



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 09:09 PM UTC

PDB ID : 7THU / pdb\_00007thu  
Title : Structure of reduced bovine cytochrome c oxidase at 1.93 Angstrom resolution  
obtained by synchrotron X-rays  
Authors : Ishigami, I.; Rousseau, D.L.; Yeh, S.-R.  
Deposited on : 2022-01-12  
Resolution : 1.93 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](mailto: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>.

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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

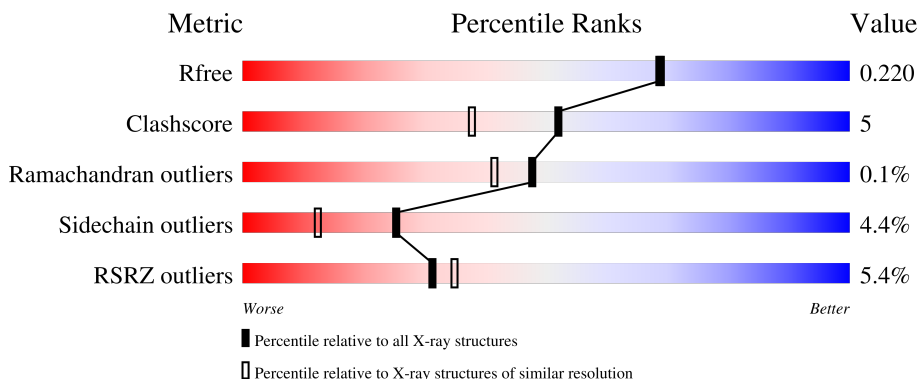
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.93 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.



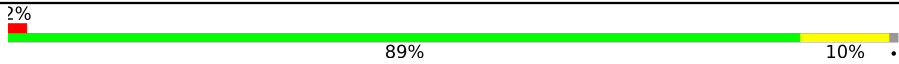
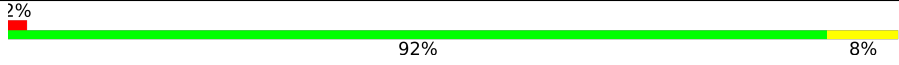
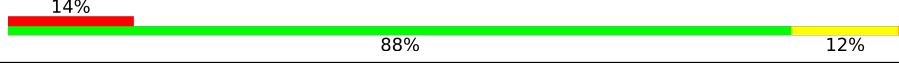
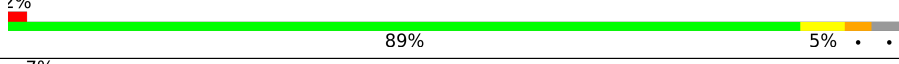
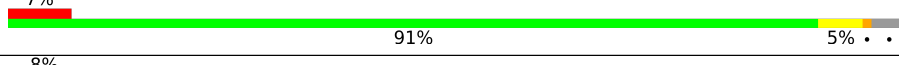
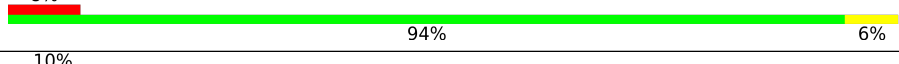


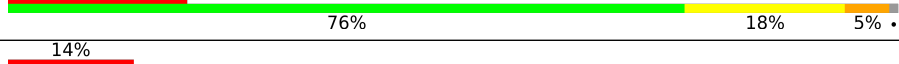


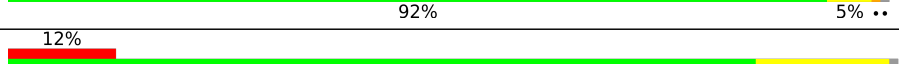

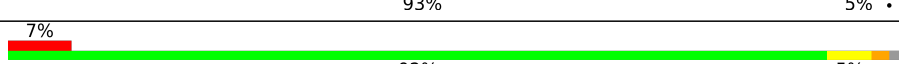
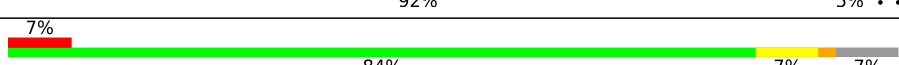
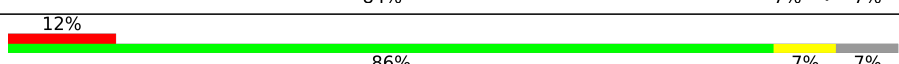
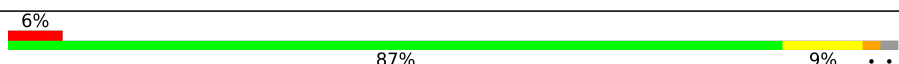
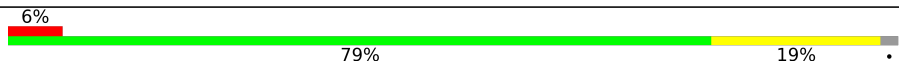
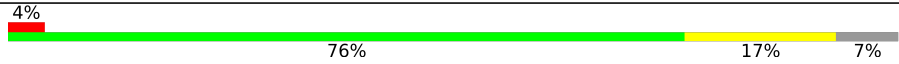


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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  $\geq 3$ , 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	 87% 13%
2	B	227	 83% 15%
2	O	227	 81% 18%
3	C	261	 90% 9%

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Mol	Chain	Length	Quality of chain
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	EDO	N	614	-	-	X	-

## 2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 32695 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
			Total	C	N	O	S			
1	A	514	4027	2691	623	678	35	0	0	0
1	N	514	4027	2691	623	678	35	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	1824	1185	281	340	18	0	0	0
2	O	227	1824	1185	281	340	18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	259	2110	1412	336	350	12	0	0	0
3	P	259	2110	1412	336	350	12	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	147	1214	788	201	221	4	0	0	0
4	Q	147	1214	788	201	221	4	0	0	0

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

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

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

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

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

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

- 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	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			
9	V	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	52	Total	C	N	O	S	0	0	0
			413	266	72	73	2			
11	X	52	Total	C	N	O	S	0	0	0
			413	266	72	73	2			

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

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

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

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

- Molecule 14 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

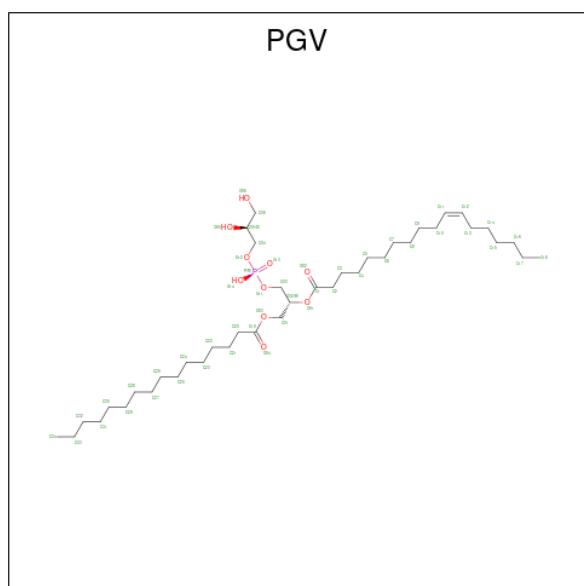
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na).

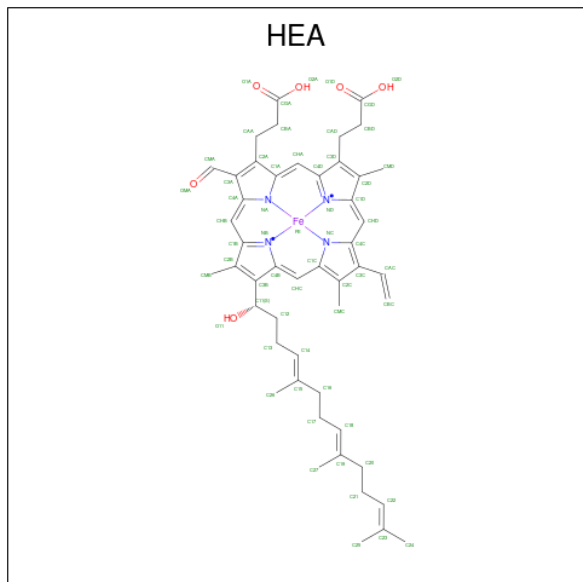
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



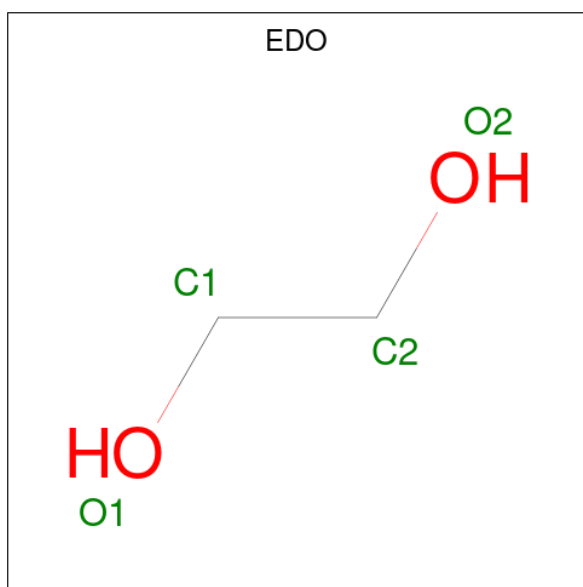
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	O	P	0	0
			51	40	10	1		
17	A	1	Total	C	O	P	0	0
			51	40	10	1		
17	C	1	Total	C	O	P	0	0
			51	40	10	1		
17	N	1	Total	C	O	P	0	0
			51	40	10	1		
17	N	1	Total	C	O	P	0	0
			51	40	10	1		
17	P	1	Total	C	O	P	0	0
			51	40	10	1		
17	T	1	Total	C	O	P	0	0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

- Molecule 18 is HEME-A (CCD ID: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 19 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



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

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

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

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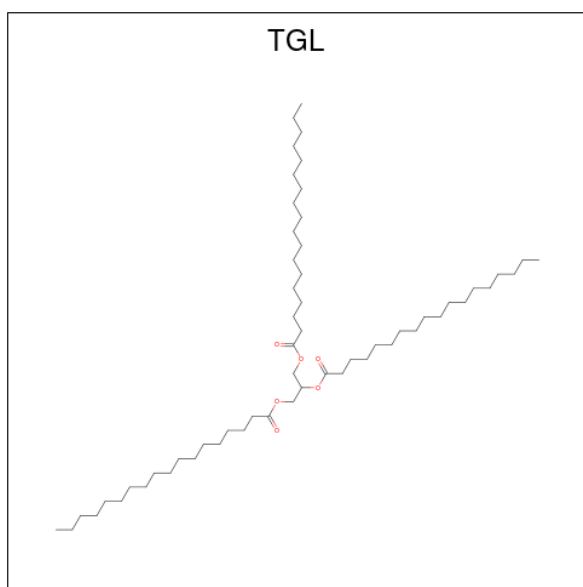
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	O	1	Total 4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

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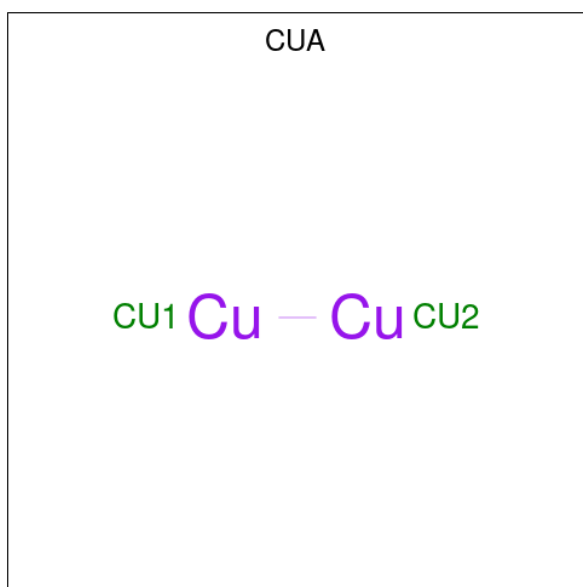
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	S	1	Total 4	C 2	O 2	0	0
19	S	1	Total 4	C 2	O 2	0	0
19	S	1	Total 4	C 2	O 2	0	0
19	S	1	Total 4	C 2	O 2	0	0
19	T	1	Total 4	C 2	O 2	0	0
19	T	1	Total 4	C 2	O 2	0	0
19	U	1	Total 4	C 2	O 2	0	0
19	V	1	Total 4	C 2	O 2	0	0
19	V	1	Total 4	C 2	O 2	0	0
19	V	1	Total 4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

- Molecule 20 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



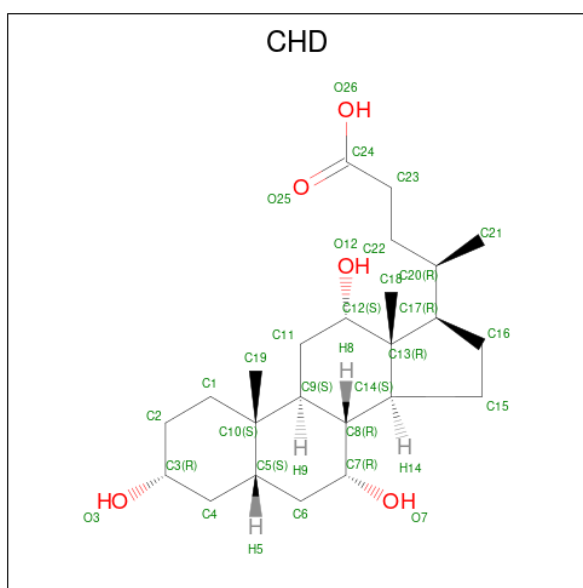
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
20	A	1	63	57	6	0	0
20	D	1	63	57	6	0	0
20	L	1	63	57	6	0	0
20	N	1	63	57	6	0	0
20	Q	1	63	57	6	0	0
20	Y	1	63	57	6	0	0

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 22 is CHOLIC ACID (CCD ID: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



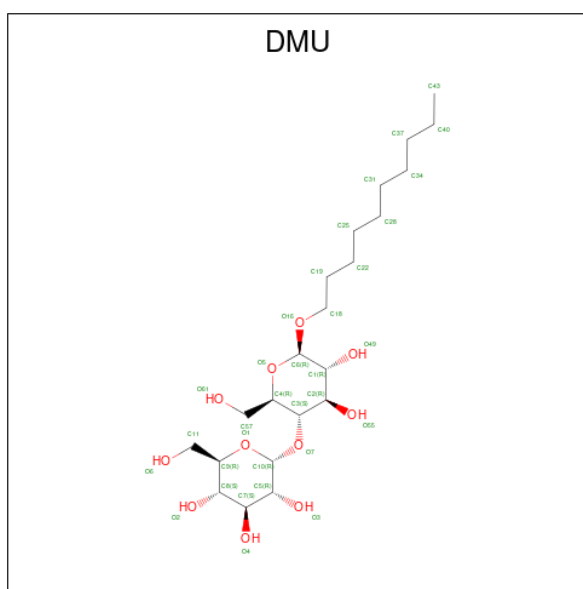
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0

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

- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula:  $C_{22}H_{42}O_{11}$ ).



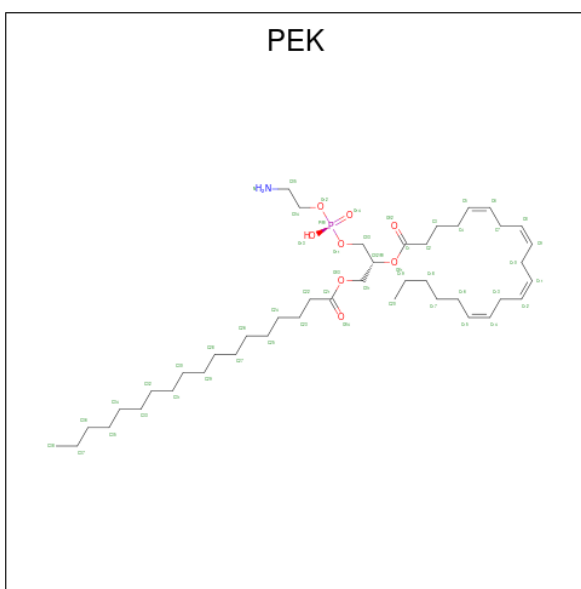
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			33	22	11		
23	C	1	Total	C	O	0	0
			33	22	11		
23	G	1	Total	C	O	0	0
			33	22	11		

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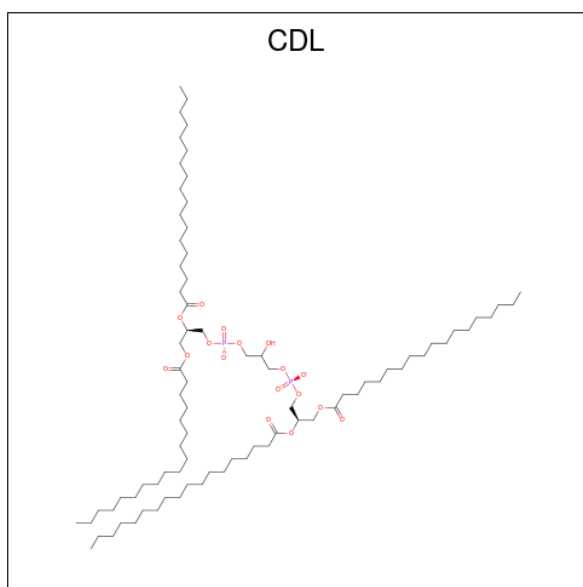
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	M	1	Total	C	O	0	0
			33	22	11		
23	P	1	Total	C	O	0	0
			33	22	11		
23	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 24 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



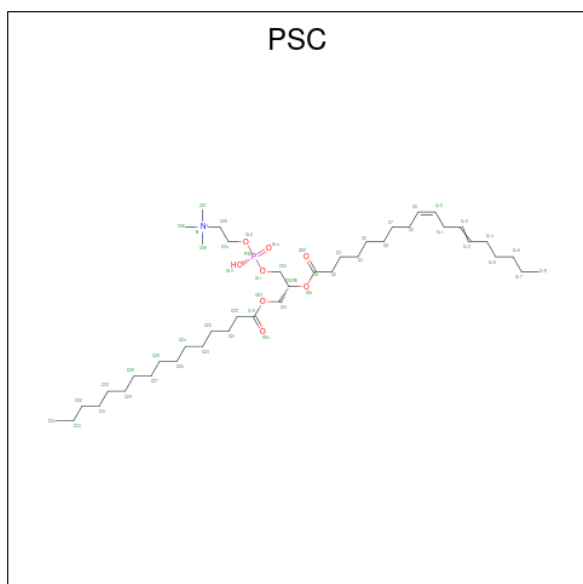
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
25	C	1	100	81	17	2	0	0
25	C	1	100	81	17	2	0	0
25	P	1	100	81	17	2	0	0
25	T	1	100	81	17	2	0	0

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).

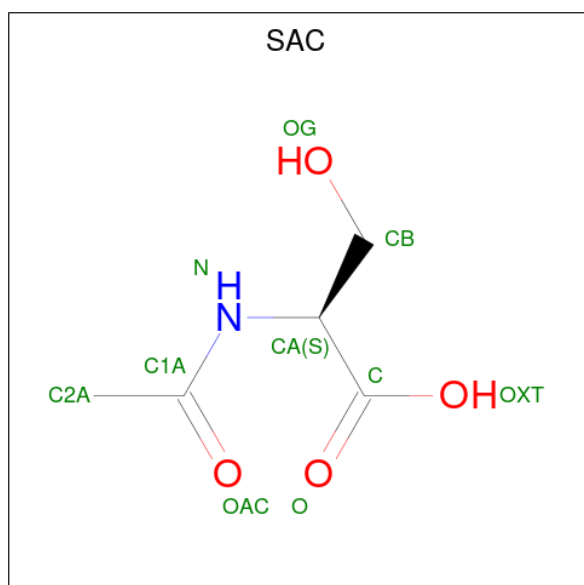


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

- Molecule 28 is N-ACETYL-SERINE (CCD ID: SAC) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	I	1	Total	C	N	O	0	0
			9	5	1	3		
28	V	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	190	Total	O	0	0
			190	190		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	B	125	Total 125	O 125	0	0
29	C	96	Total 96	O 96	0	0
29	D	68	Total 68	O 68	0	0
29	E	53	Total 53	O 53	0	0
29	F	70	Total 70	O 70	0	0
29	G	35	Total 35	O 35	0	0
29	H	39	Total 39	O 39	0	0
29	I	24	Total 24	O 24	0	0
29	J	17	Total 17	O 17	0	0
29	K	9	Total 9	O 9	0	0
29	L	21	Total 21	O 21	0	0
29	M	14	Total 14	O 14	0	0
29	N	179	Total 179	O 179	0	0
29	O	85	Total 85	O 85	0	0
29	P	80	Total 80	O 80	0	0
29	Q	46	Total 46	O 46	0	0
29	R	46	Total 46	O 46	0	0
29	S	64	Total 64	O 64	0	0
29	T	23	Total 23	O 23	0	0
29	U	30	Total 30	O 30	0	0
29	V	16	Total 16	O 16	0	0

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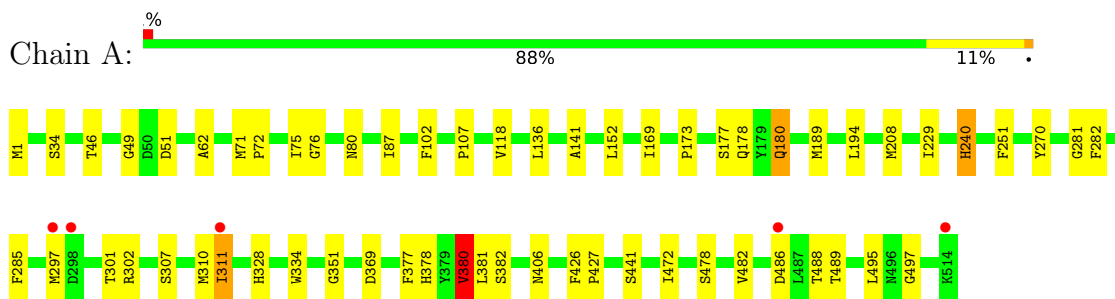
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
29	W	17	Total O 17 17	0	0
29	X	11	Total O 11 11	0	0
29	Y	18	Total O 18 18	0	0
29	Z	5	Total O 5 5	0	0

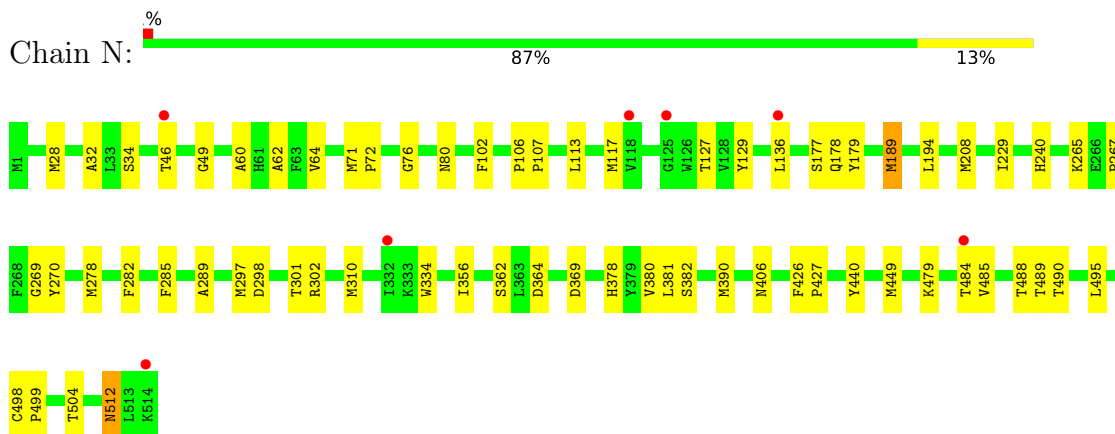
### 3 Residue-property plots [i](#)

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

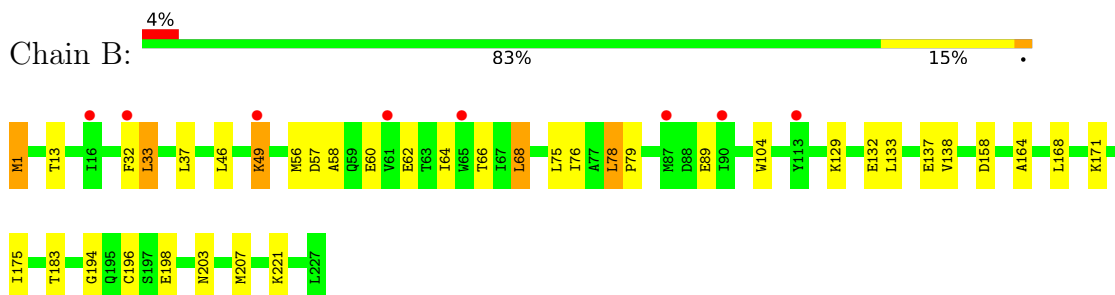
- Molecule 1: Cytochrome c oxidase subunit 1



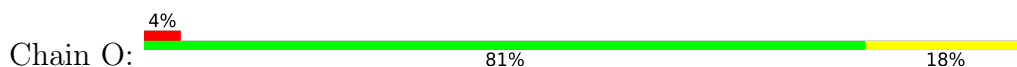
- Molecule 1: Cytochrome c oxidase subunit 1

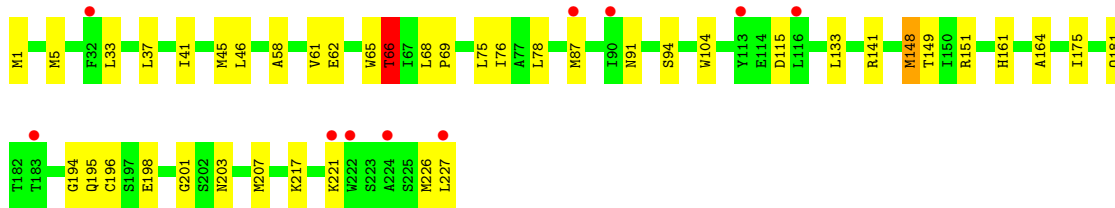


- Molecule 2: Cytochrome c oxidase subunit 2

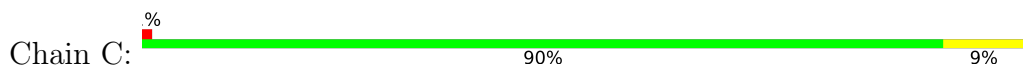


- Molecule 2: Cytochrome c oxidase subunit 2

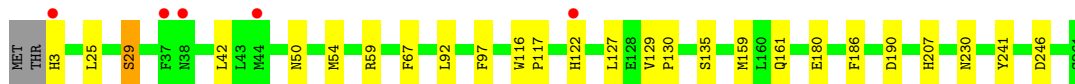
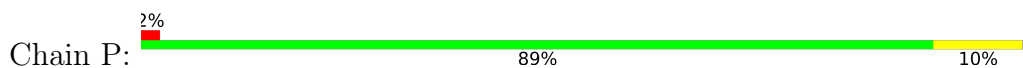




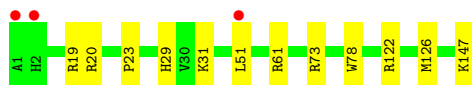
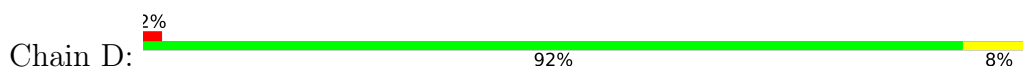
- Molecule 3: Cytochrome c oxidase subunit 3



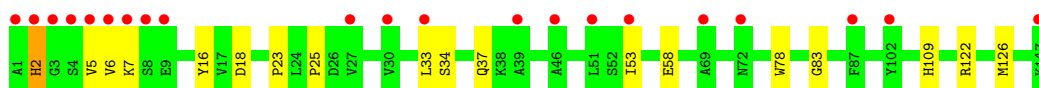
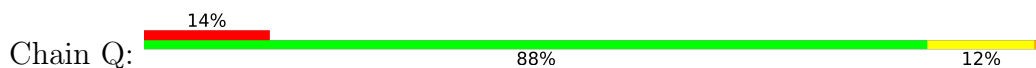
- Molecule 3: Cytochrome c oxidase subunit 3



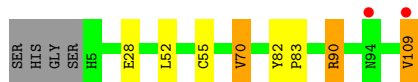
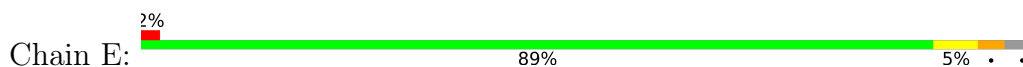
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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

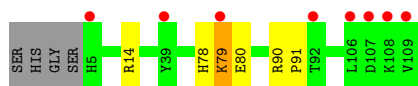


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



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

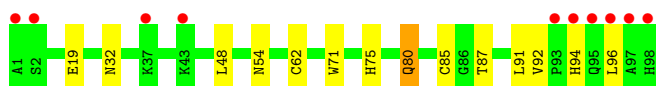
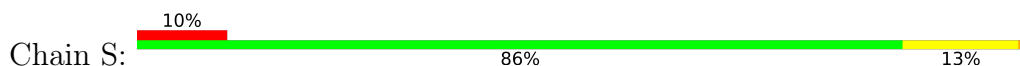




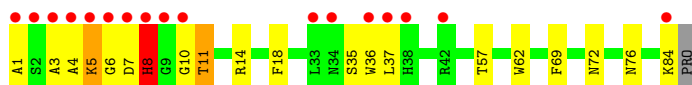
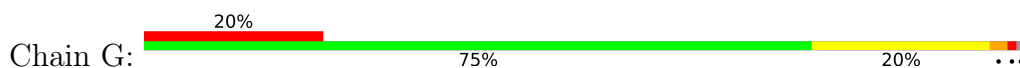
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



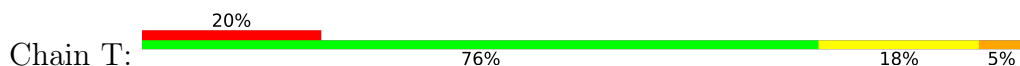
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



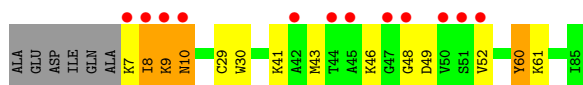
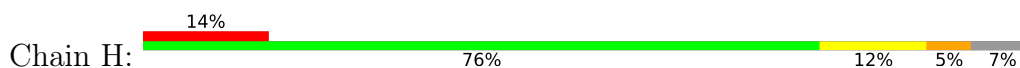
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



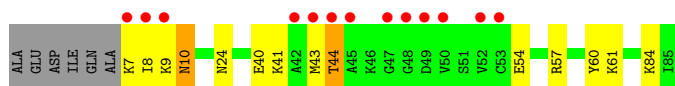
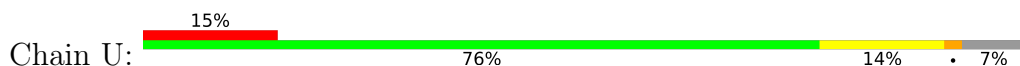
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



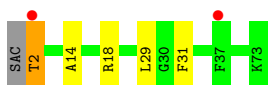
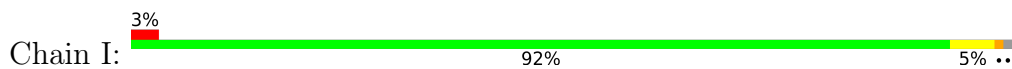
- Molecule 8: Cytochrome c oxidase subunit 6B1



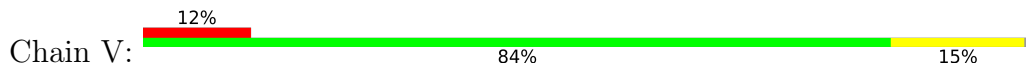
- Molecule 8: Cytochrome c oxidase subunit 6B1



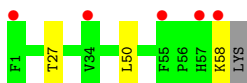
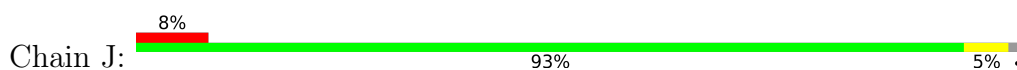
- Molecule 9: Cytochrome c oxidase subunit 6C



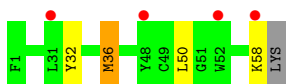
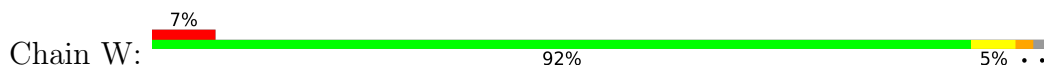
- Molecule 9: Cytochrome c oxidase subunit 6C



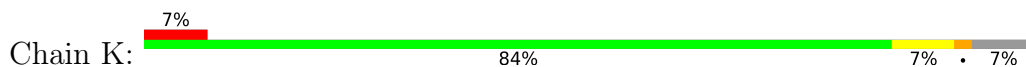
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



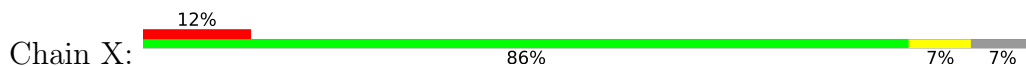
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



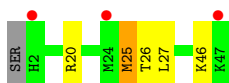
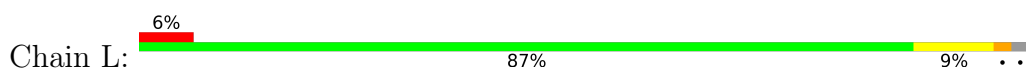
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



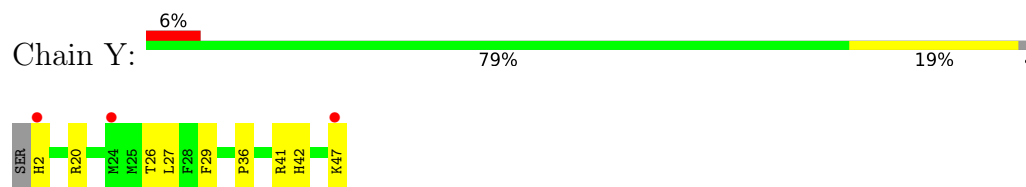
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



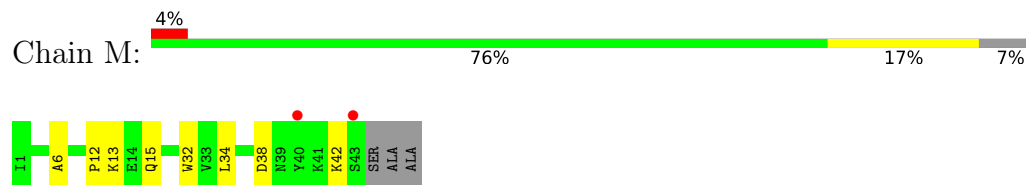
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



