



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 08:41 PM EDT

PDB ID : 3AG2 / pdb_00003ag2
Title : Bovine Heart Cytochrome c Oxidase in the Carbon Monoxide-bound Fully Reduced State at 100 K
Authors : Muramoto, K.; Ohta, K.; Shinzawa-Itoh, K.; Kanda, K.; Taniguchi, M.; Nabekura, H.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2010-03-19
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

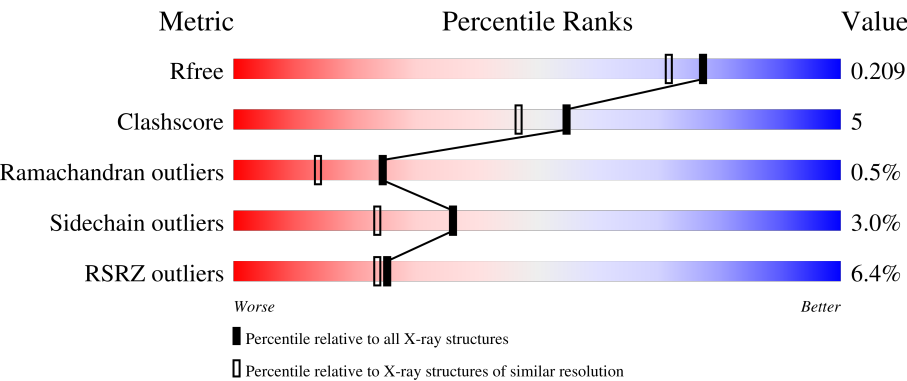
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



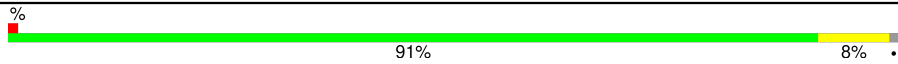
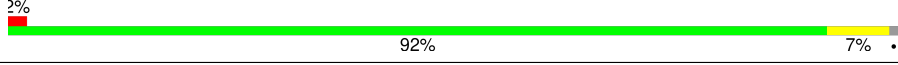
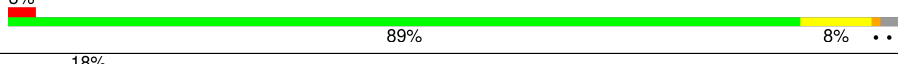
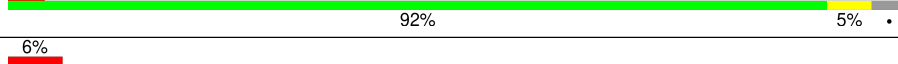
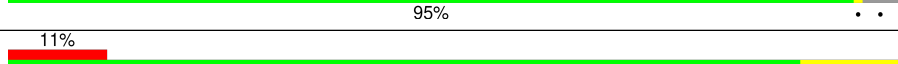
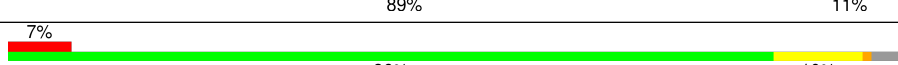
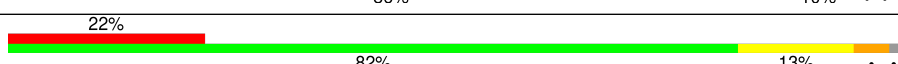
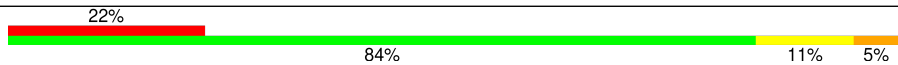
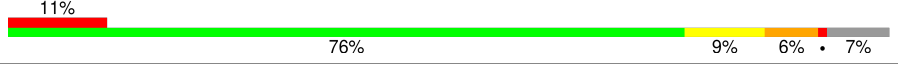
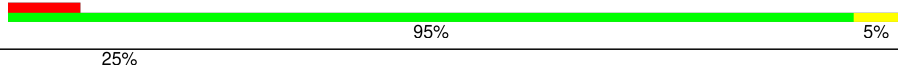
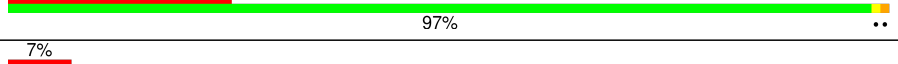
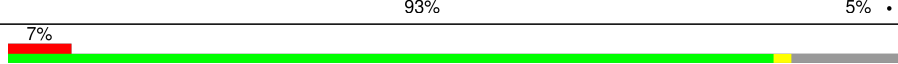
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	92%7%.
1	N	514	% 86%13%.
2	B	227	6% 85%14%
2	O	227	7% 81%18%.

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Mol	Chain	Length	Quality of chain
3	C	261	
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
21	EDO	A	619	-	-	X	-

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 33056 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	8	0
			4070	2715	631	687	37			
1	N	514	Total	C	N	O	S	0	10	0
			4074	2722	628	687	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	1	0
			1830	1191	281	340	18			
2	O	227	Total	C	N	O	S	0	2	0
			1834	1192	284	340	18			

- 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	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	2	0
			2114	1413	336	353	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	1	0
			1203	785	196	218	4			
4	Q	141	Total	C	N	O	S	0	0	0
			1175	764	193	214	4			

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

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	0	0
			852	544	144	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	0	0
			748	464	134	145	5			
6	S	95	Total	C	N	O	S	0	1	0
			726	450	129	142	5			

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

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, mitochondrial.

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, mitochondrial.

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

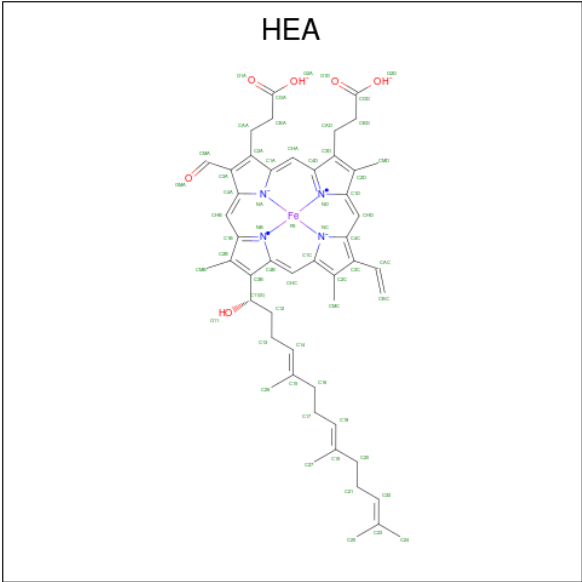
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
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, mitochondrial.

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 78	C 66	Fe 1	N 4	O 7	0	1
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 78	C 66	Fe 1	N 4	O 7	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		

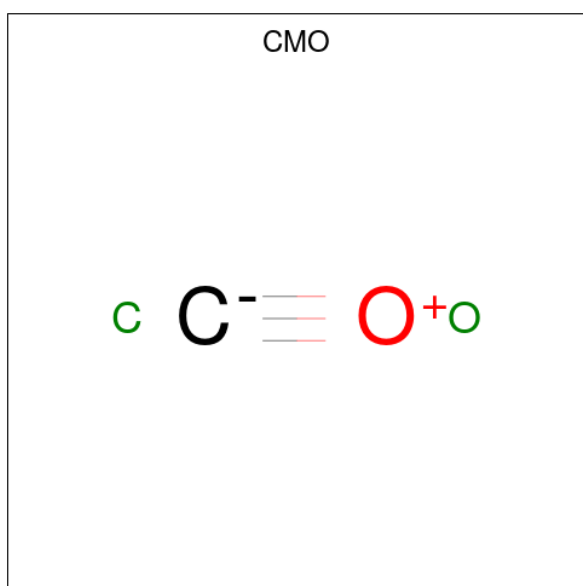
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

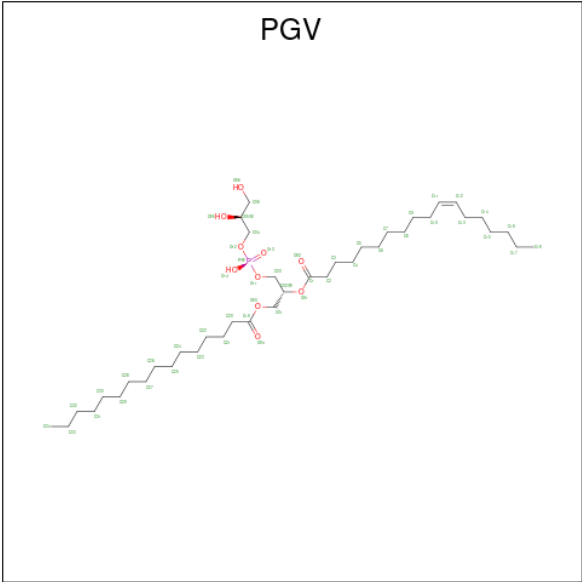
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	C	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		
17	P	1	Total	Na	0	0
			1	1		

- Molecule 18 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



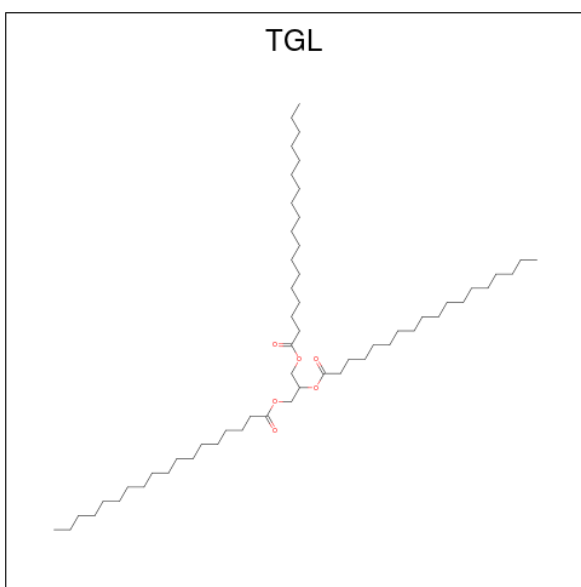
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	1
			4	2	2		
18	N	1	Total	C	O	0	1
			4	2	2		

- 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).



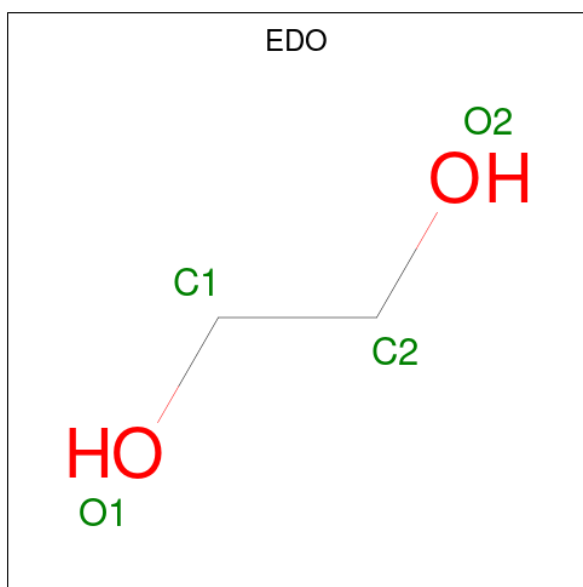
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			47	36	10	1		
19	C	1	Total	C	O	P	0	0
			49	38	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			47	38	8	1		
19	P	1	Total	C	O	P	0	0
			46	35	10	1		
19	Z	1	Total	C	O	P	0	0
			47	36	10	1		

- Molecule 20 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			59	53	6		
20	B	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			55	49	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	O	1	Total	C	O	0	0
			63	57	6		
20	Y	1	Total	C	O	0	0
			59	53	6		

- Molecule 21 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

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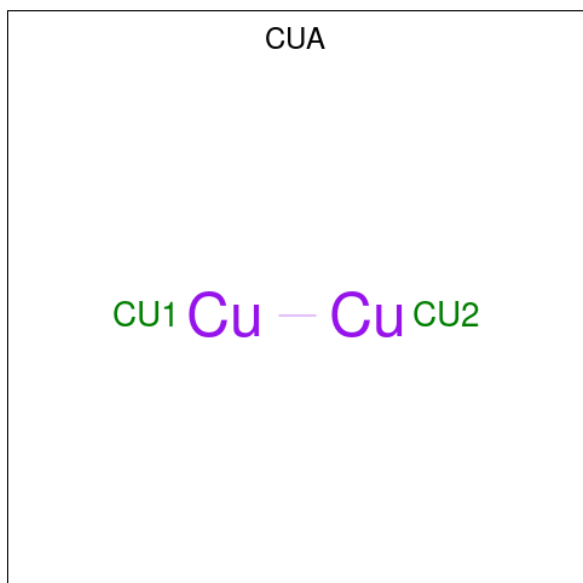
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	H	1	Total 4	C 2	O 2	0	0
21	I	1	Total 4	C 2	O 2	0	0
21	K	1	Total 4	C 2	O 2	0	0
21	L	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	Q	1	Total 4	C 2	O 2	0	0
21	Q	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	S	1	Total C O 4 2 2	0	0
21	S	1	Total C O 4 2 2	0	0
21	S	1	Total C O 4 2 2	0	0
21	S	1	Total C O 4 2 2	0	0
21	S	1	Total C O 4 2 2	0	0
21	T	1	Total C O 4 2 2	0	0
21	T	1	Total C O 4 2 2	0	0
21	U	1	Total C O 4 2 2	0	0
21	V	1	Total C O 4 2 2	0	0
21	V	1	Total C O 4 2 2	0	0

- Molecule 22 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



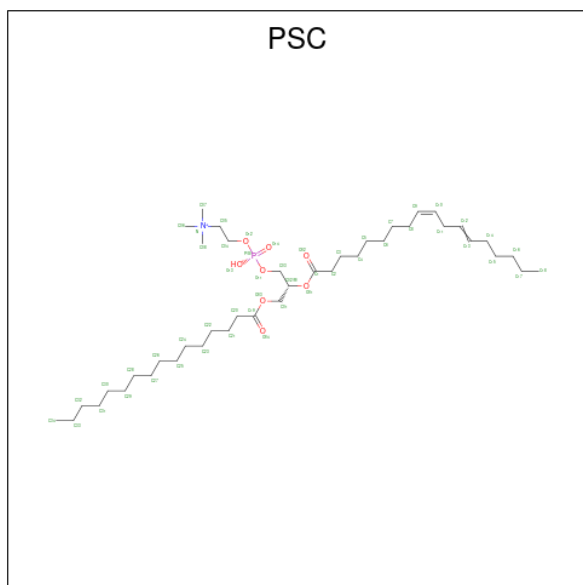
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0

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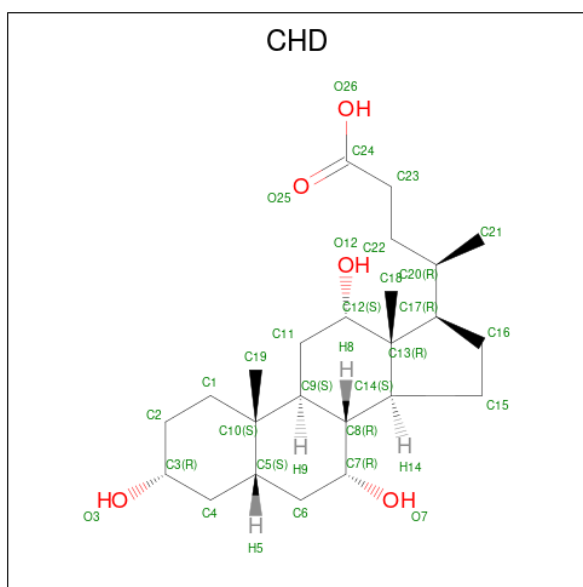
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	O	1	Total	Cu	0	0
			2	2		

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



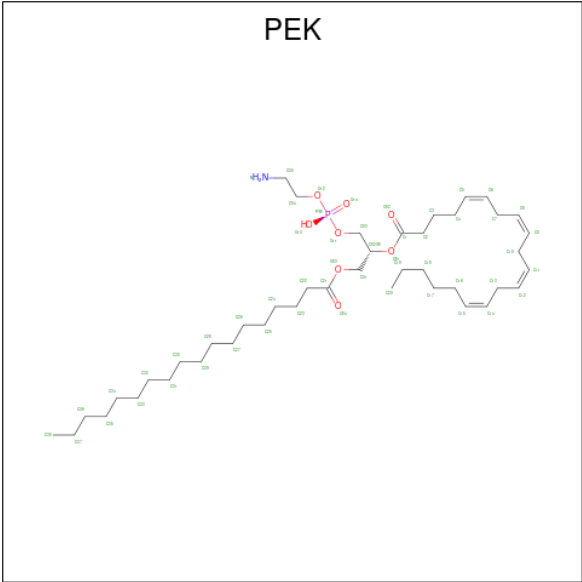
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
23	O	1	Total	C	N	O	P	0	0
			46	36	1	8	1		

- Molecule 24 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



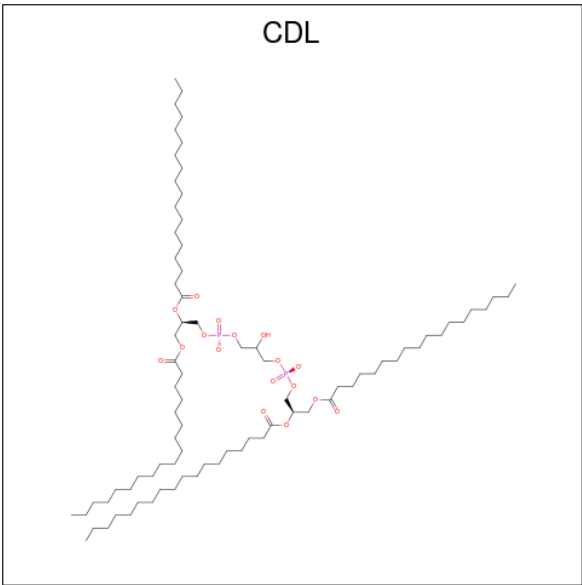
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			29	24	5		
24	C	1	Total	C	O	0	0
			29	24	5		
24	C	1	Total	C	O	0	0
			29	24	5		
24	C	1	Total	C	O	0	0
			29	24	5		
24	J	1	Total	C	O	0	0
			29	24	5		
24	O	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	Y	1	Total	C	O	0	0
			28	23	5		

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



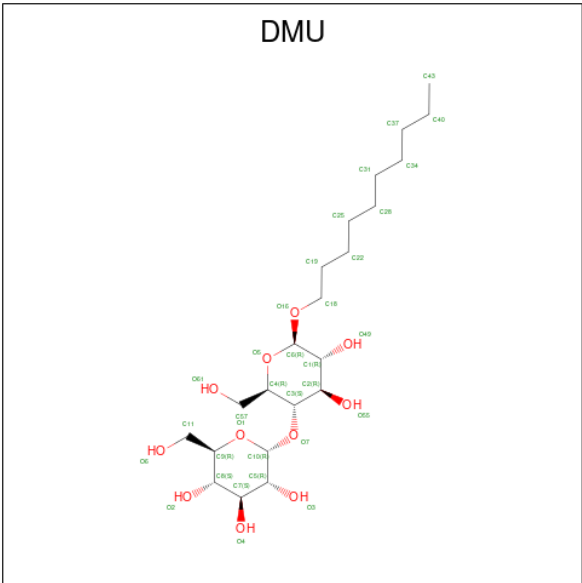
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
25	G	1	Total	C	O	P		0	0
			50	41	8	1			
25	P	1	Total	C	O	P		0	0
			40	31	8	1			
25	P	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			82	63	17	2		
26	G	1	Total	C	O	P	0	0
			88	69	17	2		
26	P	1	Total	C	O	P	0	0
			91	73	16	2		
26	T	1	Total	C	O	P	0	0
			93	74	17	2		

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O 33 22 11	0	0
27	C	1	Total C O 33 22 11	0	0
27	G	1	Total C O 33 22 11	0	0
27	L	1	Total C O 33 22 11	0	0
27	L	1	Total C O 33 22 11	0	0
27	M	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	T	1	Total C O 33 22 11	0	0
27	Z	1	Total C O 33 22 11	0	0
27	Z	1	Total C O 33 22 11	0	0

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

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	222	Total O 222 222	0	0
29	B	157	Total O 157 157	0	0
29	C	122	Total O 122 122	0	0
29	D	99	Total O 99 99	0	1
29	E	69	Total O 69 69	0	0

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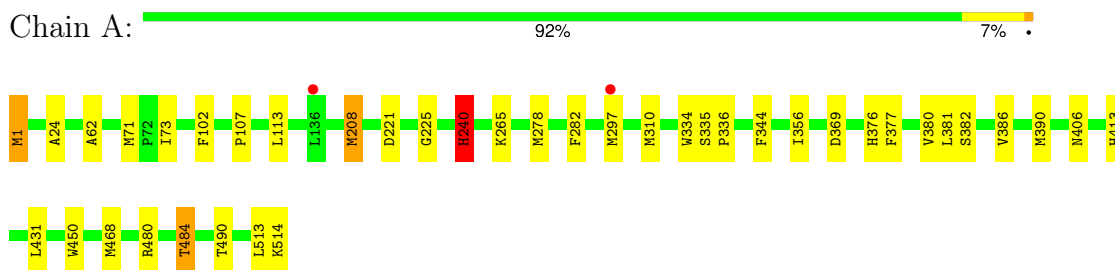
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	F	84	Total 84	O 84	0	1
29	G	42	Total 42	O 42	0	0
29	H	52	Total 52	O 52	0	0
29	I	32	Total 32	O 32	0	0
29	J	21	Total 21	O 21	0	0
29	K	21	Total 21	O 21	0	0
29	L	25	Total 25	O 25	0	0
29	M	24	Total 24	O 24	0	0
29	N	220	Total 220	O 220	0	0
29	O	121	Total 121	O 121	0	0
29	P	104	Total 104	O 104	0	0
29	Q	54	Total 54	O 54	0	0
29	R	47	Total 47	O 47	0	0
29	S	64	Total 64	O 64	0	0
29	T	54	Total 54	O 54	0	0
29	U	57	Total 57	O 57	0	0
29	V	22	Total 22	O 22	0	0
29	W	14	Total 14	O 14	0	0
29	X	17	Total 17	O 17	0	0
29	Y	12	Total 12	O 12	0	0
29	Z	9	Total 9	O 9	0	0

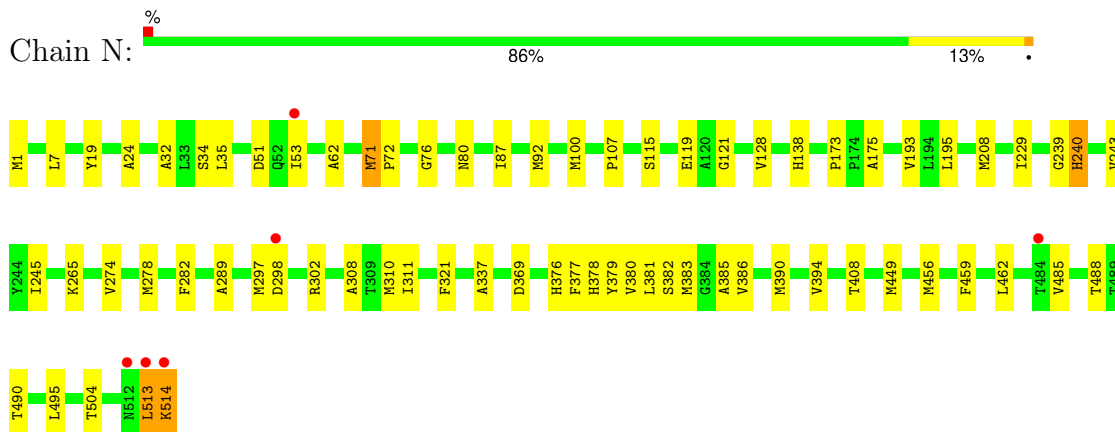
3 Residue-property plots

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.

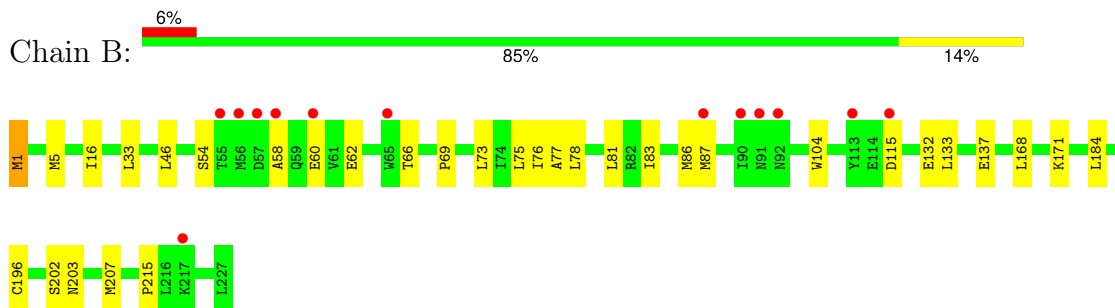
• Molecule 1: Cytochrome c oxidase subunit 1



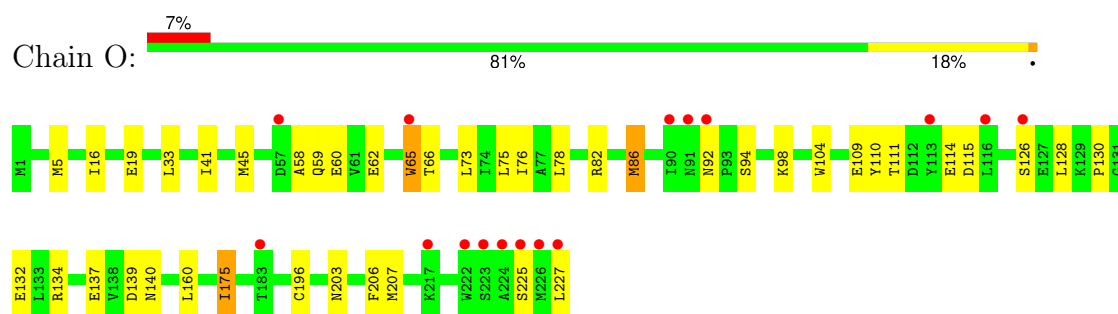
• Molecule 1: Cytochrome c oxidase subunit 1



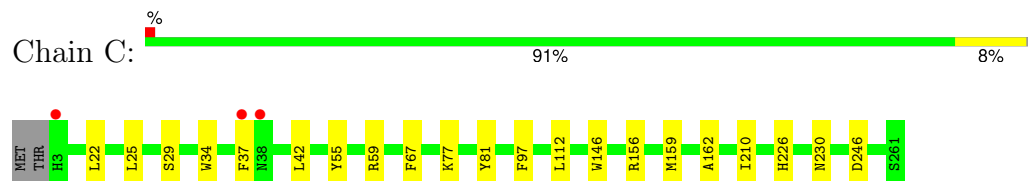
• Molecule 2: Cytochrome c oxidase subunit 2



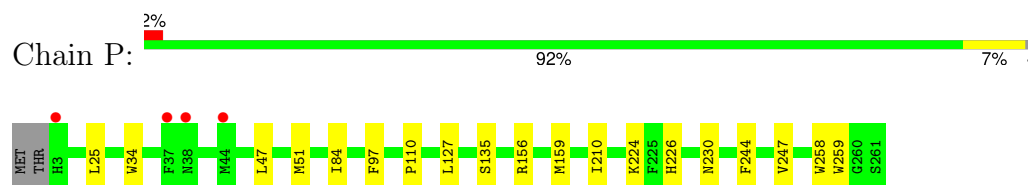
• Molecule 2: Cytochrome c oxidase subunit 2



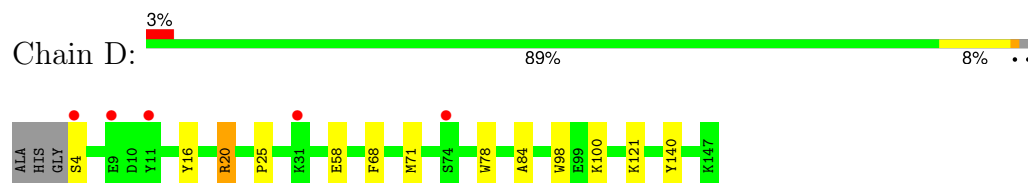
• Molecule 3: Cytochrome c oxidase subunit 3



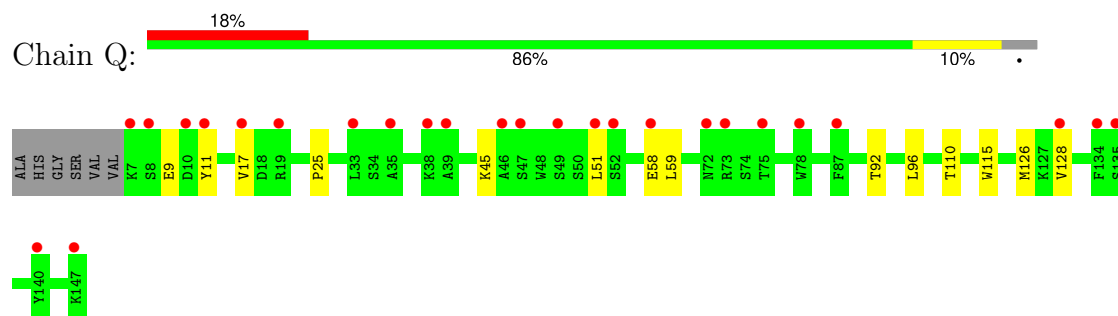
• Molecule 3: Cytochrome c oxidase subunit 3



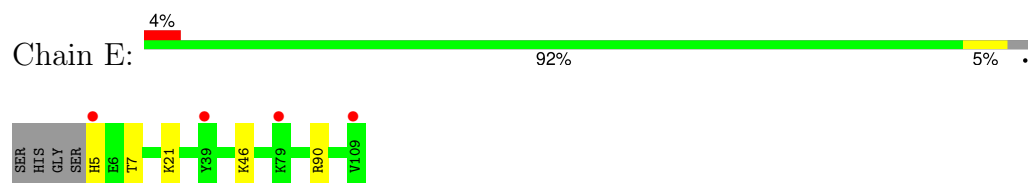
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



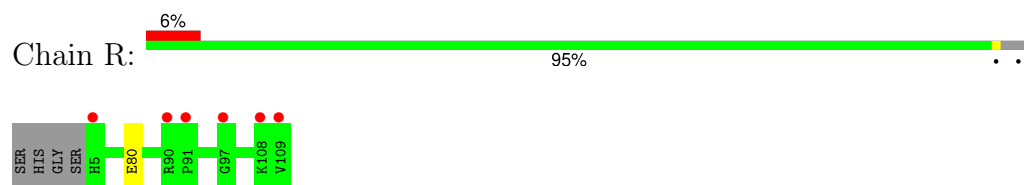
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



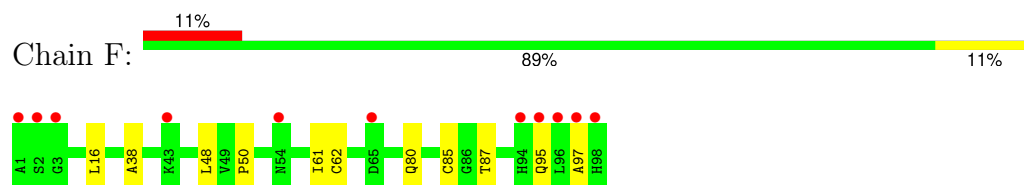
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



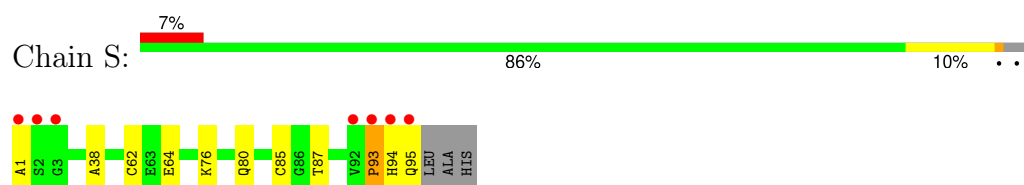
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



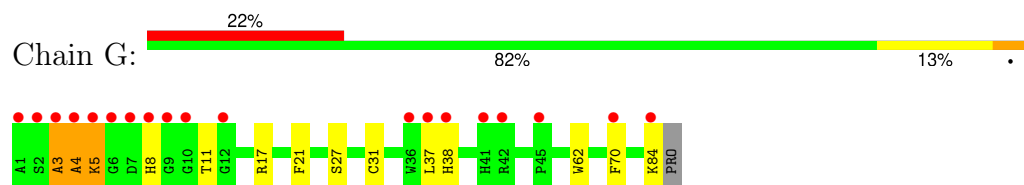
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



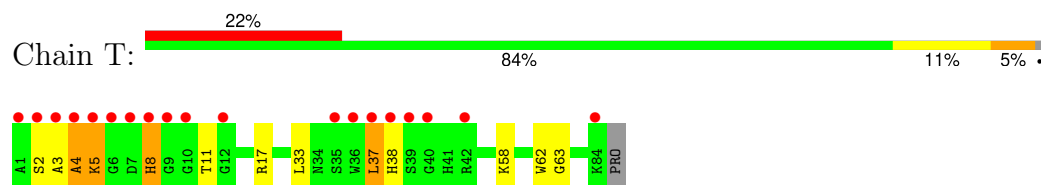
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



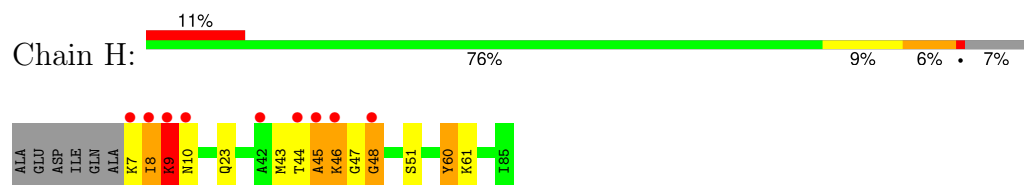
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



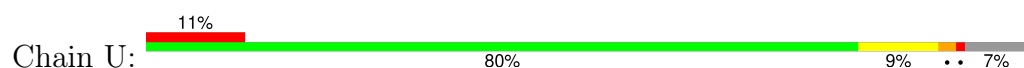
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



- Molecule 8: Cytochrome c oxidase subunit 6B1

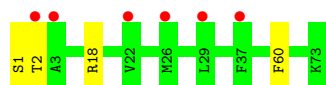


- Molecule 8: Cytochrome c oxidase subunit 6B1





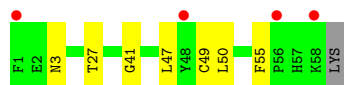
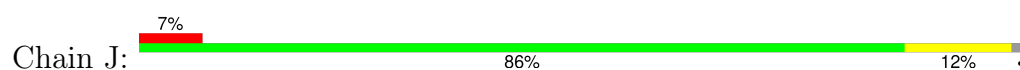
- Molecule 9: Cytochrome c oxidase subunit 6C



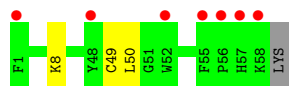
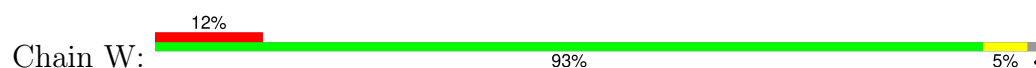
- Molecule 9: Cytochrome c oxidase subunit 6C



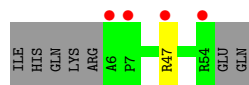
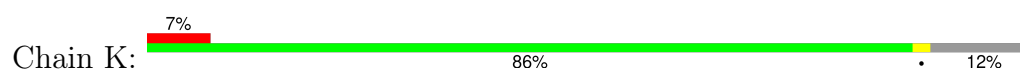
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



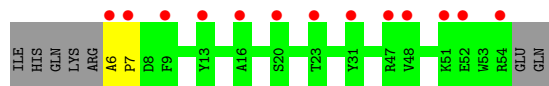
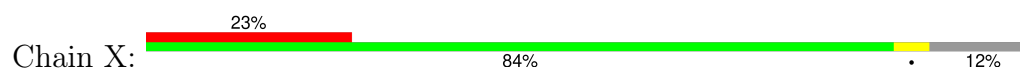
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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



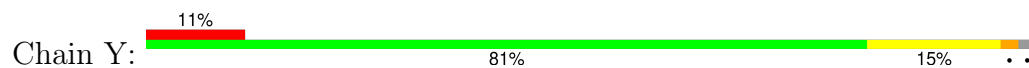
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



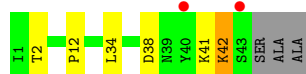
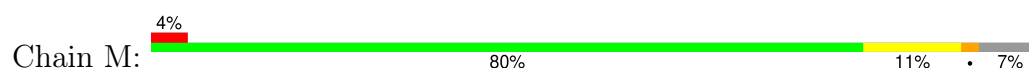
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



