



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:54 PM UTC

PDB ID : 5B3S / pdb_00005b3s
Title : Bovine heart cytochrome c oxidase in the carbon monoxide-bound mixed-valence state at 1.68 angstrom resolution (50 K)
Authors : Shimada, A.; Shinzawa-Ito, K.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2016-03-11
Resolution : 1.68 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

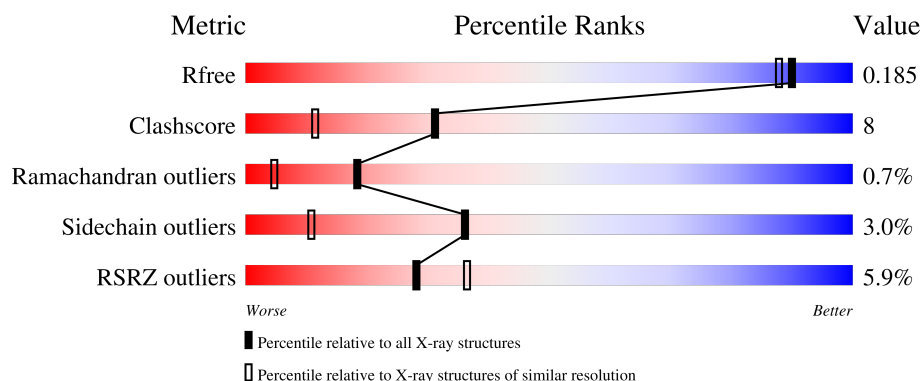
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	88% 11% .
1	N	514	86% 13%
2	B	227	7% 85% 15%
2	O	227	4% 80% 18% .
3	C	259	2% 92% 8%

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Mol	Chain	Length	Quality of chain
3	P	259	
4	D	144	
4	Q	144	
5	E	105	
5	R	105	
6	F	94	
6	S	94	
7	G	84	
7	T	84	
8	H	79	
8	U	79	
9	I	73	
9	V	73	
10	J	58	
10	W	58	
11	K	49	
11	X	49	
12	L	46	
12	Y	46	
13	M	43	
13	Z	43	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	EDO	A	622	-	-	X	-
20	EDO	M	103	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	EDO	N	618	-	-	X	-
20	EDO	U	101	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 34917 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	39	0
			4192	2793	644	712	43			
1	N	514	Total	C	N	O	S	0	36	0
			4182	2787	641	712	42			

- 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	12	0
			1858	1207	283	348	20			
2	O	227	Total	C	N	O	S	0	11	0
			1856	1205	286	346	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	7	0
			2124	1419	337	355	13			
3	P	259	Total	C	N	O	S	0	8	0
			2126	1420	337	355	14			

- 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	2	0
			1207	786	199	218	4			
4	Q	144	Total	C	N	O	S	0	1	0
			1201	780	199	218	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	94	Total	C	N	O	S	0	2	0
			721	446	128	142	5			
6	S	94	Total	C	N	O	S	0	0	0
			716	444	127	140	5			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total 676	C 431	N 129	O 114	P 1	S 1	0	0	0
7	T	84	Total 676	C 431	N 129	O 114	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
			461	297	78	83	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			461	297	78	83	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
			385	250	65	68	2			
11	X	49	Total	C	N	O	S	0	0	0
			385	250	65	68	2			

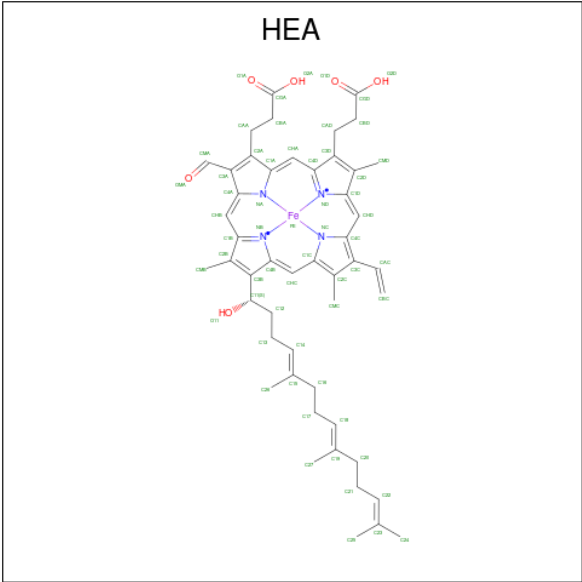
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			382	255	64	60	3			
12	Y	46	Total	C	N	O	S	0	1	0
			382	255	64	60	3			

- 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
			336	223	53	60			

- 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 79	C 67	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 79	C 67	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		

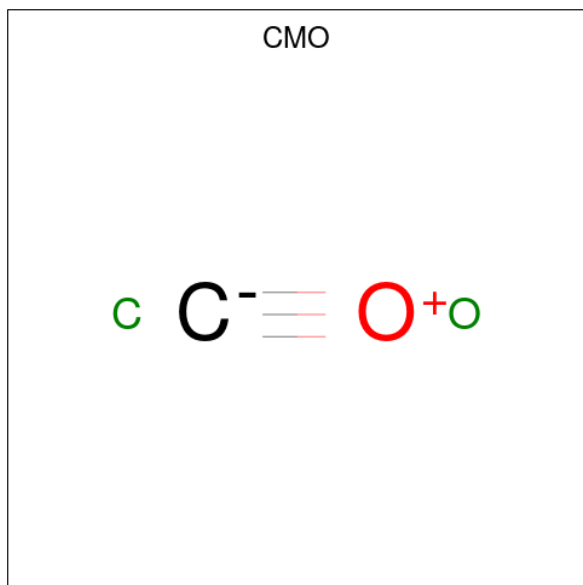
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

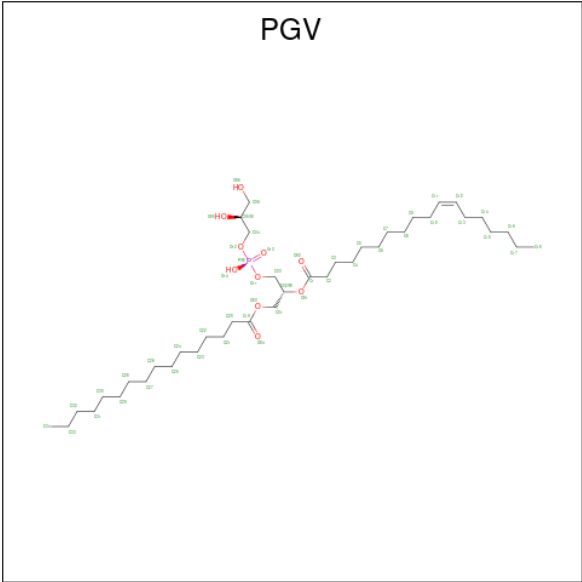
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

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



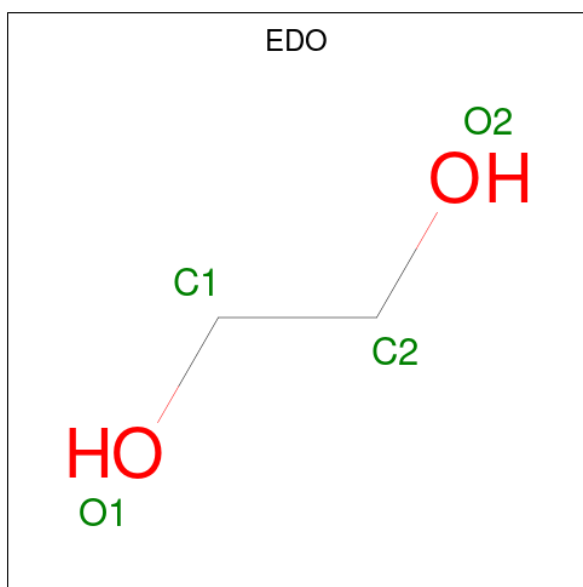
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	1
			4	2	2		
18	N	1	Total	C	O	0	1
			4	2	2		

- 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
			48	37	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			50	39	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	G	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			4	2	2		
20	B	1	Total	C	O	0	0
			4	2	2		
20	B	1	Total	C	O	0	0
			4	2	2		
20	B	1	Total	C	O	0	0
			4	2	2		
20	B	1	Total	C	O	0	0
			4	2	2		
20	C	1	Total	C	O	0	0
			4	2	2		
20	C	1	Total	C	O	0	0
			4	2	2		
20	C	1	Total	C	O	0	0
			4	2	2		
20	C	1	Total	C	O	0	0
			4	2	2		
20	C	1	Total	C	O	0	0
			4	2	2		
20	C	1	Total	C	O	0	0
			4	2	2		
20	C	1	Total	C	O	0	0
			4	2	2		
20	C	1	Total	C	O	0	0
			4	2	2		
20	D	1	Total	C	O	0	0
			4	2	2		
20	D	1	Total	C	O	0	0
			4	2	2		
20	D	1	Total	C	O	0	0
			4	2	2		
20	D	1	Total	C	O	0	0
			4	2	2		
20	E	1	Total	C	O	0	0
			4	2	2		

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

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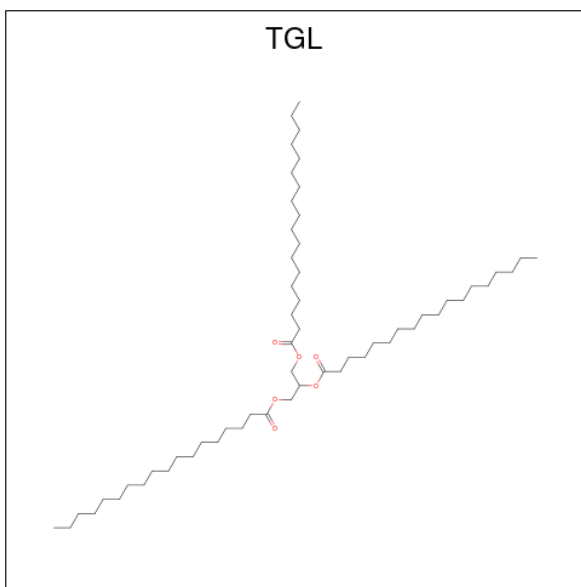
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4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

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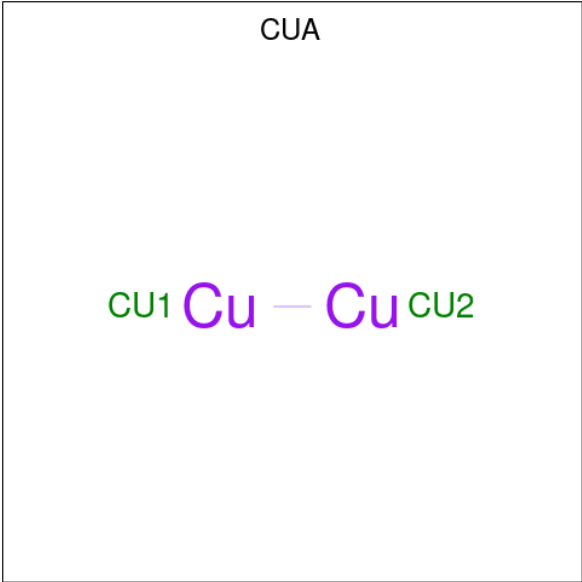
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	Q	1	Total	C	O	0	0
			4	2	2		
20	Q	1	Total	C	O	0	0
			4	2	2		
20	Q	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20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

- Molecule 21 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



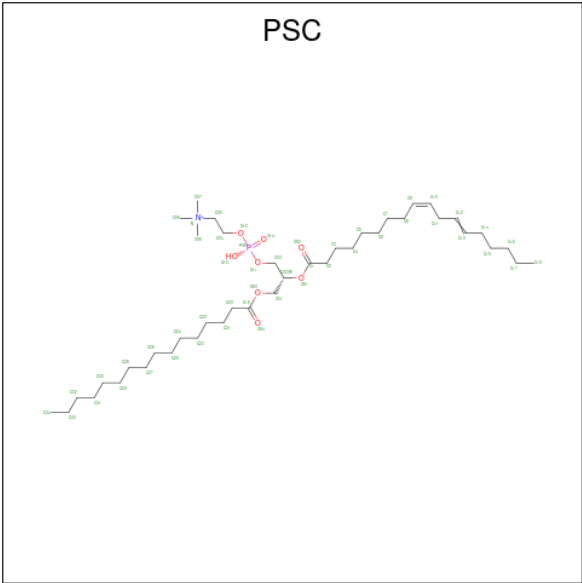
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	B	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			60	54	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			63	57	6		

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



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

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



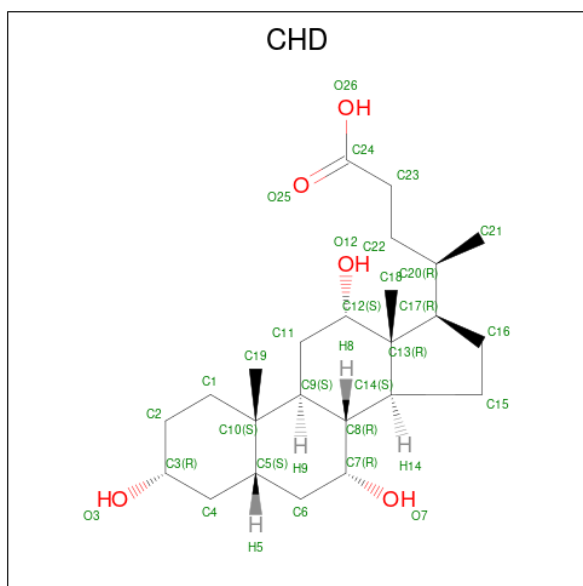
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	O	1	Total	C	O	P	0	0
			46	37	8	1		

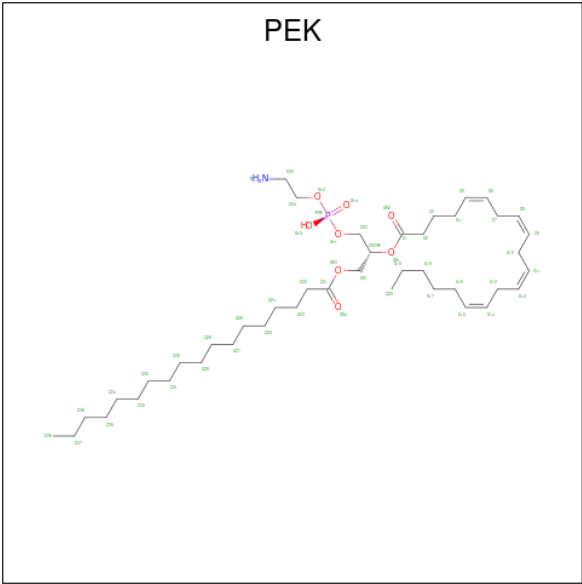
- Molecule 24 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



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

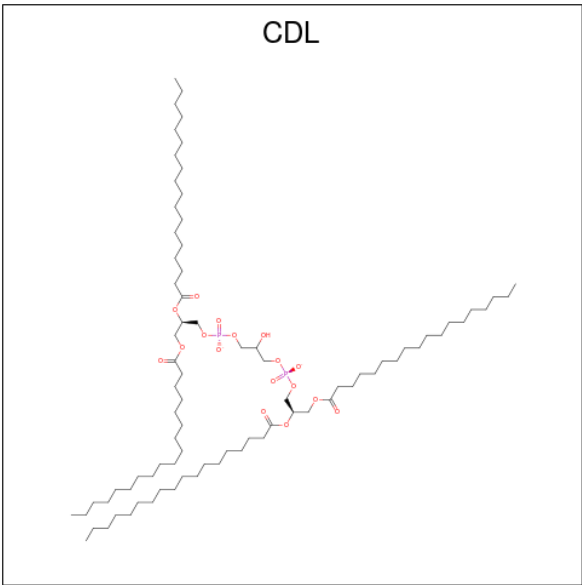
- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE

(CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



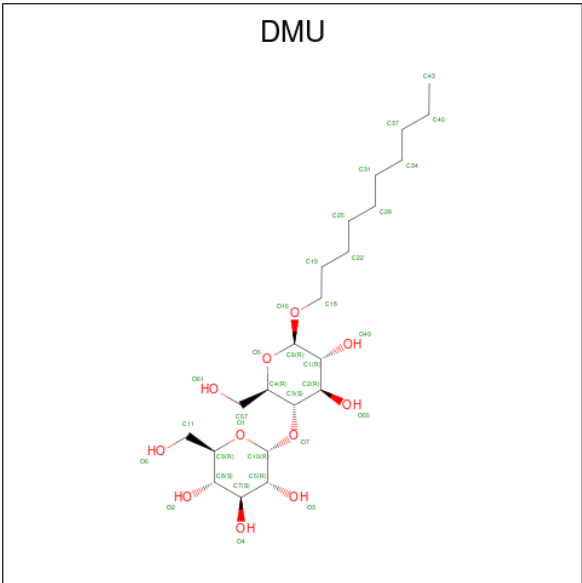
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			48	38	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			92	78	13	1		
26	G	1	Total	C	O	P	0	0
			99	80	17	2		
26	P	1	Total	C	O	P	0	0
			84	72	11	1		
26	T	1	Total	C	O	P	0	0
			96	77	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	0	0
			33	22	11		
27	C	1	Total	C	O	0	0
			33	22	11		
27	G	1	Total	C	O	0	0
			33	22	11		
27	K	1	Total	C	O	0	0
			21	16	5		
27	K	1	Total	C	O	0	0
			22	16	6		
27	K	1	Total	C	O	0	0
			33	22	11		
27	K	1	Total	C	O	0	0
			33	22	11		
27	K	1	Total	C	O	0	0
			33	22	11		
27	K	1	Total	C	O	0	0
			33	22	11		
27	L	1	Total	C	O	0	0
			33	22	11		
27	M	1	Total	C	O	0	0
			33	22	11		
27	M	1	Total	C	O	0	0
			33	22	11		
27	O	1	Total	C	O	0	0
			32	21	11		
27	P	1	Total	C	O	0	0
			33	22	11		
27	P	1	Total	C	O	0	0
			33	22	11		
27	P	1	Total	C	O	0	0
			33	22	11		
27	T	1	Total	C	O	0	0
			22	16	6		
27	X	1	Total	C	O	0	0
			33	22	11		
27	X	1	Total	C	O	0	0
			33	22	11		
27	X	1	Total	C	O	0	0
			22	16	6		
27	X	1	Total	C	O	0	0
			33	22	11		
27	X	1	Total	C	O	0	0
			22	16	6		

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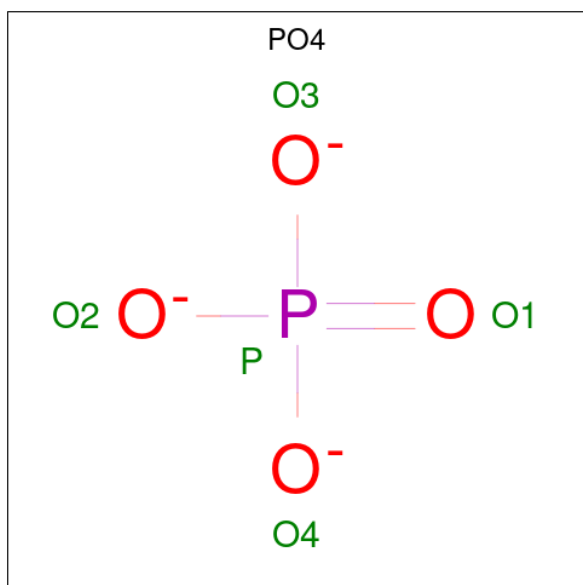
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	Z	1	Total	C	O	0	0
			33	22	11		

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

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

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



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	260	Total	O	0	4
			261	261		
30	B	220	Total	O	0	3
			222	222		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	C	154	Total 154	O 154	0	0
30	D	189	Total 189	O 189	0	0
30	E	145	Total 145	O 145	0	0
30	F	149	Total 149	O 149	0	0
30	G	93	Total 93	O 93	0	0
30	H	92	Total 92	O 92	0	0
30	I	67	Total 67	O 67	0	0
30	J	44	Total 44	O 44	0	0
30	K	41	Total 41	O 41	0	0
30	L	45	Total 45	O 45	0	1
30	M	28	Total 28	O 28	0	0
30	N	263	Total 264	O 264	0	4
30	O	181	Total 183	O 183	0	5
30	P	145	Total 145	O 145	0	0
30	Q	113	Total 113	O 113	0	0
30	R	100	Total 100	O 100	0	0
30	S	135	Total 135	O 135	0	0
30	T	77	Total 77	O 77	0	0
30	U	87	Total 87	O 87	0	0
30	V	62	Total 62	O 62	0	0
30	W	47	Total 47	O 47	0	1

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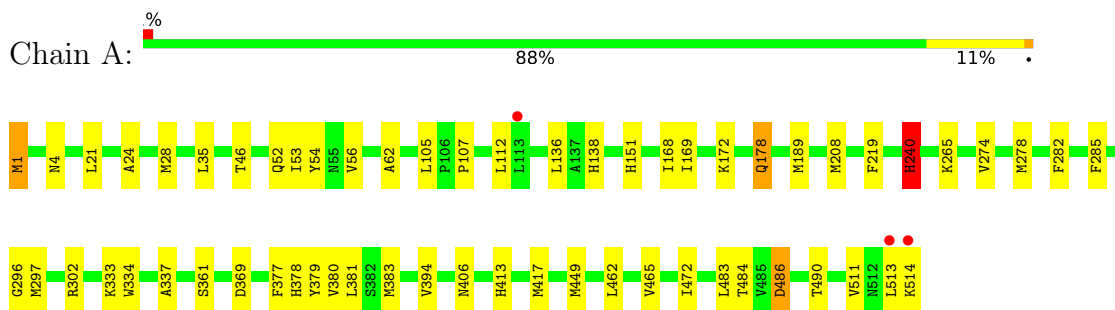
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	29	Total 29	O 29	0	0
30	Y	38	Total 38	O 38	0	1
30	Z	25	Total 25	O 25	0	2

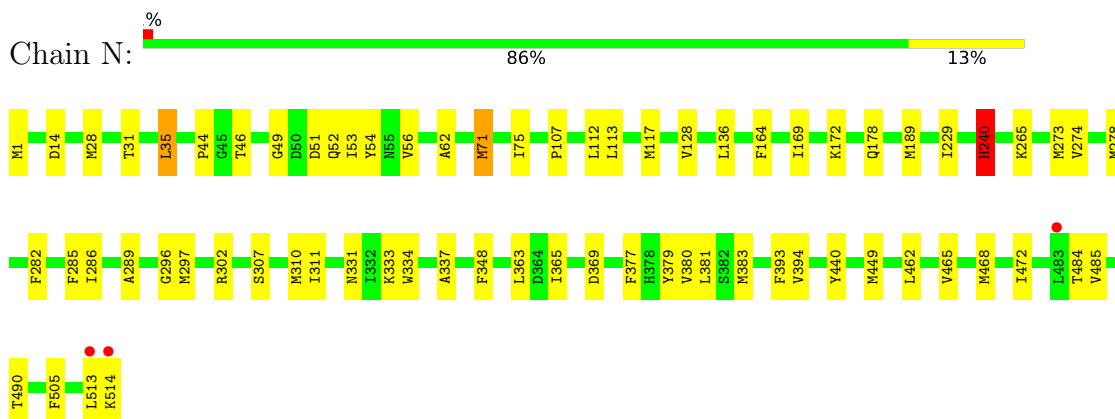
3 Residue-property plots [i](#)

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

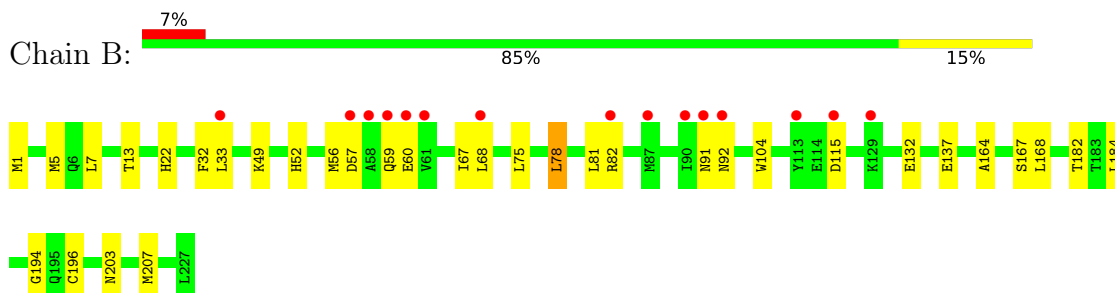
- Molecule 1: Cytochrome c oxidase subunit 1



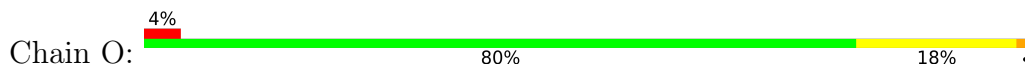
- Molecule 1: Cytochrome c oxidase subunit 1

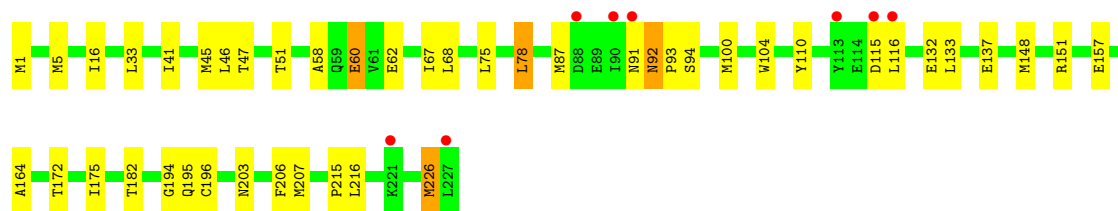


- Molecule 2: Cytochrome c oxidase subunit 2

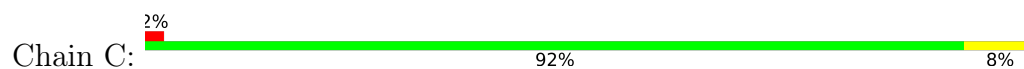


- Molecule 2: Cytochrome c oxidase subunit 2

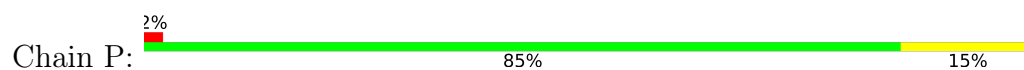




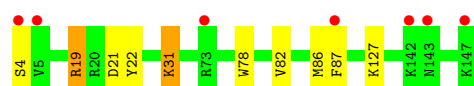
• Molecule 3: Cytochrome c oxidase subunit 3



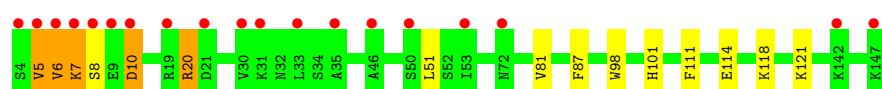
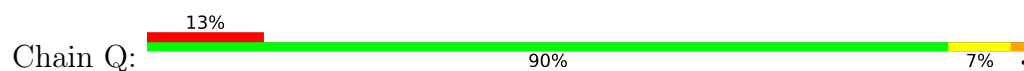
• Molecule 3: Cytochrome c oxidase subunit 3



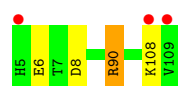
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



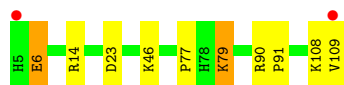
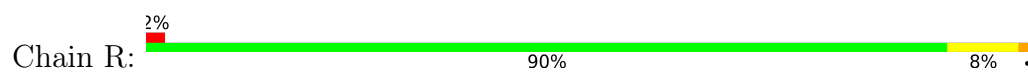
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



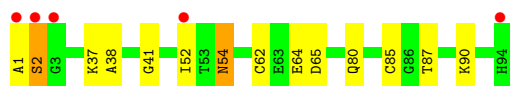
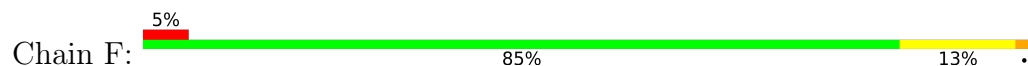
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



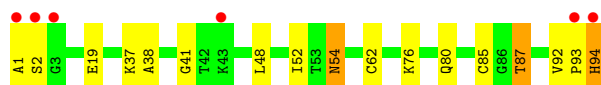
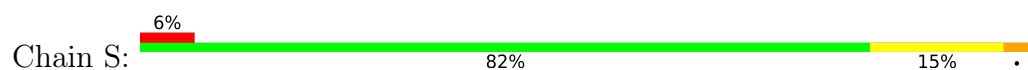
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



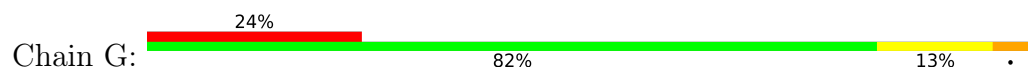
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



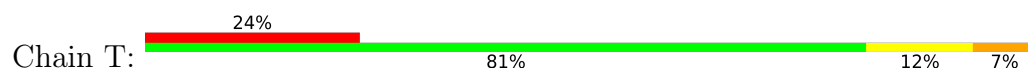
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



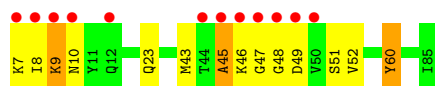
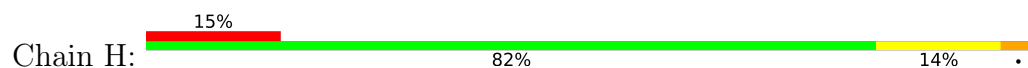
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



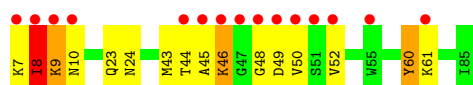
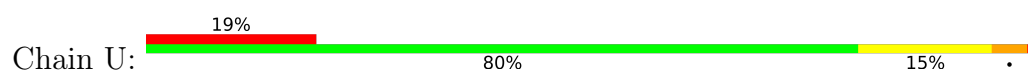
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



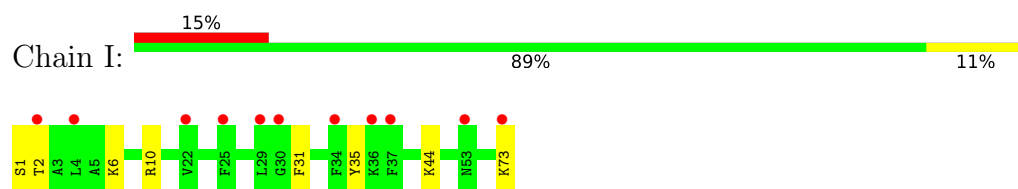
- Molecule 8: Cytochrome c oxidase subunit 6B1



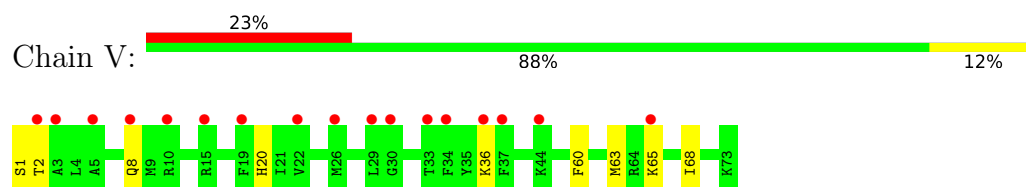
- Molecule 8: Cytochrome c oxidase subunit 6B1



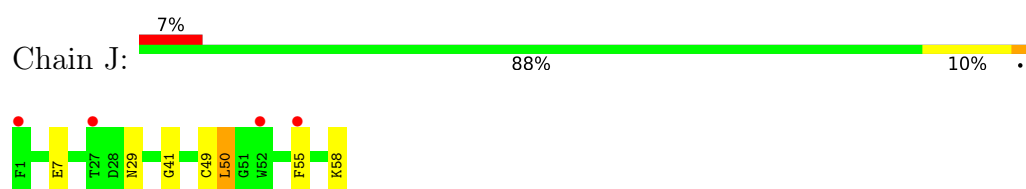
● Molecule 9: Cytochrome c oxidase subunit 6C



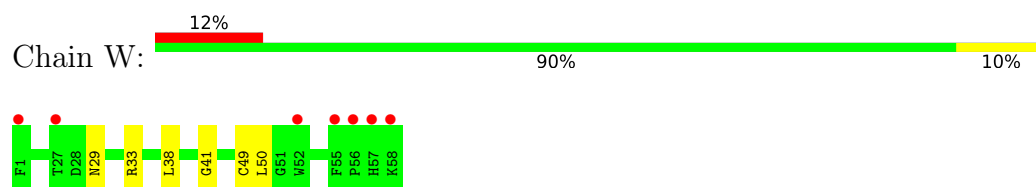
● Molecule 9: Cytochrome c oxidase subunit 6C



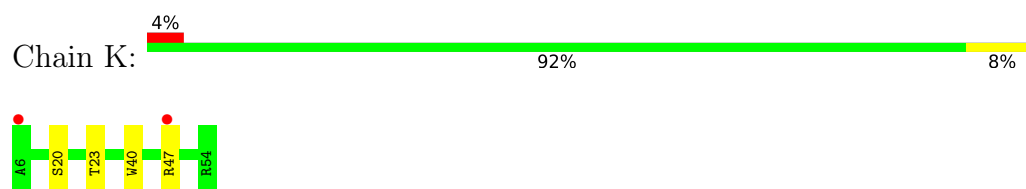
● Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



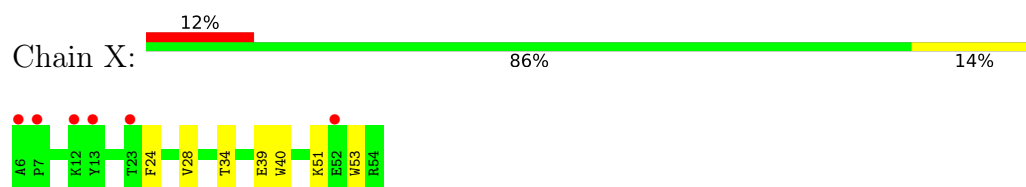
● Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



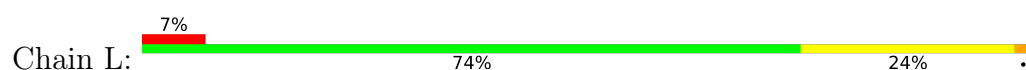
● Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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

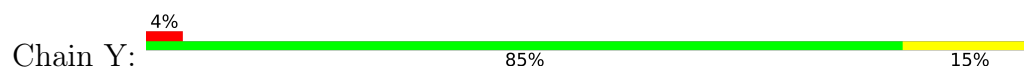


● Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

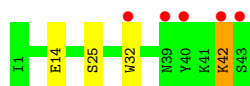




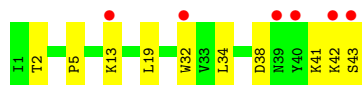
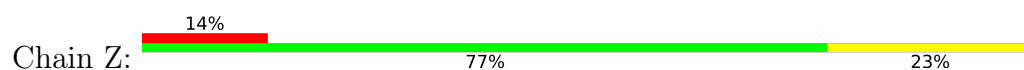
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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	181.49Å 203.30Å 177.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.62 – 1.68 39.62 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.62-1.68) 99.9 (39.62-1.68)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 1.68Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.153 , 0.177 (Not available) , 0.185	Depositor DCC
R_{free} test set	37040 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34917	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.77	0/4460	0.83	3/6086 (0.0%)
1	N	0.73	0/4433	0.80	3/6050 (0.0%)
2	B	0.71	0/1958	0.86	0/2667
2	O	0.63	0/1953	0.79	0/2660
3	C	0.68	0/2251	0.71	1/3077 (0.0%)
3	P	0.67	0/2259	0.72	0/3087
4	D	0.61	0/1252	0.74	0/1688
4	Q	0.47	0/1240	0.65	0/1672
5	E	0.57	0/871	0.65	0/1182
5	R	0.50	0/871	0.62	0/1182
6	F	0.64	0/747	0.81	0/1014
6	S	0.67	0/732	0.82	2/993 (0.2%)
7	G	0.65	0/691	0.81	0/937
7	T	0.59	0/691	0.76	0/937
8	H	0.61	0/682	0.76	0/921
8	U	0.60	0/682	0.76	0/921
9	I	0.53	0/605	0.67	0/802
9	V	0.47	0/605	0.64	0/802
10	J	0.50	0/472	0.60	0/636
10	W	0.46	0/472	0.61	0/636
11	K	0.56	0/399	0.65	0/546
11	X	0.48	0/399	0.60	0/546
12	L	0.63	0/401	0.68	0/536
12	Y	0.53	0/401	0.62	0/536
13	M	0.64	0/345	0.69	0/470
13	Z	0.51	0/346	0.62	0/470
All	All	0.65	0/30218	0.75	9/41054 (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
4	Q	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	71	MET	CG-SD-CE	-8.77	81.61	100.90
1	N	240	HIS	CA-CB-CG	-7.75	106.05	113.80
1	A	240	HIS	CA-CB-CG	-7.47	106.33	113.80
1	N	310	MET	CG-SD-CE	-6.07	87.56	100.90
1	A	511	VAL	CA-C-N	-5.57	113.04	122.67

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
4	Q	8	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4192	0	4170	68	0
1	N	4182	0	4161	76	0
2	B	1858	0	1867	25	0
2	O	1856	0	1863	31	0
3	C	2124	0	2032	19	0
3	P	2126	0	2033	37	0
4	D	1207	0	1197	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	1201	0	1192	15	0
5	E	852	0	845	2	0
5	R	852	0	845	5	0
6	F	721	0	702	11	0
6	S	716	0	697	15	0
7	G	676	0	644	12	0
7	T	676	0	643	19	0
8	H	662	0	623	16	0
8	U	662	0	623	16	0
9	I	601	0	613	9	0
9	V	601	0	613	3	0
10	J	461	0	459	9	0
10	W	461	0	459	7	0
11	K	385	0	366	4	0
11	X	385	0	366	7	0
12	L	382	0	381	19	0
12	Y	382	0	381	7	0
13	M	335	0	352	8	0
13	Z	336	0	352	8	0
14	A	139	0	111	7	0
14	N	139	0	111	6	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	4	0	0	0	0
18	N	4	0	0	0	0
19	A	99	0	143	4	0
19	C	101	0	147	5	0
19	G	51	0	76	7	0
19	N	102	0	152	6	0
19	P	51	0	76	3	0
20	A	56	0	84	10	0
20	B	24	0	36	2	0
20	C	36	0	54	1	0
20	D	20	0	30	1	0
20	E	12	0	18	0	0
20	F	20	0	30	1	0
20	G	8	0	12	0	0
20	I	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	J	8	0	12	1	0
20	L	4	0	6	3	0
20	M	16	0	24	6	0
20	N	68	0	102	15	0
20	O	16	0	24	0	0
20	P	24	0	36	0	0
20	Q	12	0	18	1	0
20	R	8	0	12	1	0
20	S	20	0	30	1	0
20	T	8	0	12	0	0
20	U	4	0	6	4	0
20	V	4	0	5	2	0
20	Y	4	0	6	0	0
21	B	126	0	220	18	0
21	L	60	0	101	13	0
21	N	63	0	110	2	0
21	Q	63	0	110	6	0
21	Y	63	0	110	9	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	51	0	75	13	0
23	O	46	0	62	4	0
24	C	29	0	39	0	0
24	G	29	0	39	0	0
24	J	58	0	78	3	0
24	P	58	0	78	2	0
24	T	29	0	39	0	0
24	W	29	0	38	1	0
24	Y	29	0	39	1	0
25	C	106	0	154	11	0
25	P	146	0	202	12	0
25	T	44	0	56	4	0
26	C	92	0	149	3	0
26	G	99	0	151	20	0
26	P	84	0	130	10	0
26	T	96	0	142	16	0
27	C	66	0	84	10	0
27	G	33	0	42	7	0
27	K	175	0	229	7	0
27	L	33	0	42	7	0
27	M	66	0	84	2	0
27	O	32	0	37	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	P	99	0	126	17	0
27	T	22	0	31	1	0
27	X	143	0	188	10	0
27	Z	33	0	42	3	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	261	0	0	17	0
30	B	222	0	0	3	0
30	C	154	0	0	4	0
30	D	189	0	0	2	0
30	E	145	0	0	1	0
30	F	149	0	0	6	0
30	G	93	0	0	3	0
30	H	92	0	0	2	0
30	I	67	0	0	4	0
30	J	44	0	0	1	0
30	K	41	0	0	0	0
30	L	45	0	0	4	0
30	M	28	0	0	0	0
30	N	264	0	0	12	0
30	O	183	0	0	6	0
30	P	145	0	0	4	0
30	Q	113	0	0	1	0
30	R	100	0	0	1	0
30	S	135	0	0	6	0
30	T	77	0	0	5	0
30	U	87	0	0	1	0
30	V	62	0	0	2	0
30	W	47	0	0	0	0
30	X	29	0	0	1	0
30	Y	38	0	0	1	0
30	Z	25	0	0	0	0
All	All	34917	0	32885	533	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 533 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)
30:N:911:HOH:O	2:O:87:MET:SD	2.25	0.94
8:U:24:ASN:HD21	20:U:101:EDO:H21	1.32	0.92
3:C:33:MET:HE2	27:C:308:DMU:H8	1.57	0.87
7:T:37:LEU:HD23	26:T:103:CDL:H371	1.56	0.87
12:L:20:ARG:HH22	21:L:101:TGL:HC61	1.39	0.85

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	552/514 (107%)	539 (98%)	13 (2%)	0	100	100
1	N	549/514 (107%)	535 (97%)	14 (3%)	0	100	100
2	B	237/227 (104%)	232 (98%)	4 (2%)	1 (0%)	30	13
2	O	236/227 (104%)	229 (97%)	6 (2%)	1 (0%)	30	13
3	C	264/259 (102%)	259 (98%)	5 (2%)	0	100	100
3	P	265/259 (102%)	260 (98%)	5 (2%)	0	100	100
4	D	144/144 (100%)	140 (97%)	4 (3%)	0	100	100
4	Q	143/144 (99%)	136 (95%)	5 (4%)	2 (1%)	9	1
5	E	103/105 (98%)	102 (99%)	0	1 (1%)	12	2
5	R	103/105 (98%)	102 (99%)	0	1 (1%)	12	2
6	F	94/94 (100%)	92 (98%)	1 (1%)	1 (1%)	11	1
6	S	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
7	G	81/84 (96%)	72 (89%)	4 (5%)	5 (6%)	1	0
7	T	81/84 (96%)	72 (89%)	5 (6%)	4 (5%)	1	0
8	H	77/79 (98%)	71 (92%)	2 (3%)	4 (5%)	1	0
8	U	77/79 (98%)	69 (90%)	6 (8%)	2 (3%)	4	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	1 (1%)	1 (1%)	9	1
10	J	56/58 (97%)	56 (100%)	0	0	100	100
10	W	56/58 (97%)	56 (100%)	0	0	100	100
11	K	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	45/46 (98%)	44 (98%)	1 (2%)	0	100	100
12	Y	45/46 (98%)	44 (98%)	1 (2%)	0	100	100
13	M	41/43 (95%)	41 (100%)	0	0	100	100
13	Z	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
All	All	3618/3550 (102%)	3513 (97%)	82 (2%)	23 (1%)	18	7

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
7	G	4	ALA
7	G	8	HIS
7	T	5	LYS
8	U	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	463/426 (109%)	456 (98%)	7 (2%)	57	34
1	N	460/426 (108%)	453 (98%)	7 (2%)	57	34
2	B	222/210 (106%)	211 (95%)	11 (5%)	22	3
2	O	221/210 (105%)	210 (95%)	11 (5%)	22	3
3	C	231/224 (103%)	228 (99%)	3 (1%)	61	39
3	P	232/224 (104%)	229 (99%)	3 (1%)	61	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	130/128 (102%)	127 (98%)	3 (2%)	44	18
4	Q	129/128 (101%)	125 (97%)	4 (3%)	35	10
5	E	92/92 (100%)	90 (98%)	2 (2%)	45	19
5	R	92/92 (100%)	87 (95%)	5 (5%)	20	2
6	F	80/78 (103%)	76 (95%)	4 (5%)	22	3
6	S	78/78 (100%)	71 (91%)	7 (9%)	9	0
7	G	67/67 (100%)	63 (94%)	4 (6%)	17	2
7	T	67/67 (100%)	63 (94%)	4 (6%)	17	2
8	H	71/71 (100%)	69 (97%)	2 (3%)	38	12
8	U	71/71 (100%)	65 (92%)	6 (8%)	10	1
9	I	57/57 (100%)	56 (98%)	1 (2%)	51	27
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	2
10	J	49/49 (100%)	47 (96%)	2 (4%)	27	5
10	W	49/49 (100%)	48 (98%)	1 (2%)	48	23
11	K	39/39 (100%)	38 (97%)	1 (3%)	40	15
11	X	39/39 (100%)	38 (97%)	1 (3%)	40	15
12	L	40/39 (103%)	39 (98%)	1 (2%)	42	16
12	Y	40/39 (103%)	38 (95%)	2 (5%)	22	3
13	M	37/37 (100%)	36 (97%)	1 (3%)	39	13
13	Z	37/37 (100%)	33 (89%)	4 (11%)	6	0
All	All	3150/3034 (104%)	3050 (97%)	100 (3%)	36	9

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	110	TYR
5	R	109	VAL
13	Z	42	LYS
2	O	226	MET
4	Q	20	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
6	S	54	ASN
8	U	37	HIS
7	T	8	HIS
8	U	25	GLN
11	X	35	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	FME	N	1	1	8,9,10	0.53	0	8,9,11	1.18	1 (12%)
1	FME	A	1	1	8,9,10	0.61	0	8,9,11	1.53	3 (37%)
2	FME	B	1	2	8,9,10	0.91	0	8,9,11	1.46	1 (12%)
2	FME	O	1	2	8,9,10	0.81	0	8,9,11	1.06	0
9	SAC	I	1	9	7,8,9	0.68	0	7,9,11	0.89	1 (14%)
9	SAC	V	1	9	7,8,9	0.59	0	7,9,11	1.39	2 (28%)
7	TPO	T	11	7	8,10,11	1.38	1 (12%)	10,14,16	1.15	2 (20%)
7	TPO	G	11	7	8,10,11	1.37	1 (12%)	10,14,16	1.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	N	1	1	-	2/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	2.88	1.59	1.50
7	G	11	TPO	P-O1P	2.83	1.59	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-2.87	104.08	112.87
7	T	11	TPO	O3P-P-OG1	2.39	115.15	105.85
7	T	11	TPO	CG2-CB-CA	2.32	117.78	113.26
9	V	1	SAC	O-C-CA	-2.32	118.81	124.77
9	V	1	SAC	C-CA-N	2.23	113.79	109.50