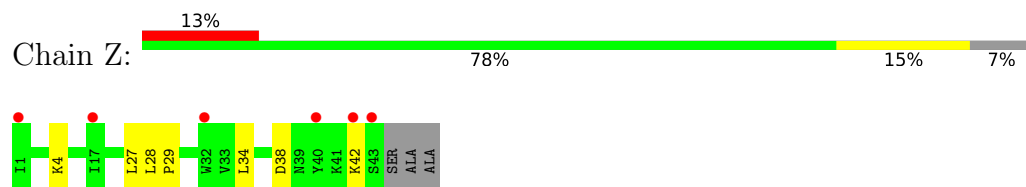
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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, $\alpha$ , $\beta$ , $\gamma$	178.18Å 182.28Å 208.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.93 40.00 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.00-1.93) 99.1 (40.00-1.93)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 1.94Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.184 , 0.212 0.194 , 0.220	Depositor DCC
$R_{free}$ test set	24681 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtrriage
Anisotropy	0.158	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.003 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	32695	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PGV, DMU, CDL, CUA, PSC, CHD, FME, PEK, CU, MG, TGL, NA, ZN, HEA, SAC, TPO, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.02	1/4156 (0.0%)	1.35	7/5678 (0.1%)
1	N	1.09	0/4156	1.28	4/5678 (0.1%)
2	B	1.09	2/1860 (0.1%)	1.36	4/2534 (0.2%)
2	O	1.04	2/1860 (0.1%)	1.35	3/2534 (0.1%)
3	C	0.99	0/2197	1.31	1/3005 (0.0%)
3	P	1.07	0/2197	1.23	4/3005 (0.1%)
4	D	1.06	0/1249	1.29	0/1685
4	Q	1.05	0/1249	1.31	0/1685
5	E	1.04	0/871	1.35	0/1182
5	R	1.01	0/871	1.41	2/1182 (0.2%)
6	F	1.08	0/765	1.26	0/1038
6	S	1.05	0/765	1.27	0/1038
7	G	1.05	0/690	1.36	3/937 (0.3%)
7	T	1.04	0/690	1.31	1/937 (0.1%)
8	H	1.03	0/682	1.47	2/921 (0.2%)
8	U	0.99	0/682	1.43	0/921
9	I	0.98	0/605	1.45	0/802
9	V	0.99	0/605	1.40	0/802
10	J	0.95	0/471	1.39	0/636
10	W	1.08	0/471	1.27	0/636
11	K	1.07	0/427	1.37	0/584
11	X	1.08	0/427	1.38	0/584
12	L	0.98	0/393	1.44	2/526 (0.4%)
12	Y	1.07	0/393	1.34	0/526
13	M	1.02	0/345	1.42	0/470
13	Z	1.03	0/345	1.42	0/470
All	All	1.05	5/29422 (0.0%)	1.33	33/39996 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	7.28	1.32	1.23
2	O	198	GLU	C-O	6.75	1.31	1.23
1	A	240	HIS	CE1-NE2	5.67	1.38	1.32
2	B	221	LYS	C-O	5.25	1.30	1.24
2	O	161	HIS	CE1-NE2	5.02	1.37	1.32

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	240	HIS	CA-CB-CG	-9.95	103.85	113.80
1	A	240	HIS	CA-CB-CG	-9.18	104.62	113.80
1	A	240	HIS	N-CA-CB	7.67	117.68	110.39
2	O	66	THR	CB-CA-C	7.57	122.79	110.83
1	A	102	PHE	CA-CB-CG	-7.23	106.57	113.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	47	0
1	N	4027	0	4001	62	0
2	B	1824	0	1833	22	0
2	O	1824	0	1833	24	0
3	C	2110	0	2027	24	0
3	P	2110	0	2027	17	0
4	D	1214	0	1201	11	0
4	Q	1214	0	1201	11	0
5	E	852	0	845	6	0
5	R	852	0	845	2	0
6	F	748	0	728	2	0
6	S	748	0	728	9	0
7	G	675	0	644	26	0
7	T	675	0	644	19	0
8	H	662	0	623	10	0
8	U	662	0	623	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	592	0	604	6	0
9	V	592	0	604	7	0
10	J	460	0	459	1	0
10	W	460	0	459	2	0
11	K	413	0	393	1	0
11	X	413	0	393	1	0
12	L	380	0	380	2	0
12	Y	380	0	380	4	0
13	M	335	0	352	5	0
13	Z	335	0	352	3	0
14	A	1	0	0	0	0
14	N	1	0	0	0	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	102	0	152	4	0
17	C	51	0	76	0	0
17	N	102	0	152	2	0
17	P	51	0	76	1	0
17	T	51	0	76	1	0
17	Z	51	0	76	2	0
18	A	120	0	108	3	0
18	N	120	0	108	5	0
19	A	48	0	72	6	0
19	B	28	0	42	0	0
19	C	20	0	30	0	0
19	D	28	0	42	0	0
19	E	16	0	24	0	0
19	F	16	0	24	1	0
19	G	16	0	24	2	0
19	I	8	0	12	0	0
19	J	16	0	24	2	0
19	K	8	0	12	0	0
19	L	4	0	6	0	0
19	M	4	0	6	0	0
19	N	48	0	72	11	0
19	O	8	0	12	0	0
19	P	12	0	18	0	0
19	Q	12	0	18	0	0
19	R	8	0	12	0	0
19	S	24	0	36	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	T	8	0	12	0	0
19	U	4	0	6	3	0
19	V	12	0	18	1	0
19	W	12	0	18	0	0
19	Z	4	0	6	0	0
20	A	63	0	110	1	0
20	D	63	0	110	7	0
20	L	63	0	110	2	0
20	N	63	0	110	0	0
20	Q	63	0	110	5	0
20	Y	63	0	110	2	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	0	0
22	C	58	0	78	1	0
22	G	29	0	39	1	0
22	J	29	0	39	0	0
22	P	58	0	78	1	0
22	T	29	0	39	7	0
22	W	29	0	39	0	0
22	Y	29	0	39	4	0
23	C	66	0	84	1	0
23	G	33	0	42	2	0
23	M	33	0	41	0	0
23	P	33	0	42	0	0
23	Z	33	0	42	1	0
24	C	159	0	231	8	0
24	P	159	0	231	6	0
25	C	200	0	312	15	0
25	P	100	0	156	4	0
25	T	100	0	156	3	0
26	E	52	0	80	5	0
26	O	52	0	80	5	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	I	9	0	8	2	0
28	V	9	0	8	1	0
29	A	190	0	0	0	0
29	B	125	0	0	1	0
29	C	96	0	0	7	0
29	D	68	0	0	0	0
29	E	53	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	F	70	0	0	0	0
29	G	35	0	0	0	0
29	H	39	0	0	1	0
29	I	24	0	0	0	0
29	J	17	0	0	0	0
29	K	9	0	0	0	0
29	L	21	0	0	2	0
29	M	14	0	0	0	0
29	N	179	0	0	7	0
29	O	85	0	0	3	0
29	P	80	0	0	1	0
29	Q	46	0	0	1	0
29	R	46	0	0	0	0
29	S	64	0	0	2	0
29	T	23	0	0	3	0
29	U	30	0	0	1	0
29	V	16	0	0	0	0
29	W	17	0	0	0	0
29	X	11	0	0	0	0
29	Y	18	0	0	1	0
29	Z	5	0	0	1	0
All	All	32695	0	32113	325	0

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

The worst 5 of 325 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)
3:C:44:MET:HG3	29:C:496:HOH:O	1.38	1.19
9:I:2:THR:N	28:I:101:SAC:HG	1.47	1.12
1:A:270:TYR:H	19:A:614:EDO:H11	1.21	1.04
24:P:305:PEK:C38	25:T:102:CDL:H271	1.91	1.00
7:T:73:PRO:HG3	7:T:84:LYS:HE2	1.49	0.94

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
1	N	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
2	B	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
2	O	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
4	D	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
4	Q	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
6	S	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
7	G	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
7	T	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	10	3
8	H	77/85 (91%)	71 (92%)	5 (6%)	1 (1%)	9	3
8	U	77/85 (91%)	71 (92%)	6 (8%)	0	100	100
9	I	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
9	V	70/73 (96%)	68 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
11	X	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3514/3614 (97%)	3412 (97%)	100 (3%)	2 (0%)	48	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	48	GLY
7	T	4	ALA

### 5.3.2 Protein sidechains [i](#)

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	426/426 (100%)	420 (99%)	6 (1%)	59	52
1	N	426/426 (100%)	415 (97%)	11 (3%)	40	28
2	B	210/210 (100%)	200 (95%)	10 (5%)	23	10
2	O	210/210 (100%)	199 (95%)	11 (5%)	21	8
3	C	224/226 (99%)	221 (99%)	3 (1%)	61	54
3	P	224/226 (99%)	219 (98%)	5 (2%)	45	35
4	D	129/129 (100%)	126 (98%)	3 (2%)	44	33
4	Q	129/129 (100%)	124 (96%)	5 (4%)	28	15
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	20
5	R	92/95 (97%)	89 (97%)	3 (3%)	33	20
6	F	81/81 (100%)	78 (96%)	3 (4%)	30	16
6	S	81/81 (100%)	76 (94%)	5 (6%)	16	5
7	G	67/68 (98%)	60 (90%)	7 (10%)	7	1
7	T	67/68 (98%)	59 (88%)	8 (12%)	5	0
8	H	71/75 (95%)	64 (90%)	7 (10%)	7	1
8	U	71/75 (95%)	62 (87%)	9 (13%)	4	0
9	I	57/57 (100%)	54 (95%)	3 (5%)	20	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	V	57/57 (100%)	52 (91%)	5 (9%)	9	2
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	14
10	W	49/50 (98%)	46 (94%)	3 (6%)	17	5
11	K	42/46 (91%)	38 (90%)	4 (10%)	8	1
11	X	42/46 (91%)	39 (93%)	3 (7%)	13	3
12	L	39/40 (98%)	36 (92%)	3 (8%)	12	3
12	Y	39/40 (98%)	34 (87%)	5 (13%)	4	0
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	1
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	2
All	All	3048/3082 (99%)	2914 (96%)	134 (4%)	25	12

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	V	29	LEU
9	V	65	LYS
12	Y	47	LYS
11	K	20	SER
11	K	12	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	181	GLN
4	Q	109	HIS
3	P	50	ASN
3	P	207	HIS
5	R	94	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

6 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
2	FME	B	1	2	8,9,10	0.77	0	8,9,11	1.15	1 (12%)
1	FME	N	1	1	8,9,10	0.56	0	8,9,11	1.11	0
7	TPO	G	11	7	8,10,11	1.37	1 (12%)	10,14,16	1.33	1 (10%)
7	TPO	T	11	7	8,10,11	0.97	1 (12%)	10,14,16	0.95	0
2	FME	O	1	2	8,9,10	0.39	0	8,9,11	0.87	0
1	FME	A	1	1	8,9,10	0.31	0	8,9,11	0.83	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	B	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-
7	TPO	G	11	7	-	6/9/11/13	-
7	TPO	T	11	7	-	5/9/11/13	-
2	FME	O	1	2	-	0/7/9/11	-
1	FME	A	1	1	-	1/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	3.23	1.65	1.59
7	T	11	TPO	P-OG1	2.14	1.63	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	11	TPO	P-OG1-CB	3.31	132.33	123.33
2	B	1	FME	O-C-CA	-2.04	119.51	124.77
1	A	1	FME	O-C-CA	-2.02	119.57	124.77

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
7	G	11	TPO	CA-CB-OG1-P

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FME	1	0
7	G	11	TPO	4	0
2	O	1	FME	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 149 ligands modelled in this entry, 8 are monoatomic - leaving 141 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	$\# Z  > 2$
19	EDO	G	1304	-	3,3,3	0.16	0	2,2,2	0.31	0
22	CHD	Y	102	-	32,32,32	0.59	0	51,51,51	0.95	3 (5%)
19	EDO	B	306	-	3,3,3	0.22	0	2,2,2	0.22	0
19	EDO	N	610	-	3,3,3	0.39	0	2,2,2	0.67	0
19	EDO	V	103	-	3,3,3	0.16	0	2,2,2	0.29	0
25	CDL	P	307	-	99,99,99	0.34	0	105,111,111	0.52	1 (0%)
19	EDO	I	102	-	3,3,3	0.10	0	2,2,2	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	EDO	P	309	-	3,3,3	0.16	0	2,2,2	0.25	0
19	EDO	K	102	-	3,3,3	0.12	0	2,2,2	0.24	0
19	EDO	N	608	-	3,3,3	0.25	0	2,2,2	0.38	0
18	HEA	N	607	1	67,67,67	2.34	24 (35%)	81,103,103	2.79	35 (43%)
21	CUA	B	301	2	0,1,1	-	-	-	-	-
19	EDO	N	618	-	3,3,3	0.17	0	2,2,2	0.07	0
19	EDO	B	308	-	3,3,3	0.08	0	2,2,2	0.04	0
19	EDO	L	102	-	3,3,3	0.25	0	2,2,2	0.33	0
19	EDO	Q	202	-	3,3,3	0.18	0	2,2,2	0.29	0
22	CHD	C	307	-	32,32,32	0.62	0	51,51,51	0.78	0
19	EDO	D	203	-	3,3,3	0.09	0	2,2,2	0.06	0
19	EDO	J	1103	-	3,3,3	0.09	0	2,2,2	0.09	0
24	PEK	P	301	-	52,52,52	0.32	0	55,57,57	0.47	0
19	EDO	N	617	-	3,3,3	0.04	0	2,2,2	0.20	0
19	EDO	U	1501	-	3,3,3	0.26	0	2,2,2	0.45	0
19	EDO	M	102	-	3,3,3	0.12	0	2,2,2	0.12	0
17	PGV	N	616	-	50,50,50	1.04	2 (4%)	53,56,56	1.06	4 (7%)
24	PEK	C	304	-	52,52,52	0.36	0	55,57,57	0.52	0
22	CHD	P	303	-	32,32,32	0.69	1 (3%)	51,51,51	0.73	0
19	EDO	V	102	-	3,3,3	0.13	0	2,2,2	0.27	0
19	EDO	A	610	-	3,3,3	0.25	0	2,2,2	0.21	0
19	EDO	C	309	-	3,3,3	0.02	0	2,2,2	0.15	0
19	EDO	N	611	-	3,3,3	0.19	0	2,2,2	0.07	0
28	SAC	V	101	-	7,8,9	0.50	0	7,9,11	1.17	1 (14%)
22	CHD	T	104	-	32,32,32	0.72	0	51,51,51	1.26	6 (11%)
19	EDO	Z	103	-	3,3,3	0.23	0	2,2,2	0.26	0
19	EDO	A	619	-	3,3,3	0.36	0	2,2,2	0.48	0
19	EDO	E	204	-	3,3,3	0.11	0	2,2,2	0.28	0
19	EDO	O	303	-	3,3,3	0.46	0	2,2,2	0.65	0
24	PEK	P	304	-	52,52,52	0.43	0	55,57,57	0.72	1 (1%)
19	EDO	C	310	-	3,3,3	0.08	0	2,2,2	0.09	0
23	DMU	P	302	-	34,34,34	1.11	2 (5%)	45,45,45	1.96	9 (20%)
19	EDO	A	613	-	3,3,3	0.38	0	2,2,2	0.35	0
19	EDO	S	2201	-	3,3,3	0.40	0	2,2,2	0.50	0
20	TGL	N	604	-	62,62,62	0.27	0	65,65,65	0.46	1 (1%)
19	EDO	A	618	-	3,3,3	0.16	0	2,2,2	0.49	0
19	EDO	S	2203	-	3,3,3	0.35	0	2,2,2	0.23	0
19	EDO	C	308	-	3,3,3	0.37	0	2,2,2	0.11	0
19	EDO	D	208	-	3,3,3	0.16	0	2,2,2	0.10	0
19	EDO	E	202	-	3,3,3	0.13	0	2,2,2	0.21	0
20	TGL	A	615	-	62,62,62	0.36	0	65,65,65	0.48	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	TGL	L	101	-	62,62,62	0.35	0	65,65,65	0.27	0
19	EDO	K	101	-	3,3,3	0.08	0	2,2,2	0.15	0
19	EDO	D	205	-	3,3,3	0.30	0	2,2,2	0.25	0
19	EDO	A	609	-	3,3,3	0.19	0	2,2,2	0.09	0
19	EDO	D	202	-	3,3,3	0.12	0	2,2,2	0.17	0
21	CUA	O	301	2	0,1,1	-	-	-	-	-
19	EDO	F	704	-	3,3,3	0.15	0	2,2,2	0.34	0
19	EDO	D	204	-	3,3,3	0.09	0	2,2,2	0.08	0
19	EDO	I	103	-	3,3,3	0.17	0	2,2,2	0.36	0
19	EDO	A	611	-	3,3,3	0.15	0	2,2,2	0.03	0
19	EDO	R	202	-	3,3,3	0.13	0	2,2,2	0.22	0
19	EDO	G	1301	-	3,3,3	0.21	0	2,2,2	0.42	0
19	EDO	B	303	-	3,3,3	0.39	0	2,2,2	0.23	0
19	EDO	E	205	-	3,3,3	0.07	0	2,2,2	0.15	0
20	TGL	Y	101	-	62,62,62	0.33	0	65,65,65	0.52	1 (1%)
17	PGV	Z	102	-	50,50,50	1.09	2 (4%)	53,56,56	1.18	5 (9%)
18	HEA	N	606	1	67,67,67	2.06	21 (31%)	81,103,103	2.71	38 (46%)
19	EDO	A	608	-	3,3,3	0.31	0	2,2,2	0.26	0
19	EDO	N	609	-	3,3,3	0.17	0	2,2,2	0.09	0
24	PEK	P	305	-	52,52,52	0.34	0	55,57,57	0.40	0
19	EDO	F	705	-	3,3,3	0.32	0	2,2,2	0.33	0
19	EDO	T	103	-	3,3,3	0.37	0	2,2,2	0.12	0
19	EDO	V	104	-	3,3,3	0.37	0	2,2,2	0.41	0
24	PEK	C	303	-	52,52,52	0.49	0	55,57,57	0.80	1 (1%)
19	EDO	N	613	-	3,3,3	0.57	0	2,2,2	0.71	0
25	CDL	C	312	-	99,99,99	0.37	0	105,111,111	0.46	0
19	EDO	D	206	-	3,3,3	0.19	0	2,2,2	0.25	0
19	EDO	E	203	-	3,3,3	0.22	0	2,2,2	0.33	0
19	EDO	A	614	-	3,3,3	0.47	0	2,2,2	0.42	0
17	PGV	N	605	-	50,50,50	0.83	2 (4%)	53,56,56	1.31	4 (7%)
17	PGV	P	306	-	50,50,50	0.77	2 (4%)	53,56,56	0.99	4 (7%)
19	EDO	P	311	-	3,3,3	0.37	0	2,2,2	0.40	0
19	EDO	F	701	-	3,3,3	0.13	0	2,2,2	0.37	0
19	EDO	A	617	-	3,3,3	0.15	0	2,2,2	0.13	0
22	CHD	W	302	-	32,32,32	0.56	0	51,51,51	0.74	0
18	HEA	A	607	1	67,67,67	2.15	23 (34%)	81,103,103	2.79	28 (34%)
24	PEK	C	315	-	52,52,52	0.43	0	55,57,57	0.57	0
26	PSC	O	302	-	51,51,51	0.42	0	57,59,59	0.42	0
19	EDO	T	105	-	3,3,3	0.04	0	2,2,2	0.28	0
18	HEA	A	606	1	67,67,67	1.99	24 (35%)	81,103,103	2.74	34 (41%)
19	EDO	G	1303	-	3,3,3	0.07	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	EDO	Q	204	-	3,3,3	0.22	0	2,2,2	0.03	0
19	EDO	S	2205	-	3,3,3	0.11	0	2,2,2	0.14	0
19	EDO	A	616	-	3,3,3	0.08	0	2,2,2	0.21	0
19	EDO	D	207	-	3,3,3	0.23	0	2,2,2	0.17	0
19	EDO	J	1101	-	3,3,3	0.47	0	2,2,2	0.32	0
19	EDO	B	309	-	3,3,3	0.11	0	2,2,2	0.22	0
28	SAC	I	101	-	7,8,9	0.54	0	7,9,11	1.14	1 (14%)
19	EDO	C	311	-	3,3,3	0.12	0	2,2,2	0.18	0
23	DMU	M	101	-	34,34,34	1.10	3 (8%)	45,45,45	1.27	5 (11%)
23	DMU	C	301	-	34,34,34	1.54	5 (14%)	45,45,45	1.86	9 (20%)
23	DMU	C	313	-	34,34,34	1.81	7 (20%)	45,45,45	1.95	10 (22%)
19	EDO	W	303	-	3,3,3	0.39	0	2,2,2	0.40	0
25	CDL	T	102	-	99,99,99	0.36	0	105,111,111	0.47	0
17	PGV	C	305	-	50,50,50	0.74	3 (6%)	53,56,56	0.82	1 (1%)
17	PGV	A	605	-	50,50,50	0.85	3 (6%)	53,56,56	1.24	2 (3%)
22	CHD	C	302	-	32,32,32	0.66	1 (3%)	51,51,51	0.78	1 (1%)
19	EDO	N	612	-	3,3,3	0.19	0	2,2,2	0.25	0
19	EDO	N	620	-	3,3,3	0.33	0	2,2,2	0.46	0
19	EDO	J	1104	-	3,3,3	0.50	0	2,2,2	0.63	0
22	CHD	J	1102	-	32,32,32	0.65	1 (3%)	51,51,51	0.78	0
19	EDO	R	201	-	3,3,3	0.11	0	2,2,2	0.12	0
19	EDO	O	304	-	3,3,3	0.25	0	2,2,2	0.30	0
19	EDO	S	2207	-	3,3,3	0.12	0	2,2,2	0.33	0
19	EDO	B	305	-	3,3,3	0.13	0	2,2,2	0.23	0
19	EDO	A	612	-	3,3,3	0.19	0	2,2,2	0.13	0
20	TGL	D	201	-	62,62,62	0.37	0	65,65,65	0.56	2 (3%)
19	EDO	S	2206	-	3,3,3	0.18	0	2,2,2	0.09	0
19	EDO	F	702	-	3,3,3	0.17	0	2,2,2	0.13	0
22	CHD	G	1305	-	32,32,32	0.57	0	51,51,51	0.81	0
23	DMU	G	1302	-	34,34,34	1.86	10 (29%)	45,45,45	1.45	7 (15%)
19	EDO	W	301	-	3,3,3	0.18	0	2,2,2	0.46	0
17	PGV	T	101	-	50,50,50	1.15	2 (4%)	53,56,56	1.21	4 (7%)
20	TGL	Q	201	-	62,62,62	0.29	0	65,65,65	0.31	0
19	EDO	S	2204	-	3,3,3	0.32	0	2,2,2	0.40	0
19	EDO	Q	203	-	3,3,3	0.21	0	2,2,2	0.09	0
19	EDO	B	304	-	3,3,3	0.22	0	2,2,2	0.20	0
22	CHD	B	302	-	32,32,32	0.62	0	51,51,51	0.86	1 (1%)
22	CHD	P	308	-	32,32,32	0.61	0	51,51,51	1.08	2 (3%)
25	CDL	C	306	-	99,99,99	0.39	0	105,111,111	0.60	2 (1%)
19	EDO	N	614	-	3,3,3	0.54	0	2,2,2	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	DMU	Z	101	-	34,34,34	1.19	4 (11%)	45,45,45	1.56	7 (15%)
19	EDO	A	620	-	3,3,3	0.28	0	2,2,2	0.06	0
19	EDO	N	619	-	3,3,3	0.10	0	2,2,2	0.13	0
19	EDO	P	310	-	3,3,3	0.31	0	2,2,2	0.23	0
26	PSC	E	201	-	51,51,51	0.45	0	57,59,59	0.52	0
19	EDO	C	314	-	3,3,3	0.11	0	2,2,2	0.11	0
19	EDO	N	615	-	3,3,3	0.11	0	2,2,2	0.24	0
19	EDO	W	304	-	3,3,3	0.18	0	2,2,2	0.17	0
17	PGV	A	604	-	50,50,50	1.19	2 (4%)	53,56,56	1.62	5 (9%)
19	EDO	J	1105	-	3,3,3	0.22	0	2,2,2	0.35	0
19	EDO	G	1306	-	3,3,3	0.12	0	2,2,2	0.18	0
19	EDO	B	307	-	3,3,3	0.16	0	2,2,2	0.16	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	G	1304	-	-	1/1/1/1	-
22	CHD	Y	102	-	-	8/9/74/74	0/4/4/4
19	EDO	B	306	-	-	1/1/1/1	-
19	EDO	N	610	-	-	0/1/1/1	-
19	EDO	V	103	-	-	0/1/1/1	-
25	CDL	P	307	-	-	49/110/110/110	-
19	EDO	I	102	-	-	1/1/1/1	-
19	EDO	P	309	-	-	1/1/1/1	-
19	EDO	K	102	-	-	1/1/1/1	-
19	EDO	N	608	-	-	1/1/1/1	-
18	HEA	N	607	1	-	4/36/76/76	-
19	EDO	N	618	-	-	0/1/1/1	-
19	EDO	B	308	-	-	1/1/1/1	-
19	EDO	L	102	-	-	0/1/1/1	-
19	EDO	Q	202	-	-	1/1/1/1	-
22	CHD	C	307	-	-	2/9/74/74	0/4/4/4
19	EDO	D	203	-	-	1/1/1/1	-
19	EDO	J	1103	-	-	0/1/1/1	-
24	PEK	P	301	-	-	29/56/56/56	-
19	EDO	N	617	-	-	0/1/1/1	-
19	EDO	U	1501	-	-	0/1/1/1	-
19	EDO	M	102	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PGV	N	616	-	-	24/55/55/55	-
24	PEK	C	304	-	-	28/56/56/56	-
22	CHD	P	303	-	-	2/9/74/74	0/4/4/4
19	EDO	V	102	-	-	1/1/1/1	-
19	EDO	A	610	-	-	0/1/1/1	-
19	EDO	C	309	-	-	1/1/1/1	-
19	EDO	N	611	-	-	0/1/1/1	-
28	SAC	V	101	-	-	3/7/8/10	-
22	CHD	T	104	-	-	6/9/74/74	0/4/4/4
19	EDO	Z	103	-	-	0/1/1/1	-
19	EDO	A	619	-	-	1/1/1/1	-
19	EDO	E	204	-	-	1/1/1/1	-
19	EDO	O	303	-	-	1/1/1/1	-
24	PEK	P	304	-	-	20/56/56/56	-
19	EDO	C	310	-	-	1/1/1/1	-
23	DMU	P	302	-	-	6/19/59/59	0/2/2/2
19	EDO	A	613	-	-	0/1/1/1	-
19	EDO	S	2201	-	-	1/1/1/1	-
20	TGL	N	604	-	-	33/65/65/65	-
19	EDO	A	618	-	-	0/1/1/1	-
19	EDO	S	2203	-	-	0/1/1/1	-
19	EDO	C	308	-	-	0/1/1/1	-
19	EDO	D	208	-	-	0/1/1/1	-
19	EDO	E	202	-	-	1/1/1/1	-
20	TGL	A	615	-	-	42/65/65/65	-
20	TGL	L	101	-	-	36/65/65/65	-
19	EDO	K	101	-	-	1/1/1/1	-
19	EDO	D	205	-	-	1/1/1/1	-
19	EDO	A	609	-	-	0/1/1/1	-
19	EDO	D	202	-	-	0/1/1/1	-
19	EDO	F	704	-	-	1/1/1/1	-
19	EDO	D	204	-	-	1/1/1/1	-
19	EDO	I	103	-	-	1/1/1/1	-
19	EDO	A	611	-	-	1/1/1/1	-
19	EDO	R	202	-	-	1/1/1/1	-
19	EDO	G	1301	-	-	0/1/1/1	-
19	EDO	B	303	-	-	0/1/1/1	-
19	EDO	E	205	-	-	1/1/1/1	-
20	TGL	Y	101	-	-	28/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PGV	Z	102	-	-	24/55/55/55	-
18	HEA	N	606	1	-	4/36/76/76	-
19	EDO	A	608	-	-	0/1/1/1	-
19	EDO	N	609	-	-	1/1/1/1	-
24	PEK	P	305	-	-	31/56/56/56	-
19	EDO	F	705	-	-	0/1/1/1	-
19	EDO	T	103	-	-	1/1/1/1	-
19	EDO	V	104	-	-	0/1/1/1	-
24	PEK	C	303	-	-	22/56/56/56	-
19	EDO	N	613	-	-	0/1/1/1	-
25	CDL	C	312	-	-	60/110/110/110	-
19	EDO	D	206	-	-	1/1/1/1	-
19	EDO	E	203	-	-	0/1/1/1	-
19	EDO	A	614	-	-	1/1/1/1	-
17	PGV	N	605	-	-	14/55/55/55	-
17	PGV	P	306	-	-	8/55/55/55	-
19	EDO	P	311	-	-	1/1/1/1	-
19	EDO	F	701	-	-	1/1/1/1	-
19	EDO	A	617	-	-	1/1/1/1	-
22	CHD	W	302	-	-	2/9/74/74	0/4/4/4
18	HEA	A	607	1	-	8/36/76/76	-
24	PEK	C	315	-	-	26/56/56/56	-
26	PSC	O	302	-	-	37/55/55/55	-
19	EDO	T	105	-	-	1/1/1/1	-
18	HEA	A	606	1	-	7/36/76/76	-
19	EDO	G	1303	-	-	1/1/1/1	-
19	EDO	Q	204	-	-	0/1/1/1	-
19	EDO	S	2205	-	-	0/1/1/1	-
19	EDO	A	616	-	-	0/1/1/1	-
19	EDO	D	207	-	-	1/1/1/1	-
19	EDO	J	1101	-	-	0/1/1/1	-
19	EDO	B	309	-	-	1/1/1/1	-
28	SAC	I	101	-	-	7/7/8/10	-
19	EDO	C	311	-	-	0/1/1/1	-
23	DMU	M	101	-	-	6/19/59/59	0/2/2/2
23	DMU	C	301	-	-	11/19/59/59	0/2/2/2
23	DMU	C	313	-	-	6/19/59/59	0/2/2/2
19	EDO	W	303	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CDL	T	102	-	-	62/110/110/110	-
17	PGV	C	305	-	-	13/55/55/55	-
17	PGV	A	605	-	-	15/55/55/55	-
22	CHD	C	302	-	-	1/9/74/74	0/4/4/4
19	EDO	N	612	-	-	1/1/1/1	-
19	EDO	N	620	-	-	1/1/1/1	-
19	EDO	J	1104	-	-	0/1/1/1	-
22	CHD	J	1102	-	-	2/9/74/74	0/4/4/4
19	EDO	R	201	-	-	1/1/1/1	-
19	EDO	O	304	-	-	0/1/1/1	-
19	EDO	S	2207	-	-	1/1/1/1	-
19	EDO	B	305	-	-	0/1/1/1	-
19	EDO	A	612	-	-	0/1/1/1	-
20	TGL	D	201	-	-	36/65/65/65	-
19	EDO	S	2206	-	-	1/1/1/1	-
19	EDO	F	702	-	-	0/1/1/1	-
22	CHD	G	1305	-	-	2/9/74/74	0/4/4/4
23	DMU	G	1302	-	-	11/19/59/59	0/2/2/2
19	EDO	W	301	-	-	1/1/1/1	-
17	PGV	T	101	-	-	25/55/55/55	-
20	TGL	Q	201	-	-	32/65/65/65	-
19	EDO	S	2204	-	-	1/1/1/1	-
19	EDO	Q	203	-	-	1/1/1/1	-
19	EDO	B	304	-	-	1/1/1/1	-
22	CHD	B	302	-	-	2/9/74/74	0/4/4/4
22	CHD	P	308	-	-	4/9/74/74	0/4/4/4
25	CDL	C	306	-	-	59/110/110/110	-
19	EDO	N	614	-	-	1/1/1/1	-
23	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
19	EDO	A	620	-	-	0/1/1/1	-
19	EDO	N	619	-	-	1/1/1/1	-
19	EDO	P	310	-	-	0/1/1/1	-
26	PSC	E	201	-	-	26/55/55/55	-
19	EDO	C	314	-	-	1/1/1/1	-
19	EDO	N	615	-	-	1/1/1/1	-
19	EDO	W	304	-	-	1/1/1/1	-
17	PGV	A	604	-	-	30/55/55/55	-
19	EDO	J	1105	-	-	1/1/1/1	-
19	EDO	G	1306	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	B	307	-	-	1/1/1/1	-

The worst 5 of 144 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	607	HEA	FE-ND	6.21	2.14	1.94
23	G	1302	DMU	O16-C6	5.88	1.50	1.40
18	N	607	HEA	C1D-ND	-5.82	1.30	1.40
23	C	313	DMU	O16-C6	5.70	1.49	1.40
18	N	607	HEA	FE-NB	5.50	2.11	1.94

The worst 5 of 236 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	607	HEA	C26-C15-C14	-8.35	102.19	123.63
18	A	607	HEA	C16-C15-C14	8.27	139.74	121.17
23	P	302	DMU	C18-O16-C6	7.82	127.05	113.68
18	A	607	HEA	C3A-C2A-C1A	-7.19	100.25	107.05
23	C	313	DMU	O1-C9-C11	7.16	124.19	106.44

There are no chirality outliers.

5 of 971 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	604	PGV	C03-O11-P-O12
17	A	604	PGV	C03-O11-P-O13
17	A	604	PGV	C03-O11-P-O14
17	A	604	PGV	C04-O12-P-O11
17	A	604	PGV	C04-O12-P-O14

There are no ring outliers.

