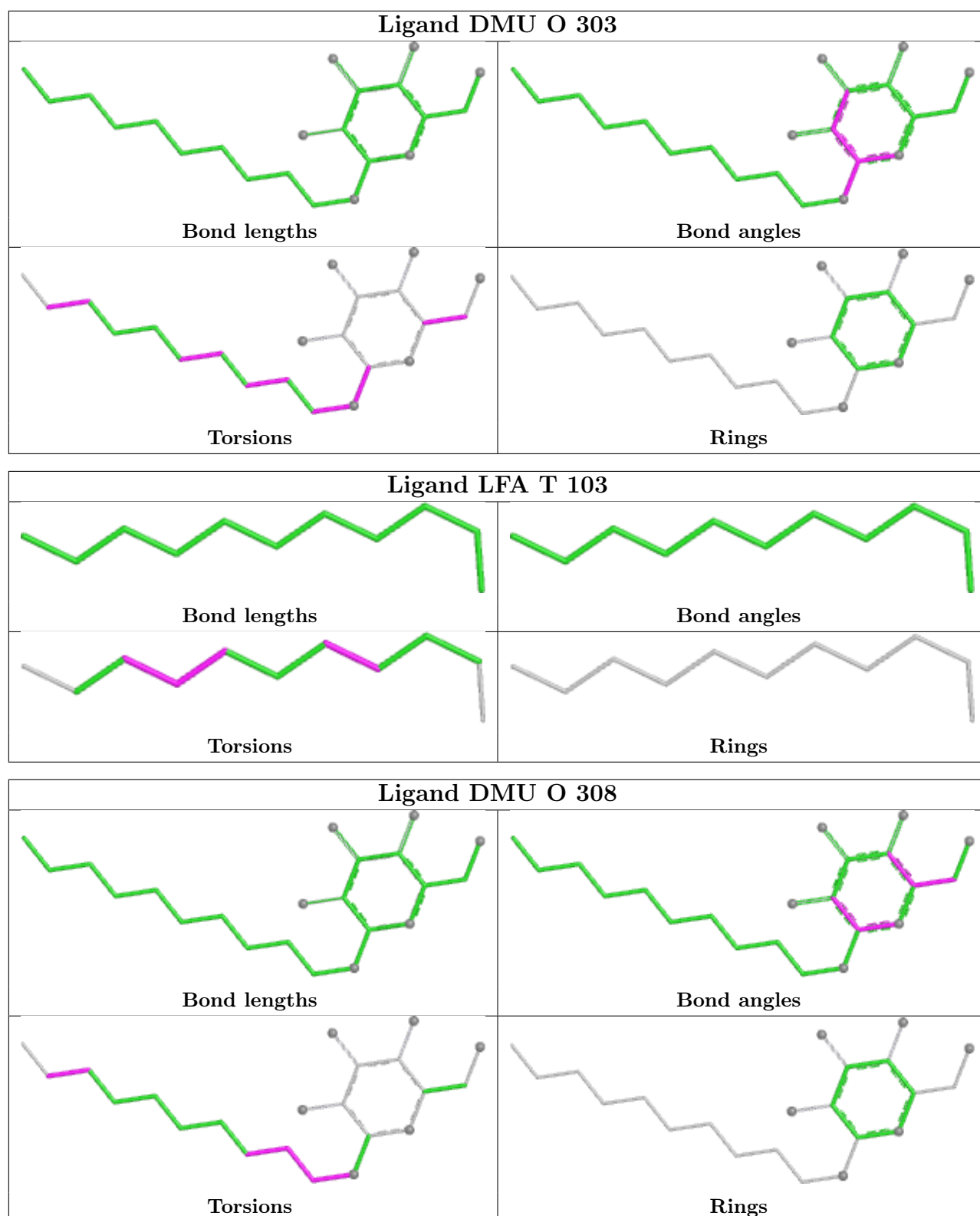
Ligand LFA C 325			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand LFA P 310			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand LFA P 312			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand DMU P 307			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

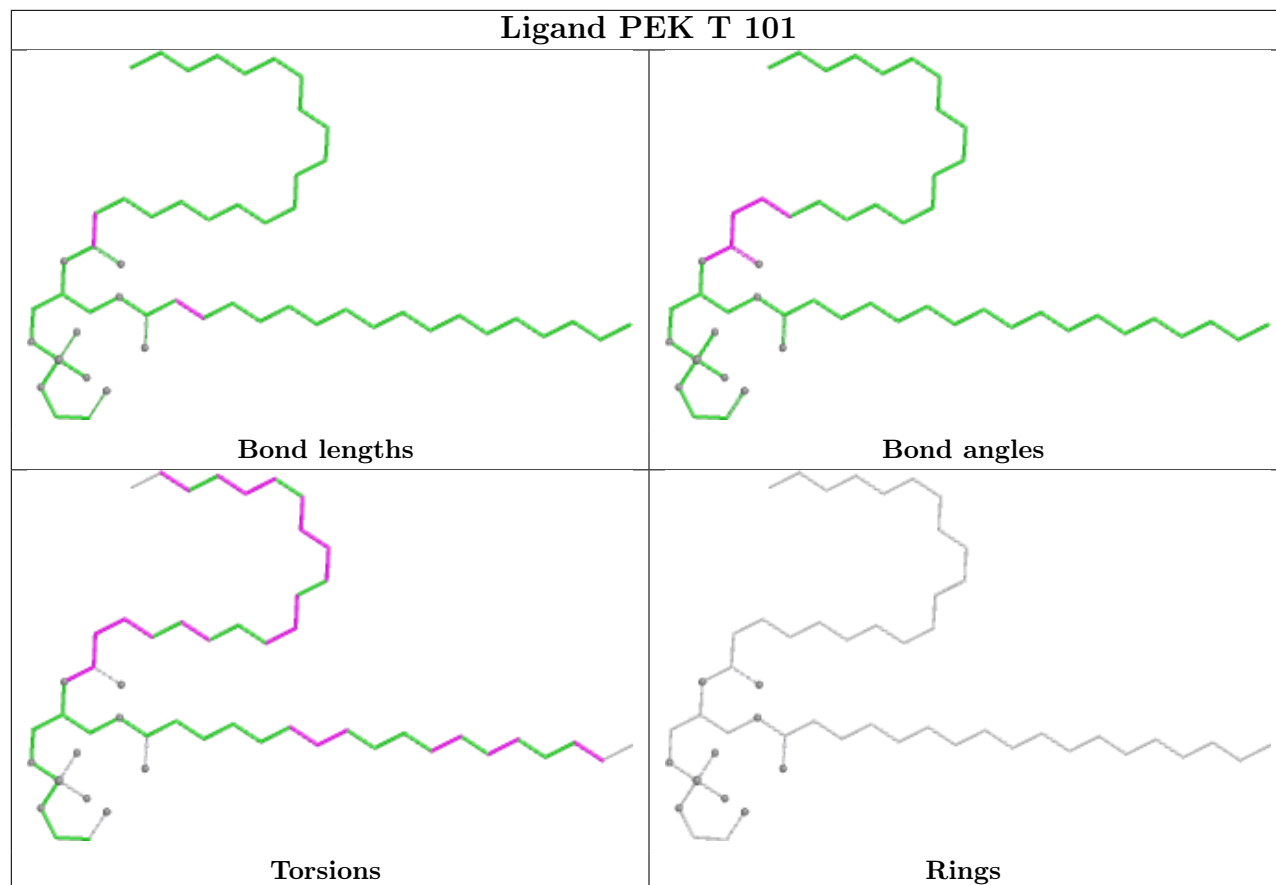
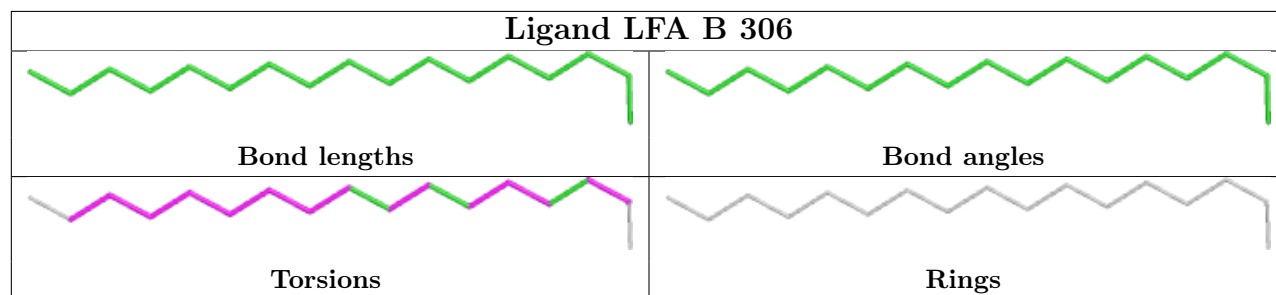
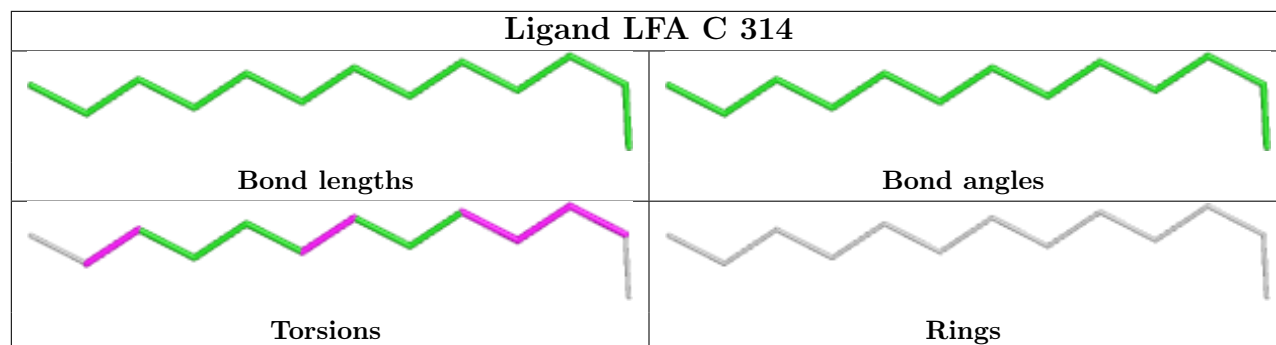
Ligand CHD P 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

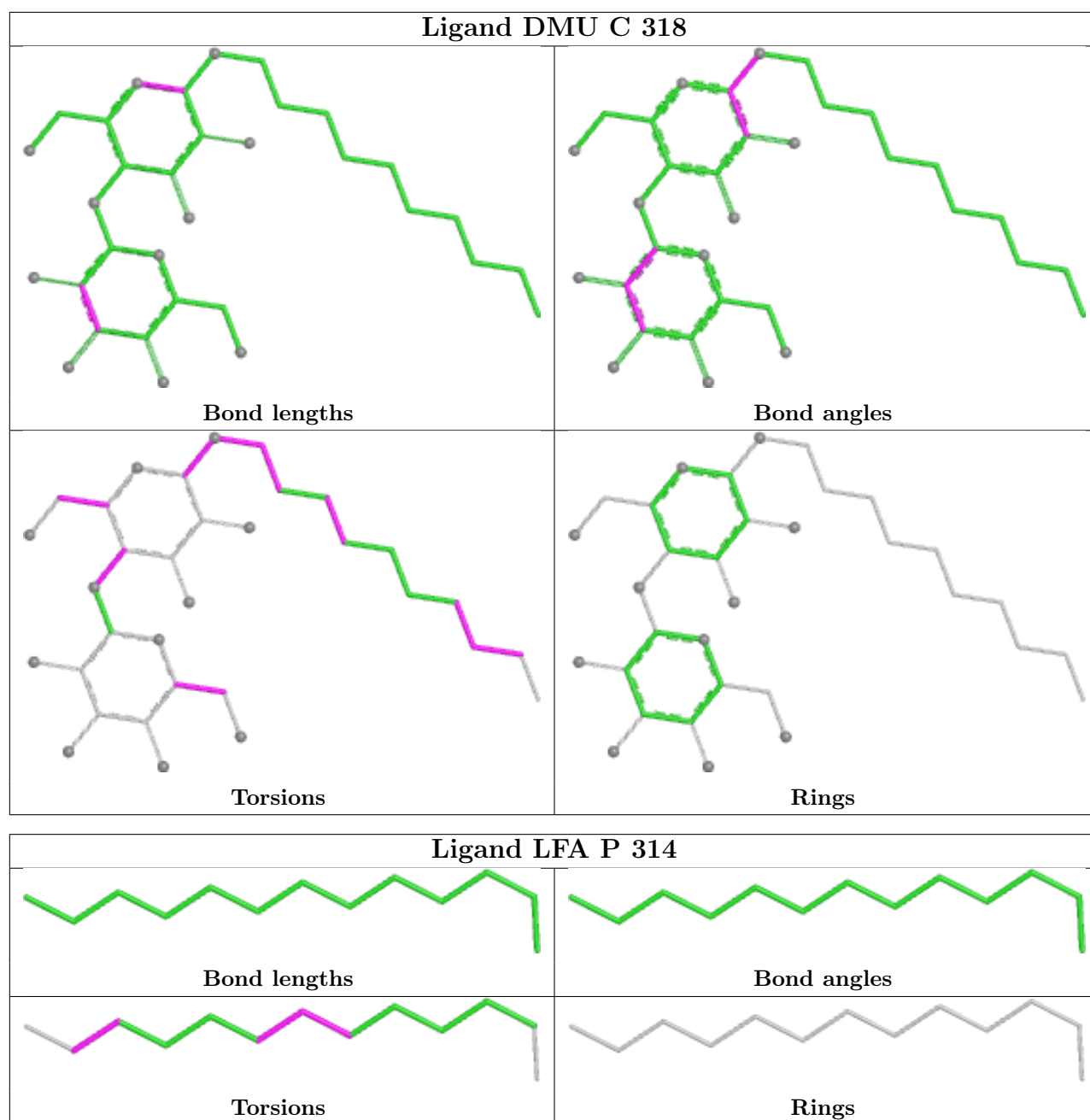
Ligand LFA N 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

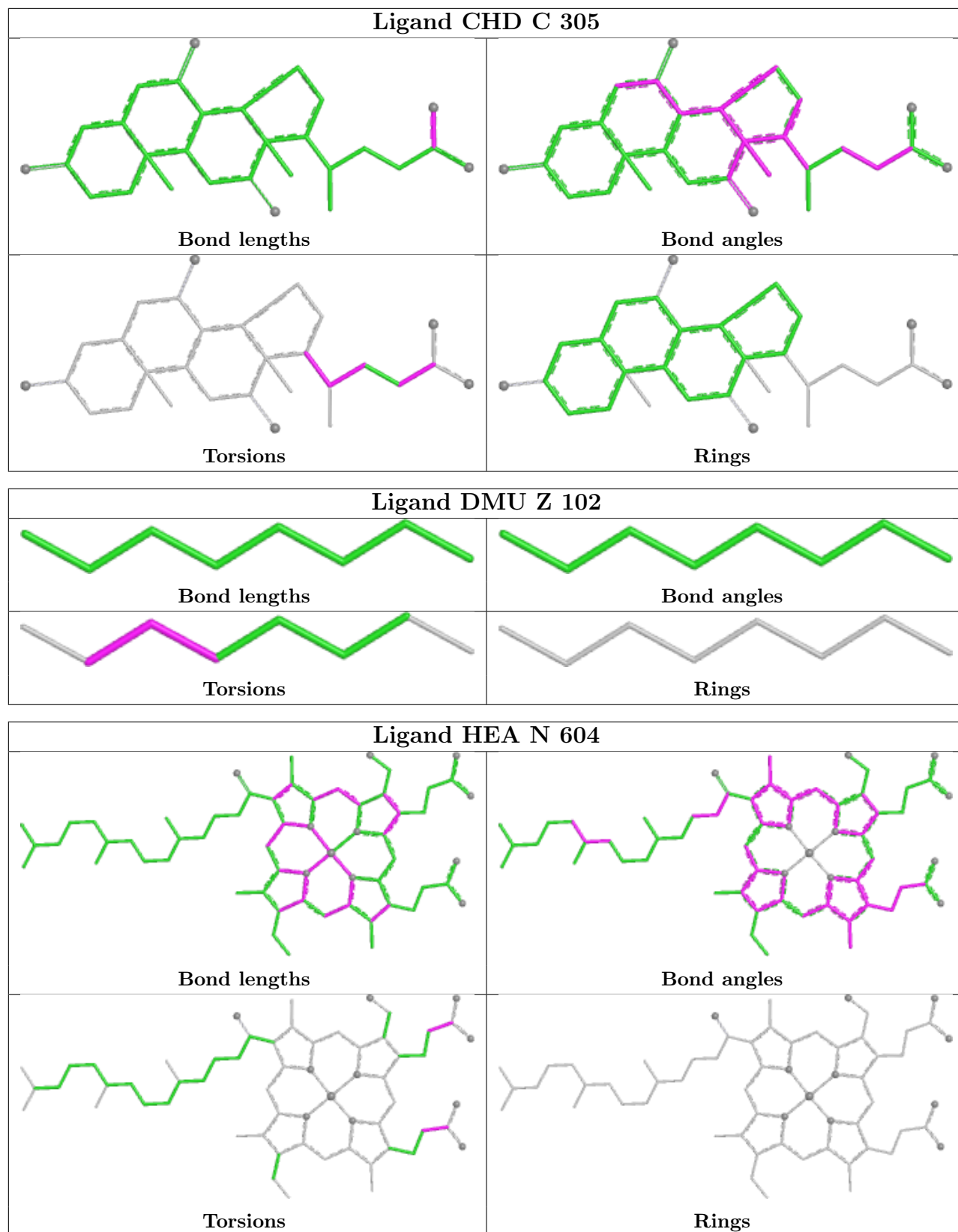
Ligand DMU P 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