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	3	0
2	O	1	FME	1	0
7	T	11	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 176 ligands modelled in this entry, 8 are monoatomic - leaving 168 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
27	DMU	X	202	-	34,34,34	0.64	1 (2%)	45,45,45	2.40	14 (31%)
20	EDO	N	625	-	3,3,3	0.59	0	2,2,2	0.51	0
14	HEA	N	601[C]	-	67,57,67	1.82	12 (17%)	81,89,103	2.31	32 (39%)
20	EDO	N	622	-	3,3,3	0.60	0	2,2,2	0.16	0
26	CDL	P	306	-	79,82,99	1.59	13 (16%)	82,87,111	1.59	11 (13%)
19	PGV	C	304	-	49,49,50	0.71	1 (2%)	52,55,56	0.88	1 (1%)
20	EDO	G	105	-	3,3,3	0.72	0	2,2,2	0.59	0
14	HEA	A	602	1	67,67,67	1.69	16 (23%)	81,103,103	1.89	25 (30%)
25	PEK	P	303	-	44,44,52	0.77	1 (2%)	47,49,57	1.31	5 (10%)
21	TGL	B	304	-	62,62,62	1.06	3 (4%)	65,65,65	1.27	10 (15%)
27	DMU	M	101	-	34,34,34	0.60	1 (2%)	45,45,45	1.12	3 (6%)
27	DMU	Z	101	-	34,34,34	0.48	0	45,45,45	1.64	9 (20%)
27	DMU	K	101	-	21,21,34	0.52	0	24,25,45	1.27	3 (12%)
25	PEK	P	304	-	52,52,52	1.08	2 (3%)	55,57,57	1.47	8 (14%)
27	DMU	K	102	-	22,22,34	0.50	0	27,27,45	1.39	5 (18%)
20	EDO	B	307	-	3,3,3	0.74	0	2,2,2	0.14	0
20	EDO	P	312	-	3,3,3	0.53	0	2,2,2	0.10	0
20	EDO	I	101	-	3,3,3	0.54	0	2,2,2	1.01	0
20	EDO	N	613	-	3,3,3	0.77	0	2,2,2	0.47	0
21	TGL	L	101	-	59,59,62	1.17	3 (5%)	62,62,65	1.45	10 (16%)
23	PSC	O	302	-	45,45,51	1.24	3 (6%)	48,50,59	1.87	8 (16%)
20	EDO	E	201	-	3,3,3	0.39	0	2,2,2	0.40	0
20	EDO	C	312	-	3,3,3	0.77	0	2,2,2	0.20	0
19	PGV	A	607	-	47,47,50	1.06	2 (4%)	50,53,56	1.09	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	O	307	-	3,3,3	0.56	0	2,2,2	0.15	0
20	EDO	J	103	-	3,3,3	0.61	0	2,2,2	0.09	0
20	EDO	R	202	-	3,3,3	0.57	0	2,2,2	0.49	0
20	EDO	S	102	-	3,3,3	0.76	0	2,2,2	0.52	0
24	CHD	P	308	-	32,32,32	0.82	1 (3%)	51,51,51	1.89	15 (29%)
20	EDO	Q	202	-	3,3,3	0.40	0	2,2,2	0.32	0
20	EDO	S	105	-	3,3,3	0.63	0	2,2,2	0.07	0
24	CHD	J	101	-	32,32,32	0.63	0	51,51,51	1.48	11 (21%)
27	DMU	G	102	-	34,34,34	0.77	1 (2%)	45,45,45	2.09	13 (28%)
20	EDO	S	106	-	3,3,3	0.39	0	2,2,2	0.78	0
20	EDO	C	317	-	3,3,3	0.49	0	2,2,2	0.41	0
20	EDO	R	201	-	3,3,3	0.30	0	2,2,2	1.08	0
21	TGL	N	608	-	62,62,62	1.05	3 (4%)	65,65,65	1.26	5 (7%)
27	DMU	P	309	-	34,34,34	0.80	1 (2%)	45,45,45	2.08	17 (37%)
20	EDO	F	105	-	3,3,3	0.78	0	2,2,2	0.36	0
20	EDO	O	304	-	3,3,3	0.80	0	2,2,2	0.59	0
24	CHD	Y	101	-	32,32,32	0.71	0	51,51,51	2.17	16 (31%)
18	CMO	N	606[A]	-	0,1,1	-	-	-	-	-
20	EDO	A	610	-	3,3,3	0.97	0	2,2,2	0.45	0
20	EDO	P	313	-	3,3,3	0.40	0	2,2,2	1.13	0
20	EDO	P	311	-	3,3,3	0.48	0	2,2,2	0.29	0
20	EDO	U	101	-	3,3,3	0.63	0	2,2,2	0.39	0
24	CHD	J	102	-	32,32,32	0.73	0	51,51,51	1.87	13 (25%)
20	EDO	M	104	-	3,3,3	0.33	0	2,2,2	0.49	0
20	EDO	C	313	-	3,3,3	0.52	0	2,2,2	0.59	0
20	EDO	Y	103	-	3,3,3	0.56	0	2,2,2	0.30	0
20	EDO	E	202	-	3,3,3	0.53	0	2,2,2	0.35	0
20	EDO	G	106	-	3,3,3	0.73	0	2,2,2	0.84	0
20	EDO	N	626	-	3,3,3	0.47	0	2,2,2	0.26	0
29	PO4	H	101	-	4,4,4	0.81	0	6,6,6	0.56	0
20	EDO	P	315	-	3,3,3	0.48	0	2,2,2	0.43	0
20	EDO	M	103	-	3,3,3	0.39	0	2,2,2	0.70	0
14	HEA	A	601[A]	-	67,67,67	1.72	18 (26%)	81,103,103	1.88	28 (34%)
19	PGV	A	608	-	50,50,50	0.86	3 (6%)	53,56,56	1.15	3 (5%)
20	EDO	V	101	-	3,3,3	0.61	0	2,2,2	1.23	0
20	EDO	C	311	-	3,3,3	0.40	0	2,2,2	0.68	0
20	EDO	N	610	-	3,3,3	0.45	0	2,2,2	0.50	0
19	PGV	G	104	-	50,50,50	1.15	2 (4%)	53,56,56	1.36	6 (11%)
20	EDO	T	105	-	3,3,3	0.70	0	2,2,2	0.85	0
20	EDO	D	202	-	3,3,3	0.45	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	DMU	C	308	-	34,34,34	0.65	1 (2%)	45,45,45	1.80	9 (20%)
20	EDO	A	617	-	3,3,3	0.20	0	2,2,2	1.08	0
20	EDO	A	620	-	3,3,3	0.68	0	2,2,2	0.18	0
20	EDO	D	204	-	3,3,3	0.75	0	2,2,2	0.45	0
20	EDO	C	316	-	3,3,3	0.47	0	2,2,2	0.20	0
27	DMU	K	104	-	34,34,34	0.65	1 (2%)	45,45,45	1.31	5 (11%)
14	HEA	N	601[A]	-	67,67,67	1.55	12 (17%)	81,103,103	1.86	25 (30%)
20	EDO	A	618	-	3,3,3	0.81	0	2,2,2	0.76	0
20	EDO	L	103	-	3,3,3	0.65	0	2,2,2	0.44	0
20	EDO	B	309	-	3,3,3	0.69	0	2,2,2	0.63	0
27	DMU	K	103	-	34,34,34	0.53	0	45,45,45	1.14	3 (6%)
14	HEA	N	602	1	67,67,67	1.88	24 (35%)	81,103,103	1.72	21 (25%)
20	EDO	N	624	-	3,3,3	0.77	0	2,2,2	0.25	0
18	CMO	A	606[A]	-	0,1,1	-	-	-	-	-
20	EDO	N	619	-	3,3,3	0.28	0	2,2,2	0.91	0
24	CHD	T	101	-	32,32,32	0.95	1 (3%)	51,51,51	1.39	9 (17%)
24	CHD	P	301	-	32,32,32	0.97	1 (3%)	51,51,51	1.25	5 (9%)
27	DMU	K	106	-	34,34,34	1.06	2 (5%)	45,45,45	1.73	14 (31%)
20	EDO	C	310	-	3,3,3	0.31	0	2,2,2	1.17	0
20	EDO	N	611	-	3,3,3	0.78	0	2,2,2	0.55	0
20	EDO	C	309	-	3,3,3	0.70	0	2,2,2	0.13	0
19	PGV	C	305	-	50,50,50	1.27	2 (4%)	53,56,56	1.80	9 (16%)
27	DMU	X	203	-	22,22,34	0.62	0	27,27,45	1.31	4 (14%)
27	DMU	X	205	-	22,22,34	0.71	1 (4%)	27,27,45	0.68	0
20	EDO	A	614	-	3,3,3	0.38	0	2,2,2	0.53	0
21	TGL	Y	102	-	62,62,62	1.09	3 (4%)	65,65,65	1.26	7 (10%)
25	PEK	C	302	-	52,52,52	0.86	2 (3%)	55,57,57	1.19	4 (7%)
19	PGV	P	305	-	50,50,50	0.66	2 (4%)	53,56,56	1.19	5 (9%)
20	EDO	A	615	-	3,3,3	0.54	0	2,2,2	0.08	0
20	EDO	B	308	-	3,3,3	0.74	0	2,2,2	0.33	0
20	EDO	N	618	-	3,3,3	0.74	0	2,2,2	0.43	0
20	EDO	S	104	-	3,3,3	0.58	0	2,2,2	0.05	0
20	EDO	A	619	-	3,3,3	0.56	0	2,2,2	0.33	0
20	EDO	N	615	-	3,3,3	0.60	0	2,2,2	0.53	0
20	EDO	A	611	-	3,3,3	0.71	0	2,2,2	0.58	0
19	PGV	N	607	-	50,50,50	1.02	2 (4%)	53,56,56	1.25	9 (16%)
20	EDO	B	305	-	3,3,3	0.62	0	2,2,2	0.30	0
20	EDO	B	306	-	3,3,3	0.78	0	2,2,2	0.15	0
20	EDO	T	106	-	3,3,3	0.50	0	2,2,2	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	N	614	-	3,3,3	0.53	0	2,2,2	0.01	0
20	EDO	A	612	-	3,3,3	0.39	0	2,2,2	0.47	0
20	EDO	A	616	-	3,3,3	0.48	0	2,2,2	0.54	0
20	EDO	N	612	-	3,3,3	0.54	0	2,2,2	0.05	0
27	DMU	T	104	-	22,22,34	0.51	0	27,27,45	1.11	3 (11%)
27	DMU	X	201	-	34,34,34	0.62	0	45,45,45	1.38	6 (13%)
22	CUA	O	301	2	0,1,1	-	-	-		
27	DMU	L	102	-	34,34,34	0.65	0	45,45,45	2.24	21 (46%)
20	EDO	B	310	-	3,3,3	0.32	0	2,2,2	0.43	0
26	CDL	T	103	-	95,95,99	1.48	12 (12%)	101,107,111	1.63	19 (18%)
20	EDO	D	201	-	3,3,3	0.51	0	2,2,2	0.72	0
27	DMU	K	105	-	34,34,34	0.60	0	45,45,45	1.75	10 (22%)
20	EDO	A	622	-	3,3,3	0.72	0	2,2,2	0.33	0
20	EDO	O	305	-	3,3,3	0.59	0	2,2,2	0.54	0
20	EDO	Q	203	-	3,3,3	0.67	0	2,2,2	0.18	0
25	PEK	C	303	-	52,52,52	1.12	2 (3%)	55,57,57	1.46	5 (9%)
27	DMU	O	303	-	31,31,34	0.54	0	36,38,45	2.94	16 (44%)
20	EDO	F	103	-	3,3,3	0.65	0	2,2,2	0.65	0
20	EDO	C	314	-	3,3,3	0.56	0	2,2,2	0.29	0
20	EDO	P	314	-	3,3,3	0.84	0	2,2,2	0.31	0
20	EDO	F	106	-	3,3,3	0.60	0	2,2,2	0.21	0
20	EDO	D	203	-	3,3,3	0.61	0	2,2,2	0.38	0
22	CUA	B	302	2	0,1,1	-	-	-		
25	PEK	T	102	-	43,43,52	1.18	2 (4%)	46,48,57	1.57	5 (10%)
20	EDO	N	623	-	3,3,3	0.62	0	2,2,2	0.26	0
27	DMU	C	307	-	34,34,34	0.47	0	45,45,45	0.93	2 (4%)
20	EDO	Q	204	-	3,3,3	0.44	0	2,2,2	0.70	0
27	DMU	P	316	-	34,34,34	1.19	2 (5%)	45,45,45	2.31	12 (26%)
20	EDO	N	616	-	3,3,3	0.31	0	2,2,2	0.09	0
20	EDO	C	315	-	3,3,3	0.57	0	2,2,2	0.17	0
20	EDO	A	621	-	3,3,3	0.68	0	2,2,2	0.43	0
20	EDO	E	203	-	3,3,3	0.52	0	2,2,2	0.64	0
18	CMO	A	606[B]	15	0,1,1	-	-	-		
21	TGL	Q	201	-	62,62,62	1.04	3 (4%)	65,65,65	1.19	6 (9%)
26	CDL	G	101	-	98,98,99	1.47	12 (12%)	104,110,111	1.43	10 (9%)
20	EDO	P	310	-	3,3,3	0.88	0	2,2,2	0.19	0
20	EDO	F	102	-	3,3,3	0.71	0	2,2,2	0.45	0
20	EDO	J	104	-	3,3,3	0.38	0	2,2,2	0.35	0
20	EDO	N	620	-	3,3,3	0.83	0	2,2,2	0.18	0
20	EDO	A	613	-	3,3,3	0.36	0	2,2,2	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	O	306	-	3,3,3	0.52	0	2,2,2	0.24	0
19	PGV	N	609	-	50,50,50	0.99	3 (6%)	53,56,56	1.12	4 (7%)
27	DMU	P	307	-	34,34,34	0.65	1 (2%)	45,45,45	1.62	11 (24%)
20	EDO	A	609	-	3,3,3	0.73	0	2,2,2	0.50	0
24	CHD	C	301	-	32,32,32	0.95	2 (6%)	51,51,51	1.31	5 (9%)
27	DMU	M	106	-	34,34,34	0.85	1 (2%)	45,45,45	1.93	12 (26%)
25	PEK	P	302	-	47,47,52	1.18	2 (4%)	50,52,57	1.46	5 (10%)
20	EDO	N	617	-	3,3,3	0.50	0	2,2,2	0.84	0
18	CMO	N	606[B]	15	0,1,1	-	-	-		
20	EDO	F	104	-	3,3,3	0.68	0	2,2,2	0.23	0
29	PO4	U	102	-	4,4,4	0.74	0	6,6,6	0.59	0
14	HEA	A	601[C]	-	67,57,67	2.09	19 (28%)	81,89,103	2.44	33 (40%)
20	EDO	M	105	-	3,3,3	0.67	0	2,2,2	0.21	0
27	DMU	X	204	-	34,34,34	0.59	1 (2%)	45,45,45	1.00	3 (6%)
20	EDO	N	621	-	3,3,3	0.62	0	2,2,2	0.33	0
24	CHD	W	101	-	32,32,32	0.88	0	51,51,51	3.52	23 (45%)
20	EDO	D	205	-	3,3,3	0.50	0	2,2,2	0.19	0
21	TGL	B	301	-	62,62,62	1.11	3 (4%)	65,65,65	1.42	6 (9%)
23	PSC	B	303	-	50,50,51	1.21	3 (6%)	56,58,59	1.47	7 (12%)
26	CDL	C	306	-	90,90,99	1.61	15 (16%)	95,97,111	1.97	17 (17%)
24	CHD	G	103	-	32,32,32	0.88	0	51,51,51	1.41	11 (21%)
20	EDO	M	102	-	3,3,3	0.43	0	2,2,2	0.72	0
20	EDO	S	103	-	3,3,3	0.80	0	2,2,2	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DMU	X	202	-	-	13/19/59/59	0/2/2/2
20	EDO	N	625	-	-	1/1/1/1	-
14	HEA	N	601[C]	-	-	8/36/60/76	-
20	EDO	N	622	-	-	0/1/1/1	-
26	CDL	P	306	-	-	31/83/85/110	-
19	PGV	C	304	-	-	10/54/54/55	-
20	EDO	G	105	-	-	0/1/1/1	-
14	HEA	A	602	1	-	4/36/76/76	-
25	PEK	P	303	-	-	7/48/48/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	TGL	B	304	-	-	25/65/65/65	-
27	DMU	M	101	-	-	6/19/59/59	0/2/2/2
27	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
27	DMU	K	101	-	-	10/13/29/59	0/1/1/2
25	PEK	P	304	-	-	23/56/56/56	-
27	DMU	K	102	-	-	7/13/33/59	0/1/1/2
20	EDO	B	307	-	-	0/1/1/1	-
20	EDO	P	312	-	-	0/1/1/1	-
20	EDO	I	101	-	-	1/1/1/1	-
20	EDO	N	613	-	-	0/1/1/1	-
21	TGL	L	101	-	-	33/62/62/65	-
23	PSC	O	302	-	-	18/49/49/55	-
20	EDO	E	201	-	-	0/1/1/1	-
20	EDO	C	312	-	-	0/1/1/1	-
19	PGV	A	607	-	-	21/52/52/55	-
20	EDO	O	307	-	-	0/1/1/1	-
20	EDO	J	103	-	-	0/1/1/1	-
20	EDO	R	202	-	-	0/1/1/1	-
20	EDO	S	102	-	-	0/1/1/1	-
24	CHD	P	308	-	-	5/9/74/74	0/4/4/4
20	EDO	Q	202	-	-	0/1/1/1	-
20	EDO	S	105	-	-	0/1/1/1	-
24	CHD	J	101	-	-	4/9/74/74	0/4/4/4
27	DMU	G	102	-	-	12/19/59/59	0/2/2/2
20	EDO	S	106	-	-	0/1/1/1	-
20	EDO	C	317	-	-	1/1/1/1	-
20	EDO	R	201	-	-	0/1/1/1	-
21	TGL	N	608	-	-	20/65/65/65	-
27	DMU	P	309	-	-	10/19/59/59	0/2/2/2
20	EDO	F	105	-	-	1/1/1/1	-
20	EDO	O	304	-	-	0/1/1/1	-
24	CHD	Y	101	-	-	4/9/74/74	0/4/4/4
20	EDO	A	610	-	-	0/1/1/1	-
20	EDO	P	313	-	-	1/1/1/1	-
20	EDO	P	311	-	-	0/1/1/1	-
20	EDO	U	101	-	-	1/1/1/1	-
24	CHD	J	102	-	-	4/9/74/74	0/4/4/4
20	EDO	M	104	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	C	313	-	-	0/1/1/1	-
20	EDO	Y	103	-	-	1/1/1/1	-
20	EDO	E	202	-	-	1/1/1/1	-
20	EDO	G	106	-	-	0/1/1/1	-
20	EDO	N	626	-	-	0/1/1/1	-
20	EDO	P	315	-	-	1/1/1/1	-
20	EDO	M	103	-	-	0/1/1/1	-
14	HEA	A	601[A]	-	-	5/36/76/76	-
19	PGV	A	608	-	-	10/55/55/55	-
20	EDO	V	101	-	-	1/1/1/1	-
20	EDO	C	311	-	-	1/1/1/1	-
20	EDO	N	610	-	-	0/1/1/1	-
19	PGV	G	104	-	-	17/55/55/55	-
20	EDO	T	105	-	-	0/1/1/1	-
20	EDO	D	202	-	-	0/1/1/1	-
27	DMU	C	308	-	-	8/19/59/59	0/2/2/2
20	EDO	A	617	-	-	1/1/1/1	-
20	EDO	A	620	-	-	1/1/1/1	-
20	EDO	D	204	-	-	0/1/1/1	-
20	EDO	C	316	-	-	0/1/1/1	-
27	DMU	K	104	-	-	6/19/59/59	0/2/2/2
14	HEA	N	601[A]	-	-	5/36/76/76	-
20	EDO	A	618	-	-	0/1/1/1	-
20	EDO	L	103	-	-	0/1/1/1	-
20	EDO	B	309	-	-	1/1/1/1	-
27	DMU	K	103	-	-	9/19/59/59	0/2/2/2
14	HEA	N	602	1	-	4/36/76/76	-
20	EDO	N	624	-	-	0/1/1/1	-
20	EDO	N	619	-	-	0/1/1/1	-
24	CHD	T	101	-	-	2/9/74/74	0/4/4/4
27	DMU	K	106	-	-	10/19/59/59	0/2/2/2
24	CHD	P	301	-	-	2/9/74/74	0/4/4/4
20	EDO	C	310	-	-	1/1/1/1	-
20	EDO	N	611	-	-	0/1/1/1	-
20	EDO	C	309	-	-	0/1/1/1	-
19	PGV	C	305	-	-	15/55/55/55	-
27	DMU	X	203	-	-	8/13/33/59	0/1/1/2
27	DMU	X	205	-	-	3/13/33/59	0/1/1/2
20	EDO	A	614	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	TGL	Y	102	-	-	34/65/65/65	-
25	PEK	C	302	-	-	12/56/56/56	-
19	PGV	P	305	-	-	9/55/55/55	-
20	EDO	A	615	-	-	0/1/1/1	-
20	EDO	B	308	-	-	0/1/1/1	-
20	EDO	N	618	-	-	0/1/1/1	-
20	EDO	S	104	-	-	0/1/1/1	-
20	EDO	A	619	-	-	0/1/1/1	-
20	EDO	N	615	-	-	0/1/1/1	-
20	EDO	A	611	-	-	1/1/1/1	-
19	PGV	N	607	-	-	24/55/55/55	-
20	EDO	B	305	-	-	0/1/1/1	-
20	EDO	B	306	-	-	0/1/1/1	-
20	EDO	T	106	-	-	0/1/1/1	-
20	EDO	N	614	-	-	0/1/1/1	-
20	EDO	A	612	-	-	1/1/1/1	-
20	EDO	A	616	-	-	0/1/1/1	-
20	EDO	N	612	-	-	1/1/1/1	-
27	DMU	T	104	-	-	10/13/33/59	0/1/1/2
27	DMU	X	201	-	-	12/19/59/59	0/2/2/2
27	DMU	L	102	-	-	13/19/59/59	0/2/2/2
20	EDO	B	310	-	-	0/1/1/1	-
26	CDL	T	103	-	-	40/106/106/110	-
20	EDO	D	201	-	-	1/1/1/1	-
27	DMU	K	105	-	-	8/19/59/59	0/2/2/2
20	EDO	A	622	-	-	1/1/1/1	-
20	EDO	O	305	-	-	1/1/1/1	-
20	EDO	Q	203	-	-	1/1/1/1	-
25	PEK	C	303	-	-	22/56/56/56	-
27	DMU	O	303	-	-	12/27/47/59	0/1/1/2
20	EDO	F	103	-	-	0/1/1/1	-
20	EDO	C	314	-	-	1/1/1/1	-
20	EDO	P	314	-	-	0/1/1/1	-
20	EDO	F	106	-	-	1/1/1/1	-
20	EDO	D	203	-	-	0/1/1/1	-
25	PEK	T	102	-	-	25/47/47/56	-
20	EDO	N	623	-	-	0/1/1/1	-
27	DMU	C	307	-	-	6/19/59/59	0/2/2/2
20	EDO	Q	204	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DMU	P	316	-	-	10/19/59/59	0/2/2/2
20	EDO	N	616	-	-	0/1/1/1	-
20	EDO	C	315	-	-	0/1/1/1	-
20	EDO	A	621	-	-	0/1/1/1	-
20	EDO	E	203	-	-	0/1/1/1	-
21	TGL	Q	201	-	-	23/65/65/65	-
26	CDL	G	101	-	-	37/109/109/110	-
20	EDO	P	310	-	-	0/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
20	EDO	J	104	-	-	1/1/1/1	-
20	EDO	N	620	-	-	1/1/1/1	-
20	EDO	A	613	-	-	0/1/1/1	-
20	EDO	O	306	-	-	0/1/1/1	-
19	PGV	N	609	-	-	6/55/55/55	-
27	DMU	P	307	-	-	5/19/59/59	0/2/2/2
20	EDO	A	609	-	-	0/1/1/1	-
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
27	DMU	M	106	-	-	9/19/59/59	0/2/2/2
25	PEK	P	302	-	-	19/51/51/56	-
20	EDO	N	617	-	-	1/1/1/1	-
20	EDO	F	104	-	-	0/1/1/1	-
14	HEA	A	601[C]	-	-	7/36/60/76	-
20	EDO	M	105	-	-	1/1/1/1	-
27	DMU	X	204	-	-	11/19/59/59	0/2/2/2
20	EDO	N	621	-	-	0/1/1/1	-
24	CHD	W	101	-	-	9/9/74/74	0/4/4/4
20	EDO	D	205	-	-	0/1/1/1	-
21	TGL	B	301	-	-	18/65/65/65	-
23	PSC	B	303	-	-	28/54/54/55	-
26	CDL	C	306	-	-	52/94/94/110	-
24	CHD	G	103	-	-	2/9/74/74	0/4/4/4
20	EDO	M	102	-	-	1/1/1/1	-
20	EDO	S	103	-	-	0/1/1/1	-

The worst 5 of 224 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[C]	HEA	C18-C19	10.14	1.56	1.33
14	N	601[C]	HEA	C18-C19	8.25	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	305	PGV	O03-C19	5.88	1.50	1.33
25	C	303	PEK	O03-C21	5.47	1.49	1.33
26	C	306	CDL	OA8-CA7	5.42	1.49	1.33

The worst 5 of 656 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	W	101	CHD	C14-C8-C9	-8.82	97.43	109.75
14	A	601[C]	HEA	C13-C12-C11	-8.75	100.41	114.39
26	C	306	CDL	OA8-CA6-CA4	8.53	132.98	108.40
24	W	101	CHD	C10-C9-C8	8.40	121.20	111.84
14	A	601[C]	HEA	C17-C18-C19	7.61	145.05	127.62

There are no chirality outliers.

5 of 878 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[C]	HEA	C17-C18-C19-C20
14	A	601[C]	HEA	C17-C18-C19-C27
14	N	601[A]	HEA	C2A-C3A-CMA-OMA
14	N	601[C]	HEA	C2A-C3A-CMA-OMA
19	A	607	PGV	C03-O11-P-O12

There are no ring outliers.

80 monomers are involved in 288 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	X	202	DMU	4	0
20	N	625	EDO	2	0
26	P	306	CDL	10	0
19	C	304	PGV	1	0
14	A	602	HEA	2	0
21	B	304	TGL	11	0
27	Z	101	DMU	3	0
25	P	304	PEK	6	0
27	K	102	DMU	1	0
21	L	101	TGL	13	0
23	O	302	PSC	4	0
19	A	607	PGV	4	0
24	P	308	CHD	2	0
20	Q	202	EDO	1	0

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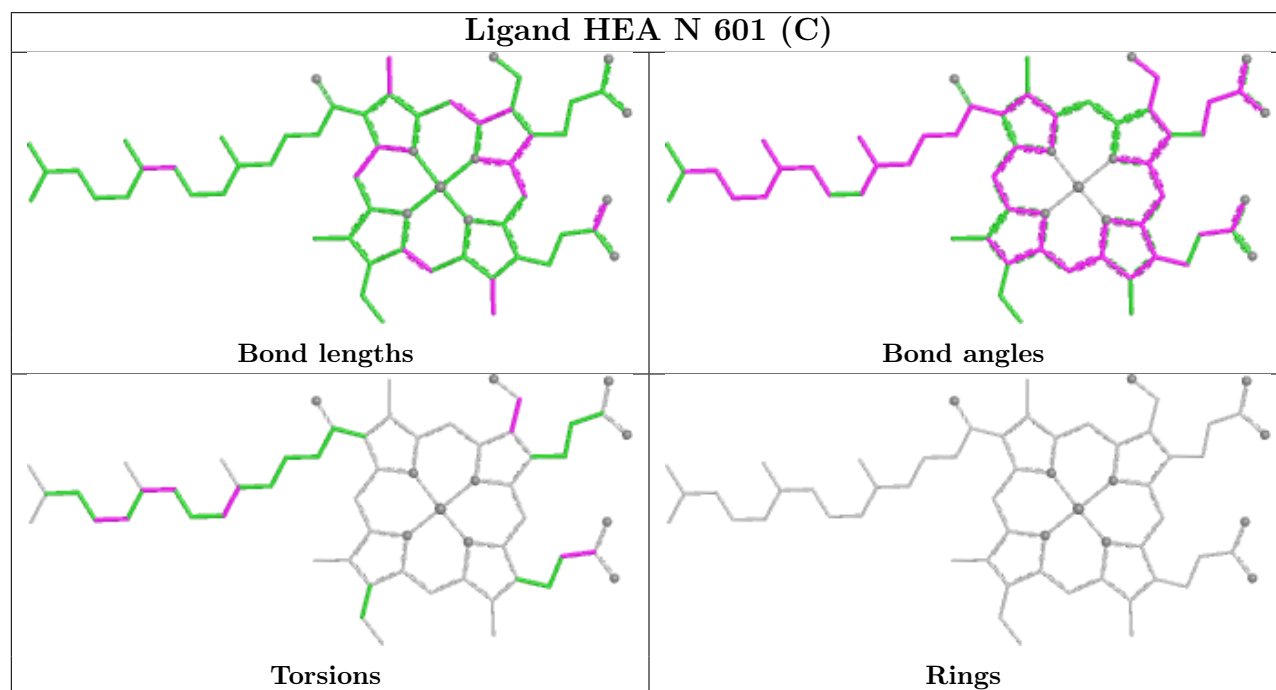
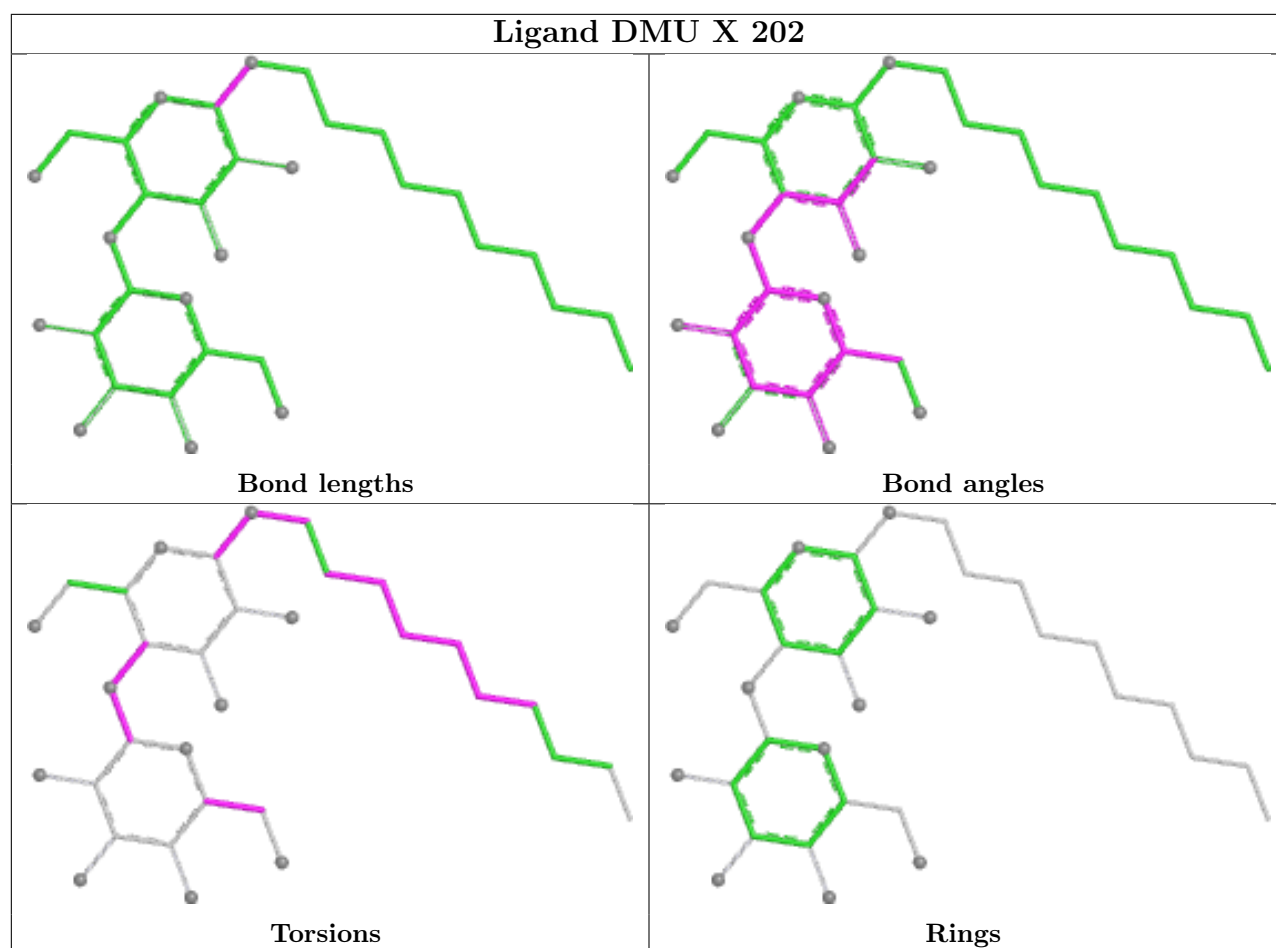
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	J	101	CHD	1	0
27	G	102	DMU	7	0
20	R	201	EDO	1	0
21	N	608	TGL	2	0
27	P	309	DMU	4	0
24	Y	101	CHD	1	0
20	U	101	EDO	4	0
24	J	102	CHD	2	0
20	N	626	EDO	2	0
20	M	103	EDO	5	0
14	A	601[A]	HEA	3	0
20	V	101	EDO	2	0
19	G	104	PGV	7	0
20	D	202	EDO	1	0
27	C	308	DMU	6	0
20	A	617	EDO	3	0
27	K	104	DMU	1	0
14	N	601[A]	HEA	2	0
20	L	103	EDO	3	0
20	B	309	EDO	1	0
27	K	103	DMU	1	0
14	N	602	HEA	2	0
27	K	106	DMU	5	0
19	C	305	PGV	4	0
27	X	203	DMU	3	0
27	X	205	DMU	1	0
21	Y	102	TGL	9	0
25	C	302	PEK	5	0
19	P	305	PGV	3	0
20	N	618	EDO	5	0
20	S	104	EDO	1	0
20	A	611	EDO	1	0
19	N	607	PGV	6	0
20	N	612	EDO	2	0
27	T	104	DMU	1	0
27	X	201	DMU	2	0
27	L	102	DMU	7	0
20	B	310	EDO	1	0
26	T	103	CDL	16	0
27	K	105	DMU	1	0
20	A	622	EDO	4	0
25	C	303	PEK	6	0

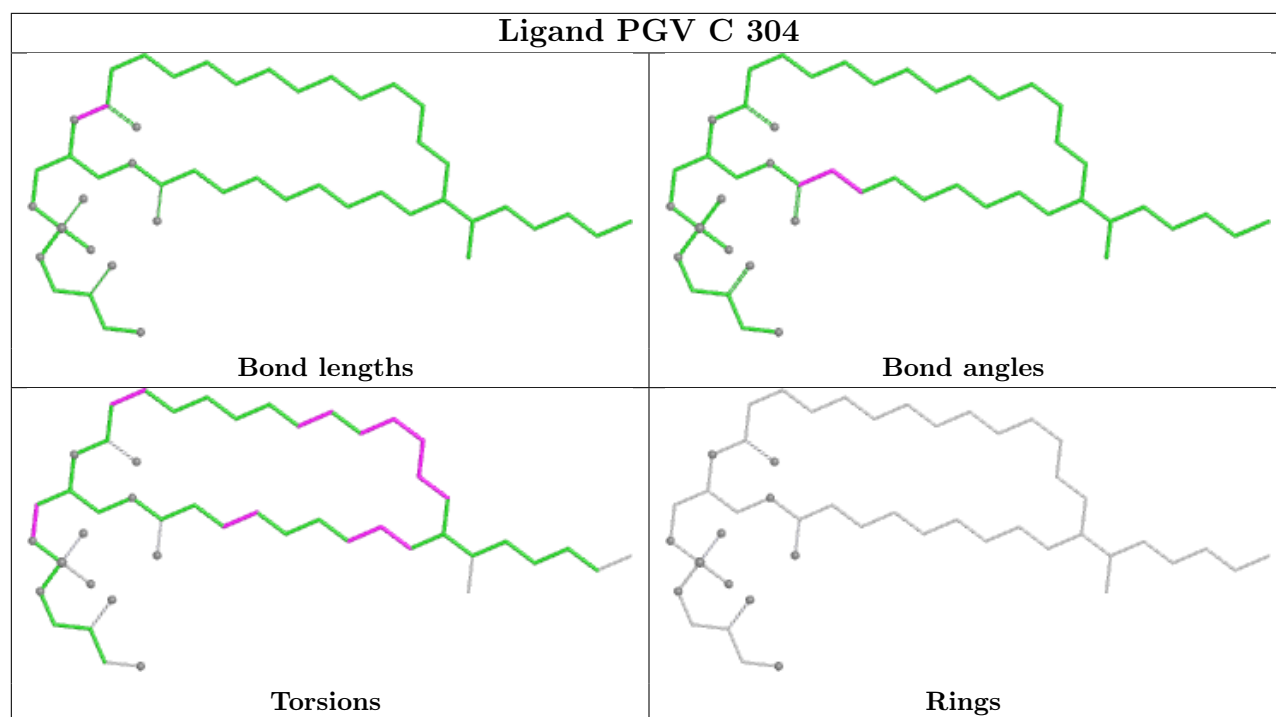
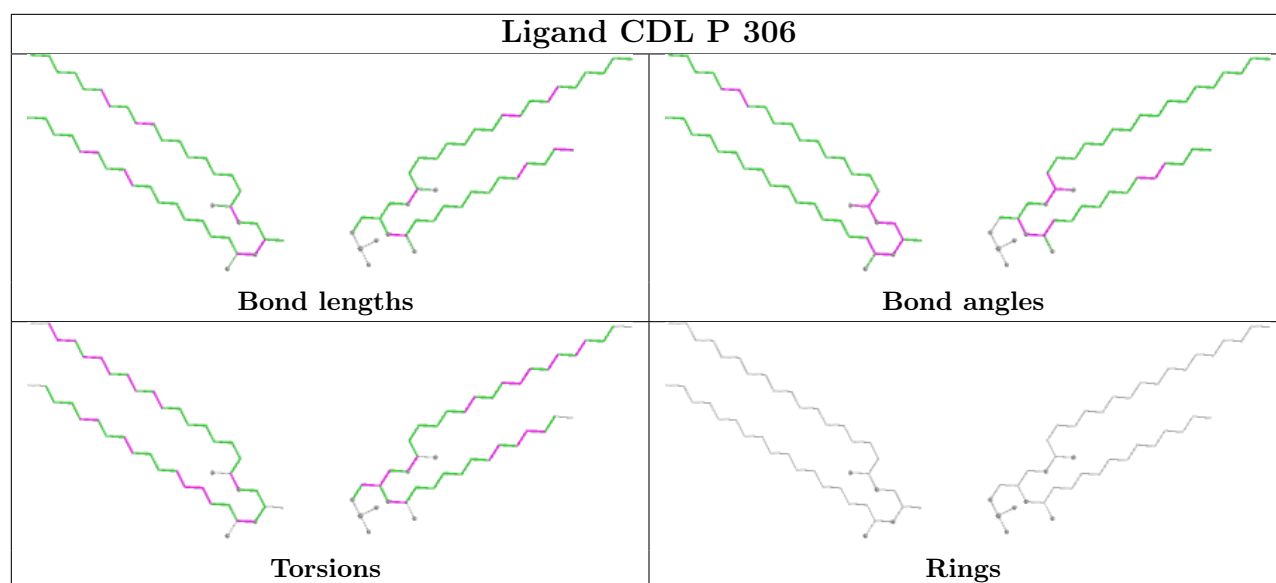
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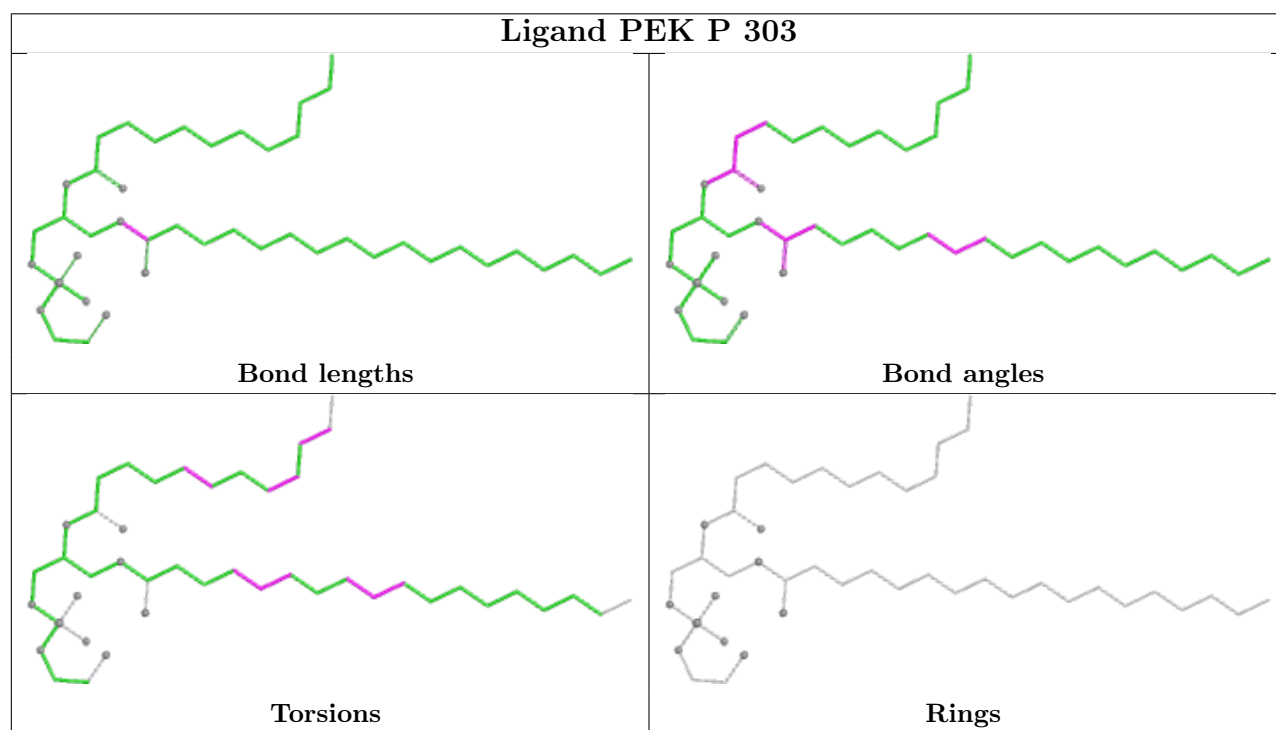
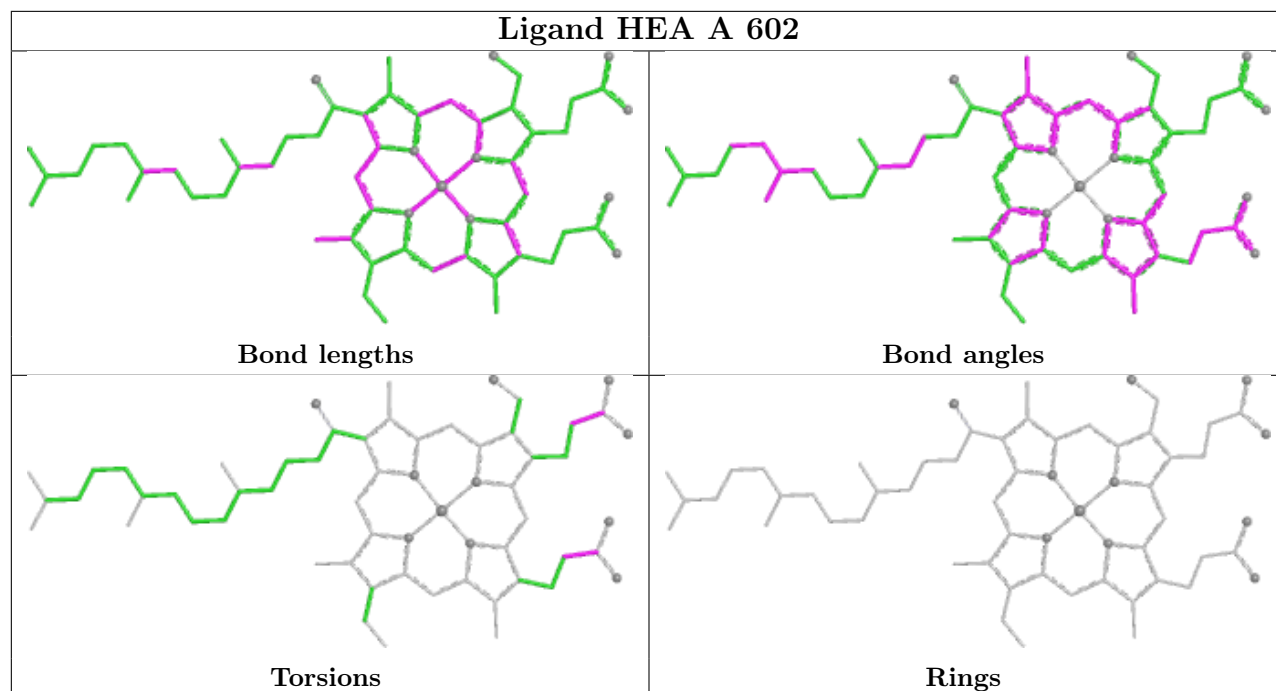
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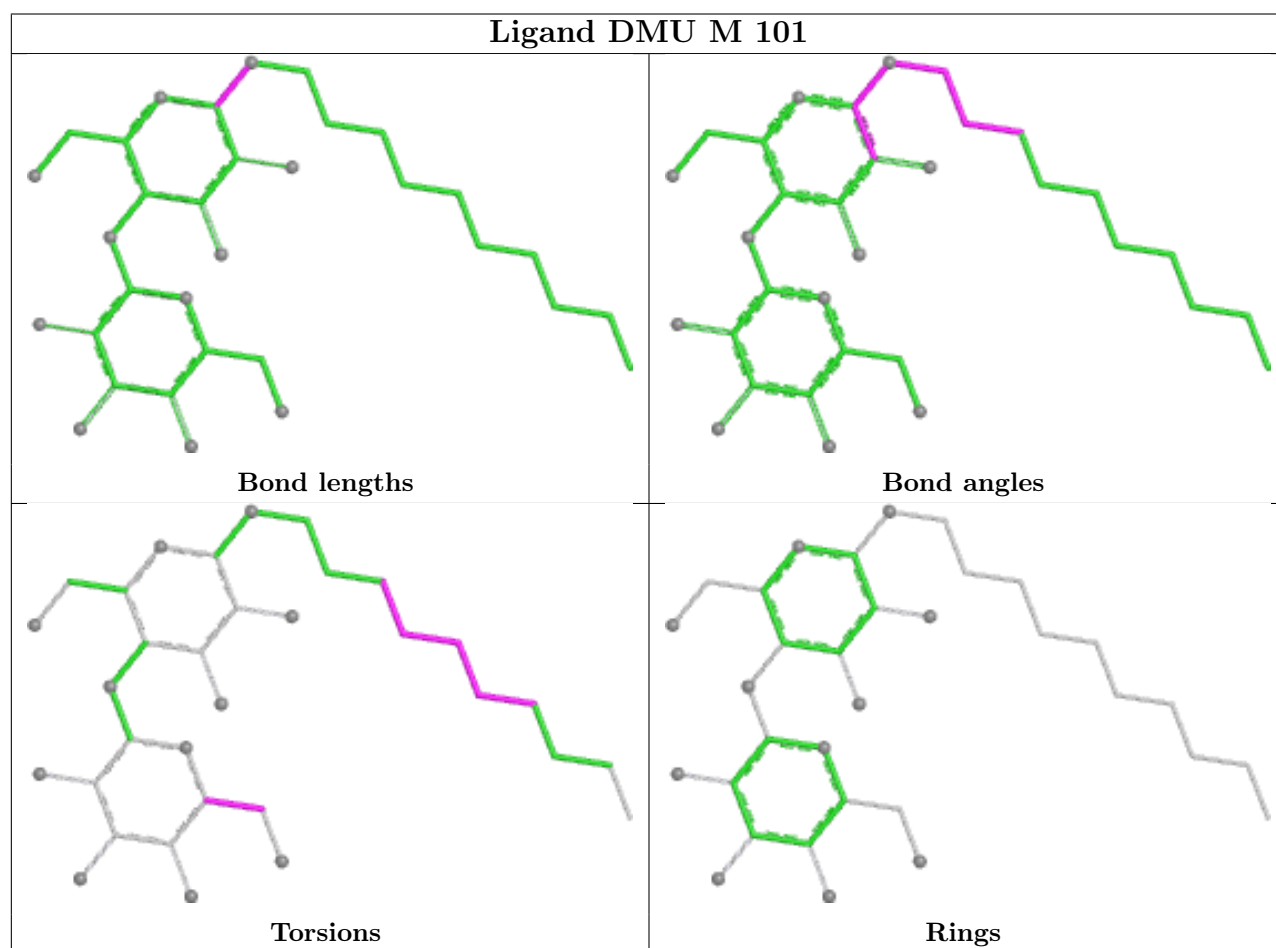
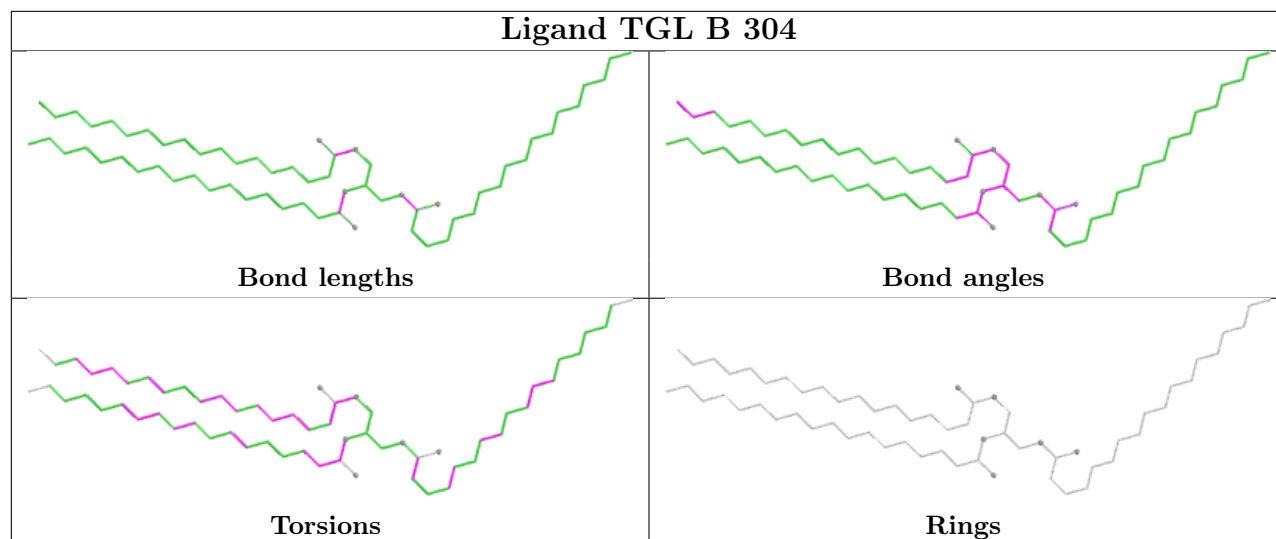
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	O	303	DMU	1	0
20	F	106	EDO	1	0
25	T	102	PEK	4	0
27	C	307	DMU	4	0
20	Q	204	EDO	1	0
27	P	316	DMU	8	0
20	N	616	EDO	2	0
20	C	315	EDO	1	0
20	A	621	EDO	1	0
21	Q	201	TGL	6	0
26	G	101	CDL	20	0
20	J	104	EDO	1	0
20	A	613	EDO	1	0
27	P	307	DMU	5	0
27	M	106	DMU	2	0
25	P	302	PEK	6	0
20	N	617	EDO	3	0
14	A	601[C]	HEA	1	0
20	M	105	EDO	1	0
27	X	204	DMU	1	0
24	W	101	CHD	1	0
21	B	301	TGL	7	0
23	B	303	PSC	13	0
26	C	306	CDL	3	0

