



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:27 AM UTC

PDB ID : 7Y44 / pdb_00007y44
Title : Re-refinement of damage free X-ray structure of bovine cytochrome c oxidase at 1.9 angstrom resolution
Authors : Tsukihara, T.; Hirata, K.; Ago, H.
Deposited on : 2022-06-14
Resolution : 1.90 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

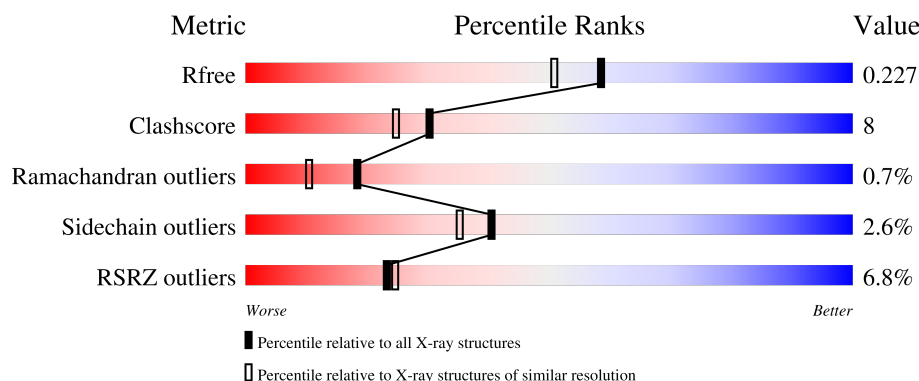
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	
1	N	514	
2	B	227	
2	O	227	
3	C	261	

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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
20	EDO	A	612	-	-	X	-
20	EDO	N	613	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	EDO	S	107	-	-	X	-
26	CDL	C	304	-	-	X	-
26	CDL	G	101	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 34120 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	514	Total	C	N	O	S	0	10	0
			4051	2710	623	681	37			
1	N	514	Total	C	N	O	S	0	7	0
			4046	2708	623	678	37			

- 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	3	0
			1834	1190	281	344	19			
2	O	227	Total	C	N	O	S	0	4	0
			1844	1200	283	342	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	3	0
			2117	1416	336	350	15			
3	P	259	Total	C	N	O	S	0	2	0
			2115	1415	336	350	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	1	0
			1201	783	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	1	0
			860	549	147	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	1	0
			750	465	134	146	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0
7	T	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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

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			

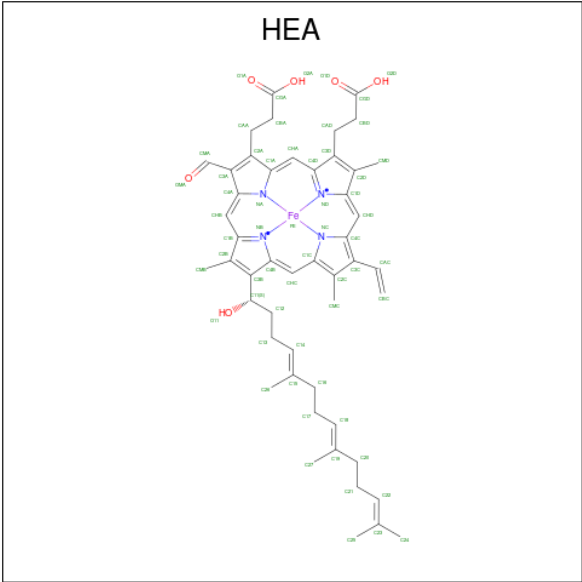
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			383	256	64	60	3			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

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



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

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

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

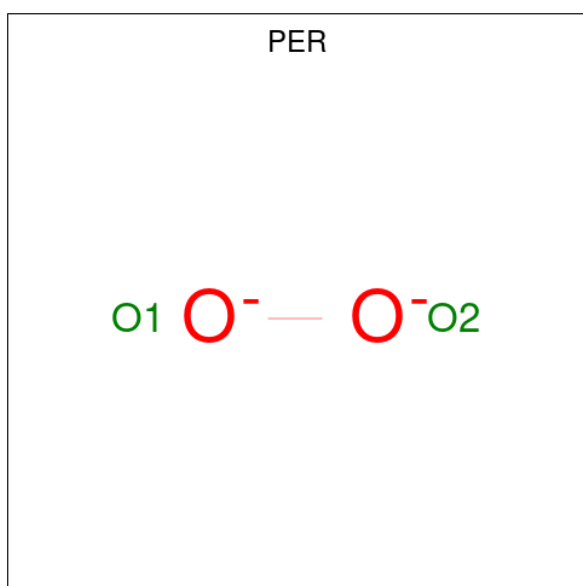
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

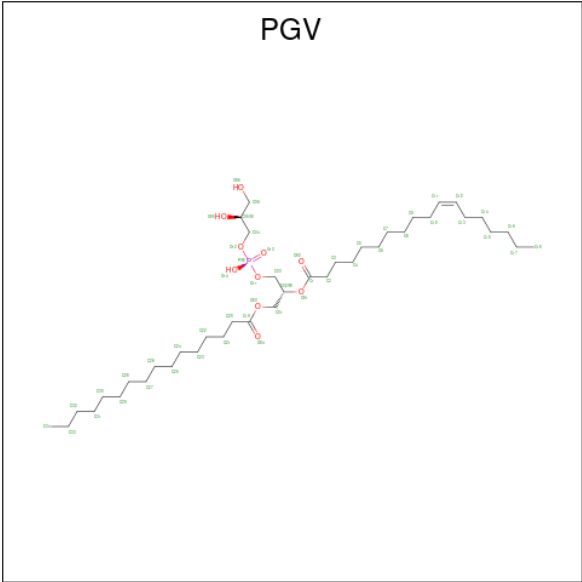
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0
17	P	1	Total Na 1 1	0	0

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



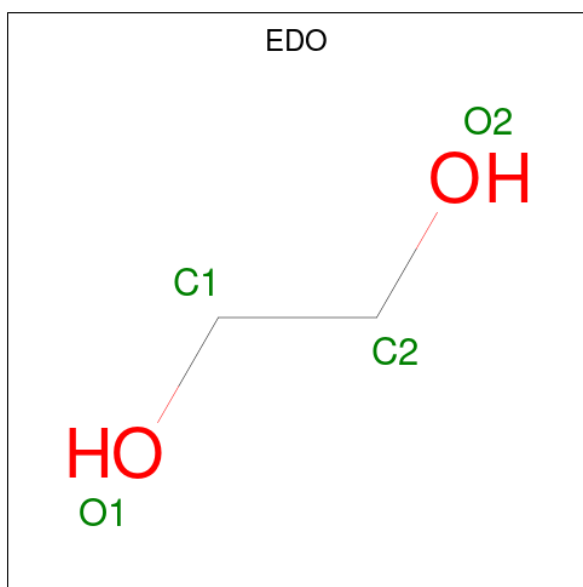
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total O 2 2	0	0
18	N	1	Total O 2 2	0	0

- Molecule 19 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
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 20 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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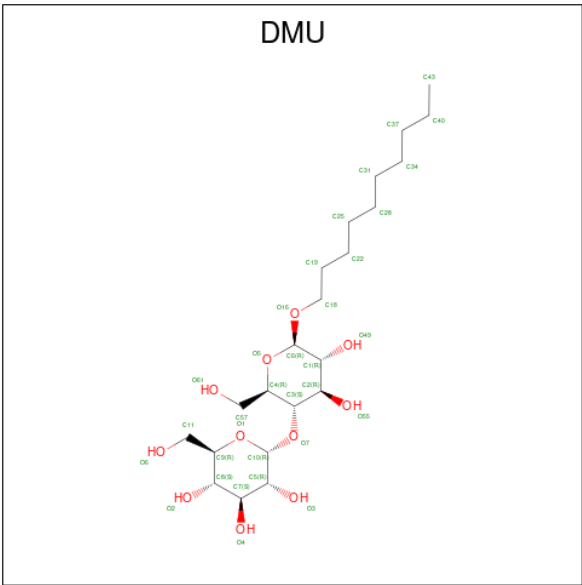
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	F	1	Total 4	C 2	O 2	0	0
20	G	1	Total 4	C 2	O 2	0	0
20	L	1	Total 4	C 2	O 2	0	0
20	L	1	Total 4	C 2	O 2	0	0
20	M	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	Q	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	W	1	Total	C	O	0	0
			4	2	2		
20	W	1	Total	C	O	0	0
			4	2	2		
20	Y	1	Total	C	O	0	0
			4	2	2		

- Molecule 21 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



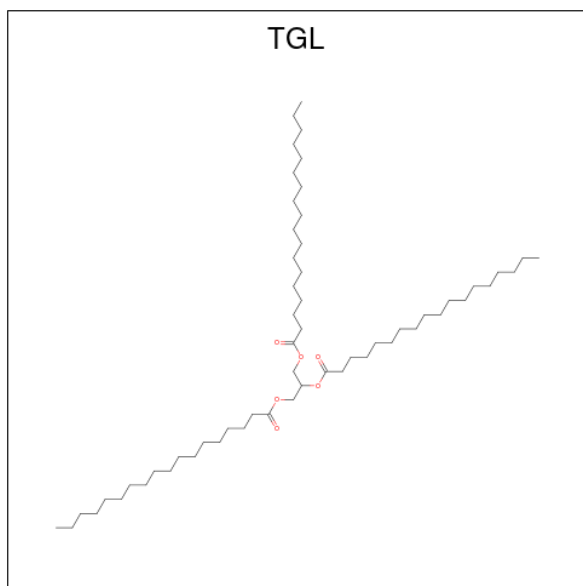
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			33	22	11		
21	B	1	Total	C	O	0	0
			33	22	11		
21	C	1	Total	C	O	0	0
			33	22	11		
21	D	1	Total	C	O	0	0
			33	22	11		
21	G	1	Total	C	O	0	0
			33	22	11		
21	K	1	Total	C	O	0	0
			33	22	11		
21	K	1	Total	C	O	0	0
			33	22	11		
21	K	1	Total	C	O	0	0
			33	22	11		
21	K	1	Total	C	O	0	0
			33	22	11		
21	K	1	Total	C	O	0	0
			33	22	11		
21	L	1	Total	C	O	0	0
			33	22	11		
21	M	1	Total	C	O	0	0
			33	22	11		
21	O	1	Total	C	O	0	0
			33	22	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	P	1	Total	C	O	0	0
			33	22	11		
21	P	1	Total	C	O	0	0
			33	22	11		
21	Q	1	Total	C	O	0	0
			33	22	11		
21	T	1	Total	C	O	0	0
			33	22	11		
21	X	1	Total	C	O	0	0
			33	22	11		
21	X	1	Total	C	O	0	0
			22	16	6		
21	X	1	Total	C	O	0	0
			22	16	6		
21	X	1	Total	C	O	0	0
			22	16	6		
21	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 22 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



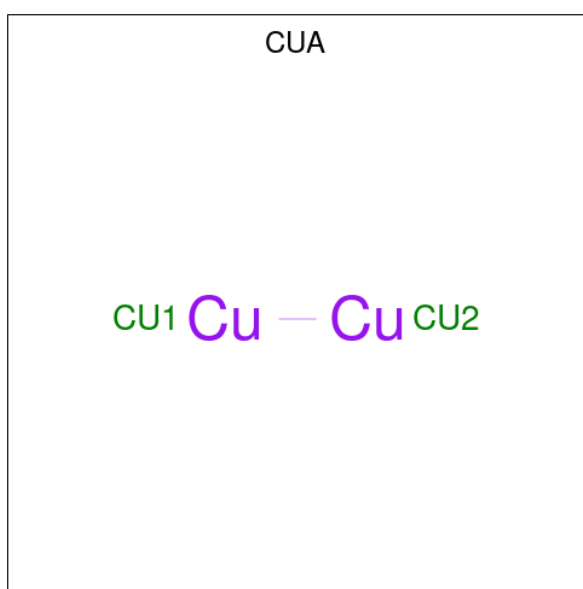
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			63	57	6		
22	D	1	Total	C	O	0	0
			63	57	6		

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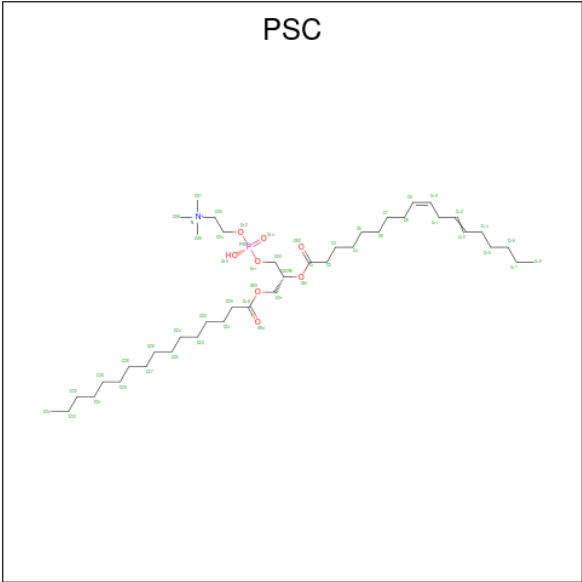
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	L	1	Total	C	O	0	0
			63	57	6		
22	O	1	Total	C	O	0	0
			63	57	6		
22	Q	1	Total	C	O	0	0
			63	57	6		
22	Y	1	Total	C	O	0	0
			63	57	6		

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



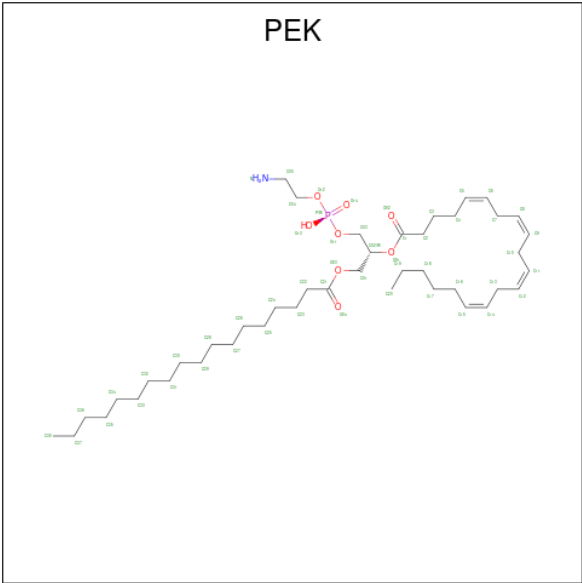
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	B	1	Total	Cu	0	0
			2	2		
23	O	1	Total	Cu	0	0
			2	2		

- Molecule 24 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
24	N	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 25 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYL)OXY]METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



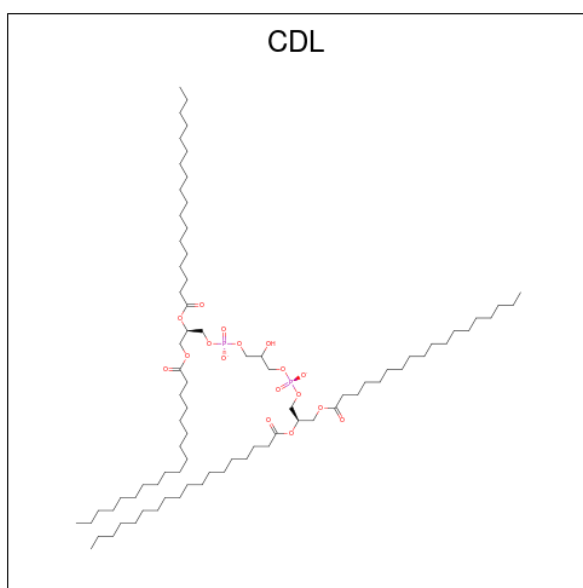
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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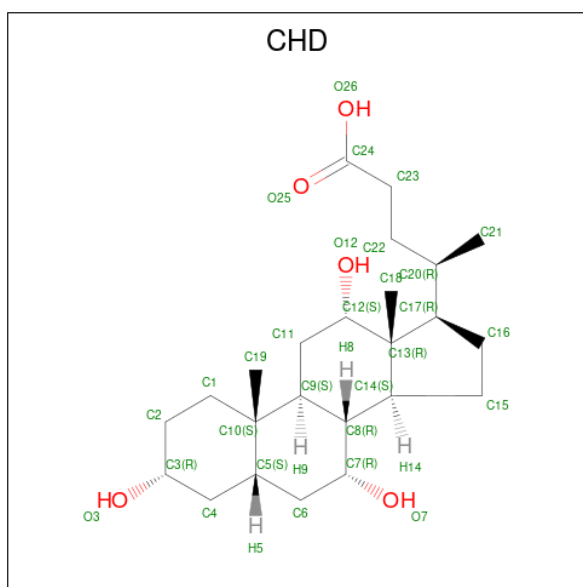
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- 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
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 27 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	C	1	Total	C	O	0	0
			29	24	5		
27	C	1	Total	C	O	0	0
			29	24	5		
27	G	1	Total	C	O	0	0
			29	24	5		
27	J	1	Total	C	O	0	0
			29	24	5		
27	L	1	Total	C	O	0	0
			29	24	5		
27	P	1	Total	C	O	0	0
			29	24	5		
27	P	1	Total	C	O	0	0
			29	24	5		
27	T	1	Total	C	O	0	0
			29	24	5		
27	W	1	Total	C	O	0	0
			29	24	5		
27	X	1	Total	C	O	0	0
			29	24	5		
27	Y	1	Total	C	O	0	0
			29	24	5		

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

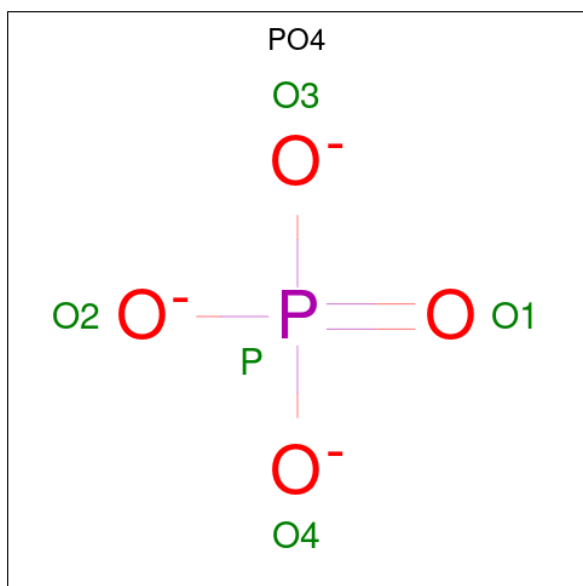
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	F	1	Total	Zn	0	0
			1	1		

Continued on next page...

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

- Molecule 29 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	H	1	Total	O	P	0	0
			5	4	1		
29	U	1	Total	O	P	0	0
			5	4	1		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	263	Total	O	0	0
			263	263		
30	B	176	Total	O	0	2
			176	176		
30	C	128	Total	O	0	0
			128	128		
30	D	154	Total	O	0	0
			154	154		
30	E	124	Total	O	0	0
			124	124		
30	F	114	Total	O	0	0
			114	114		

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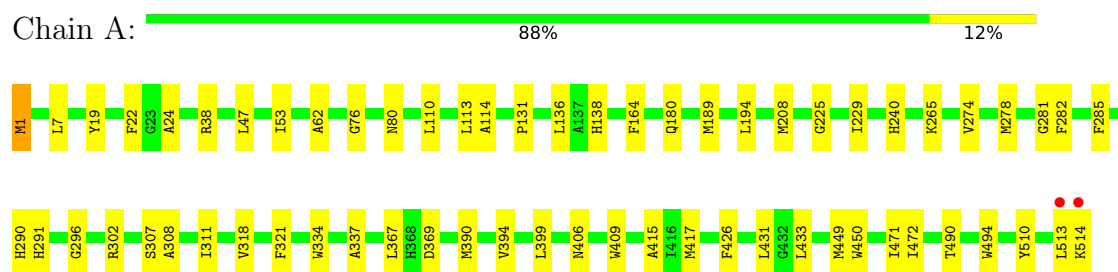
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	G	69	Total 69	O 69	0	0
30	H	69	Total 69	O 69	0	0
30	I	60	Total 60	O 60	0	0
30	J	33	Total 33	O 33	0	0
30	K	32	Total 32	O 32	0	0
30	L	31	Total 31	O 31	0	0
30	M	29	Total 29	O 29	0	0
30	N	239	Total 239	O 239	0	0
30	O	154	Total 154	O 154	0	0
30	P	131	Total 131	O 131	0	0
30	Q	91	Total 91	O 91	0	0
30	R	93	Total 93	O 93	0	0
30	S	108	Total 108	O 108	0	0
30	T	61	Total 61	O 61	0	0
30	U	50	Total 50	O 50	0	0
30	V	41	Total 41	O 41	0	0
30	W	39	Total 39	O 39	0	0
30	X	31	Total 31	O 31	0	0
30	Y	31	Total 31	O 31	0	0
30	Z	24	Total 24	O 24	0	0

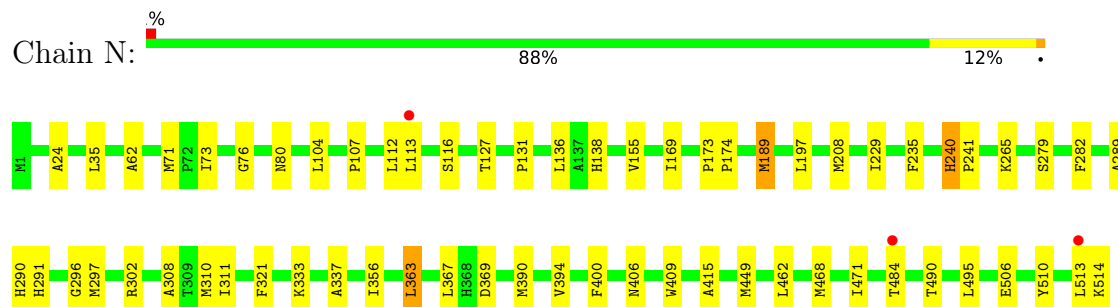
3 Residue-property plots

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.

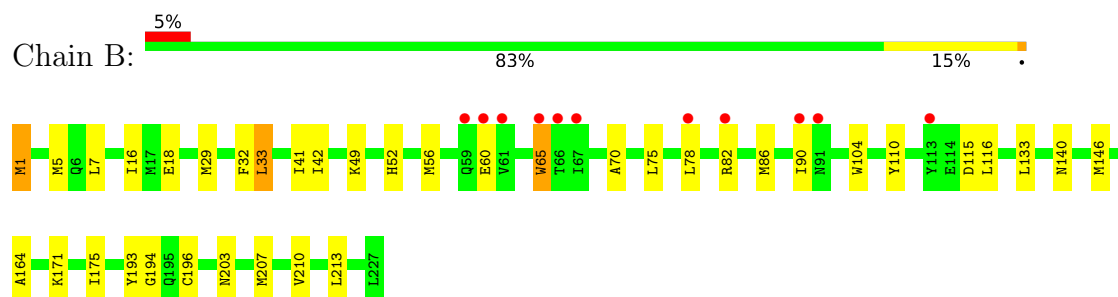
• Molecule 1: Cytochrome c oxidase subunit 1



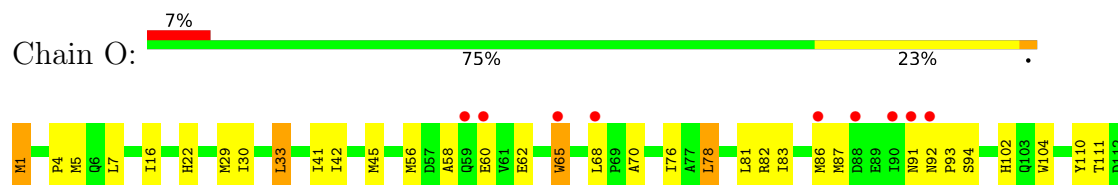
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2

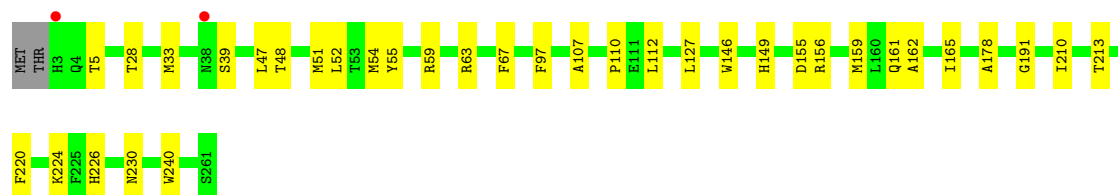
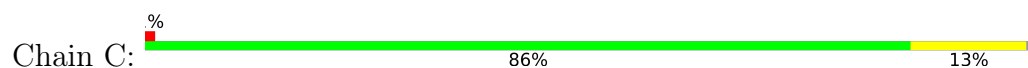


• Molecule 2: Cytochrome c oxidase subunit 2

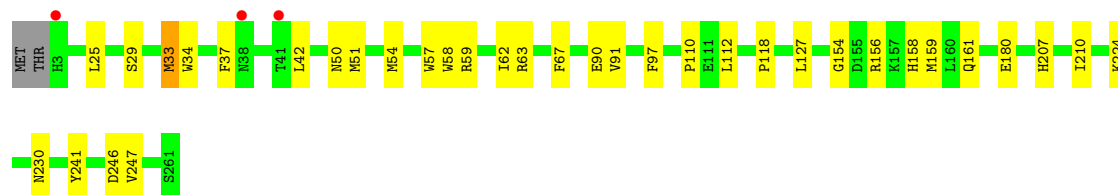
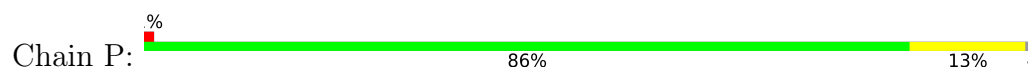




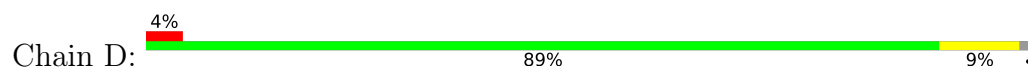
• Molecule 3: Cytochrome c oxidase subunit 3



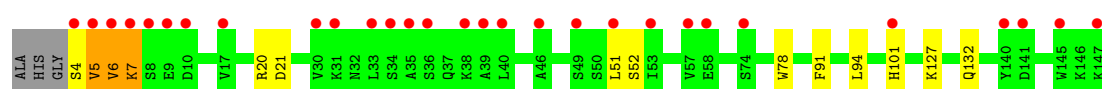
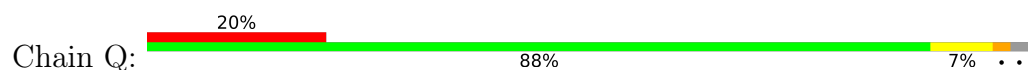
• Molecule 3: Cytochrome c oxidase subunit 3



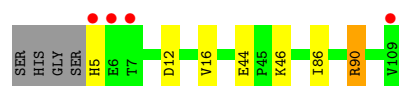
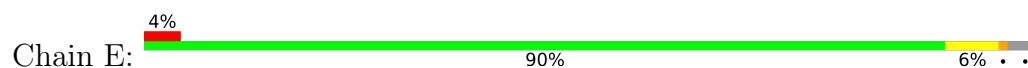
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



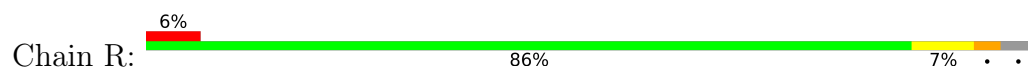
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



• Molecule 5: Cytochrome c oxidase subunit 5A

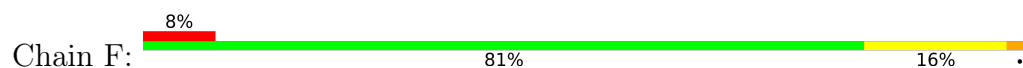


• Molecule 5: Cytochrome c oxidase subunit 5A

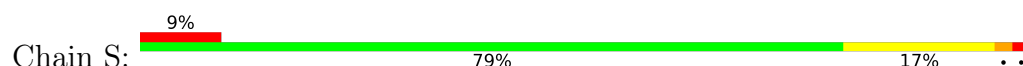




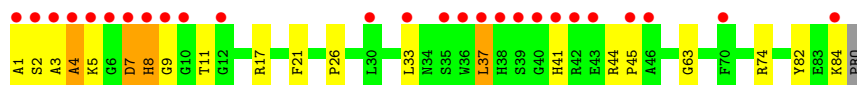
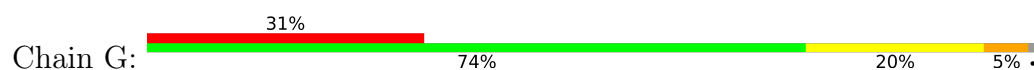
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



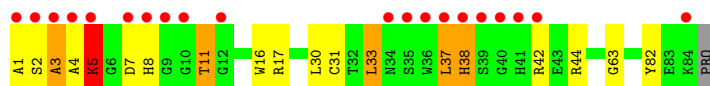
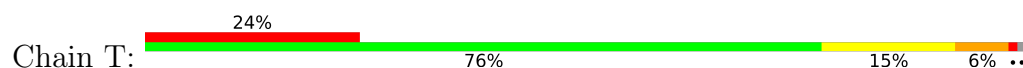
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



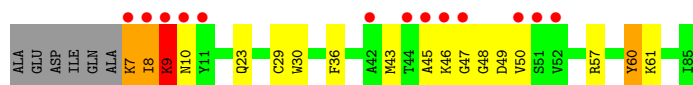
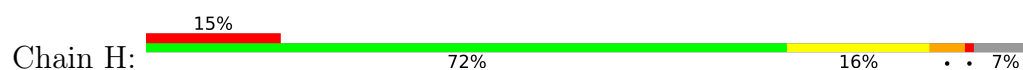
- Molecule 7: Cytochrome c oxidase subunit 6A2



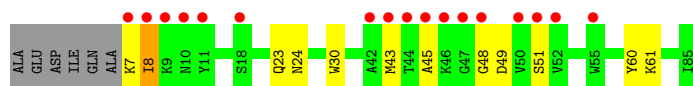
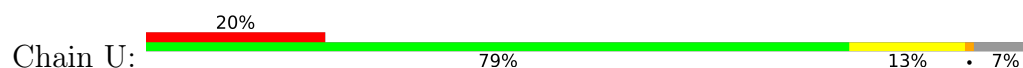
- Molecule 7: Cytochrome c oxidase subunit 6A2



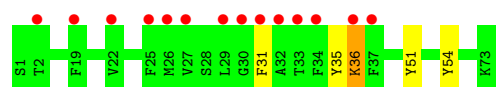
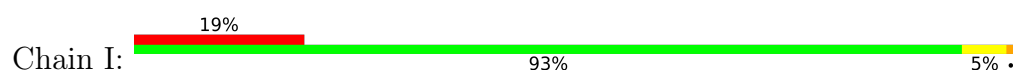
- Molecule 8: Cytochrome c oxidase subunit 6B1



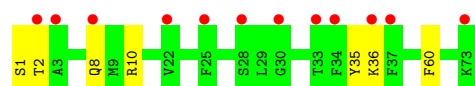
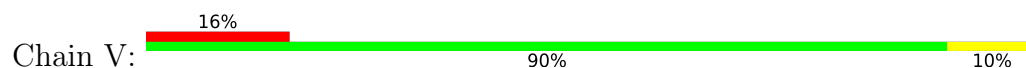
- Molecule 8: Cytochrome c oxidase subunit 6B1



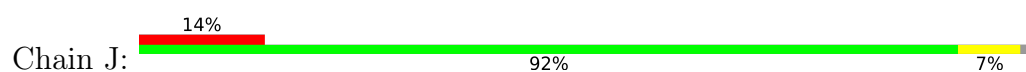
- Molecule 9: Cytochrome c oxidase subunit 6C



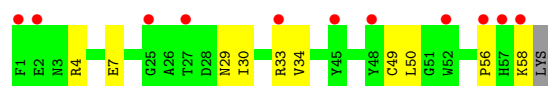
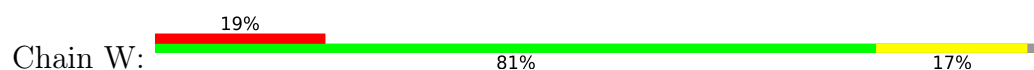
- Molecule 9: Cytochrome c oxidase subunit 6C



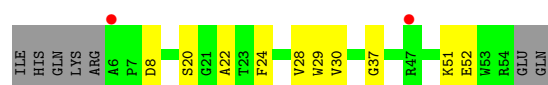
- Molecule 10: Cytochrome c oxidase subunit 7A1



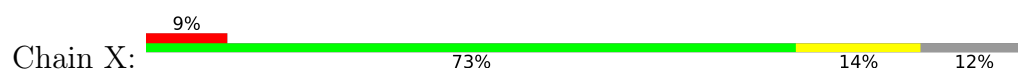
- Molecule 10: Cytochrome c oxidase subunit 7A1



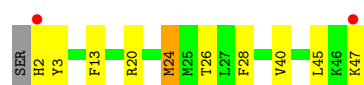
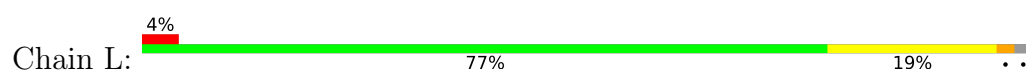
- Molecule 11: Cytochrome c oxidase subunit 7B



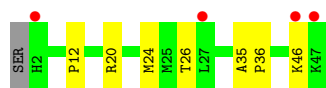
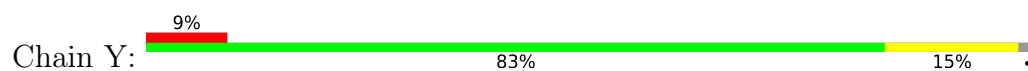
- Molecule 11: Cytochrome c oxidase subunit 7B



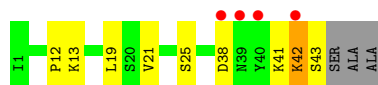
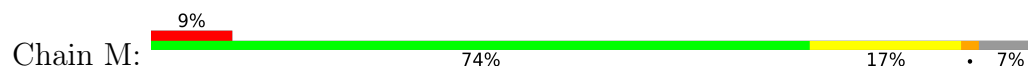
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



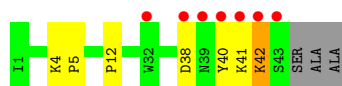
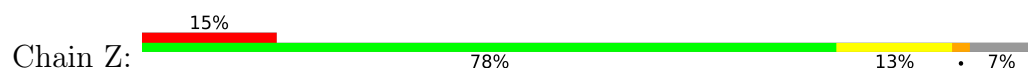
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.60Å 204.51Å 178.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.31 – 1.90 27.31 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (27.31-1.90) 96.0 (27.31-1.90)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.89Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.185 , 0.227 0.185 , 0.227	Depositor DCC
R_{free} test set	25229 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 83.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34120	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PSC, MG, CDL, FME, EDO, HEA, NA, SAC, CUA, DMU, PEK, PGV, TPO, PO4, CU, PER, TGL, ZN, CHD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.97	0/4233	0.87	2/5782 (0.0%)
1	N	0.89	0/4211	0.84	1/5752 (0.0%)
2	B	0.80	0/1885	0.87	1/2567 (0.0%)
2	O	0.71	0/1900	0.82	1/2587 (0.0%)
3	C	0.85	0/2221	0.74	0/3035
3	P	0.79	0/2213	0.74	0/3025
4	D	0.77	0/1241	0.75	0/1674
4	Q	0.54	0/1229	0.65	0/1658
5	E	0.76	0/871	0.70	0/1182
5	R	0.62	0/882	0.68	0/1196
6	F	0.74	0/772	0.85	0/1048
6	S	0.72	0/765	0.89	3/1038 (0.3%)
7	G	0.71	0/690	0.75	0/937
7	T	0.64	0/690	0.79	0/937
8	H	0.68	0/682	0.74	0/921
8	U	0.58	0/682	0.72	0/921
9	I	0.58	0/605	0.70	0/802
9	V	0.51	0/605	0.69	0/802
10	J	0.58	0/471	0.72	0/636
10	W	0.60	0/471	0.70	0/636
11	K	0.62	0/398	0.66	0/546
11	X	0.43	0/398	0.63	0/546
12	L	0.80	0/401	0.78	0/536
12	Y	0.65	0/393	0.67	0/526
13	M	0.67	0/345	0.72	0/470
13	Z	0.55	0/345	0.55	0/470
All	All	0.78	0/29599	0.78	8/40230 (0.0%)

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	N	0	1
6	F	0	1
6	S	0	2
8	H	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	HIS	CA-CB-CG	-6.54	107.26	113.80
6	S	95	GLN	CA-C-N	6.28	133.01	121.70
6	S	95	GLN	C-N-CA	6.28	133.01	121.70
2	O	65	TRP	CA-CB-CG	6.22	125.42	113.60
2	B	65	TRP	CA-CB-CG	5.41	123.88	113.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	94	HIS	Peptide
8	H	9	LYS	Peptide
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide
6	S	94	HIS	Peptide

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	4051	0	4040	57	0
1	N	4046	0	4040	54	0
2	B	1834	0	1840	31	0
2	O	1844	0	1852	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2117	0	2034	41	0
3	P	2115	0	2033	45	0
4	D	1201	0	1188	16	0
4	Q	1195	0	1183	16	0
5	E	852	0	845	4	0
5	R	860	0	858	7	0
6	F	750	0	731	20	0
6	S	748	0	728	21	0
7	G	675	0	643	18	0
7	T	675	0	643	23	0
8	H	662	0	623	10	0
8	U	662	0	623	11	0
9	I	601	0	613	4	0
9	V	601	0	613	4	0
10	J	460	0	459	5	0
10	W	460	0	459	6	0
11	K	384	0	366	9	0
11	X	384	0	366	9	0
12	L	383	0	389	15	0
12	Y	380	0	380	9	0
13	M	335	0	352	7	0
13	Z	335	0	352	6	0
14	A	129	0	88	2	0
14	N	129	0	88	4	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	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	1	0
19	A	102	0	152	9	0
19	C	102	0	152	6	0
19	N	51	0	76	6	0
19	P	153	0	228	9	0
20	A	28	0	42	5	0
20	B	8	0	12	0	0
20	C	8	0	12	1	0
20	F	16	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	G	4	0	6	0	0
20	L	8	0	12	0	0
20	M	4	0	6	1	0
20	N	48	0	72	9	0
20	O	8	0	12	0	0
20	P	20	0	30	1	0
20	Q	4	0	6	1	0
20	R	4	0	6	0	0
20	S	24	0	36	5	0
20	W	8	0	12	6	0
20	Y	4	0	6	1	0
21	A	33	0	42	1	0
21	B	33	0	41	0	0
21	C	33	0	42	0	0
21	D	33	0	42	1	0
21	G	33	0	42	2	0
21	K	198	0	252	12	0
21	L	33	0	42	3	0
21	M	33	0	42	1	0
21	O	33	0	42	2	0
21	P	66	0	84	10	0
21	Q	33	0	41	1	0
21	T	33	0	42	2	0
21	X	99	0	135	4	0
21	Z	33	0	42	0	0
22	B	63	0	110	6	0
22	D	63	0	110	10	0
22	L	63	0	108	12	0
22	O	63	0	110	1	0
22	Q	63	0	110	6	0
22	Y	63	0	110	7	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	52	0	80	9	0
24	N	52	0	80	12	0
25	C	159	0	231	20	0
25	G	53	0	77	4	0
25	P	106	0	154	8	0
26	C	100	0	156	24	0
26	G	100	0	156	21	0
26	P	100	0	156	17	0
26	T	100	0	156	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	C	58	0	78	1	0
27	G	29	0	39	0	0
27	J	29	0	39	4	0
27	L	29	0	39	1	0
27	P	58	0	78	3	0
27	T	29	0	39	0	0
27	W	29	0	38	1	0
27	X	29	0	39	5	0
27	Y	29	0	39	3	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	263	0	0	3	0
30	B	176	0	0	2	0
30	C	128	0	0	2	0
30	D	154	0	0	3	0
30	E	124	0	0	1	0
30	F	114	0	0	1	0
30	G	69	0	0	5	0
30	H	69	0	0	1	0
30	I	60	0	0	0	0
30	J	33	0	0	1	0
30	K	32	0	0	1	0
30	L	31	0	0	1	0
30	M	29	0	0	0	0
30	N	239	0	0	5	0
30	O	154	0	0	3	0
30	P	131	0	0	3	0
30	Q	91	0	0	4	0
30	R	93	0	0	0	0
30	S	108	0	0	2	0
30	T	61	0	0	0	0
30	U	50	0	0	0	0
30	V	41	0	0	2	0
30	W	39	0	0	1	0
30	X	31	0	0	3	0
30	Y	31	0	0	1	0
30	Z	24	0	0	0	0
All	All	34120	0	32594	541	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 8.

