



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 10:24 PM UTC

PDB ID : 7EV7 / pdb_00007ev7
Title : Bovine heart cytochrome c oxidase in the carbon monoxide-bound fully reduced state at a 50 K
Authors : Shimada, A.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2021-05-20
Resolution : 1.70 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

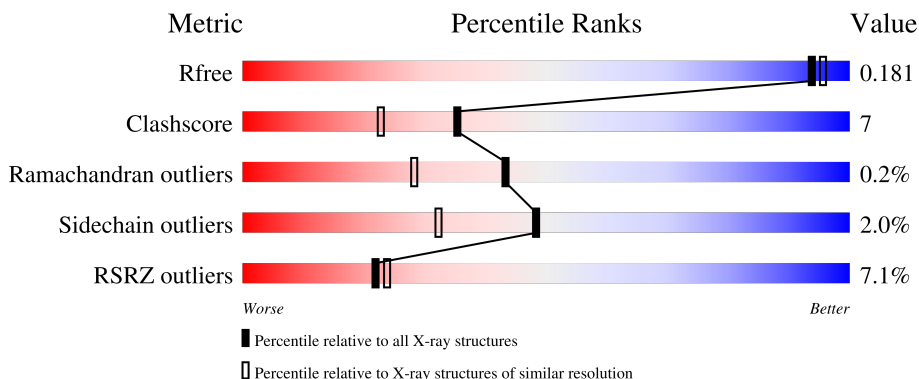
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



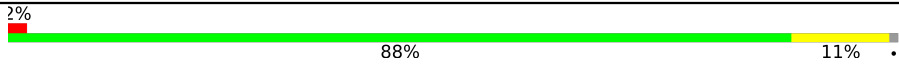
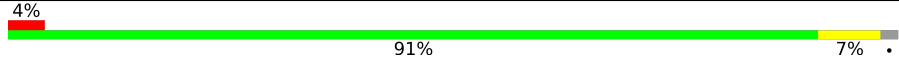
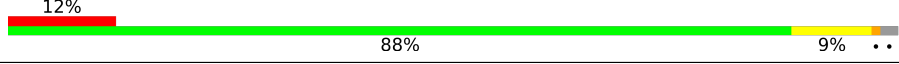
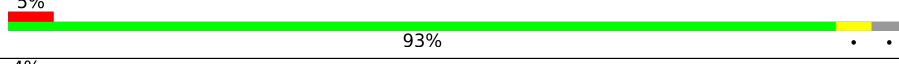
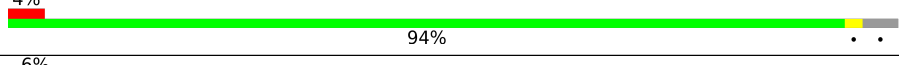
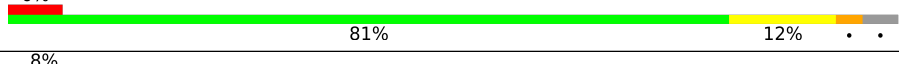


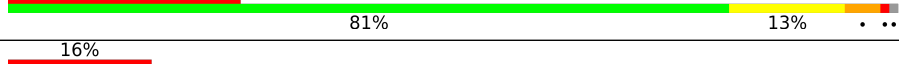


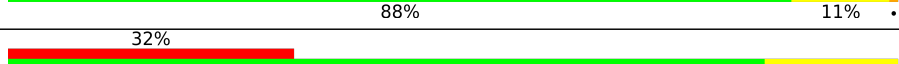

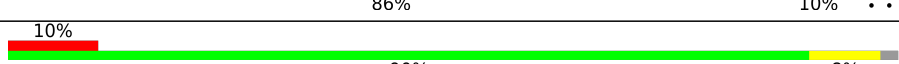
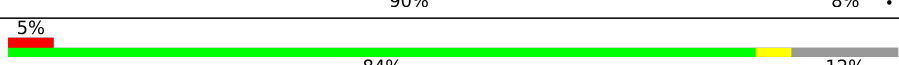
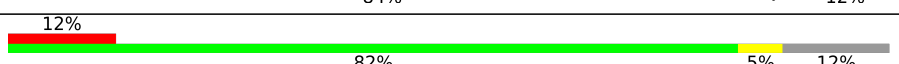
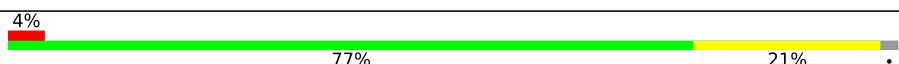
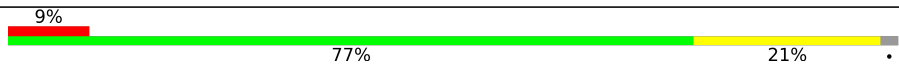
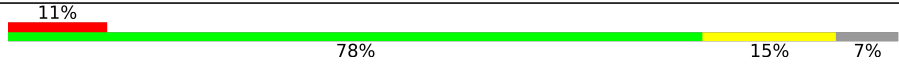


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	514	 88% 11%
1	N	514	 87% 13%
2	B	227	 82% 17%
2	O	227	 81% 19%
3	C	261	 92% 8%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	EDO	B	309	-	-	-	X
20	EDO	B	314	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	EDO	D	206	-	-	-	X
20	EDO	H	103	-	-	X	-
20	EDO	N	612	-	-	X	-
20	EDO	N	630	-	-	-	X
20	EDO	O	305	-	-	-	X
20	EDO	W	104	-	-	-	X

2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 34489 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	4124	2750	635	698	41	0	30	0
1	N	514	4116	2741	635	699	41	0	28	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	1869	1218	284	348	19	0	11	0
2	O	227	1865	1216	284	346	19	0	10	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	2131	1422	337	357	15	0	9	0
3	P	259	2141	1428	341	357	15	0	11	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	144	1214	787	202	221	4	0	5	0
4	Q	144	1206	785	199	218	4	0	3	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	94	Total	C	N	O	S	0	3	0
			723	447	129	142	5			
6	S	94	Total	C	N	O	S	0	3	0
			723	448	128	141	6			

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

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	1	0
			678	432	129	115	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	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

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

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

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

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

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

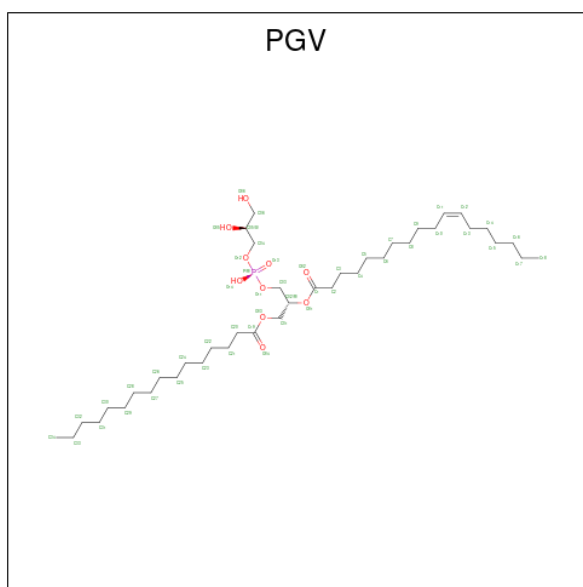
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	2	0
			388	259	66	60	3			
12	Y	46	Total	C	N	O	S	0	4	0
			394	261	66	64	3			

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

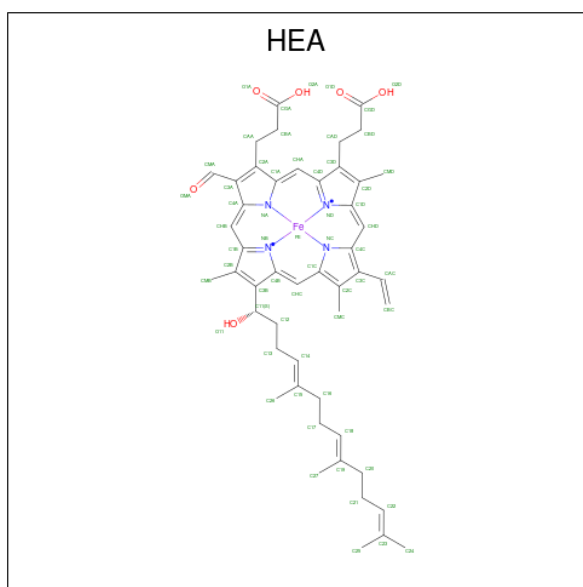
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



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

- Molecule 15 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	
15	A	1	Total	79	67	1	4	7	0	1
15	A	1	Total	60	49	1	4	6	0	0
15	N	1	Total	79	67	1	4	7	0	1
15	N	1	Total	60	49	1	4	6	0	0

- Molecule 16 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

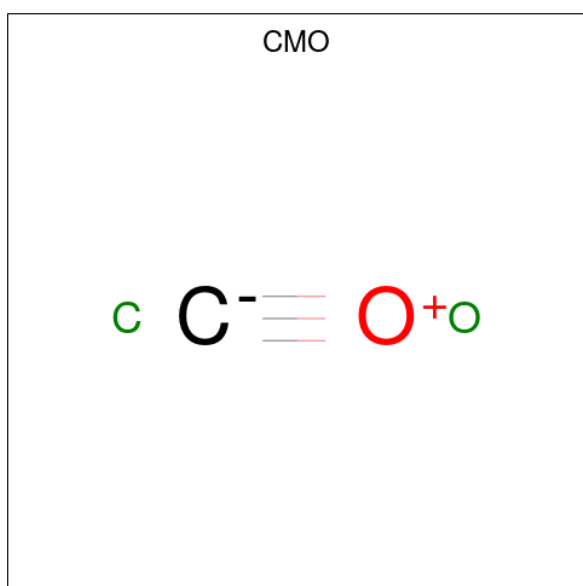
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (CCD ID: NA) (formula: Na).

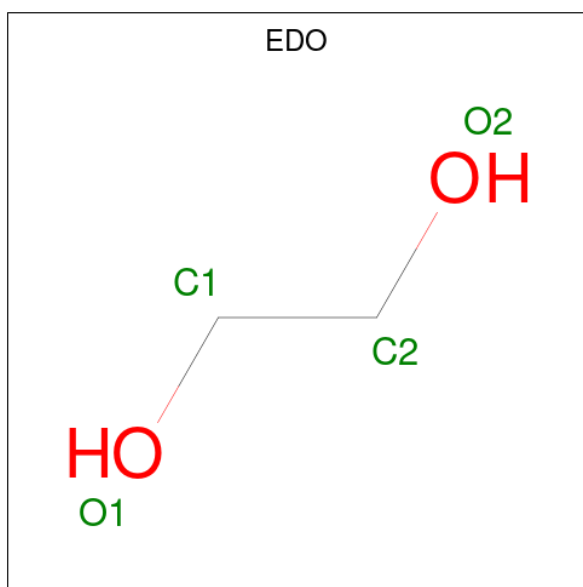
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Na	0	0
			1	1		
18	C	1	Total	Na	0	0
			1	1		
18	N	1	Total	Na	0	0
			1	1		
18	P	1	Total	Na	0	0
			1	1		

- Molecule 19 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

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



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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	H	1	Total 4	C 2	O 2	0	0
20	H	1	Total 4	C 2	O 2	0	0
20	H	1	Total 4	C 2	O 2	0	0
20	J	1	Total 4	C 2	O 2	0	0
20	J	1	Total 4	C 2	O 2	0	0
20	K	1	Total 4	C 2	O 2	0	0
20	K	1	Total 4	C 2	O 2	0	0
20	L	1	Total 4	C 2	O 2	0	0
20	L	1	Total 4	C 2	O 2	0	0
20	L	1	Total 4	C 2	O 2	0	0
20	L	1	Total 4	C 2	O 2	0	0
20	M	1	Total 4	C 2	O 2	0	0
20	M	1	Total 4	C 2	O 2	0	0
20	M	1	Total 4	C 2	O 2	0	0
20	M	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0

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

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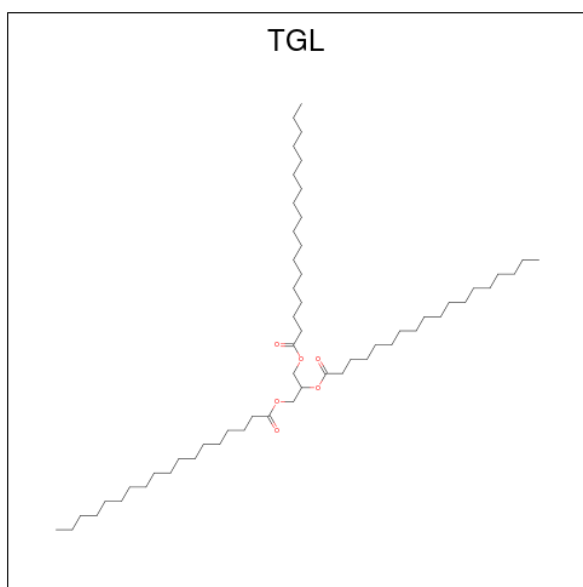
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20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

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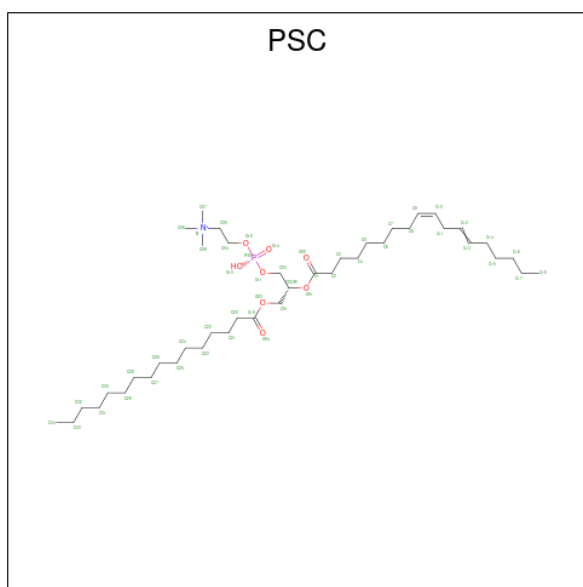
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	S	1	Total C O 4 2 2	0	0
20	S	1	Total C O 4 2 2	0	0
20	S	1	Total C O 4 2 2	0	0
20	S	1	Total C O 4 2 2	0	0
20	S	1	Total C O 4 2 2	0	0
20	S	1	Total C O 4 2 2	0	0
20	S	1	Total C O 4 2 2	0	0
20	T	1	Total C O 4 2 2	0	0
20	T	1	Total C O 4 2 2	0	0
20	U	1	Total C O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

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



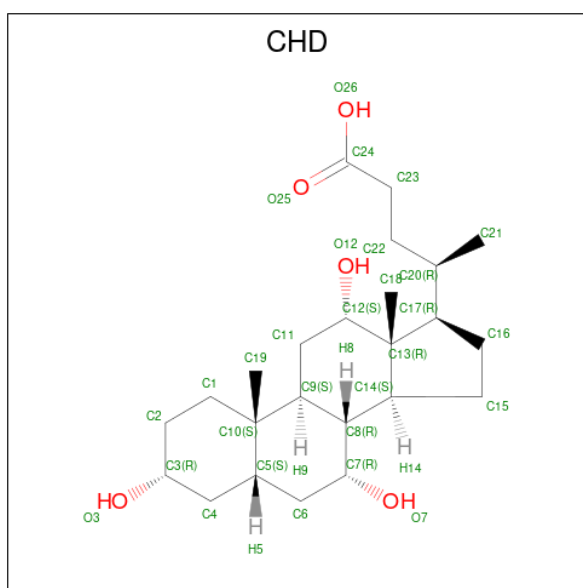
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



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

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



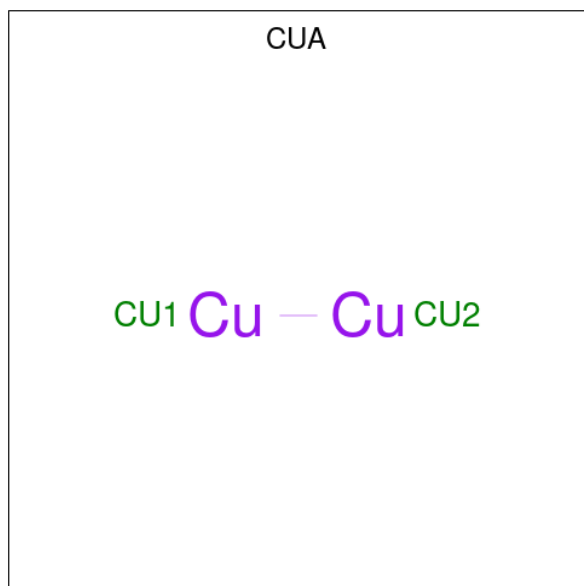
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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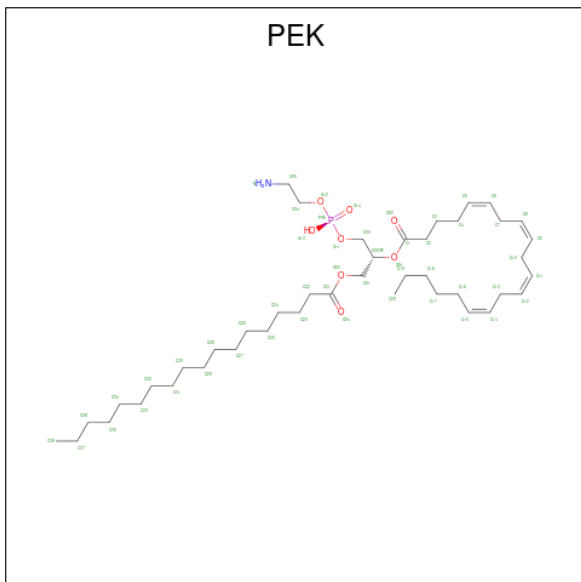
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	C	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	G	1	Total C O 29 24 5	0	0
23	J	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	W	1	Total C O 29 24 5	0	0
23	Y	1	Total C O 29 24 5	0	0

- Molecule 24 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



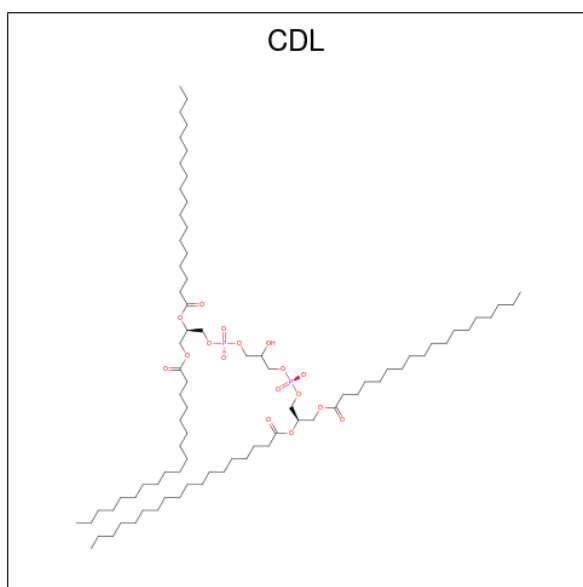
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total Cu 2 2	0	0
24	O	1	Total Cu 2 2	0	0

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



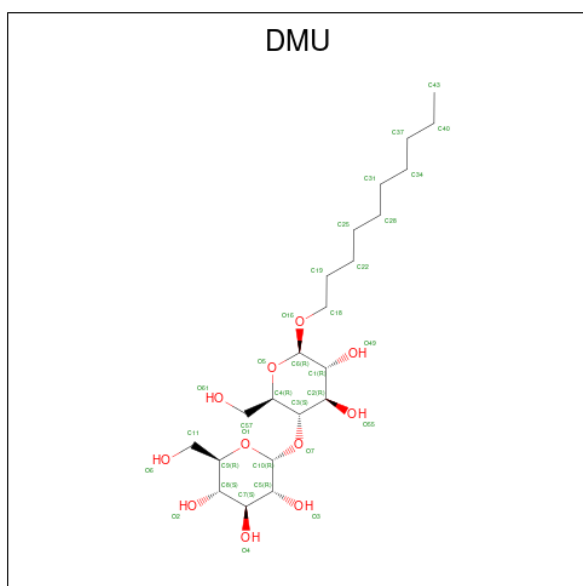
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
	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

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



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

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

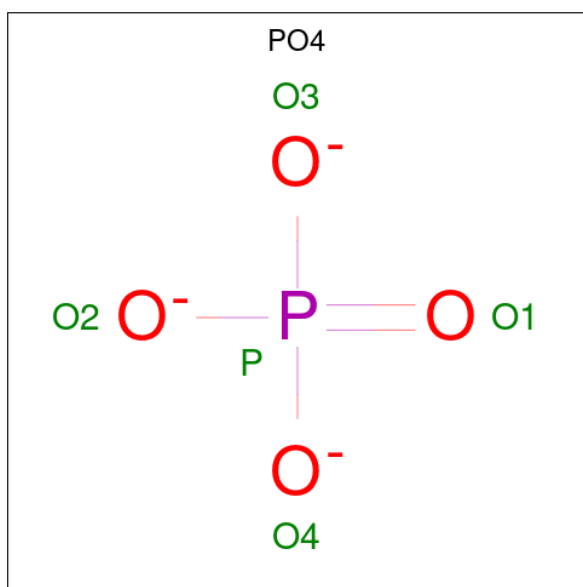


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	C	1	Total	C	O	0	0
			33	22	11		
27	C	1	Total	C	O	0	0
			33	22	11		
27	G	1	Total	C	O	0	0
			33	22	11		
27	M	1	Total	C	O	0	0
			33	22	11		
27	M	1	Total	C	O	0	0
			33	22	11		
27	P	1	Total	C	O	0	0
			33	22	11		
27	P	1	Total	C	O	0	0
			33	22	11		
27	P	1	Total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

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

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

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



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	255	Total	O	0	0
			255	255		
30	B	194	Total	O	0	2
			195	195		
30	C	142	Total	O	0	0
			142	142		
30	D	167	Total	O	0	0
			167	167		
30	E	120	Total	O	0	0
			120	120		
30	F	130	Total	O	0	0
			130	130		
30	G	67	Total	O	0	0
			67	67		
30	H	78	Total	O	0	0
			78	78		
30	I	53	Total	O	0	0
			53	53		
30	J	39	Total	O	0	0
			39	39		

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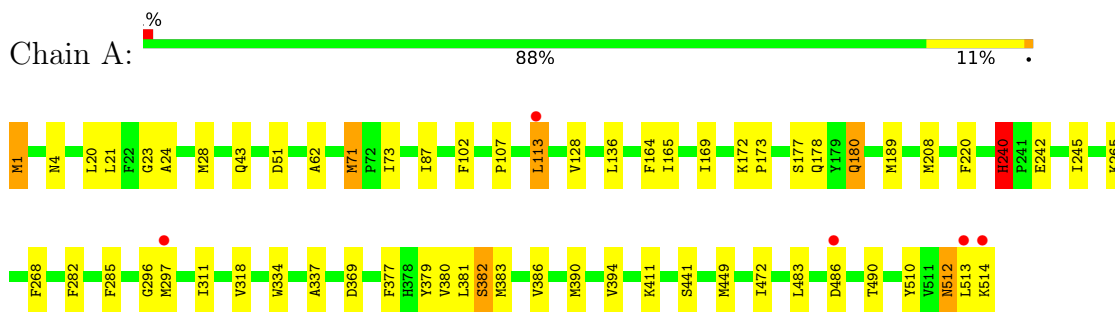
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	K	43	Total O 43 43	0	0
30	L	38	Total O 38 38	0	0
30	M	32	Total O 32 32	0	0
30	N	240	Total O 240 240	0	0
30	O	163	Total O 164 164	0	1
30	P	138	Total O 138 138	0	0
30	Q	85	Total O 85 85	0	0
30	R	96	Total O 96 96	0	0
30	S	129	Total O 129 129	0	0
30	T	65	Total O 65 65	0	0
30	U	72	Total O 72 72	0	0
30	V	40	Total O 40 40	0	0
30	W	45	Total O 45 45	0	0
30	X	33	Total O 33 33	0	0
30	Y	27	Total O 27 27	0	0
30	Z	21	Total O 21 21	0	0

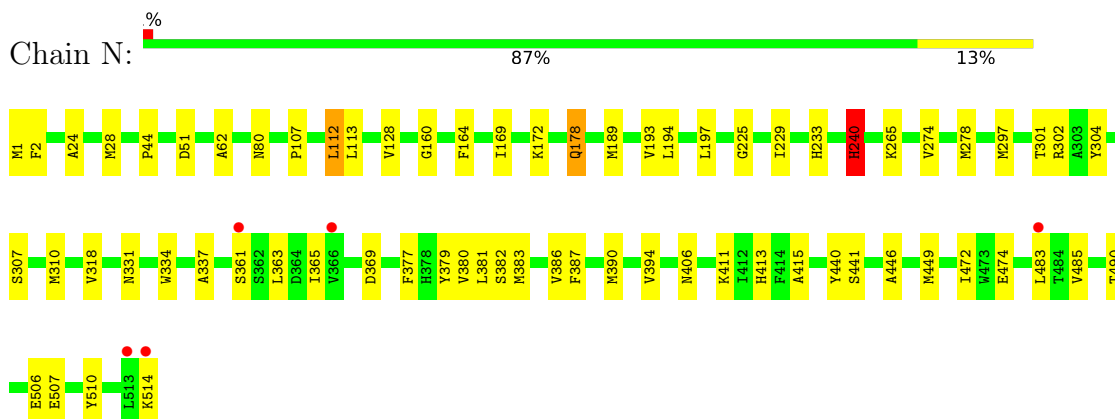
3 Residue-property plots [i](#)

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.

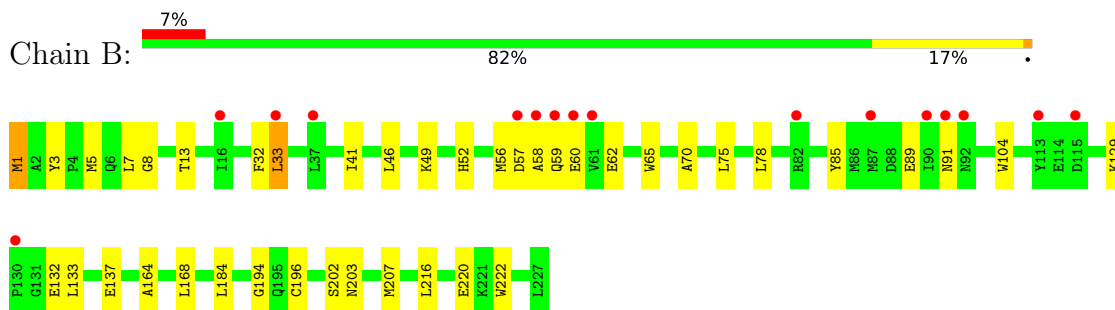
- Molecule 1: Cytochrome c oxidase subunit 1



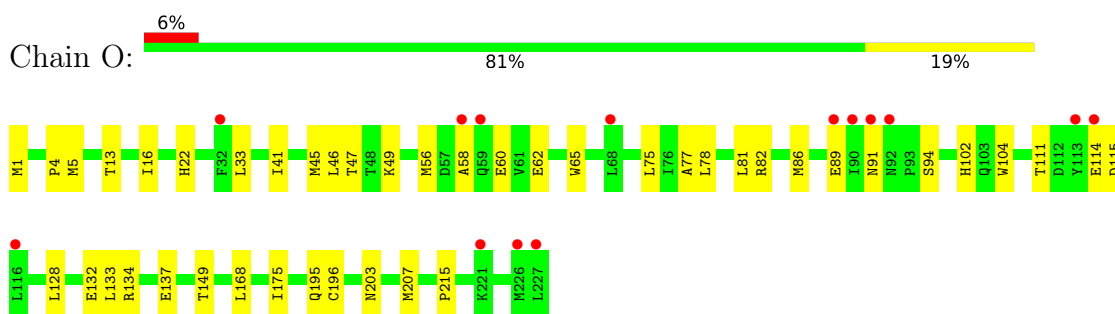
- Molecule 1: Cytochrome c oxidase subunit 1



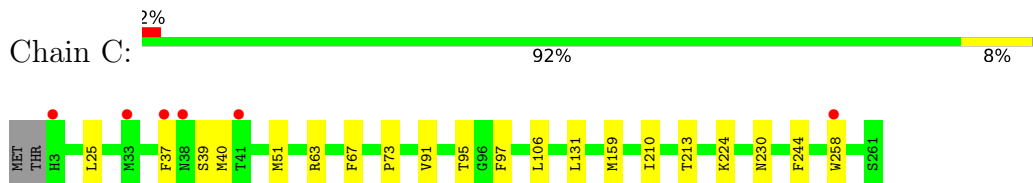
- Molecule 2: Cytochrome c oxidase subunit 2



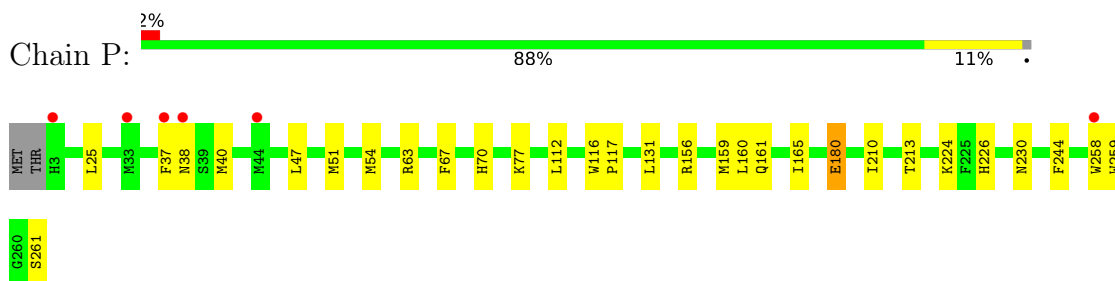
- Molecule 2: Cytochrome c oxidase subunit 2



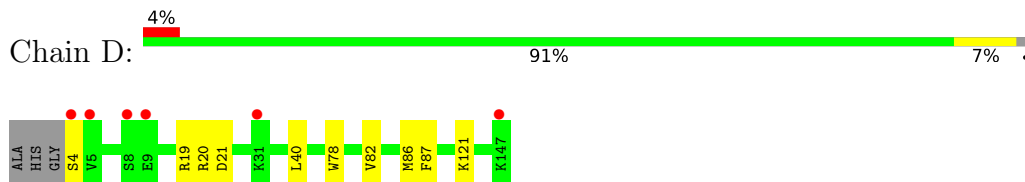
- Molecule 3: Cytochrome c oxidase subunit 3