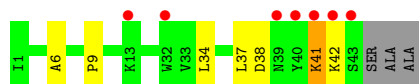
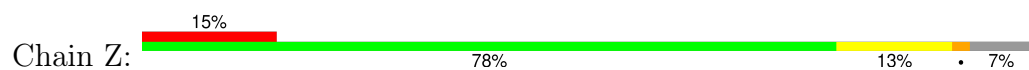
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.83Å 206.93Å 178.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.44 – 1.80 39.44 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.44-1.80) 99.5 (39.44-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.81Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.176 , 0.208 0.177 , 0.209	Depositor DCC
R_{free} test set	30375 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33056	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.06	2/4222 (0.0%)	0.92	7/5765 (0.1%)
1	N	0.83	0/4234	0.82	4/5783 (0.1%)
2	B	0.90	0/1872	0.91	0/2550
2	O	0.74	1/1883 (0.1%)	0.84	1/2564 (0.0%)
3	C	0.82	0/2197	0.80	0/3005
3	P	0.75	0/2211	0.75	0/3024
4	D	0.80	0/1241	0.78	1/1674 (0.1%)
4	Q	0.52	0/1209	0.62	0/1630
5	E	0.73	0/871	0.72	0/1182
5	R	0.54	0/871	0.66	0/1182
6	F	0.83	0/765	0.94	2/1038 (0.2%)
6	S	0.71	0/747	0.84	2/1015 (0.2%)
7	G	0.65	0/690	0.75	0/937
7	T	0.63	0/690	0.76	0/937
8	H	0.74	0/682	0.80	0/921
8	U	0.62	0/682	0.74	2/921 (0.2%)
9	I	0.65	0/605	0.73	0/802
9	V	0.48	0/605	0.67	0/802
10	J	0.52	0/471	0.69	0/636
10	W	0.53	0/471	0.63	0/636
11	K	0.75	0/398	0.76	0/546
11	X	0.52	0/398	0.57	0/546
12	L	0.84	0/393	0.82	0/526
12	Y	0.59	0/393	0.69	0/526
13	M	0.82	0/345	0.78	0/470
13	Z	0.54	0/345	0.66	0/470
All	All	0.79	3/29491 (0.0%)	0.80	19/40088 (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	A	0	1
1	N	0	1
8	H	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	175	ILE	CA-C	-11.56	1.42	1.52
1	A	480	ARG	CD-NE	5.93	1.54	1.46
1	A	484	THR	CB-OG1	5.45	1.52	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	MET	CG-SD-CE	-8.46	82.28	100.90
6	S	93	PRO	CA-C-N	8.21	137.21	121.54
6	S	93	PRO	C-N-CA	8.21	137.21	121.54
6	F	97	ALA	CA-C-N	6.42	133.25	121.70
6	F	97	ALA	C-N-CA	6.42	133.25	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
8	H	9	LYS	Peptide
1	N	240	HIS	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4070	0	4039	34	0
1	N	4074	0	4057	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1830	0	1838	21	0
2	O	1834	0	1839	23	0
3	C	2110	0	2027	20	0
3	P	2114	0	2028	17	0
4	D	1203	0	1192	9	0
4	Q	1175	0	1160	8	0
5	E	852	0	845	2	0
5	R	852	0	845	0	0
6	F	748	0	728	6	0
6	S	726	0	708	6	0
7	G	675	0	644	9	0
7	T	675	0	644	13	0
8	H	662	0	623	7	0
8	U	662	0	623	6	0
9	I	601	0	613	1	0
9	V	601	0	613	3	0
10	J	460	0	459	5	0
10	W	460	0	459	2	0
11	K	384	0	366	0	0
11	X	384	0	366	1	0
12	L	380	0	380	12	0
12	Y	380	0	380	8	0
13	M	335	0	352	4	0
13	Z	335	0	352	3	0
14	A	138	0	112	8	0
14	N	138	0	112	7	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	4	0	0	0	0
18	N	4	0	0	0	0
19	A	102	0	152	8	0
19	C	96	0	132	5	0
19	N	51	0	76	2	0
19	P	93	0	132	3	0
19	Z	47	0	65	1	0
20	A	59	0	95	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	63	0	110	1	0
20	D	55	0	88	3	0
20	N	63	0	110	2	0
20	O	63	0	110	2	0
20	Y	59	0	99	3	0
21	A	52	0	78	5	0
21	B	8	0	12	0	0
21	C	16	0	24	2	0
21	D	16	0	24	3	0
21	E	16	0	24	1	0
21	F	20	0	30	0	0
21	G	8	0	12	0	0
21	H	8	0	12	0	0
21	I	4	0	6	0	0
21	K	4	0	6	0	0
21	L	4	0	6	1	0
21	N	24	0	36	1	0
21	O	12	0	18	1	0
21	P	12	0	18	0	0
21	Q	8	0	12	1	0
21	R	8	0	12	0	0
21	S	24	0	36	0	0
21	T	8	0	12	0	0
21	U	4	0	6	0	0
21	V	8	0	12	0	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	50	0	71	3	0
23	O	46	0	62	0	0
24	B	29	0	39	0	0
24	C	87	0	117	3	0
24	J	29	0	39	2	0
24	O	29	0	39	2	0
24	P	87	0	117	10	0
24	Y	28	0	33	4	0
25	C	99	0	137	4	0
25	G	50	0	71	4	0
25	P	145	0	197	4	0
26	C	82	0	111	8	0
26	G	88	0	126	5	0
26	P	91	0	134	7	0
26	T	93	0	136	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	C	66	0	84	5	0
27	G	33	0	42	2	0
27	L	66	0	84	9	0
27	M	33	0	42	1	0
27	P	66	0	84	1	0
27	T	33	0	42	8	0
27	Z	66	0	84	2	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	222	0	0	6	0
29	B	157	0	0	1	0
29	C	122	0	0	1	0
29	D	99	0	0	3	0
29	E	69	0	0	1	0
29	F	84	0	0	1	0
29	G	42	0	0	0	0
29	H	52	0	0	0	0
29	I	32	0	0	0	0
29	J	21	0	0	0	0
29	K	21	0	0	1	0
29	L	25	0	0	0	0
29	M	24	0	0	0	0
29	N	220	0	0	0	0
29	O	121	0	0	1	0
29	P	104	0	0	1	0
29	Q	54	0	0	0	0
29	R	47	0	0	0	0
29	S	64	0	0	0	0
29	T	54	0	0	2	0
29	U	57	0	0	0	0
29	V	22	0	0	1	0
29	W	14	0	0	0	0
29	X	17	0	0	0	0
29	Y	12	0	0	0	0
29	Z	9	0	0	0	0
All	All	33056	0	31860	303	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 303 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASN:HD21	19:A:607:PGV:H21	1.45	0.80
7:T:37:LEU:HD23	26:T:102:CDL:H381	1.63	0.80
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.68	0.75
21:D:204:EDO:H11	29:D:320:HOH:O	1.87	0.75
7:T:63:GLY:HA2	27:T:101:DMU:H34	1.70	0.74

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	521/514 (101%)	508 (98%)	13 (2%)	0	100	100
1	N	523/514 (102%)	514 (98%)	9 (2%)	0	100	100
2	B	226/227 (100%)	221 (98%)	5 (2%)	0	100	100
2	O	227/227 (100%)	218 (96%)	7 (3%)	2 (1%)	14	5
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	259/261 (99%)	254 (98%)	5 (2%)	0	100	100
4	D	143/147 (97%)	140 (98%)	3 (2%)	0	100	100
4	Q	139/147 (95%)	133 (96%)	6 (4%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	93 (97%)	2 (2%)	1 (1%)	12	4
6	S	94/98 (96%)	89 (95%)	4 (4%)	1 (1%)	11	3
7	G	81/85 (95%)	69 (85%)	9 (11%)	3 (4%)	2	0
7	T	81/85 (95%)	69 (85%)	9 (11%)	3 (4%)	2	0
8	H	77/85 (91%)	69 (90%)	3 (4%)	5 (6%)	1	0
8	U	77/85 (91%)	74 (96%)	2 (3%)	1 (1%)	9	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	71/73 (97%)	69 (97%)	2 (3%)	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%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	0	1 (2%)	4	1
All	All	3525/3614 (98%)	3415 (97%)	93 (3%)	17 (0%)	24	14

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
8	H	10	ASN
6	S	94	HIS
8	U	8	ILE
8	H	8	ILE

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	434/426 (102%)	432 (100%)	2 (0%)	81	80
1	N	436/426 (102%)	425 (98%)	11 (2%)	42	30
2	B	211/210 (100%)	202 (96%)	9 (4%)	26	13
2	O	212/210 (101%)	201 (95%)	11 (5%)	21	9
3	C	224/226 (99%)	221 (99%)	3 (1%)	61	54
3	P	226/226 (100%)	223 (99%)	3 (1%)	61	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	129/129 (100%)	127 (98%)	2 (2%)	55	47
4	Q	125/129 (97%)	121 (97%)	4 (3%)	34	22
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	21
5	R	92/95 (97%)	91 (99%)	1 (1%)	65	60
6	F	81/81 (100%)	79 (98%)	2 (2%)	42	30
6	S	80/81 (99%)	78 (98%)	2 (2%)	42	30
7	G	67/68 (98%)	63 (94%)	4 (6%)	17	7
7	T	67/68 (98%)	63 (94%)	4 (6%)	17	7
8	H	71/75 (95%)	65 (92%)	6 (8%)	10	3
8	U	71/75 (95%)	66 (93%)	5 (7%)	14	4
9	I	57/57 (100%)	55 (96%)	2 (4%)	32	19
9	V	57/57 (100%)	56 (98%)	1 (2%)	51	43
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	15
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	38
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	28
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	39/40 (98%)	36 (92%)	3 (8%)	12	3
12	Y	39/40 (98%)	36 (92%)	3 (8%)	12	3
13	M	37/38 (97%)	34 (92%)	3 (8%)	11	3
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	3
All	All	3060/3082 (99%)	2969 (97%)	91 (3%)	36	24

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	66	THR
5	R	80	GLU
2	O	78	LEU
3	P	159	MET
7	T	5	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	76	GLN
5	R	78	HIS
4	Q	143	ASN
7	T	34	ASN
6	F	54	ASN

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	$\# Z > 2$
7	TPO	G	11	7	8,10,11	1.35	1 (12%)	10,14,16	0.95	1 (10%)
2	FME	B	1	2	8,9,10	1.00	0	8,9,11	1.71	2 (25%)
9	SAC	I	1	9	7,8,9	0.92	0	7,9,11	1.26	1 (14%)
9	SAC	V	1	9	7,8,9	0.65	0	7,9,11	0.84	0
2	FME	O	1	2	8,9,10	0.63	0	8,9,11	1.07	0
1	FME	N	1	1	8,9,10	0.51	0	8,9,11	1.15	1 (12%)
7	TPO	T	11	7	8,10,11	1.38	1 (12%)	10,14,16	0.81	0
1	FME	A	1	1	8,9,10	0.78	0	8,9,11	1.33	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TPO	G	11	7	-	6/9/11/13	-
2	FME	B	1	2	-	0/7/9/11	-

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	2.98	1.59	1.50
7	G	11	TPO	P-O1P	2.96	1.59	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-3.03	103.59	112.87
1	A	1	FME	O1-CN-N	-2.48	118.91	125.32
9	I	1	SAC	O-C-CA	-2.45	118.46	124.77
2	B	1	FME	O1-CN-N	-2.39	119.15	125.32
7	G	11	TPO	P-OG1-CB	-2.16	117.47	123.33

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	O-C-CA-CB
7	G	11	TPO	CA-CB-OG1-P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 135 ligands modelled in this entry, 10 are monoatomic - leaving 125 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PEK	C	303	-	52,52,52	0.87	2 (3%)	55,57,57	1.63	7 (12%)
21	EDO	T	104	-	3,3,3	0.42	0	2,2,2	0.40	0
21	EDO	C	310	-	3,3,3	0.46	0	2,2,2	0.35	0
21	EDO	I	101	-	3,3,3	0.69	0	2,2,2	0.12	0
21	EDO	N	612	-	3,3,3	0.63	0	2,2,2	0.56	0
21	EDO	S	105	-	3,3,3	0.38	0	2,2,2	0.54	0
25	PEK	P	305	-	51,51,52	0.83	2 (3%)	54,56,57	1.46	6 (11%)
27	DMU	C	313	-	34,34,34	0.61	1 (2%)	45,45,45	1.30	6 (13%)
19	PGV	C	305	-	47,47,50	1.38	4 (8%)	47,51,56	1.54	4 (8%)
22	CUA	B	301	2	0,1,1	-	-	-	-	-
21	EDO	G	104	-	3,3,3	0.69	0	2,2,2	0.21	0
21	EDO	D	203	-	3,3,3	0.41	0	2,2,2	0.58	0
23	PSC	O	304	-	45,45,51	1.17	3 (6%)	48,50,59	1.27	3 (6%)
19	PGV	N	608	-	50,50,50	0.93	2 (4%)	53,56,56	1.37	5 (9%)
20	TGL	Y	101	-	58,58,62	1.25	3 (5%)	61,61,65	1.43	7 (11%)
26	CDL	T	102	-	92,92,99	1.47	12 (13%)	98,104,111	1.46	12 (12%)
27	DMU	P	313	-	34,34,34	0.46	0	45,45,45	1.51	8 (17%)
24	CHD	O	301	-	32,32,32	0.97	1 (3%)	51,51,51	1.42	4 (7%)
21	EDO	G	105	-	3,3,3	0.66	0	2,2,2	0.35	0
21	EDO	A	621	-	3,3,3	0.90	0	2,2,2	0.77	0
21	EDO	E	203	-	3,3,3	0.49	0	2,2,2	0.17	0
23	PSC	B	303	-	48,48,51	1.16	3 (6%)	51,54,59	1.05	2 (3%)
26	CDL	P	308	-	89,89,99	1.45	12 (13%)	95,99,111	1.66	14 (14%)
21	EDO	O	305	-	3,3,3	0.47	0	2,2,2	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	A	619	-	3,3,3	0.15	0	2,2,2	0.25	0
27	DMU	L	102	-	34,34,34	0.72	1 (2%)	45,45,45	1.29	4 (8%)
14	HEA	N	601[B]	-	67,67,67	1.74	17 (25%)	81,103,103	2.11	20 (24%)
21	EDO	A	620	-	3,3,3	0.58	0	2,2,2	0.82	0
21	EDO	N	613	-	3,3,3	0.48	0	2,2,2	0.38	0
21	EDO	N	614	-	3,3,3	0.48	0	2,2,2	0.22	0
21	EDO	N	610	-	3,3,3	0.61	0	2,2,2	0.45	0
21	EDO	D	205	-	3,3,3	0.62	0	2,2,2	0.18	0
21	EDO	P	311	-	3,3,3	0.75	0	2,2,2	0.49	0
27	DMU	L	103	-	34,34,34	0.76	1 (2%)	45,45,45	1.09	4 (8%)
21	EDO	V	102	-	3,3,3	0.57	0	2,2,2	0.15	0
21	EDO	P	312	-	3,3,3	0.68	0	2,2,2	0.21	0
21	EDO	T	103	-	3,3,3	0.53	0	2,2,2	0.62	0
19	PGV	C	304	-	46,46,50	0.84	1 (2%)	49,52,56	1.12	5 (10%)
21	EDO	E	204	-	3,3,3	0.48	0	2,2,2	0.35	0
25	PEK	P	306	-	52,52,52	1.04	2 (3%)	55,57,57	1.17	4 (7%)
21	EDO	O	306	-	3,3,3	0.51	0	2,2,2	0.07	0
21	EDO	B	305	-	3,3,3	0.64	0	2,2,2	0.67	0
25	PEK	P	301	-	39,39,52	1.13	2 (5%)	42,44,57	1.76	7 (16%)
21	EDO	D	202	-	3,3,3	0.50	0	2,2,2	0.19	0
27	DMU	Z	103	-	34,34,34	0.55	0	45,45,45	0.98	2 (4%)
24	CHD	C	315	-	32,32,32	0.82	1 (3%)	51,51,51	2.26	15 (29%)
27	DMU	T	101	-	34,34,34	0.57	0	45,45,45	2.44	11 (24%)
21	EDO	N	611	-	3,3,3	0.51	0	2,2,2	0.38	0
14	HEA	A	602	1	67,67,67	2.14	20 (29%)	81,103,103	2.38	33 (40%)
18	CMO	N	606[B]	15	0,1,1	-	-	-	-	-
27	DMU	Z	102	-	34,34,34	0.50	0	45,45,45	1.06	6 (13%)
19	PGV	A	607	-	50,50,50	0.97	2 (4%)	53,56,56	1.32	5 (9%)
18	CMO	A	606[B]	15	0,1,1	-	-	-	-	-
21	EDO	F	104	-	3,3,3	0.63	0	2,2,2	0.64	0
21	EDO	A	617	-	3,3,3	0.37	0	2,2,2	0.74	0
21	EDO	V	101	-	3,3,3	0.64	0	2,2,2	0.25	0
21	EDO	N	609	-	3,3,3	0.81	0	2,2,2	0.65	0
21	EDO	A	611	-	3,3,3	0.54	0	2,2,2	0.93	0
21	EDO	S	107	-	3,3,3	0.55	0	2,2,2	0.59	0
14	HEA	A	601[A]	-	67,67,67	1.98	22 (32%)	81,103,103	2.15	30 (37%)
21	EDO	O	307	-	3,3,3	0.76	0	2,2,2	0.19	0
21	EDO	L	101	-	3,3,3	0.90	0	2,2,2	0.28	0
14	HEA	N	602	1	67,67,67	1.82	22 (32%)	81,103,103	1.92	22 (27%)
21	EDO	A	612	-	3,3,3	0.91	0	2,2,2	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	S	102	-	3,3,3	0.75	0	2,2,2	0.79	0
21	EDO	E	202	-	3,3,3	0.62	0	2,2,2	0.24	0
14	HEA	N	601[A]	-	67,67,67	1.74	17 (25%)	81,103,103	2.02	25 (30%)
24	CHD	J	101	-	32,32,32	0.72	0	51,51,51	1.77	10 (19%)
21	EDO	H	102	-	3,3,3	0.44	0	2,2,2	0.42	0
19	PGV	Z	101	-	46,46,50	1.01	2 (4%)	49,52,56	1.40	6 (12%)
26	CDL	G	103	-	87,87,99	1.41	10 (11%)	93,99,111	1.30	6 (6%)
21	EDO	R	202	-	3,3,3	0.50	0	2,2,2	0.29	0
20	TGL	D	201	-	54,54,62	1.24	4 (7%)	57,57,65	1.16	7 (12%)
21	EDO	A	614	-	3,3,3	0.71	0	2,2,2	0.94	0
21	EDO	F	105	-	3,3,3	0.59	0	2,2,2	0.56	0
21	EDO	F	102	-	3,3,3	0.88	0	2,2,2	0.46	0
19	PGV	P	302	-	46,46,50	1.12	2 (4%)	49,51,56	1.75	7 (14%)
22	CUA	O	302	2	0,1,1	-	-	-	-	-
24	CHD	P	315	-	32,32,32	0.85	0	51,51,51	2.47	20 (39%)
21	EDO	A	618	-	3,3,3	0.67	0	2,2,2	0.34	0
21	EDO	Q	202	-	3,3,3	0.33	0	2,2,2	0.27	0
21	EDO	Q	201	-	3,3,3	0.28	0	2,2,2	0.70	0
27	DMU	G	101	-	34,34,34	0.77	1 (2%)	45,45,45	2.25	12 (26%)
21	EDO	P	310	-	3,3,3	0.20	0	2,2,2	0.70	0
18	CMO	A	606[A]	-	0,1,1	-	-	-	-	-
24	CHD	P	309	-	32,32,32	0.93	1 (3%)	51,51,51	2.00	18 (35%)
21	EDO	F	103	-	3,3,3	0.74	0	2,2,2	0.17	0
21	EDO	S	103	-	3,3,3	0.57	0	2,2,2	1.26	0
27	DMU	C	314	-	34,34,34	0.60	1 (2%)	45,45,45	1.00	1 (2%)
27	DMU	P	314	-	34,34,34	0.58	1 (2%)	45,45,45	1.12	4 (8%)
24	CHD	B	304	-	32,32,32	1.05	2 (6%)	51,51,51	1.64	13 (25%)
19	PGV	P	307	-	45,45,50	0.83	2 (4%)	48,51,56	1.13	3 (6%)
25	PEK	G	102	-	49,49,52	1.05	3 (6%)	52,54,57	1.40	5 (9%)
24	CHD	P	304	-	32,32,32	0.86	0	51,51,51	1.70	12 (23%)
21	EDO	F	106	-	3,3,3	0.54	0	2,2,2	0.45	0
21	EDO	C	311	-	3,3,3	0.47	0	2,2,2	0.28	0
19	PGV	A	608	-	50,50,50	1.09	5 (10%)	53,56,56	1.29	7 (13%)
21	EDO	K	101	-	3,3,3	0.64	0	2,2,2	0.35	0
21	EDO	U	101	-	3,3,3	0.44	0	2,2,2	0.61	0
21	EDO	A	615	-	3,3,3	0.64	0	2,2,2	0.19	0
24	CHD	Y	102	-	30,30,32	0.85	1 (3%)	45,47,51	2.30	15 (33%)
21	EDO	R	201	-	3,3,3	0.60	0	2,2,2	0.34	0
20	TGL	B	302	-	62,62,62	1.12	3 (4%)	65,65,65	1.23	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	DMU	M	101	-	34,34,34	0.50	0	45,45,45	1.63	10 (22%)
20	TGL	O	303	-	62,62,62	1.09	3 (4%)	65,65,65	1.17	5 (7%)
20	TGL	A	609	-	57,57,62	1.18	3 (5%)	59,59,65	1.60	9 (15%)
25	PEK	C	308	-	45,45,52	1.07	2 (4%)	48,50,57	1.10	3 (6%)
21	EDO	C	309	-	3,3,3	0.65	0	2,2,2	0.32	0
21	EDO	D	204	-	3,3,3	0.49	0	2,2,2	0.34	0
21	EDO	S	104	-	3,3,3	0.66	0	2,2,2	0.16	0
21	EDO	H	101	-	3,3,3	0.47	0	2,2,2	0.18	0
20	TGL	N	607	-	62,62,62	1.06	3 (4%)	65,65,65	1.17	7 (10%)
21	EDO	A	613	-	3,3,3	0.60	0	2,2,2	0.08	0
26	CDL	C	306	-	81,81,99	1.37	9 (11%)	87,93,111	1.61	17 (19%)
18	CMO	N	606[A]	-	0,1,1	-	-	-	-	-
21	EDO	A	610	-	3,3,3	1.04	0	2,2,2	0.54	0
21	EDO	A	622	-	3,3,3	0.44	0	2,2,2	0.29	0
14	HEA	A	601[B]	-	67,67,67	1.99	22 (32%)	81,103,103	2.30	32 (39%)
21	EDO	A	616	-	3,3,3	0.86	0	2,2,2	0.47	0
21	EDO	C	312	-	3,3,3	0.64	0	2,2,2	0.32	0
24	CHD	C	307	-	32,32,32	0.76	0	51,51,51	1.24	4 (7%)
21	EDO	B	306	-	3,3,3	0.52	0	2,2,2	0.20	0
21	EDO	S	106	-	3,3,3	0.58	0	2,2,2	0.28	0
24	CHD	C	301	-	32,32,32	1.36	4 (12%)	51,51,51	1.51	11 (21%)
21	EDO	E	201	-	3,3,3	0.41	0	2,2,2	0.53	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
25	PEK	C	303	-	-	20/56/56/56	-
21	EDO	T	104	-	-	0/1/1/1	-
21	EDO	C	310	-	-	0/1/1/1	-
21	EDO	I	101	-	-	1/1/1/1	-
21	EDO	N	612	-	-	0/1/1/1	-
21	EDO	S	105	-	-	1/1/1/1	-
25	PEK	P	305	-	-	9/55/55/56	-
27	DMU	C	313	-	-	4/19/59/59	0/2/2/2
19	PGV	C	305	-	-	18/49/49/55	-
21	EDO	G	104	-	-	1/1/1/1	-
21	EDO	D	203	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSC	O	304	-	-	14/49/49/55	-
19	PGV	N	608	-	-	11/55/55/55	-
20	TGL	Y	101	-	-	28/61/61/65	-
26	CDL	T	102	-	-	33/103/103/110	-
27	DMU	P	313	-	-	6/19/59/59	0/2/2/2
24	CHD	O	301	-	-	2/9/74/74	0/4/4/4
21	EDO	G	105	-	-	0/1/1/1	-
21	EDO	A	621	-	-	0/1/1/1	-
21	EDO	E	203	-	-	0/1/1/1	-
23	PSC	B	303	-	-	16/49/49/55	-
26	CDL	P	308	-	-	50/95/95/110	-
21	EDO	O	305	-	-	0/1/1/1	-
21	EDO	A	619	-	-	0/1/1/1	-
27	DMU	L	102	-	-	5/19/59/59	0/2/2/2
14	HEA	N	601[B]	-	-	5/36/76/76	-
21	EDO	A	620	-	-	1/1/1/1	-
21	EDO	N	613	-	-	0/1/1/1	-
21	EDO	N	614	-	-	1/1/1/1	-
21	EDO	N	610	-	-	0/1/1/1	-
21	EDO	D	205	-	-	0/1/1/1	-
21	EDO	P	311	-	-	1/1/1/1	-
27	DMU	L	103	-	-	10/19/59/59	0/2/2/2
21	EDO	V	102	-	-	0/1/1/1	-
21	EDO	P	312	-	-	1/1/1/1	-
21	EDO	T	103	-	-	0/1/1/1	-
19	PGV	C	304	-	-	8/51/51/55	-
21	EDO	E	204	-	-	0/1/1/1	-
25	PEK	P	306	-	-	25/56/56/56	-
21	EDO	O	306	-	-	0/1/1/1	-
21	EDO	B	305	-	-	0/1/1/1	-
25	PEK	P	301	-	-	17/41/41/56	-
21	EDO	D	202	-	-	1/1/1/1	-
27	DMU	Z	103	-	-	9/19/59/59	0/2/2/2
24	CHD	C	315	-	-	3/9/74/74	0/4/4/4
27	DMU	T	101	-	-	8/19/59/59	0/2/2/2
21	EDO	N	611	-	-	0/1/1/1	-
14	HEA	A	602	1	-	6/36/76/76	-
27	DMU	Z	102	-	-	5/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PGV	A	607	-	-	32/55/55/55	-
21	EDO	V	101	-	-	1/1/1/1	-
21	EDO	F	104	-	-	0/1/1/1	-
21	EDO	A	617	-	-	0/1/1/1	-
21	EDO	N	609	-	-	0/1/1/1	-
21	EDO	A	611	-	-	1/1/1/1	-
21	EDO	S	107	-	-	0/1/1/1	-
14	HEA	A	601[A]	-	-	9/36/76/76	-
21	EDO	O	307	-	-	0/1/1/1	-
21	EDO	L	101	-	-	1/1/1/1	-
14	HEA	N	602	1	-	5/36/76/76	-
21	EDO	A	612	-	-	0/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
21	EDO	E	202	-	-	1/1/1/1	-
14	HEA	N	601[A]	-	-	7/36/76/76	-
24	CHD	J	101	-	-	8/9/74/74	0/4/4/4
21	EDO	H	102	-	-	0/1/1/1	-
19	PGV	Z	101	-	-	12/51/51/55	-
26	CDL	G	103	-	-	36/98/98/110	-
21	EDO	R	202	-	-	0/1/1/1	-
20	TGL	D	201	-	-	18/57/57/65	-
21	EDO	A	614	-	-	0/1/1/1	-
21	EDO	F	105	-	-	0/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
19	PGV	P	302	-	-	12/50/50/55	-
24	CHD	P	315	-	-	3/9/74/74	0/4/4/4
21	EDO	A	618	-	-	0/1/1/1	-
21	EDO	Q	202	-	-	0/1/1/1	-
21	EDO	Q	201	-	-	1/1/1/1	-
27	DMU	G	101	-	-	14/19/59/59	0/2/2/2
21	EDO	P	310	-	-	1/1/1/1	-
24	CHD	P	309	-	-	4/9/74/74	0/4/4/4
21	EDO	F	103	-	-	0/1/1/1	-
21	EDO	S	103	-	-	1/1/1/1	-
27	DMU	C	314	-	-	4/19/59/59	0/2/2/2
27	DMU	P	314	-	-	7/19/59/59	0/2/2/2
24	CHD	B	304	-	-	2/9/74/74	0/4/4/4
19	PGV	P	307	-	-	6/50/50/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEK	G	102	-	-	25/51/51/56	-
24	CHD	P	304	-	-	1/9/74/74	0/4/4/4
21	EDO	F	106	-	-	0/1/1/1	-
21	EDO	C	311	-	-	0/1/1/1	-
19	PGV	A	608	-	-	6/55/55/55	-
21	EDO	K	101	-	-	0/1/1/1	-
21	EDO	U	101	-	-	1/1/1/1	-
21	EDO	A	615	-	-	0/1/1/1	-
24	CHD	Y	102	-	-	2/12/67/74	0/3/3/4
21	EDO	R	201	-	-	0/1/1/1	-
20	TGL	B	302	-	-	20/65/65/65	-
27	DMU	M	101	-	-	5/19/59/59	0/2/2/2
20	TGL	O	303	-	-	27/65/65/65	-
20	TGL	A	609	-	-	28/57/57/65	-
25	PEK	C	308	-	-	16/49/49/56	-
21	EDO	C	309	-	-	0/1/1/1	-
21	EDO	D	204	-	-	1/1/1/1	-
21	EDO	S	104	-	-	0/1/1/1	-
21	EDO	H	101	-	-	0/1/1/1	-
20	TGL	N	607	-	-	22/65/65/65	-
21	EDO	A	613	-	-	1/1/1/1	-
26	CDL	C	306	-	-	46/92/92/110	-
21	EDO	A	610	-	-	1/1/1/1	-
21	EDO	A	622	-	-	0/1/1/1	-
14	HEA	A	601[B]	-	-	6/36/76/76	-
21	EDO	A	616	-	-	0/1/1/1	-
21	EDO	C	312	-	-	0/1/1/1	-
24	CHD	C	307	-	-	4/9/74/74	0/4/4/4
21	EDO	B	306	-	-	0/1/1/1	-
21	EDO	S	106	-	-	1/1/1/1	-
24	CHD	C	301	-	-	1/9/74/74	0/4/4/4
21	EDO	E	201	-	-	1/1/1/1	-

The worst 5 of 237 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	305	PGV	O01-C1	5.84	1.45	1.33
20	Y	101	TGL	OG2-CB1	5.52	1.49	1.34
14	A	602	HEA	C4A-NA	-5.48	1.29	1.39
20	A	609	TGL	OG2-CB1	5.23	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	303	PSC	O01-C1	5.22	1.49	1.34

The worst 5 of 518 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601[B]	HEA	C13-C12-C11	-7.59	102.26	114.39
27	T	101	DMU	O4-C7-C5	-7.34	93.06	110.38
19	P	302	PGV	O01-C1-C2	7.24	127.14	111.48
25	P	301	PEK	O01-C1-C2	6.62	125.81	111.48
19	C	305	PGV	O01-C1-O02	-6.56	117.29	125.70

There are no chirality outliers.

5 of 721 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	N	601[A]	HEA	C2A-C3A-CMA-OMA
14	N	601[B]	HEA	C2A-C3A-CMA-OMA
19	A	607	PGV	C03-O11-P-O12

There are no ring outliers.

55 monomers are involved in 152 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	303	PEK	2	0
27	C	313	DMU	2	0
19	C	305	PGV	4	0
21	D	203	EDO	1	0
19	N	608	PGV	2	0
20	Y	101	TGL	3	0
26	T	102	CDL	11	0
27	P	313	DMU	1	0
24	O	301	CHD	2	0
21	E	203	EDO	1	0
23	B	303	PSC	3	0
26	P	308	CDL	7	0
21	O	305	EDO	1	0
21	A	619	EDO	5	0
27	L	102	DMU	5	0
27	L	103	DMU	4	0

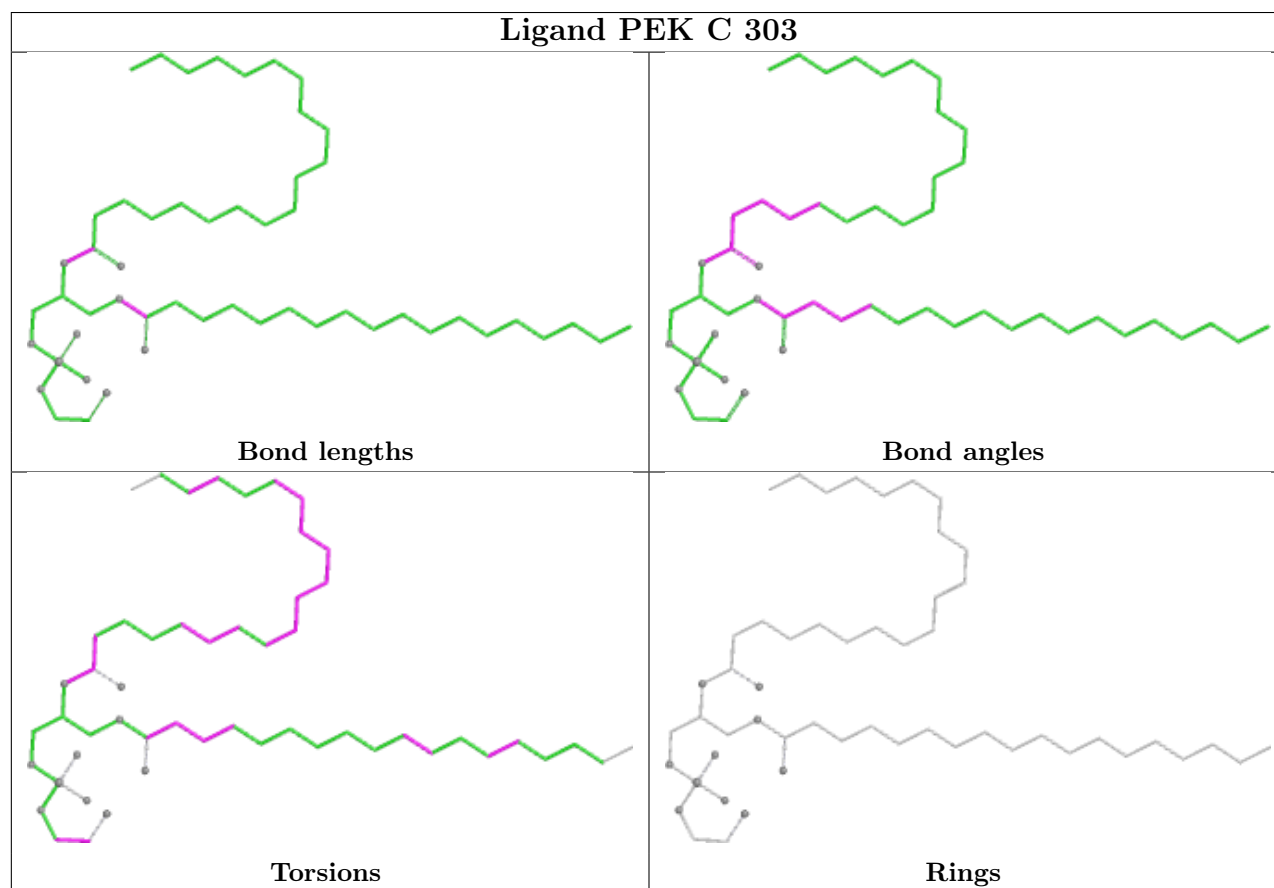
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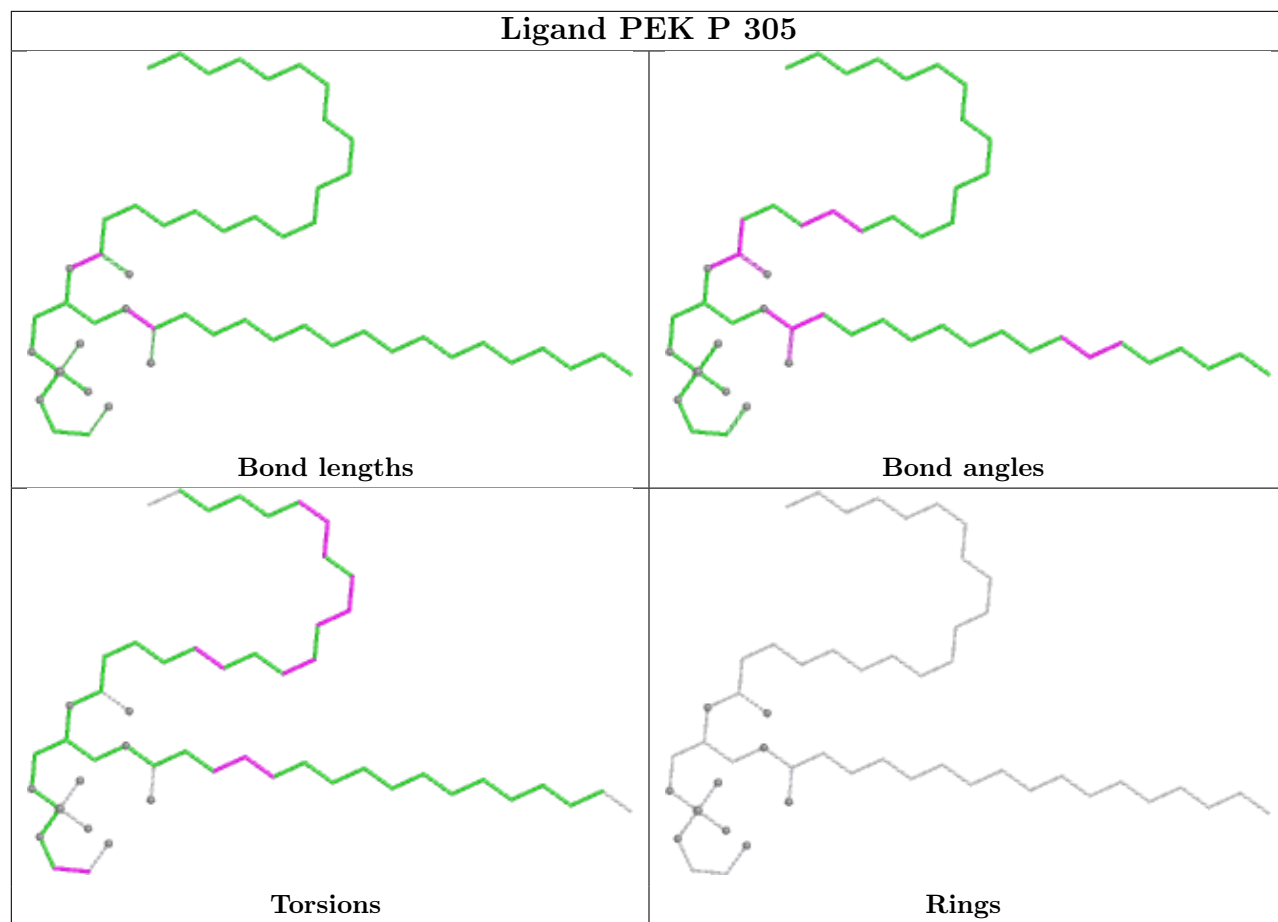
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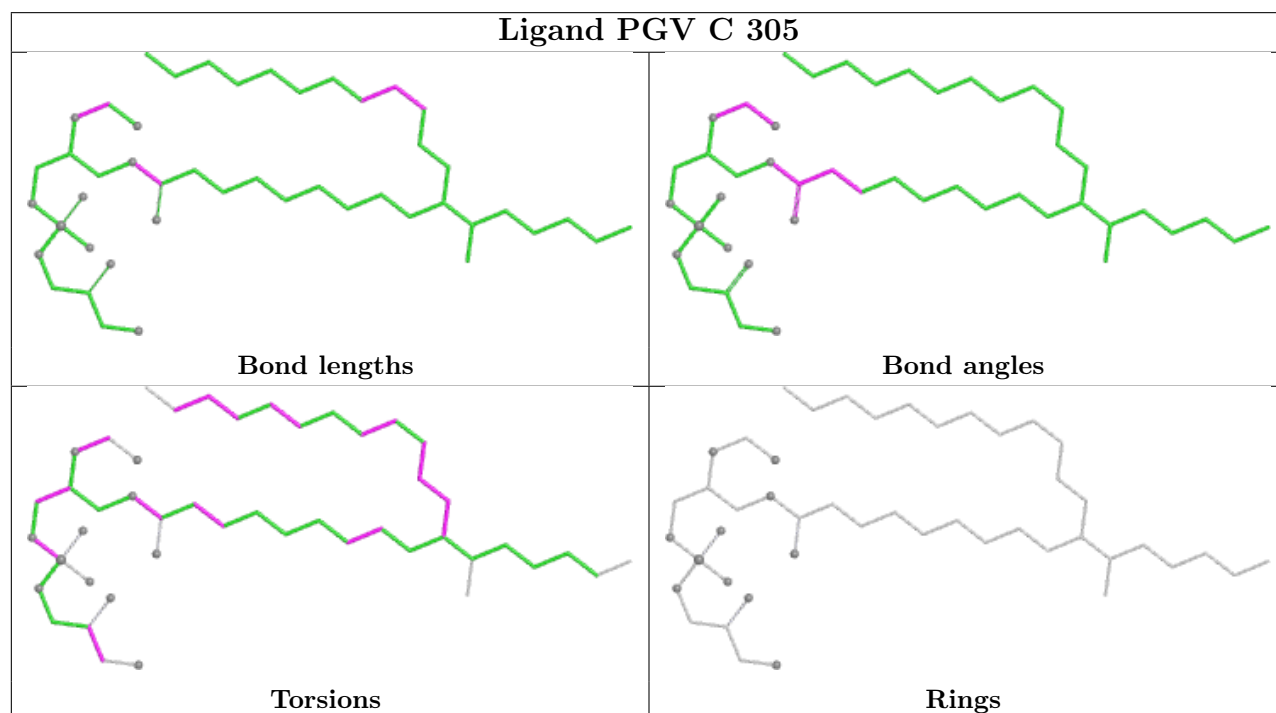
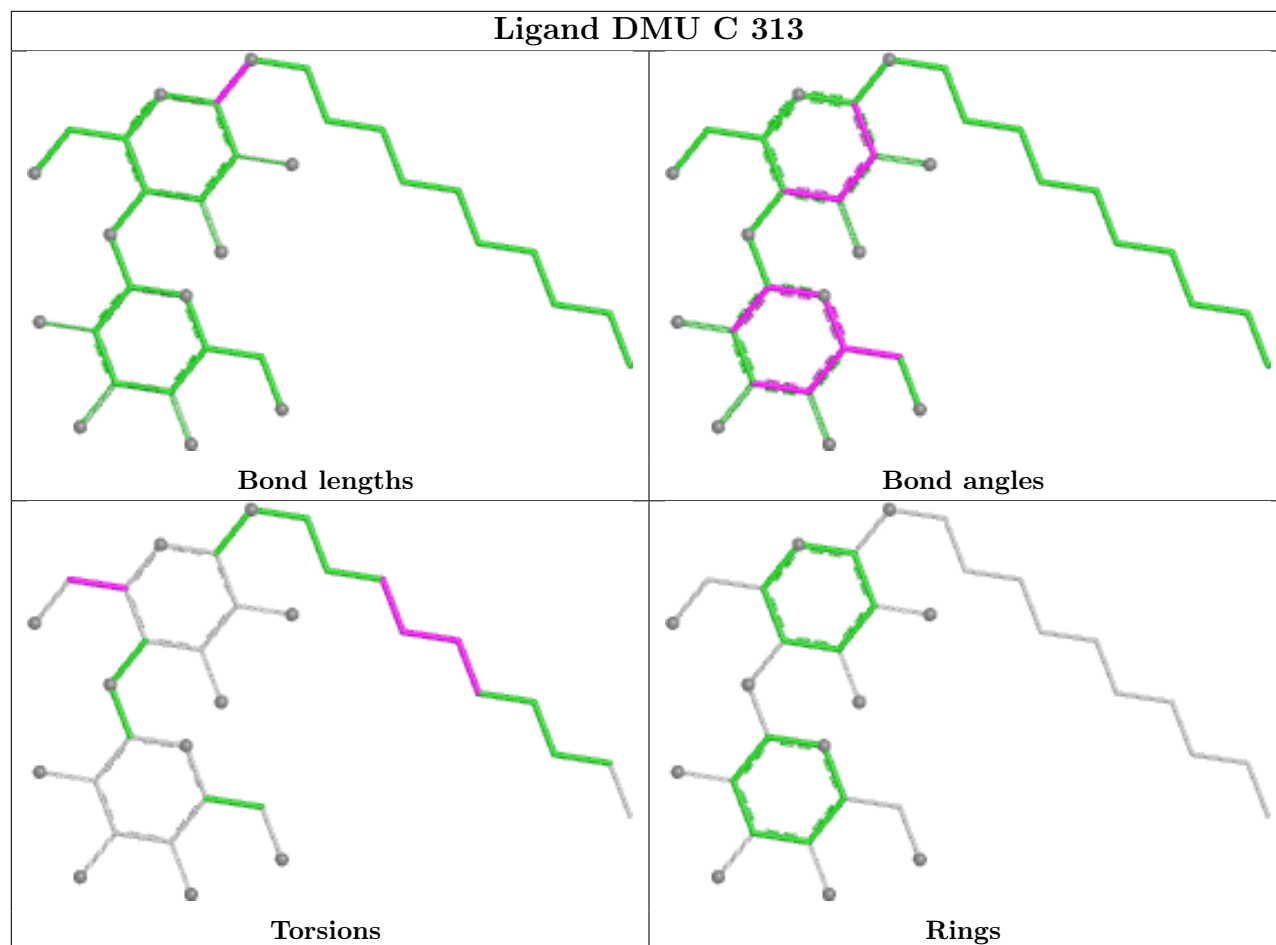
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	304	PGV	1	0
25	P	306	PEK	1	0
25	P	301	PEK	3	0
27	Z	103	DMU	2	0
24	C	315	CHD	2	0
27	T	101	DMU	8	0
21	N	611	EDO	1	0
14	A	602	HEA	2	0
19	A	607	PGV	8	0
14	A	601[A]	HEA	2	0
21	L	101	EDO	1	0
14	N	602	HEA	4	0
14	N	601[A]	HEA	3	0
24	J	101	CHD	2	0
19	Z	101	PGV	1	0
26	G	103	CDL	5	0
20	D	201	TGL	3	0
19	P	302	PGV	2	0
24	P	315	CHD	7	0
21	Q	202	EDO	1	0
21	Q	201	EDO	1	0
27	G	101	DMU	2	0
24	P	309	CHD	3	0
27	C	314	DMU	4	0
19	P	307	PGV	1	0
25	G	102	PEK	4	0
24	Y	102	CHD	4	0
20	B	302	TGL	1	0
27	M	101	DMU	1	0
20	O	303	TGL	2	0
20	A	609	TGL	3	0
25	C	308	PEK	2	0
21	C	309	EDO	1	0
21	D	204	EDO	2	0
20	N	607	TGL	2	0
26	C	306	CDL	8	0
14	A	601[B]	HEA	4	0
21	C	312	EDO	1	0
24	C	307	CHD	1	0