The worst 5 of 541 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:606:PER:O2	18:A:606:PER:O1	1.55	1.23
18:N:606:PER:O2	18:N:606:PER:O1	1.55	1.20
20:N:613:EDO:H21	6:S:36:PRO:HD3	1.38	1.03
25:C:307:PEK:H041	7:G:17:ARG:HH22	1.23	1.03
3:C:67:PHE:HE1	26:C:304:CDL:H1	1.26	0.96

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	522/514 (102%)	508 (97%)	14 (3%)	0	100	100
1	N	519/514 (101%)	505 (97%)	14 (3%)	0	100	100
2	B	228/227 (100%)	220 (96%)	8 (4%)	0	100	100
2	O	229/227 (101%)	219 (96%)	9 (4%)	1 (0%)	30	22
3	C	260/261 (100%)	254 (98%)	6 (2%)	0	100	100
3	P	259/261 (99%)	254 (98%)	5 (2%)	0	100	100
4	D	143/147 (97%)	139 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	136 (96%)	5 (4%)	1 (1%)	18	10
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	104/109 (95%)	104 (100%)	0	0	100	100
6	F	97/98 (99%)	93 (96%)	2 (2%)	2 (2%)	5	1
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	3	0
7	G	81/85 (95%)	71 (88%)	5 (6%)	5 (6%)	1	0
7	T	81/85 (95%)	70 (86%)	7 (9%)	4 (5%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	2	0
8	U	77/85 (91%)	69 (90%)	6 (8%)	2 (3%)	4	1
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	47 (100%)	0	0	100	100
12	L	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	4	1
13	Z	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	4	1
All	All	3537/3614 (98%)	3411 (96%)	103 (3%)	23 (1%)	18	10

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	8	HIS
8	H	8	ILE
6	S	94	HIS
7	T	5	LYS

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	436/426 (102%)	430 (99%)	6 (1%)	59	59
1	N	433/426 (102%)	426 (98%)	7 (2%)	55	54
2	B	213/210 (101%)	203 (95%)	10 (5%)	23	15
2	O	214/210 (102%)	205 (96%)	9 (4%)	26	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	227/226 (100%)	225 (99%)	2 (1%)	70	73
3	P	226/226 (100%)	222 (98%)	4 (2%)	51	50
4	D	129/129 (100%)	127 (98%)	2 (2%)	55	54
4	Q	128/129 (99%)	125 (98%)	3 (2%)	44	40
5	E	92/95 (97%)	90 (98%)	2 (2%)	45	42
5	R	93/95 (98%)	88 (95%)	5 (5%)	20	12
6	F	82/81 (101%)	79 (96%)	3 (4%)	30	22
6	S	81/81 (100%)	79 (98%)	2 (2%)	42	37
7	G	67/68 (98%)	66 (98%)	1 (2%)	57	56
7	T	67/68 (98%)	62 (92%)	5 (8%)	12	6
8	H	71/75 (95%)	66 (93%)	5 (7%)	14	7
8	U	71/75 (95%)	70 (99%)	1 (1%)	59	59
9	I	57/57 (100%)	56 (98%)	1 (2%)	51	50
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	12
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	46
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	46
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	40/40 (100%)	37 (92%)	3 (8%)	12	6
12	Y	39/40 (98%)	38 (97%)	1 (3%)	40	35
13	M	37/38 (97%)	35 (95%)	2 (5%)	20	12
13	Z	37/38 (97%)	35 (95%)	2 (5%)	20	12
All	All	3073/3082 (100%)	2992 (97%)	81 (3%)	40	35

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	230	ASN
7	T	38	HIS
4	Q	7	LYS
5	R	109	VAL
9	V	8	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	103	GLN
6	S	28	GLN
11	X	35	GLN
4	Q	76	ASN
6	S	95	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	0.45	0	8,9,11	0.97	0
1	FME	A	1	1	8,9,10	0.40	0	8,9,11	1.32	1 (12%)
7	TPO	T	11	7	8,10,11	1.62	1 (12%)	10,14,16	1.41	1 (10%)
2	FME	B	1	2	8,9,10	0.91	0	8,9,11	1.97	4 (50%)
9	SAC	I	1	9	7,8,9	0.60	0	7,9,11	0.82	0
2	FME	O	1	2	8,9,10	0.80	0	8,9,11	1.61	1 (12%)
7	TPO	G	11	7	8,10,11	1.29	1 (12%)	10,14,16	1.15	0
9	SAC	V	1	9	7,8,9	0.60	0	7,9,11	0.91	1 (14%)

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	-	2/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TPO	T	11	7	-	6/9/11/13	-
2	FME	B	1	2	-	2/7/9/11	-
9	SAC	I	1	9	-	1/7/8/10	-
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
9	SAC	V	1	9	-	4/7/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	3.50	1.61	1.50
7	G	11	TPO	P-O1P	2.57	1.58	1.50

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	11	TPO	CG2-CB-CA	3.95	120.96	113.26
2	O	1	FME	CG-CB-CA	-3.46	102.27	112.87
2	B	1	FME	O-C-CA	-2.85	117.45	124.77
1	A	1	FME	C-CA-N	2.85	114.99	109.50
2	B	1	FME	C-CA-N	-2.54	104.60	109.50

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
9	I	1	SAC	O-C-CA-CB
1	N	1	FME	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	2	0
7	T	11	TPO	1	0
2	B	1	FME	2	0
2	O	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 131 ligands modelled in this entry, 10 are monoatomic - leaving 121 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	EDO	S	104	-	3,3,3	0.51	0	2,2,2	0.53	0
20	EDO	P	312	-	3,3,3	0.47	0	2,2,2	1.13	0
20	EDO	N	610	-	3,3,3	0.78	0	2,2,2	0.39	0
27	CHD	L	103	-	32,32,32	0.70	0	51,51,51	2.72	20 (39%)
20	EDO	N	615	-	3,3,3	0.35	0	2,2,2	0.80	0
22	TGL	Y	101	-	62,62,62	1.12	3 (4%)	65,65,65	1.42	7 (10%)
19	PGV	C	308	-	50,50,50	1.09	2 (4%)	53,56,56	1.67	8 (15%)
20	EDO	F	104	-	3,3,3	0.32	0	2,2,2	0.63	0
21	DMU	L	102	-	34,34,34	0.54	1 (2%)	45,45,45	1.07	2 (4%)
29	PO4	U	101	-	4,4,4	1.06	0	6,6,6	0.61	0
22	TGL	D	201	-	62,62,62	1.17	4 (6%)	65,65,65	1.05	5 (7%)
20	EDO	W	102	-	3,3,3	0.41	0	2,2,2	0.33	0
18	PER	A	606	14,15	1,1,1	0.90	0	-	-	-
24	PSC	N	608	-	51,51,51	1.16	3 (5%)	57,59,59	1.55	7 (12%)
23	CUA	O	302	2	0,1,1	-	-	-	-	-
20	EDO	A	610	-	3,3,3	0.59	0	2,2,2	0.58	0
25	PEK	C	302	-	52,52,52	0.98	2 (3%)	55,57,57	1.14	4 (7%)
25	PEK	P	309	-	52,52,52	1.06	2 (3%)	55,57,57	1.52	4 (7%)
20	EDO	N	619	-	3,3,3	0.48	0	2,2,2	0.10	0
19	PGV	P	302	-	50,50,50	1.03	2 (4%)	53,56,56	1.28	6 (11%)
20	EDO	P	315	-	3,3,3	0.35	0	2,2,2	1.05	0
26	CDL	C	304	-	99,99,99	1.46	13 (13%)	105,111,111	1.44	12 (11%)
20	EDO	S	106	-	3,3,3	0.64	0	2,2,2	0.69	0
26	CDL	P	306	-	99,99,99	1.47	12 (12%)	105,111,111	1.54	19 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CDL	T	102	-	99,99,99	1.40	12 (12%)	105,111,111	1.33	7 (6%)
20	EDO	A	612	-	3,3,3	0.33	0	2,2,2	0.30	0
20	EDO	F	105	-	3,3,3	0.47	0	2,2,2	0.72	0
21	DMU	K	104	-	34,34,34	0.52	0	45,45,45	1.20	6 (13%)
20	EDO	C	311	-	3,3,3	0.33	0	2,2,2	0.79	0
21	DMU	A	616	-	34,34,34	0.48	0	45,45,45	1.09	3 (6%)
27	CHD	P	307	-	32,32,32	0.75	0	51,51,51	1.45	10 (19%)
27	CHD	C	305	-	32,32,32	0.83	1 (3%)	51,51,51	1.40	8 (15%)
14	HEA	N	602	1,18	67,67,67	1.92	23 (34%)	81,103,103	1.94	25 (30%)
14	HEA	N	601[B]	-	67,67,67	1.65	17 (25%)	81,103,103	1.82	21 (25%)
27	CHD	G	103	-	32,32,32	0.98	2 (6%)	51,51,51	1.52	9 (17%)
19	PGV	N	607	-	50,50,50	0.98	2 (4%)	53,56,56	1.31	8 (15%)
21	DMU	P	316	-	34,34,34	0.79	1 (2%)	45,45,45	2.40	16 (35%)
22	TGL	L	101	-	62,62,62	1.17	4 (6%)	65,65,65	1.58	8 (12%)
20	EDO	N	617	-	3,3,3	0.33	0	2,2,2	1.09	0
25	PEK	C	307	-	52,52,52	1.00	2 (3%)	55,57,57	1.53	8 (14%)
27	CHD	P	308	-	32,32,32	0.72	0	51,51,51	1.35	6 (11%)
21	DMU	Z	101	-	34,34,34	0.60	1 (2%)	45,45,45	0.97	3 (6%)
20	EDO	A	613	-	3,3,3	0.73	0	2,2,2	0.11	0
20	EDO	N	612	-	3,3,3	0.50	0	2,2,2	0.05	0
22	TGL	Q	201	-	62,62,62	1.07	3 (4%)	65,65,65	1.00	5 (7%)
20	EDO	S	103	-	3,3,3	0.60	0	2,2,2	0.13	0
25	PEK	C	309	-	52,52,52	1.01	2 (3%)	55,57,57	1.40	6 (10%)
20	EDO	Y	103	-	3,3,3	0.39	0	2,2,2	0.17	0
21	DMU	D	202	-	34,34,34	0.53	0	45,45,45	1.10	3 (6%)
25	PEK	P	304	-	52,52,52	0.85	2 (3%)	55,57,57	1.24	5 (9%)
27	CHD	Y	102	-	32,32,32	0.73	0	51,51,51	2.17	15 (29%)
20	EDO	N	614	-	3,3,3	0.57	0	2,2,2	0.12	0
14	HEA	A	601[B]	-	67,67,67	1.91	23 (34%)	81,103,103	1.82	27 (33%)
20	EDO	R	201	-	3,3,3	0.34	0	2,2,2	0.34	0
18	PER	N	606	14,15	1,1,1	0.91	0	-		
20	EDO	L	105	-	3,3,3	0.46	0	2,2,2	0.25	0
26	CDL	G	101	-	99,99,99	1.43	12 (12%)	105,111,111	1.48	13 (12%)
20	EDO	B	304	-	3,3,3	0.61	0	2,2,2	0.25	0
27	CHD	W	101	-	32,32,32	0.78	0	51,51,51	2.35	17 (33%)
21	DMU	X	102	-	22,22,34	0.70	1 (4%)	27,27,45	1.60	6 (22%)
14	HEA	N	601[A]	-	67,67,67	1.67	17 (25%)	81,103,103	1.83	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	DMU	T	103	-	34,34,34	0.56	0	45,45,45	1.23	7 (15%)
27	CHD	J	101	-	32,32,32	0.63	0	51,51,51	2.36	20 (39%)
20	EDO	N	613	-	3,3,3	0.36	0	2,2,2	0.42	0
19	PGV	A	607	-	50,50,50	1.03	2 (4%)	53,56,56	1.27	4 (7%)
22	TGL	O	301	-	62,62,62	1.12	3 (4%)	65,65,65	1.16	5 (7%)
21	DMU	K	106	-	34,34,34	0.55	1 (2%)	45,45,45	1.46	6 (13%)
27	CHD	T	101	-	32,32,32	0.86	1 (3%)	51,51,51	1.56	10 (19%)
20	EDO	C	310	-	3,3,3	0.72	0	2,2,2	0.55	0
19	PGV	C	303	-	50,50,50	0.84	2 (4%)	53,56,56	1.07	4 (7%)
22	TGL	B	301	-	62,62,62	1.09	3 (4%)	65,65,65	1.26	4 (6%)
20	EDO	M	102	-	3,3,3	0.35	0	2,2,2	0.42	0
20	EDO	S	105	-	3,3,3	0.48	0	2,2,2	0.21	0
21	DMU	K	101	-	34,34,34	0.54	1 (2%)	45,45,45	1.55	10 (22%)
20	EDO	P	310	-	3,3,3	0.60	0	2,2,2	0.15	0
20	EDO	O	304	-	3,3,3	0.59	0	2,2,2	0.27	0
20	EDO	N	616	-	3,3,3	0.44	0	2,2,2	0.46	0
20	EDO	N	609	-	3,3,3	0.78	0	2,2,2	0.67	0
29	PO4	H	101	-	4,4,4	0.87	0	6,6,6	0.45	0
14	HEA	A	601[A]	-	67,67,67	1.91	23 (34%)	81,103,103	1.83	26 (32%)
21	DMU	C	312	-	34,34,34	0.48	0	45,45,45	1.46	8 (17%)
20	EDO	F	103	-	3,3,3	0.64	0	2,2,2	0.62	0
27	CHD	X	105	-	32,32,32	0.77	0	51,51,51	1.68	13 (25%)
20	EDO	A	611	-	3,3,3	0.37	0	2,2,2	0.14	0
24	PSC	B	303	-	51,51,51	1.10	3 (5%)	57,59,59	1.42	7 (12%)
21	DMU	P	314	-	34,34,34	0.56	0	45,45,45	1.35	4 (8%)
20	EDO	F	102	-	3,3,3	0.48	0	2,2,2	0.84	0
20	EDO	A	615	-	3,3,3	0.87	0	2,2,2	0.62	0
20	EDO	A	609	-	3,3,3	0.40	0	2,2,2	0.83	0
20	EDO	L	104	-	3,3,3	0.48	0	2,2,2	0.43	0
21	DMU	X	101	-	34,34,34	0.59	1 (2%)	45,45,45	1.79	10 (22%)
20	EDO	N	618	-	3,3,3	0.33	0	2,2,2	0.51	0
25	PEK	G	102	-	52,52,52	1.03	2 (3%)	55,57,57	1.07	4 (7%)
23	CUA	B	302	2	0,1,1	-	-	-	-	-
20	EDO	S	107	-	3,3,3	0.38	0	2,2,2	0.45	0
21	DMU	G	104	-	34,34,34	0.57	0	45,45,45	1.47	8 (17%)
21	DMU	M	101	-	34,34,34	0.46	0	45,45,45	1.17	4 (8%)
20	EDO	P	311	-	3,3,3	0.59	0	2,2,2	0.08	0
20	EDO	S	102	-	3,3,3	0.81	0	2,2,2	0.37	0
20	EDO	Q	202	-	3,3,3	0.38	0	2,2,2	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	A	602	1,18	67,67,67	1.71	19 (28%)	81,103,103	1.82	26 (32%)
19	PGV	P	305	-	50,50,50	0.83	2 (4%)	53,56,56	1.13	4 (7%)
21	DMU	K	102	-	34,34,34	0.56	1 (2%)	45,45,45	1.41	7 (15%)
20	EDO	N	620	-	3,3,3	0.37	0	2,2,2	0.37	0
21	DMU	X	104	-	22,22,34	0.52	0	27,27,45	0.60	0
20	EDO	O	303	-	3,3,3	0.71	0	2,2,2	0.63	0
20	EDO	N	611	-	3,3,3	0.46	0	2,2,2	0.31	0
20	EDO	A	614	-	3,3,3	0.56	0	2,2,2	0.14	0
19	PGV	P	301	-	50,50,50	0.99	2 (4%)	53,56,56	1.30	4 (7%)
20	EDO	G	105	-	3,3,3	0.49	0	2,2,2	0.08	0
20	EDO	B	305	-	3,3,3	0.44	0	2,2,2	0.47	0
21	DMU	X	103	-	22,22,34	0.55	0	27,27,45	0.66	0
21	DMU	B	306	-	34,34,34	0.85	1 (2%)	45,45,45	2.61	17 (37%)
20	EDO	P	313	-	3,3,3	0.46	0	2,2,2	0.50	0
21	DMU	O	305	-	34,34,34	0.55	0	45,45,45	1.71	12 (26%)
19	PGV	A	608	-	50,50,50	1.07	2 (4%)	53,56,56	1.13	4 (7%)
21	DMU	Q	203	-	34,34,34	0.78	1 (2%)	45,45,45	2.66	18 (40%)
21	DMU	K	103	-	34,34,34	0.53	0	45,45,45	1.35	6 (13%)
21	DMU	K	105	-	34,34,34	0.49	0	45,45,45	1.33	6 (13%)
27	CHD	C	306	-	32,32,32	0.94	1 (3%)	51,51,51	1.38	7 (13%)
20	EDO	W	103	-	3,3,3	0.53	0	2,2,2	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	S	104	-	-	1/1/1/1	-
20	EDO	P	312	-	-	1/1/1/1	-
20	EDO	N	610	-	-	0/1/1/1	-
27	CHD	L	103	-	-	5/9/74/74	0/4/4/4
20	EDO	N	615	-	-	1/1/1/1	-
22	TGL	Y	101	-	-	29/65/65/65	-
19	PGV	C	308	-	-	20/55/55/55	-
20	EDO	F	104	-	-	1/1/1/1	-
21	DMU	L	102	-	-	9/19/59/59	0/2/2/2
22	TGL	D	201	-	-	26/65/65/65	-
20	EDO	W	102	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSC	N	608	-	-	27/55/55/55	-
20	EDO	A	610	-	-	0/1/1/1	-
25	PEK	C	302	-	-	14/56/56/56	-
25	PEK	P	309	-	-	30/56/56/56	-
20	EDO	N	619	-	-	0/1/1/1	-
19	PGV	P	302	-	-	18/55/55/55	-
20	EDO	P	315	-	-	1/1/1/1	-
26	CDL	C	304	-	-	45/110/110/110	-
20	EDO	S	106	-	-	0/1/1/1	-
26	CDL	P	306	-	-	43/110/110/110	-
26	CDL	T	102	-	-	42/110/110/110	-
20	EDO	A	612	-	-	0/1/1/1	-
20	EDO	F	105	-	-	0/1/1/1	-
21	DMU	K	104	-	-	12/19/59/59	0/2/2/2
20	EDO	C	311	-	-	1/1/1/1	-
21	DMU	A	616	-	-	8/19/59/59	0/2/2/2
27	CHD	P	307	-	-	5/9/74/74	0/4/4/4
27	CHD	C	305	-	-	5/9/74/74	0/4/4/4
14	HEA	N	602	1,18	-	6/36/76/76	-
14	HEA	N	601[B]	-	-	9/36/76/76	-
27	CHD	G	103	-	-	2/9/74/74	0/4/4/4
19	PGV	N	607	-	-	22/55/55/55	-
21	DMU	P	316	-	-	14/19/59/59	0/2/2/2
22	TGL	L	101	-	-	34/65/65/65	-
20	EDO	N	617	-	-	1/1/1/1	-
25	PEK	C	307	-	-	26/56/56/56	-
27	CHD	P	308	-	-	2/9/74/74	0/4/4/4
21	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
20	EDO	A	613	-	-	0/1/1/1	-
20	EDO	N	612	-	-	0/1/1/1	-
22	TGL	Q	201	-	-	32/65/65/65	-
20	EDO	S	103	-	-	0/1/1/1	-
25	PEK	C	309	-	-	22/56/56/56	-
20	EDO	Y	103	-	-	0/1/1/1	-
21	DMU	D	202	-	-	8/19/59/59	0/2/2/2
25	PEK	P	304	-	-	6/56/56/56	-
27	CHD	Y	102	-	-	0/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	614	-	-	0/1/1/1	-
14	HEA	A	601[B]	-	-	9/36/76/76	-
20	EDO	R	201	-	-	0/1/1/1	-
20	EDO	L	105	-	-	0/1/1/1	-
26	CDL	G	101	-	-	38/110/110/110	-
20	EDO	B	304	-	-	0/1/1/1	-
27	CHD	W	101	-	-	6/9/74/74	0/4/4/4
21	DMU	X	102	-	-	8/13/33/59	0/1/1/2
14	HEA	N	601[A]	-	-	6/36/76/76	-
21	DMU	T	103	-	-	8/19/59/59	0/2/2/2
27	CHD	J	101	-	-	7/9/74/74	0/4/4/4
20	EDO	N	613	-	-	1/1/1/1	-
19	PGV	A	607	-	-	5/55/55/55	-
22	TGL	O	301	-	-	30/65/65/65	-
21	DMU	K	106	-	-	10/19/59/59	0/2/2/2
27	CHD	T	101	-	-	2/9/74/74	0/4/4/4
20	EDO	C	310	-	-	0/1/1/1	-
19	PGV	C	303	-	-	14/55/55/55	-
22	TGL	B	301	-	-	27/65/65/65	-
20	EDO	M	102	-	-	1/1/1/1	-
20	EDO	S	105	-	-	0/1/1/1	-
21	DMU	K	101	-	-	7/19/59/59	0/2/2/2
20	EDO	P	310	-	-	0/1/1/1	-
20	EDO	O	304	-	-	1/1/1/1	-
20	EDO	N	616	-	-	1/1/1/1	-
20	EDO	N	609	-	-	0/1/1/1	-
14	HEA	A	601[A]	-	-	7/36/76/76	-
21	DMU	C	312	-	-	10/19/59/59	0/2/2/2
20	EDO	F	103	-	-	0/1/1/1	-
27	CHD	X	105	-	-	7/9/74/74	0/4/4/4
20	EDO	A	611	-	-	0/1/1/1	-
24	PSC	B	303	-	-	25/55/55/55	-
21	DMU	P	314	-	-	7/19/59/59	0/2/2/2
20	EDO	F	102	-	-	0/1/1/1	-
20	EDO	A	615	-	-	0/1/1/1	-
20	EDO	A	609	-	-	1/1/1/1	-
20	EDO	L	104	-	-	1/1/1/1	-
21	DMU	X	101	-	-	11/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	618	-	-	1/1/1/1	-
25	PEK	G	102	-	-	15/56/56/56	-
20	EDO	S	107	-	-	1/1/1/1	-
21	DMU	G	104	-	-	11/19/59/59	0/2/2/2
21	DMU	M	101	-	-	4/19/59/59	0/2/2/2
20	EDO	P	311	-	-	1/1/1/1	-
20	EDO	S	102	-	-	0/1/1/1	-
20	EDO	Q	202	-	-	1/1/1/1	-
14	HEA	A	602	1,18	-	7/36/76/76	-
19	PGV	P	305	-	-	5/55/55/55	-
21	DMU	K	102	-	-	11/19/59/59	0/2/2/2
20	EDO	N	620	-	-	1/1/1/1	-
21	DMU	X	104	-	-	6/13/33/59	0/1/1/2
20	EDO	O	303	-	-	0/1/1/1	-
20	EDO	N	611	-	-	0/1/1/1	-
20	EDO	A	614	-	-	1/1/1/1	-
19	PGV	P	301	-	-	8/55/55/55	-
20	EDO	G	105	-	-	0/1/1/1	-
20	EDO	B	305	-	-	0/1/1/1	-
21	DMU	X	103	-	-	6/13/33/59	0/1/1/2
21	DMU	B	306	-	-	14/19/59/59	0/2/2/2
20	EDO	P	313	-	-	0/1/1/1	-
21	DMU	O	305	-	-	10/19/59/59	0/2/2/2
19	PGV	A	608	-	-	22/55/55/55	-
21	DMU	Q	203	-	-	17/19/59/59	0/2/2/2
21	DMU	K	103	-	-	10/19/59/59	0/2/2/2
21	DMU	K	105	-	-	9/19/59/59	0/2/2/2
27	CHD	C	306	-	-	2/9/74/74	0/4/4/4
20	EDO	W	103	-	-	1/1/1/1	-

The worst 5 of 240 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	308	PGV	O03-C19	5.27	1.48	1.33
22	L	101	TGL	OG2-CB1	5.26	1.49	1.34
22	Y	101	TGL	OG2-CB1	5.15	1.48	1.34
22	O	301	TGL	OG3-CC1	5.05	1.48	1.33
19	A	608	PGV	O03-C19	5.04	1.48	1.33

The worst 5 of 614 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	306	DMU	O4-C7-C5	-7.16	93.49	110.38
26	G	101	CDL	OA6-CA5-C11	7.02	126.66	111.48
27	J	101	CHD	C10-C9-C8	6.85	119.48	111.84
21	B	306	DMU	C10-O1-C9	6.71	126.82	113.72
27	W	101	CHD	C13-C17-C20	6.50	127.36	119.48

There are no chirality outliers.

5 of 948 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C2A-C3A-CMA-OMA
14	A	601[B]	HEA	C2A-C3A-CMA-OMA
14	A	601[B]	HEA	C18-C19-C20-C21
14	N	602	HEA	C2A-C3A-CMA-OMA
19	A	608	PGV	C04-O12-P-O14

There are no ring outliers.

75 monomers are involved in 293 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	L	103	CHD	1	0
22	Y	101	TGL	7	0
19	C	308	PGV	3	0
21	L	102	DMU	3	0
22	D	201	TGL	10	0
20	W	102	EDO	3	0
18	A	606	PER	1	0
24	N	608	PSC	12	0
25	C	302	PEK	3	0
25	P	309	PEK	5	0
19	P	302	PGV	2	0
20	P	315	EDO	1	0
26	C	304	CDL	24	0
26	P	306	CDL	17	0
26	T	102	CDL	19	0
20	A	612	EDO	4	0
21	K	104	DMU	1	0
20	C	311	EDO	1	0
21	A	616	DMU	1	0
27	P	307	CHD	2	0
27	C	305	CHD	1	0

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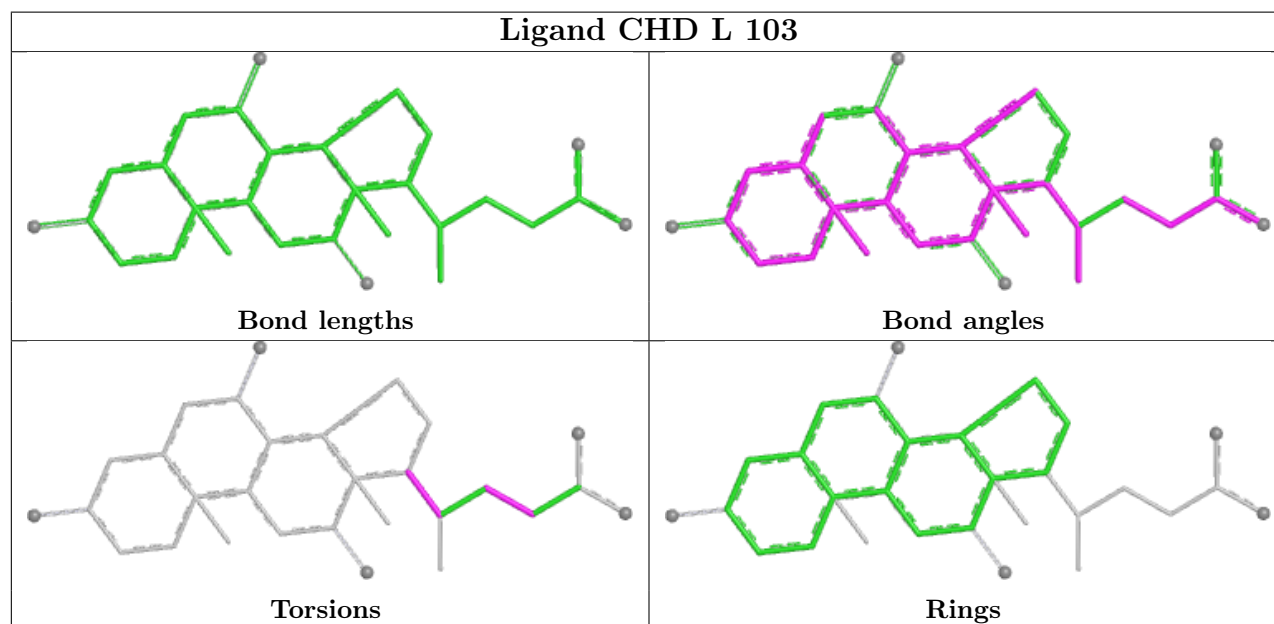
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	602	HEA	2	0
14	N	601[B]	HEA	1	0
19	N	607	PGV	6	0
21	P	316	DMU	10	0
22	L	101	TGL	12	0
20	N	617	EDO	2	0
25	C	307	PEK	13	0
27	P	308	CHD	1	0
20	N	612	EDO	1	0
22	Q	201	TGL	6	0
25	C	309	PEK	4	0
20	Y	103	EDO	1	0
21	D	202	DMU	1	0
25	P	304	PEK	3	0
27	Y	102	CHD	3	0
14	A	601[B]	HEA	1	0
18	N	606	PER	1	0
26	G	101	CDL	21	0
27	W	101	CHD	1	0
21	X	102	DMU	2	0
14	N	601[A]	HEA	1	0
21	T	103	DMU	2	0
27	J	101	CHD	4	0
20	N	613	EDO	4	0
19	A	607	PGV	1	0
22	O	301	TGL	1	0
21	K	106	DMU	1	0
19	C	303	PGV	3	0
22	B	301	TGL	6	0
20	M	102	EDO	1	0
20	S	105	EDO	1	0
21	K	101	DMU	3	0
20	N	616	EDO	1	0
14	A	601[A]	HEA	1	0
27	X	105	CHD	5	0
20	A	611	EDO	1	0
24	B	303	PSC	9	0
21	X	101	DMU	1	0
20	N	618	EDO	1	0
25	G	102	PEK	4	0
20	S	107	EDO	4	0
21	G	104	DMU	2	0

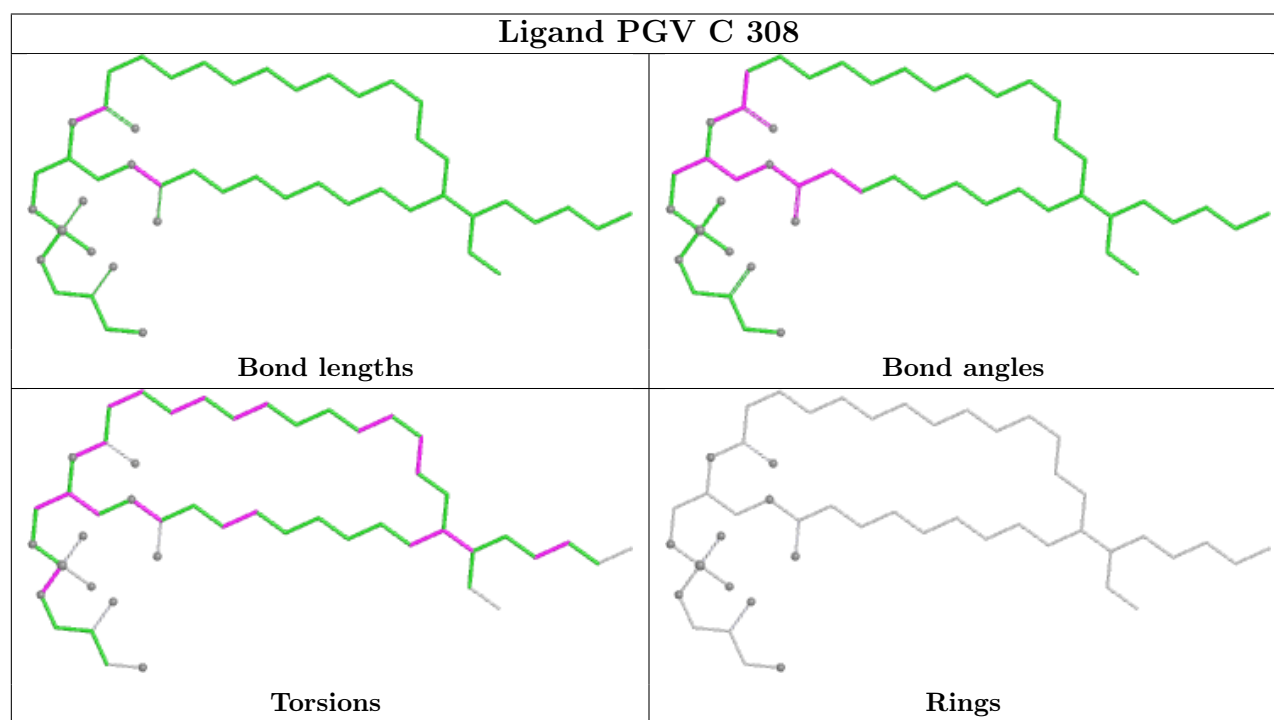
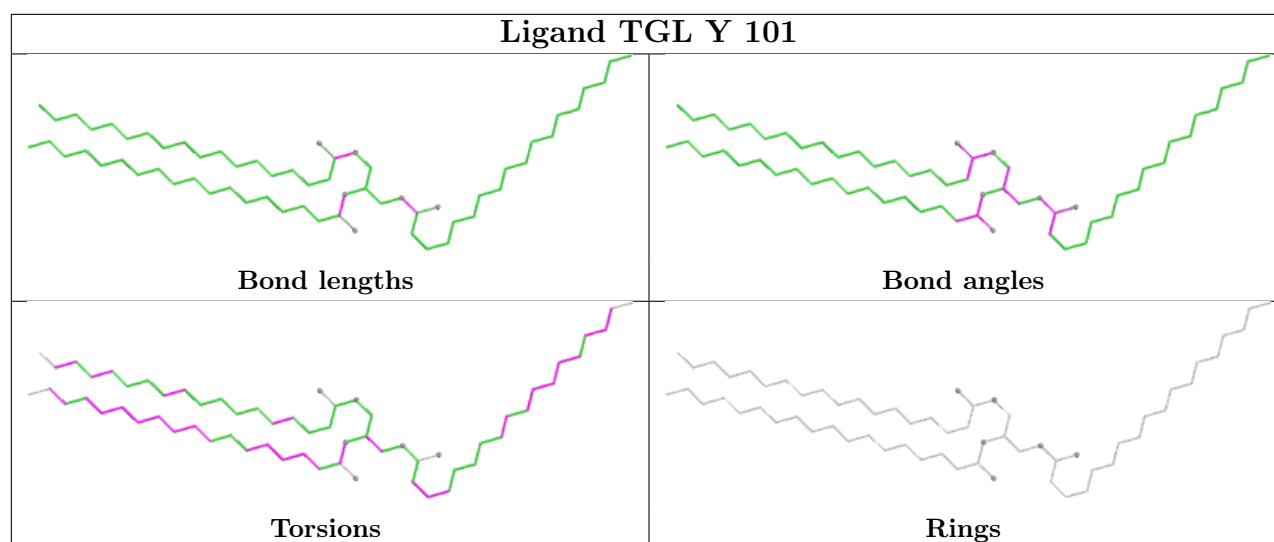
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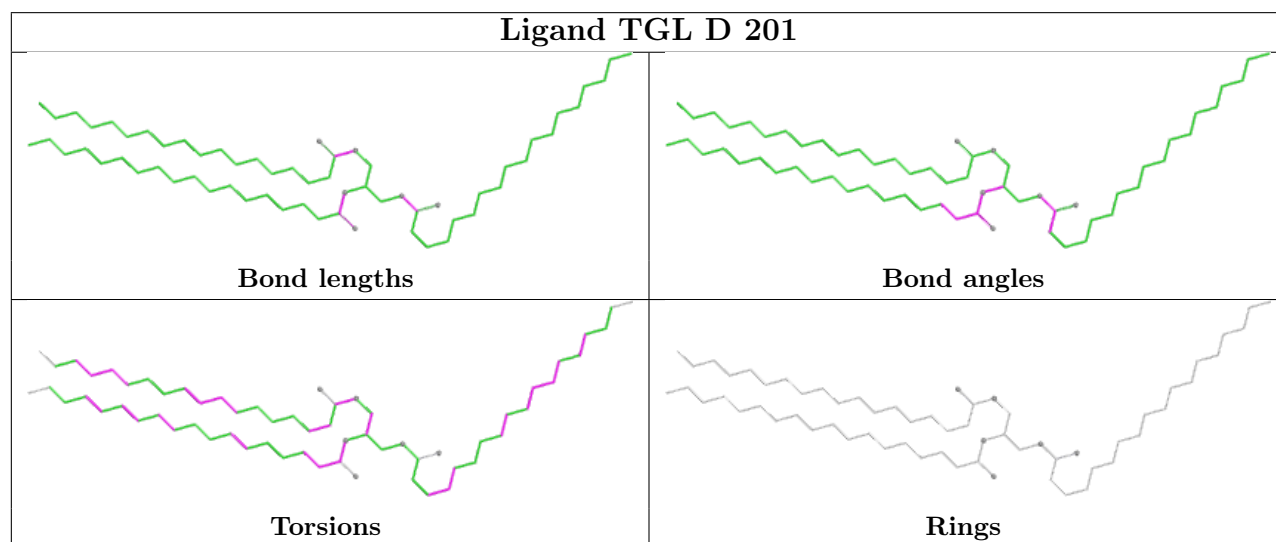
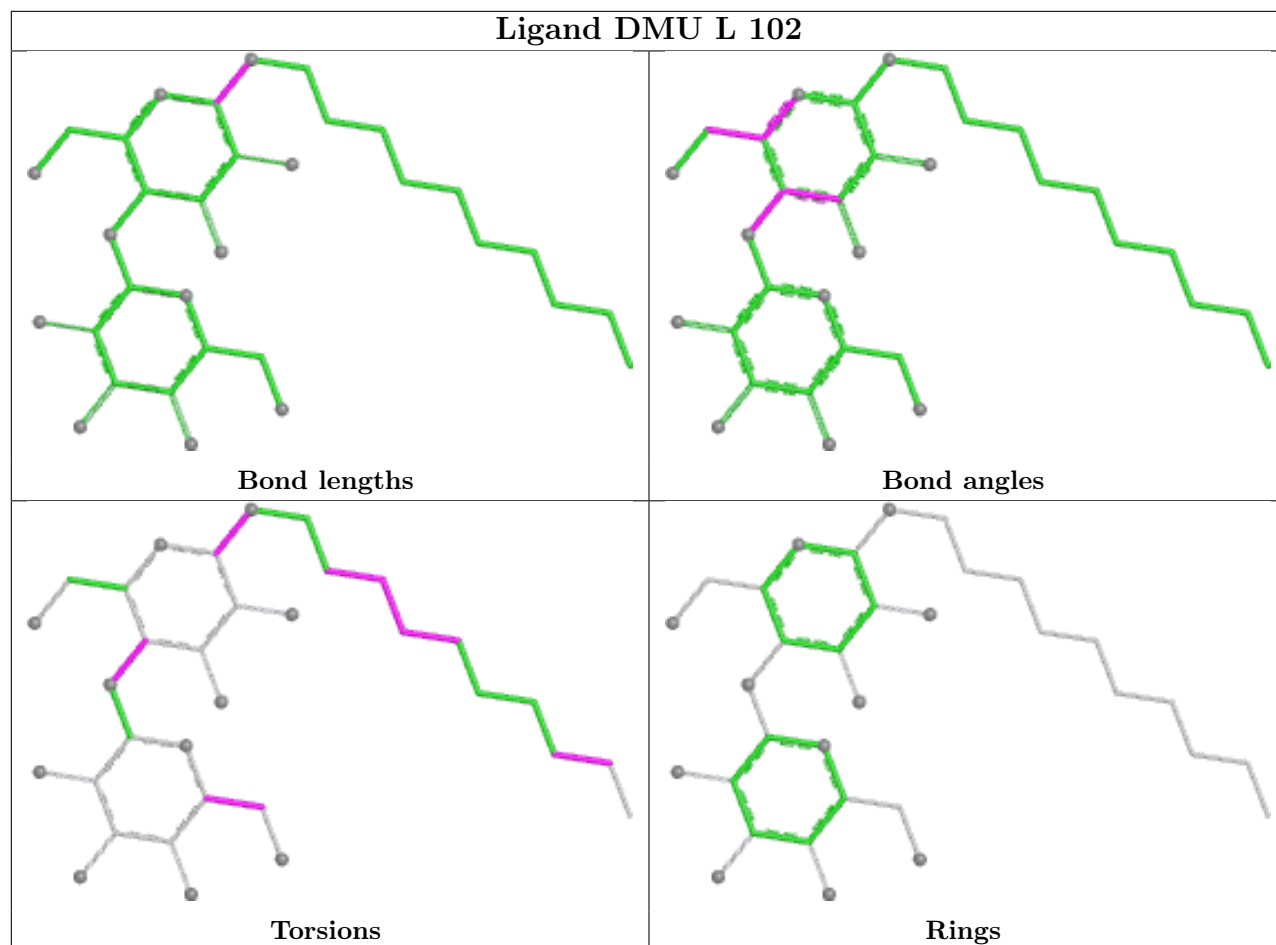
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	M	101	DMU	1	0
20	Q	202	EDO	1	0
19	P	305	PGV	5	0
21	K	102	DMU	1	0
19	P	301	PGV	3	0
21	X	103	DMU	1	0
21	O	305	DMU	2	0
19	A	608	PGV	8	0
21	Q	203	DMU	1	0
21	K	103	DMU	3	0
21	K	105	DMU	5	0
20	W	103	EDO	3	0

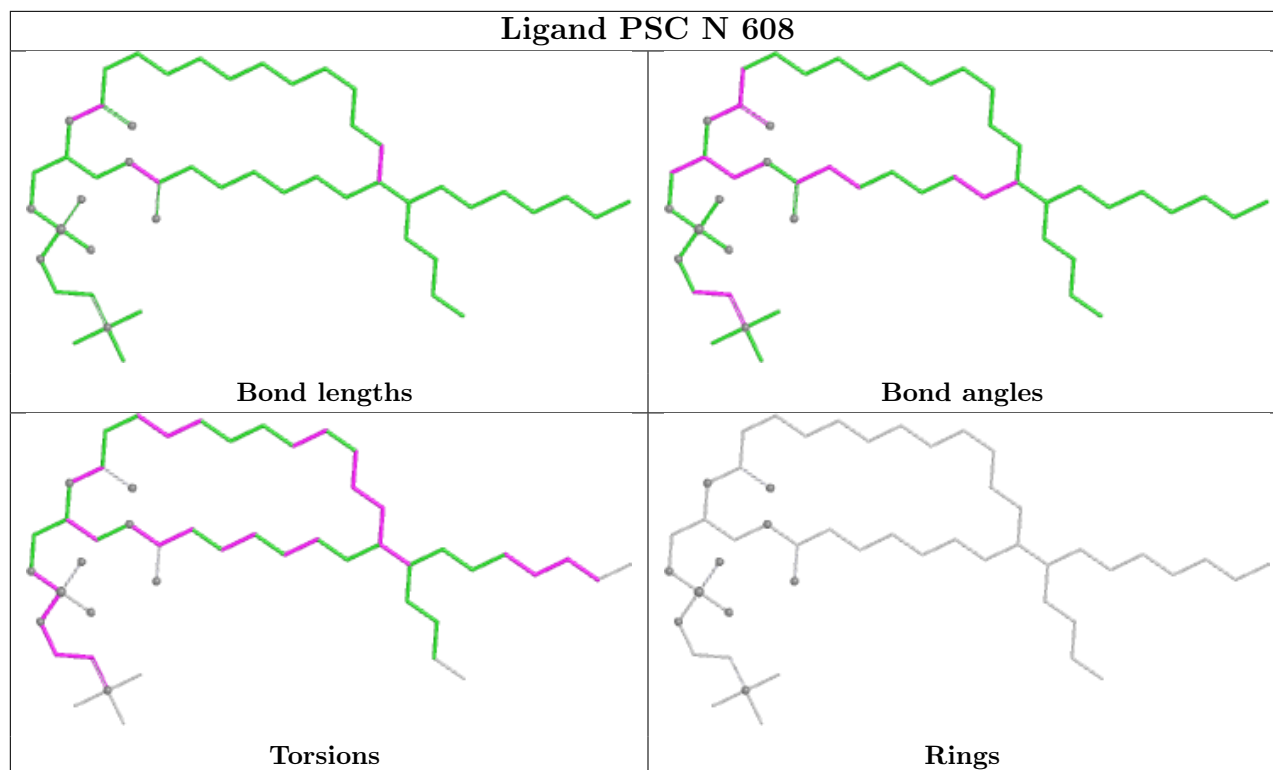
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