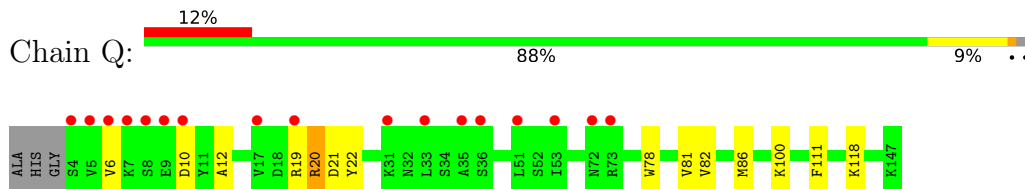
- Molecule 3: Cytochrome c oxidase subunit 3



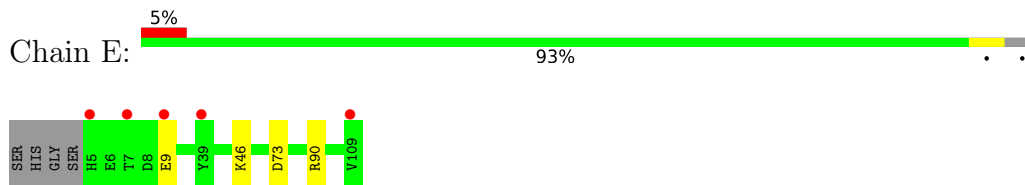
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



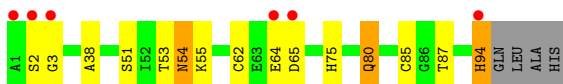
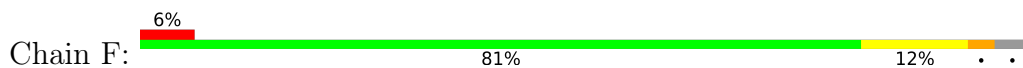
- Molecule 5: Cytochrome c oxidase subunit 5A



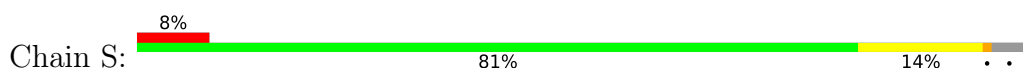
- Molecule 5: Cytochrome c oxidase subunit 5A



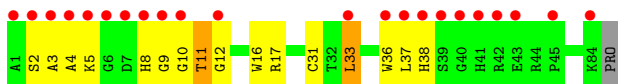
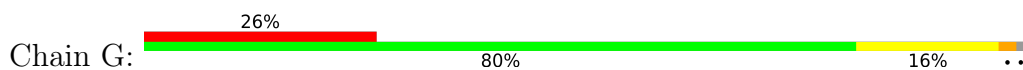
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



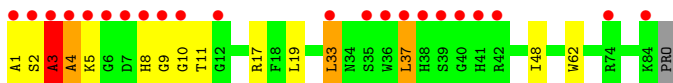
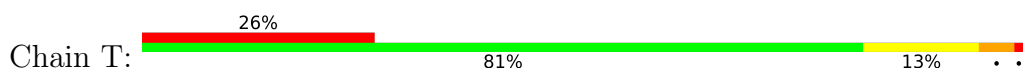
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



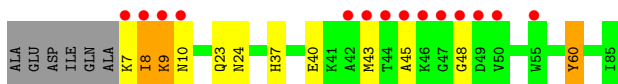
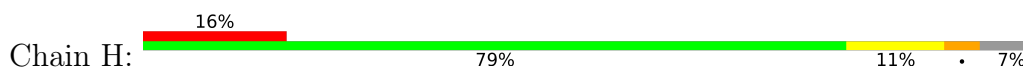
- Molecule 7: Cytochrome c oxidase subunit 6A2



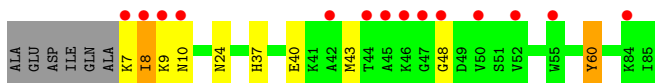
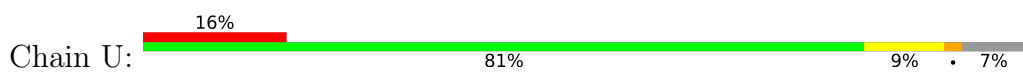
- Molecule 7: Cytochrome c oxidase subunit 6A2



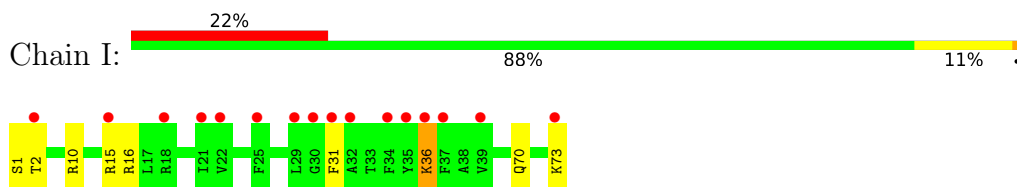
- Molecule 8: Cytochrome c oxidase subunit 6B1



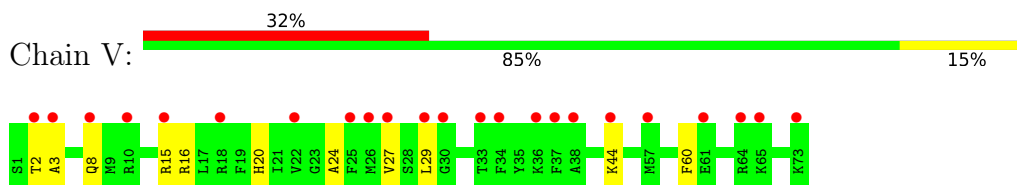
- Molecule 8: Cytochrome c oxidase subunit 6B1



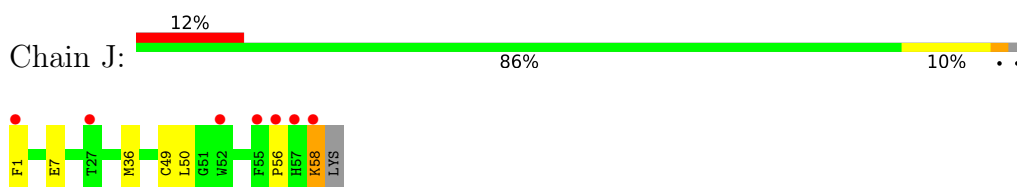
- Molecule 9: Cytochrome c oxidase subunit 6C



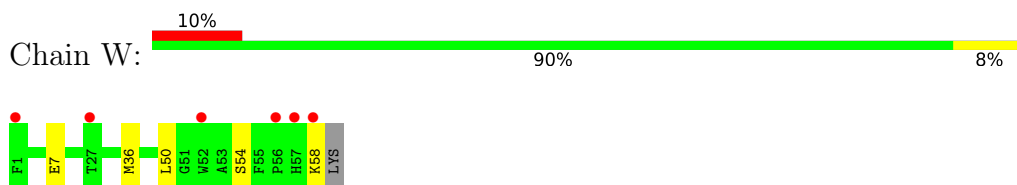
- Molecule 9: Cytochrome c oxidase subunit 6C



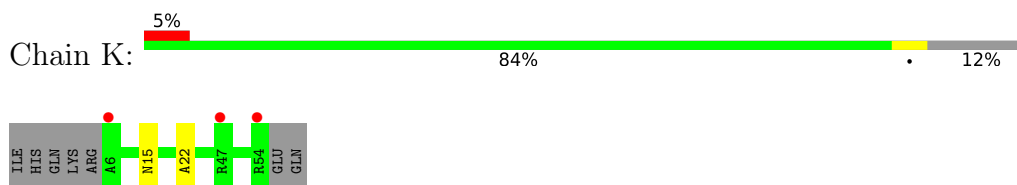
- Molecule 10: Cytochrome c oxidase subunit 7A1



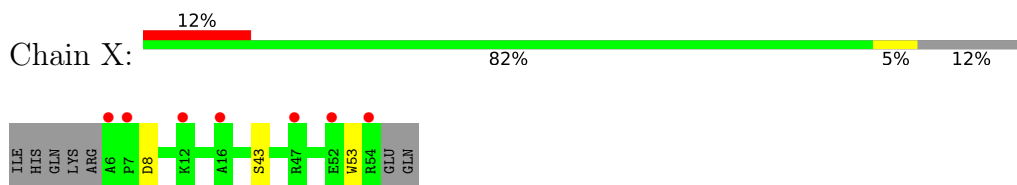
- Molecule 10: Cytochrome c oxidase subunit 7A1



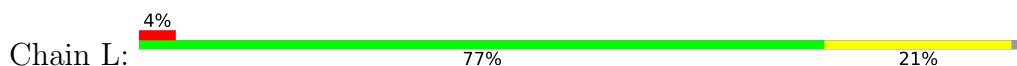
- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 11: Cytochrome c oxidase subunit 7B

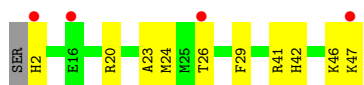
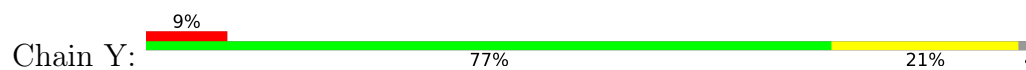


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

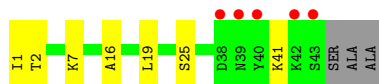
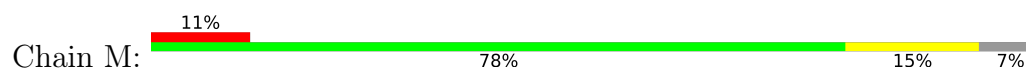




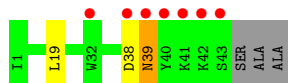
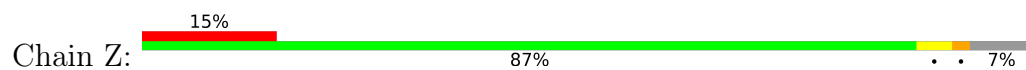
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.54Å 203.66Å 177.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.74 – 1.70 39.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.74-1.70) 99.6 (39.74-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 1.70Å)	Xtrriage
Refinement program	PHENIX (1.13-2998-000)	Depositor
R, R_{free}	0.159 , 0.178 0.163 , 0.181	Depositor DCC
R_{free} test set	35759 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtrriage
Anisotropy	0.782	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.005 for l,-k,h	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34489	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.99	0/4390	0.97	5/5989 (0.1%)
1	N	0.91	0/4371	0.90	1/5964 (0.0%)
2	B	0.85	0/1961	0.94	0/2672
2	O	0.76	0/1952	0.85	0/2660
3	C	0.88	0/2268	0.84	0/3099
3	P	0.92	0/2289	0.84	0/3126
4	D	0.76	0/1273	0.78	0/1716
4	Q	0.55	0/1258	0.64	0/1696
5	E	0.72	0/871	0.71	0/1182
5	R	0.58	0/871	0.63	0/1182
6	F	0.81	0/755	0.89	0/1026
6	S	0.76	0/755	0.81	0/1025
7	G	0.75	0/690	0.70	0/937
7	T	0.67	0/698	0.75	2/948 (0.2%)
8	H	0.79	0/682	0.81	0/921
8	U	0.66	0/682	0.73	0/921
9	I	0.63	0/605	0.71	0/802
9	V	0.51	0/605	0.62	0/802
10	J	0.63	0/471	0.66	0/636
10	W	0.54	0/471	0.63	0/636
11	K	0.70	0/398	0.71	0/546
11	X	0.52	0/398	0.55	0/546
12	L	0.82	0/412	0.77	0/551
12	Y	0.68	0/430	0.67	0/575
13	M	0.76	0/345	0.74	0/470
13	Z	0.61	0/345	0.62	0/470
All	All	0.82	0/30246	0.83	8/41098 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	MET	CG-SD-CE	-13.06	72.16	100.90
1	N	240	HIS	CA-CB-CG	-7.80	106.00	113.80
1	A	240	HIS	CA-CB-CG	-7.22	106.58	113.80
1	A	102	PHE	CA-CB-CG	-5.97	107.83	113.80
7	T	3	ALA	CA-C-N	5.60	131.78	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4124	0	4092	62	0
1	N	4116	0	4070	67	0
2	B	1869	0	1872	37	0
2	O	1865	0	1874	39	0
3	C	2131	0	2039	23	0
3	P	2141	0	2056	43	0
4	D	1214	0	1205	17	0
4	Q	1206	0	1196	16	0
5	E	852	0	845	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	852	0	845	1	0
6	F	723	0	702	9	0
6	S	723	0	705	14	0
7	G	675	0	644	20	0
7	T	678	0	644	14	0
8	H	662	0	623	8	0
8	U	662	0	623	8	0
9	I	601	0	613	7	0
9	V	601	0	613	9	0
10	J	460	0	459	6	0
10	W	460	0	459	3	0
11	K	384	0	366	4	0
11	X	384	0	366	3	0
12	L	388	0	389	14	0
12	Y	394	0	385	9	0
13	M	335	0	352	9	0
13	Z	335	0	352	2	0
14	A	102	0	152	3	0
14	C	102	0	152	4	0
14	N	102	0	152	4	0
14	P	102	0	152	8	0
15	A	139	0	112	5	0
15	N	139	0	112	3	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	C	1	0	0	0	0
18	N	1	0	0	0	0
18	P	1	0	0	1	0
19	A	4	0	0	0	0
19	N	4	0	0	0	0
20	A	76	0	114	9	0
20	B	40	0	60	10	2
20	C	28	0	42	3	0
20	D	24	0	33	3	2
20	E	12	0	18	0	0
20	F	24	0	36	1	0
20	G	20	0	30	4	0
20	H	12	0	18	5	0
20	J	8	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	K	8	0	12	2	0
20	L	16	0	24	0	0
20	M	16	0	24	3	0
20	N	84	0	126	13	0
20	O	20	0	30	2	0
20	P	44	0	66	5	0
20	Q	8	0	12	0	0
20	R	20	0	30	1	0
20	S	44	0	66	3	0
20	T	8	0	12	0	0
20	U	4	0	6	1	0
20	V	4	0	6	0	0
20	W	12	0	18	2	0
20	Y	8	0	12	0	0
21	B	63	0	110	4	0
21	D	63	0	110	9	0
21	L	63	0	110	11	0
21	N	63	0	110	2	0
21	Q	63	0	110	7	0
21	Y	63	0	110	11	0
22	B	52	0	80	10	0
22	O	52	0	80	5	0
23	B	29	0	39	0	0
23	C	87	0	117	3	0
23	G	29	0	39	1	0
23	J	29	0	39	3	0
23	P	87	0	117	9	0
23	W	29	0	39	3	0
23	Y	29	0	39	4	0
24	B	2	0	0	0	0
24	O	2	0	0	0	0
25	C	159	0	231	8	0
25	P	159	0	231	15	0
26	C	100	0	156	13	0
26	G	100	0	156	18	0
26	P	100	0	156	20	0
26	T	100	0	156	11	0
27	C	66	0	84	3	0
27	G	33	0	42	1	0
27	M	66	0	84	0	0
27	P	99	0	124	8	0
27	V	33	0	42	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	Z	66	0	84	1	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	255	0	0	7	0
30	B	195	0	0	3	2
30	C	142	0	0	1	0
30	D	167	0	0	1	2
30	E	120	0	0	1	0
30	F	130	0	0	2	0
30	G	67	0	0	1	0
30	H	78	0	0	1	0
30	I	53	0	0	1	0
30	J	39	0	0	1	0
30	K	43	0	0	0	0
30	L	38	0	0	1	0
30	M	32	0	0	0	0
30	N	240	0	0	5	0
30	O	164	0	0	3	0
30	P	138	0	0	4	0
30	Q	85	0	0	5	0
30	R	96	0	0	1	0
30	S	129	0	0	6	0
30	T	65	0	0	0	0
30	U	72	0	0	2	0
30	V	40	0	0	1	0
30	W	45	0	0	3	0
30	X	33	0	0	1	0
30	Y	27	0	0	1	0
30	Z	21	0	0	0	0
All	All	34489	0	32823	482	4

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 7.

The worst 5 of 482 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:24:ASN:HD21	20:H:103:EDO:H21	1.24	0.98
6:F:75:HIS:H	6:F:80[A]:GLN:HE22	1.12	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:178[B]:GLN:NE2	30:N:701:HOH:O	1.99	0.95
6:S:75:HIS:H	6:S:80[A]:GLN:HE22	1.14	0.93
25:P:305:PEK:H041	7:T:17:ARG:HH22	1.32	0.93

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:314:EDO:C2	20:D:206:EDO:C1[2_584]	1.49	0.71
30:B:479:HOH:O	30:D:306:HOH:O[2_584]	1.96	0.24
20:B:314:EDO:O2	20:D:206:EDO:C1[2_584]	1.97	0.23
30:B:551:HOH:O	30:D:426:HOH:O[2_584]	2.17	0.03

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	543/514 (106%)	532 (98%)	11 (2%)	0	100	100
1	N	541/514 (105%)	532 (98%)	9 (2%)	0	100	100
2	B	236/227 (104%)	231 (98%)	5 (2%)	0	100	100
2	O	235/227 (104%)	228 (97%)	7 (3%)	0	100	100
3	C	266/261 (102%)	260 (98%)	6 (2%)	0	100	100
3	P	268/261 (103%)	263 (98%)	5 (2%)	0	100	100
4	D	147/147 (100%)	144 (98%)	3 (2%)	0	100	100
4	Q	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	95/98 (97%)	94 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
7	G	81/85 (95%)	73 (90%)	7 (9%)	1 (1%)	10	2
7	T	82/85 (96%)	73 (89%)	6 (7%)	3 (4%)	2	0
8	H	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	2	0
8	U	77/85 (91%)	74 (96%)	2 (3%)	1 (1%)	9	2
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
12	Y	47/47 (100%)	46 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3616/3614 (100%)	3521 (97%)	87 (2%)	8 (0%)	43	28

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	T	4	ALA
7	G	10	GLY
8	H	8	ILE
8	H	9	LYS
7	T	3	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	455/426 (107%)	447 (98%)	8 (2%)	51	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	453/426 (106%)	445 (98%)	8 (2%)	51	36
2	B	221/210 (105%)	214 (97%)	7 (3%)	34	17
2	O	220/210 (105%)	212 (96%)	8 (4%)	31	14
3	C	233/226 (103%)	231 (99%)	2 (1%)	70	62
3	P	235/226 (104%)	231 (98%)	4 (2%)	53	38
4	D	133/129 (103%)	132 (99%)	1 (1%)	73	65
4	Q	131/129 (102%)	129 (98%)	2 (2%)	57	43
5	E	92/95 (97%)	91 (99%)	1 (1%)	65	54
5	R	92/95 (97%)	91 (99%)	1 (1%)	65	54
6	F	81/81 (100%)	75 (93%)	6 (7%)	13	3
6	S	81/81 (100%)	79 (98%)	2 (2%)	42	24
7	G	67/68 (98%)	65 (97%)	2 (3%)	36	19
7	T	68/68 (100%)	65 (96%)	3 (4%)	25	10
8	H	71/75 (95%)	69 (97%)	2 (3%)	38	21
8	U	71/75 (95%)	69 (97%)	2 (3%)	38	21
9	I	57/57 (100%)	54 (95%)	3 (5%)	20	7
9	V	57/57 (100%)	55 (96%)	2 (4%)	32	15
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	11
10	W	49/50 (98%)	47 (96%)	2 (4%)	27	11
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	41/40 (102%)	41 (100%)	0	100	100
12	Y	43/40 (108%)	39 (91%)	4 (9%)	8	2
13	M	37/38 (97%)	37 (100%)	0	100	100
13	Z	37/38 (97%)	35 (95%)	2 (5%)	20	6
All	All	3152/3082 (102%)	3078 (98%)	74 (2%)	48	27

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	S	80[A]	GLN
12	Y	47	LYS
7	T	5	LYS

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Mol	Chain	Res	Type
9	V	29	LEU
6	F	94	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
7	T	8	HIS
9	V	8	GLN
8	U	10	ASN
8	U	31	GLN
8	H	25	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
9	SAC	V	1	9	7,8,9	0.65	0	7,9,11	0.86	0
7	TPO	T	11	7	8,10,11	1.36	1 (12%)	10,14,16	0.85	0
1	FME	N	1	1	8,9,10	0.44	0	8,9,11	1.16	1 (12%)
2	FME	B	1	2	8,9,10	0.94	0	8,9,11	1.33	1 (12%)
1	FME	A	1	1	8,9,10	0.48	0	8,9,11	1.60	1 (12%)
9	SAC	I	1	9	7,8,9	0.68	0	7,9,11	1.03	1 (14%)
2	FME	O	1	2	8,9,10	0.88	0	8,9,11	0.95	0
7	TPO	G	11	7	8,10,11	1.37	1 (12%)	10,14,16	0.91	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
9	SAC	V	1	9	-	4/7/8/10	-
7	TPO	T	11	7	-	5/9/11/13	-
1	FME	N	1	1	-	2/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
9	SAC	I	1	9	-	0/7/8/10	-
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	G	11	7	-	3/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	2.94	1.59	1.50
7	G	11	TPO	P-O1P	2.93	1.59	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	C-CA-N	3.32	115.91	109.50
2	B	1	FME	O-C-CA	-2.23	119.03	124.77
1	N	1	FME	O-C-CA	-2.05	119.50	124.77
9	I	1	SAC	O-C-CA	-2.02	119.57	124.77