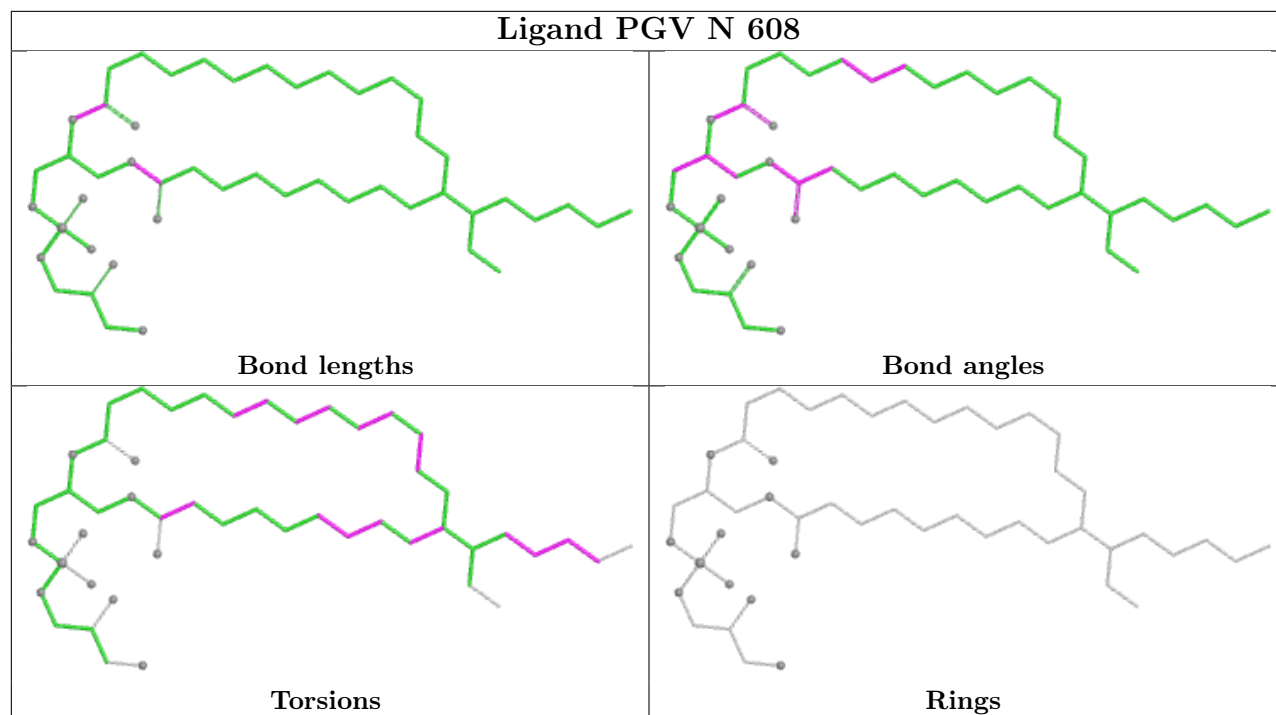
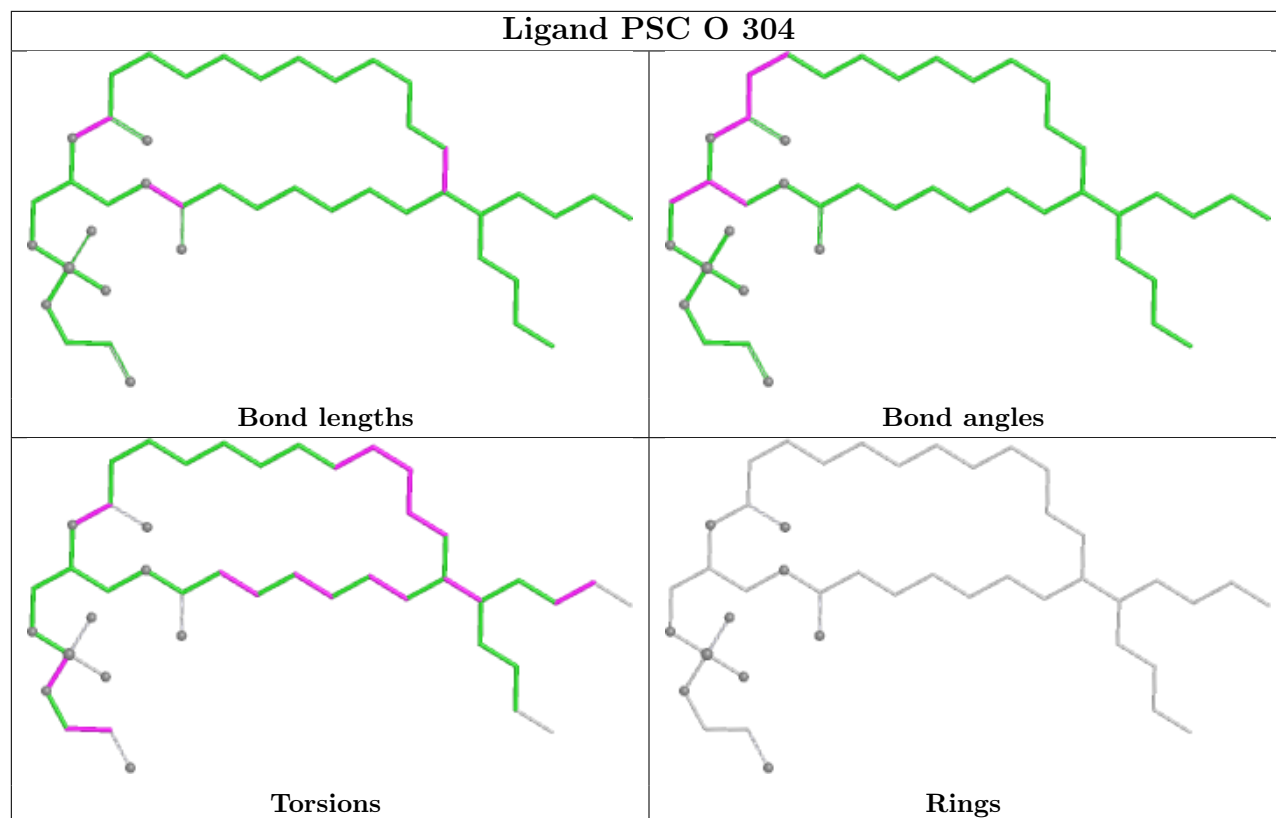
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

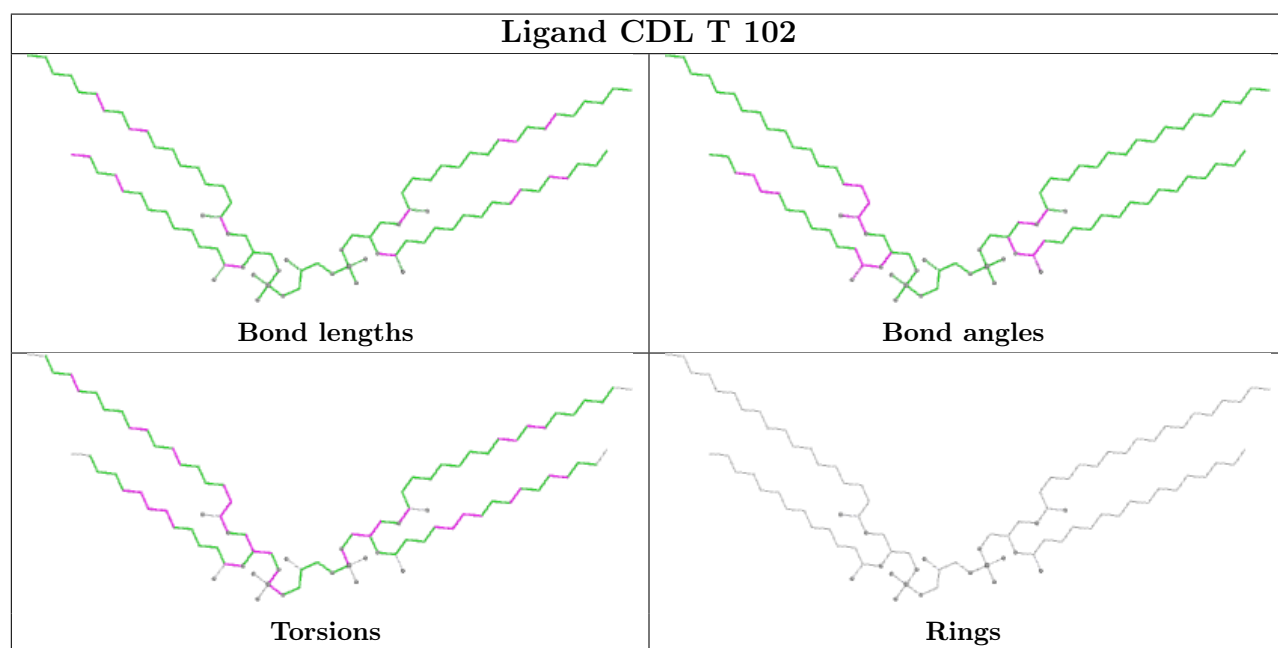
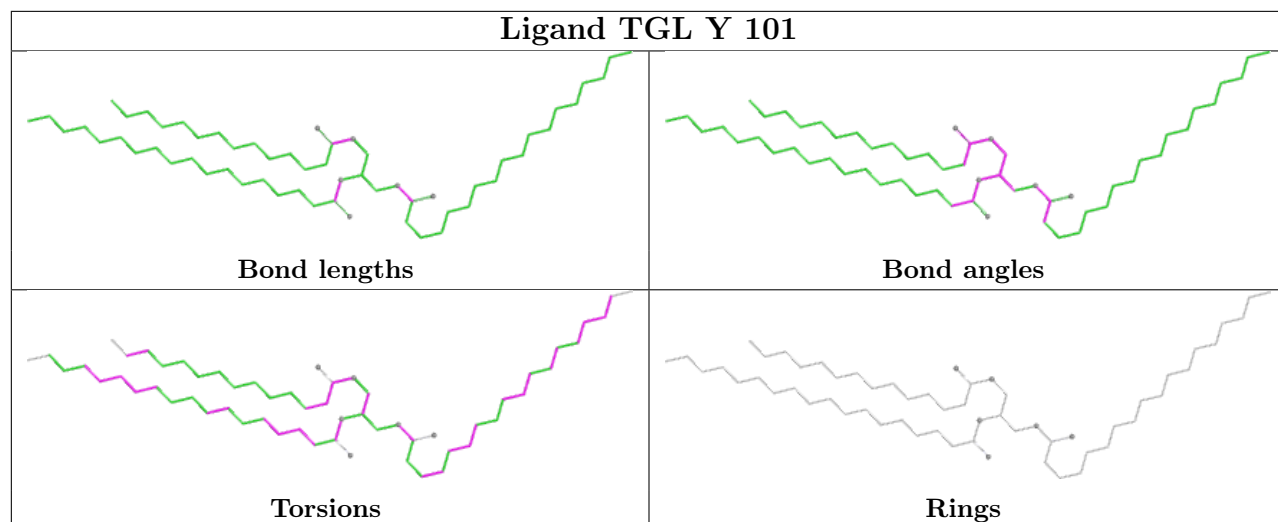
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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

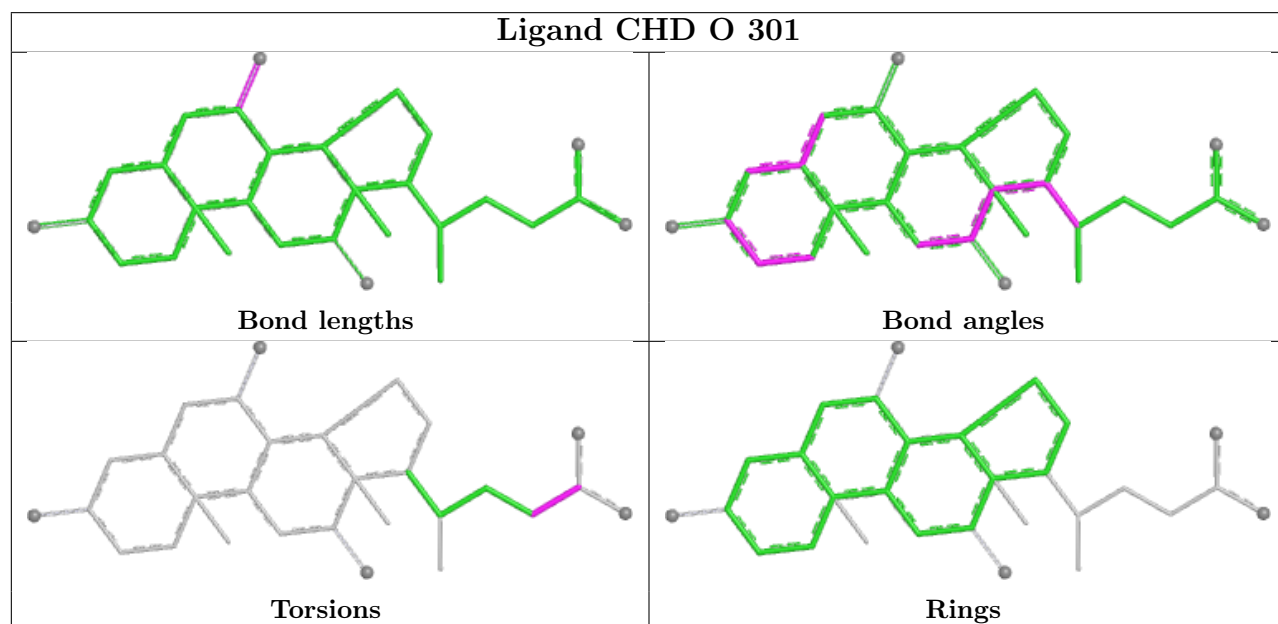
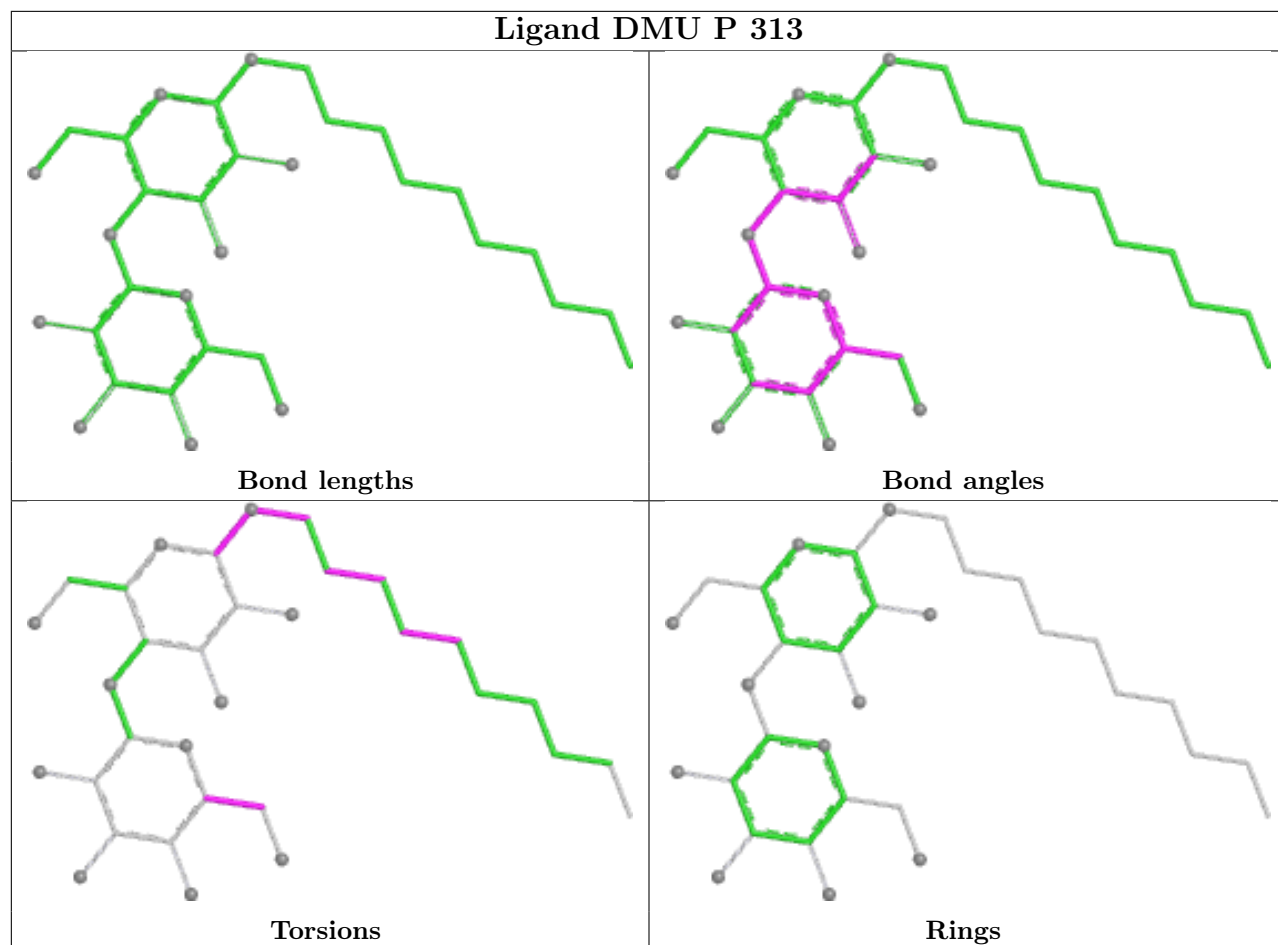


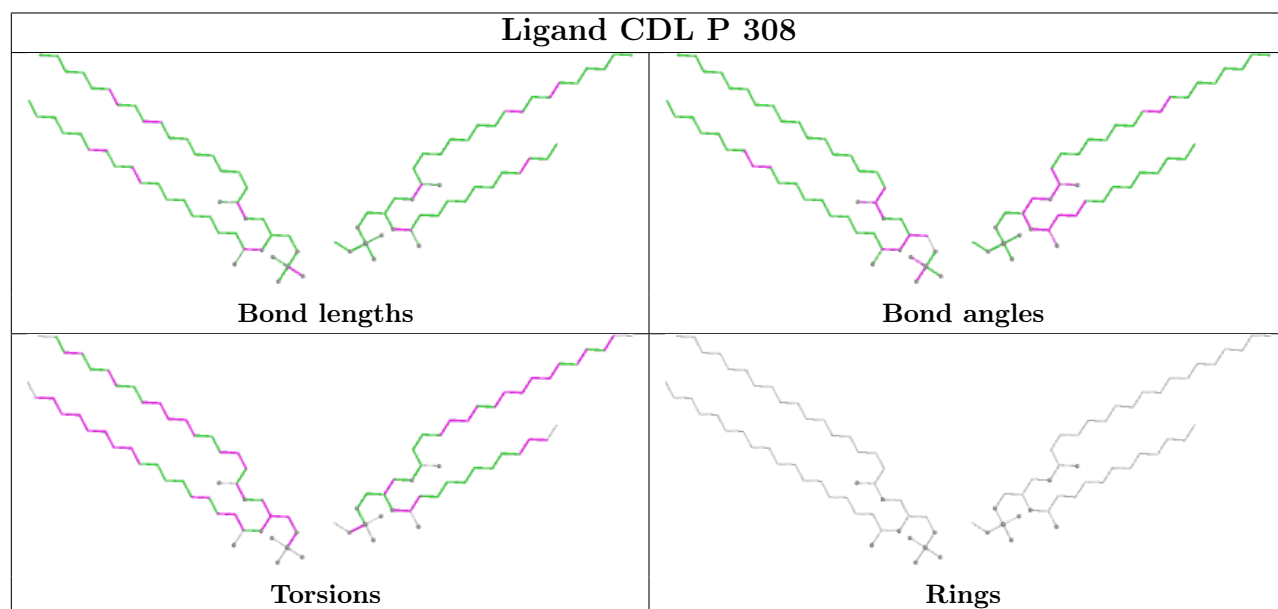
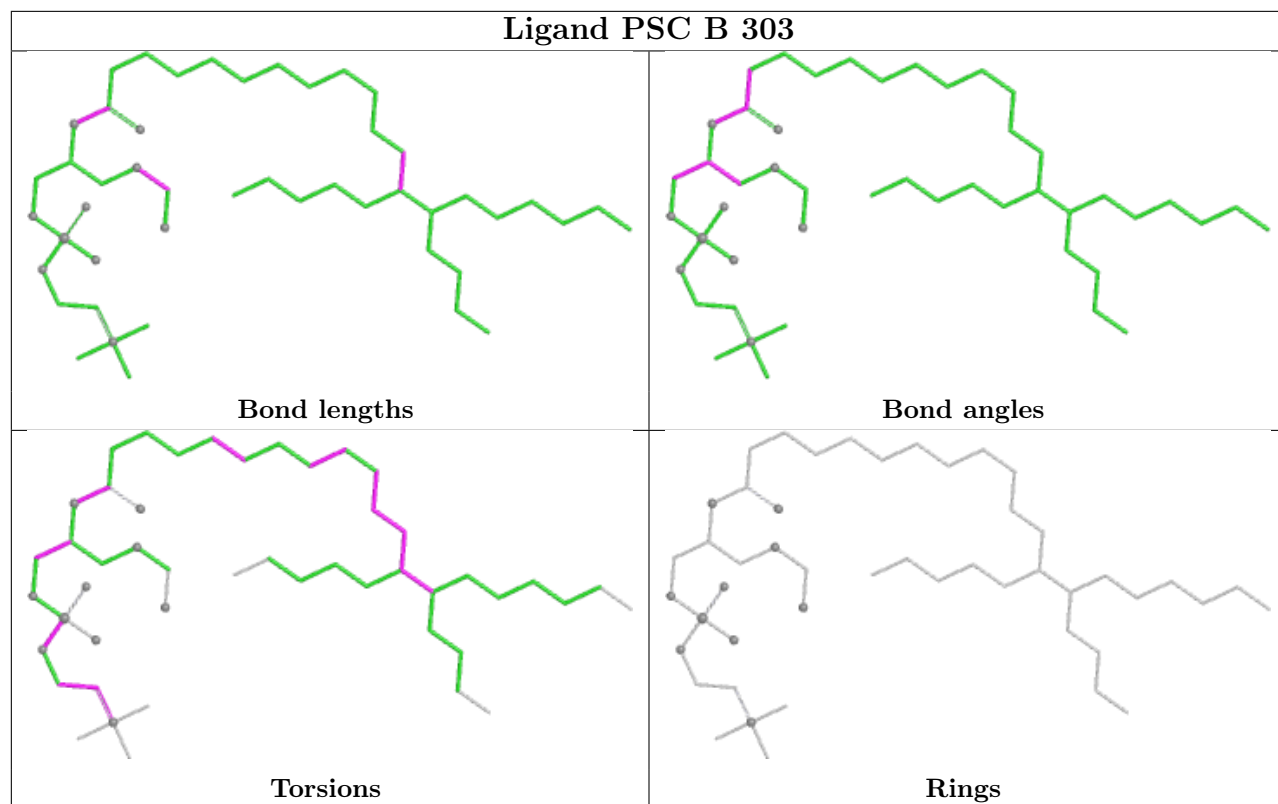


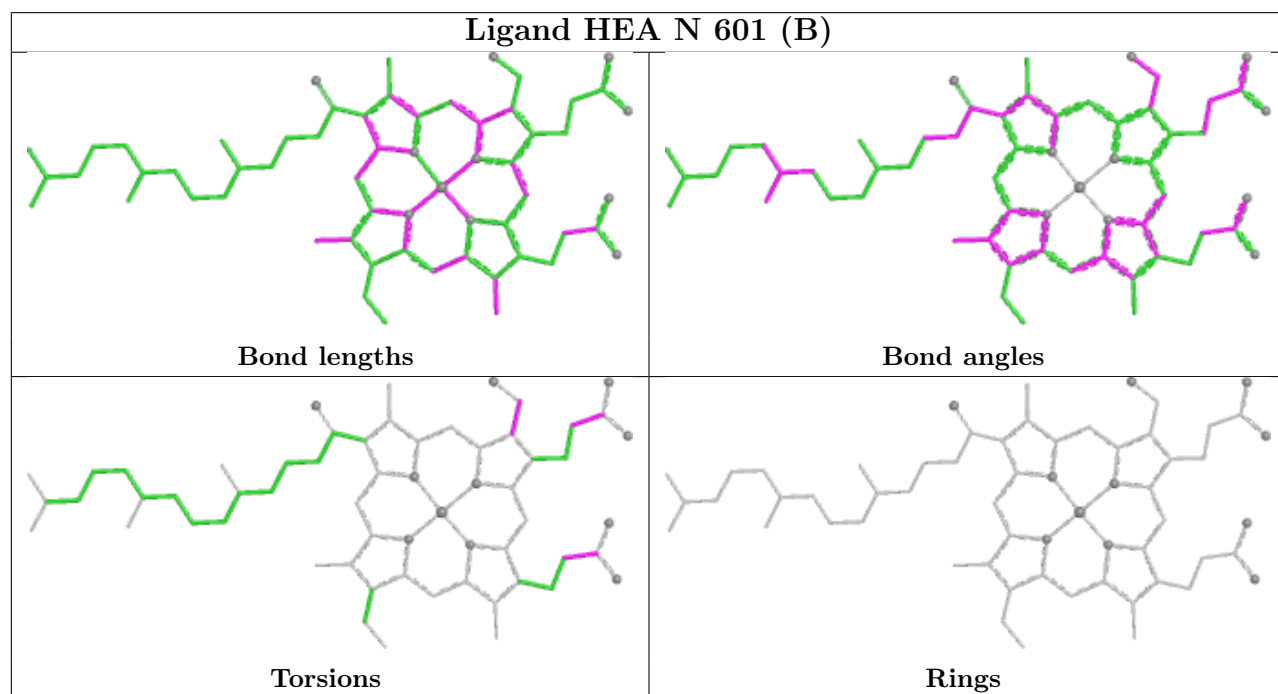
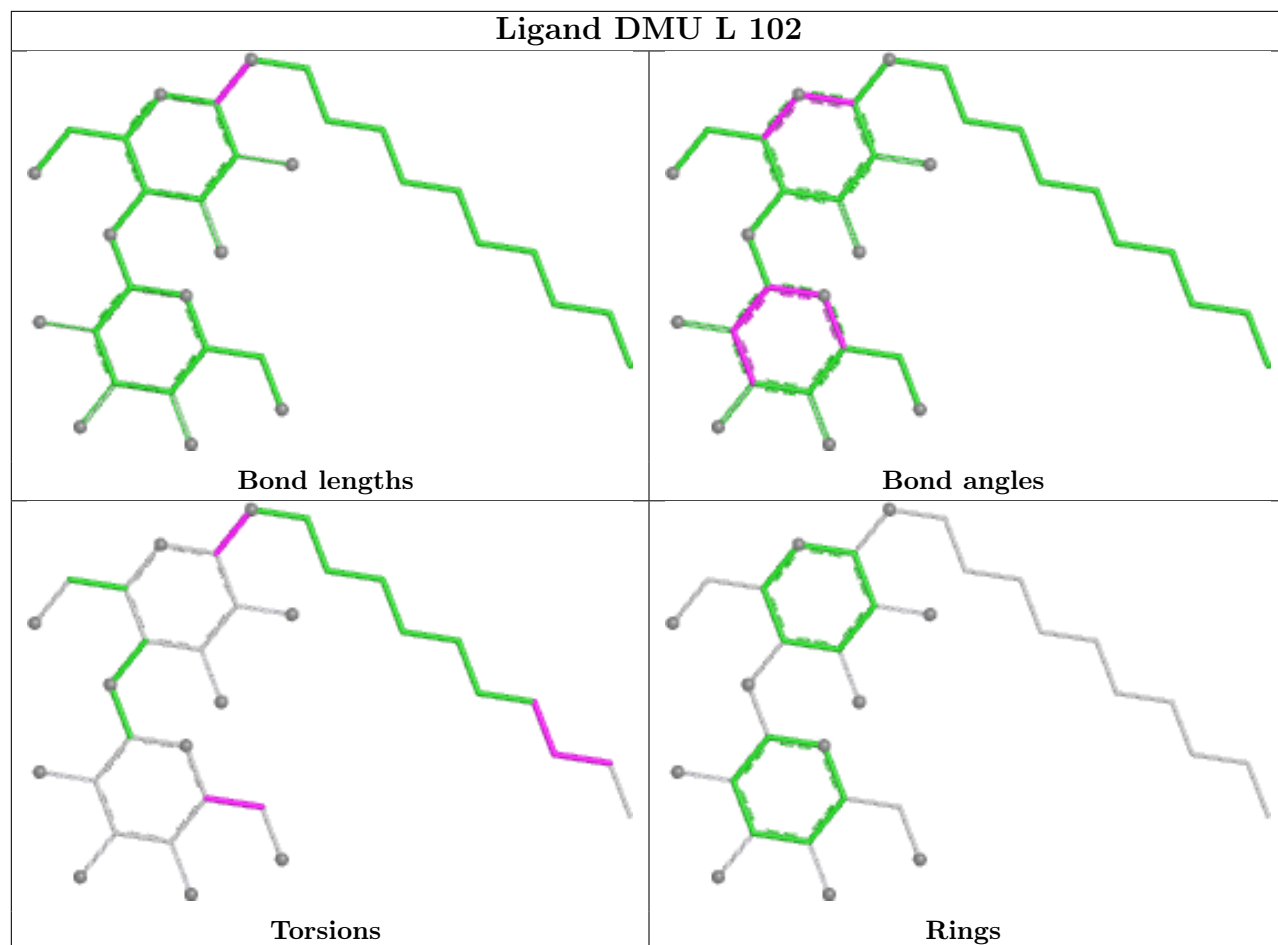


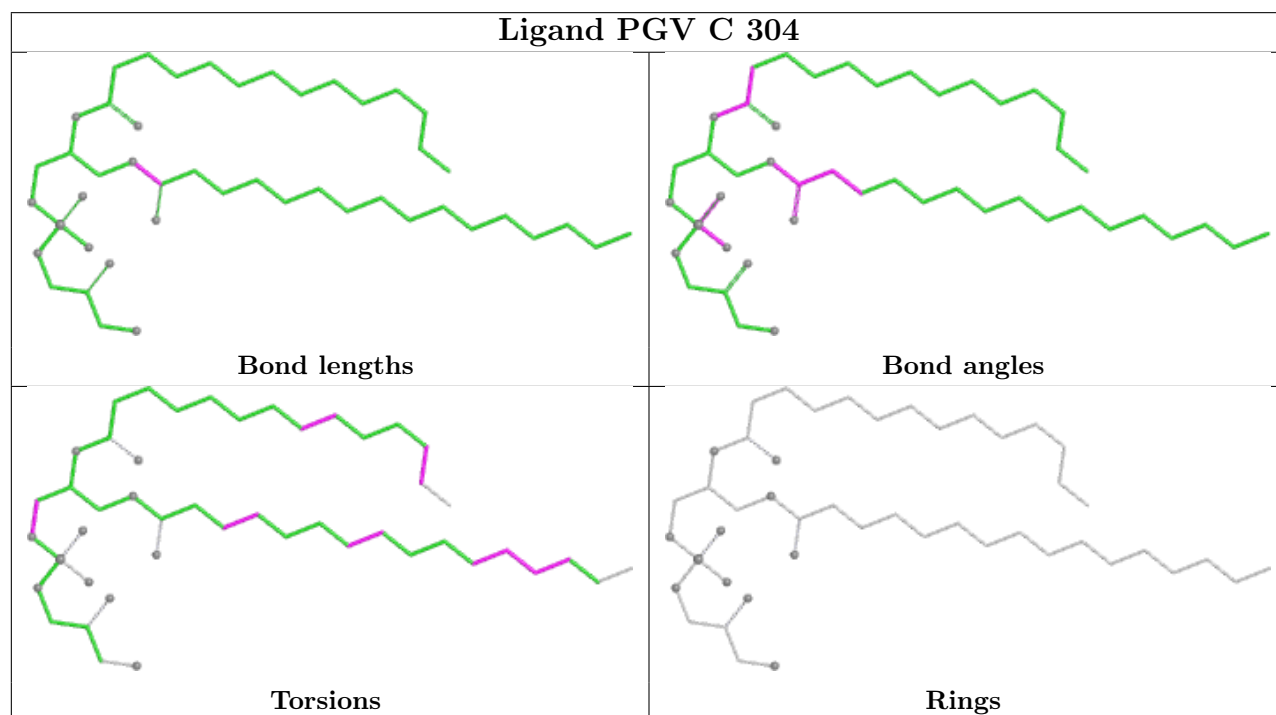
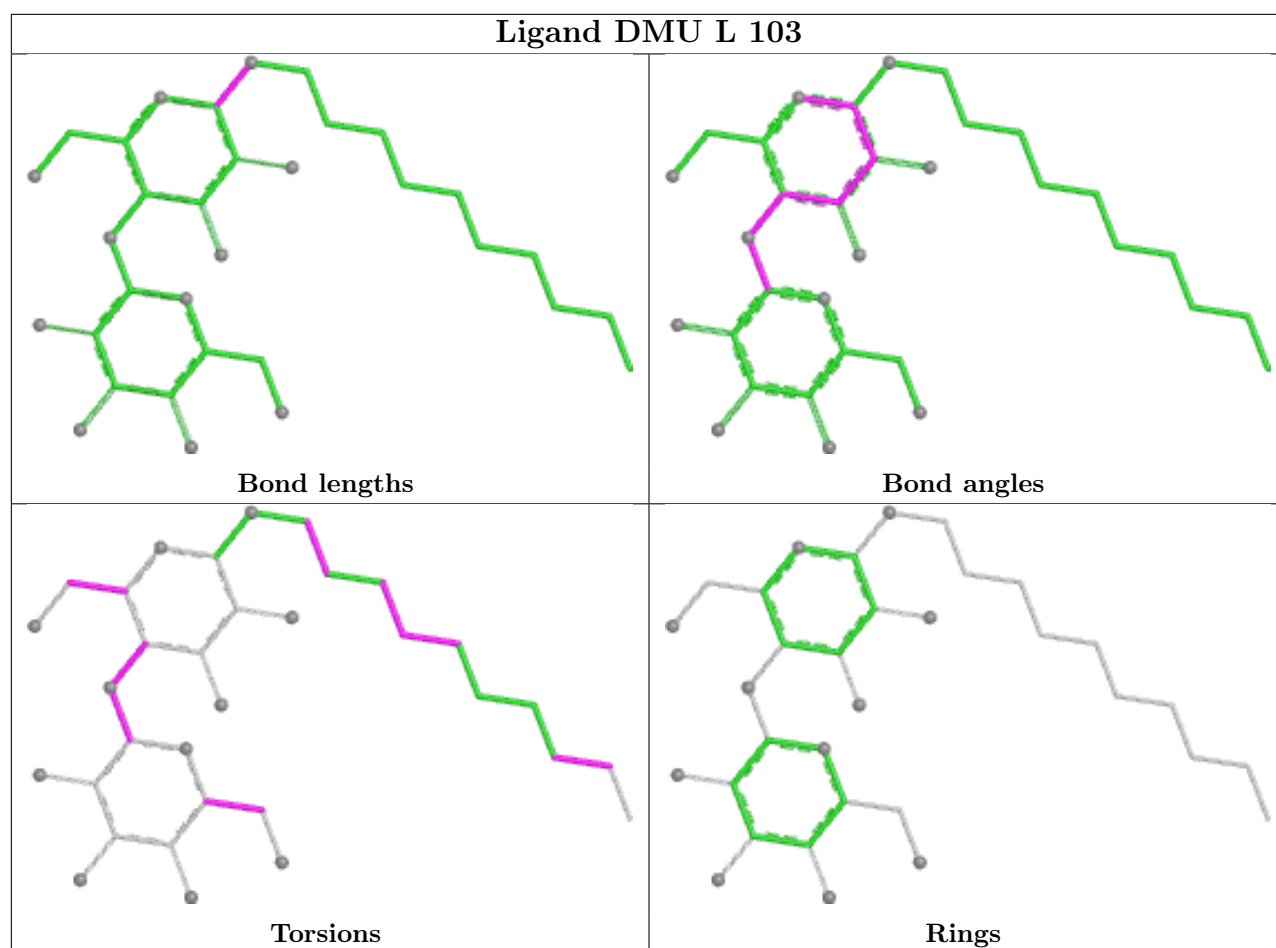