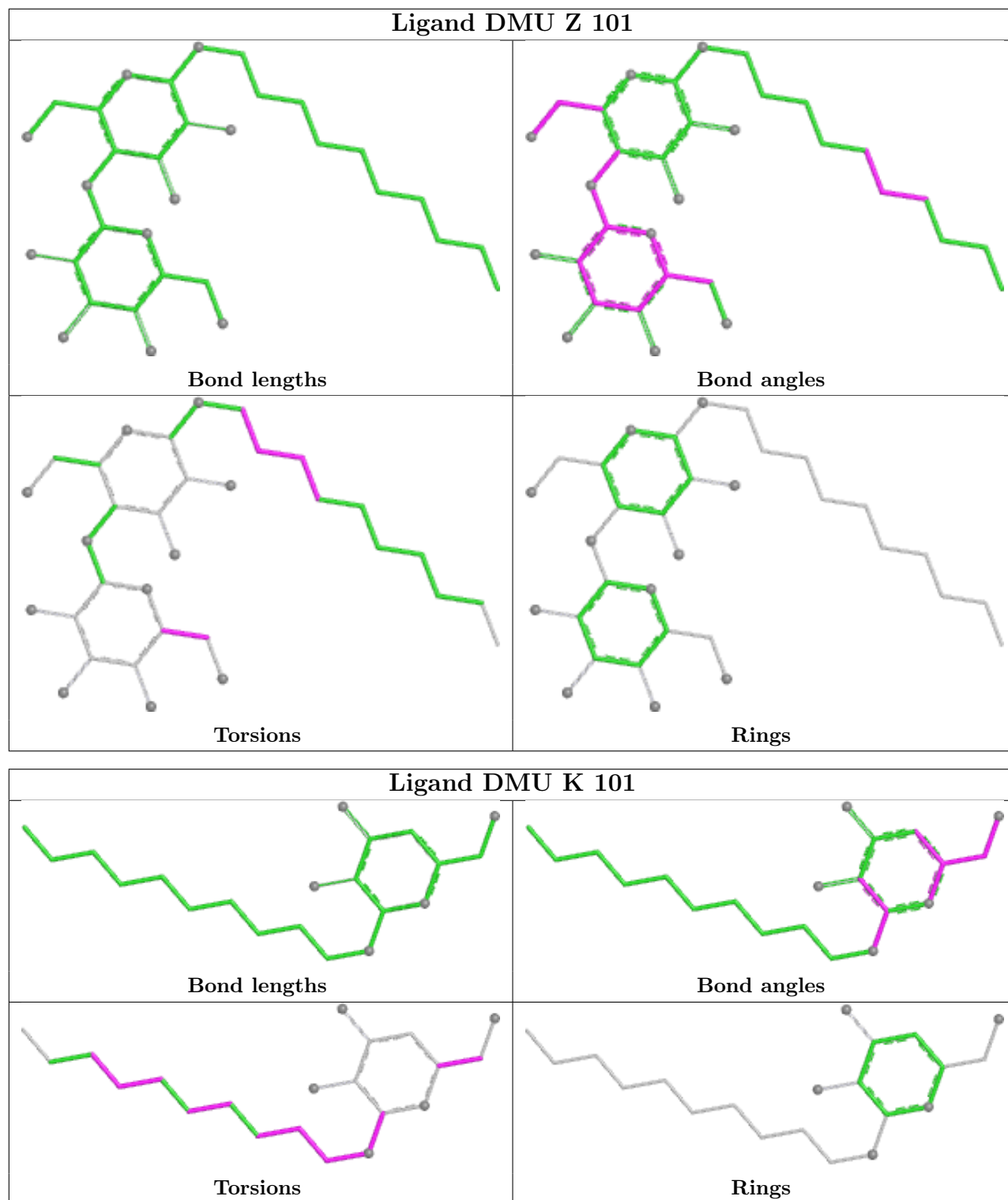
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

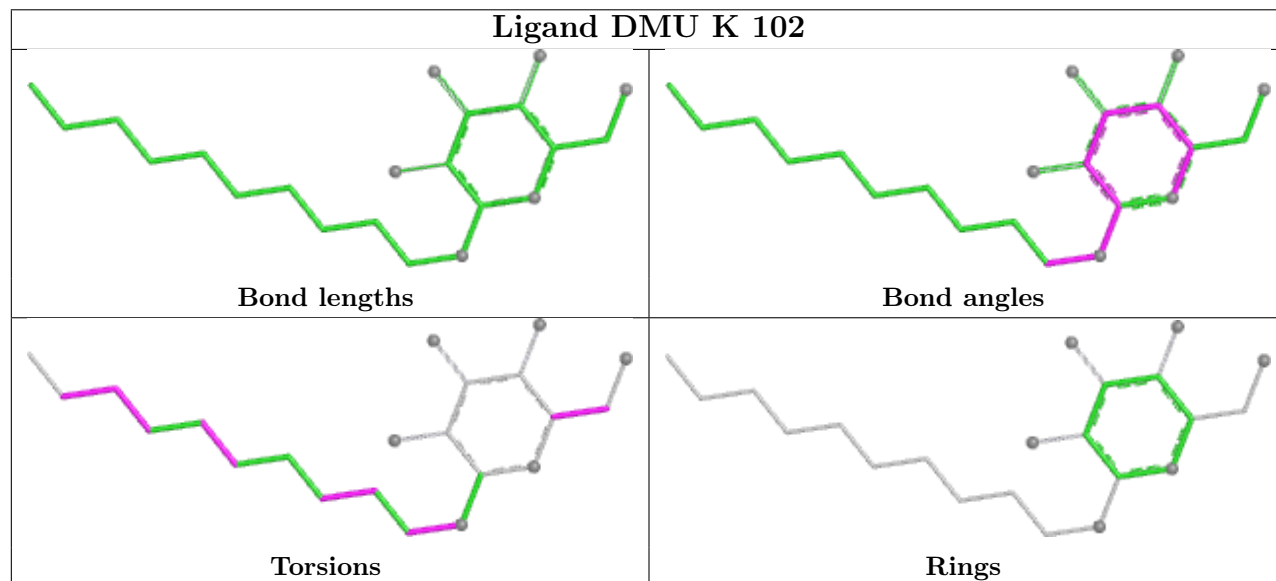
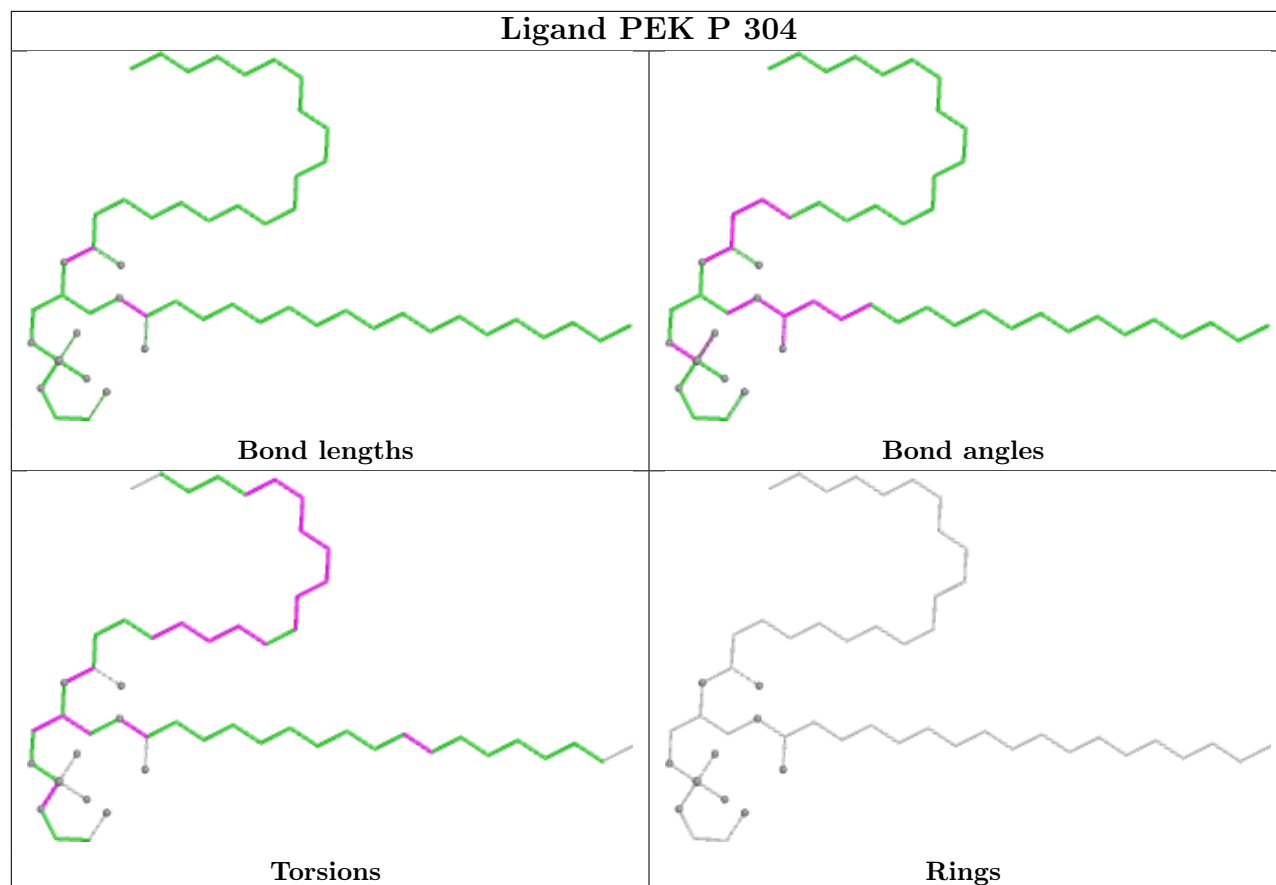


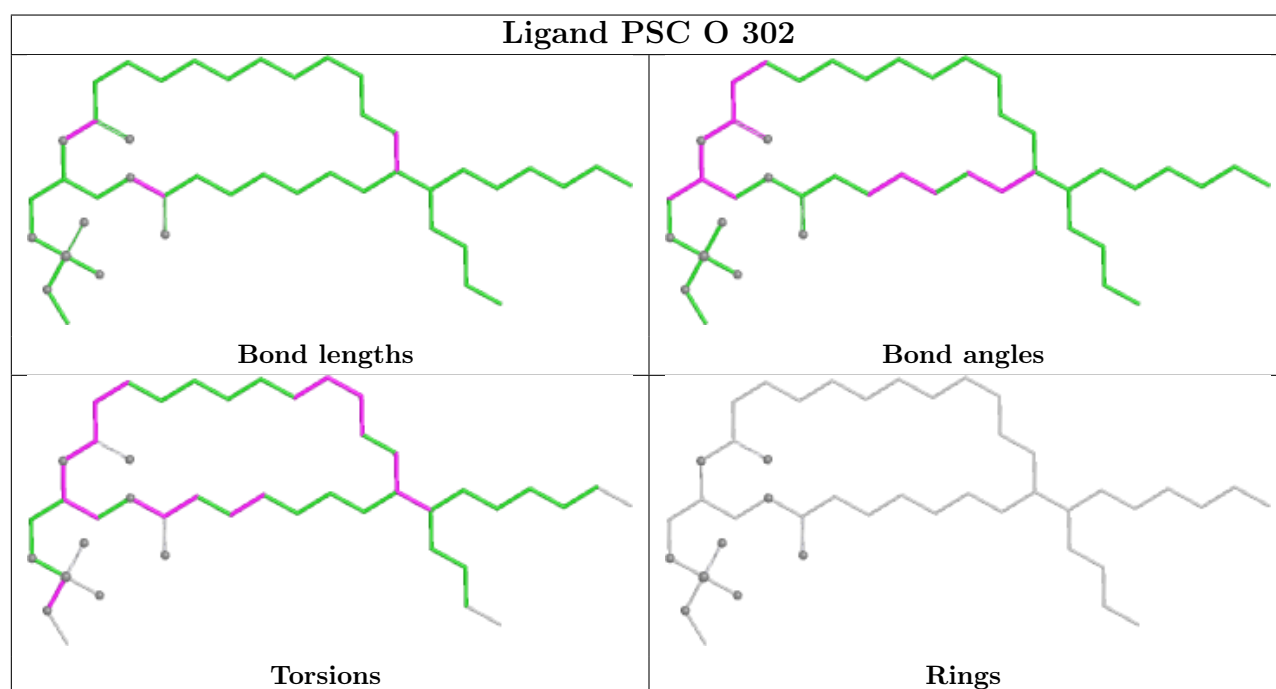
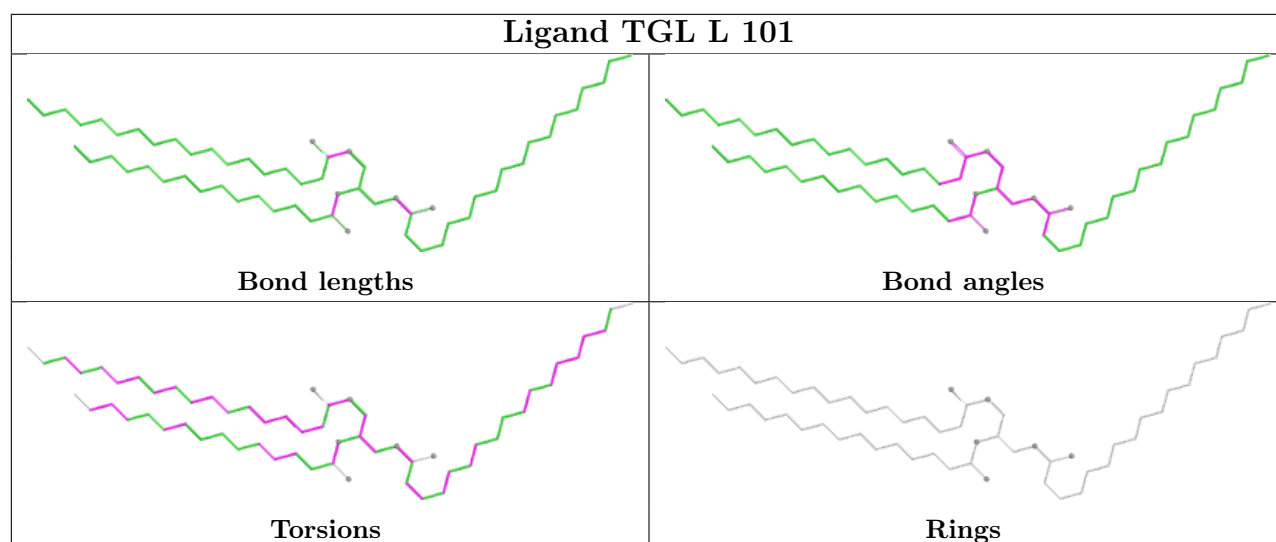


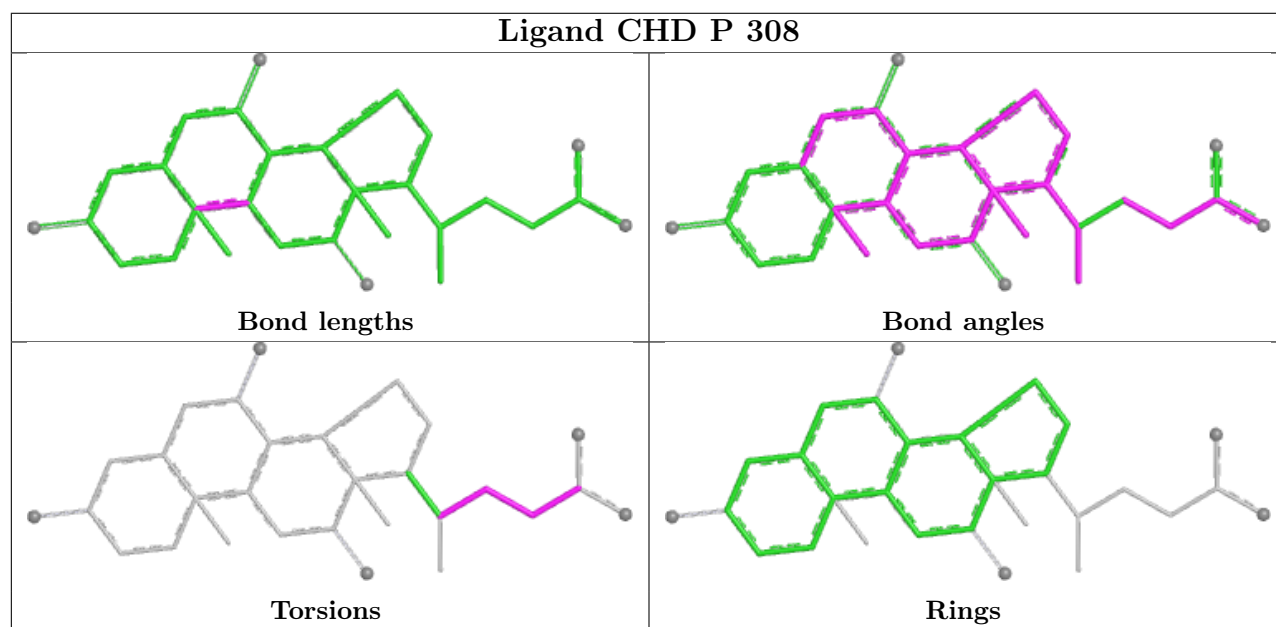
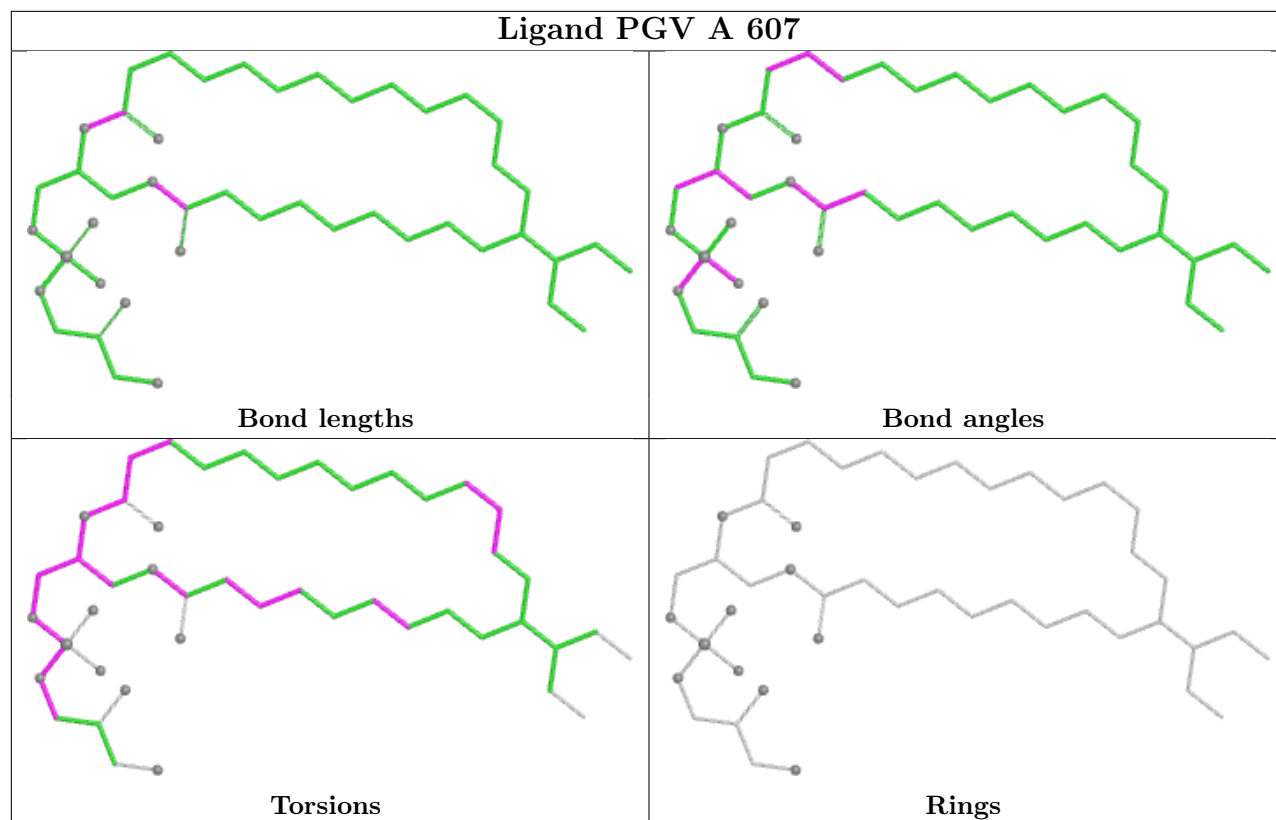




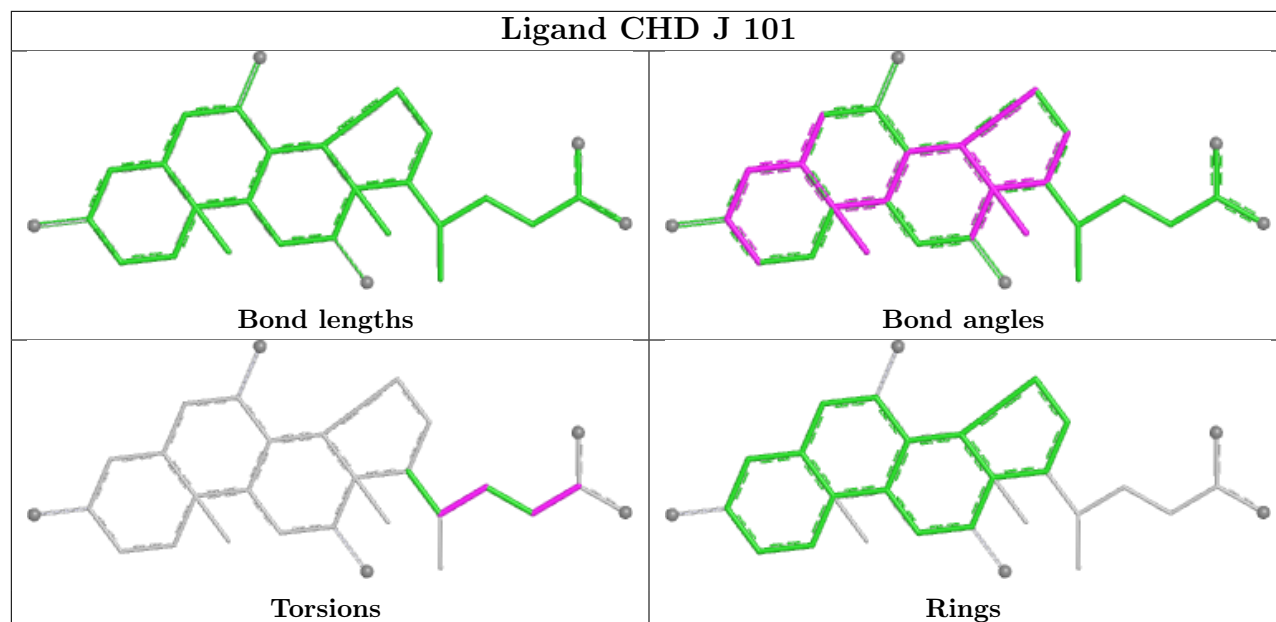




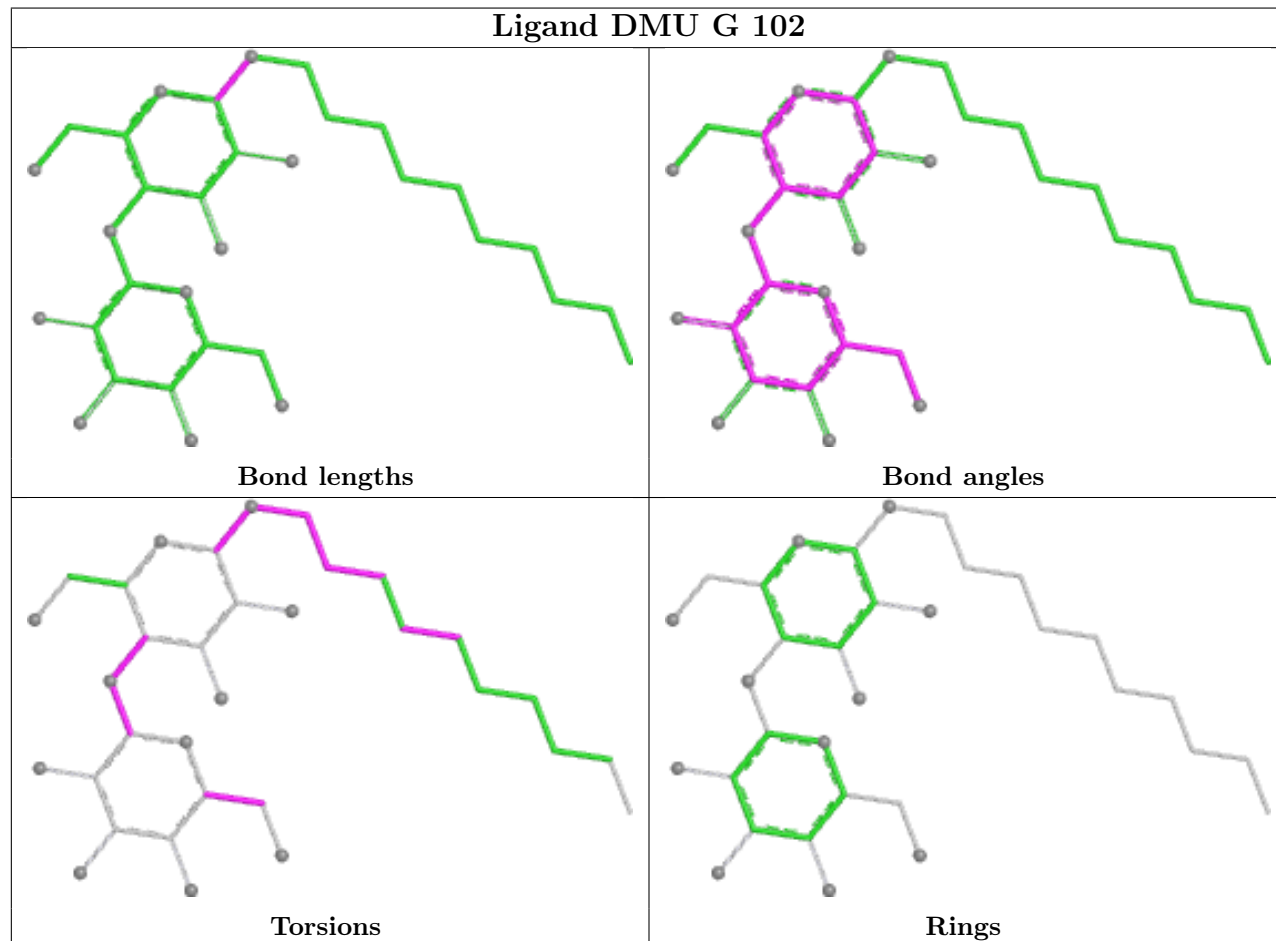


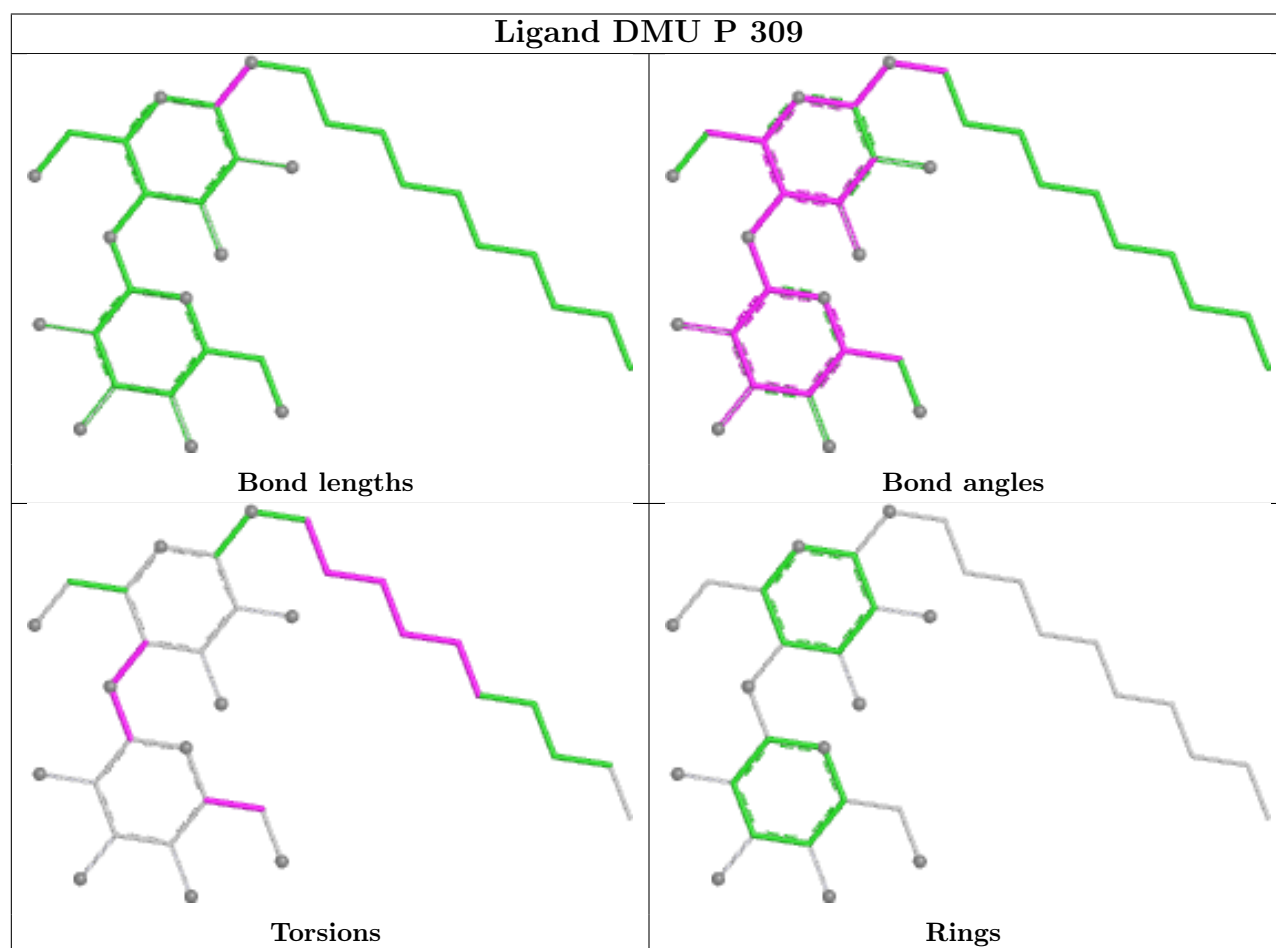
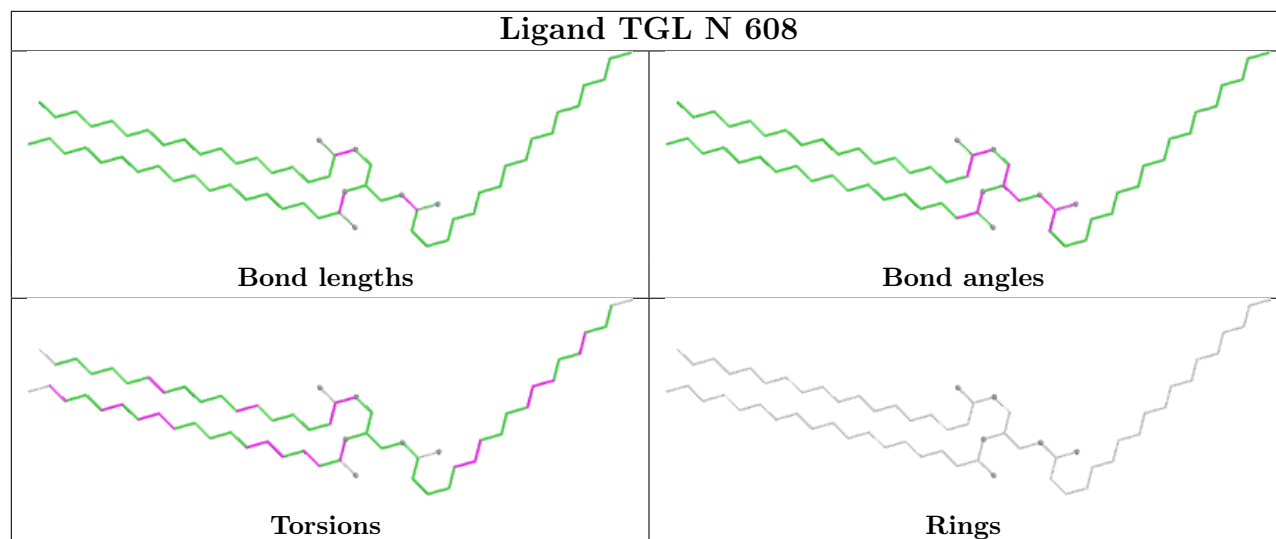


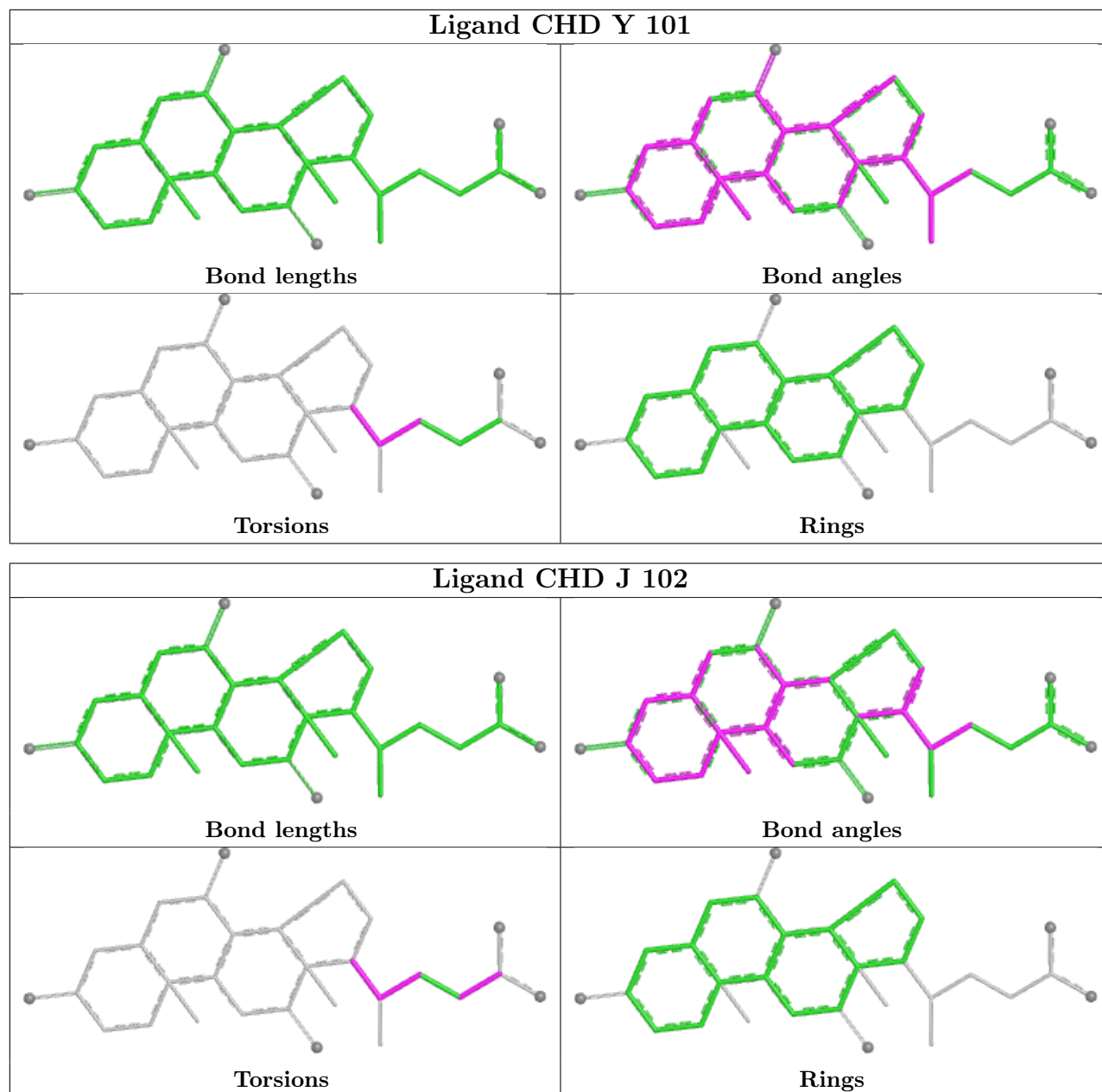
Ligand CHD J 101

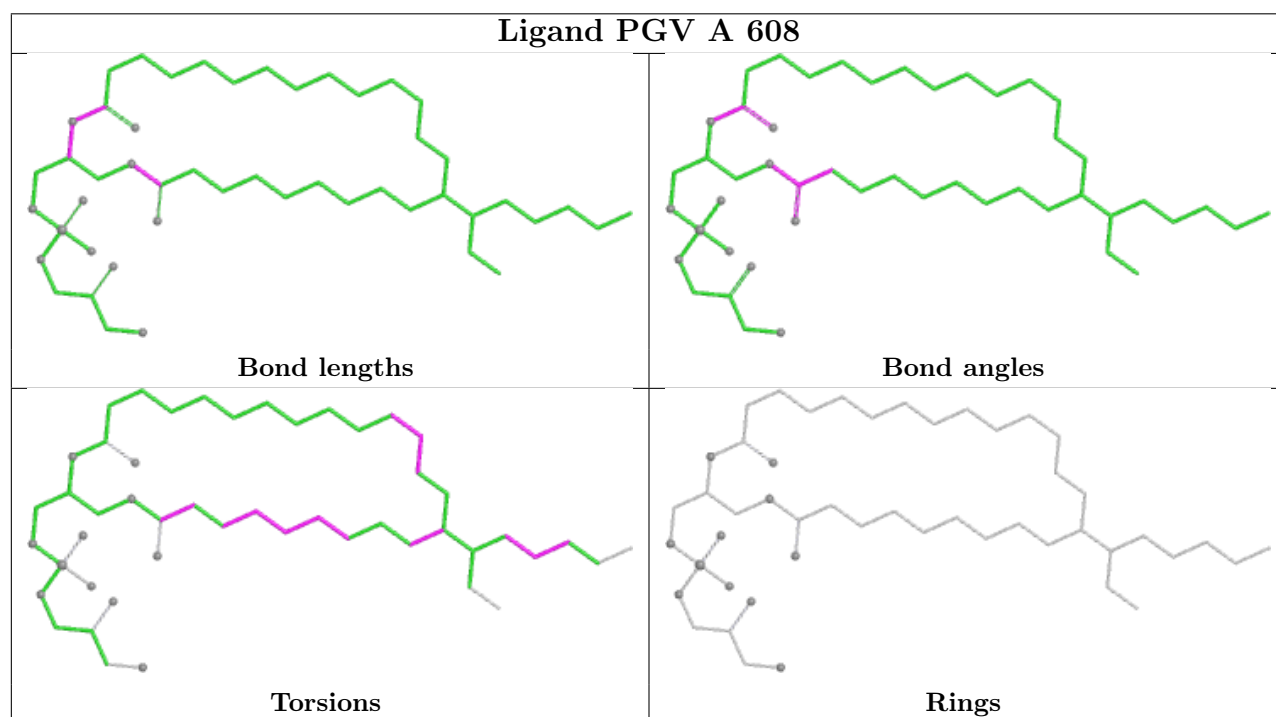
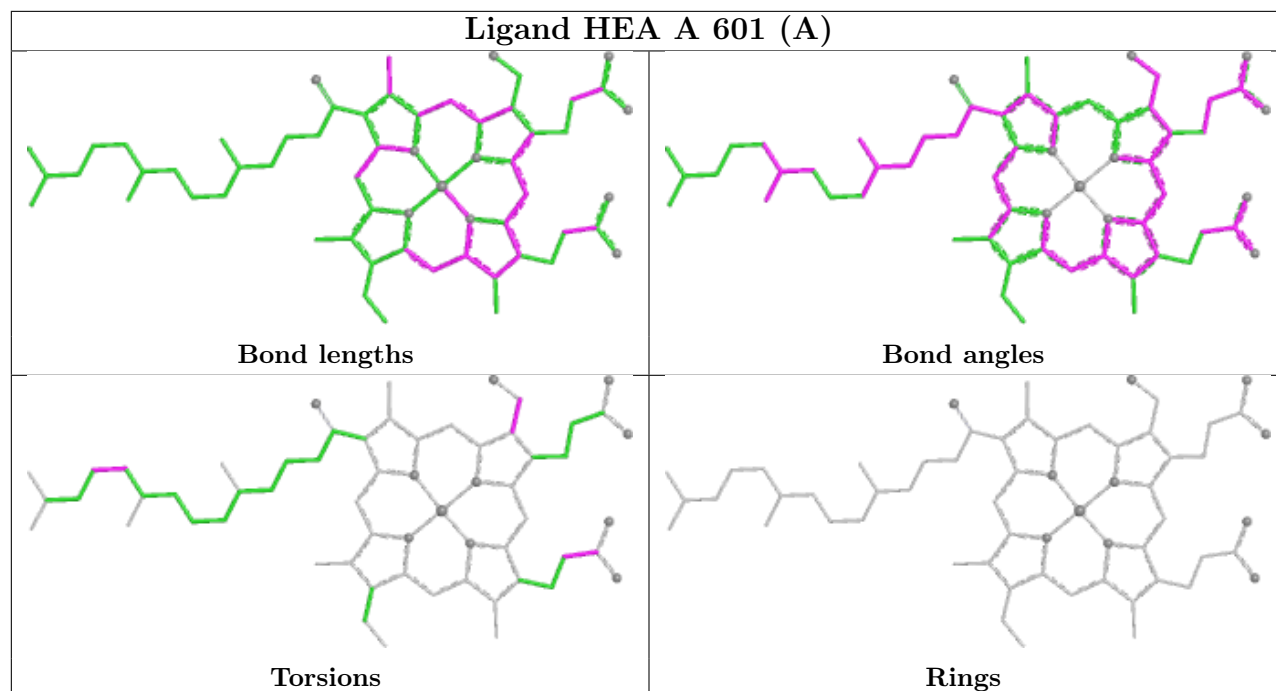