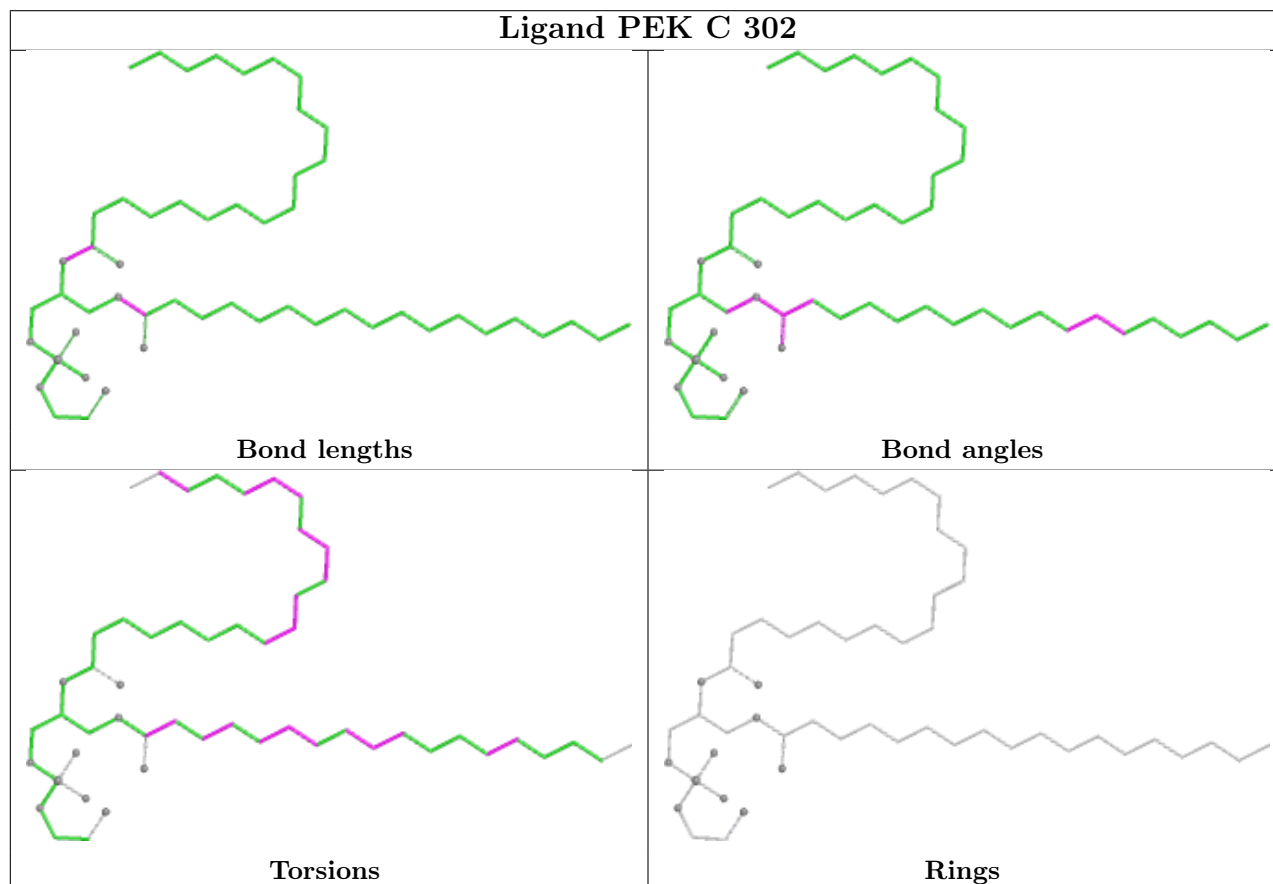




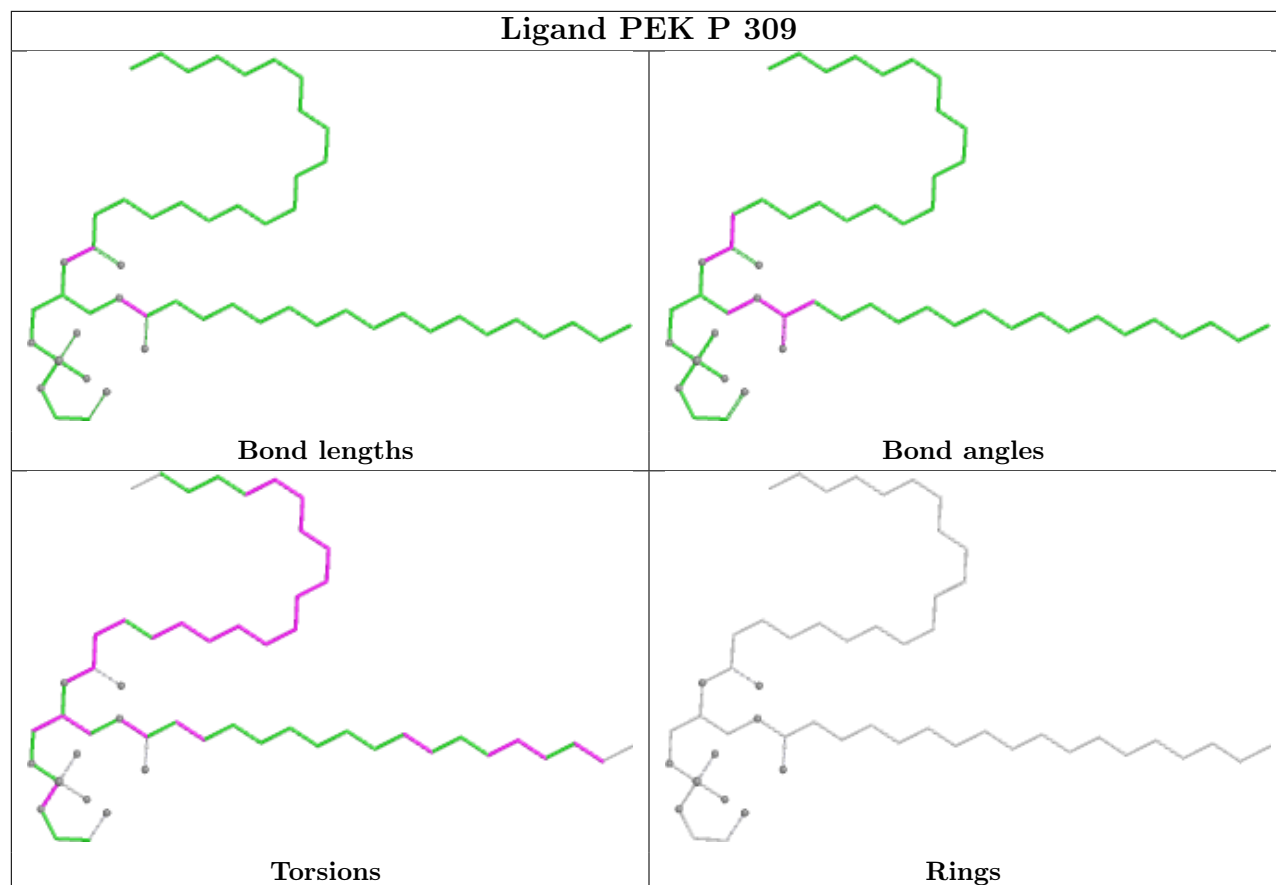
Ligand PSC N 608



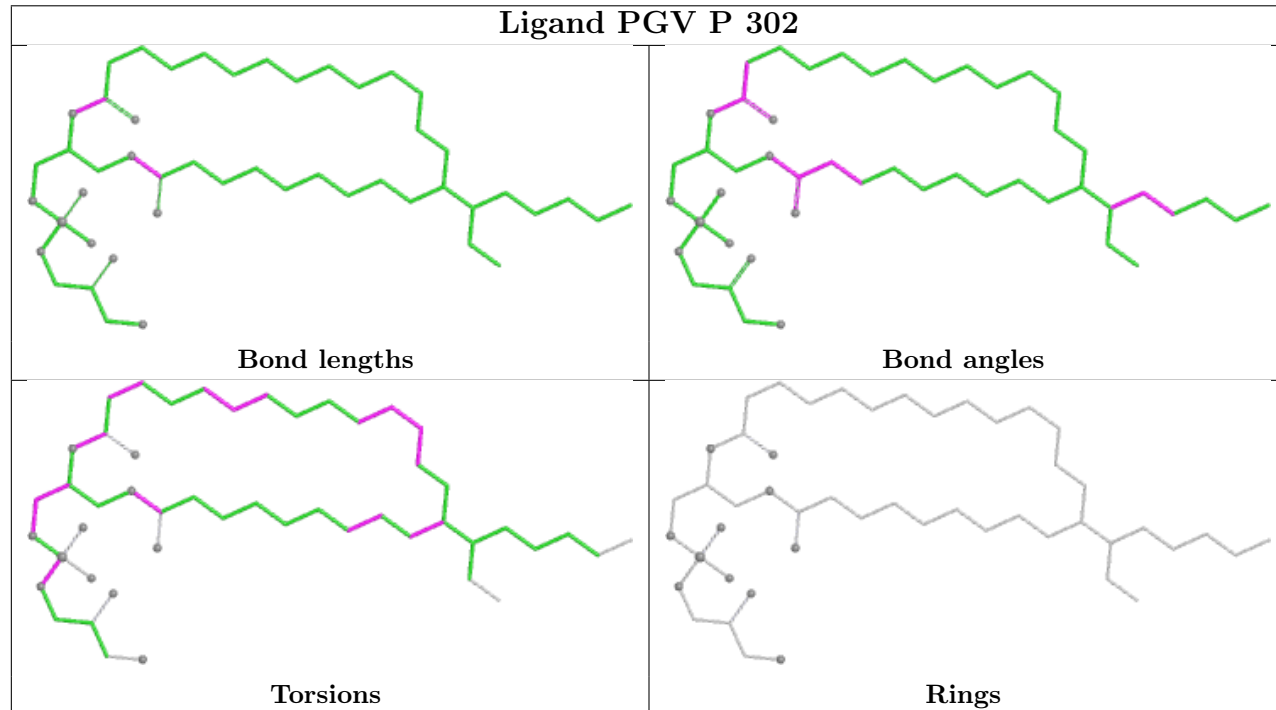
Ligand PEK C 302

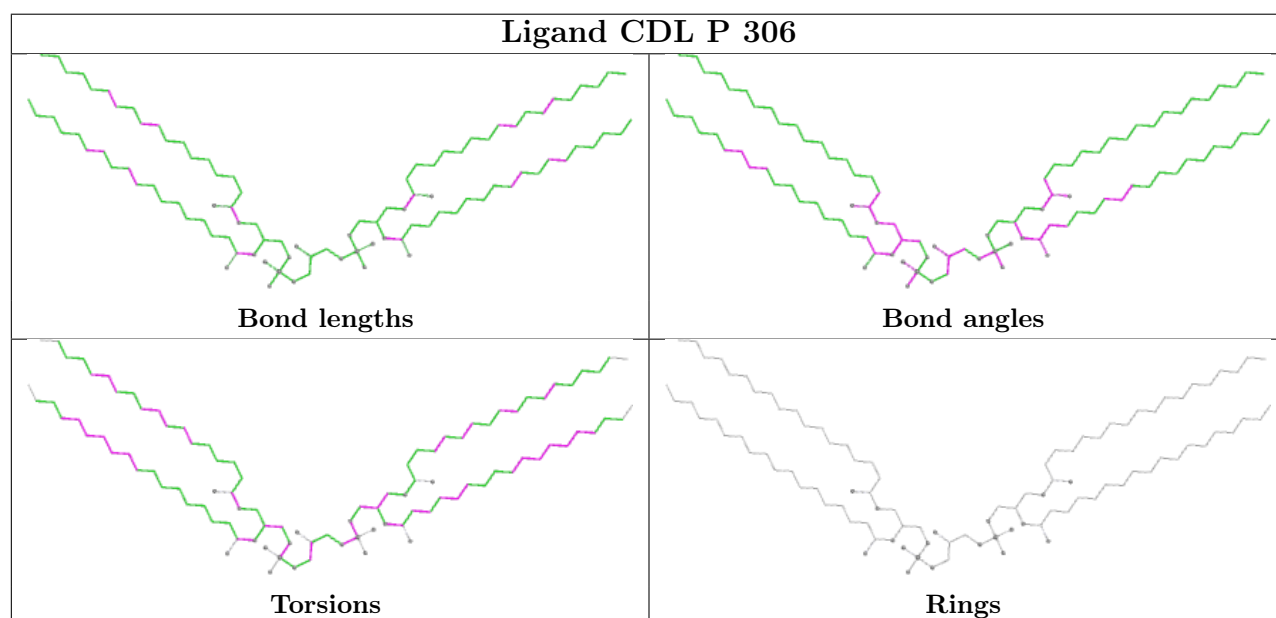
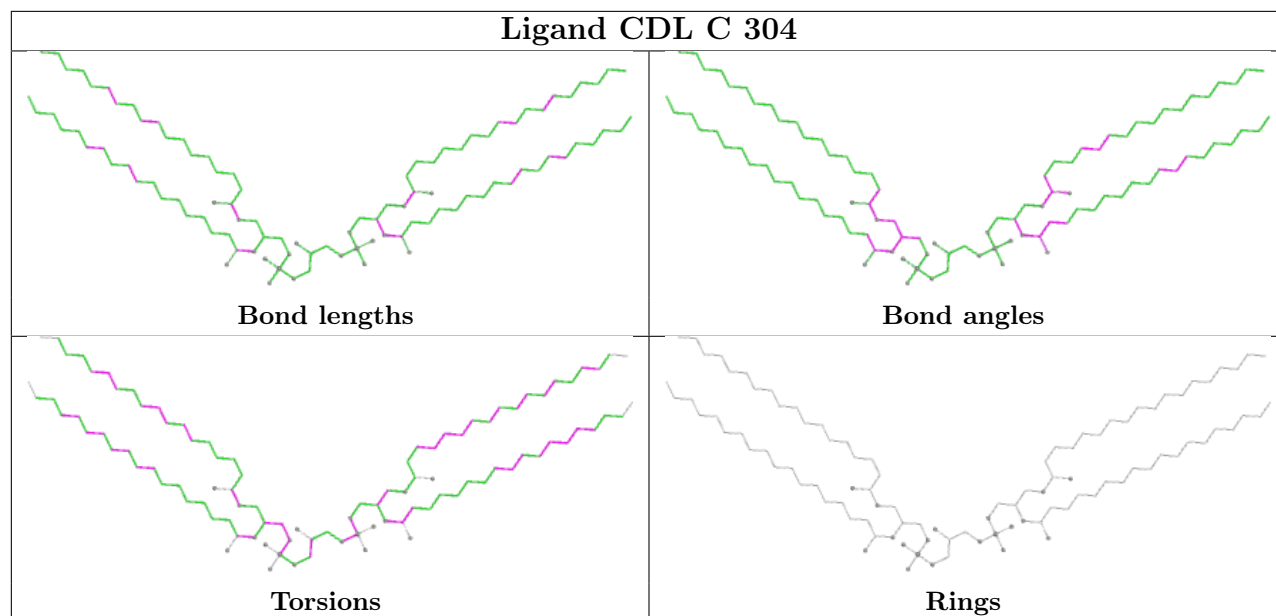


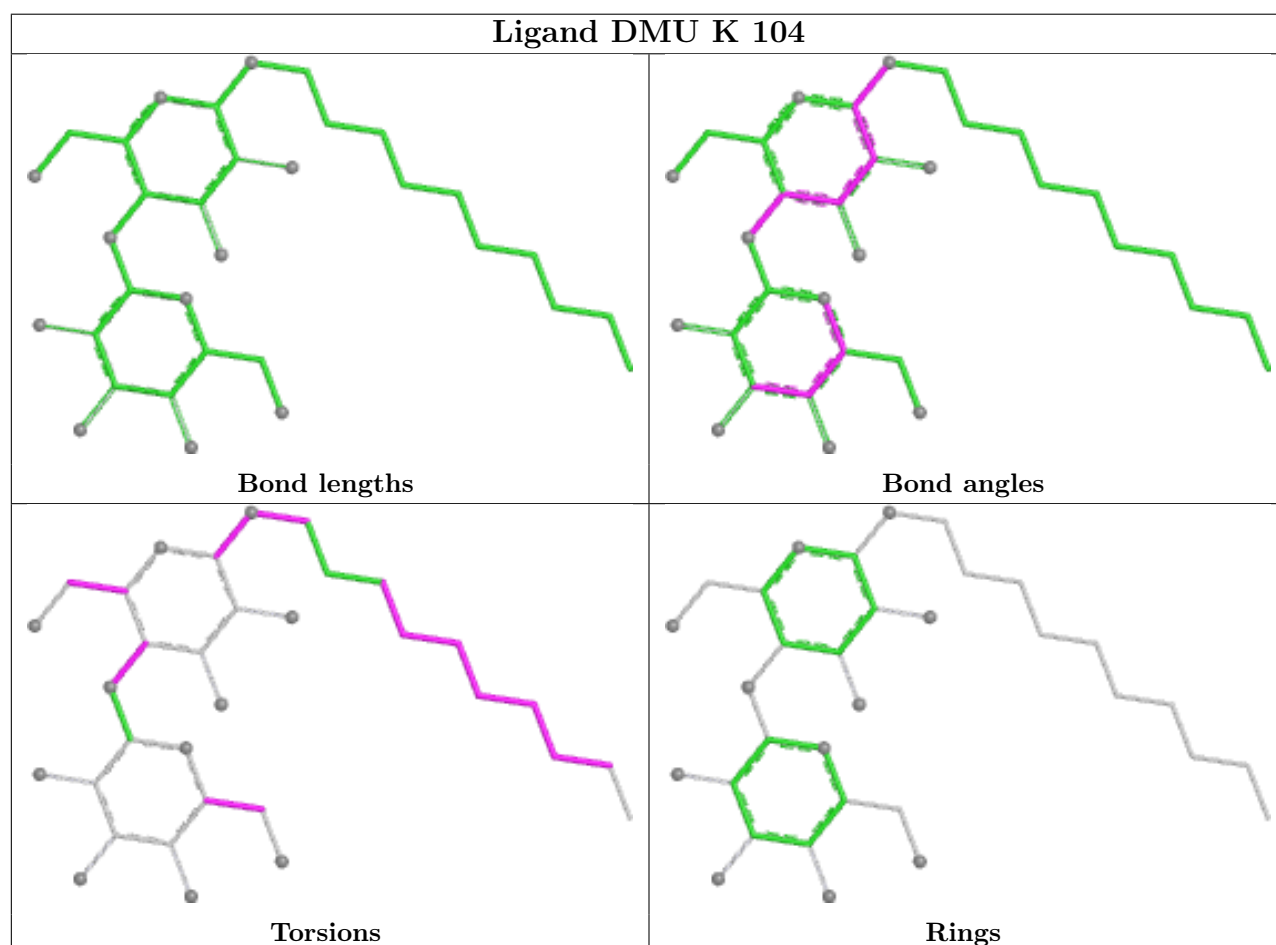
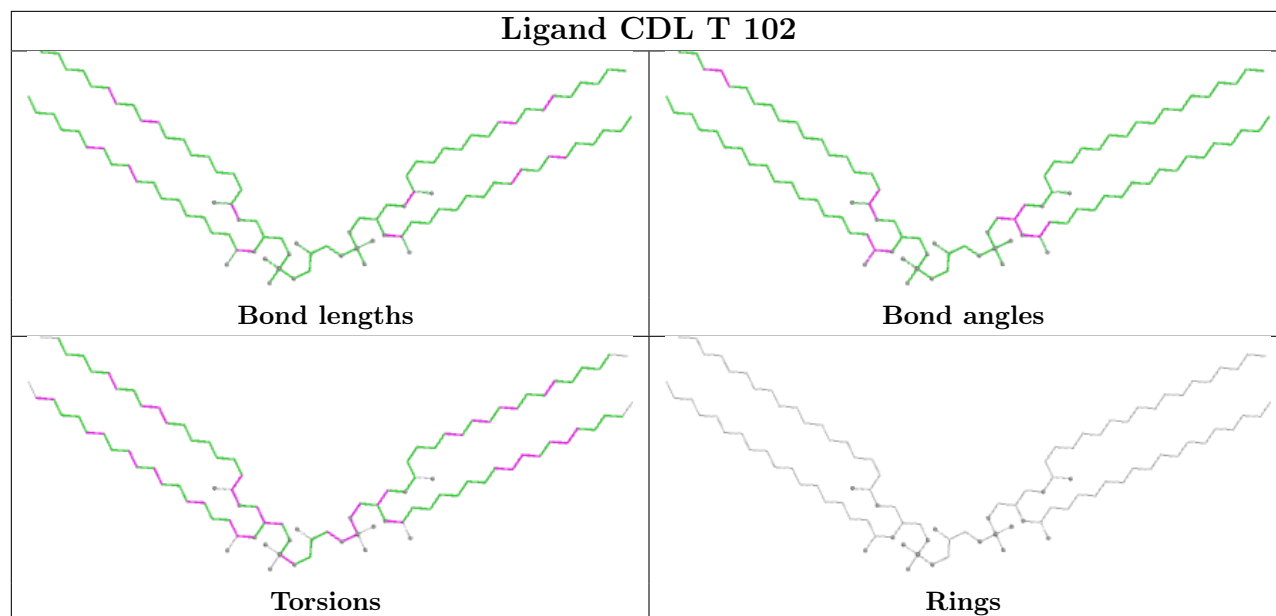
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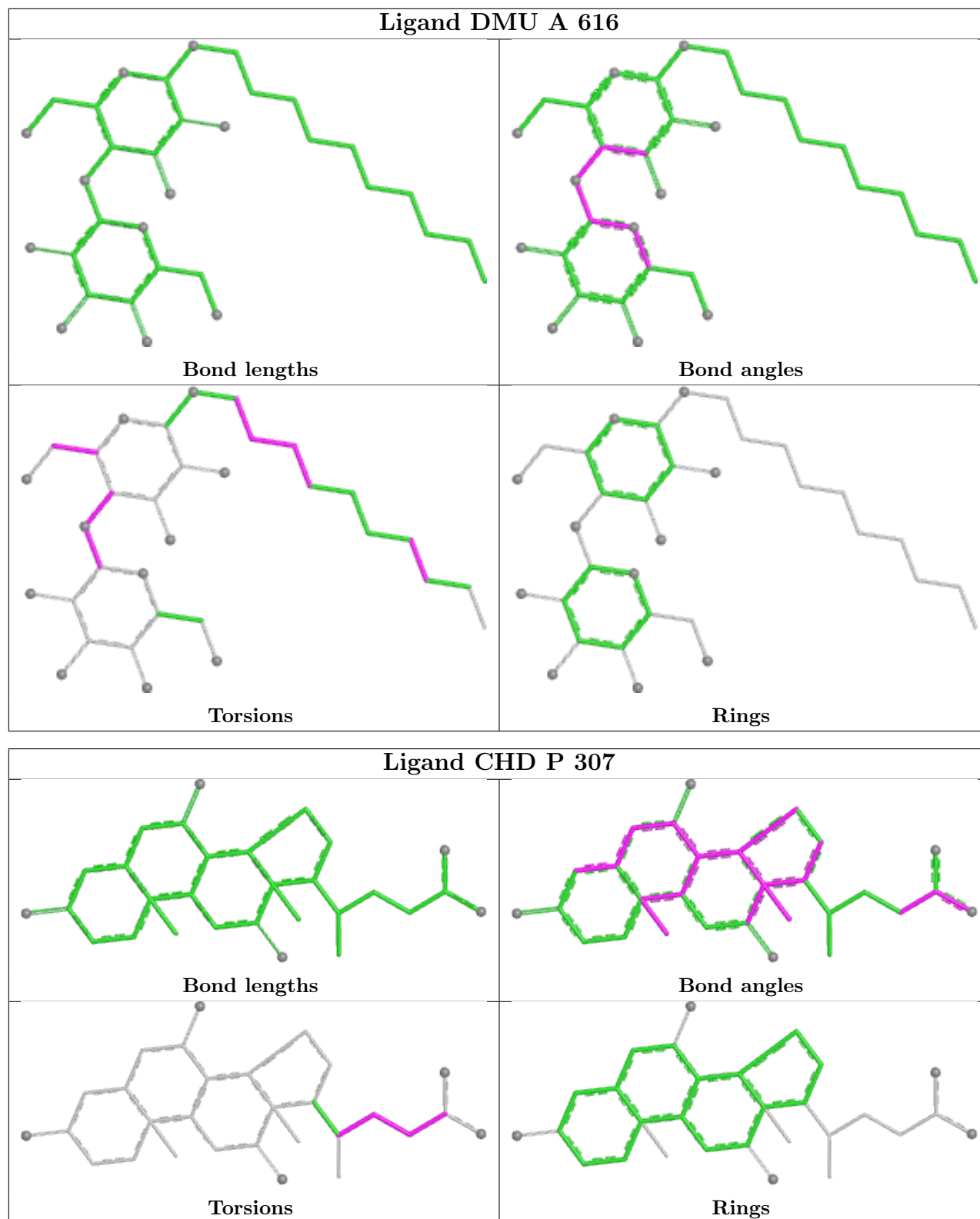


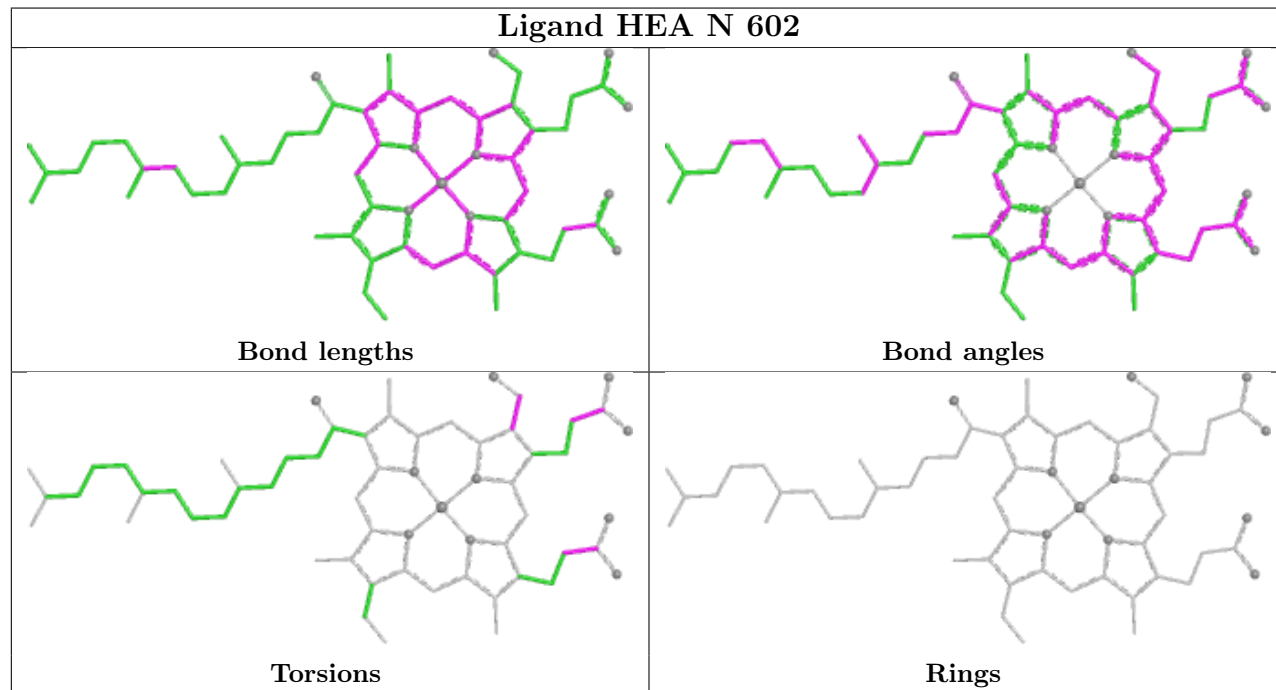
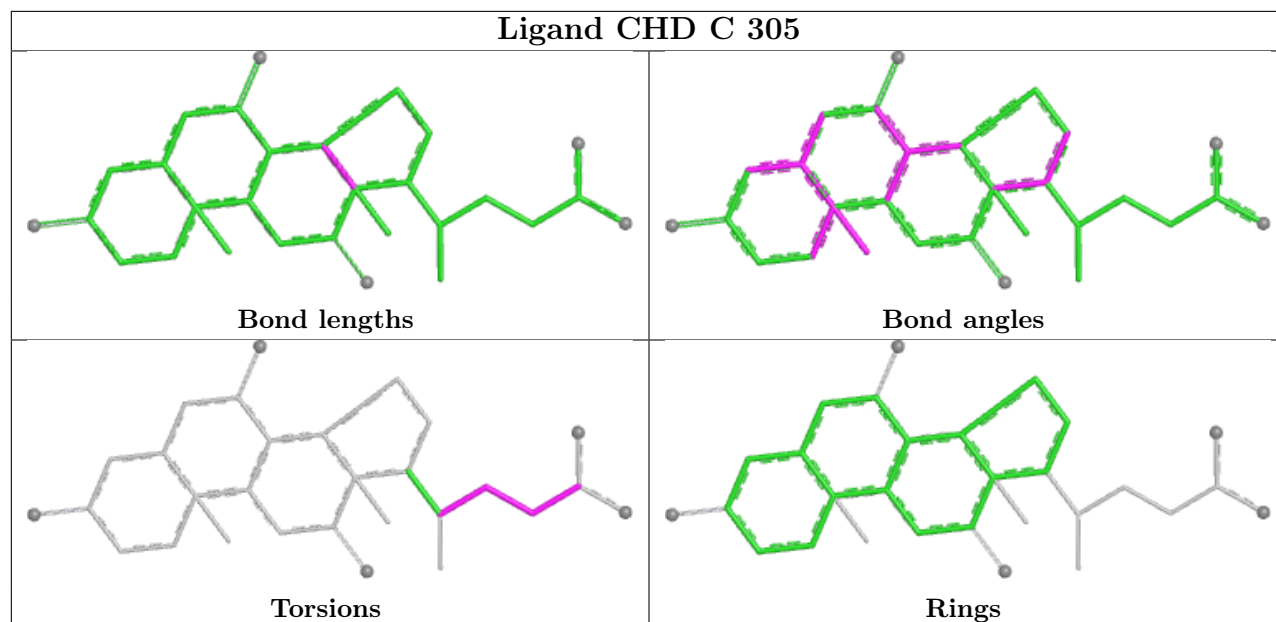
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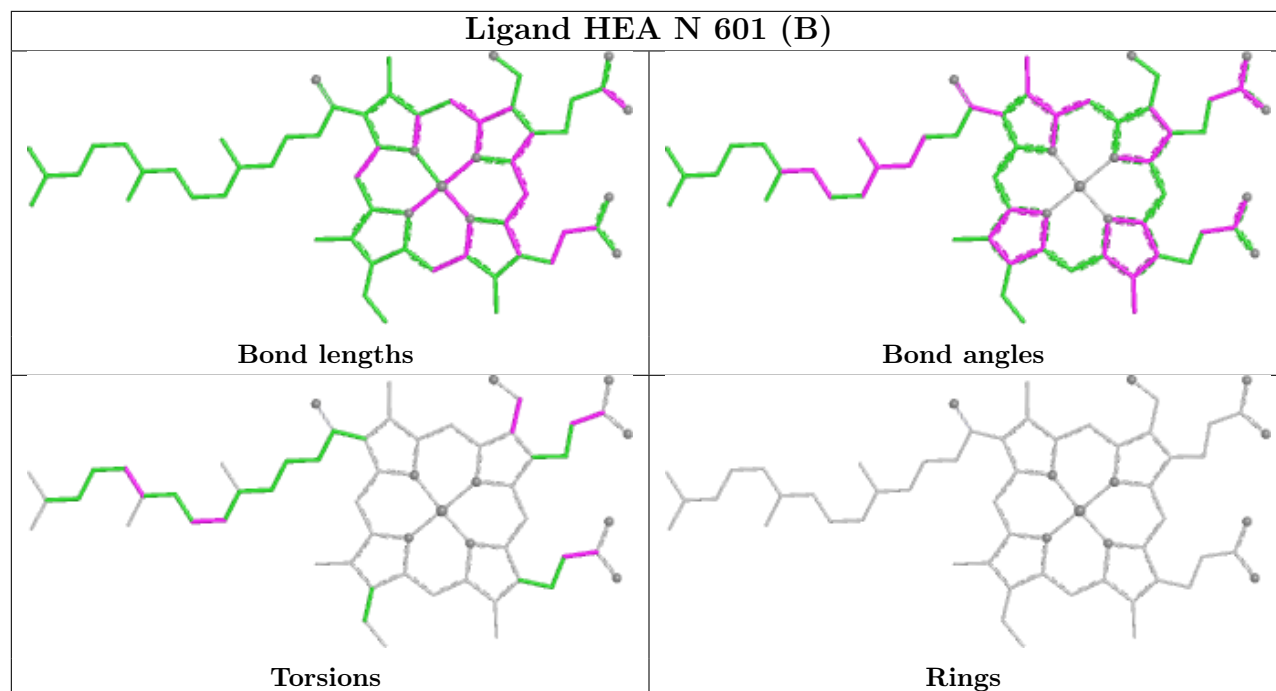
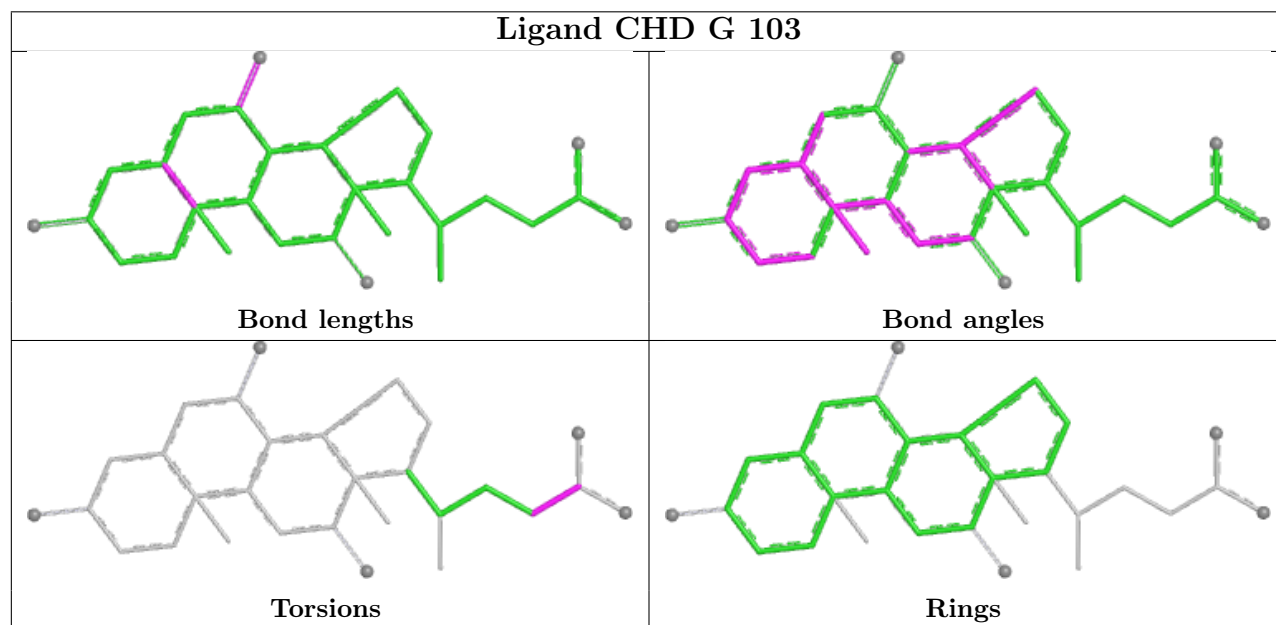


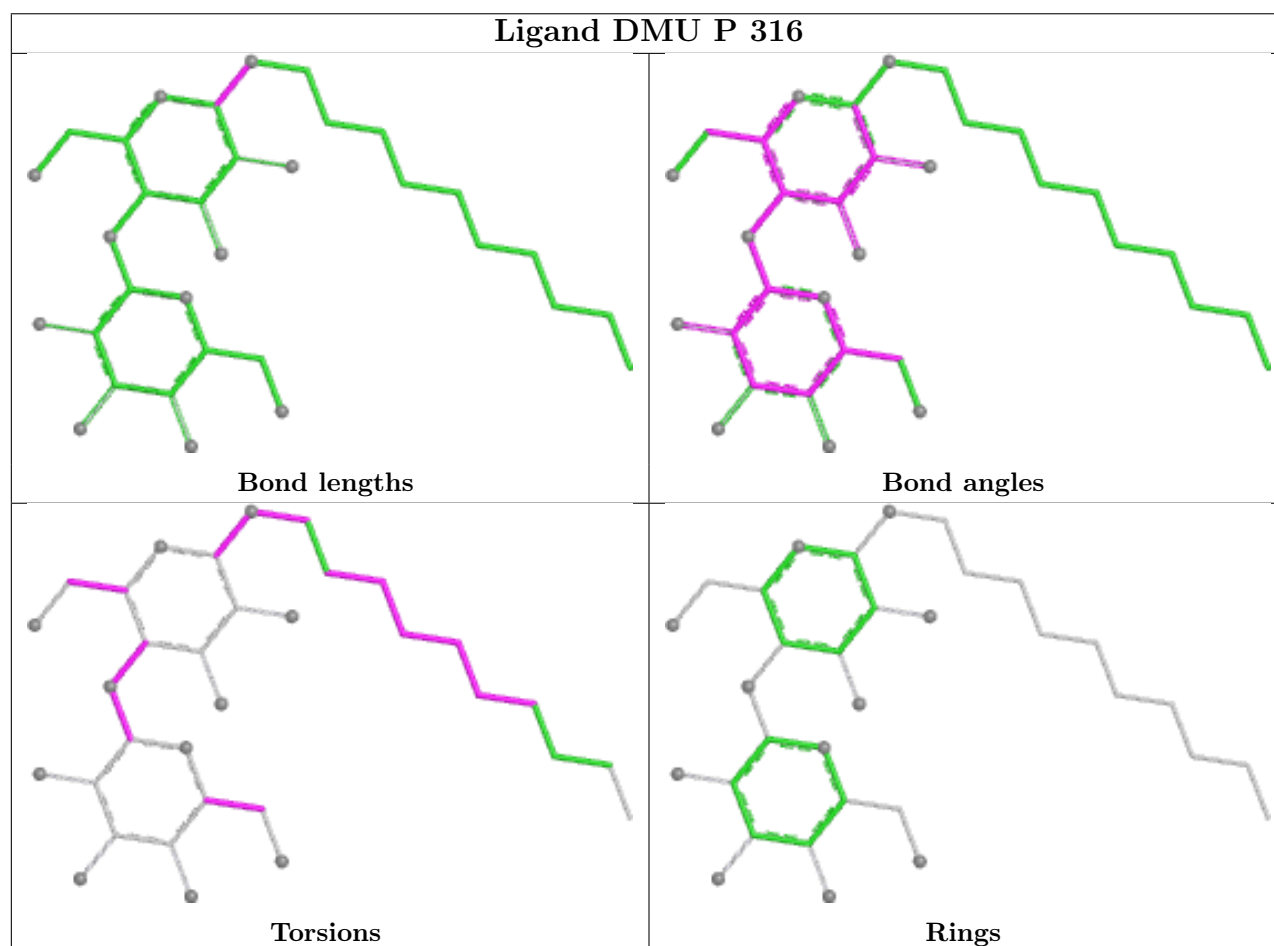
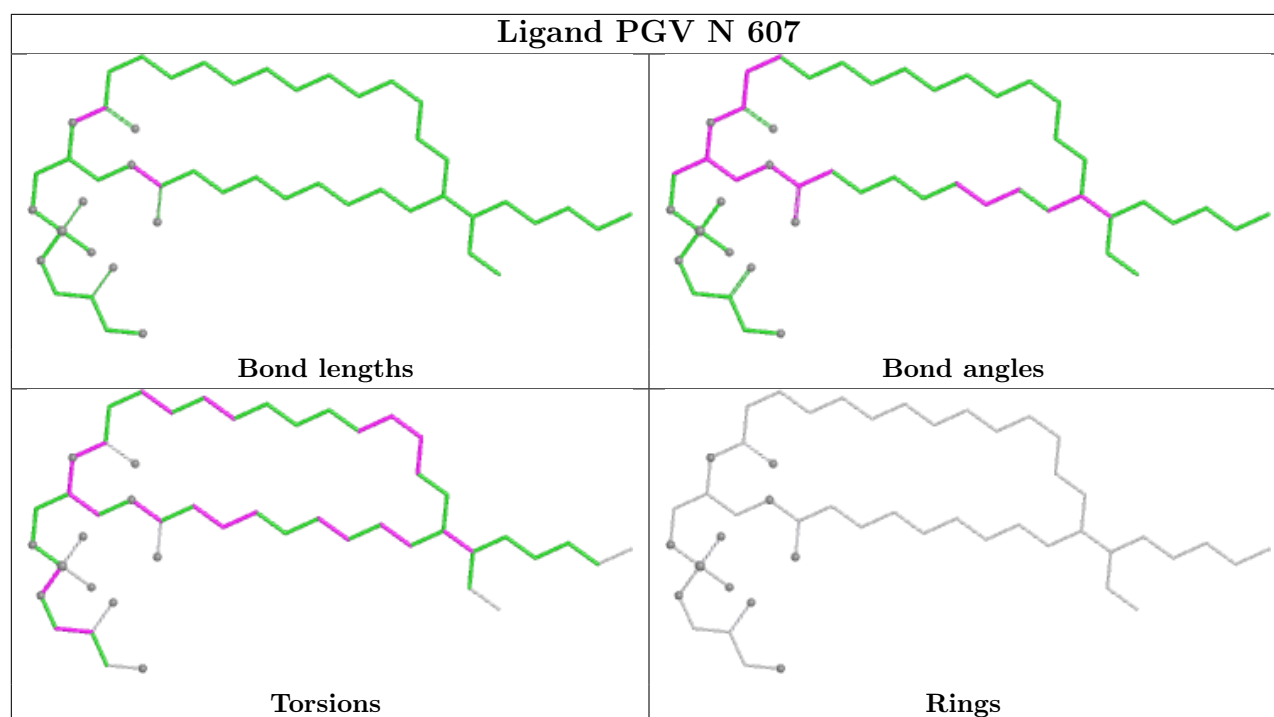


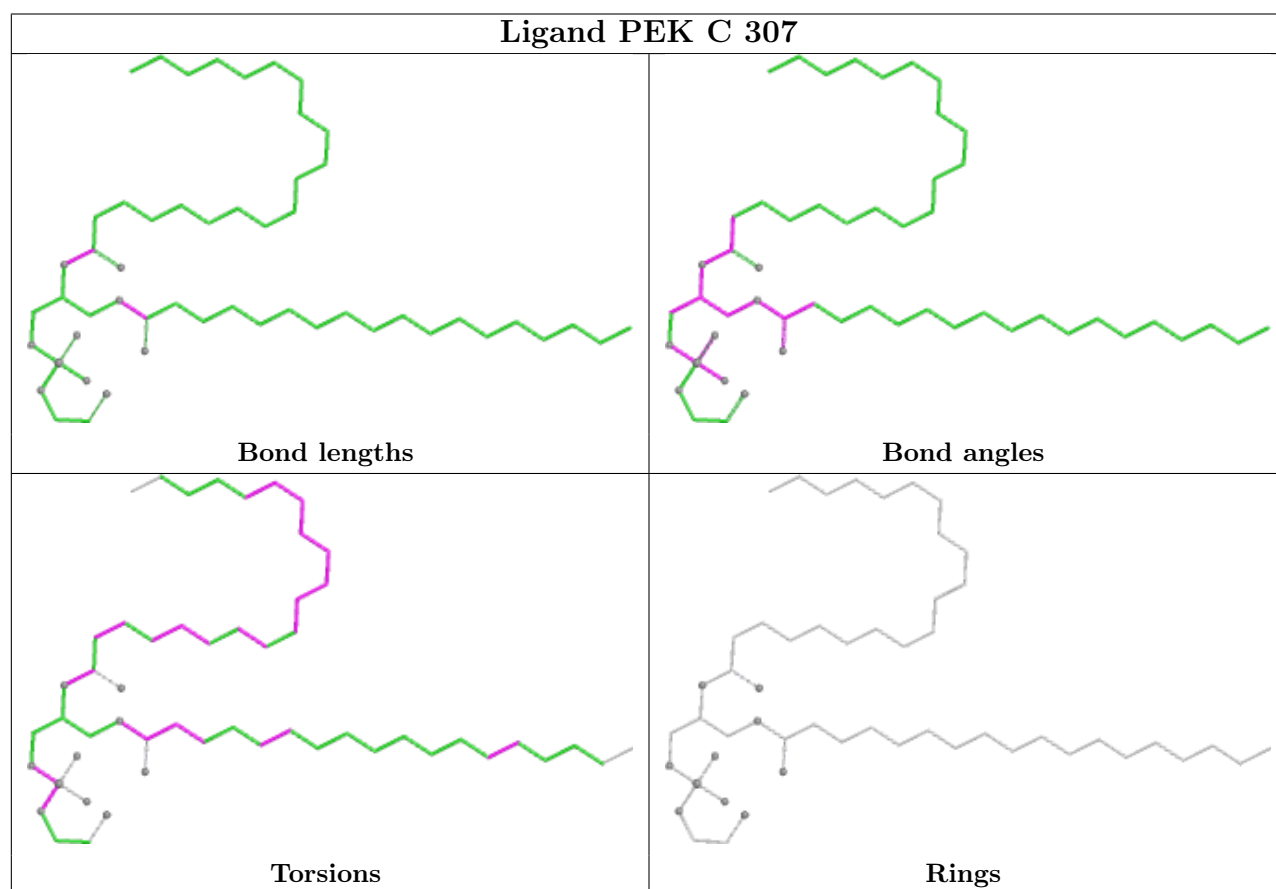
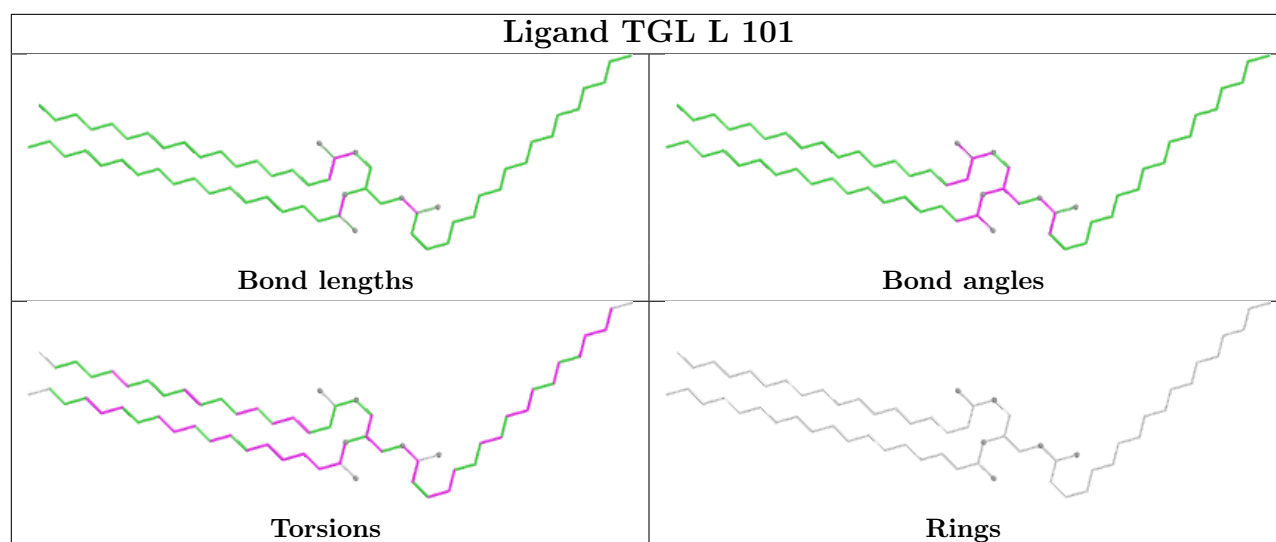


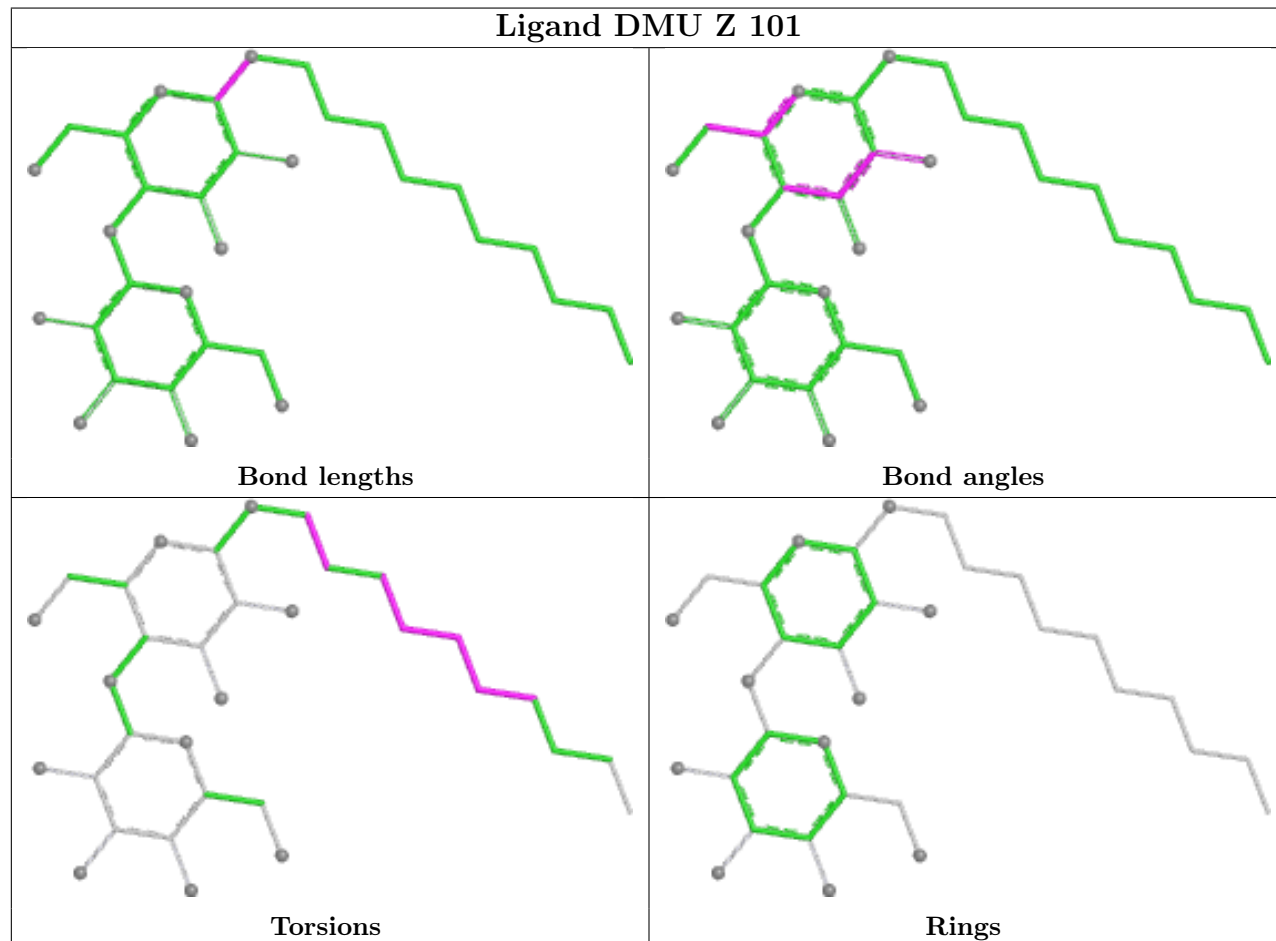
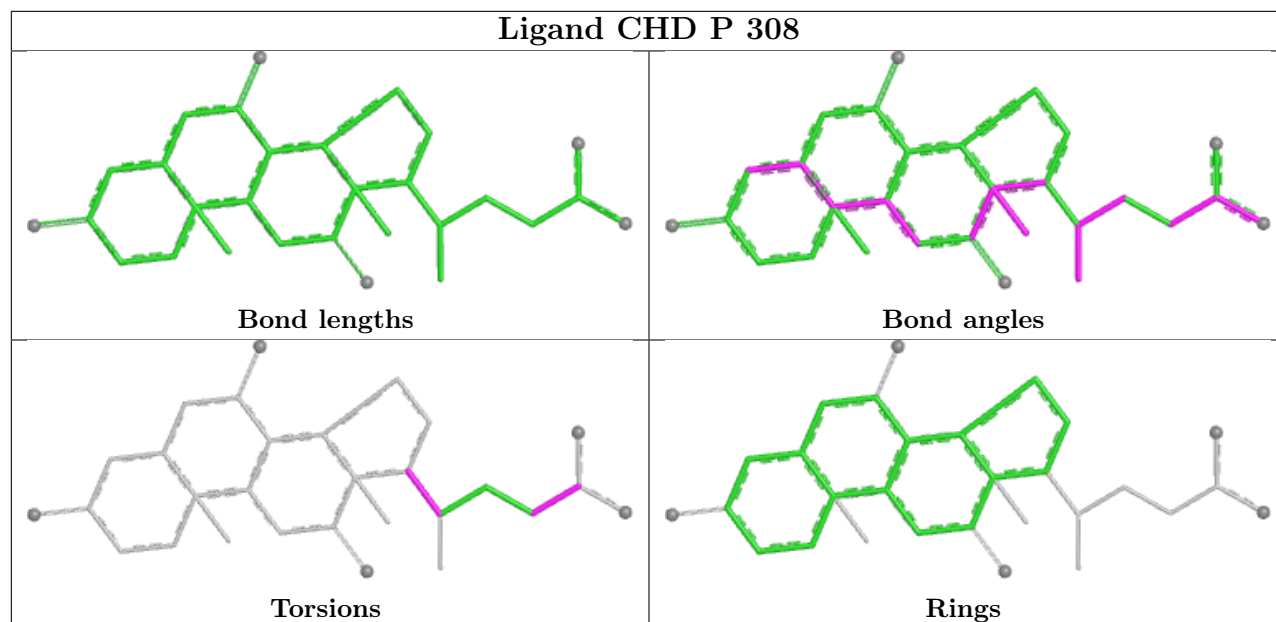