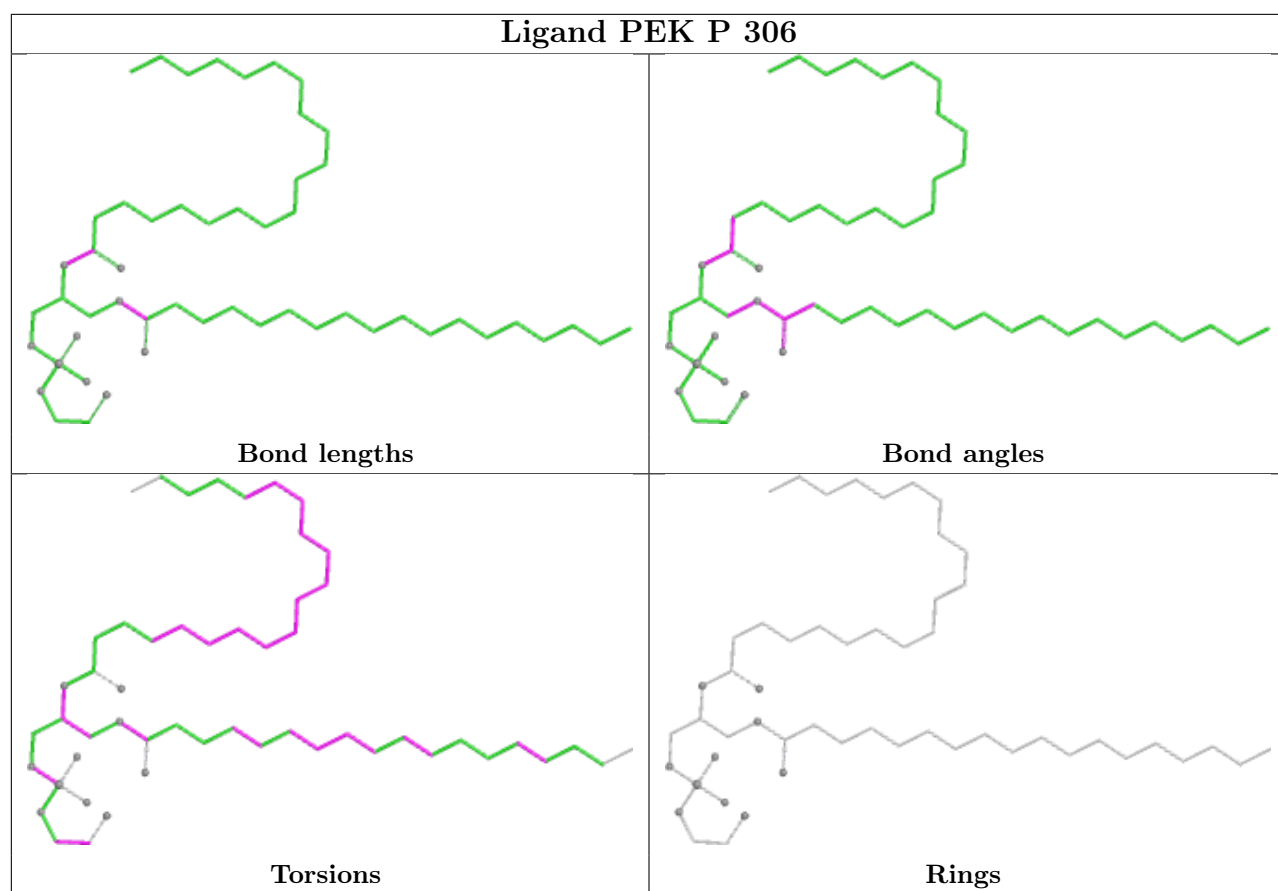


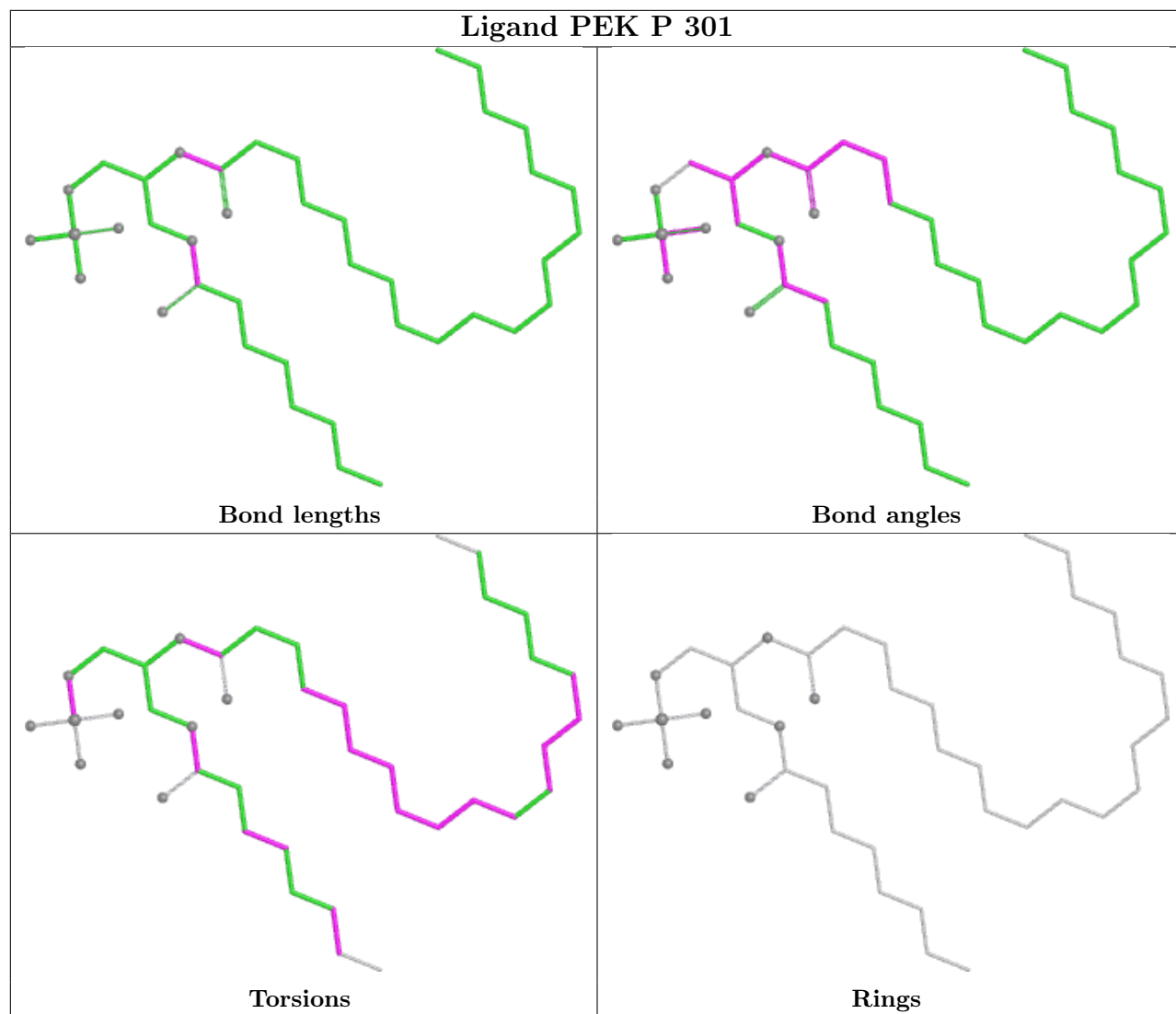


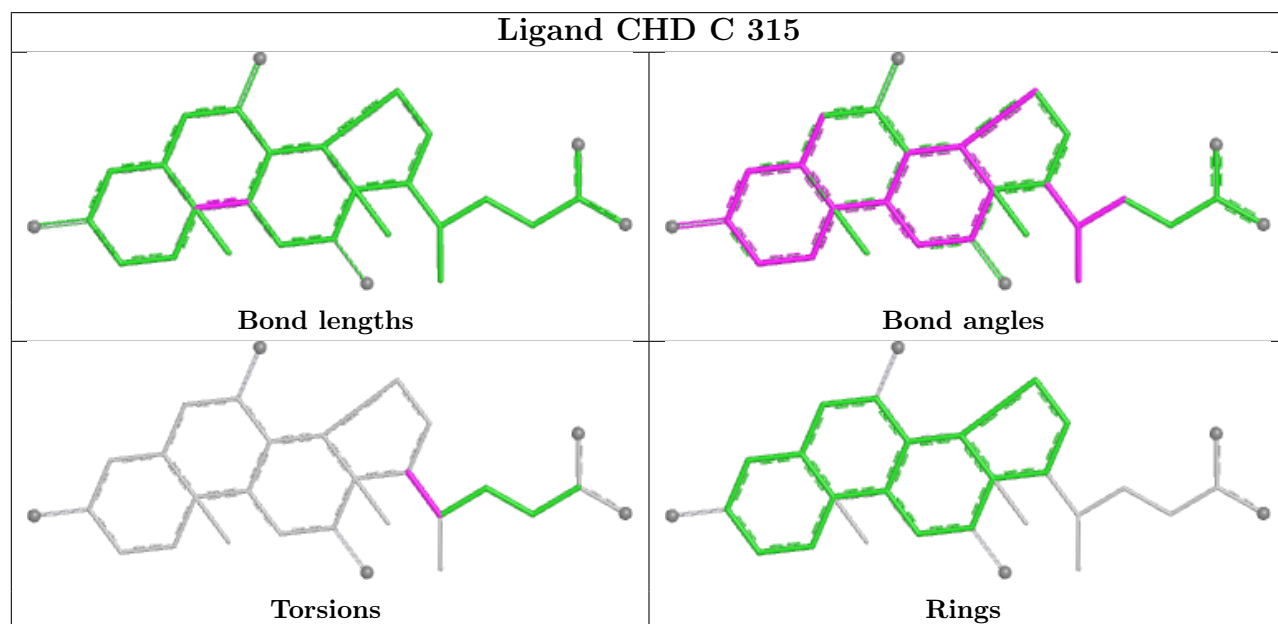
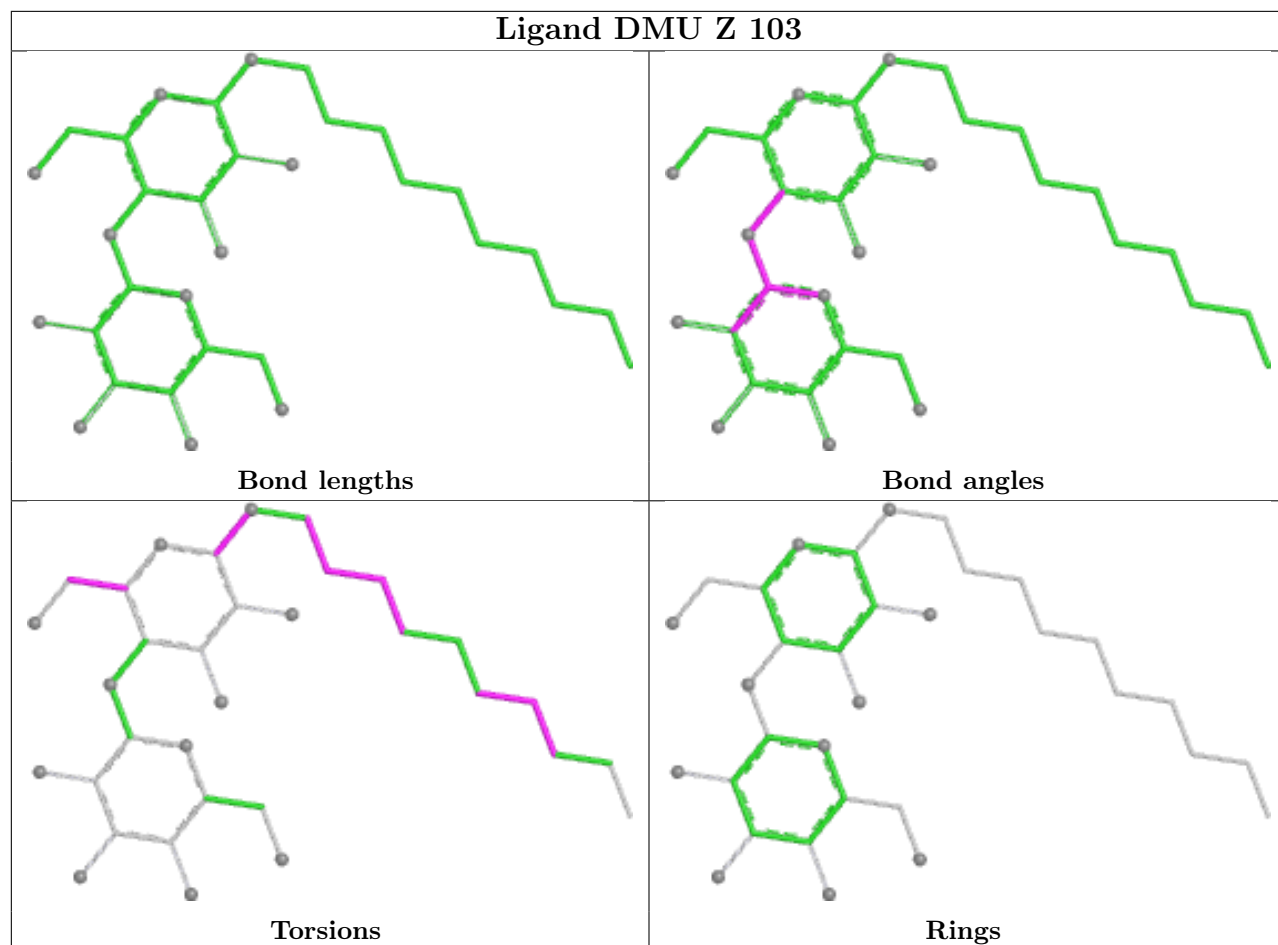


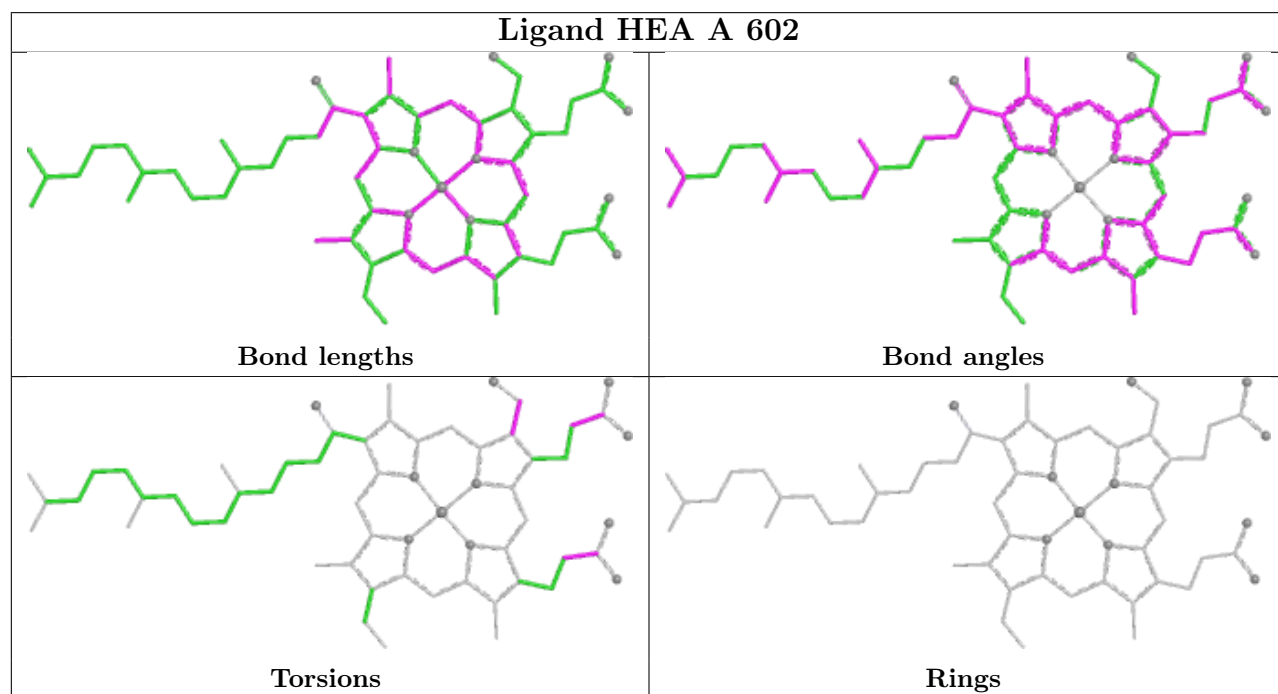
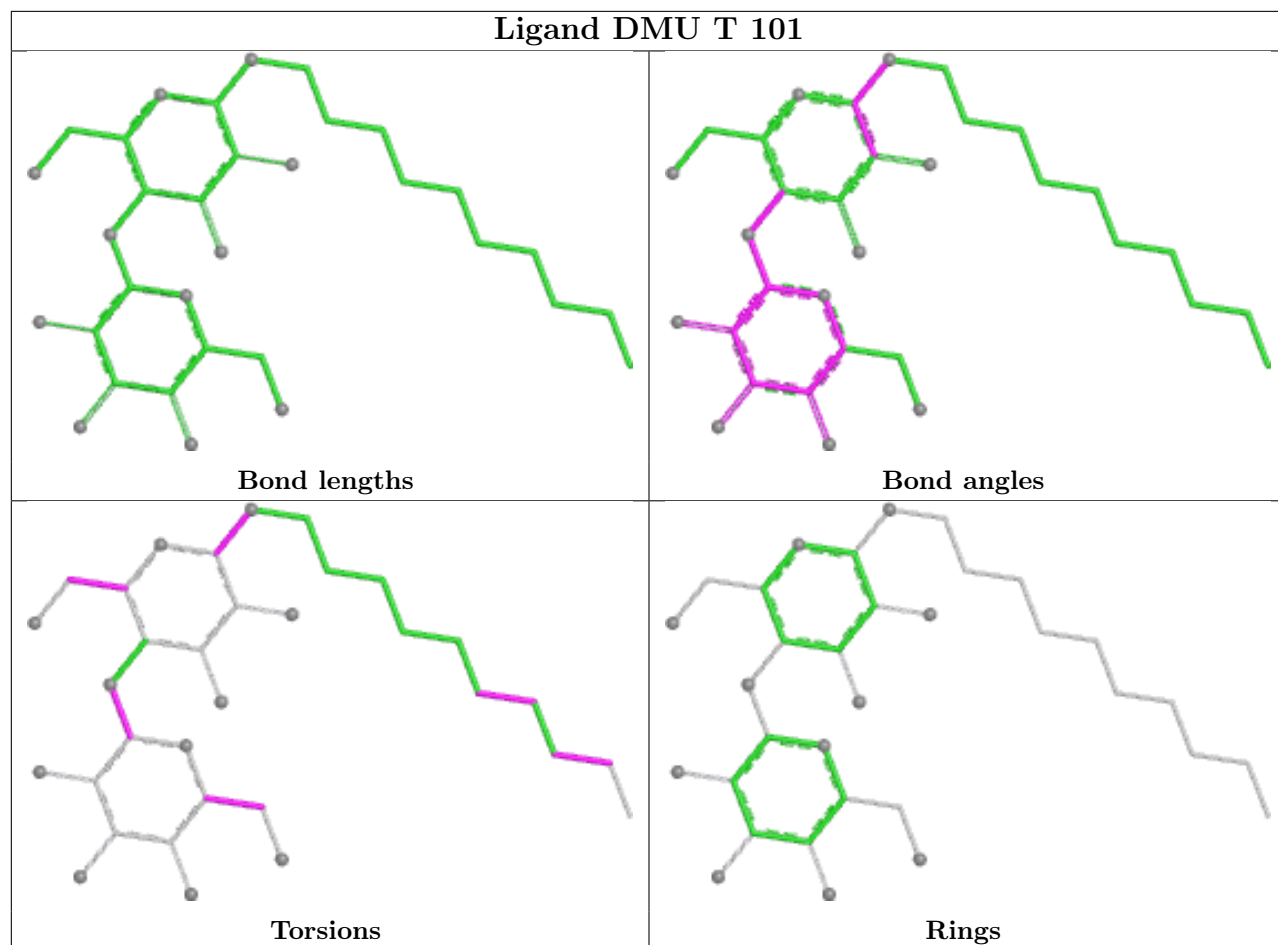


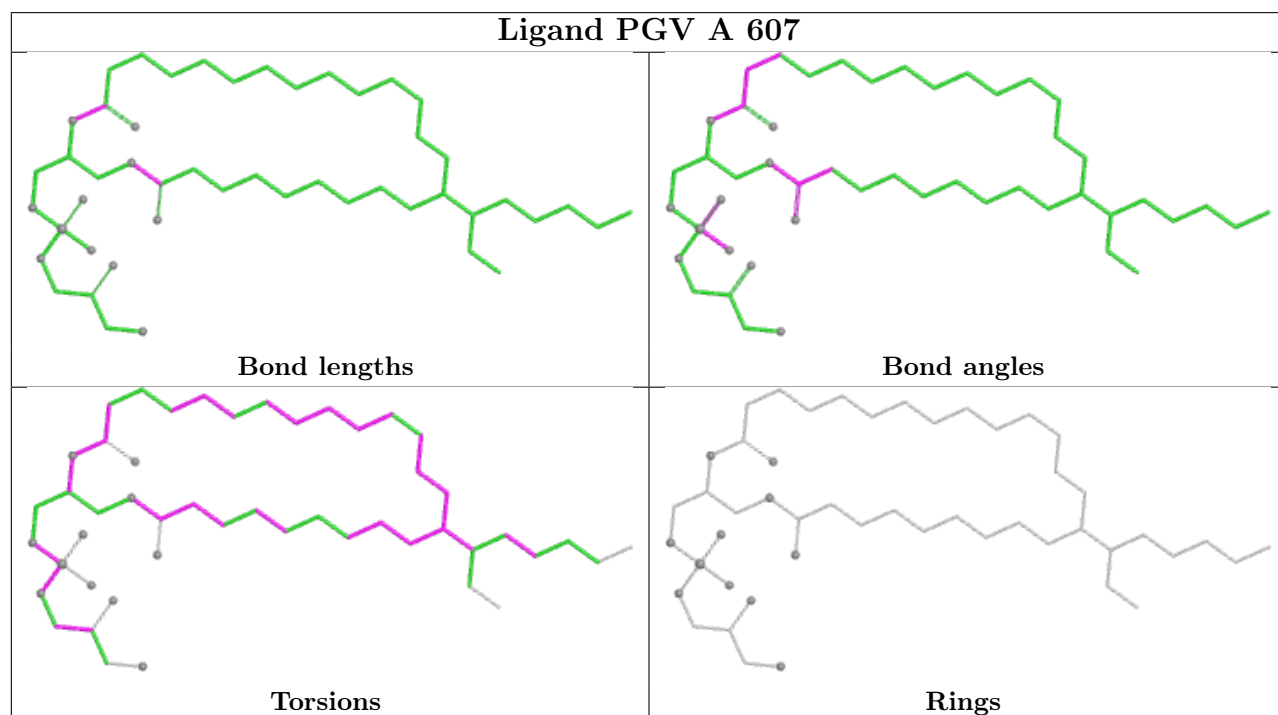
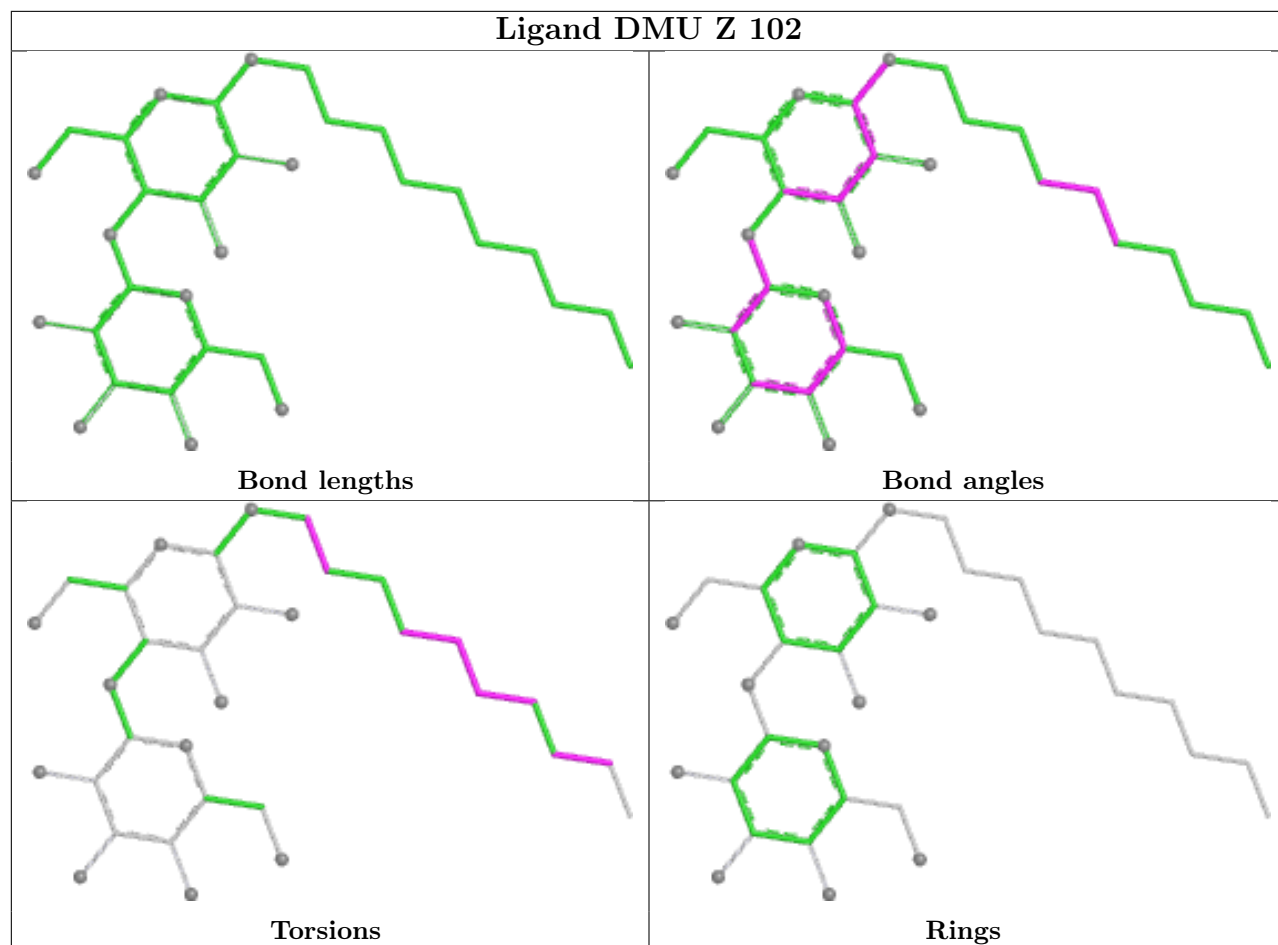


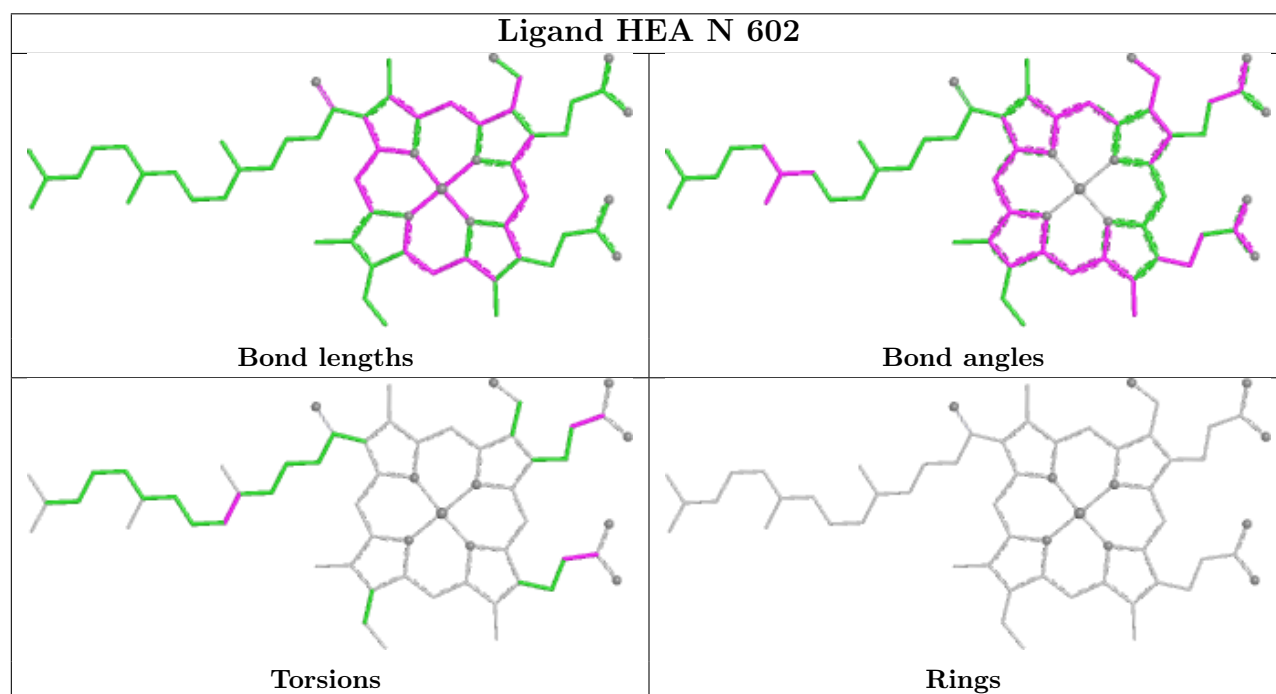
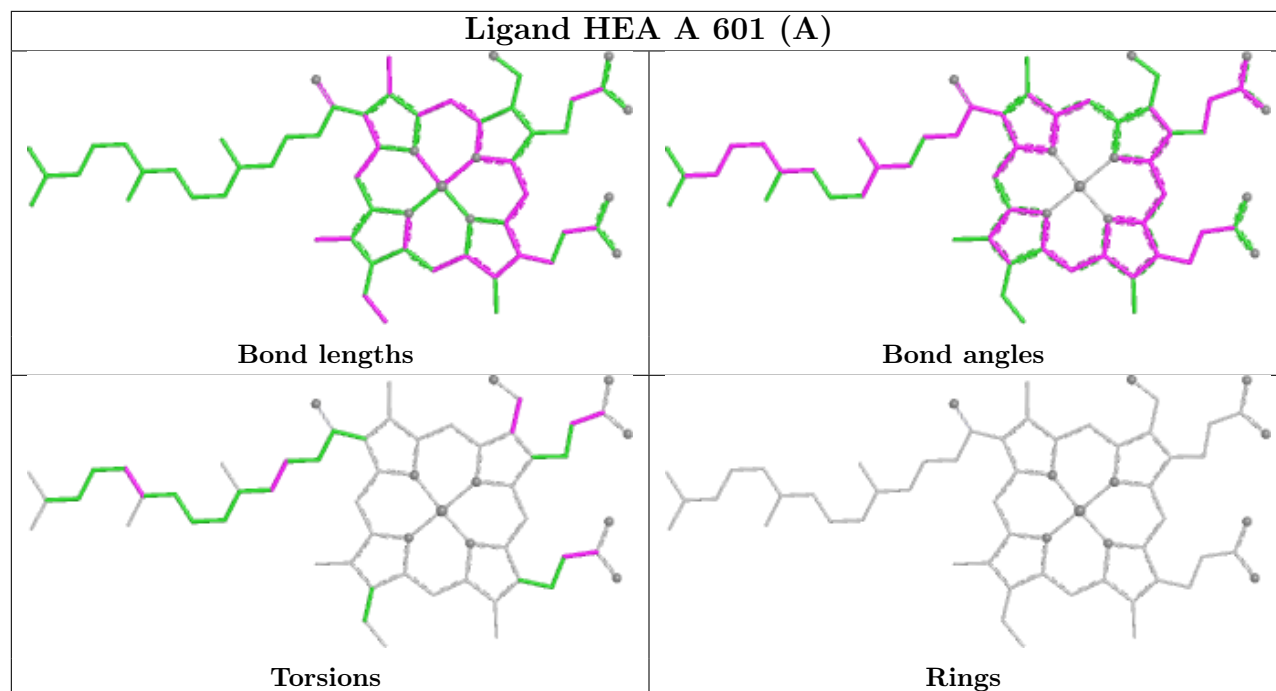