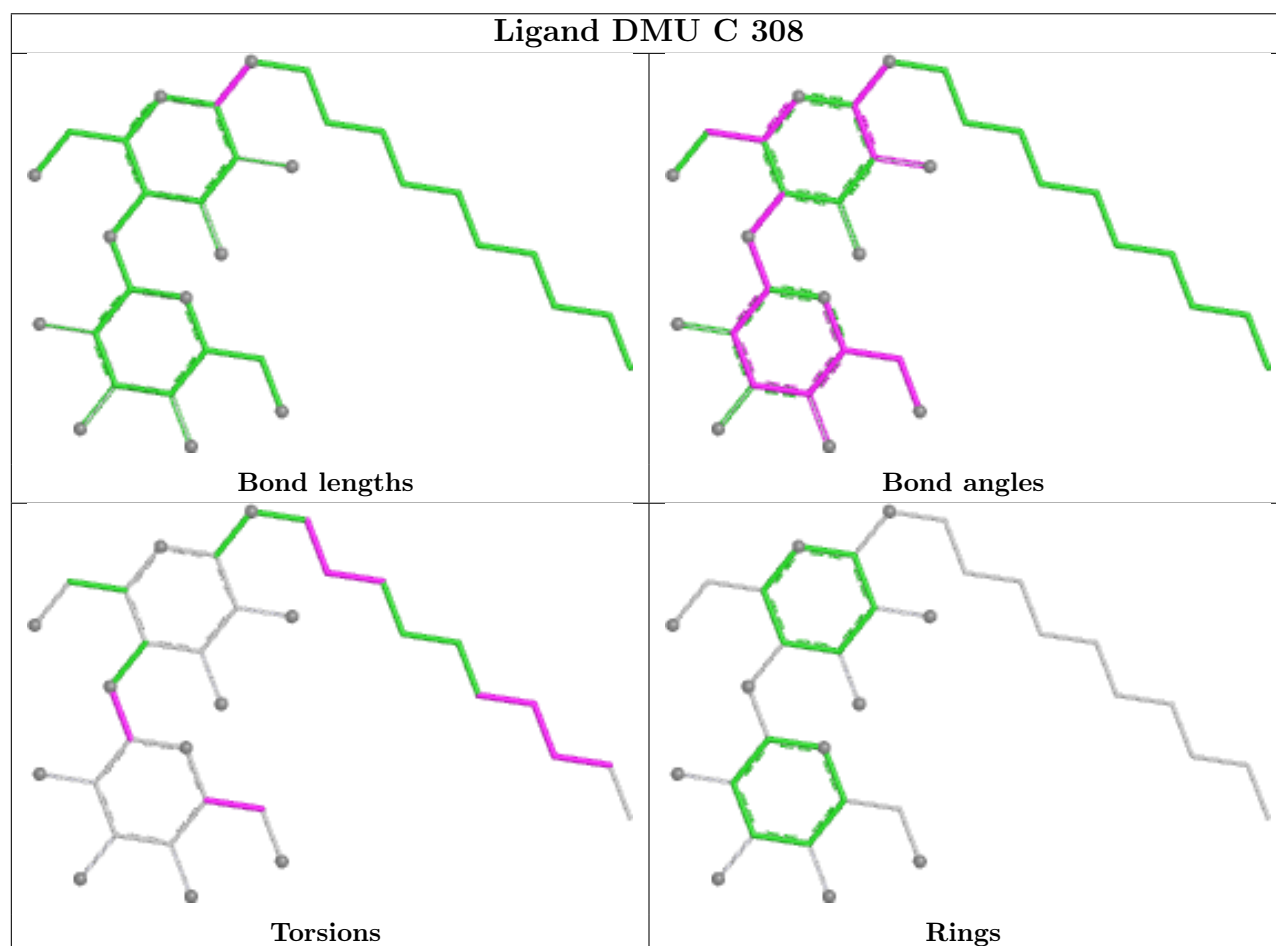
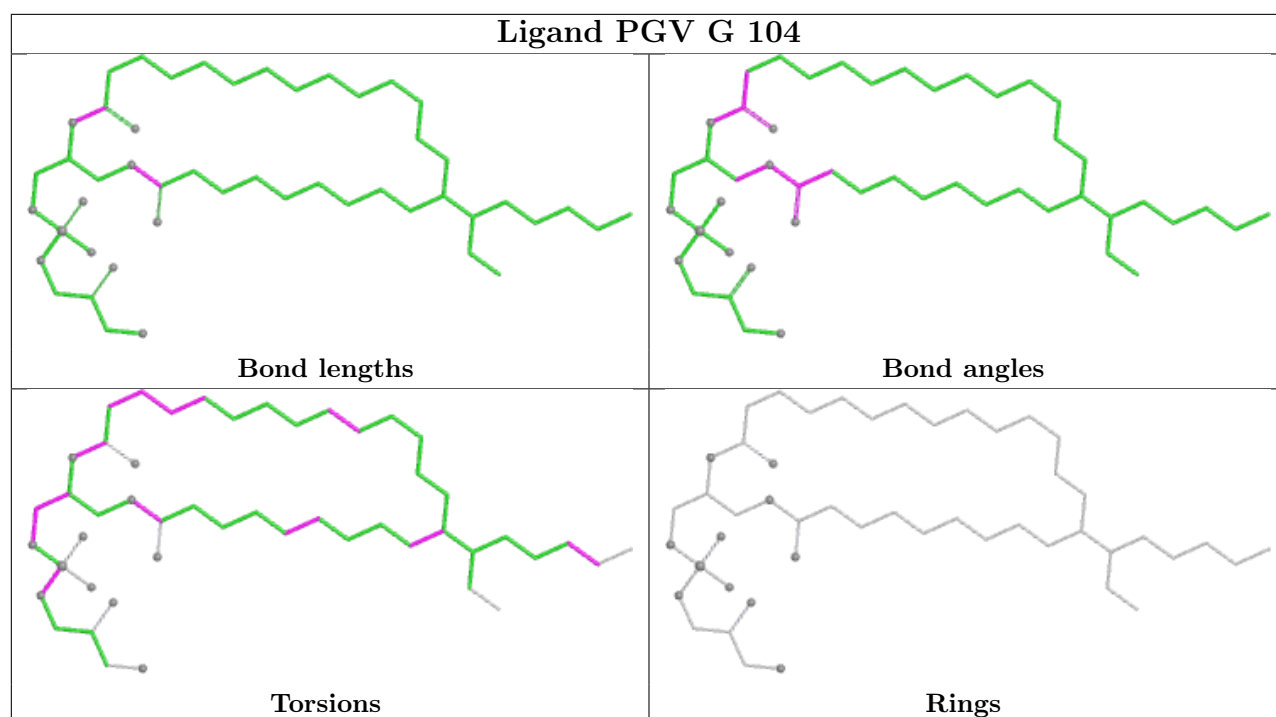
Ligand DMU G 102

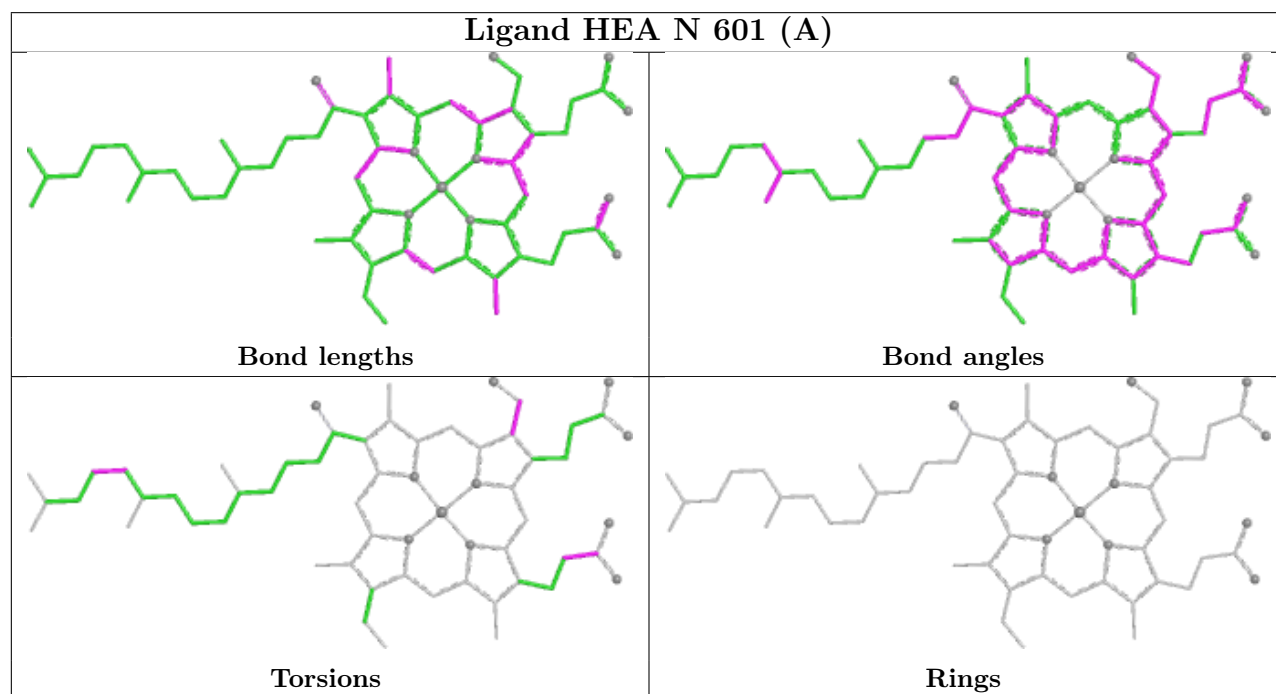
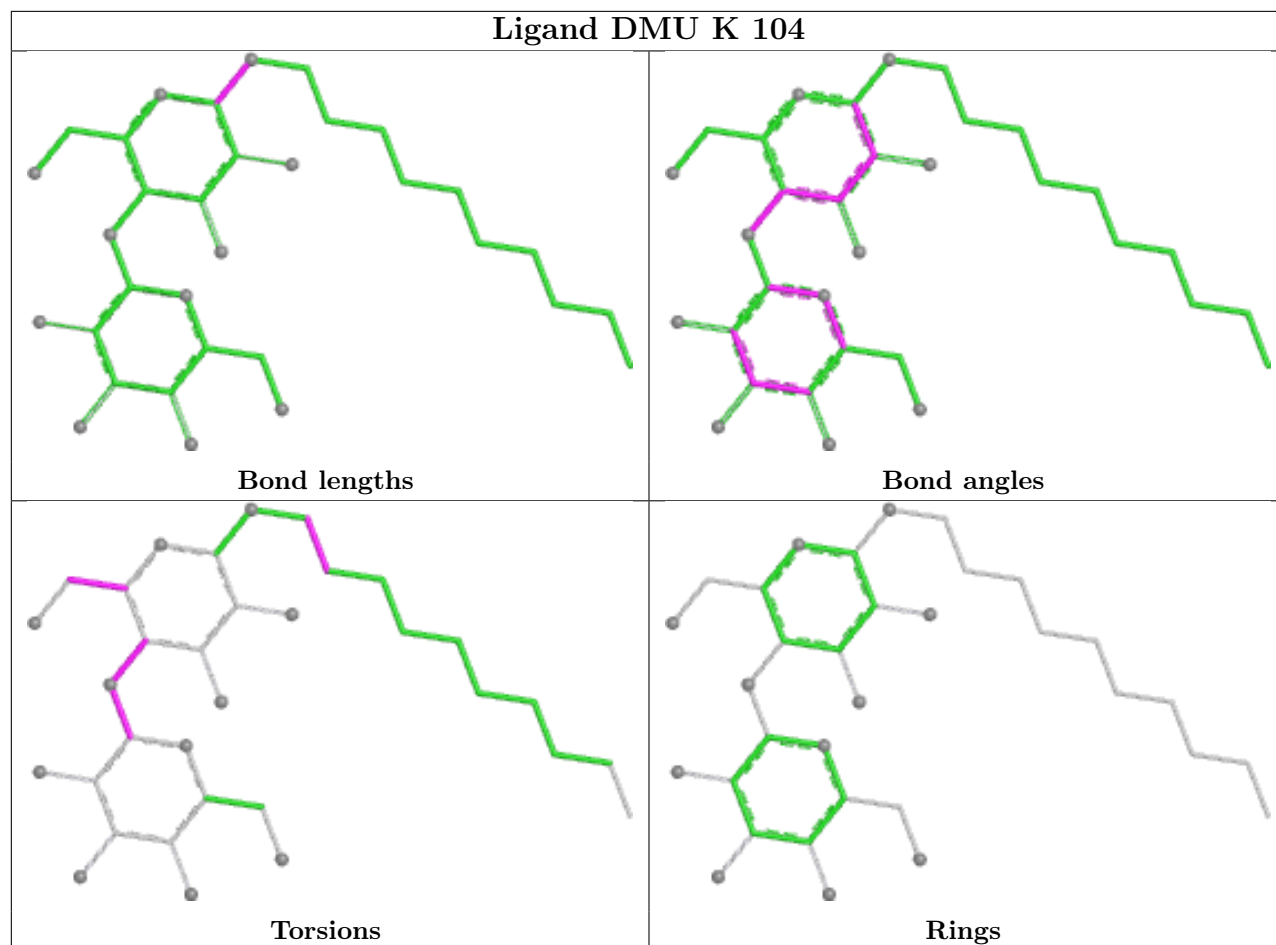


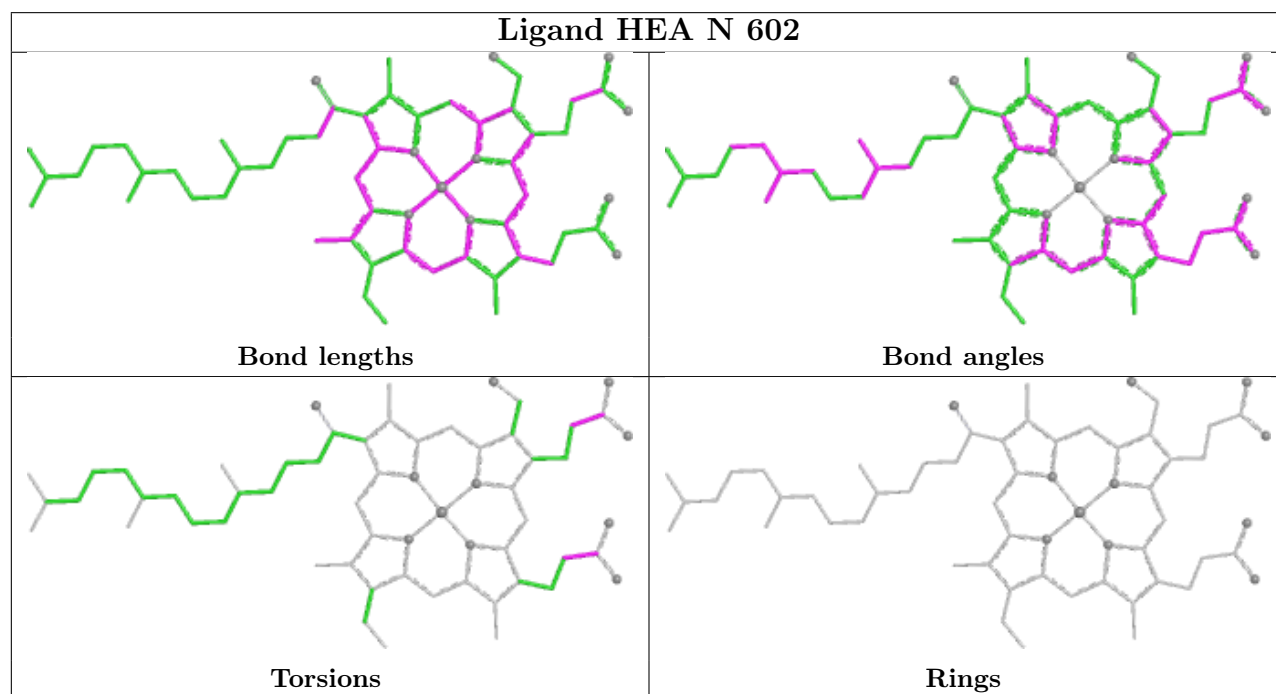
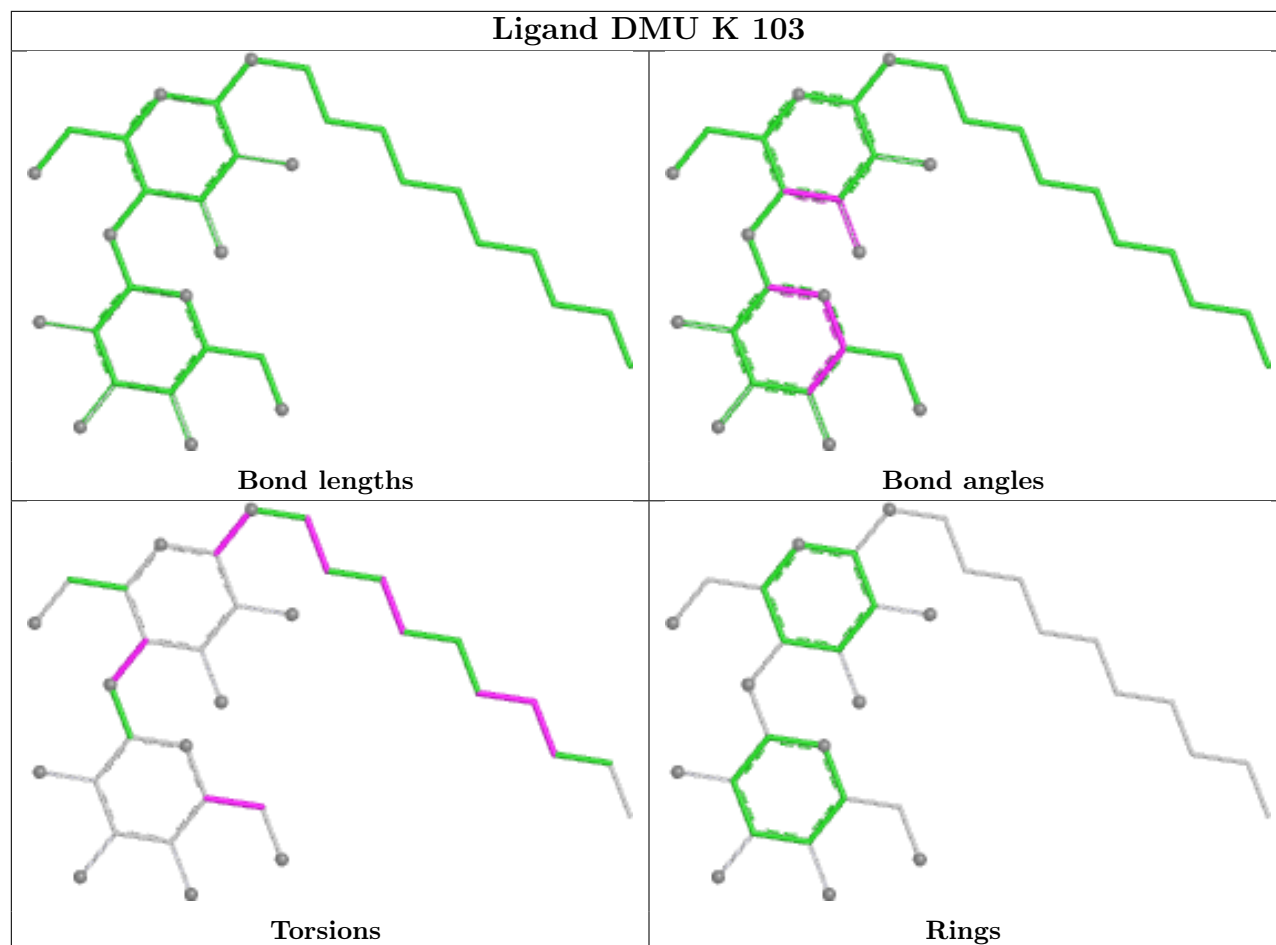


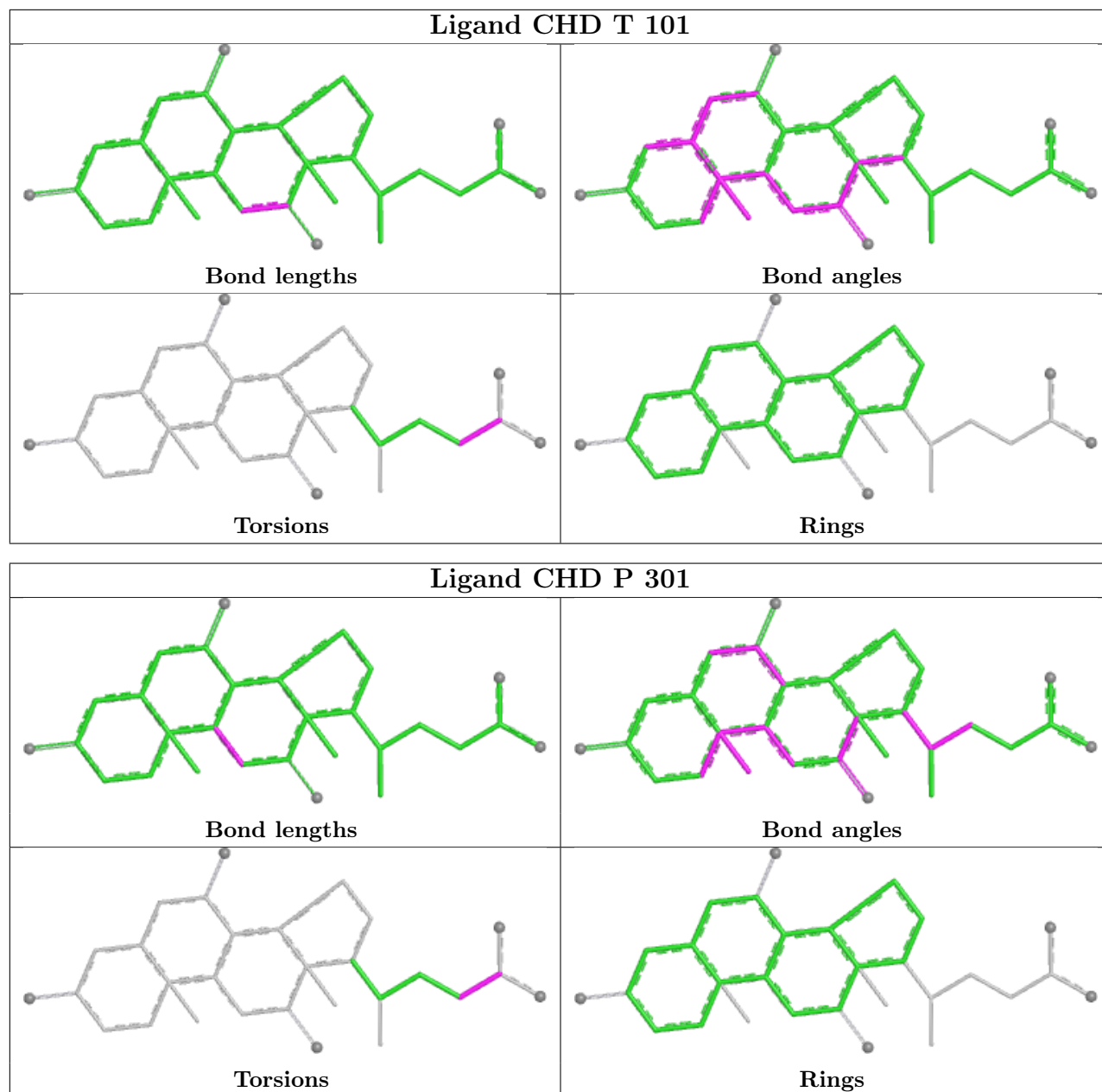


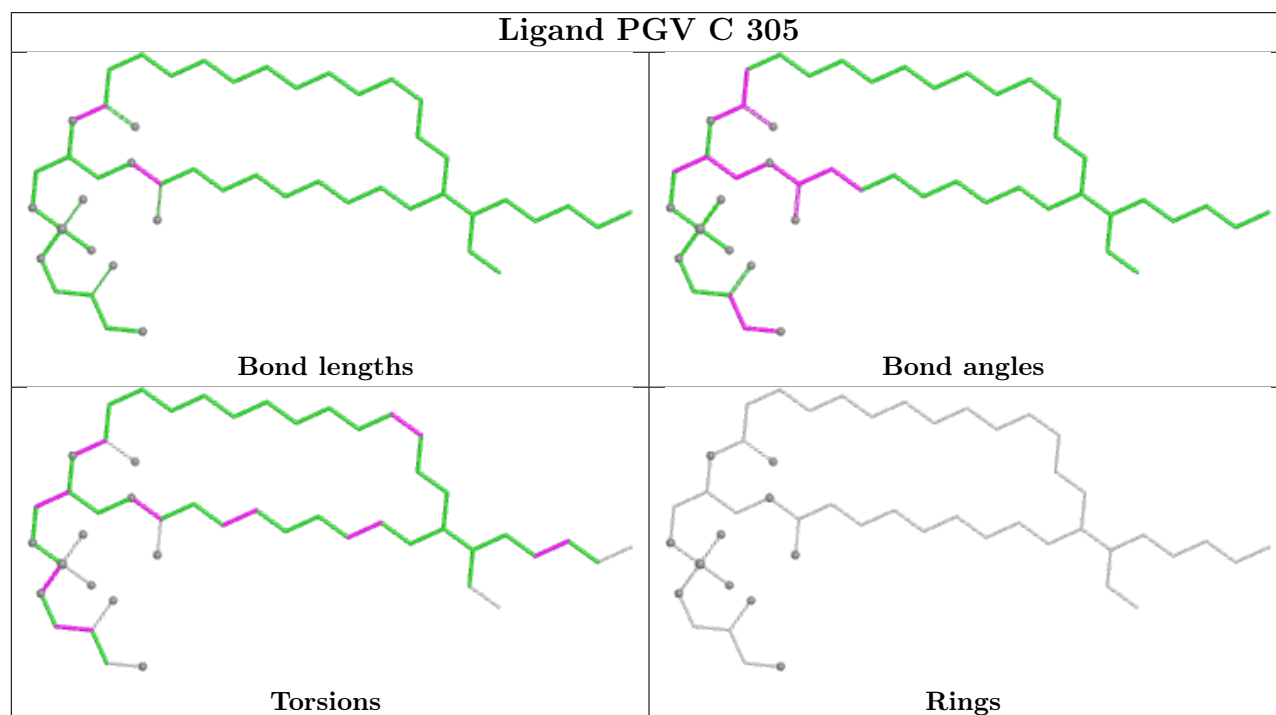
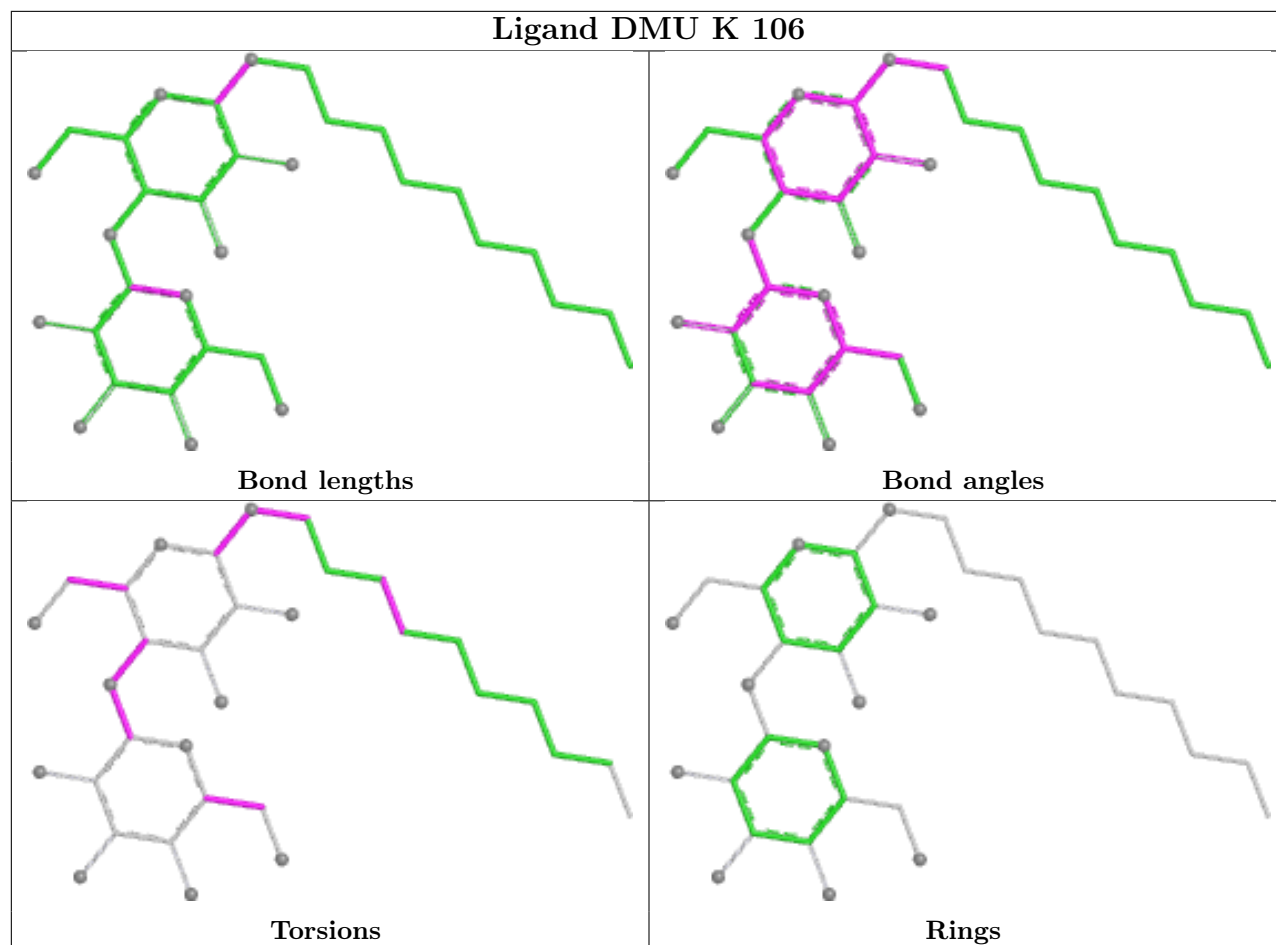


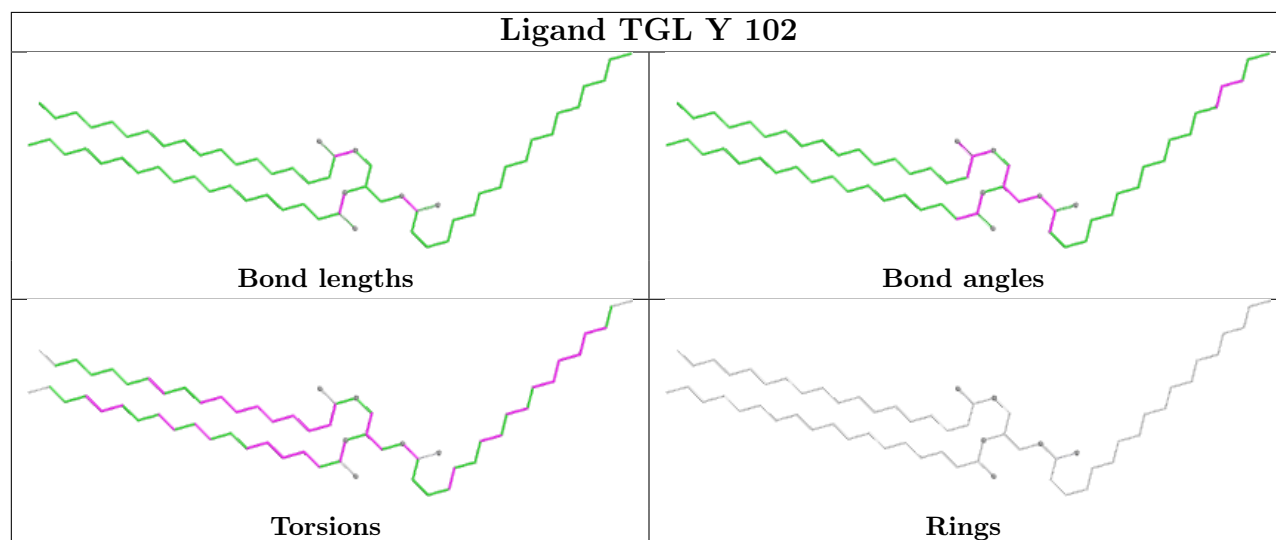
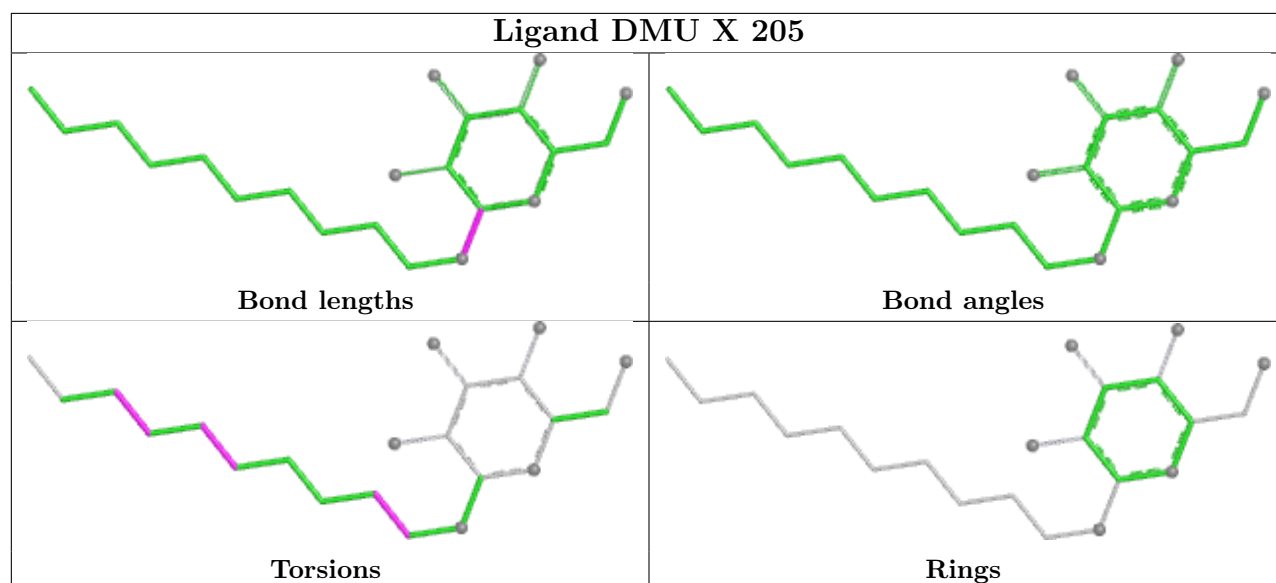
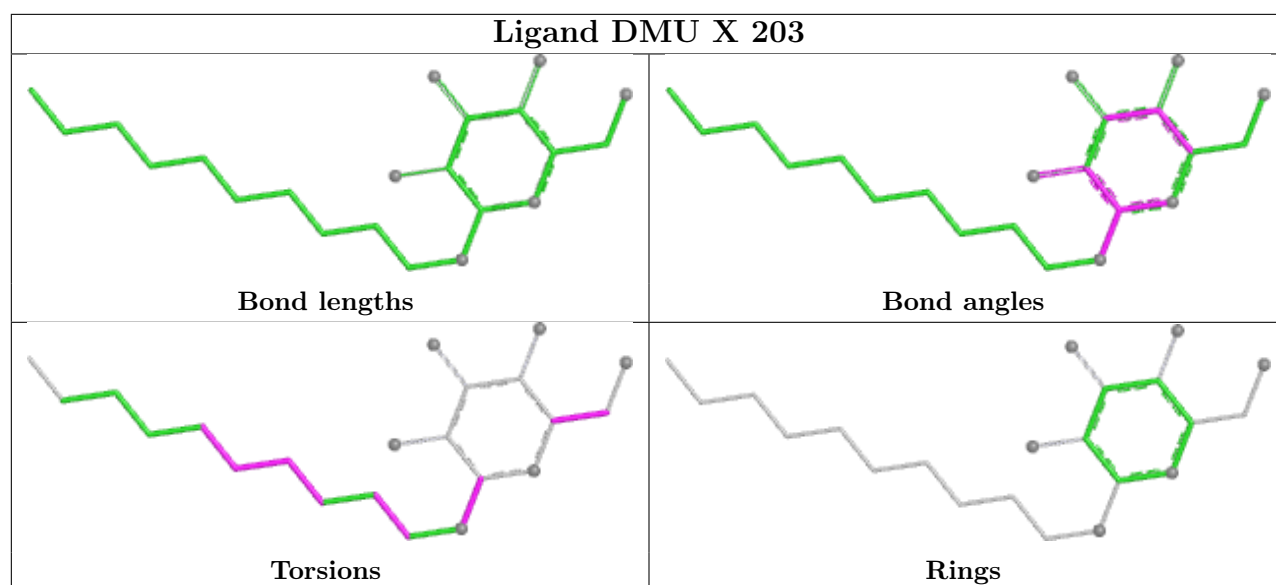