50 monomers are involved in 128 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	Y	102	CHD	4	0
19	V	103	EDO	1	0
25	P	307	CDL	4	0
18	N	607	HEA	4	0
19	U	1501	EDO	3	0
17	N	616	PGV	1	0
24	C	304	PEK	2	0

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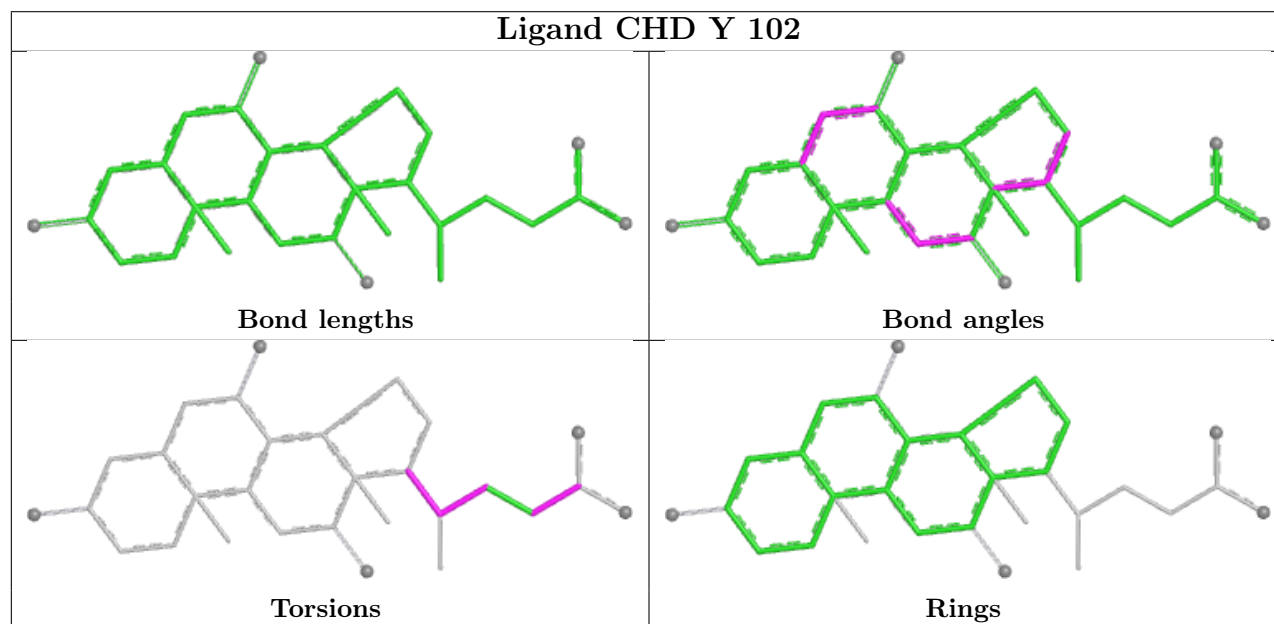
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	V	101	SAC	1	0
22	T	104	CHD	7	0
24	P	304	PEK	1	0
19	A	613	EDO	1	0
19	S	2201	EDO	3	0
20	A	615	TGL	1	0
20	L	101	TGL	2	0
20	Y	101	TGL	2	0
17	Z	102	PGV	2	0
18	N	606	HEA	1	0
19	A	608	EDO	1	0
24	P	305	PEK	5	0
24	C	303	PEK	4	0
19	N	613	EDO	1	0
25	C	312	CDL	13	0
19	A	614	EDO	3	0
17	N	605	PGV	1	0
17	P	306	PGV	1	0
18	A	607	HEA	3	0
24	C	315	PEK	2	0
26	O	302	PSC	5	0
19	G	1303	EDO	2	0
19	A	616	EDO	1	0
19	J	1101	EDO	1	0
28	I	101	SAC	2	0
23	C	313	DMU	1	0
25	T	102	CDL	3	0
22	C	302	CHD	1	0
19	J	1104	EDO	1	0
20	D	201	TGL	7	0
19	S	2206	EDO	1	0
19	F	702	EDO	1	0
22	G	1305	CHD	1	0
23	G	1302	DMU	2	0
17	T	101	PGV	1	0
20	Q	201	TGL	5	0
22	P	308	CHD	1	0
25	C	306	CDL	2	0
19	N	614	EDO	9	0
23	Z	101	DMU	1	0
19	N	619	EDO	1	0
26	E	201	PSC	5	0

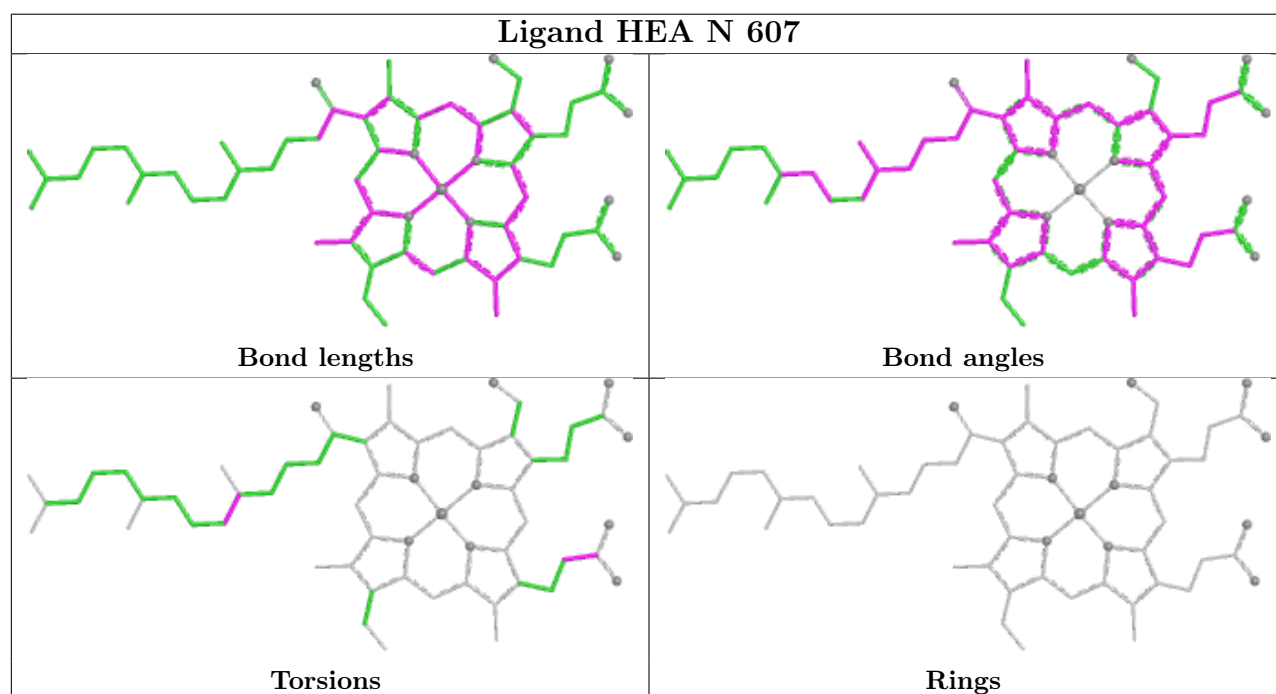
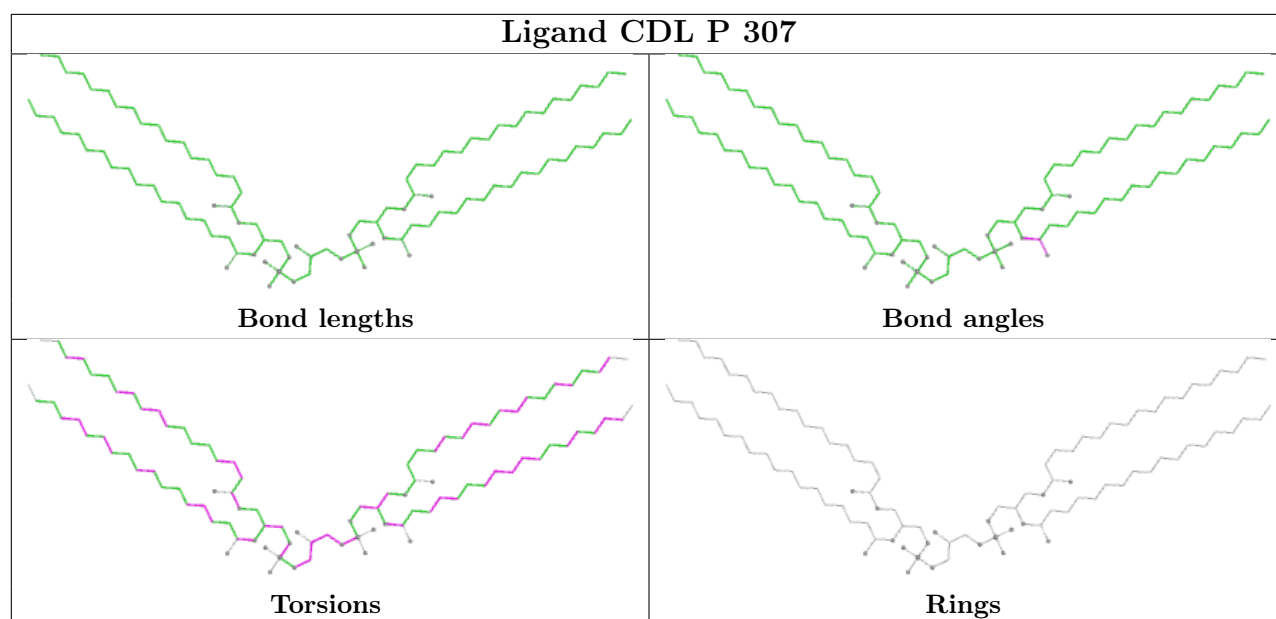
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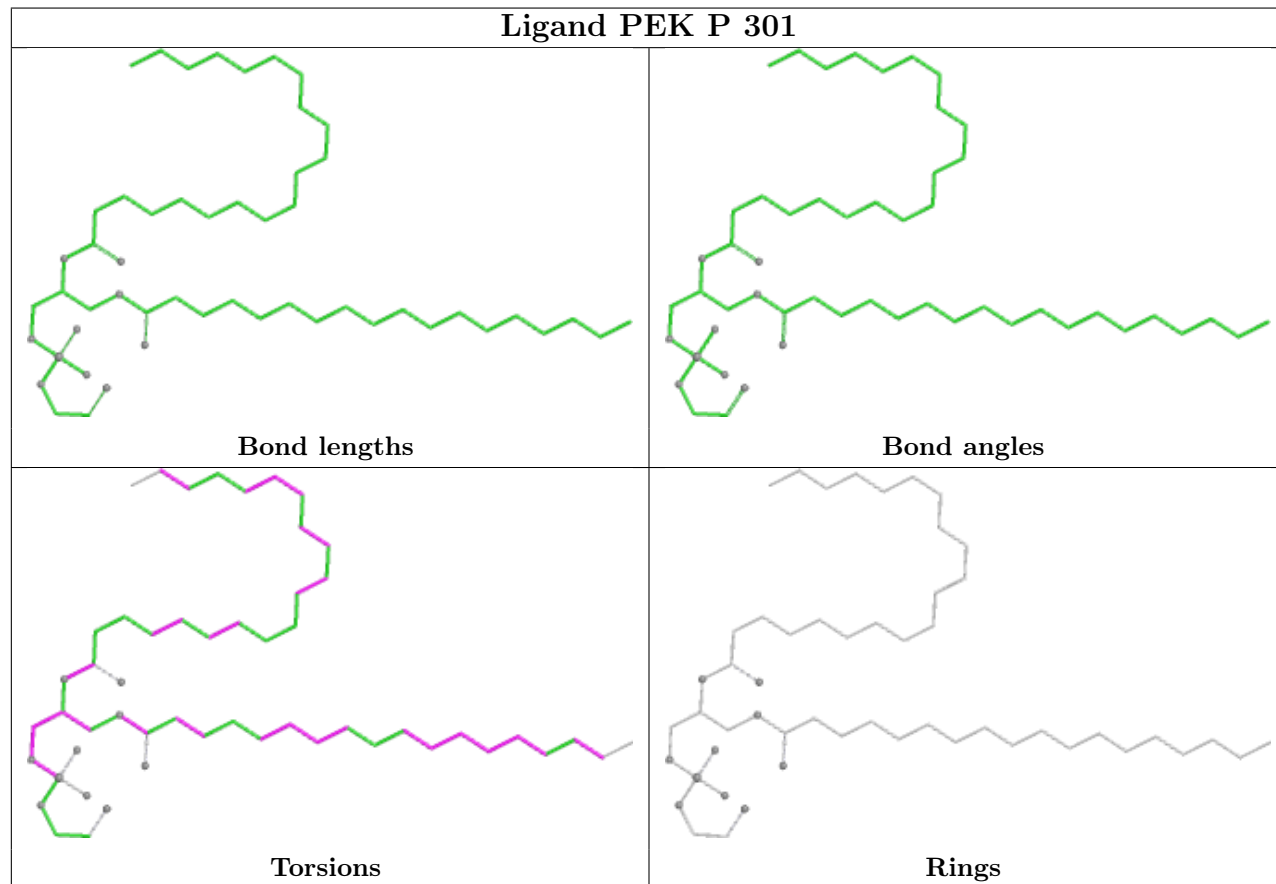
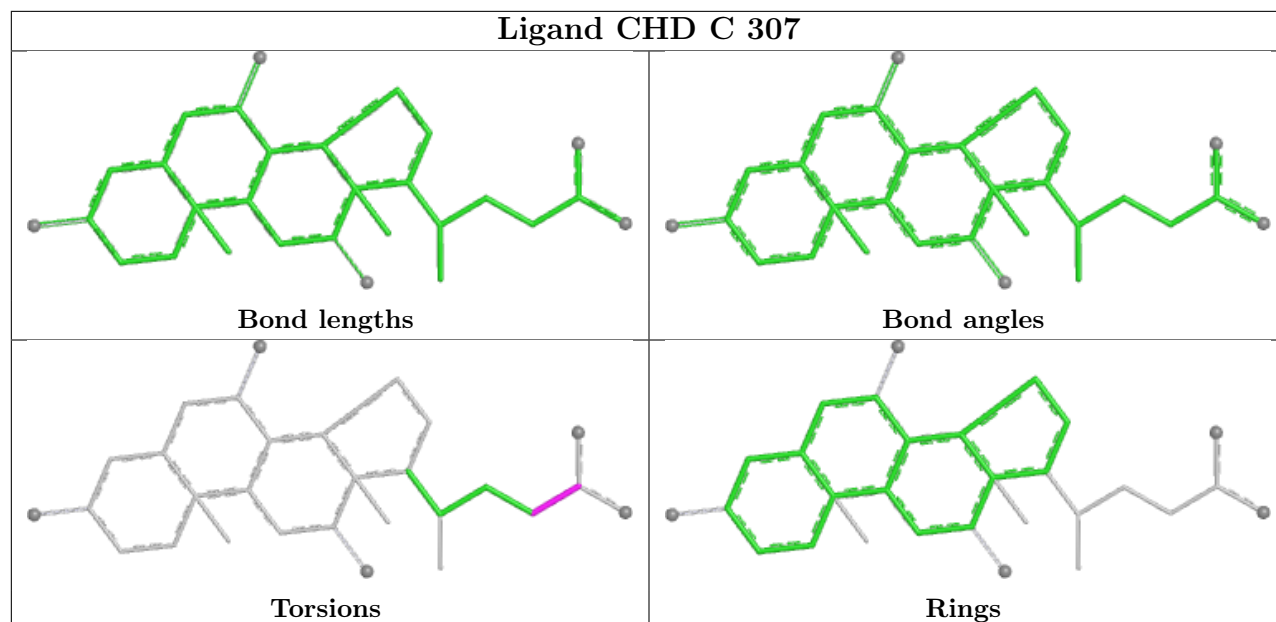
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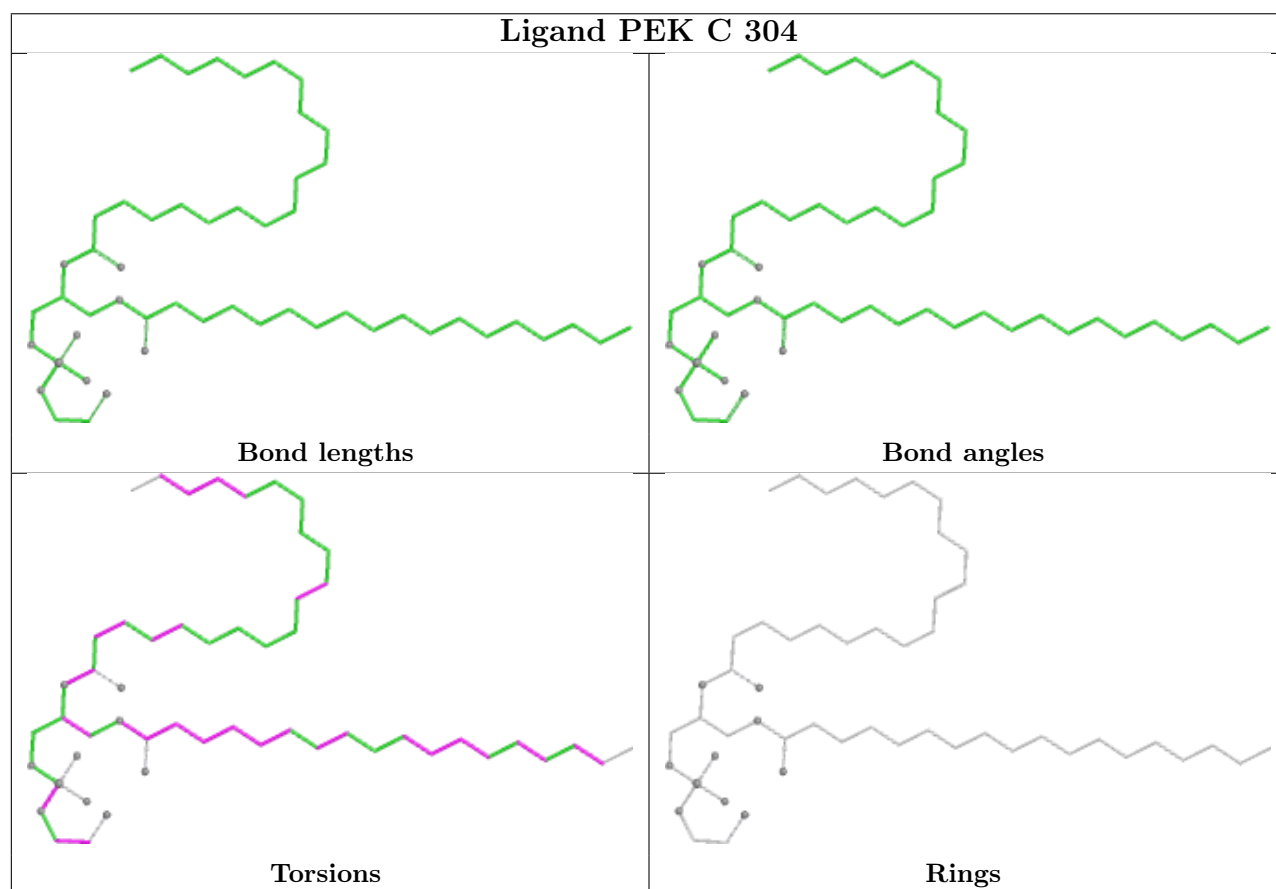
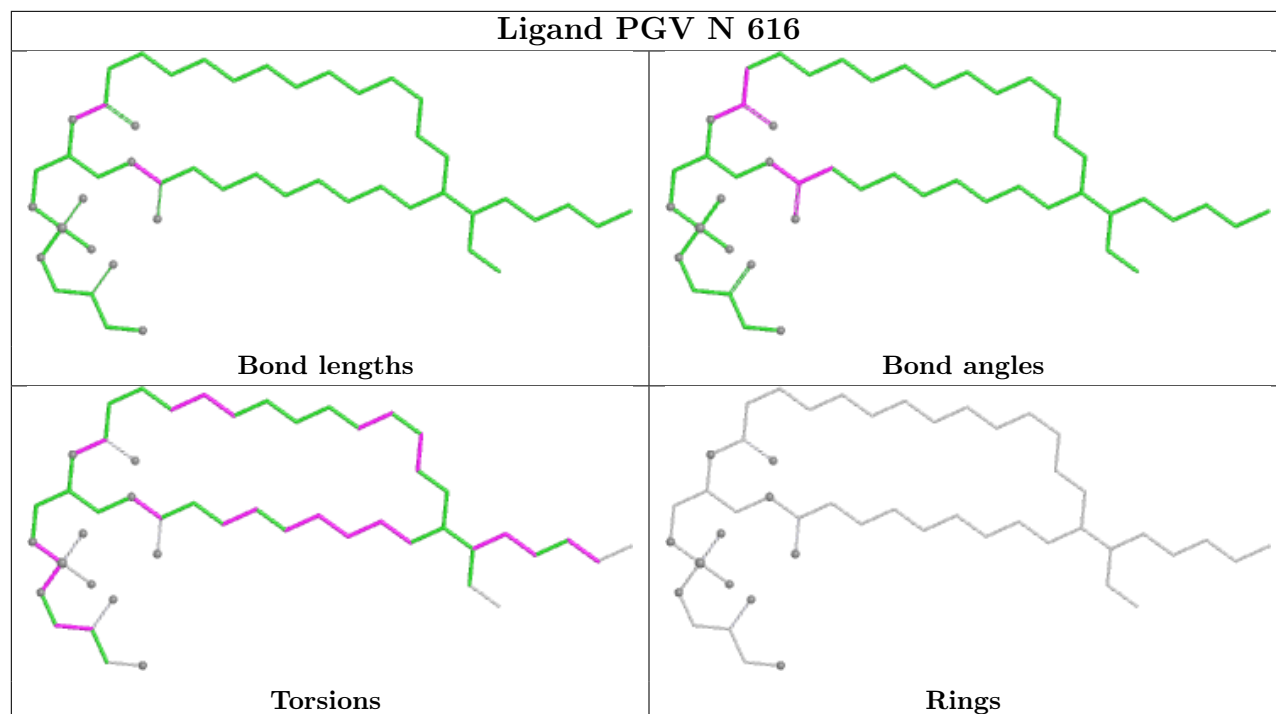
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	604	PGV	4	0

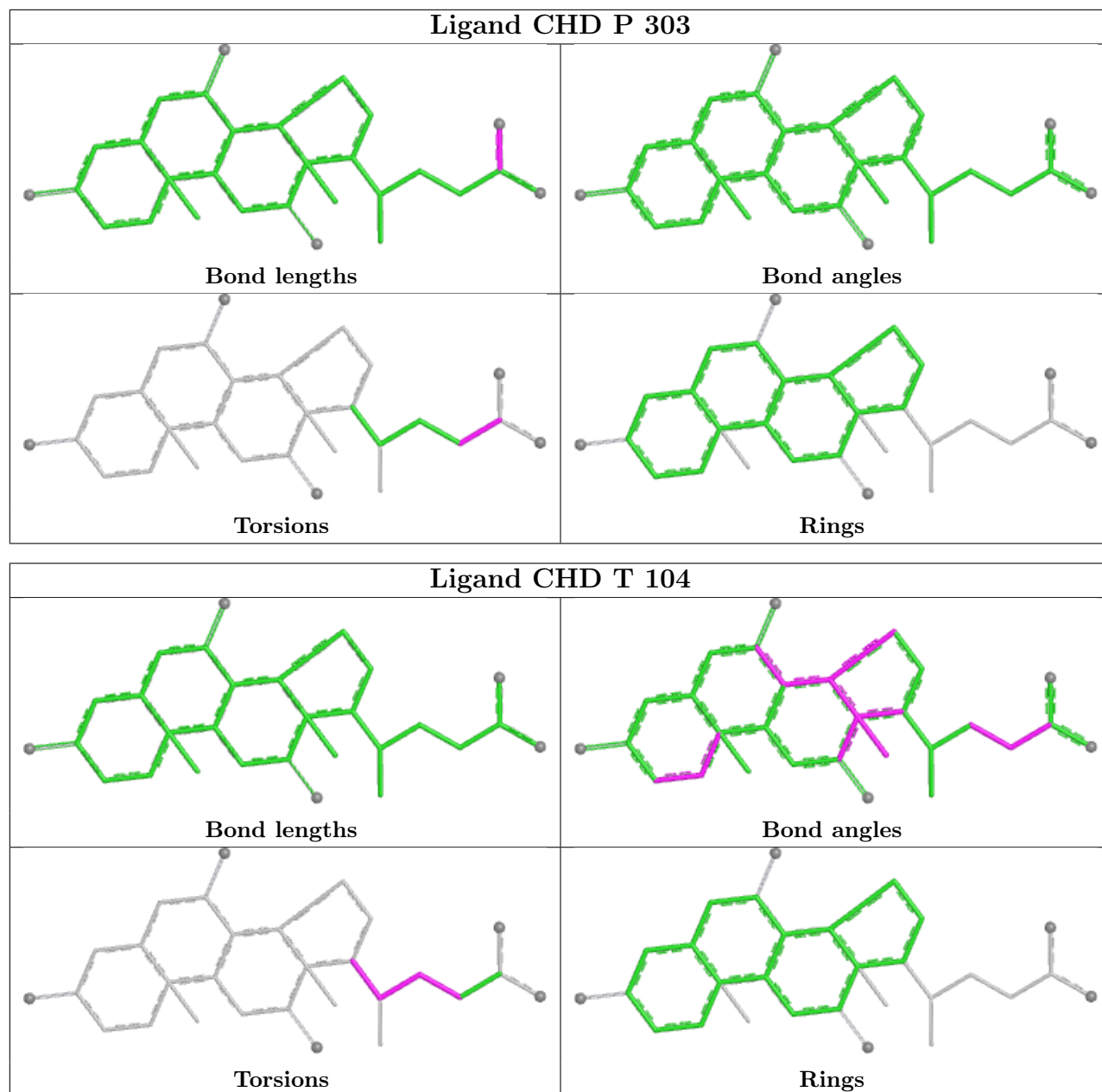
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

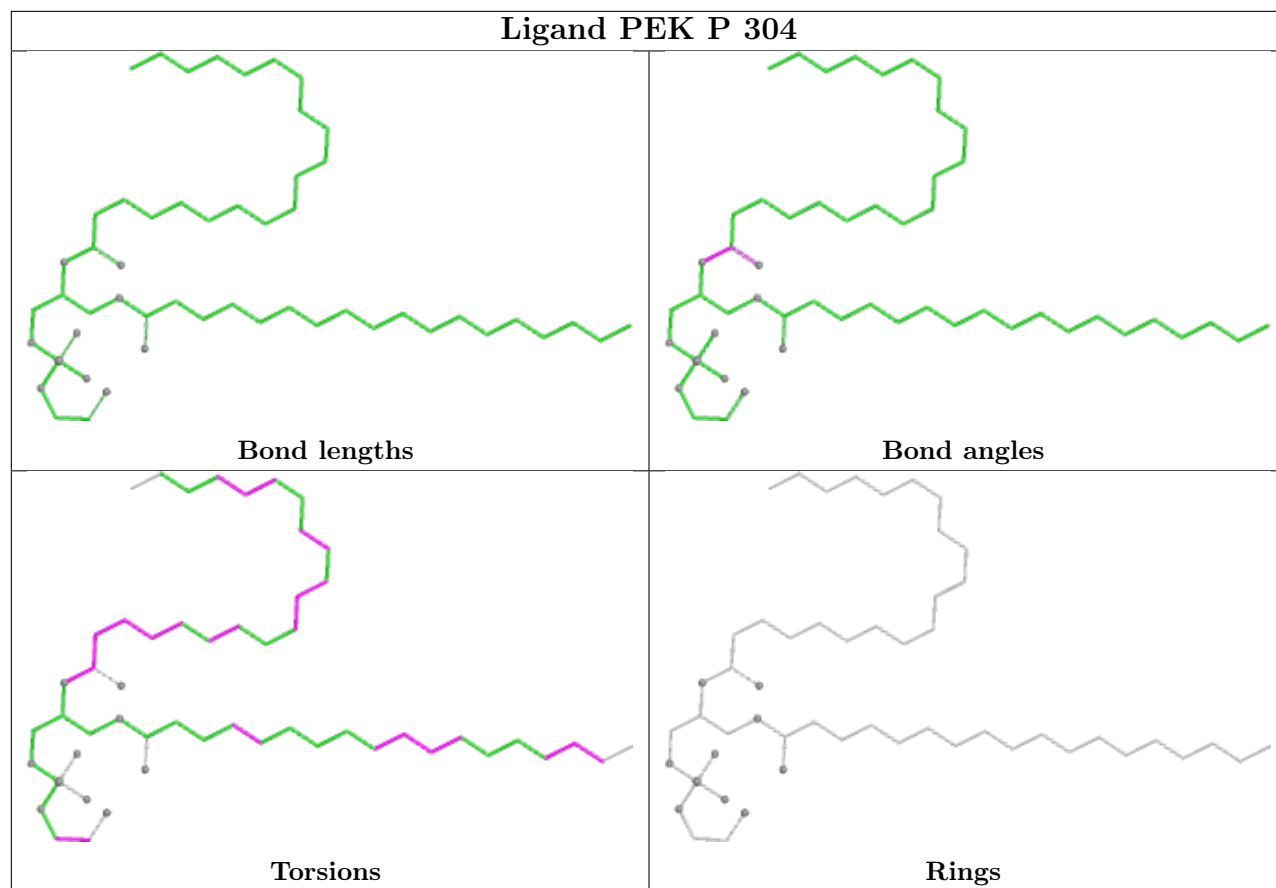


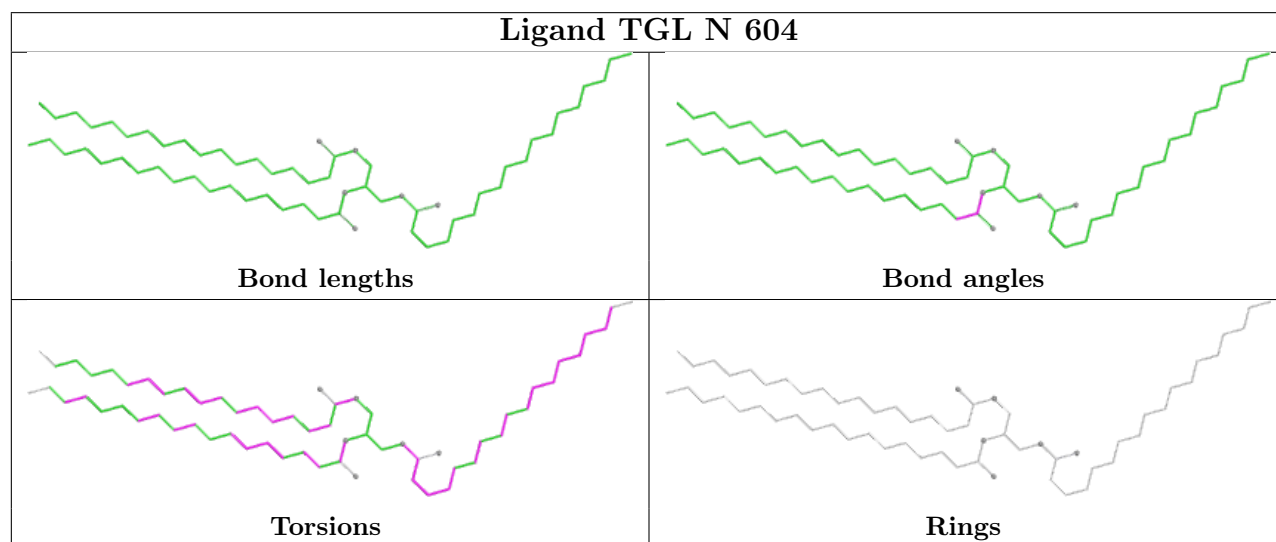
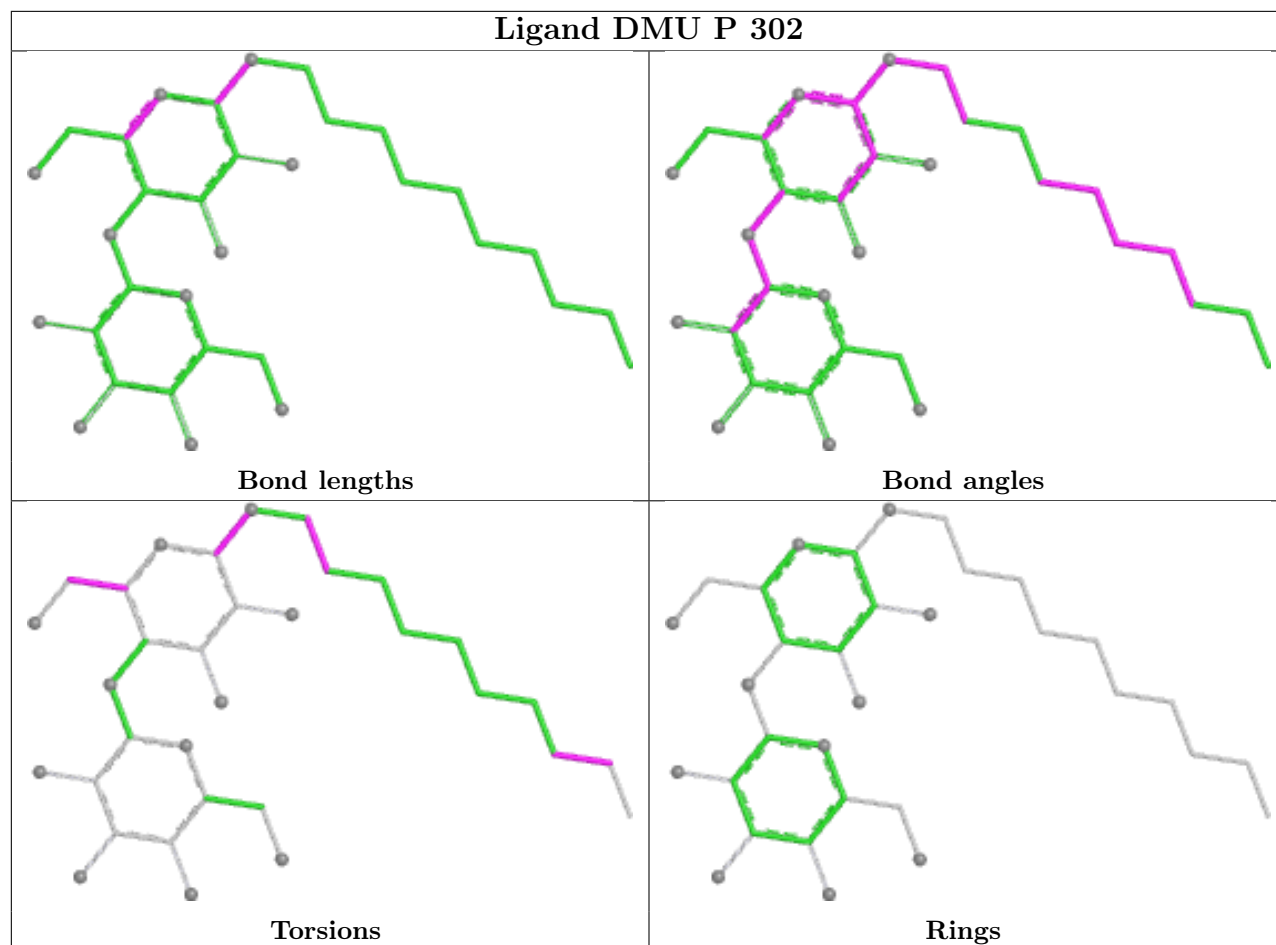


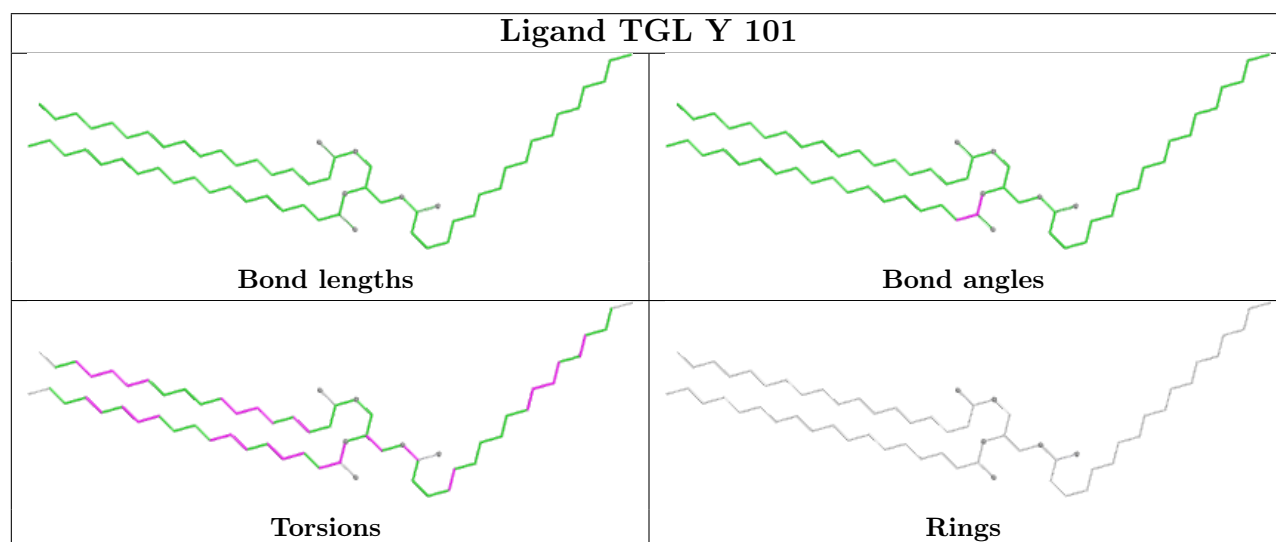
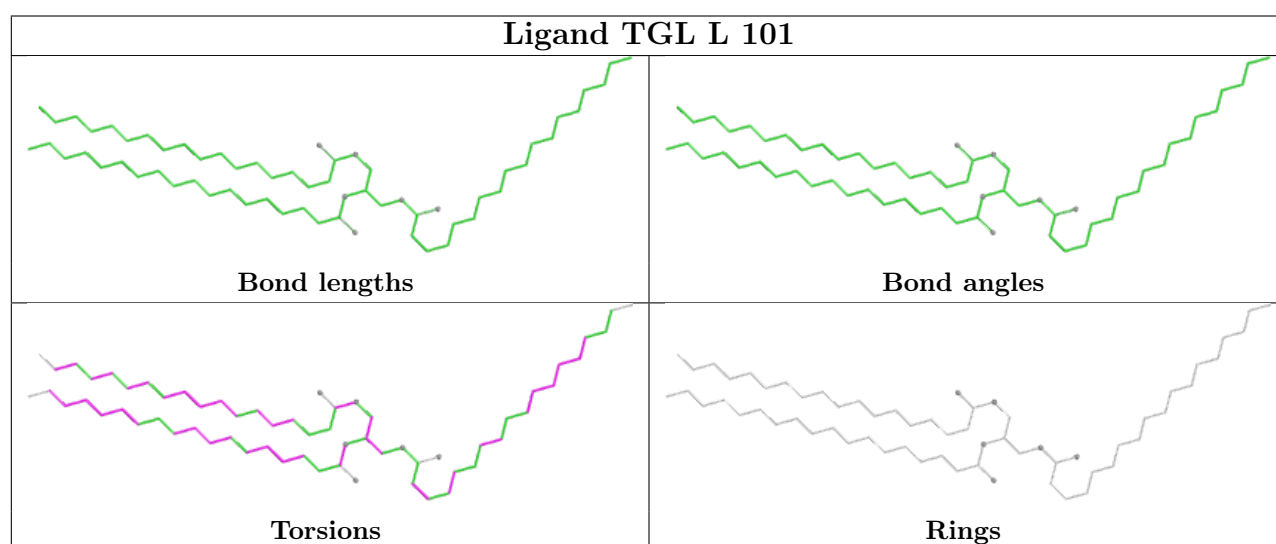
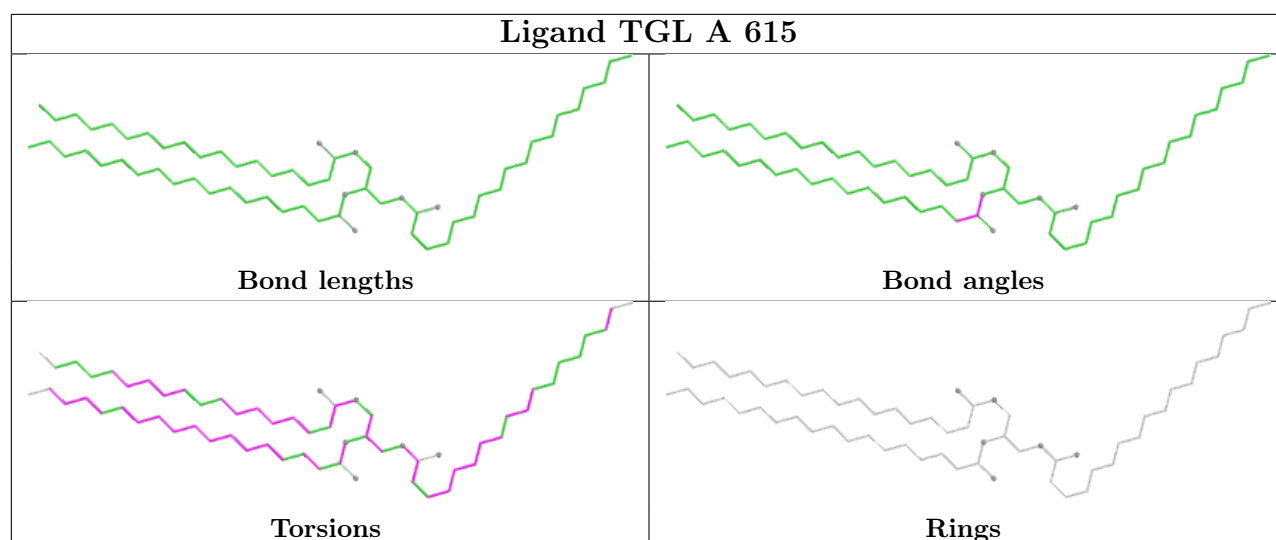