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 209 ligands modelled in this entry, 10 are monoatomic - leaving 199 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	EDO	S	108	-	3,3,3	0.70	0	2,2,2	0.39	0
20	EDO	M	104	-	3,3,3	0.61	0	2,2,2	0.51	0
23	CHD	G	102	-	32,32,32	0.97	0	51,51,51	1.38	7 (13%)
20	EDO	S	112	-	3,3,3	0.47	0	2,2,2	1.61	1 (50%)
20	EDO	B	306	-	3,3,3	0.77	0	2,2,2	0.38	0
20	EDO	B	313	-	3,3,3	0.53	0	2,2,2	0.40	0
26	CDL	G	101	-	99,99,99	1.41	12 (12%)	105,111,111	1.47	12 (11%)
20	EDO	B	309	-	3,3,3	0.39	0	2,2,2	0.15	0
20	EDO	R	204	-	3,3,3	0.48	0	2,2,2	0.30	0
27	DMU	V	102	-	34,34,34	0.55	1 (2%)	45,45,45	1.05	3 (6%)
26	CDL	P	308	-	99,99,99	1.43	12 (12%)	105,111,111	1.34	9 (8%)
20	EDO	K	101	-	3,3,3	0.66	0	2,2,2	0.17	0
20	EDO	F	107	-	3,3,3	0.34	0	2,2,2	0.60	0
20	EDO	A	615	-	3,3,3	0.61	0	2,2,2	0.11	0
20	EDO	O	305	-	3,3,3	0.44	0	2,2,2	0.17	0
20	EDO	P	322	-	3,3,3	0.50	0	2,2,2	0.28	0
23	CHD	C	301	-	32,32,32	1.13	4 (12%)	51,51,51	1.54	8 (15%)
20	EDO	P	321	-	3,3,3	0.56	0	2,2,2	0.53	0
20	EDO	A	623	-	3,3,3	0.57	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	D	202	-	3,3,3	0.57	0	2,2,2	0.18	0
20	EDO	A	624	-	3,3,3	0.37	0	2,2,2	0.66	0
20	EDO	L	103	-	3,3,3	0.55	0	2,2,2	0.16	0
20	EDO	S	111	-	3,3,3	0.74	0	2,2,2	0.22	0
21	TGL	B	301	-	62,62,62	1.13	3 (4%)	65,65,65	1.30	6 (9%)
20	EDO	N	613	-	3,3,3	0.41	0	2,2,2	0.50	0
20	EDO	S	110	-	3,3,3	0.60	0	2,2,2	0.69	0
20	EDO	F	106	-	3,3,3	0.86	0	2,2,2	0.46	0
20	EDO	H	102	-	3,3,3	0.50	0	2,2,2	0.21	0
20	EDO	A	617	-	3,3,3	0.65	0	2,2,2	0.12	0
20	EDO	N	623	-	3,3,3	0.49	0	2,2,2	0.41	0
20	EDO	N	629	-	3,3,3	0.38	0	2,2,2	0.39	0
14	PGV	N	609	-	50,50,50	1.03	5 (10%)	53,56,56	1.14	3 (5%)
27	DMU	Z	102	-	34,34,34	0.48	0	45,45,45	1.15	3 (6%)
20	EDO	C	317	-	3,3,3	0.37	0	2,2,2	0.05	0
20	EDO	M	105	-	3,3,3	1.15	0	2,2,2	0.62	0
20	EDO	P	317	-	3,3,3	0.64	0	2,2,2	0.19	0
20	EDO	C	316	-	3,3,3	0.87	0	2,2,2	0.57	0
20	EDO	P	320	-	3,3,3	0.44	0	2,2,2	0.34	0
20	EDO	H	101	-	3,3,3	0.40	0	2,2,2	0.56	0
20	EDO	N	617	-	3,3,3	0.30	0	2,2,2	0.82	0
21	TGL	Y	101	-	62,62,62	1.03	3 (4%)	65,65,65	1.16	4 (6%)
20	EDO	P	316	-	3,3,3	0.63	0	2,2,2	0.35	0
20	EDO	P	318	-	3,3,3	0.70	0	2,2,2	0.15	0
20	EDO	C	314	-	3,3,3	0.51	0	2,2,2	0.42	0
20	EDO	A	621	-	3,3,3	0.58	0	2,2,2	0.42	0
20	EDO	J	103	-	3,3,3	0.37	0	2,2,2	0.52	0
20	EDO	P	313	-	3,3,3	0.41	0	2,2,2	0.34	0
23	CHD	Y	104	-	32,32,32	0.86	1 (3%)	51,51,51	1.78	13 (25%)
20	EDO	D	206	20	3,3,3	0.40	0	2,2,2	0.44	0
20	EDO	Y	103	-	3,3,3	0.40	0	2,2,2	0.29	0
15	HEA	A	602[B]	-	67,67,67	1.80	18 (26%)	81,103,103	1.83	21 (25%)
20	EDO	P	312	-	3,3,3	0.43	0	2,2,2	1.02	0
20	EDO	N	612	-	3,3,3	0.51	0	2,2,2	0.65	0
20	EDO	D	205	-	3,3,3	0.65	0	2,2,2	0.35	0
20	EDO	S	105	-	3,3,3	0.50	0	2,2,2	0.18	0
20	EDO	F	105	-	3,3,3	0.50	0	2,2,2	0.17	0
24	CUA	O	302	2	0,1,1	-	-	-	-	-
19	CMO	N	607[A]	-	0,1,1	-	-	-	-	-
20	EDO	A	625	-	3,3,3	0.51	0	2,2,2	0.84	0
20	EDO	L	102	-	3,3,3	0.51	0	2,2,2	0.14	0
20	EDO	B	311	-	3,3,3	0.51	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	DMU	Z	101	-	34,34,34	0.38	0	45,45,45	0.87	2 (4%)
20	EDO	G	106	-	3,3,3	0.59	0	2,2,2	0.71	0
20	EDO	W	103	-	3,3,3	0.82	0	2,2,2	0.38	0
20	EDO	A	620	-	3,3,3	0.61	0	2,2,2	1.04	0
20	EDO	F	104	-	3,3,3	0.86	0	2,2,2	0.11	0
20	EDO	H	103	-	3,3,3	0.48	0	2,2,2	0.17	0
20	EDO	A	616	-	3,3,3	0.39	0	2,2,2	0.67	0
15	HEA	N	602[B]	-	67,67,67	1.76	21 (31%)	81,103,103	2.08	24 (29%)
20	EDO	F	103	-	3,3,3	0.41	0	2,2,2	0.21	0
20	EDO	F	102	-	3,3,3	0.94	0	2,2,2	0.59	0
29	PO4	H	104	-	4,4,4	0.97	0	6,6,6	0.39	0
20	EDO	B	314	20	3,3,3	0.44	0	2,2,2	0.43	0
20	EDO	D	207	-	3,3,3	0.46	0	2,2,2	0.79	0
21	TGL	L	101	-	62,62,62	1.06	3 (4%)	65,65,65	1.21	8 (12%)
23	CHD	C	309	-	32,32,32	0.73	0	51,51,51	1.11	4 (7%)
20	EDO	G	105	-	3,3,3	0.51	0	2,2,2	0.08	0
25	PEK	C	303	-	52,52,52	0.93	2 (3%)	55,57,57	1.32	5 (9%)
21	TGL	Q	201	-	62,62,62	1.04	3 (4%)	65,65,65	1.02	6 (9%)
20	EDO	N	622	-	3,3,3	0.52	0	2,2,2	0.55	0
20	EDO	B	310	-	3,3,3	0.42	0	2,2,2	0.29	0
20	EDO	N	619	-	3,3,3	0.52	0	2,2,2	0.20	0
20	EDO	N	624	-	3,3,3	0.59	0	2,2,2	0.32	0
14	PGV	N	601	-	50,50,50	0.93	2 (4%)	53,56,56	1.21	5 (9%)
20	EDO	V	101	-	3,3,3	0.45	0	2,2,2	0.45	0
14	PGV	P	306	-	50,50,50	0.78	1 (2%)	53,56,56	1.25	4 (7%)
20	EDO	A	619	-	3,3,3	0.36	0	2,2,2	0.86	0
14	PGV	C	307	-	50,50,50	0.96	2 (4%)	53,56,56	1.60	8 (15%)
27	DMU	P	323	-	34,34,34	0.45	0	45,45,45	0.90	3 (6%)
23	CHD	P	310	-	32,32,32	0.82	1 (3%)	51,51,51	1.87	11 (21%)
20	EDO	O	306	-	3,3,3	0.49	0	2,2,2	0.16	0
14	PGV	A	601	-	50,50,50	0.96	2 (4%)	53,56,56	1.09	4 (7%)
20	EDO	N	630	-	3,3,3	0.36	0	2,2,2	0.14	0
20	EDO	A	618	-	3,3,3	0.41	0	2,2,2	0.52	0
20	EDO	N	614	-	3,3,3	0.78	0	2,2,2	0.35	0
20	EDO	R	201	-	3,3,3	0.57	0	2,2,2	0.52	0
20	EDO	K	102	-	3,3,3	0.46	0	2,2,2	0.26	0
15	HEA	A	603	1	67,67,67	1.82	16 (23%)	81,103,103	1.92	21 (25%)
22	PSC	B	302	-	51,51,51	1.10	3 (5%)	57,59,59	1.35	7 (12%)
20	EDO	A	610	-	3,3,3	0.90	0	2,2,2	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PEK	P	303	-	52,52,52	0.94	2 (3%)	55,57,57	1.16	5 (9%)
23	CHD	P	301	-	32,32,32	0.96	2 (6%)	51,51,51	1.42	10 (19%)
27	DMU	C	319	-	34,34,34	0.47	0	45,45,45	1.06	6 (13%)
20	EDO	S	102	-	3,3,3	0.90	0	2,2,2	0.79	0
20	EDO	O	307	-	3,3,3	0.45	0	2,2,2	0.31	0
23	CHD	B	303	-	32,32,32	1.20	2 (6%)	51,51,51	1.75	11 (21%)
24	CUA	B	304	2	0,1,1	-	-	-	-	-
20	EDO	C	313	-	3,3,3	0.74	0	2,2,2	0.23	0
20	EDO	M	103	-	3,3,3	0.42	0	2,2,2	0.19	0
20	EDO	S	103	-	3,3,3	0.78	0	2,2,2	0.09	0
20	EDO	B	307	-	3,3,3	0.57	0	2,2,2	0.27	0
20	EDO	M	102	-	3,3,3	0.43	0	2,2,2	0.38	0
26	CDL	T	101	-	99,99,99	1.40	12 (12%)	105,111,111	1.12	6 (5%)
14	PGV	C	306	-	50,50,50	0.81	2 (4%)	53,56,56	0.95	3 (5%)
20	EDO	E	202	-	3,3,3	0.62	0	2,2,2	0.12	0
20	EDO	A	622	-	3,3,3	0.30	0	2,2,2	0.60	0
20	EDO	O	303	-	3,3,3	0.83	0	2,2,2	0.50	0
27	DMU	G	108	-	34,34,34	0.49	0	45,45,45	1.17	3 (6%)
20	EDO	E	203	-	3,3,3	0.52	0	2,2,2	0.54	0
14	PGV	A	608	-	50,50,50	0.89	2 (4%)	53,56,56	0.89	1 (1%)
20	EDO	S	106	-	3,3,3	0.42	0	2,2,2	0.59	0
20	EDO	Y	102	-	3,3,3	0.50	0	2,2,2	0.42	0
20	EDO	N	620	-	3,3,3	0.56	0	2,2,2	0.46	0
20	EDO	P	314	-	3,3,3	0.38	0	2,2,2	0.80	0
20	EDO	B	308	-	3,3,3	0.56	0	2,2,2	0.40	0
21	TGL	D	201	-	62,62,62	1.21	4 (6%)	65,65,65	0.95	5 (7%)
20	EDO	E	201	-	3,3,3	0.38	0	2,2,2	0.50	0
20	EDO	J	102	-	3,3,3	0.37	0	2,2,2	0.39	0
19	CMO	A	607[B]	16	0,1,1	-	-	-	-	-
29	PO4	U	102	-	4,4,4	1.02	0	6,6,6	0.43	0
15	HEA	N	602[A]	-	67,67,67	1.73	20 (29%)	81,103,103	2.22	26 (32%)
27	DMU	P	309	-	34,34,34	0.47	0	45,45,45	0.71	0
20	EDO	D	203	-	3,3,3	0.47	0	2,2,2	0.19	0
23	CHD	J	101	-	32,32,32	0.77	1 (3%)	51,51,51	1.72	13 (25%)
20	EDO	Q	202	-	3,3,3	0.39	0	2,2,2	0.38	0
20	EDO	S	107	-	3,3,3	0.46	0	2,2,2	0.39	0
26	CDL	C	308	-	99,99,99	1.41	12 (12%)	105,111,111	1.24	9 (8%)
27	DMU	C	310	-	34,34,34	0.43	0	45,45,45	0.89	1 (2%)
20	EDO	N	628	-	3,3,3	0.42	0	2,2,2	1.08	0
25	PEK	C	304	-	52,52,52	0.86	2 (3%)	55,57,57	1.07	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	N	610	-	3,3,3	1.10	0	2,2,2	0.55	0
20	EDO	S	109	-	3,3,3	0.43	0	2,2,2	0.47	0
27	DMU	P	324	-	34,34,34	0.55	0	45,45,45	0.75	1 (2%)
23	CHD	P	311	-	32,32,32	0.79	0	51,51,51	1.16	5 (9%)
20	EDO	N	616	-	3,3,3	0.50	0	2,2,2	0.43	0
23	CHD	C	311	-	32,32,32	0.85	1 (3%)	51,51,51	1.77	10 (19%)
20	EDO	G	104	-	3,3,3	0.41	0	2,2,2	0.55	0
25	PEK	P	305	-	52,52,52	0.96	2 (3%)	55,57,57	1.24	5 (9%)
20	EDO	N	611	-	3,3,3	0.64	0	2,2,2	0.58	0
20	EDO	G	107	-	3,3,3	0.70	0	2,2,2	0.18	0
20	EDO	N	615	-	3,3,3	0.49	0	2,2,2	0.41	0
20	EDO	N	627	-	3,3,3	0.41	0	2,2,2	0.52	0
20	EDO	A	627	-	3,3,3	0.82	0	2,2,2	0.49	0
20	EDO	G	103	-	3,3,3	0.52	0	2,2,2	0.26	0
20	EDO	N	621	-	3,3,3	0.56	0	2,2,2	0.28	0
20	EDO	A	613	-	3,3,3	0.69	0	2,2,2	0.40	0
20	EDO	Q	203	-	3,3,3	0.40	0	2,2,2	0.44	0
20	EDO	C	312	-	3,3,3	0.71	0	2,2,2	0.17	0
20	EDO	C	315	-	3,3,3	0.57	0	2,2,2	0.45	0
15	HEA	N	603	1	67,67,67	1.76	18 (26%)	81,103,103	1.77	23 (28%)
20	EDO	A	609	-	3,3,3	0.42	0	2,2,2	0.46	0
20	EDO	C	318	-	3,3,3	0.68	0	2,2,2	0.15	0
20	EDO	U	101	-	3,3,3	0.58	0	2,2,2	0.20	0
15	HEA	A	602[A]	-	67,67,67	1.75	18 (26%)	81,103,103	1.97	21 (25%)
20	EDO	L	105	-	3,3,3	0.54	0	2,2,2	0.33	0
22	PSC	O	301	-	51,51,51	1.11	3 (5%)	57,59,59	1.27	5 (8%)
20	EDO	A	611	-	3,3,3	0.65	0	2,2,2	0.62	0
27	DMU	M	101	-	34,34,34	0.51	0	45,45,45	1.10	4 (8%)
27	DMU	M	106	-	34,34,34	0.59	1 (2%)	45,45,45	1.21	5 (11%)
20	EDO	A	626	-	3,3,3	0.64	0	2,2,2	1.02	0
20	EDO	N	618	-	3,3,3	0.75	0	2,2,2	1.02	0
20	EDO	N	625	-	3,3,3	0.70	0	2,2,2	0.24	0
20	EDO	R	205	-	3,3,3	0.50	0	2,2,2	0.23	0
20	EDO	A	614	-	3,3,3	0.44	0	2,2,2	0.23	0
20	EDO	R	203	-	3,3,3	0.52	0	2,2,2	0.29	0
20	EDO	B	312	-	3,3,3	0.55	0	2,2,2	0.17	0
25	PEK	P	304	-	52,52,52	0.70	2 (3%)	55,57,57	1.13	5 (9%)
20	EDO	W	102	-	3,3,3	0.27	0	2,2,2	0.70	0
20	EDO	R	202	-	3,3,3	0.58	0	2,2,2	0.27	0
20	EDO	S	104	-	3,3,3	0.76	0	2,2,2	0.75	0
20	EDO	T	102	-	3,3,3	0.64	0	2,2,2	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	W	104	-	3,3,3	0.49	0	2,2,2	0.33	0
20	EDO	T	103	-	3,3,3	0.54	0	2,2,2	0.53	0
23	CHD	W	101	-	32,32,32	0.73	1 (3%)	51,51,51	1.59	7 (13%)
25	PEK	C	305	-	52,52,52	0.95	2 (3%)	55,57,57	1.20	5 (9%)
20	EDO	P	315	-	3,3,3	1.03	0	2,2,2	0.47	0
20	EDO	A	612	-	3,3,3	0.58	0	2,2,2	0.68	0
21	TGL	N	608	-	62,62,62	1.02	3 (4%)	65,65,65	1.21	4 (6%)
20	EDO	L	104	-	3,3,3	0.79	0	2,2,2	0.20	0
20	EDO	N	626	-	3,3,3	0.33	0	2,2,2	0.38	0
19	CMO	A	607[A]	-	0,1,1	-	-	-	-	-
19	CMO	N	607[B]	16	0,1,1	-	-	-	-	-
20	EDO	O	304	-	3,3,3	0.47	0	2,2,2	0.18	0
20	EDO	P	319	-	3,3,3	0.92	0	2,2,2	0.42	0
20	EDO	B	305	-	3,3,3	0.44	0	2,2,2	0.70	0
14	PGV	P	307	-	50,50,50	0.98	2 (4%)	53,56,56	1.38	8 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	S	108	-	-	1/1/1/1	-
20	EDO	M	104	-	-	1/1/1/1	-
23	CHD	G	102	-	-	2/9/74/74	0/4/4/4
20	EDO	S	112	-	-	1/1/1/1	-
20	EDO	B	306	-	-	0/1/1/1	-
20	EDO	B	313	-	-	1/1/1/1	-
26	CDL	G	101	-	-	29/110/110/110	-
20	EDO	B	309	-	-	0/1/1/1	-
20	EDO	R	204	-	-	1/1/1/1	-
27	DMU	V	102	-	-	11/19/59/59	0/2/2/2
26	CDL	P	308	-	-	34/110/110/110	-
20	EDO	K	101	-	-	0/1/1/1	-
20	EDO	F	107	-	-	1/1/1/1	-
20	EDO	A	615	-	-	0/1/1/1	-
20	EDO	O	305	-	-	1/1/1/1	-
20	EDO	P	322	-	-	1/1/1/1	-
23	CHD	C	301	-	-	1/9/74/74	0/4/4/4
20	EDO	P	321	-	-	1/1/1/1	-
20	EDO	A	623	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	D	202	-	-	1/1/1/1	-
20	EDO	A	624	-	-	0/1/1/1	-
20	EDO	L	103	-	-	0/1/1/1	-
20	EDO	S	111	-	-	1/1/1/1	-
21	TGL	B	301	-	-	20/65/65/65	-
20	EDO	N	613	-	-	0/1/1/1	-
20	EDO	S	110	-	-	0/1/1/1	-
20	EDO	F	106	-	-	0/1/1/1	-
20	EDO	H	102	-	-	0/1/1/1	-
20	EDO	A	617	-	-	1/1/1/1	-
20	EDO	N	623	-	-	1/1/1/1	-
20	EDO	N	629	-	-	1/1/1/1	-
14	PGV	N	609	-	-	5/55/55/55	-
27	DMU	Z	102	-	-	9/19/59/59	0/2/2/2
20	EDO	C	317	-	-	0/1/1/1	-
20	EDO	M	105	-	-	1/1/1/1	-
20	EDO	P	317	-	-	0/1/1/1	-
20	EDO	C	316	-	-	0/1/1/1	-
20	EDO	P	320	-	-	0/1/1/1	-
20	EDO	H	101	-	-	0/1/1/1	-
20	EDO	N	617	-	-	0/1/1/1	-
21	TGL	Y	101	-	-	30/65/65/65	-
20	EDO	P	316	-	-	1/1/1/1	-
20	EDO	P	318	-	-	0/1/1/1	-
20	EDO	C	314	-	-	0/1/1/1	-
20	EDO	A	621	-	-	0/1/1/1	-
20	EDO	J	103	-	-	1/1/1/1	-
20	EDO	P	313	-	-	1/1/1/1	-
23	CHD	Y	104	-	-	7/9/74/74	0/4/4/4
20	EDO	D	206	20	-	0/1/1/1	-
20	EDO	Y	103	-	-	0/1/1/1	-
15	HEA	A	602[B]	-	-	5/36/76/76	-
20	EDO	P	312	-	-	0/1/1/1	-
20	EDO	N	612	-	-	1/1/1/1	-
20	EDO	D	205	-	-	1/1/1/1	-
20	EDO	S	105	-	-	0/1/1/1	-
20	EDO	F	105	-	-	0/1/1/1	-
20	EDO	A	625	-	-	0/1/1/1	-
20	EDO	L	102	-	-	1/1/1/1	-
20	EDO	B	311	-	-	0/1/1/1	-
27	DMU	Z	101	-	-	2/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	G	106	-	-	0/1/1/1	-
20	EDO	W	103	-	-	1/1/1/1	-
20	EDO	A	620	-	-	1/1/1/1	-
20	EDO	F	104	-	-	0/1/1/1	-
20	EDO	H	103	-	-	0/1/1/1	-
20	EDO	A	616	-	-	0/1/1/1	-
15	HEA	N	602[B]	-	-	4/36/76/76	-
20	EDO	F	103	-	-	0/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
20	EDO	B	314	20	-	0/1/1/1	-
20	EDO	D	207	-	-	0/1/1/1	-
21	TGL	L	101	-	-	29/65/65/65	-
23	CHD	C	309	-	-	5/9/74/74	0/4/4/4
20	EDO	G	105	-	-	0/1/1/1	-
25	PEK	C	303	-	-	21/56/56/56	-
21	TGL	Q	201	-	-	21/65/65/65	-
20	EDO	N	622	-	-	1/1/1/1	-
20	EDO	B	310	-	-	0/1/1/1	-
20	EDO	N	619	-	-	0/1/1/1	-
20	EDO	N	624	-	-	1/1/1/1	-
14	PGV	N	601	-	-	20/55/55/55	-
20	EDO	V	101	-	-	0/1/1/1	-
14	PGV	P	306	-	-	8/55/55/55	-
20	EDO	A	619	-	-	0/1/1/1	-
14	PGV	C	307	-	-	12/55/55/55	-
27	DMU	P	323	-	-	3/19/59/59	0/2/2/2
23	CHD	P	310	-	-	1/9/74/74	0/4/4/4
20	EDO	O	306	-	-	1/1/1/1	-
14	PGV	A	601	-	-	11/55/55/55	-
20	EDO	N	630	-	-	0/1/1/1	-
20	EDO	A	618	-	-	0/1/1/1	-
20	EDO	N	614	-	-	0/1/1/1	-
20	EDO	R	201	-	-	0/1/1/1	-
20	EDO	K	102	-	-	0/1/1/1	-
15	HEA	A	603	1	-	4/36/76/76	-
22	PSC	B	302	-	-	20/55/55/55	-
20	EDO	A	610	-	-	0/1/1/1	-
25	PEK	P	303	-	-	18/56/56/56	-
23	CHD	P	301	-	-	2/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DMU	C	319	-	-	9/19/59/59	0/2/2/2
20	EDO	S	102	-	-	0/1/1/1	-
20	EDO	O	307	-	-	0/1/1/1	-
23	CHD	B	303	-	-	2/9/74/74	0/4/4/4
20	EDO	C	313	-	-	0/1/1/1	-
20	EDO	M	103	-	-	0/1/1/1	-
20	EDO	S	103	-	-	0/1/1/1	-
20	EDO	B	307	-	-	1/1/1/1	-
20	EDO	M	102	-	-	0/1/1/1	-
26	CDL	T	101	-	-	34/110/110/110	-
14	PGV	C	306	-	-	10/55/55/55	-
20	EDO	E	202	-	-	0/1/1/1	-
20	EDO	A	622	-	-	0/1/1/1	-
20	EDO	O	303	-	-	0/1/1/1	-
27	DMU	G	108	-	-	6/19/59/59	0/2/2/2
20	EDO	E	203	-	-	0/1/1/1	-
14	PGV	A	608	-	-	8/55/55/55	-
20	EDO	S	106	-	-	0/1/1/1	-
20	EDO	Y	102	-	-	0/1/1/1	-
20	EDO	N	620	-	-	0/1/1/1	-
20	EDO	P	314	-	-	0/1/1/1	-
20	EDO	B	308	-	-	0/1/1/1	-
21	TGL	D	201	-	-	19/65/65/65	-
20	EDO	E	201	-	-	0/1/1/1	-
20	EDO	J	102	-	-	0/1/1/1	-
15	HEA	N	602[A]	-	-	3/36/76/76	-
27	DMU	P	309	-	-	5/19/59/59	0/2/2/2
20	EDO	D	203	-	-	0/1/1/1	-
23	CHD	J	101	-	-	9/9/74/74	0/4/4/4
20	EDO	Q	202	-	-	1/1/1/1	-
20	EDO	S	107	-	-	1/1/1/1	-
26	CDL	C	308	-	-	34/110/110/110	-
27	DMU	C	310	-	-	4/19/59/59	0/2/2/2
20	EDO	N	628	-	-	1/1/1/1	-
25	PEK	C	304	-	-	12/56/56/56	-
20	EDO	N	610	-	-	0/1/1/1	-
20	EDO	S	109	-	-	0/1/1/1	-
27	DMU	P	324	-	-	13/19/59/59	0/2/2/2
23	CHD	P	311	-	-	5/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	616	-	-	1/1/1/1	-
23	CHD	C	311	-	-	1/9/74/74	0/4/4/4
20	EDO	G	104	-	-	0/1/1/1	-
20	EDO	N	611	-	-	0/1/1/1	-
20	EDO	G	107	-	-	0/1/1/1	-
20	EDO	N	615	-	-	0/1/1/1	-
20	EDO	N	627	-	-	0/1/1/1	-
20	EDO	A	627	-	-	0/1/1/1	-
20	EDO	G	103	-	-	1/1/1/1	-
20	EDO	N	621	-	-	0/1/1/1	-
20	EDO	A	613	-	-	0/1/1/1	-
20	EDO	Q	203	-	-	1/1/1/1	-
20	EDO	C	312	-	-	0/1/1/1	-
20	EDO	C	315	-	-	0/1/1/1	-
15	HEA	N	603	1	-	5/36/76/76	-
20	EDO	A	609	-	-	1/1/1/1	-
20	EDO	C	318	-	-	0/1/1/1	-
20	EDO	U	101	-	-	0/1/1/1	-
15	HEA	A	602[A]	-	-	7/36/76/76	-
20	EDO	L	105	-	-	0/1/1/1	-
22	PSC	O	301	-	-	19/55/55/55	-
20	EDO	A	611	-	-	0/1/1/1	-
27	DMU	M	101	-	-	7/19/59/59	0/2/2/2
27	DMU	M	106	-	-	7/19/59/59	0/2/2/2
20	EDO	A	626	-	-	1/1/1/1	-
20	EDO	N	618	-	-	1/1/1/1	-
20	EDO	N	625	-	-	1/1/1/1	-
20	EDO	R	205	-	-	0/1/1/1	-
20	EDO	A	614	-	-	0/1/1/1	-
20	EDO	R	203	-	-	0/1/1/1	-
20	EDO	B	312	-	-	0/1/1/1	-
25	PEK	P	304	-	-	9/56/56/56	-
20	EDO	W	102	-	-	1/1/1/1	-
20	EDO	R	202	-	-	0/1/1/1	-
20	EDO	S	104	-	-	0/1/1/1	-
20	EDO	T	102	-	-	0/1/1/1	-
20	EDO	W	104	-	-	1/1/1/1	-
20	EDO	T	103	-	-	1/1/1/1	-
23	CHD	W	101	-	-	8/9/74/74	0/4/4/4
25	PEK	C	305	-	-	19/56/56/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	P	315	-	-	0/1/1/1	-
20	EDO	A	612	-	-	0/1/1/1	-
21	TGL	N	608	-	-	19/65/65/65	-
20	EDO	L	104	-	-	1/1/1/1	-
20	EDO	N	626	-	-	0/1/1/1	-
20	EDO	P	319	-	-	0/1/1/1	-
25	PEK	P	305	-	-	21/56/56/56	-
20	EDO	O	304	-	-	0/1/1/1	-
20	EDO	B	305	-	-	0/1/1/1	-
14	PGV	P	307	-	-	9/55/55/55	-

The worst 5 of 229 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	201	TGL	OG2-CB1	5.05	1.48	1.34
21	B	301	TGL	OG3-CC1	4.92	1.47	1.33
21	B	301	TGL	OG1-CA1	4.84	1.47	1.33
26	G	101	CDL	OA8-CA7	4.63	1.46	1.33
14	A	601	PGV	O03-C19	4.61	1.46	1.33

The worst 5 of 413 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	602[A]	HEA	C13-C12-C11	-7.80	101.93	114.39
23	P	310	CHD	C13-C14-C8	-6.52	106.46	114.72
15	A	602[A]	HEA	C13-C12-C11	-6.15	104.56	114.39
15	N	602[A]	HEA	C2B-C1B-NB	6.12	116.97	109.90
15	N	602[B]	HEA	C2B-C1B-NB	6.12	116.97	109.90

There are no chirality outliers.

5 of 679 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601	PGV	O04-C19-O03-C01
14	A	601	PGV	C20-C19-O03-C01
14	C	307	PGV	C04-O12-P-O11
14	C	307	PGV	C04-O12-P-O13
14	C	307	PGV	O04-C19-O03-C01

There are no ring outliers.

90 monomers are involved in 269 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	M	104	EDO	2	0
23	G	102	CHD	1	0
26	G	101	CDL	18	0
20	B	309	EDO	2	0
27	V	102	DMU	4	0
26	P	308	CDL	20	0
20	A	623	EDO	1	0
20	D	202	EDO	1	0
20	A	624	EDO	1	0
21	B	301	TGL	4	0
20	H	102	EDO	1	0
20	N	623	EDO	1	0
14	N	609	PGV	1	0
27	Z	102	DMU	1	0
20	C	317	EDO	2	0
20	C	316	EDO	1	0
20	P	320	EDO	1	0
21	Y	101	TGL	11	0
20	J	103	EDO	1	0
23	Y	104	CHD	4	0
20	D	206	EDO	0	2
20	N	612	EDO	5	0
20	D	205	EDO	1	0
20	B	311	EDO	1	0
20	A	620	EDO	1	0
20	H	103	EDO	4	0
20	F	103	EDO	1	0
20	B	314	EDO	0	2
20	D	207	EDO	1	0
21	L	101	TGL	11	0
23	C	309	CHD	1	0
25	C	303	PEK	3	0
21	Q	201	TGL	7	0
20	B	310	EDO	3	0
20	N	619	EDO	1	0
14	N	601	PGV	3	0
14	P	306	PGV	5	0
20	A	619	EDO	1	0
14	C	307	PGV	2	0
27	P	323	DMU	1	0
23	P	310	CHD	7	0
20	O	306	EDO	2	0
14	A	601	PGV	3	0

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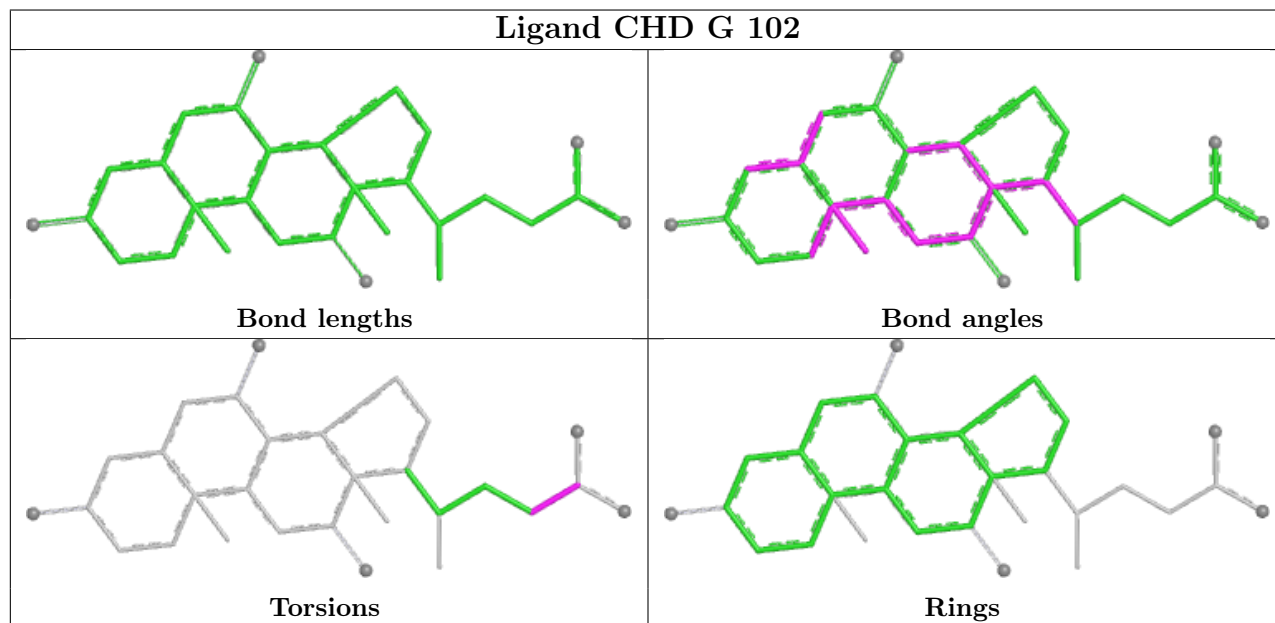
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	N	630	EDO	3	0
20	K	102	EDO	2	0
15	A	603	HEA	2	0
22	B	302	PSC	10	0
25	P	303	PEK	3	0
27	C	319	DMU	1	0
20	M	103	EDO	1	0
20	S	103	EDO	1	0
26	T	101	CDL	11	0
14	C	306	PGV	2	0
27	G	108	DMU	1	0
20	P	314	EDO	1	0
20	B	308	EDO	1	0
21	D	201	TGL	9	0
20	J	102	EDO	1	0
15	N	602[A]	HEA	2	0
27	P	309	DMU	3	0
23	J	101	CHD	3	0
20	S	107	EDO	2	0
26	C	308	CDL	13	0
27	C	310	DMU	2	0
25	C	304	PEK	1	0
27	P	324	DMU	4	0
23	P	311	CHD	2	0
23	C	311	CHD	2	0
20	G	104	EDO	2	0
25	P	305	PEK	9	0
20	G	107	EDO	1	0
20	A	627	EDO	1	0
20	G	103	EDO	1	0
15	N	603	HEA	1	0
20	A	609	EDO	3	0
20	U	101	EDO	1	0
15	A	602[A]	HEA	3	0
22	O	301	PSC	5	0
20	N	618	EDO	3	0
20	A	614	EDO	1	0
20	R	203	EDO	1	0
20	B	312	EDO	3	0
25	P	304	PEK	3	0
20	W	104	EDO	2	0
23	W	101	CHD	3	0