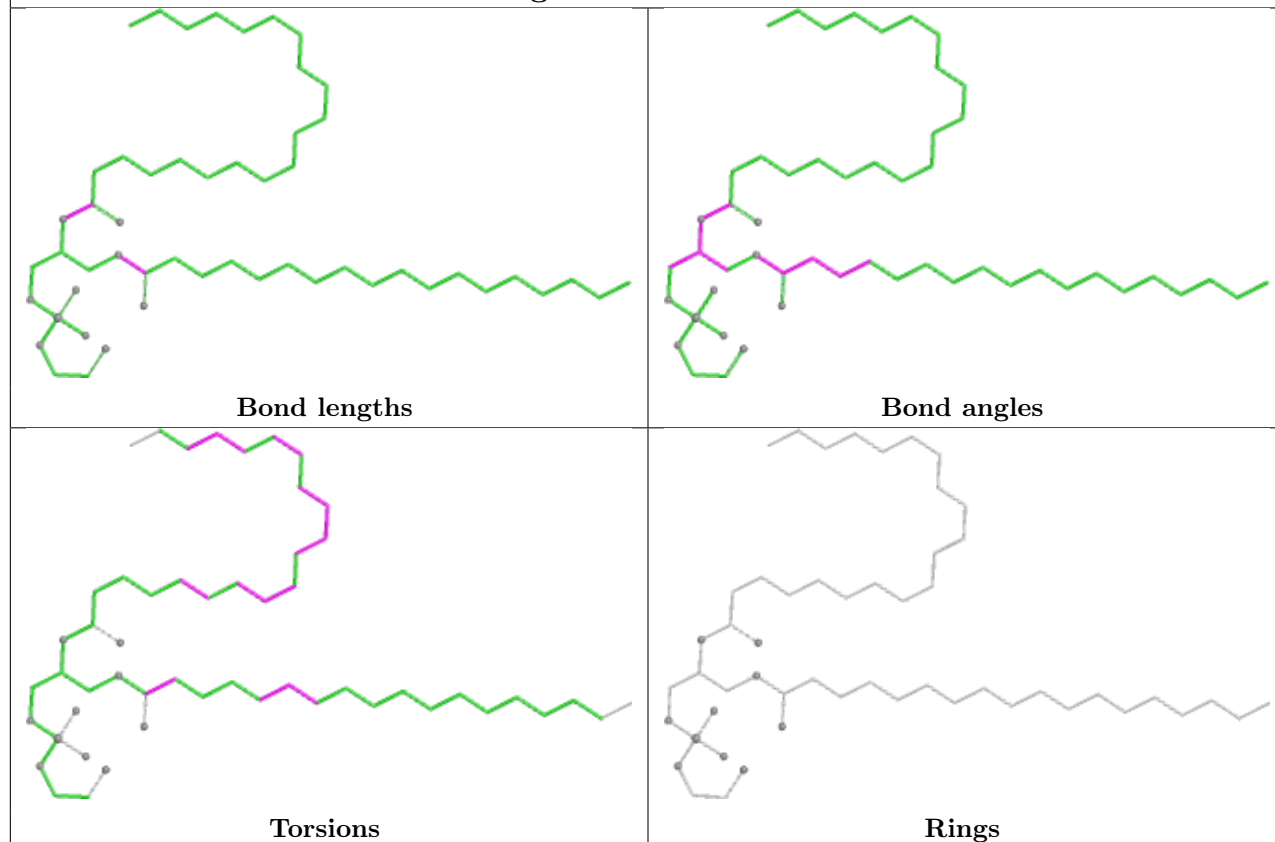




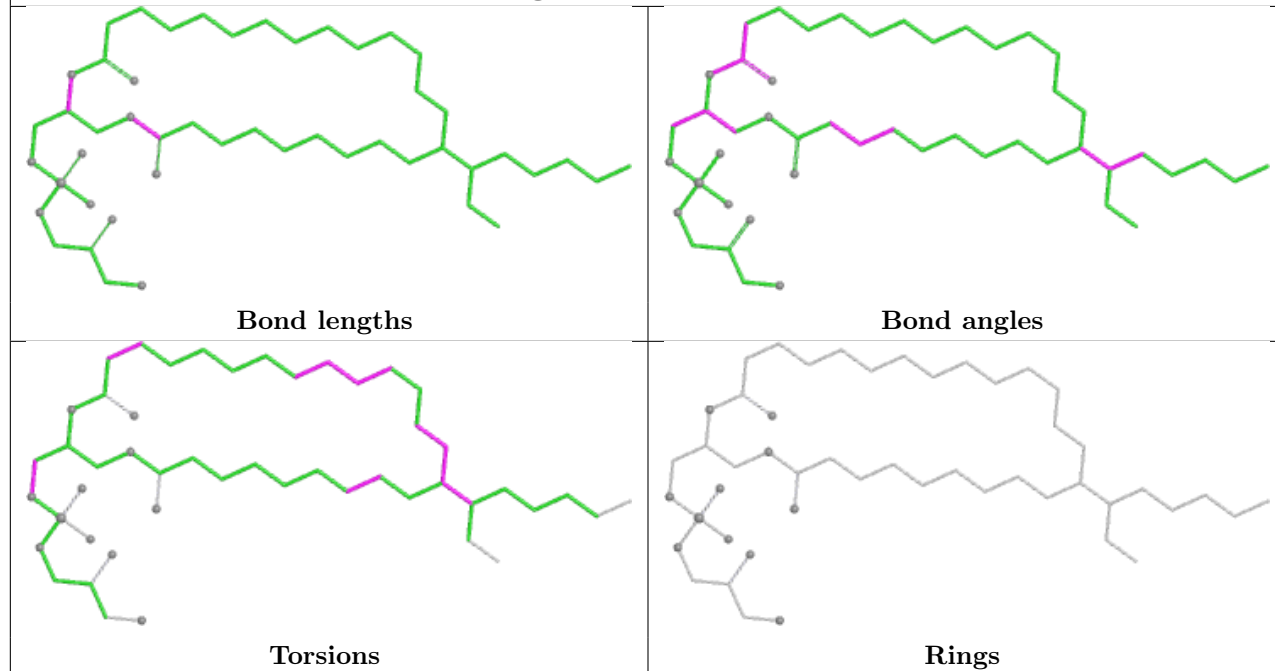


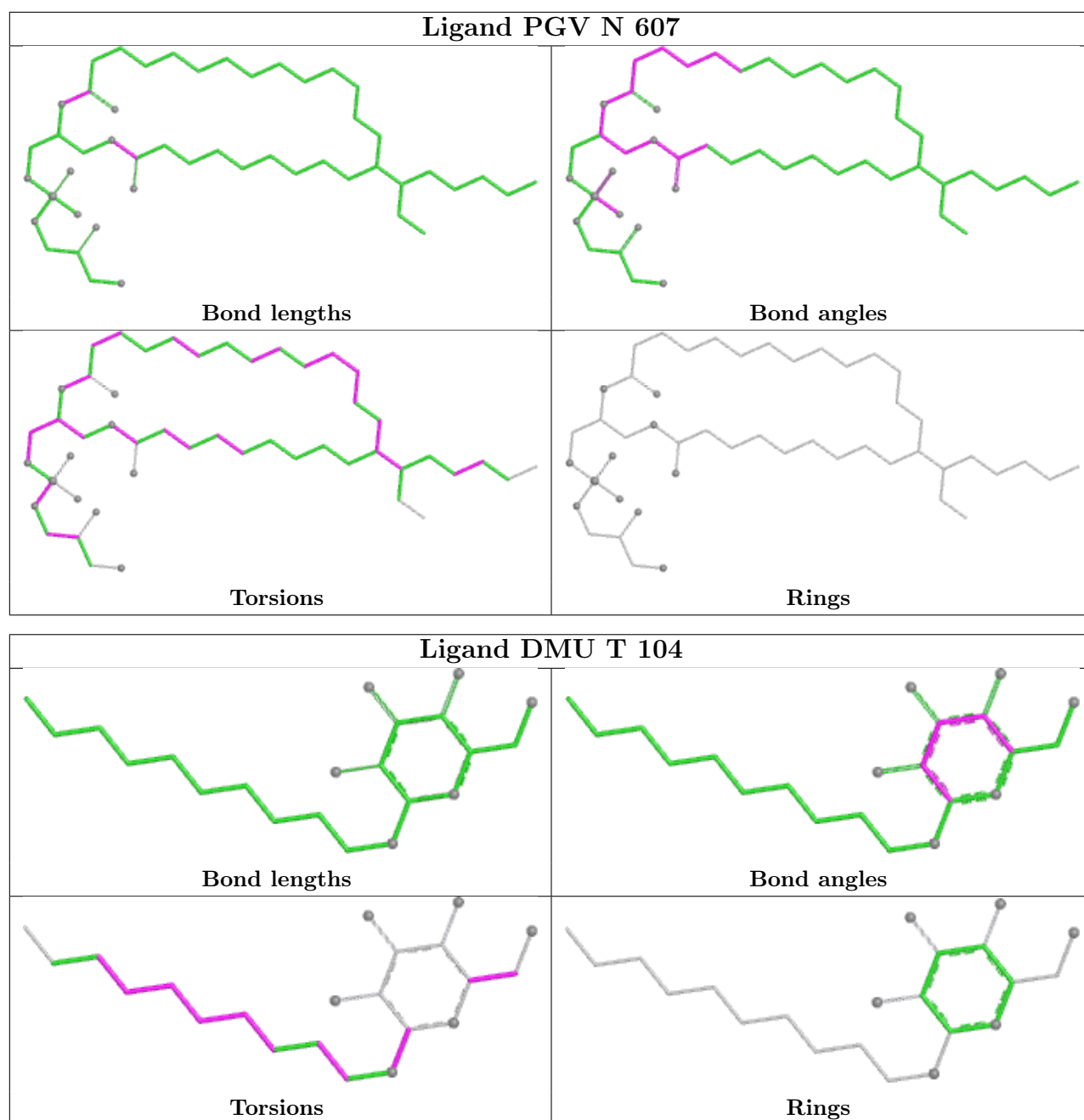


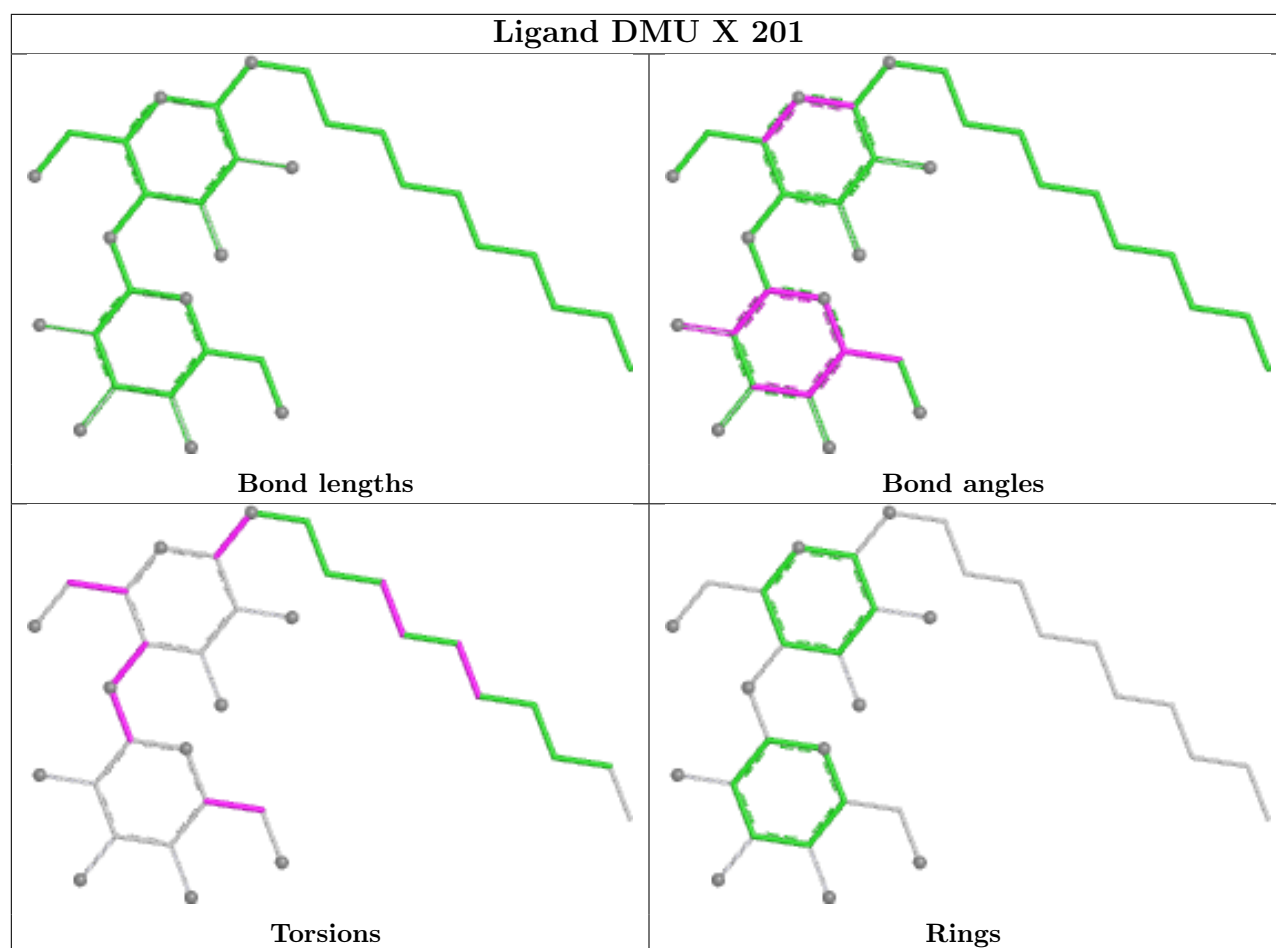
Ligand PEK C 302

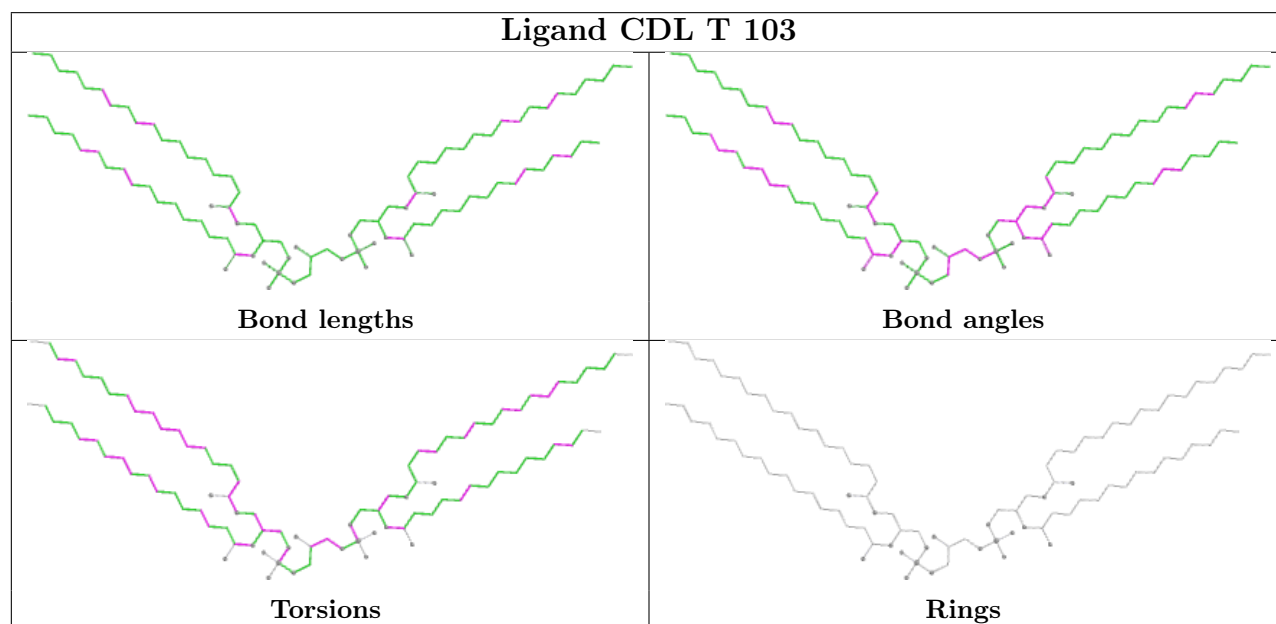
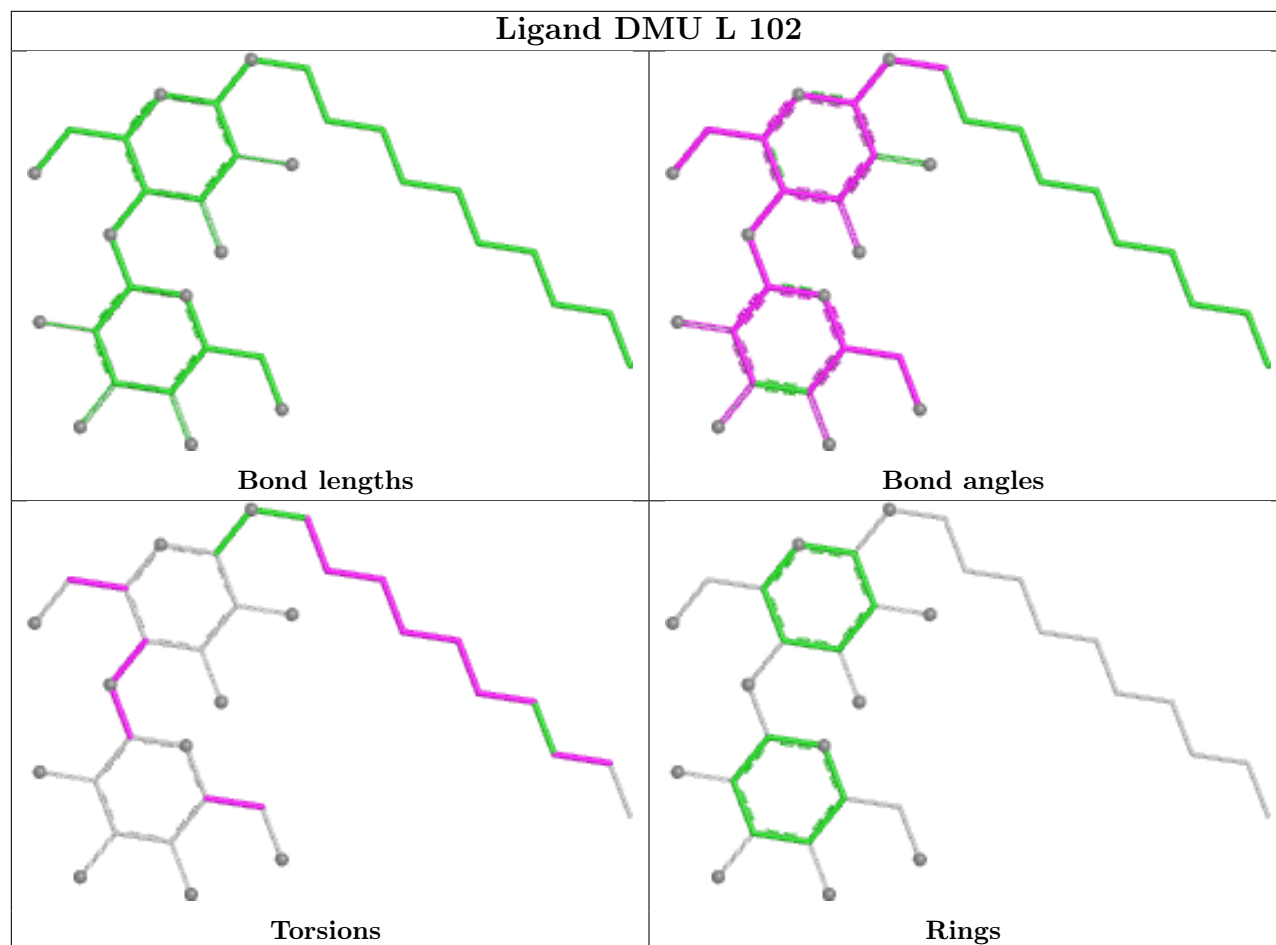


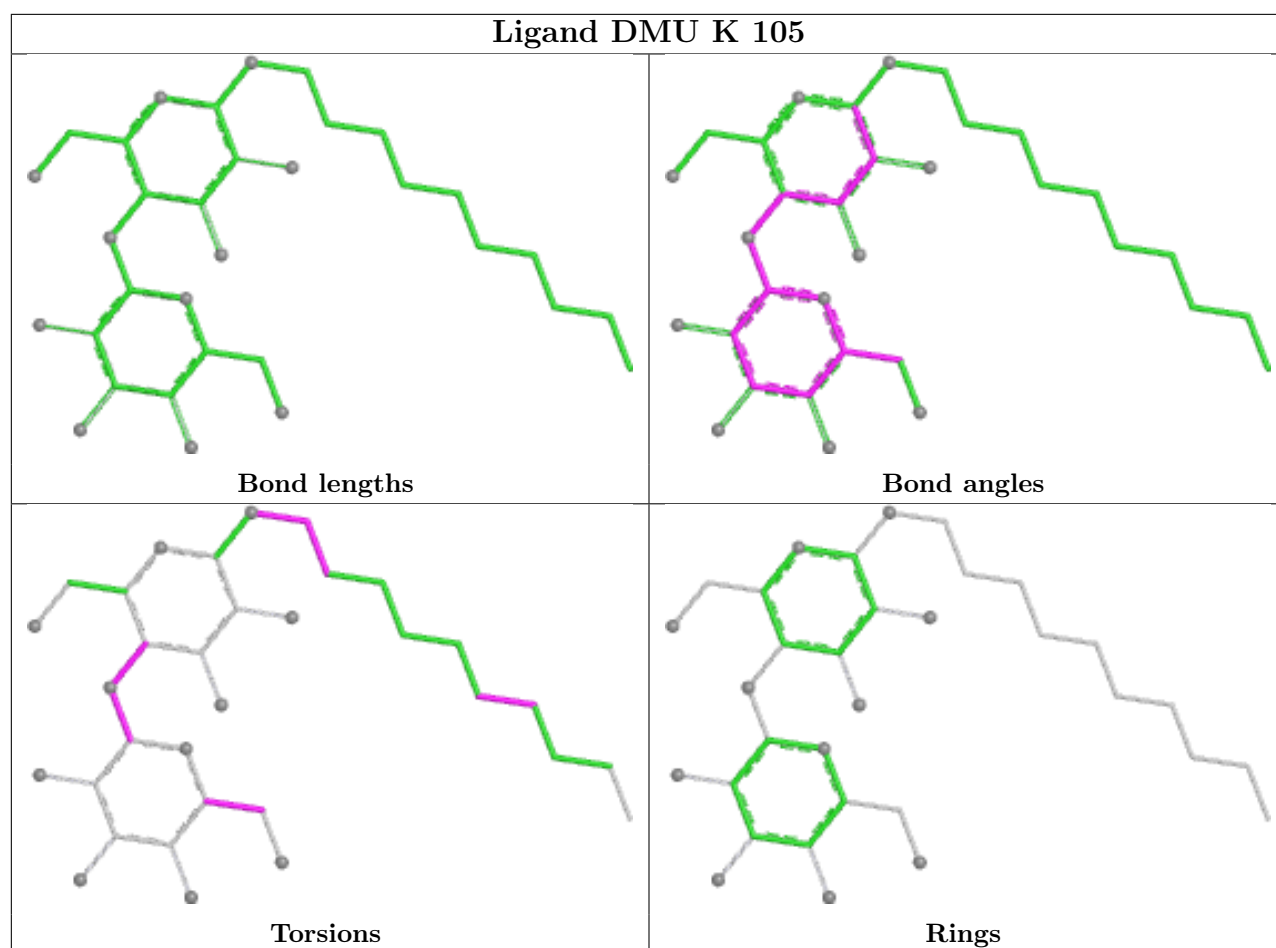
Ligand PGV P 305

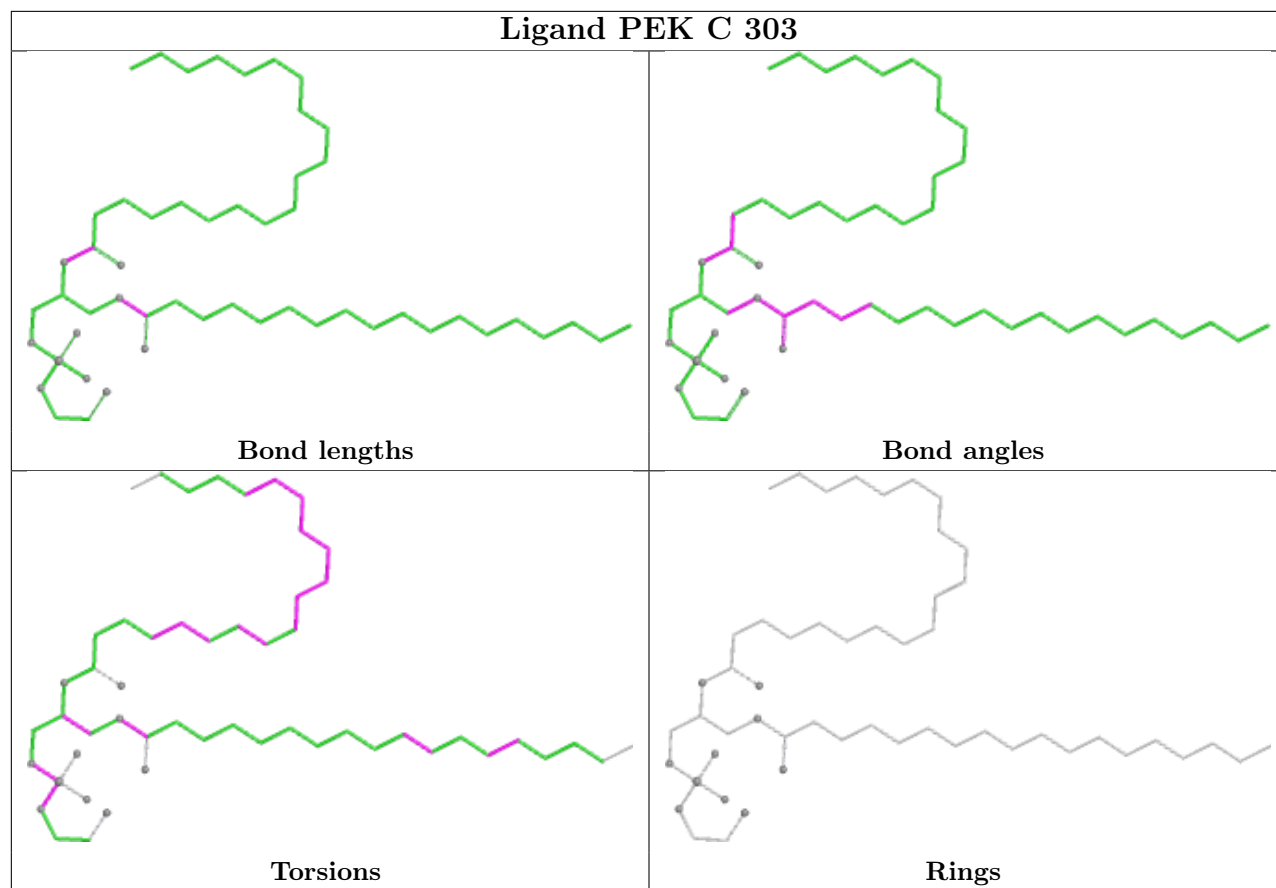


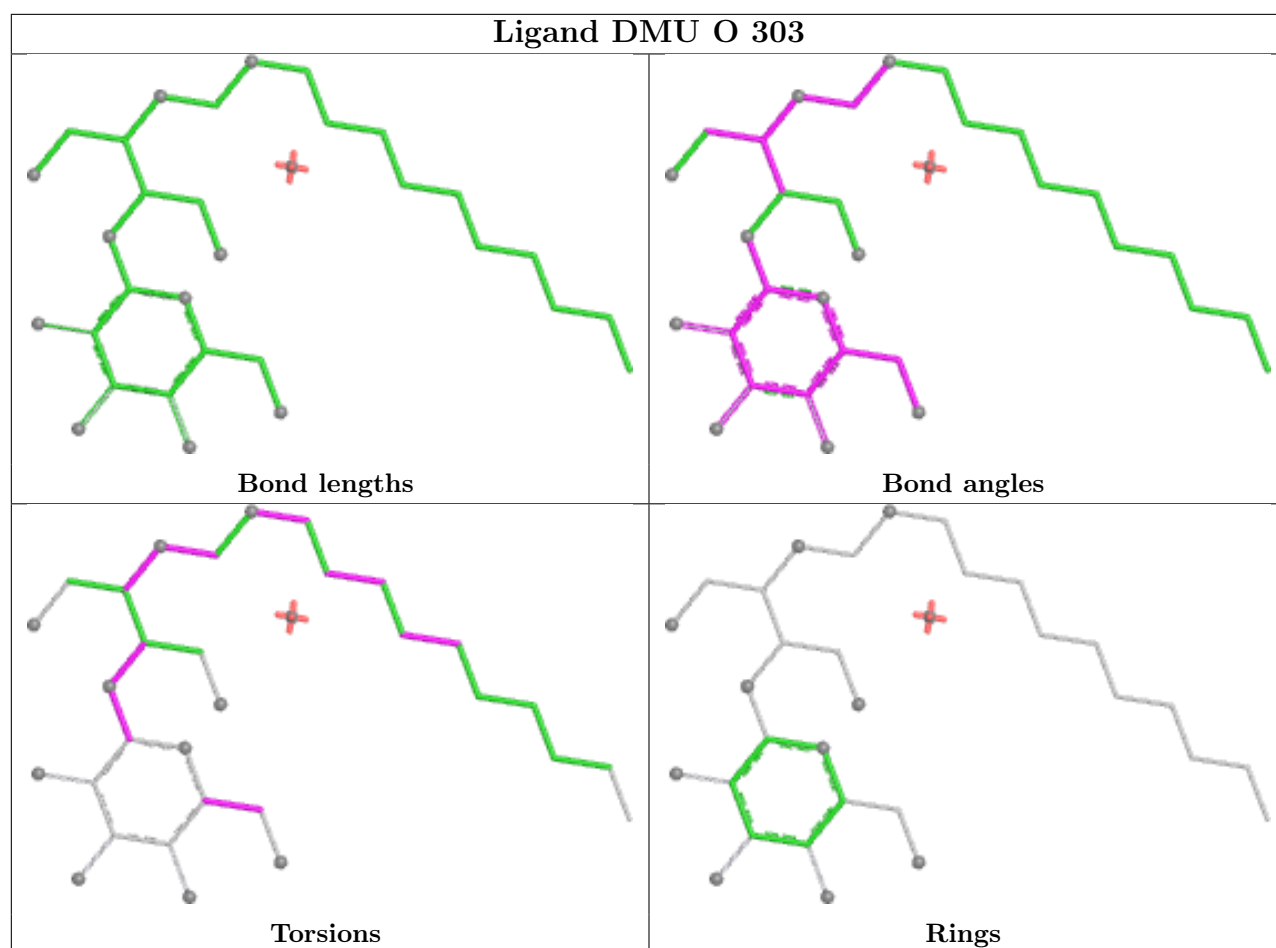


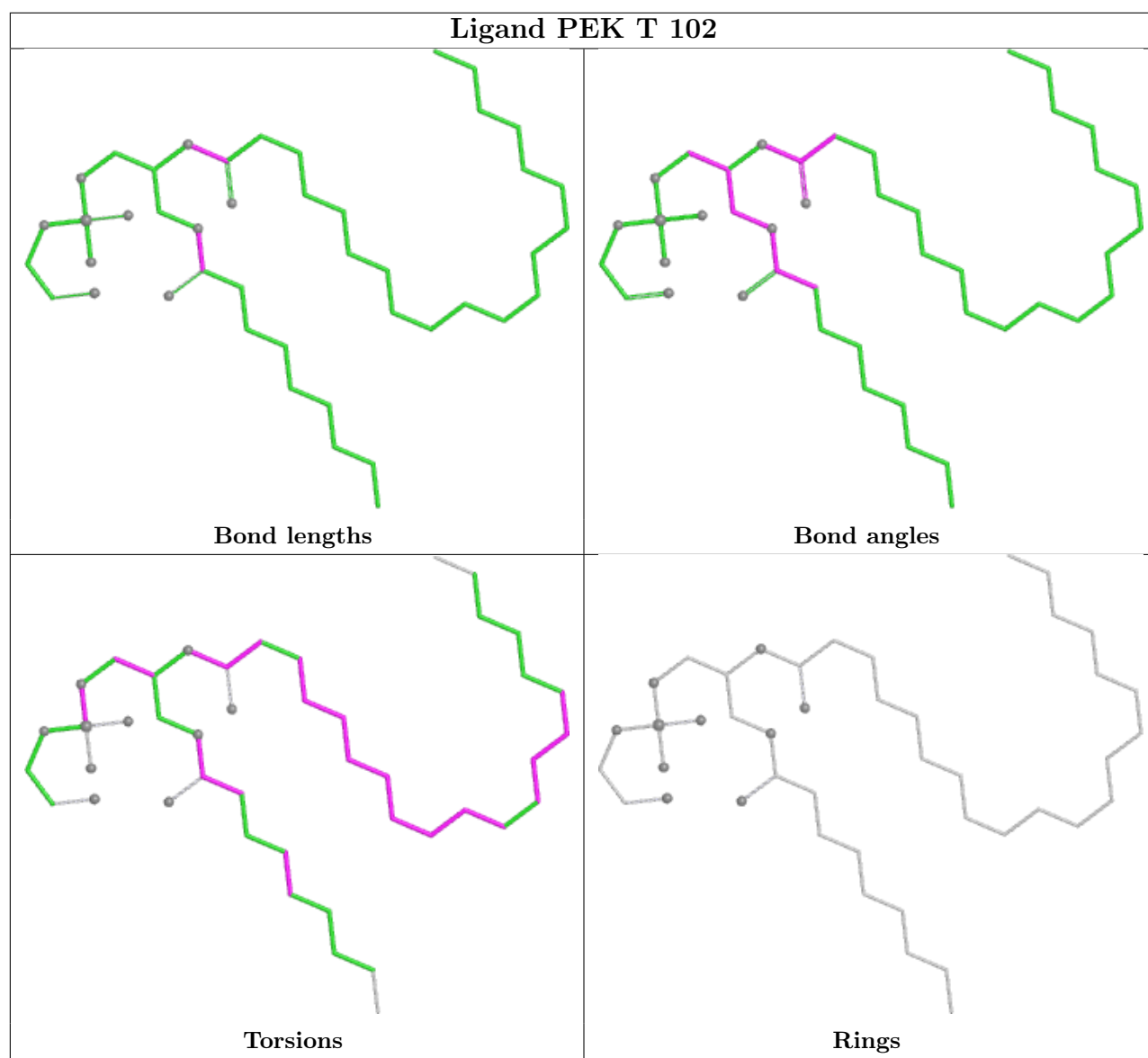


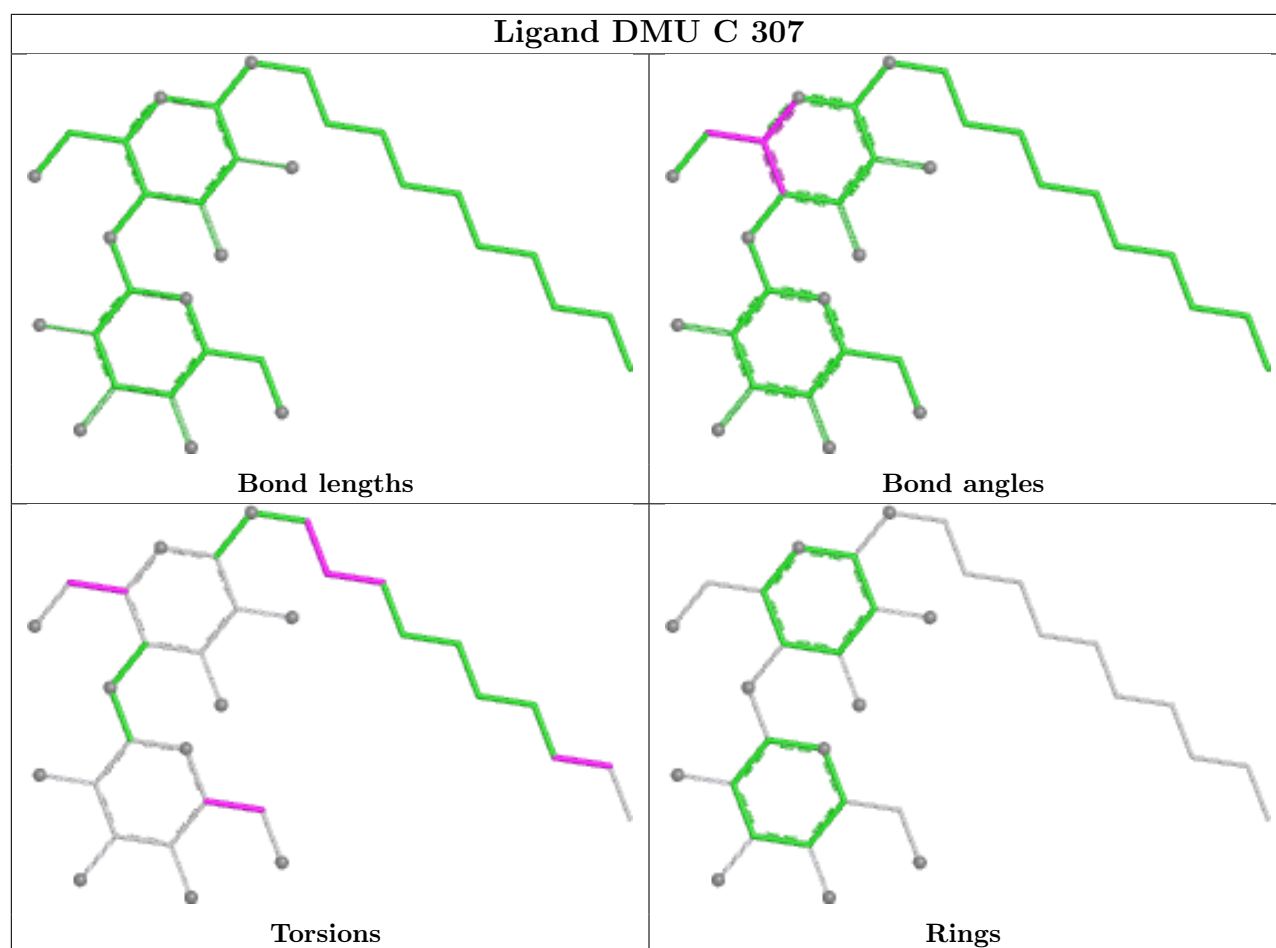


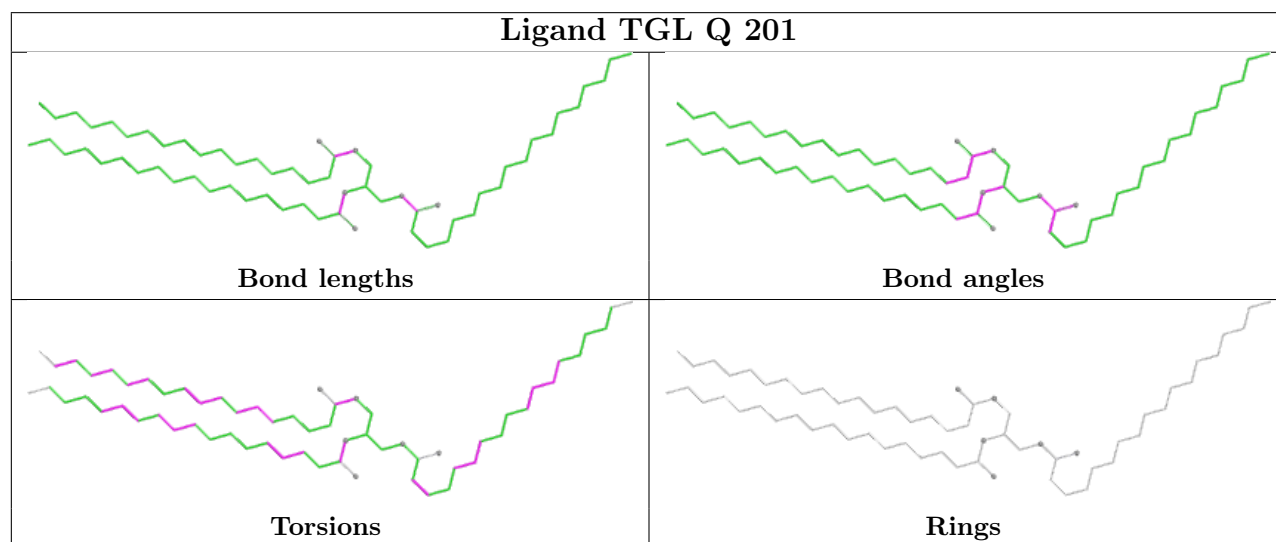
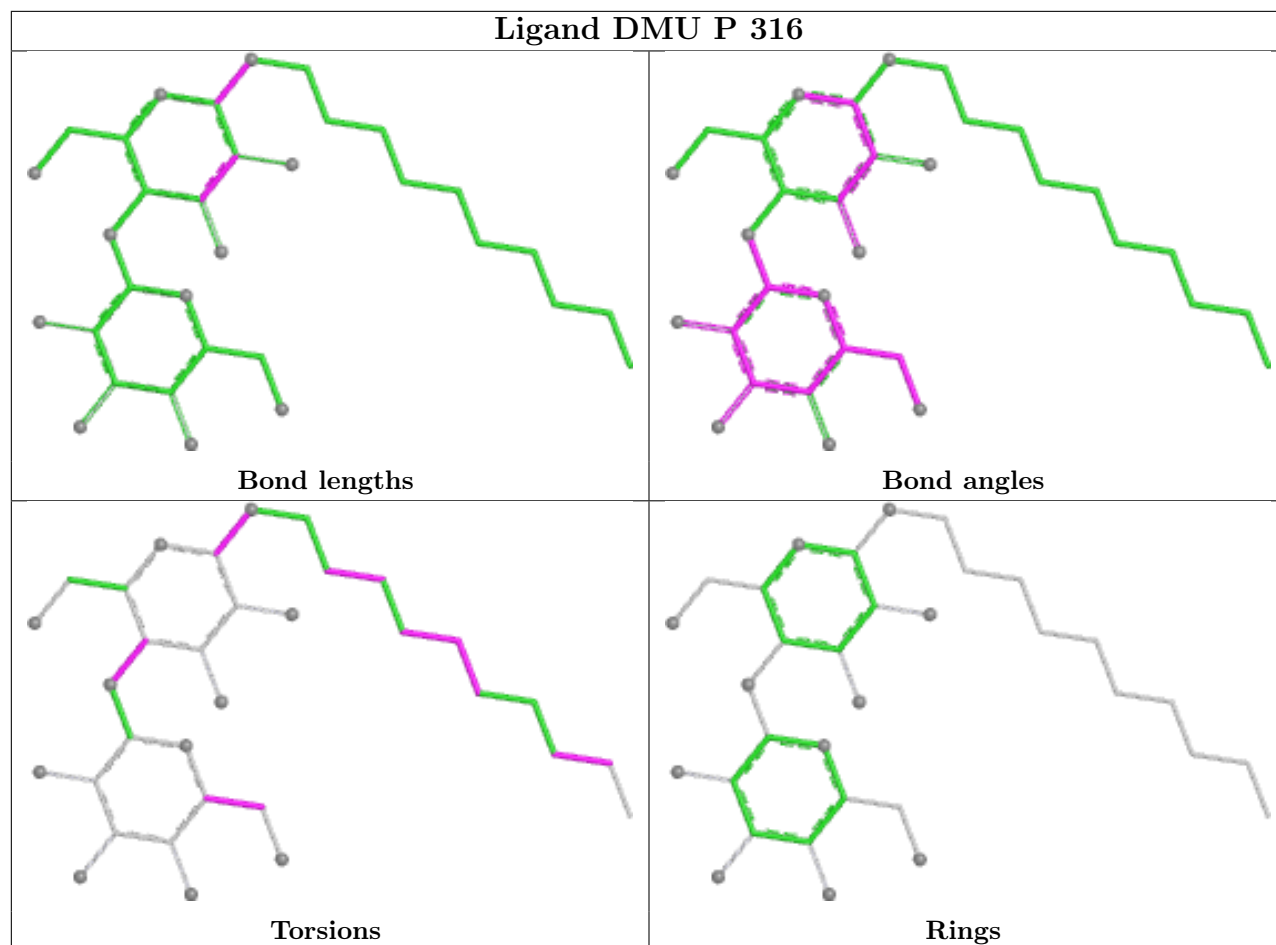


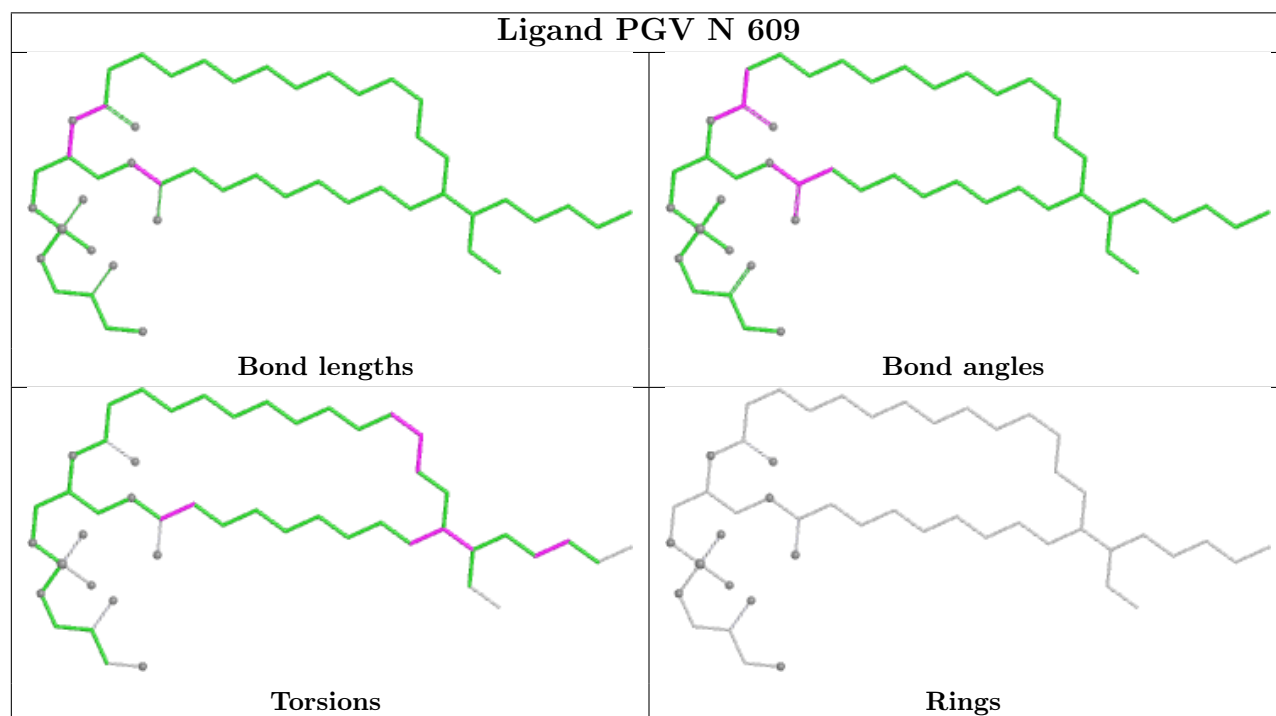
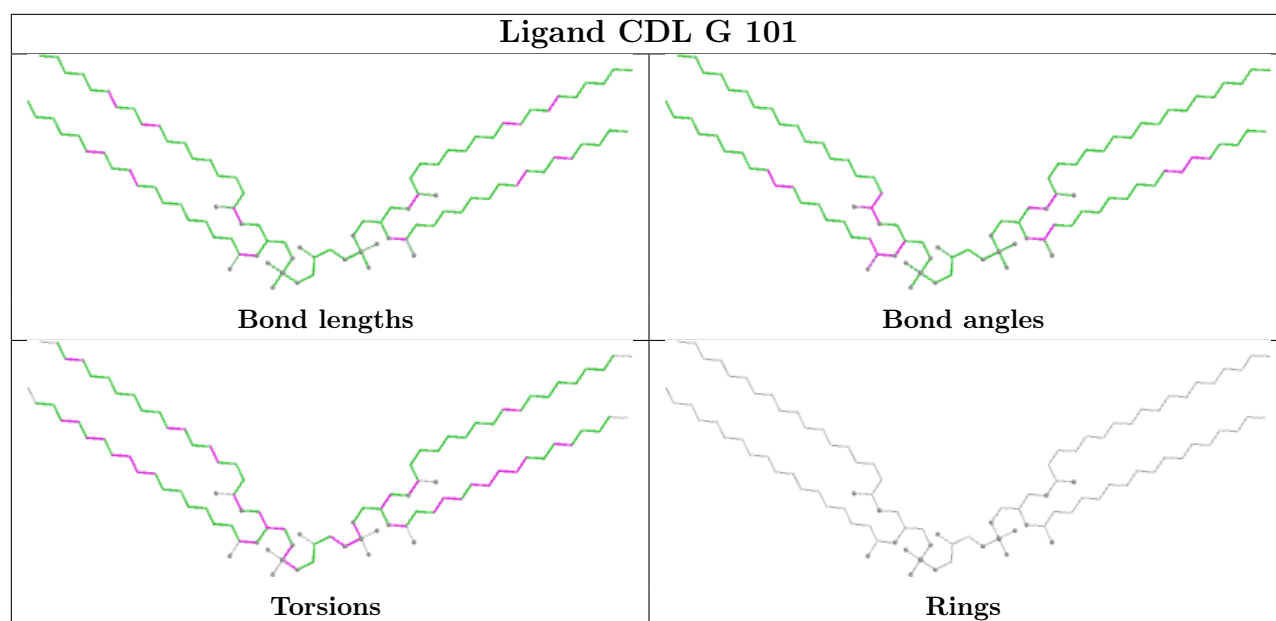