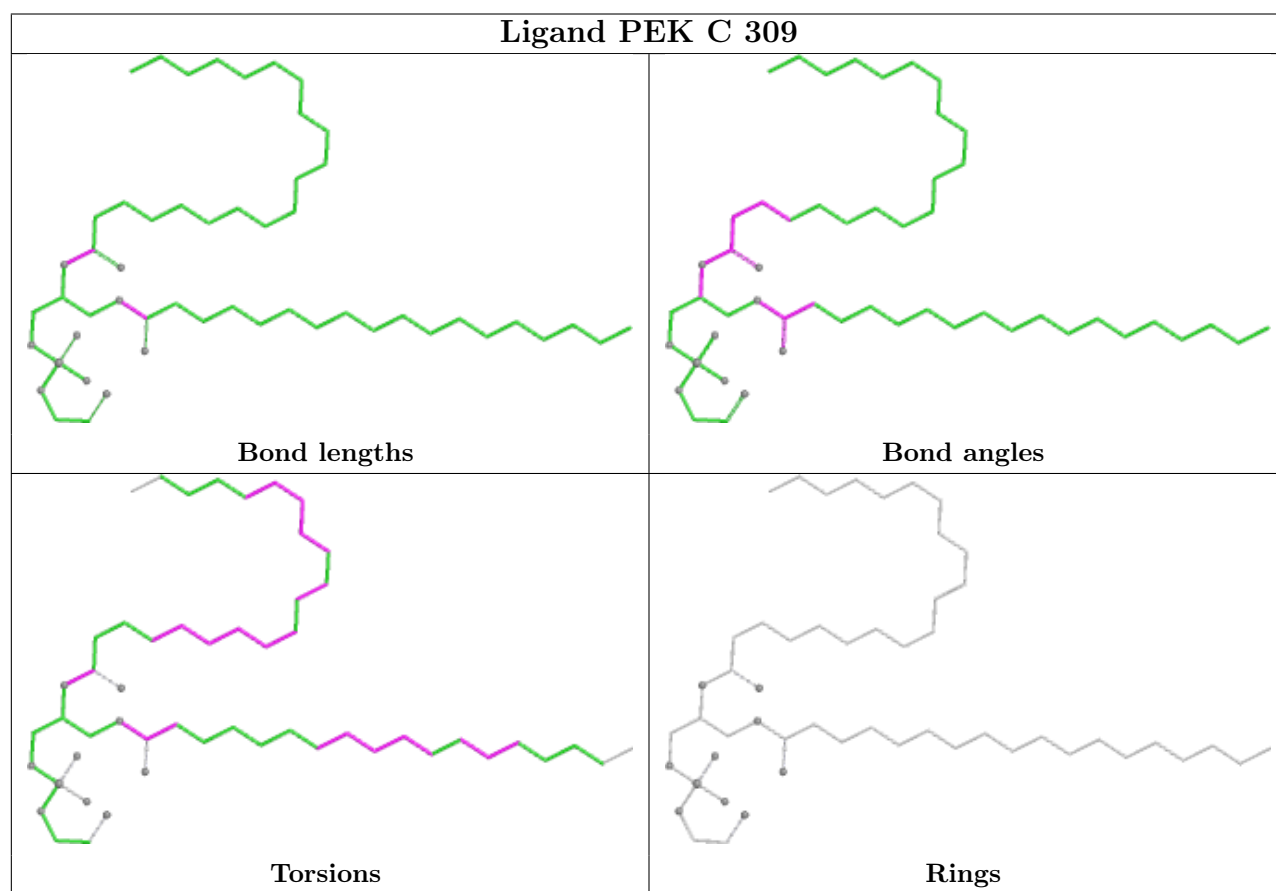
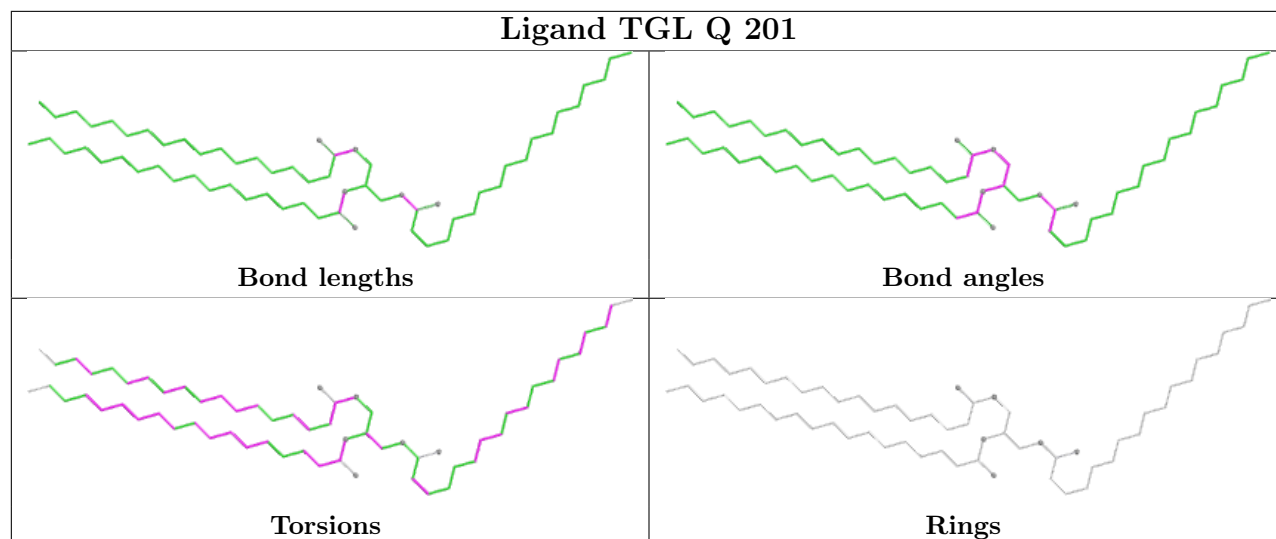


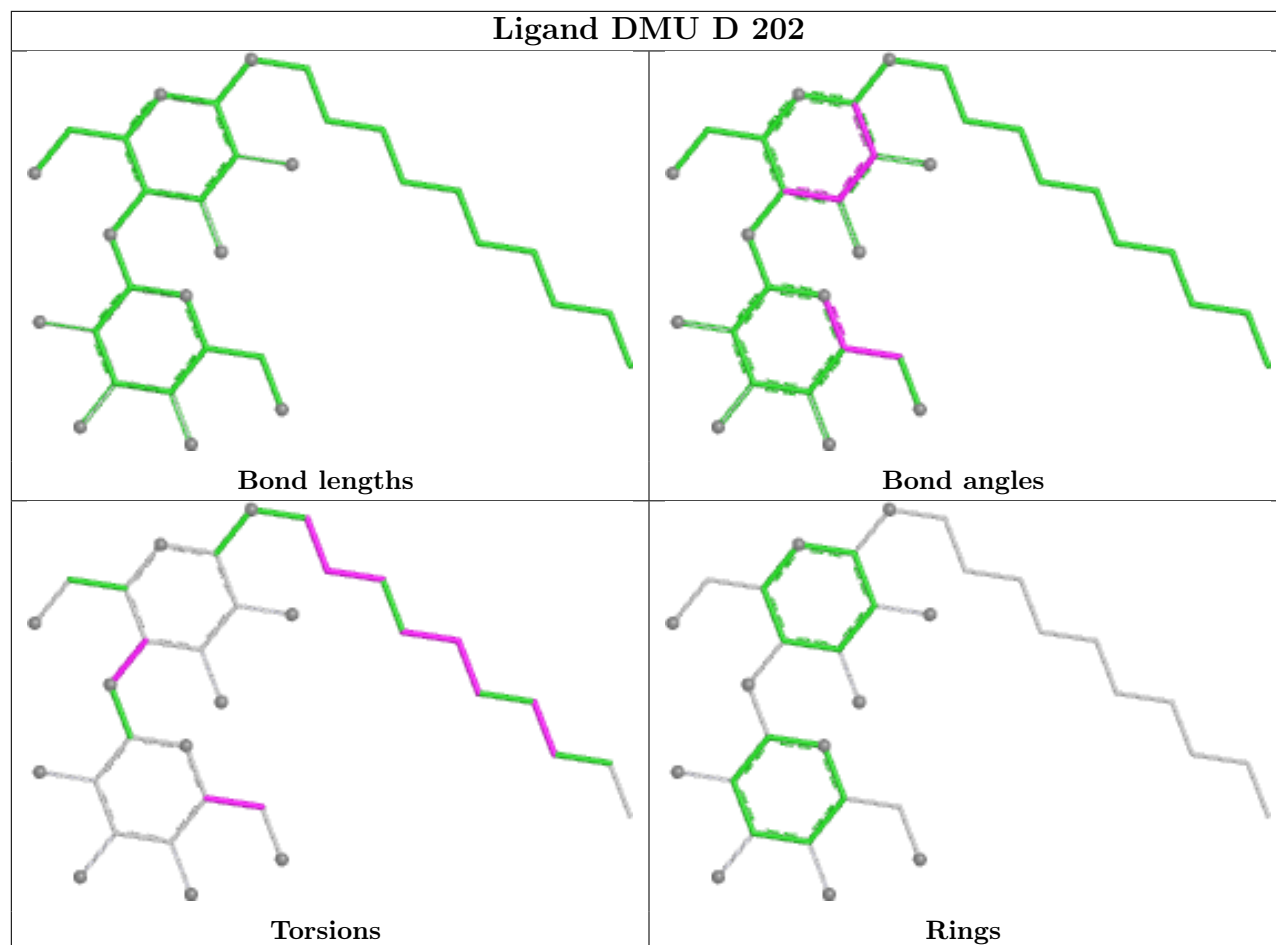
Ligand HEA N 601 (B)**Ligand CHD G 103**



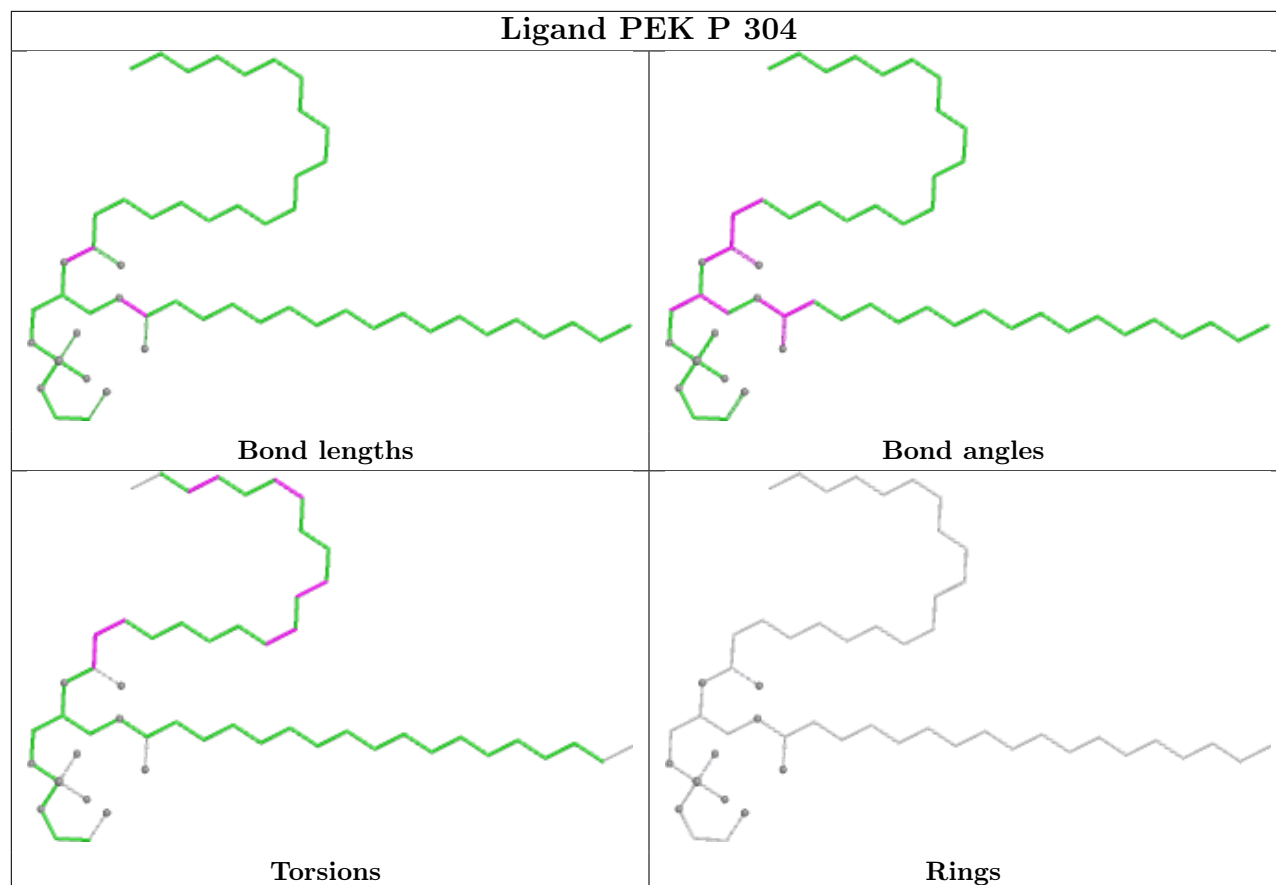




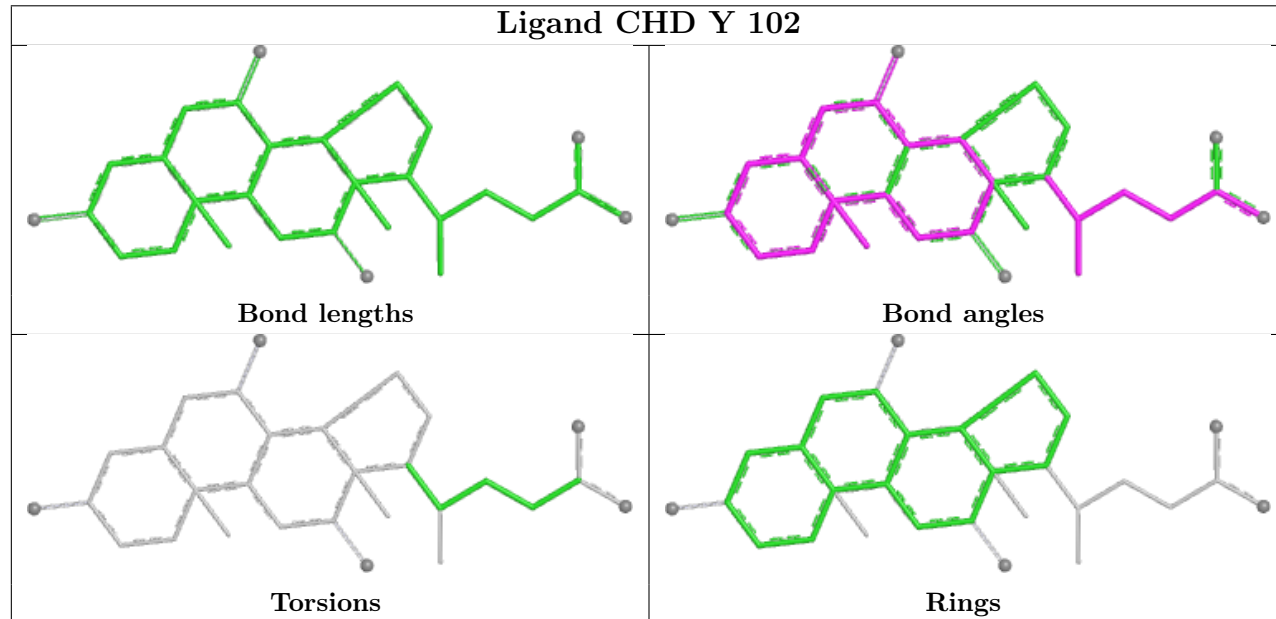


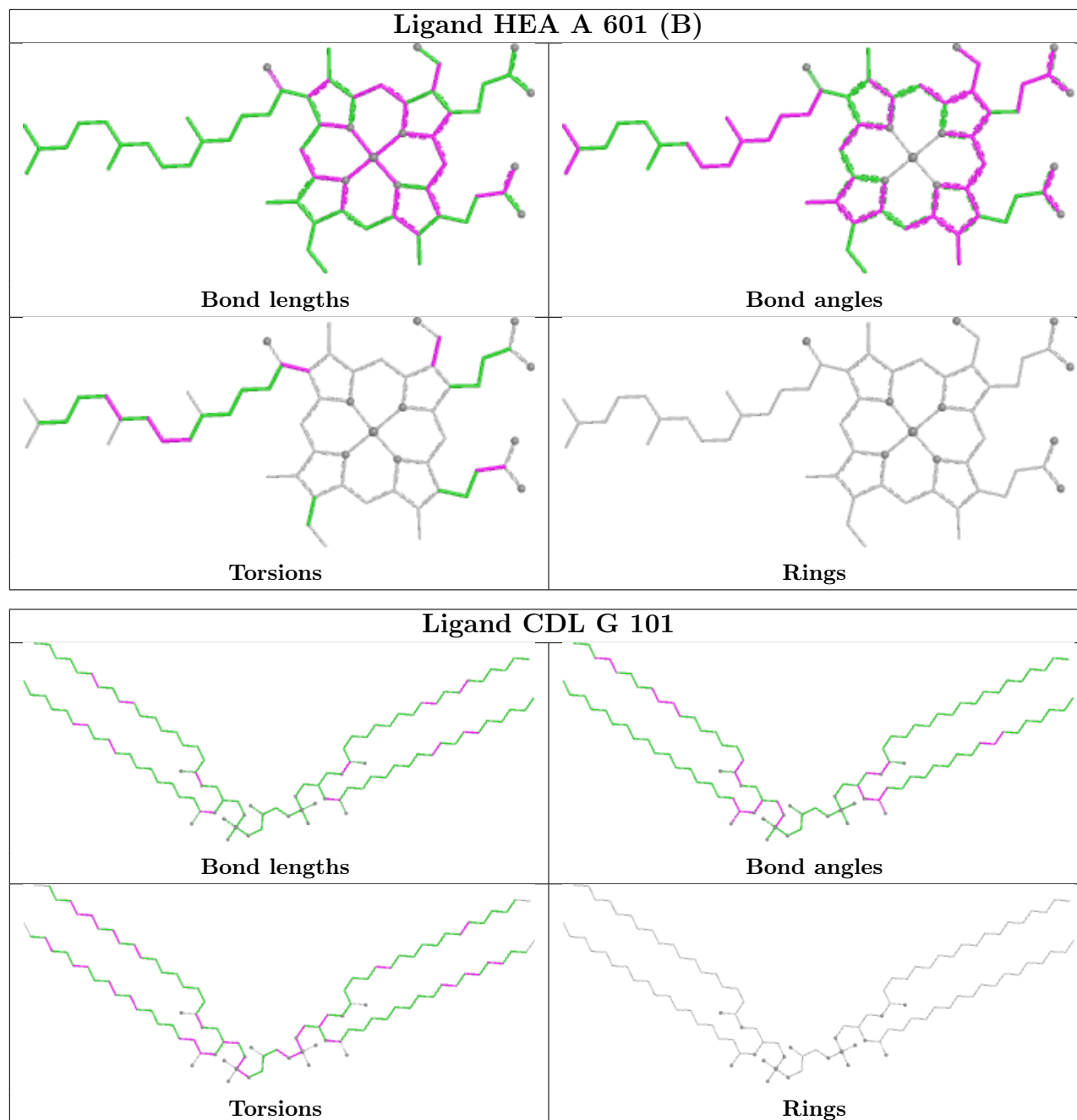


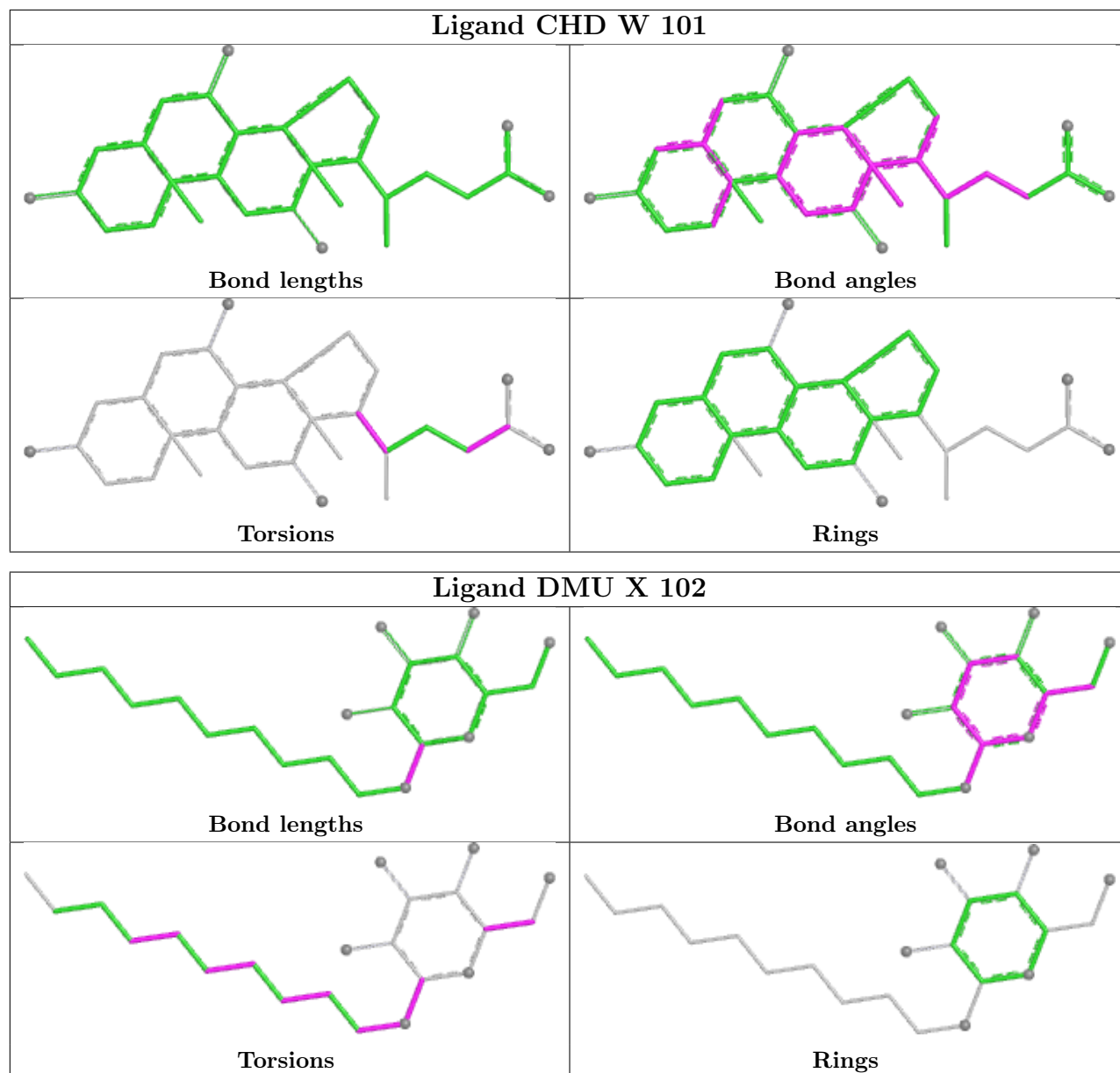
Ligand PEK P 304

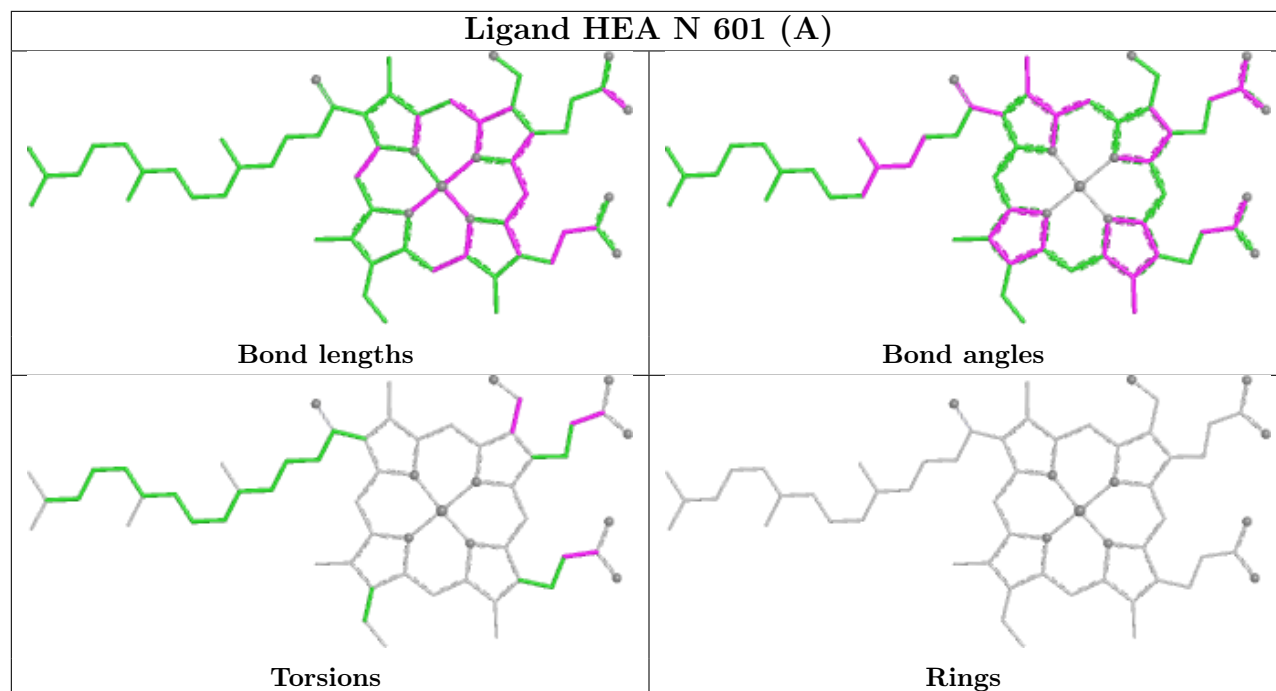
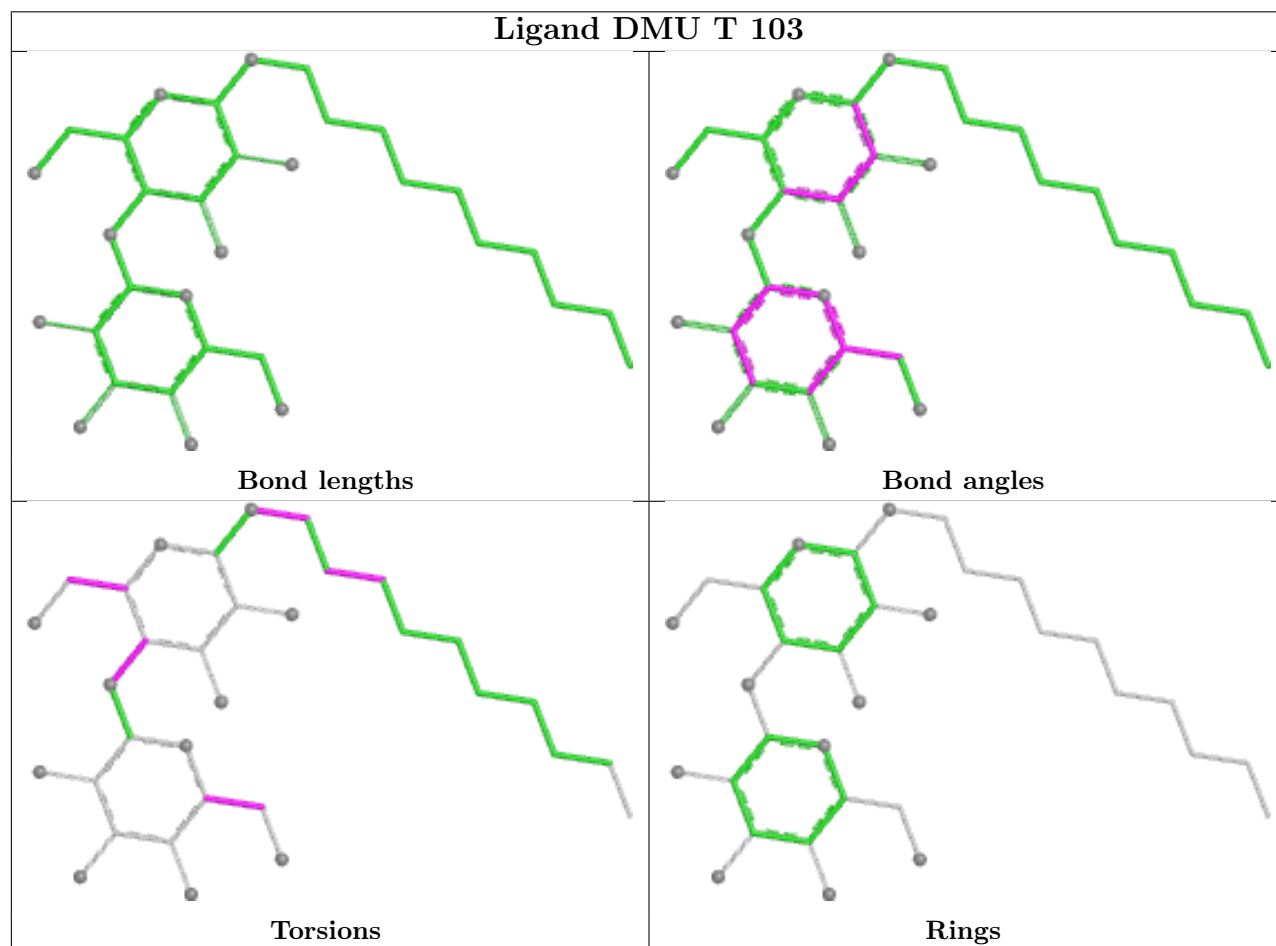


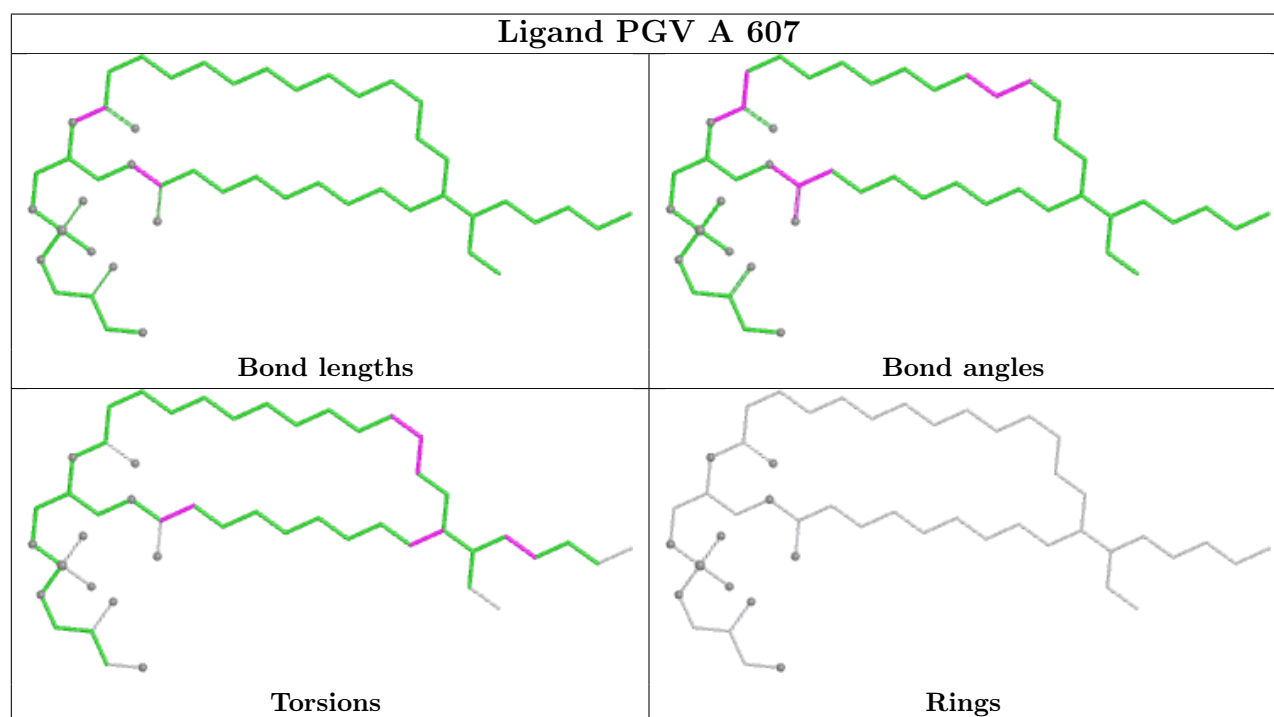
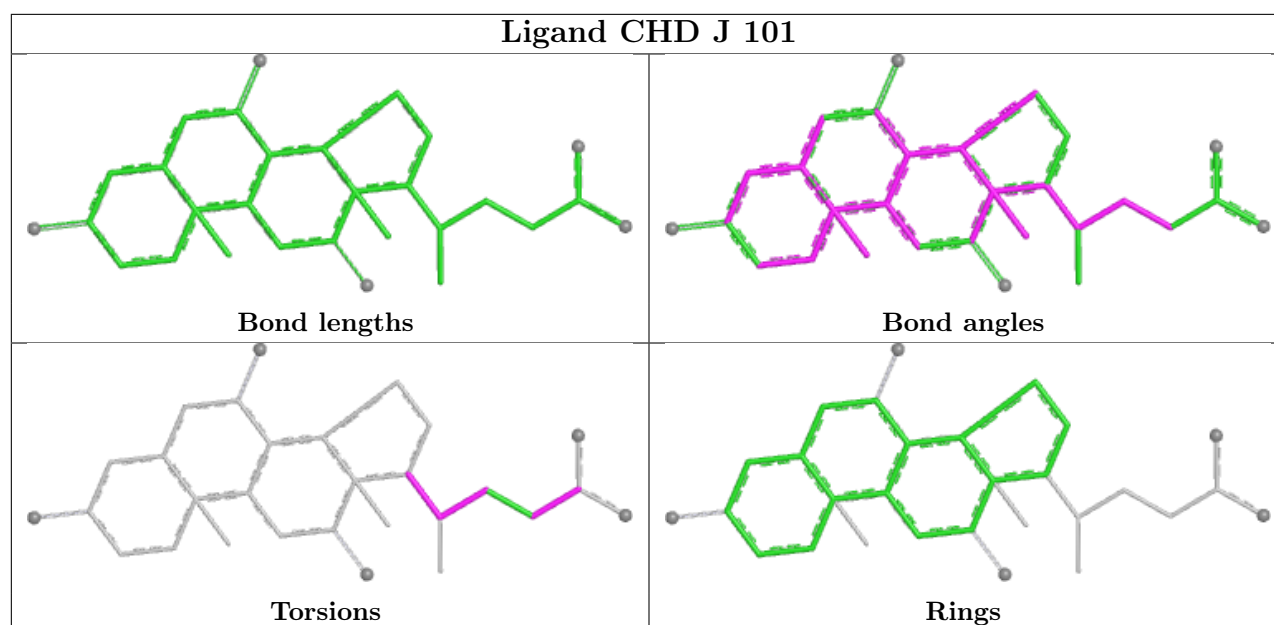
Ligand CHD Y 102

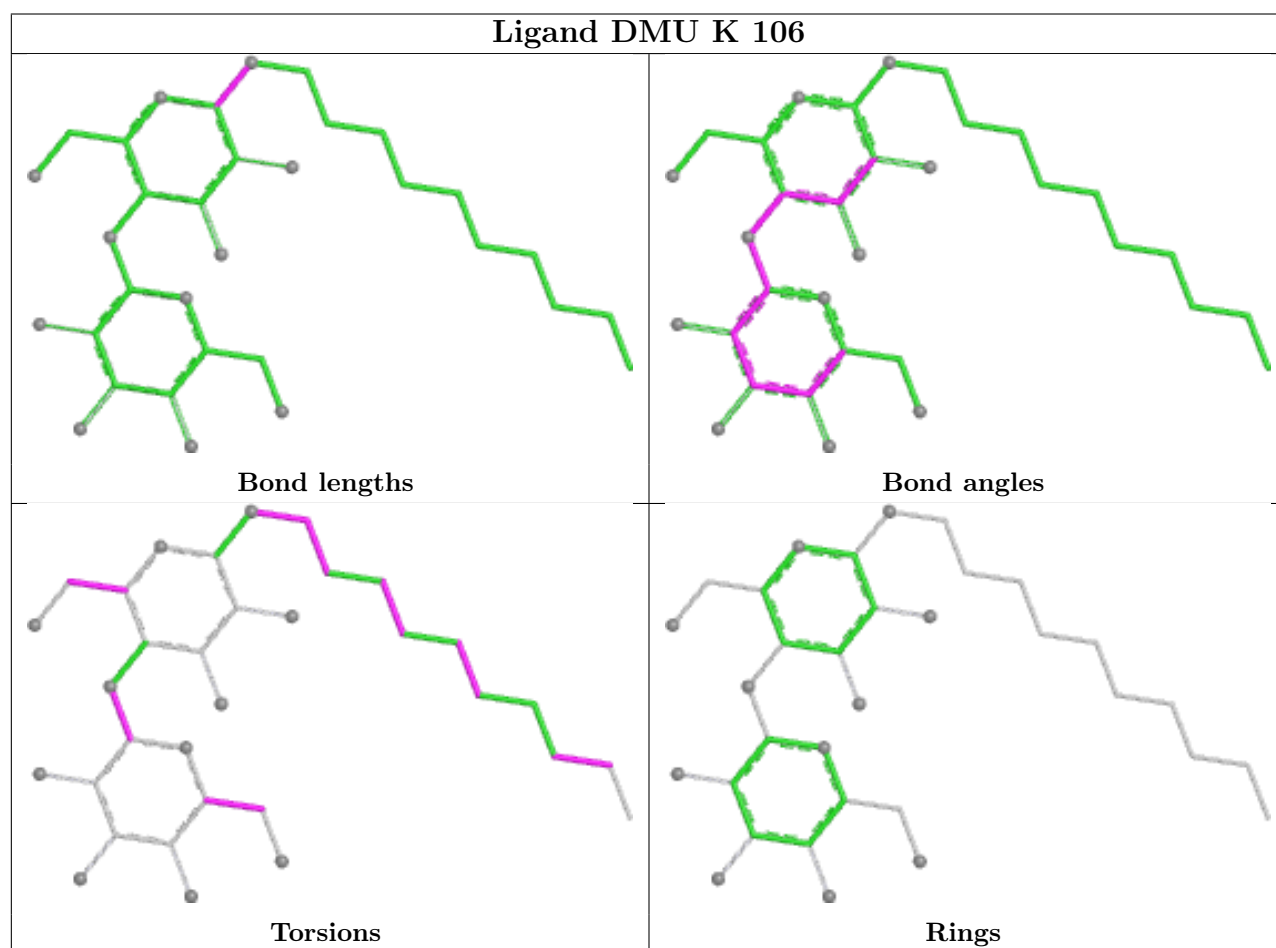
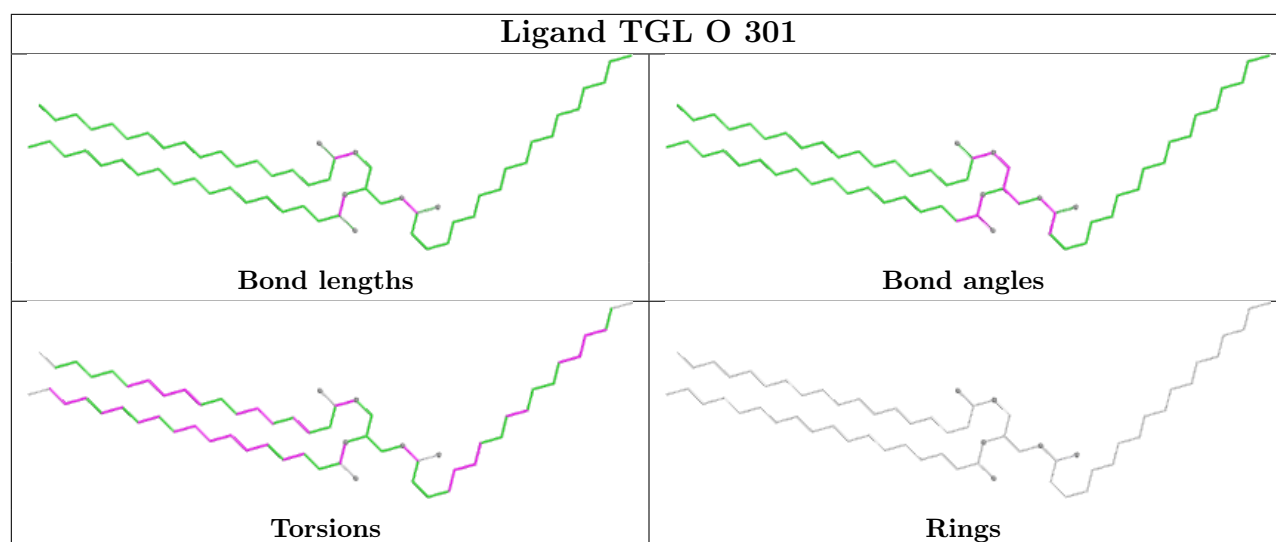


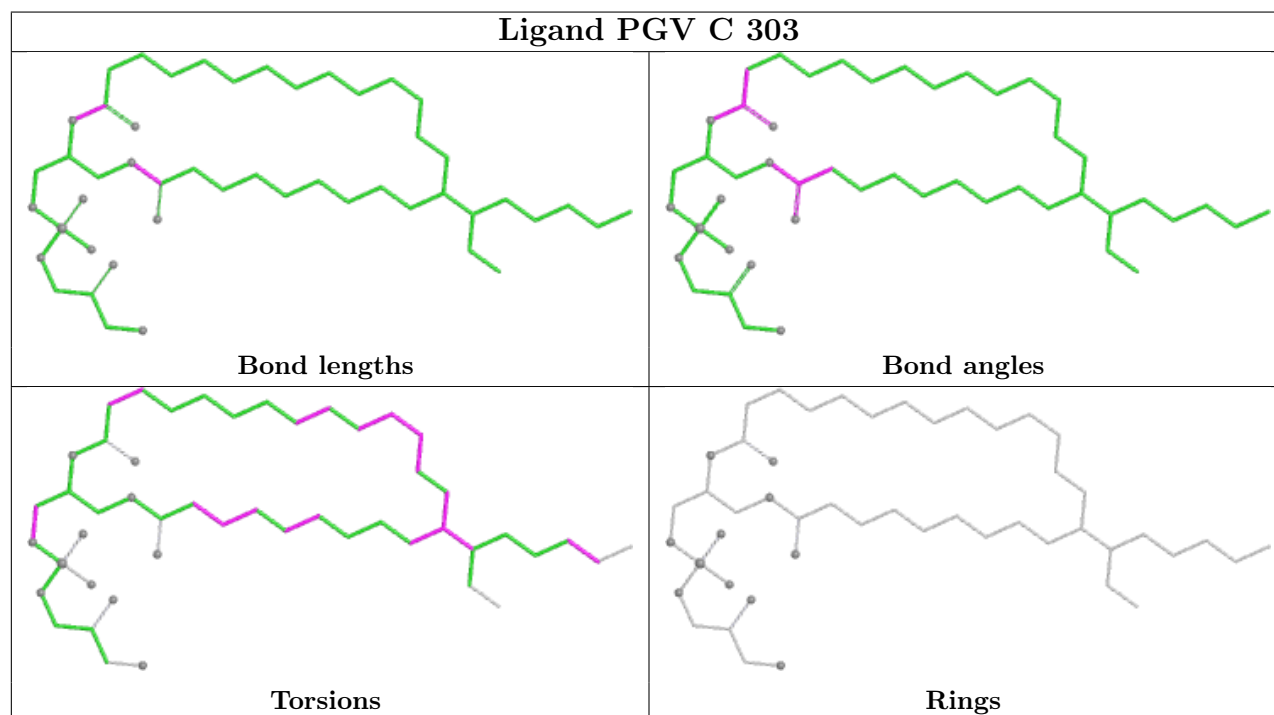
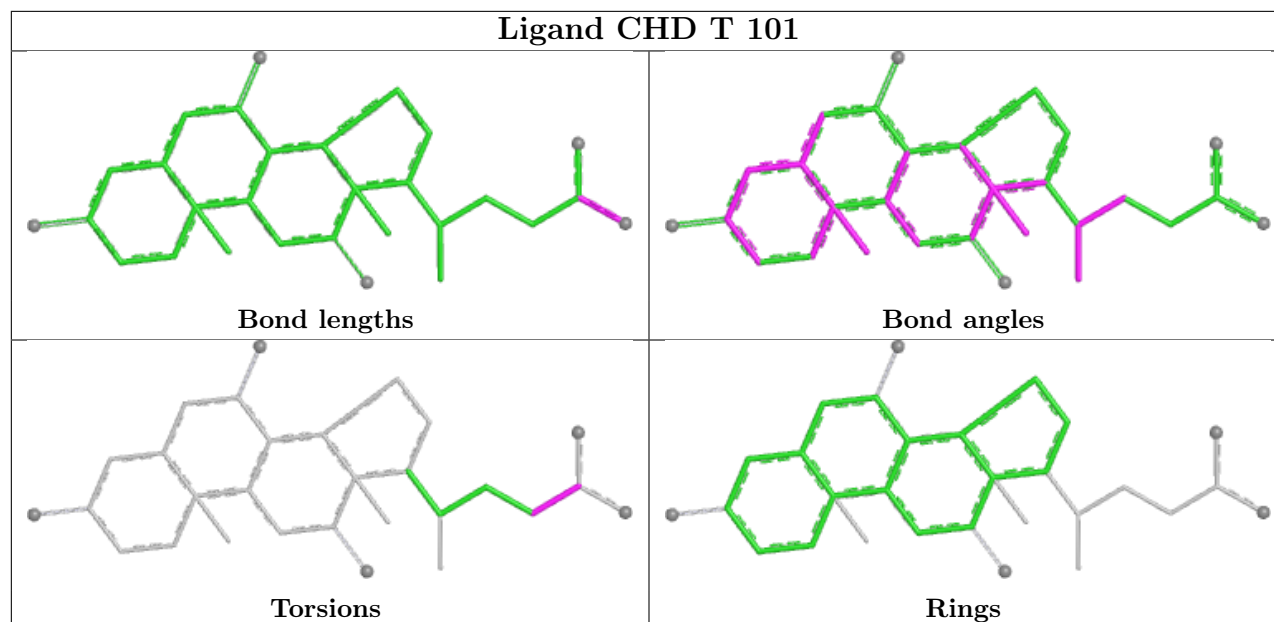