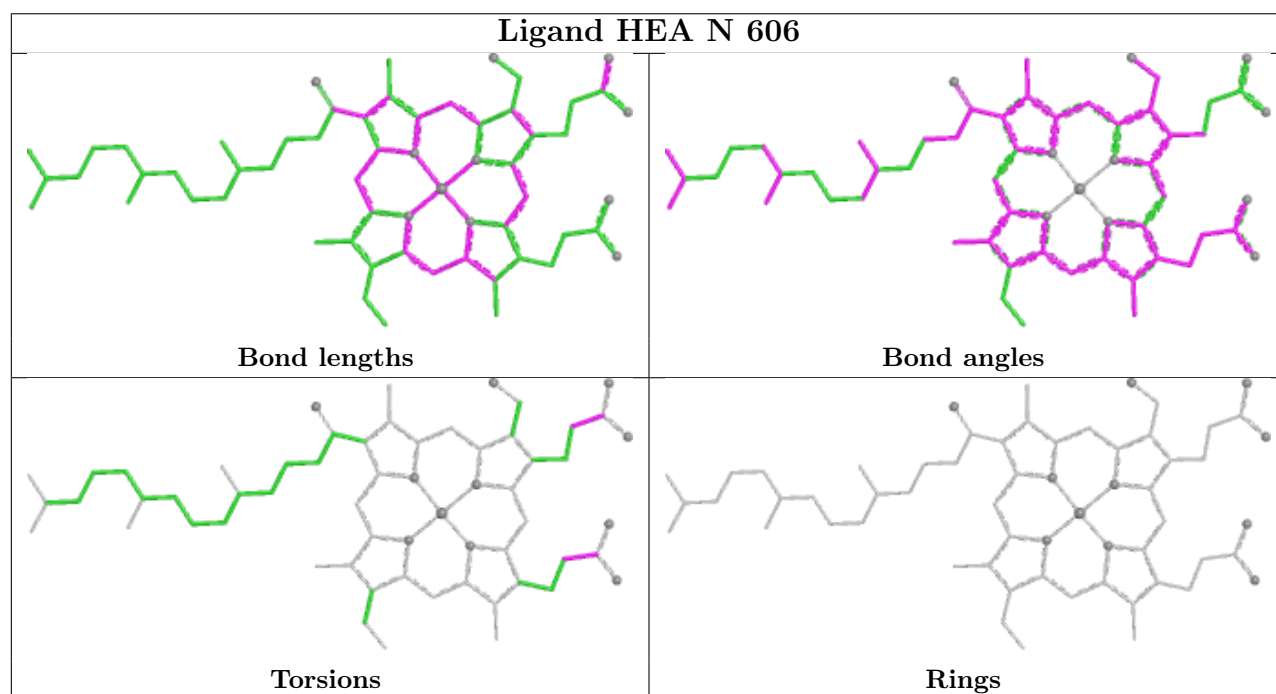
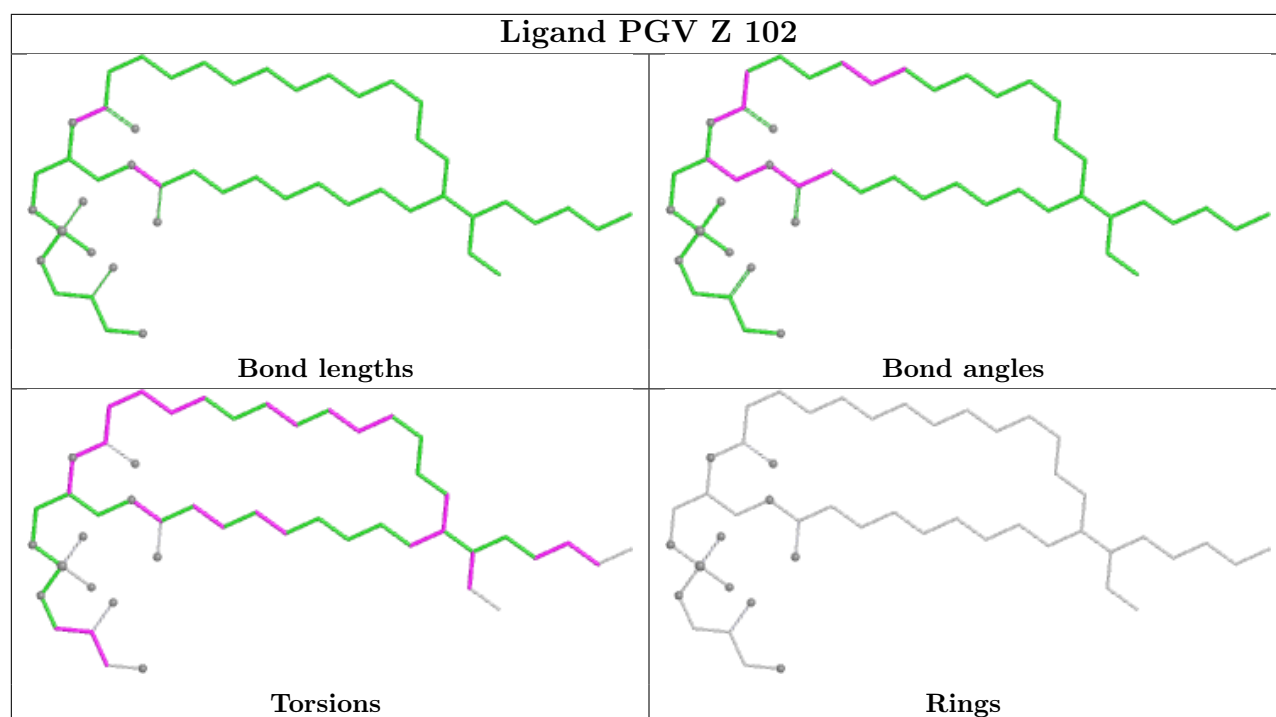


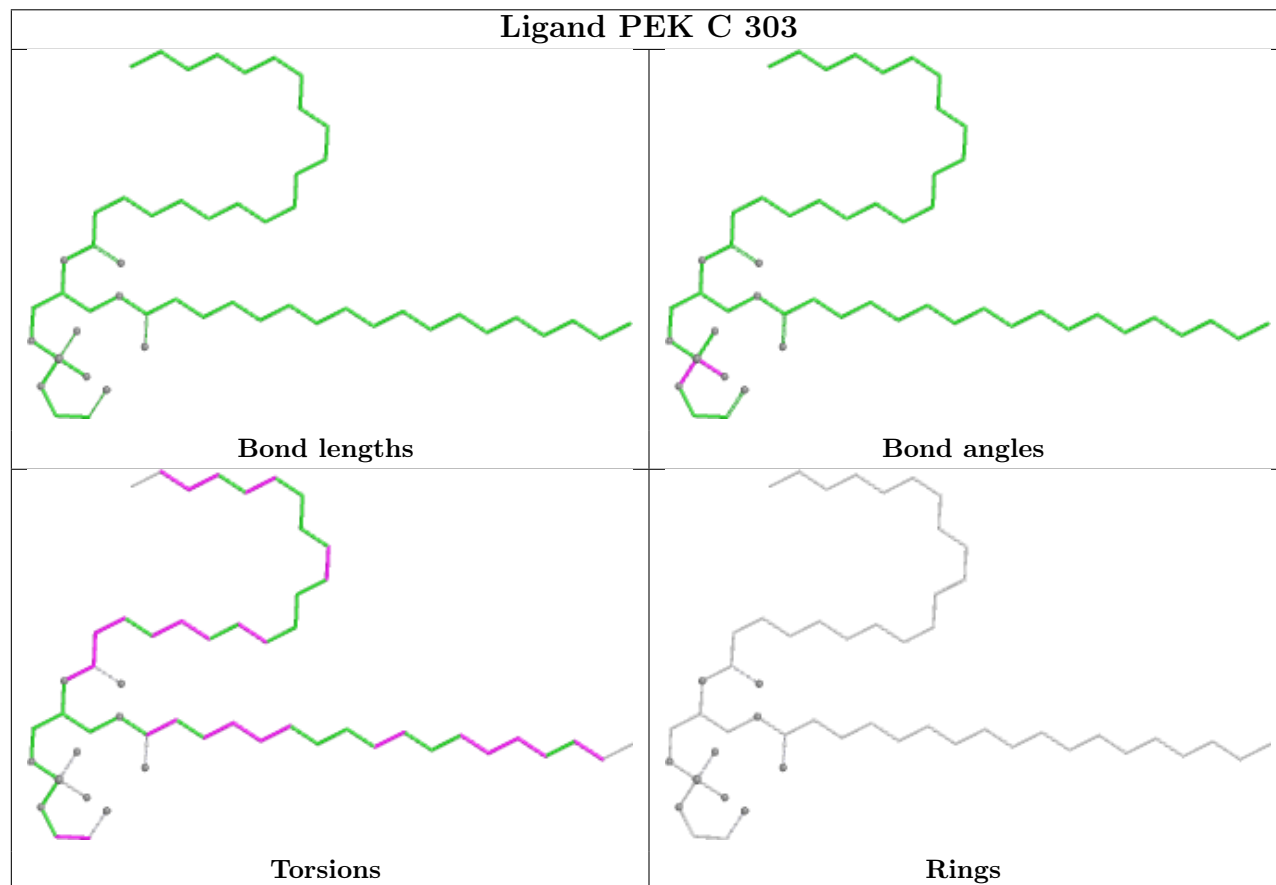
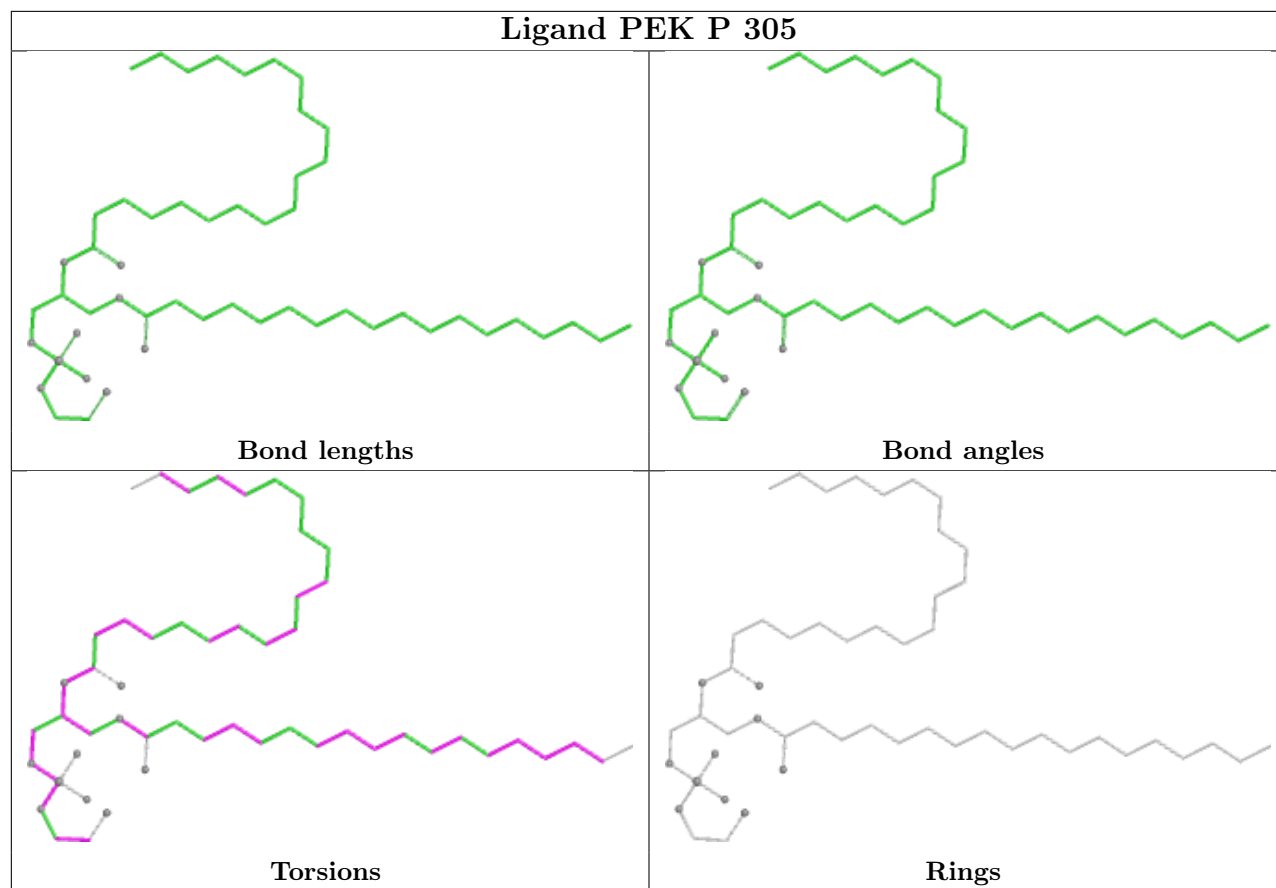


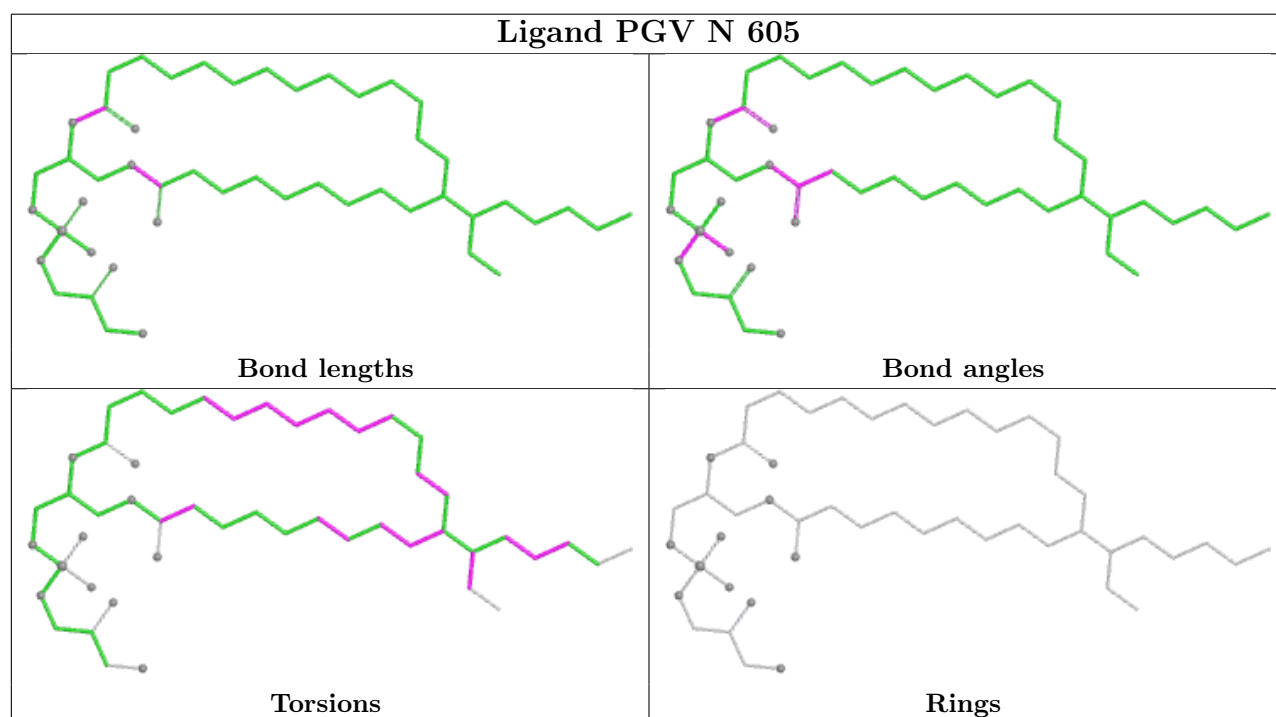
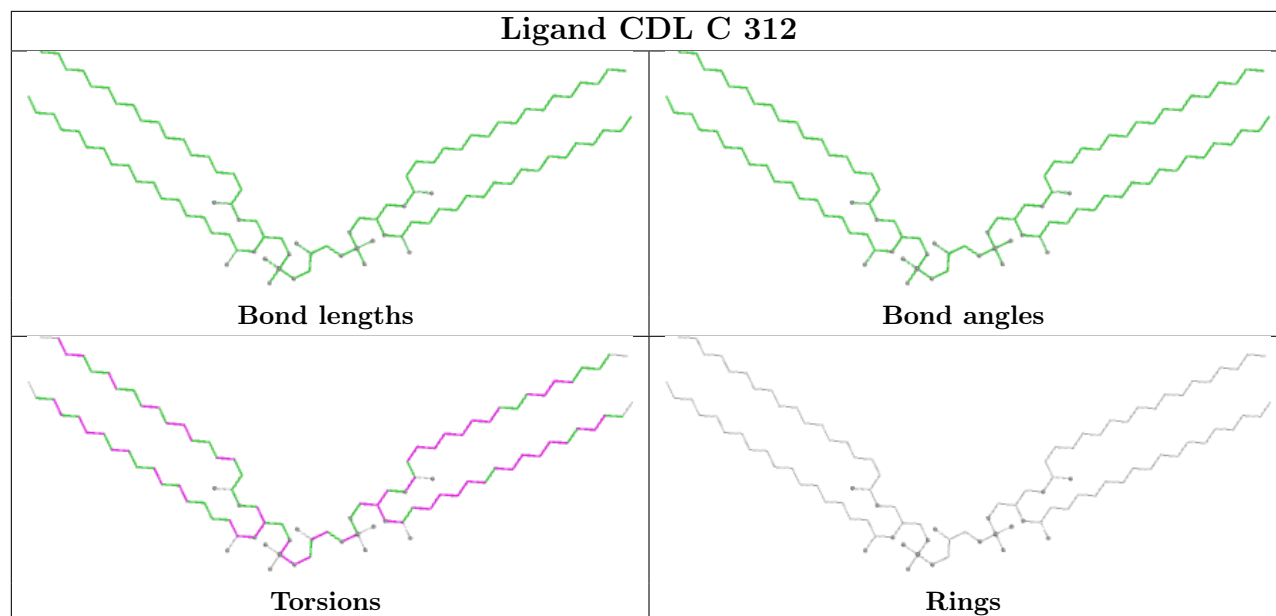


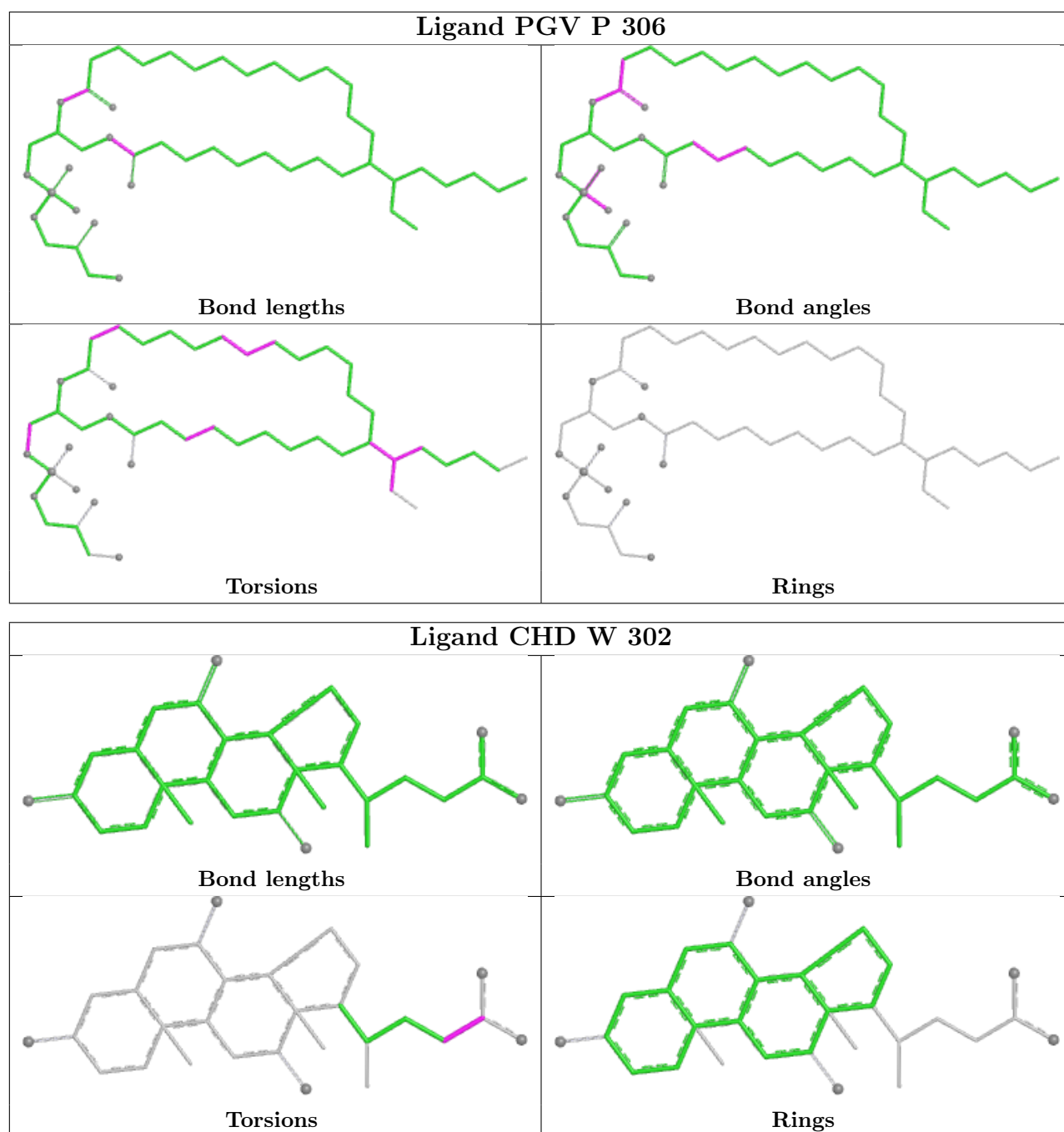


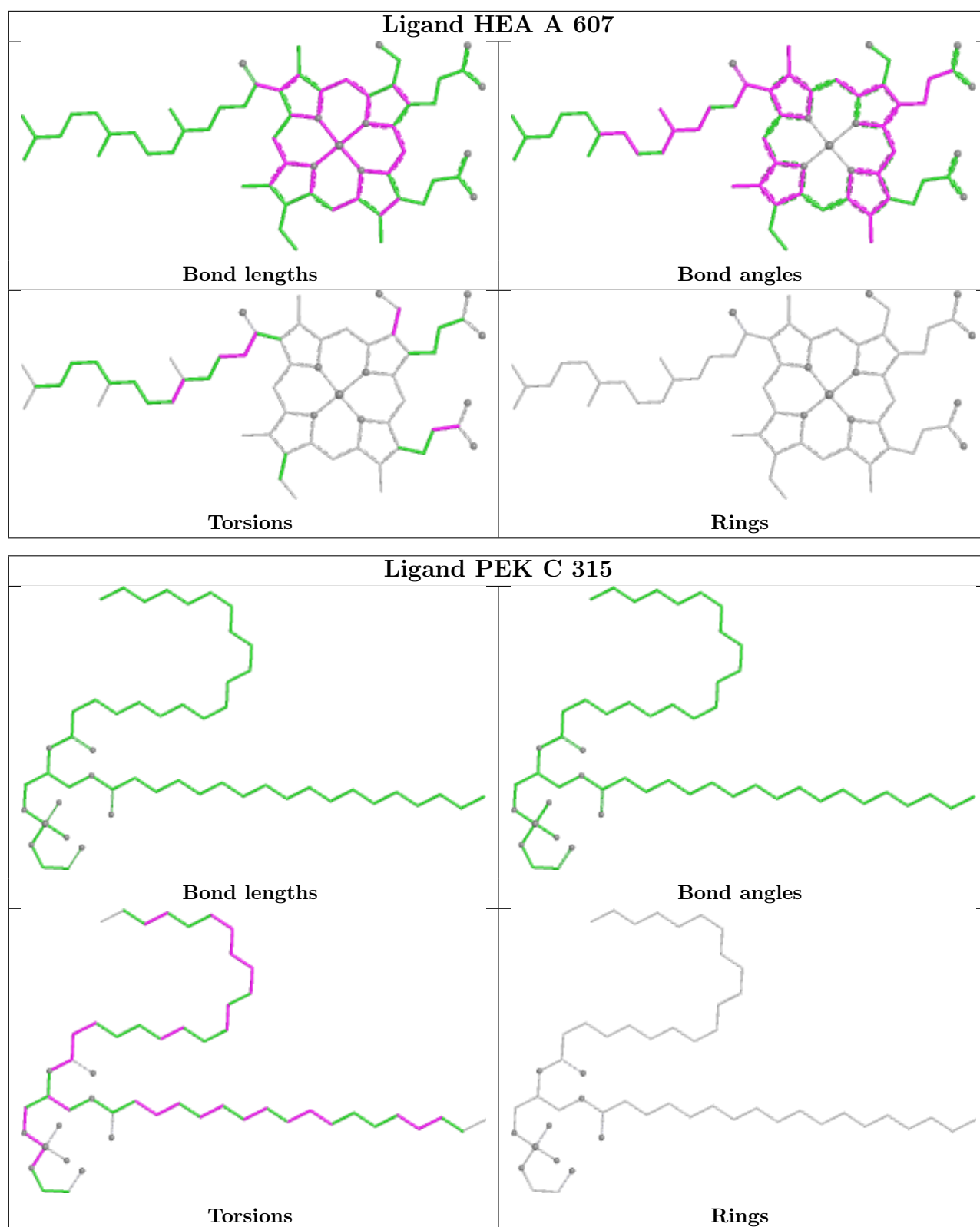


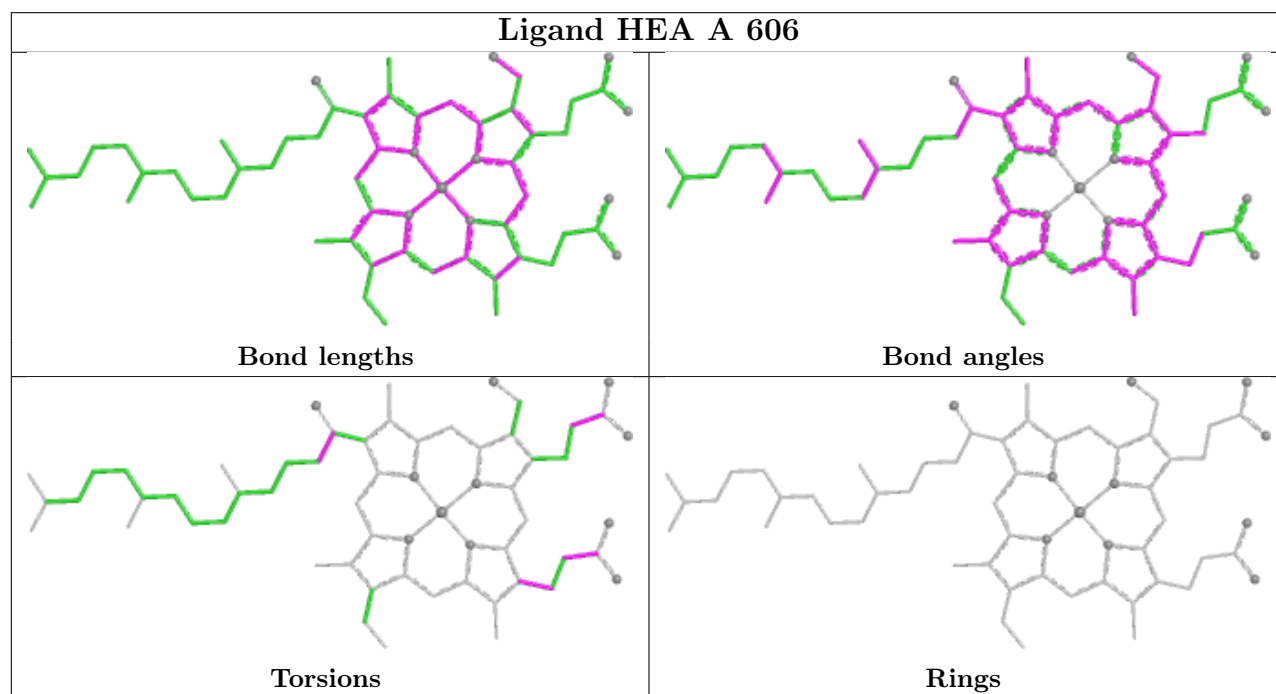
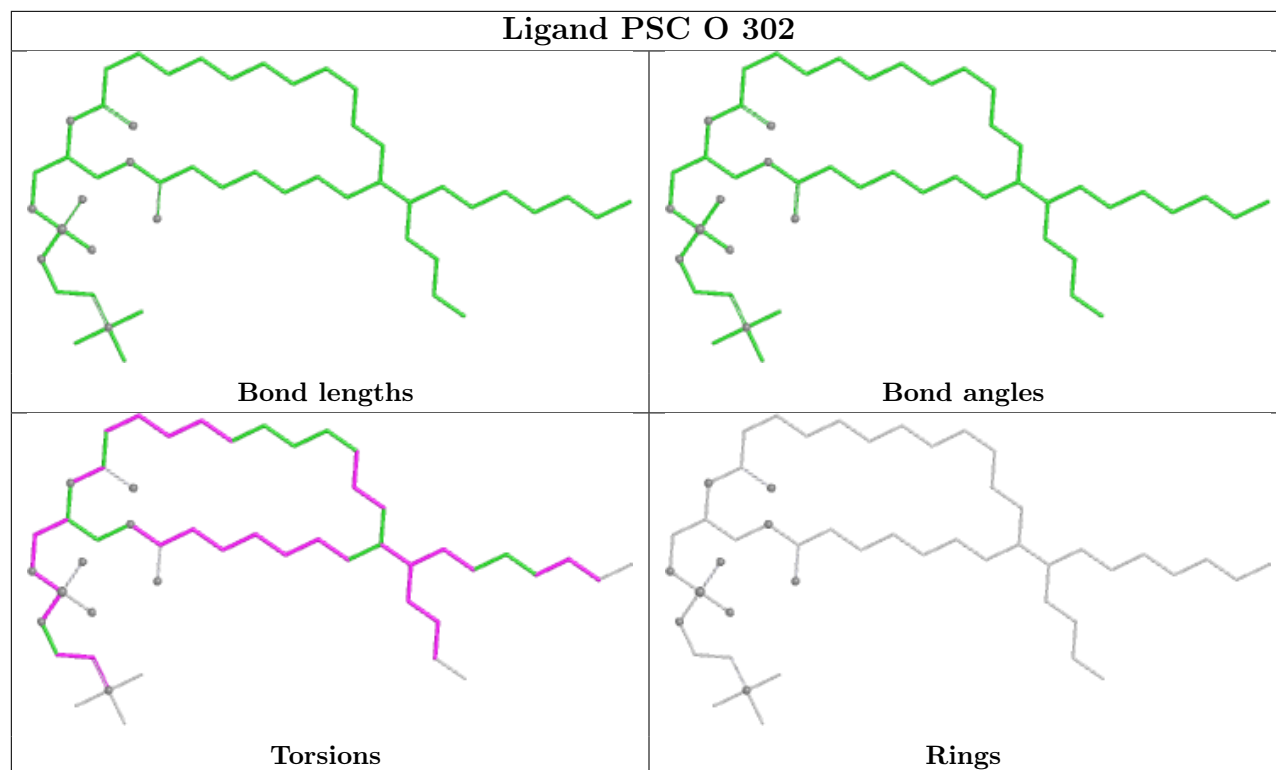