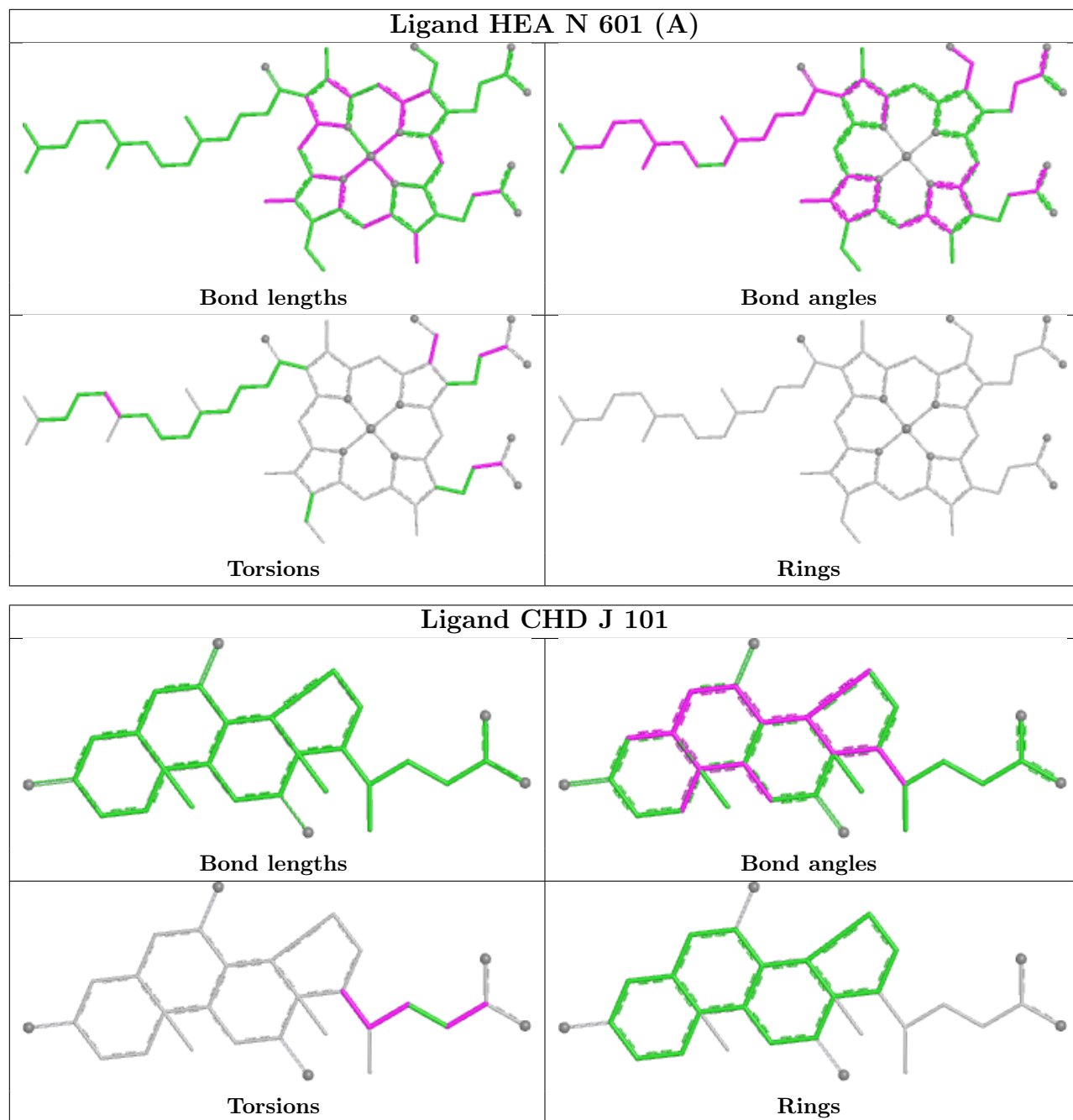


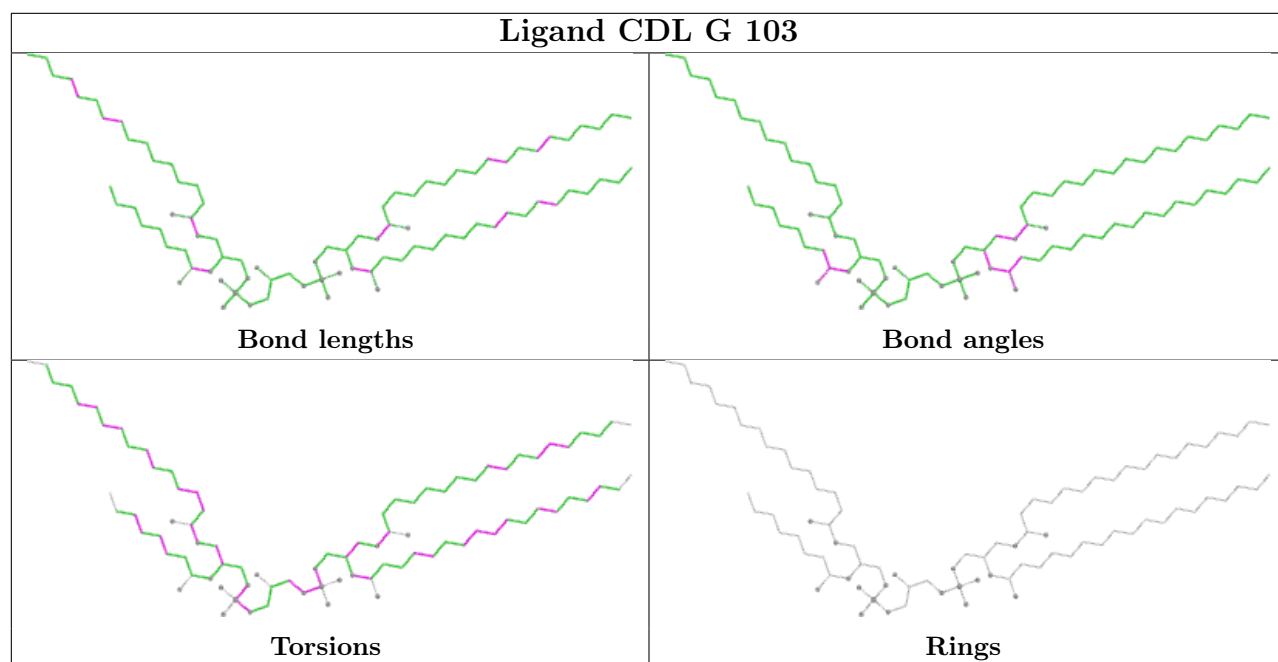
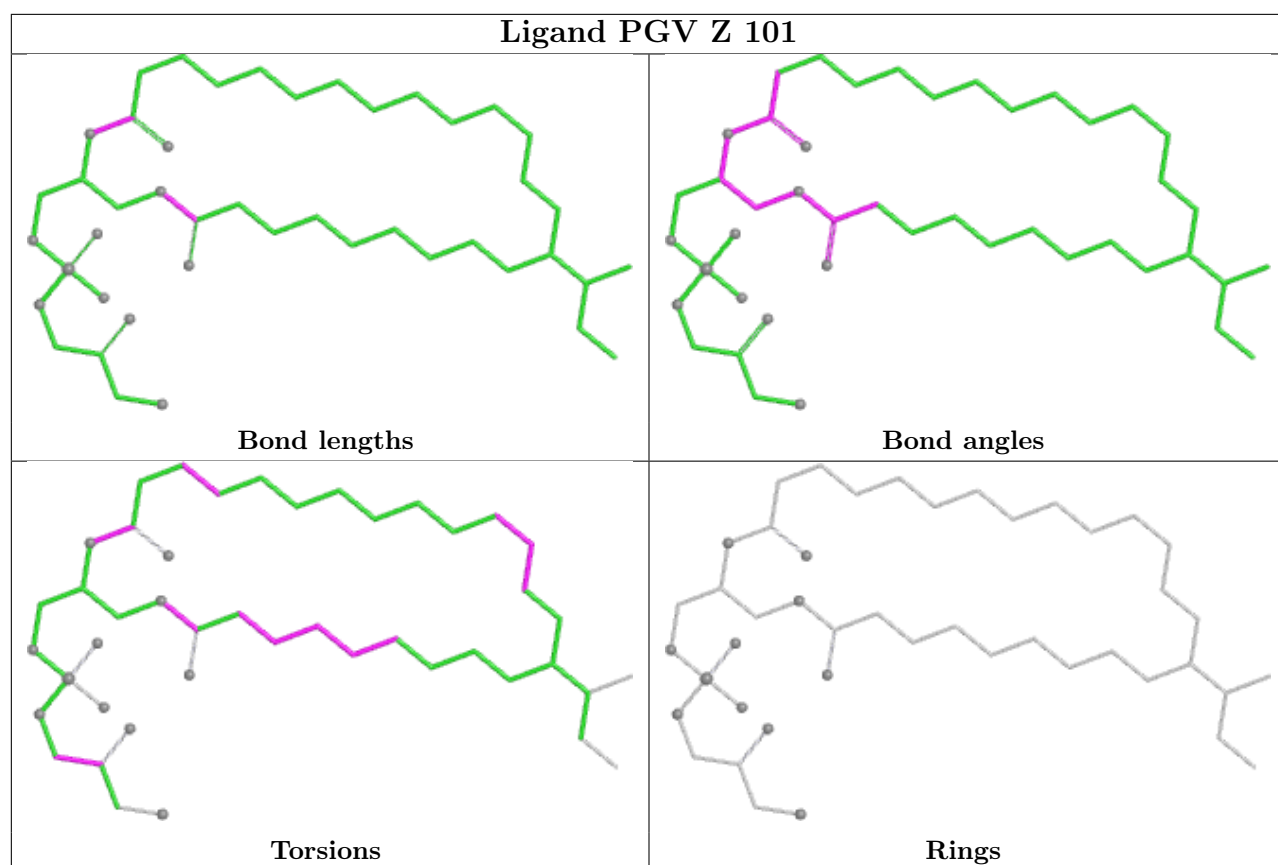


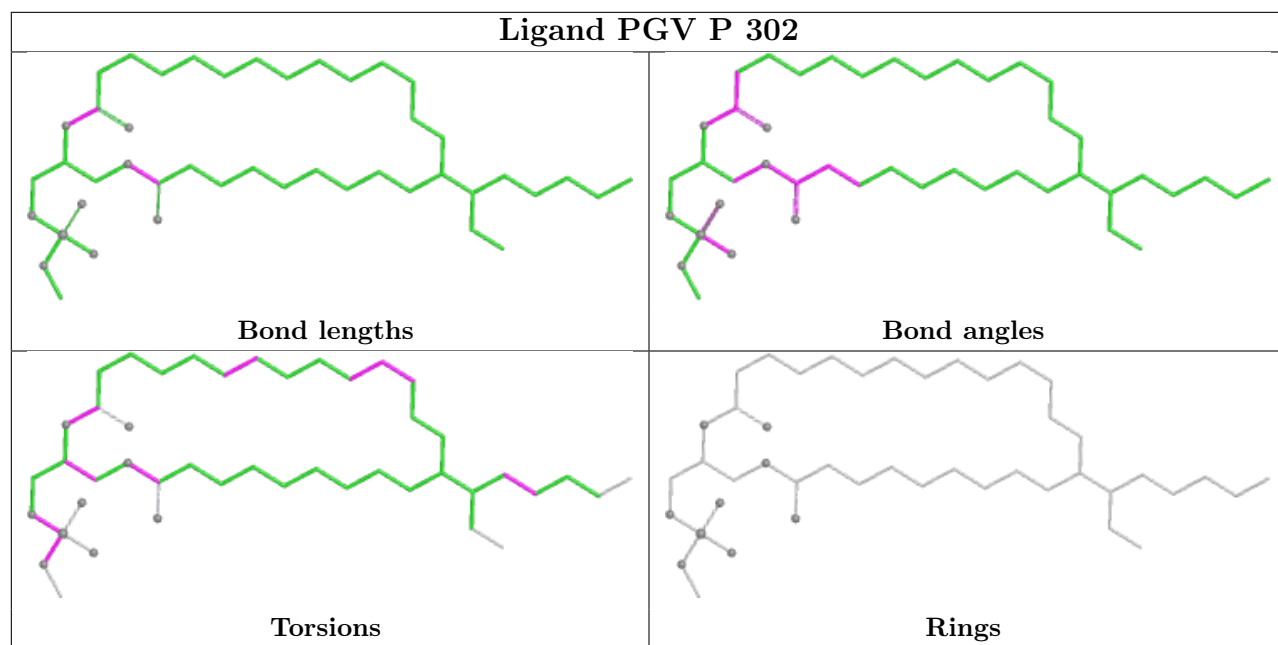
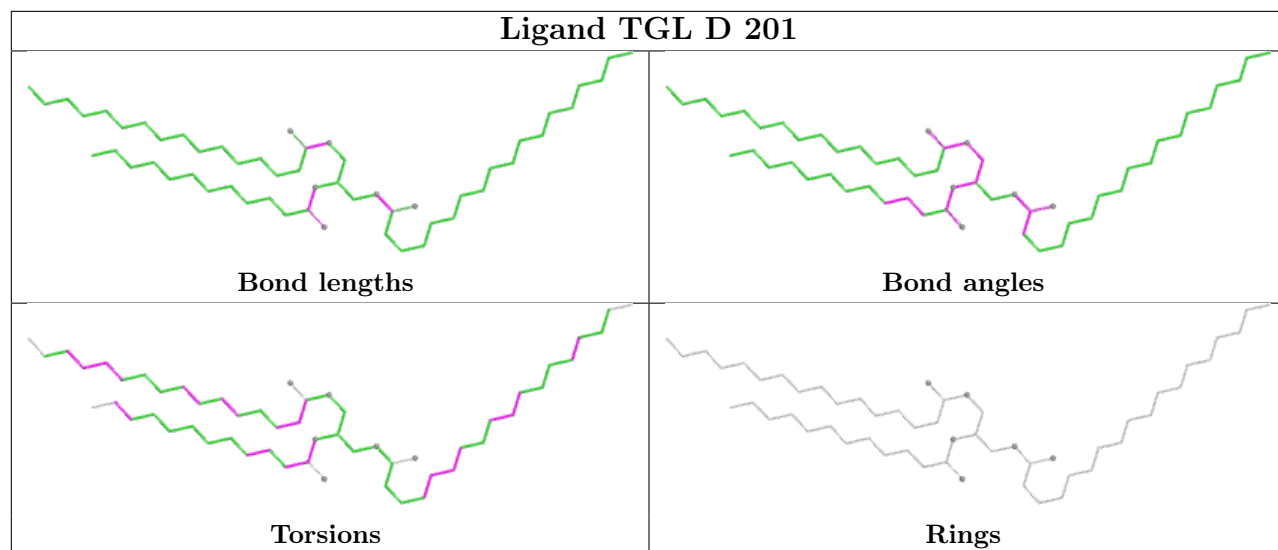


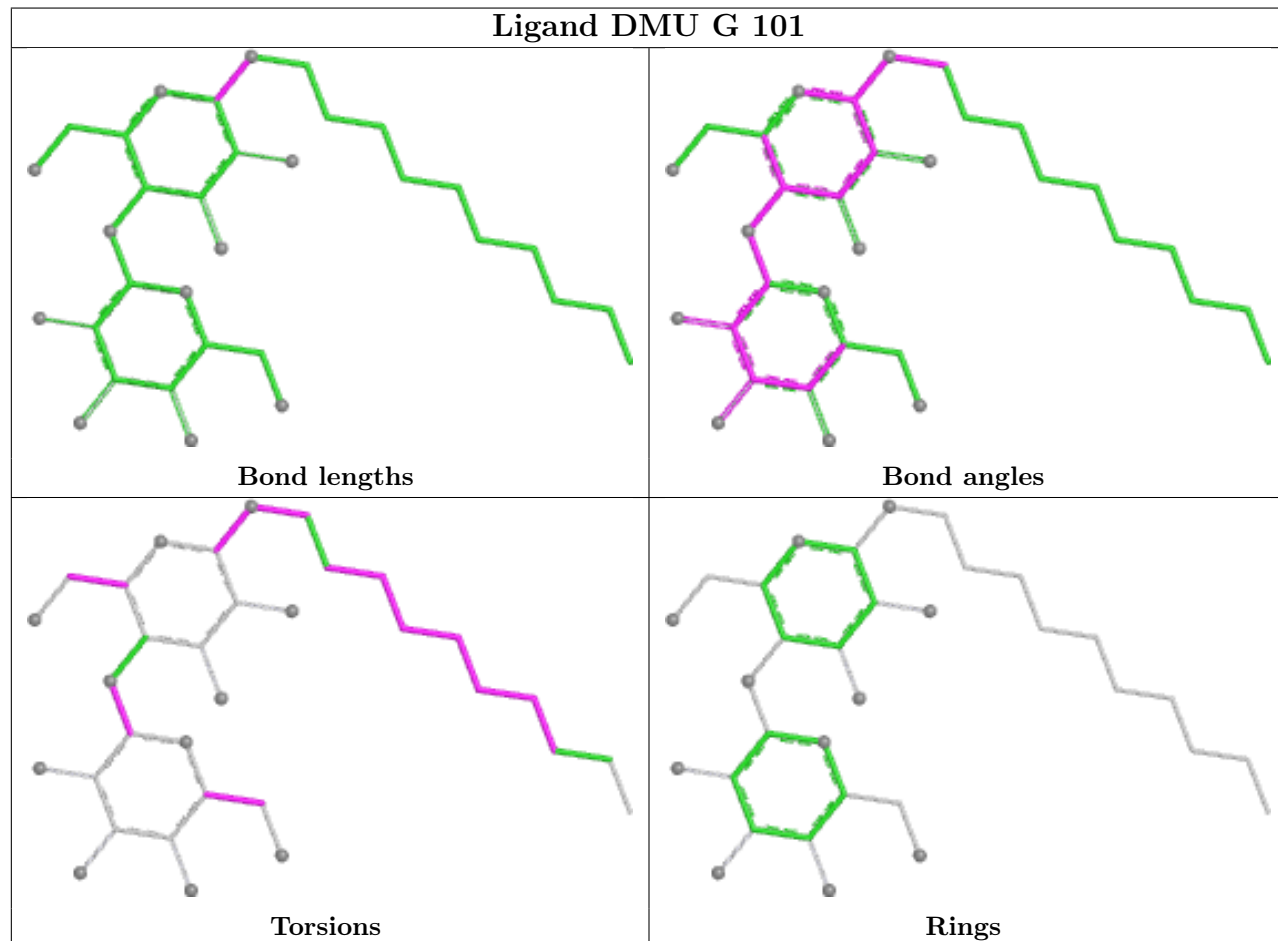
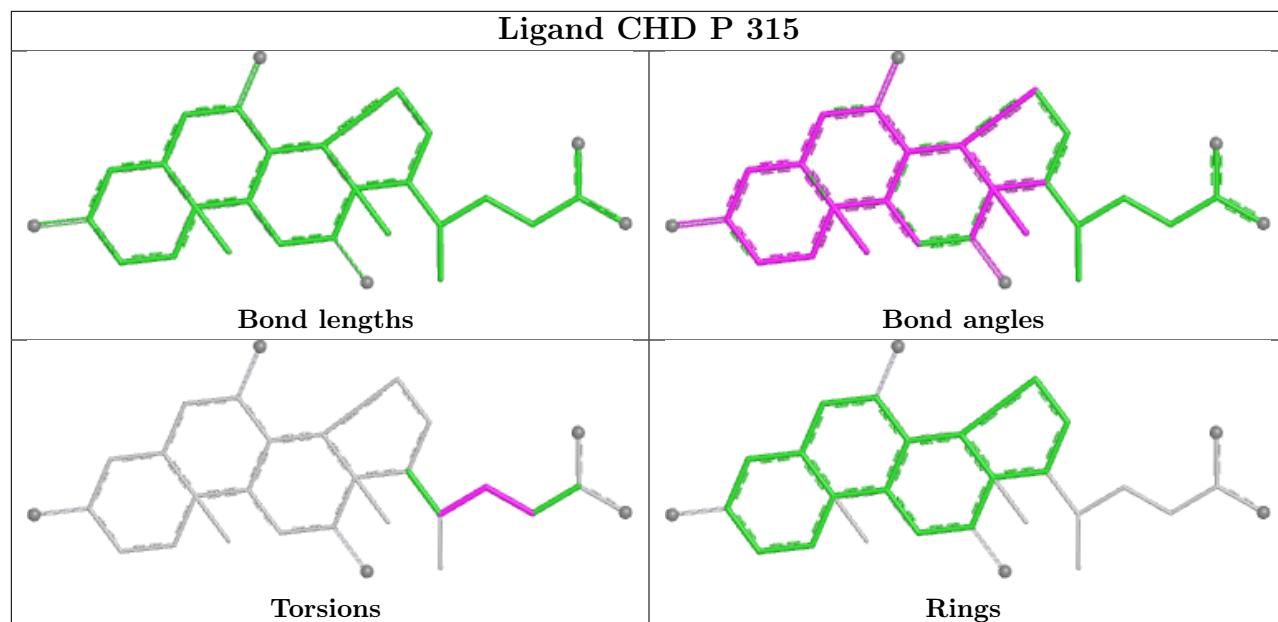


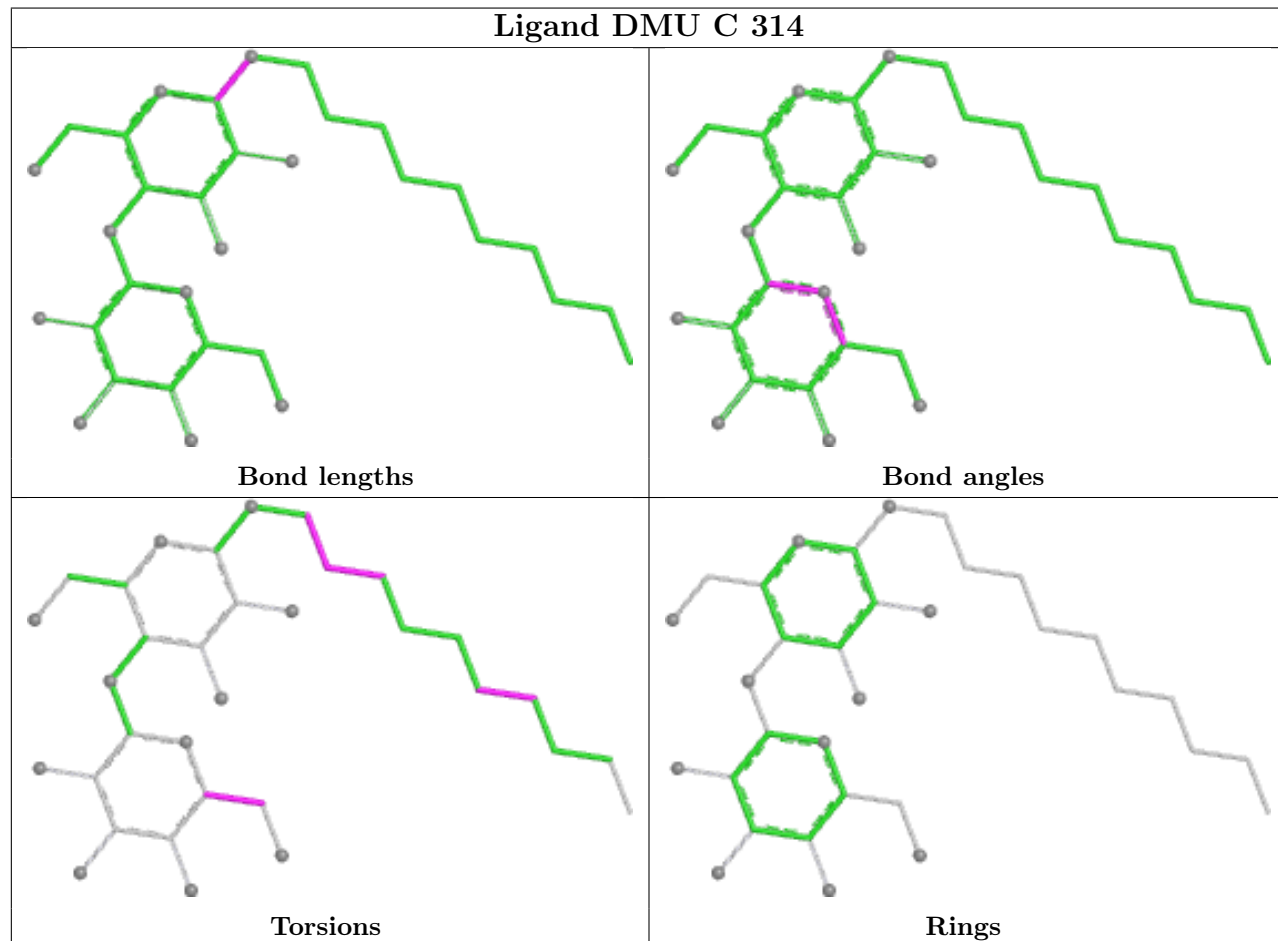
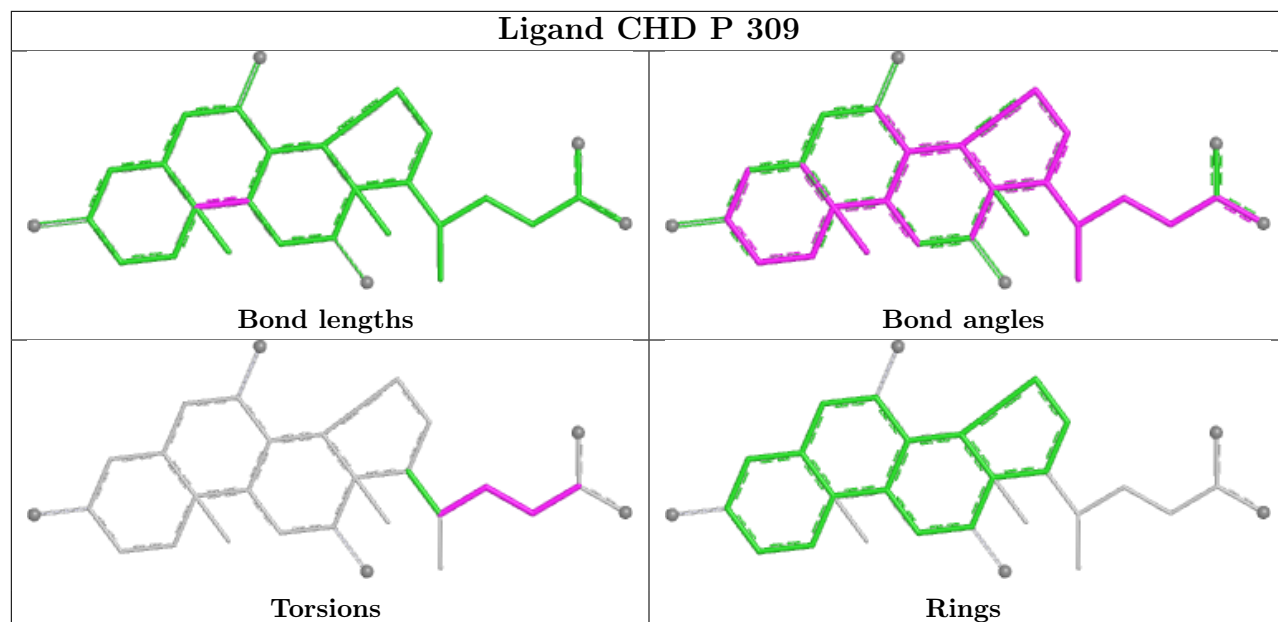


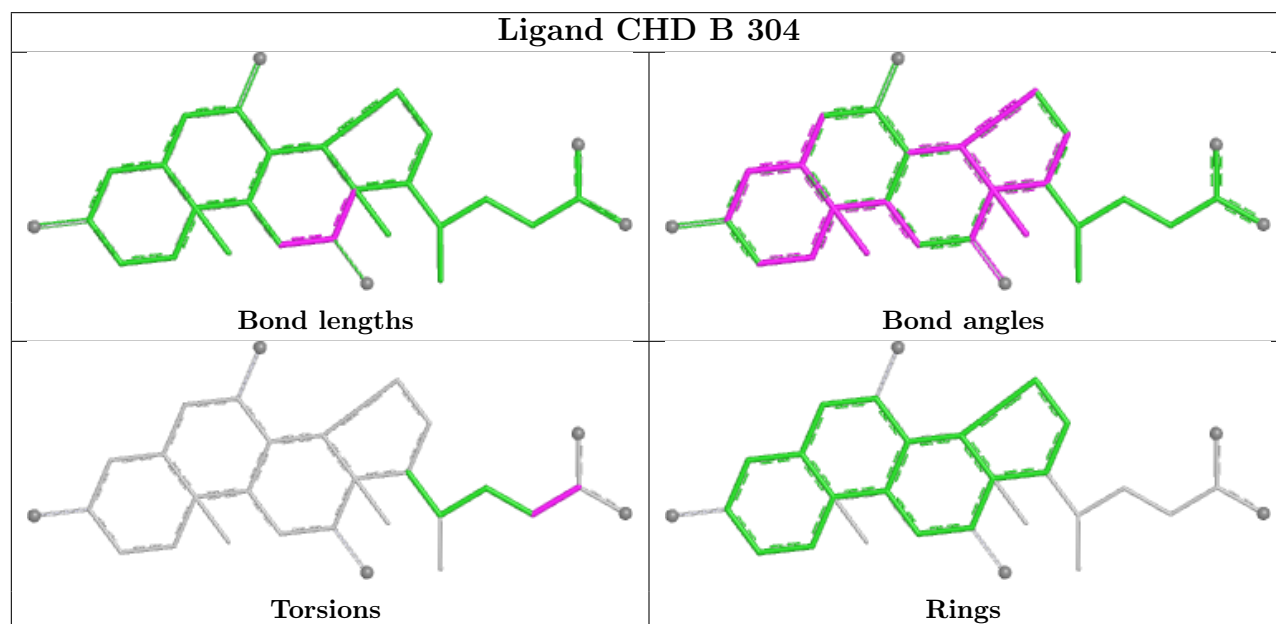
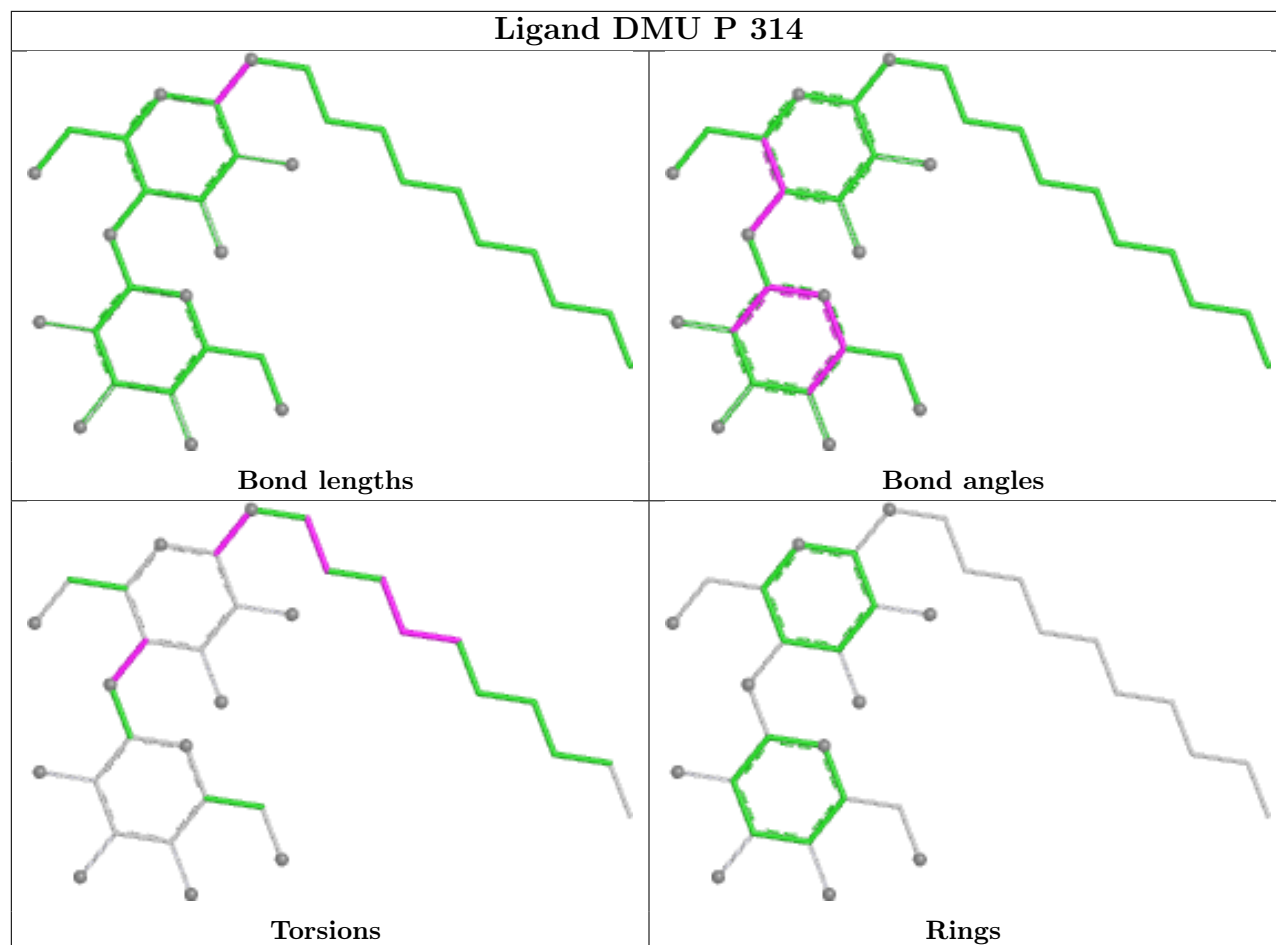


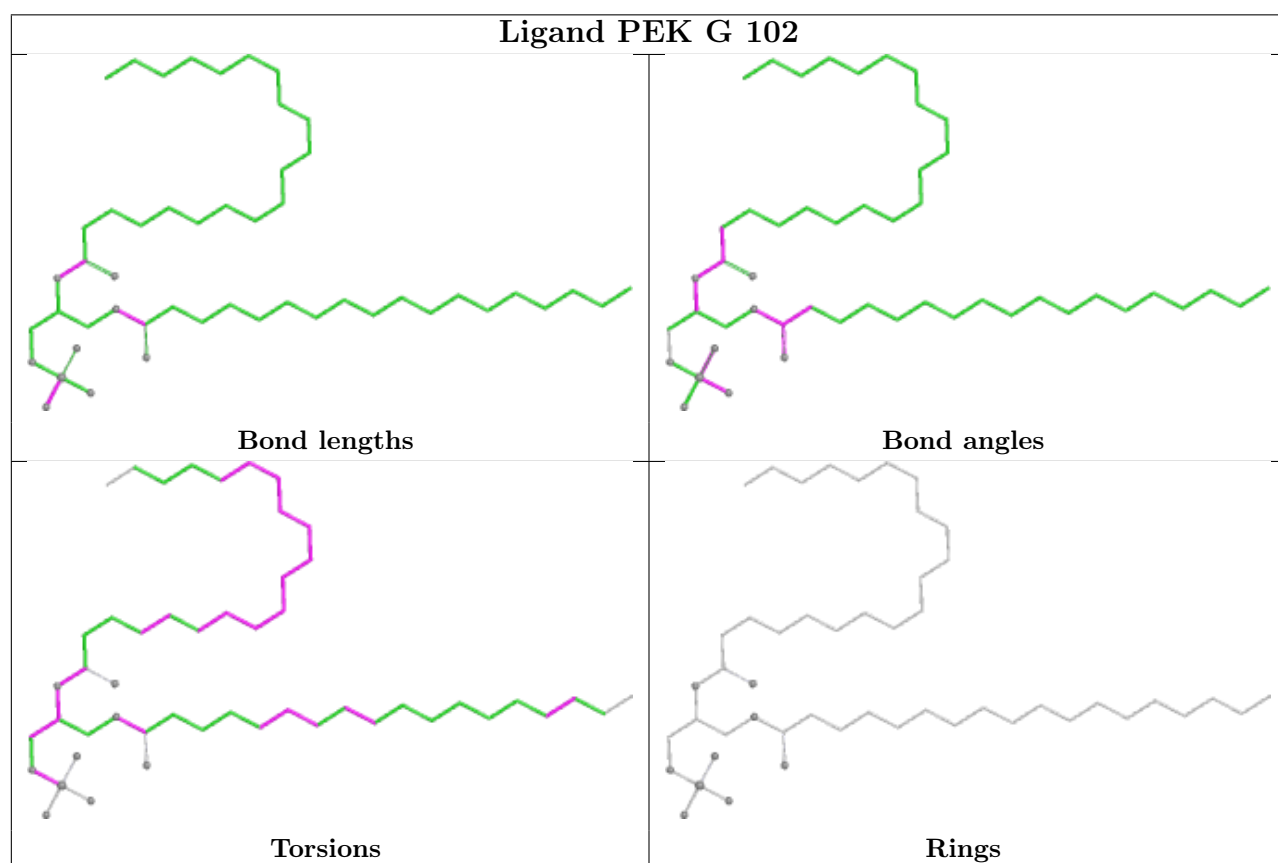
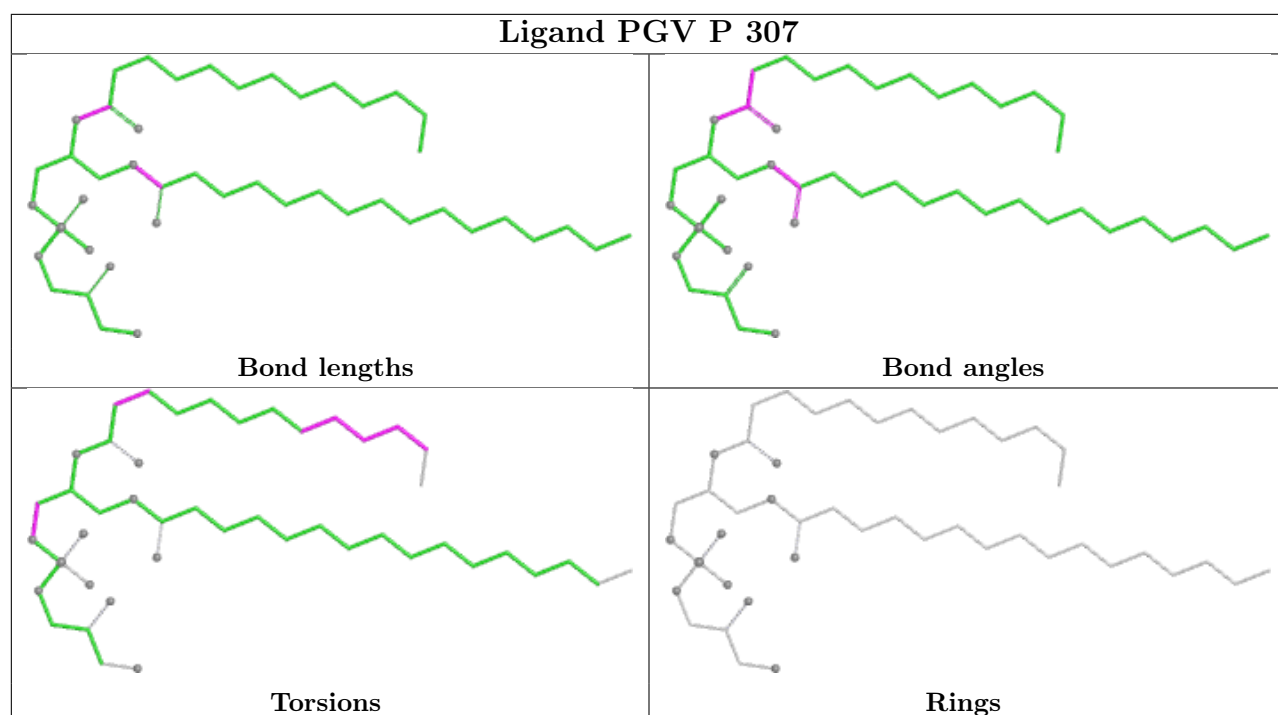


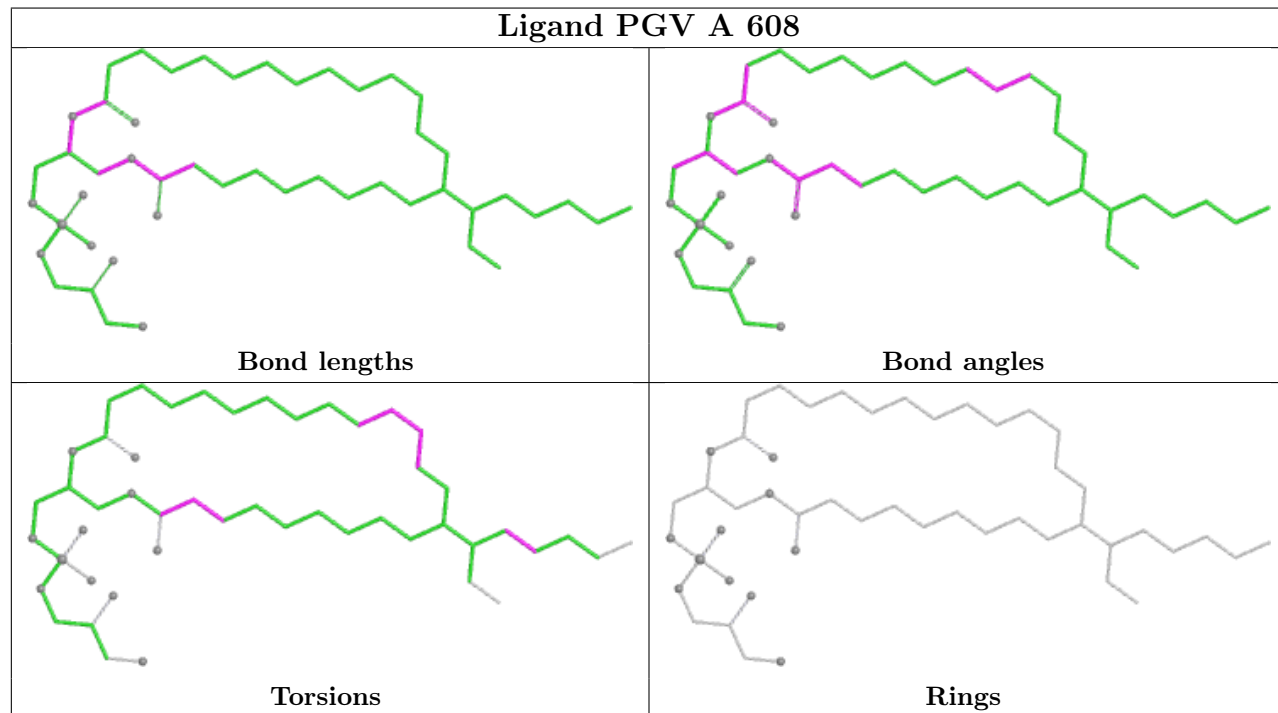
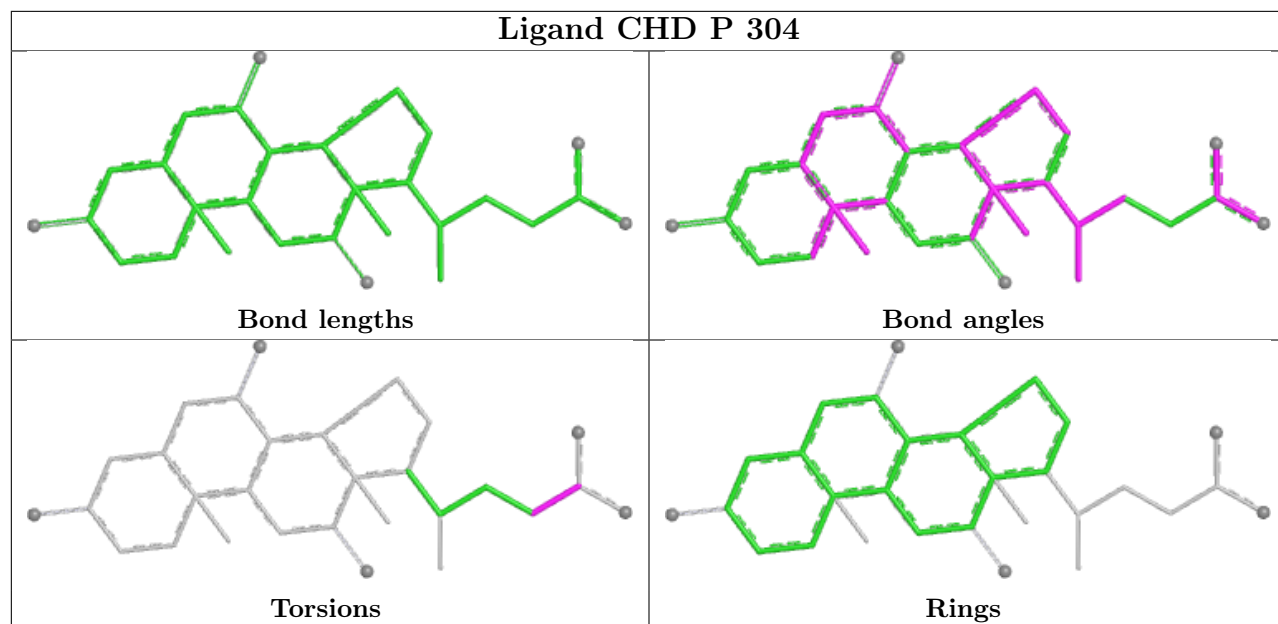