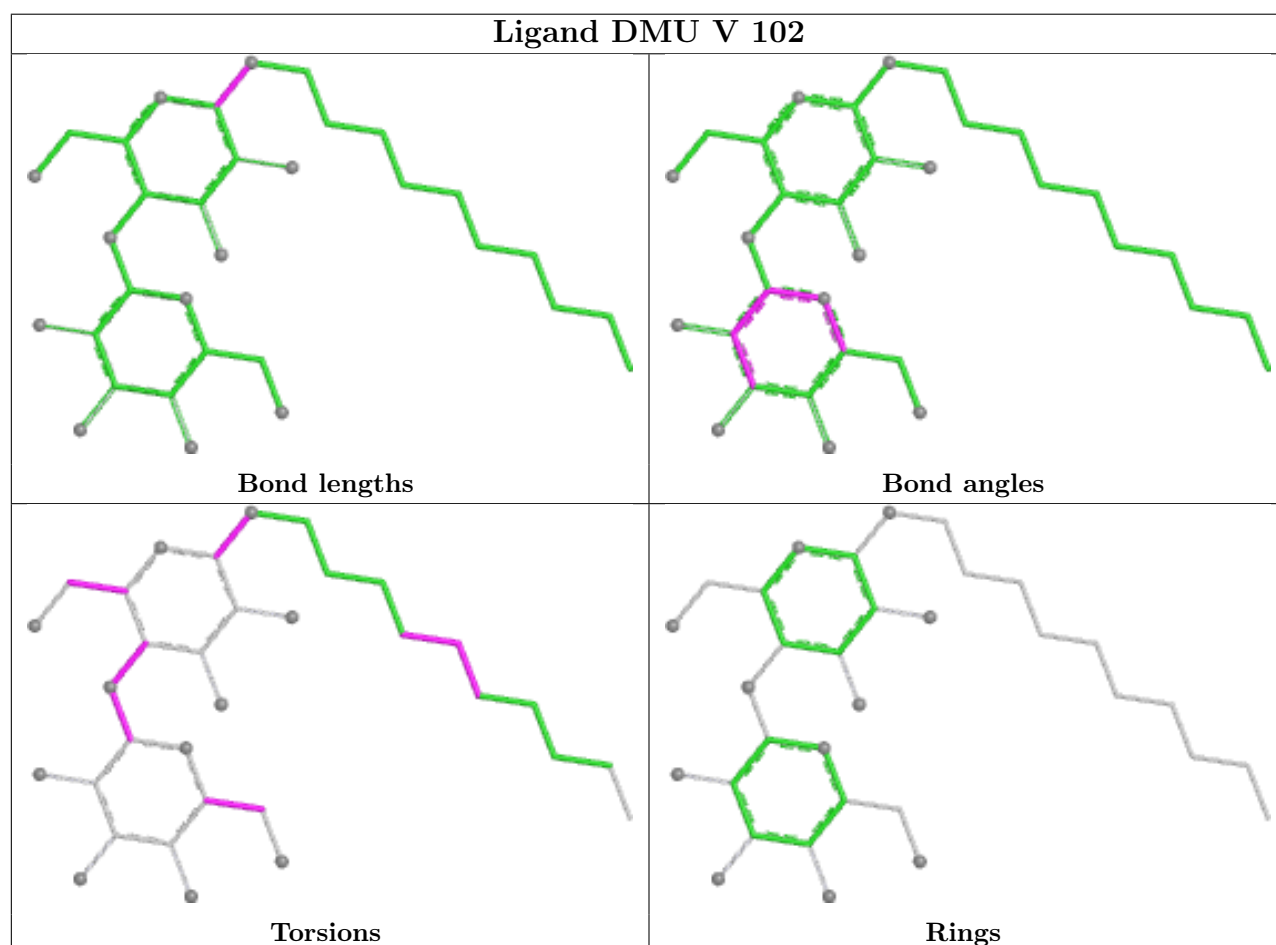
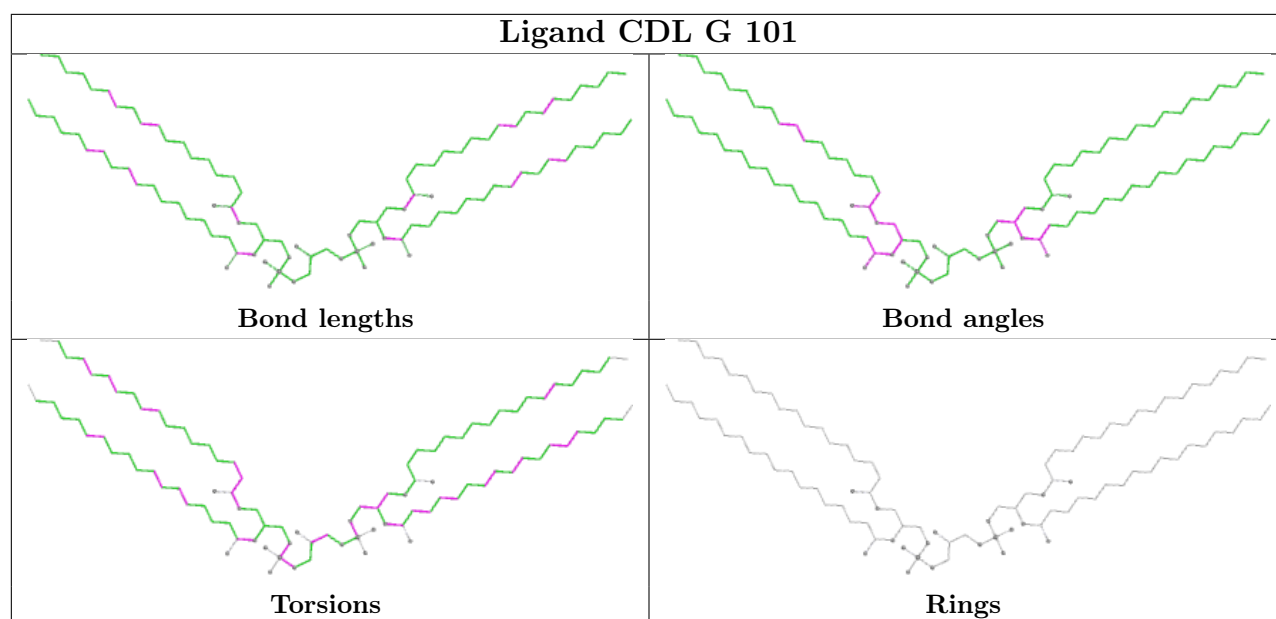
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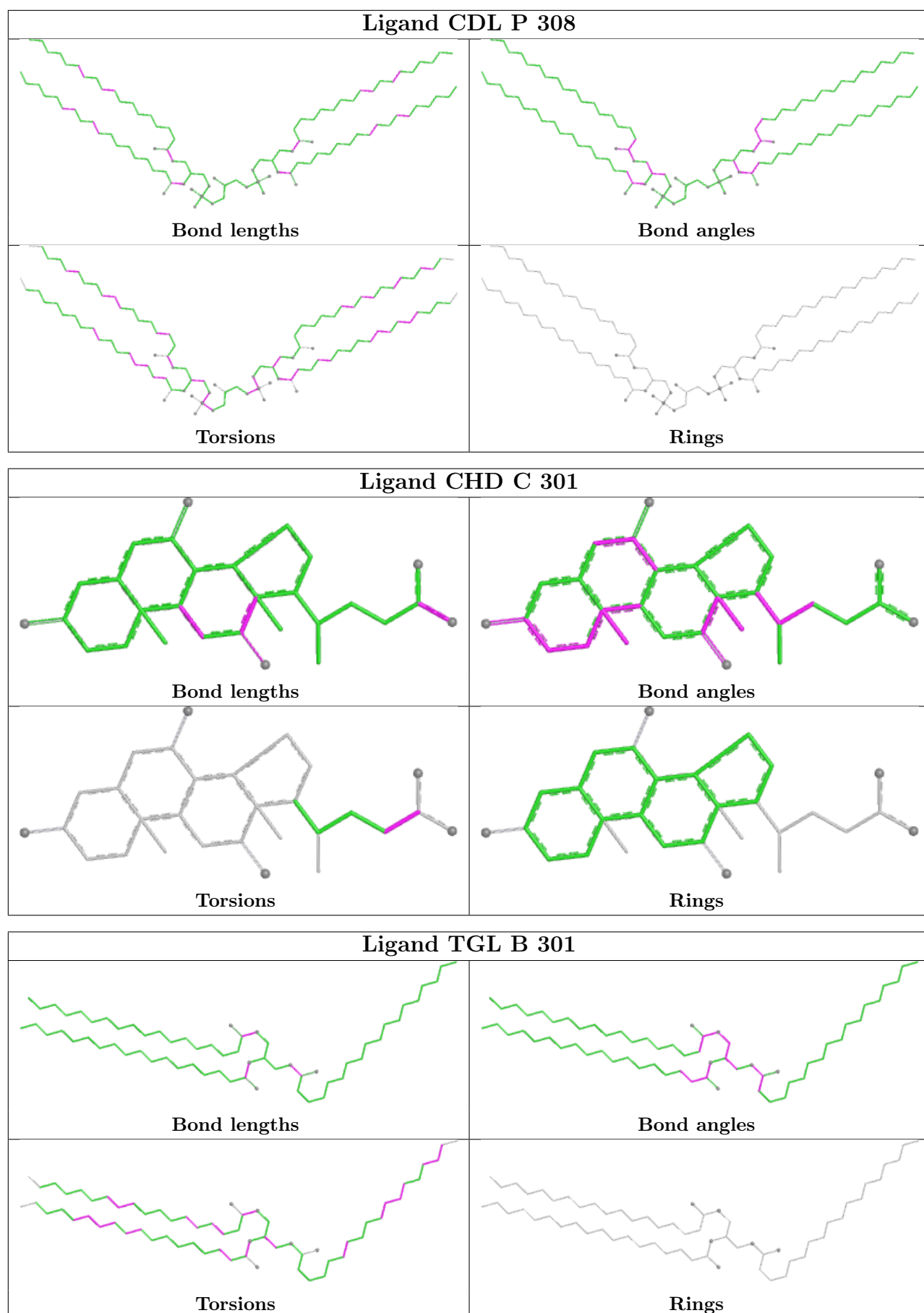
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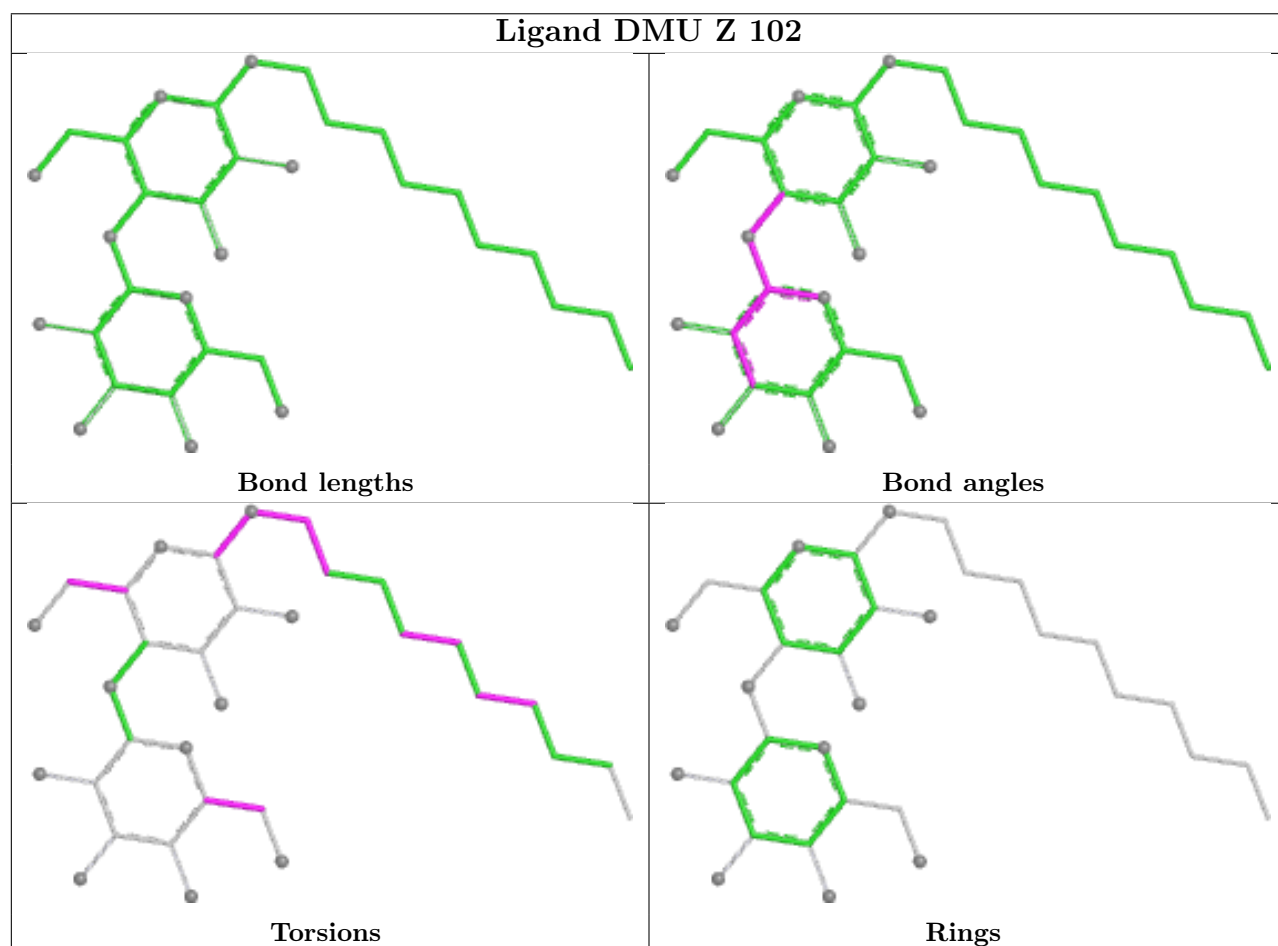
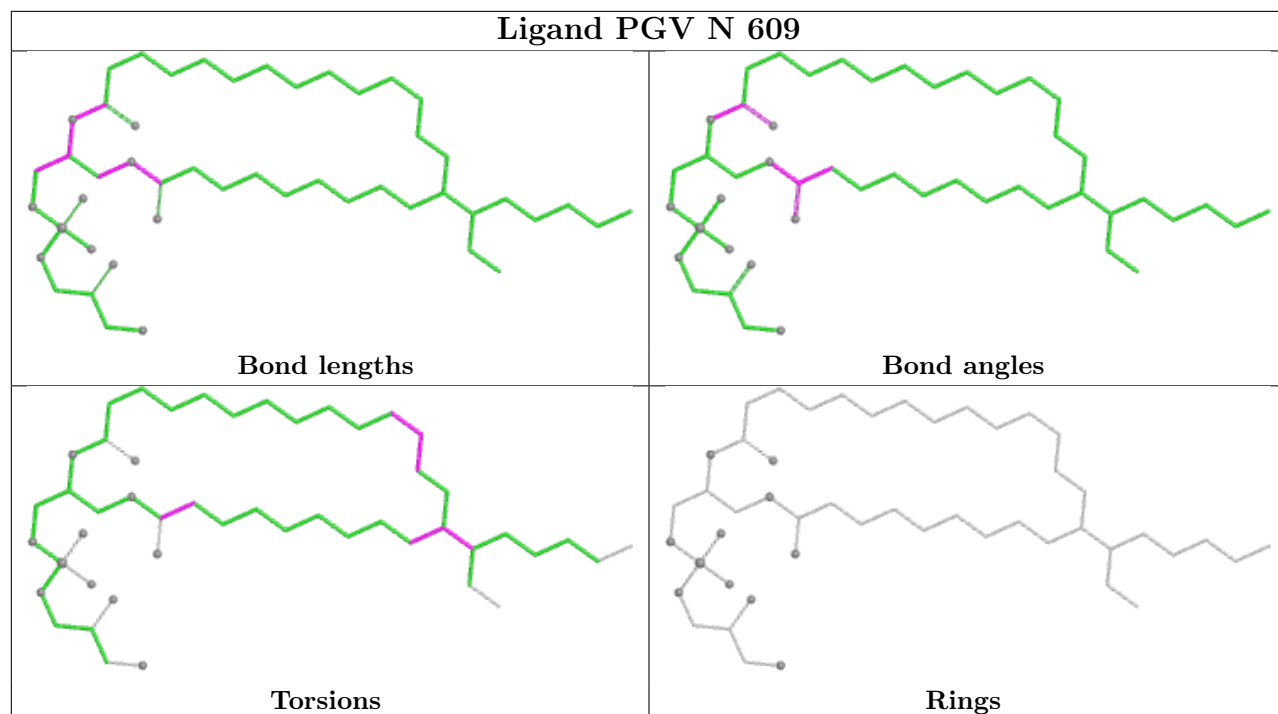
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	305	PEK	4	0
20	P	315	EDO	1	0
21	N	608	TGL	2	0
20	P	319	EDO	2	0
14	P	307	PGV	3	0

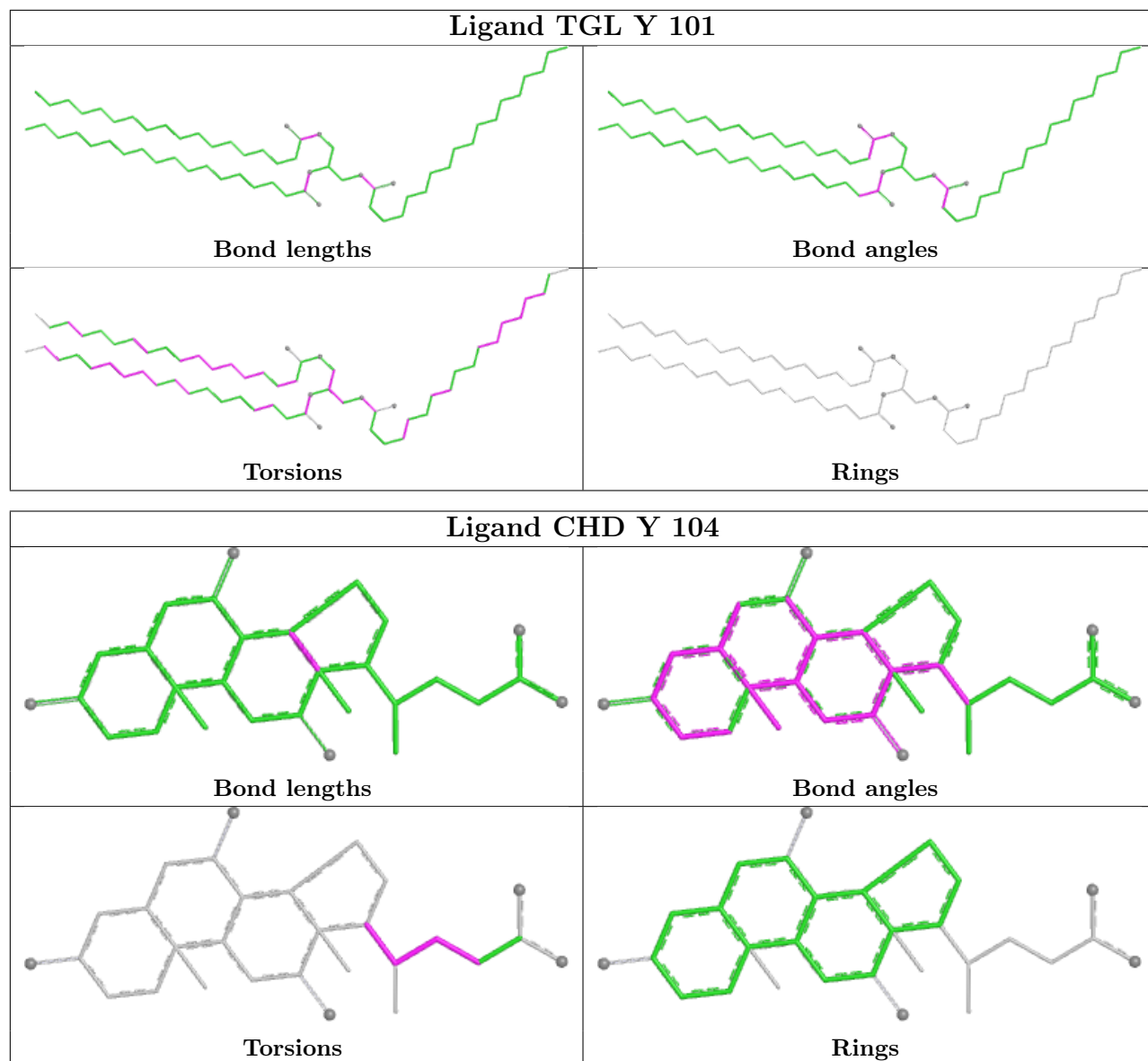
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

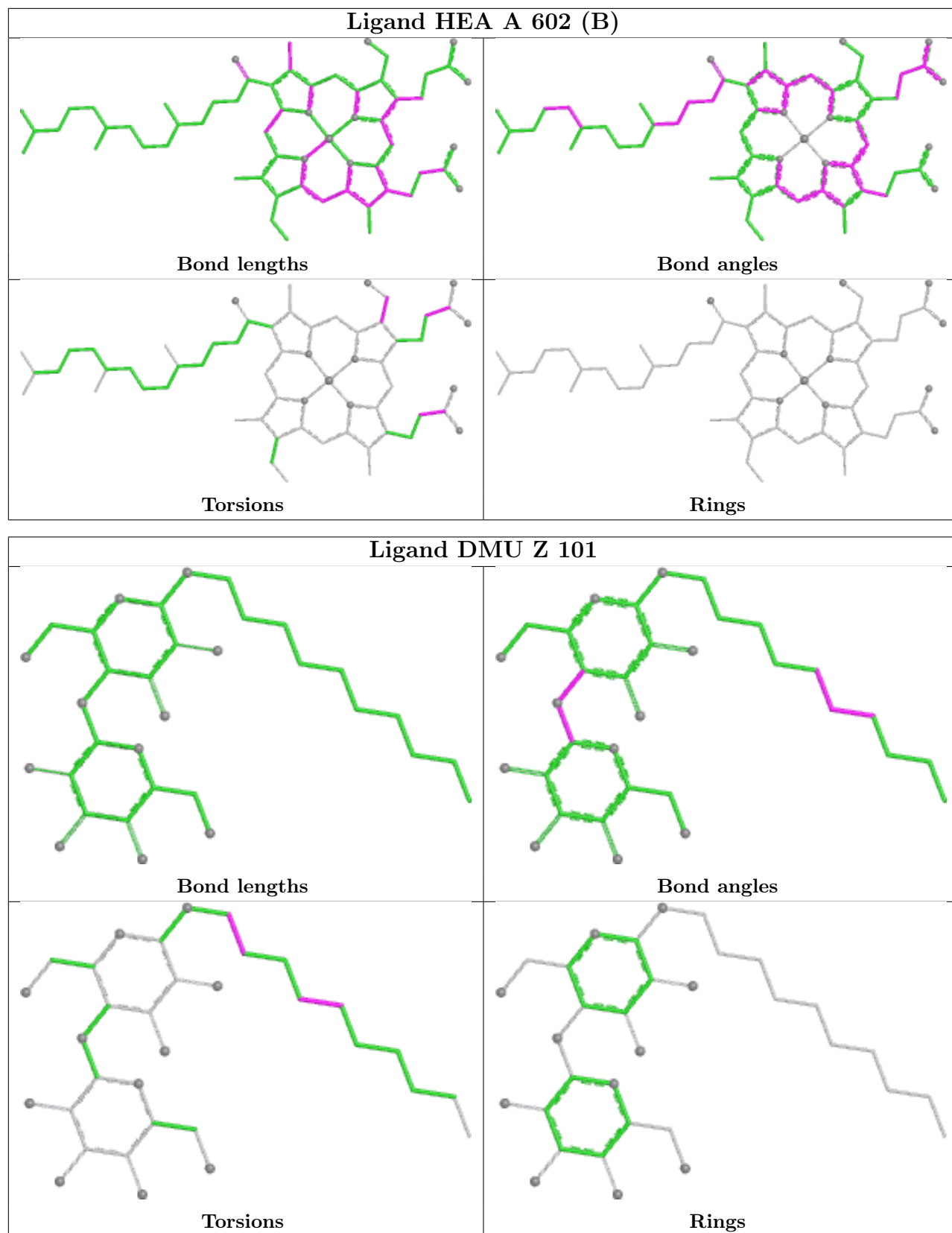


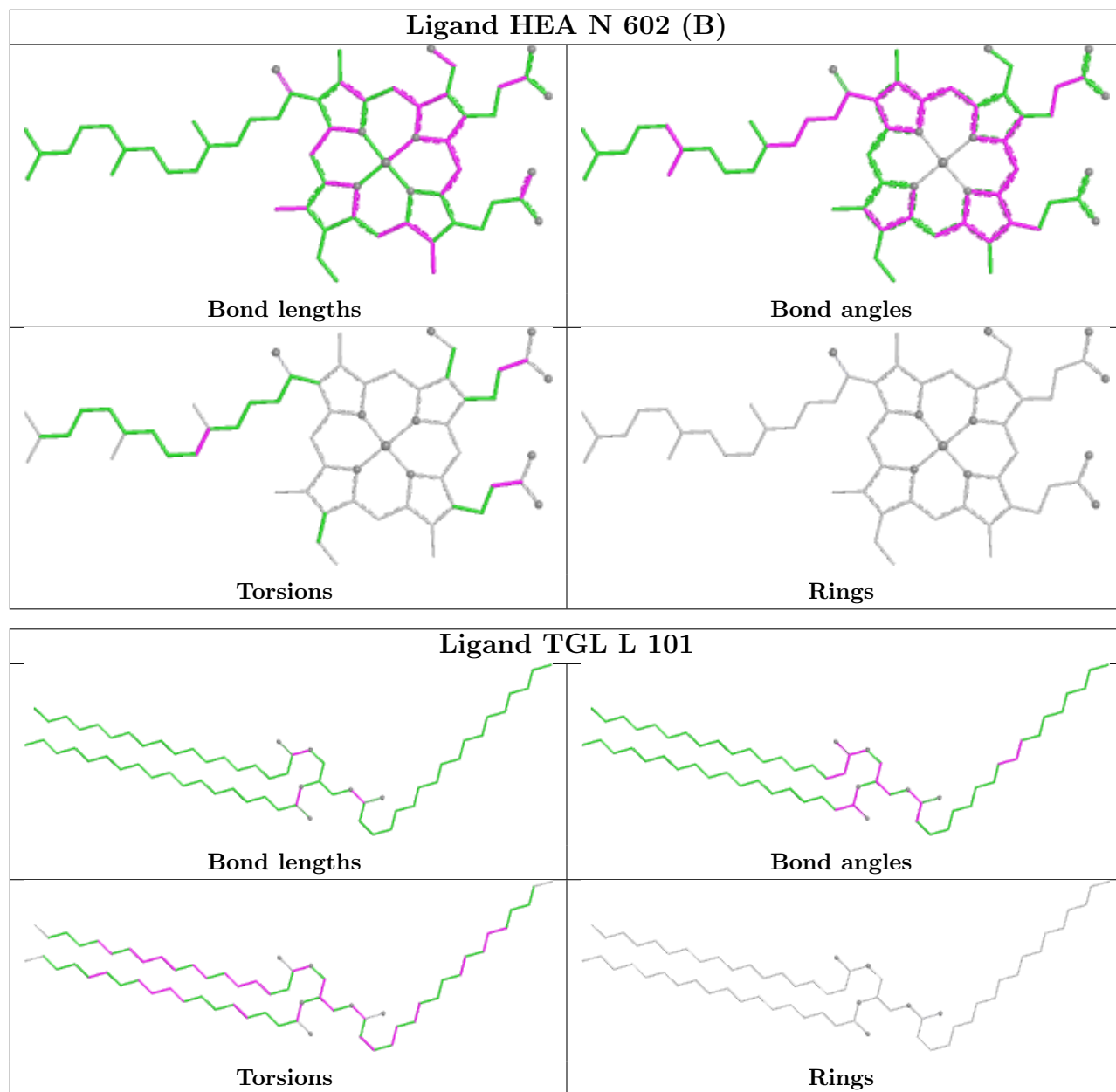


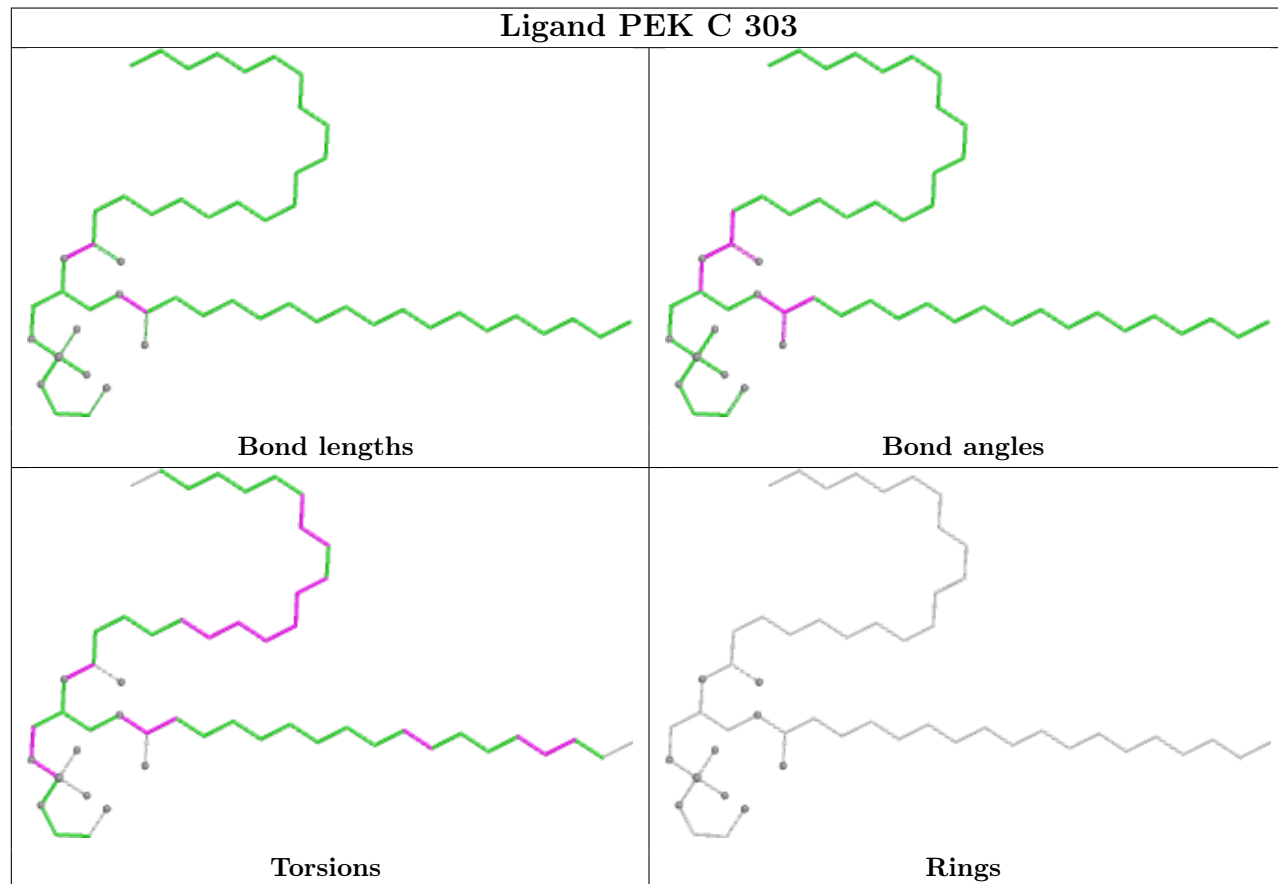
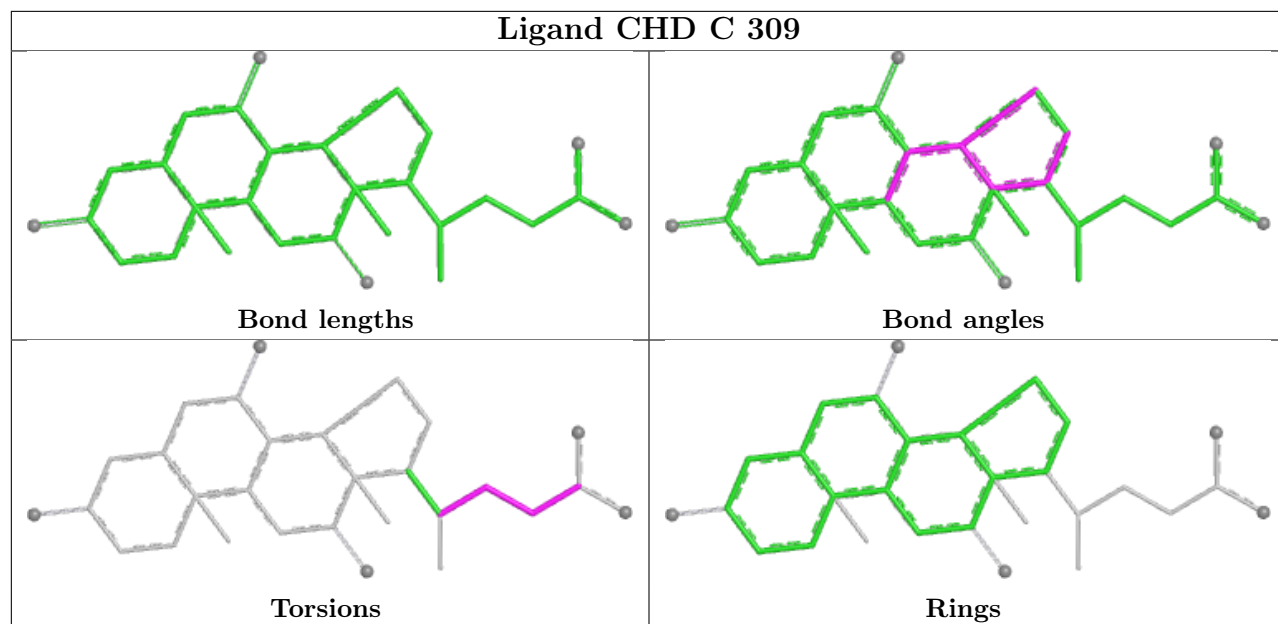