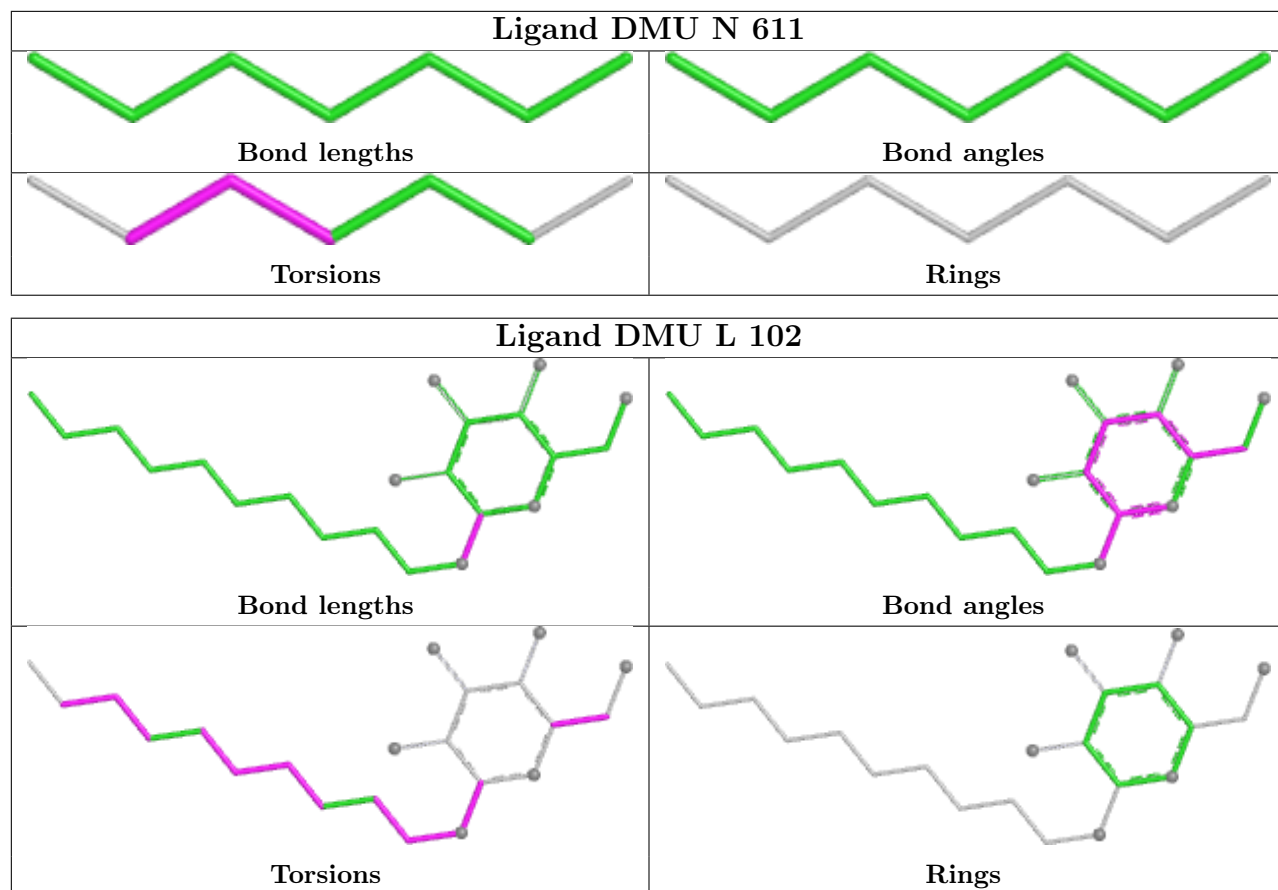


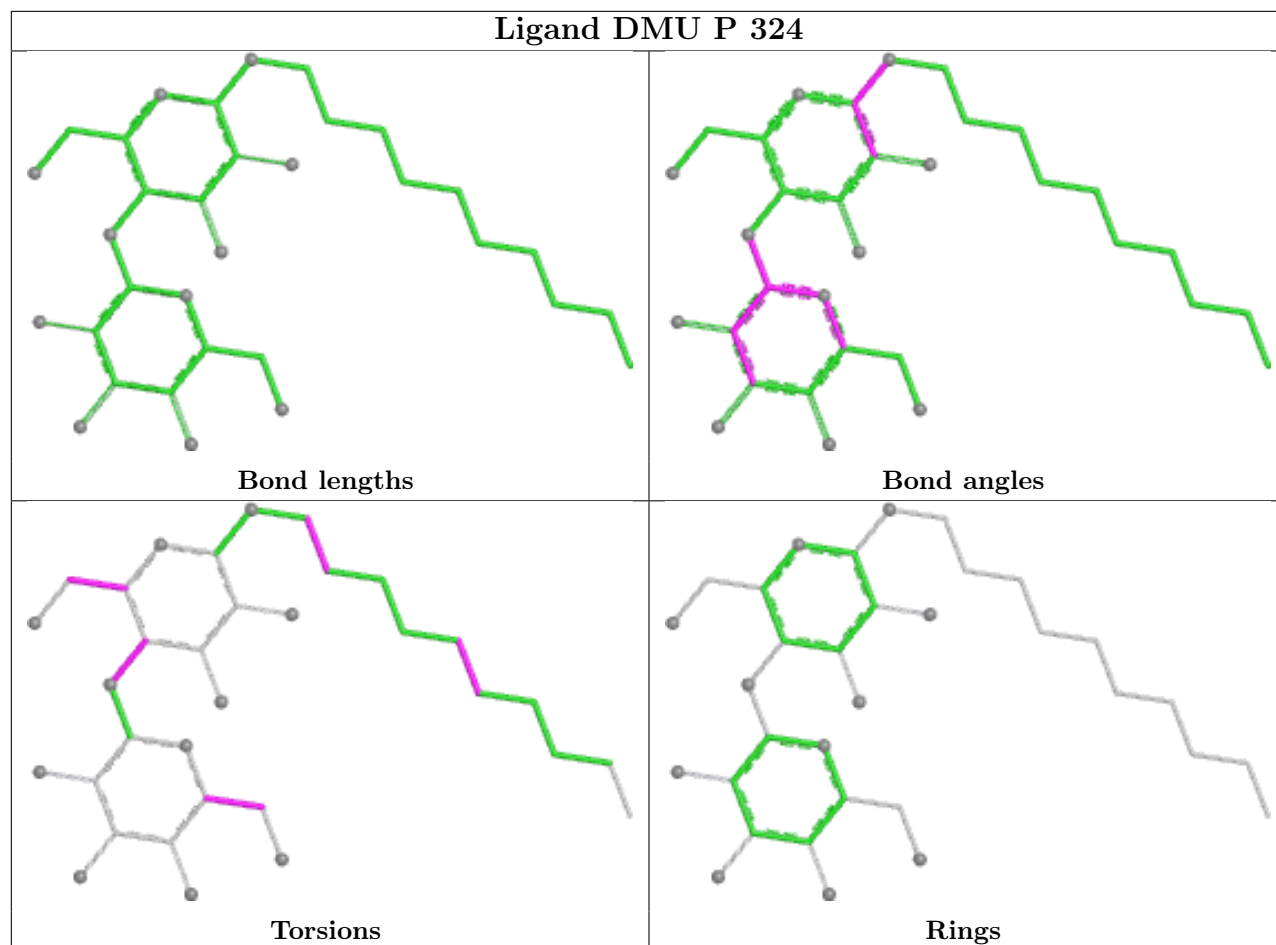












5.7 Other polymers [i](#)

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%)	-0.27	4 (0%)	82 85	15, 31, 39, 57	15 (2%)
1	N	512/514 (99%)	-0.04	6 (1%)	76 80	17, 36, 47, 66	15 (2%)
2	B	226/227 (99%)	0.14	15 (6%)	24 26	19, 37, 57, 81	5 (2%)
2	O	226/227 (99%)	0.32	9 (3%)	42 46	23, 47, 74, 84	5 (2%)
3	C	258/261 (98%)	-0.10	4 (1%)	70 75	16, 35, 47, 62	9 (3%)
3	P	258/261 (98%)	0.01	1 (0%)	88 90	16, 37, 49, 76	9 (3%)
4	D	143/147 (97%)	0.06	2 (1%)	73 77	19, 40, 56, 70	1 (0%)
4	Q	137/147 (93%)	0.59	9 (6%)	24 26	24, 59, 85, 104	1 (0%)
5	E	102/109 (93%)	-0.11	1 (0%)	79 82	33, 39, 56, 74	0
5	R	102/109 (93%)	0.12	2 (1%)	65 69	37, 48, 64, 82	0
6	F	91/98 (92%)	0.18	2 (2%)	62 66	20, 42, 65, 79	2 (2%)
6	S	91/98 (92%)	0.32	2 (2%)	62 66	19, 41, 66, 79	2 (2%)
7	G	72/85 (84%)	0.41	6 (8%)	17 18	20, 41, 96, 108	1 (1%)
7	T	72/85 (84%)	0.47	5 (6%)	23 25	22, 46, 94, 105	1 (1%)
8	H	75/85 (88%)	0.42	6 (8%)	18 19	34, 45, 89, 110	0
8	U	75/85 (88%)	0.49	3 (4%)	42 46	42, 50, 89, 114	0
9	I	70/73 (95%)	0.45	5 (7%)	22 24	36, 48, 72, 91	0
9	V	70/73 (95%)	0.72	5 (7%)	22 24	37, 61, 79, 101	0
10	J	56/59 (94%)	0.35	4 (7%)	22 24	36, 45, 66, 78	0
10	W	56/59 (94%)	0.61	5 (8%)	15 16	40, 51, 75, 83	0
11	K	49/56 (87%)	0.43	3 (6%)	27 29	38, 45, 60, 76	0
11	X	49/56 (87%)	0.82	2 (4%)	41 45	50, 60, 76, 100	0
12	L	44/47 (93%)	0.05	1 (2%)	61 65	32, 37, 50, 60	0
12	Y	44/47 (93%)	0.43	1 (2%)	61 65	41, 49, 65, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	40/46 (86%)	0.27	1 (2%) 58 62	34, 38, 74, 89	0
13	Z	40/46 (86%)	0.90	4 (10%) 12 13	47, 54, 94, 101	0
All	All	3470/3614 (96%)	0.13	108 (3%) 51 55	15, 39, 68, 114	66 (1%)

The worst 5 of 108 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	93	PRO	7.1
7	T	36	TRP	6.6
2	B	59	GLN	5.5
6	F	3	GLY	5.5
2	O	113	TYR	5.5

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	0.91	0.14	42,50,91,118	0
1	FME	N	1	10/11	0.95	0.16	48,54,98,107	0
2	FME	B	1	10/11	0.97	0.09	32,35,45,85	0
2	FME	O	1	10/11	0.98	0.07	40,49,57,73	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
20	DMU	C	317	22/33	0.68	0.33	42,65,78,85	22

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	LFA	P	311	11/20	0.72	0.39	59,67,76,82	11
20	DMU	P	317	22/33	0.72	0.32	50,66,82,91	22
20	DMU	N	611	7/33	0.78	0.44	72,76,81,93	7
20	DMU	C	318	33/33	0.78	0.35	46,55,68,81	33
20	DMU	P	319	33/33	0.78	0.28	55,74,82,94	33
19	LFA	C	308	6/20	0.79	0.45	49,51,55,59	6
20	DMU	A	609	7/33	0.81	0.39	61,69,77,86	7
19	LFA	C	325	15/20	0.81	0.40	57,66,74,75	15
19	LFA	C	310	11/20	0.81	0.32	59,70,85,90	11
21	EDO	P	322	4/4	0.81	0.27	32,36,40,42	4
20	DMU	M	102	8/33	0.82	0.26	48,51,58,60	8
20	DMU	P	318	33/33	0.82	0.34	52,62,77,100	33
19	LFA	P	312	11/20	0.82	0.33	47,59,70,74	11
21	EDO	C	322	4/4	0.82	0.31	36,36,37,38	4
20	DMU	P	315	33/33	0.82	0.27	45,54,67,71	33
19	LFA	C	312	11/20	0.83	0.33	53,59,73,76	11
20	DMU	C	324	33/33	0.83	0.22	39,54,72,82	33
20	DMU	P	324	33/33	0.83	0.23	50,63,84,91	33
20	DMU	P	316	7/33	0.83	0.32	62,66,71,72	7
21	EDO	E	201	4/4	0.83	0.32	39,41,48,51	4
19	LFA	O	302	11/20	0.83	0.30	49,56,73,80	11
19	LFA	C	311	14/20	0.84	0.33	40,62,72,75	14
19	LFA	C	313	15/20	0.84	0.29	44,52,70,73	15
21	EDO	C	320	4/4	0.84	0.32	53,57,58,71	4
20	DMU	C	319	33/33	0.84	0.24	43,71,86,87	33
19	LFA	P	310	18/20	0.84	0.28	43,52,62,69	18
20	DMU	C	315	33/33	0.84	0.26	43,56,69,70	33
20	DMU	O	306	11/33	0.85	0.29	44,47,72,75	11
19	LFA	P	308	11/20	0.85	0.31	36,52,58,59	11
20	DMU	B	307	22/33	0.85	0.26	61,71,81,85	22
19	LFA	P	309	6/20	0.85	0.34	45,51,54,55	6
19	LFA	N	601	17/20	0.85	0.28	41,60,75,78	17
19	LFA	N	610	14/20	0.85	0.27	42,51,71,72	14
19	LFA	C	307	11/20	0.85	0.32	41,52,64,70	11
19	LFA	P	313	15/20	0.85	0.24	48,53,63,66	15
19	LFA	P	314	13/20	0.85	0.29	46,63,74,76	13
19	LFA	T	102	14/20	0.85	0.36	42,70,86,87	14
20	DMU	O	303	22/33	0.85	0.27	51,76,86,88	22
19	LFA	A	607	14/20	0.86	0.28	36,51,76,78	14
20	DMU	A	615	11/33	0.86	0.28	54,63,68,71	11
26	CDL	C	304	87/100	0.86	0.20	46,81,122,135	0
26	CDL	O	304	64/100	0.86	0.17	62,91,140,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	LFA	C	314	13/20	0.87	0.25	56,59,77,86	13
21	EDO	A	612	4/4	0.87	0.25	35,41,50,53	4
20	DMU	C	323	22/33	0.87	0.28	50,62,70,83	22
20	DMU	C	316	7/33	0.87	0.29	47,51,63,69	7
19	LFA	P	301	15/20	0.87	0.28	51,57,62,64	15
19	LFA	T	103	11/20	0.87	0.29	55,59,73,75	11
20	DMU	N	612	33/33	0.87	0.23	40,55,75,86	33
26	CDL	I	101	64/100	0.87	0.17	54,87,129,158	0
20	DMU	N	619	33/33	0.87	0.23	35,49,63,66	33
26	CDL	P	305	87/100	0.87	0.19	50,86,130,152	0
26	CDL	Y	101	94/100	0.87	0.17	57,95,141,156	0
20	DMU	P	323	22/33	0.88	0.22	46,60,70,77	22
20	DMU	H	101	33/33	0.88	0.20	31,45,59,68	33
20	DMU	Q	201	33/33	0.88	0.21	39,57,69,89	33
20	DMU	W	101	11/33	0.88	0.36	68,74,76,78	11
20	DMU	Y	102	22/33	0.88	0.33	55,63,76,86	22
21	EDO	A	611	4/4	0.88	0.17	27,29,29,33	4
19	LFA	A	608	14/20	0.88	0.27	37,50,62,63	14
20	DMU	A	617	11/33	0.88	0.32	47,60,69,72	11
25	UNX	P	303	1/1	0.89	0.24	55,55,55,55	0
19	LFA	B	306	17/20	0.89	0.28	43,59,87,90	17
20	DMU	A	610	33/33	0.89	0.19	31,42,53,63	33
20	DMU	N	602	11/33	0.89	0.31	52,67,72,75	11
21	EDO	N	614	4/4	0.89	0.20	39,40,50,50	4
19	LFA	N	609	14/20	0.89	0.24	40,50,68,71	14
20	DMU	B	302	11/33	0.90	0.24	47,58,64,68	11
24	CHD	P	306	29/29	0.90	0.12	54,60,72,86	0
19	LFA	C	309	18/20	0.90	0.18	37,45,54,56	18
20	DMU	J	101	11/33	0.90	0.35	63,68,71,82	11
20	DMU	O	308	22/33	0.90	0.18	46,52,59,63	22
21	EDO	F	102	4/4	0.90	0.19	23,24,31,31	4
20	DMU	L	102	22/33	0.90	0.30	49,59,67,70	22
21	EDO	N	617	4/4	0.90	0.18	31,39,39,43	4
24	CHD	C	305	29/29	0.91	0.12	50,58,77,111	0
21	EDO	N	613	4/4	0.91	0.17	31,37,37,39	4
21	EDO	P	320	4/4	0.91	0.26	53,60,63,73	4
20	DMU	C	306	11/33	0.91	0.27	59,63,70,72	11
20	DMU	B	303	22/33	0.92	0.19	50,61,72,75	22
21	EDO	G	102	4/4	0.92	0.17	30,34,35,38	4
26	CDL	L	101	94/100	0.92	0.15	44,85,129,155	0
20	DMU	Z	101	33/33	0.92	0.12	56,67,90,94	0
20	DMU	Z	102	8/33	0.92	0.23	51,57,61,62	8

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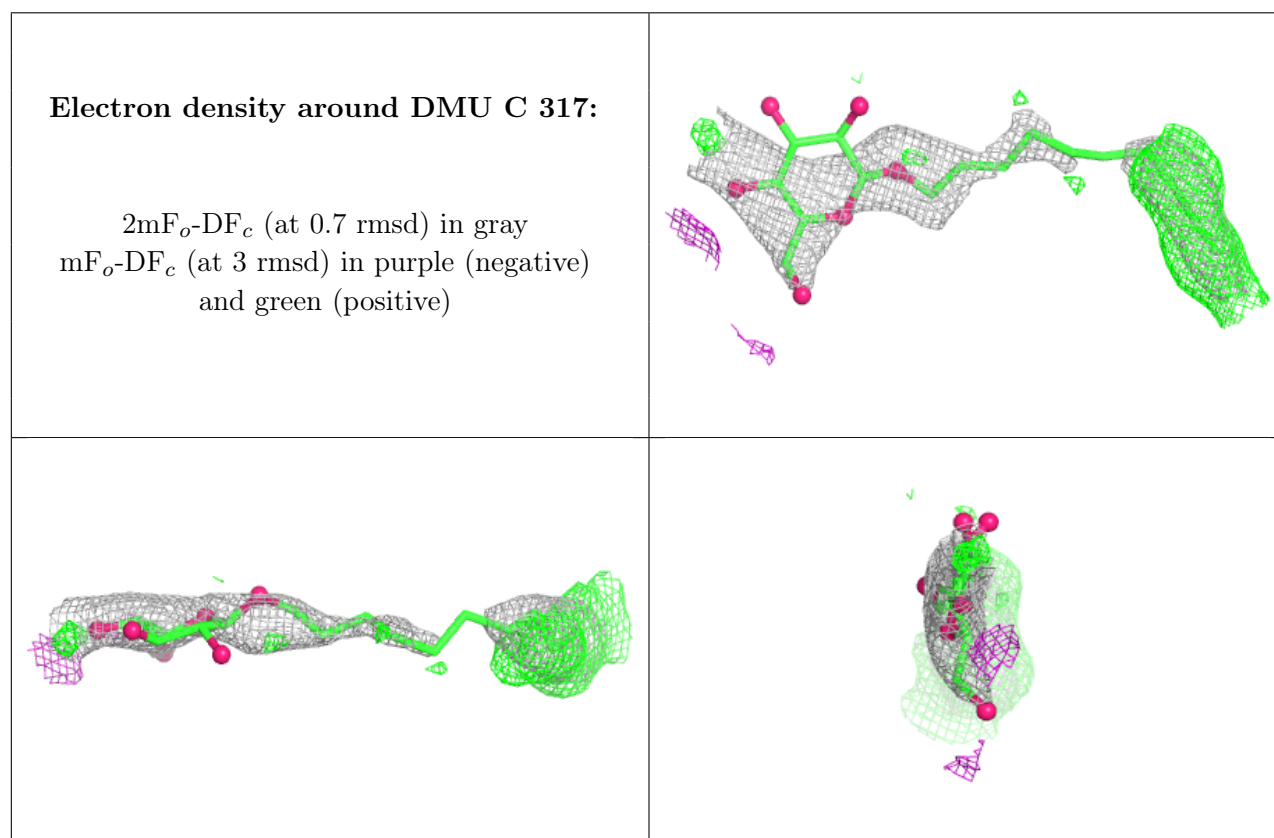
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	DMU	D	201	33/33	0.92	0.15	28,44,51,78	33
21	EDO	O	309	4/4	0.93	0.16	36,37,39,40	4
21	EDO	E	202	4/4	0.93	0.24	35,35,37,39	4
20	DMU	P	307	11/33	0.93	0.25	52,53,61,63	11
20	DMU	O	307	11/33	0.93	0.24	47,55,65,70	11
21	EDO	A	614	4/4	0.94	0.12	37,39,40,44	4
21	EDO	N	615	4/4	0.94	0.21	31,32,32,33	4
21	EDO	S	102	4/4	0.94	0.11	25,25,31,31	4
21	EDO	E	203	4/4	0.95	0.21	34,35,41,42	4
21	EDO	C	321	4/4	0.95	0.16	37,37,39,40	4
24	CHD	C	301	29/29	0.95	0.07	32,35,40,43	0
21	EDO	N	616	4/4	0.95	0.15	37,39,42,45	4
28	PEK	T	101	53/53	0.95	0.13	38,62,110,159	0
24	CHD	P	302	29/29	0.96	0.07	32,37,41,45	0
21	EDO	A	613	4/4	0.96	0.18	27,28,28,29	4
21	EDO	T	104	4/4	0.96	0.10	36,37,39,40	4
20	DMU	M	101	33/33	0.96	0.08	41,52,78,83	0
21	EDO	R	202	4/4	0.96	0.15	38,39,41,41	4
21	EDO	R	201	4/4	0.97	0.26	63,63,64,70	4
21	EDO	P	321	4/4	0.97	0.12	42,42,45,45	4
22	PGV	N	618	51/51	0.97	0.09	33,46,79,92	0
28	PEK	G	101	53/53	0.97	0.11	33,56,90,112	0
24	CHD	B	305	29/29	0.97	0.07	30,36,41,50	0
21	EDO	R	203	4/4	0.98	0.16	44,49,51,58	4
22	PGV	P	304	51/51	0.98	0.09	34,43,102,119	0
21	EDO	B	304	4/4	0.98	0.08	25,26,27,30	4
21	EDO	S	103	4/4	0.98	0.13	32,36,37,37	4
21	EDO	F	103	4/4	0.98	0.08	32,34,37,38	4
24	CHD	O	301	29/29	0.98	0.06	32,36,39,47	0
22	PGV	A	616	51/51	0.98	0.08	29,41,80,92	0
22	PGV	C	303	51/51	0.98	0.09	32,41,90,108	0
25	UNX	C	302	1/1	0.98	0.19	56,56,56,56	0
14	HEA	A	601[A]	60/60	0.99	0.05	25,28,41,47	9
14	HEA	A	601[B]	60/60	0.99	0.05	25,28,45,51	9
14	HEA	A	602	60/60	0.99	0.05	24,27,36,41	0
14	HEA	N	603[A]	60/60	0.99	0.05	31,35,46,52	9
14	HEA	N	603[B]	60/60	0.99	0.05	31,35,49,53	9
14	HEA	N	604	60/60	0.99	0.06	28,32,40,43	0
16	MG	A	604	1/1	0.99	0.02	30,30,30,30	0
18	PER	A	606	2/2	0.99	0.05	29,29,29,34	0
18	PER	N	608	2/2	0.99	0.07	33,33,33,40	0
15	CU	N	605	1/1	1.00	0.01	32,32,32,32	0