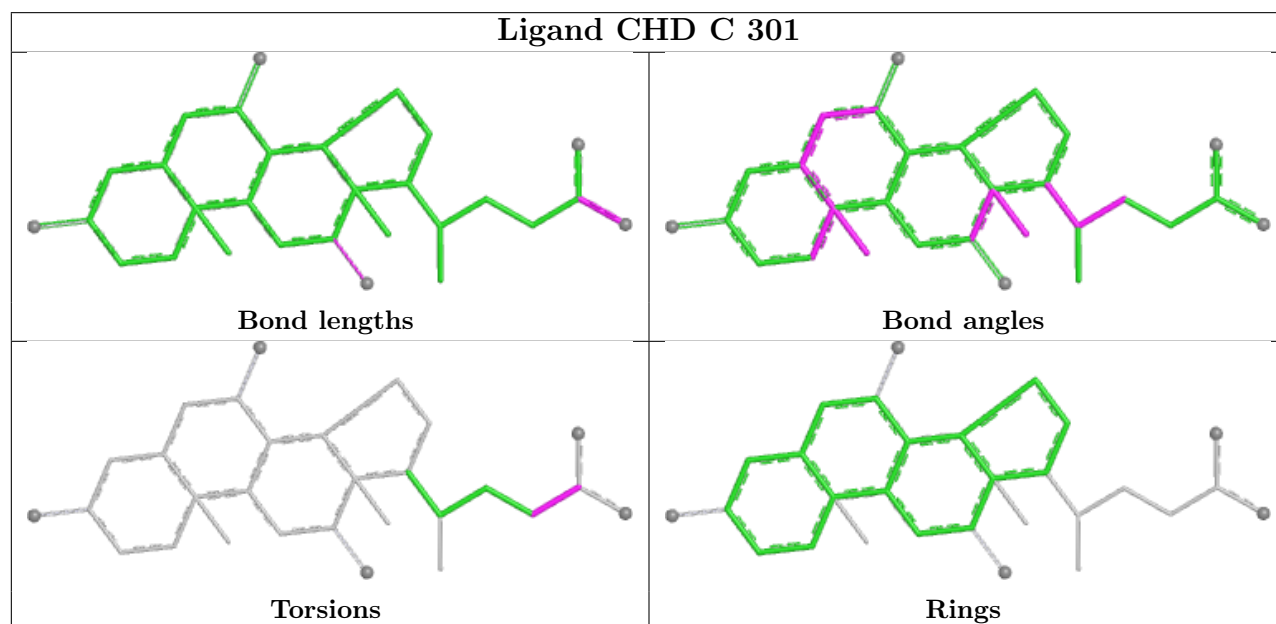
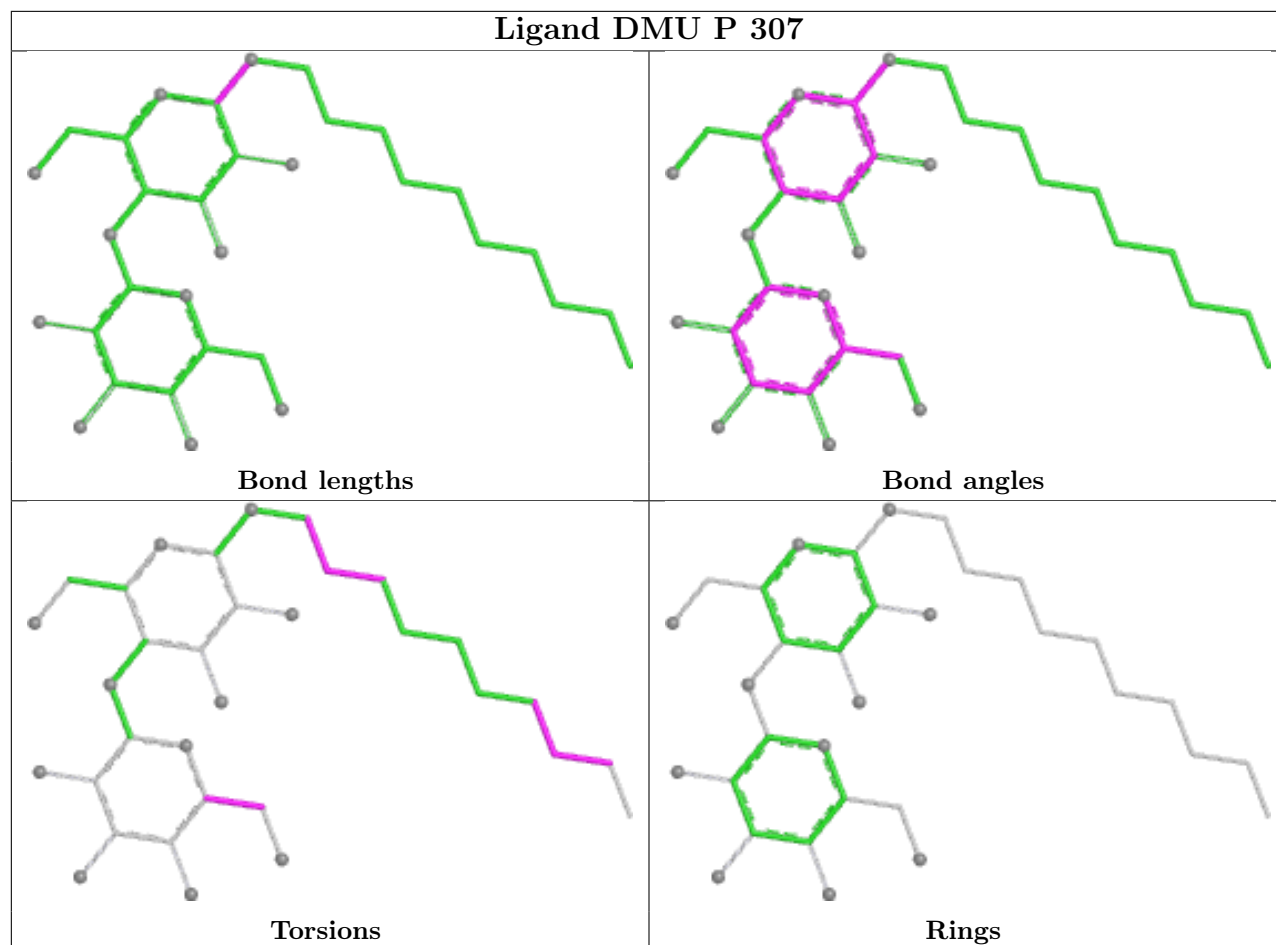


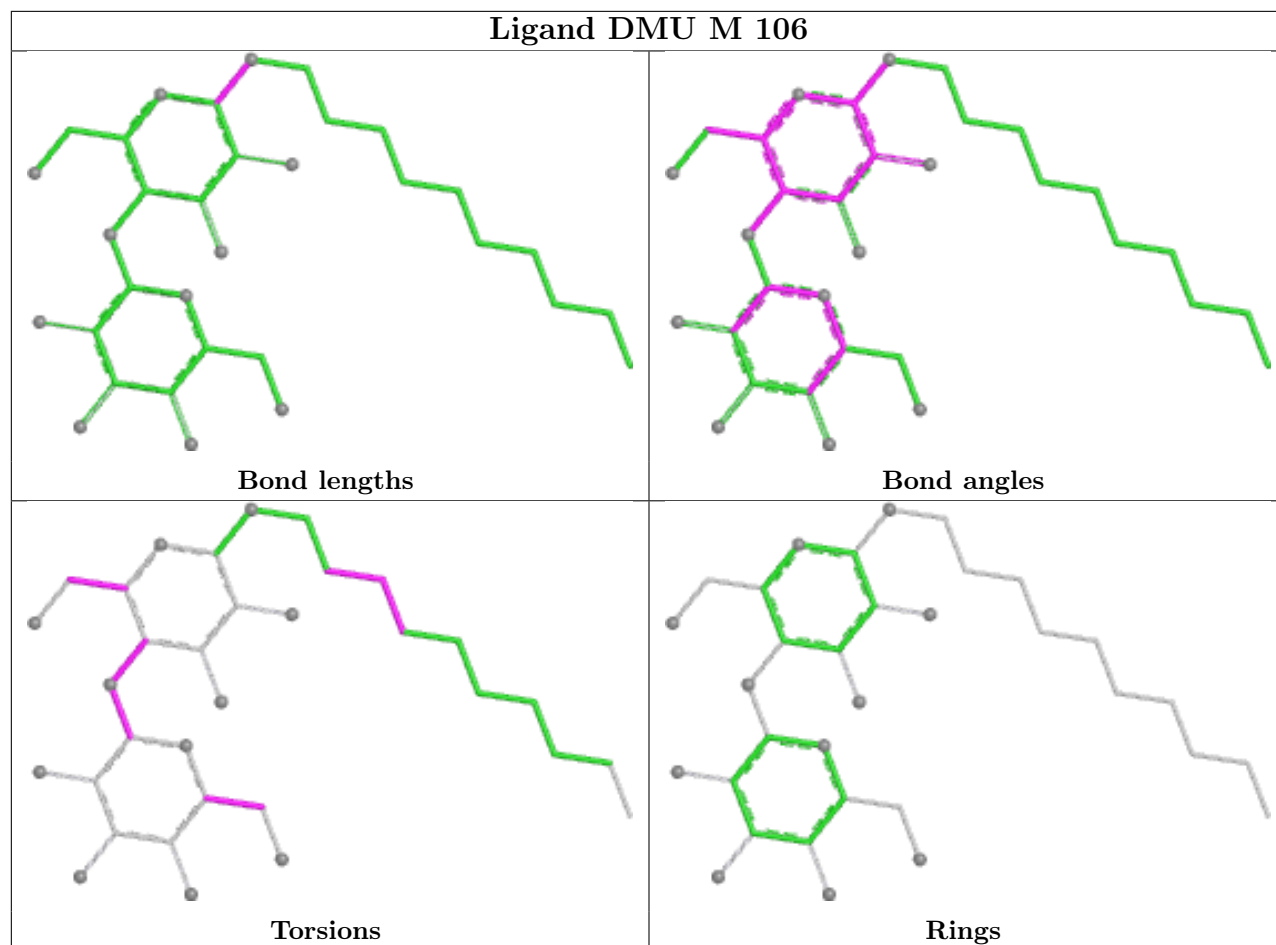


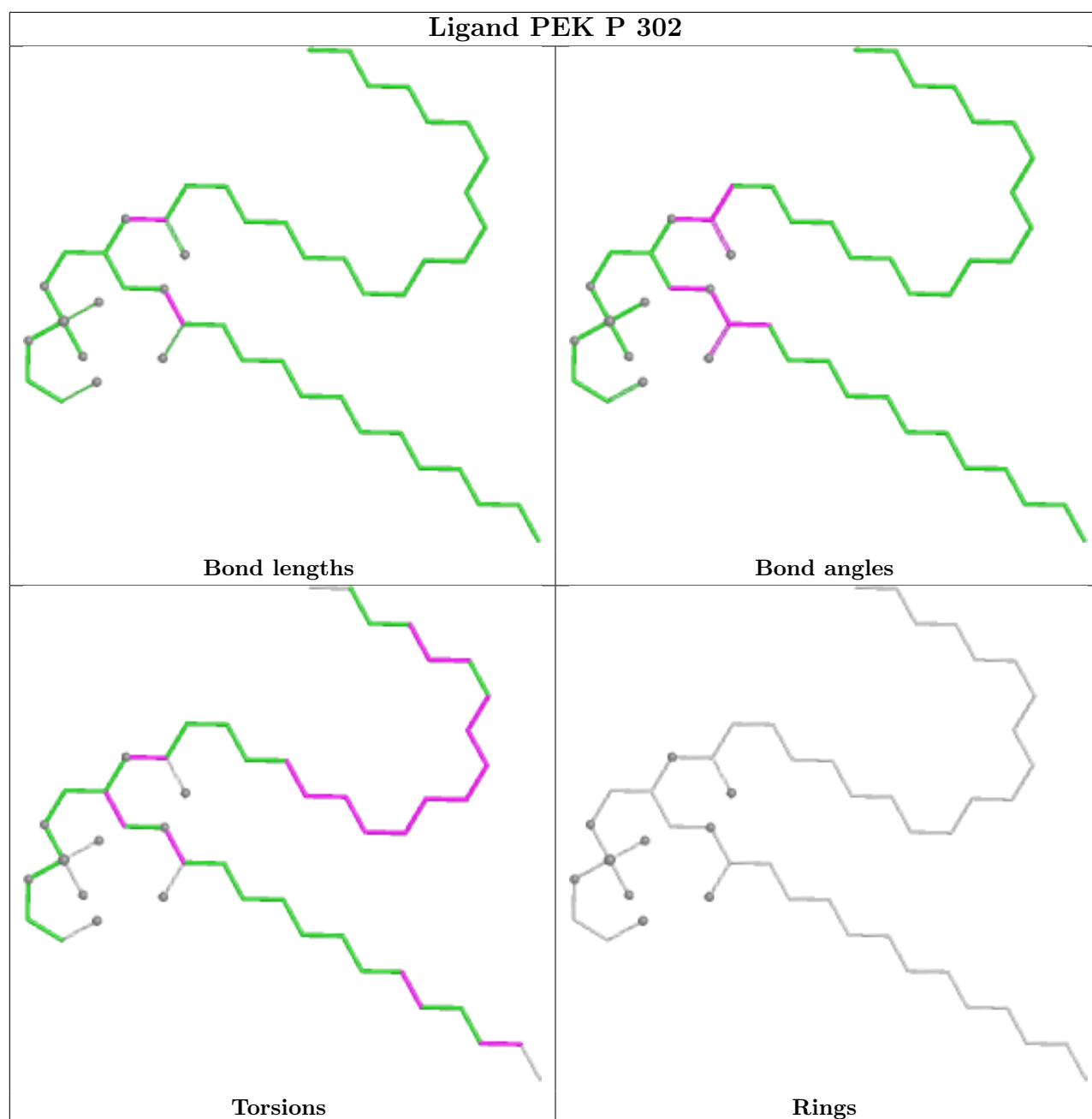




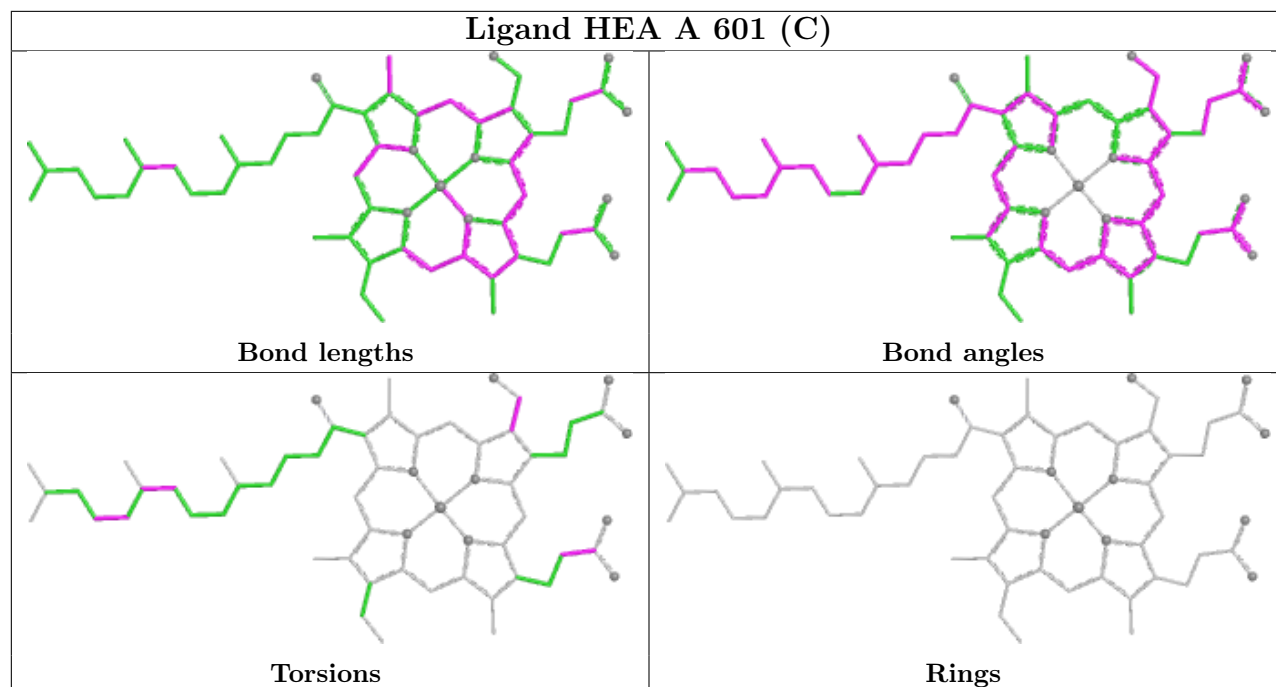




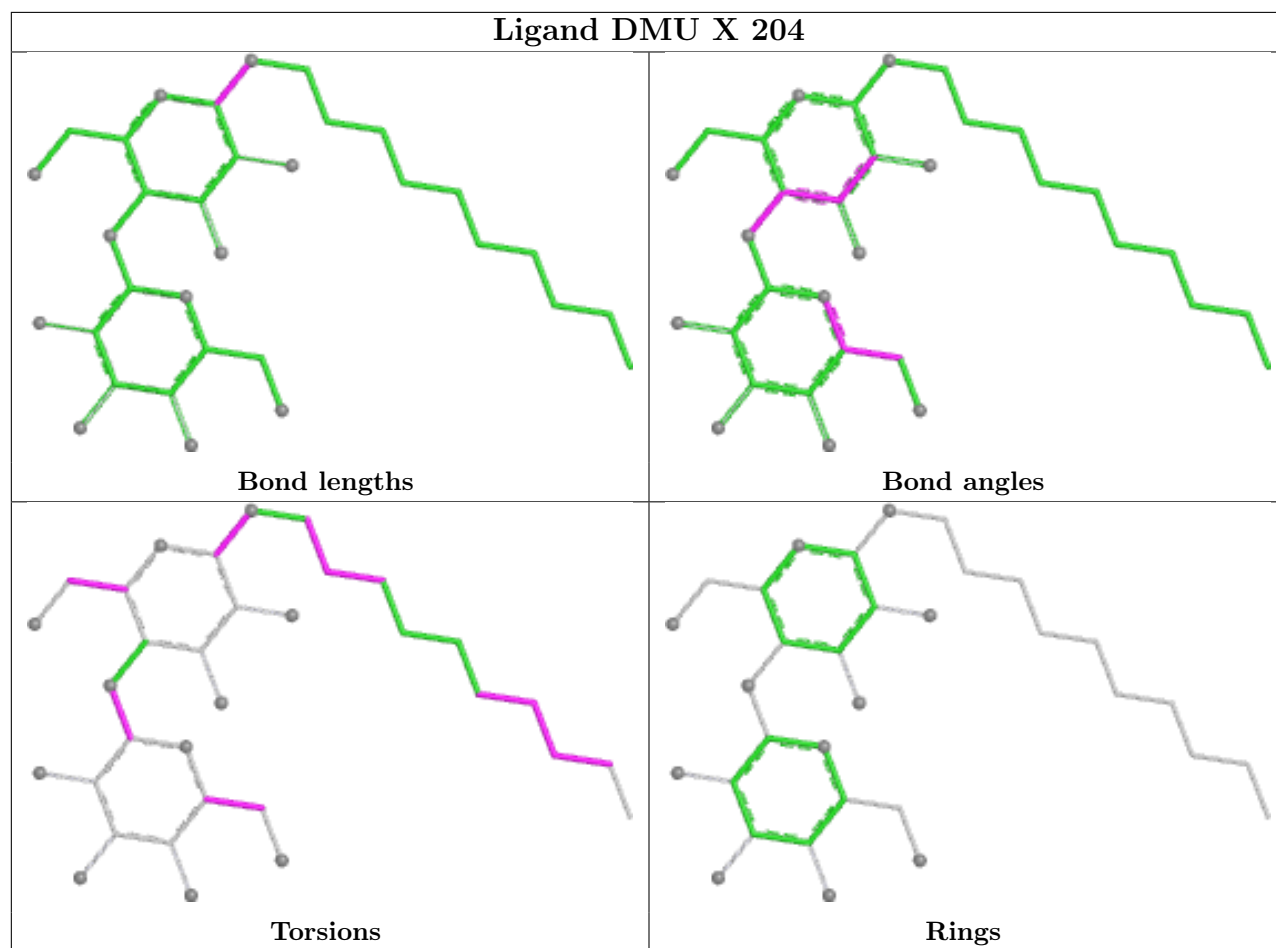


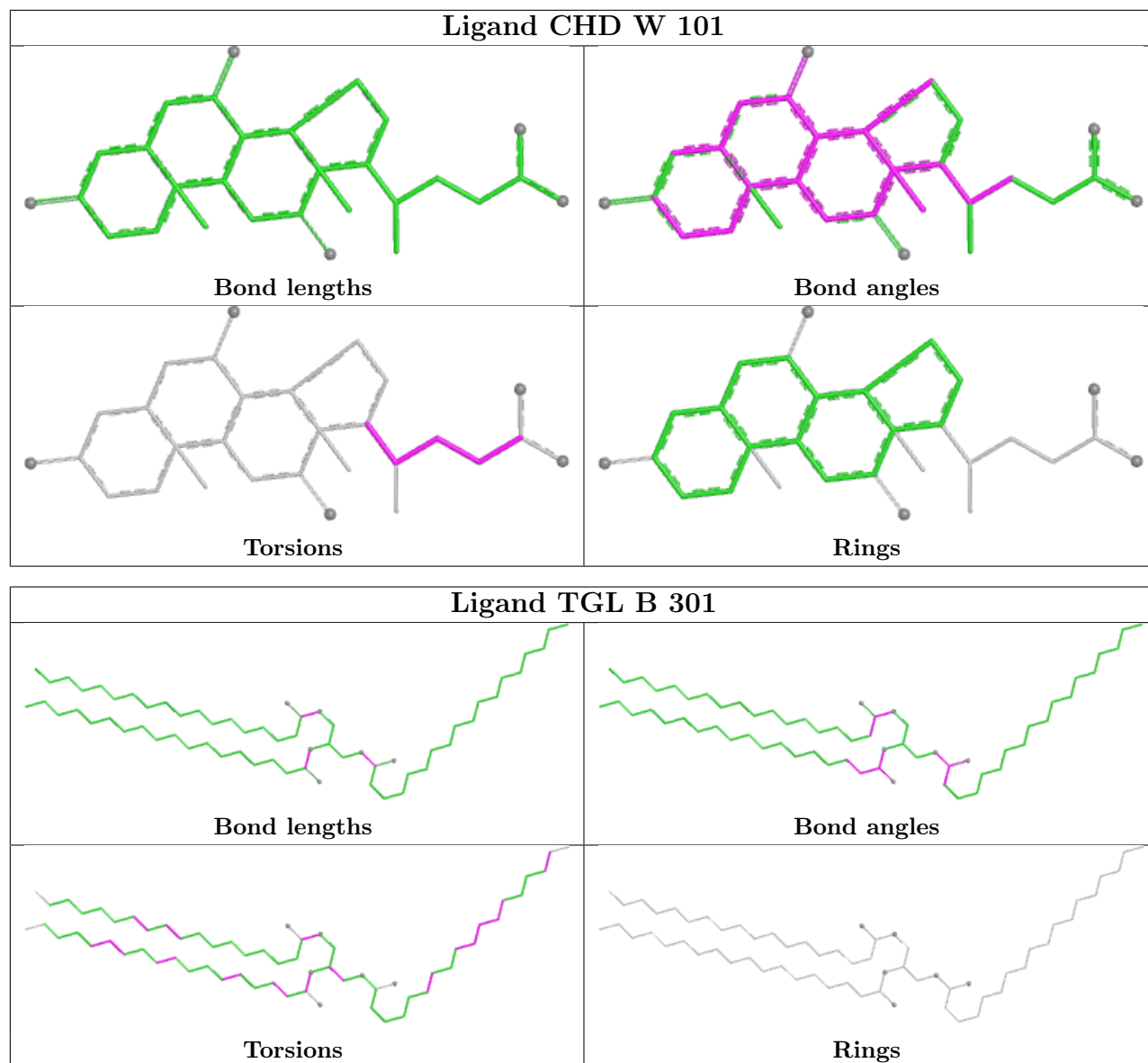


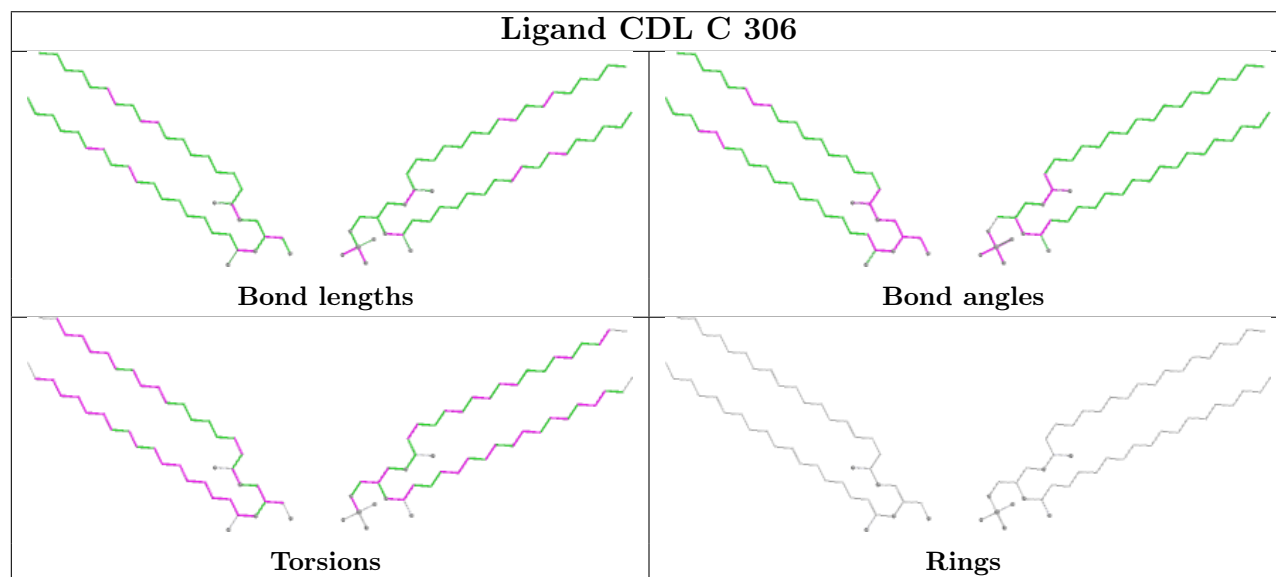
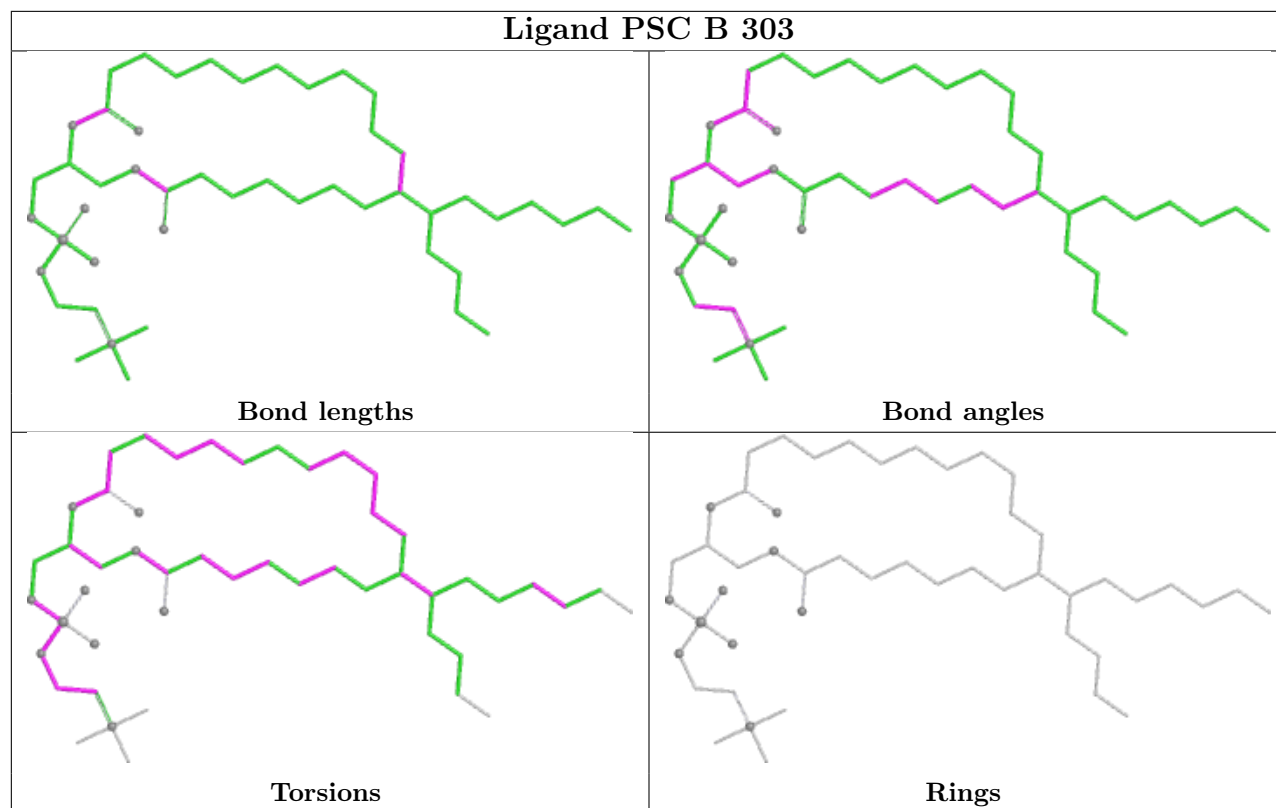
Ligand HEA A 601 (C)

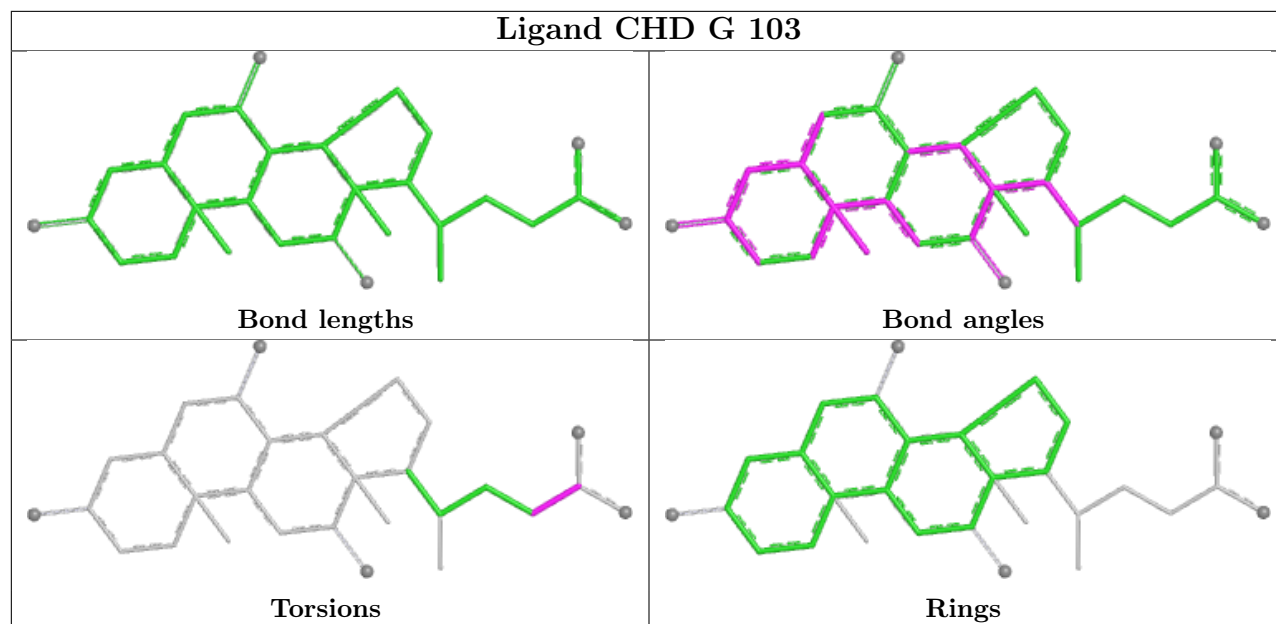


Ligand DMU X 204









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%)	-0.49	3 (0%) 85 92	10, 23, 30, 89	39 (7%)
1	N	513/514 (99%)	-0.43	3 (0%) 85 92	11, 25, 33, 78	36 (7%)
2	B	226/227 (99%)	0.07	15 (6%) 24 30	21, 29, 53, 128	12 (5%)
2	O	226/227 (99%)	0.12	8 (3%) 47 55	23, 33, 70, 109	11 (4%)
3	C	259/259 (100%)	-0.24	5 (1%) 66 74	18, 26, 41, 102	7 (2%)
3	P	259/259 (100%)	-0.22	4 (1%) 72 80	17, 27, 41, 93	8 (3%)
4	D	144/144 (100%)	0.03	7 (4%) 35 43	21, 33, 54, 97	2 (1%)
4	Q	144/144 (100%)	0.91	19 (13%) 7 9	30, 45, 96, 266	1 (0%)
5	E	105/105 (100%)	0.02	3 (2%) 53 60	26, 32, 64, 139	0
5	R	105/105 (100%)	0.28	2 (1%) 66 74	27, 38, 76, 133	0
6	F	94/94 (100%)	0.28	5 (5%) 32 40	22, 33, 64, 125	2 (2%)
6	S	94/94 (100%)	0.32	6 (6%) 25 32	22, 32, 63, 150	0
7	G	83/84 (98%)	1.25	20 (24%) 2 2	25, 35, 135, 234	0
7	T	83/84 (98%)	1.17	20 (24%) 2 2	24, 36, 122, 189	0
8	H	79/79 (100%)	0.72	12 (15%) 5 6	26, 37, 112, 126	0
8	U	79/79 (100%)	0.78	15 (18%) 3 4	30, 39, 111, 141	0
9	I	72/73 (98%)	0.84	11 (15%) 5 6	29, 43, 76, 96	0
9	V	72/73 (98%)	1.20	17 (23%) 2 2	28, 50, 89, 234	0
10	J	58/58 (100%)	0.53	4 (6%) 23 29	27, 38, 87, 134	0
10	W	58/58 (100%)	0.64	7 (12%) 8 11	28, 39, 98, 181	0
11	K	49/49 (100%)	0.51	2 (4%) 41 49	29, 37, 57, 67	0
11	X	49/49 (100%)	0.82	6 (12%) 8 11	35, 45, 79, 82	0
12	L	46/46 (100%)	0.12	3 (6%) 25 31	24, 29, 53, 124	1 (2%)
12	Y	46/46 (100%)	0.38	2 (4%) 40 48	28, 35, 61, 120	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/43 (100%)	0.41	5 (11%) 9 12	25, 29, 70, 121	0
13	Z	43/43 (100%)	0.89	6 (13%) 6 7	32, 38, 81, 170	0
All	All	3542/3550 (99%)	0.10	210 (5%) 28 36	10, 30, 72, 266	120 (3%)

The worst 5 of 210 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	3	ALA	10.6
6	S	1	ALA	10.5
7	T	3	ALA	9.8
7	G	36	TRP	9.7
4	Q	5	VAL	9.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.30	0.21	167,216,240,253	0
9	SAC	I	1	9/10	0.40	0.26	113,144,171,199	0
7	TPO	G	11	11/12	0.62	0.31	139,175,198,204	0
7	TPO	T	11	11/12	0.75	0.23	55,128,192,194	0
1	FME	N	1	10/11	0.92	0.14	35,41,72,108	0
1	FME	A	1	10/11	0.95	0.09	34,44,63,88	0
2	FME	B	1	10/11	0.96	0.12	28,29,36,113	0
2	FME	O	1	10/11	0.97	0.11	32,34,39,104	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	DMU	K	104	33/33	0.51	0.18	74,126,182,201	0
27	DMU	K	106	33/33	0.57	0.23	43,88,108,118	0
27	DMU	X	204	33/33	0.61	0.18	63,144,182,202	0
27	DMU	P	316	33/33	0.67	0.19	53,60,74,79	0
24	CHD	Y	101	29/29	0.71	0.25	67,92,145,156	0
24	CHD	W	101	29/29	0.72	0.23	46,119,204,206	0
19	PGV	G	104	51/51	0.73	0.23	40,82,127,155	0
24	CHD	P	308	29/29	0.73	0.19	56,77,138,177	0
20	EDO	N	615	4/4	0.74	0.18	56,57,58,67	0
27	DMU	M	106	33/33	0.74	0.19	49,76,103,112	0
25	PEK	P	304	53/53	0.75	0.23	42,77,136,186	0
27	DMU	K	105	33/33	0.75	0.20	47,125,201,217	0
27	DMU	X	202	33/33	0.75	0.18	43,142,216,227	0
27	DMU	X	203	22/33	0.75	0.20	64,96,171,186	0
25	PEK	T	102	44/53	0.75	0.21	43,96,157,183	0
27	DMU	X	201	33/33	0.76	0.18	53,106,180,192	0
25	PEK	C	303	53/53	0.76	0.22	40,78,139,158	0
27	DMU	P	307	33/33	0.76	0.20	52,103,149,183	0
24	CHD	J	101	29/29	0.76	0.19	56,80,126,169	0
19	PGV	C	305	51/51	0.77	0.24	42,80,129,135	0
20	EDO	M	102	4/4	0.77	0.14	52,58,71,72	0
24	CHD	J	102	29/29	0.77	0.20	52,94,162,199	0
26	CDL	T	103	96/100	0.77	0.22	45,82,125,176	0
27	DMU	C	307	33/33	0.77	0.20	48,109,157,171	0
27	DMU	X	205	22/33	0.77	0.20	65,104,160,162	0
27	DMU	K	103	33/33	0.78	0.18	55,114,190,202	0
20	EDO	A	610	4/4	0.78	0.25	34,47,71,82	0
26	CDL	G	101	99/100	0.78	0.22	36,85,129,181	0
20	EDO	A	622	4/4	0.79	0.20	46,55,59,71	0
27	DMU	G	102	33/33	0.79	0.19	54,105,156,157	0
19	PGV	N	607	51/51	0.80	0.22	43,79,130,161	0
21	TGL	B	304	63/63	0.80	0.22	26,66,132,168	0
23	PSC	O	302	46/52	0.80	0.23	32,76,132,166	0
27	DMU	K	101	21/33	0.80	0.24	41,110,189,196	0
25	PEK	P	302	48/53	0.81	0.20	43,76,148,161	0
27	DMU	O	303	32/33	0.81	0.17	42,102,173,202	0
21	TGL	N	608	63/63	0.81	0.21	40,76,128,162	0
20	EDO	P	311	4/4	0.82	0.19	54,71,82,98	0
21	TGL	B	301	63/63	0.82	0.22	37,65,131,160	0
26	CDL	C	306	92/100	0.82	0.19	40,77,112,123	0
20	EDO	I	101	4/4	0.82	0.19	39,49,57,69	0
20	EDO	L	103	4/4	0.82	0.19	33,64,68,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	PGV	A	607	48/51	0.82	0.19	31,60,116,157	0
20	EDO	D	202	4/4	0.82	0.26	54,67,104,106	0
20	EDO	N	618	4/4	0.83	0.19	30,37,43,48	0
20	EDO	F	106	4/4	0.83	0.20	44,52,65,74	0
27	DMU	P	309	33/33	0.83	0.19	31,78,157,181	0
20	EDO	G	106	4/4	0.83	0.29	35,45,83,104	0
20	EDO	N	612	4/4	0.83	0.19	45,59,71,81	0
20	EDO	A	613	4/4	0.83	0.17	60,63,78,80	0
21	TGL	Q	201	63/63	0.83	0.22	44,74,134,171	0
27	DMU	L	102	33/33	0.83	0.17	54,103,152,159	0
23	PSC	B	303	51/52	0.83	0.21	39,79,158,184	0
20	EDO	S	104	4/4	0.84	0.24	59,108,114,122	0
20	EDO	N	620	4/4	0.84	0.26	46,53,64,68	0
20	EDO	J	103	4/4	0.84	0.19	49,51,69,73	0
26	CDL	P	306	84/100	0.84	0.23	37,79,134,142	0
27	DMU	K	102	22/33	0.84	0.18	53,109,188,214	0
29	PO4	U	102	5/5	0.84	0.10	52,53,95,97	0
20	EDO	T	106	4/4	0.85	0.23	44,62,75,86	0
20	EDO	C	315	4/4	0.85	0.14	42,65,69,70	0
20	EDO	A	615	4/4	0.85	0.27	50,58,69,100	0
20	EDO	M	105	4/4	0.85	0.15	41,50,55,99	0
20	EDO	Q	203	4/4	0.86	0.22	53,60,62,90	0
21	TGL	Y	102	63/63	0.86	0.23	40,73,135,230	0
21	TGL	L	101	60/63	0.86	0.24	31,62,180,229	0
27	DMU	T	104	22/33	0.86	0.14	50,84,149,169	0
20	EDO	C	311	4/4	0.86	0.16	71,76,87,88	0
27	DMU	C	308	33/33	0.87	0.18	28,76,162,192	0
20	EDO	M	103	4/4	0.87	0.25	40,72,86,94	0
20	EDO	C	317	4/4	0.87	0.14	48,65,69,69	0
20	EDO	C	316	4/4	0.87	0.15	51,55,65,78	0
20	EDO	P	315	4/4	0.87	0.14	57,59,84,96	0
20	EDO	D	203	4/4	0.87	0.18	45,56,56,60	0
20	EDO	Q	204	4/4	0.87	0.14	45,50,55,56	0
20	EDO	A	616	4/4	0.88	0.19	45,51,54,55	0
20	EDO	A	614	4/4	0.88	0.16	46,67,71,71	0
20	EDO	N	626	4/4	0.88	0.17	60,67,68,69	0
20	EDO	J	104	4/4	0.88	0.17	42,61,62,75	0
20	EDO	D	204	4/4	0.89	0.18	36,41,53,81	0
20	EDO	V	101	4/4	0.89	0.31	19,38,52,86	0
20	EDO	C	314	4/4	0.89	0.18	43,62,63,92	0
20	EDO	B	309	4/4	0.89	0.17	32,55,55,70	0
27	DMU	Z	101	33/33	0.89	0.13	36,50,67,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	PO4	H	101	5/5	0.89	0.10	52,61,77,97	0
20	EDO	B	308	4/4	0.89	0.13	45,45,66,70	0
20	EDO	O	307	4/4	0.90	0.14	44,51,62,77	0
20	EDO	A	620	4/4	0.90	0.18	43,54,56,84	0
20	EDO	P	314	4/4	0.90	0.13	34,40,42,42	0
20	EDO	Y	103	4/4	0.90	0.16	48,52,65,81	0
20	EDO	E	203	4/4	0.90	0.14	40,55,56,65	0
20	EDO	C	312	4/4	0.90	0.18	31,40,46,69	0
20	EDO	N	614	4/4	0.90	0.11	46,48,63,86	0
20	EDO	R	201	4/4	0.92	0.20	62,63,82,93	0
20	EDO	F	104	4/4	0.92	0.13	33,36,44,57	0
20	EDO	C	313	4/4	0.92	0.13	39,62,68,79	0
20	EDO	U	101	4/4	0.92	0.14	38,44,54,65	0
20	EDO	P	312	4/4	0.92	0.14	49,63,65,77	0
20	EDO	P	313	4/4	0.92	0.12	52,62,63,68	0
20	EDO	D	201	4/4	0.92	0.15	47,47,59,72	0
27	DMU	M	101	33/33	0.92	0.11	33,43,61,83	0
20	EDO	N	624	4/4	0.92	0.20	32,33,47,92	0
20	EDO	A	621	4/4	0.92	0.11	39,39,48,49	0
20	EDO	O	306	4/4	0.92	0.11	43,54,61,70	0
20	EDO	B	306	4/4	0.93	0.13	29,42,43,56	0
20	EDO	N	617	4/4	0.93	0.15	32,38,48,75	0
20	EDO	F	105	4/4	0.93	0.13	42,43,47,68	0
20	EDO	S	106	4/4	0.93	0.19	36,51,71,84	0
20	EDO	M	104	4/4	0.93	0.14	50,65,66,70	0
20	EDO	N	622	4/4	0.93	0.11	44,52,53,58	0
25	PEK	P	303	45/53	0.94	0.13	26,42,78,93	0
20	EDO	N	619	4/4	0.94	0.15	39,48,54,63	0
20	EDO	B	310	4/4	0.94	0.12	41,47,47,55	0
20	EDO	D	205	4/4	0.94	0.10	35,40,61,70	0
20	EDO	T	105	4/4	0.95	0.09	28,31,36,38	0
20	EDO	E	202	4/4	0.95	0.08	36,40,42,43	0
20	EDO	Q	202	4/4	0.95	0.11	28,46,50,69	0
20	EDO	B	307	4/4	0.95	0.10	34,45,48,48	0
20	EDO	N	625	4/4	0.95	0.15	33,44,48,82	0
24	CHD	C	301	29/29	0.95	0.08	24,27,35,38	0
20	EDO	A	612	4/4	0.95	0.15	28,38,78,85	0
20	EDO	O	304	4/4	0.95	0.09	29,29,30,31	0
20	EDO	O	305	4/4	0.95	0.11	37,48,52,54	0
20	EDO	N	623	4/4	0.96	0.09	35,39,42,48	0
25	PEK	C	302	53/53	0.96	0.13	25,40,84,114	0
20	EDO	A	611	4/4	0.96	0.10	30,38,39,68	0