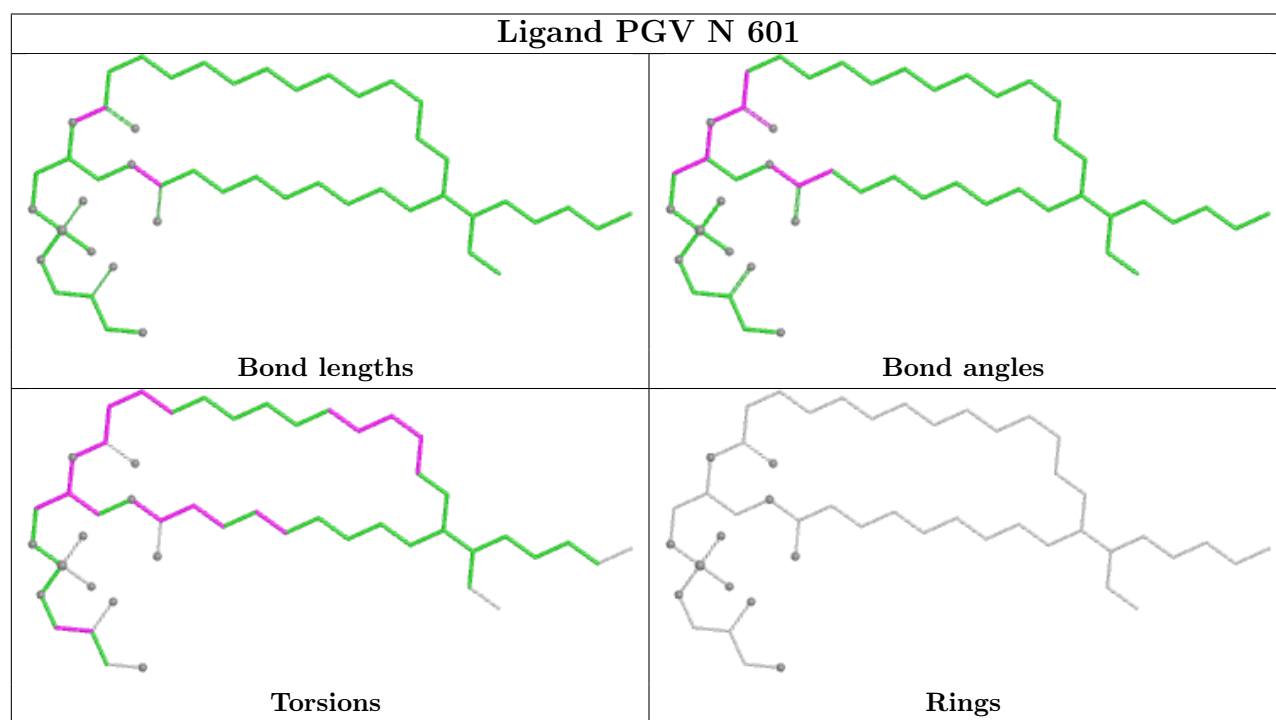
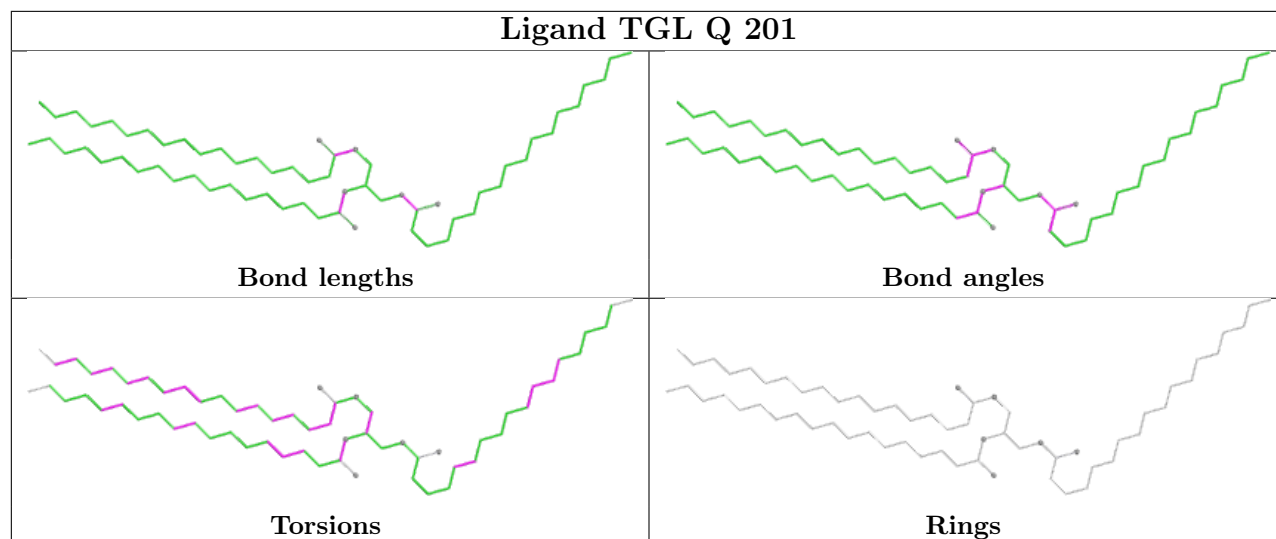


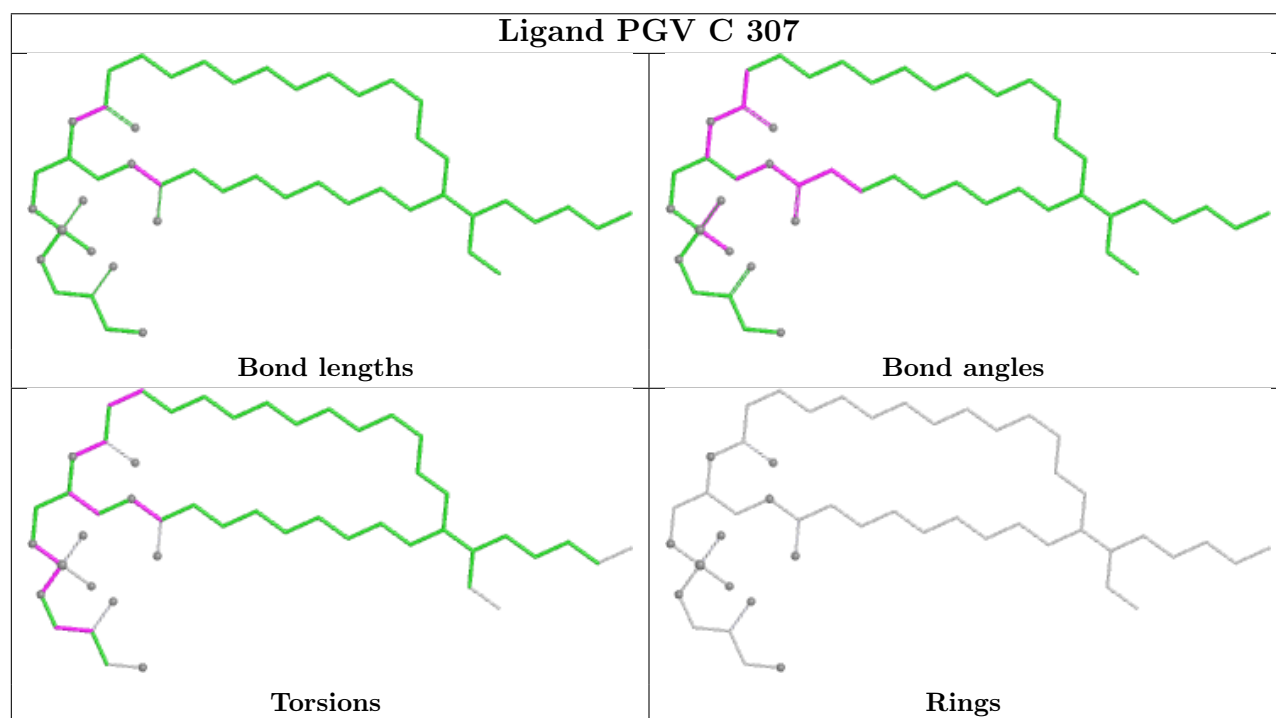
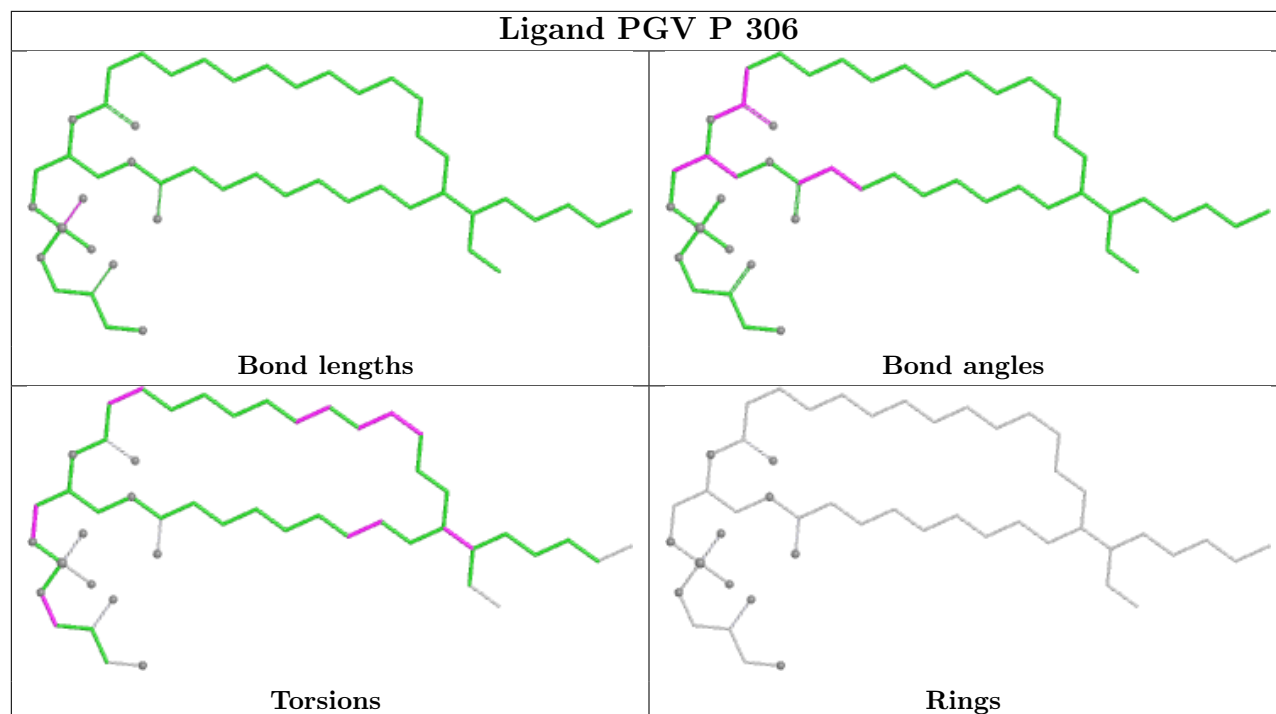


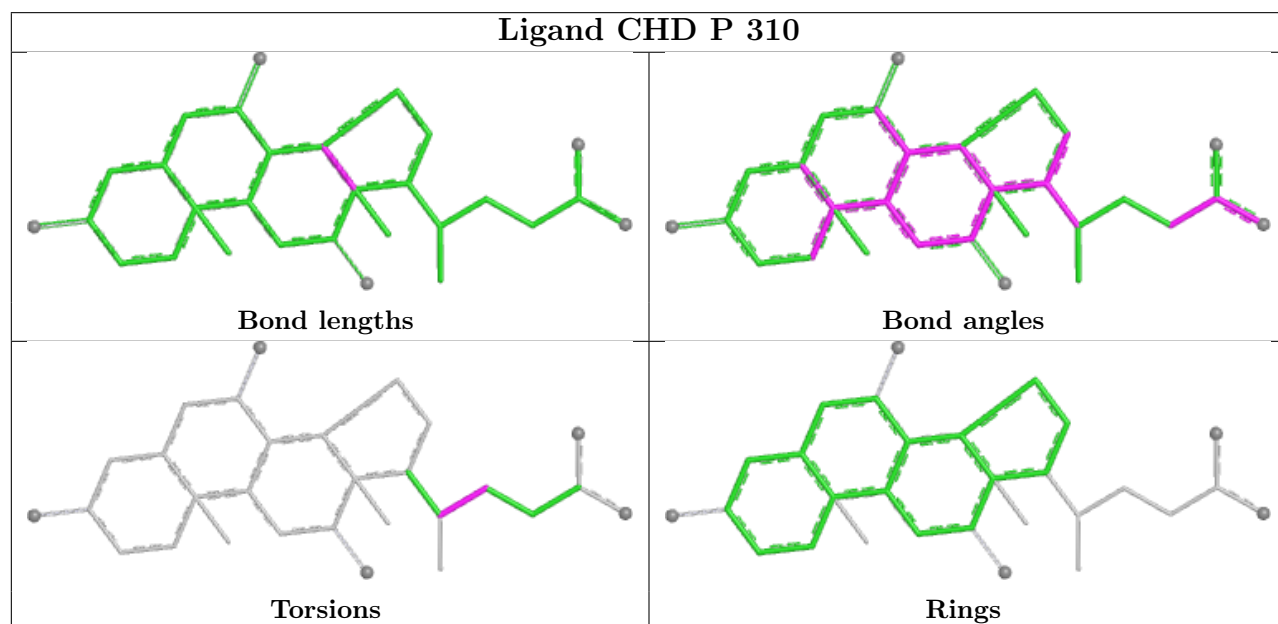
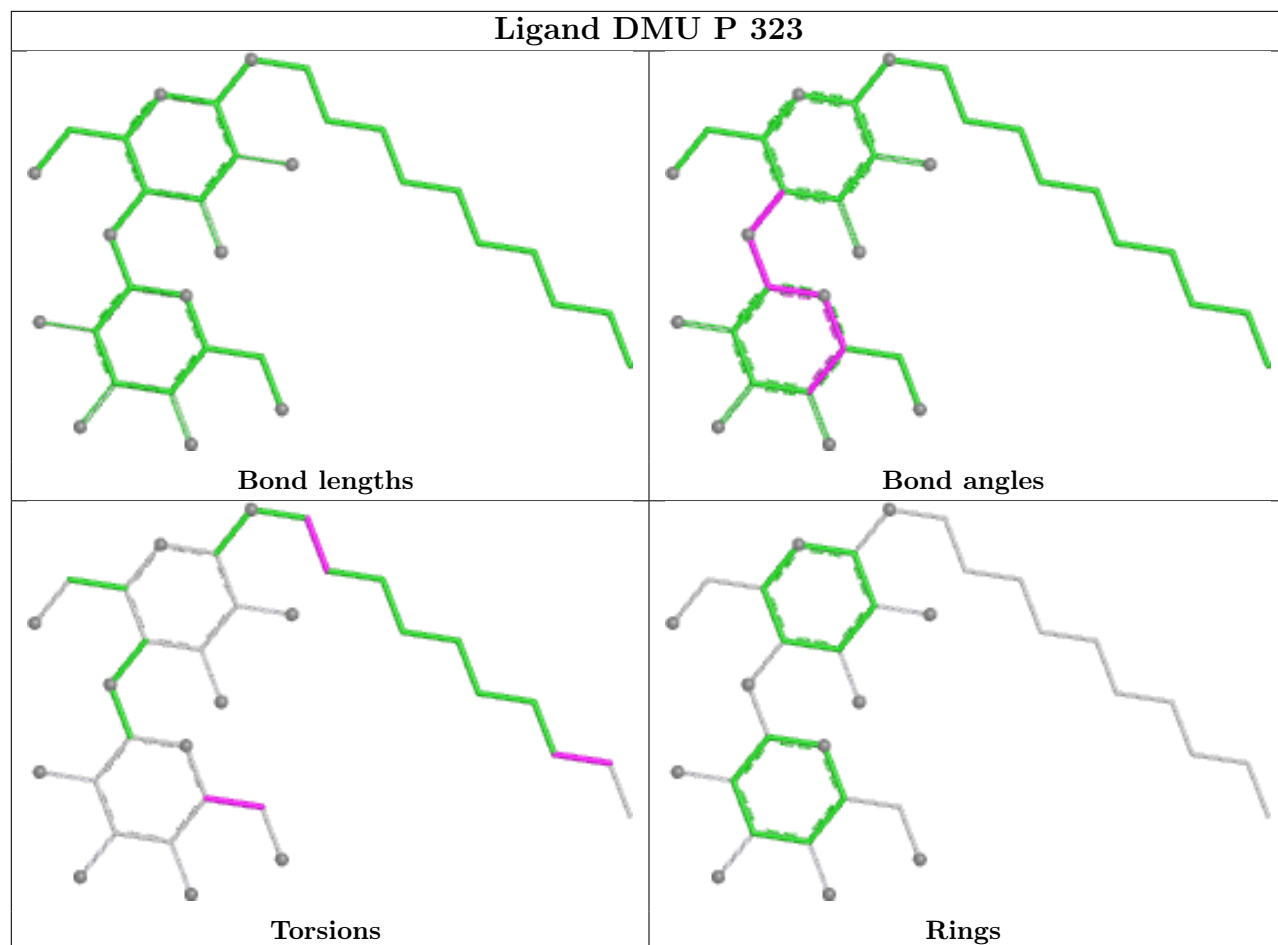


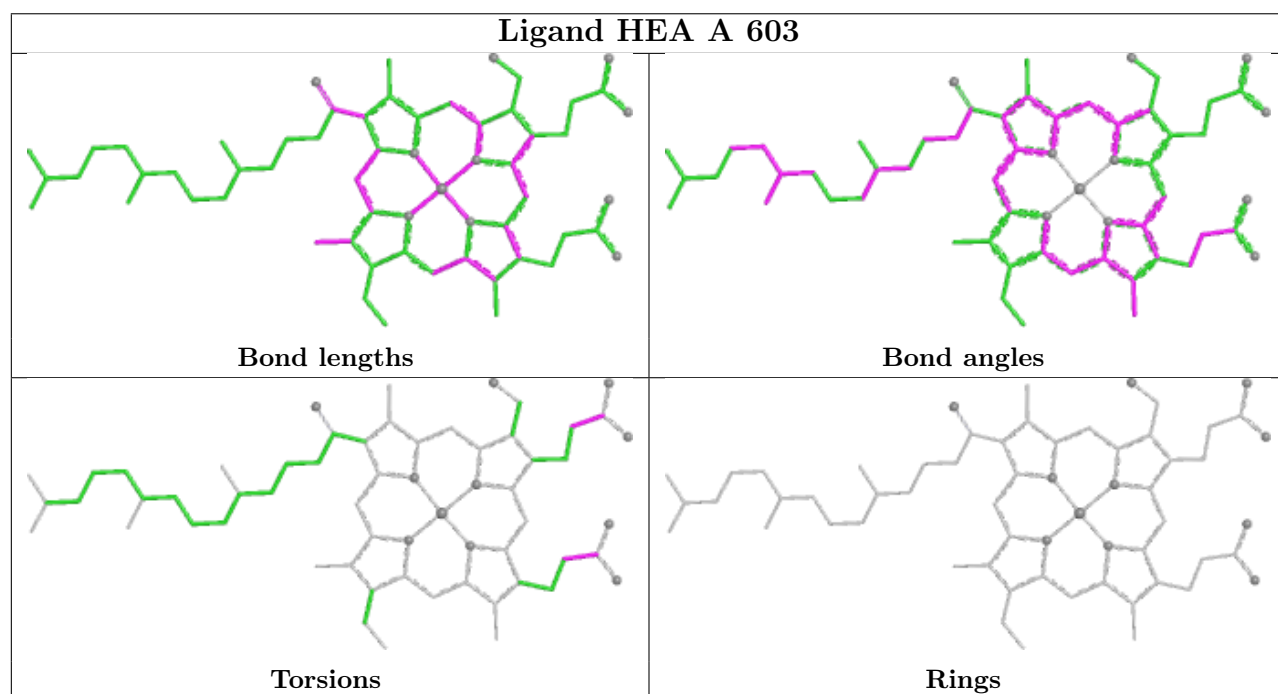
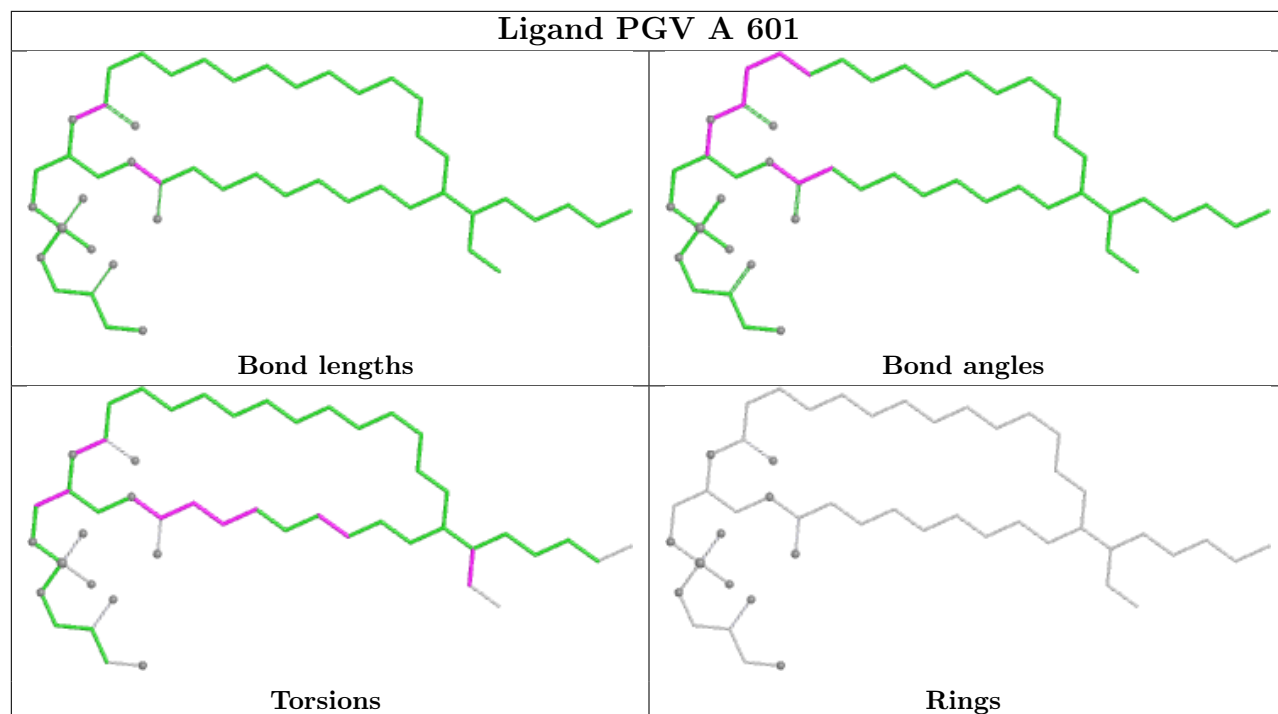


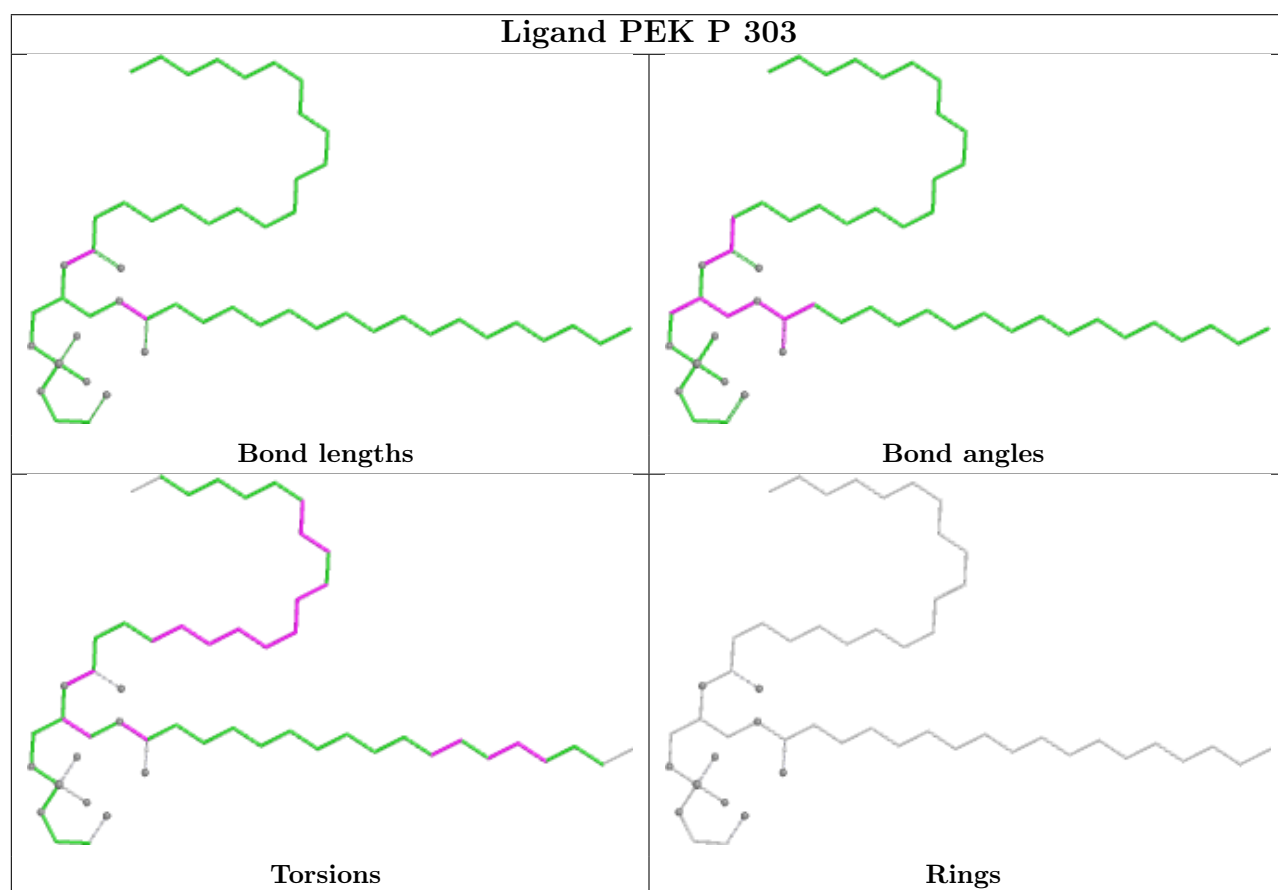
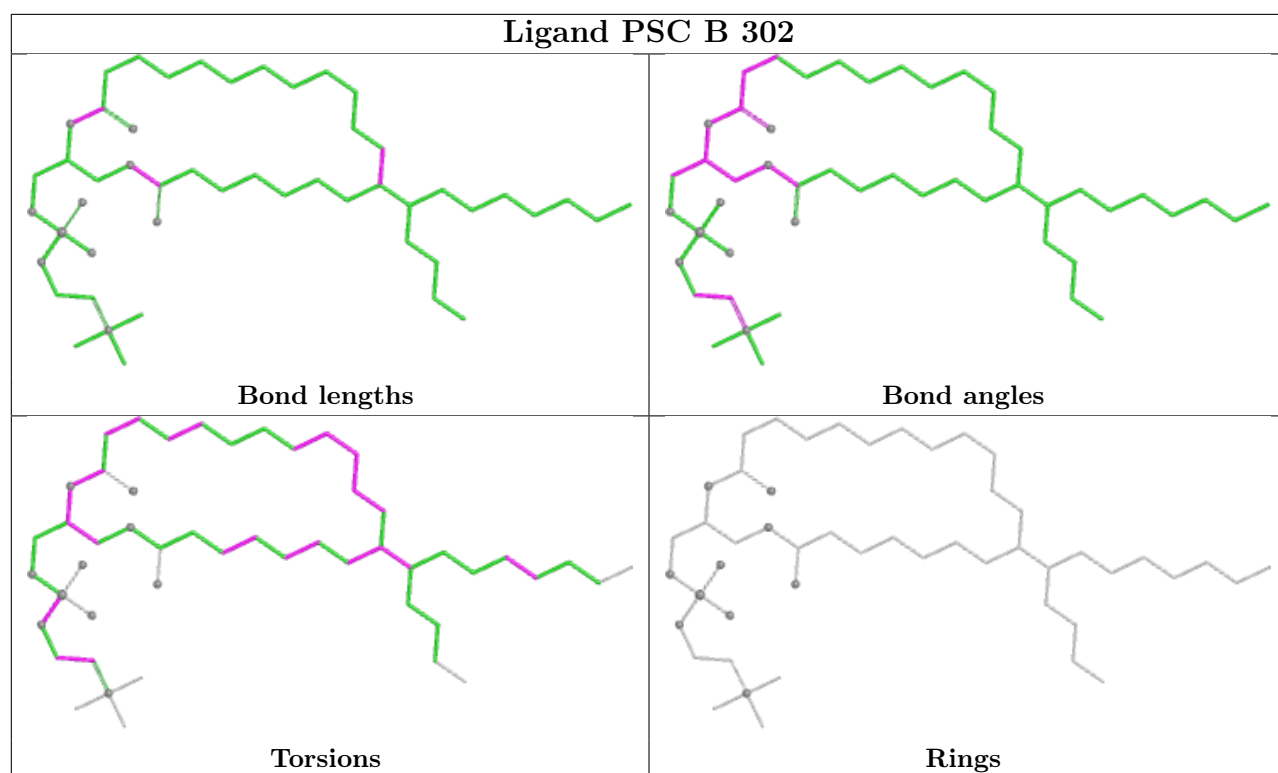