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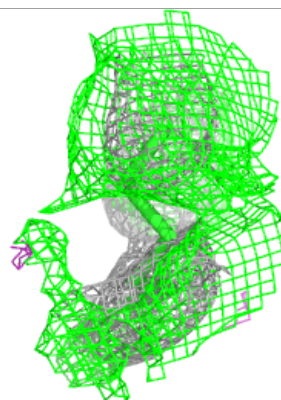
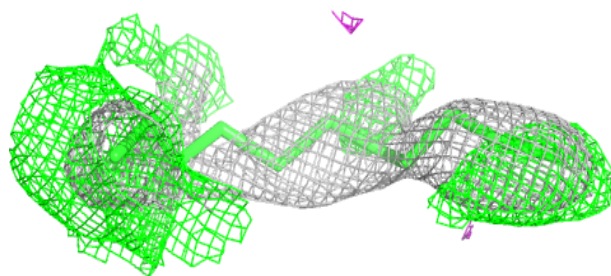
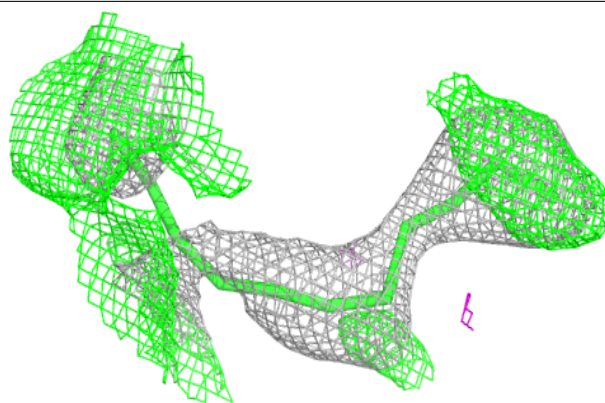
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CU	A	603	1/1	1.00	0.02	28,28,28,28	0
16	MG	N	606	1/1	1.00	0.02	37,37,37,37	0
23	CUA	B	301	2/2	1.00	0.02	29,29,29,30	0
23	CUA	O	305	2/2	1.00	0.02	39,39,39,40	0
27	ZN	F	101	1/1	1.00	0.01	36,36,36,36	0
27	ZN	S	101	1/1	1.00	0.03	37,37,37,37	0
17	CA	A	605	1/1	1.00	0.02	33,33,33,33	0
17	CA	N	607	1/1	1.00	0.02	45,45,45,45	0

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

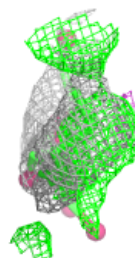
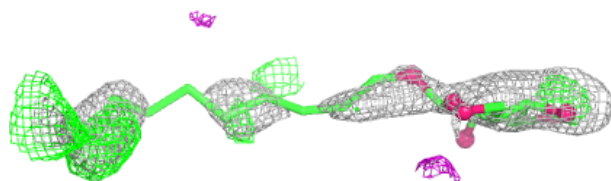
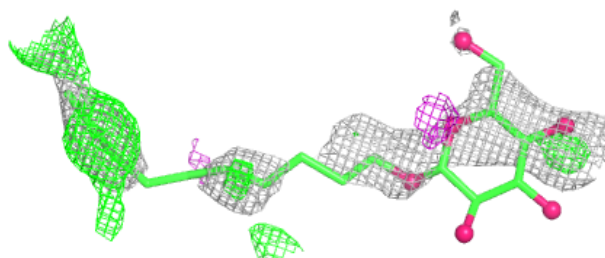


Electron density around LFA P 311:

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

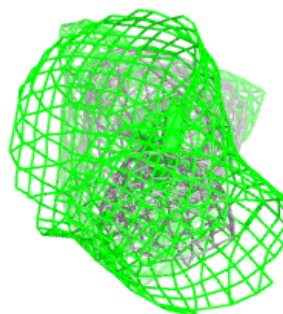
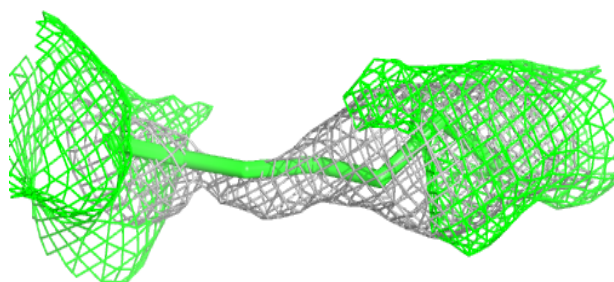
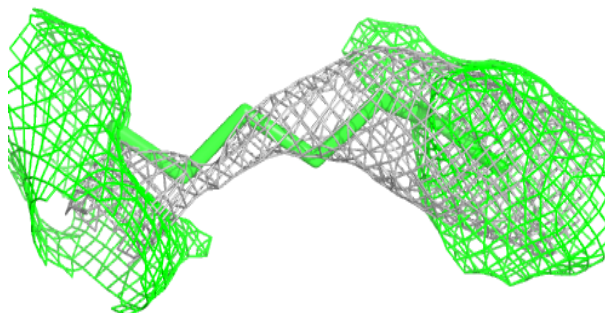
**Electron density around DMU P 317:**

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

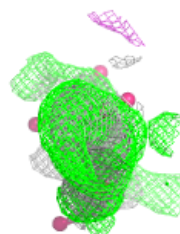
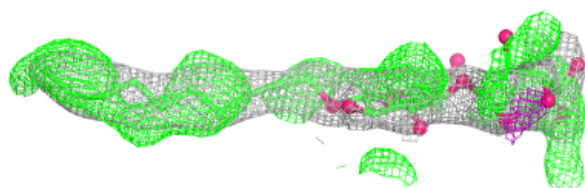
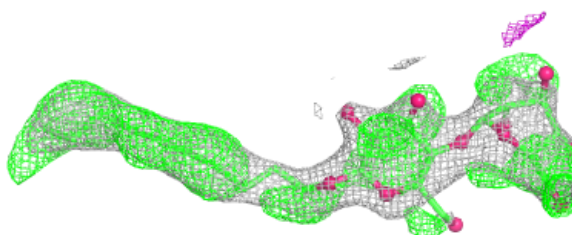


Electron density around DMU N 611:

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

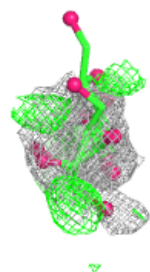
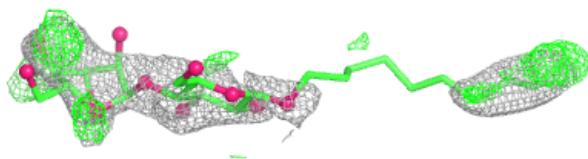
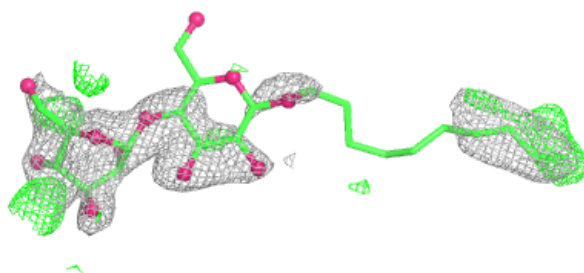
**Electron density around DMU C 318:**

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

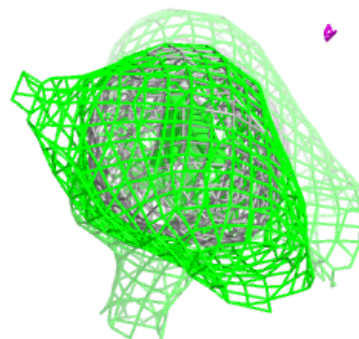
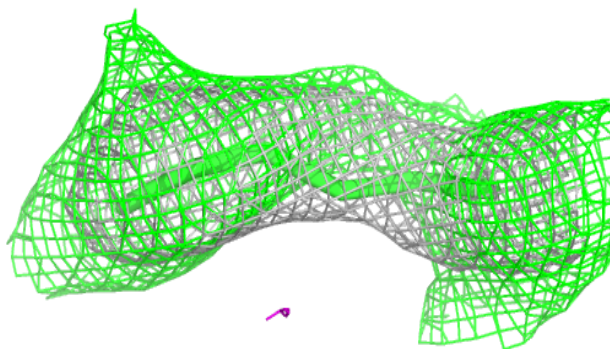
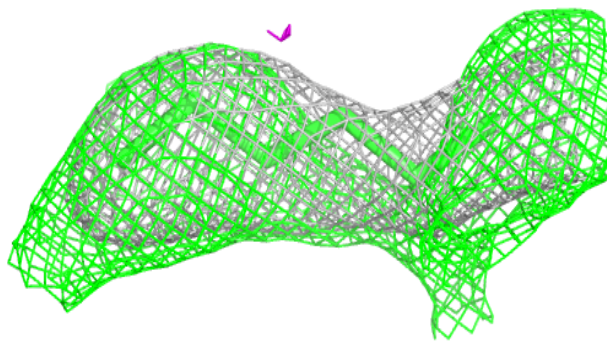


Electron density around DMU P 319:

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

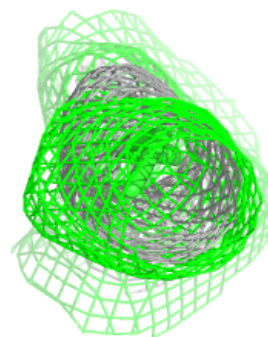
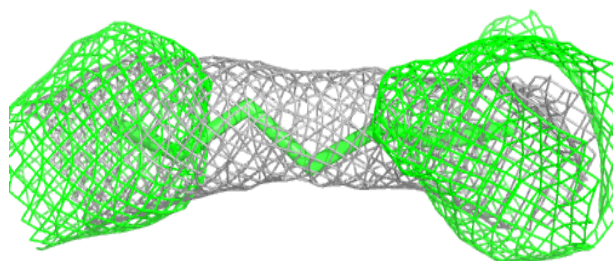
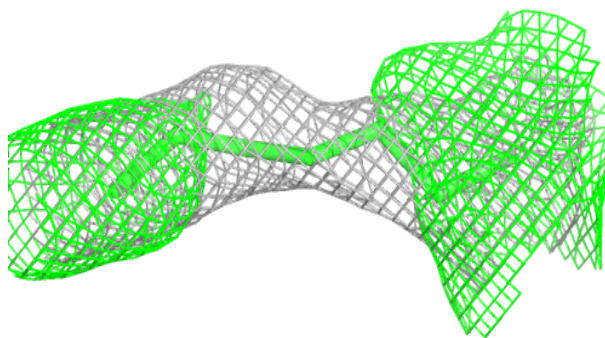
**Electron density around LFA C 308:**

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

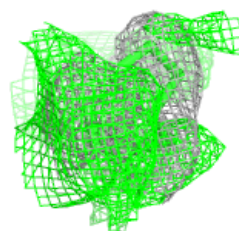
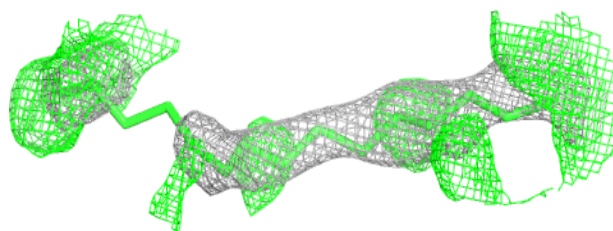
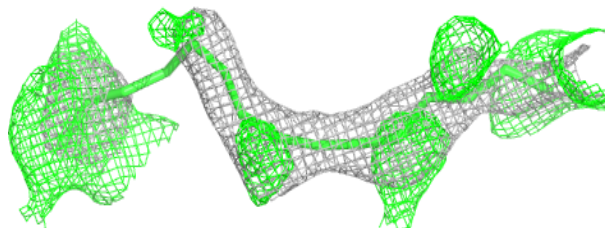


Electron density around DMU A 609:

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

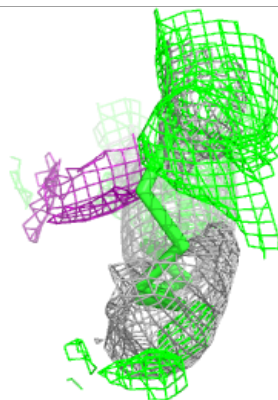
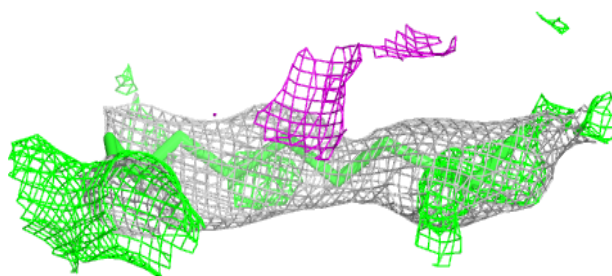
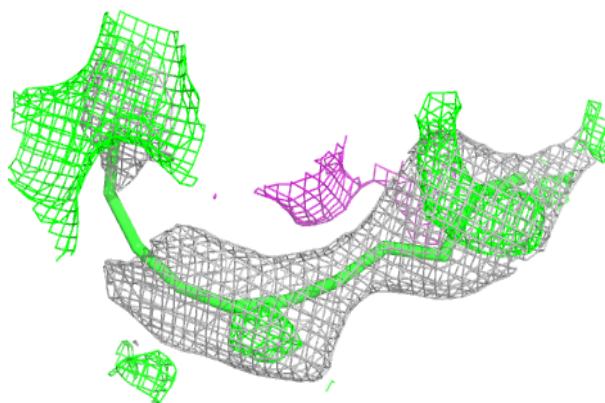
**Electron density around LFA C 325:**

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

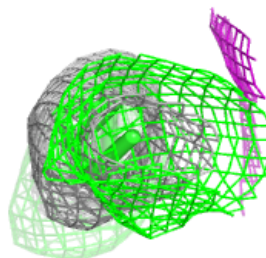
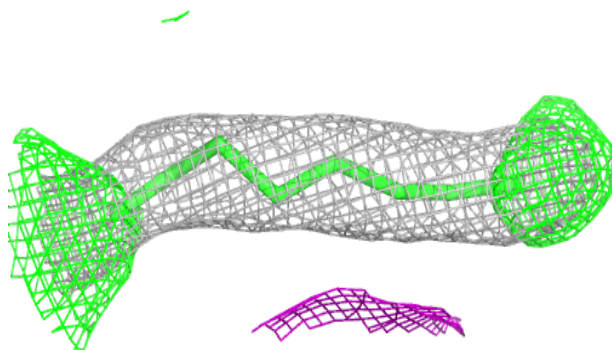
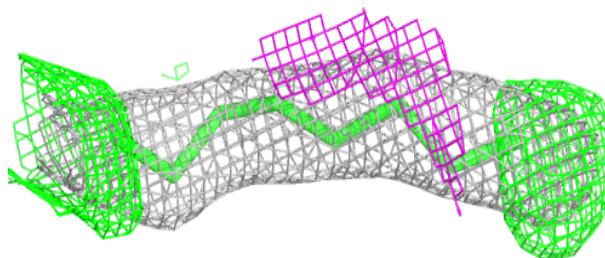


Electron density around LFA C 310:

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

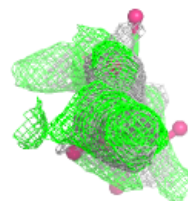
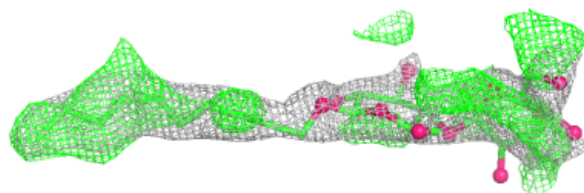
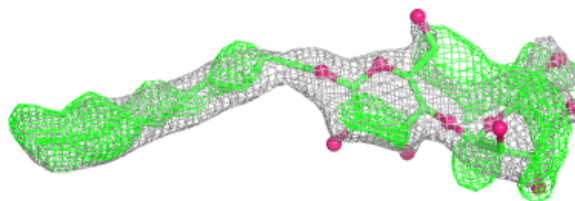
**Electron density around DMU M 102:**

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

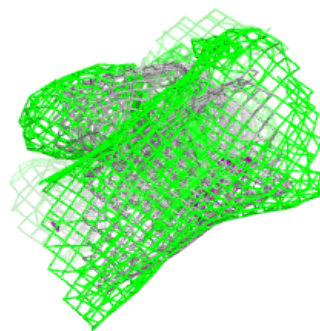
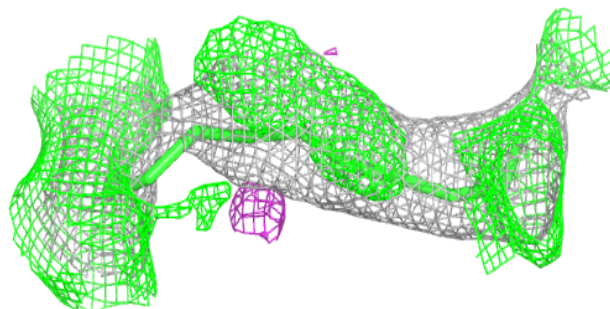
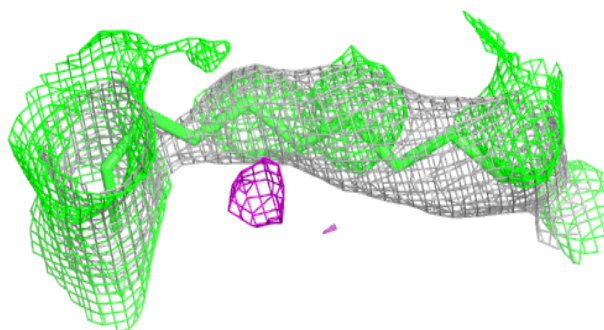


Electron density around DMU P 318:

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

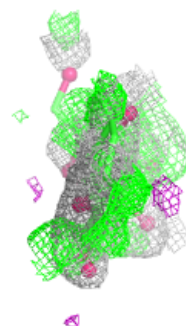
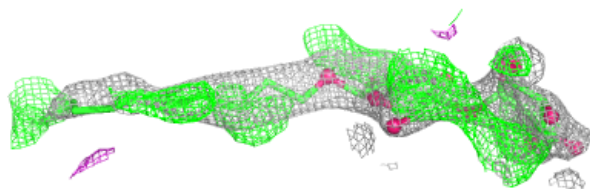
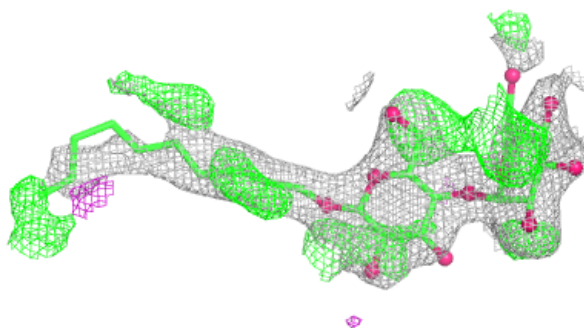
**Electron density around LFA P 312:**

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

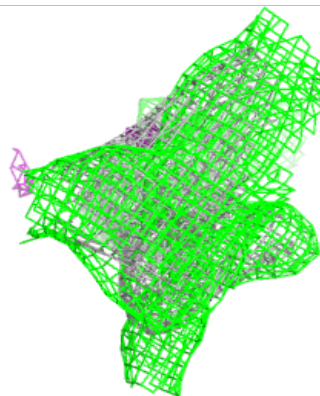
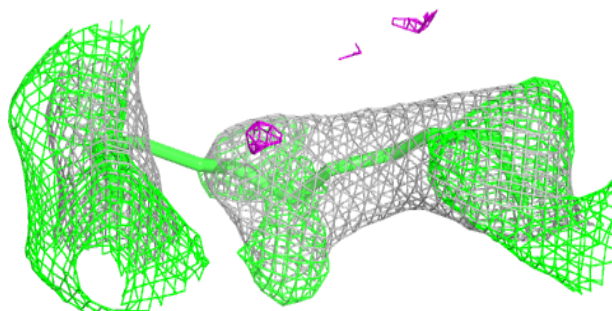
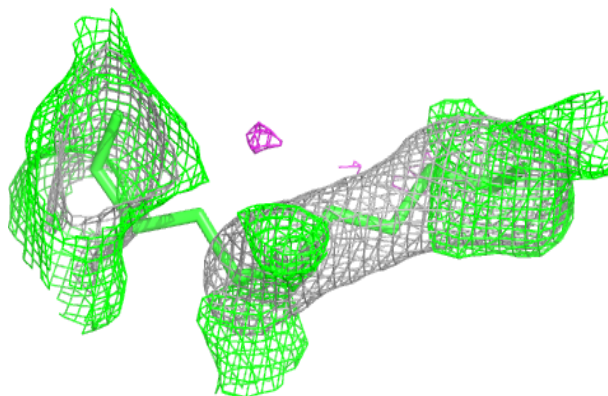


Electron density around DMU P 315:

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

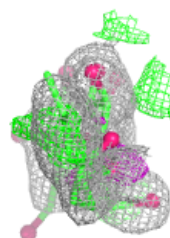
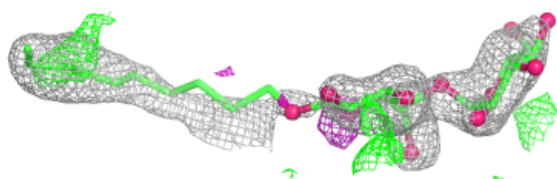
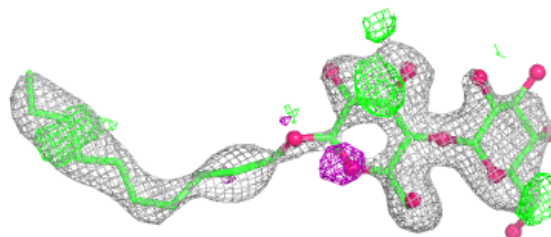
**Electron density around LFA C 312:**

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

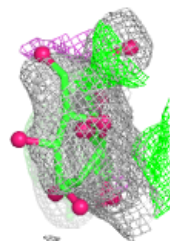
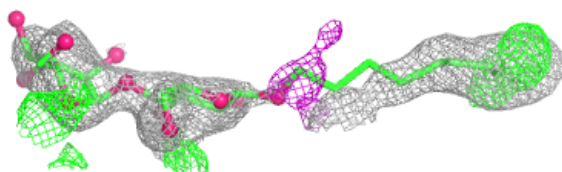
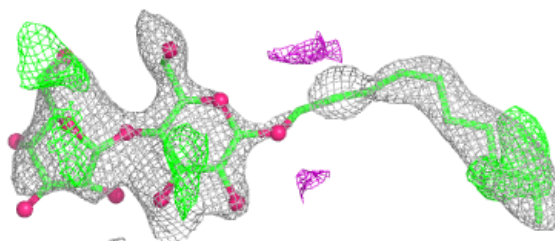