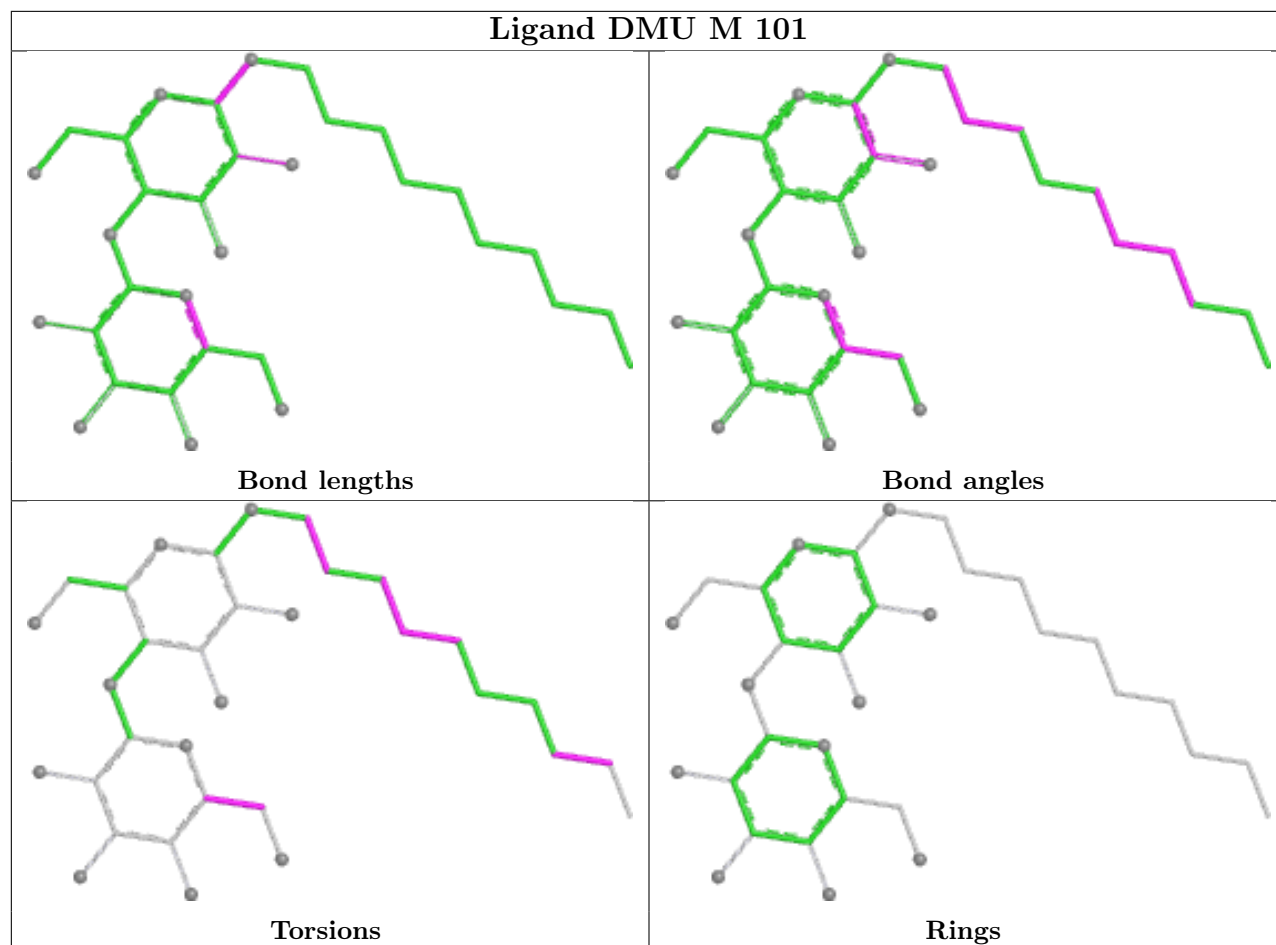


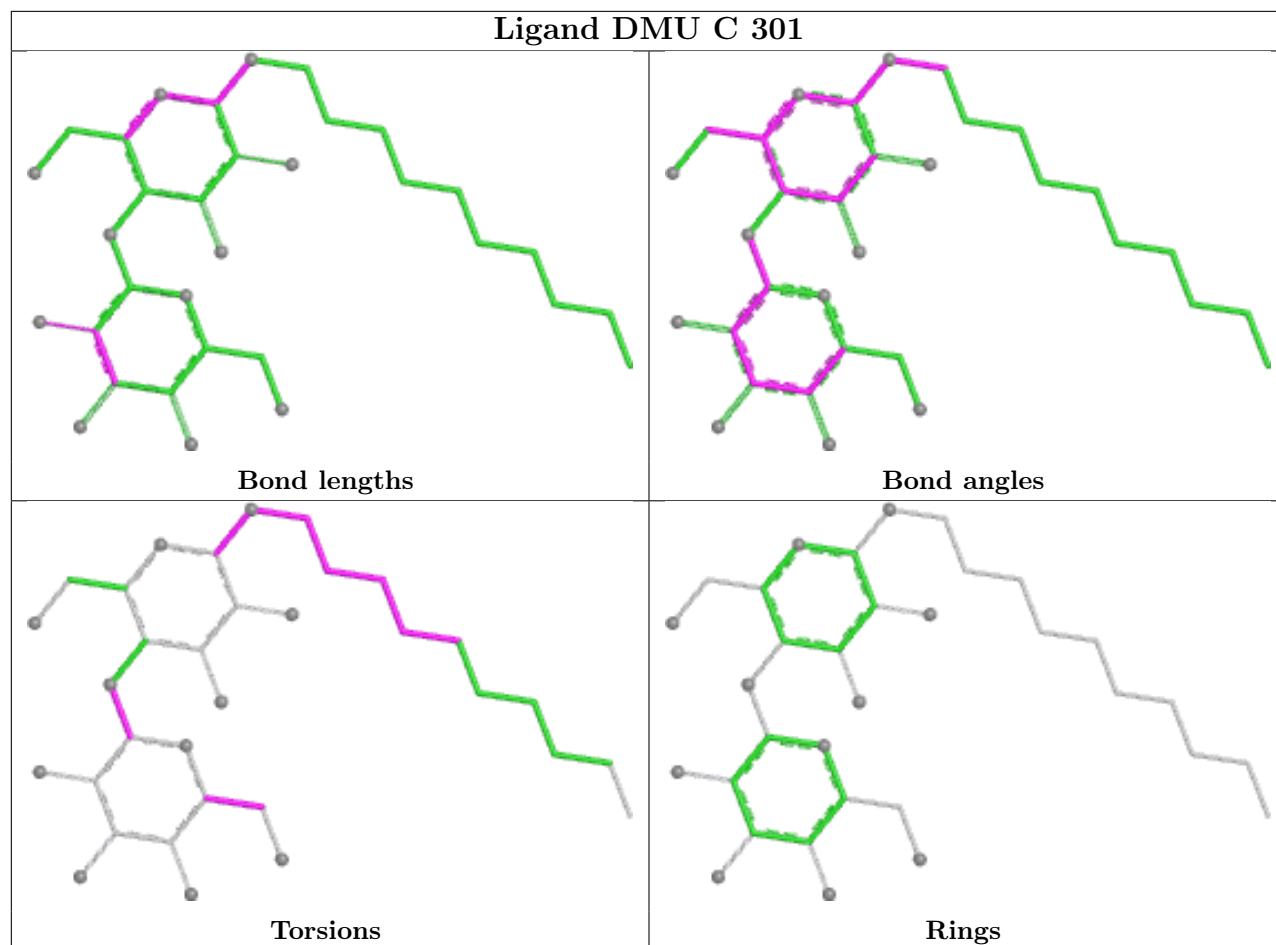


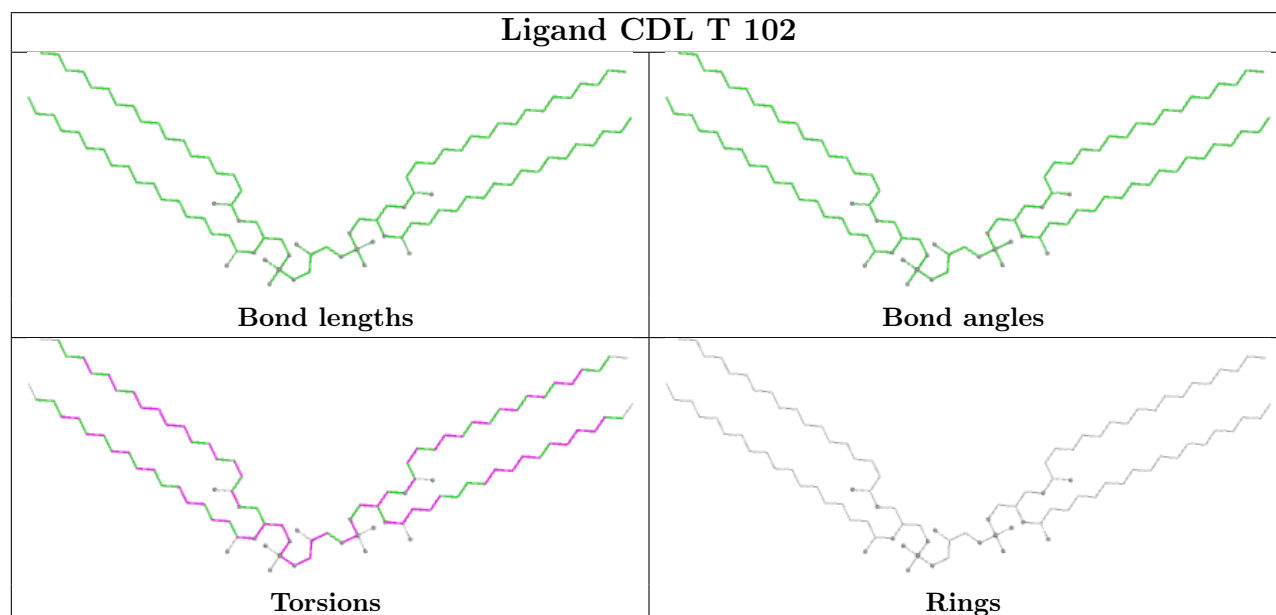
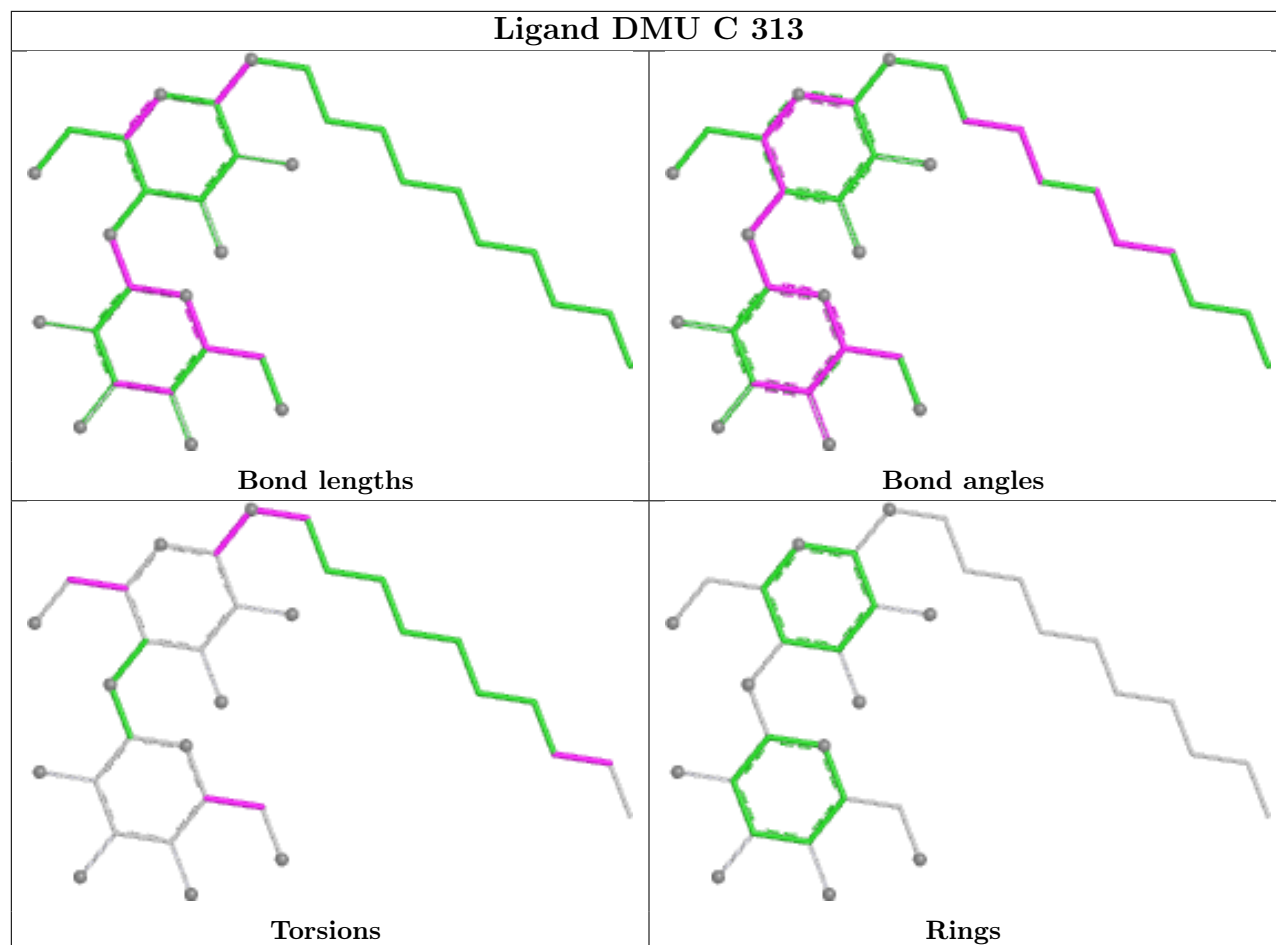


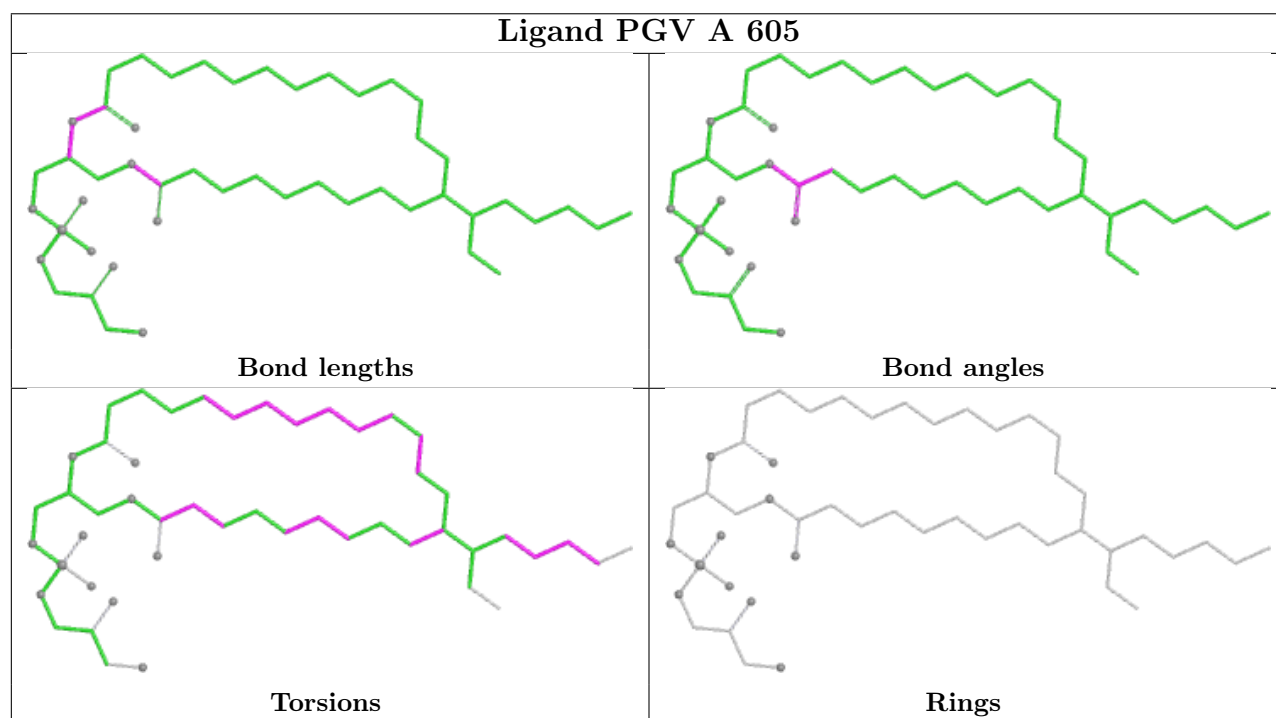
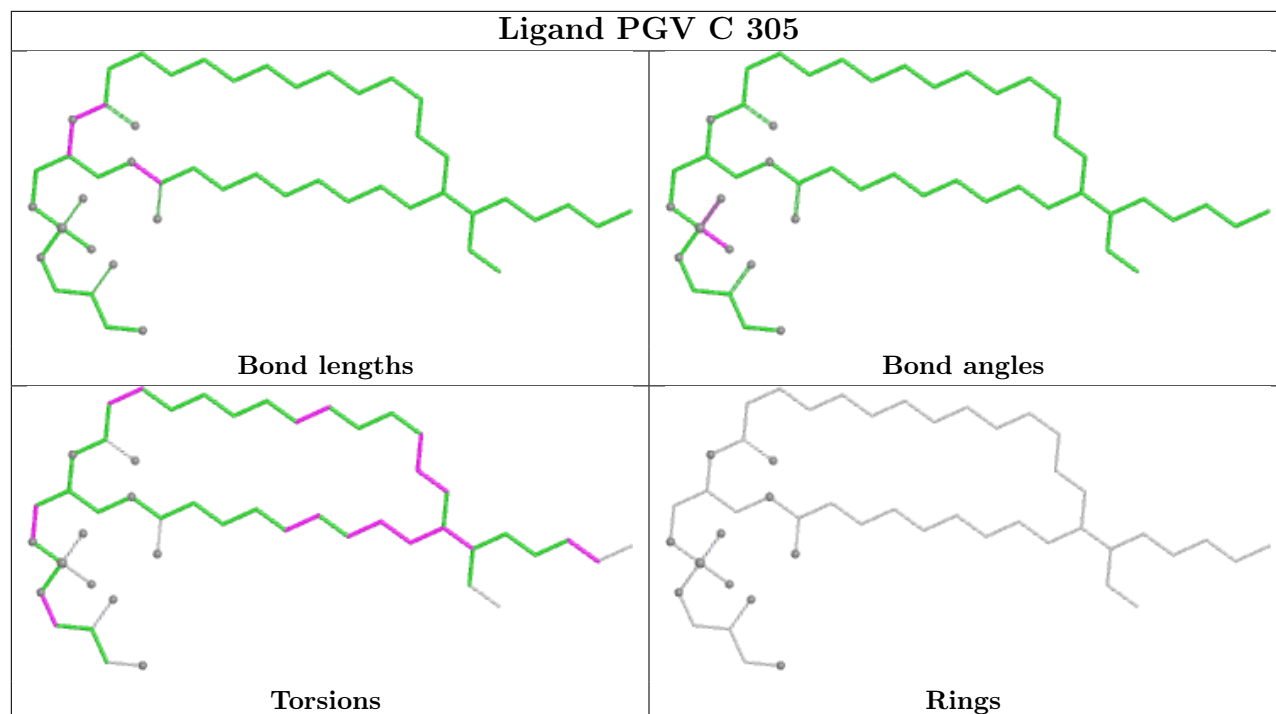


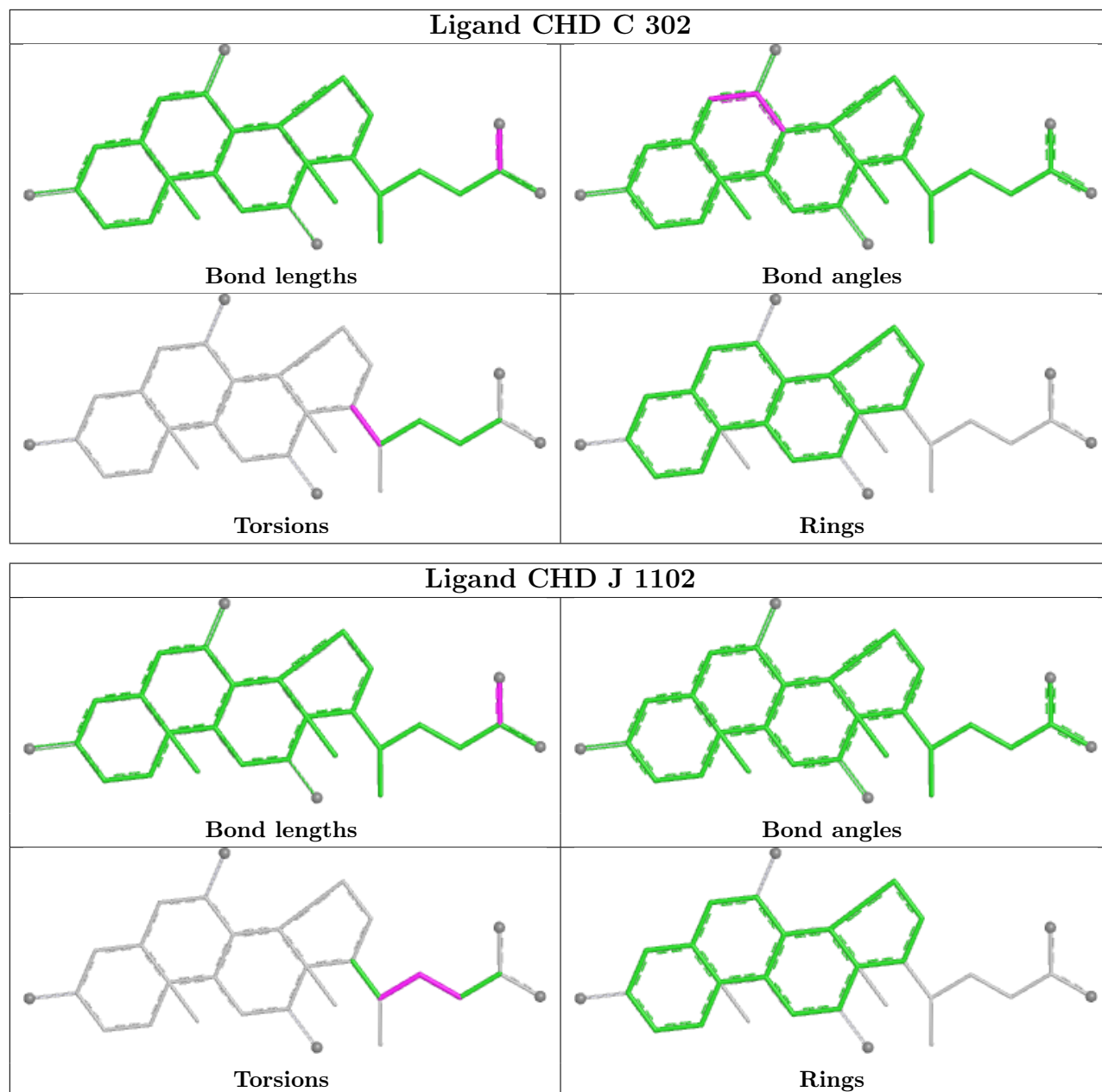


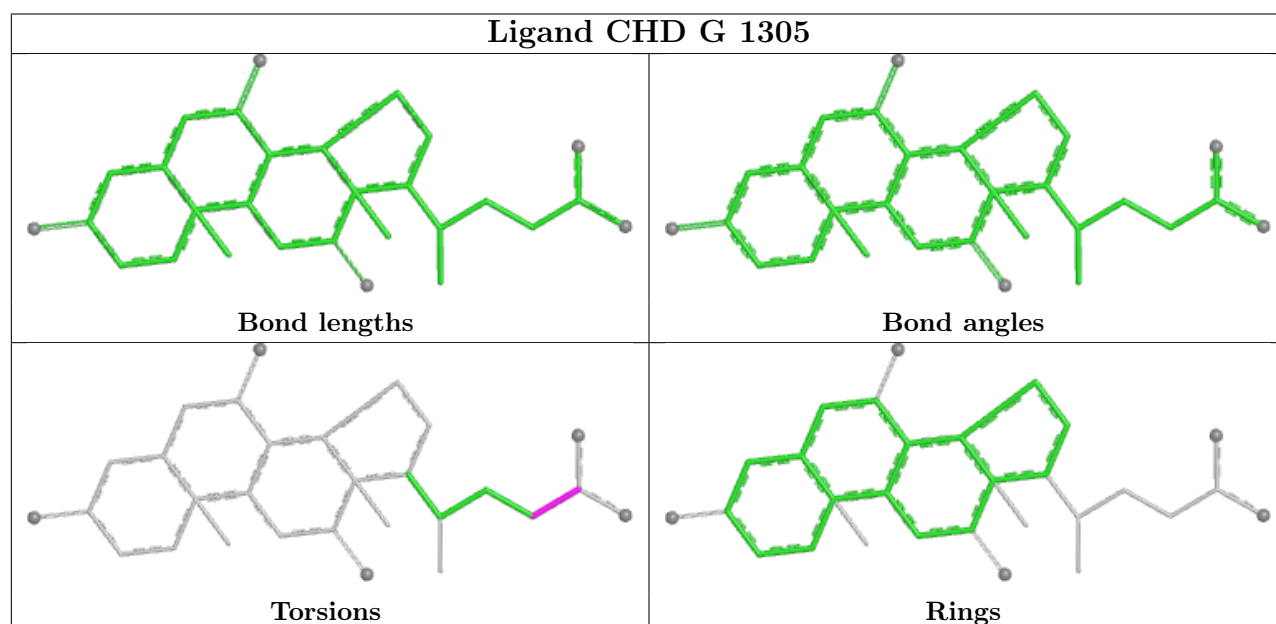
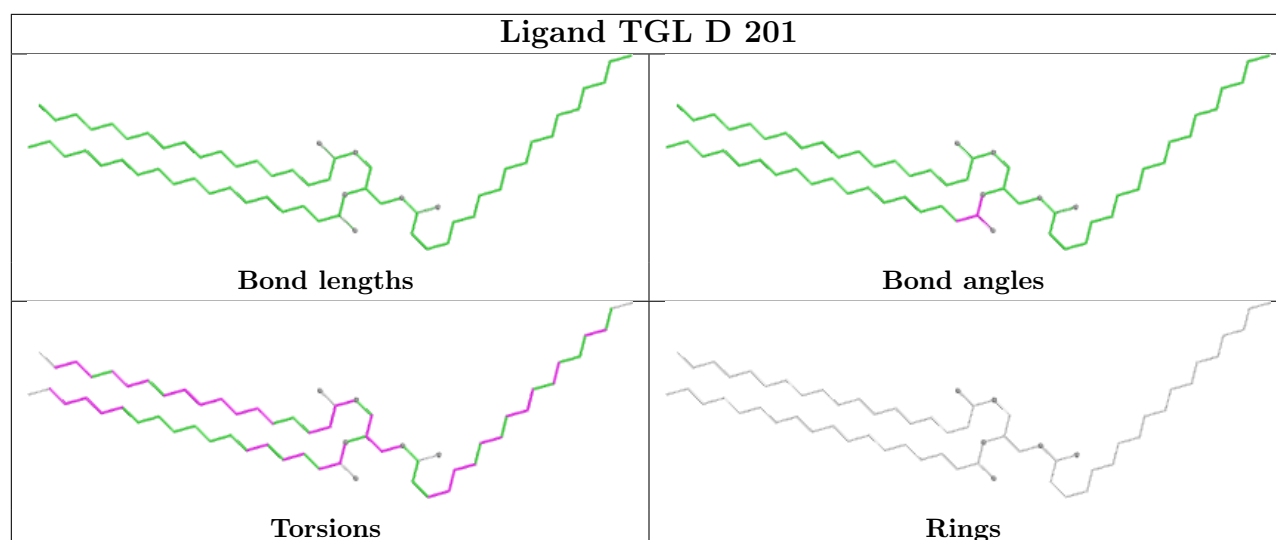


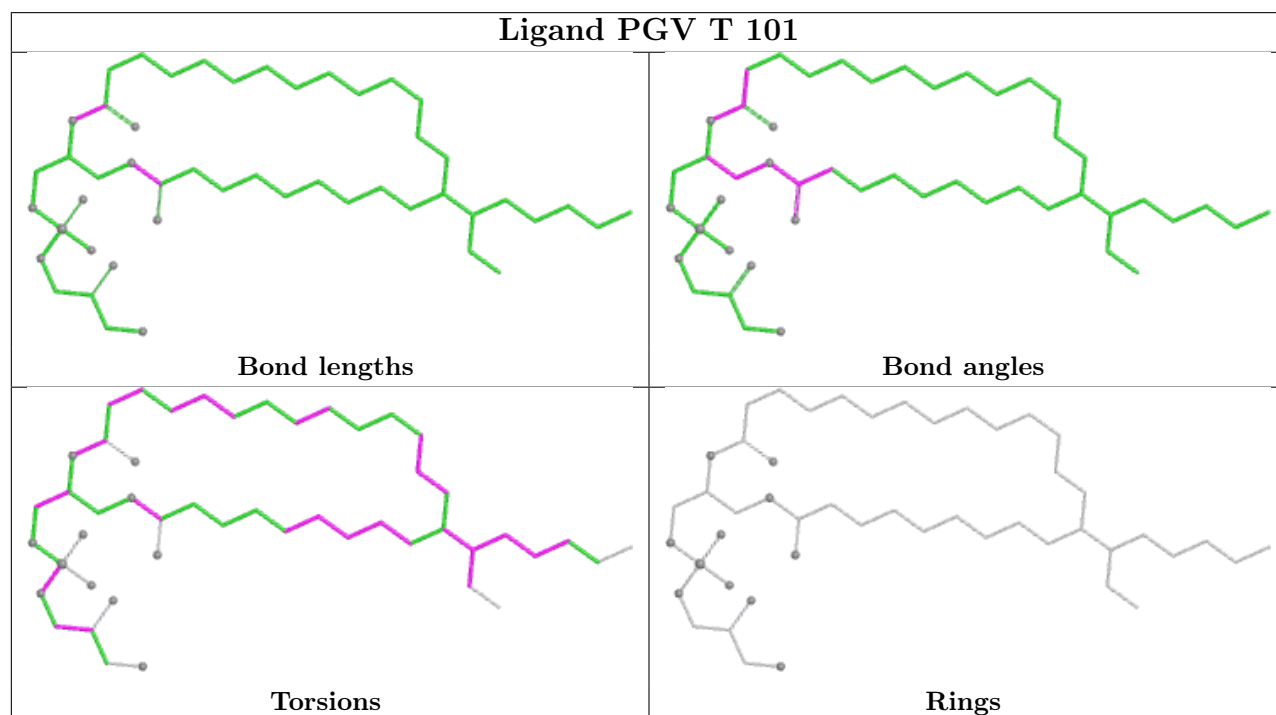
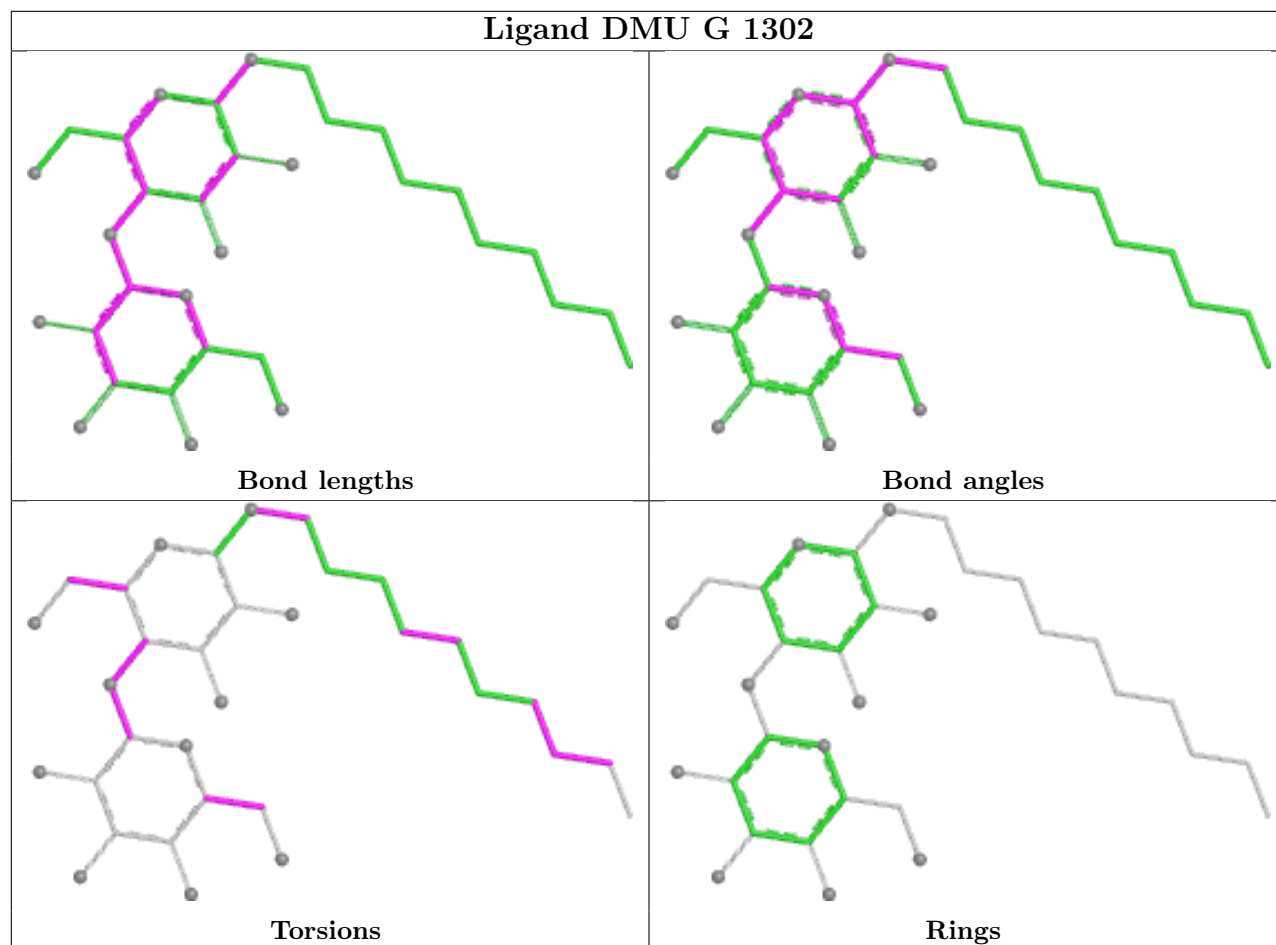