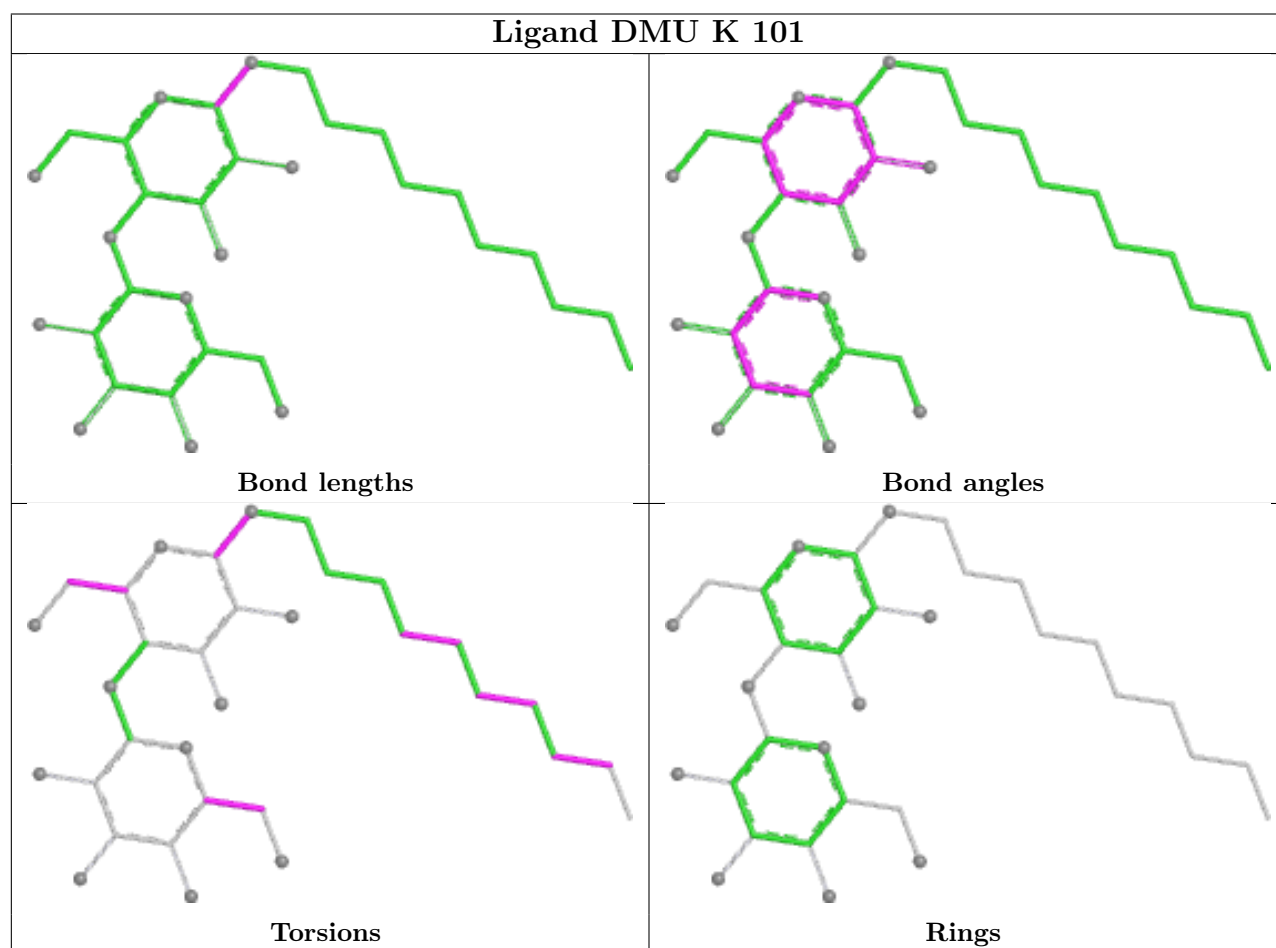
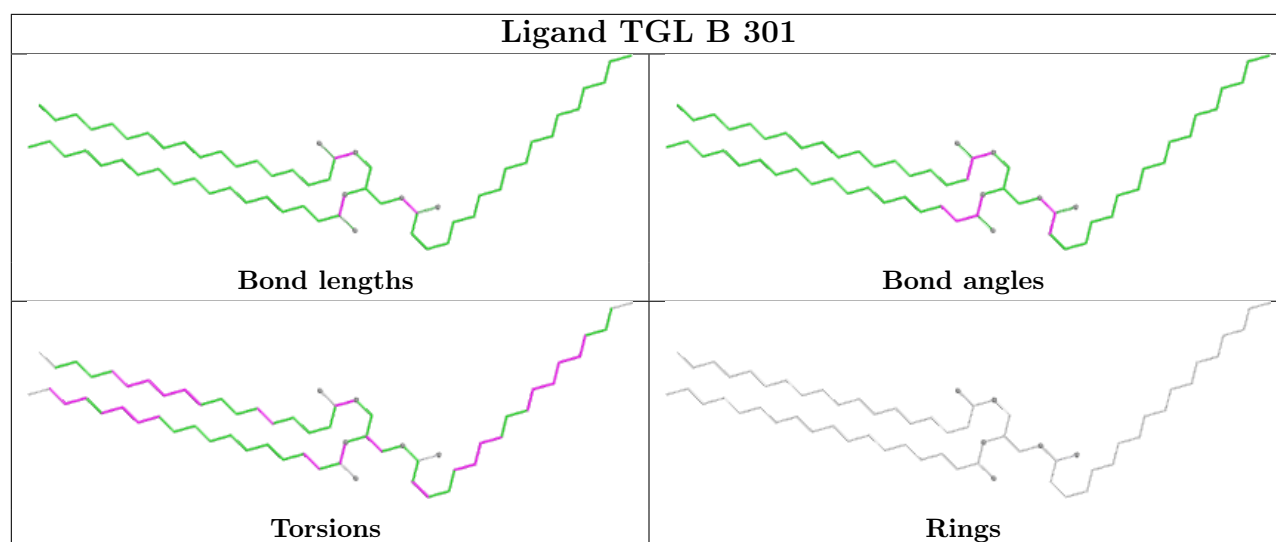


Ligand HEA N 601 (A)**Ligand DMU T 103**

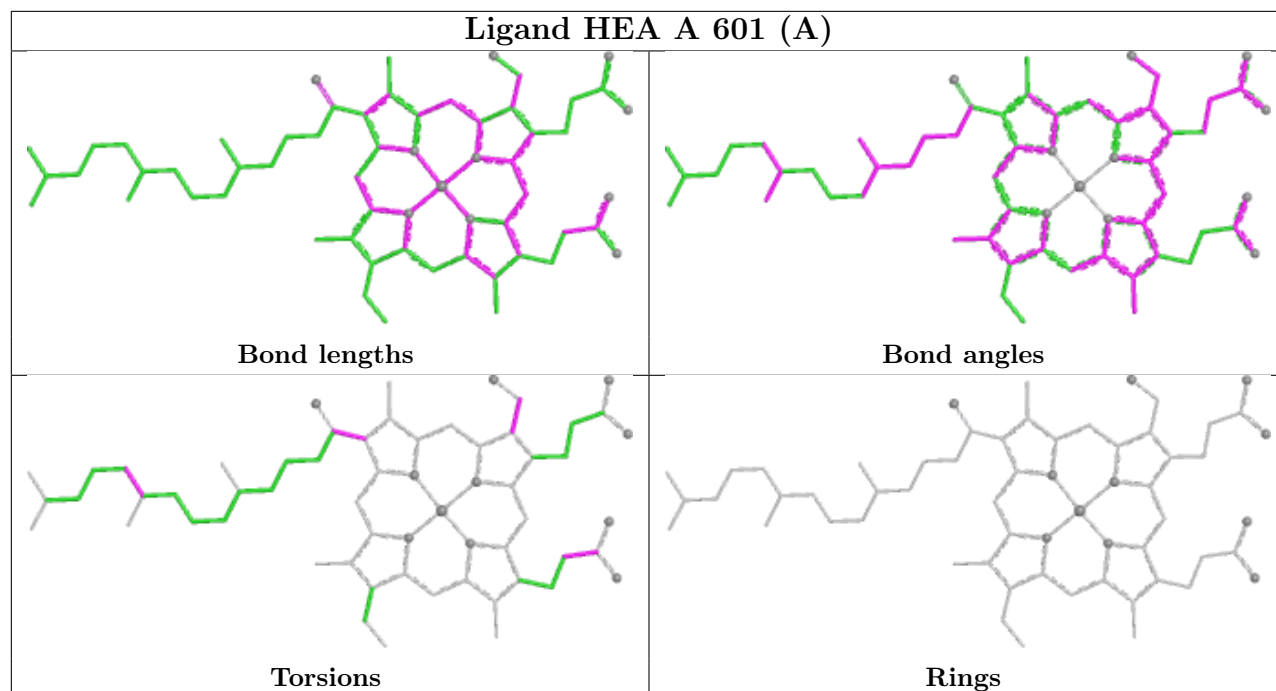




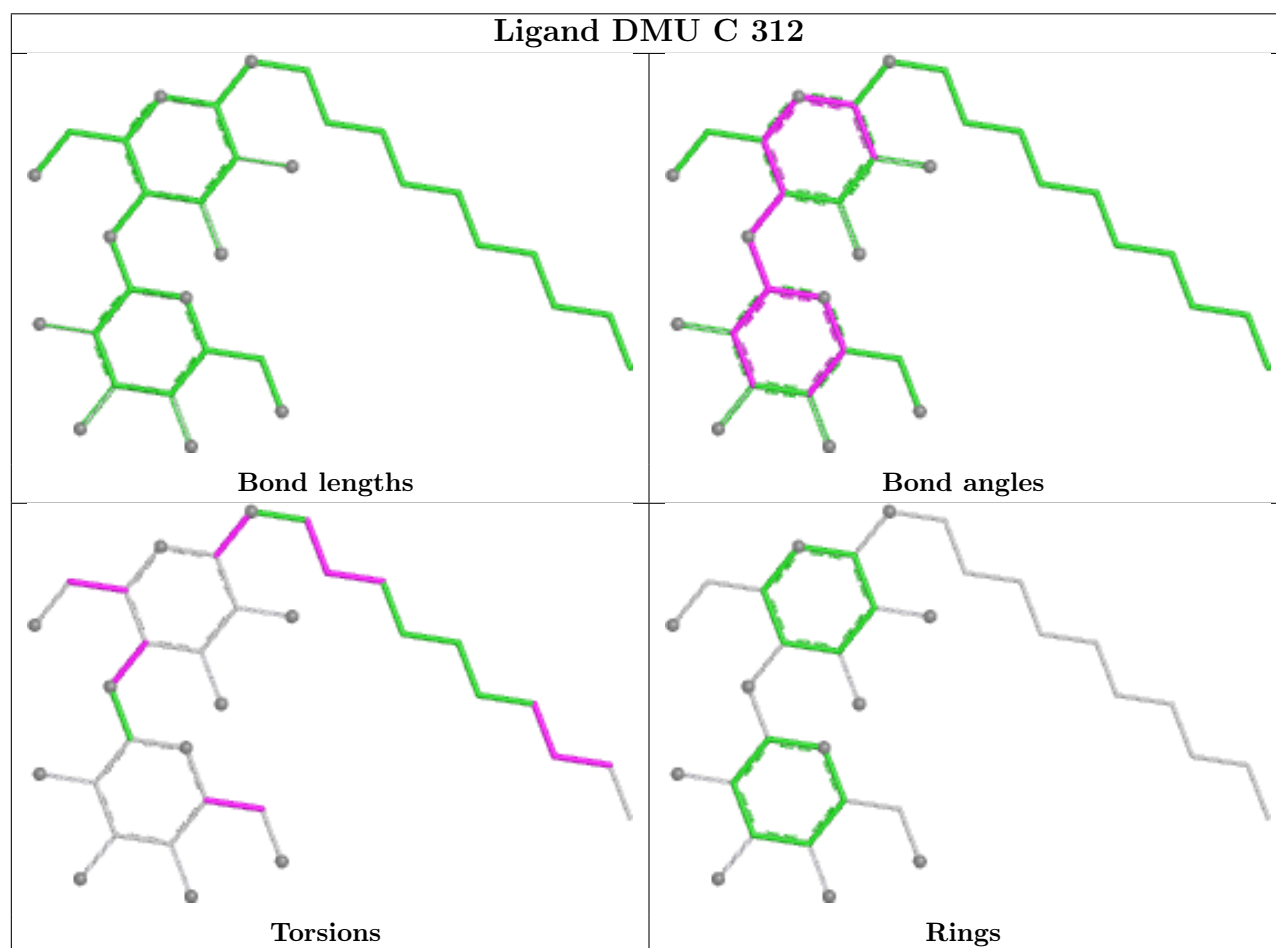


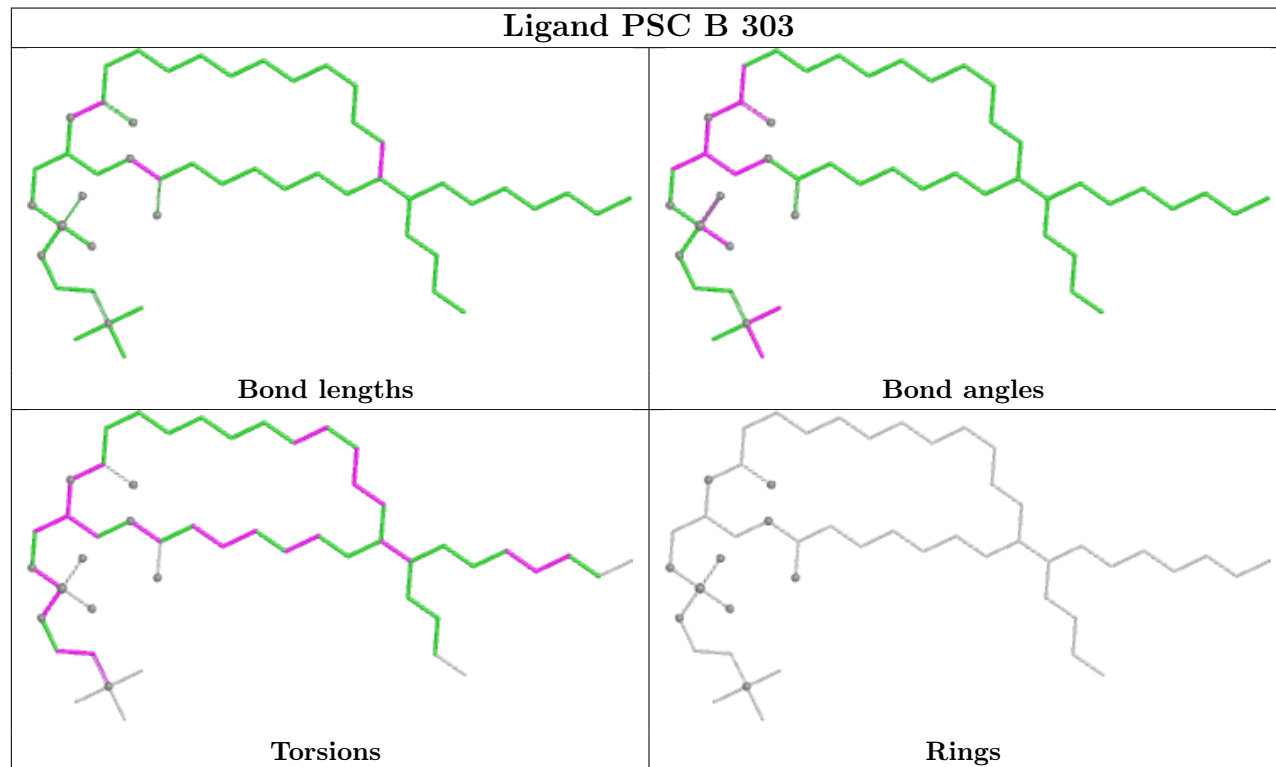
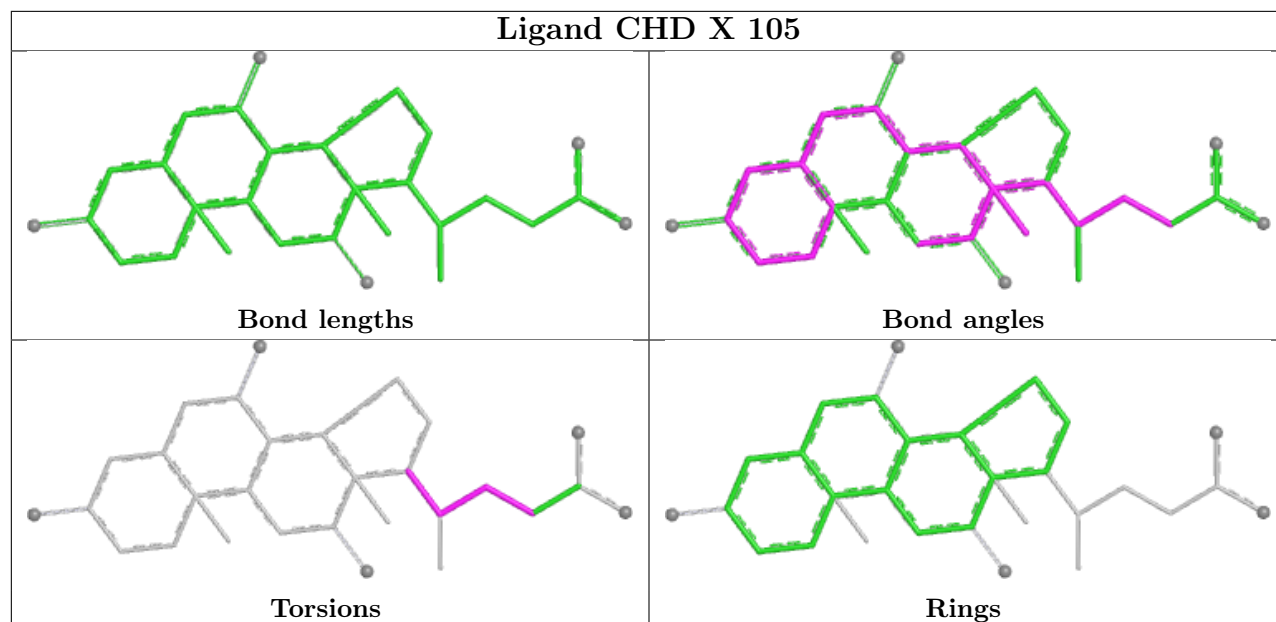


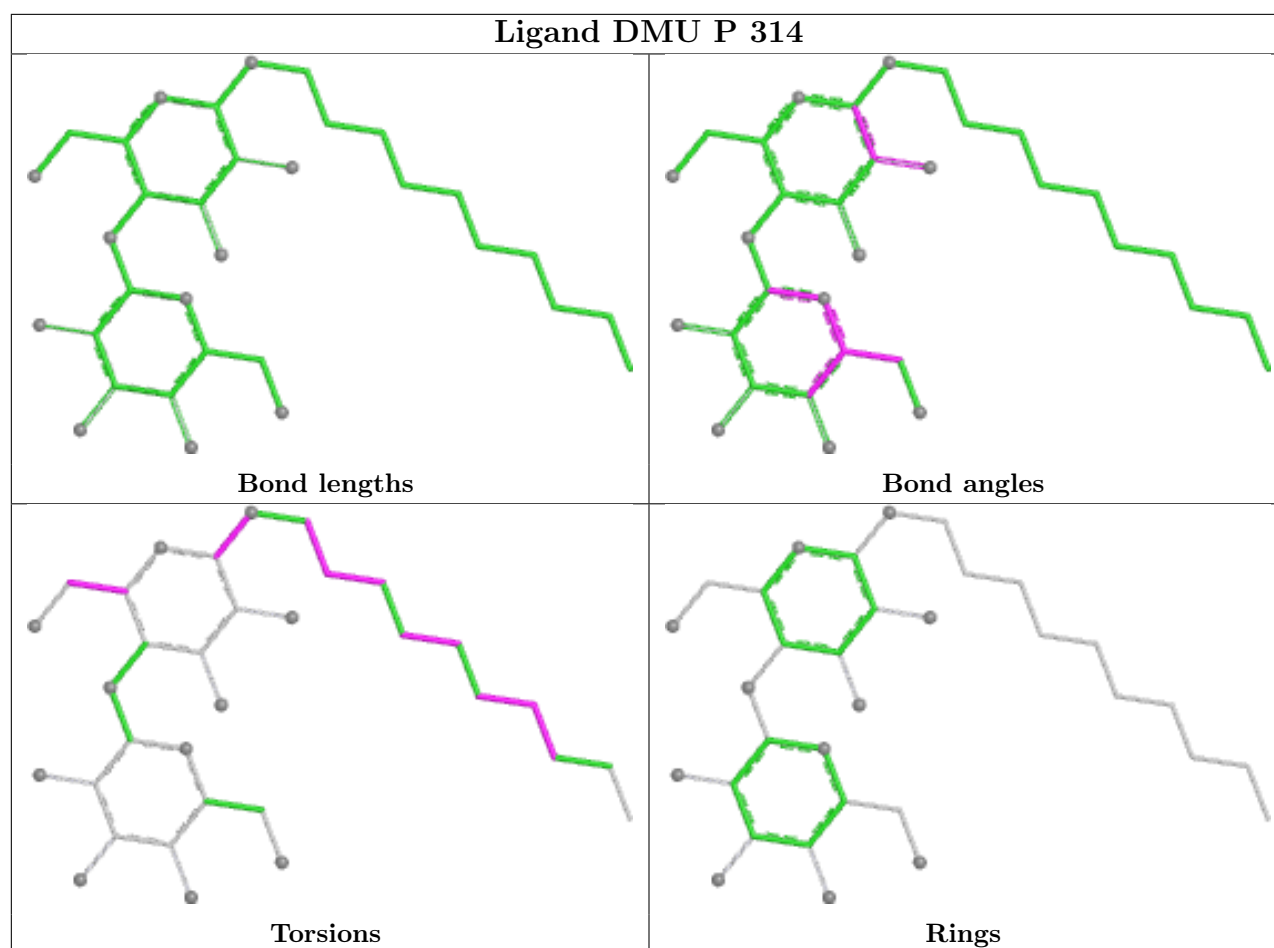
Ligand HEA A 601 (A)

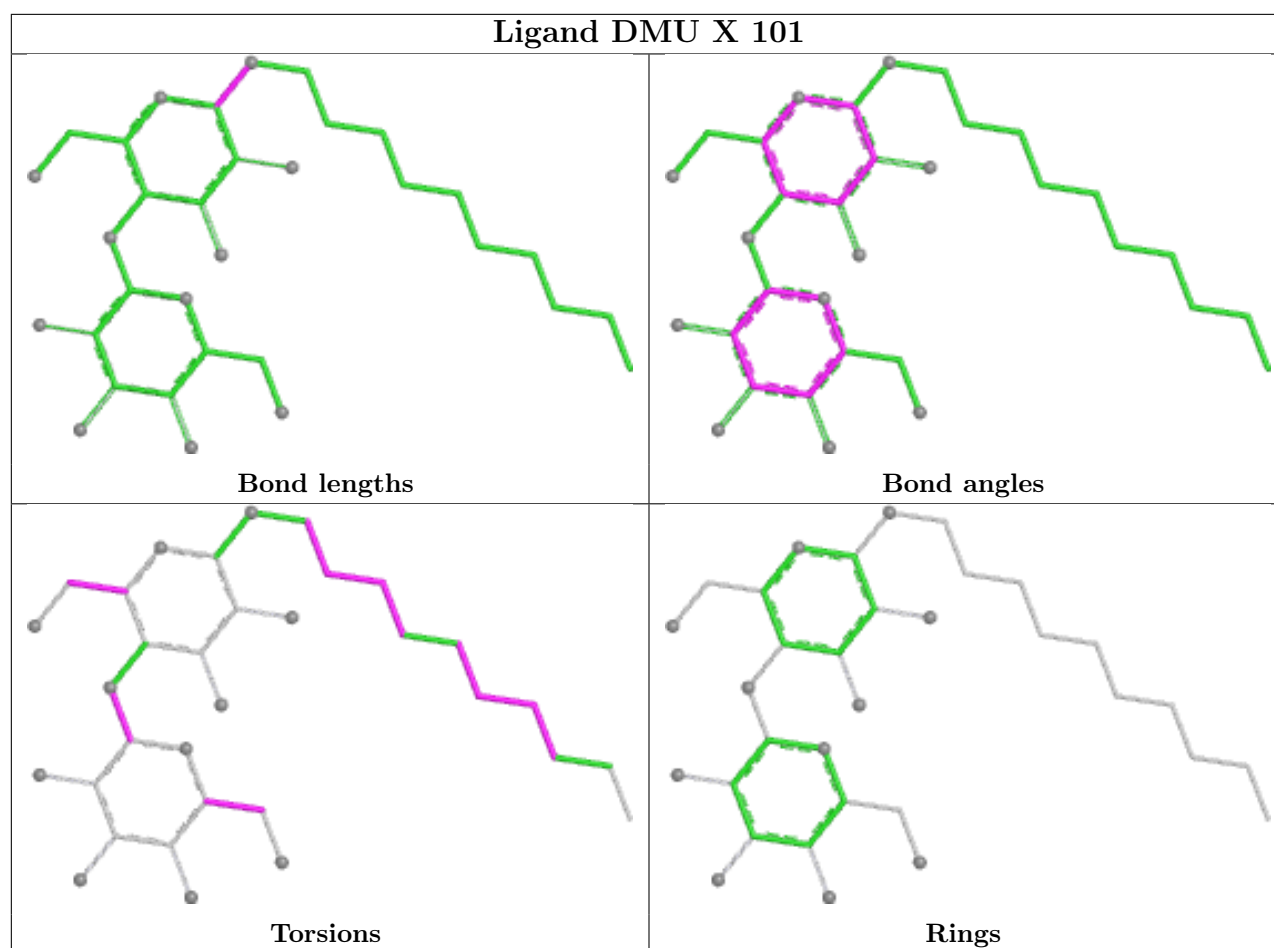


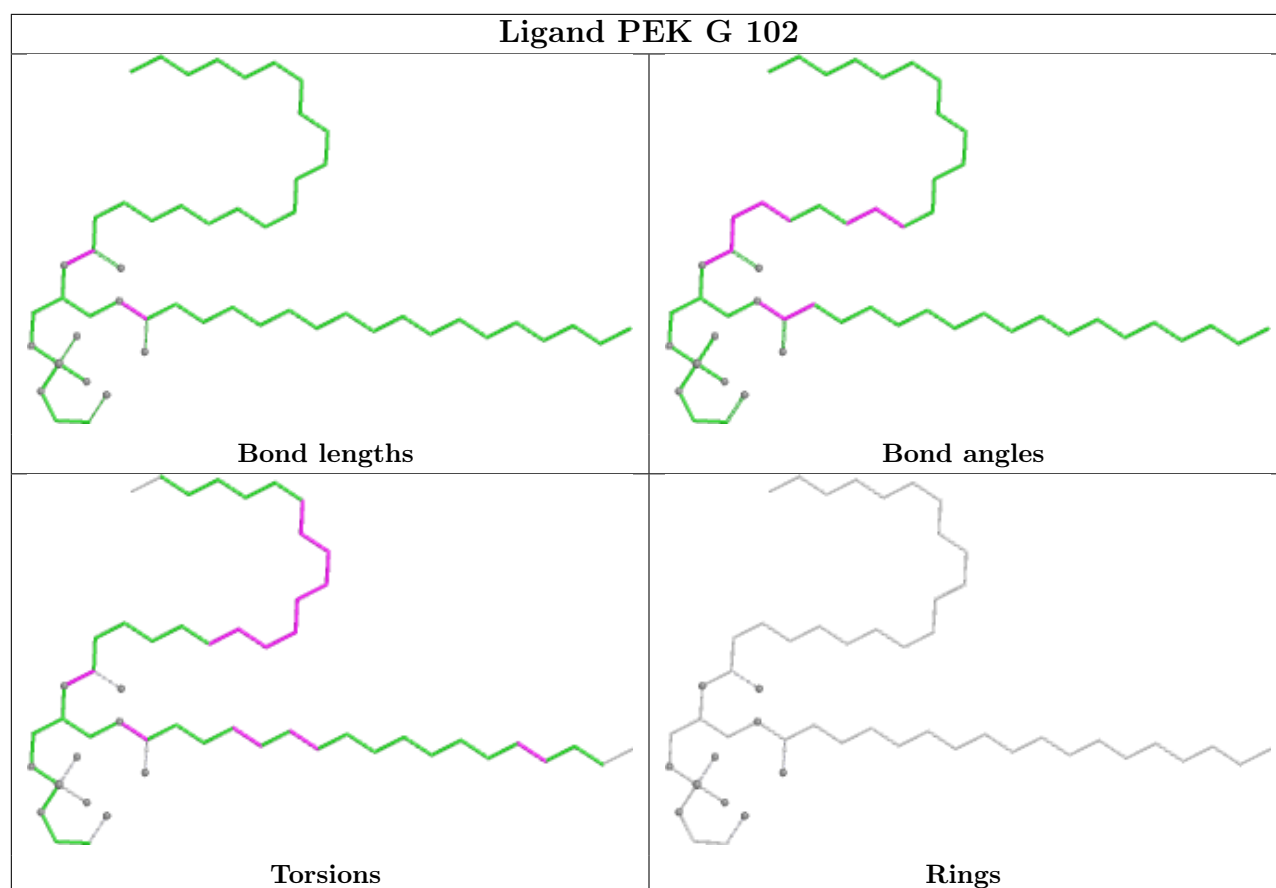
Ligand DMU C 312

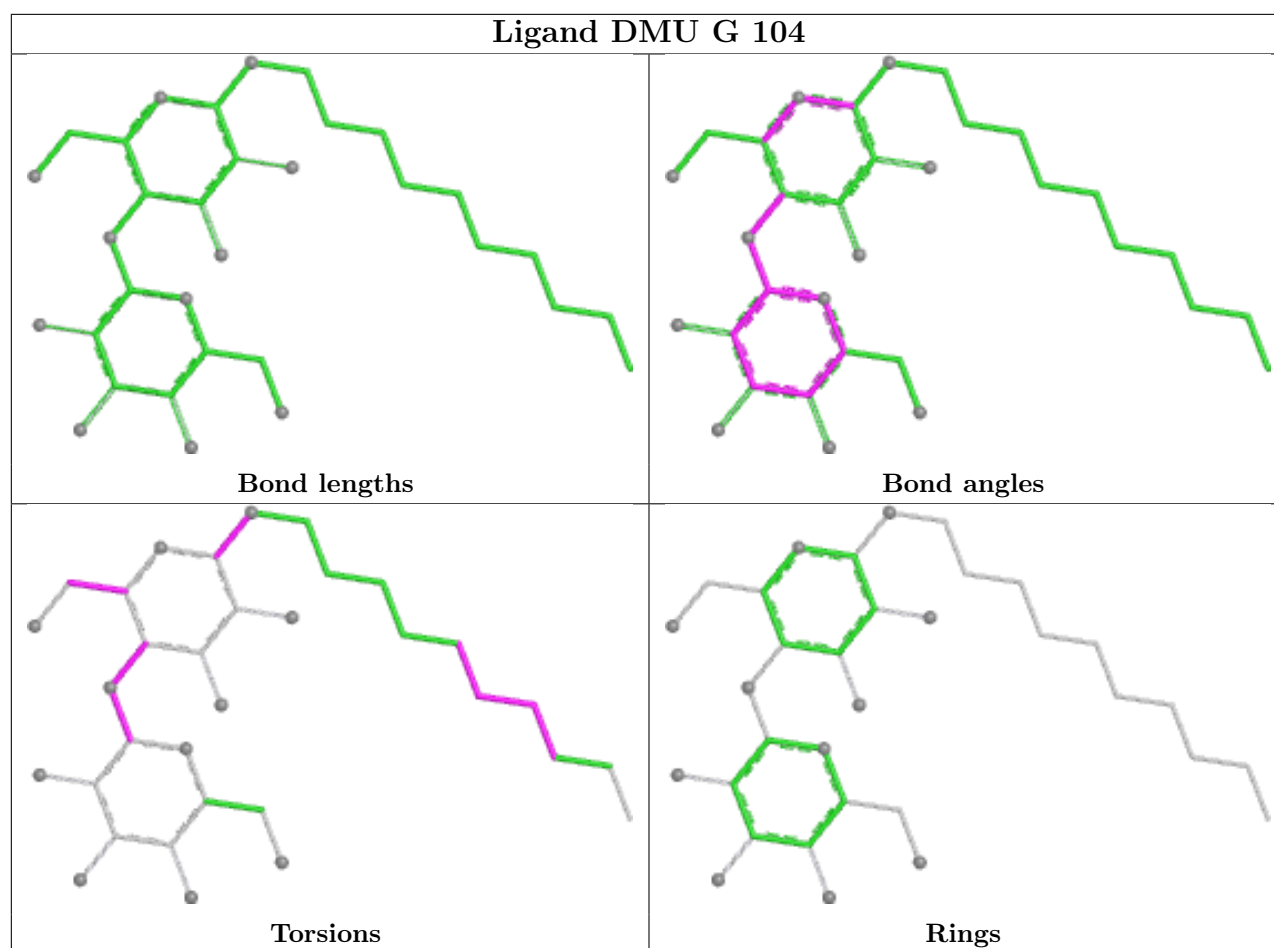


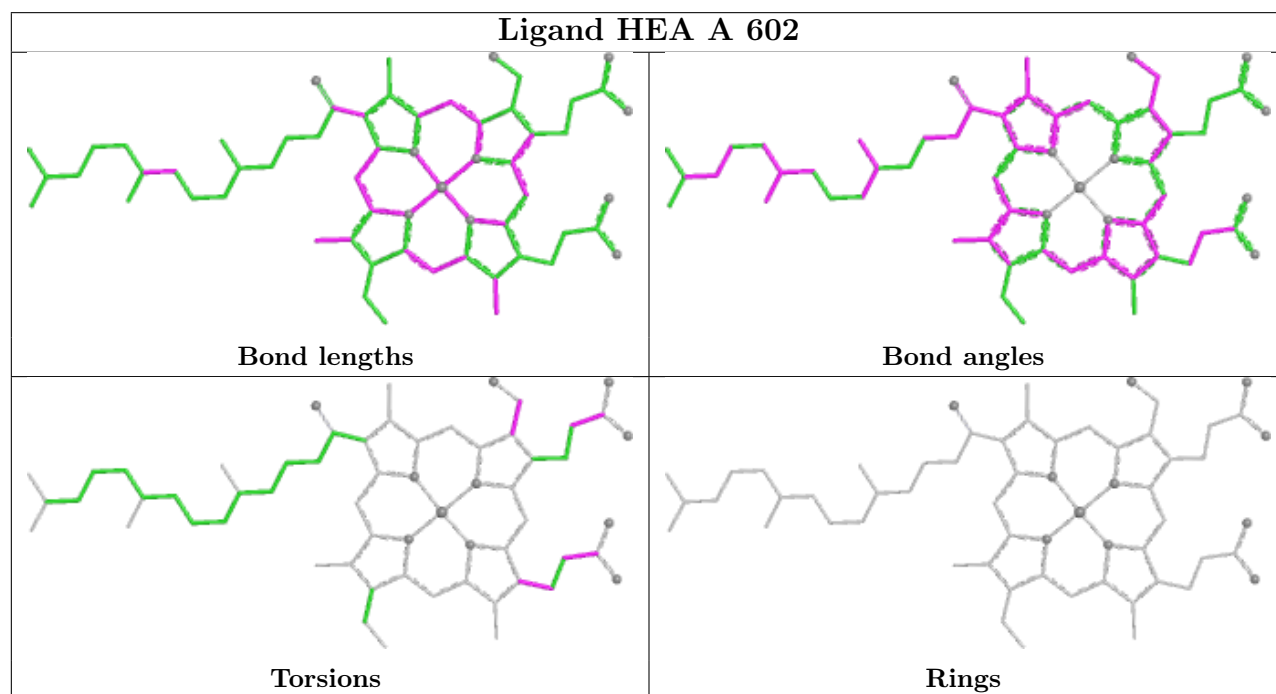
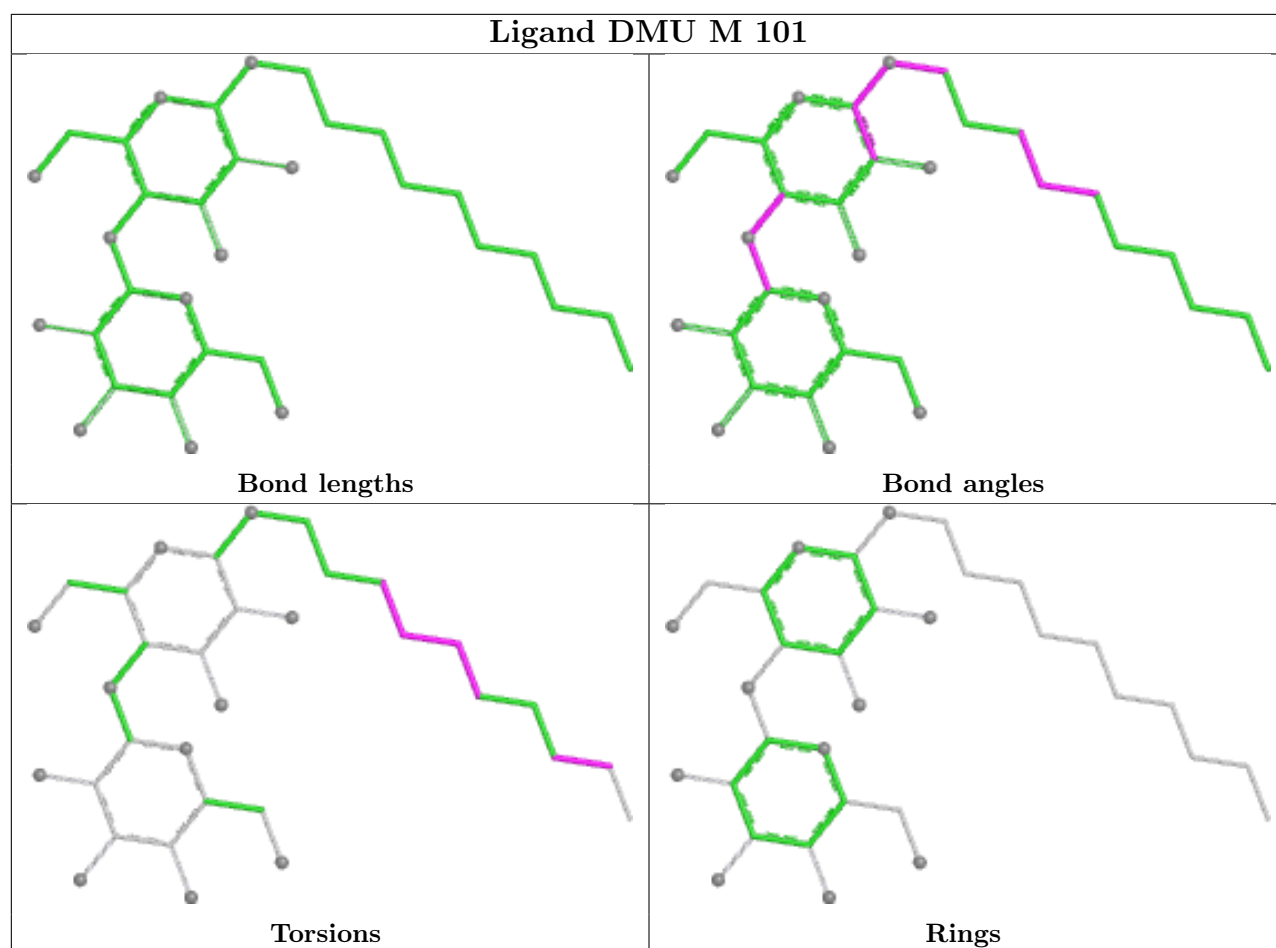


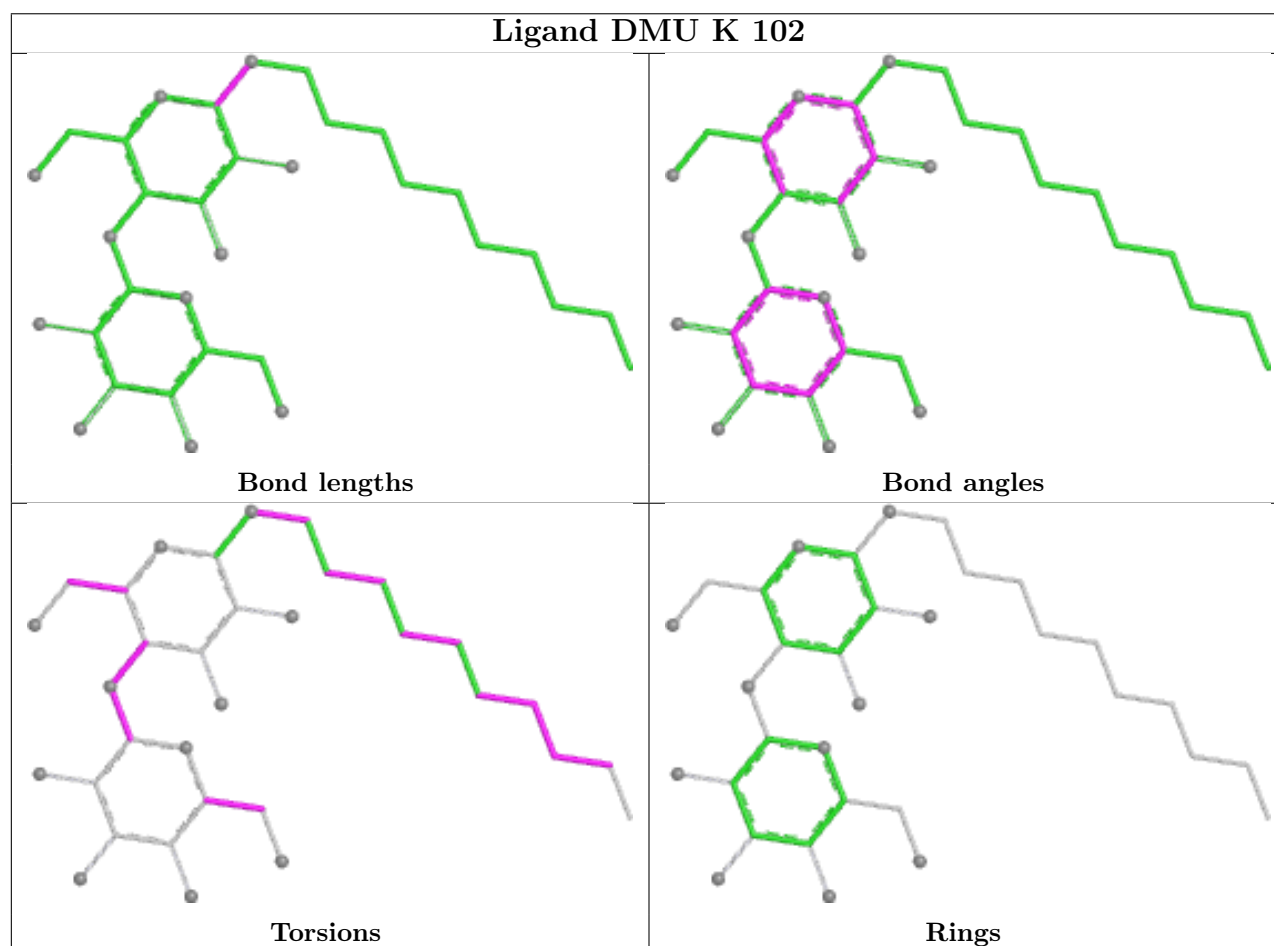
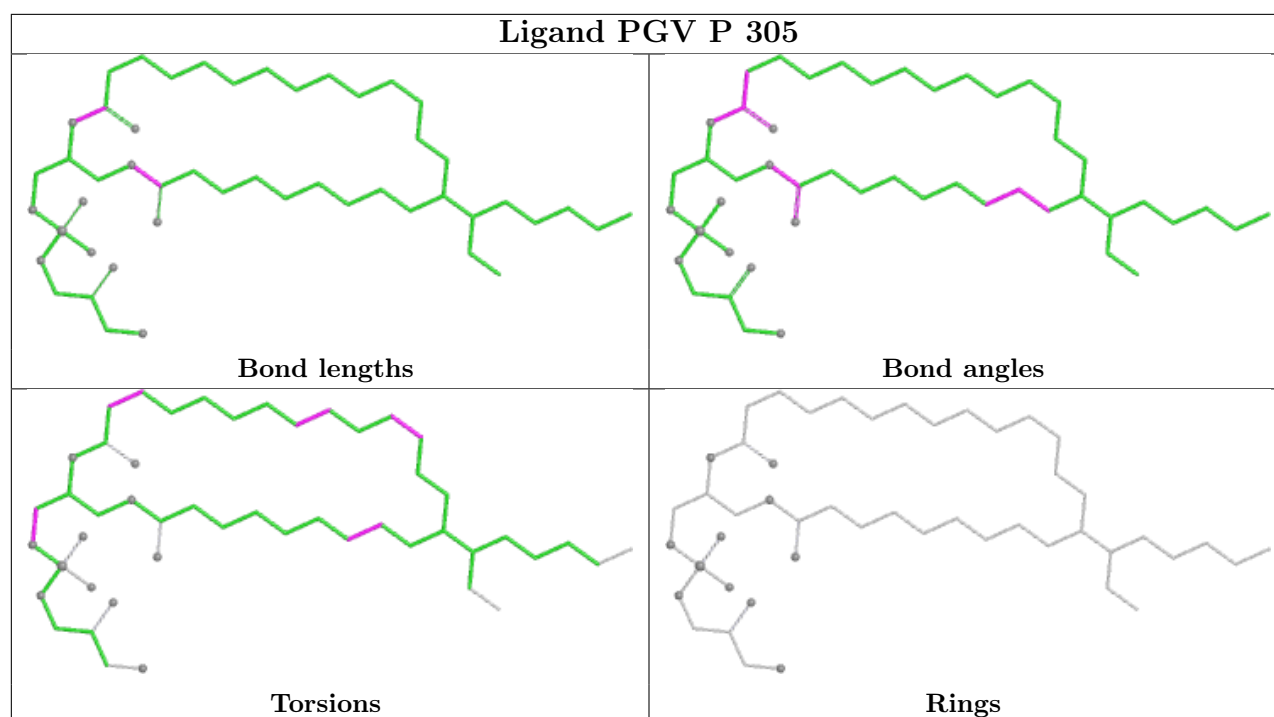