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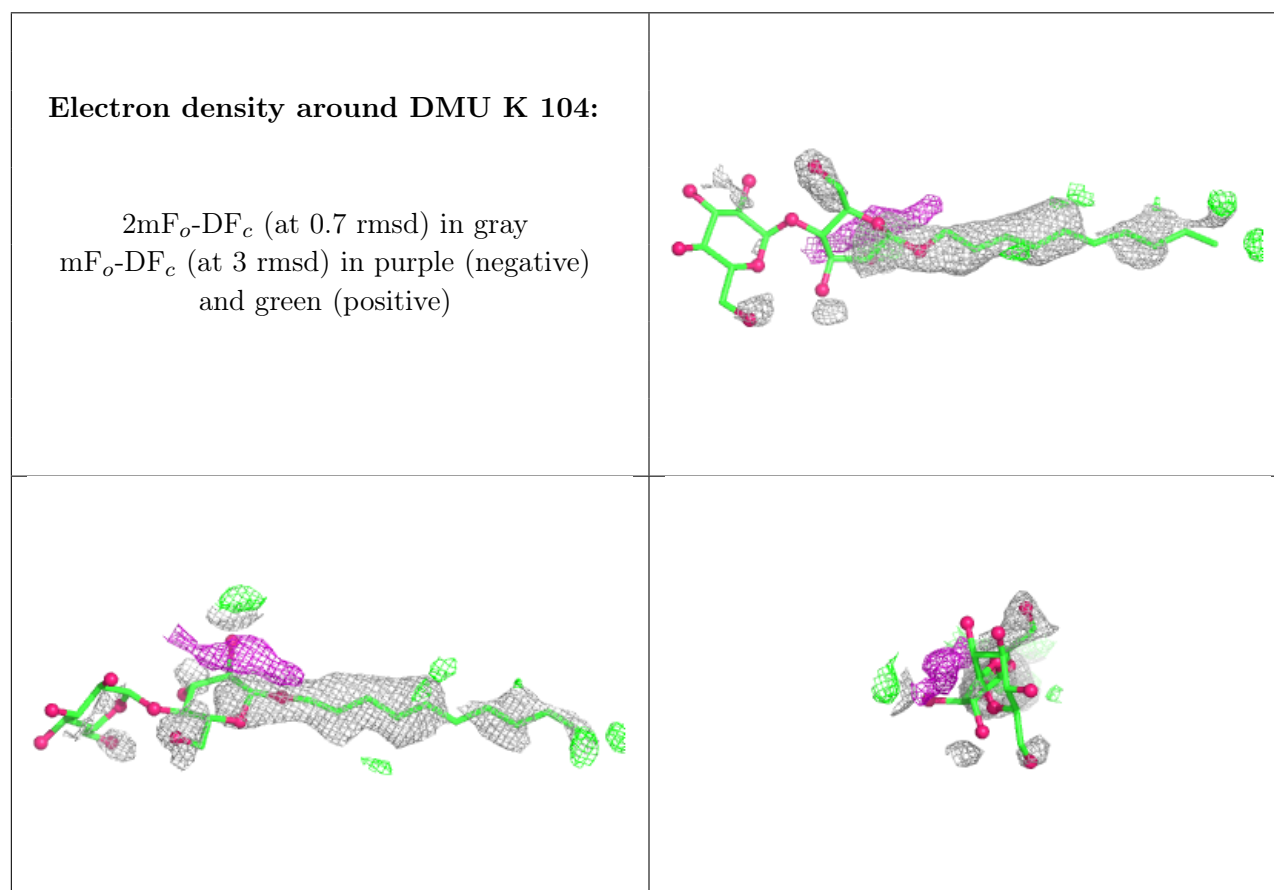
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	EDO	C	310	4/4	0.96	0.11	27,32,44,57	0
20	EDO	A	617	4/4	0.96	0.10	29,36,37,88	0
20	EDO	A	618	4/4	0.96	0.10	26,28,30,34	0
20	EDO	N	613	4/4	0.96	0.09	36,38,42,44	0
20	EDO	N	621	4/4	0.96	0.08	31,40,41,43	0
20	EDO	B	305	4/4	0.96	0.09	22,26,27,29	0
24	CHD	P	301	29/29	0.96	0.07	23,29,34,36	0
20	EDO	P	310	4/4	0.96	0.11	33,36,37,40	0
20	EDO	R	202	4/4	0.96	0.10	40,42,43,45	0
19	PGV	A	608	51/51	0.97	0.10	22,28,69,77	0
19	PGV	N	609	51/51	0.97	0.10	22,29,65,89	0
19	PGV	P	305	51/51	0.97	0.10	22,31,85,100	0
20	EDO	N	616	4/4	0.97	0.12	33,35,55,74	0
24	CHD	T	101	29/29	0.97	0.05	22,25,30,40	0
19	PGV	C	304	50/51	0.97	0.09	22,30,86,98	0
20	EDO	C	309	4/4	0.97	0.08	30,33,33,35	0
20	EDO	G	105	4/4	0.97	0.07	27,30,34,34	0
20	EDO	S	103	4/4	0.97	0.09	29,30,30,35	0
20	EDO	A	619	4/4	0.97	0.16	27,38,40,46	0
20	EDO	N	610	4/4	0.97	0.07	22,27,28,30	0
20	EDO	N	611	4/4	0.97	0.07	25,26,28,30	0
20	EDO	E	201	4/4	0.97	0.08	39,40,42,43	0
24	CHD	G	103	29/29	0.97	0.06	21,24,30,37	0
20	EDO	A	609	4/4	0.98	0.05	22,23,24,27	0
20	EDO	S	105	4/4	0.98	0.06	33,37,41,44	0
20	EDO	S	102	4/4	0.98	0.06	22,23,24,24	0
20	EDO	F	103	4/4	0.98	0.11	27,29,33,35	0
14	HEA	A	602	60/60	0.99	0.05	18,20,26,31	0
14	HEA	N	601[A]	60/60	0.99	0.06	21,24,34,40	18
14	HEA	N	601[B]	52/60	0.99	0.06	20,23,30,36	10
14	HEA	N	601[C]	51/60	0.99	0.06	20,23,29,37	9
14	HEA	N	602	60/60	0.99	0.05	18,22,27,30	0
16	MG	A	604	1/1	0.99	0.04	20,20,20,20	0
16	MG	N	604	1/1	0.99	0.04	21,21,21,21	0
17	NA	A	605	1/1	0.99	0.03	24,24,24,24	0
17	NA	N	605	1/1	0.99	0.03	29,29,29,29	0
18	CMO	A	606[A]	2/2	0.99	0.06	17,17,17,18	2
20	EDO	F	102	4/4	0.99	0.04	22,23,24,25	0
18	CMO	A	606[B]	2/2	0.99	0.06	16,16,16,16	2
18	CMO	N	606[A]	2/2	0.99	0.10	19,19,19,19	2
18	CMO	N	606[B]	2/2	0.99	0.10	17,17,17,20	2
14	HEA	A	601[A]	60/60	0.99	0.05	17,20,33,36	18

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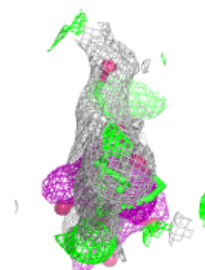
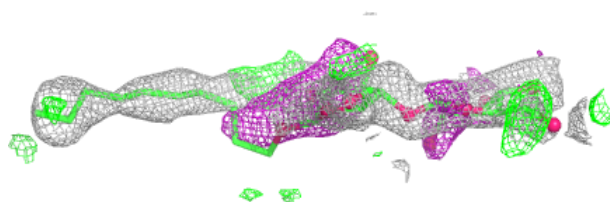
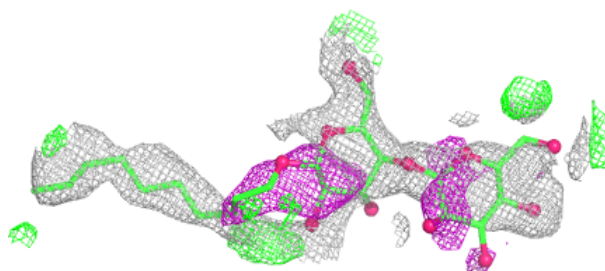
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	HEA	A	601[B]	52/60	0.99	0.05	17,20,26,34	10
14	HEA	A	601[C]	51/60	0.99	0.05	17,20,32,33	9
22	CUA	B	302	2/2	1.00	0.01	22,22,22,23	0
22	CUA	O	301	2/2	1.00	0.01	25,25,25,26	0
28	ZN	F	101	1/1	1.00	0.03	26,26,26,26	0
28	ZN	S	101	1/1	1.00	0.03	26,26,26,26	0
15	CU	A	603	1/1	1.00	0.01	21,21,21,21	0
15	CU	N	603	1/1	1.00	0.01	22,22,22,22	0

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

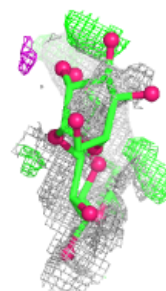
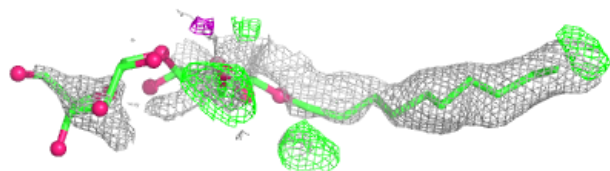
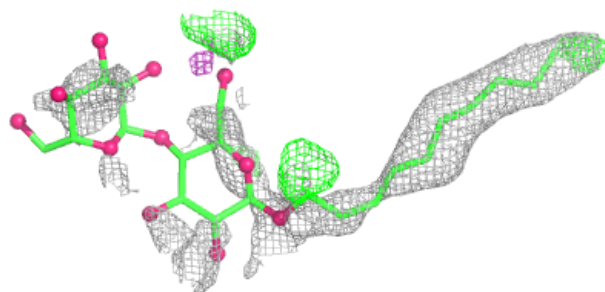


Electron density around DMU K 106:

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

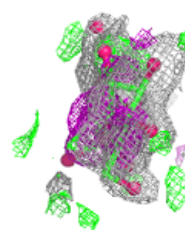
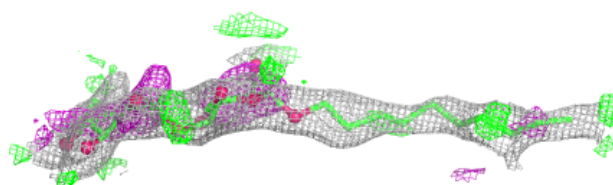
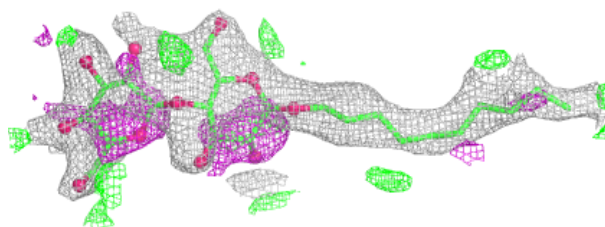
**Electron density around DMU X 204:**

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

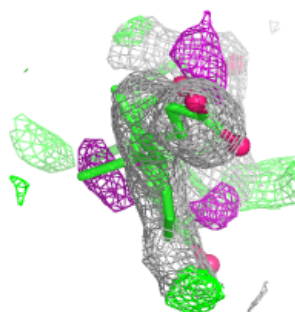
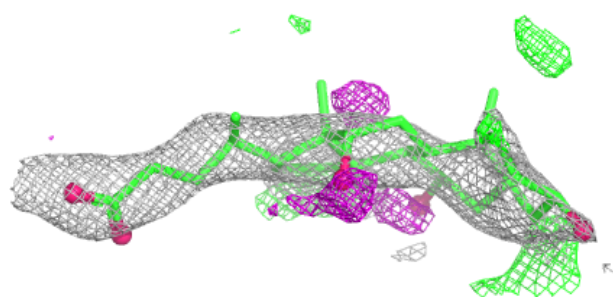
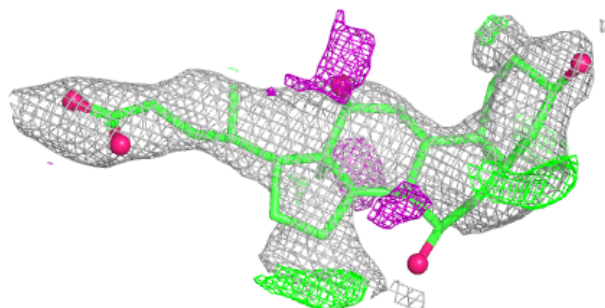


Electron density around DMU P 316:

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

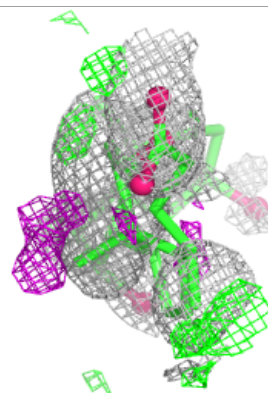
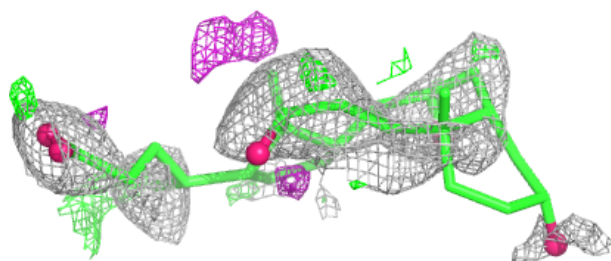
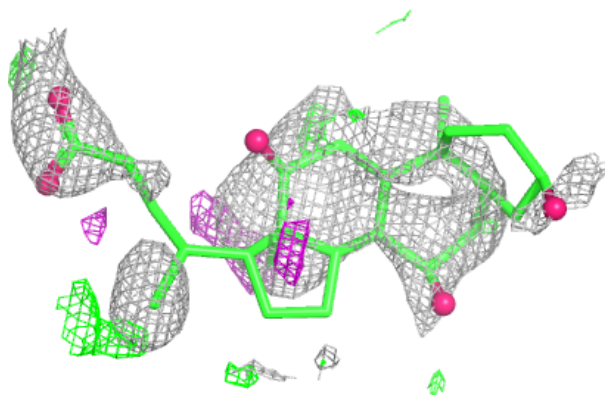
**Electron density around CHD Y 101:**

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

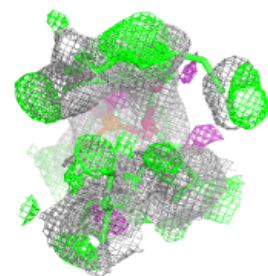
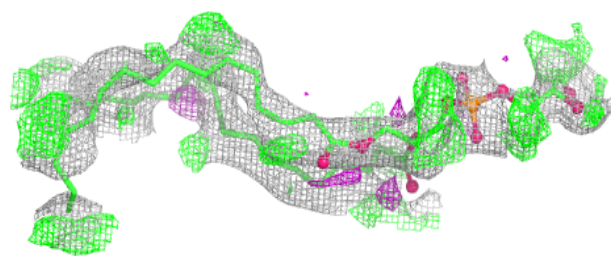
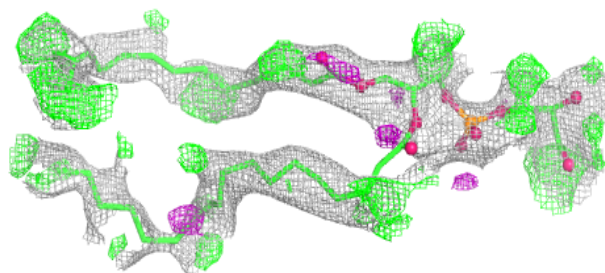


Electron density around CHD W 101:

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

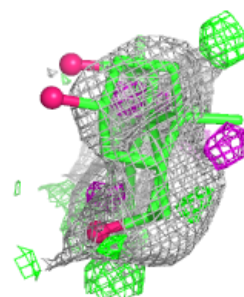
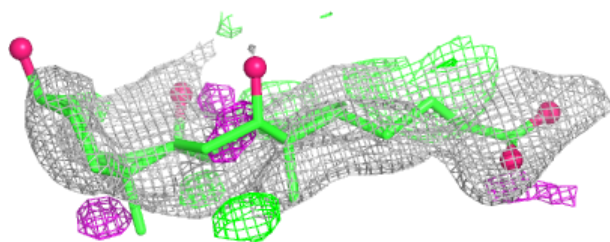
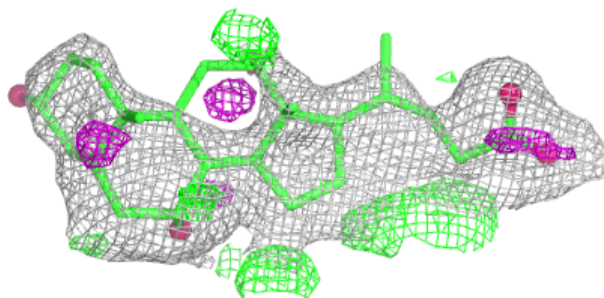
**Electron density around PGV G 104:**

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

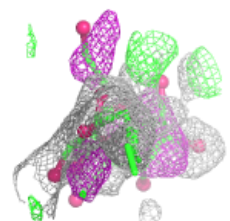
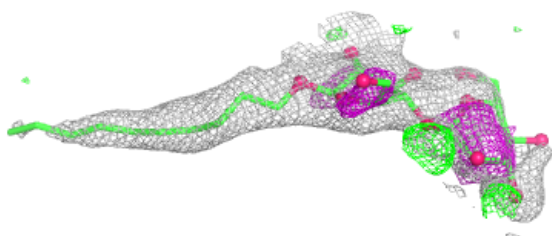
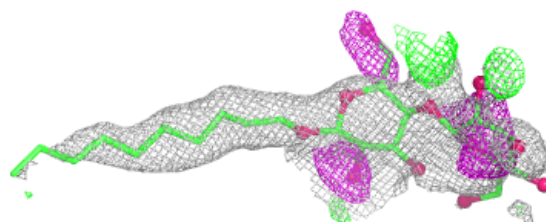


Electron density around CHD P 308:

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

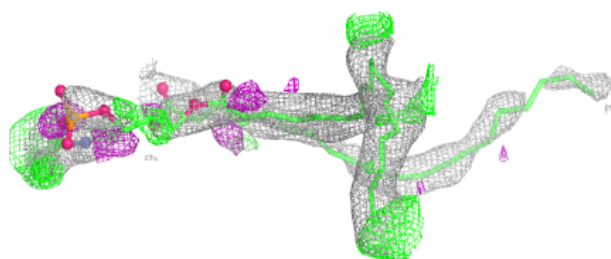
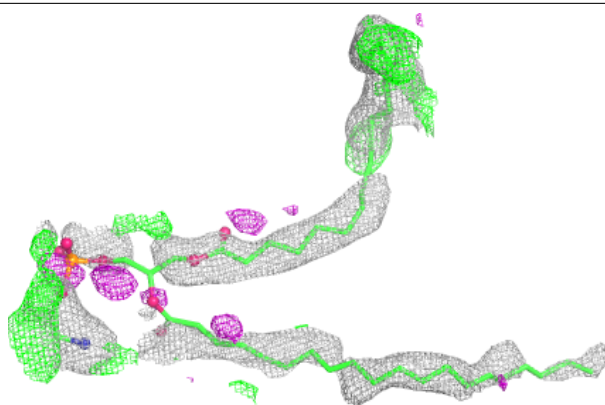
**Electron density around DMU M 106:**

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

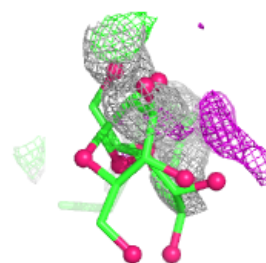
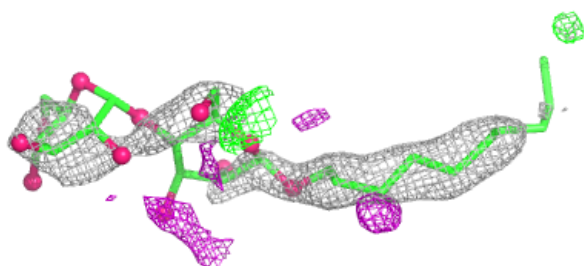
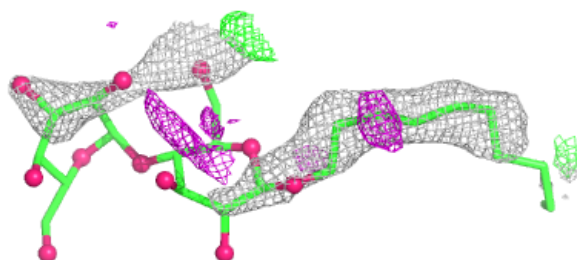


Electron density around PEK P 304:

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

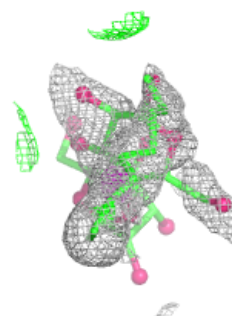
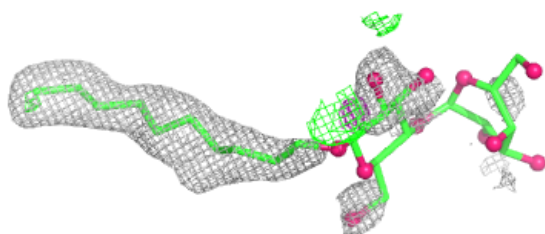
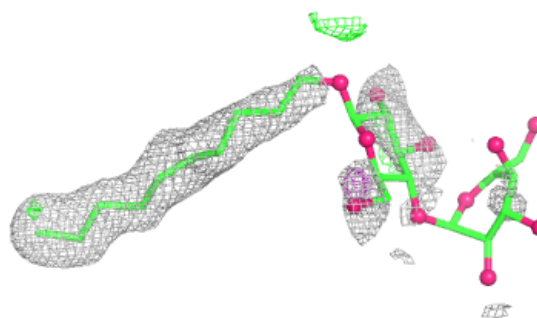
**Electron density around DMU K 105:**

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

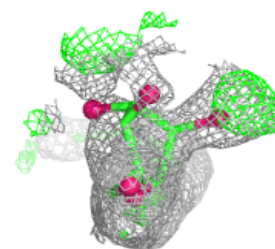
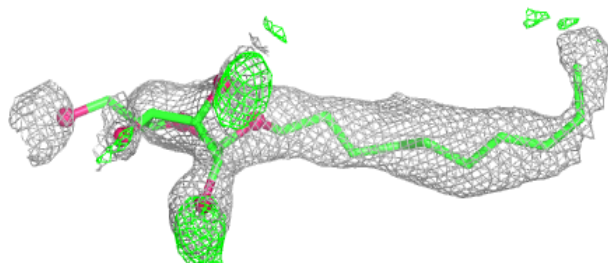
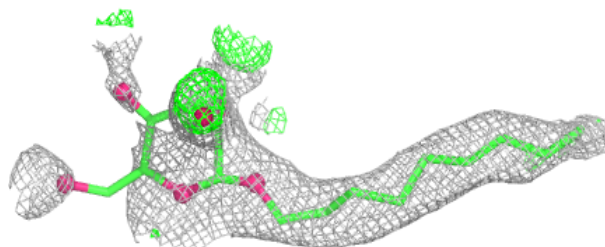


Electron density around DMU X 202:

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

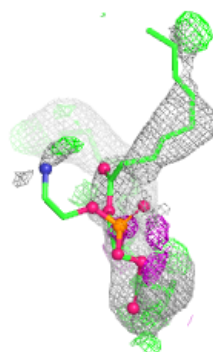
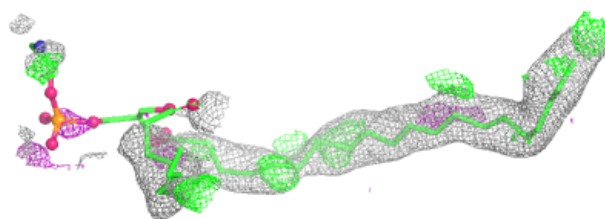
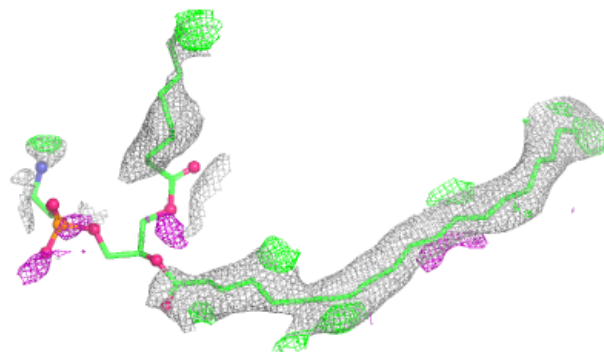
**Electron density around DMU X 203:**

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

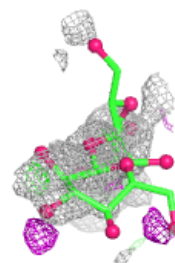
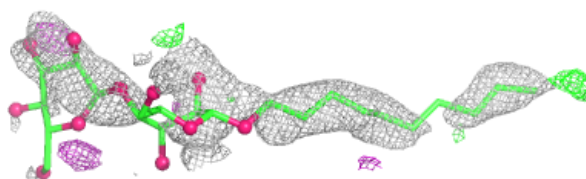
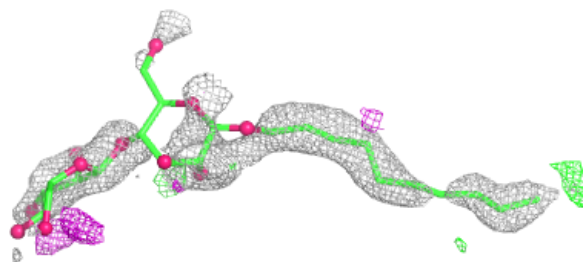


Electron density around PEK T 102:

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

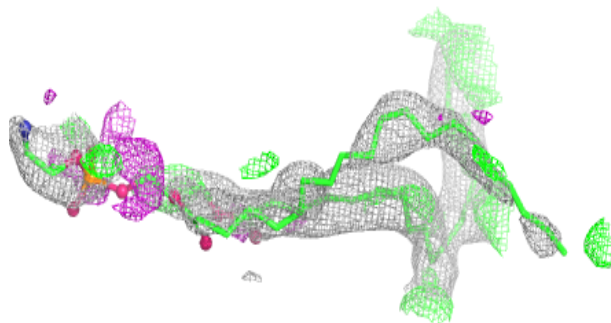
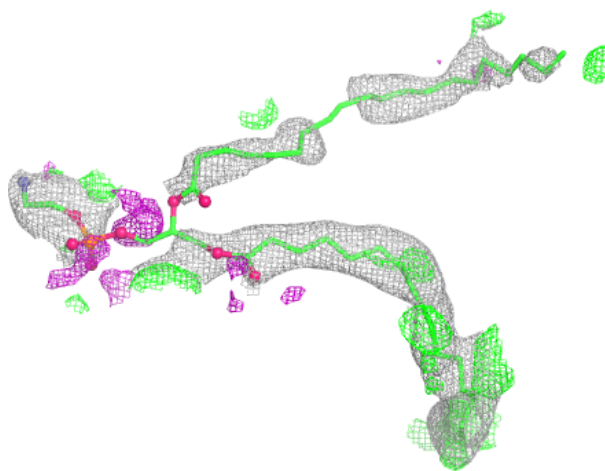
**Electron density around DMU X 201:**

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



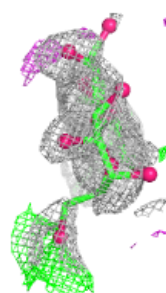
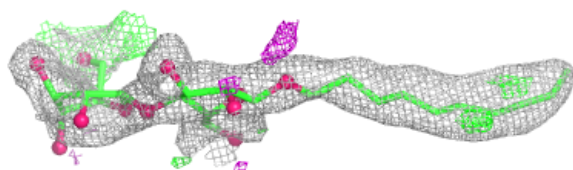
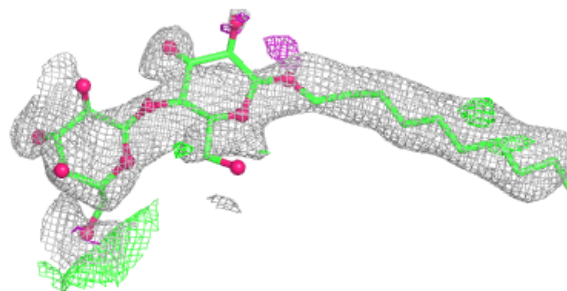
Electron density around PEK C 303:

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

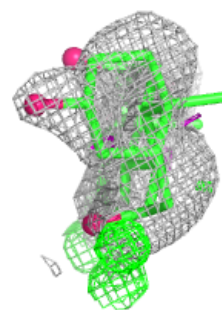
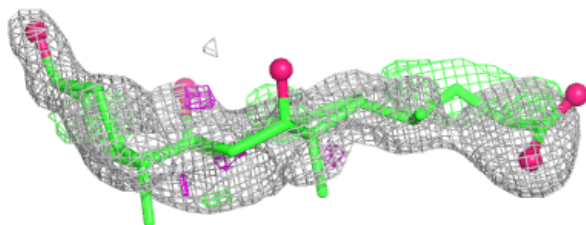
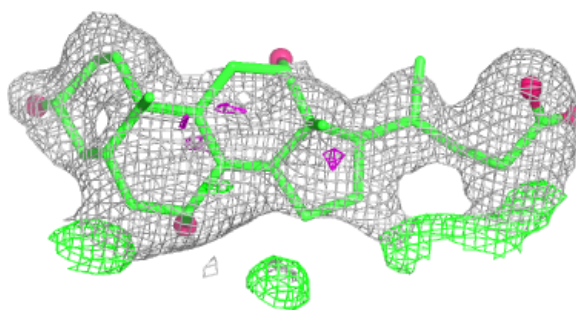


Electron density around DMU P 307:

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

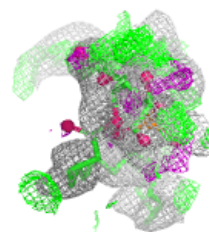
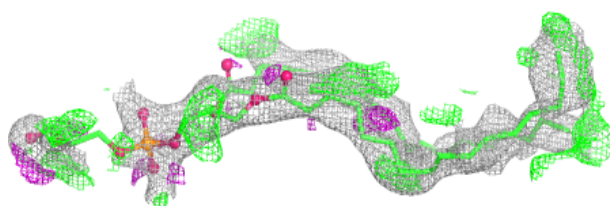
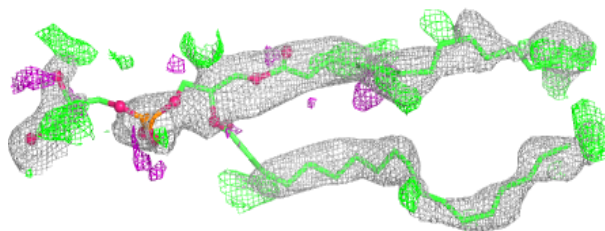
**Electron density around CHD J 101:**

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

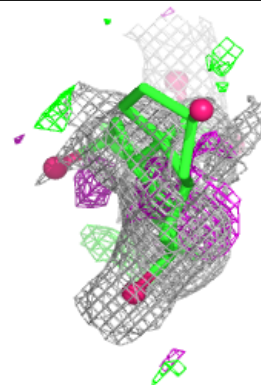
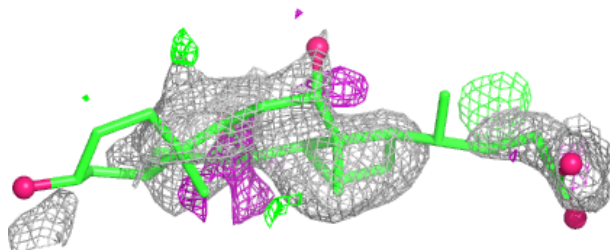
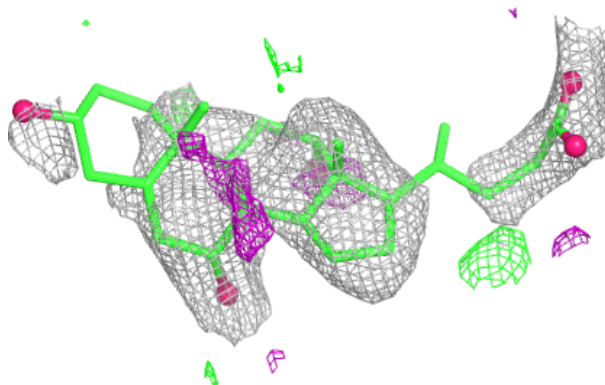


Electron density around PGV C 305:

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

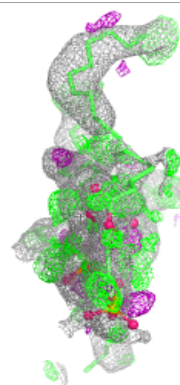
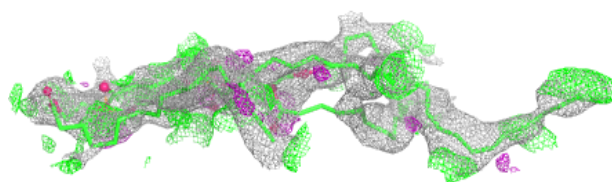
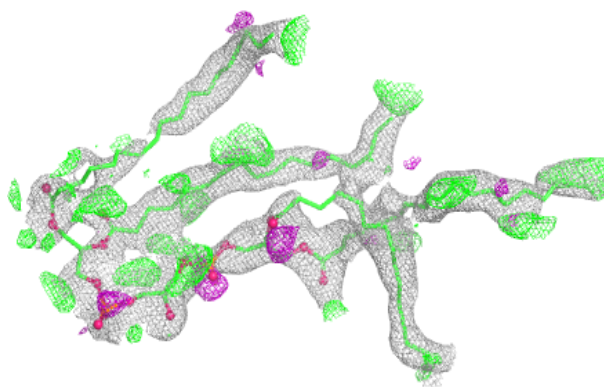
**Electron density around CHD J 102:**

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

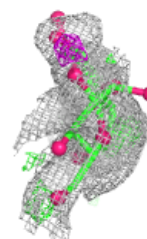
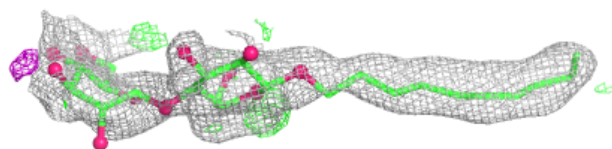
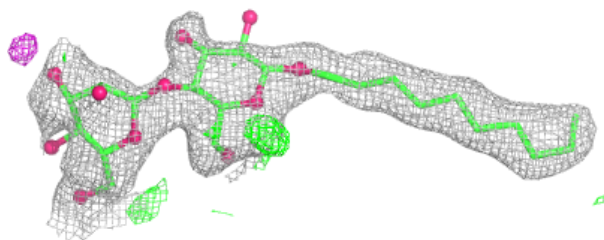


Electron density around CDL T 103:

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

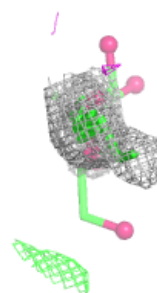
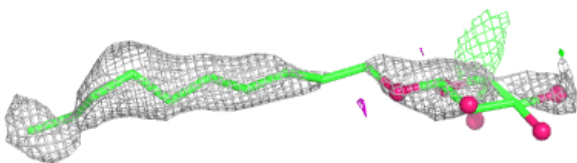
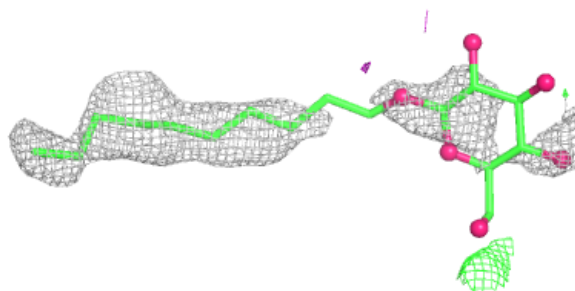
**Electron density around DMU C 307:**

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

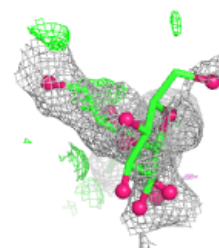
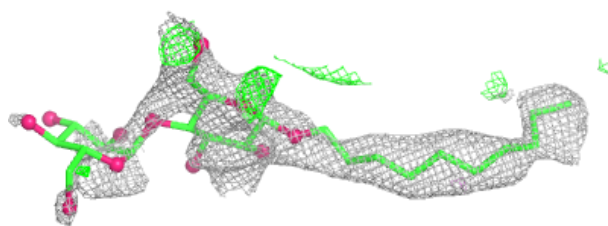
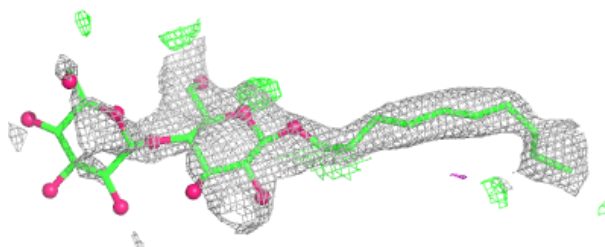


Electron density around DMU X 205:

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

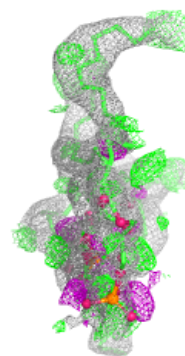
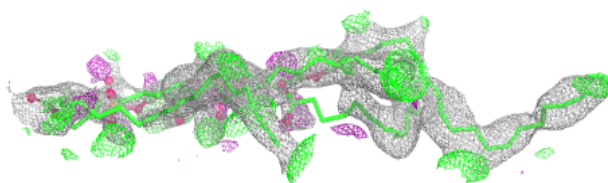
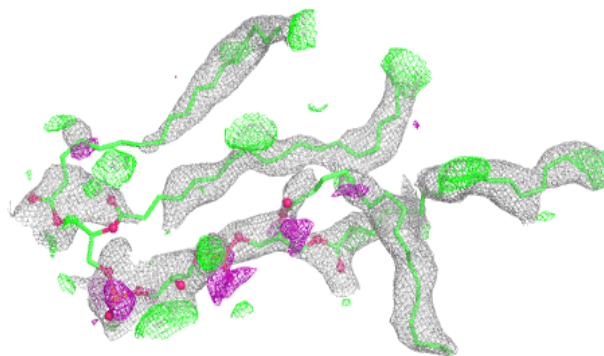
**Electron density around DMU K 103:**

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

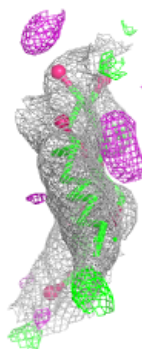
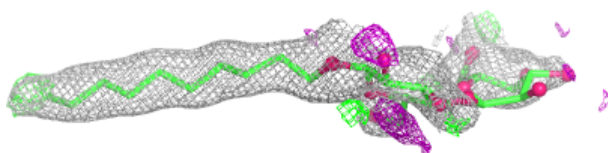
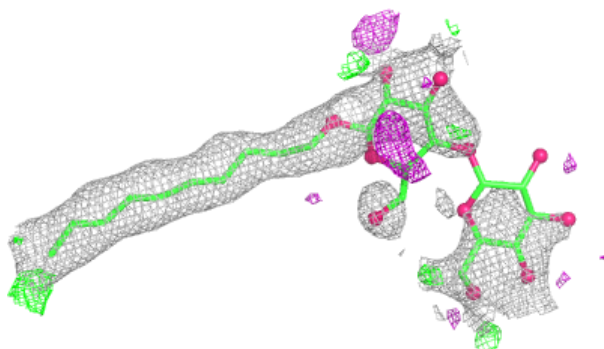


Electron density around CDL G 101:

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

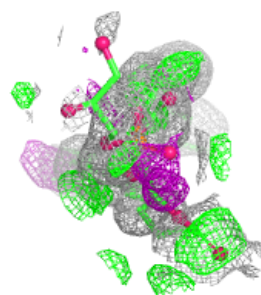
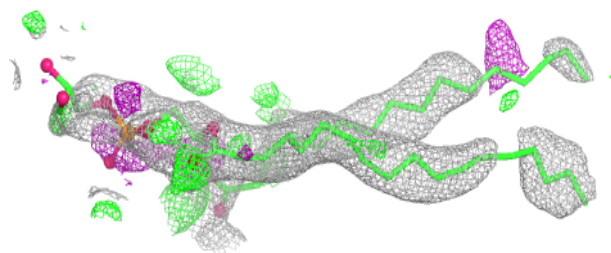
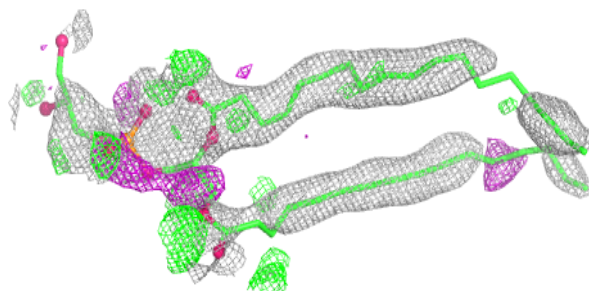
**Electron density around DMU G 102:**

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

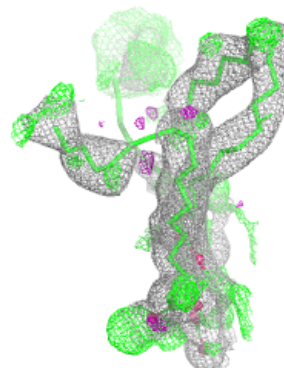
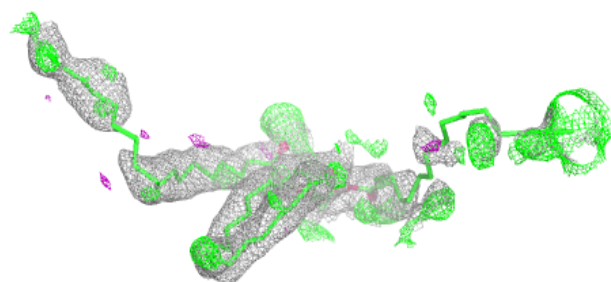
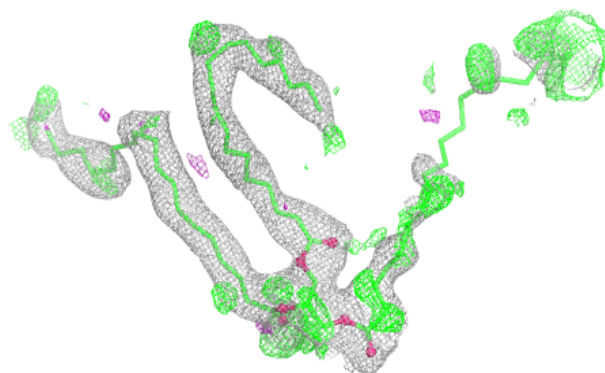


Electron density around PGV N 607:

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

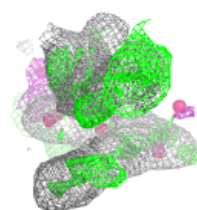
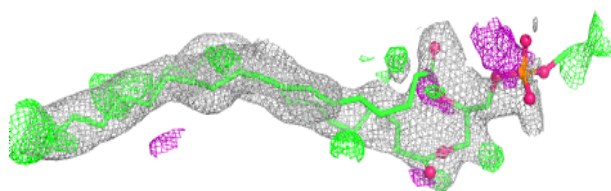
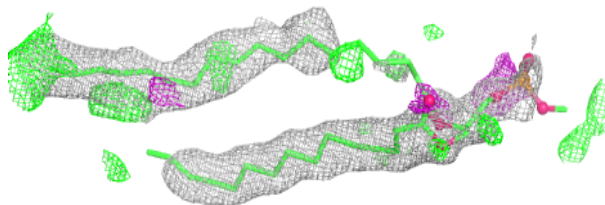
**Electron density around TGL B 304:**

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

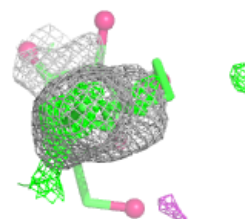
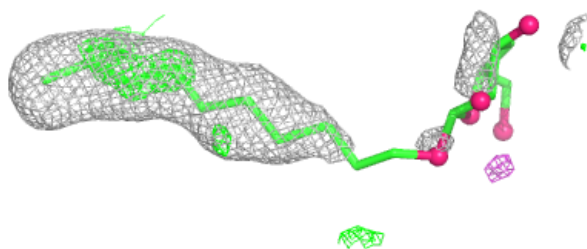
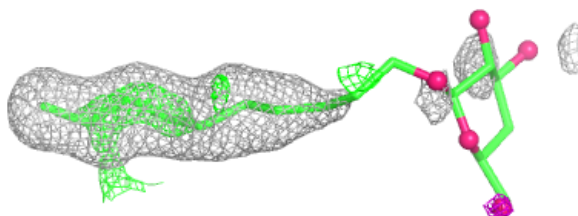


Electron density around PSC O 302:

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

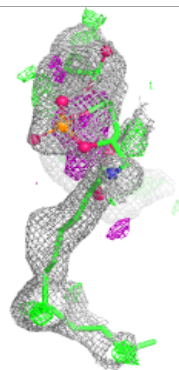
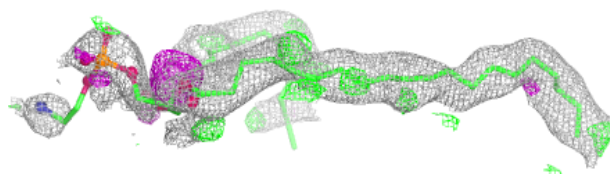
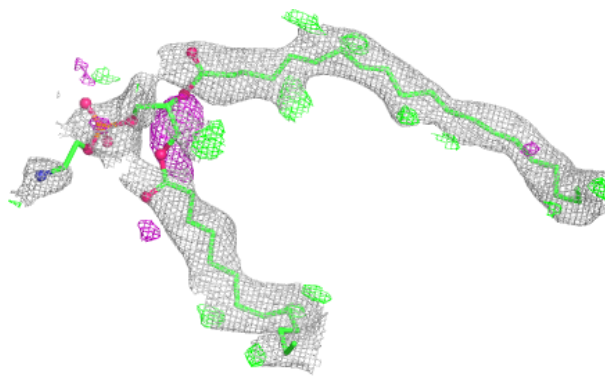
**Electron density around DMU K 101:**

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

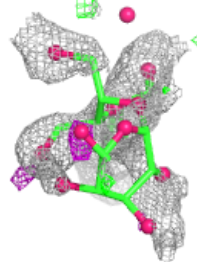
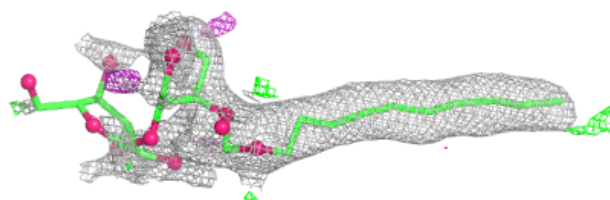
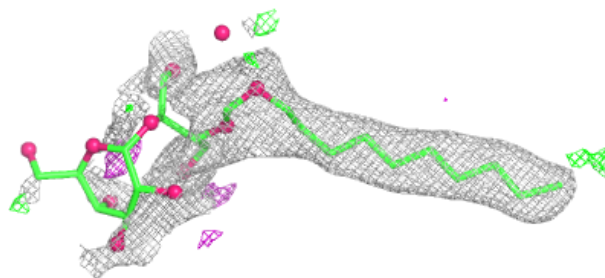


Electron density around PEK P 302:

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

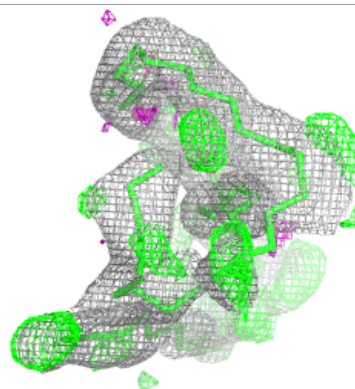
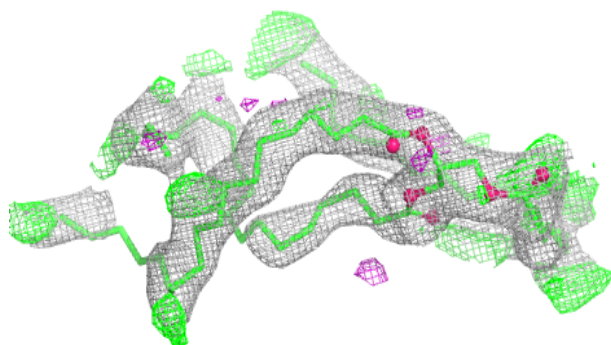
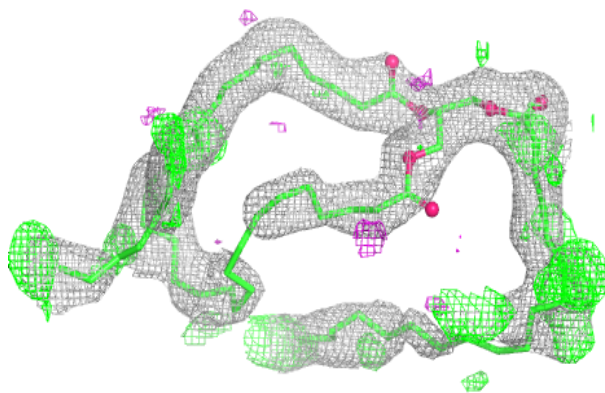
**Electron density around DMU O 303:**