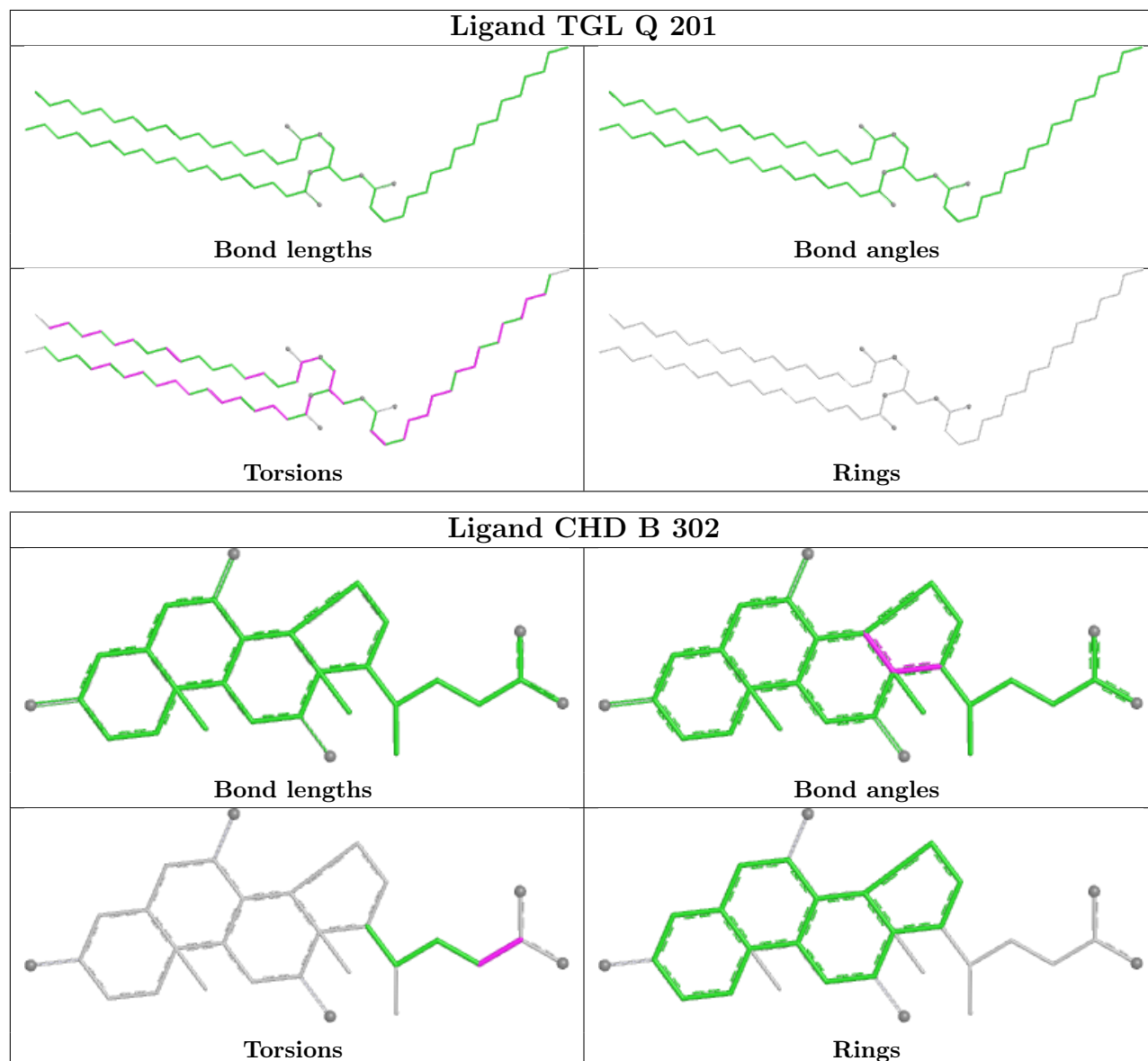


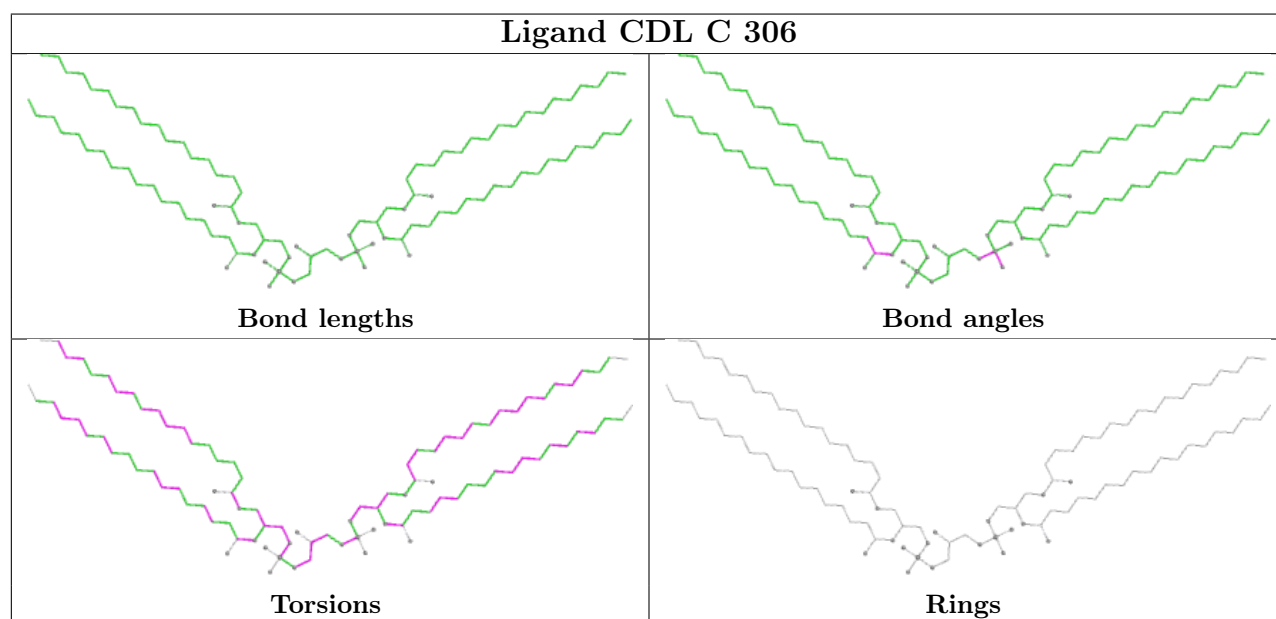
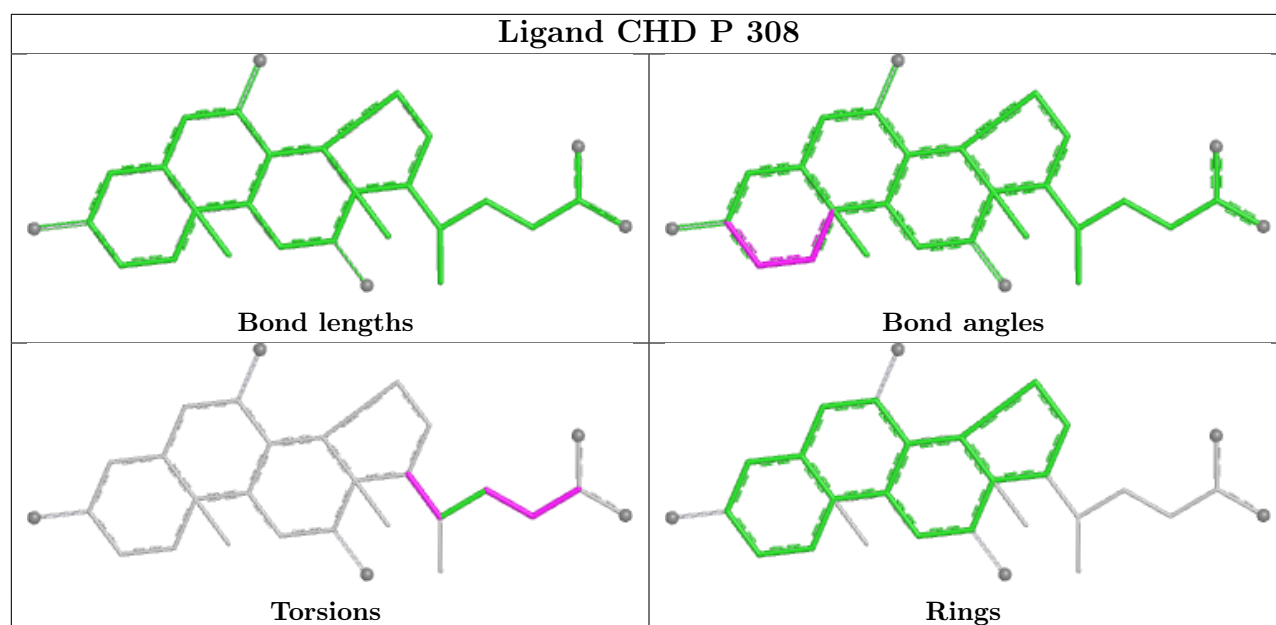


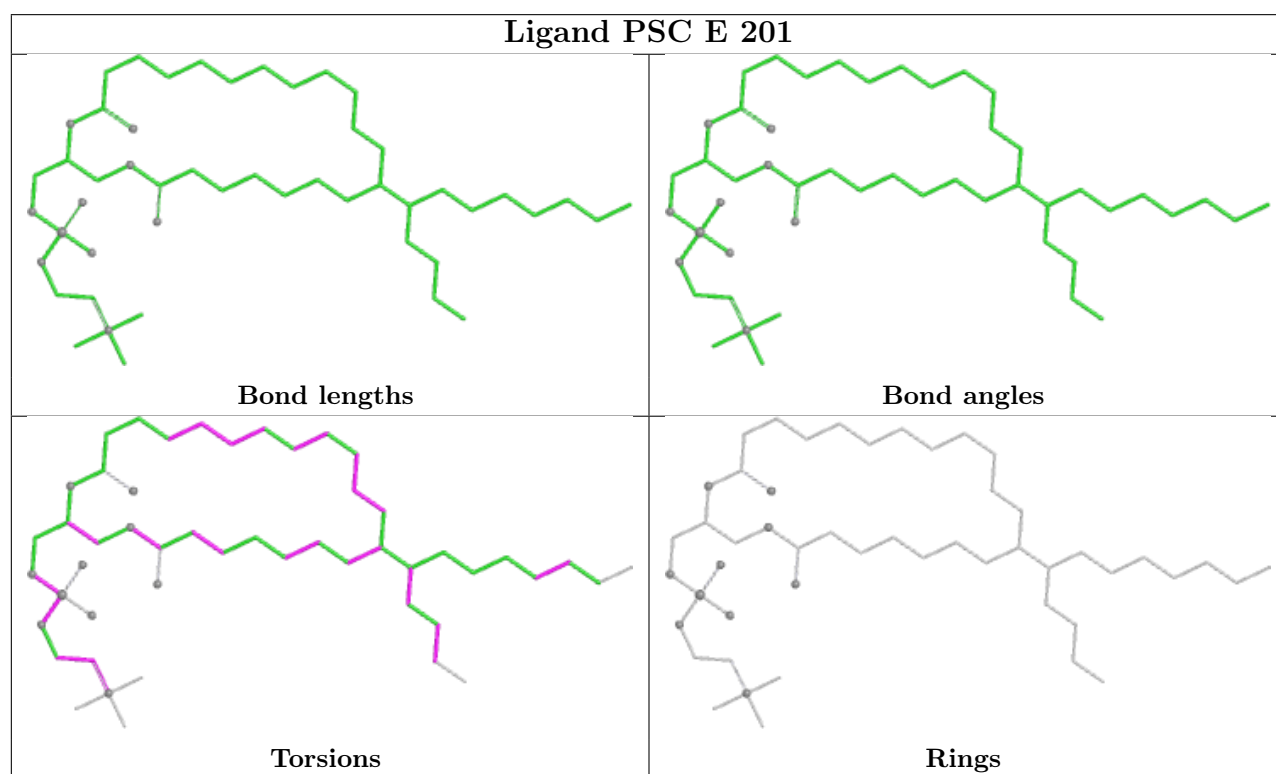
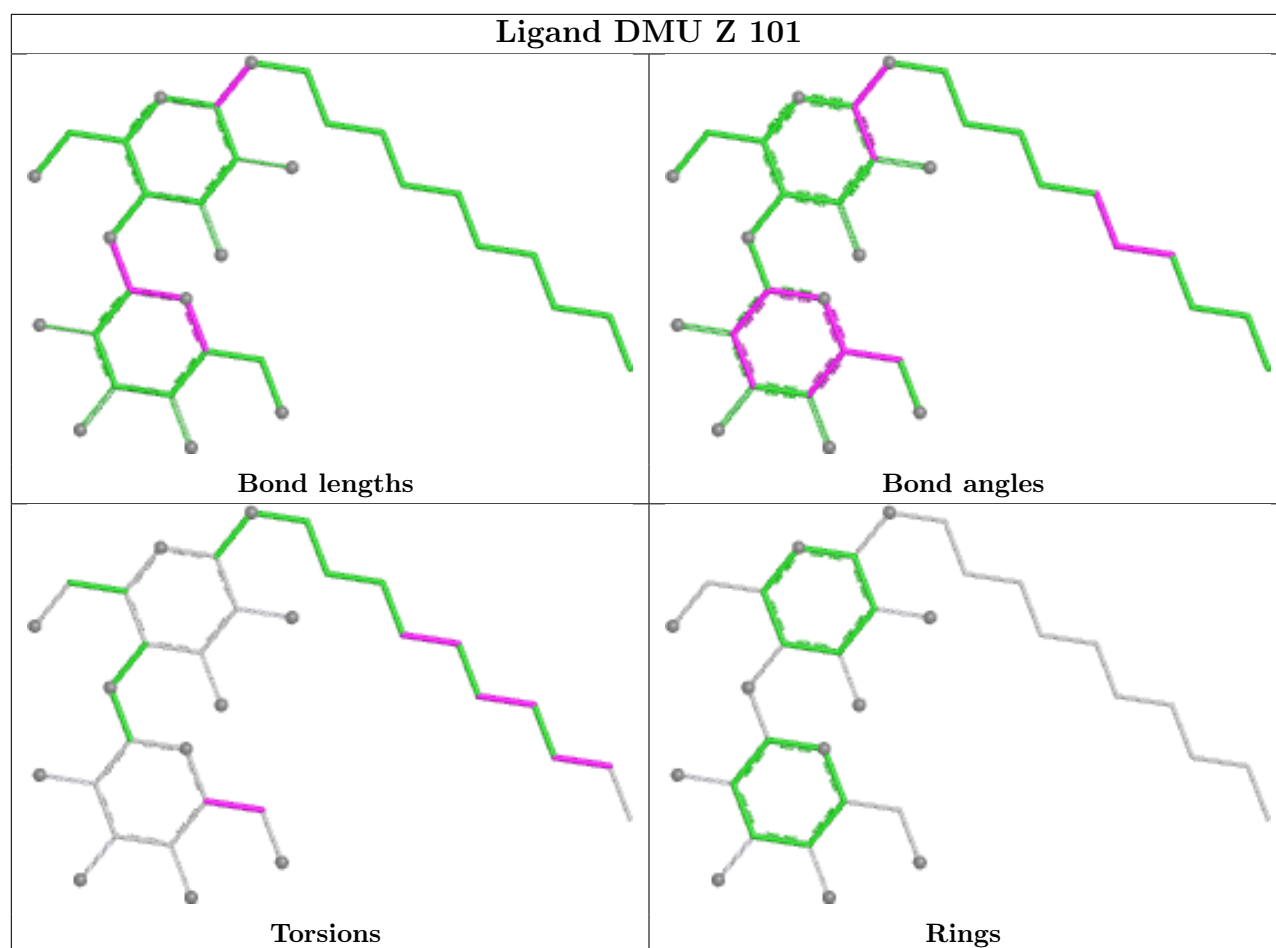


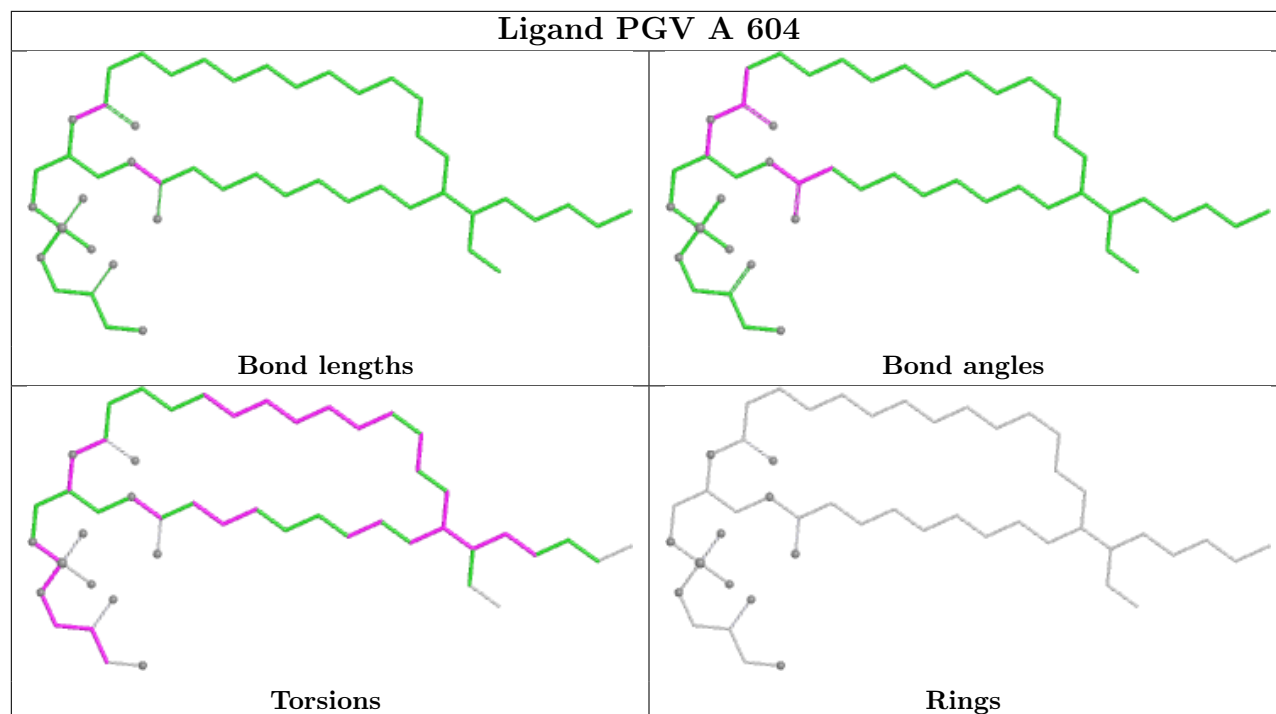












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	-0.21	5 (0%) 79 84	27, 33, 42, 79	0
1	N	513/514 (99%)	0.19	7 (1%) 73 79	32, 39, 51, 84	0
2	B	226/227 (99%)	0.22	8 (3%) 47 53	28, 38, 61, 99	0
2	O	226/227 (99%)	0.52	10 (4%) 39 43	36, 46, 73, 103	0
3	C	259/261 (99%)	-0.03	2 (0%) 82 87	30, 37, 49, 83	0
3	P	259/261 (99%)	0.21	5 (1%) 66 72	32, 41, 55, 87	0
4	D	147/147 (100%)	0.27	3 (2%) 65 72	35, 43, 59, 90	0
4	Q	147/147 (100%)	1.20	21 (14%) 6 7	41, 57, 98, 154	0
5	E	105/109 (96%)	0.34	2 (1%) 66 72	37, 45, 69, 123	0
5	R	105/109 (96%)	0.80	8 (7%) 20 22	42, 53, 75, 124	0
6	F	98/98 (100%)	0.45	8 (8%) 17 19	32, 43, 85, 138	0
6	S	98/98 (100%)	0.68	10 (10%) 12 13	37, 48, 82, 117	0
7	G	83/85 (97%)	1.23	17 (20%) 2 2	34, 44, 108, 122	0
7	T	83/85 (97%)	1.28	17 (20%) 2 2	36, 50, 104, 130	0
8	H	79/85 (92%)	0.87	12 (15%) 5 6	35, 48, 97, 110	0
8	U	79/85 (92%)	1.07	13 (16%) 4 4	42, 53, 114, 127	0
9	I	72/73 (98%)	0.56	2 (2%) 55 62	36, 51, 67, 86	0
9	V	72/73 (98%)	0.95	9 (12%) 8 9	40, 57, 80, 99	0
10	J	58/59 (98%)	0.58	5 (8%) 16 18	36, 47, 72, 122	0
10	W	58/59 (98%)	0.98	4 (6%) 23 26	41, 53, 84, 123	0
11	K	52/56 (92%)	0.83	4 (7%) 19 22	37, 46, 65, 111	0
11	X	52/56 (92%)	1.06	7 (13%) 7 7	50, 59, 104, 120	0
12	L	46/47 (97%)	0.23	3 (6%) 25 28	33, 39, 62, 93	0
12	Y	46/47 (97%)	0.80	3 (6%) 25 28	42, 49, 73, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	0.45	2 (4%) 36 41	36, 40, 71, 105	0
13	Z	43/46 (93%)	1.10	6 (13%) 6 7	45, 53, 84, 143	0
All	All	3562/3614 (98%)	0.40	193 (5%) 31 35	27, 42, 76, 154	0

The worst 5 of 193 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	3	ALA	10.2
4	Q	6	VAL	8.7
4	Q	5	VAL	7.5
7	T	9	GLY	7.5
7	T	10	GLY	7.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	TPO	G	11	11/12	0.70	0.21	47,87,130,139	0
7	TPO	T	11	11/12	0.71	0.17	54,119,161,165	0
1	FME	N	1	10/11	0.94	0.12	51,59,89,92	0
1	FME	A	1	10/11	0.94	0.11	45,53,79,101	0
2	FME	O	1	10/11	0.96	0.12	40,48,59,62	0
2	FME	B	1	10/11	0.97	0.08	36,41,50,58	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
28	SAC	V	101	9/10	0.31	0.19	129,139,152,154	0
22	CHD	T	104	29/29	0.68	0.27	81,147,172,175	0
28	SAC	I	101	9/10	0.69	0.22	83,101,110,116	0
24	PEK	C	315	53/53	0.70	0.29	60,85,124,172	0
19	EDO	R	202	4/4	0.73	0.20	78,85,89,96	0
19	EDO	P	310	4/4	0.73	0.32	61,83,84,90	0
23	DMU	C	301	33/33	0.73	0.21	87,130,143,153	0
22	CHD	Y	102	29/29	0.74	0.25	96,138,156,166	0
17	PGV	Z	102	51/51	0.75	0.27	50,90,154,168	0
25	CDL	C	312	100/100	0.75	0.34	68,105,138,150	0
24	PEK	P	301	53/53	0.76	0.23	64,88,161,171	0
26	PSC	O	302	52/52	0.77	0.26	47,95,173,185	0
17	PGV	A	604	51/51	0.78	0.27	51,83,114,126	0
19	EDO	C	310	4/4	0.78	0.19	80,89,92,100	0
26	PSC	E	201	52/52	0.78	0.29	46,92,184,199	0
23	DMU	C	313	33/33	0.78	0.14	57,89,100,105	0
24	PEK	C	304	53/53	0.78	0.28	64,89,138,146	0
19	EDO	N	613	4/4	0.78	0.29	61,65,69,80	0
19	EDO	W	304	4/4	0.79	0.23	88,88,91,100	0
23	DMU	G	1302	33/33	0.79	0.19	62,110,125,125	0
17	PGV	T	101	51/51	0.79	0.26	56,90,115,134	0
19	EDO	D	204	4/4	0.79	0.18	60,76,76,78	0
19	EDO	F	702	4/4	0.79	0.20	70,84,89,96	0
19	EDO	J	1103	4/4	0.80	0.20	77,77,78,85	0
20	TGL	N	604	63/63	0.80	0.28	65,97,118,130	0
19	EDO	A	611	4/4	0.80	0.24	63,81,82,84	0
19	EDO	A	614	4/4	0.81	0.24	41,44,46,52	0
23	DMU	P	302	33/33	0.81	0.16	73,106,128,133	0
19	EDO	C	311	4/4	0.81	0.23	83,85,90,99	0
20	TGL	A	615	63/63	0.81	0.28	59,87,139,151	0
19	EDO	G	1306	4/4	0.81	0.20	90,90,93,95	0
17	PGV	N	616	51/51	0.82	0.23	66,87,140,156	0
25	CDL	T	102	100/100	0.82	0.28	67,112,154,170	0
19	EDO	V	103	4/4	0.82	0.20	81,81,90,95	0
20	TGL	D	201	63/63	0.83	0.25	55,86,101,108	0
19	EDO	N	617	4/4	0.83	0.20	87,88,92,93	0
19	EDO	S	2201	4/4	0.83	0.22	58,63,63,78	0
24	PEK	P	305	53/53	0.83	0.25	59,92,159,171	0
19	EDO	T	103	4/4	0.83	0.21	57,66,69,71	0
19	EDO	S	2206	4/4	0.84	0.17	55,60,63,70	0
19	EDO	S	2207	4/4	0.84	0.22	75,81,84,85	0
20	TGL	Q	201	63/63	0.84	0.25	67,91,111,119	0
20	TGL	Y	101	63/63	0.84	0.26	55,79,120,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
19	EDO	B	309	4/4	0.84	0.23	75,91,97,105	0
25	CDL	P	307	100/100	0.85	0.23	52,96,128,136	0
19	EDO	V	104	4/4	0.85	0.20	50,74,76,77	0
19	EDO	I	102	4/4	0.85	0.19	88,88,94,94	0
19	EDO	S	2204	4/4	0.86	0.18	50,66,66,68	0
19	EDO	Z	103	4/4	0.86	0.16	86,94,94,96	0
19	EDO	P	309	4/4	0.86	0.15	81,82,85,87	0
20	TGL	L	101	63/63	0.87	0.22	47,77,104,109	0
19	EDO	B	308	4/4	0.87	0.18	59,62,69,85	0
25	CDL	C	306	100/100	0.87	0.21	48,89,122,127	0
19	EDO	W	303	4/4	0.87	0.19	60,74,75,76	0
19	EDO	G	1303	4/4	0.87	0.17	71,83,83,89	0
19	EDO	D	205	4/4	0.88	0.16	64,77,78,81	0
19	EDO	D	206	4/4	0.88	0.17	74,79,83,88	0
19	EDO	J	1105	4/4	0.88	0.14	56,73,74,88	0
19	EDO	N	611	4/4	0.88	0.17	67,71,73,81	0
19	EDO	N	612	4/4	0.88	0.18	67,73,74,82	0
19	EDO	E	204	4/4	0.88	0.17	73,75,75,78	0
19	EDO	U	1501	4/4	0.88	0.20	55,66,68,72	0
19	EDO	A	610	4/4	0.88	0.16	38,43,46,50	0
19	EDO	O	303	4/4	0.88	0.16	53,74,76,77	0
19	EDO	D	202	4/4	0.88	0.15	62,72,77,81	0
19	EDO	A	612	4/4	0.88	0.18	55,56,56,62	0
19	EDO	Q	204	4/4	0.88	0.17	73,73,75,75	0
19	EDO	B	306	4/4	0.89	0.22	70,76,78,81	0
19	EDO	F	704	4/4	0.89	0.19	61,61,69,71	0
19	EDO	N	614	4/4	0.89	0.26	41,45,46,47	0
23	DMU	Z	101	33/33	0.89	0.14	54,72,82,84	0
22	CHD	J	1102	29/29	0.89	0.13	59,74,86,97	0
19	EDO	C	309	4/4	0.89	0.17	75,80,83,84	0
19	EDO	N	620	4/4	0.89	0.19	65,66,69,79	0
19	EDO	B	304	4/4	0.89	0.15	51,59,64,72	0
19	EDO	L	102	4/4	0.90	0.17	68,69,72,75	0
19	EDO	B	307	4/4	0.90	0.19	65,67,68,84	0
19	EDO	S	2205	4/4	0.90	0.14	56,59,69,70	0
19	EDO	E	205	4/4	0.90	0.20	81,82,82,86	0
22	CHD	P	308	29/29	0.90	0.12	57,64,73,78	0
19	EDO	A	616	4/4	0.90	0.15	54,66,68,68	0
19	EDO	E	203	4/4	0.91	0.11	51,52,57,59	0
22	CHD	W	302	29/29	0.91	0.12	78,88,98,106	0
22	CHD	C	307	29/29	0.91	0.11	53,60,67,73	0
19	EDO	A	618	4/4	0.91	0.14	56,62,64,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
19	EDO	G	1304	4/4	0.91	0.18	75,79,80,80	0
19	EDO	V	102	4/4	0.92	0.18	78,79,80,83	0
19	EDO	C	314	4/4	0.92	0.14	62,70,71,79	0
19	EDO	P	311	4/4	0.92	0.14	42,51,51,60	0
19	EDO	Q	202	4/4	0.92	0.14	44,56,58,60	0
19	EDO	M	102	4/4	0.92	0.13	72,75,80,83	0
19	EDO	D	208	4/4	0.93	0.16	62,64,70,74	0
19	EDO	Q	203	4/4	0.93	0.15	73,77,82,86	0
19	EDO	A	620	4/4	0.93	0.11	45,47,52,52	0
19	EDO	N	618	4/4	0.93	0.13	54,56,62,64	0
24	PEK	P	304	53/53	0.93	0.18	41,64,101,108	0
19	EDO	W	301	4/4	0.93	0.16	62,74,75,76	0
19	EDO	N	610	4/4	0.93	0.14	52,55,58,59	0
19	EDO	I	103	4/4	0.94	0.11	58,63,64,67	0
19	EDO	A	613	4/4	0.94	0.14	45,52,57,59	0
19	EDO	A	608	4/4	0.94	0.14	50,56,63,68	0
19	EDO	K	101	4/4	0.94	0.13	74,75,76,77	0
19	EDO	D	203	4/4	0.94	0.15	61,66,75,83	0
19	EDO	A	619	4/4	0.94	0.16	66,67,70,78	0
19	EDO	N	609	4/4	0.94	0.13	50,53,54,55	0
19	EDO	N	619	4/4	0.94	0.12	51,60,68,77	0
19	EDO	R	201	4/4	0.94	0.10	54,54,55,56	0
24	PEK	C	303	53/53	0.95	0.15	37,62,93,113	0
22	CHD	C	302	29/29	0.95	0.08	35,38,41,42	0
19	EDO	A	617	4/4	0.95	0.14	56,61,62,69	0
19	EDO	S	2203	4/4	0.95	0.12	35,36,37,40	0
19	EDO	J	1104	4/4	0.95	0.13	55,55,58,62	0
19	EDO	E	202	4/4	0.95	0.09	51,52,52,54	0
17	PGV	A	605	51/51	0.95	0.13	28,48,85,90	0
19	EDO	N	615	4/4	0.95	0.15	55,68,73,83	0
19	EDO	B	305	4/4	0.95	0.10	44,54,60,62	0
19	EDO	T	105	4/4	0.95	0.13	44,46,47,49	0
17	PGV	N	605	51/51	0.95	0.14	34,49,85,93	0
23	DMU	M	101	33/33	0.95	0.09	46,54,68,74	0
19	EDO	D	207	4/4	0.95	0.12	60,63,63,70	0
19	EDO	J	1101	4/4	0.95	0.10	52,61,64,68	0
17	PGV	P	306	51/51	0.96	0.12	35,49,96,106	0
16	NA	A	603	1/1	0.96	0.12	35,35,35,35	0
19	EDO	N	608	4/4	0.96	0.08	42,42,45,50	0
22	CHD	P	303	29/29	0.96	0.07	35,40,44,46	0
19	EDO	C	308	4/4	0.96	0.11	43,49,53,61	0
19	EDO	K	102	4/4	0.96	0.10	66,68,74,75	0

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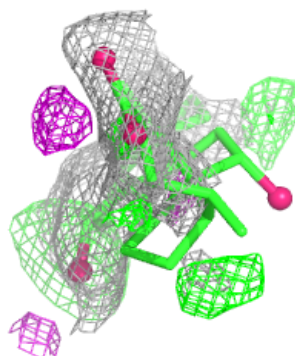
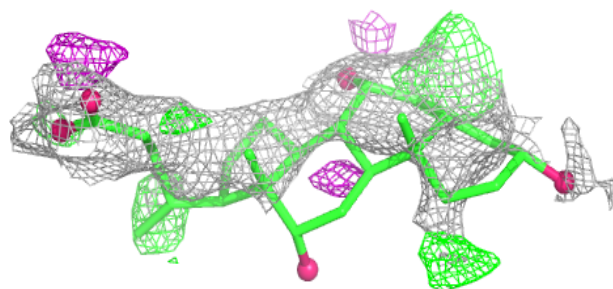
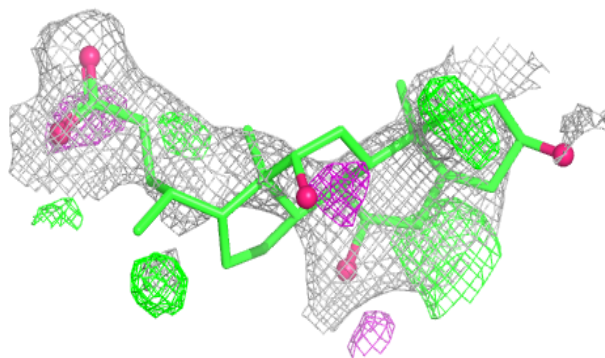
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
19	EDO	O	304	4/4	0.96	0.19	44,45,48,50	0
17	PGV	C	305	51/51	0.97	0.12	32,43,94,101	0
19	EDO	A	609	4/4	0.97	0.07	33,34,35,36	0
22	CHD	B	302	29/29	0.97	0.07	33,37,43,46	0
19	EDO	F	701	4/4	0.97	0.09	46,48,50,55	0
15	MG	A	602	1/1	0.97	0.04	32,32,32,32	0
22	CHD	G	1305	29/29	0.97	0.07	35,39,43,46	0
16	NA	N	603	1/1	0.97	0.11	49,49,49,49	0
19	EDO	B	303	4/4	0.97	0.14	32,33,34,37	0
18	HEA	N	606	60/60	0.98	0.06	27,34,43,49	0
19	EDO	F	705	4/4	0.98	0.09	34,36,37,37	0
19	EDO	G	1301	4/4	0.98	0.07	39,40,49,51	0
18	HEA	N	607	60/60	0.98	0.07	31,36,53,61	0
15	MG	N	602	1/1	0.98	0.05	39,39,39,39	0
18	HEA	A	607	60/60	0.99	0.06	24,29,48,55	0
27	ZN	F	703	1/1	0.99	0.03	38,38,38,38	0
18	HEA	A	606	60/60	0.99	0.05	24,29,37,43	0
21	CUA	O	301	2/2	0.99	0.02	37,37,37,38	0
21	CUA	B	301	2/2	1.00	0.02	30,30,30,30	0
27	ZN	S	2202	1/1	1.00	0.03	42,42,42,42	0
14	CU	N	601	1/1	1.00	0.02	35,35,35,35	0
14	CU	A	601	1/1	1.00	0.01	29,29,29,29	0

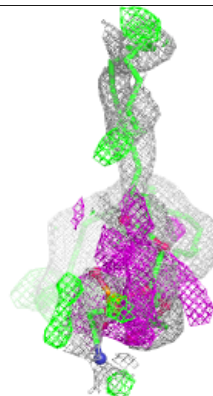
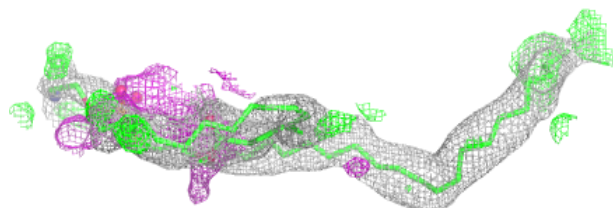
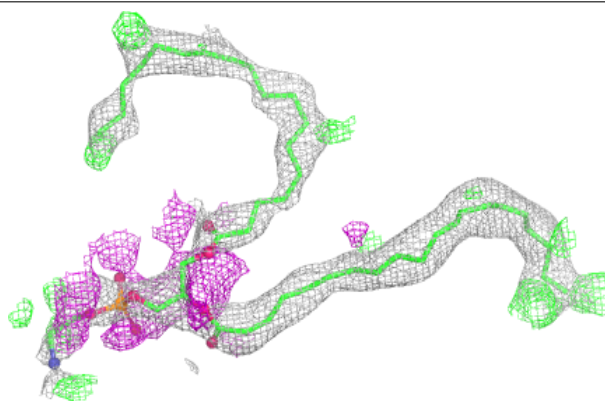
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around CHD 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)

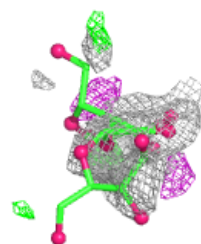
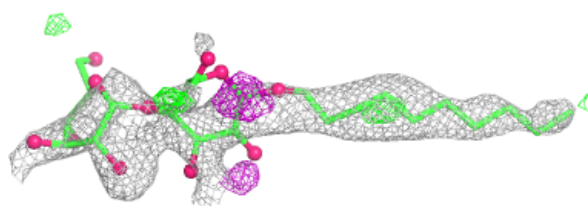
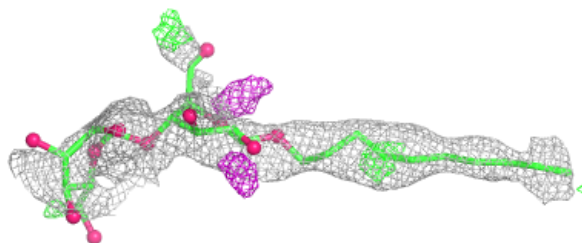
**Electron density around PEK C 315:**