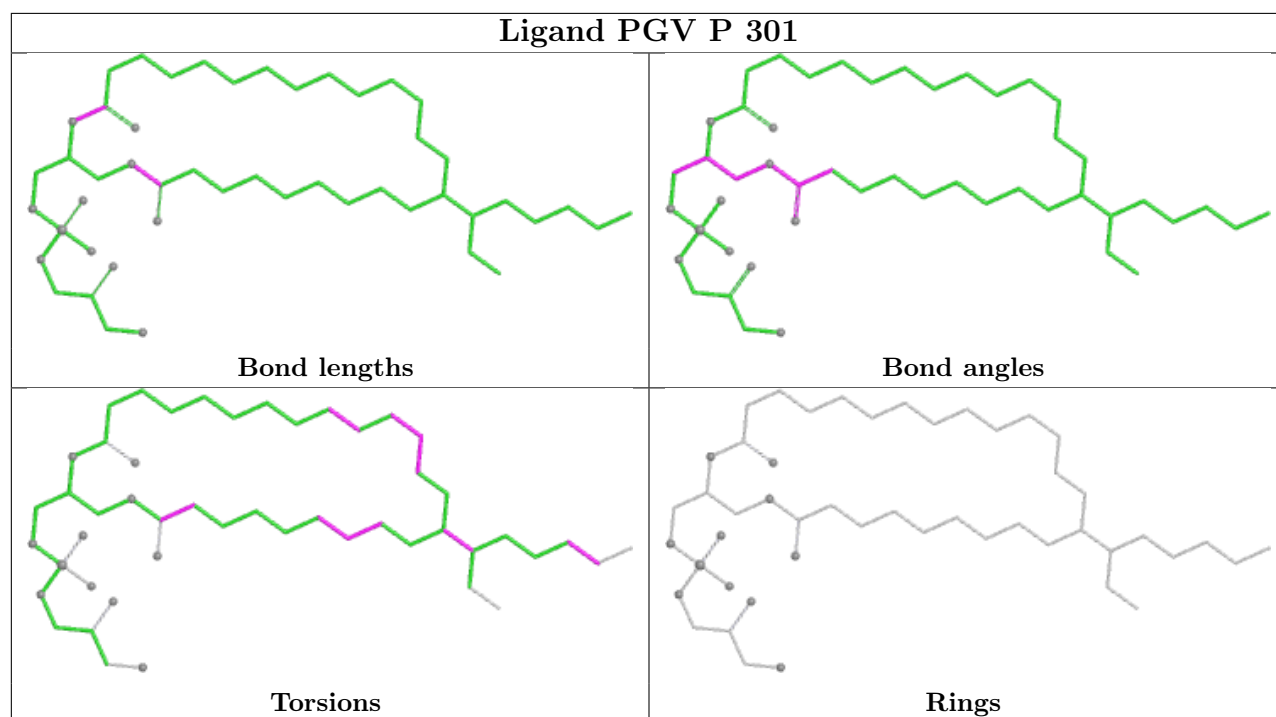
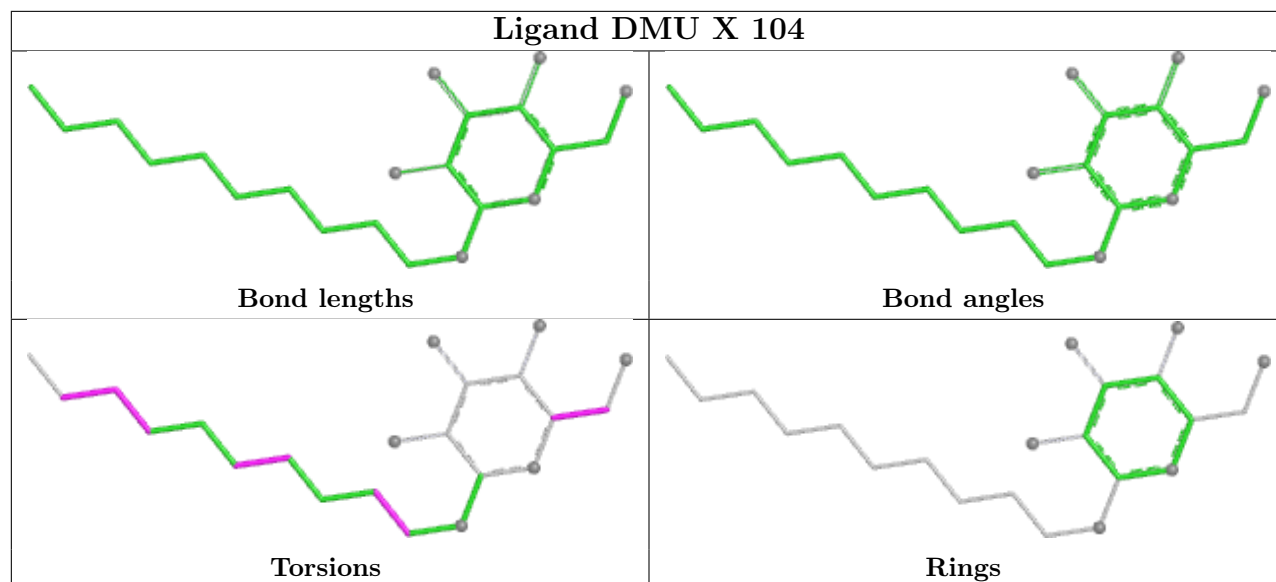


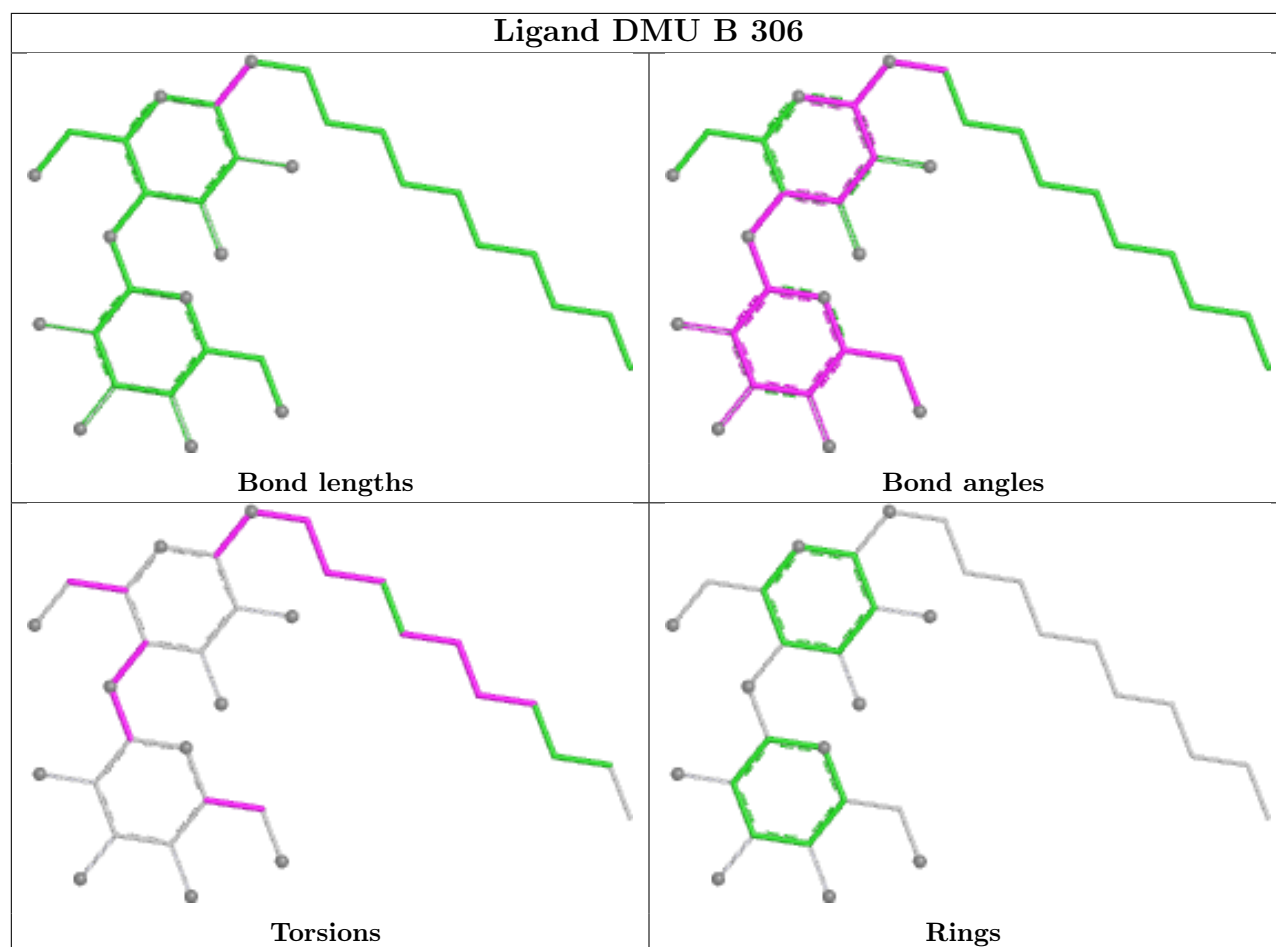
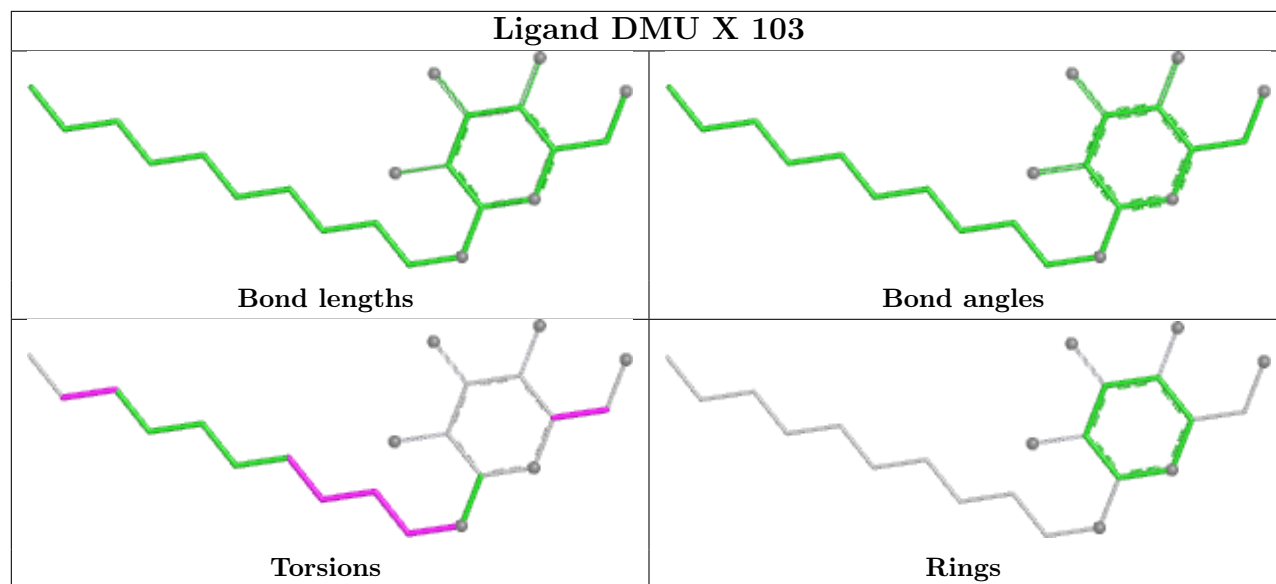


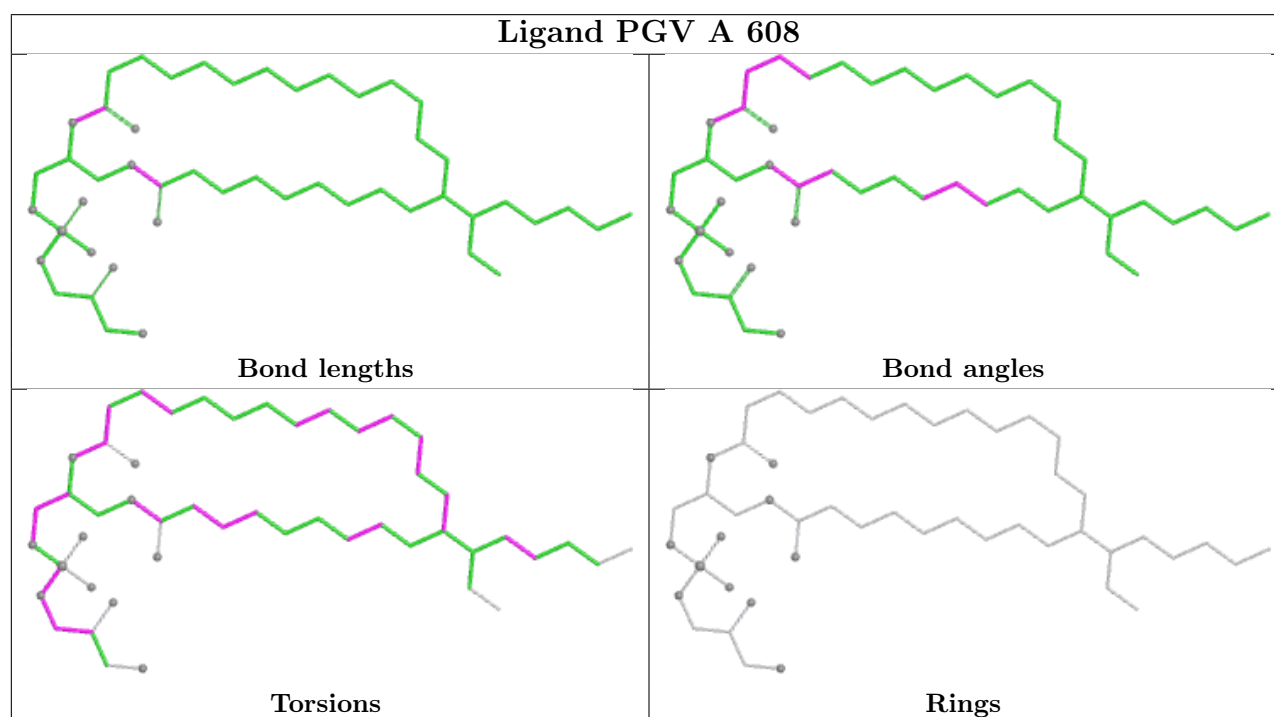
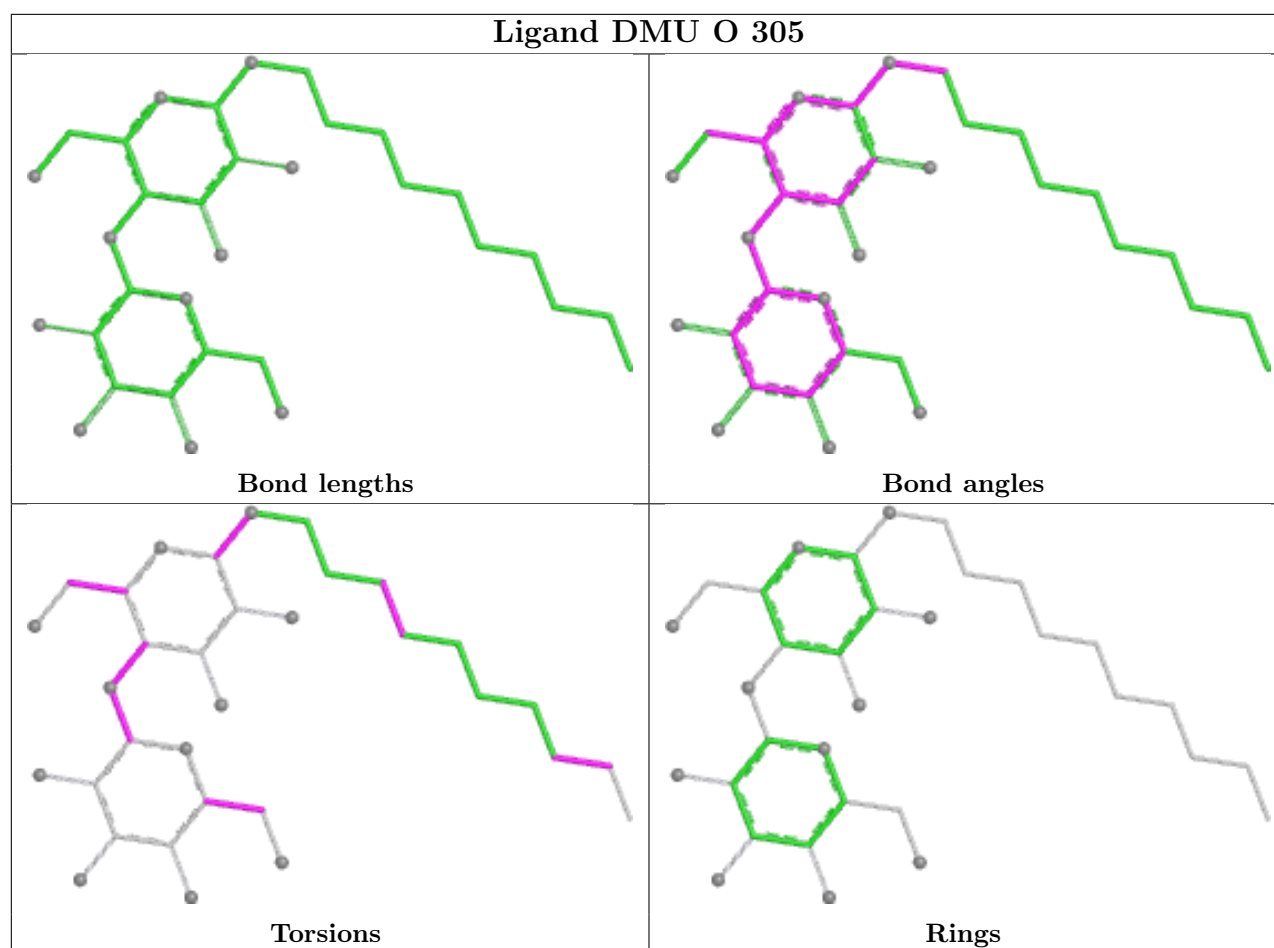


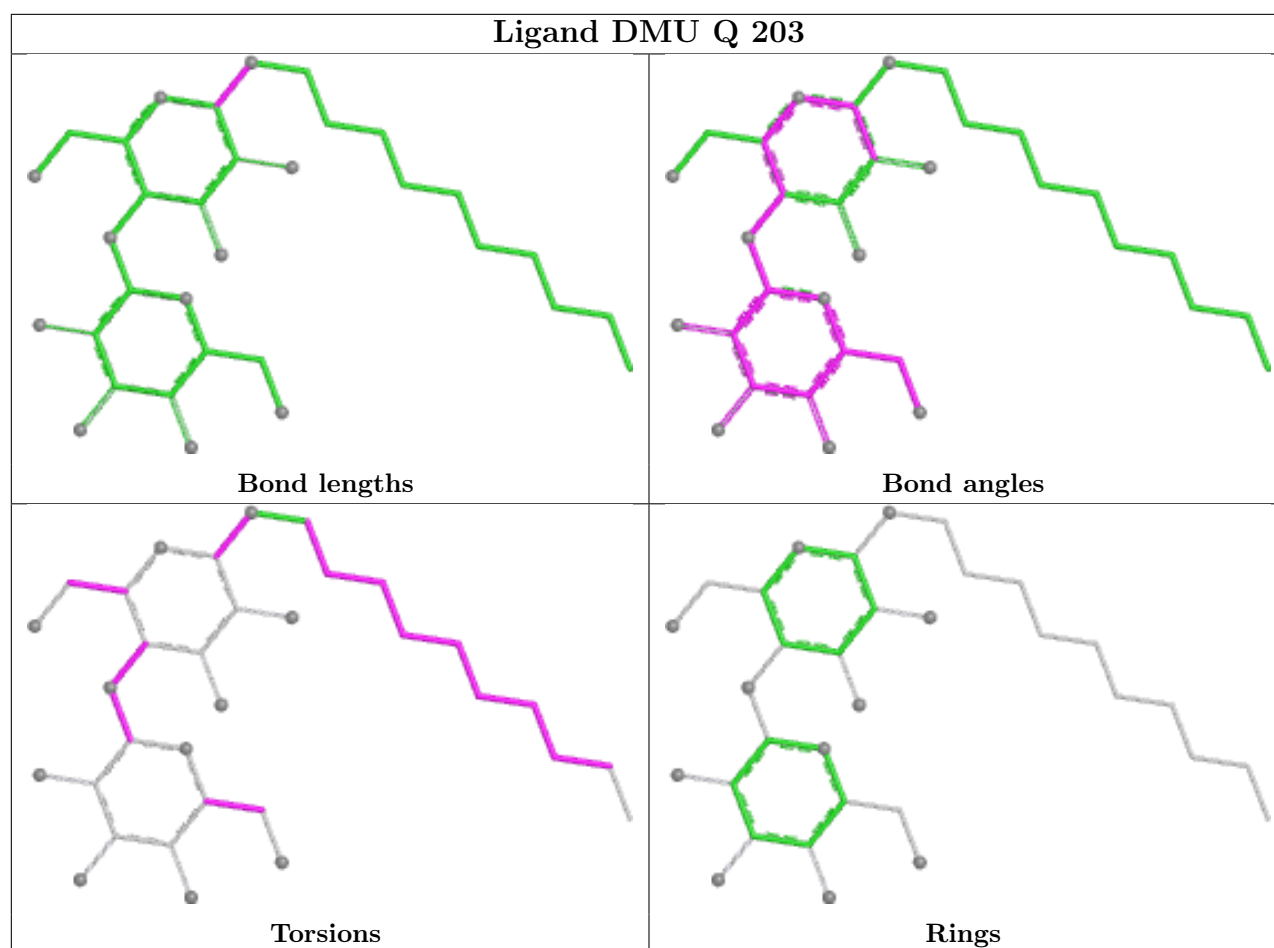


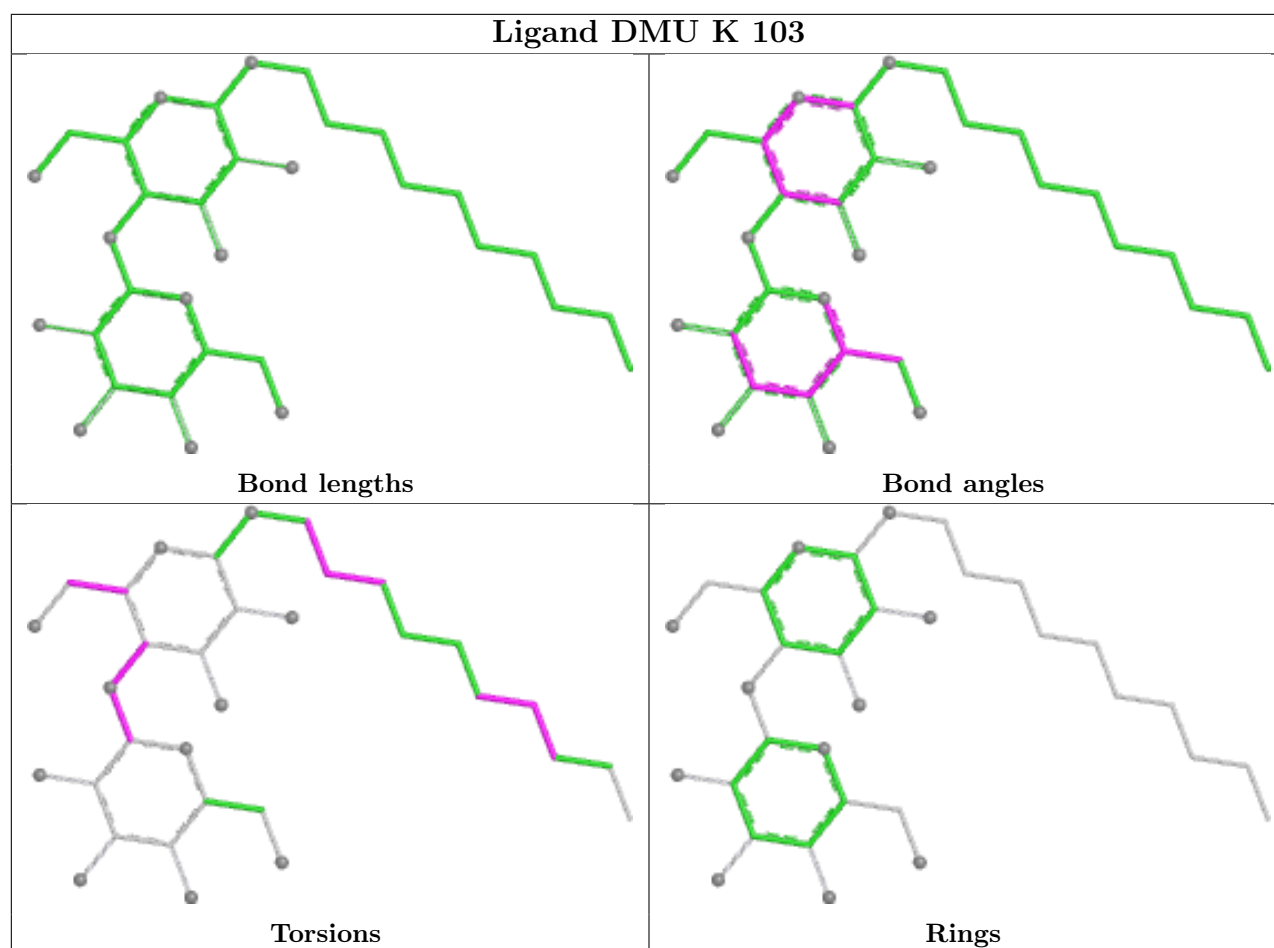


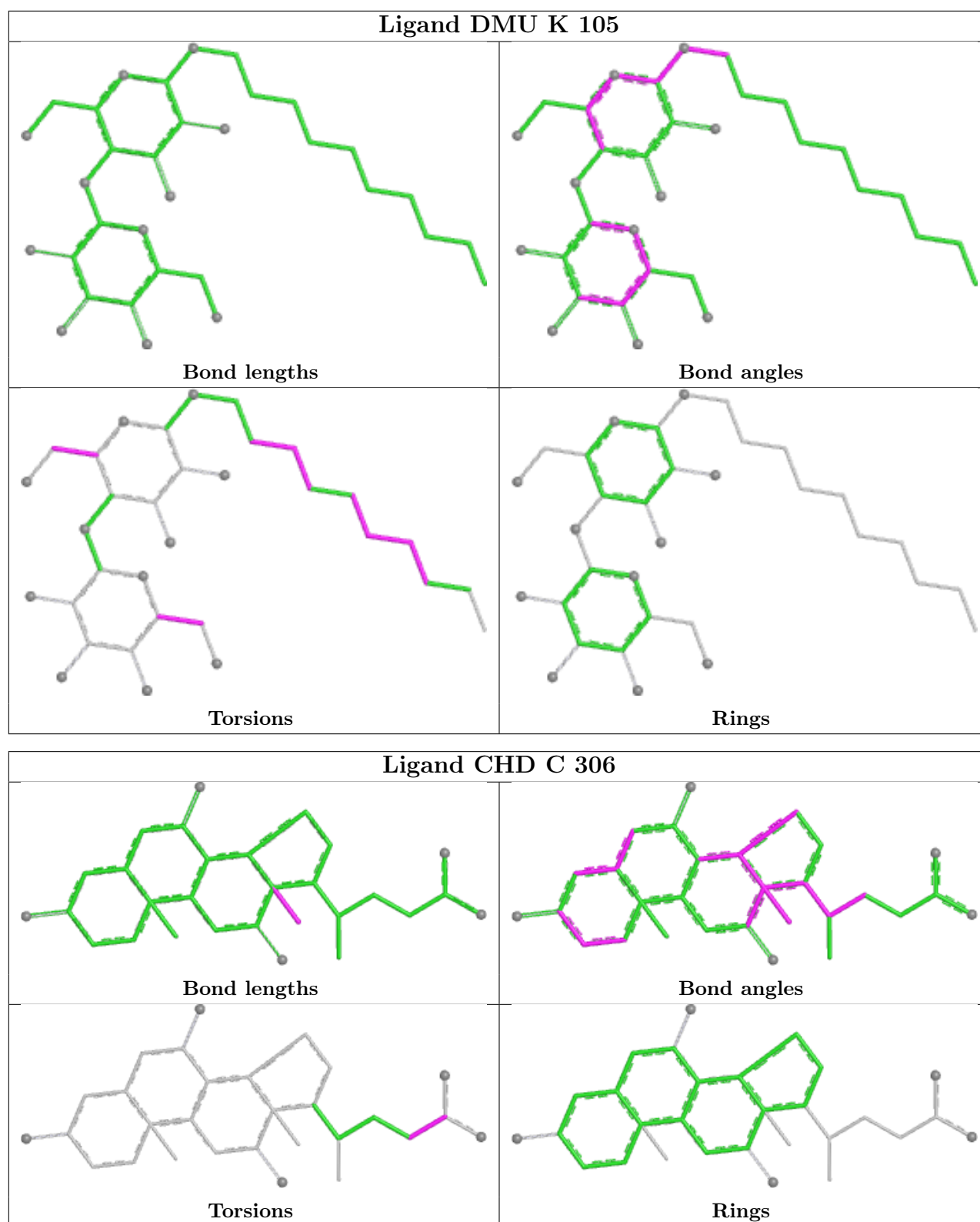












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	513/514 (99%)	-0.49	2 (0%) 88 90	13, 19, 28, 75	10 (1%)
1	N	513/514 (99%)	-0.36	3 (0%) 85 87	15, 22, 32, 67	7 (1%)
2	B	226/227 (99%)	0.07	11 (4%) 35 37	17, 26, 52, 93	3 (1%)
2	O	226/227 (99%)	0.32	15 (6%) 24 26	20, 31, 68, 124	4 (1%)
3	C	259/261 (99%)	-0.23	2 (0%) 82 85	17, 23, 37, 79	3 (1%)
3	P	259/261 (99%)	-0.18	3 (1%) 76 79	17, 24, 41, 80	2 (0%)
4	D	144/147 (97%)	0.16	6 (4%) 40 43	19, 28, 50, 95	1 (0%)
4	Q	144/147 (97%)	1.21	29 (20%) 3 2	26, 42, 87, 227	0
5	E	105/109 (96%)	0.10	4 (3%) 44 47	19, 28, 57, 141	0
5	R	105/109 (96%)	0.43	6 (5%) 29 31	24, 36, 61, 137	1 (0%)
6	F	98/98 (100%)	0.54	8 (8%) 17 18	18, 29, 105, 151	1 (1%)
6	S	98/98 (100%)	0.58	9 (9%) 14 15	19, 28, 94, 185	0
7	G	83/85 (97%)	1.28	26 (31%) 1 1	20, 32, 124, 163	0
7	T	83/85 (97%)	1.19	20 (24%) 2 1	20, 34, 114, 165	0
8	H	79/85 (92%)	0.97	13 (16%) 4 4	23, 35, 106, 153	0
8	U	79/85 (92%)	1.07	17 (21%) 2 2	27, 38, 131, 184	0
9	I	72/73 (98%)	1.00	14 (19%) 3 3	26, 39, 70, 87	0
9	V	72/73 (98%)	1.16	12 (16%) 4 4	25, 50, 75, 134	0
10	J	58/59 (98%)	0.68	8 (13%) 6 6	23, 34, 69, 106	0
10	W	58/59 (98%)	0.88	11 (18%) 3 3	24, 37, 78, 157	0
11	K	49/56 (87%)	0.49	2 (4%) 41 44	24, 35, 58, 62	0
11	X	49/56 (87%)	1.11	5 (10%) 12 12	36, 44, 65, 82	0
12	L	46/47 (97%)	0.17	2 (4%) 40 42	20, 26, 47, 94	1 (2%)
12	Y	46/47 (97%)	0.45	4 (8%) 16 17	23, 32, 69, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.24	4 (9%) 14 15	20, 26, 68, 101	0
13	Z	43/46 (93%)	0.77	7 (16%) 4 4	29, 36, 86, 126	0
All	All	3550/3614 (98%)	0.19	243 (6%) 23 24	13, 27, 67, 227	33 (0%)

The worst 5 of 243 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	1	ALA	10.7
6	S	1	ALA	9.0
8	H	44	THR	8.9
4	Q	5	VAL	8.8
4	Q	6	VAL	8.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
9	SAC	V	1	9/10	0.46	0.25	168,196,204,213	0
9	SAC	I	1	9/10	0.68	0.25	64,103,134,151	0
7	TPO	G	11	11/12	0.70	0.29	102,138,168,184	0
7	TPO	T	11	11/12	0.84	0.21	37,90,131,149	0
1	FME	N	1	10/11	0.91	0.12	30,45,72,79	0
1	FME	A	1	10/11	0.93	0.10	30,35,87,99	0
2	FME	B	1	10/11	0.96	0.10	15,24,35,116	0
2	FME	O	1	10/11	0.97	0.09	25,35,45,96	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
21	DMU	B	306	33/33	0.57	0.18	46,75,90,95	0
27	CHD	X	105	29/29	0.60	0.28	91,122,143,147	0
21	DMU	K	105	33/33	0.62	0.25	45,140,194,202	0
21	DMU	A	616	33/33	0.64	0.21	56,130,180,189	0
21	DMU	X	101	33/33	0.66	0.23	45,136,220,232	0
27	CHD	J	101	29/29	0.69	0.23	36,97,125,132	0
21	DMU	K	104	33/33	0.70	0.22	55,109,174,183	0
21	DMU	P	316	33/33	0.71	0.21	45,72,87,88	0
27	CHD	W	101	29/29	0.71	0.22	48,87,120,129	0
21	DMU	X	103	22/33	0.71	0.24	44,114,175,179	0
21	DMU	C	312	33/33	0.72	0.23	40,102,147,166	0
27	CHD	L	103	29/29	0.72	0.23	43,92,143,156	0
21	DMU	Q	203	33/33	0.72	0.18	50,70,87,89	0
21	DMU	X	104	22/33	0.72	0.20	50,86,128,134	0
21	DMU	K	103	33/33	0.73	0.23	46,125,193,196	0
21	DMU	D	202	33/33	0.73	0.19	45,120,185,206	0
27	CHD	Y	102	29/29	0.74	0.25	51,96,128,136	0
19	PGV	C	308	51/51	0.75	0.21	38,73,130,148	0
21	DMU	O	305	33/33	0.76	0.19	39,118,177,200	0
19	PGV	P	302	51/51	0.78	0.20	39,75,131,156	0
21	DMU	X	102	22/33	0.78	0.23	51,87,176,183	0
25	PEK	C	309	53/53	0.78	0.23	38,89,140,147	0
26	CDL	G	101	100/100	0.78	0.21	37,78,128,171	0
26	CDL	T	102	100/100	0.78	0.21	36,85,128,174	0
25	PEK	C	307	53/53	0.79	0.21	30,67,125,163	0
22	TGL	Q	201	63/63	0.80	0.20	34,64,99,123	0
24	PSC	B	303	52/52	0.80	0.22	29,85,150,174	0
21	DMU	P	314	33/33	0.80	0.21	44,95,145,181	0
21	DMU	T	103	33/33	0.80	0.18	43,92,177,189	0
25	PEK	G	102	53/53	0.80	0.22	35,84,135,144	0
19	PGV	N	607	51/51	0.80	0.21	29,74,124,175	0
21	DMU	L	102	33/33	0.81	0.20	45,90,142,145	0
25	PEK	P	309	53/53	0.81	0.22	31,69,134,199	0
27	CHD	P	307	29/29	0.81	0.16	37,57,80,101	0
20	EDO	A	609	4/4	0.82	0.17	34,65,68,70	0
21	DMU	K	101	33/33	0.82	0.20	41,96,158,172	0
21	DMU	K	102	33/33	0.82	0.19	40,137,212,226	0
20	EDO	N	614	4/4	0.82	0.13	38,46,50,53	0
20	EDO	S	105	4/4	0.82	0.17	50,56,81,100	0
21	DMU	G	104	33/33	0.83	0.17	44,93,162,176	0
22	TGL	D	201	63/63	0.83	0.19	25,56,92,141	0
20	EDO	P	310	4/4	0.83	0.17	36,41,65,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	PGV	A	608	51/51	0.83	0.20	24,62,119,169	0
21	DMU	K	106	33/33	0.84	0.20	37,128,202,207	0
24	PSC	N	608	52/52	0.84	0.20	26,80,141,151	0
27	CHD	C	305	29/29	0.84	0.14	38,56,79,104	0
20	EDO	O	304	4/4	0.85	0.14	40,61,63,67	0
26	CDL	C	304	100/100	0.85	0.18	15,70,122,136	0
22	TGL	L	101	63/63	0.85	0.18	23,52,106,155	0
26	CDL	P	306	100/100	0.85	0.19	21,78,136,154	0
20	EDO	P	313	4/4	0.86	0.15	28,43,51,66	0
22	TGL	O	301	63/63	0.86	0.18	29,69,101,117	0
20	EDO	N	618	4/4	0.86	0.17	49,51,55,101	0
22	TGL	Y	101	63/63	0.86	0.18	29,62,103,122	0
20	EDO	F	105	4/4	0.86	0.17	45,45,75,75	0
22	TGL	B	301	63/63	0.86	0.16	26,59,100,113	0
20	EDO	F	104	4/4	0.86	0.19	45,45,67,73	0
29	PO4	H	101	5/5	0.86	0.11	58,61,79,149	0
29	PO4	U	101	5/5	0.86	0.12	48,52,113,186	0
20	EDO	B	304	4/4	0.88	0.15	31,56,61,72	0
20	EDO	N	619	4/4	0.88	0.17	45,52,58,70	0
20	EDO	W	103	4/4	0.88	0.17	45,47,50,68	0
20	EDO	Y	103	4/4	0.88	0.13	53,59,59,70	0
20	EDO	P	312	4/4	0.88	0.13	40,50,56,61	0
20	EDO	N	615	4/4	0.89	0.16	28,52,52,53	0
20	EDO	L	104	4/4	0.89	0.12	45,45,51,58	0
20	EDO	M	102	4/4	0.90	0.10	44,46,46,67	0
20	EDO	A	613	4/4	0.90	0.13	30,42,53,62	0
20	EDO	N	620	4/4	0.92	0.16	45,47,56,72	0
20	EDO	L	105	4/4	0.92	0.13	45,52,55,62	0
21	DMU	Z	101	33/33	0.92	0.10	25,52,70,76	0
20	EDO	R	201	4/4	0.92	0.13	45,45,50,50	0
20	EDO	S	104	4/4	0.92	0.13	28,37,45,46	0
21	DMU	M	101	33/33	0.92	0.10	27,38,63,68	0
20	EDO	F	103	4/4	0.92	0.11	33,33,38,51	0
20	EDO	N	617	4/4	0.93	0.12	44,48,53,81	0
20	EDO	N	613	4/4	0.93	0.21	31,38,40,103	0
20	EDO	G	105	4/4	0.93	0.14	45,45,45,45	0
20	EDO	S	106	4/4	0.93	0.10	34,35,46,54	0
20	EDO	S	107	4/4	0.93	0.14	45,51,52,55	0
20	EDO	W	102	4/4	0.93	0.10	52,52,66,80	0
17	NA	P	303	1/1	0.93	0.07	42,42,42,42	0
20	EDO	O	303	4/4	0.94	0.08	20,21,27,32	0
20	EDO	A	614	4/4	0.94	0.10	37,41,48,59	0

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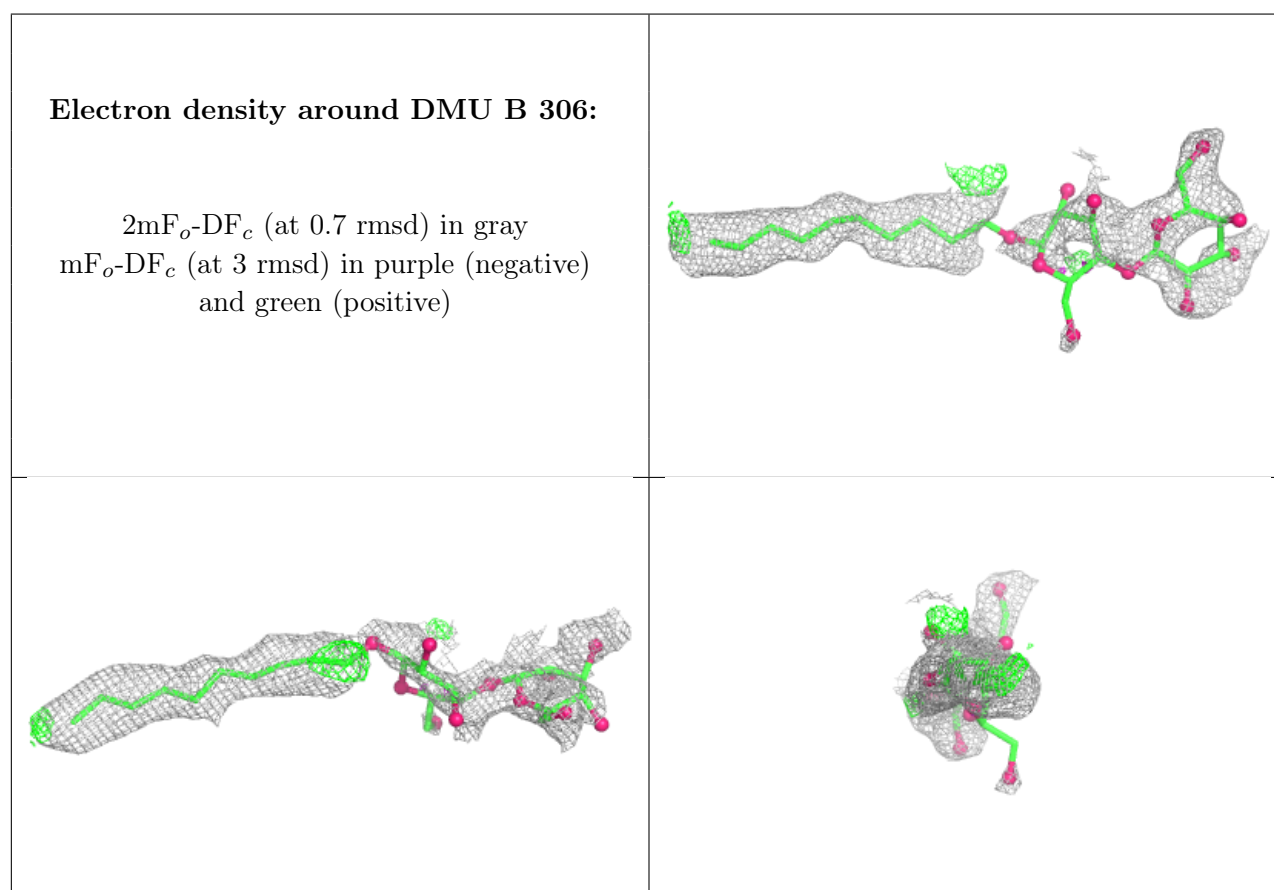
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	CHD	P	308	29/29	0.94	0.07	17,25,33,42	0
25	PEK	C	302	53/53	0.94	0.12	19,37,81,96	0
20	EDO	P	315	4/4	0.94	0.13	45,45,45,48	0
17	NA	C	301	1/1	0.94	0.15	58,58,58,58	0
20	EDO	P	311	4/4	0.94	0.18	34,36,43,44	0
25	PEK	P	304	53/53	0.94	0.12	22,39,106,120	0
27	CHD	C	306	29/29	0.95	0.07	18,26,33,37	0
20	EDO	N	609	4/4	0.95	0.07	19,25,27,28	0
20	EDO	N	611	4/4	0.95	0.09	31,32,38,47	0
20	EDO	N	616	4/4	0.95	0.08	32,38,39,48	0
20	EDO	C	311	4/4	0.95	0.11	23,27,47,49	0
19	PGV	C	303	51/51	0.96	0.09	15,26,67,85	0
27	CHD	G	103	29/29	0.96	0.06	16,21,28,36	0
20	EDO	B	305	4/4	0.96	0.07	17,19,25,30	0
20	EDO	C	310	4/4	0.96	0.07	26,31,32,34	0
20	EDO	N	610	4/4	0.96	0.08	24,25,31,40	0
19	PGV	A	607	51/51	0.96	0.09	17,30,63,68	0
20	EDO	A	611	4/4	0.96	0.11	25,31,56,74	0
20	EDO	A	612	4/4	0.96	0.14	24,26,62,82	0
17	NA	N	605	1/1	0.96	0.05	25,25,25,25	0
19	PGV	P	301	51/51	0.96	0.10	17,32,72,81	0
20	EDO	A	615	4/4	0.96	0.07	22,26,27,37	0
19	PGV	P	305	51/51	0.97	0.08	13,27,75,97	0
27	CHD	T	101	29/29	0.97	0.06	16,22,26,39	0
18	PER	N	606	2/2	0.97	0.10	17,17,17,18	0
18	PER	A	606	2/2	0.97	0.09	12,12,12,15	0
20	EDO	Q	202	4/4	0.97	0.11	25,35,53,70	0
20	EDO	N	612	4/4	0.97	0.09	27,34,37,65	0
20	EDO	S	103	4/4	0.97	0.08	27,31,36,39	0
14	HEA	N	602	60/60	0.98	0.06	13,18,27,30	0
20	EDO	S	102	4/4	0.98	0.05	19,19,19,20	0
16	MG	N	604	1/1	0.98	0.05	16,16,16,16	0
17	NA	A	605	1/1	0.98	0.03	20,20,20,20	0
14	HEA	A	602	60/60	0.98	0.05	11,17,23,27	0
14	HEA	N	601[A]	60/60	0.98	0.06	12,20,30,35	9
20	EDO	A	610	4/4	0.98	0.06	19,22,22,23	0
14	HEA	N	601[B]	60/60	0.98	0.06	12,21,47,59	9
20	EDO	F	102	4/4	0.99	0.03	16,18,21,21	0
16	MG	A	604	1/1	0.99	0.06	13,13,13,13	0
14	HEA	A	601[A]	60/60	0.99	0.05	10,16,32,46	9
14	HEA	A	601[B]	60/60	0.99	0.05	10,16,35,64	9
15	CU	N	603	1/1	1.00	0.01	18,18,18,18	0

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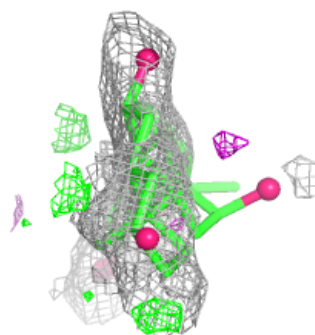
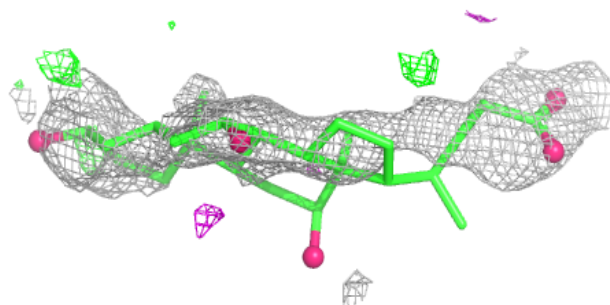
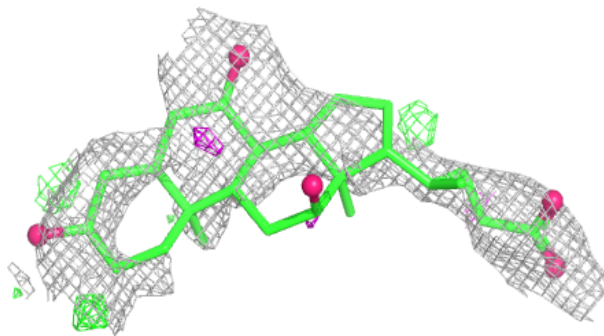
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CUA	B	302	2/2	1.00	0.01	18,18,18,19	0
28	ZN	F	101	1/1	1.00	0.02	22,22,22,22	0
28	ZN	S	101	1/1	1.00	0.02	22,22,22,22	0
23	CUA	O	302	2/2	1.00	0.02	22,22,22,22	0
15	CU	A	603	1/1	1.00	0.01	17,17,17,17	0

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.