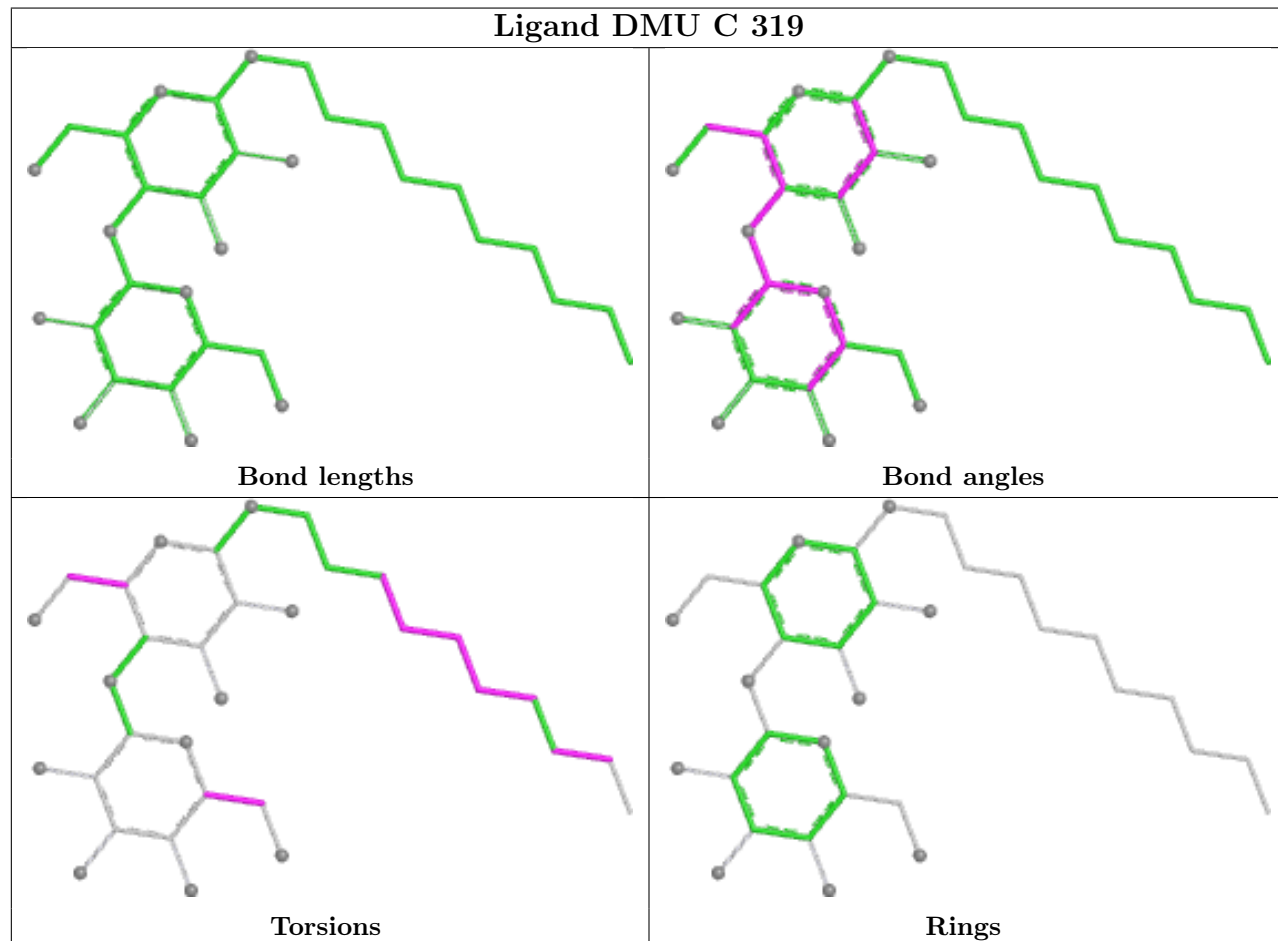
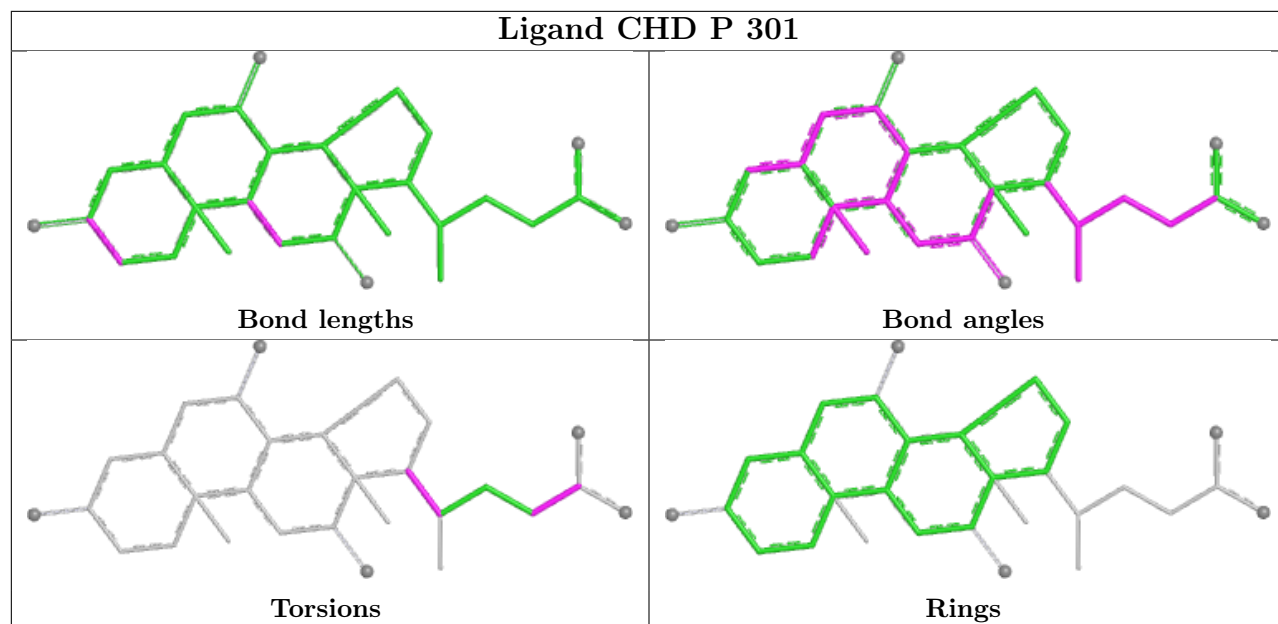


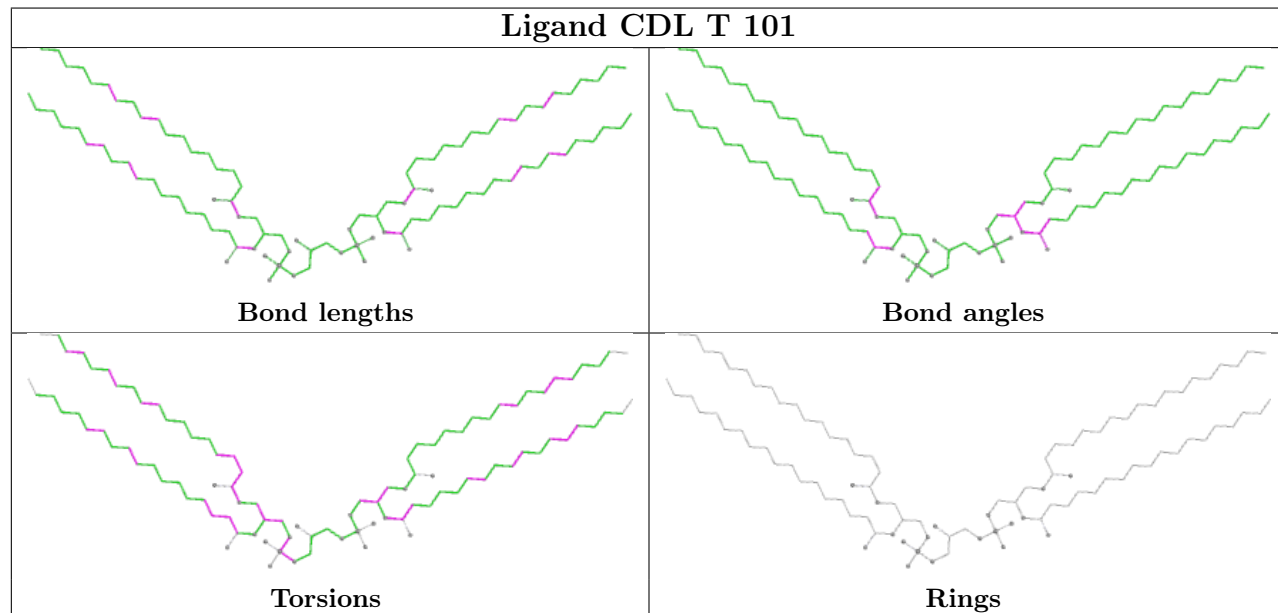
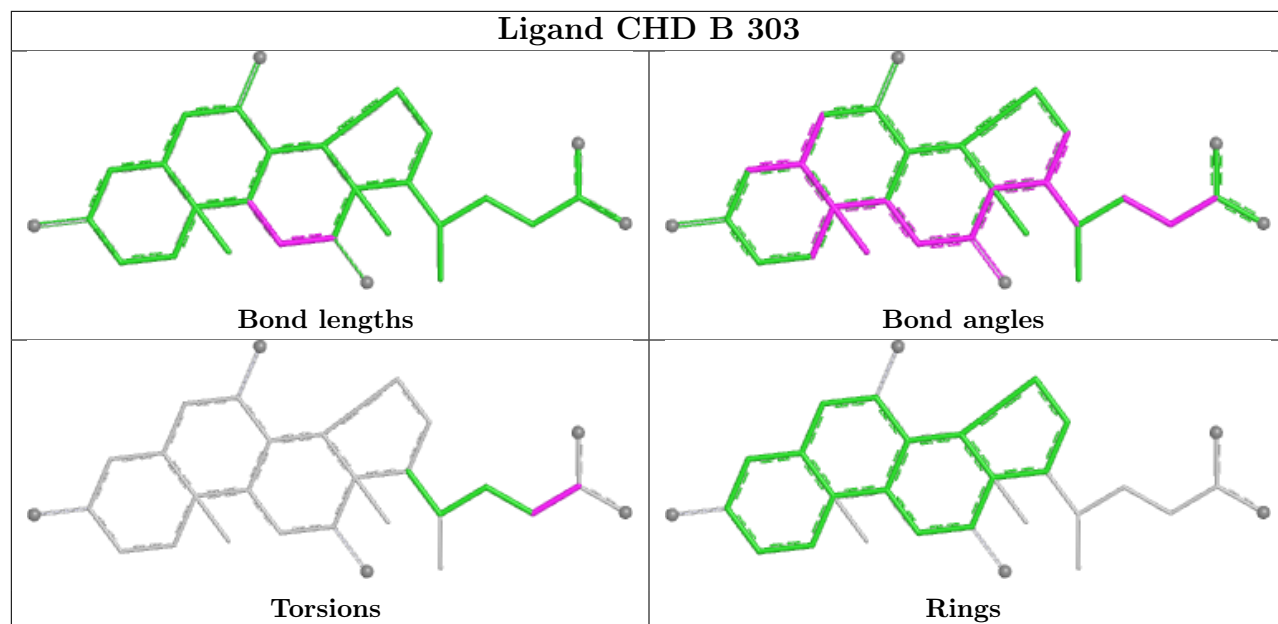


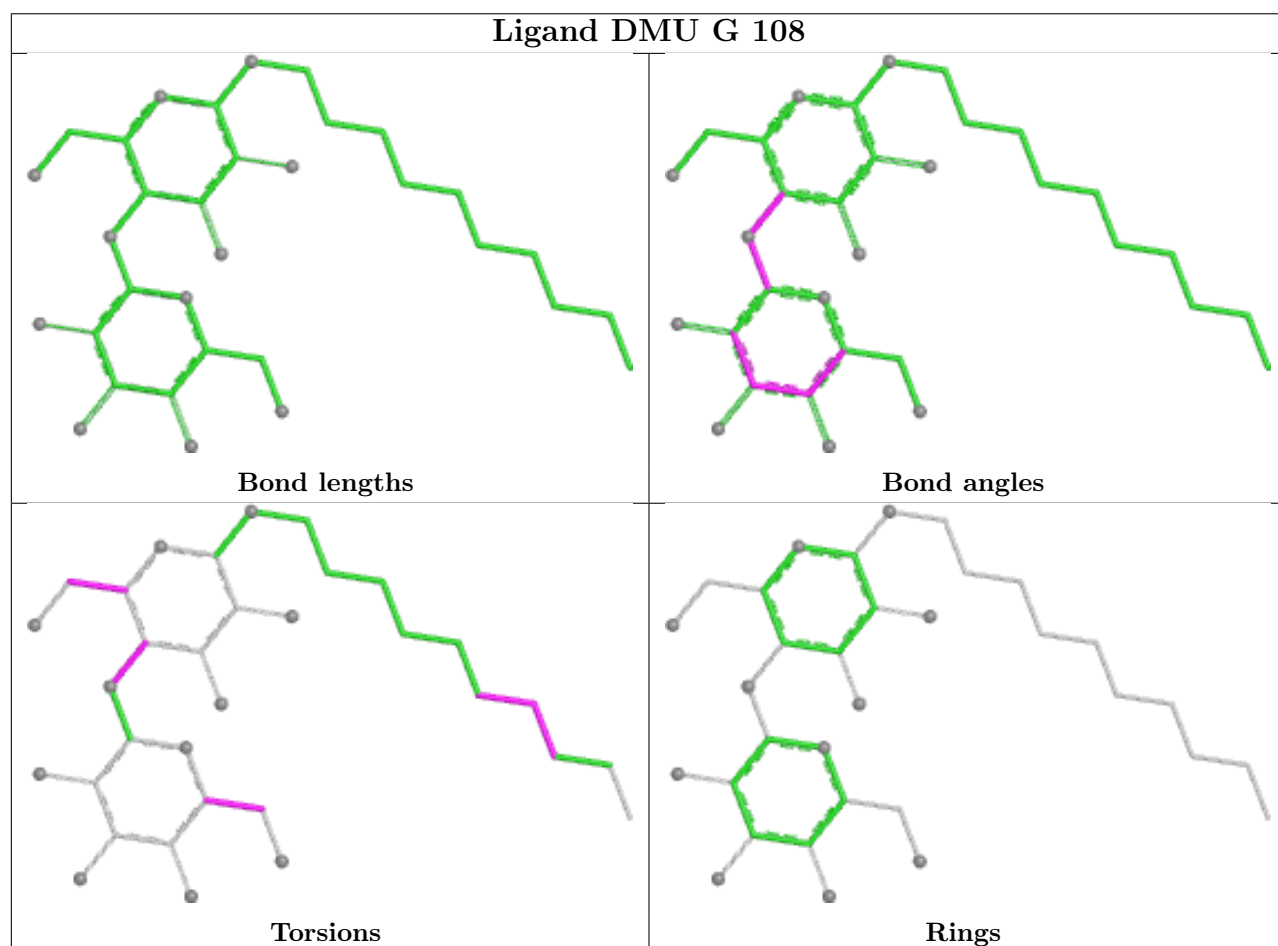
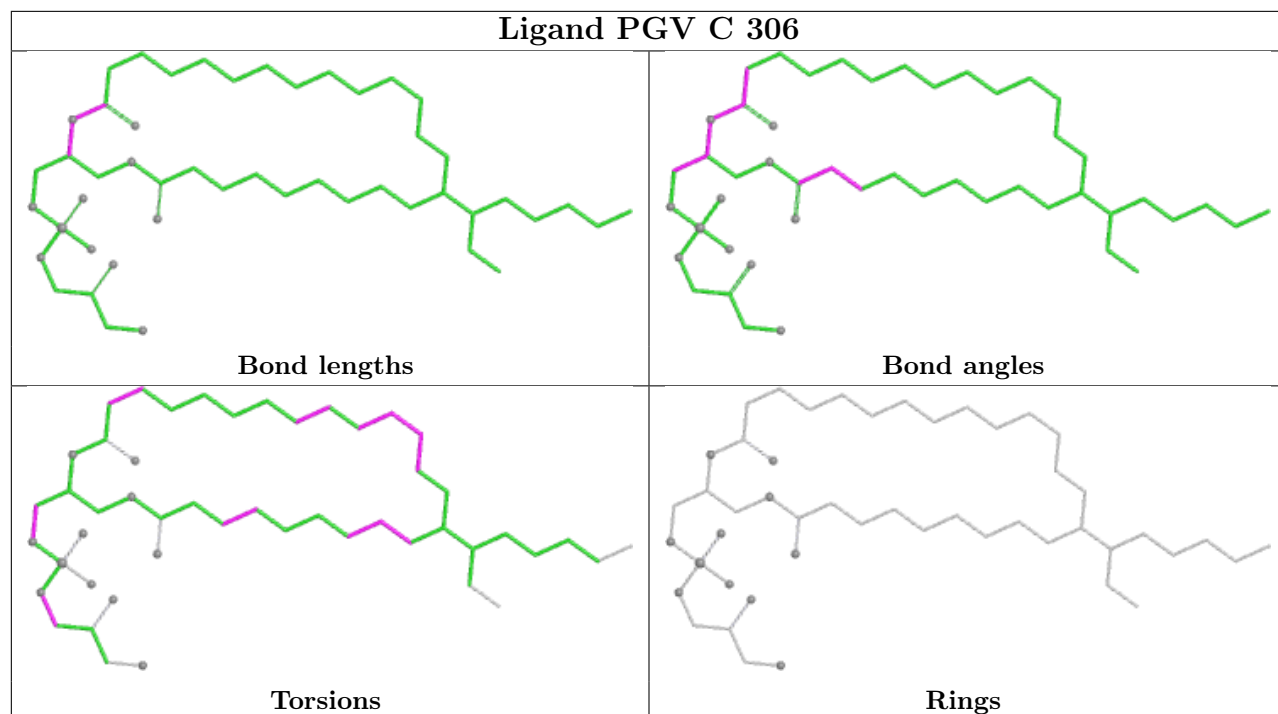


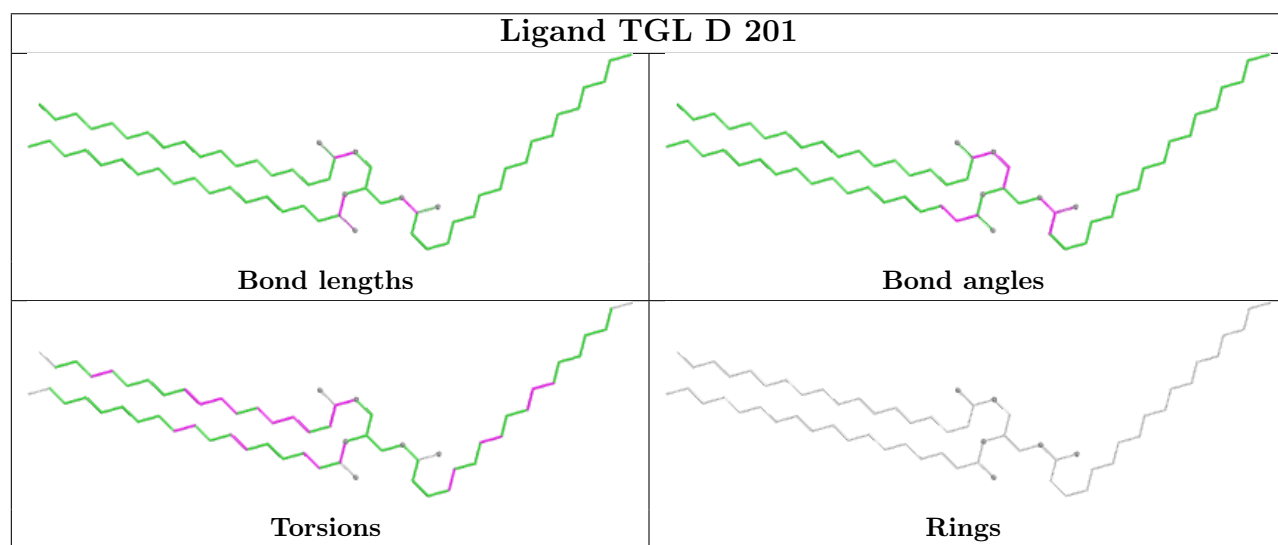
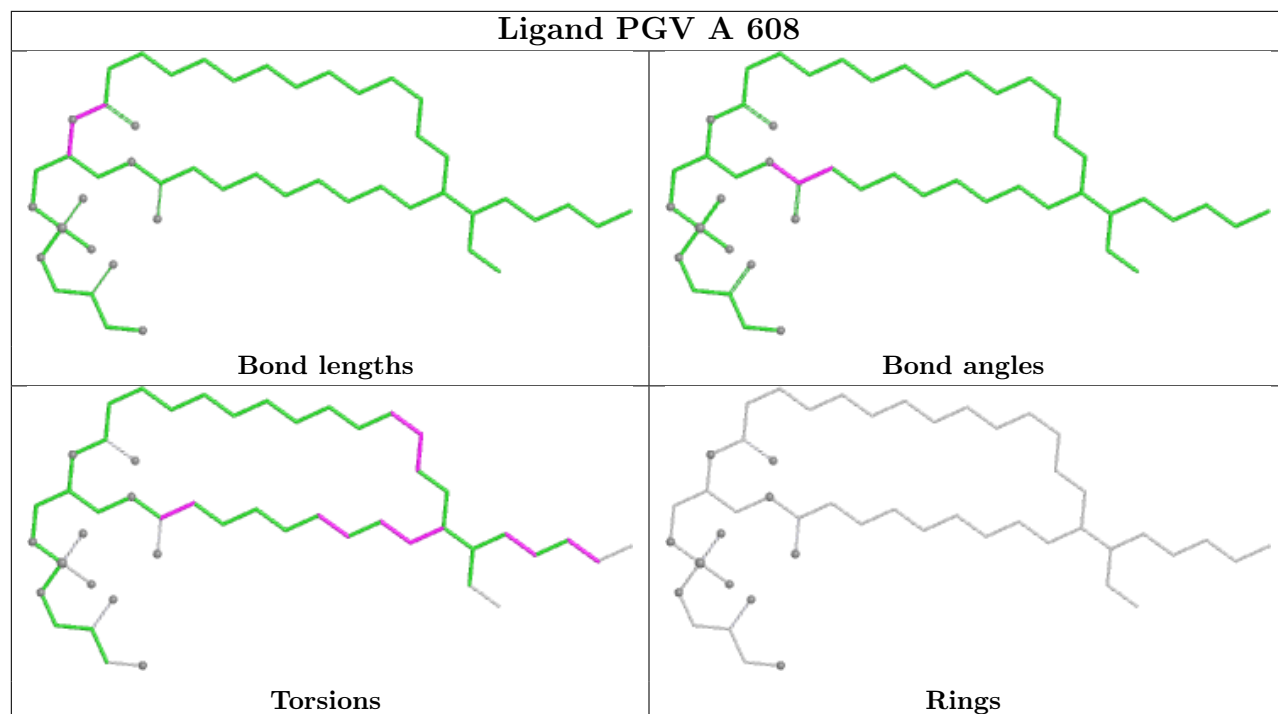