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

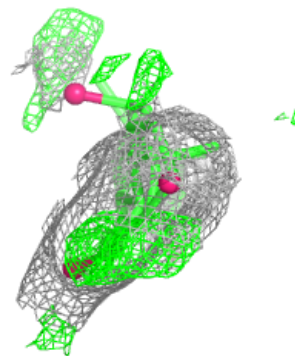
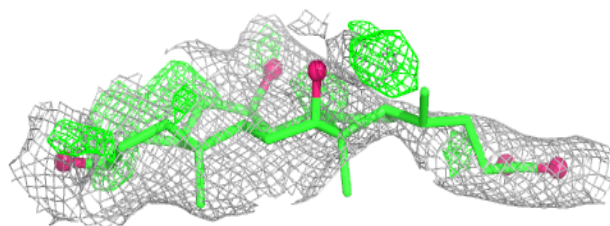
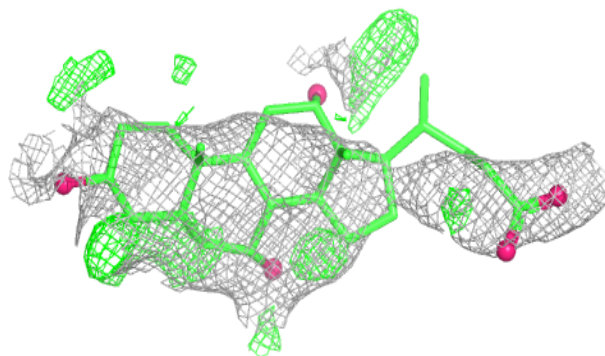


**Electron density around DMU C 301:**

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

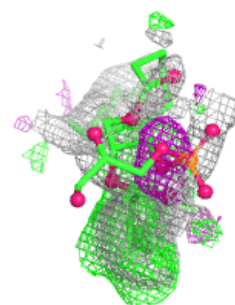
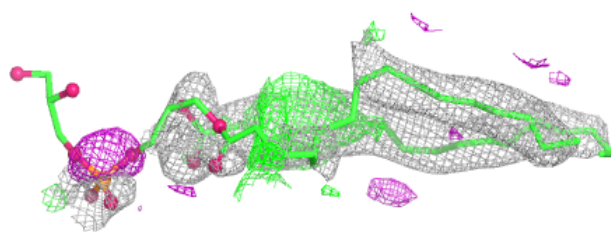
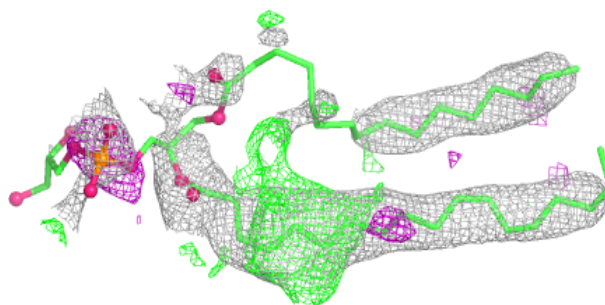
**Electron density around CHD Y 102:**

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

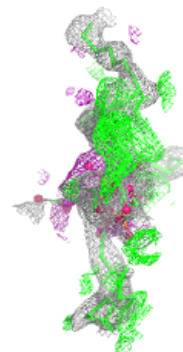
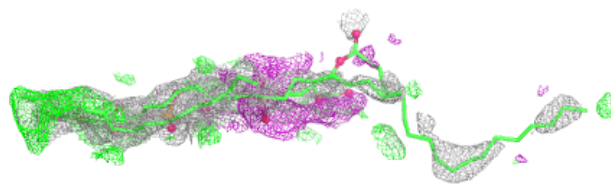
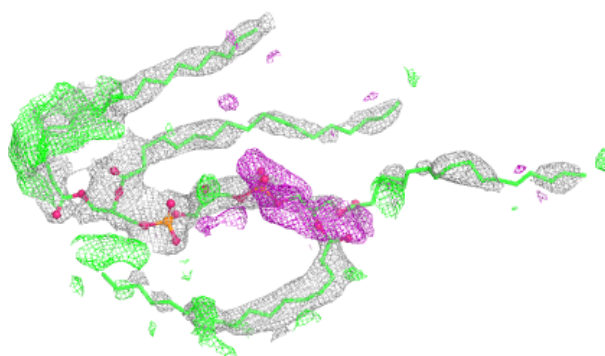


**Electron density around PGV Z 102:**

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

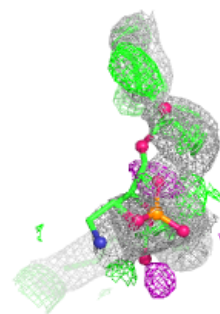
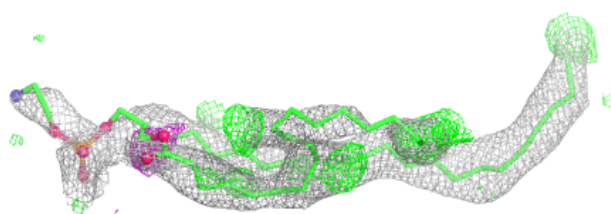
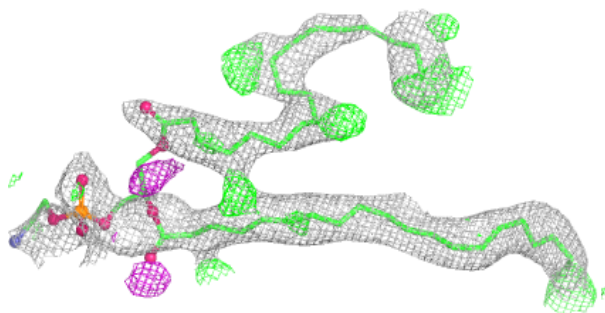
**Electron density around CDL C 312:**

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

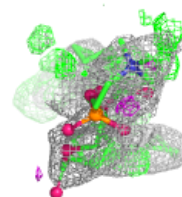
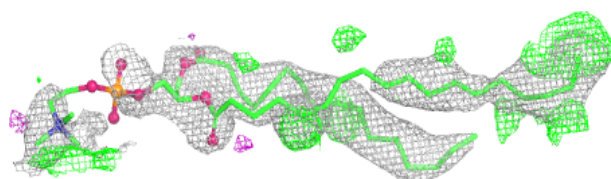
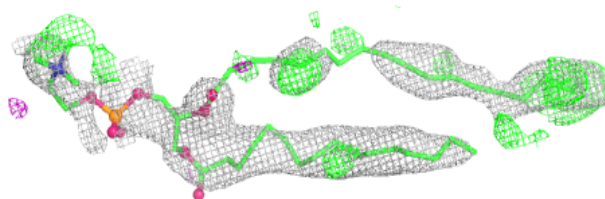


**Electron density around PEK P 301:**

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

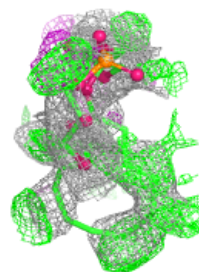
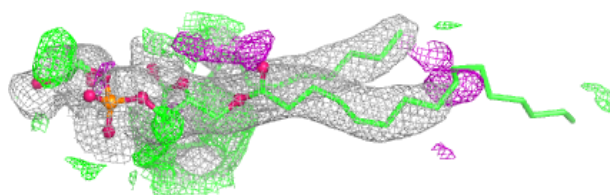
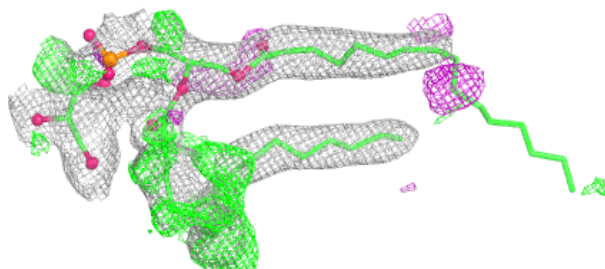
**Electron density around PSC O 302:**

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

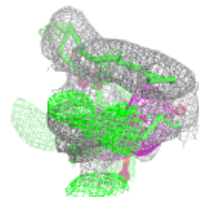
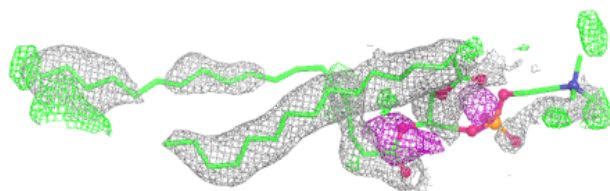
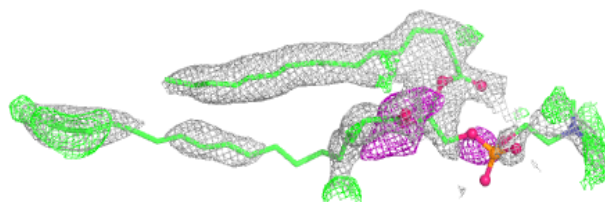


**Electron density around PGV A 604:**

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

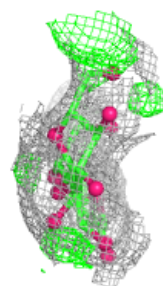
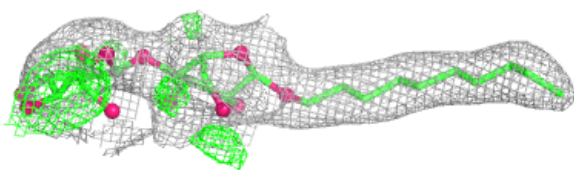
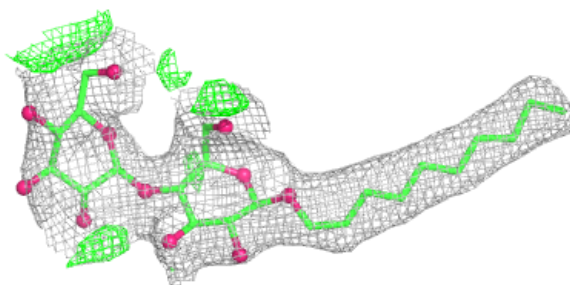
**Electron density around PSC E 201:**

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

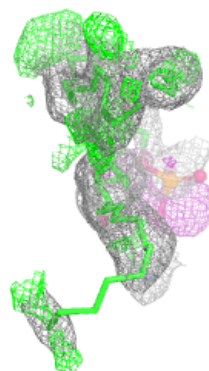
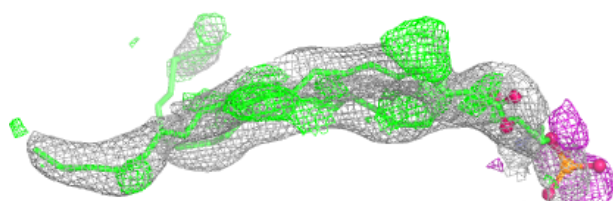
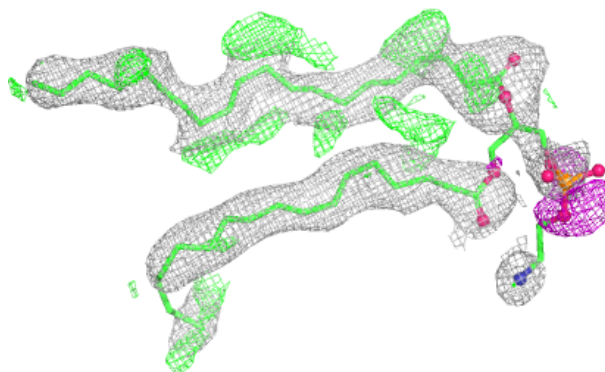


**Electron density around DMU C 313:**

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

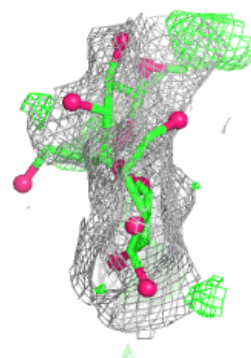
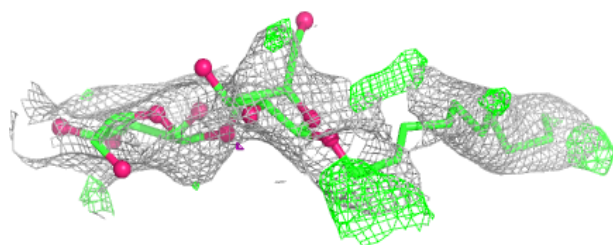
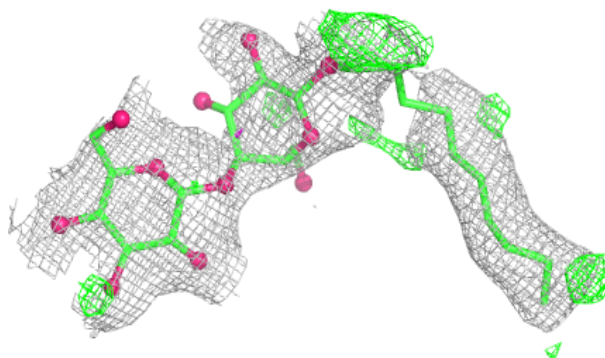
**Electron density around PEK C 304:**

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

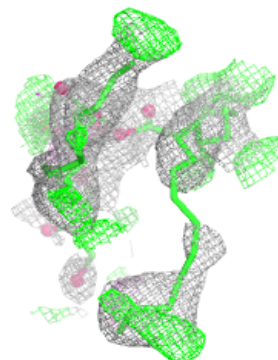
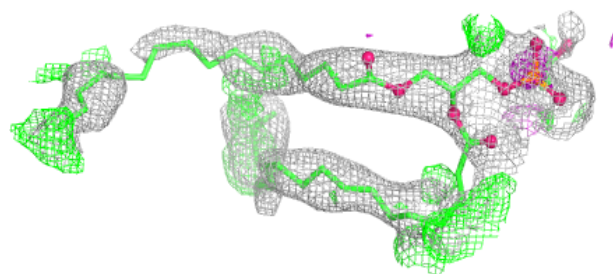
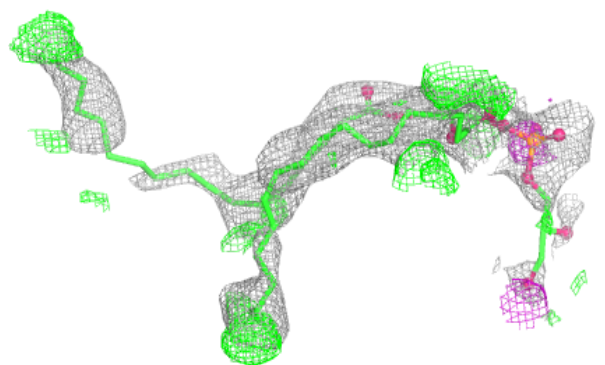


**Electron density around DMU G 1302:**

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

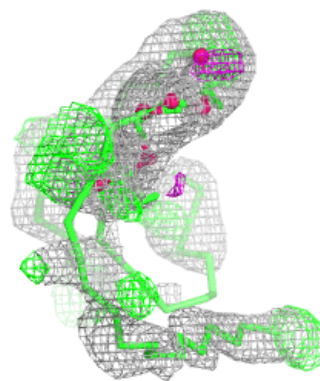
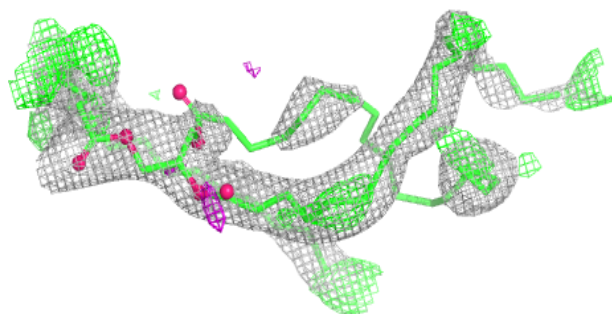
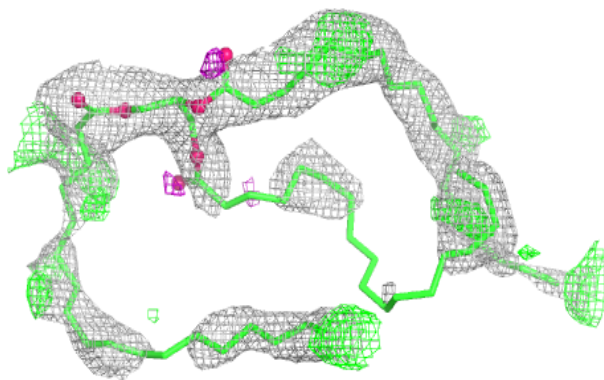
**Electron density around PGV T 101:**

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

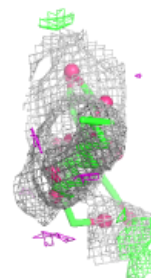
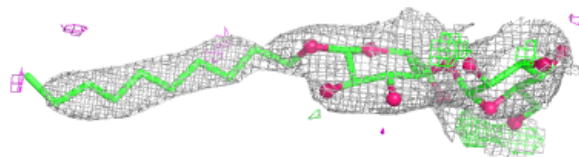
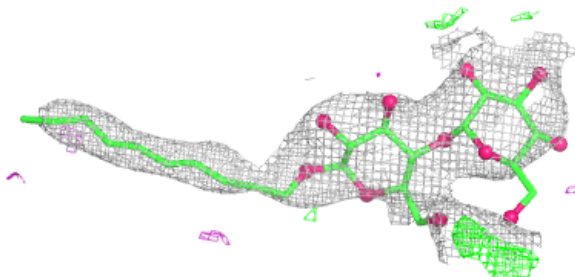


**Electron density around TGL N 604:**

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

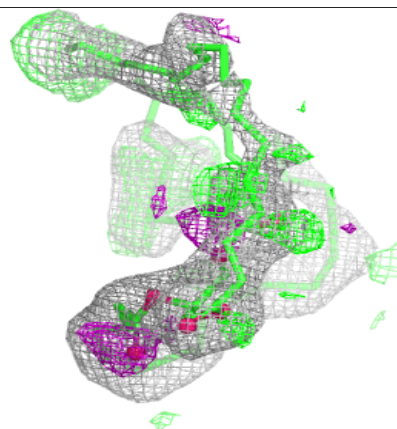
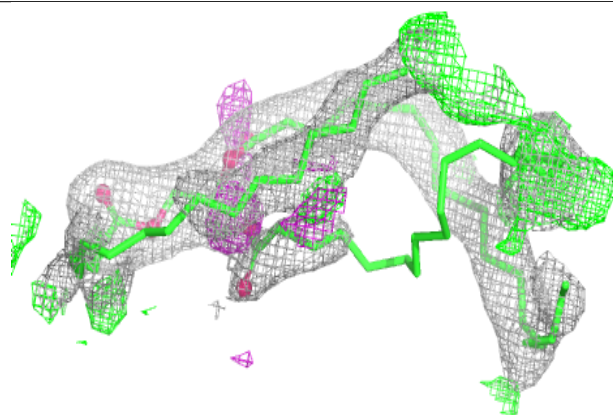
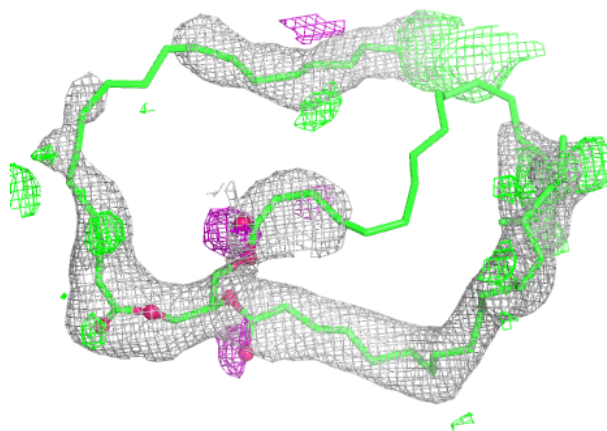
**Electron density around DMU P 302:**

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

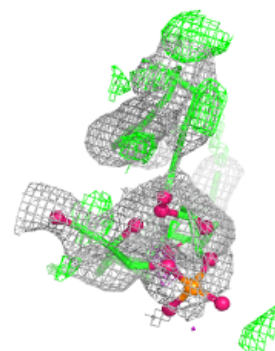
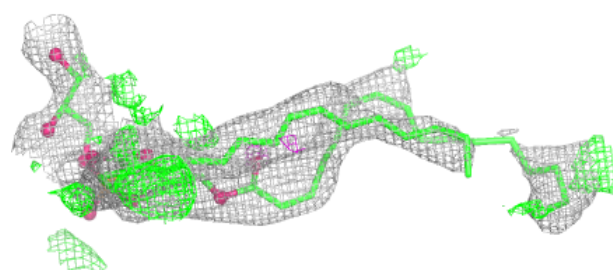
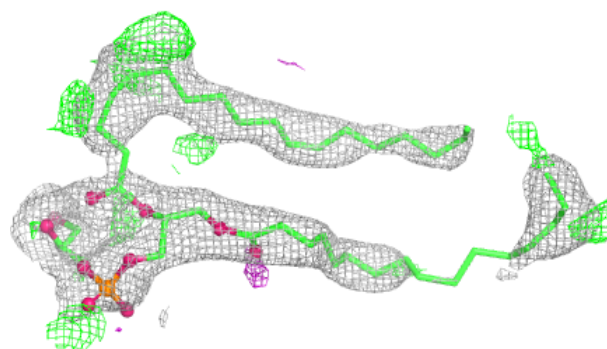


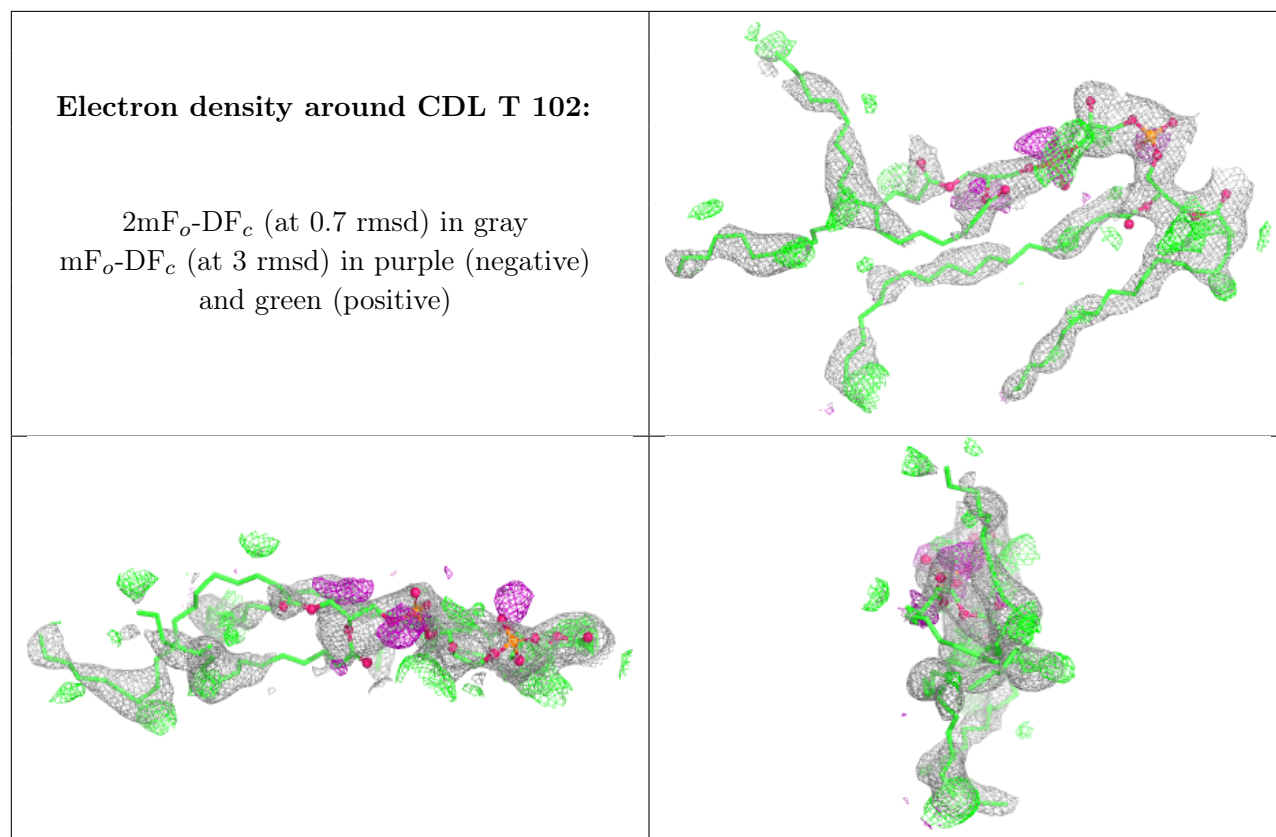
**Electron density around TGL A 615:**

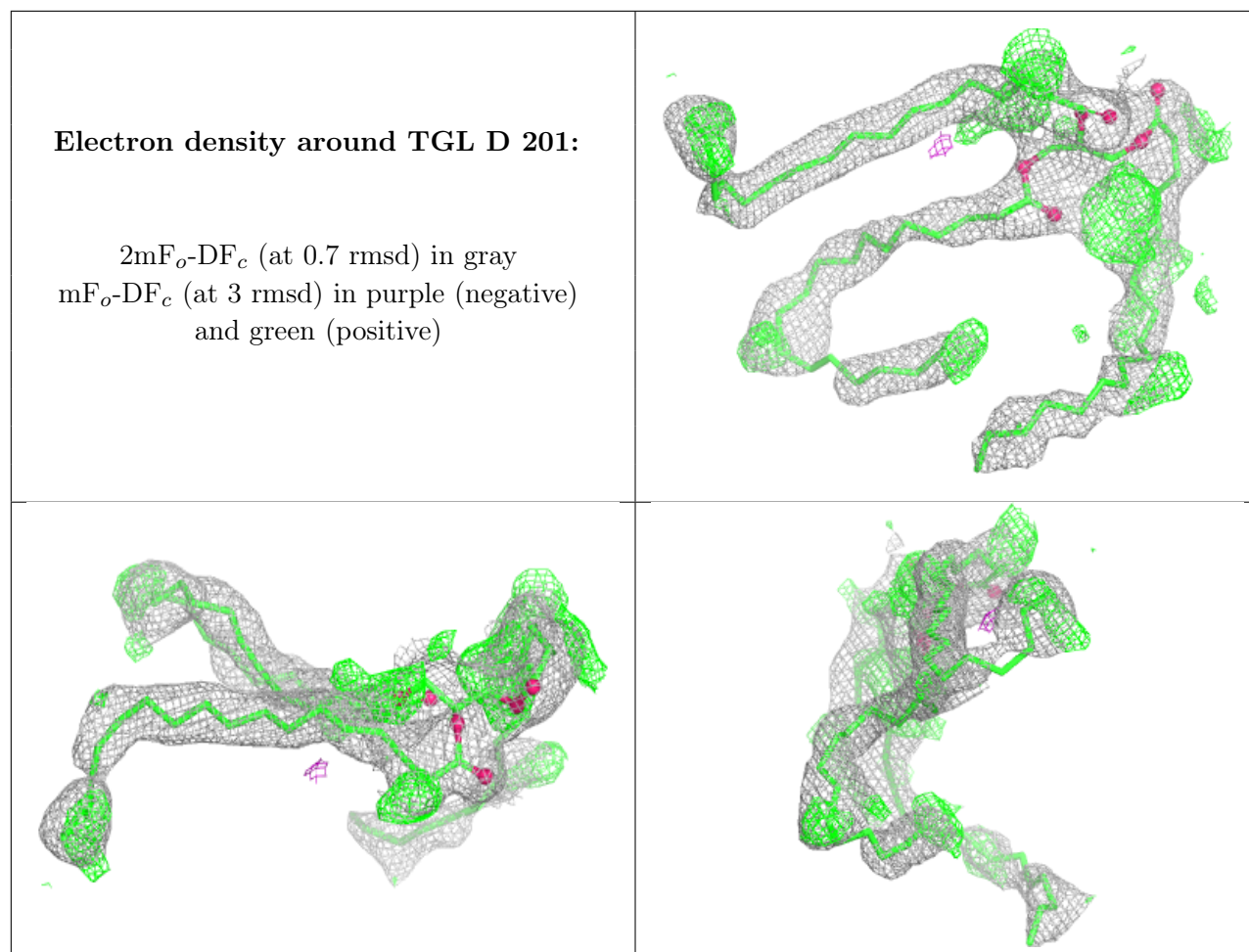
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PGV N 616:**

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

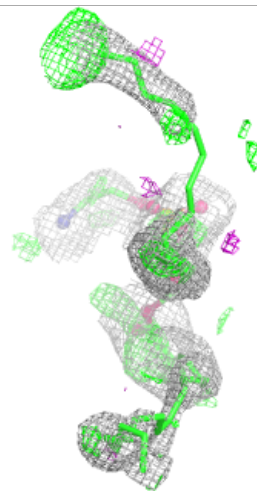
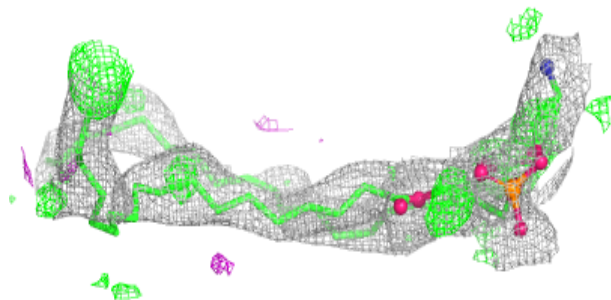
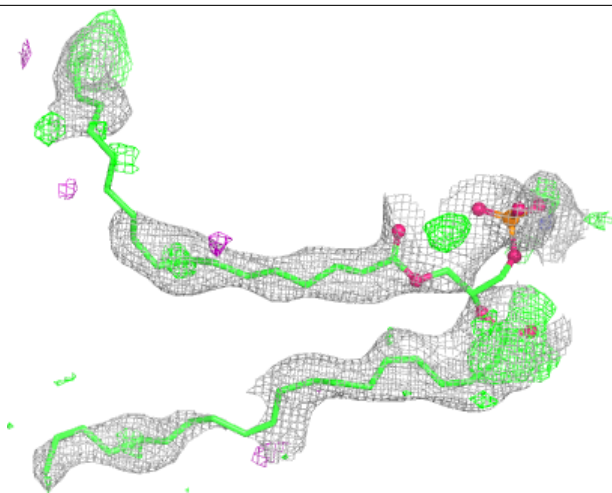


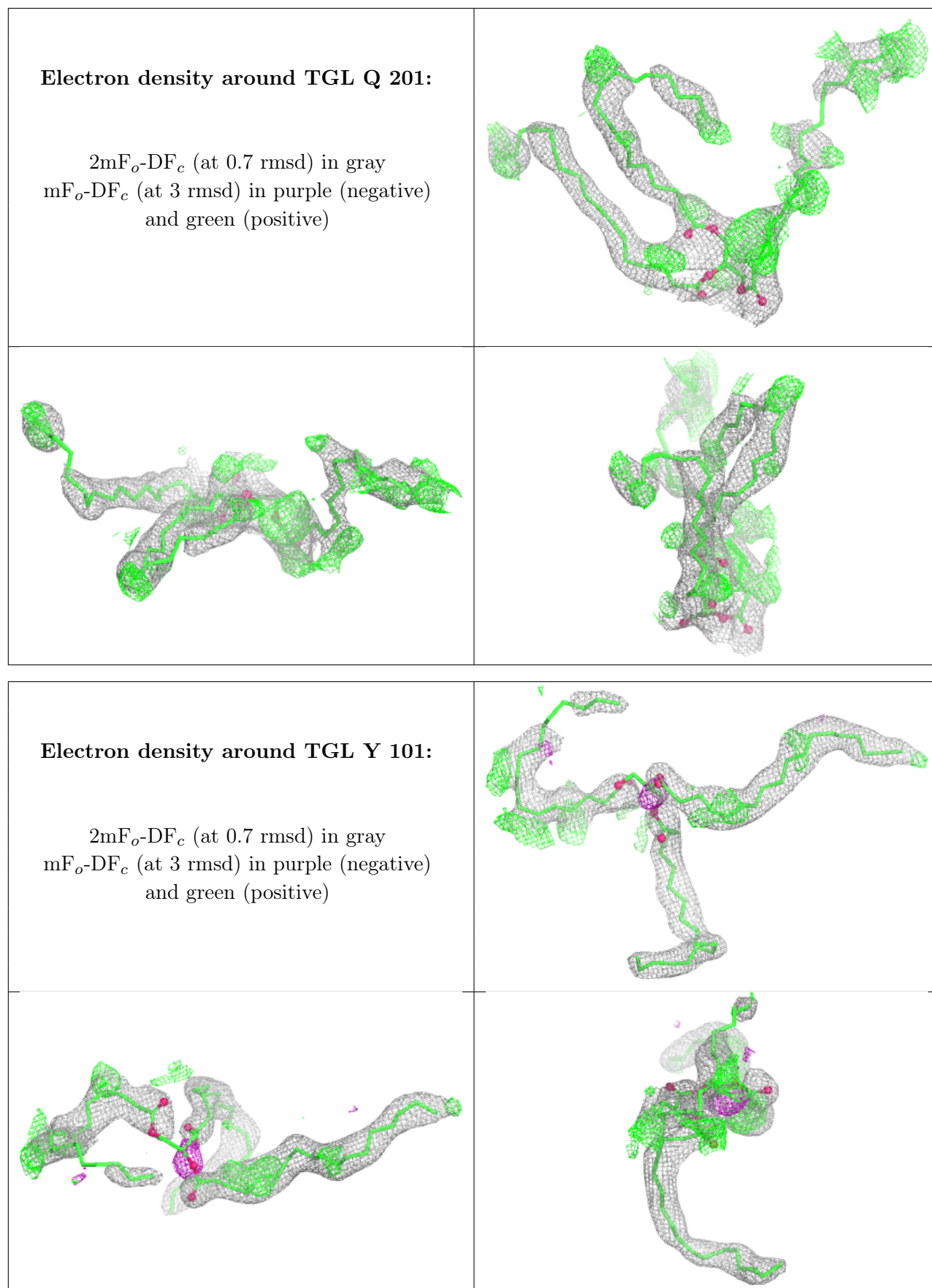




**Electron density around PEK P 305:**

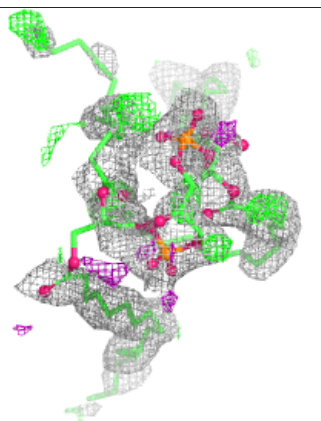
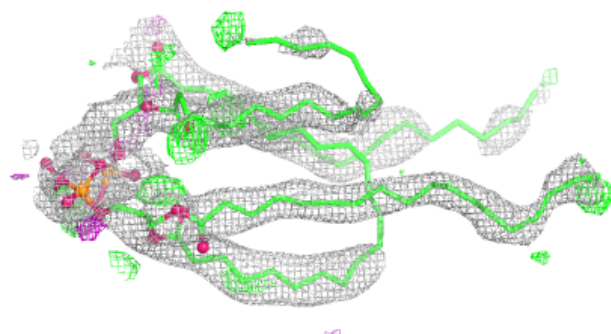
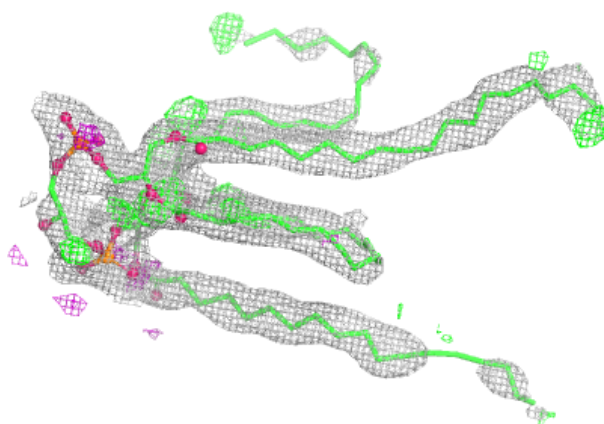
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