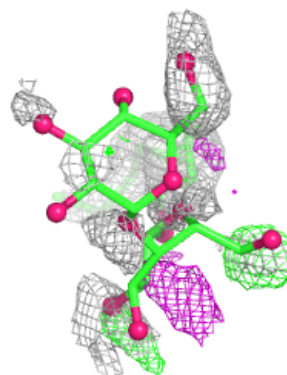
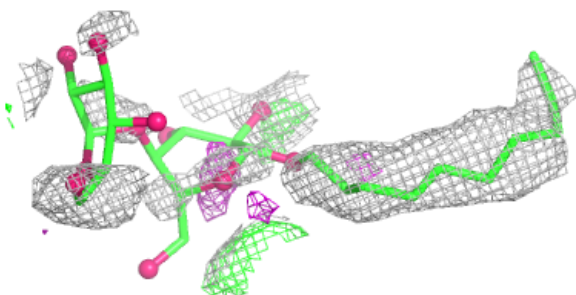
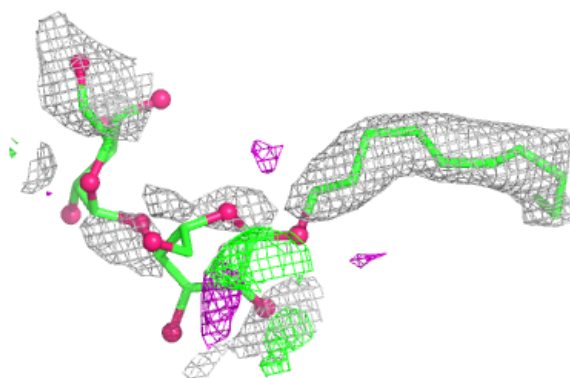


Electron density around CHD X 105:

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

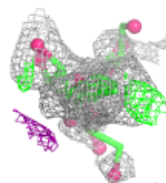
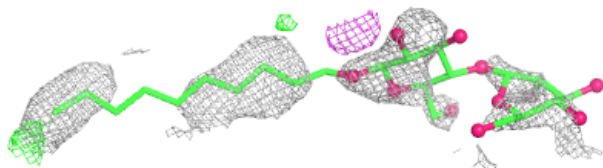
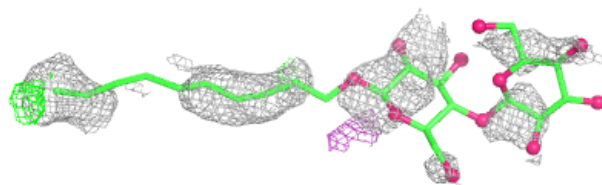
**Electron density around DMU K 105:**

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

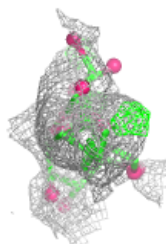
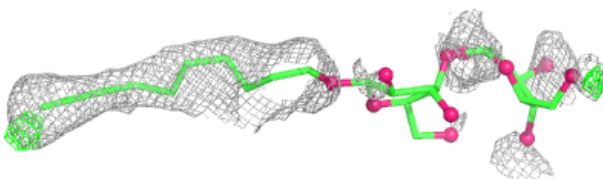
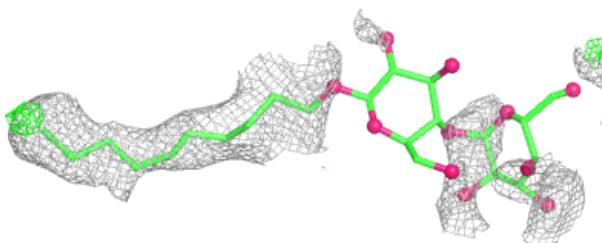


Electron density around DMU A 616:

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

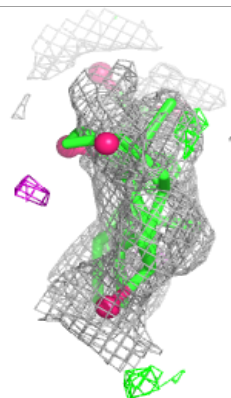
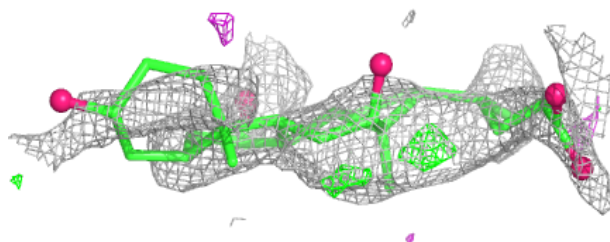
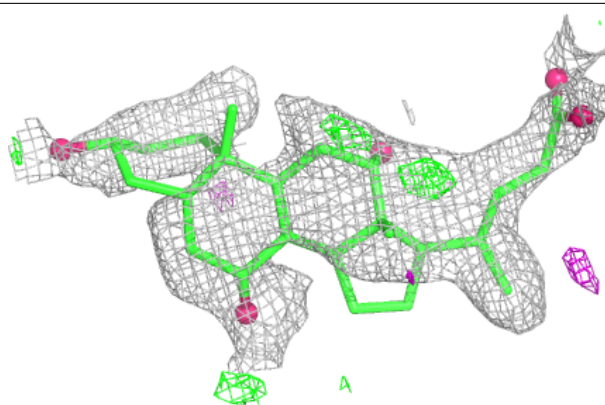
**Electron density around DMU X 101:**

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

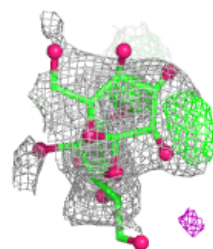
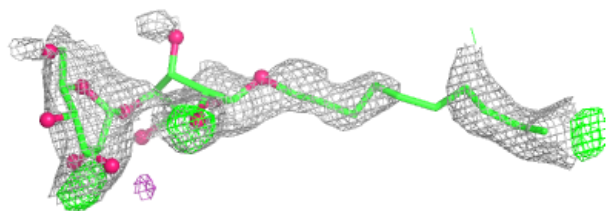
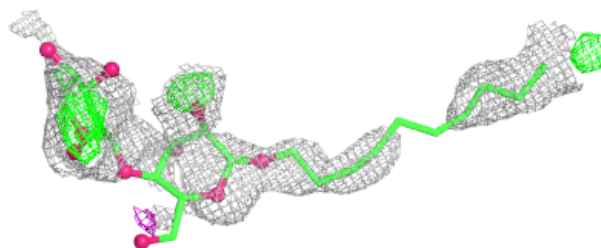


Electron density around CHD J 101:

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

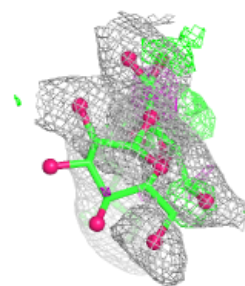
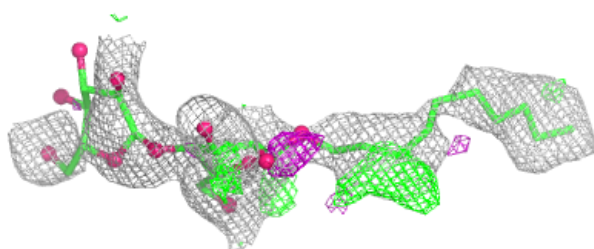
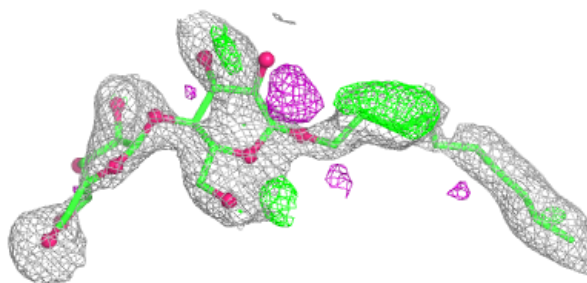
**Electron density around DMU K 104:**

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

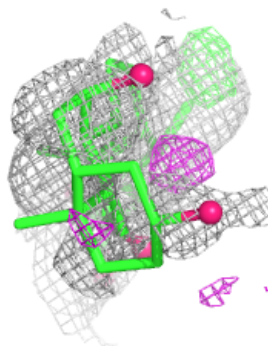
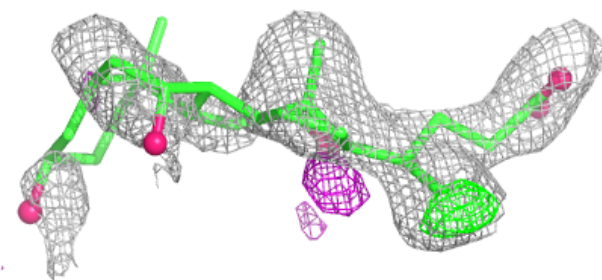
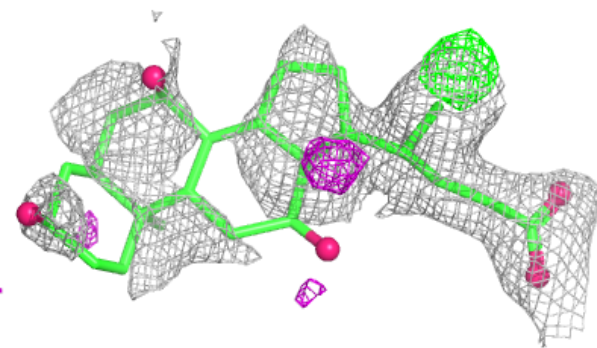


Electron density around DMU P 316:

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

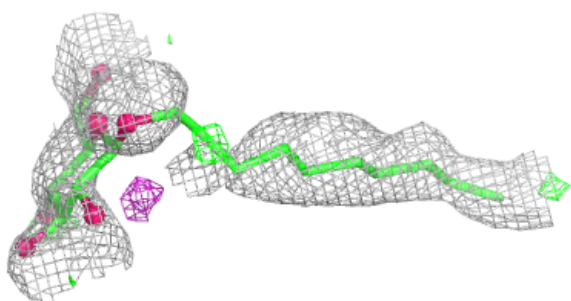
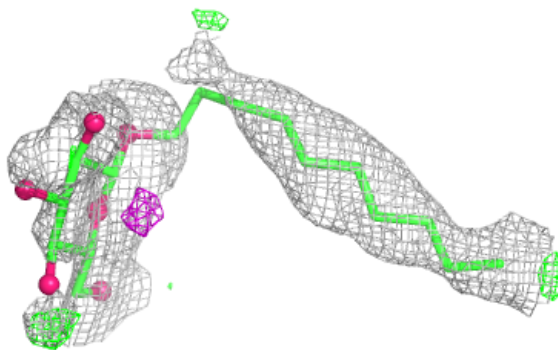
**Electron density around CHD W 101:**

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

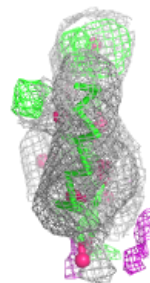
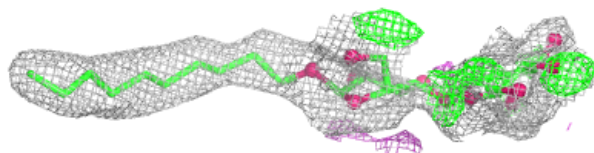
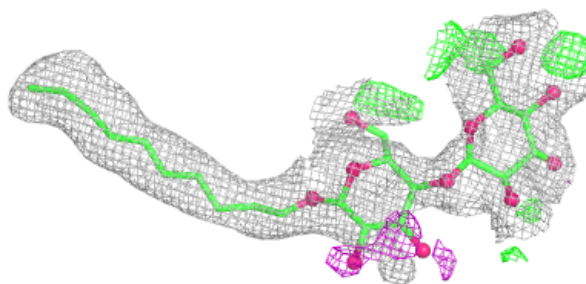


Electron density around DMU X 103:

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

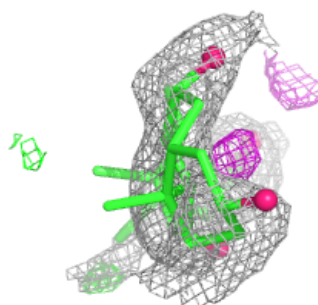
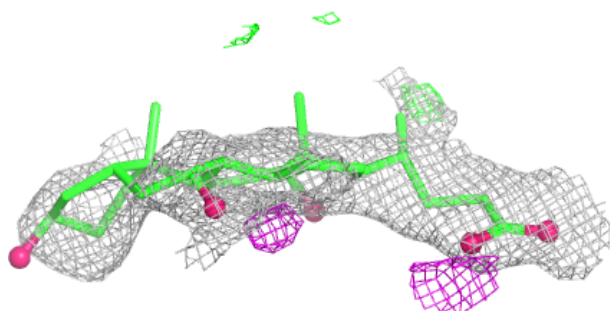
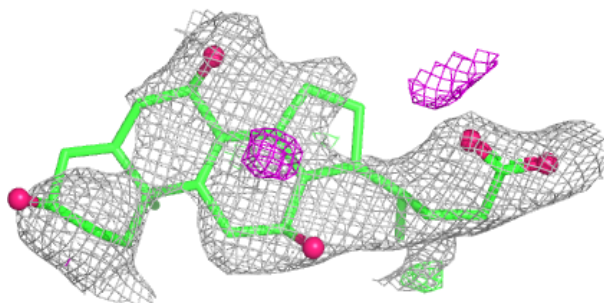
**Electron density around DMU C 312:**

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

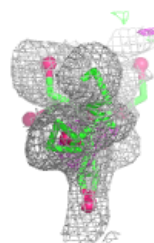
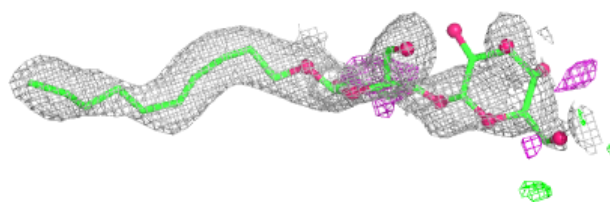
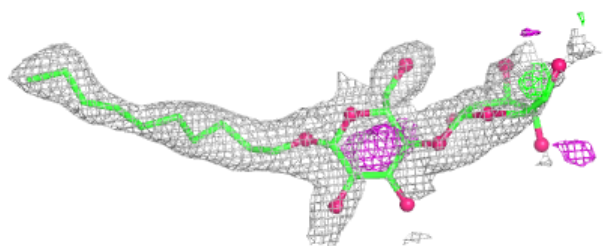


Electron density around CHD L 103:

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

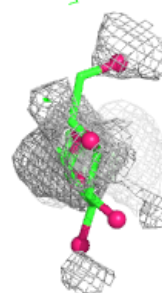
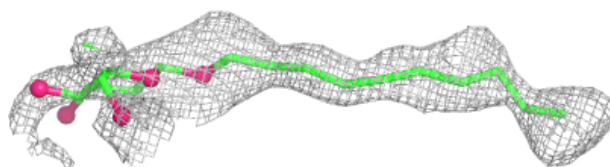
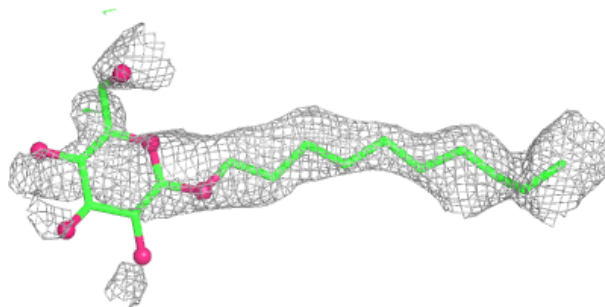
**Electron density around DMU Q 203:**

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

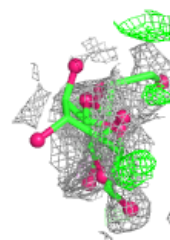
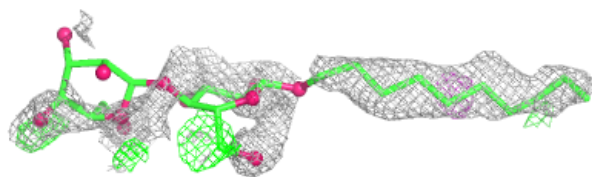
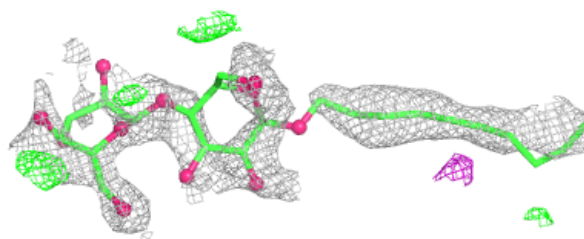


Electron density around DMU X 104:

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

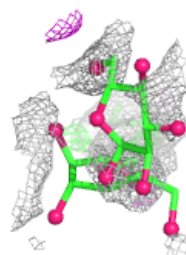
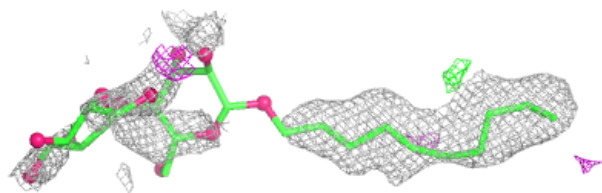
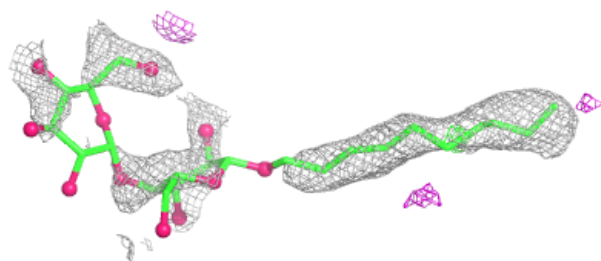
**Electron density around DMU K 103:**

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

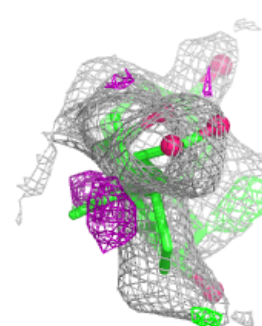
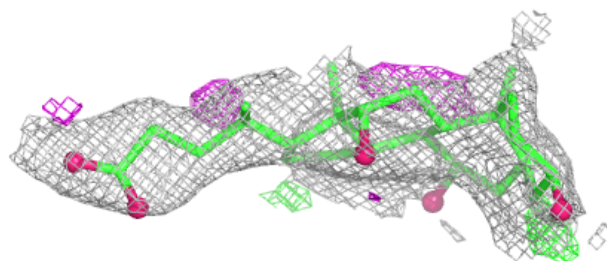
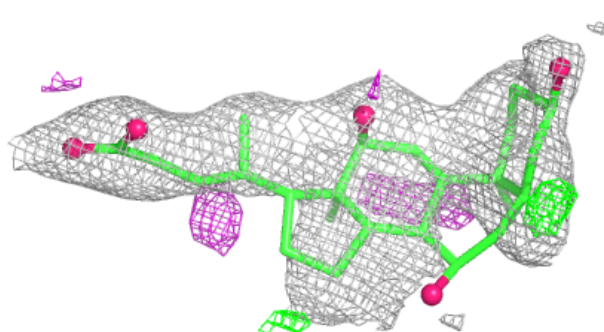


Electron density around DMU D 202:

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

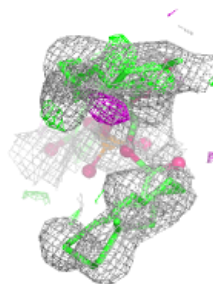
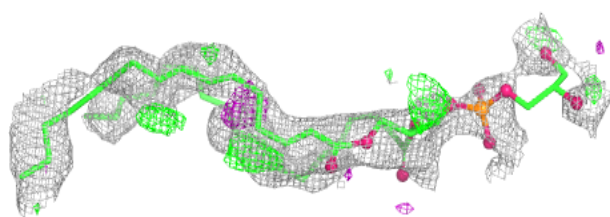
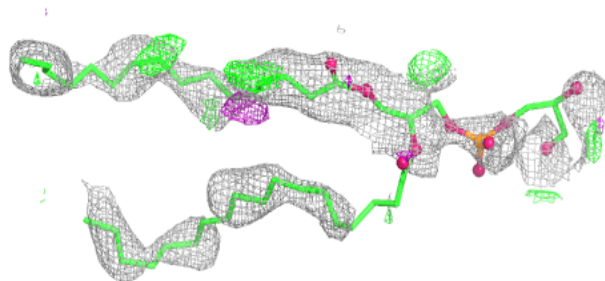
**Electron density around CHD Y 102:**

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

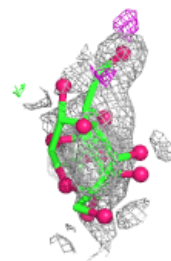
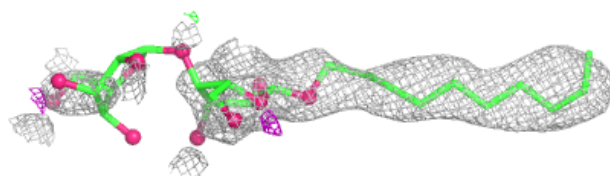
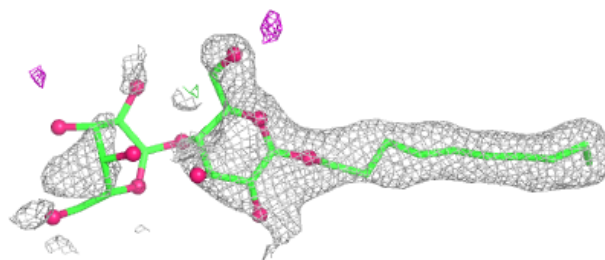


Electron density around PGV C 308:

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

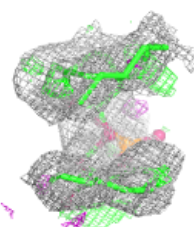
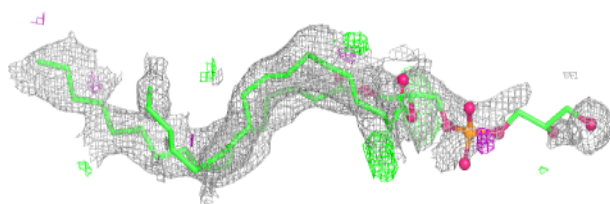
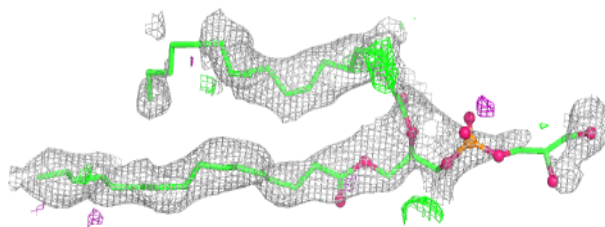
**Electron density around DMU O 305:**

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

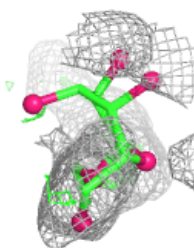
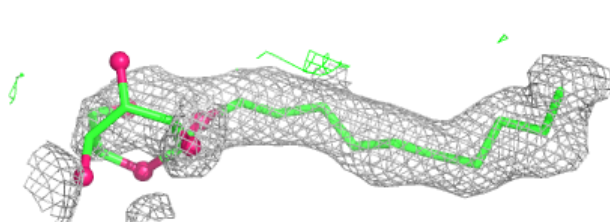
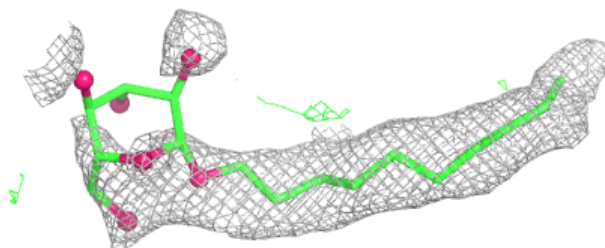


Electron density around PGV P 302:

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

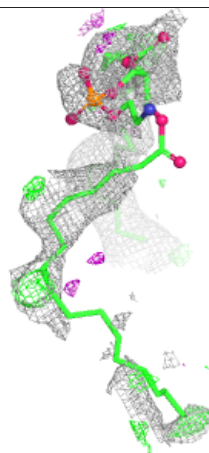
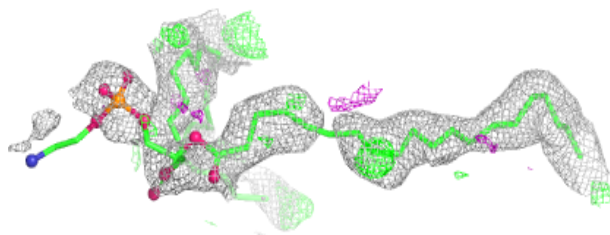
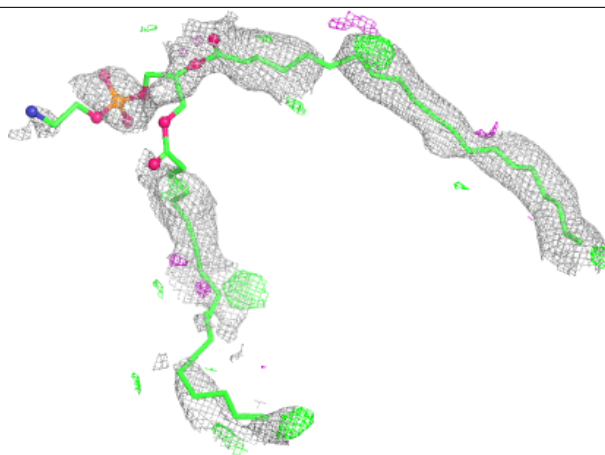
**Electron density around DMU X 102:**

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

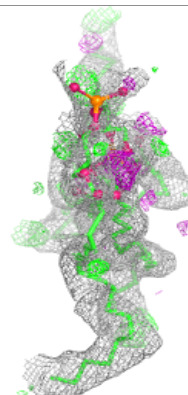
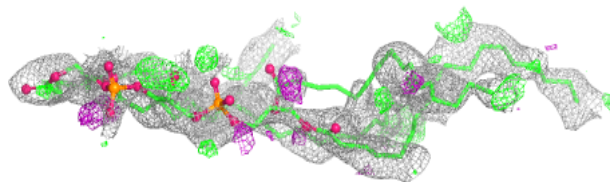
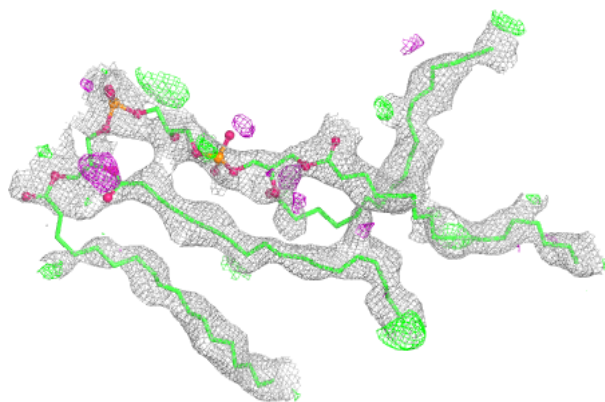


Electron density around PEK C 309:

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

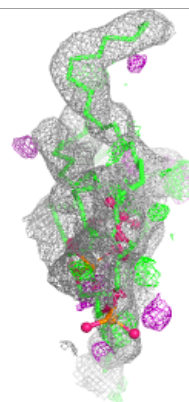
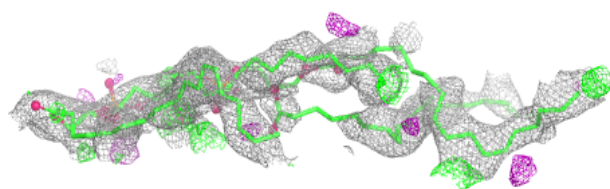
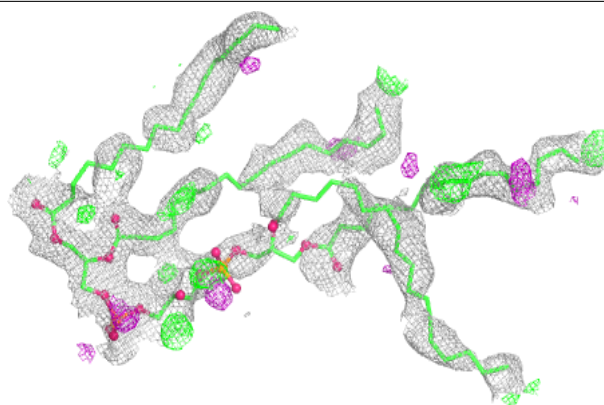
**Electron density around CDL G 101:**

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



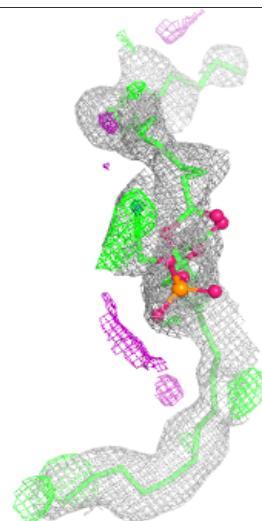
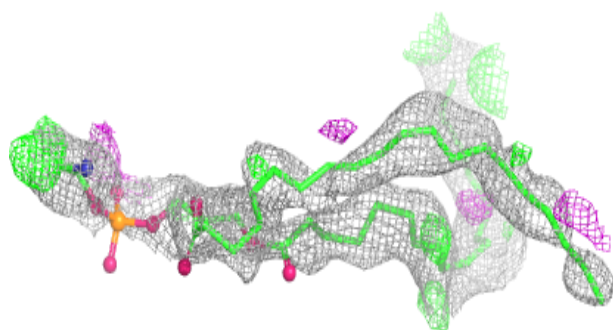
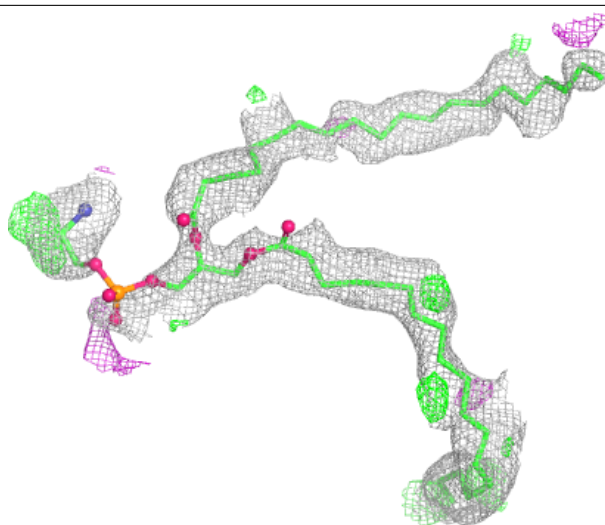
Electron density around CDL T 102:

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



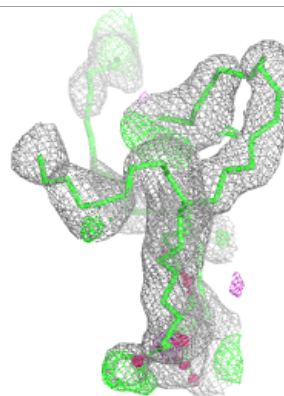
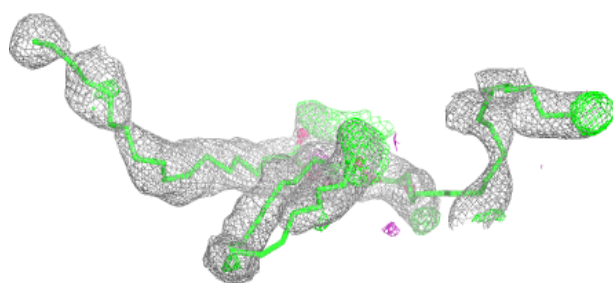
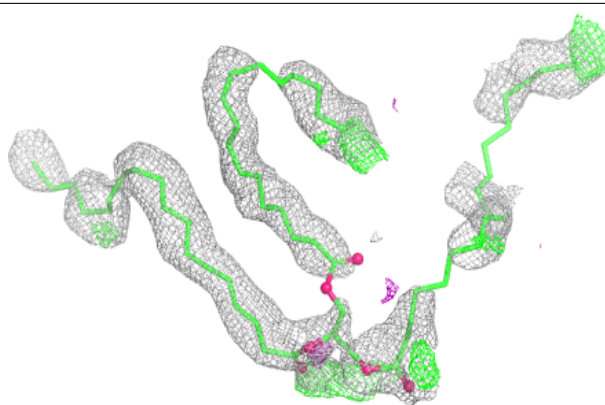
Electron density around PEK C 307:

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

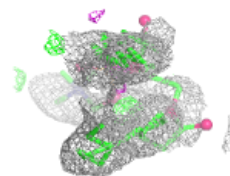
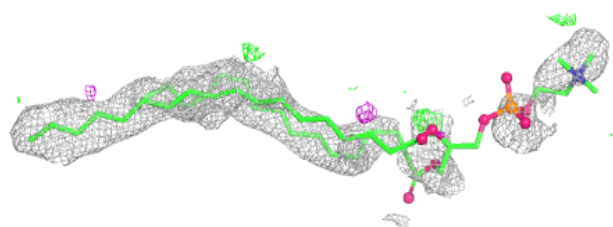
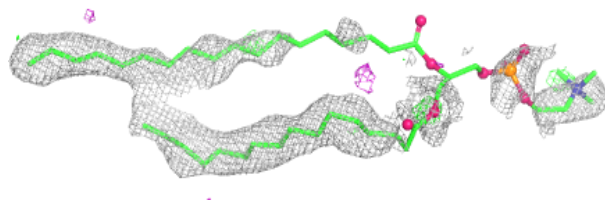


Electron density around TGL Q 201:

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

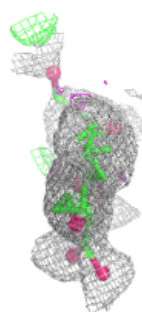
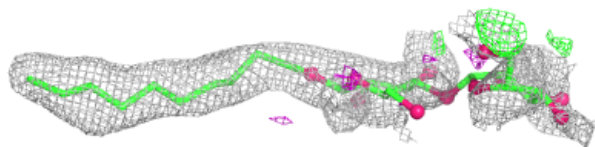
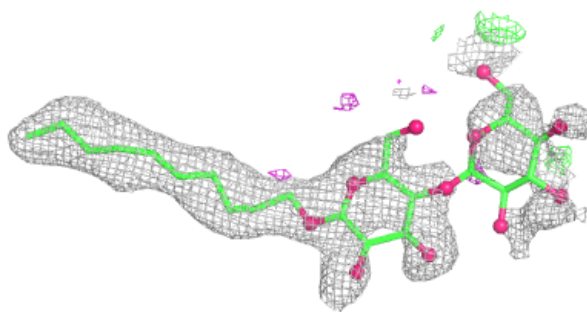
**Electron density around PSC B 303:**

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

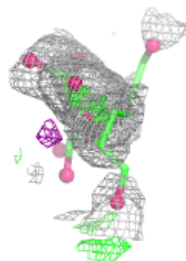
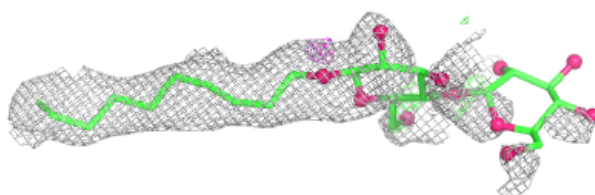
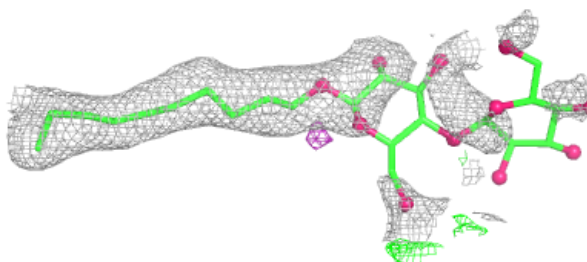


Electron density around DMU P 314:

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

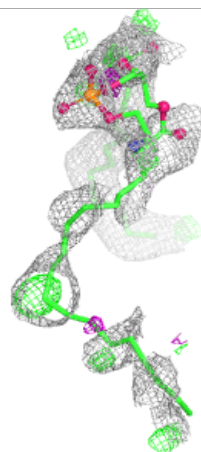
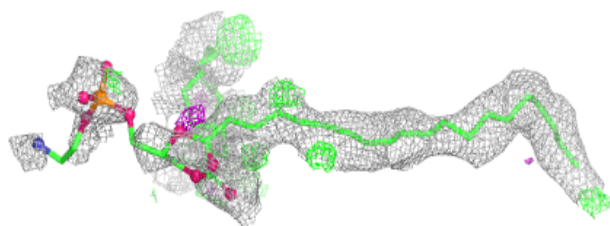
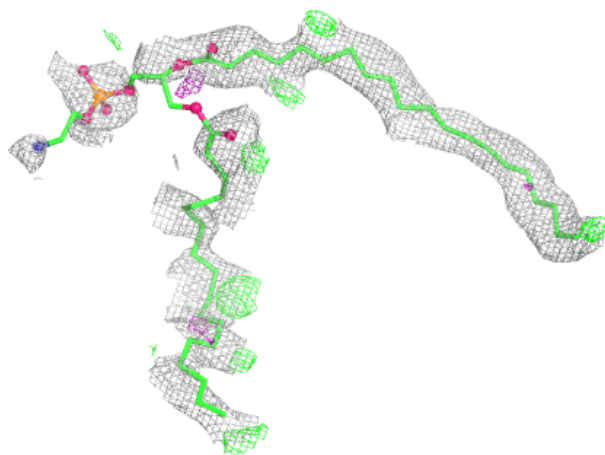
**Electron density around DMU T 103:**

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



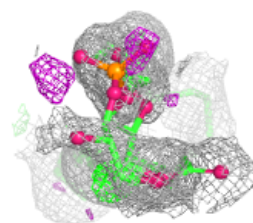
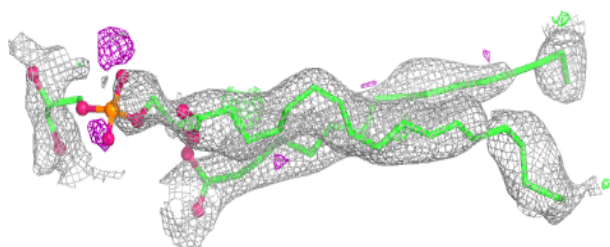
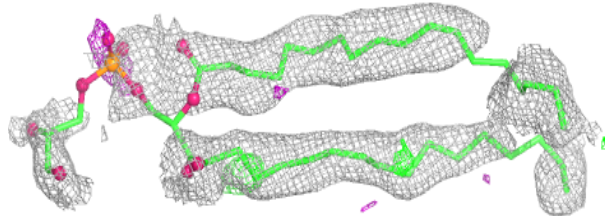
Electron density around PEK G 102:

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

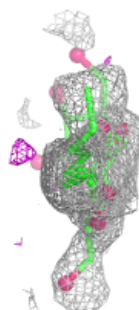
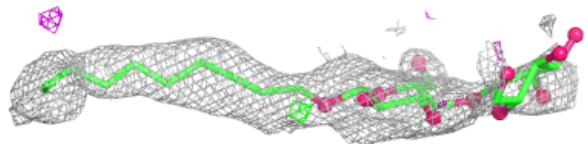
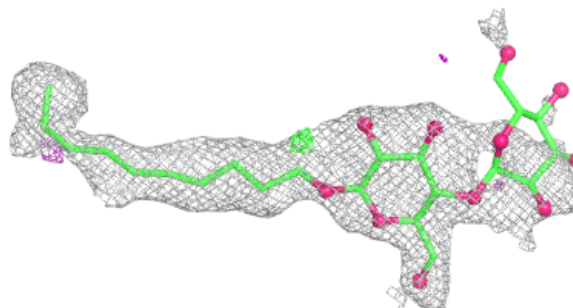


Electron density around PGV N 607:

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

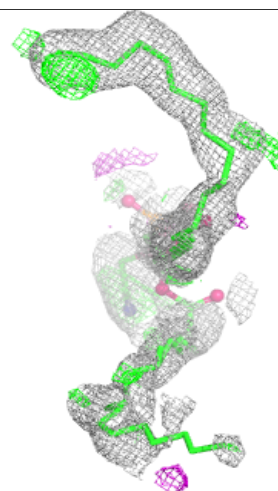
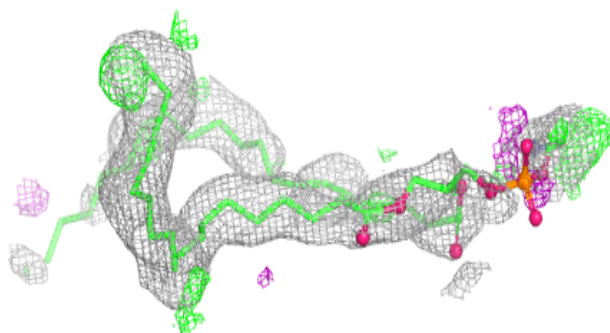
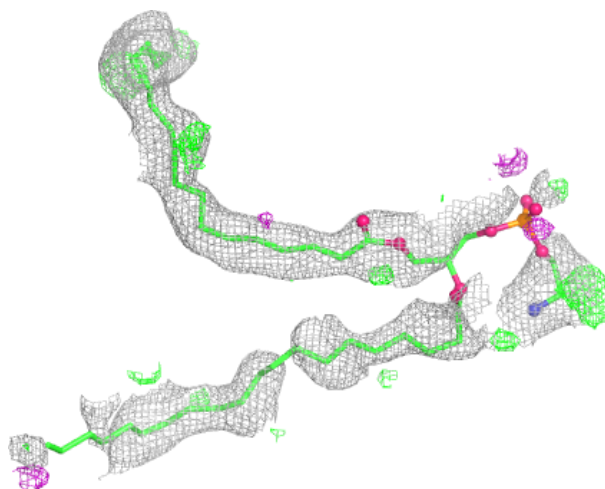
**Electron density around DMU L 102:**

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



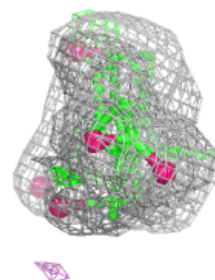
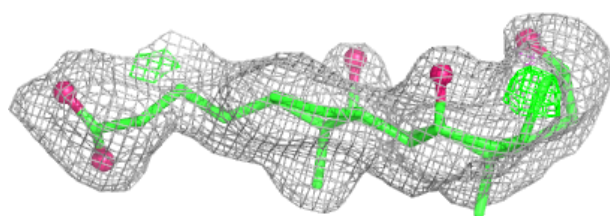
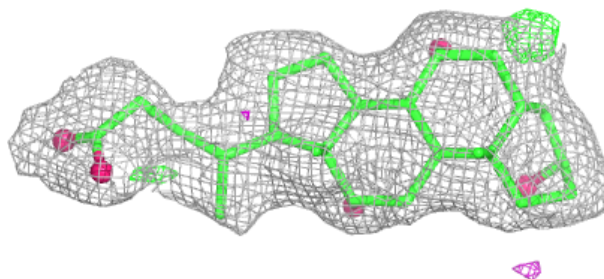
Electron density around PEK P 309:

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

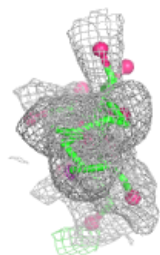
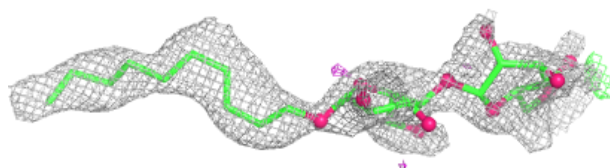
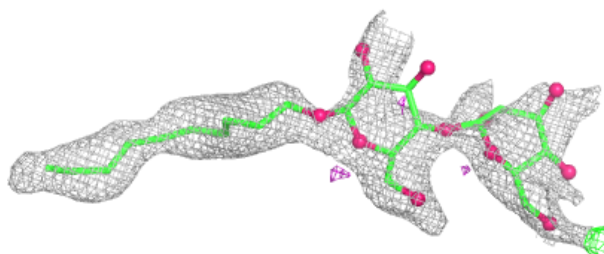


Electron density around CHD P 307:

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

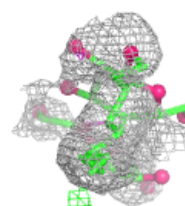
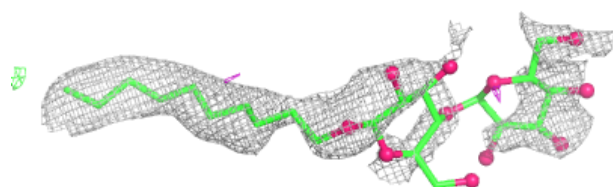
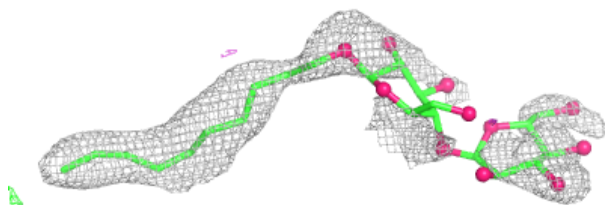
**Electron density around DMU K 101:**