Electron density around DMU C 324:

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

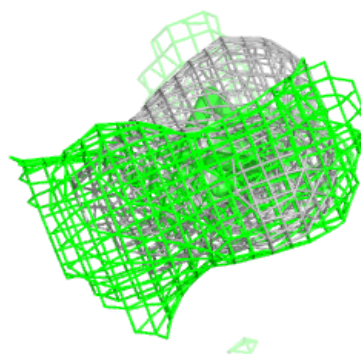
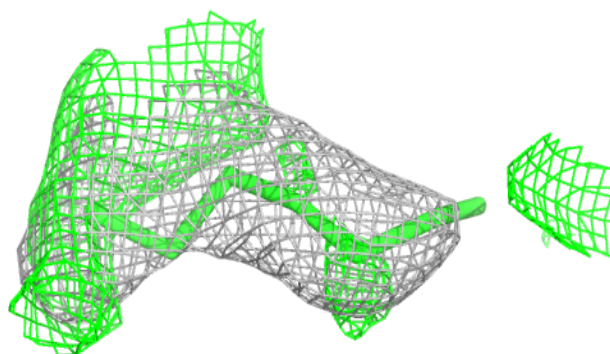
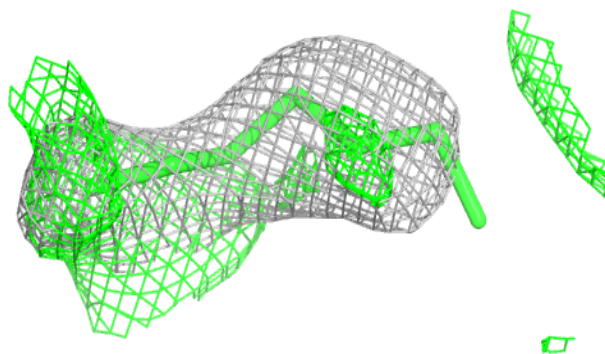
**Electron density around DMU P 324:**

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

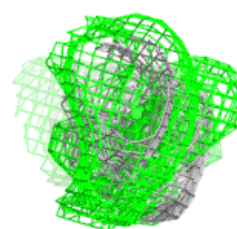
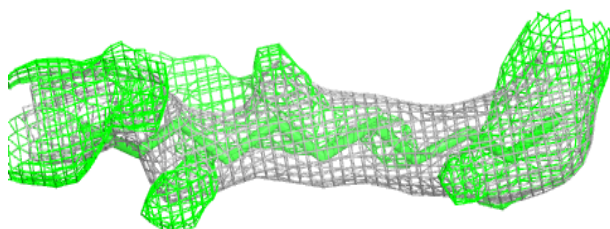
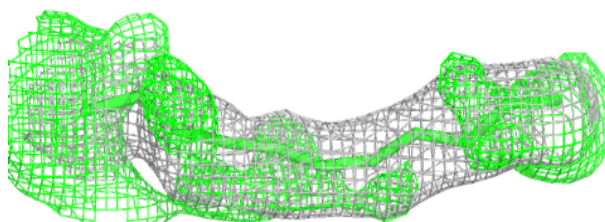


Electron density around DMU P 316:

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

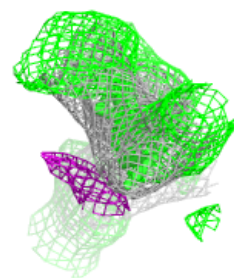
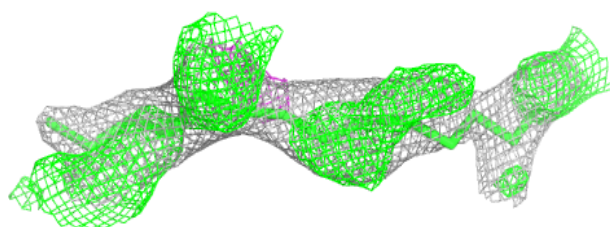
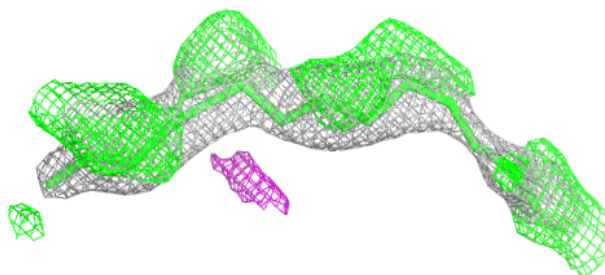
**Electron density around LFA O 302:**

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

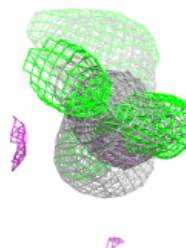
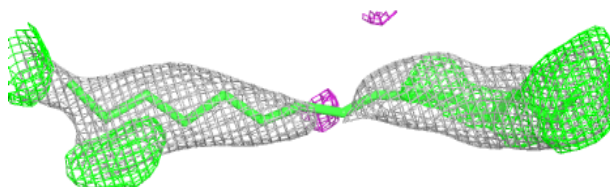
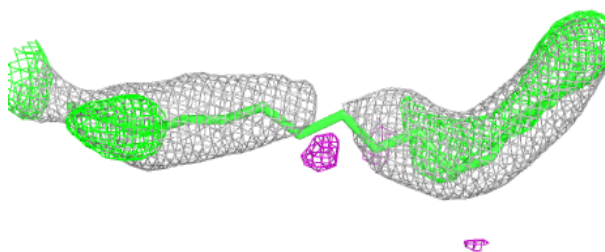


Electron density around LFA C 311:

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

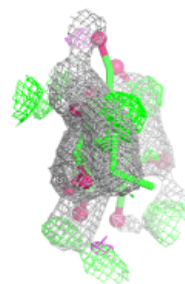
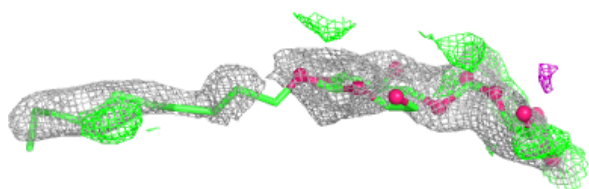
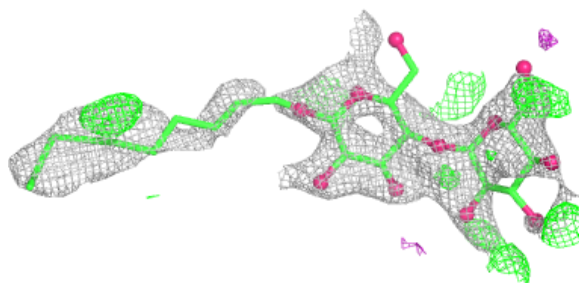
**Electron density around LFA C 313:**

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

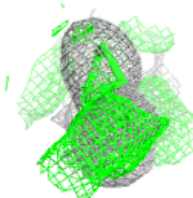
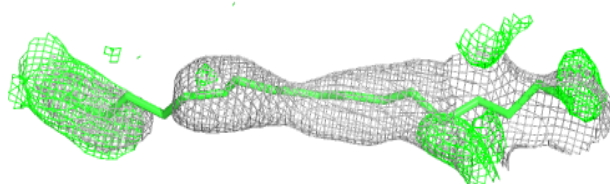
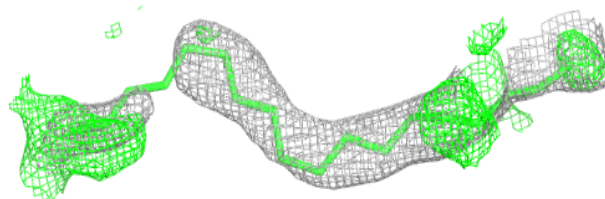


Electron density around DMU C 319:

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

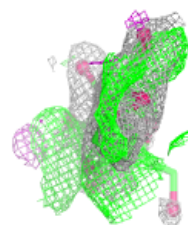
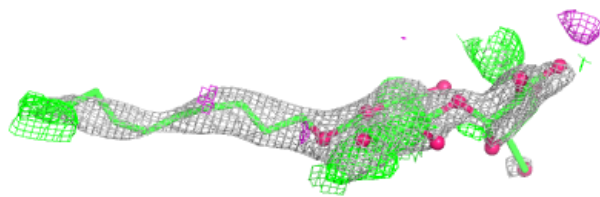
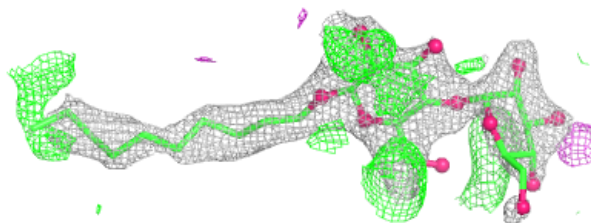
**Electron density around LFA P 310:**

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

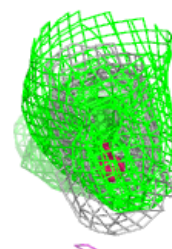
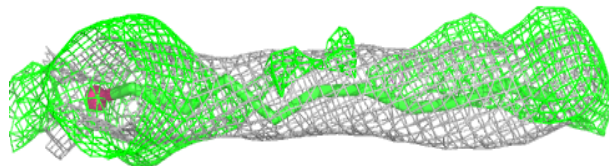
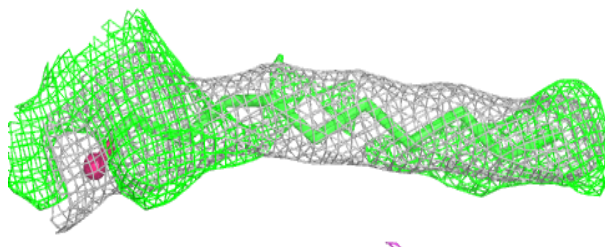


Electron density around DMU C 315:

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

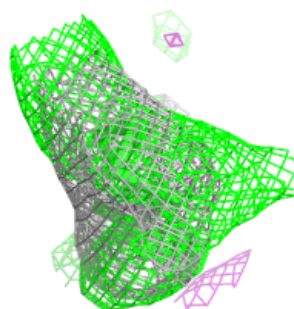
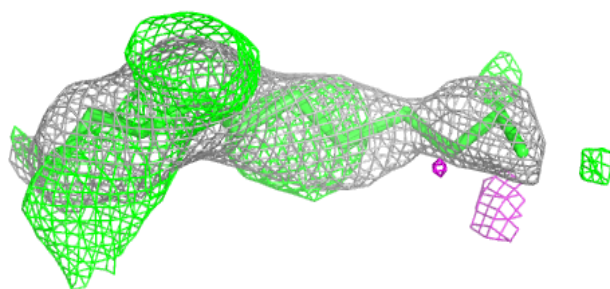
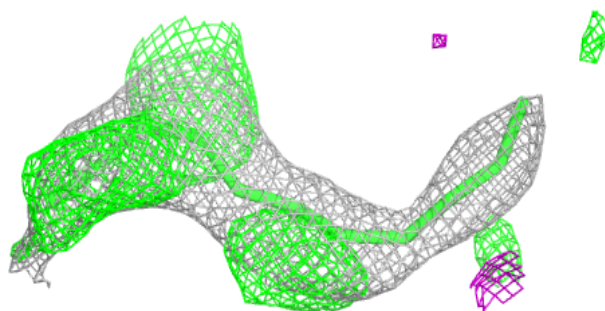
**Electron density around DMU O 306:**

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

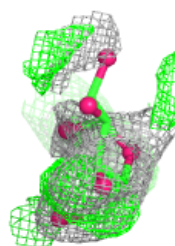
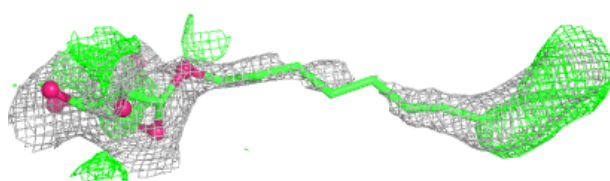
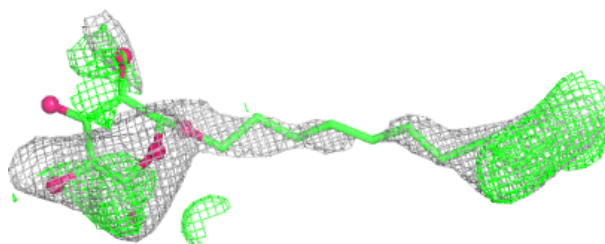


Electron density around LFA P 308:

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

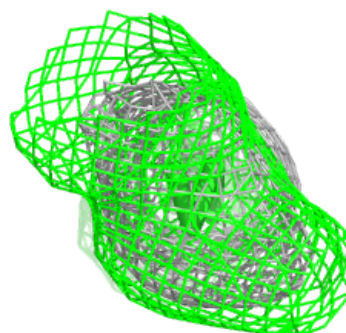
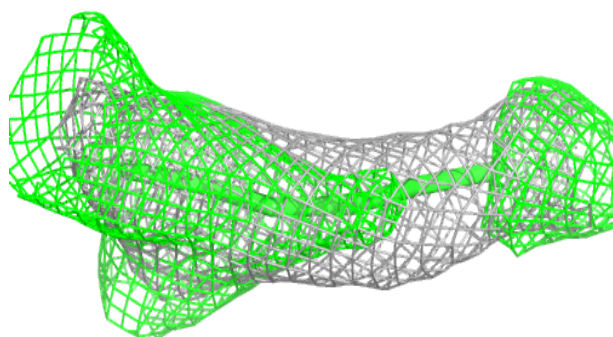
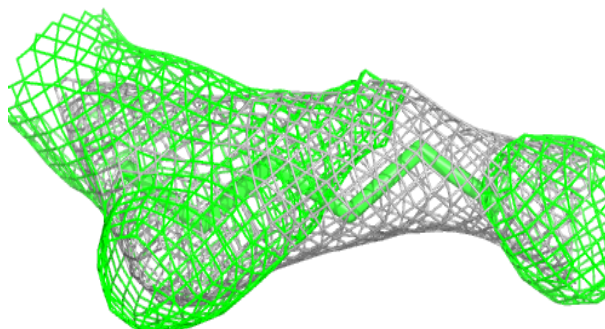
**Electron density around DMU B 307:**

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

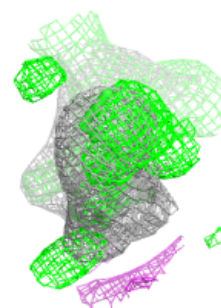
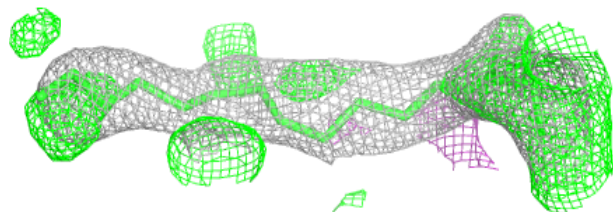
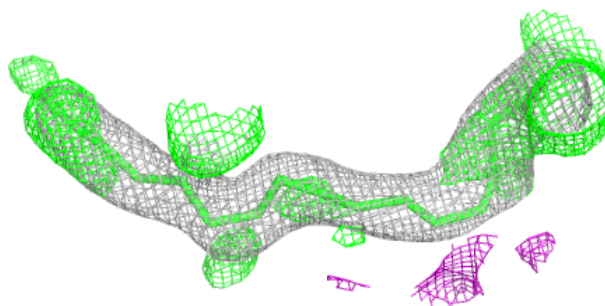


Electron density around LFA P 309:

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

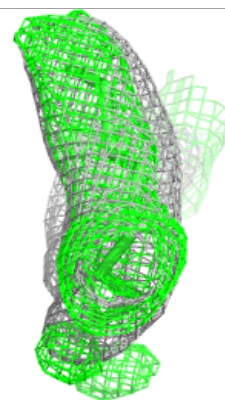
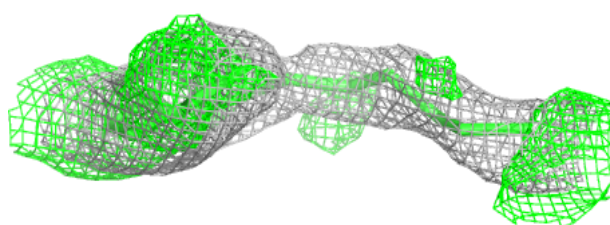
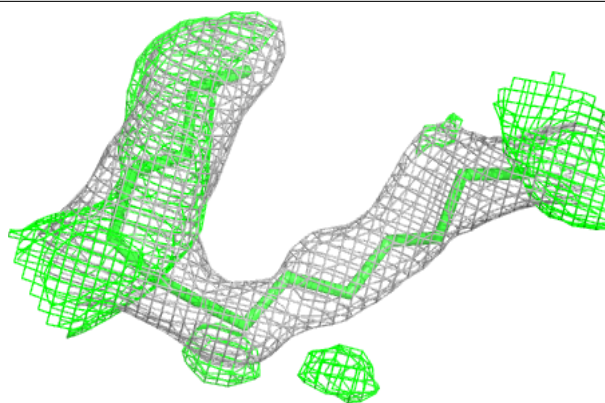
**Electron density around LFA N 601:**

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

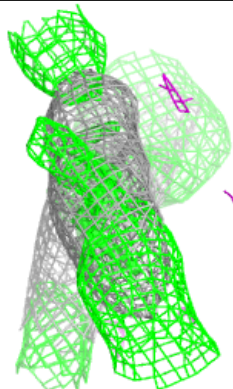
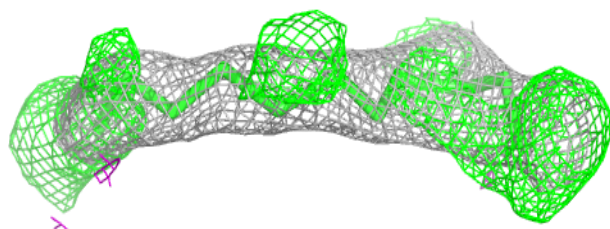
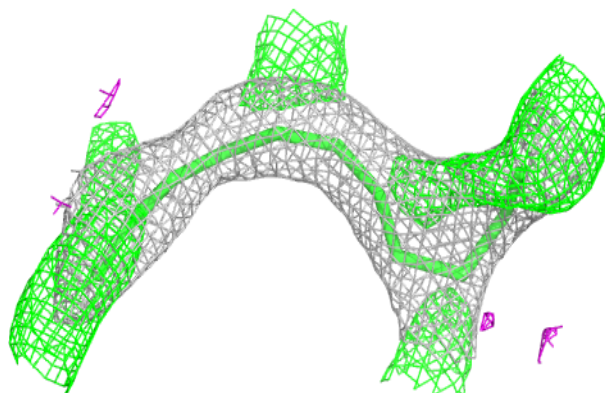


Electron density around LFA N 610:

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

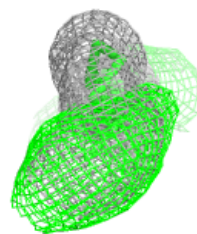
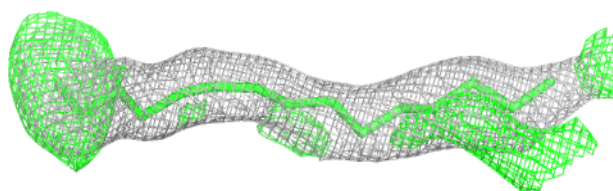
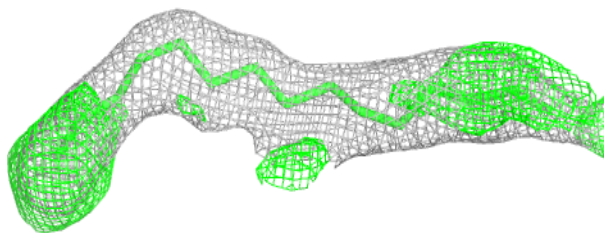
**Electron density around LFA C 307:**

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

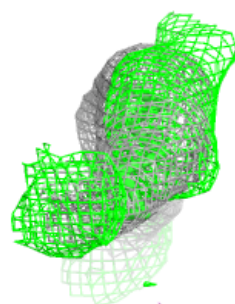
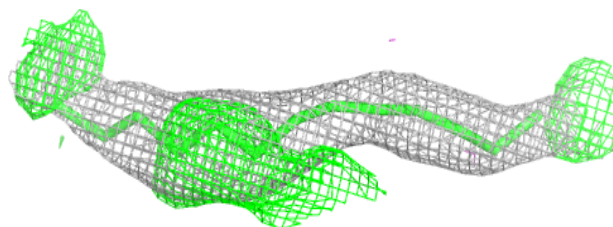
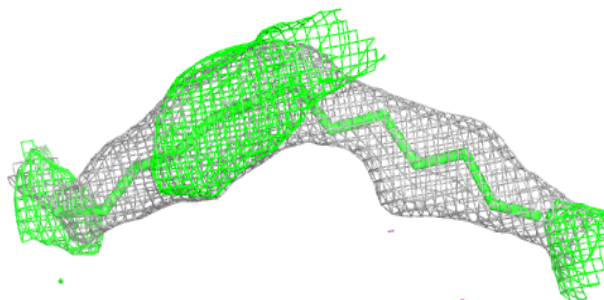


Electron density around LFA P 313:

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

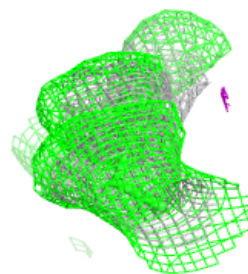
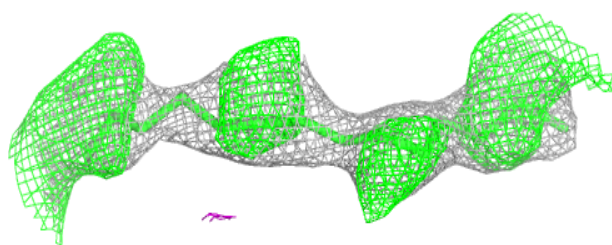
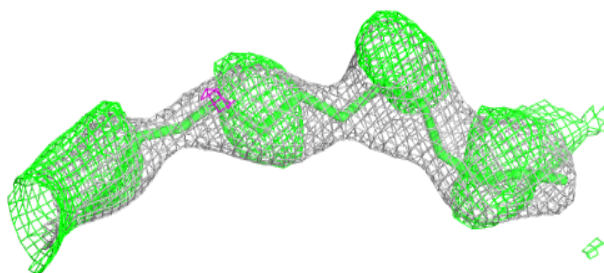
**Electron density around LFA P 314:**

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

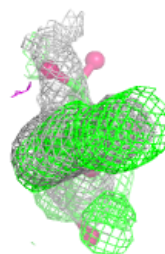
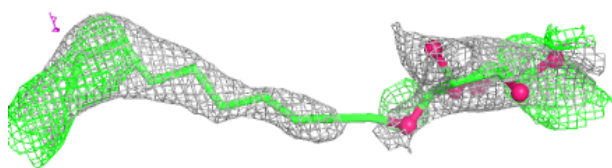
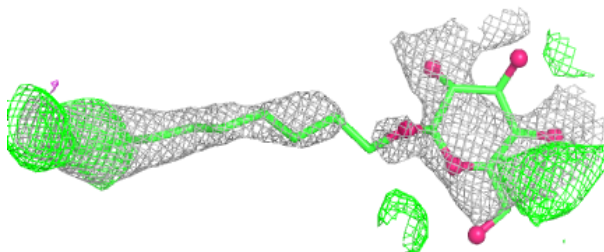


Electron density around LFA T 102:

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

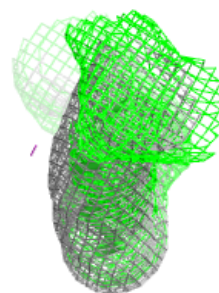
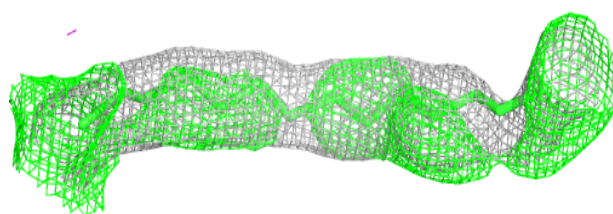
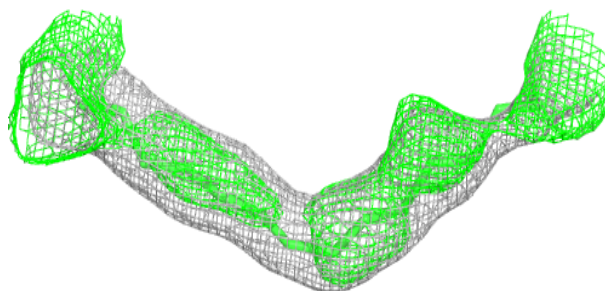
**Electron density around DMU O 303:**

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

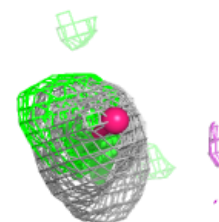
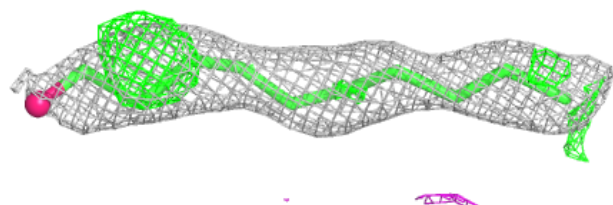
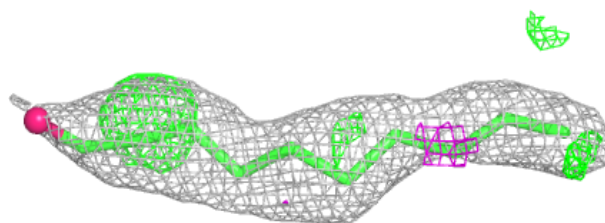


Electron density around LFA A 607:

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

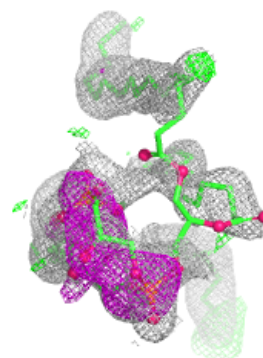
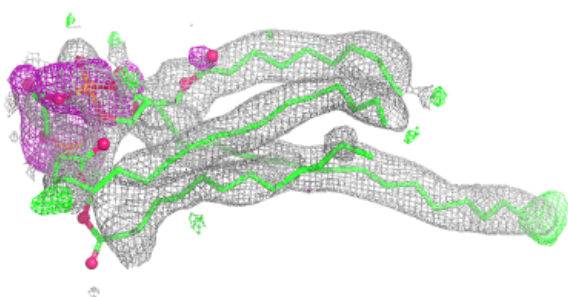
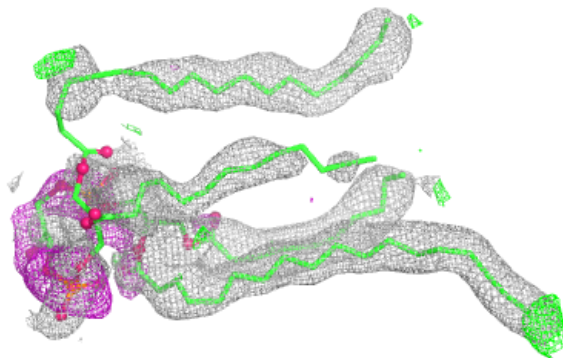
**Electron density around DMU A 615:**

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

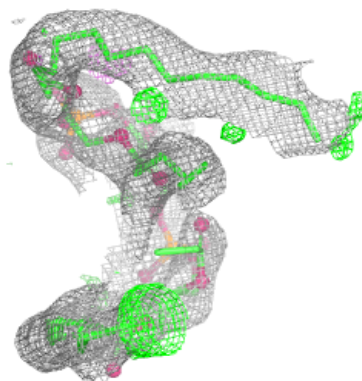
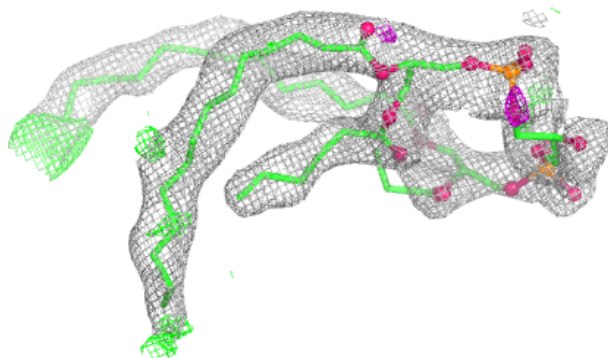
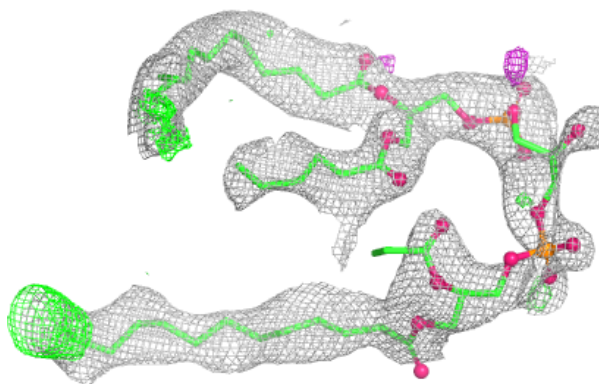


Electron density around CDL C 304:

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

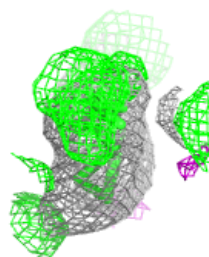
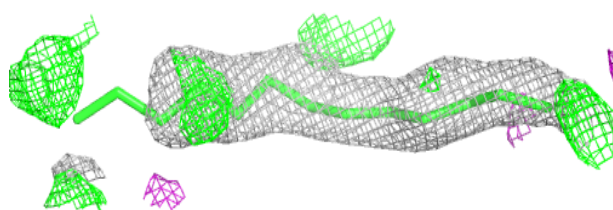
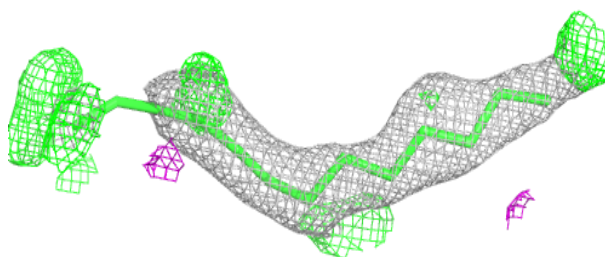
**Electron density around CDL O 304:**

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

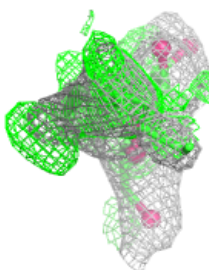
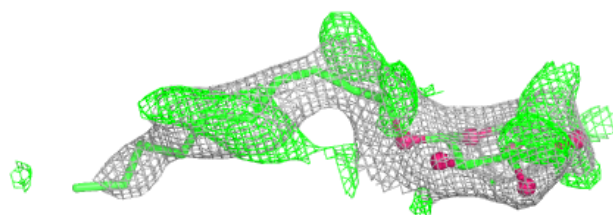
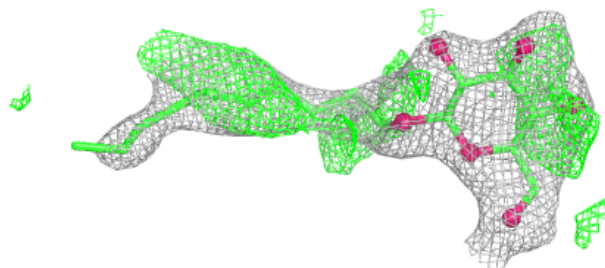


Electron density around LFA C 314:

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

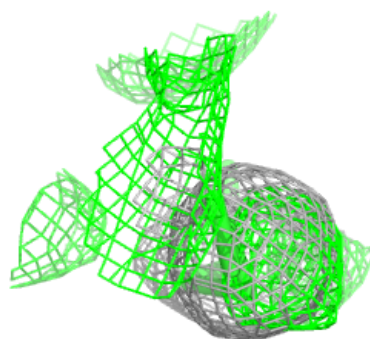
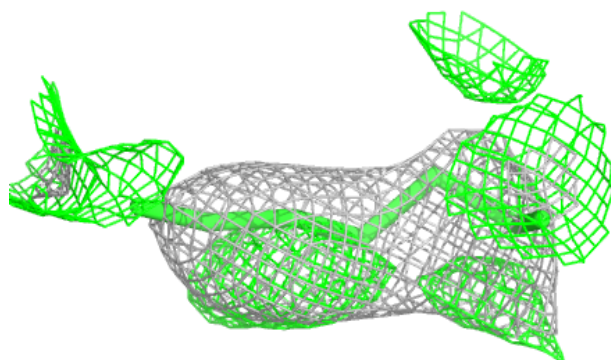
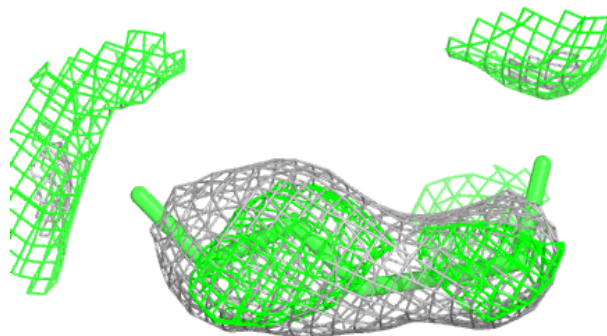
**Electron density around DMU C 323:**

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

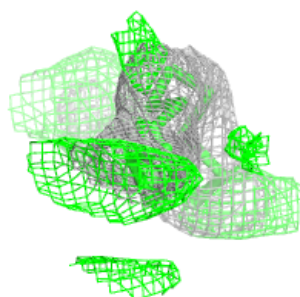
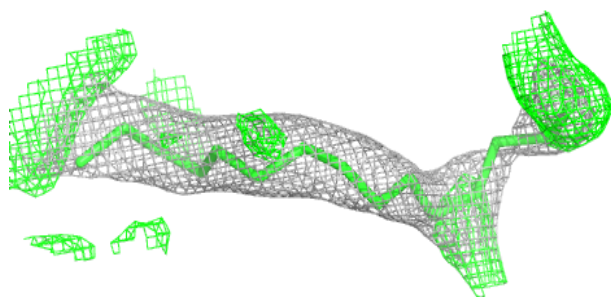
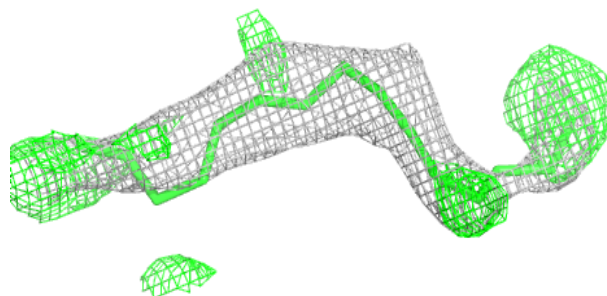


Electron density around DMU C 316:

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

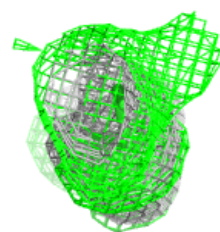
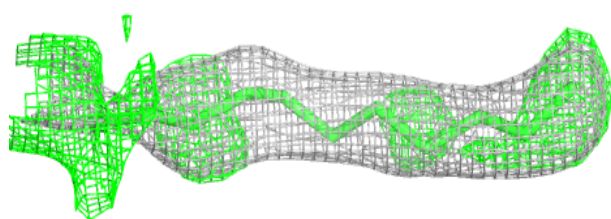
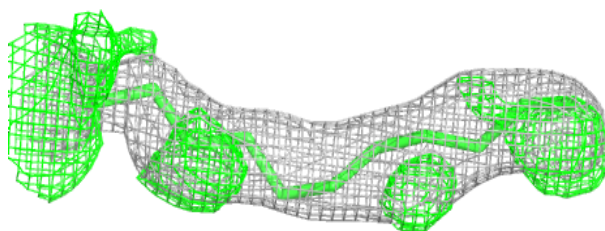
**Electron density around LFA P 301:**

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

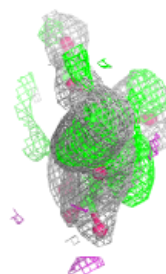
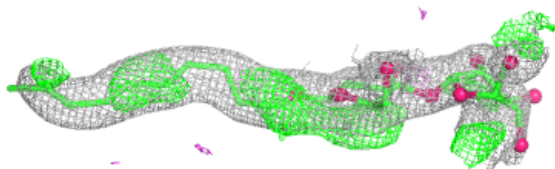
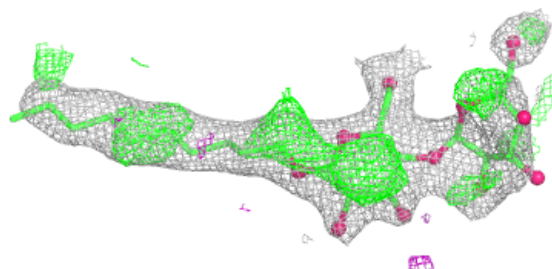


Electron density around LFA T 103:

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

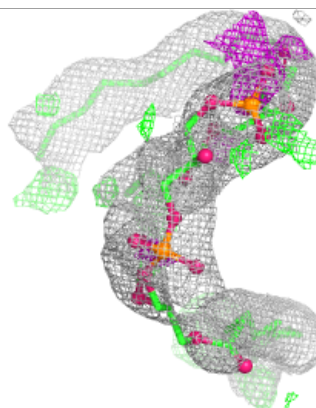
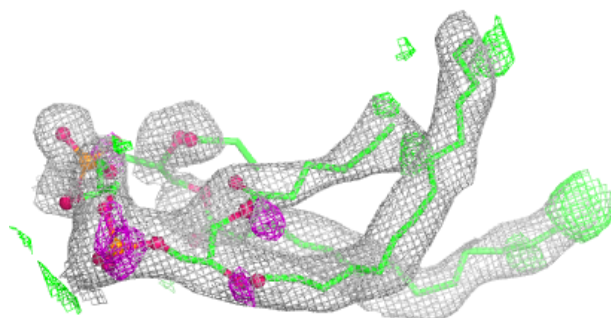
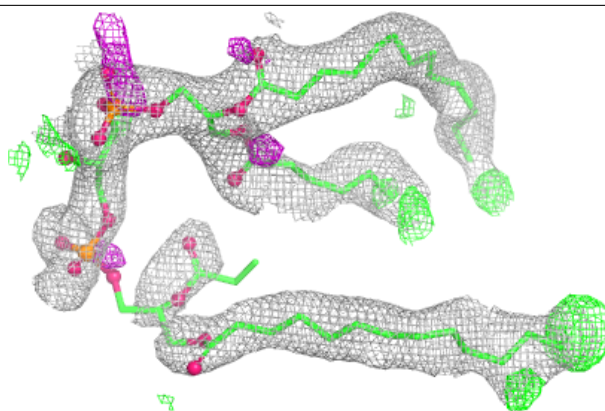
**Electron density around DMU N 612:**

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

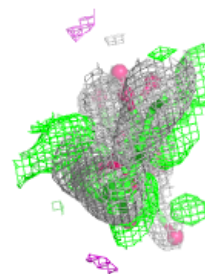
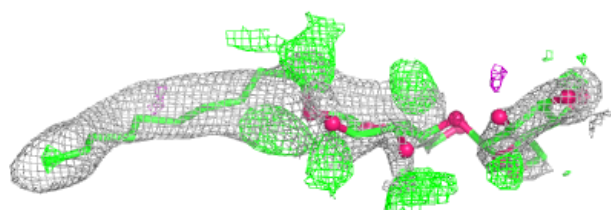
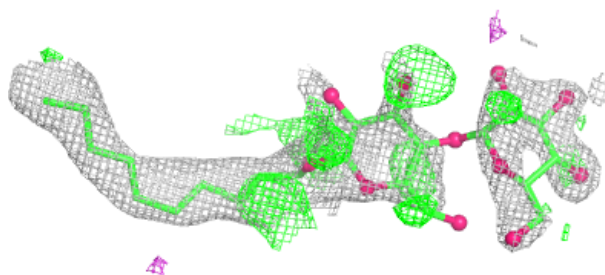


Electron density around CDL I 101:

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

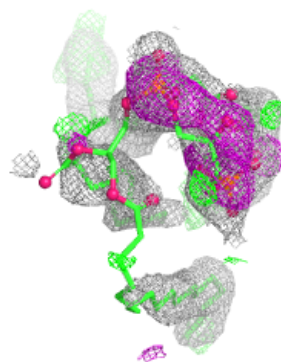
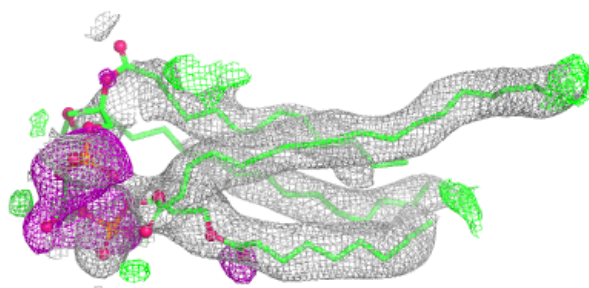
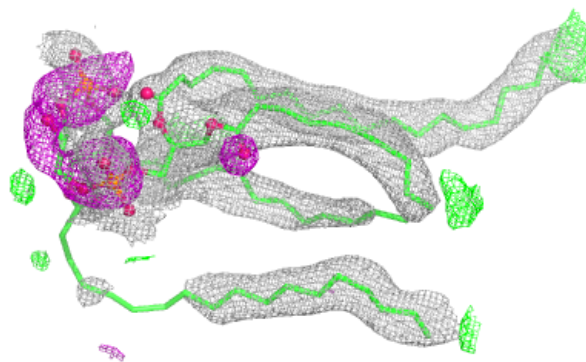
**Electron density around DMU N 619:**