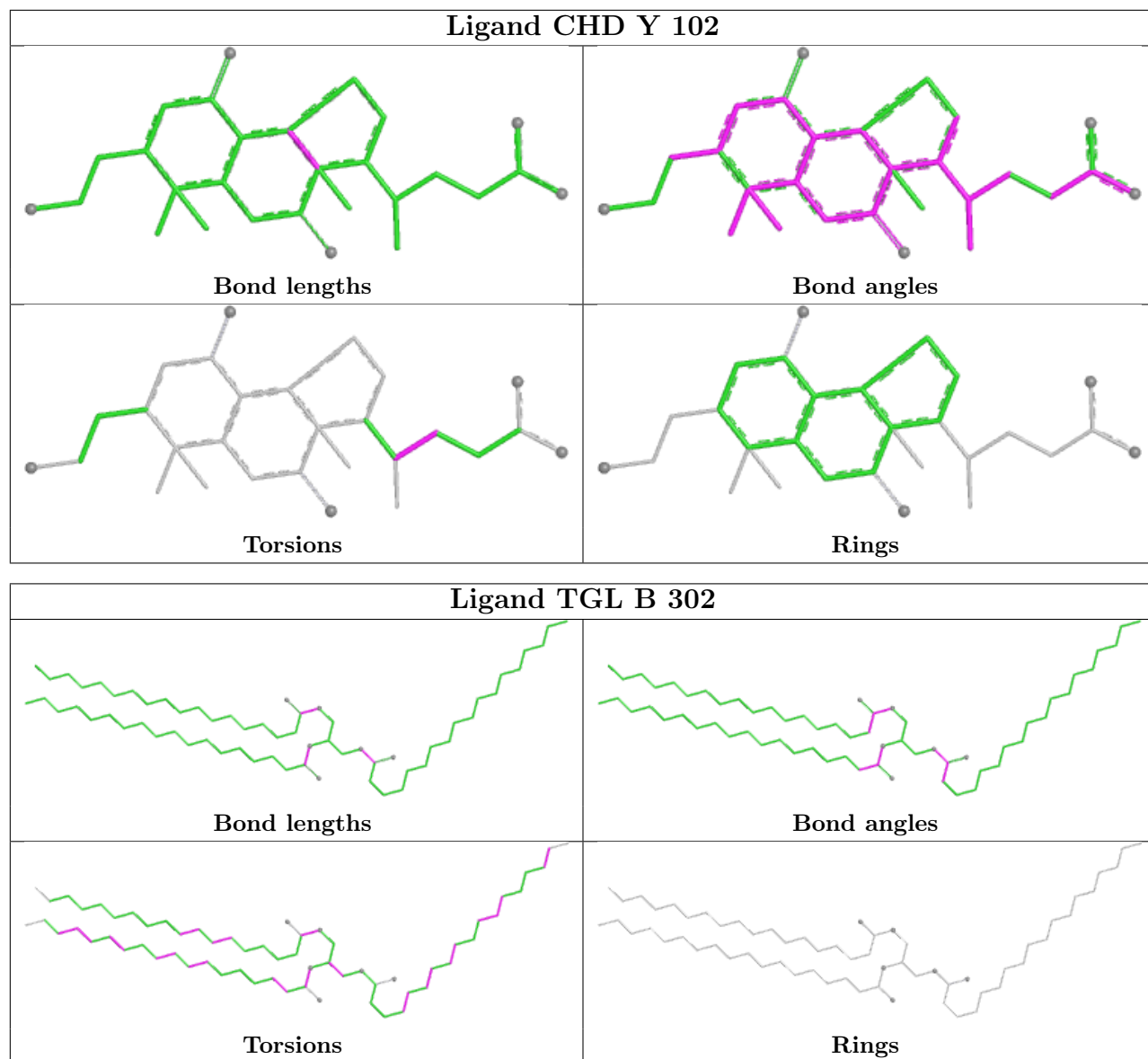


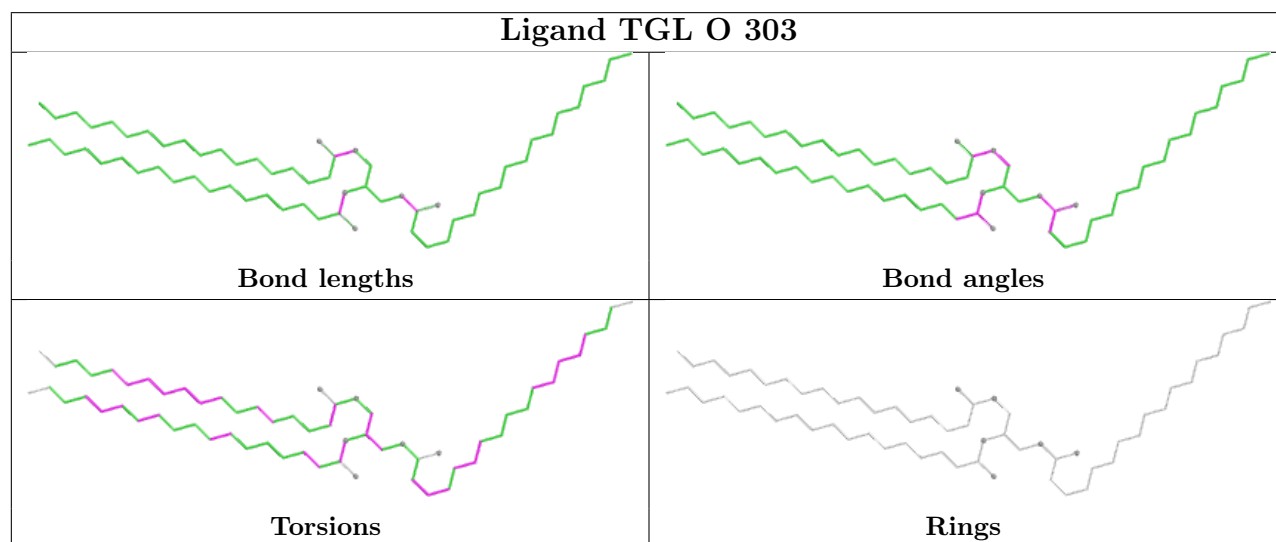
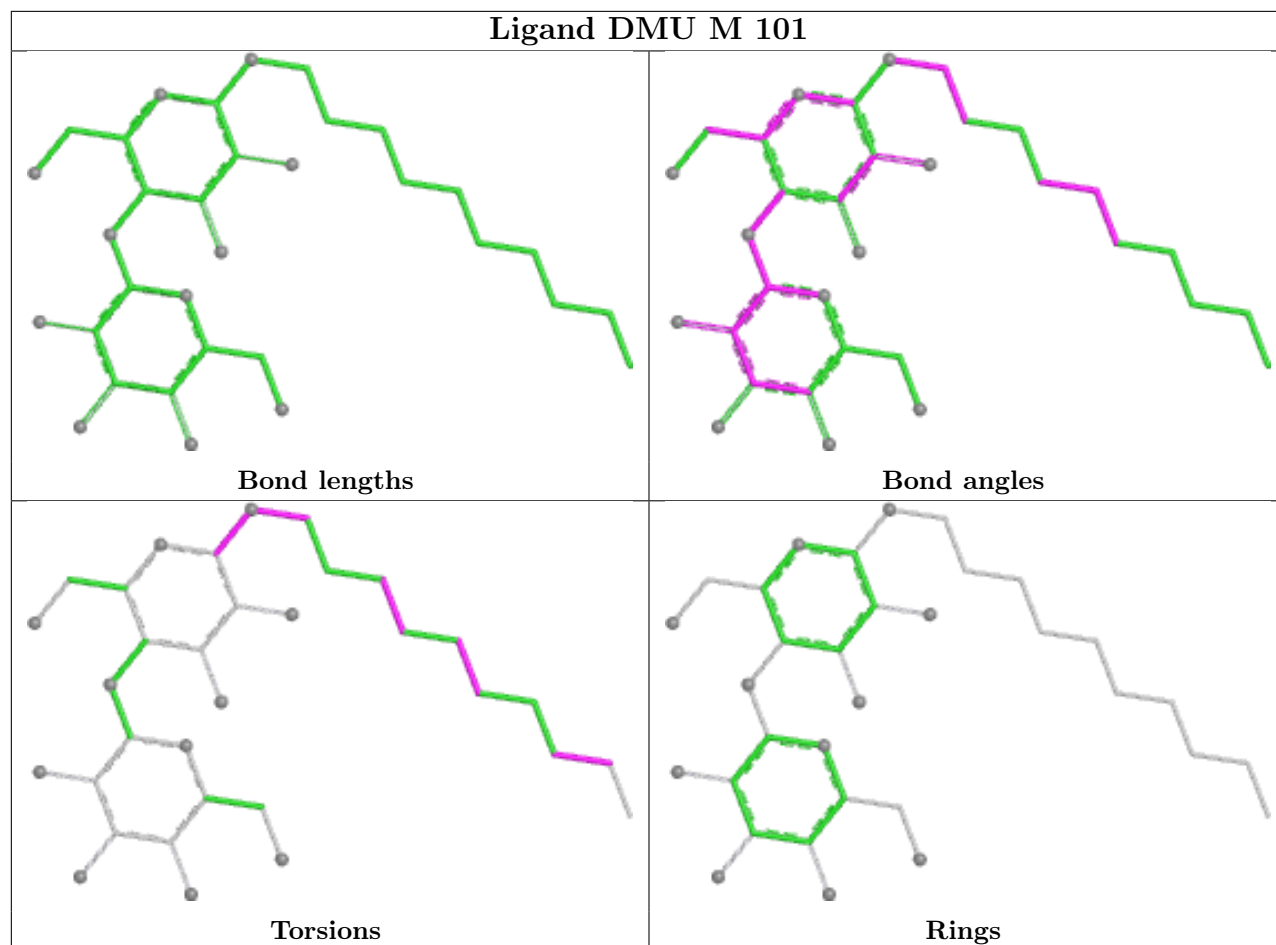


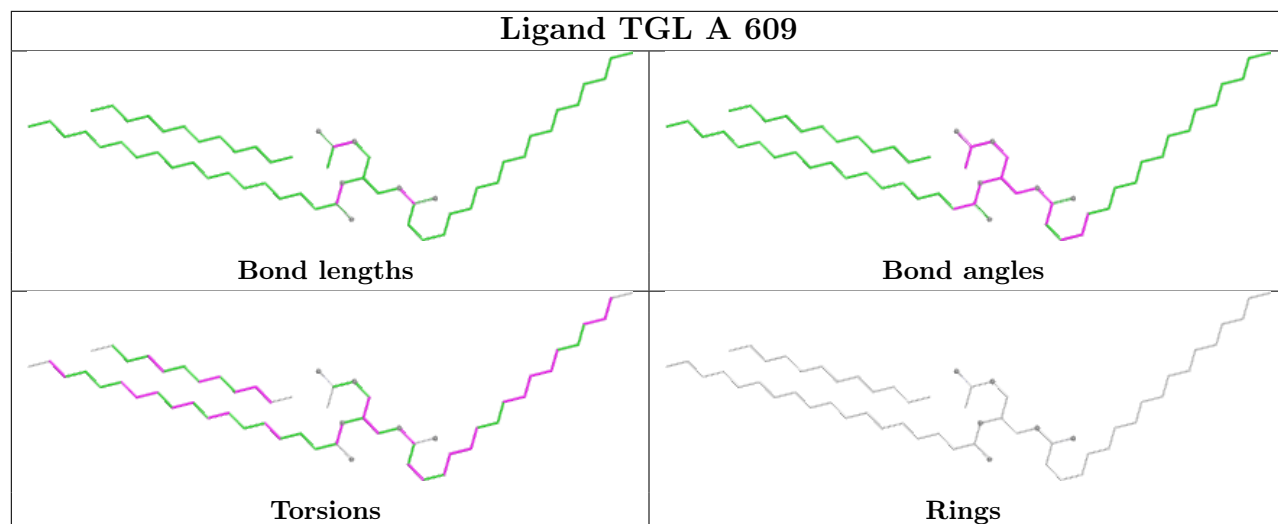


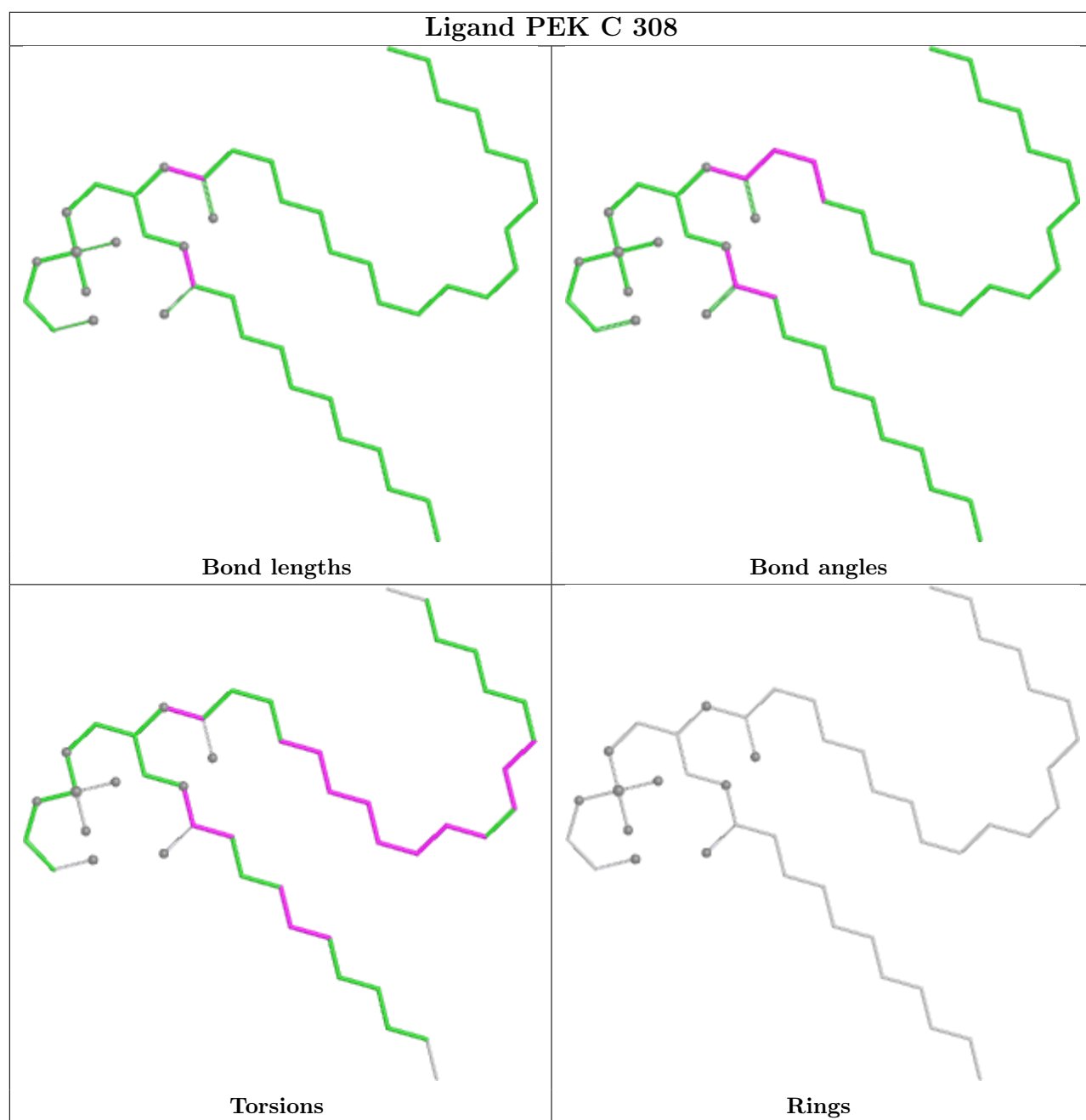


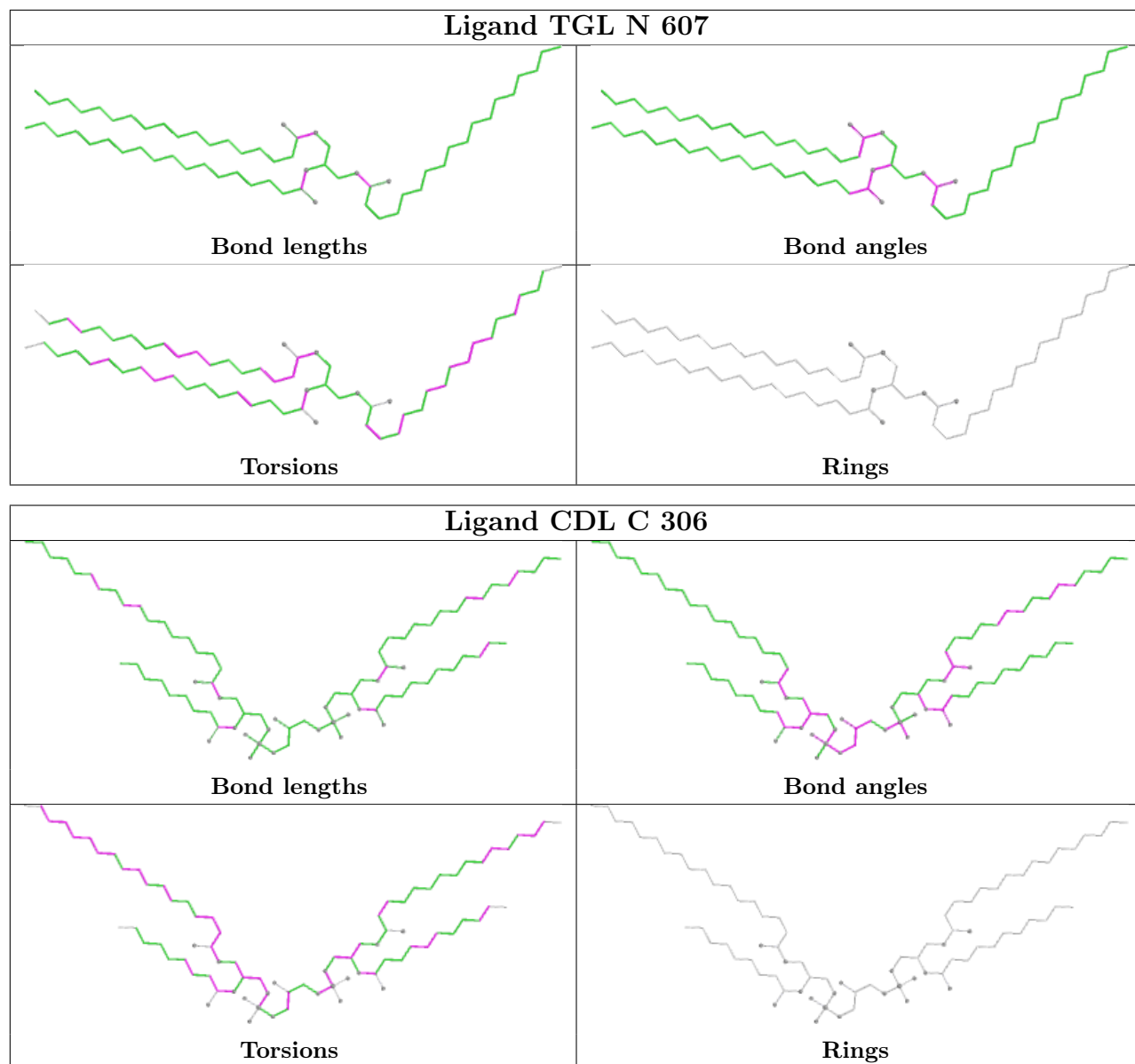




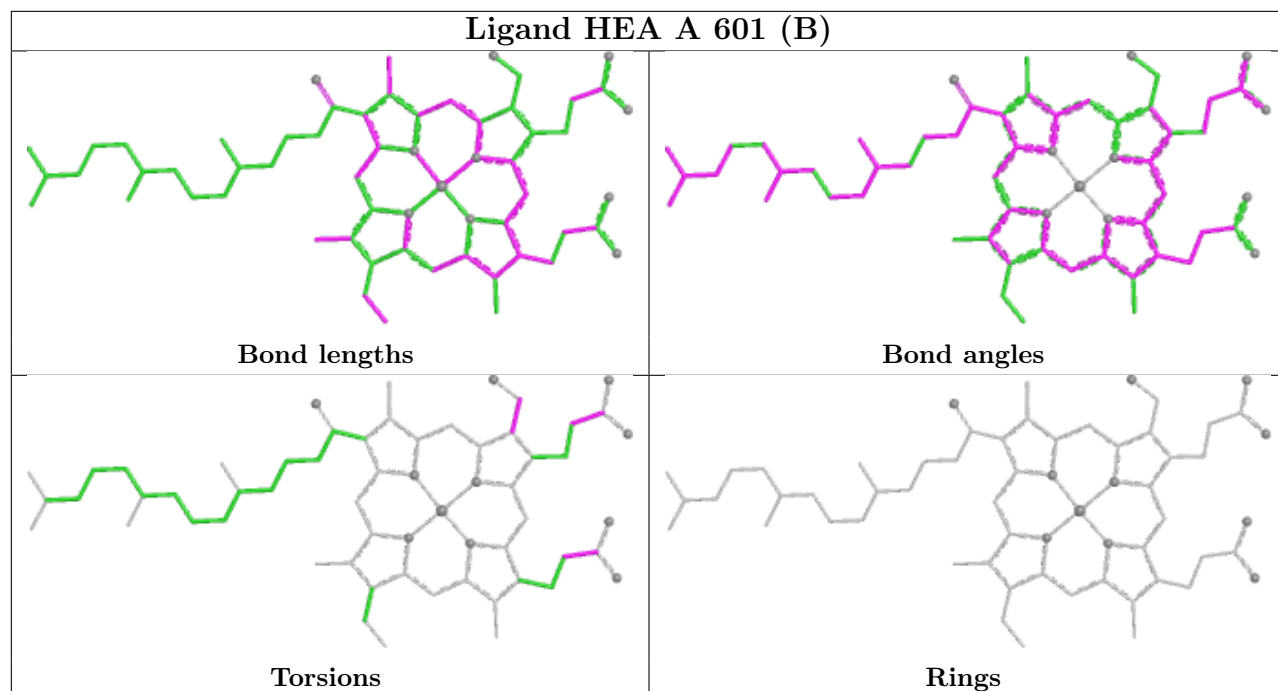




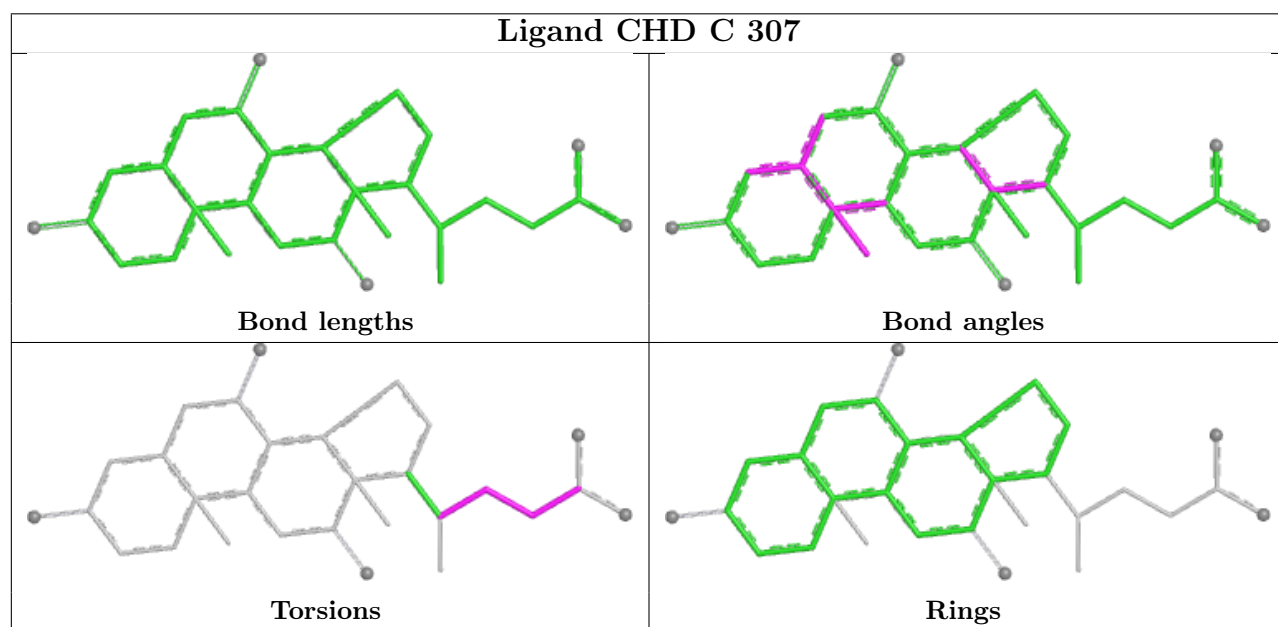


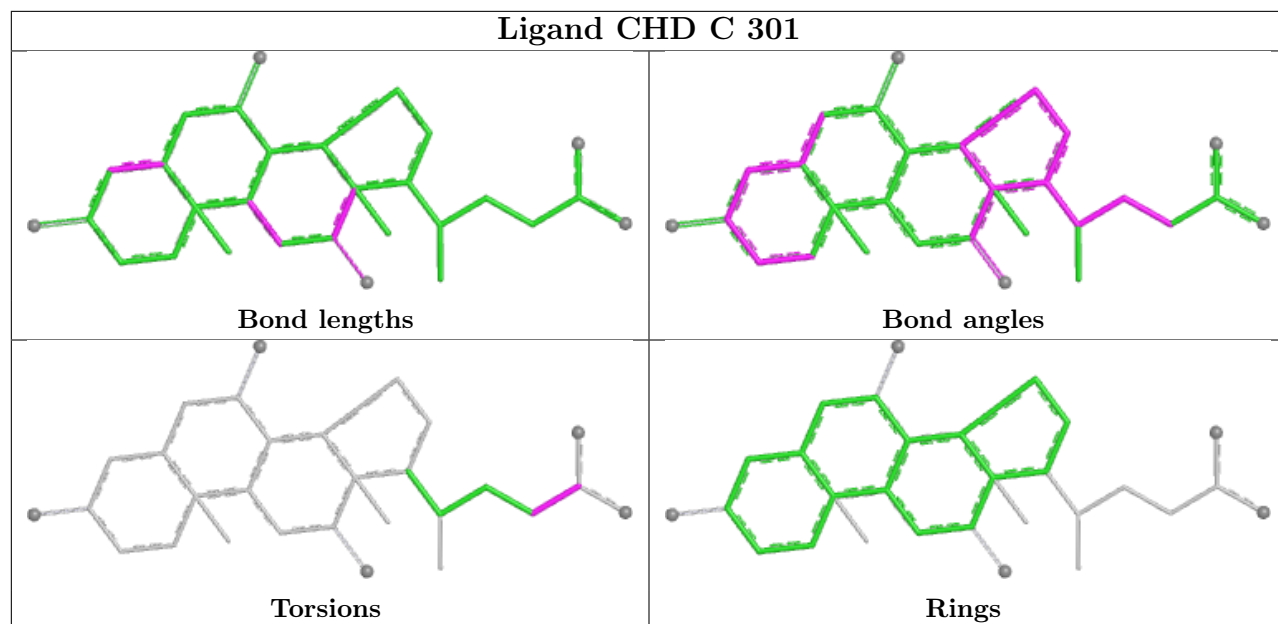


Ligand HEA A 601 (B)



Ligand CHD C 307





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.60	2 (0%) 88 89	12, 28, 38, 87	8 (1%)
1	N	513/514 (99%)	-0.37	6 (1%) 76 77	16, 35, 49, 99	10 (1%)
2	B	226/227 (99%)	-0.09	13 (5%) 29 27	24, 35, 74, 120	1 (0%)
2	O	226/227 (99%)	0.35	16 (7%) 22 20	30, 45, 96, 173	2 (0%)
3	C	259/261 (99%)	-0.33	3 (1%) 76 77	25, 33, 54, 113	0
3	P	259/261 (99%)	-0.28	4 (1%) 72 72	22, 35, 54, 130	2 (0%)
4	D	144/147 (97%)	0.15	5 (3%) 47 47	20, 41, 74, 120	1 (0%)
4	Q	141/147 (95%)	1.27	26 (18%) 3 2	41, 61, 112, 228	0
5	E	105/109 (96%)	0.26	4 (3%) 44 44	36, 45, 88, 160	0
5	R	105/109 (96%)	0.64	6 (5%) 29 28	40, 56, 98, 174	0
6	F	98/98 (100%)	0.36	11 (11%) 10 8	27, 42, 151, 193	0
6	S	95/98 (96%)	0.49	7 (7%) 20 19	32, 44, 97, 198	1 (1%)
7	G	83/85 (97%)	1.01	19 (22%) 2 1	31, 42, 160, 182	0
7	T	83/85 (97%)	0.97	19 (22%) 2 1	28, 45, 139, 207	0
8	H	79/85 (92%)	0.55	9 (11%) 10 8	31, 43, 133, 161	0
8	U	79/85 (92%)	0.70	9 (11%) 10 8	38, 48, 144, 170	0
9	I	72/73 (98%)	0.65	6 (8%) 17 15	35, 52, 92, 157	0
9	V	72/73 (98%)	1.22	18 (25%) 2 1	43, 67, 111, 166	0
10	J	58/59 (98%)	0.36	4 (6%) 23 21	35, 46, 100, 140	0
10	W	58/59 (98%)	0.56	7 (12%) 8 7	38, 50, 113, 173	0
11	K	49/56 (87%)	0.40	4 (8%) 17 15	34, 42, 78, 119	0
11	X	49/56 (87%)	1.18	13 (26%) 1 1	49, 62, 124, 139	0
12	L	46/47 (97%)	0.01	3 (6%) 25 23	27, 34, 66, 116	0
12	Y	46/47 (97%)	0.51	5 (10%) 10 9	38, 45, 100, 138	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.12	2 (4%) 36 35	31, 35, 98, 161	0
13	Z	43/46 (93%)	0.82	7 (16%) 4 3	43, 51, 120, 241	0
All	All	3544/3614 (98%)	0.11	228 (6%) 25 24	12, 39, 96, 241	25 (0%)

The worst 5 of 228 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	3	ALA	7.9
7	T	36	TRP	7.8
6	F	96	LEU	7.0
2	O	113	TYR	6.9
8	H	8	ILE	6.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	-0.04	0.20	183,230,258,263	0
9	SAC	I	1	9/10	0.64	0.18	113,138,176,201	0
7	TPO	T	11	11/12	0.70	0.28	113,188,264,274	0
7	TPO	G	11	11/12	0.70	0.28	133,196,252,264	0
1	FME	N	1	10/11	0.92	0.12	41,59,101,103	0
1	FME	A	1	10/11	0.93	0.11	41,54,85,120	0
2	FME	O	1	10/11	0.97	0.09	34,43,53,70	0
2	FME	B	1	10/11	0.98	0.08	31,35,41,111	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	CHD	Y	102	28/29	0.60	0.28	69,133,187,220	0
24	CHD	J	101	29/29	0.68	0.21	73,152,246,260	0
21	EDO	D	205	4/4	0.71	0.27	52,77,109,114	0
24	CHD	C	315	29/29	0.71	0.28	47,113,216,236	0
24	CHD	P	315	29/29	0.74	0.23	54,105,213,227	0
27	DMU	Z	103	33/33	0.74	0.17	57,104,162,167	0
27	DMU	P	314	33/33	0.75	0.16	58,119,191,241	0
21	EDO	O	307	4/4	0.76	0.20	48,65,75,87	0
27	DMU	C	313	33/33	0.77	0.14	54,104,173,187	0
21	EDO	A	611	4/4	0.78	0.27	47,48,75,86	0
21	EDO	S	103	4/4	0.78	0.32	46,50,91,138	0
25	PEK	P	301	40/53	0.78	0.21	49,80,243,289	0
19	PGV	P	302	47/51	0.79	0.24	43,83,176,216	0
25	PEK	C	308	46/53	0.79	0.24	49,88,237,256	0
27	DMU	T	101	33/33	0.80	0.18	57,117,233,237	0
27	DMU	L	103	33/33	0.81	0.18	49,89,213,237	0
21	EDO	V	102	4/4	0.81	0.18	71,87,100,102	0
20	TGL	A	609	59/63	0.81	0.24	37,62,180,255	0
27	DMU	G	101	33/33	0.81	0.17	59,100,205,249	0
20	TGL	B	302	63/63	0.82	0.20	41,71,128,147	0
21	EDO	F	104	4/4	0.82	0.32	54,54,65,140	0
19	PGV	Z	101	47/51	0.82	0.20	40,91,183,222	0
21	EDO	R	202	4/4	0.82	0.21	68,76,116,136	0
25	PEK	P	306	53/53	0.82	0.22	40,84,194,289	0
26	CDL	G	103	88/100	0.82	0.26	54,100,223,283	0
23	PSC	O	304	46/52	0.83	0.24	40,92,231,329	0
25	PEK	G	102	50/53	0.83	0.22	45,87,241,290	0
24	CHD	P	309	29/29	0.83	0.17	67,120,177,198	0
27	DMU	P	313	33/33	0.83	0.19	49,111,196,214	0
24	CHD	C	307	29/29	0.83	0.18	59,124,188,226	0
23	PSC	B	303	50/52	0.83	0.21	44,106,211,318	0
26	CDL	T	102	93/100	0.83	0.25	46,97,196,240	0
21	EDO	A	619	4/4	0.84	0.26	61,62,69,166	0
21	EDO	C	311	4/4	0.84	0.15	50,57,70,84	0
19	PGV	C	305	49/51	0.84	0.24	48,81,199,279	0
21	EDO	A	616	4/4	0.84	0.27	52,53,57,101	0
27	DMU	L	102	33/33	0.84	0.16	52,105,200,217	0
20	TGL	O	303	63/63	0.85	0.20	49,78,150,203	0
21	EDO	I	101	4/4	0.85	0.17	57,65,72,90	0
21	EDO	L	101	4/4	0.85	0.18	49,52,61,84	0
21	EDO	N	614	4/4	0.85	0.14	63,65,69,78	0
20	TGL	N	607	63/63	0.85	0.21	52,77,148,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	A	613	4/4	0.86	0.20	50,61,72,78	0
19	PGV	A	607	51/51	0.86	0.21	31,78,182,264	0
26	CDL	P	308	91/100	0.86	0.22	41,88,197,256	0
20	TGL	D	201	55/63	0.87	0.21	37,71,132,200	0
21	EDO	H	101	4/4	0.87	0.22	47,78,84,105	0
21	EDO	S	106	4/4	0.87	0.17	53,60,63,90	0
21	EDO	U	101	4/4	0.87	0.25	51,62,106,158	0
21	EDO	O	305	4/4	0.88	0.15	52,70,74,80	0
21	EDO	D	202	4/4	0.88	0.21	49,59,98,118	0
21	EDO	H	102	4/4	0.88	0.19	29,64,86,98	0
21	EDO	A	620	4/4	0.88	0.18	47,67,67,76	0
20	TGL	Y	101	59/63	0.88	0.21	45,71,181,274	0
21	EDO	G	104	4/4	0.88	0.20	44,54,67,104	0
21	EDO	S	107	4/4	0.89	0.17	42,54,82,89	0
21	EDO	F	106	4/4	0.89	0.21	42,67,70,120	0
21	EDO	K	101	4/4	0.89	0.19	48,60,62,117	0
26	CDL	C	306	82/100	0.89	0.20	40,90,223,304	0
21	EDO	A	610	4/4	0.89	0.23	40,60,63,93	0
21	EDO	Q	202	4/4	0.90	0.16	49,60,63,68	0
21	EDO	E	201	4/4	0.90	0.14	58,66,74,78	0
27	DMU	C	314	33/33	0.90	0.14	42,84,148,224	0
21	EDO	P	311	4/4	0.90	0.15	55,58,63,74	0
27	DMU	Z	102	33/33	0.90	0.12	46,66,102,181	0
21	EDO	V	101	4/4	0.90	0.16	51,67,83,115	0
21	EDO	T	104	4/4	0.91	0.15	47,54,63,77	0
21	EDO	R	201	4/4	0.91	0.19	60,73,75,85	0
21	EDO	A	621	4/4	0.91	0.20	30,57,83,118	0
21	EDO	C	312	4/4	0.91	0.19	45,70,88,158	0
21	EDO	P	312	4/4	0.91	0.14	48,56,59,68	0
21	EDO	B	306	4/4	0.91	0.14	44,49,50,81	0
27	DMU	M	101	33/33	0.92	0.10	34,53,80,98	0
21	EDO	A	618	4/4	0.92	0.16	41,42,68,71	0
21	EDO	E	204	4/4	0.92	0.17	56,56,71,75	0
21	EDO	D	204	4/4	0.93	0.14	46,64,73,79	0
21	EDO	A	622	4/4	0.93	0.19	46,64,67,125	0
21	EDO	E	202	4/4	0.94	0.09	46,46,47,55	0
21	EDO	A	615	4/4	0.94	0.10	36,49,50,62	0
21	EDO	A	614	4/4	0.94	0.13	34,35,43,58	0
21	EDO	O	306	4/4	0.94	0.13	47,63,68,72	0
21	EDO	S	105	4/4	0.95	0.11	48,54,66,74	0
21	EDO	Q	201	4/4	0.95	0.10	41,48,52,80	0
21	EDO	N	611	4/4	0.95	0.14	48,54,55,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	PEK	C	303	53/53	0.95	0.14	32,49,123,160	0
21	EDO	N	613	4/4	0.95	0.11	49,58,66,68	0
21	EDO	D	203	4/4	0.95	0.10	43,50,54,82	0
21	EDO	N	610	4/4	0.95	0.13	38,56,57,101	0
25	PEK	P	305	52/53	0.95	0.14	32,52,124,204	0
21	EDO	F	103	4/4	0.96	0.09	40,42,55,61	0
21	EDO	S	104	4/4	0.96	0.10	47,47,55,58	0
21	EDO	P	310	4/4	0.96	0.12	35,40,51,54	0
19	PGV	N	608	51/51	0.96	0.10	26,41,69,88	0
21	EDO	N	612	4/4	0.96	0.07	27,34,36,39	0
24	CHD	P	304	29/29	0.96	0.07	28,36,42,47	0
21	EDO	F	105	4/4	0.96	0.10	38,45,48,57	0
21	EDO	C	309	4/4	0.96	0.09	37,43,45,46	0
21	EDO	C	310	4/4	0.96	0.10	38,47,50,59	0
21	EDO	N	609	4/4	0.96	0.16	35,38,46,58	0
21	EDO	A	617	4/4	0.97	0.12	44,48,55,110	0
19	PGV	A	608	51/51	0.97	0.10	24,37,69,99	0
19	PGV	P	307	46/51	0.97	0.09	27,40,63,76	0
21	EDO	S	102	4/4	0.97	0.10	34,34,35,37	0
19	PGV	C	304	47/51	0.97	0.10	27,38,66,94	0
17	NA	N	605	1/1	0.97	0.12	41,41,41,41	0
17	NA	C	302	1/1	0.97	0.05	42,42,42,42	0
24	CHD	C	301	29/29	0.97	0.06	27,32,39,40	0
21	EDO	B	305	4/4	0.97	0.08	27,29,29,35	0
21	EDO	G	105	4/4	0.98	0.06	36,39,45,47	0
24	CHD	O	301	29/29	0.98	0.06	24,34,46,48	0
21	EDO	A	612	4/4	0.98	0.07	27,29,30,33	0
18	CMO	N	606[A]	2/2	0.98	0.12	21,21,21,22	2
18	CMO	N	606[B]	2/2	0.98	0.12	15,15,15,29	2
24	CHD	B	304	29/29	0.98	0.04	25,32,43,49	0
21	EDO	T	103	4/4	0.98	0.07	37,39,43,57	0
21	EDO	E	203	4/4	0.98	0.06	41,46,49,50	0
17	NA	P	303	1/1	0.98	0.08	38,38,38,38	0
21	EDO	F	102	4/4	0.99	0.06	29,29,31,39	0
18	CMO	A	606[B]	2/2	0.99	0.10	10,10,10,16	2
14	HEA	N	601[A]	60/60	0.99	0.07	16,33,62,79	18
14	HEA	N	601[B]	60/60	0.99	0.07	27,33,47,59	18
14	HEA	N	602	60/60	0.99	0.05	21,30,38,42	0
16	MG	A	604	1/1	0.99	0.06	21,21,21,21	0
16	MG	N	604	1/1	0.99	0.08	24,24,24,24	0
17	NA	A	605	1/1	0.99	0.06	32,32,32,32	0
14	HEA	A	601[A]	60/60	0.99	0.05	14,23,53,77	18