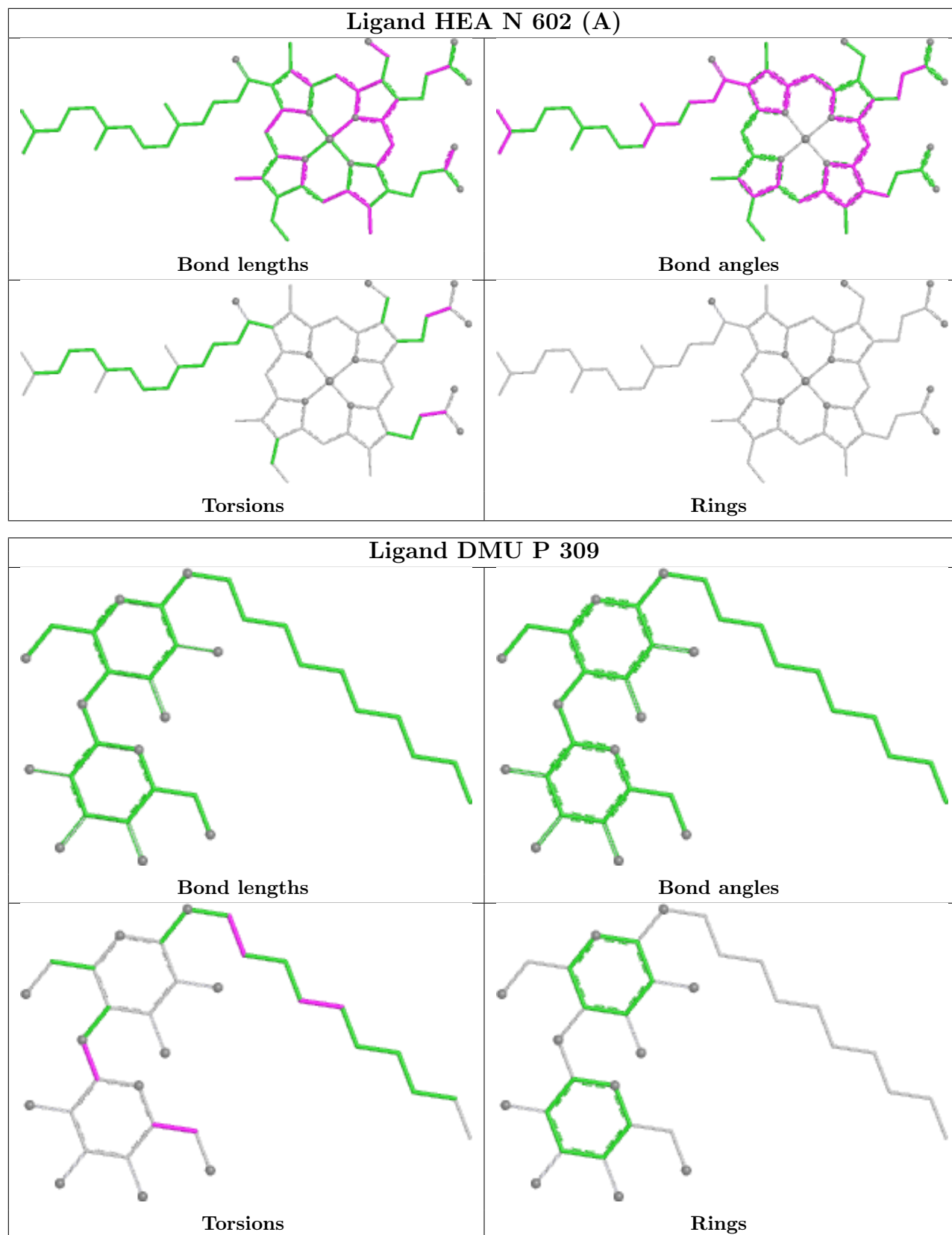


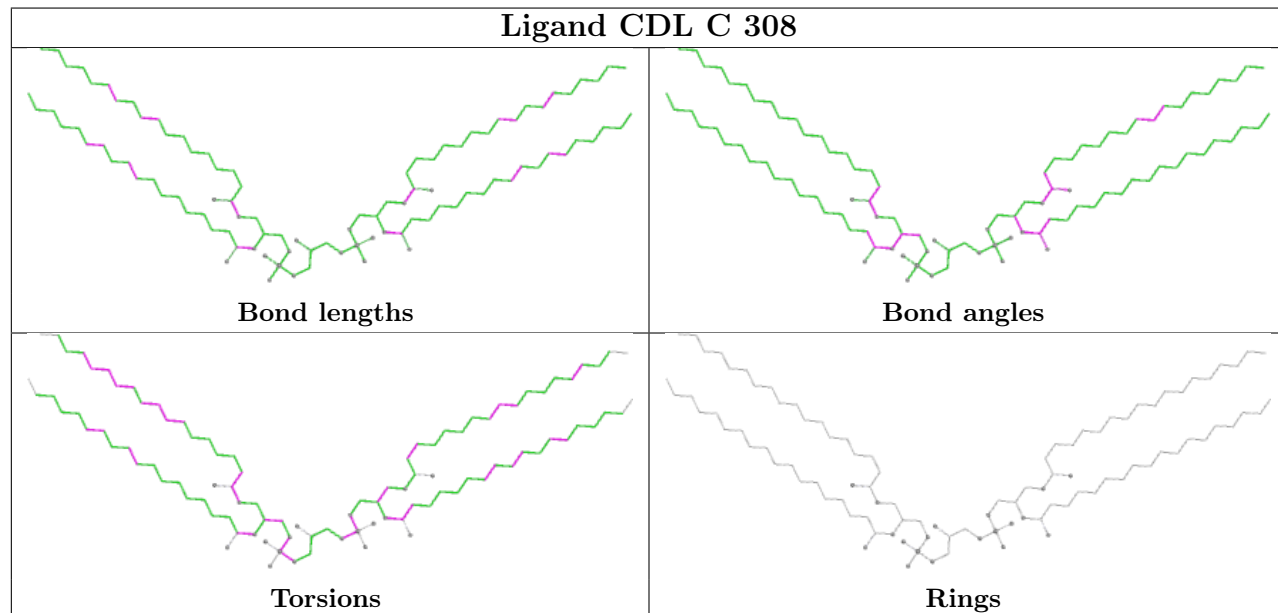


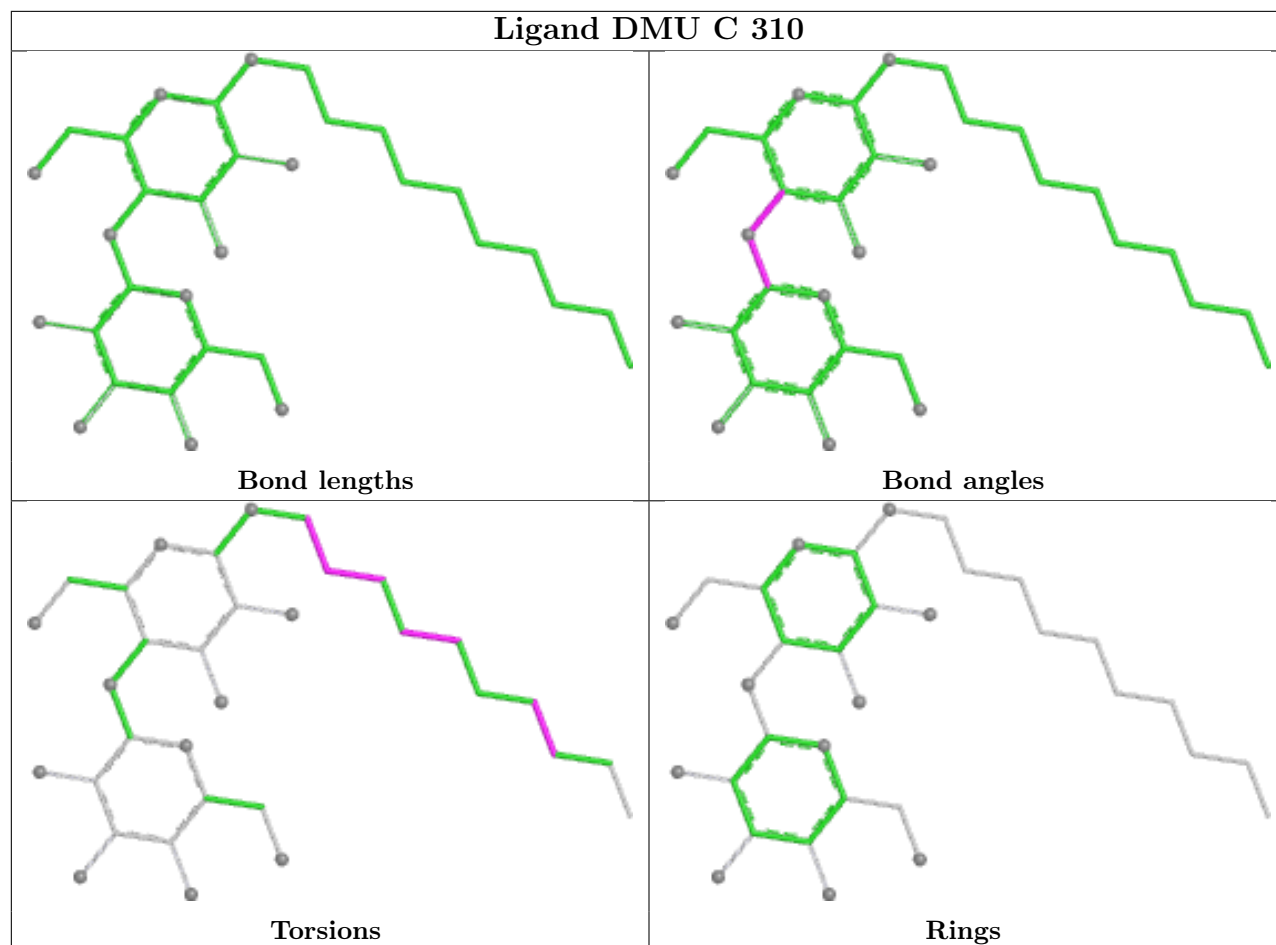


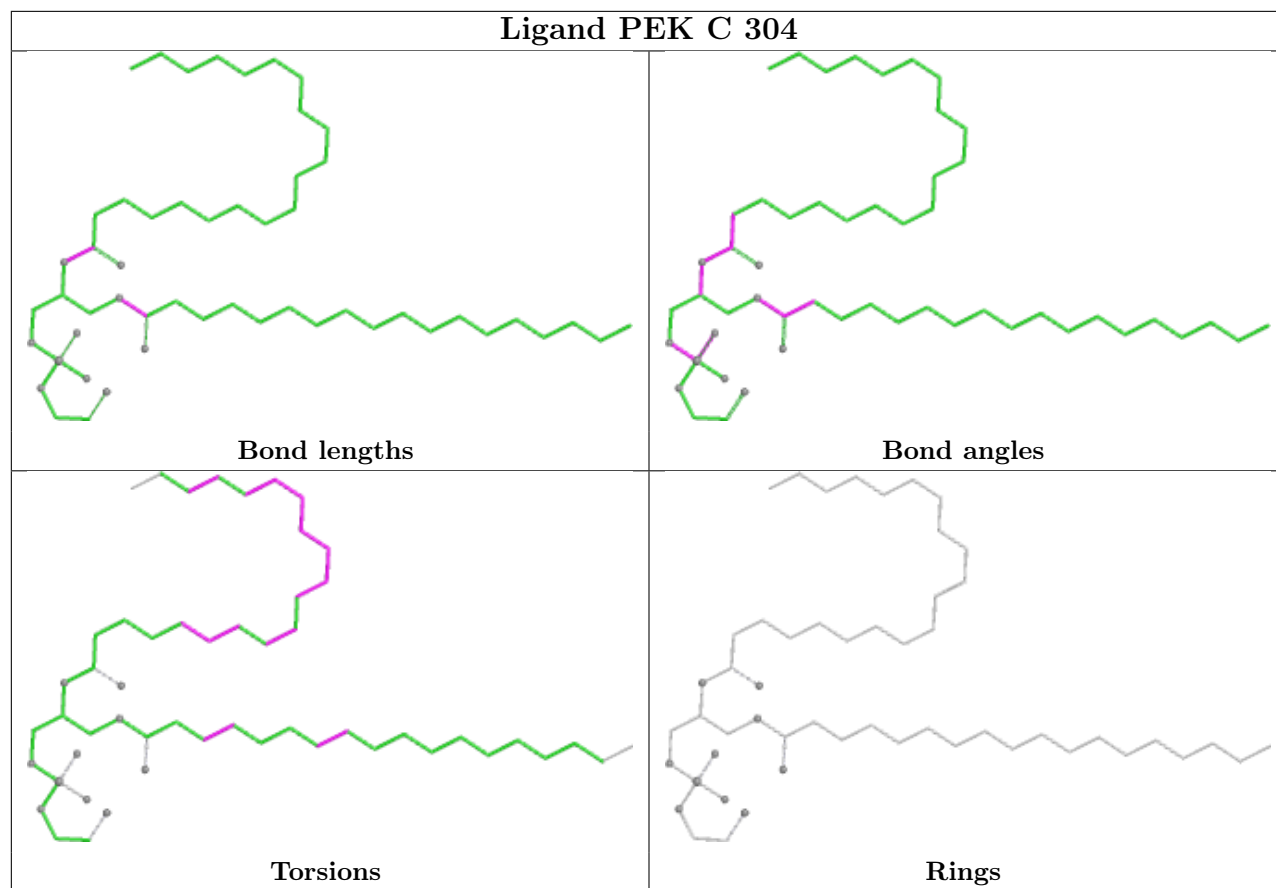


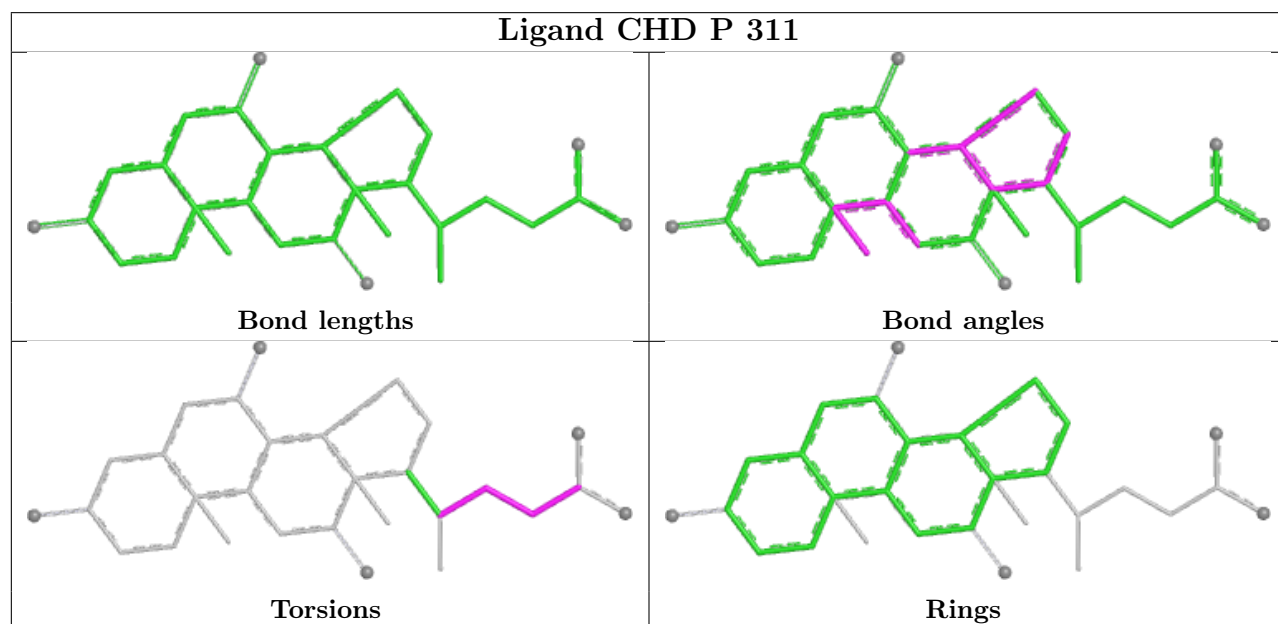
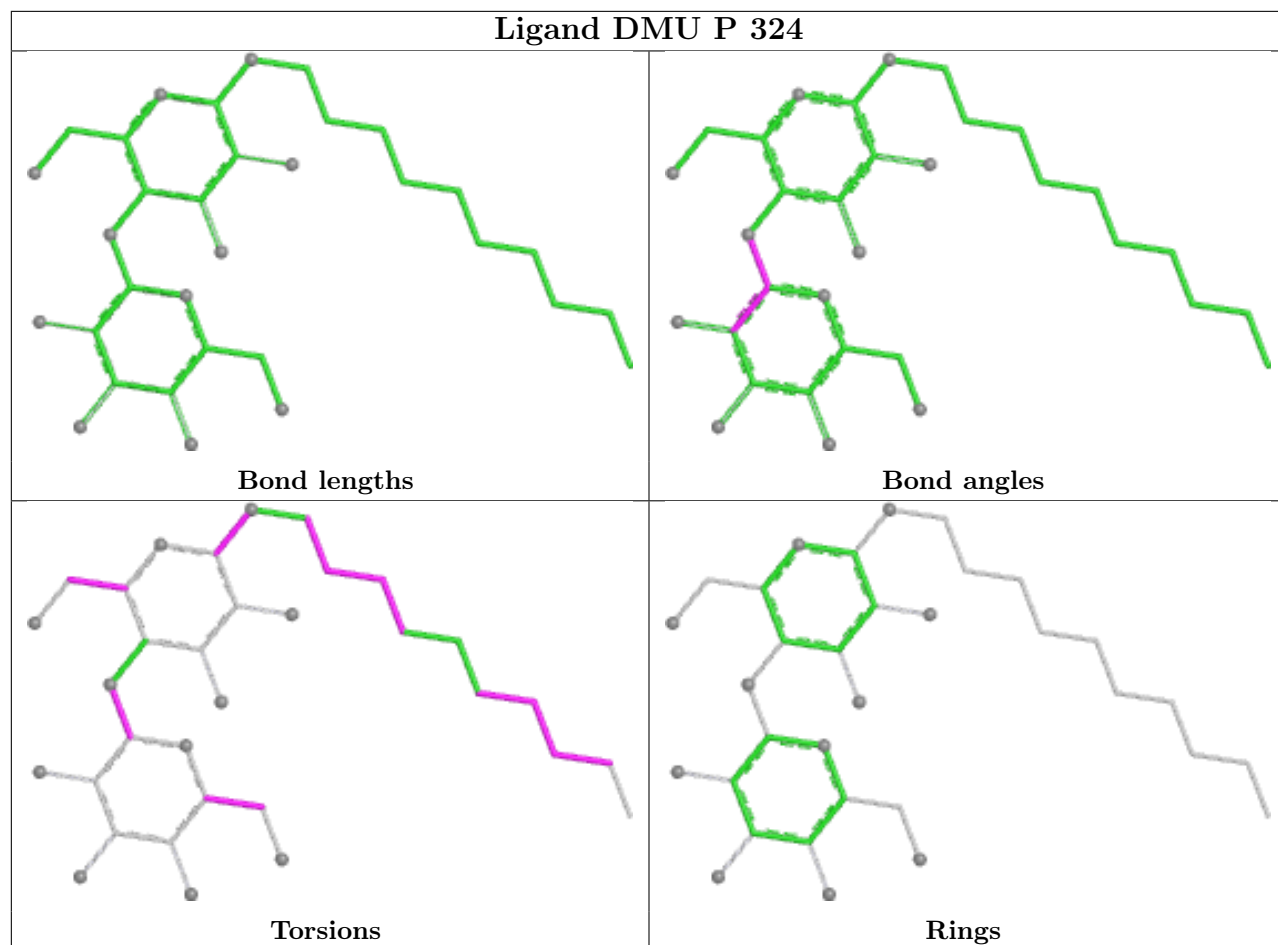


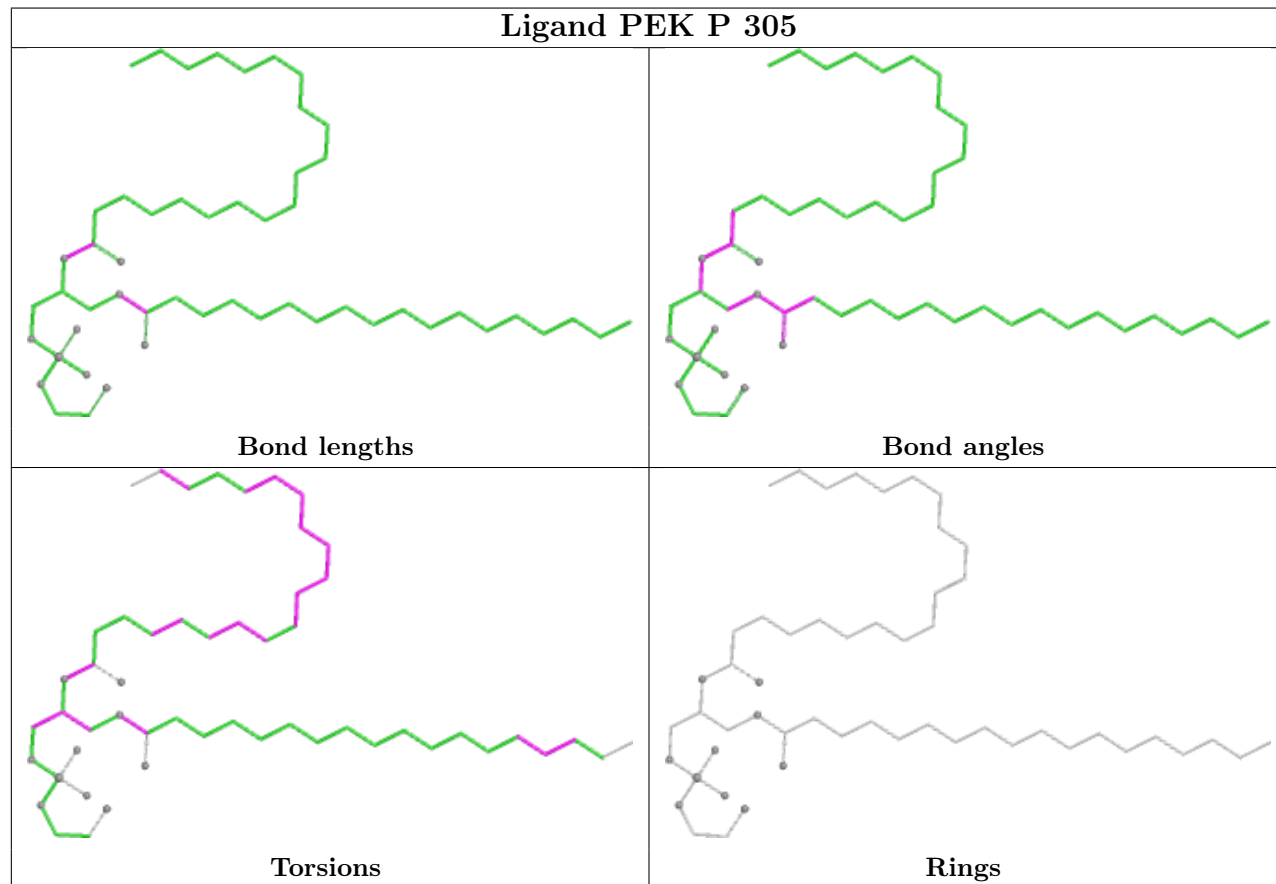
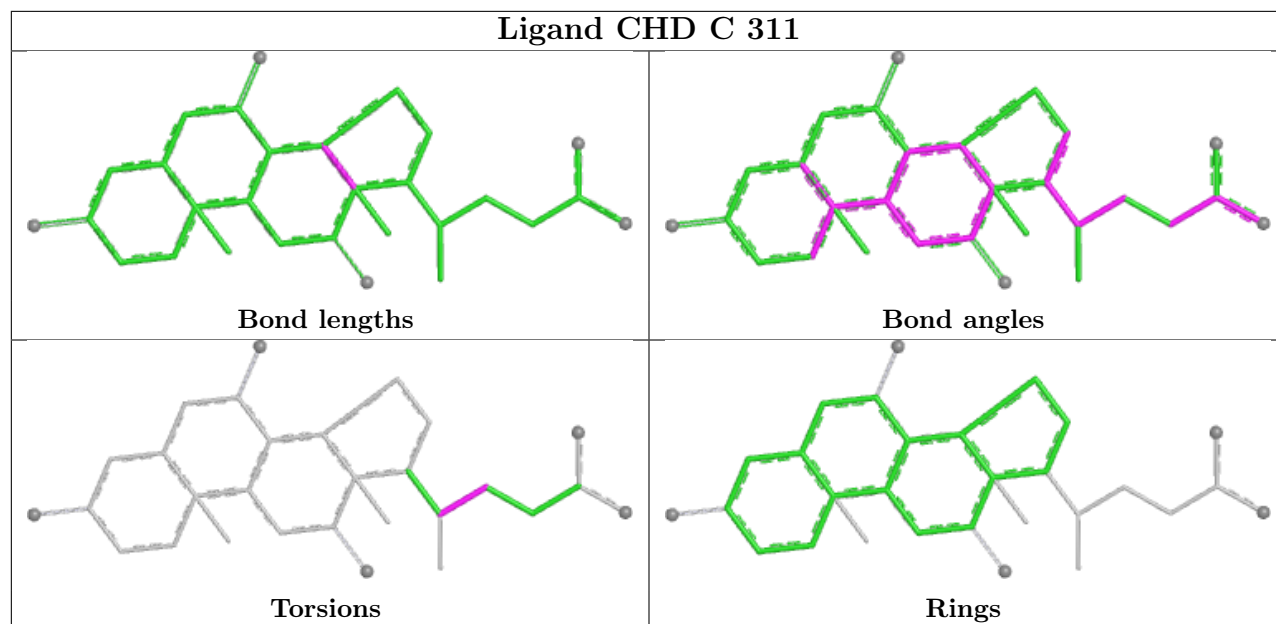


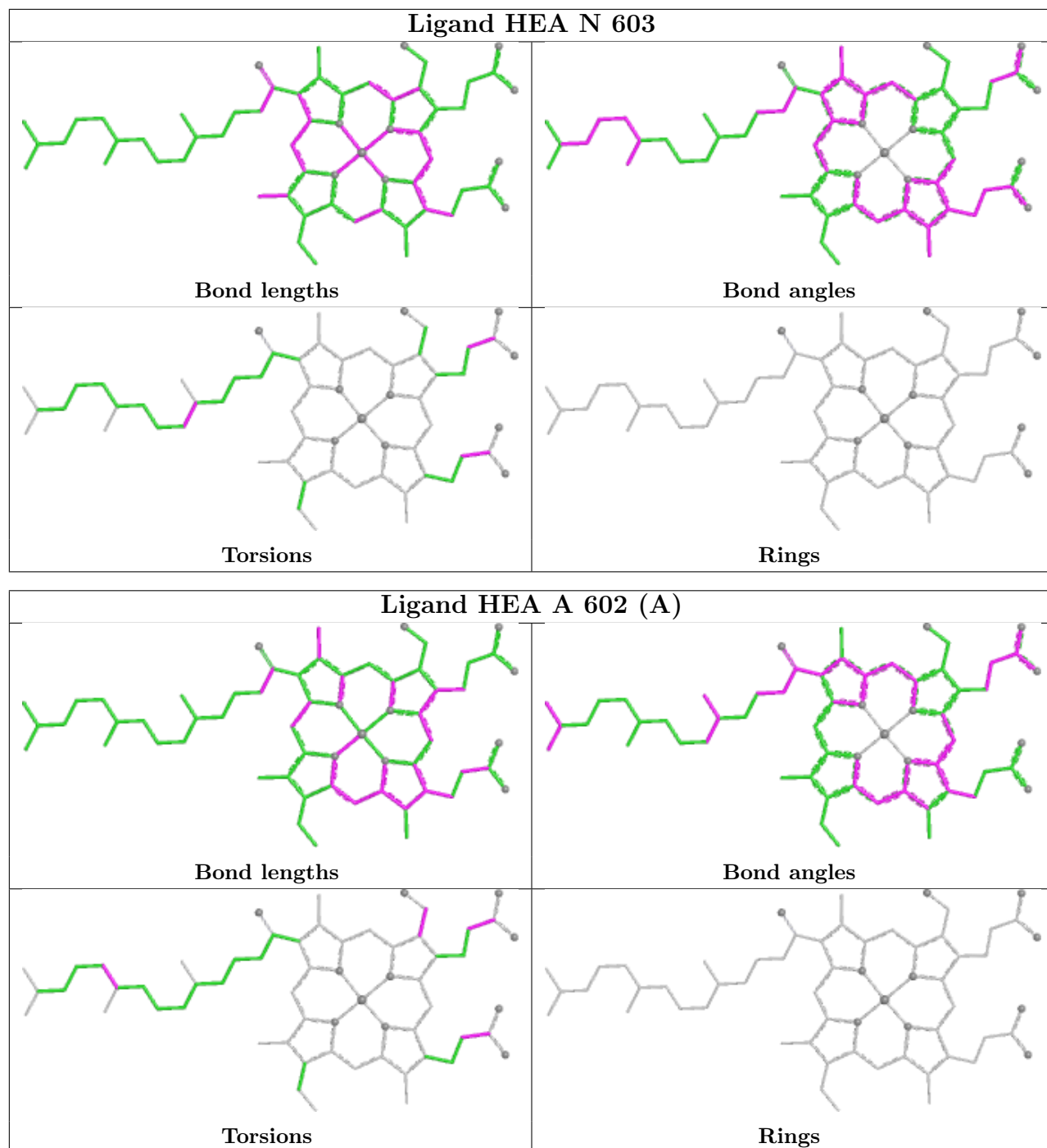


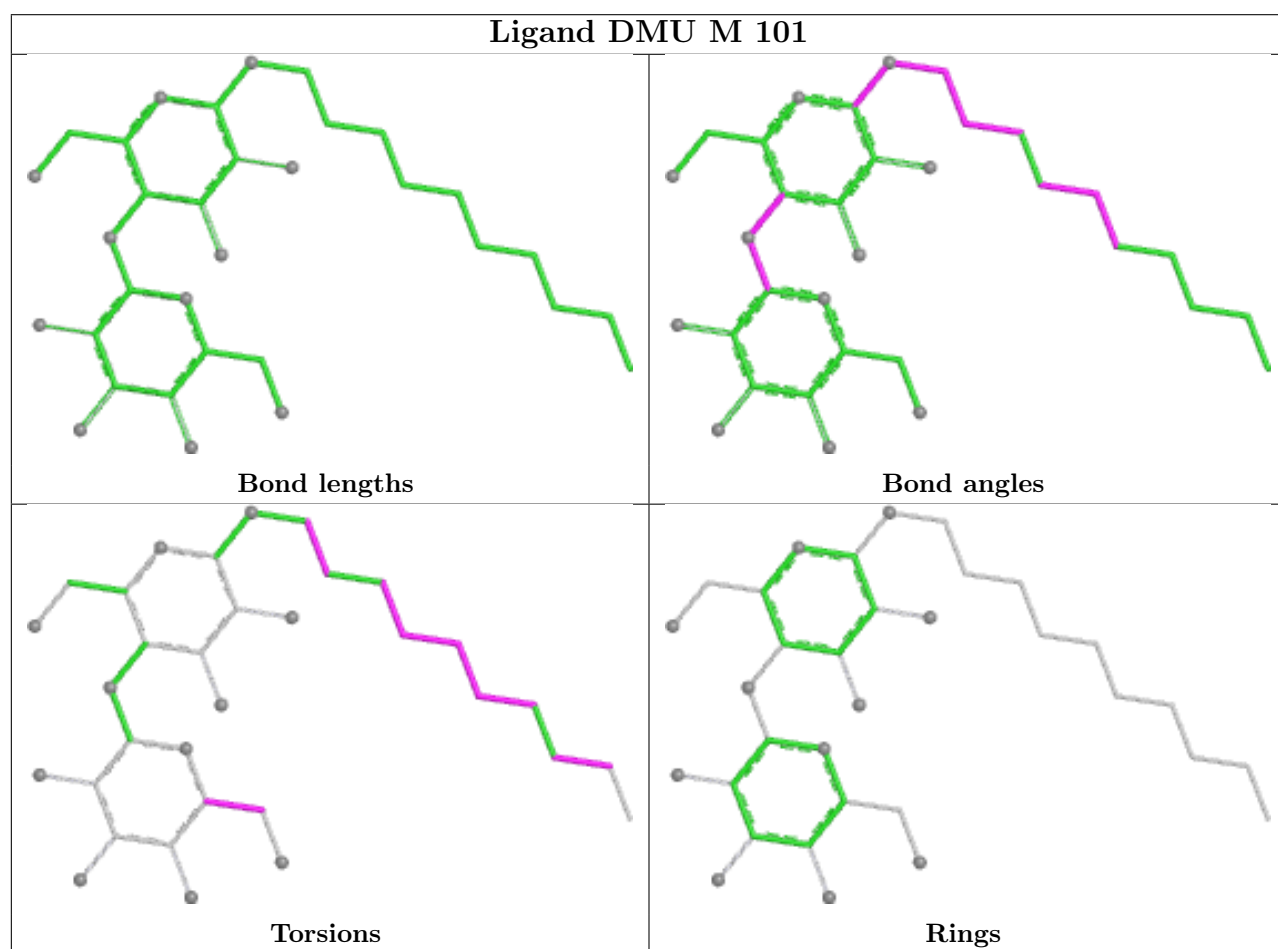
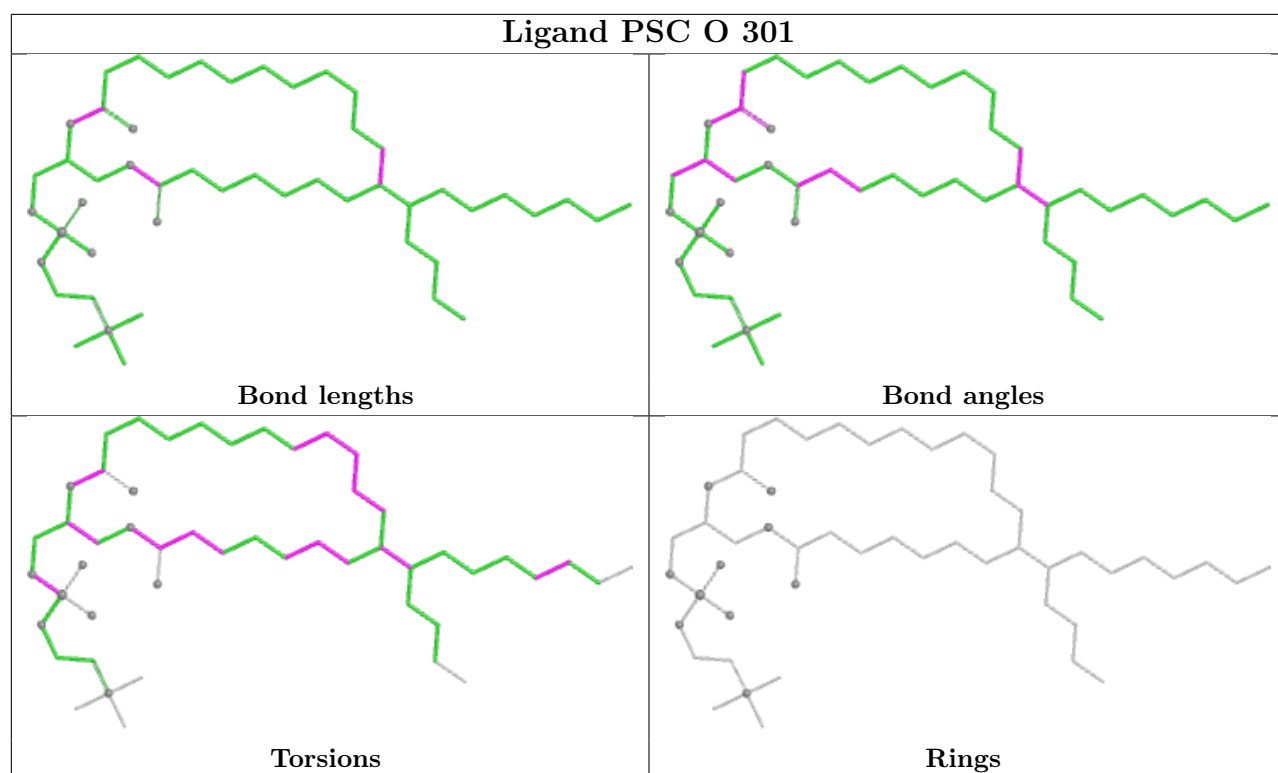