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

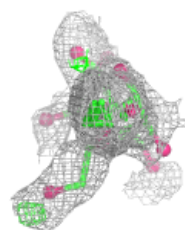
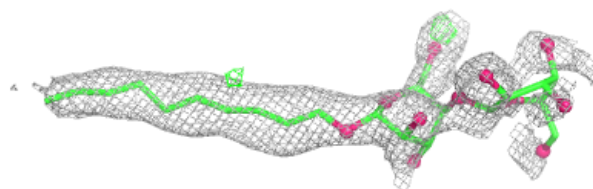
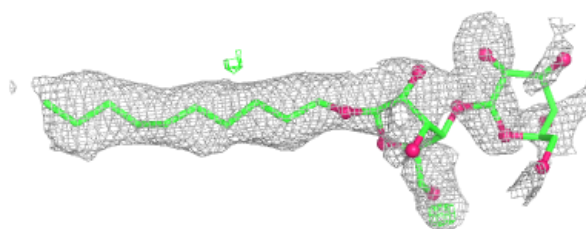


Electron density around DMU K 102:

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

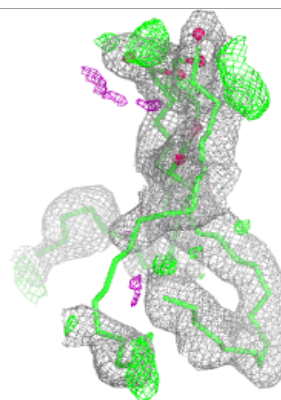
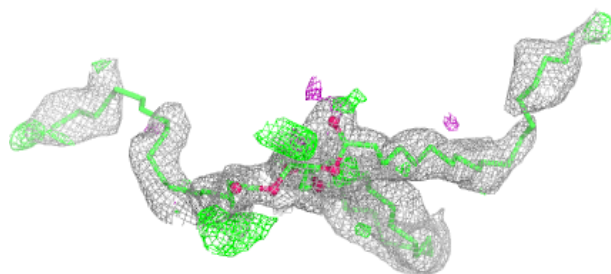
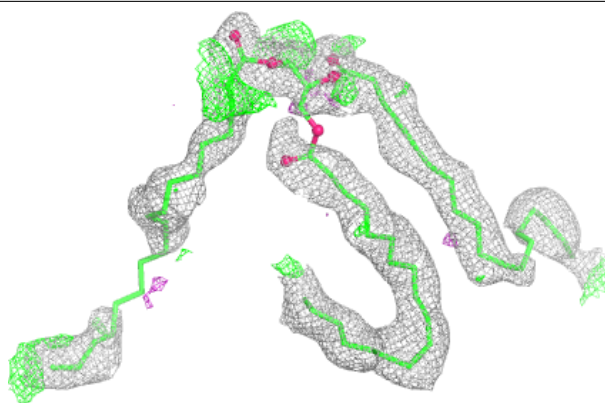
**Electron density around DMU G 104:**

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

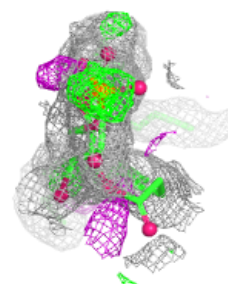
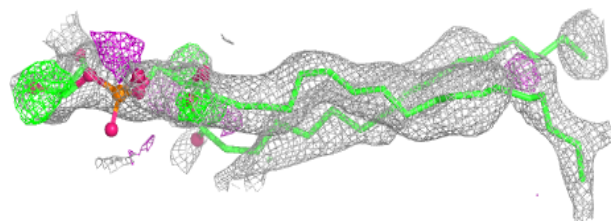
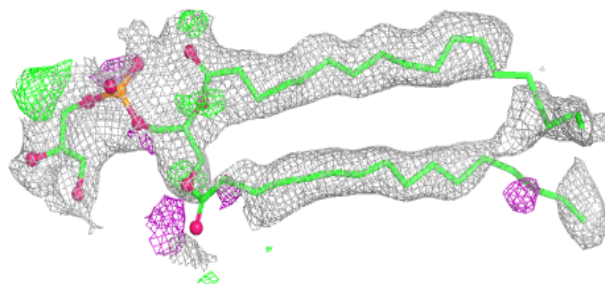


Electron density around TGL D 201:

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

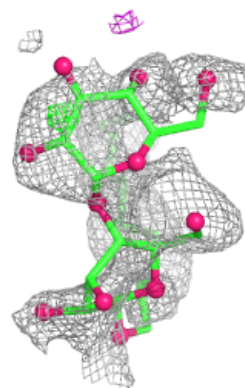
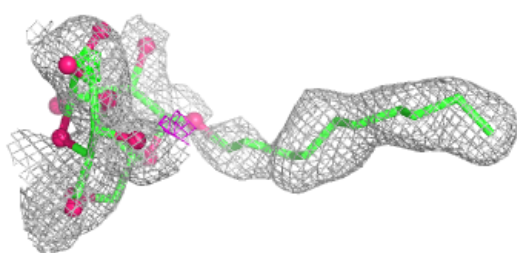
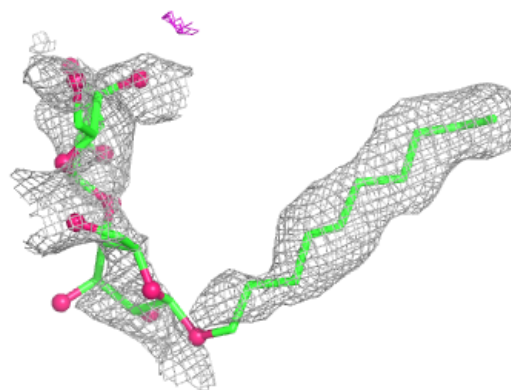
**Electron density around PGV A 608:**

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

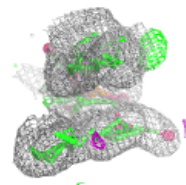
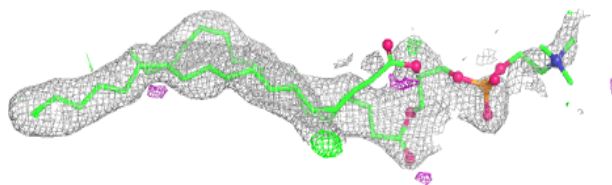
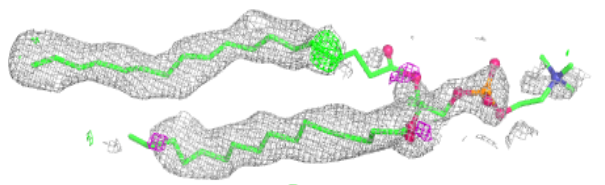


Electron density around DMU K 106:

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

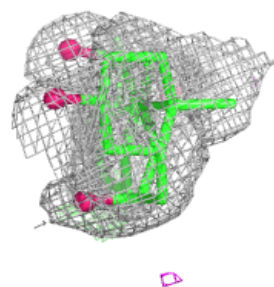
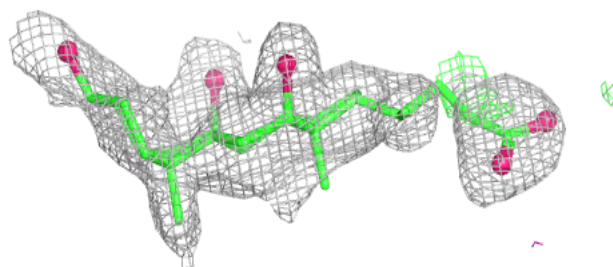
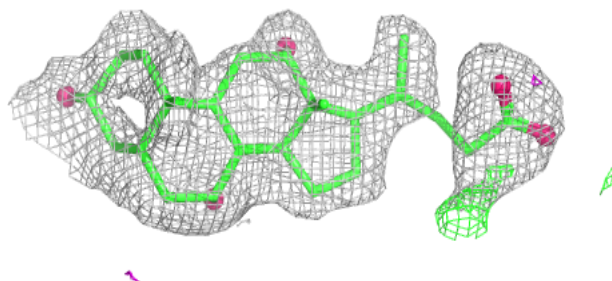
**Electron density around PSC N 608:**

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

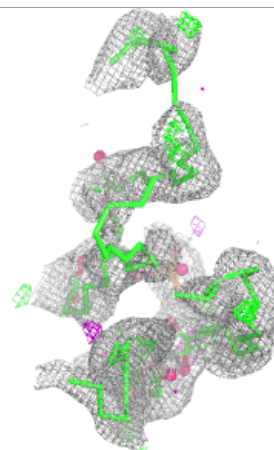
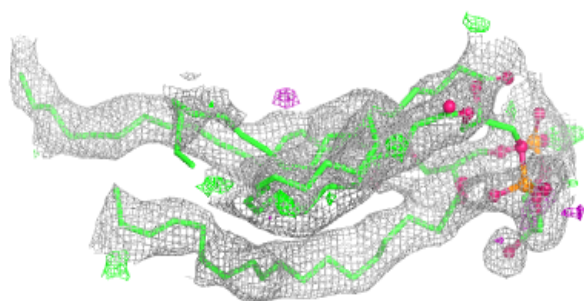
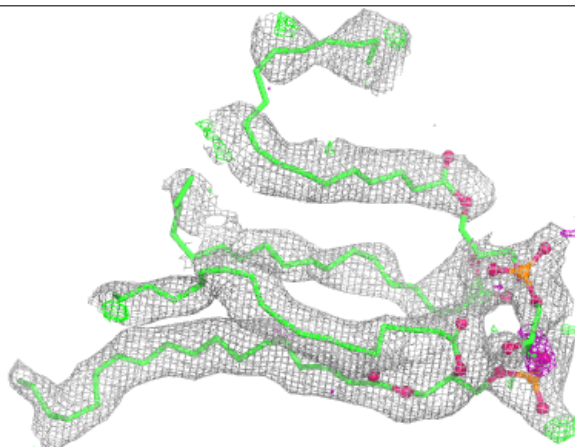


Electron density around CHD C 305:

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

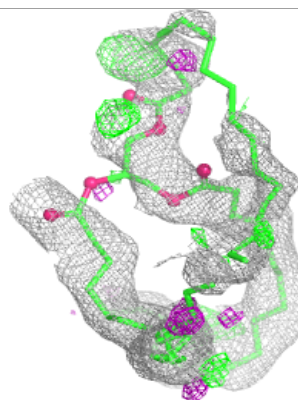
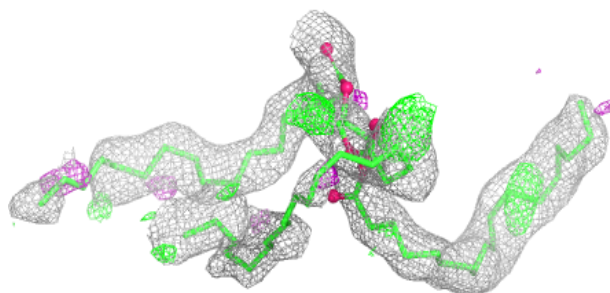
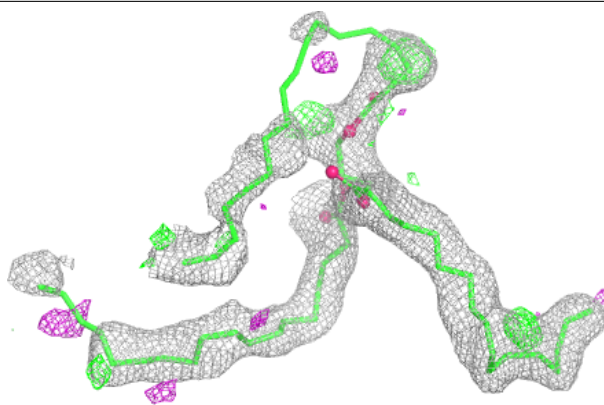
**Electron density around CDL C 304:**

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



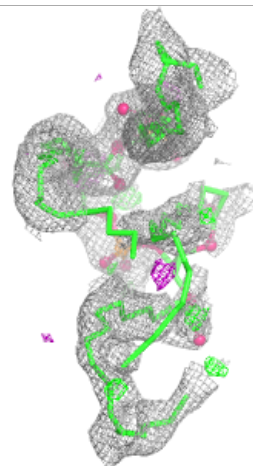
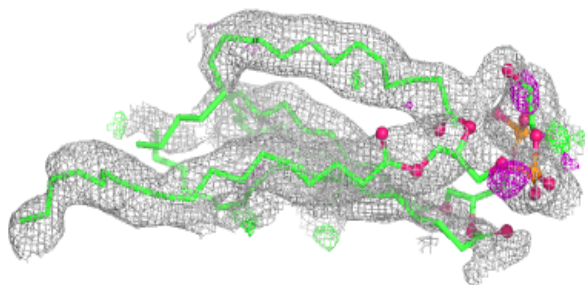
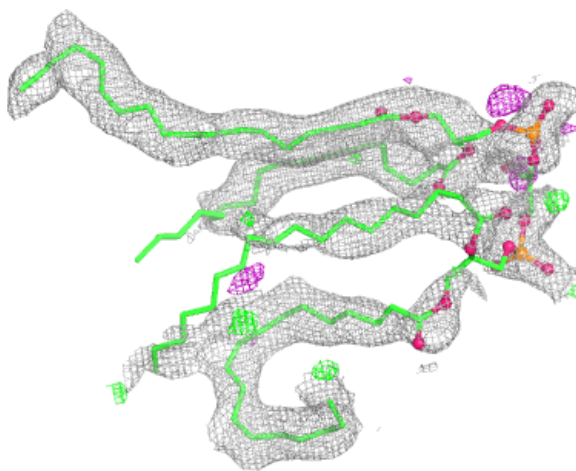
Electron density around TGL L 101:

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



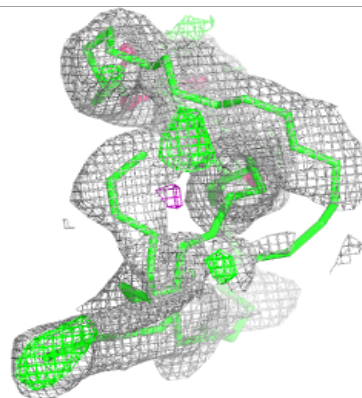
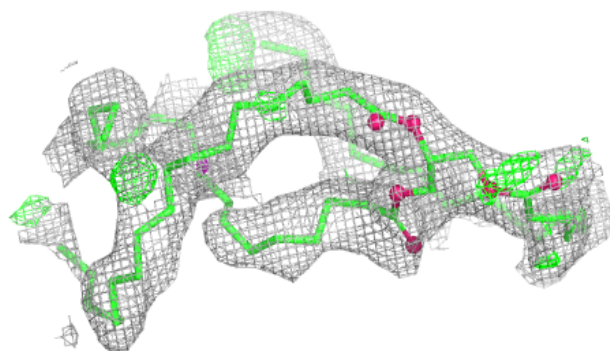
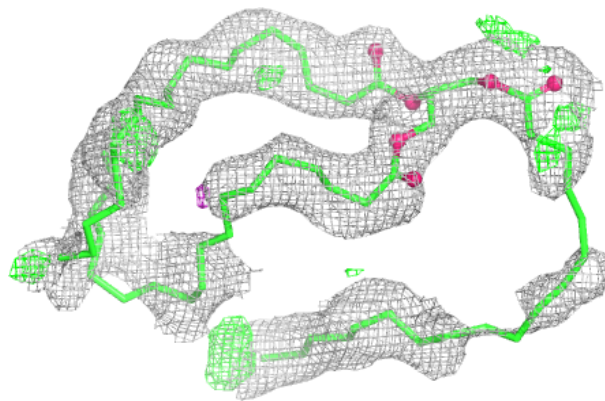
Electron density around CDL P 306:

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

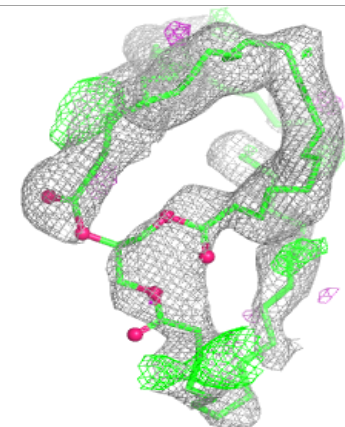
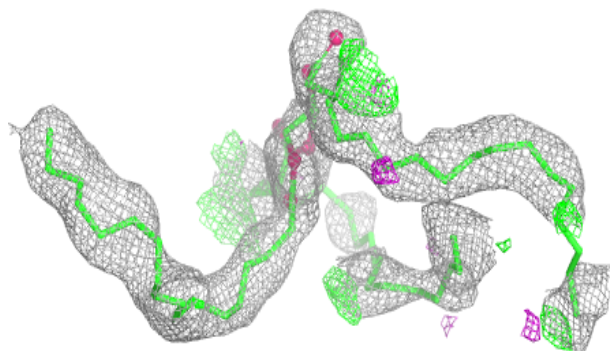
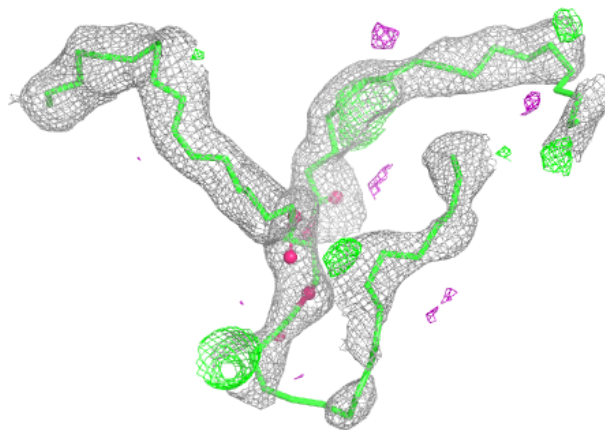


Electron density around TGL O 301:

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

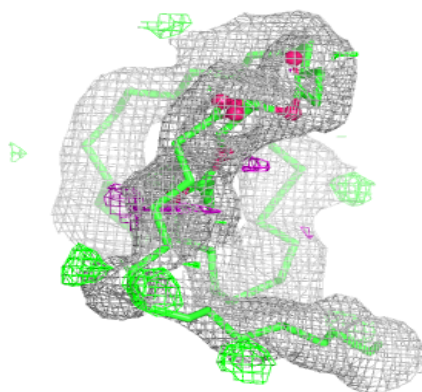
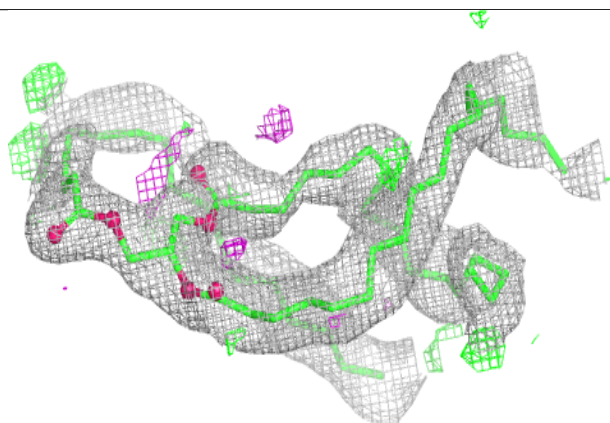
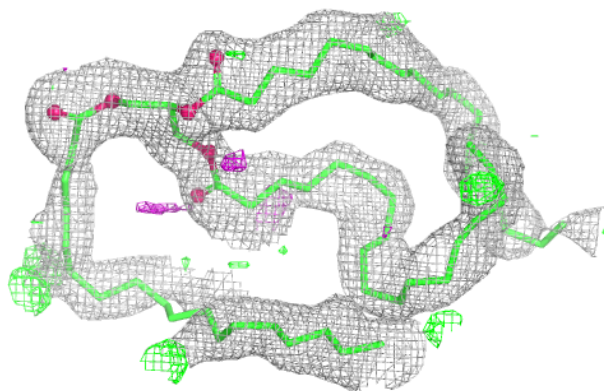
**Electron density around TGL Y 101:**

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

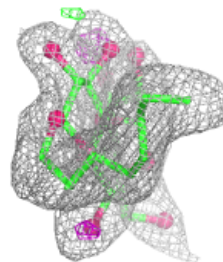
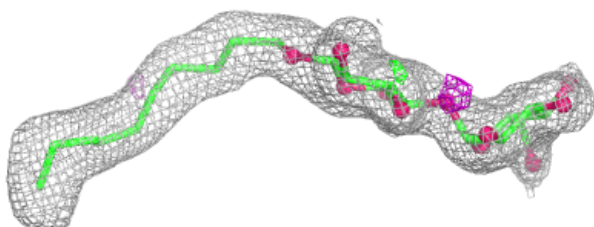
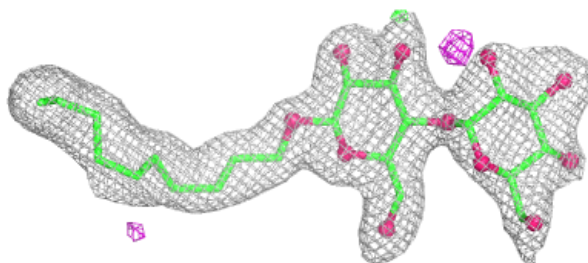


Electron density around TGL B 301:

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

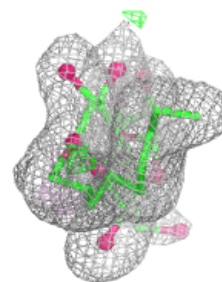
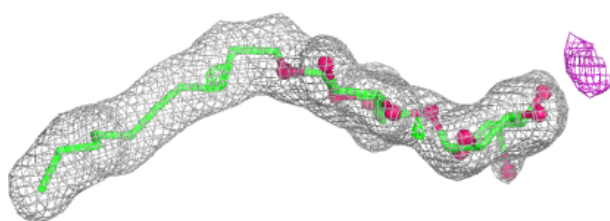
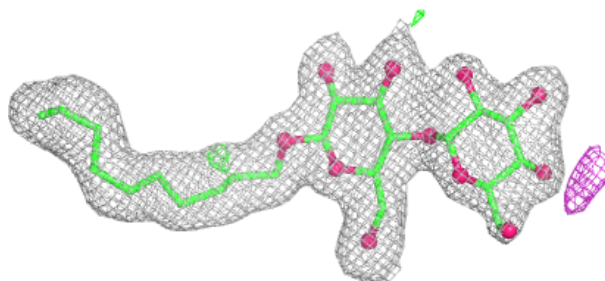
**Electron density around DMU Z 101:**

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

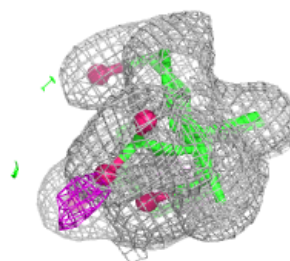
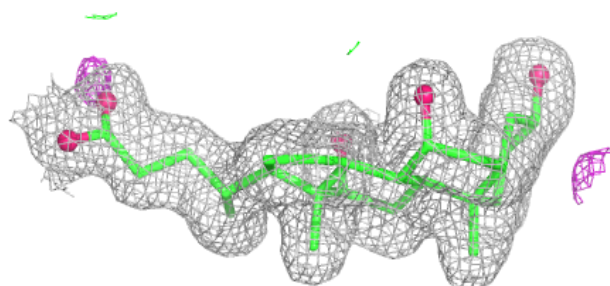
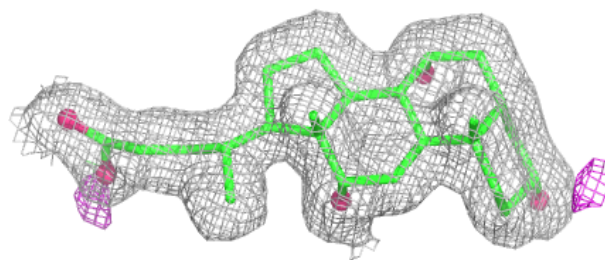


Electron density around DMU M 101:

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

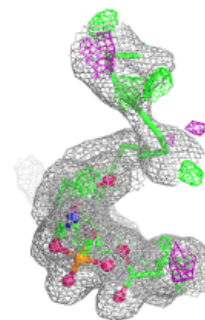
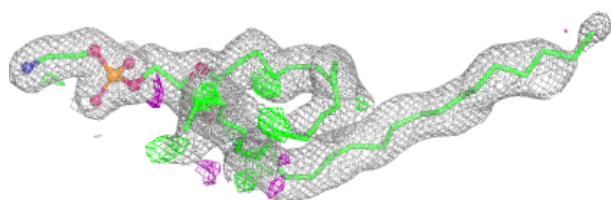
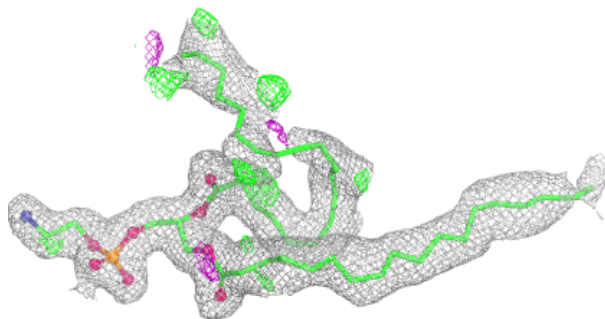
**Electron density around CHD P 308:**

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

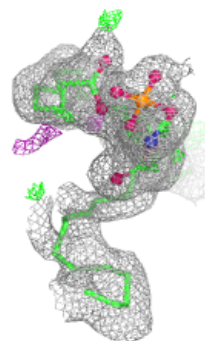
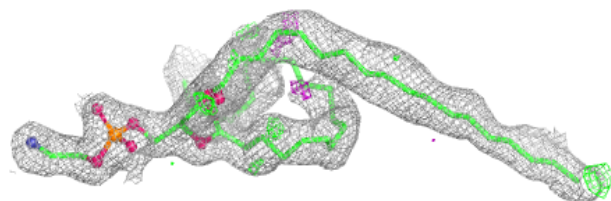
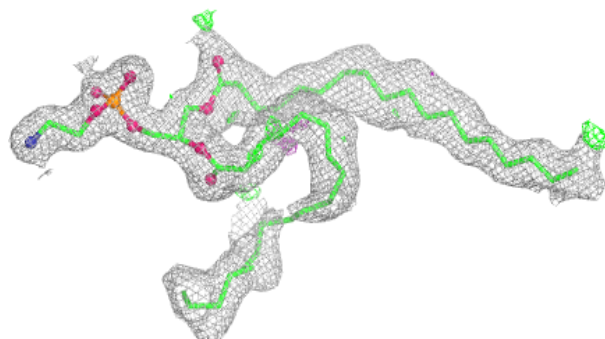


Electron density around PEK C 302:

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

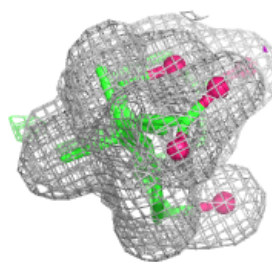
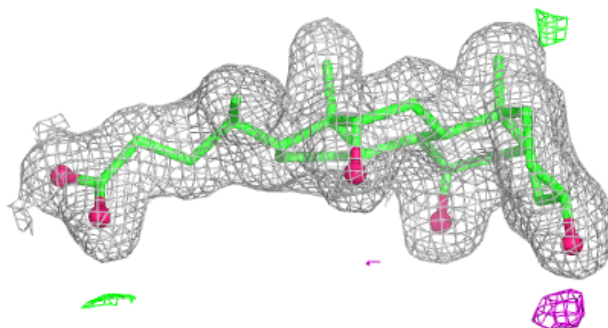
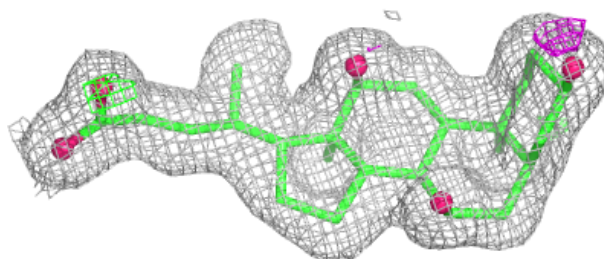
**Electron density around PEK P 304:**

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

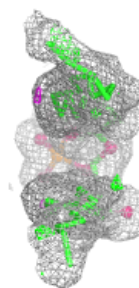
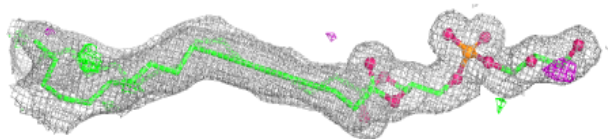
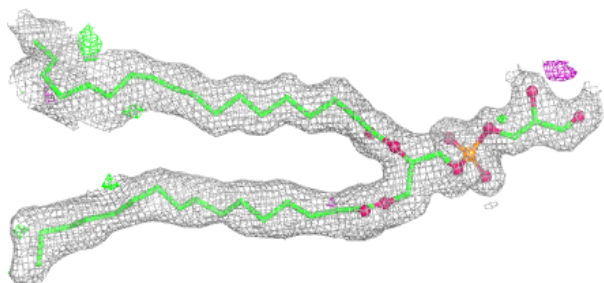


Electron density around CHD C 306:

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

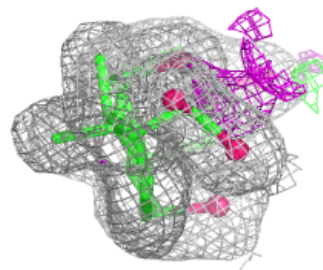
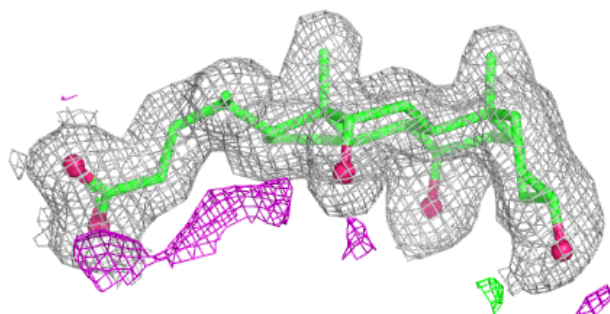
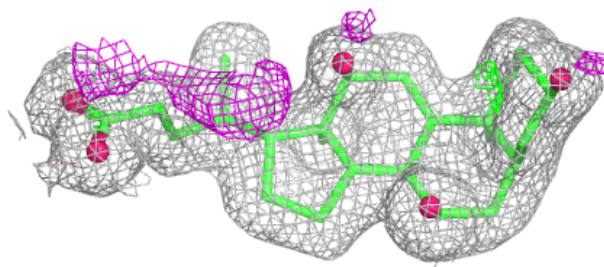
**Electron density around PGV C 303:**

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

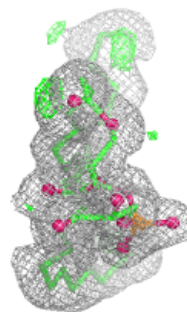
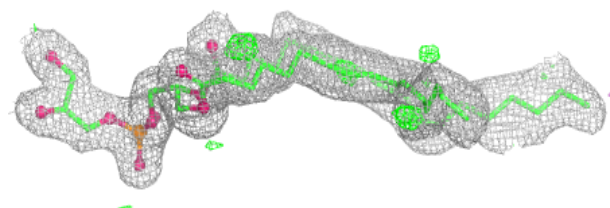
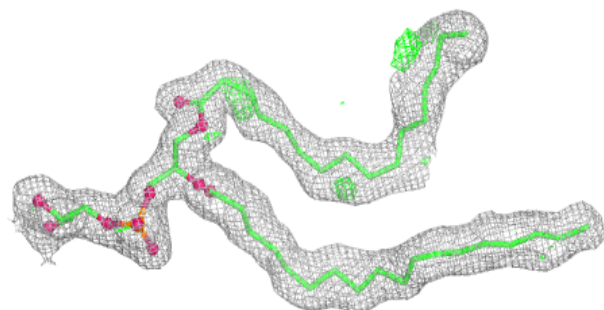


Electron density around CHD G 103:

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

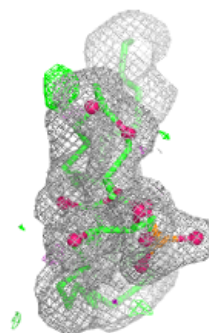
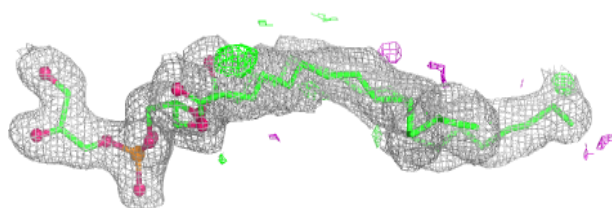
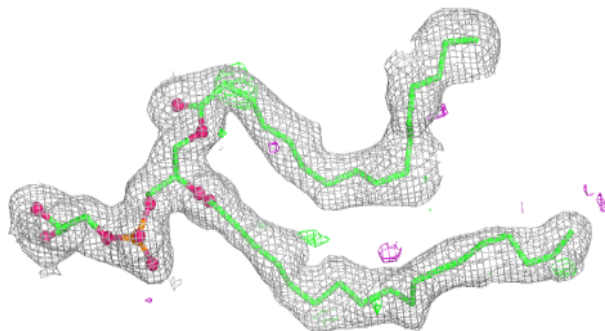
**Electron density around PGV A 607:**

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

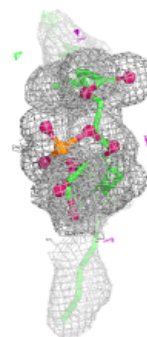
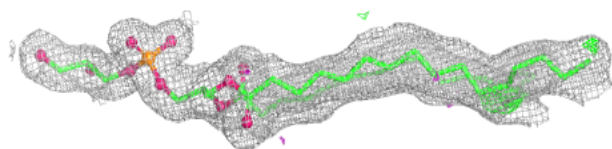
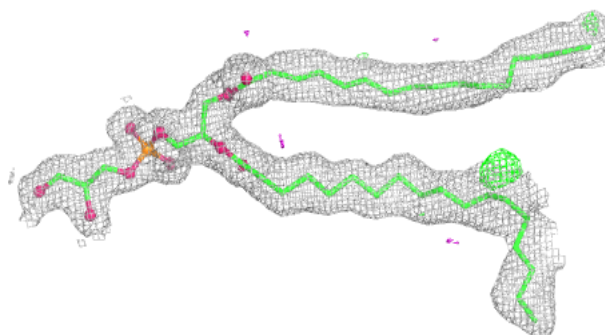


Electron density around PGV P 301:

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

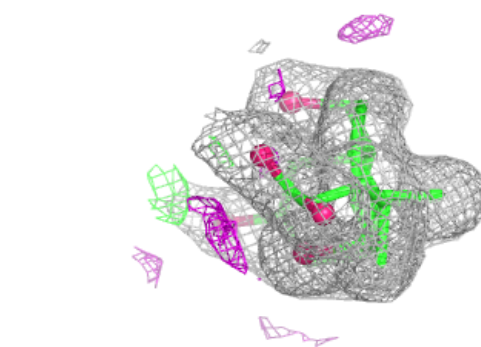
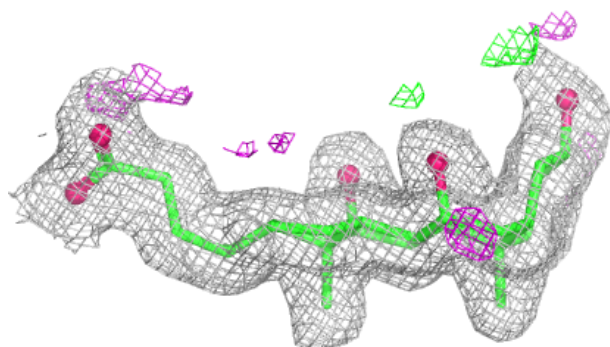
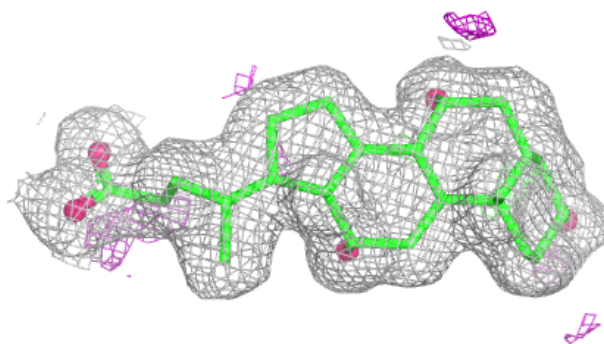
**Electron density around PGV P 305:**

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

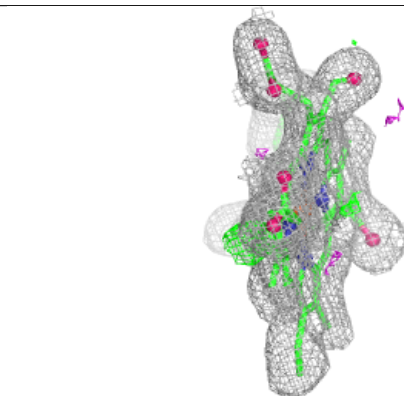
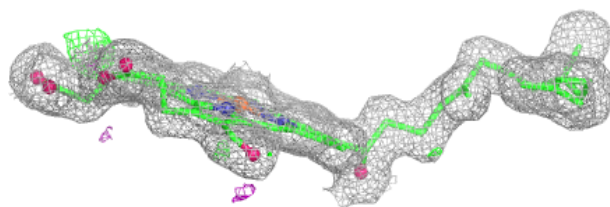
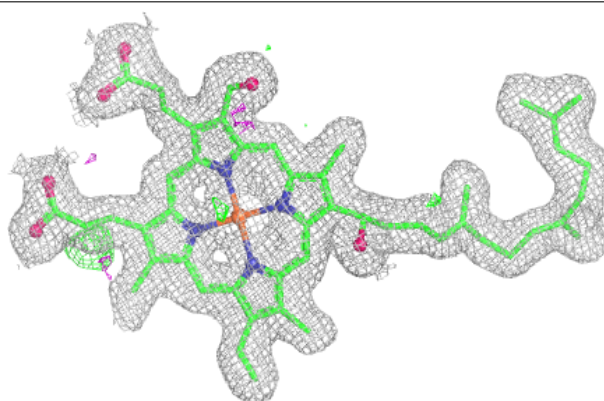


Electron density around CHD T 101:

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

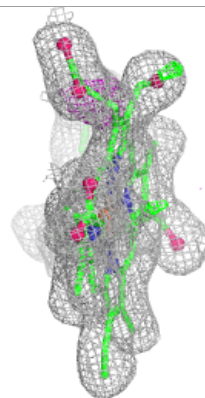
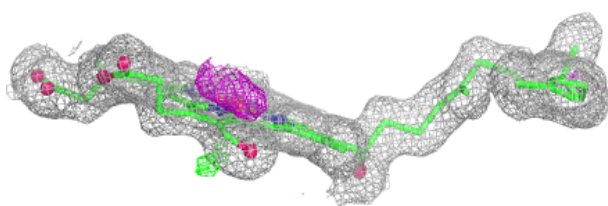
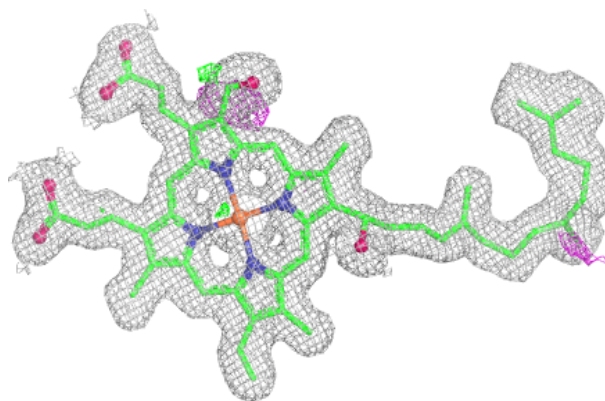
**Electron density around HEA N 602:**

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

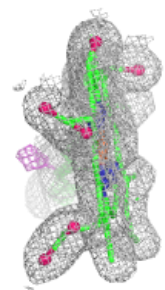
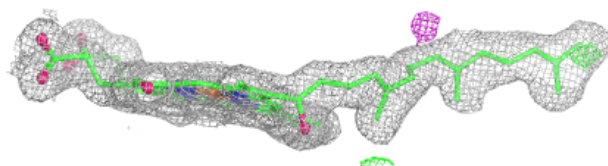
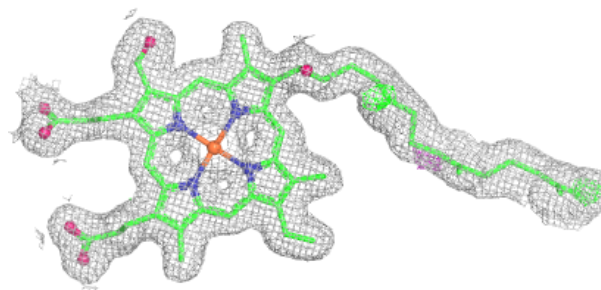


Electron density around HEA A 602:

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

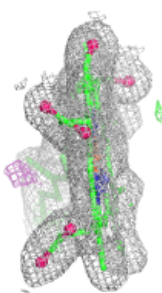
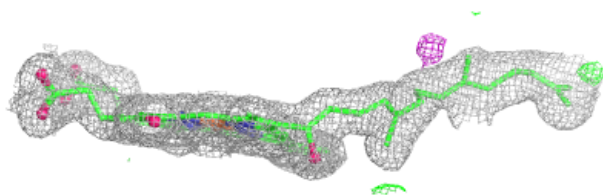
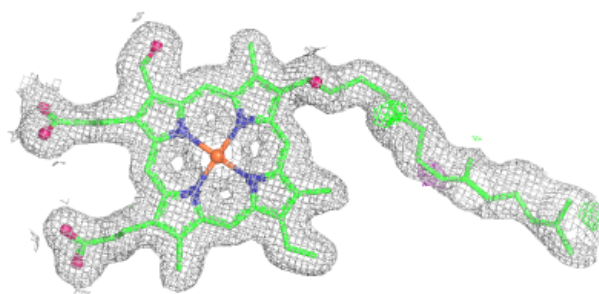
**Electron density around HEA N 601 (A):**

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

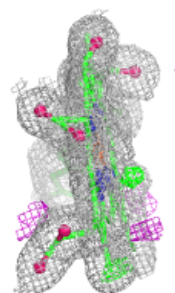
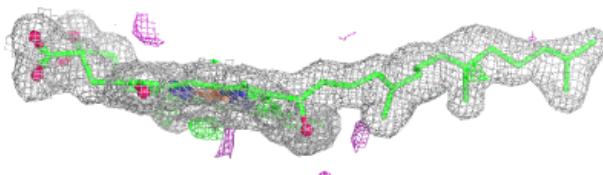
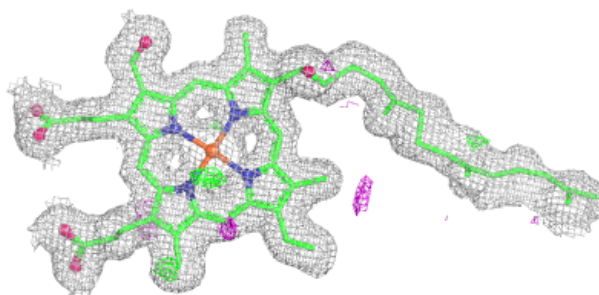


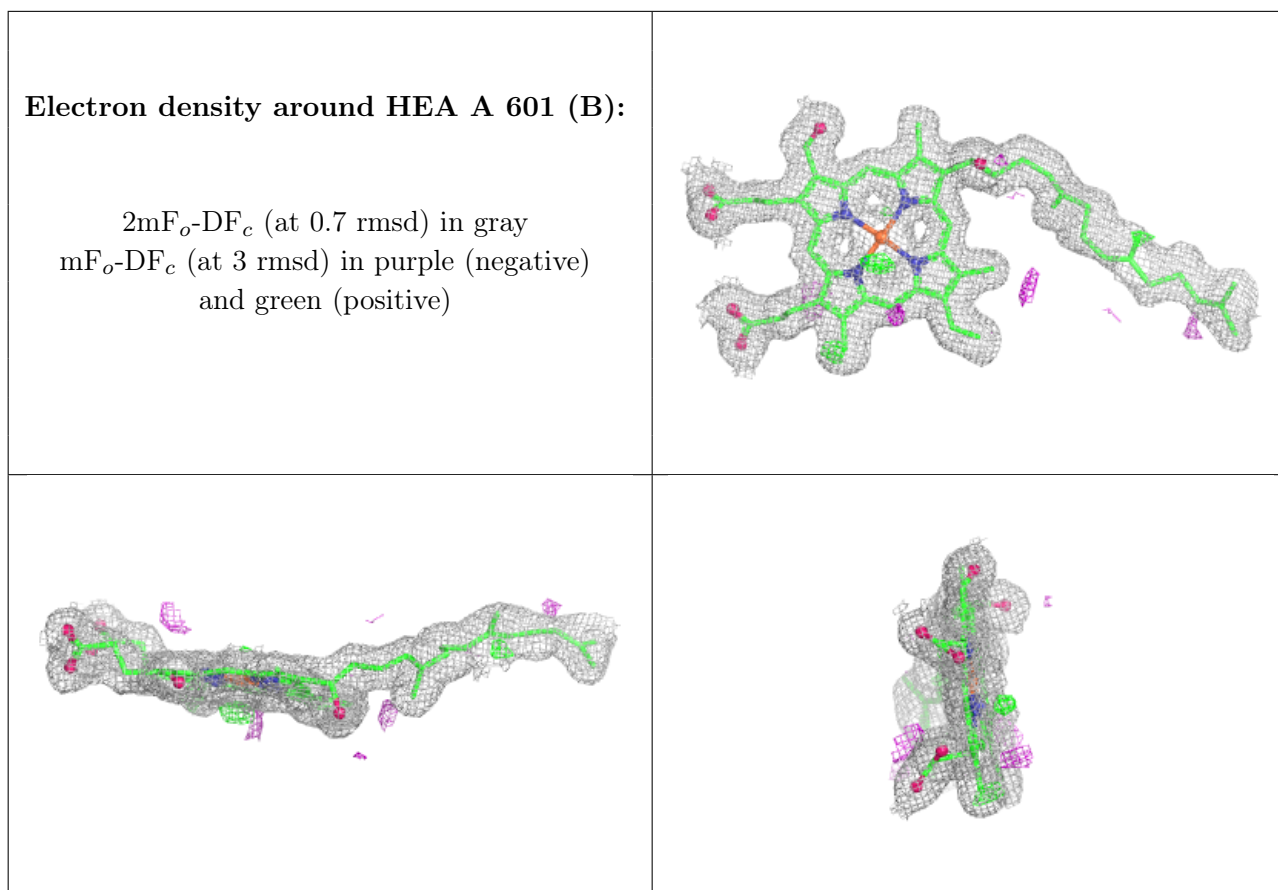
Electron density around HEA N 601 (B):

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

**Electron density around HEA A 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.