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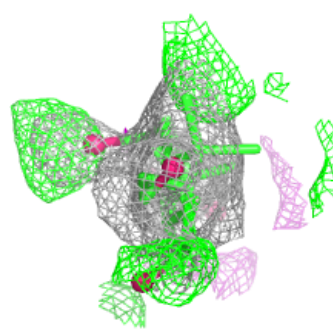
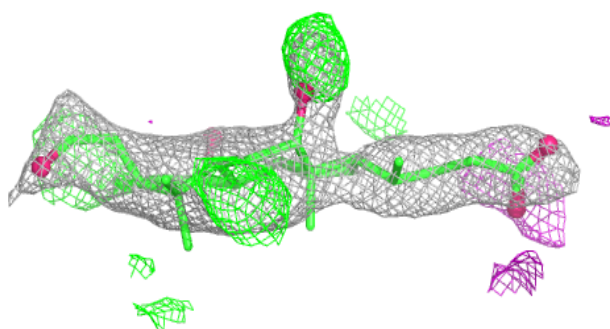
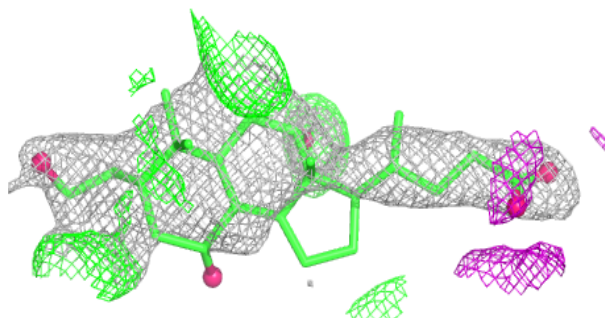
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	HEA	A	601[B]	60/60	0.99	0.05	19,23,35,50	18
14	HEA	A	602	60/60	0.99	0.05	17,24,33,40	0
18	CMO	A	606[A]	2/2	0.99	0.10	18,18,18,26	2
28	ZN	S	101	1/1	0.99	0.02	40,40,40,40	0
22	CUA	B	301	2/2	1.00	0.01	25,25,25,26	0
22	CUA	O	302	2/2	1.00	0.04	32,32,32,32	0
15	CU	A	603	1/1	1.00	0.01	25,25,25,25	0
28	ZN	F	101	1/1	1.00	0.03	32,32,32,32	0
15	CU	N	603	1/1	1.00	0.01	28,28,28,28	0

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

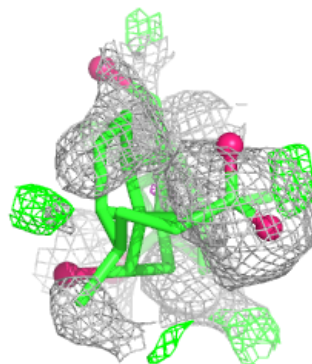
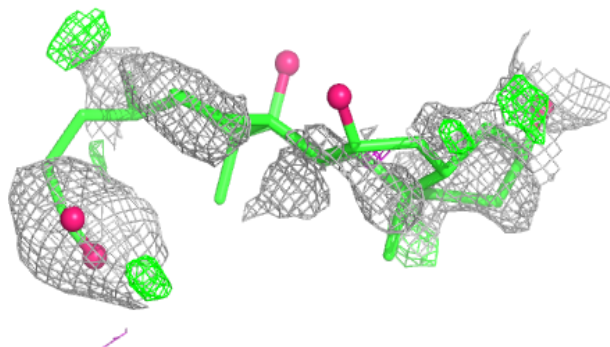
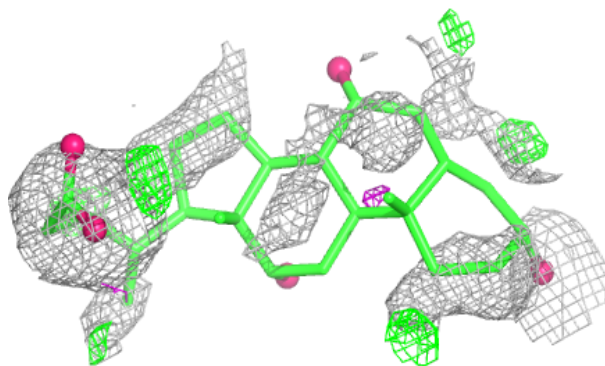
Electron density around CHD Y 102:

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

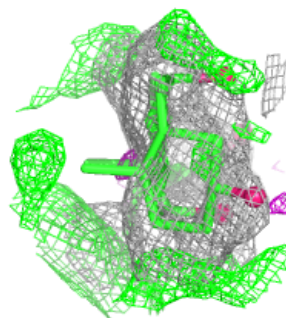
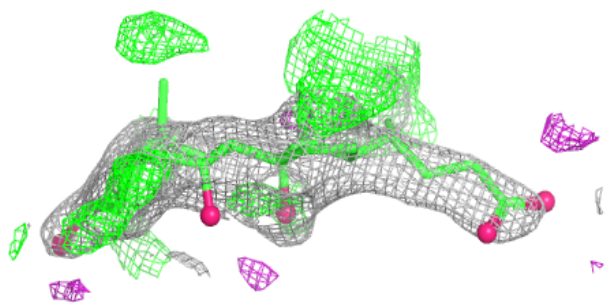
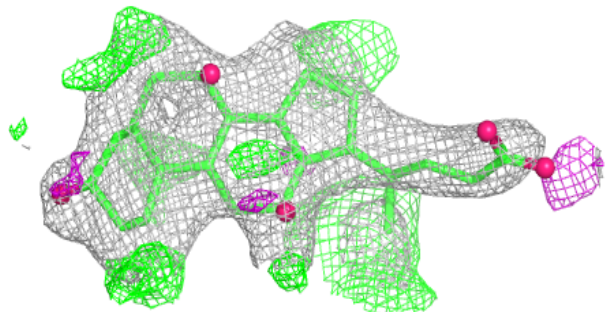


Electron density around CHD J 101:

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

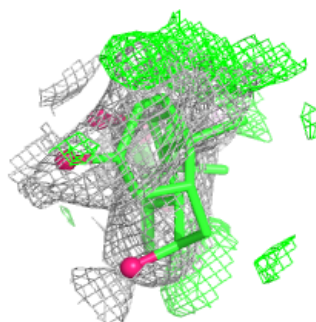
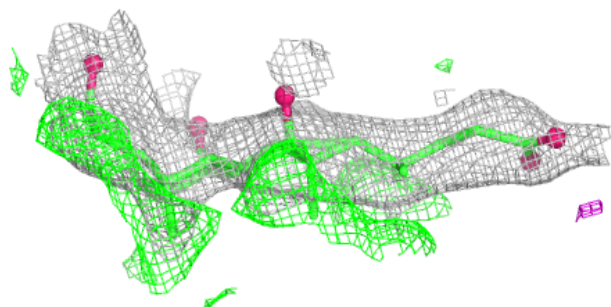
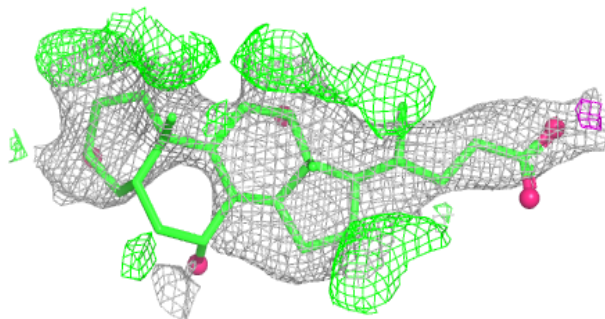
**Electron density around CHD C 315:**

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

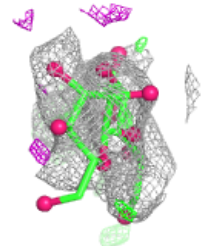
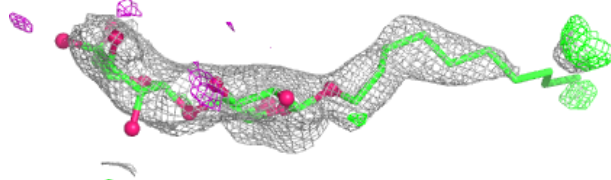
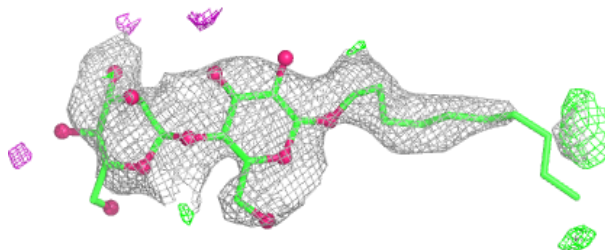


Electron density around CHD P 315:

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

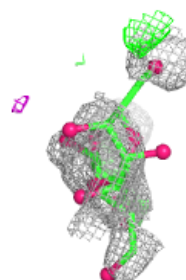
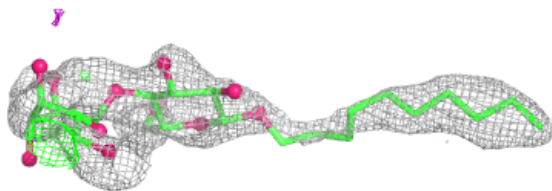
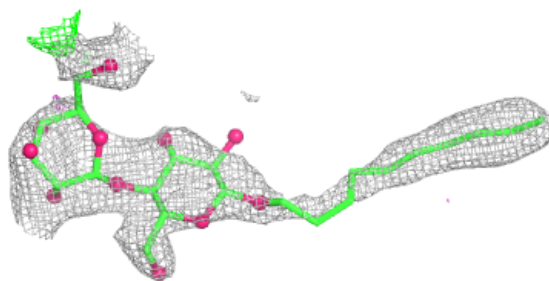
**Electron density around DMU Z 103:**

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

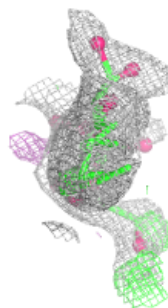
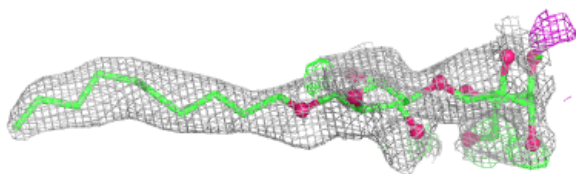
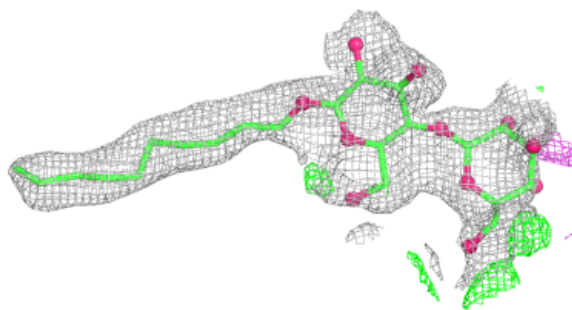


Electron density around DMU P 314:

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

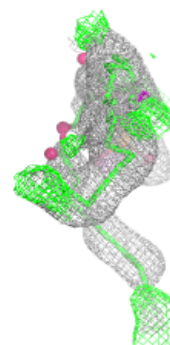
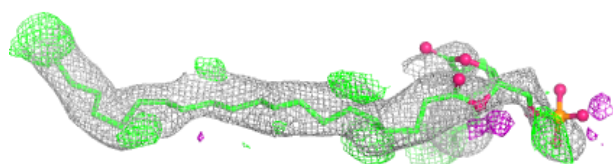
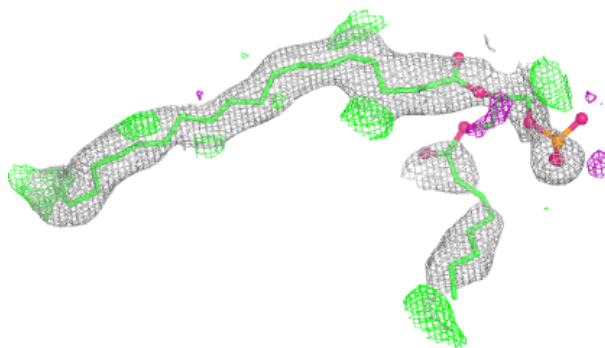
**Electron density around DMU C 313:**

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

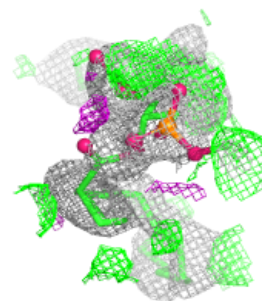
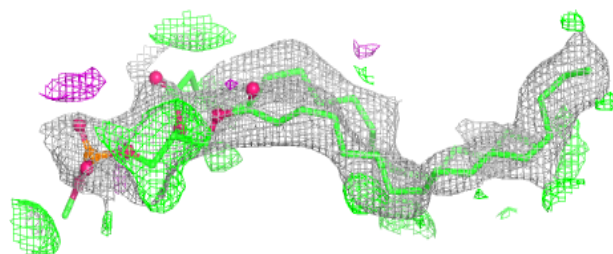
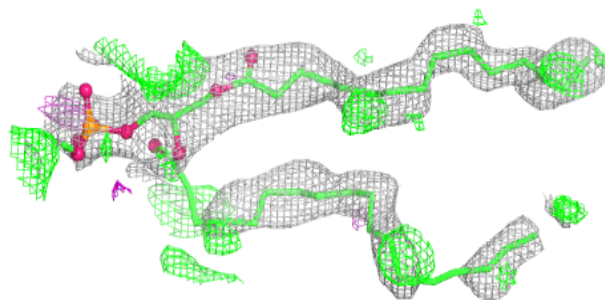


Electron density around PEK P 301:

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

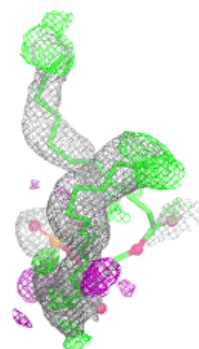
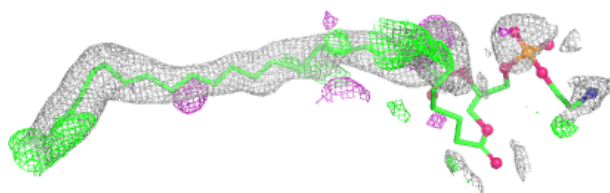
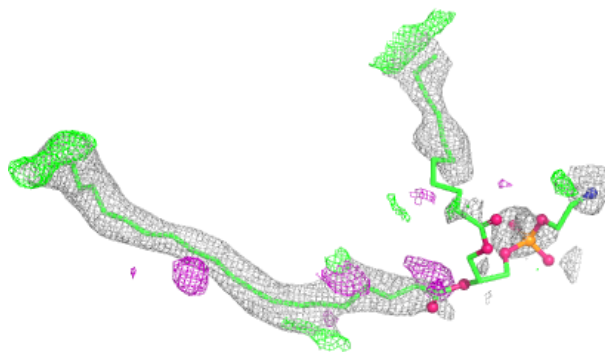
**Electron density around PGV P 302:**

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

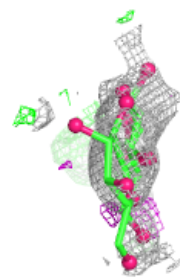
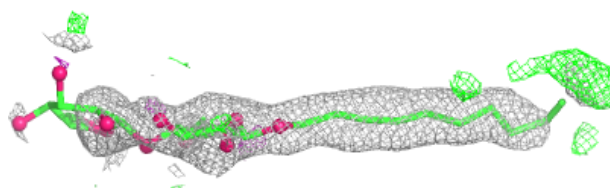
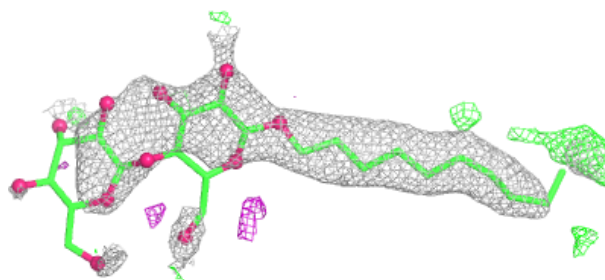


Electron density around PEK C 308:

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

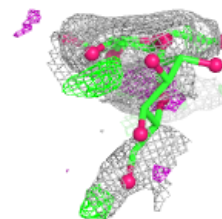
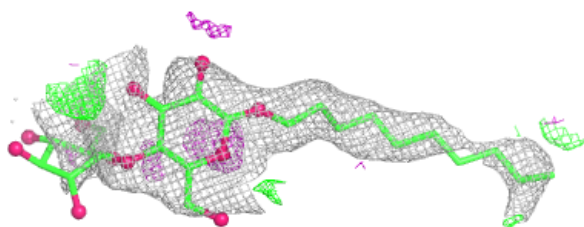
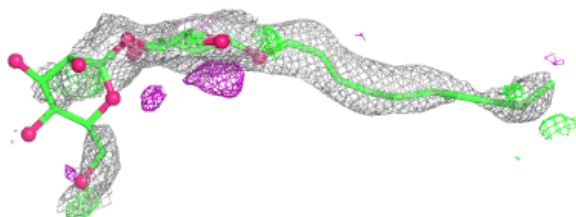
**Electron density around DMU T 101:**

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



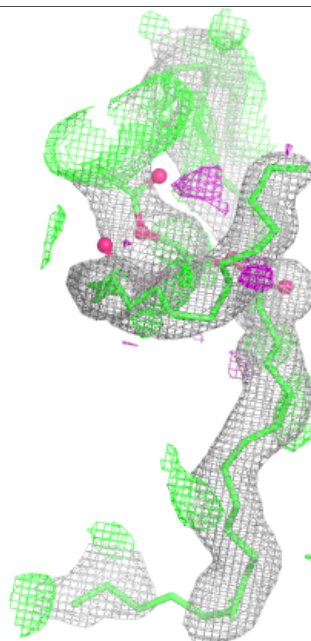
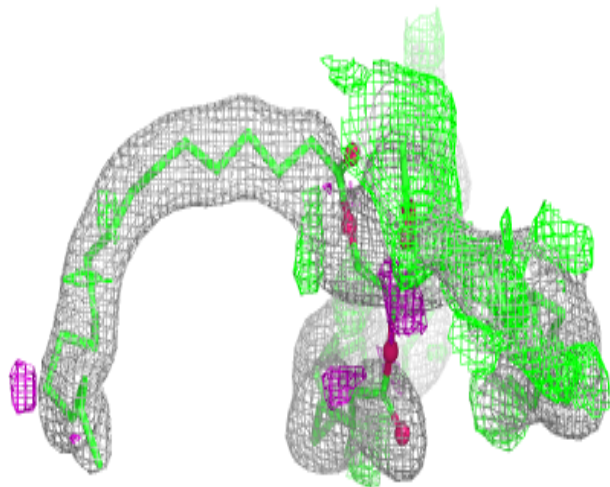
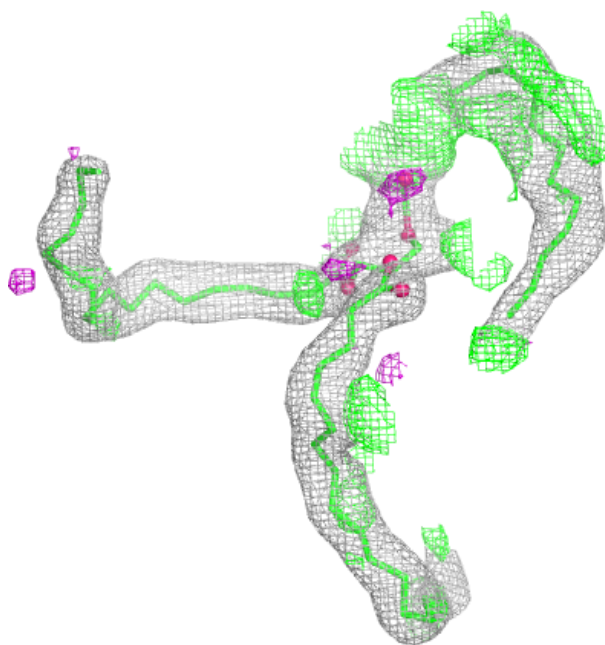
Electron density around DMU L 103:

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



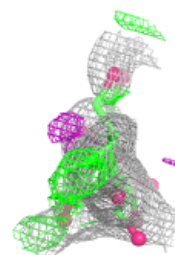
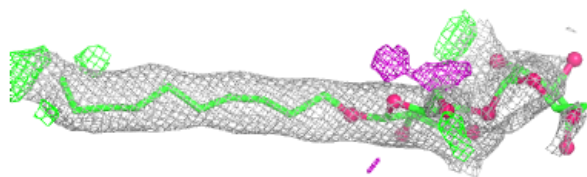
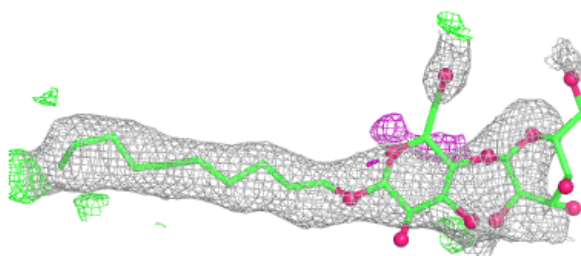
Electron density around TGL A 609:

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

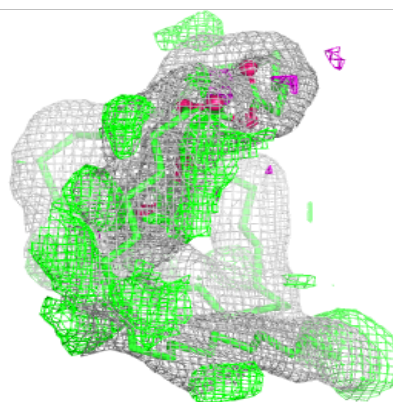
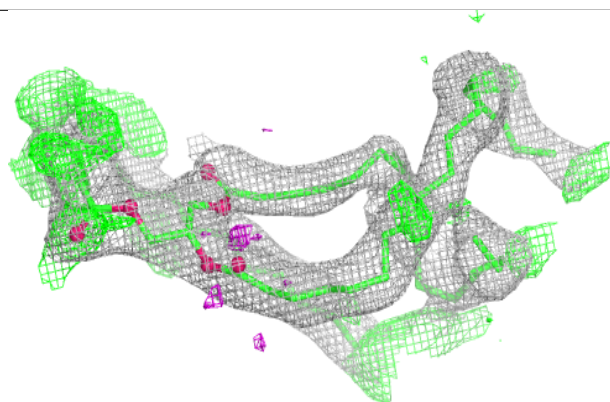
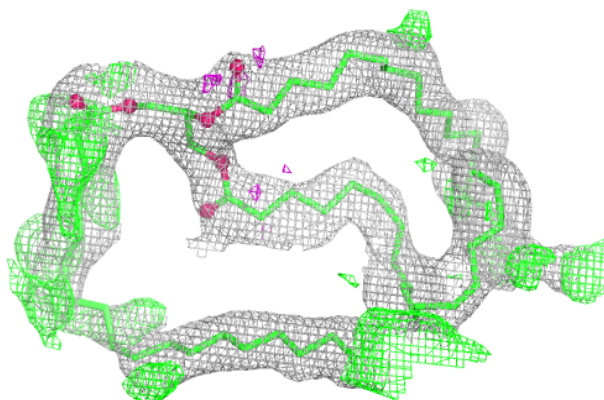


Electron density around DMU G 101:

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

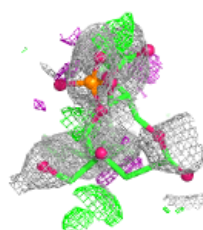
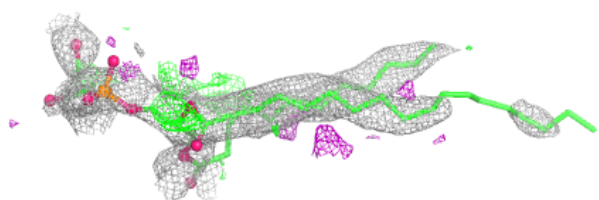
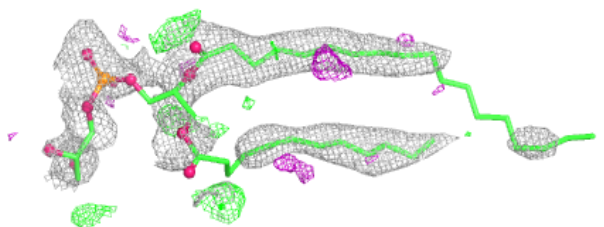
**Electron density around TGL B 302:**

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

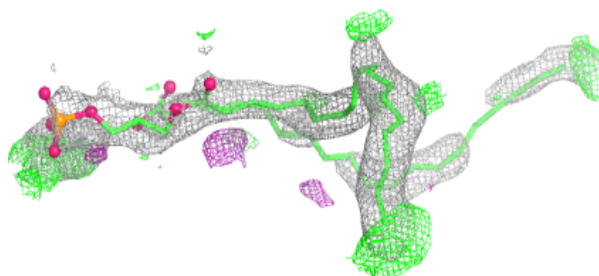
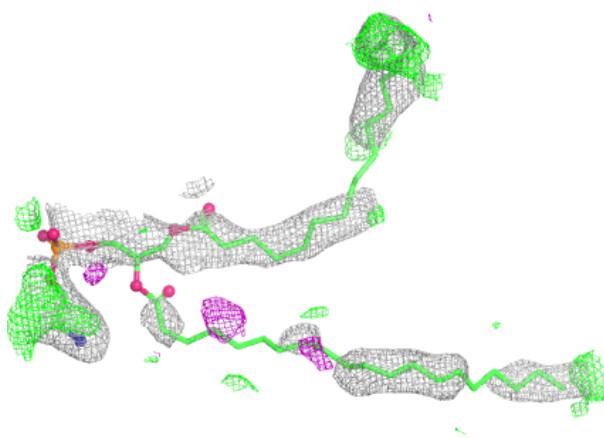


Electron density around PGV Z 101:

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

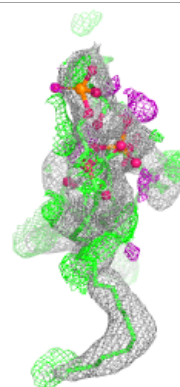
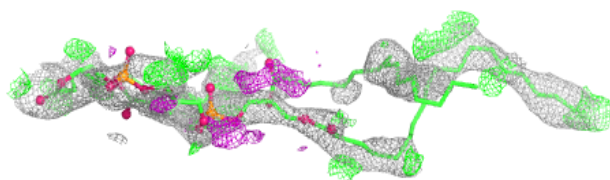
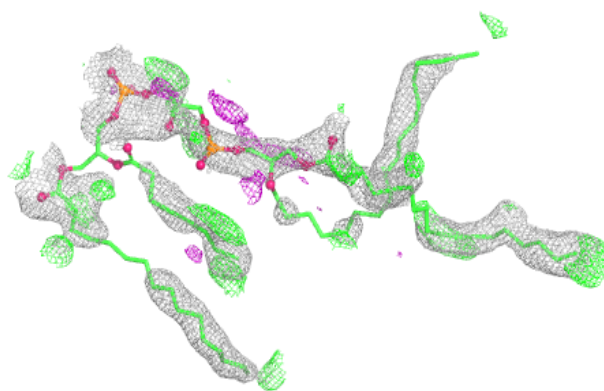
**Electron density around PEK P 306:**

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

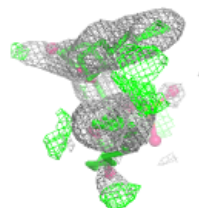
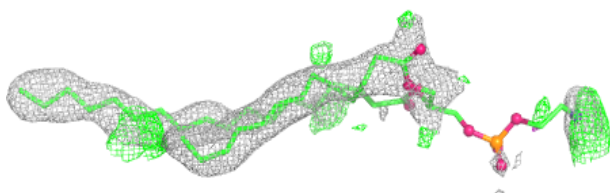
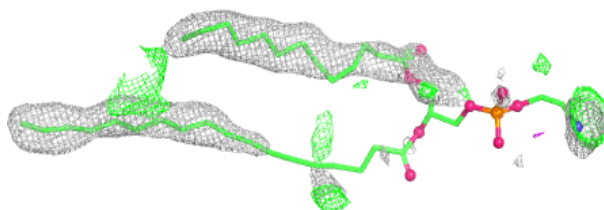


Electron density around CDL G 103:

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

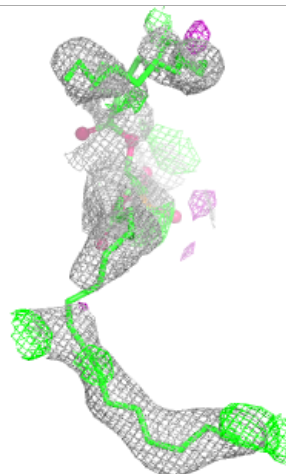
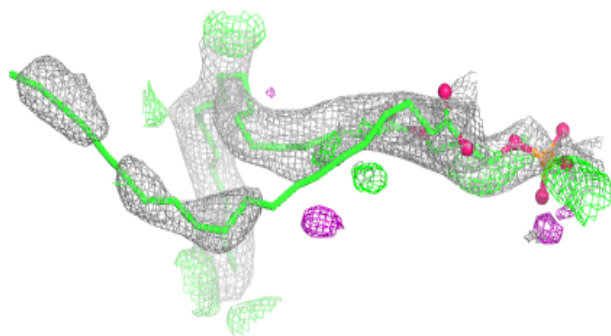
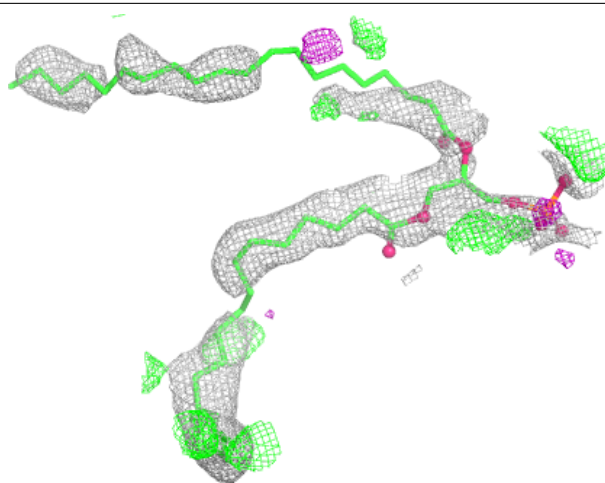
**Electron density around PSC O 304:**

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



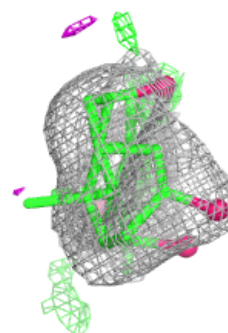
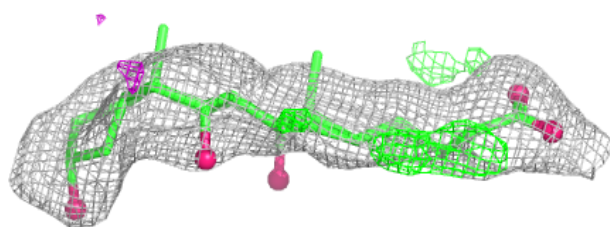
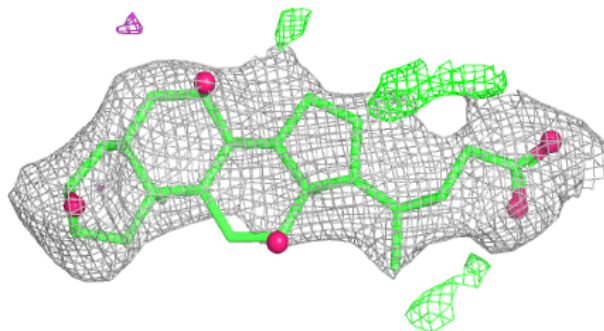
Electron density around PEK G 102:

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

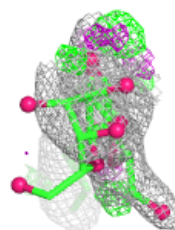
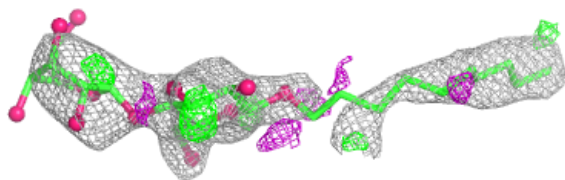
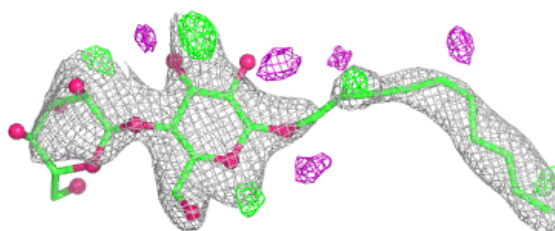


Electron density around CHD P 309:

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

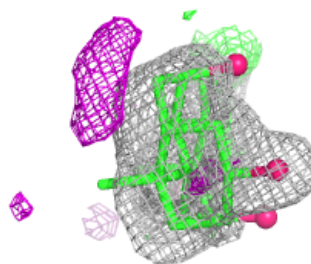
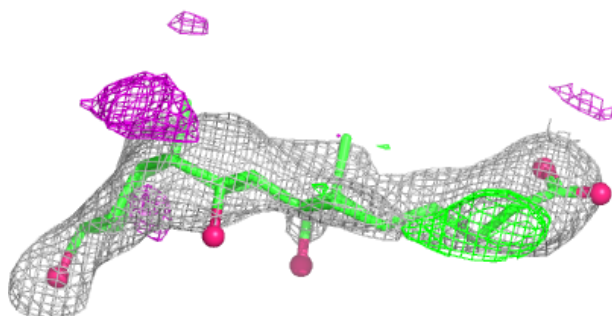
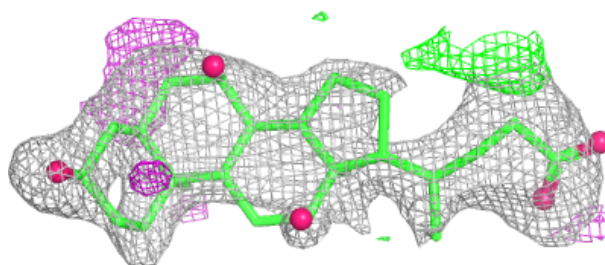
**Electron density around DMU P 313:**

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

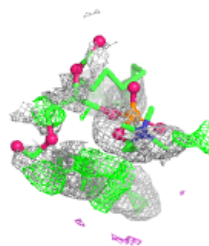
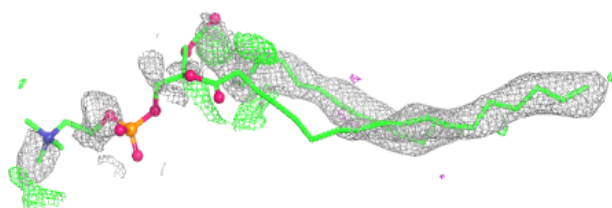
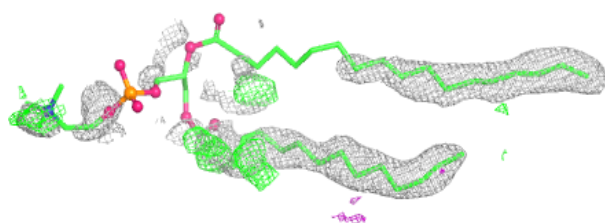


Electron density around CHD C 307:

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

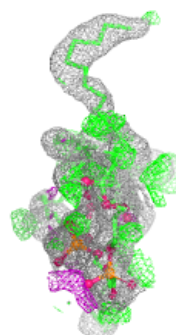
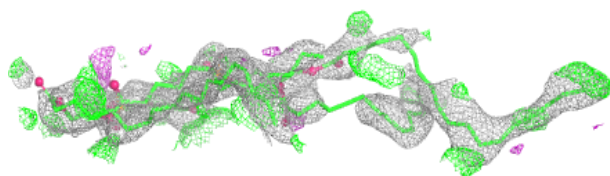
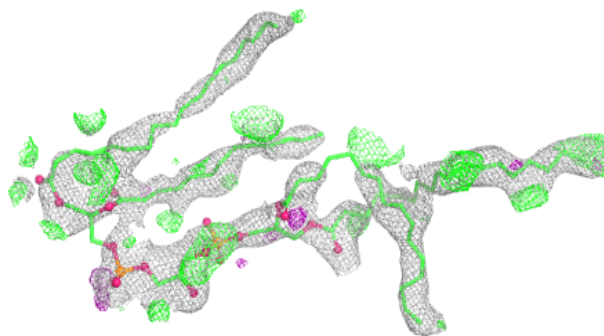
**Electron density around PSC B 303:**