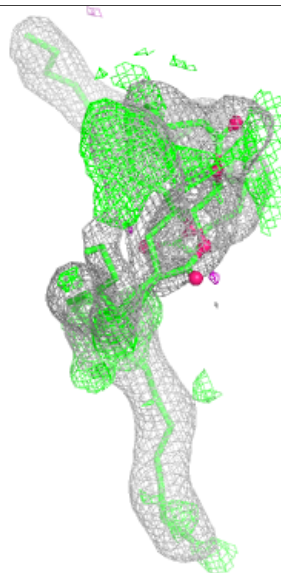
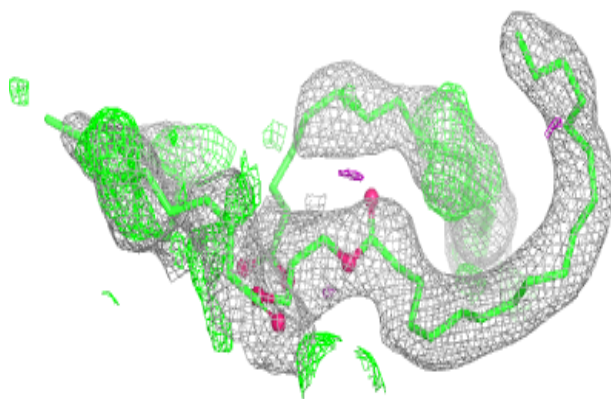
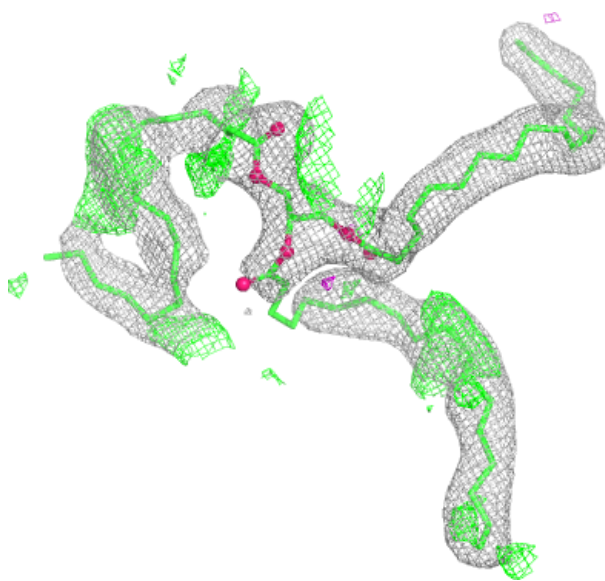
**Electron density around CDL P 307:**

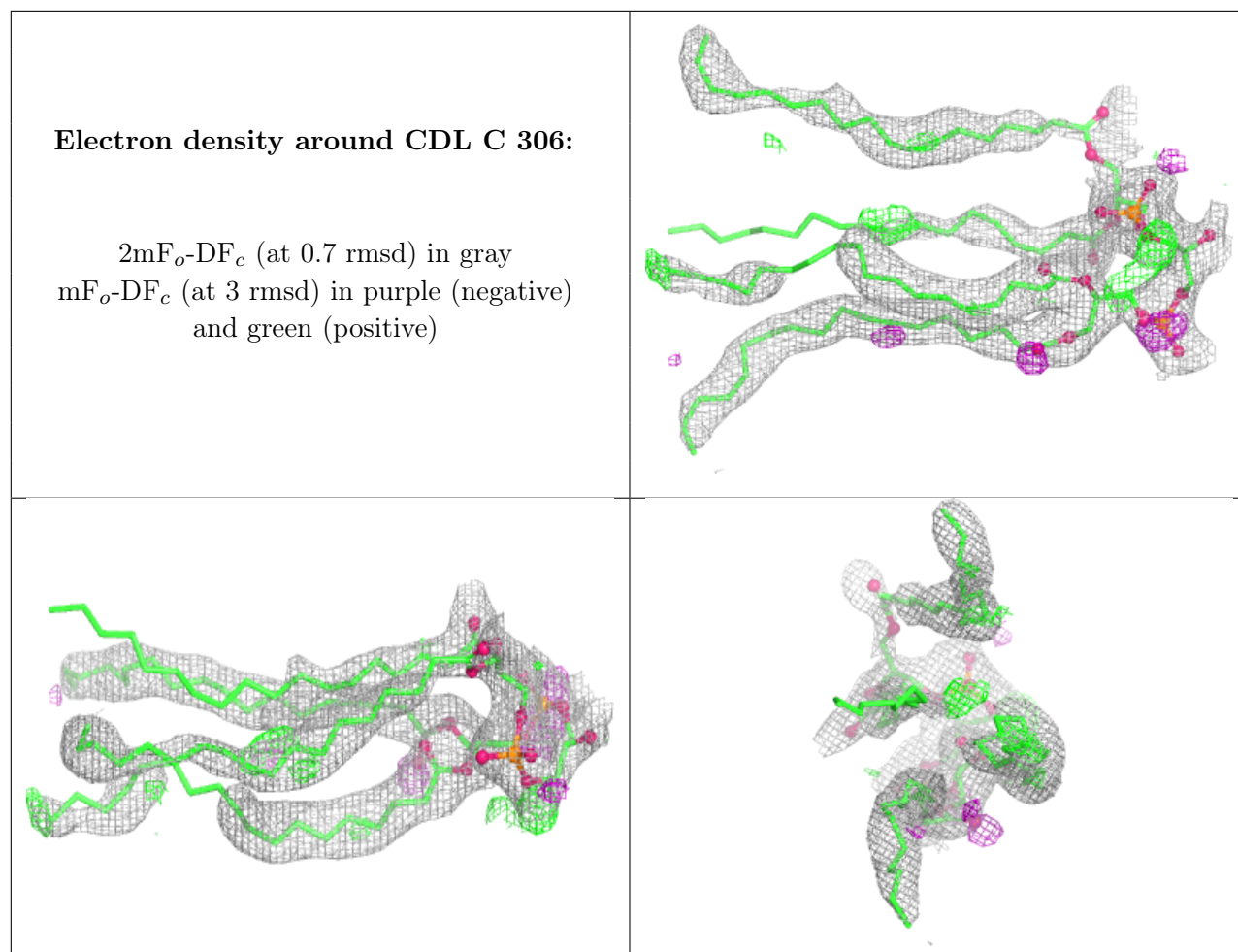
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around TGL L 101:**

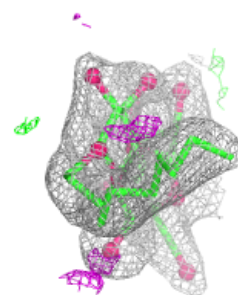
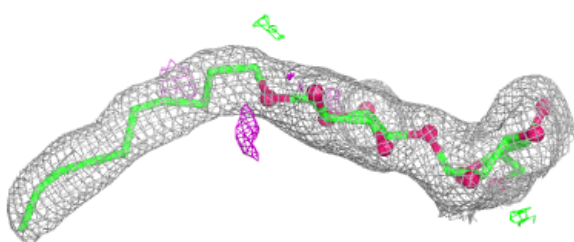
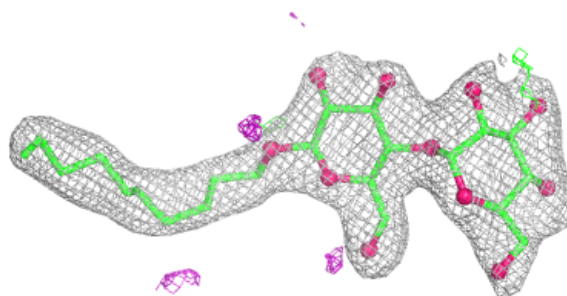
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



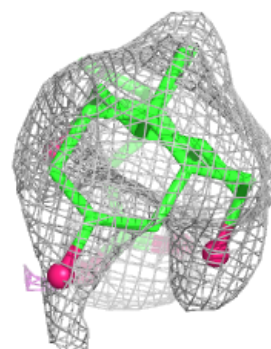
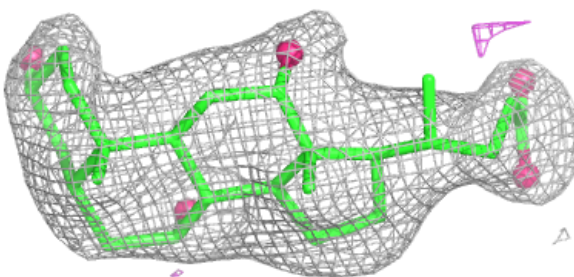
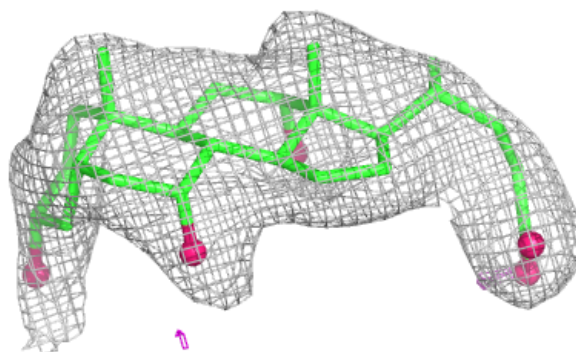


**Electron density around DMU Z 101:**

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

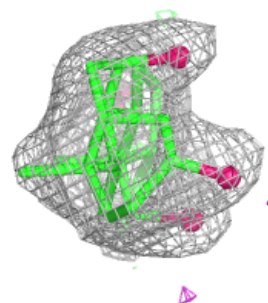
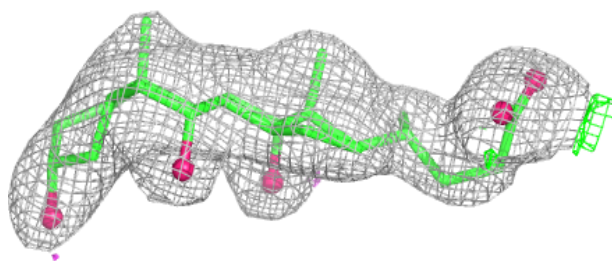
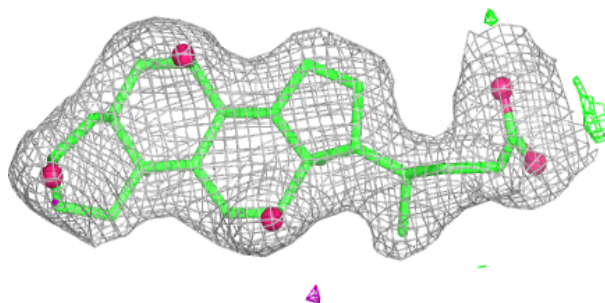
**Electron density around CHD J 1102:**

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

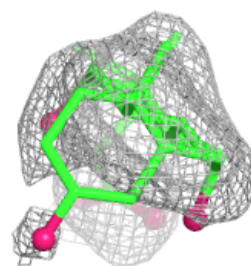
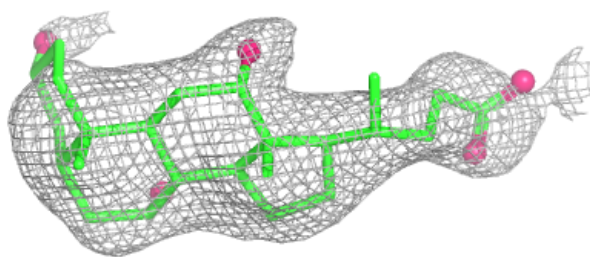
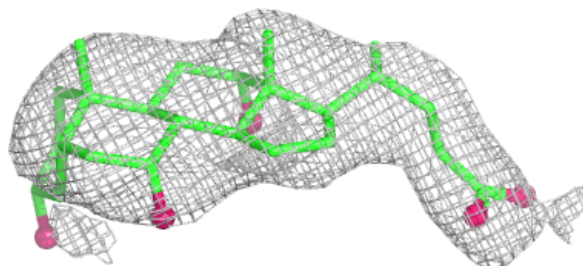


**Electron density around CHD P 308:**

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

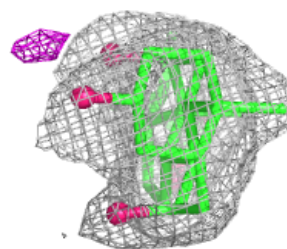
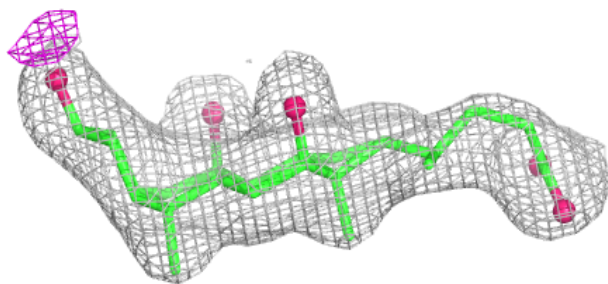
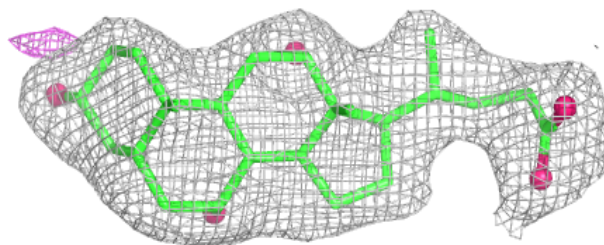
**Electron density around CHD W 302:**

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

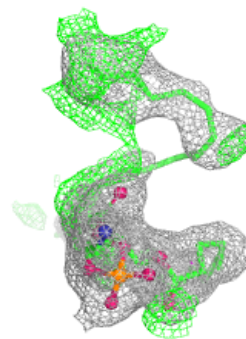
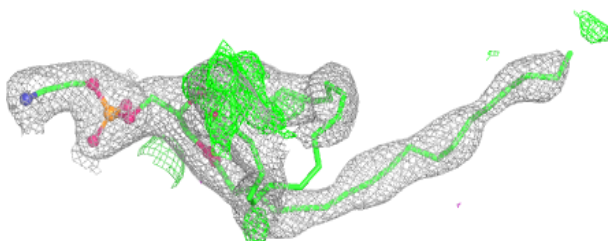
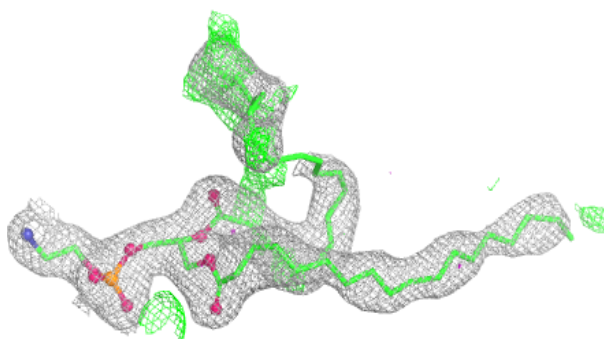


**Electron density around CHD C 307:**

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

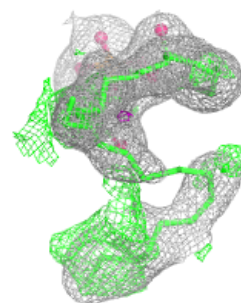
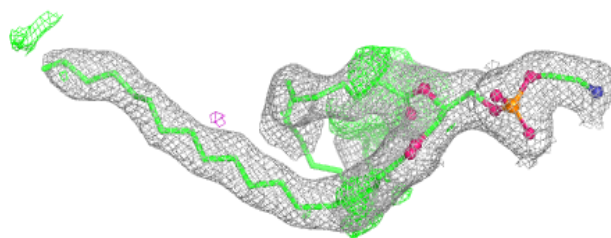
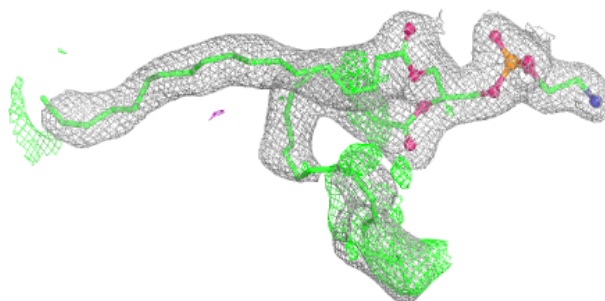
**Electron density around PEK P 304:**

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

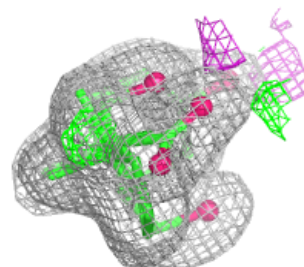
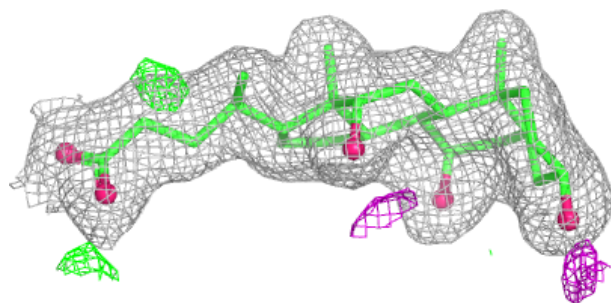
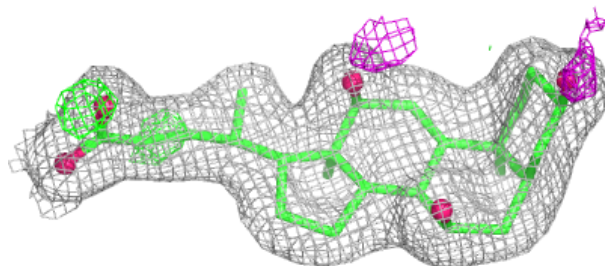


**Electron density around PEK C 303:**

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

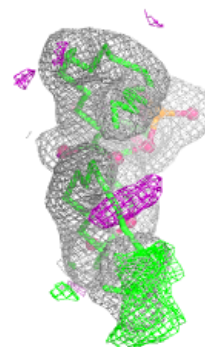
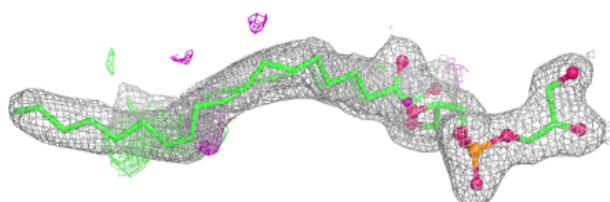
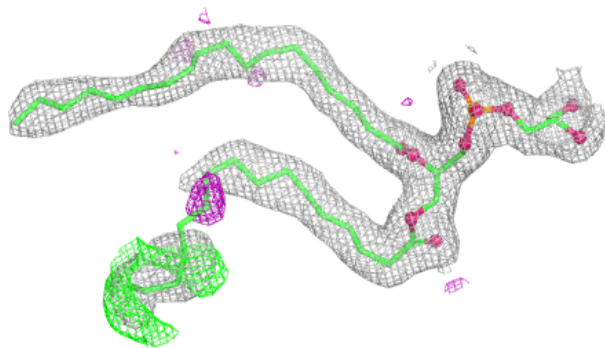
**Electron density around CHD C 302:**

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

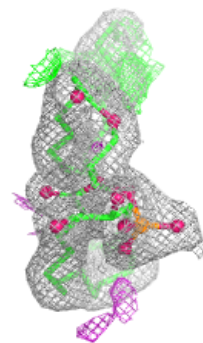
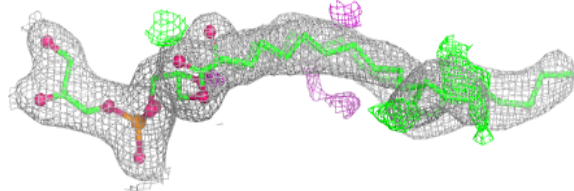
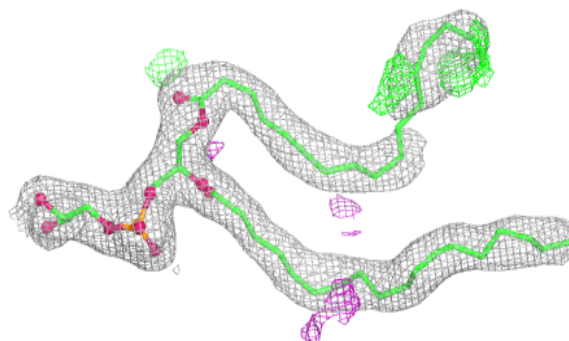


**Electron density around PGV A 605:**

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

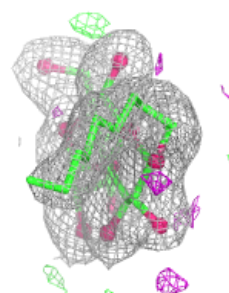
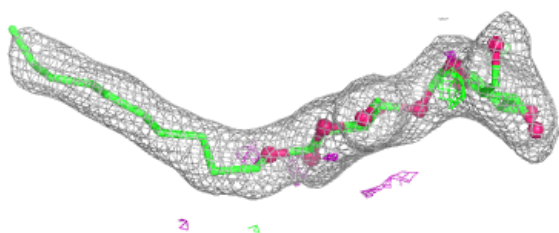
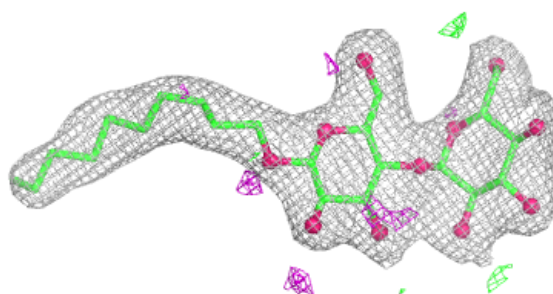
**Electron density around PGV N 605:**

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

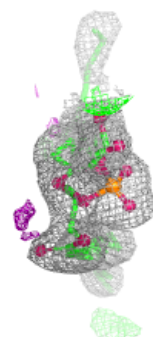
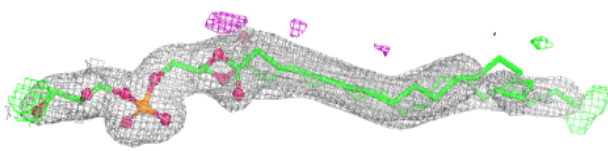
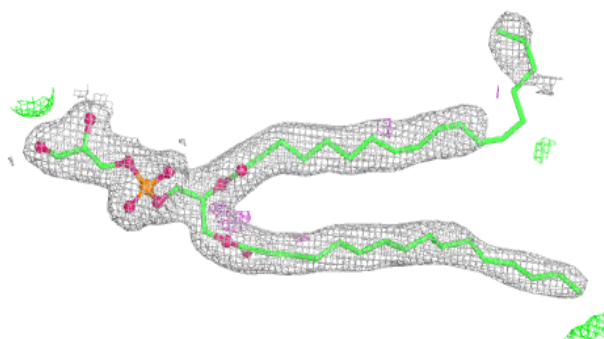


**Electron density around DMU M 101:**

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

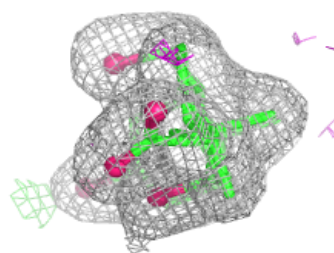
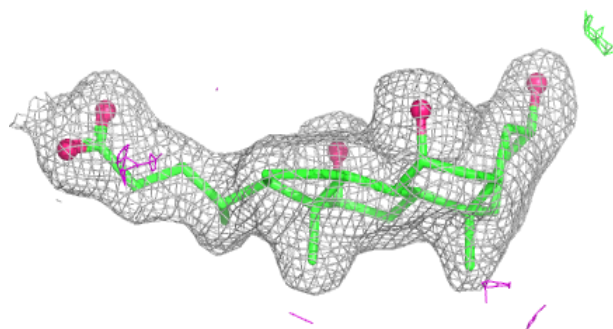
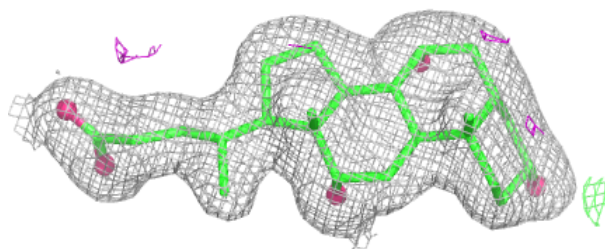
**Electron density around PGV P 306:**

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

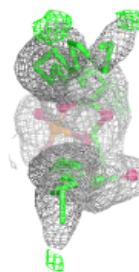
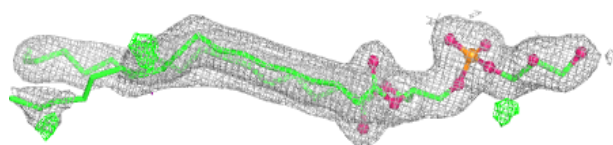
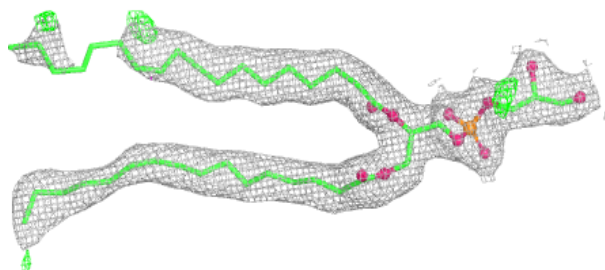


**Electron density around CHD P 303:**

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

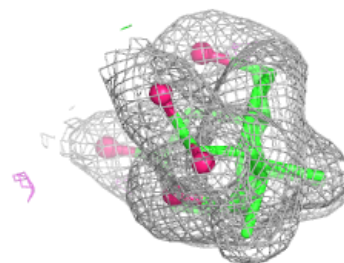
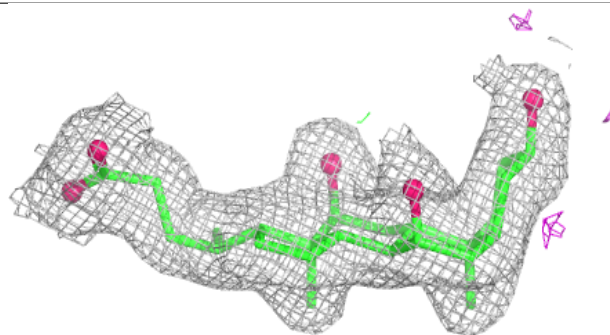
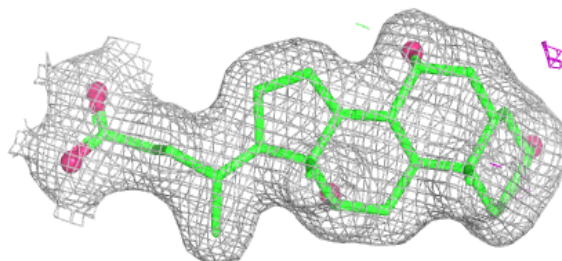
**Electron density around PGV C 305:**

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

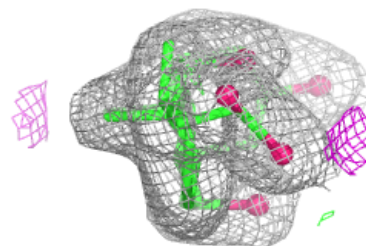
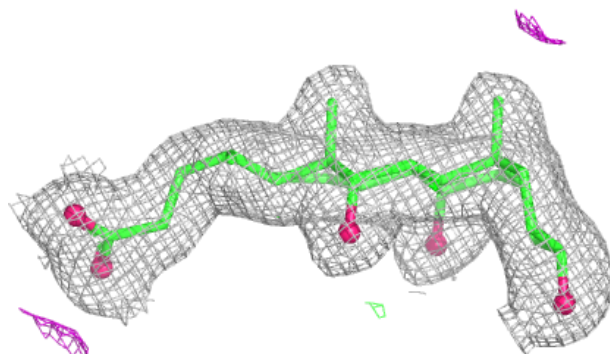
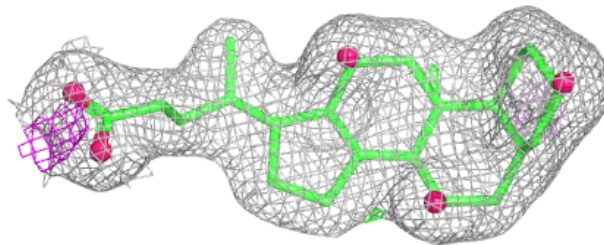


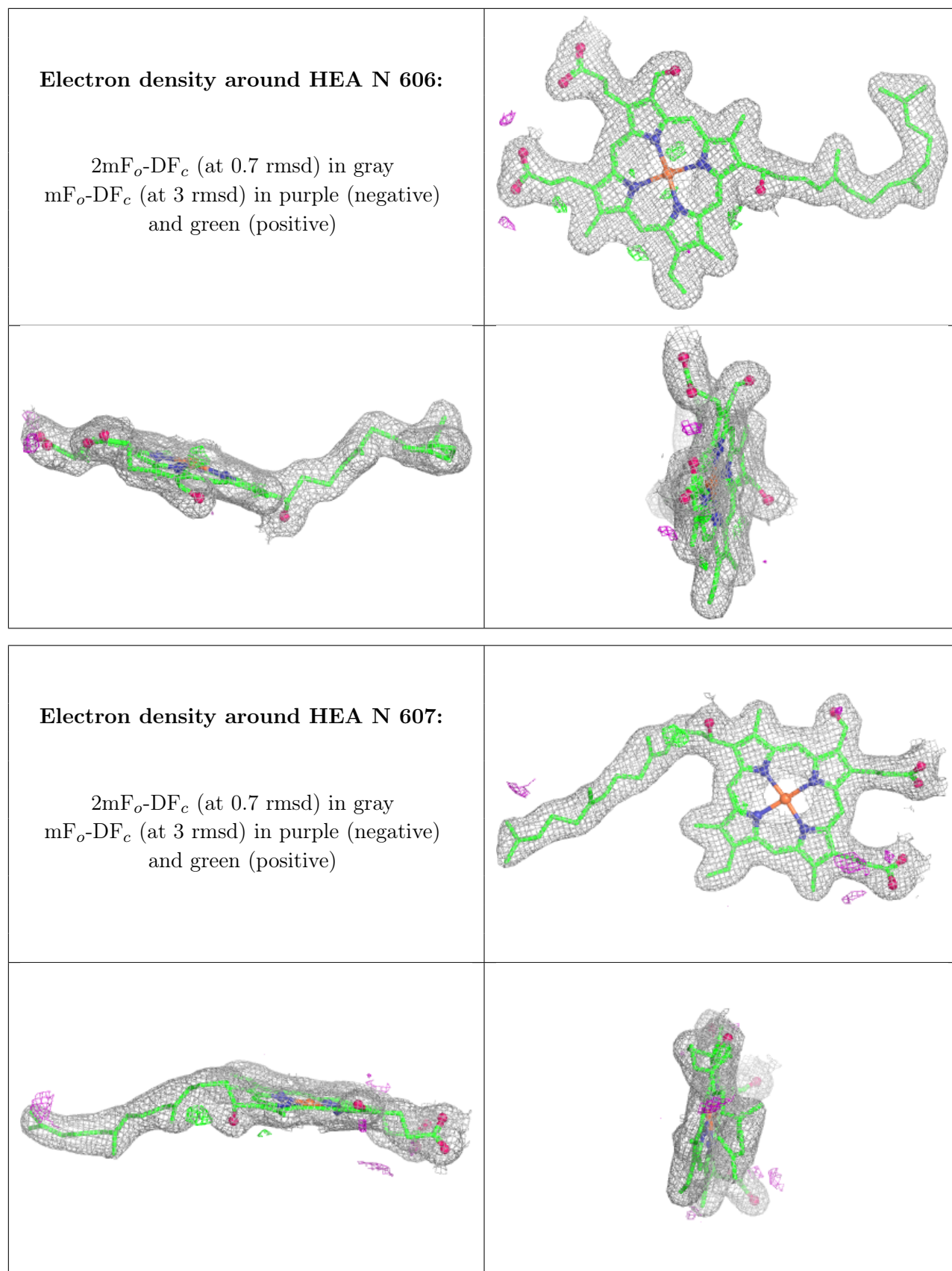
**Electron density around CHD B 302:**

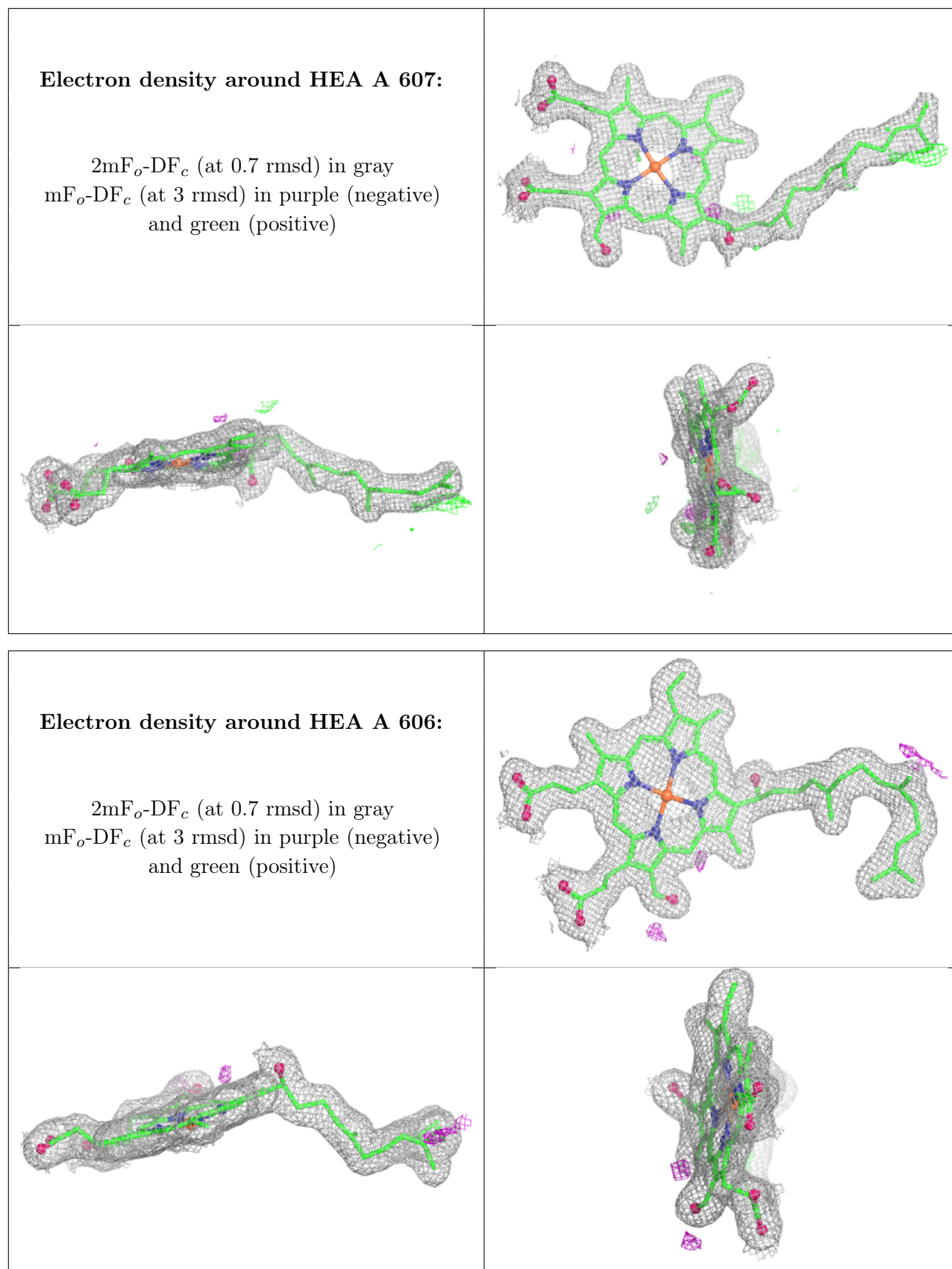
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CHD G 1305:**

$2mF_o-DF_c$  (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.