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



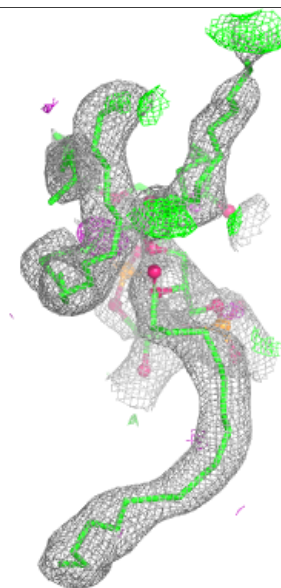
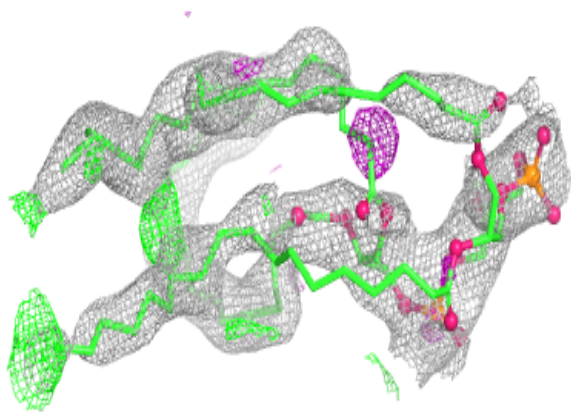
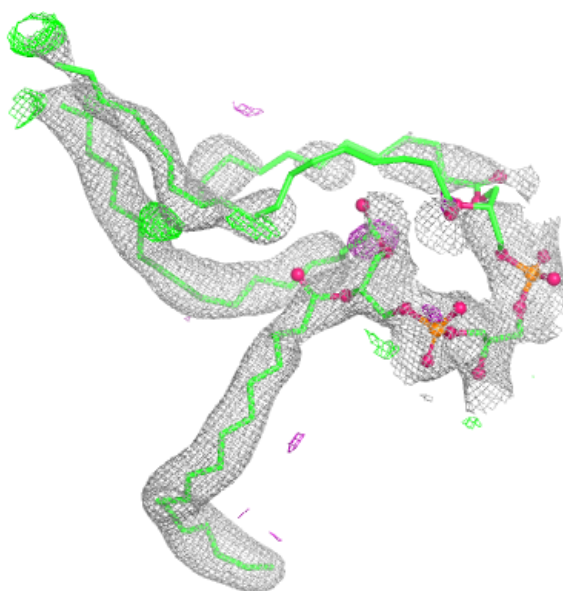
Electron density around CDL P 305:

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



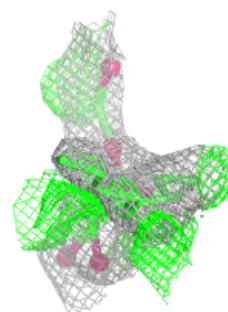
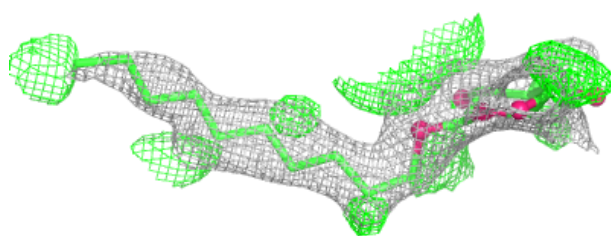
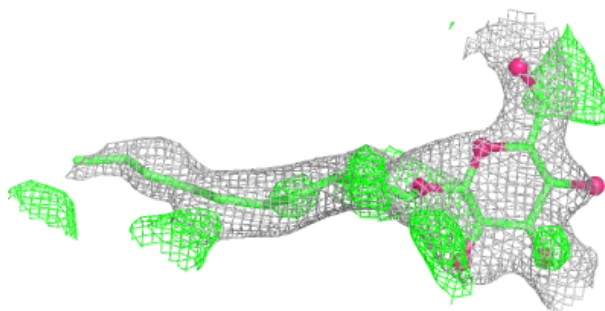
Electron density around CDL Y 101:

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

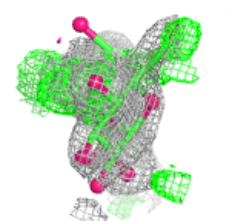
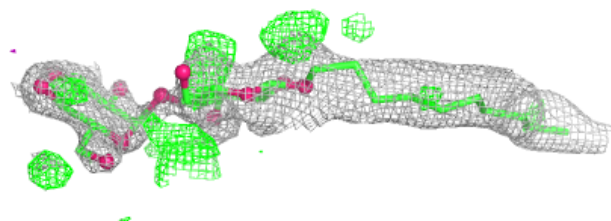
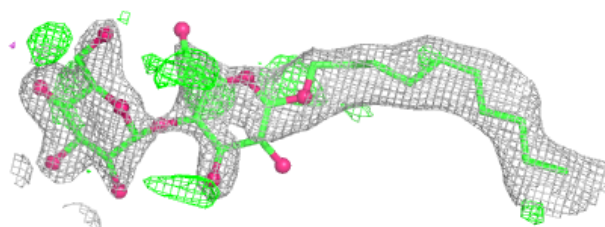


Electron density around DMU P 323:

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

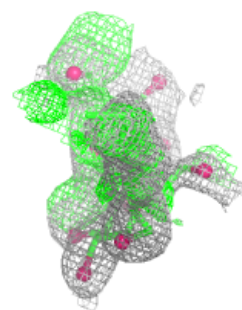
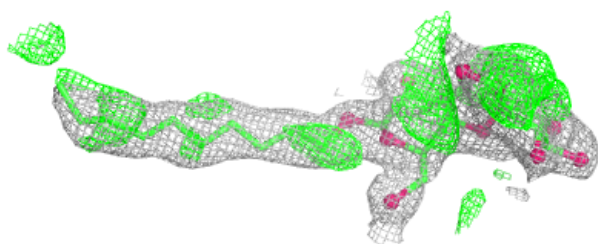
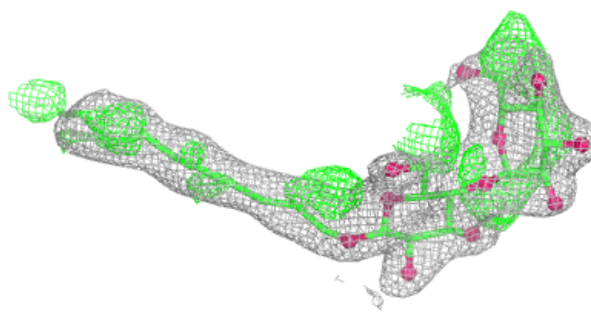
**Electron density around DMU H 101:**

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

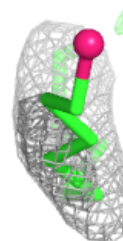
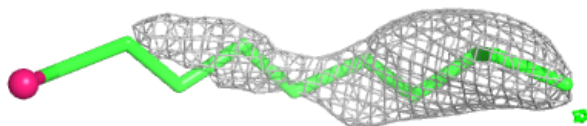
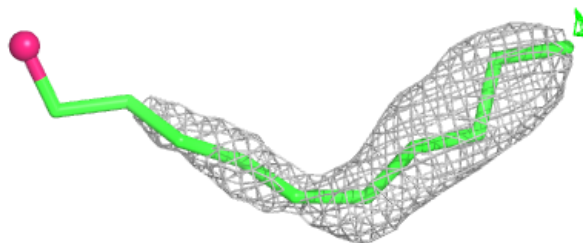


Electron density around DMU Q 201:

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

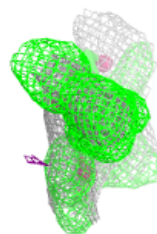
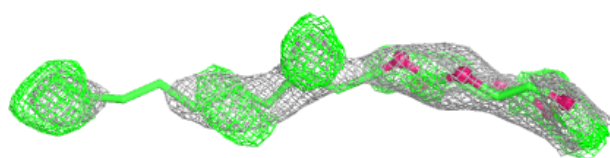
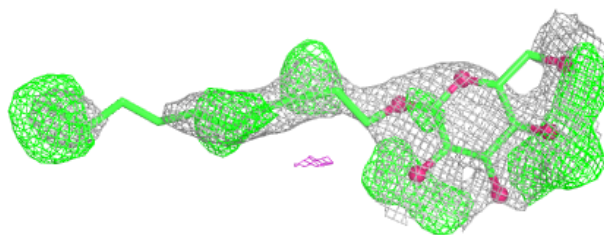
**Electron density around DMU W 101:**

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

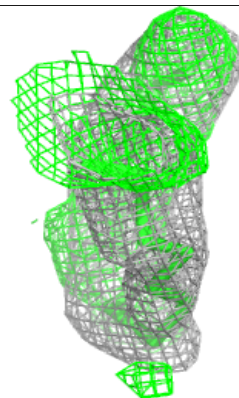
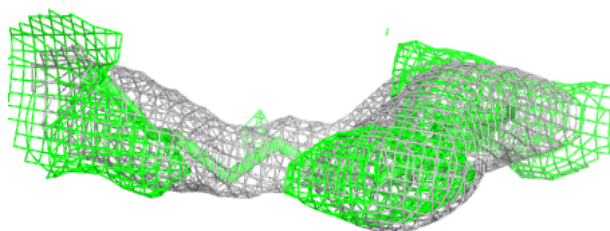
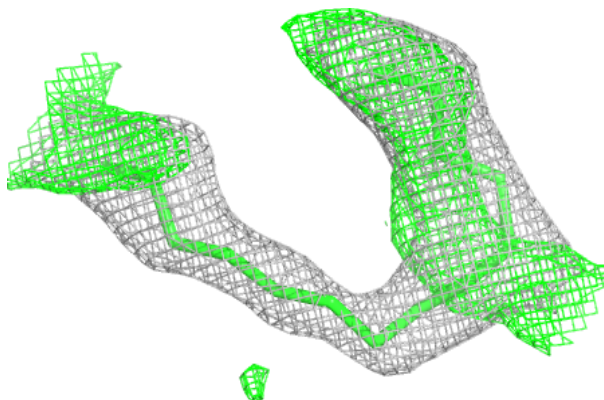


Electron density around DMU Y 102:

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

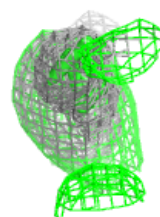
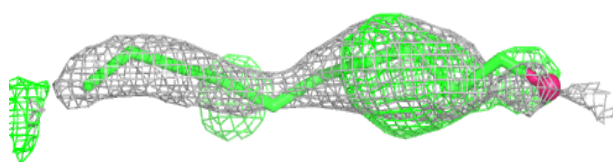
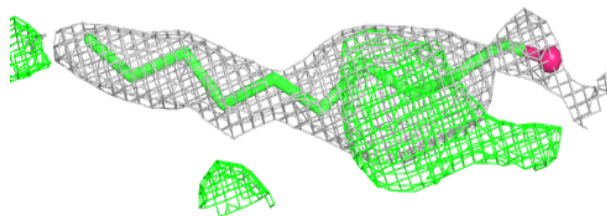
**Electron density around LFA A 608:**

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

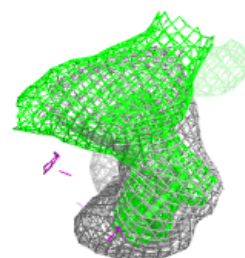
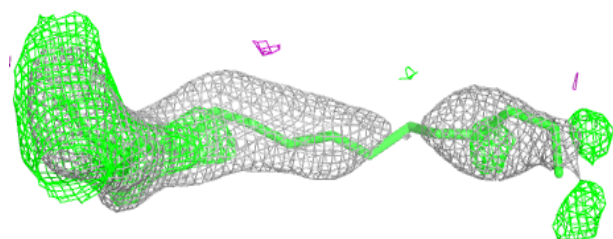
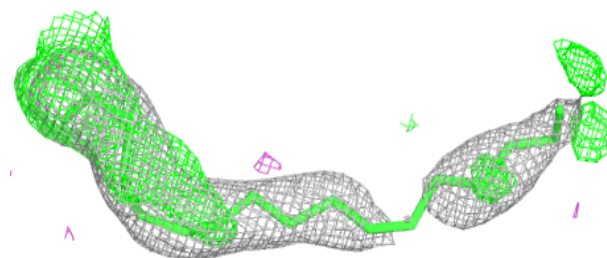


Electron density around DMU A 617:

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

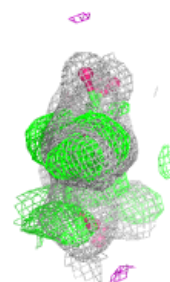
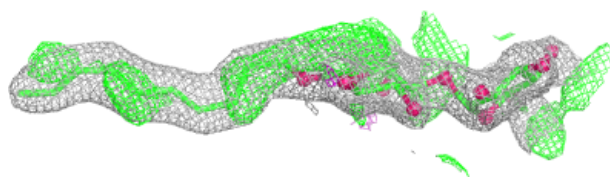
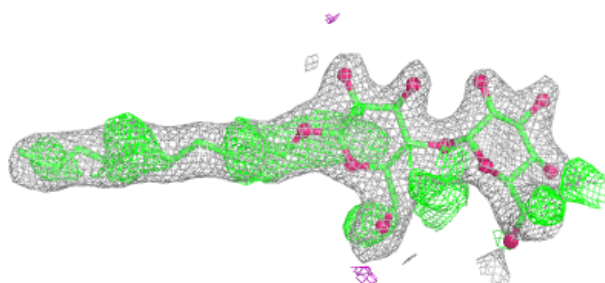
**Electron density around LFA B 306:**

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

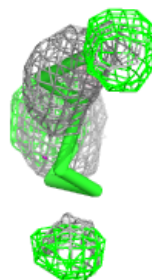
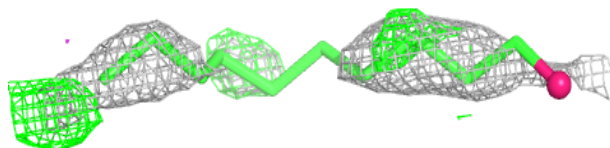
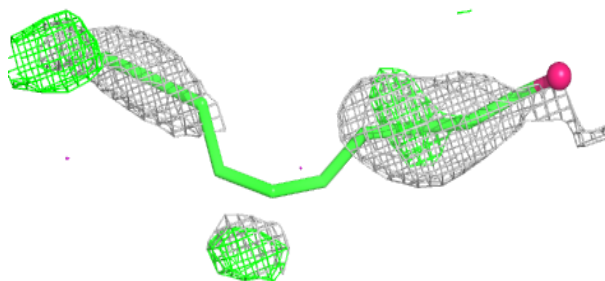


Electron density around DMU A 610:

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

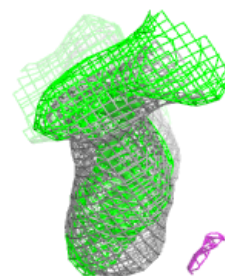
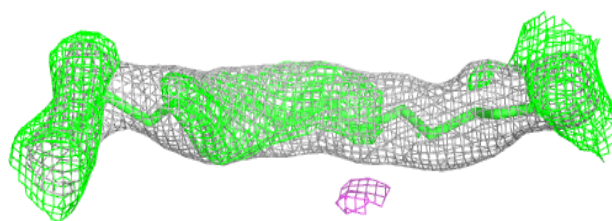
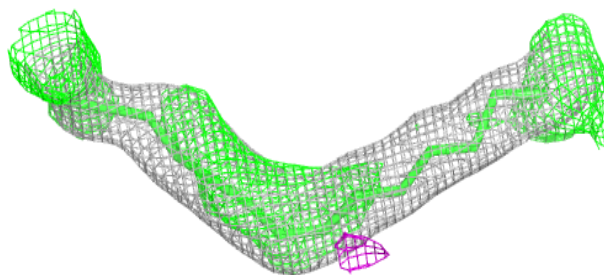
**Electron density around DMU N 602:**

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

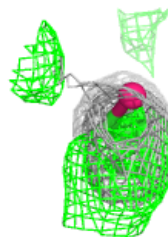
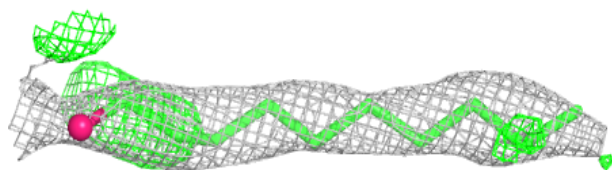
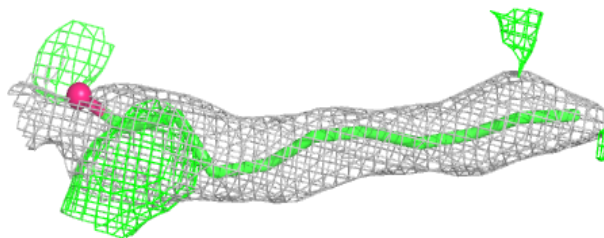


Electron density around LFA N 609:

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

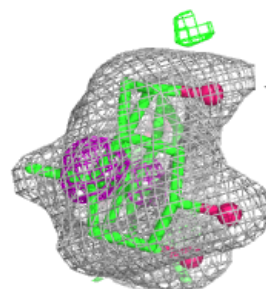
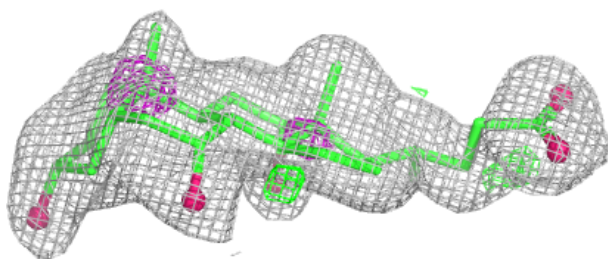
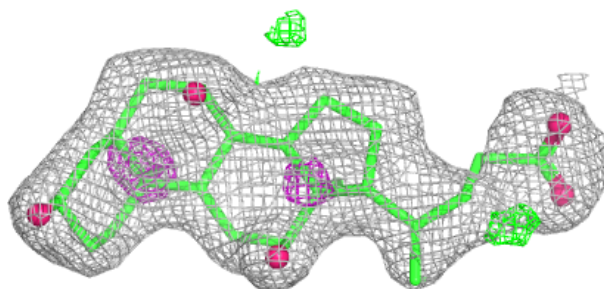
**Electron density around DMU B 302:**

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

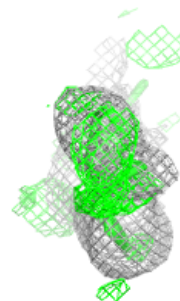
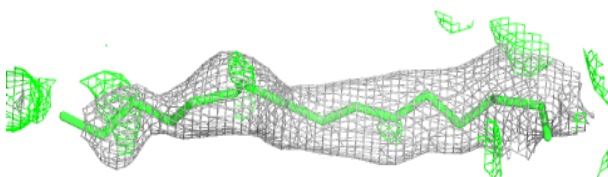
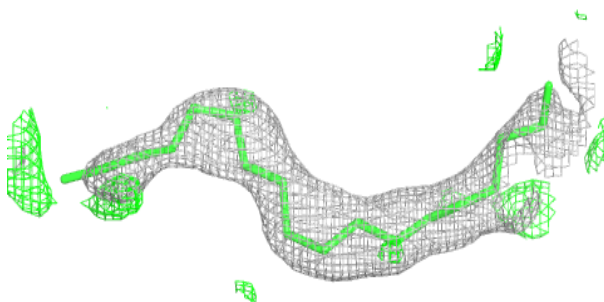


Electron density around CHD P 306:

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

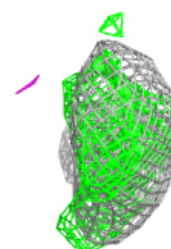
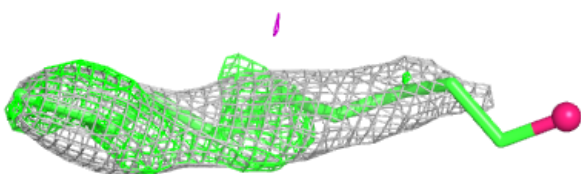
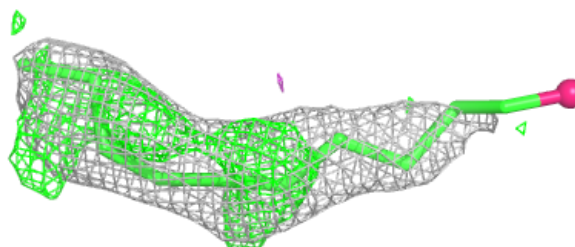
**Electron density around LFA C 309:**

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

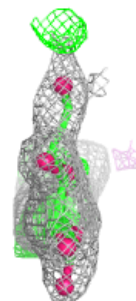
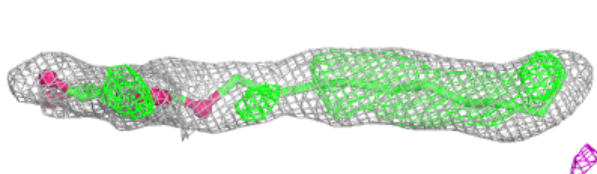
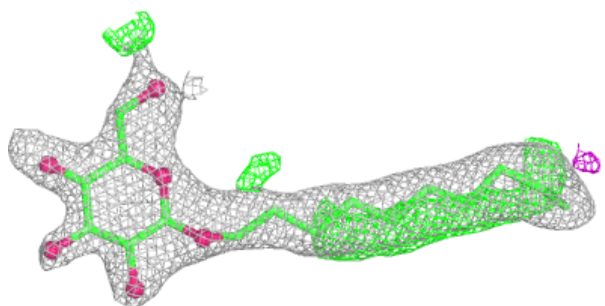


Electron density around DMU J 101:

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

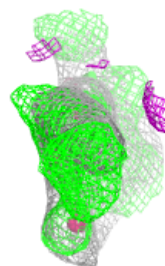
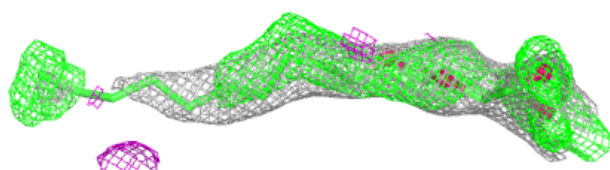
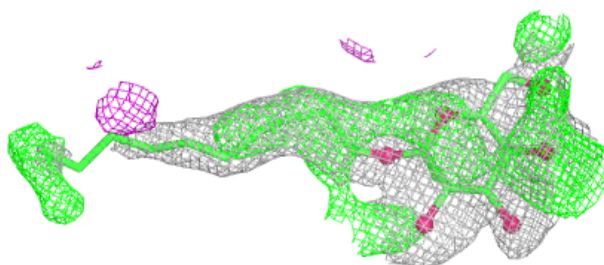
**Electron density around DMU O 308:**

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

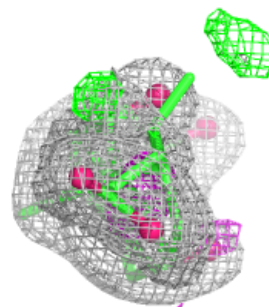
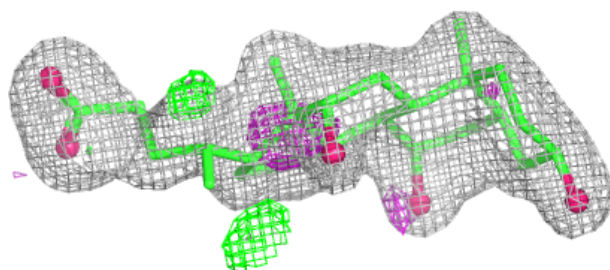
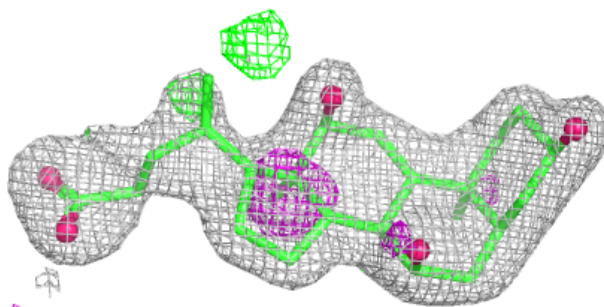


Electron density around DMU L 102:

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

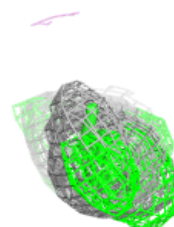
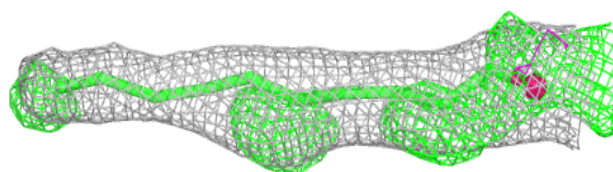
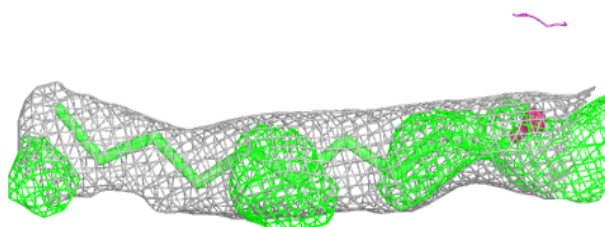
**Electron density around CHD C 305:**

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

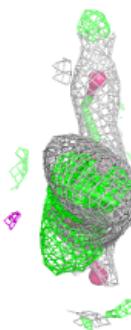
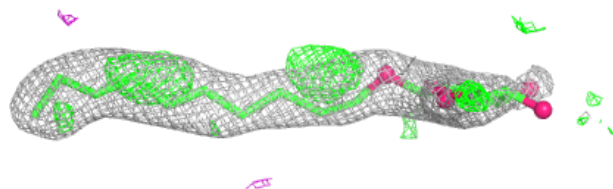
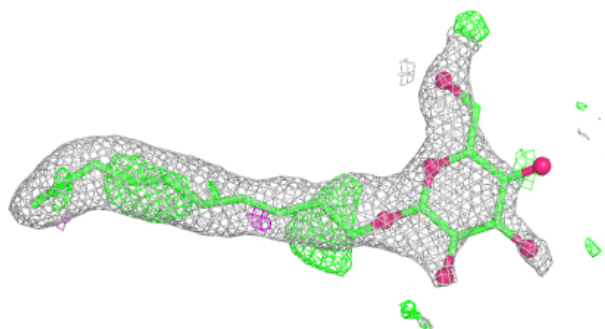


Electron density around DMU C 306:

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

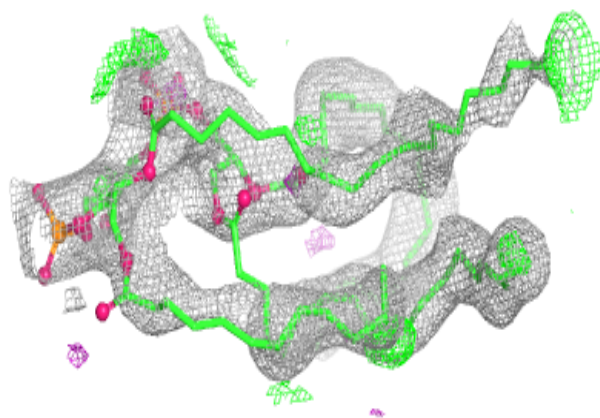
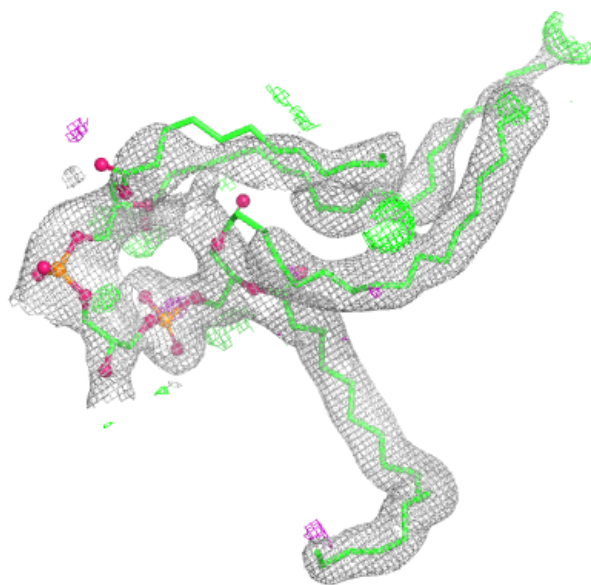
**Electron density around DMU B 303:**

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



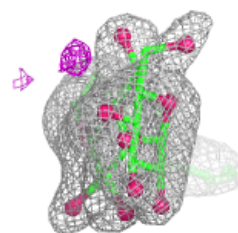
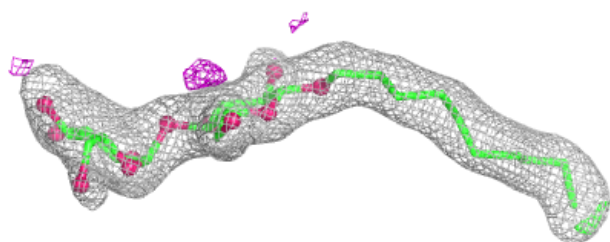
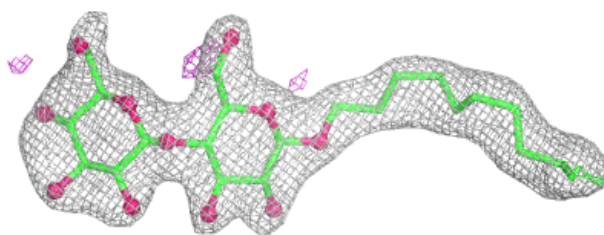
Electron density around CDL L 101:

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

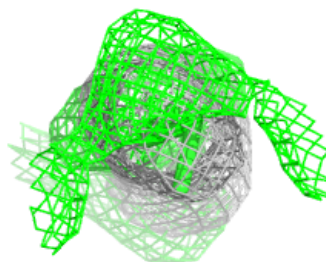
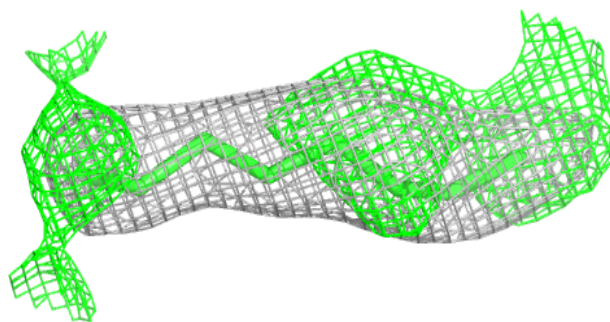
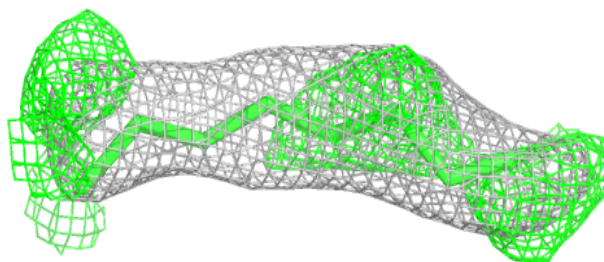


Electron density around DMU Z 101:

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

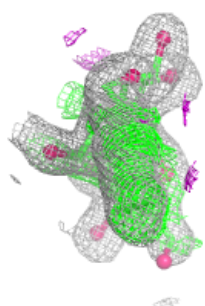
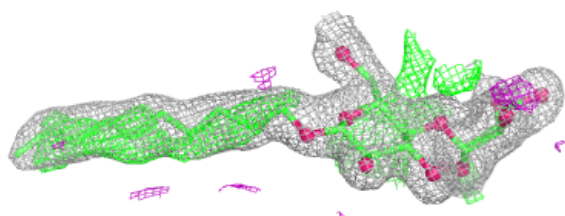
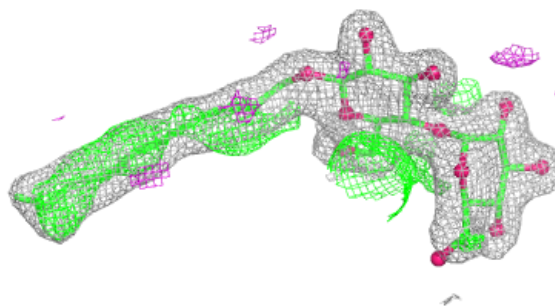
**Electron density around DMU Z 102:**

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

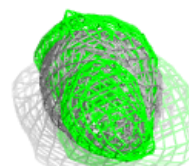
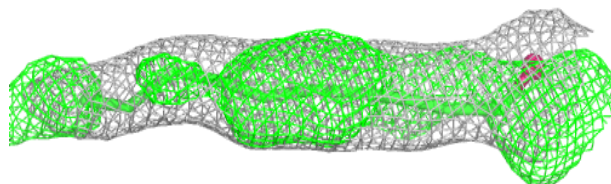
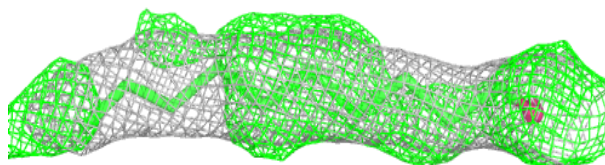


Electron density around DMU D 201:

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

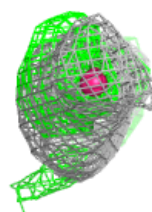
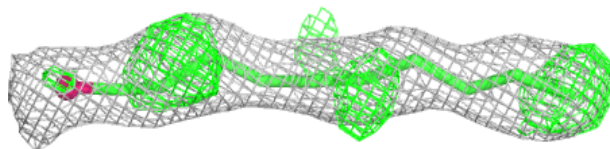
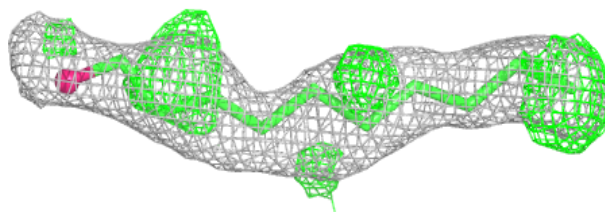
**Electron density around DMU P 307:**

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

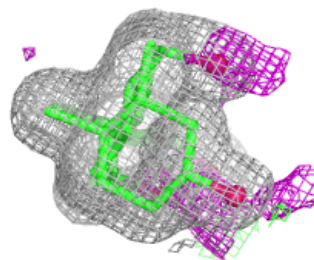
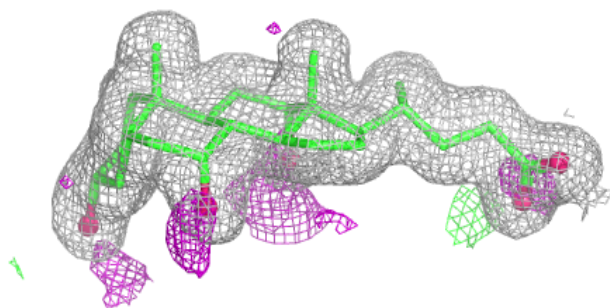
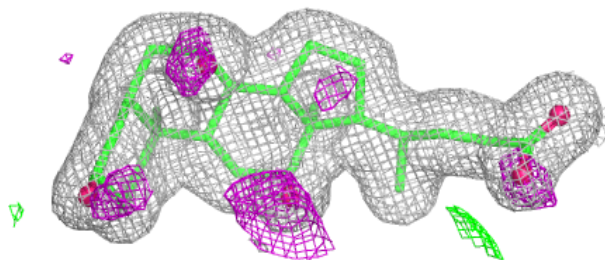


Electron density around DMU O 307:

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

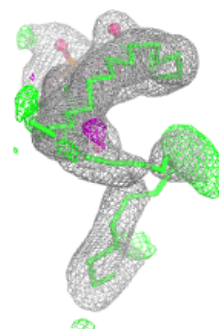
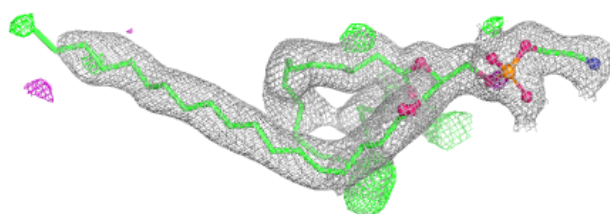
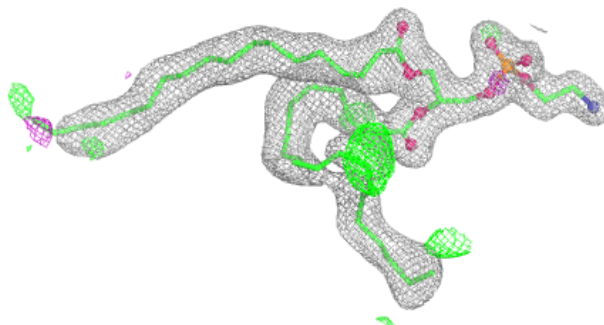
**Electron density around CHD C 301:**

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

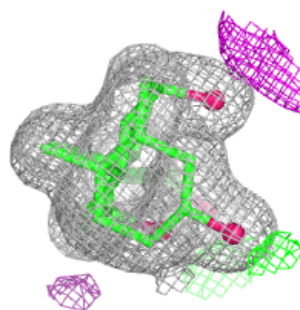
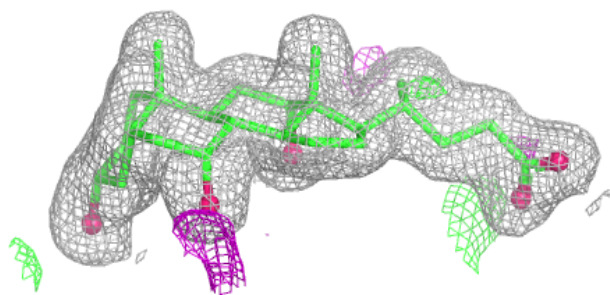
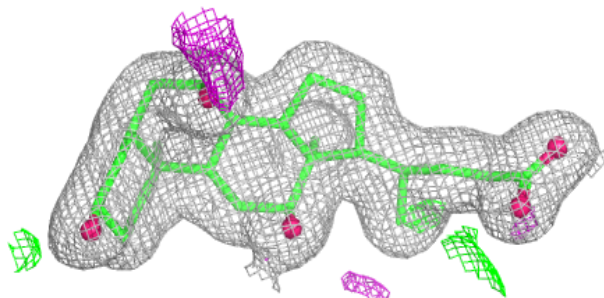


Electron density around PEK T 101:

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

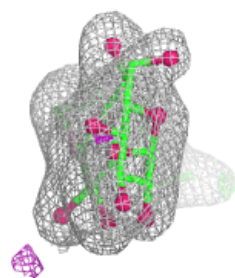
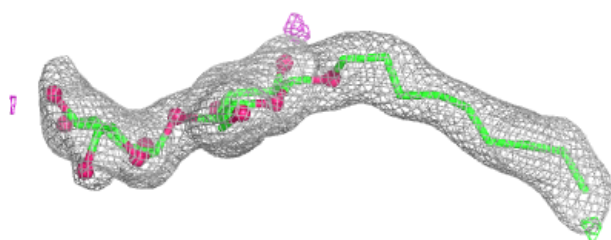
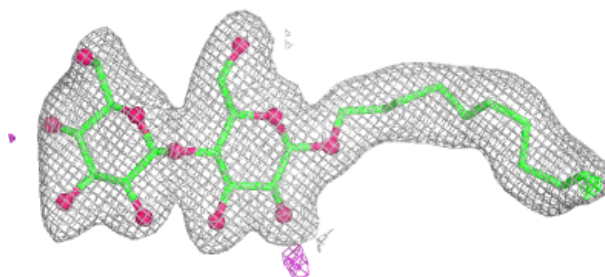
**Electron density around CHD P 302:**

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

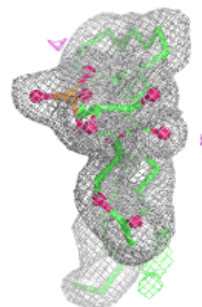
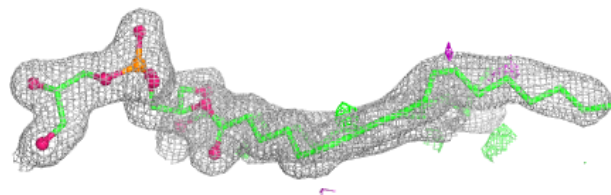
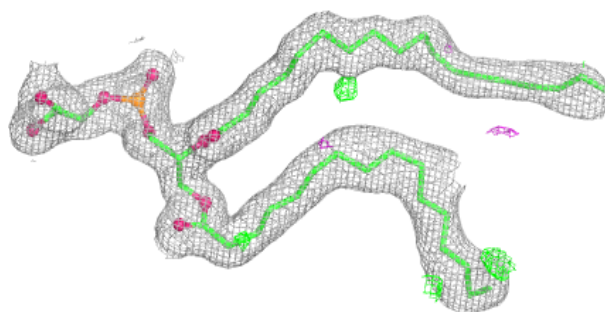


Electron density around DMU M 101:

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

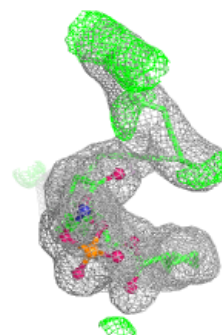
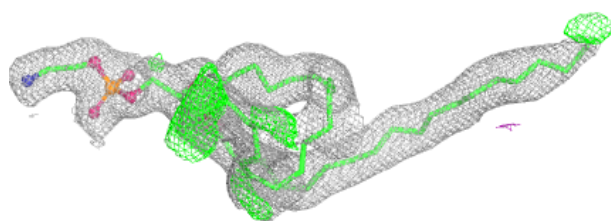
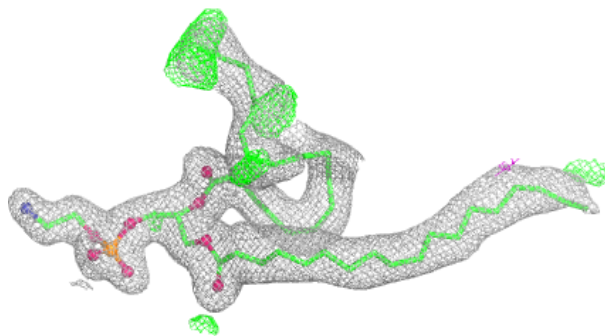
**Electron density around PGV N 618:**

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

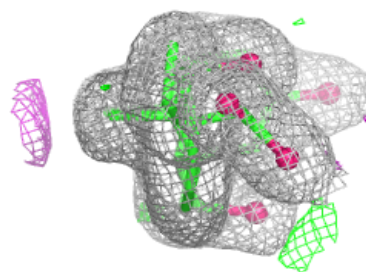
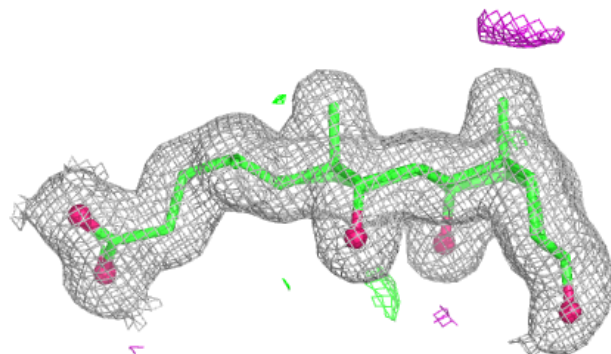
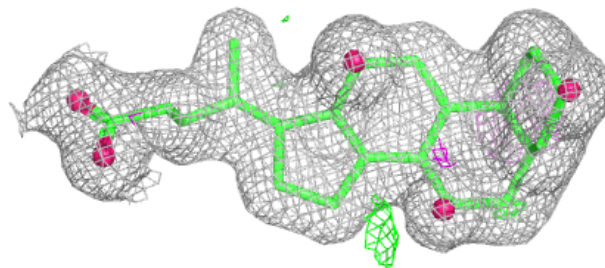