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

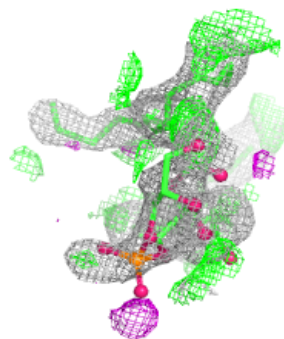
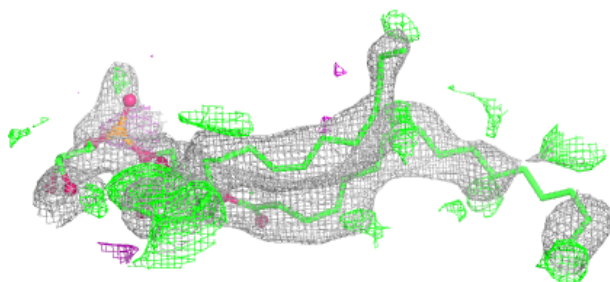
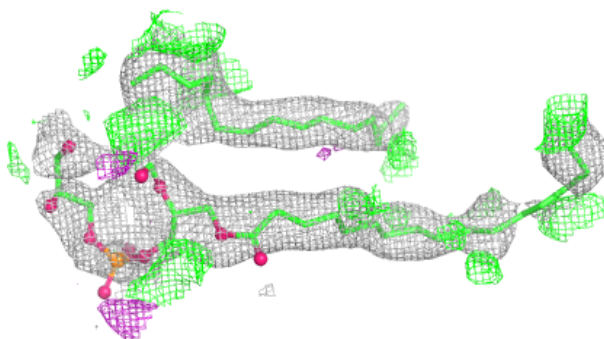


Electron density around CDL T 102:

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

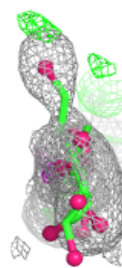
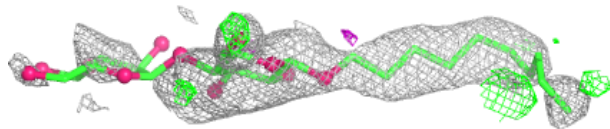
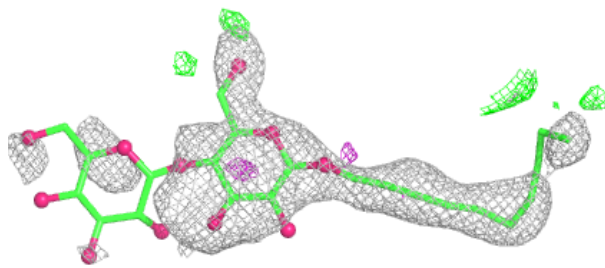
**Electron density around PGV C 305:**

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

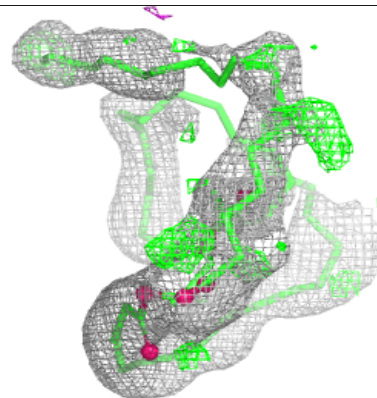
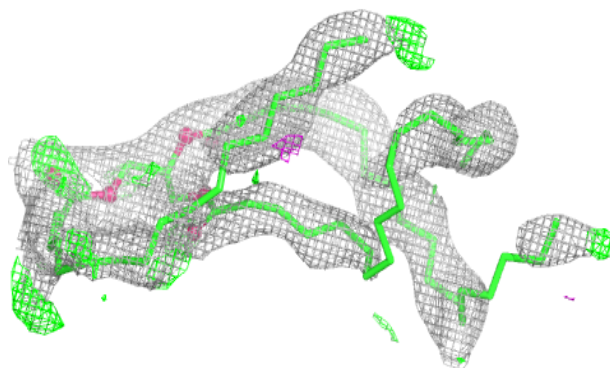
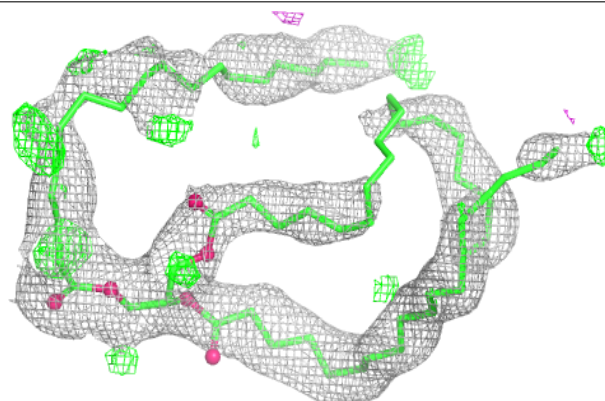


Electron density around DMU L 102:

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

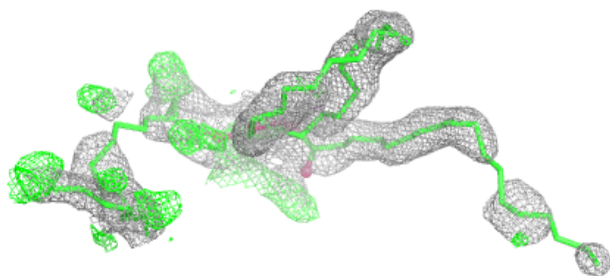
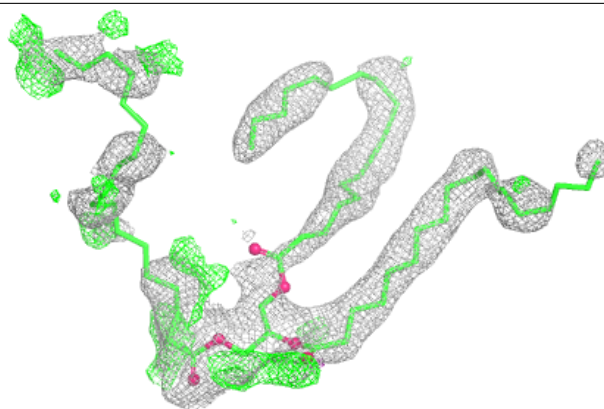
**Electron density around TGL O 303:**

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

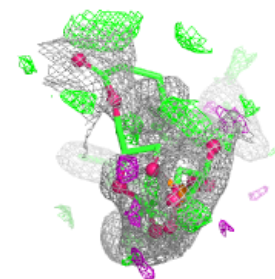
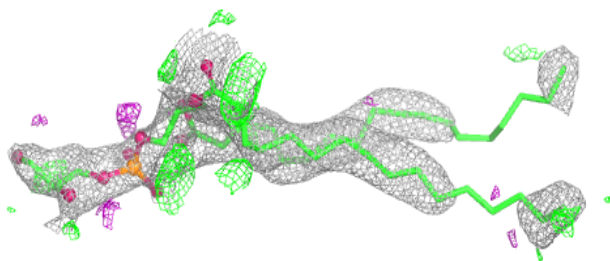
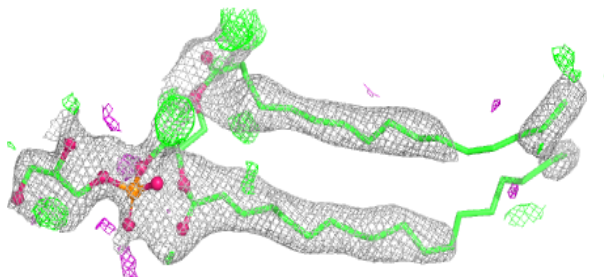


Electron density around TGL N 607:

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

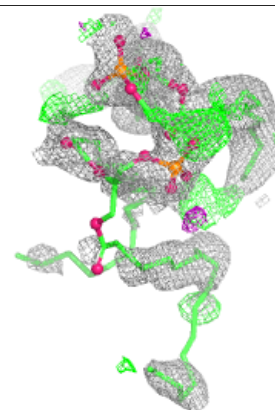
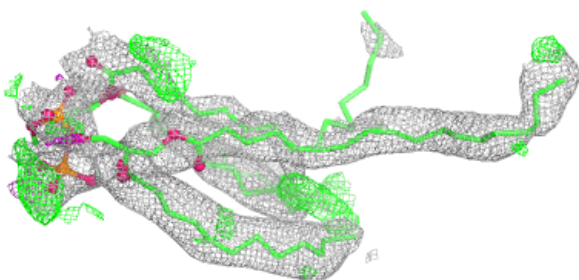
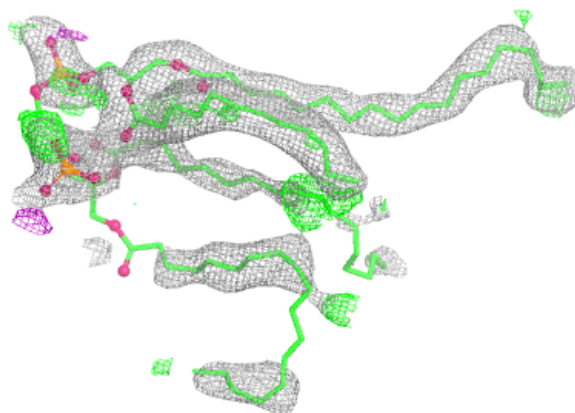
**Electron density around PGV A 607:**

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



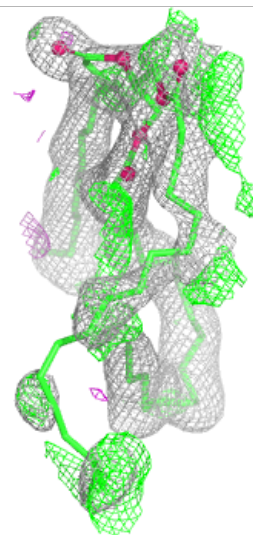
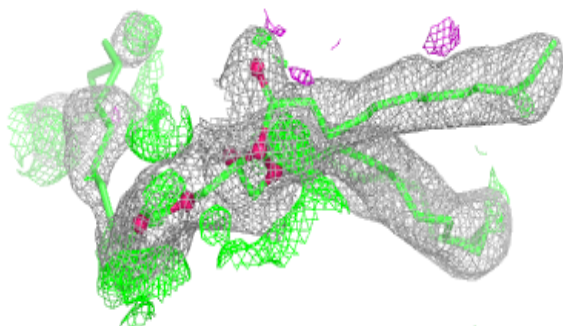
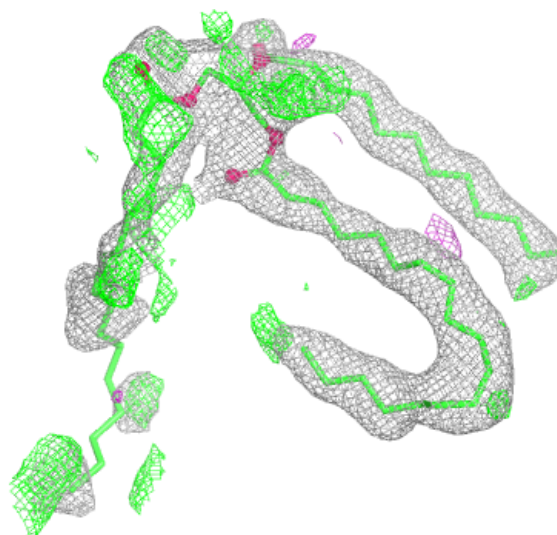
Electron density around CDL P 308:

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



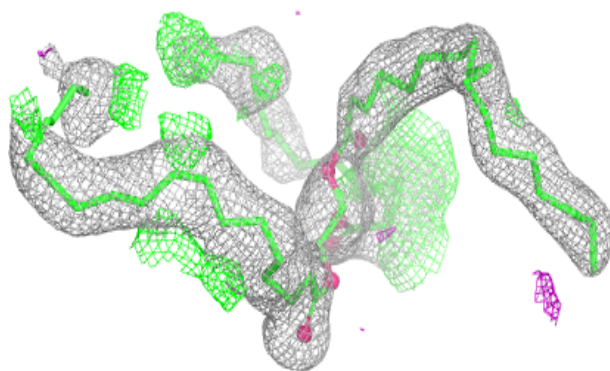
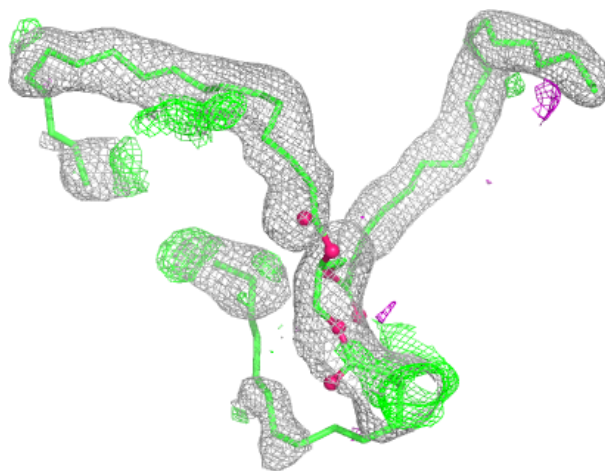
Electron density around TGL D 201:

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



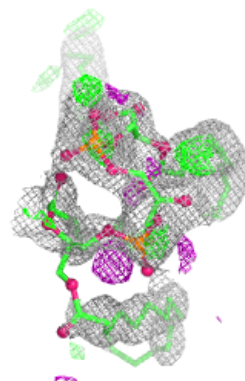
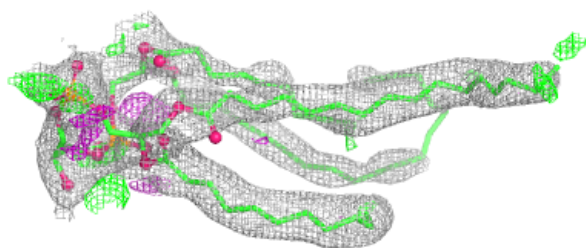
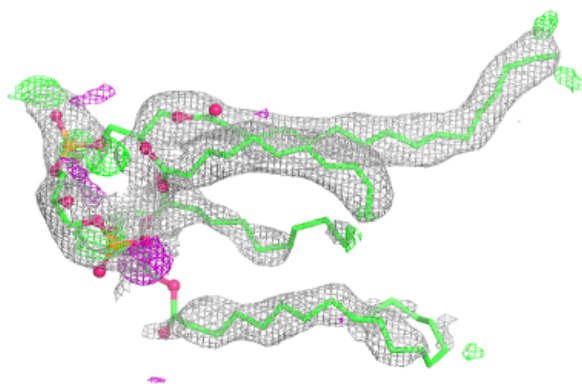
Electron density around TGL Y 101:

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

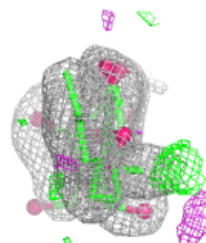
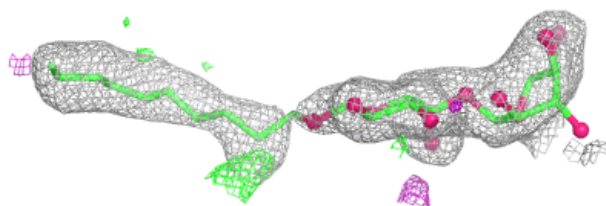
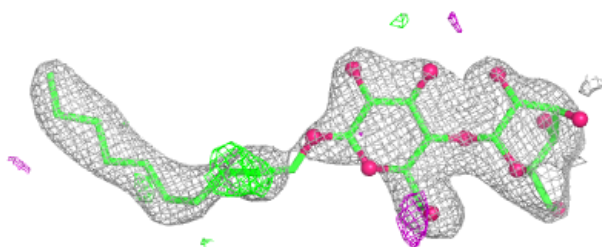


Electron density around CDL C 306:

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

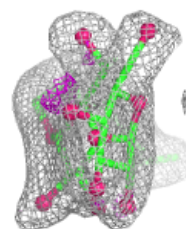
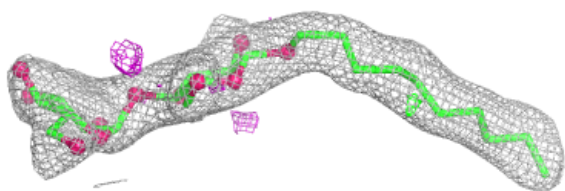
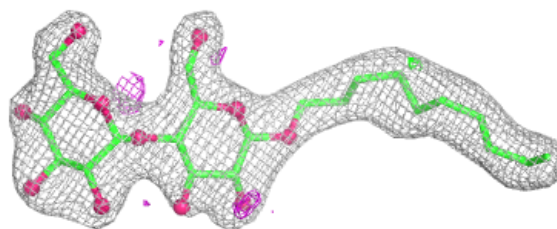
**Electron density around DMU C 314:**

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

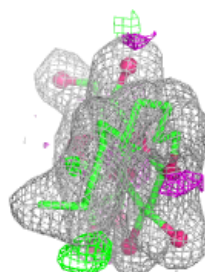
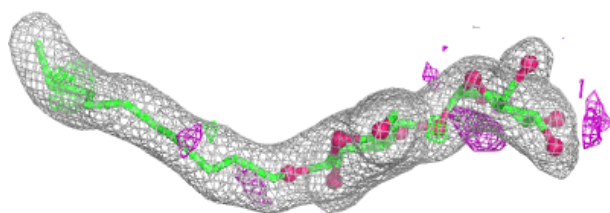
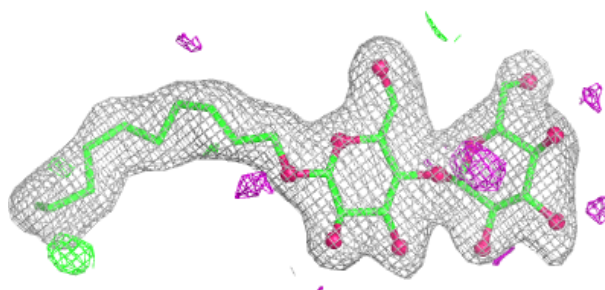


Electron density around DMU Z 102:

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

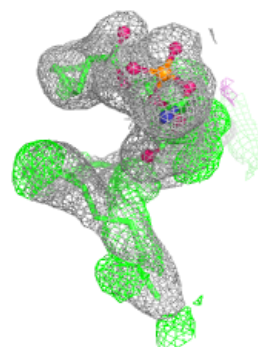
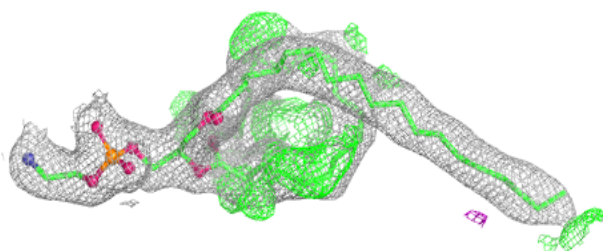
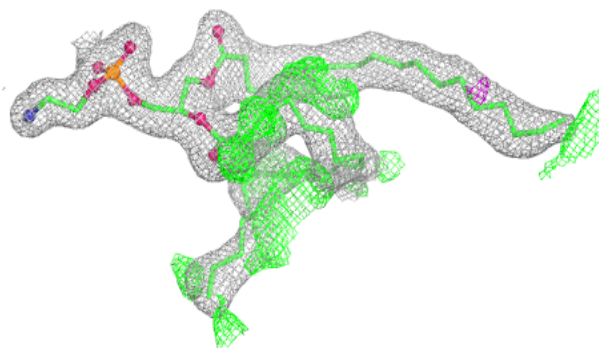
**Electron density around DMU M 101:**

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

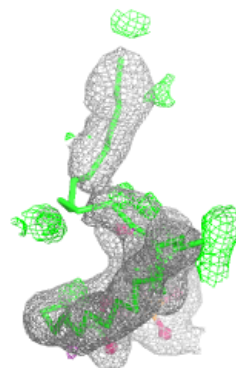
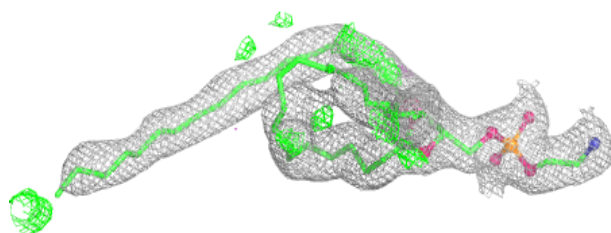
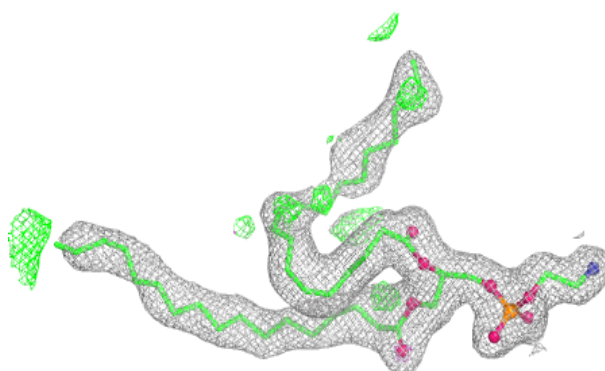


Electron density around PEK C 303:

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

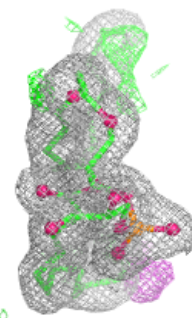
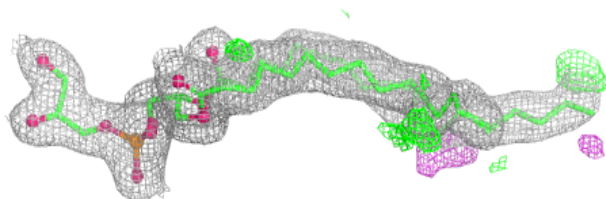
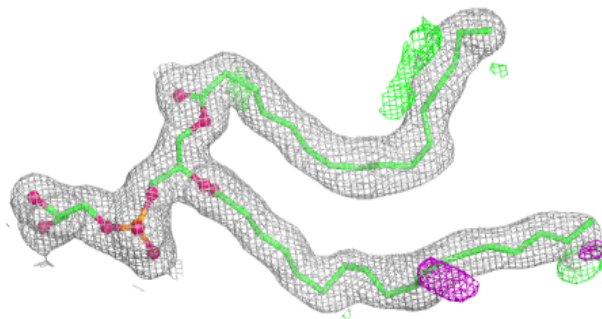
**Electron density around PEK P 305:**

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

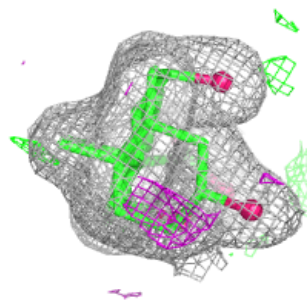
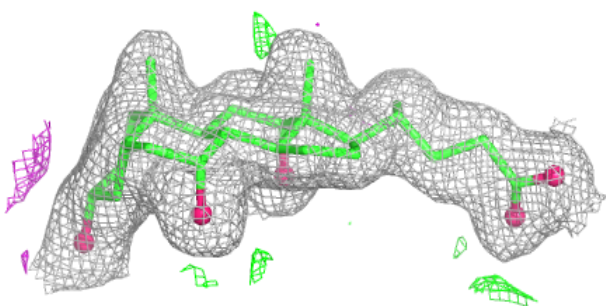
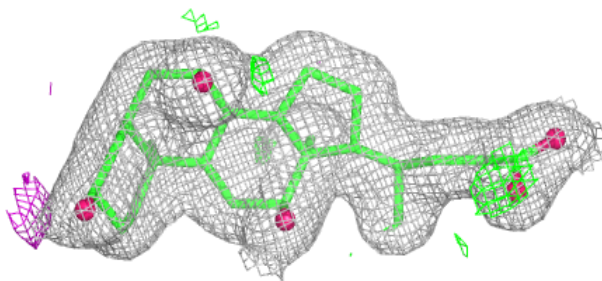


Electron density around PGV N 608:

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

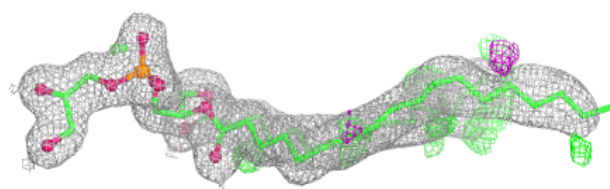
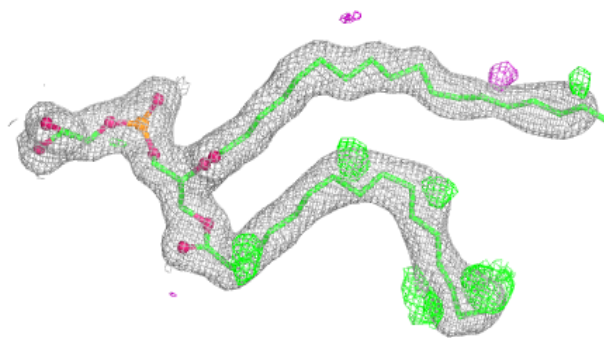
**Electron density around CHD P 304:**

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

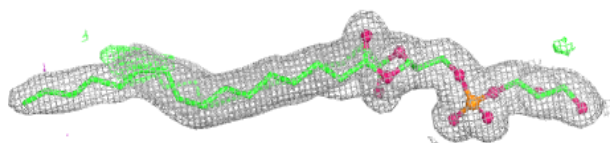
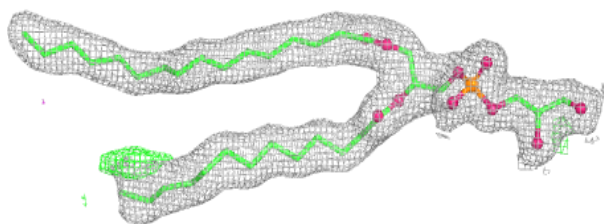


Electron density around PGV A 608:

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

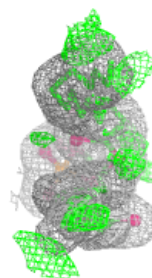
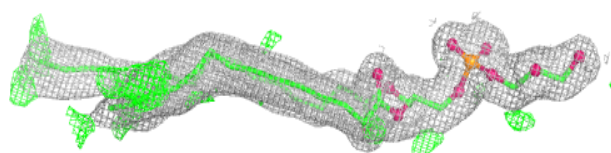
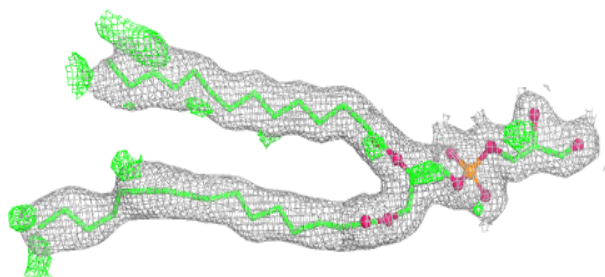
**Electron density around PGV P 307:**

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

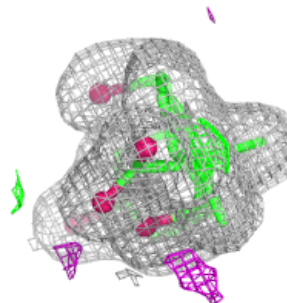
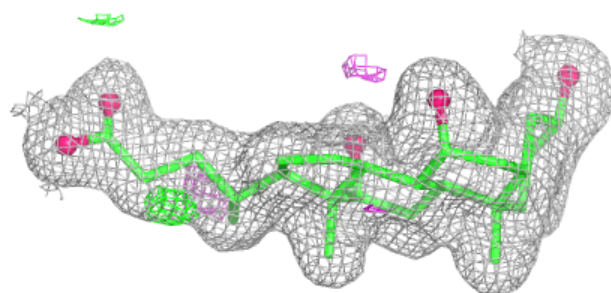
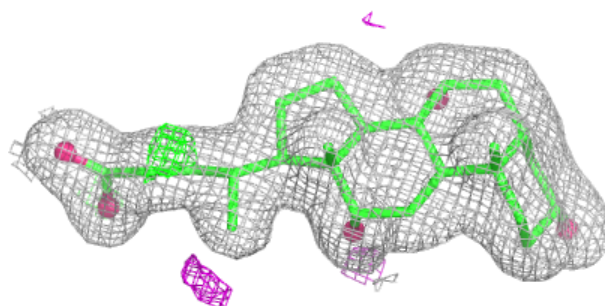


Electron density around PGV C 304:

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

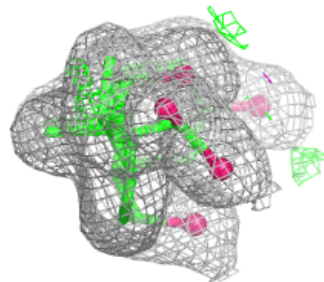
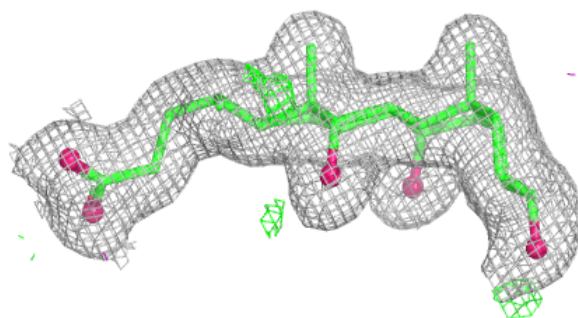
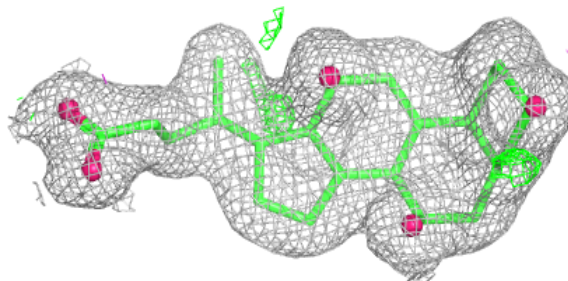
**Electron density around CHD C 301:**

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

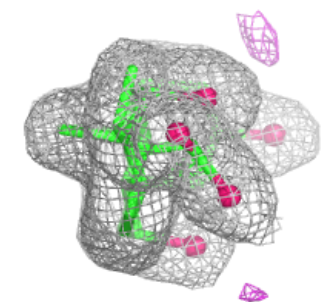
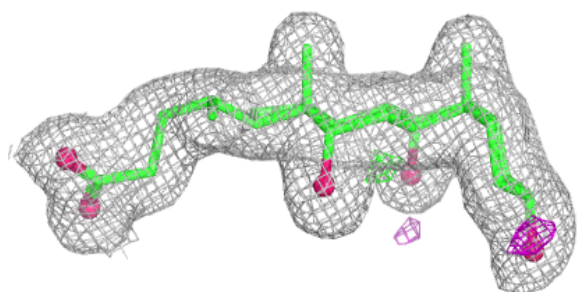
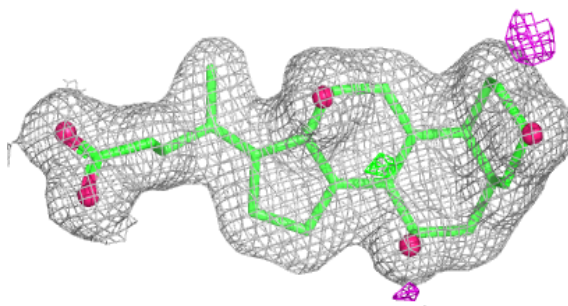


Electron density around CHD O 301:

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

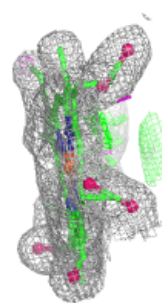
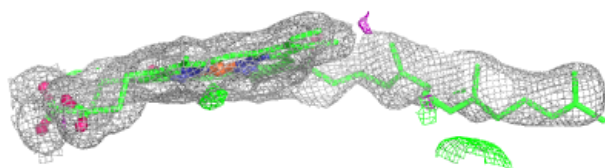
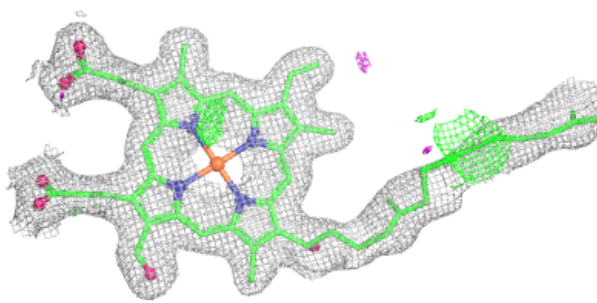
**Electron density around CHD B 304:**

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

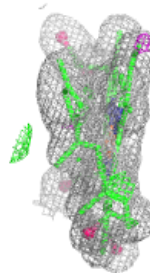
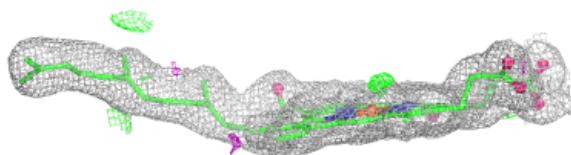
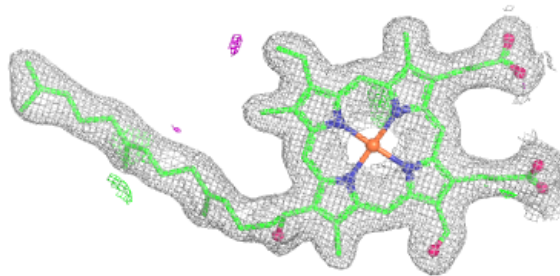


Electron density around HEA N 601 (A):

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

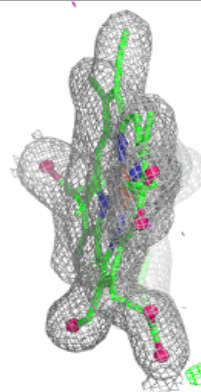
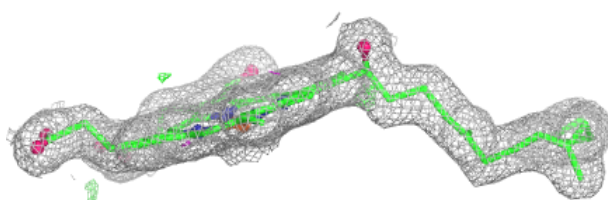
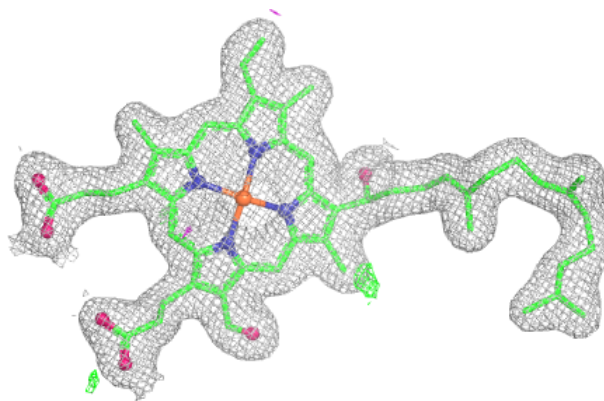
**Electron density around HEA N 601 (B):**

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

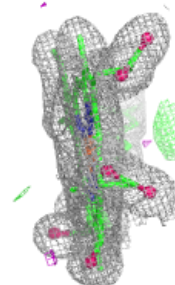
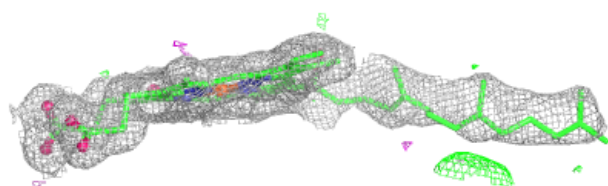
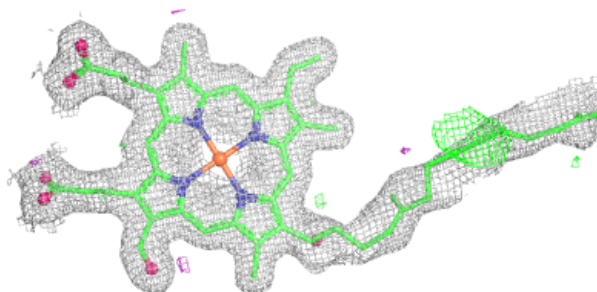


Electron density around HEA N 602:

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

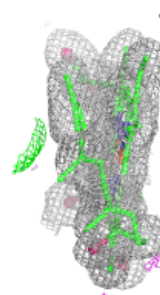
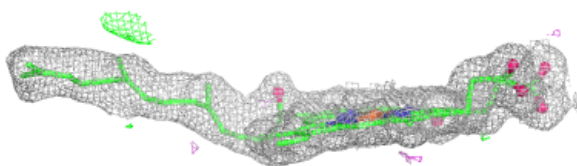
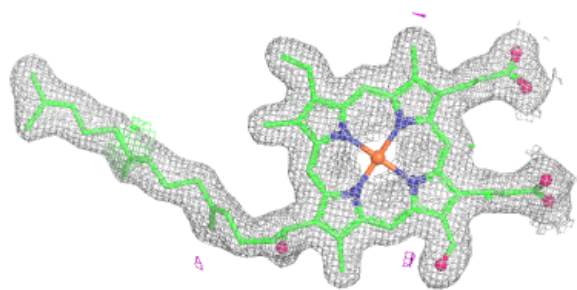
**Electron density around HEA A 601 (A):**

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

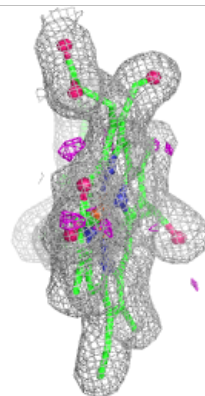
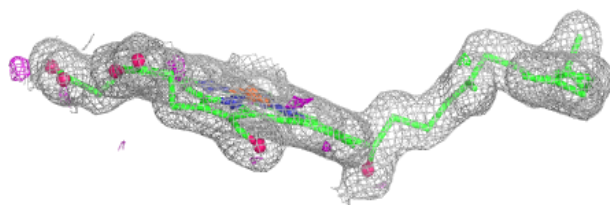
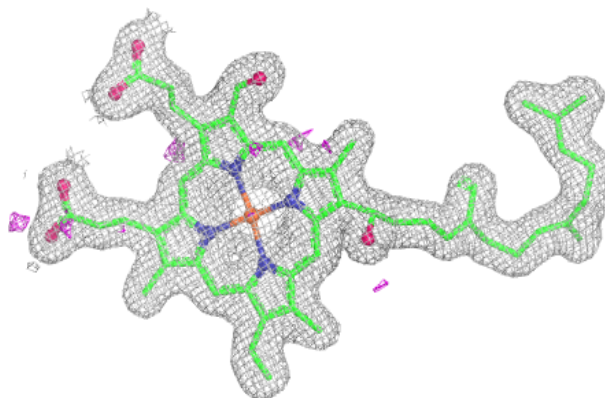


Electron density around HEA A 601 (B):

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

**Electron density around HEA A 602:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.