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

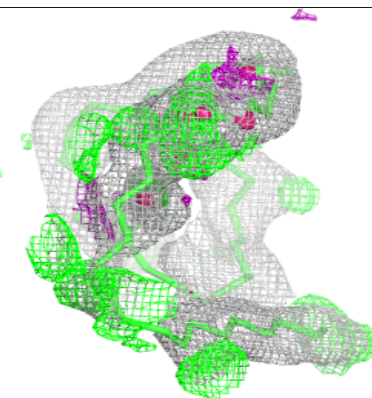
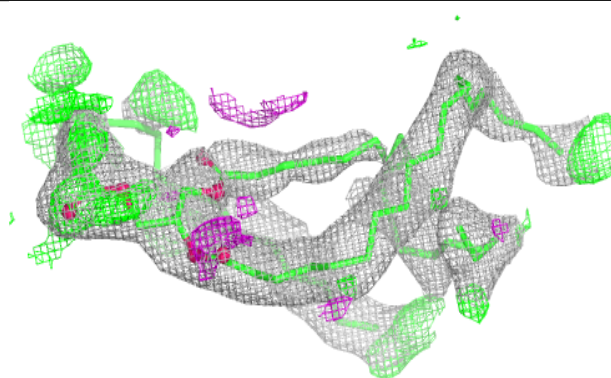
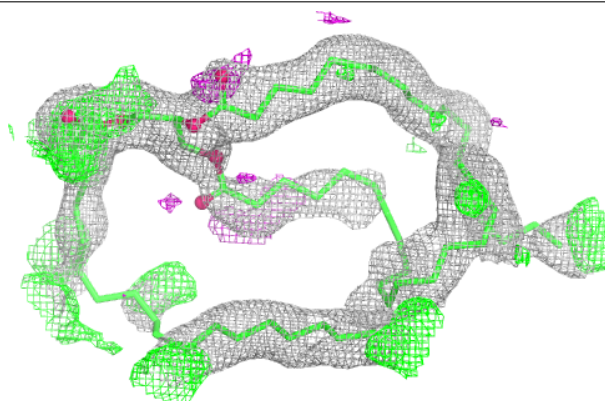


Electron density around TGL N 608:

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

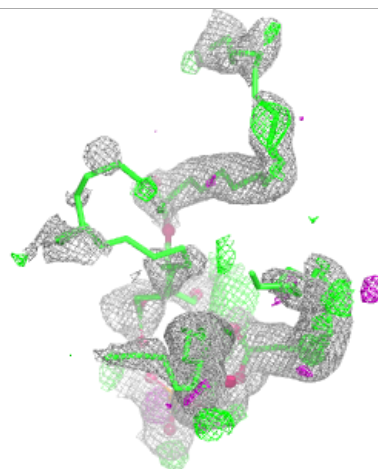
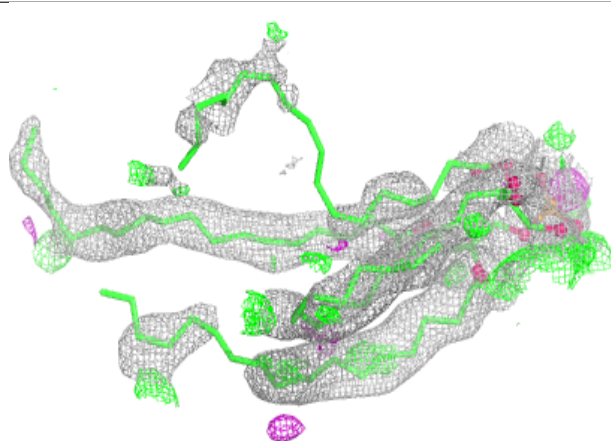
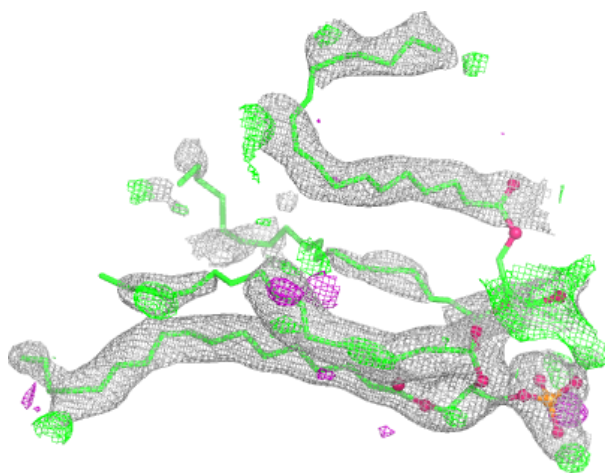
**Electron density around TGL B 301:**

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



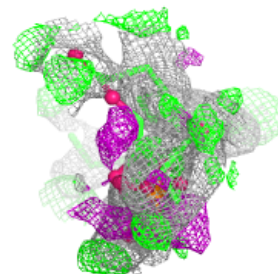
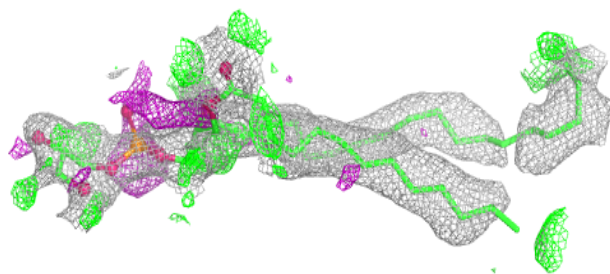
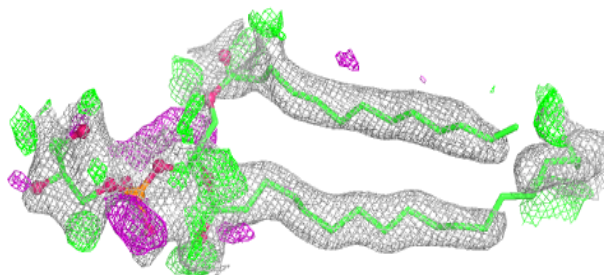
Electron density around CDL C 306:

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

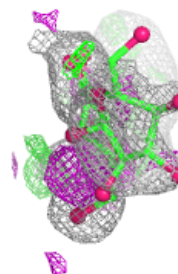
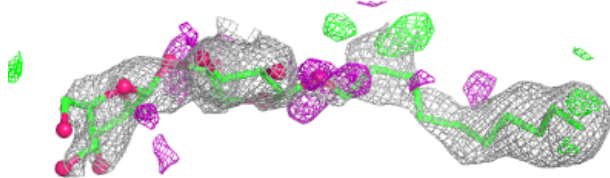
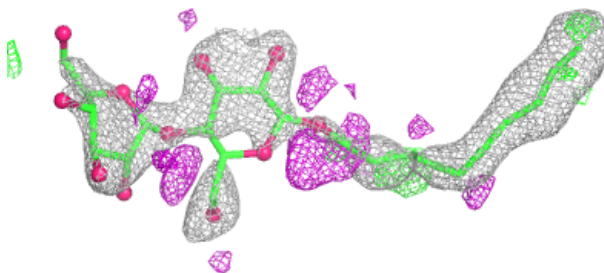


Electron density around PGV A 607:

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

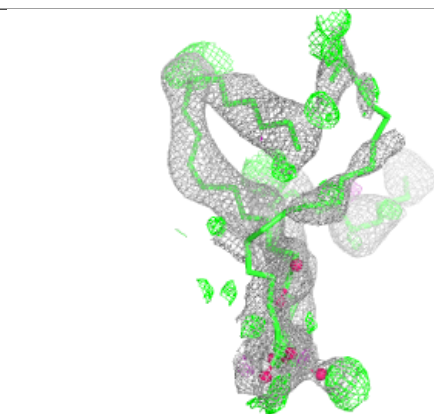
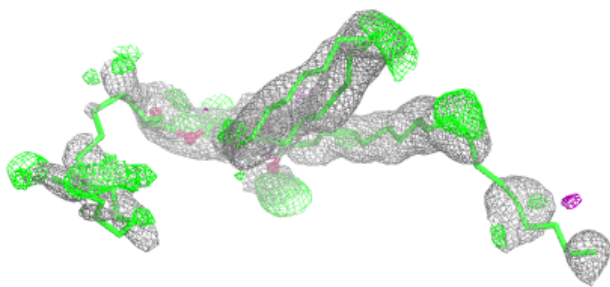
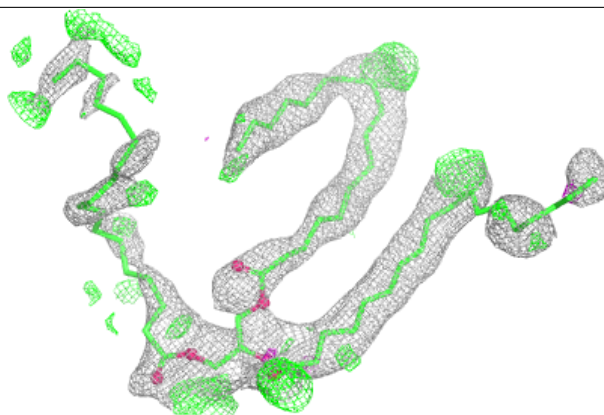
**Electron density around DMU P 309:**

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

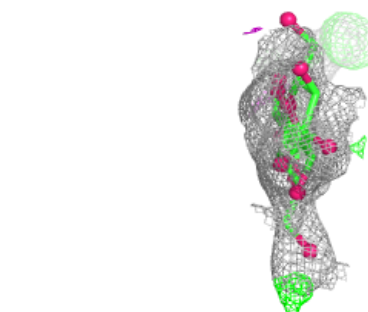
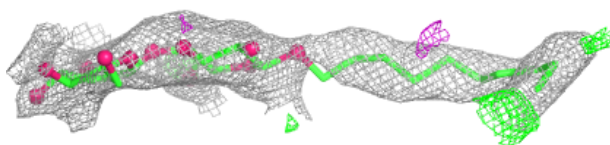
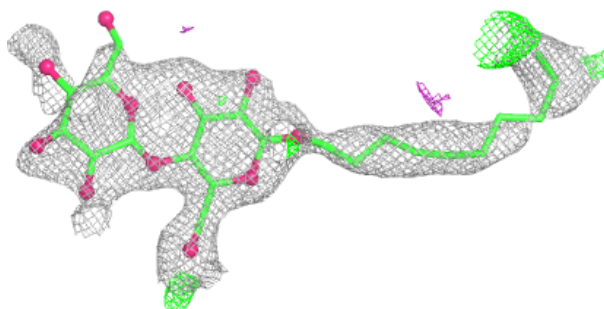


Electron density around TGL Q 201:

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

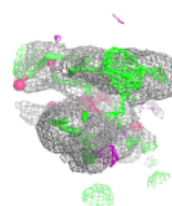
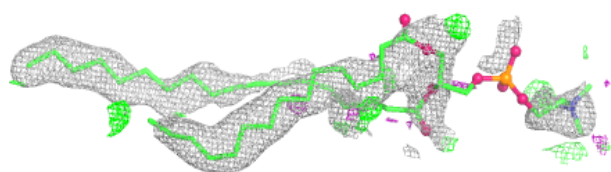
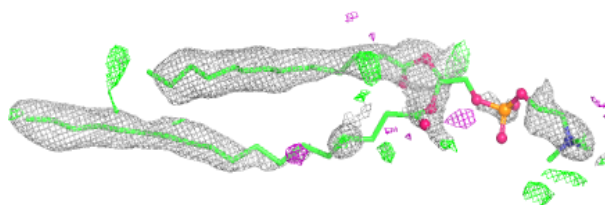
**Electron density around DMU L 102:**

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

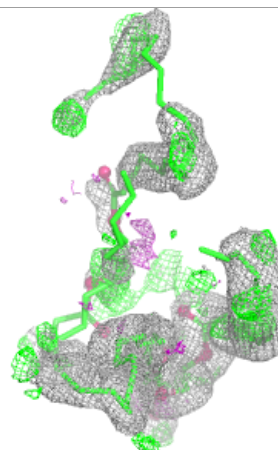
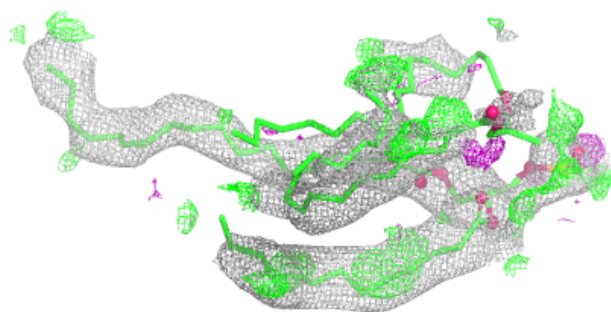
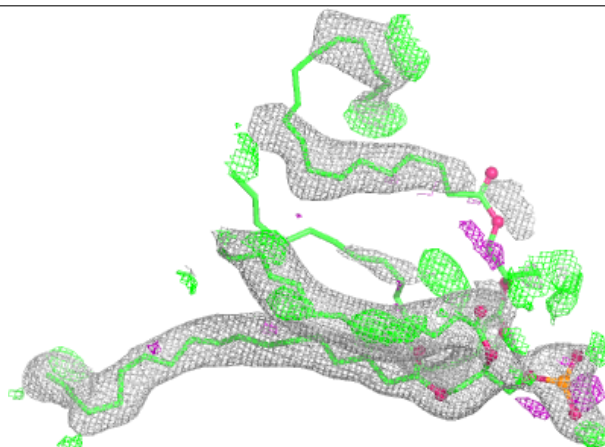


Electron density around PSC B 303:

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

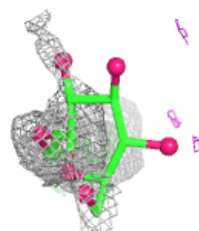
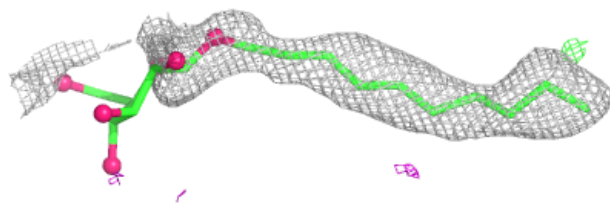
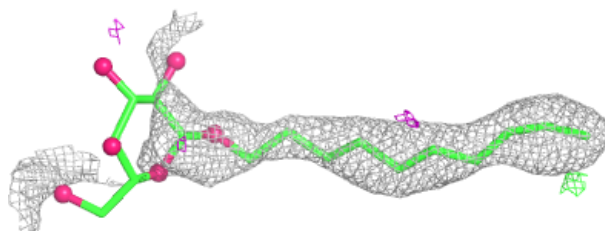
**Electron density around CDL P 306:**

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



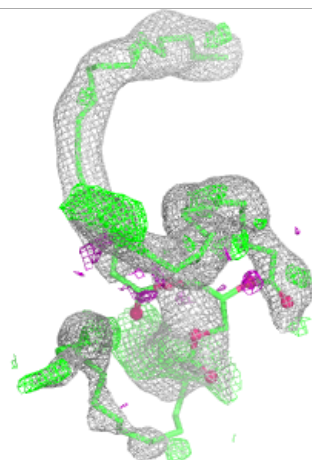
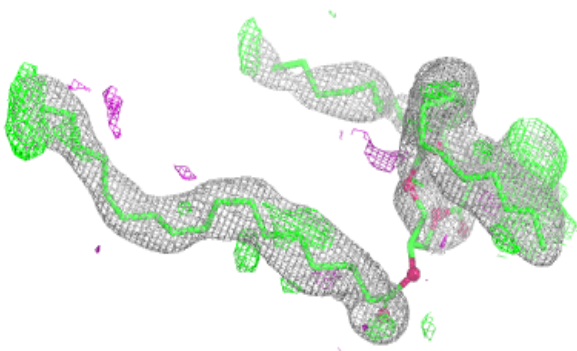
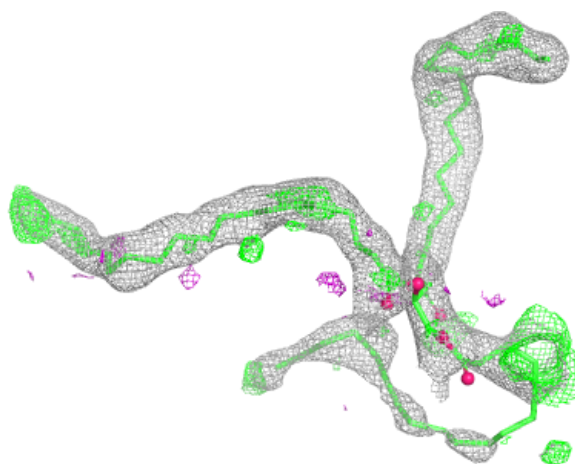
Electron density around DMU K 102:

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



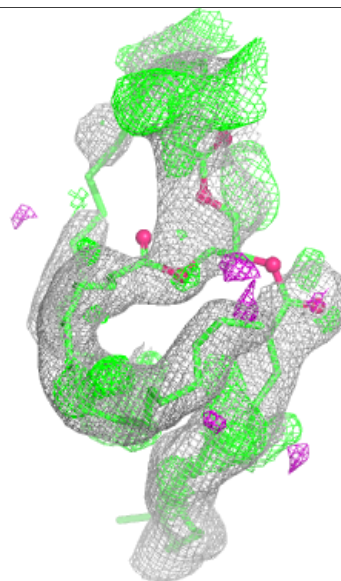
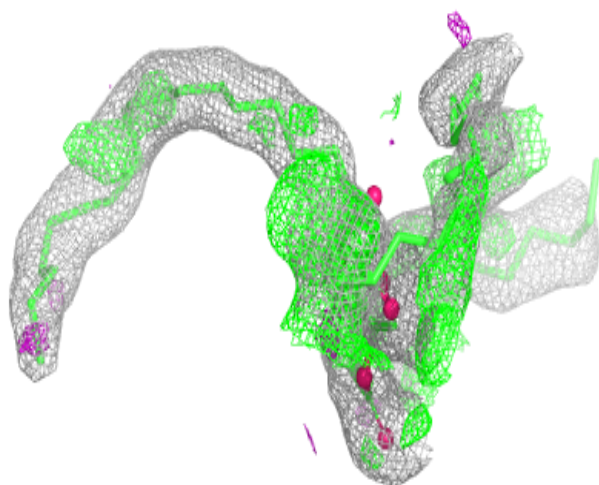
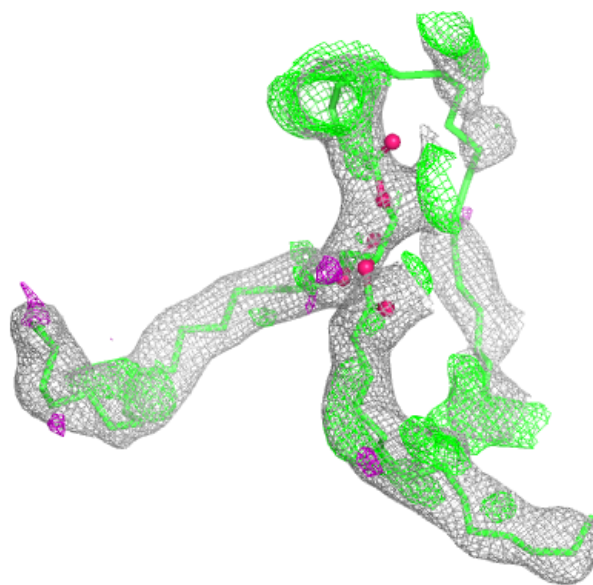
Electron density around TGL Y 102:

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



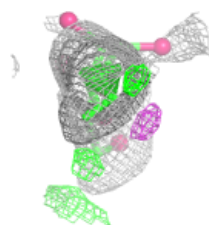
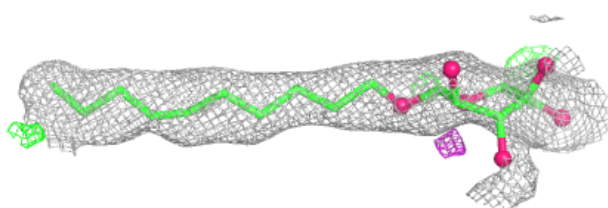
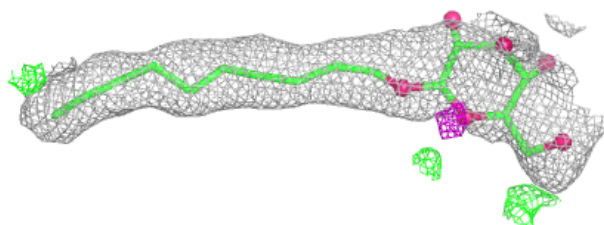
Electron density around TGL L 101:

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

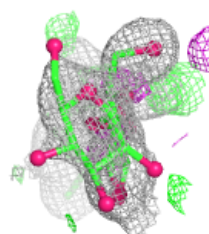
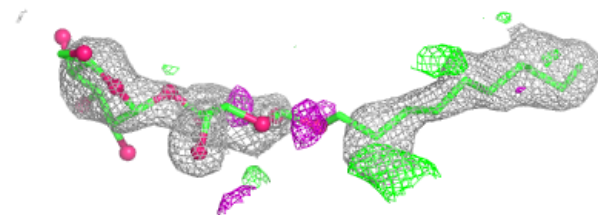
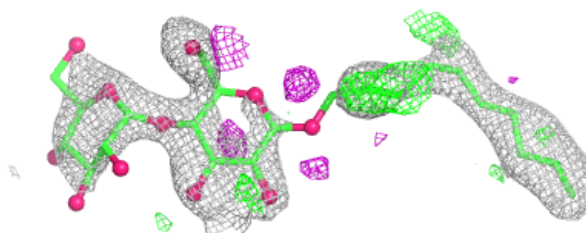


Electron density around DMU T 104:

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

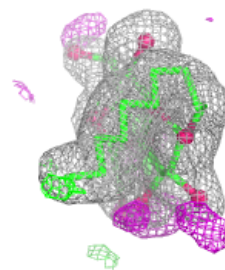
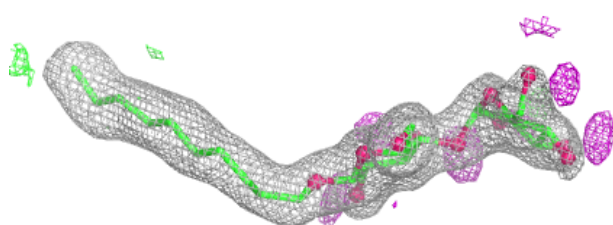
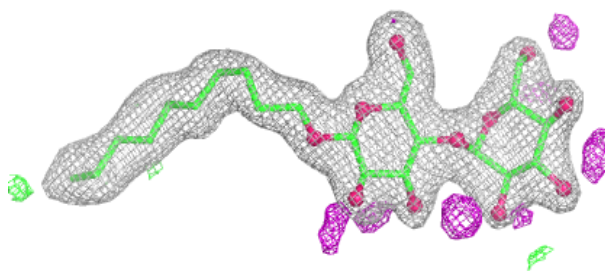
**Electron density around DMU C 308:**

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

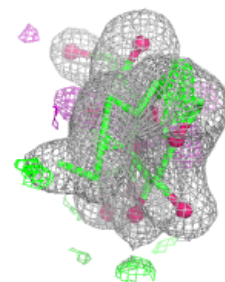
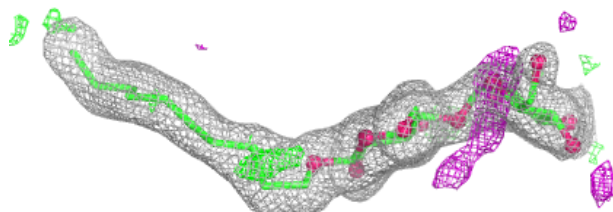
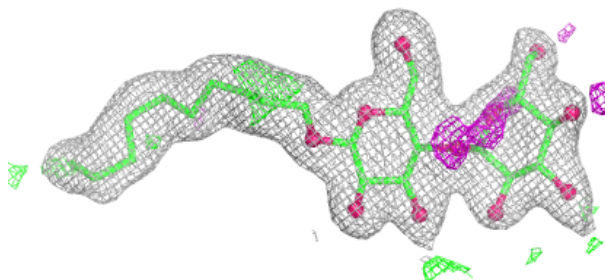


Electron density around DMU Z 101:

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

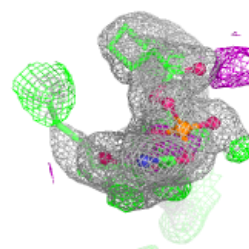
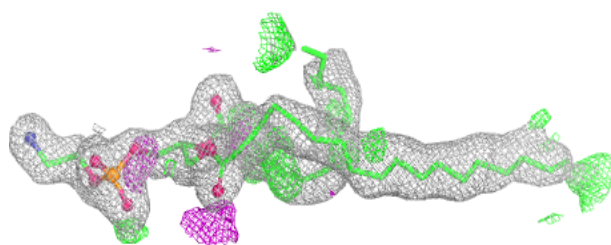
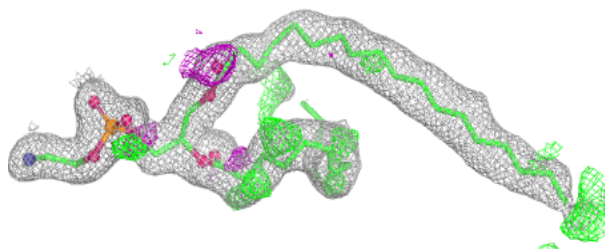
**Electron density around DMU M 101:**

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

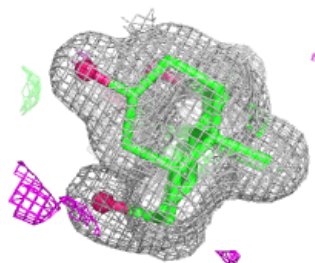
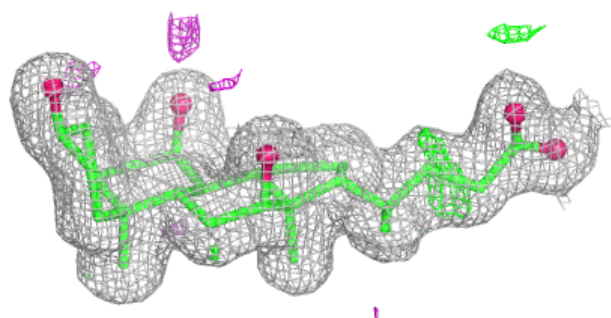
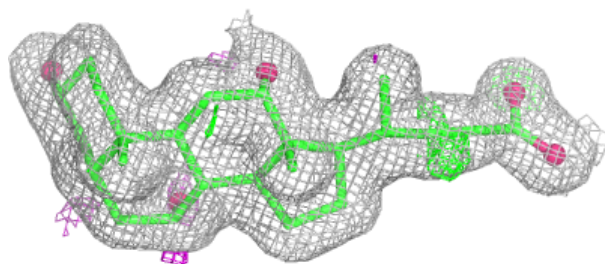


Electron density around PEK P 303:

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

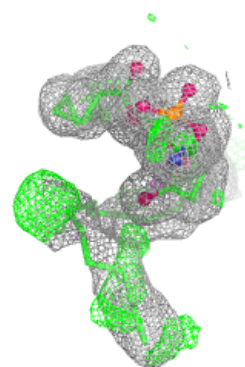
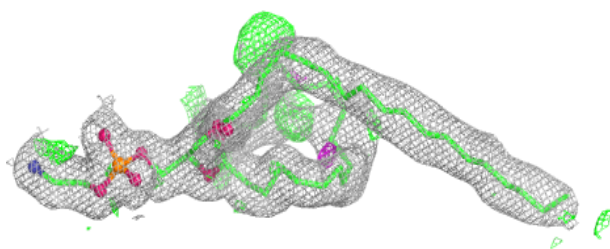
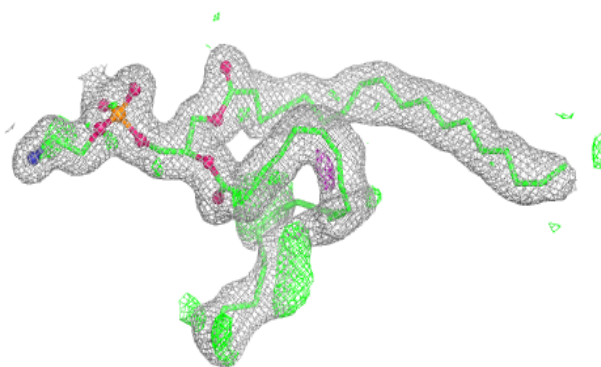
**Electron density around CHD C 301:**

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

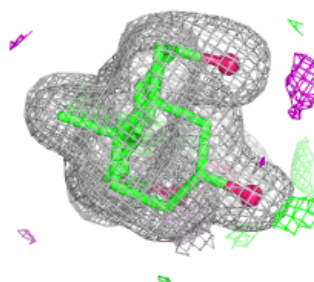
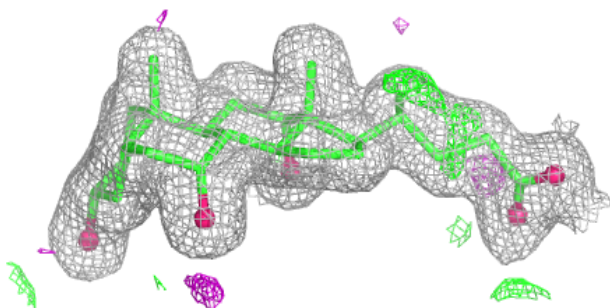
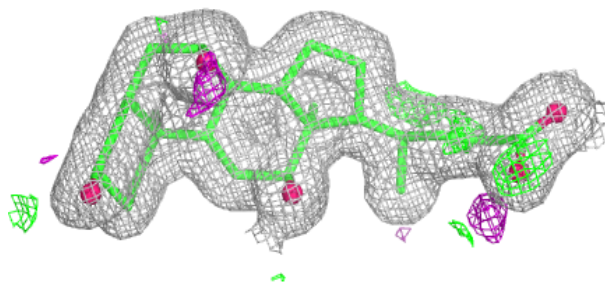


Electron density around PEK C 302:

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

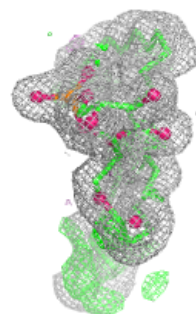
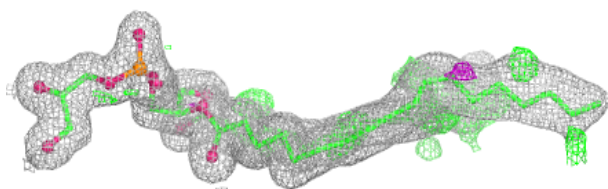
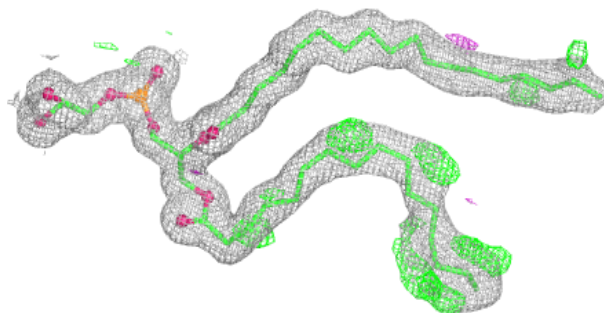
**Electron density around CHD P 301:**

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

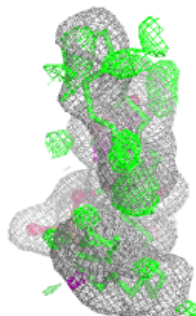
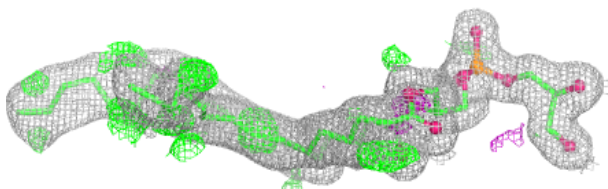
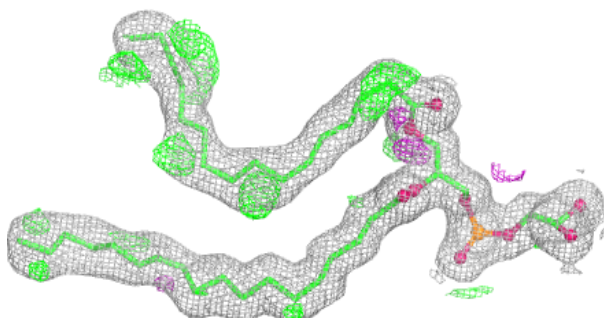


Electron density around PGV A 608:

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

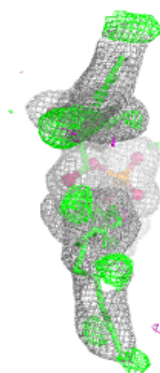
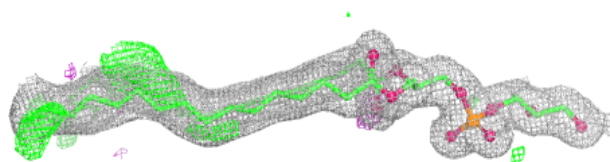
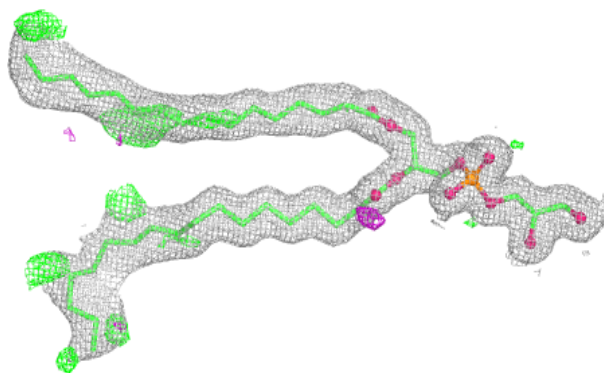
**Electron density around PGV N 609:**

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

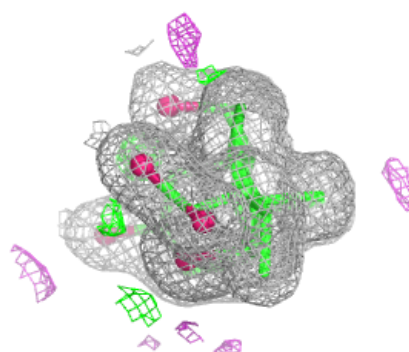
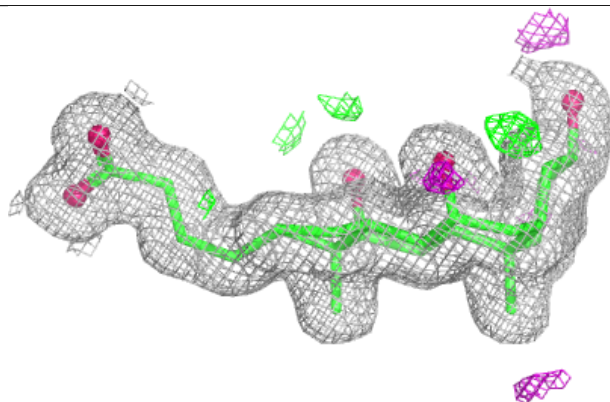
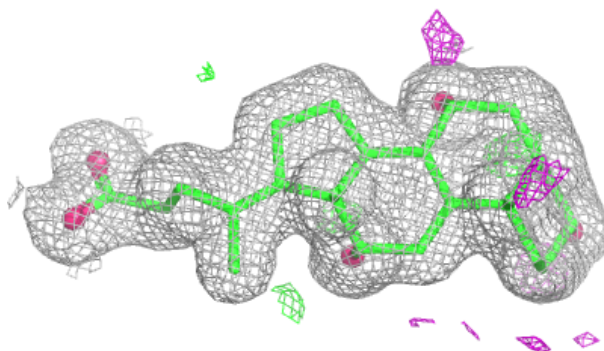


Electron density around PGV P 305:

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

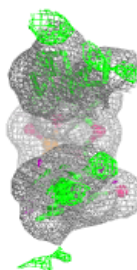
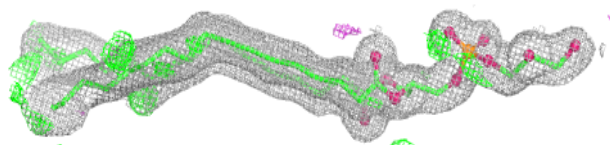
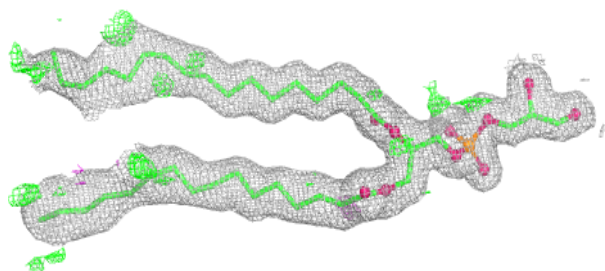
**Electron density around CHD T 101:**

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

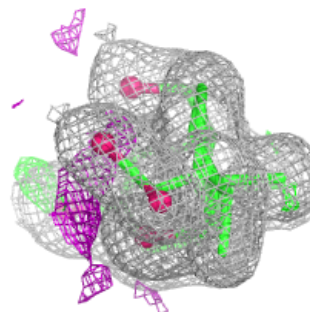
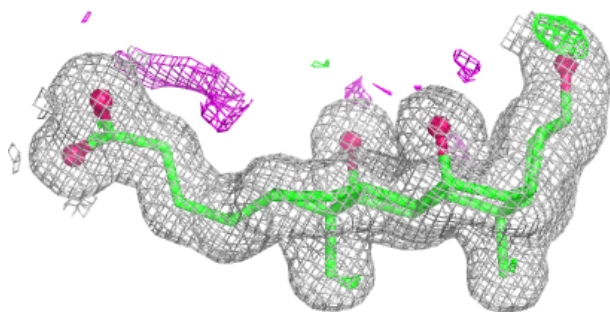
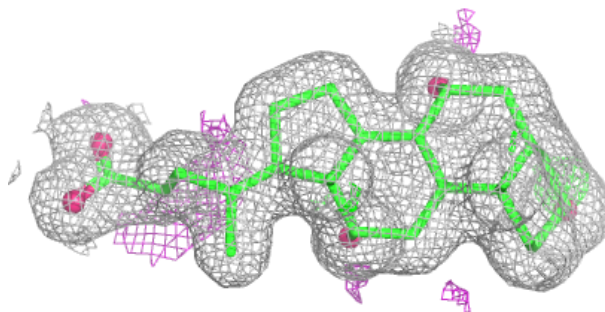


Electron density around PGV C 304:

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

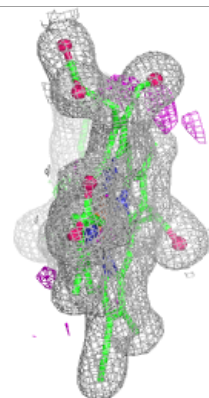
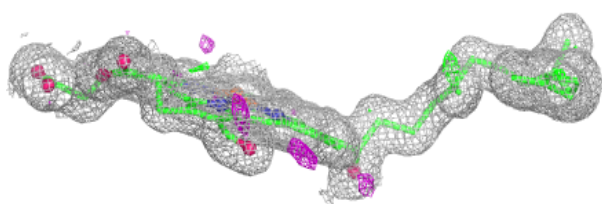
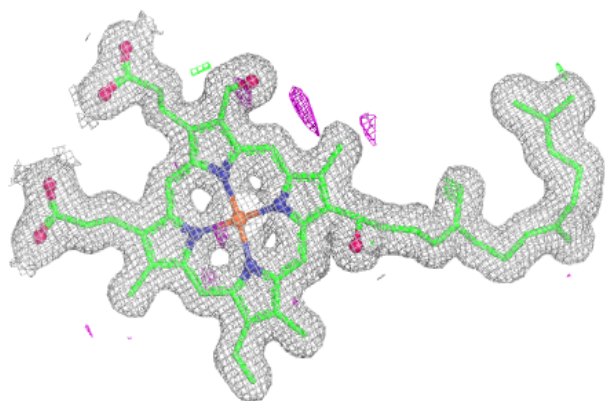
**Electron density around CHD G 103:**

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

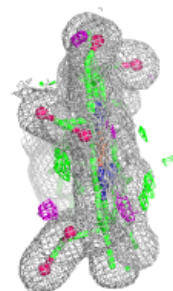
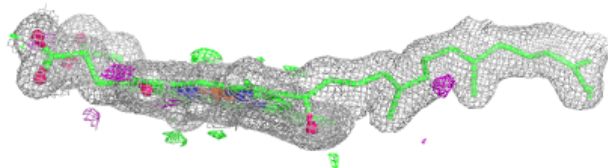
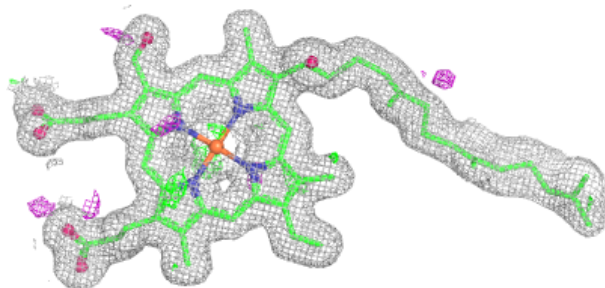


Electron density around HEA A 602:

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

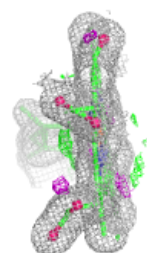
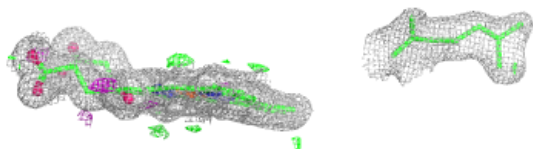
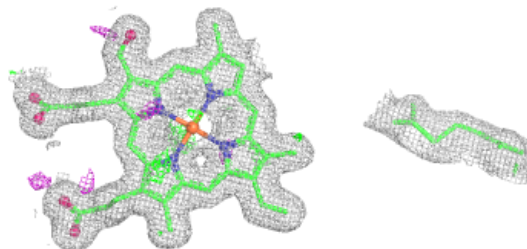
**Electron density around HEA N 601 (A):**

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

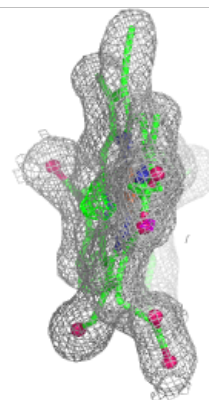
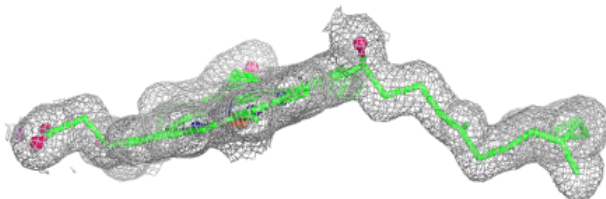
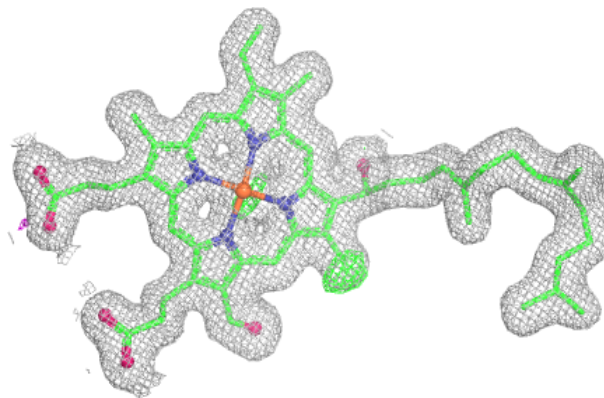


Electron density around HEA N 601 (C):

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

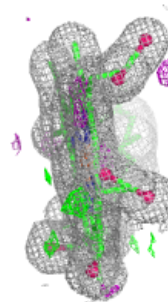
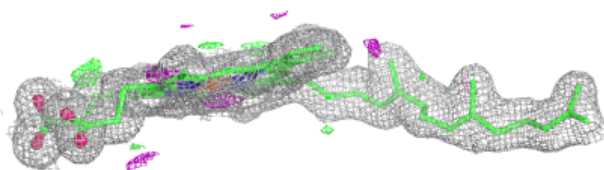
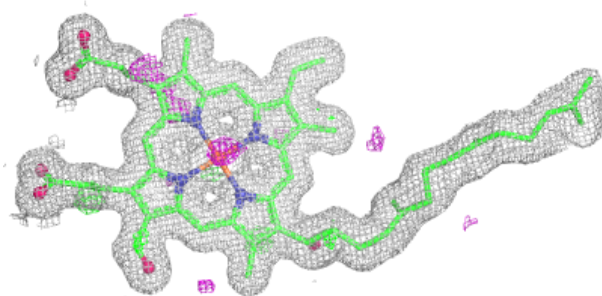
**Electron density around HEA N 602:**

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

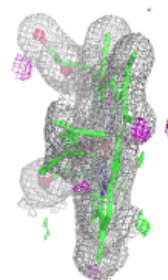
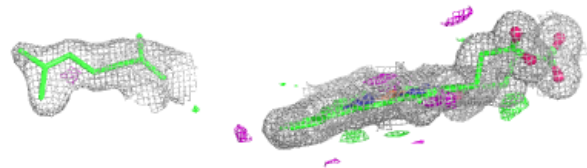
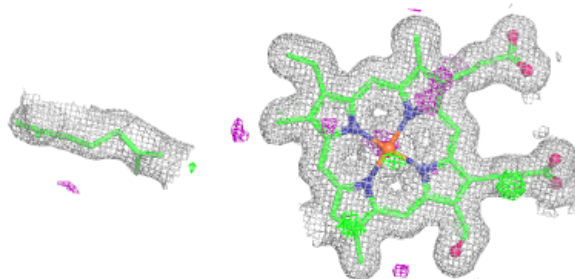


Electron density around HEA A 601 (A):

$2mF_o-DF_c$ (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 (C):**

$2mF_o-DF_c$ (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.