Electron density around PEK G 101:

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

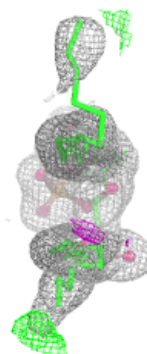
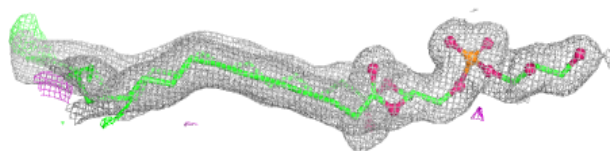
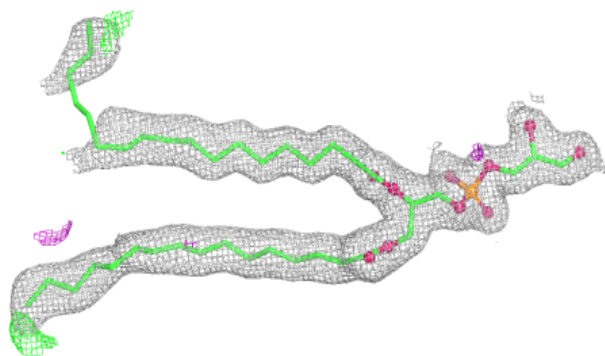
**Electron density around CHD B 305:**

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

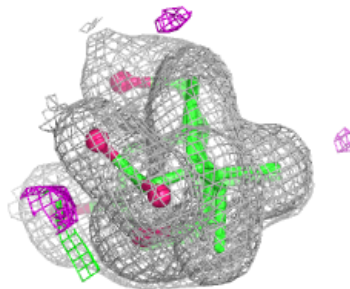
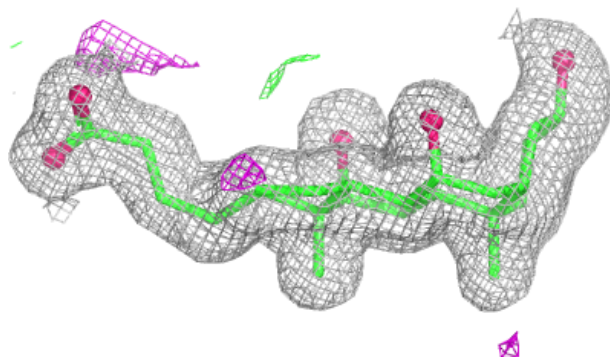
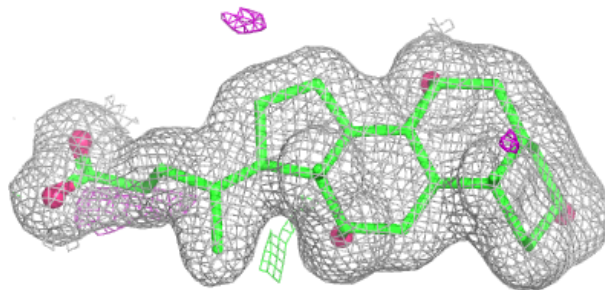


Electron density around PGV P 304:

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

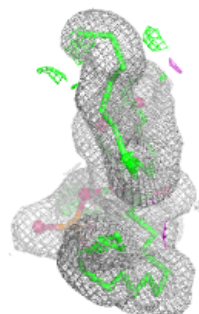
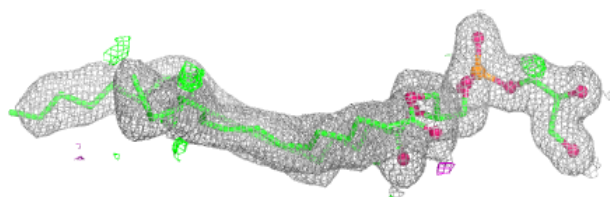
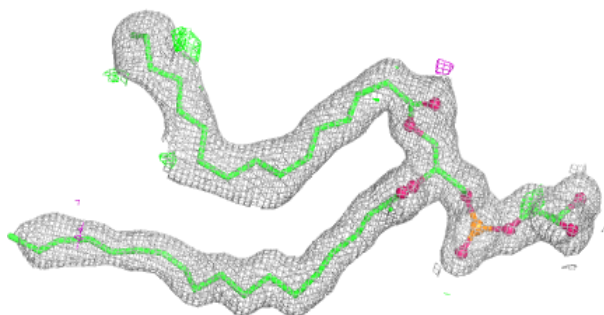
**Electron density around CHD O 301:**

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

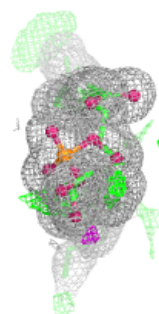
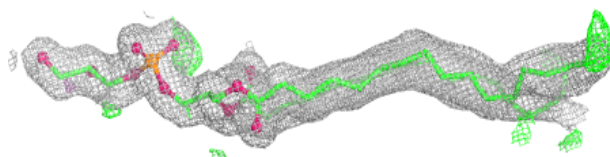
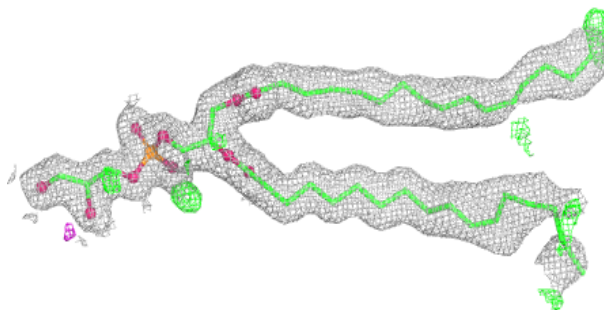


Electron density around PGV A 616:

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

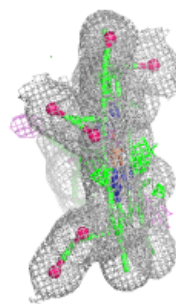
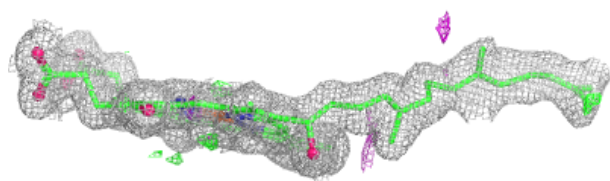
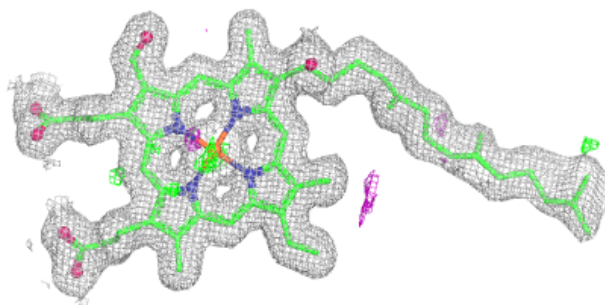
**Electron density around PGV C 303:**

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

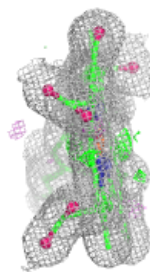
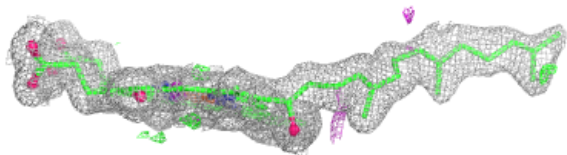
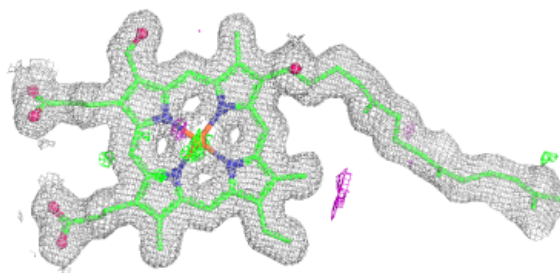


Electron density around HEA A 601 (A):

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

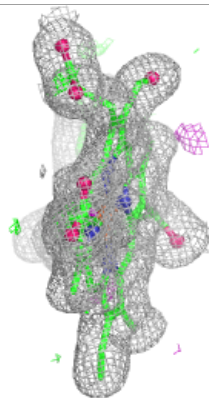
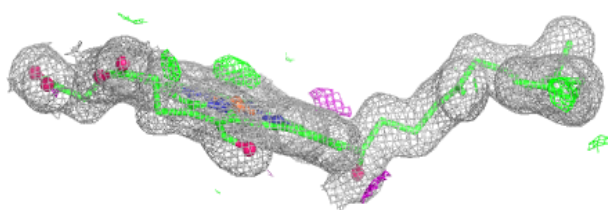
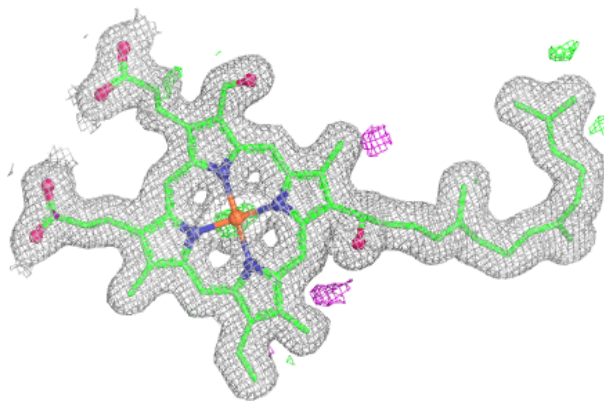
**Electron density around HEA A 601 (B):**

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

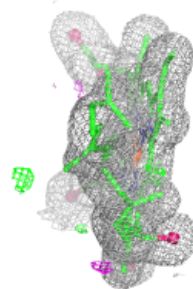
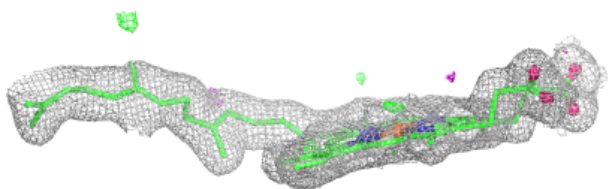
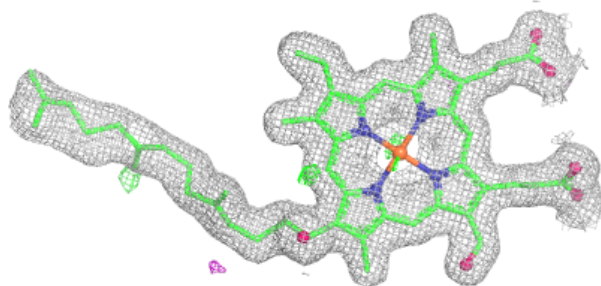


Electron density around HEA A 602:

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

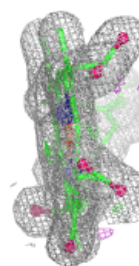
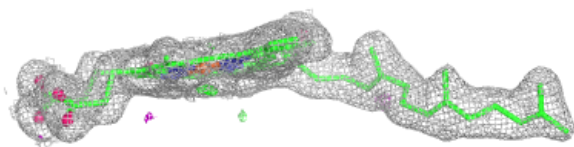
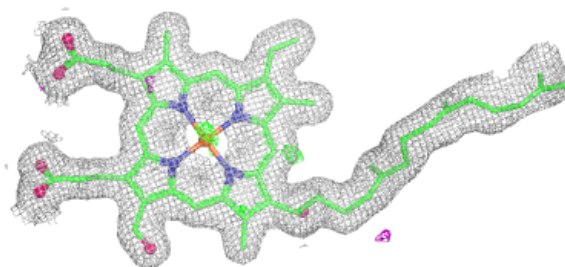
**Electron density around HEA N 603 (A):**

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

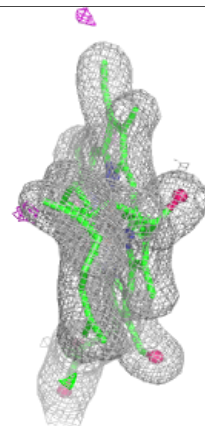
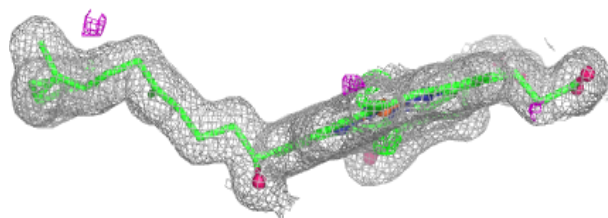
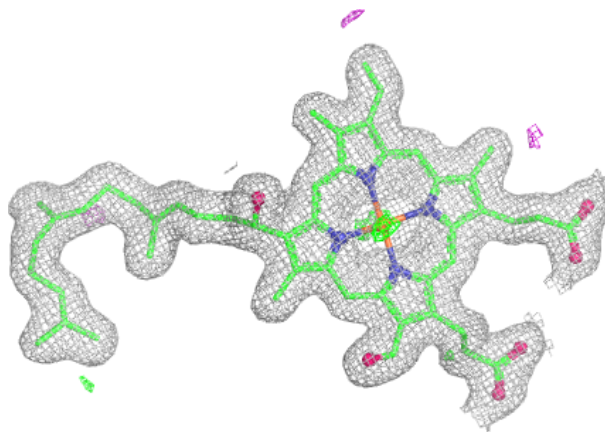


Electron density around HEA N 603 (B):

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

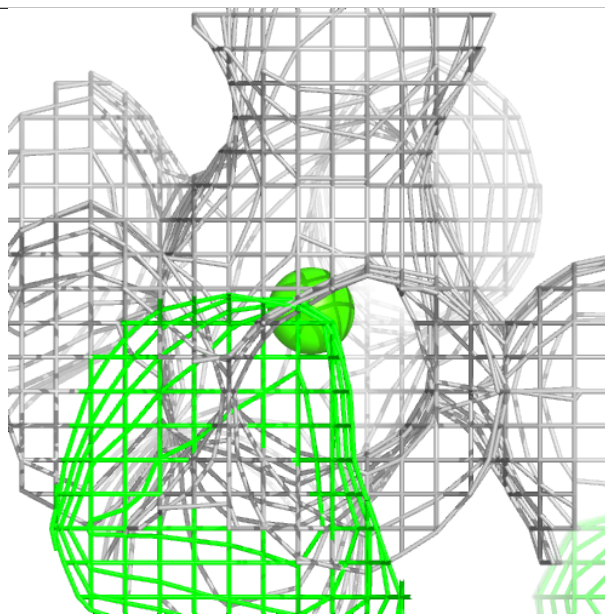
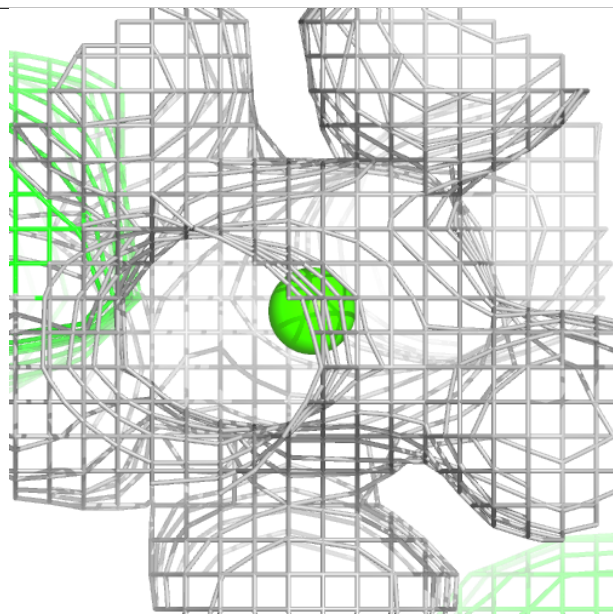
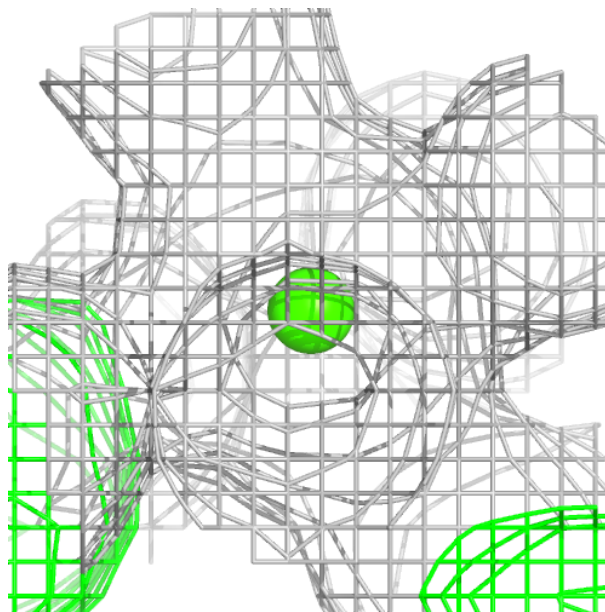
**Electron density around HEA N 604:**

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



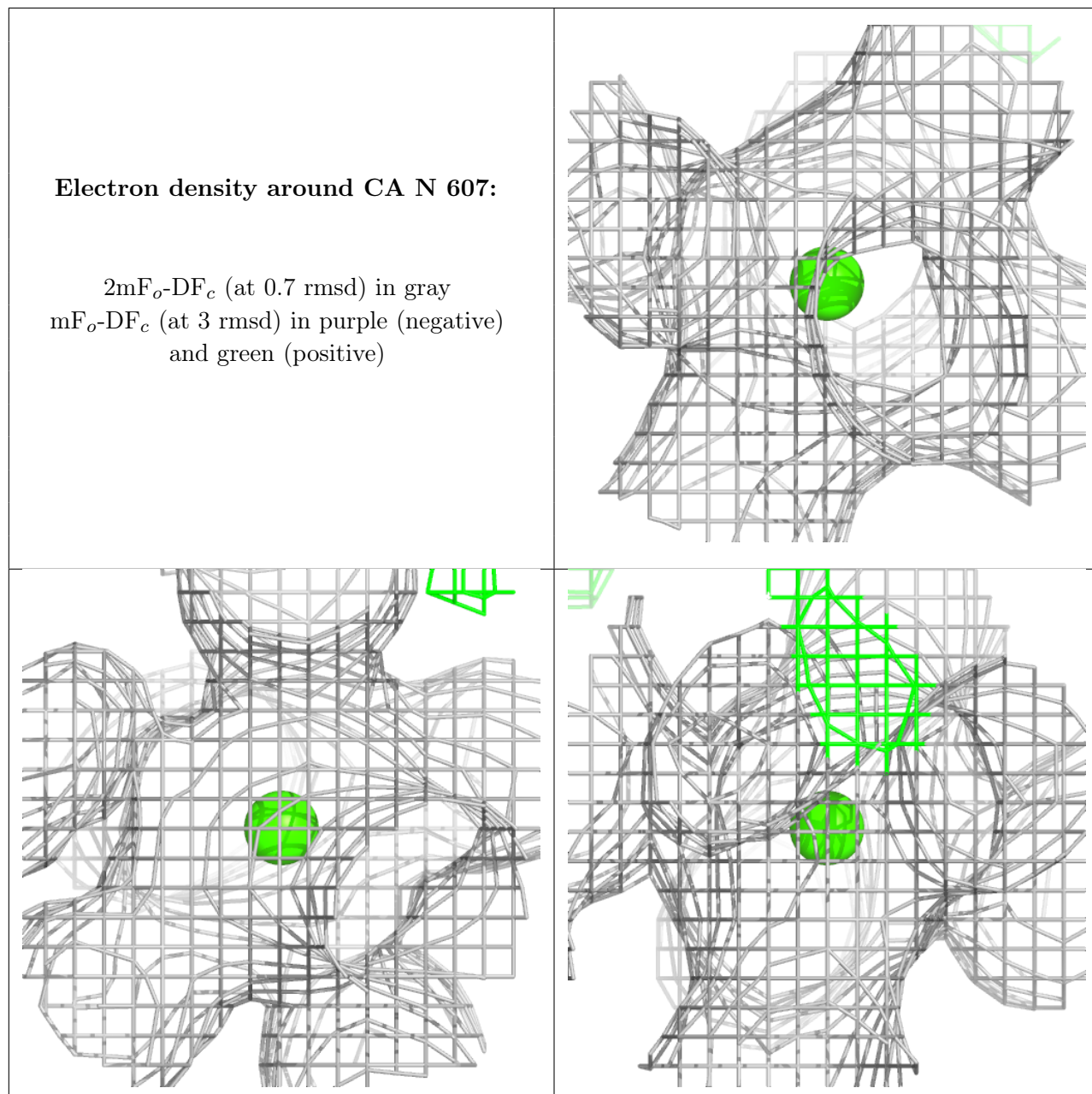
Electron density around CA A 605:

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



Electron density around CA N 607:

$2mF_o-DF_c$ (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.