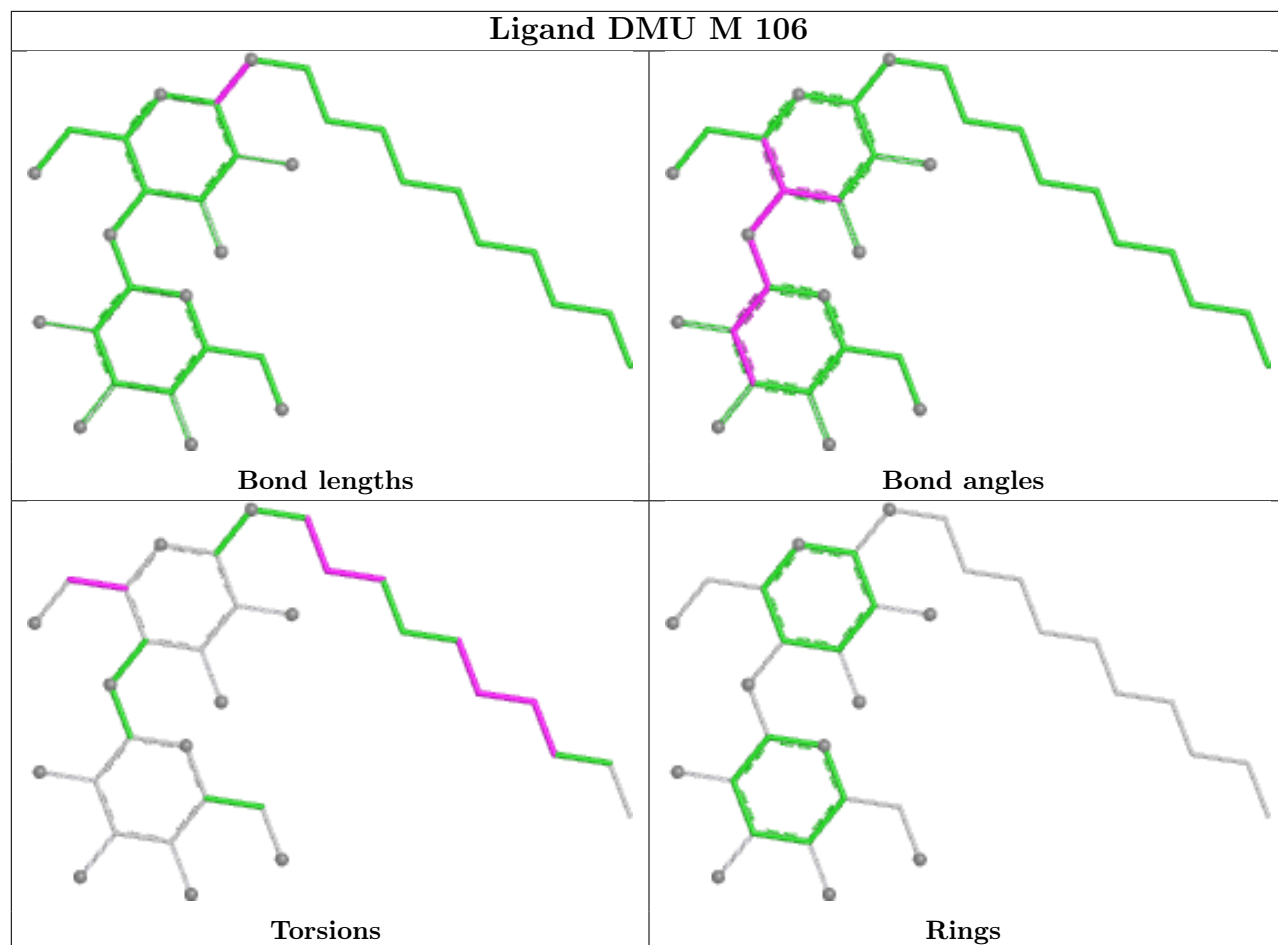


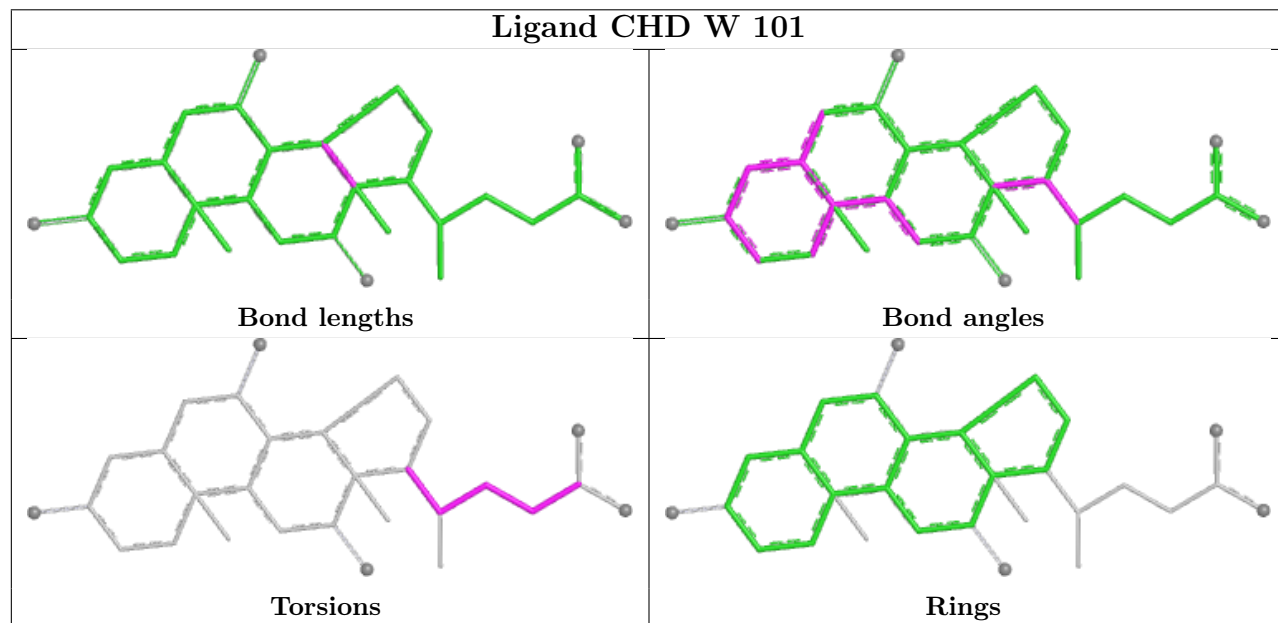
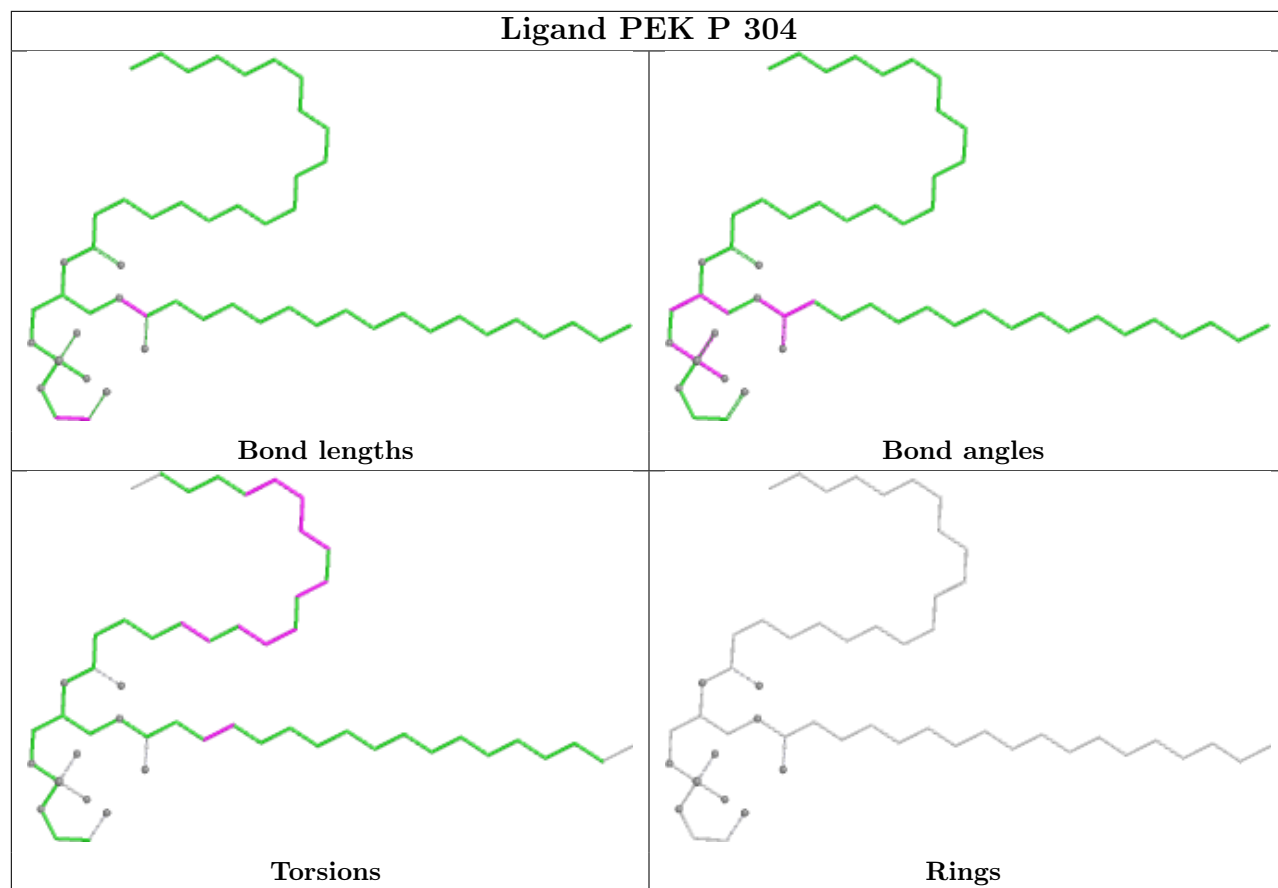


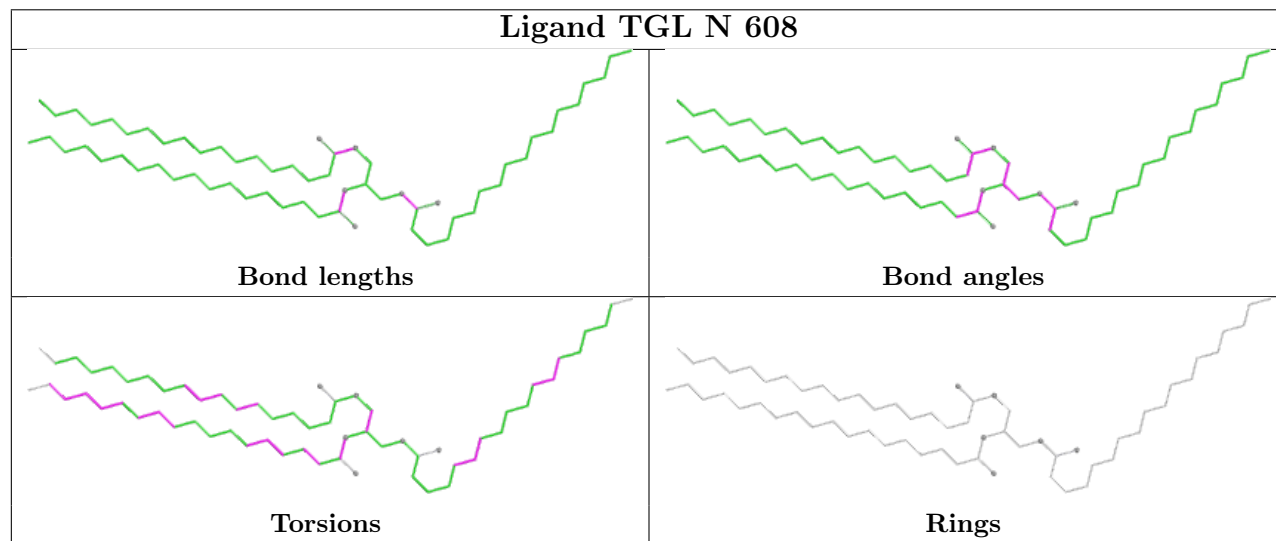
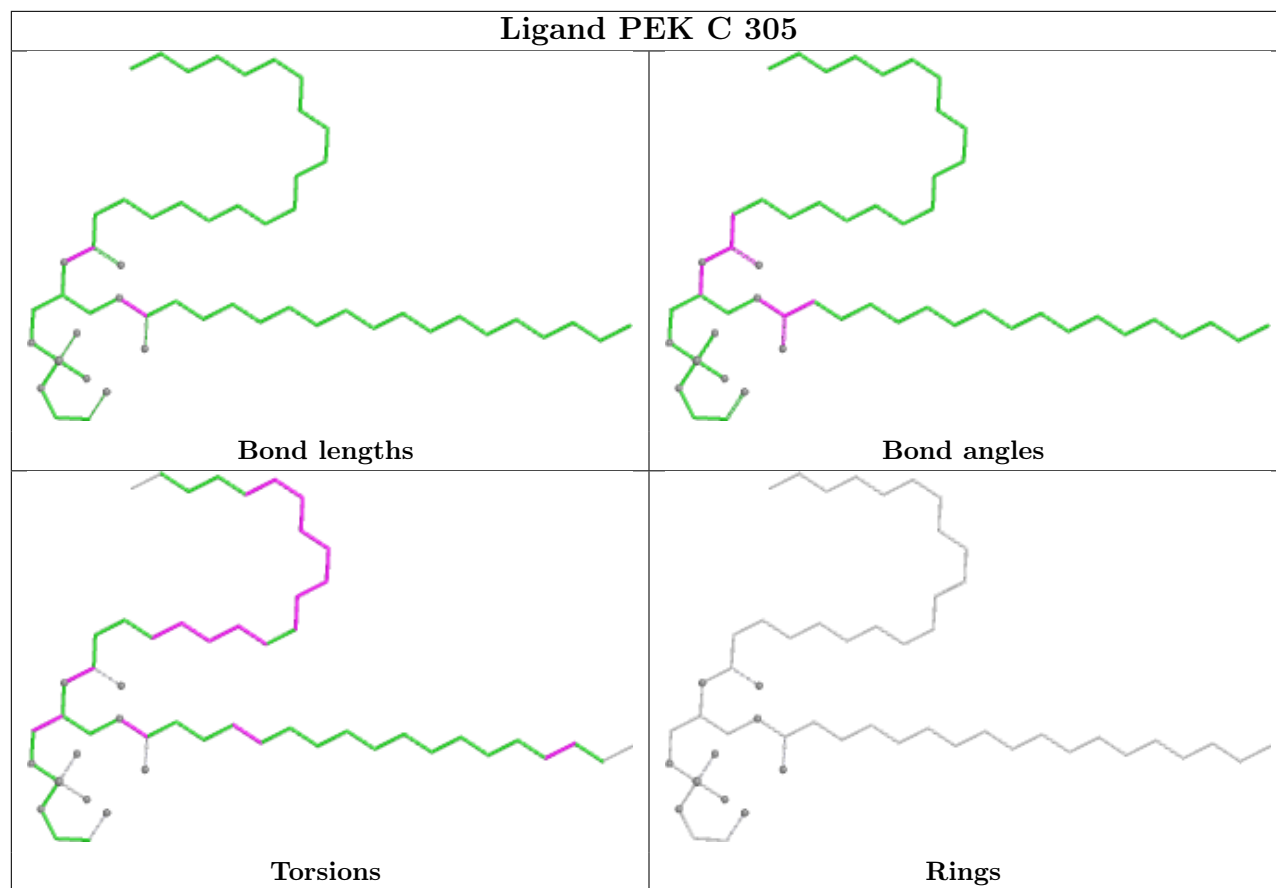


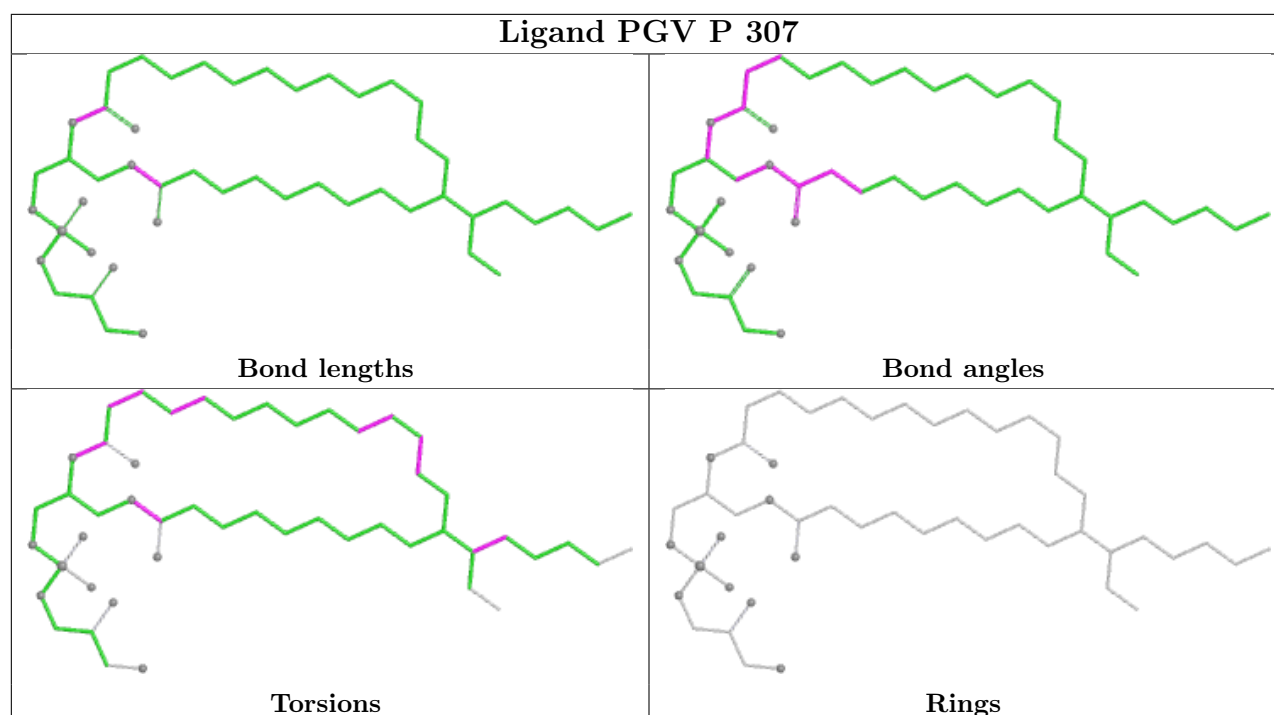












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.34	5 (0%) 79 82	10, 23, 29, 74	30 (5%)
1	N	513/514 (99%)	-0.27	5 (0%) 79 82	11, 25, 33, 69	28 (5%)
2	B	226/227 (99%)	0.29	16 (7%) 22 24	20, 29, 46, 108	11 (4%)
2	O	226/227 (99%)	0.29	14 (6%) 26 29	18, 34, 62, 118	10 (4%)
3	C	259/261 (99%)	0.02	6 (2%) 61 65	17, 26, 38, 84	9 (3%)
3	P	259/261 (99%)	0.19	6 (2%) 61 65	17, 27, 39, 108	11 (4%)
4	D	144/147 (97%)	0.19	6 (4%) 40 45	18, 32, 50, 86	5 (3%)
4	Q	144/147 (97%)	1.04	17 (11%) 9 9	28, 44, 89, 254	3 (2%)
5	E	105/109 (96%)	0.17	5 (4%) 35 39	26, 31, 57, 134	0
5	R	105/109 (96%)	0.37	4 (3%) 44 48	26, 38, 64, 127	0
6	F	94/98 (95%)	0.48	6 (6%) 25 27	22, 32, 61, 160	3 (3%)
6	S	94/98 (95%)	0.52	8 (8%) 16 17	22, 31, 58, 169	3 (3%)
7	G	83/85 (97%)	1.80	22 (26%) 1 1	25, 33, 142, 185	0
7	T	83/85 (97%)	1.77	22 (26%) 1 1	24, 36, 125, 185	1 (1%)
8	H	79/85 (92%)	1.02	14 (17%) 4 3	26, 35, 117, 150	0
8	U	79/85 (92%)	1.06	14 (17%) 4 3	30, 40, 135, 187	0
9	I	72/73 (98%)	1.01	16 (22%) 2 2	28, 42, 71, 85	0
9	V	72/73 (98%)	1.38	23 (31%) 1 1	28, 49, 81, 147	0
10	J	58/59 (98%)	0.95	7 (12%) 8 8	26, 36, 78, 150	0
10	W	58/59 (98%)	0.67	6 (10%) 12 12	27, 37, 80, 213	0
11	K	49/56 (87%)	0.68	3 (6%) 27 29	28, 36, 50, 82	0
11	X	49/56 (87%)	1.04	7 (14%) 6 5	35, 44, 76, 96	0
12	L	46/47 (97%)	0.16	2 (4%) 40 44	24, 28, 44, 108	2 (4%)
12	Y	46/47 (97%)	0.40	4 (8%) 16 17	27, 33, 63, 135	4 (8%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.46	5 (11%) 9 9	24, 29, 69, 120	0
13	Z	43/46 (93%)	0.93	7 (16%) 4 4	31, 37, 96, 250	0
All	All	3542/3614 (98%)	0.31	250 (7%) 22 24	10, 30, 66, 254	120 (3%)

The worst 5 of 250 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	1	ALA	14.8
7	G	3	ALA	13.7
7	G	4	ALA	13.7
6	F	1	ALA	12.6
7	T	3	ALA	12.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.24	0.23	179,194,204,205	0
7	TPO	T	11	11/12	0.41	0.35	140,173,213,214	0
7	TPO	G	11	11/12	0.45	0.29	130,158,180,180	0
9	SAC	I	1	9/10	0.55	0.27	124,152,158,159	0
1	FME	A	1	10/11	0.93	0.11	35,41,68,72	0
1	FME	N	1	10/11	0.94	0.12	35,41,68,69	0
2	FME	B	1	10/11	0.96	0.09	27,29,34,51	0
2	FME	O	1	10/11	0.97	0.09	34,36,41,51	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	EDO	D	206	4/4	0.60	0.48	167,169,170,172	0
20	EDO	B	314	4/4	0.62	0.42	167,168,169,169	0
23	CHD	C	311	29/29	0.63	0.37	104,140,160,162	0
27	DMU	V	102	33/33	0.66	0.23	71,155,170,171	0
23	CHD	P	310	29/29	0.67	0.35	92,136,146,150	0
23	CHD	Y	104	29/29	0.68	0.28	94,123,130,131	0
20	EDO	W	104	4/4	0.68	0.46	80,83,86,86	0
27	DMU	P	324	33/33	0.69	0.25	56,122,149,154	0
20	EDO	S	105	4/4	0.69	0.29	84,88,90,91	0
20	EDO	N	623	4/4	0.70	0.36	90,91,93,94	0
27	DMU	G	108	33/33	0.70	0.23	61,124,156,158	0
20	EDO	A	623	4/4	0.71	0.27	51,66,75,81	0
20	EDO	N	619	4/4	0.72	0.36	85,86,89,89	0
27	DMU	M	106	33/33	0.72	0.21	59,101,127,131	0
27	DMU	Z	102	33/33	0.72	0.24	75,102,117,127	0
14	PGV	P	307	51/51	0.73	0.30	65,96,161,165	0
20	EDO	D	202	4/4	0.73	0.40	83,91,98,99	0
25	PEK	P	305	53/53	0.73	0.33	39,89,206,231	0
26	CDL	P	308	100/100	0.73	0.33	43,112,160,168	0
20	EDO	P	316	4/4	0.73	0.32	53,58,65,66	0
20	EDO	R	205	4/4	0.73	0.26	68,73,75,76	0
14	PGV	C	307	51/51	0.73	0.31	51,91,167,179	0
20	EDO	L	104	4/4	0.73	0.18	58,59,60,60	0
20	EDO	N	618	4/4	0.73	0.25	41,41,44,47	0
27	DMU	C	319	33/33	0.74	0.21	50,98,119,120	0
23	CHD	P	311	29/29	0.74	0.24	80,96,107,109	0
20	EDO	D	205	4/4	0.74	0.25	60,62,71,74	0
25	PEK	C	303	53/53	0.74	0.26	46,134,181,186	0
20	EDO	C	313	4/4	0.74	0.34	56,66,73,73	0
20	EDO	B	309	4/4	0.74	0.42	98,99,99,100	0
20	EDO	S	111	4/4	0.75	0.24	49,52,60,60	0
20	EDO	P	319	4/4	0.75	0.29	47,54,56,58	0
21	TGL	L	101	63/63	0.75	0.29	30,76,115,139	0
20	EDO	P	320	4/4	0.75	0.31	85,85,87,88	0
20	EDO	S	108	4/4	0.75	0.25	43,53,63,69	0
26	CDL	T	101	100/100	0.75	0.30	58,102,162,185	0
20	EDO	K	102	4/4	0.76	0.33	97,97,98,99	0
20	EDO	B	307	4/4	0.76	0.25	60,61,66,67	0
29	PO4	U	102	5/5	0.76	0.23	157,157,158,159	0
20	EDO	B	312	4/4	0.77	0.28	59,63,64,66	0
20	EDO	O	305	4/4	0.77	0.42	89,94,97,99	0
21	TGL	N	608	63/63	0.77	0.24	52,73,109,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
21	TGL	Q	201	63/63	0.77	0.26	53,80,101,104	0
25	PEK	P	303	53/53	0.77	0.26	47,94,170,176	0
23	CHD	C	309	29/29	0.77	0.21	68,78,95,97	0
26	CDL	G	101	100/100	0.77	0.29	55,112,187,207	0
14	PGV	N	601	51/51	0.77	0.26	45,87,144,151	0
20	EDO	U	101	4/4	0.78	0.24	67,70,71,72	0
20	EDO	W	103	4/4	0.78	0.20	47,49,56,57	0
25	PEK	C	305	53/53	0.78	0.26	47,79,141,144	0
20	EDO	P	321	4/4	0.78	0.22	53,61,65,68	0
22	PSC	O	301	52/52	0.78	0.31	35,100,221,227	0
20	EDO	N	617	4/4	0.79	0.25	61,65,70,71	0
20	EDO	J	102	4/4	0.79	0.36	111,111,113,114	0
20	EDO	P	322	4/4	0.79	0.19	57,58,58,60	0
21	TGL	Y	101	63/63	0.79	0.26	42,68,122,141	0
20	EDO	A	614	4/4	0.79	0.36	108,110,111,113	0
14	PGV	A	601	51/51	0.79	0.30	32,79,182,190	0
20	EDO	N	630	4/4	0.79	0.49	94,94,94,97	0
20	EDO	M	103	4/4	0.79	0.27	91,92,94,96	0
20	EDO	P	315	4/4	0.79	0.28	32,50,59,60	0
20	EDO	M	104	4/4	0.79	0.25	57,58,58,66	0
20	EDO	N	616	4/4	0.79	0.17	61,62,63,65	0
21	TGL	B	301	63/63	0.79	0.24	45,67,109,115	0
23	CHD	J	101	29/29	0.80	0.24	101,111,135,139	0
22	PSC	B	302	52/52	0.80	0.31	44,121,206,217	0
20	EDO	N	612	4/4	0.80	0.24	42,50,50,54	0
26	CDL	C	308	100/100	0.80	0.27	41,94,151,153	0
23	CHD	W	101	29/29	0.80	0.22	97,102,131,133	0
20	EDO	D	203	4/4	0.80	0.30	85,87,90,91	0
20	EDO	O	307	4/4	0.80	0.26	85,87,88,89	0
20	EDO	S	110	4/4	0.81	0.16	51,53,58,58	0
20	EDO	G	104	4/4	0.81	0.39	107,109,111,112	0
21	TGL	D	201	63/63	0.81	0.24	36,71,99,104	0
20	EDO	A	622	4/4	0.81	0.20	63,65,67,67	0
27	DMU	C	310	33/33	0.81	0.20	48,101,111,113	0
20	EDO	M	105	4/4	0.81	0.23	35,47,53,56	0
20	EDO	J	103	4/4	0.82	0.19	57,61,65,72	0
20	EDO	G	107	4/4	0.82	0.18	35,50,57,58	0
20	EDO	B	311	4/4	0.82	0.23	79,80,81,82	0
27	DMU	P	309	33/33	0.83	0.19	46,101,136,137	0
27	DMU	P	323	33/33	0.83	0.15	51,88,98,100	0
20	EDO	R	203	4/4	0.83	0.28	60,64,66,68	0
20	EDO	O	306	4/4	0.84	0.30	73,80,80,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	EDO	Y	103	4/4	0.84	0.21	57,57,61,63	0
20	EDO	N	627	4/4	0.84	0.20	64,65,67,70	0
20	EDO	B	310	4/4	0.84	0.34	89,94,97,99	0
18	NA	C	302	1/1	0.84	0.33	809,809,809,809	0
20	EDO	A	624	4/4	0.85	0.13	58,59,60,64	0
20	EDO	A	625	4/4	0.85	0.16	50,54,60,61	0
20	EDO	T	103	4/4	0.85	0.16	40,46,48,51	0
20	EDO	H	101	4/4	0.85	0.22	56,57,62,63	0
20	EDO	P	314	4/4	0.85	0.20	49,50,55,55	0
20	EDO	A	621	4/4	0.85	0.22	40,47,52,55	0
20	EDO	C	316	4/4	0.85	0.19	31,39,40,41	0
20	EDO	F	105	4/4	0.85	0.22	65,68,73,75	0
20	EDO	G	105	4/4	0.86	0.26	74,75,75,77	0
20	EDO	Y	102	4/4	0.86	0.13	59,59,61,65	0
20	EDO	C	318	4/4	0.86	0.16	39,53,59,60	0
20	EDO	V	101	4/4	0.86	0.21	60,65,68,71	0
20	EDO	W	102	4/4	0.86	0.20	58,59,62,67	0
20	EDO	Q	202	4/4	0.86	0.19	65,67,71,77	0
20	EDO	D	204[A]	4/4	0.87	0.17	46,55,59,64	1
20	EDO	Q	203	4/4	0.87	0.17	47,58,58,61	0
20	EDO	P	318	4/4	0.87	0.14	38,42,46,46	0
20	EDO	N	629	4/4	0.87	0.40	110,114,115,115	0
20	EDO	P	313	4/4	0.87	0.15	60,62,63,63	0
20	EDO	C	317	4/4	0.87	0.22	75,78,78,79	0
29	PO4	H	104	5/5	0.87	0.14	90,91,95,96	0
20	EDO	A	617	4/4	0.87	0.25	52,56,61,62	0
20	EDO	R	204	4/4	0.88	0.18	68,68,69,70	0
20	EDO	N	625	4/4	0.88	0.22	54,56,58,59	0
20	EDO	L	105	4/4	0.88	0.15	53,55,57,59	0
20	EDO	S	106	4/4	0.88	0.18	40,51,51,56	0
27	DMU	Z	101	33/33	0.88	0.12	37,45,63,69	0
20	EDO	N	628	4/4	0.88	0.17	33,42,47,50	0
20	EDO	R	202	4/4	0.88	0.18	60,61,61,67	0
20	EDO	B	305	4/4	0.88	0.19	50,52,54,54	0
20	EDO	E	202	4/4	0.89	0.18	53,54,56,60	0
20	EDO	B	308	4/4	0.89	0.14	46,50,51,52	0
20	EDO	L	103	4/4	0.89	0.13	56,58,59,64	0
20	EDO	F	107	4/4	0.89	0.14	43,45,57,66	0
20	EDO	D	207	4/4	0.89	0.14	44,44,49,54	0
20	EDO	M	102	4/4	0.90	0.14	61,67,68,69	0
20	EDO	S	112	4/4	0.90	0.15	39,43,45,46	0
20	EDO	S	107	4/4	0.90	0.16	56,62,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	EDO	N	621	4/4	0.90	0.15	47,49,49,50	0
20	EDO	C	314	4/4	0.90	0.17	54,57,62,63	0
20	EDO	N	626	4/4	0.91	0.15	59,60,63,65	0
20	EDO	C	315	4/4	0.91	0.15	29,34,42,48	0
20	EDO	H	102	4/4	0.91	0.14	50,50,54,55	0
20	EDO	G	103	4/4	0.91	0.17	45,49,51,54	0
20	EDO	B	313	4/4	0.91	0.14	39,44,47,48	0
20	EDO	F	103	4/4	0.91	0.15	38,52,57,58	0
20	EDO	L	102	4/4	0.91	0.16	68,70,71,73	0
20	EDO	A	626	4/4	0.91	0.16	30,36,48,52	0
27	DMU	M	101	33/33	0.91	0.10	34,40,57,62	0
20	EDO	A	609	4/4	0.92	0.17	32,46,54,57	0
20	EDO	F	104	4/4	0.92	0.13	32,37,37,42	0
20	EDO	N	615	4/4	0.92	0.14	55,57,57,61	0
20	EDO	A	615	4/4	0.93	0.17	36,41,50,51	0
20	EDO	N	624	4/4	0.93	0.14	29,40,56,67	0
20	EDO	A	613	4/4	0.93	0.14	37,40,48,50	0
20	EDO	H	103	4/4	0.93	0.18	34,38,43,45	0
20	EDO	A	619	4/4	0.93	0.13	33,35,47,48	0
20	EDO	A	620	4/4	0.93	0.12	37,40,42,47	0
20	EDO	S	109	4/4	0.93	0.12	28,39,46,47	0
20	EDO	A	612	4/4	0.93	0.14	39,41,42,42	0
20	EDO	A	627	4/4	0.93	0.15	27,31,37,41	0
18	NA	P	302	1/1	0.94	0.30	17,17,17,17	1
20	EDO	A	618	4/4	0.94	0.14	30,42,54,61	0
20	EDO	E	201	4/4	0.94	0.14	59,62,66,68	0
20	EDO	N	611	4/4	0.95	0.10	36,39,40,41	0
20	EDO	K	101	4/4	0.95	0.09	49,49,50,53	0
20	EDO	P	312	4/4	0.95	0.10	28,34,39,47	0
20	EDO	N	614	4/4	0.95	0.09	36,37,41,44	0
25	PEK	C	304	53/53	0.95	0.14	26,43,87,91	0
20	EDO	A	610	4/4	0.95	0.10	27,27,31,32	0
20	EDO	O	303	4/4	0.95	0.09	29,29,30,30	0
25	PEK	P	304	53/53	0.95	0.13	25,44,95,99	0
23	CHD	C	301	29/29	0.95	0.07	23,27,31,33	0
20	EDO	O	304	4/4	0.95	0.10	40,40,44,46	0
20	EDO	P	317	4/4	0.95	0.14	36,39,40,42	0
20	EDO	N	620	4/4	0.95	0.10	37,38,41,42	0
20	EDO	T	102	4/4	0.95	0.10	31,31,36,38	0
20	EDO	R	201	4/4	0.96	0.08	40,40,41,41	0
14	PGV	C	306	51/51	0.96	0.12	21,28,77,81	0
20	EDO	C	312	4/4	0.96	0.08	31,34,34,35	0

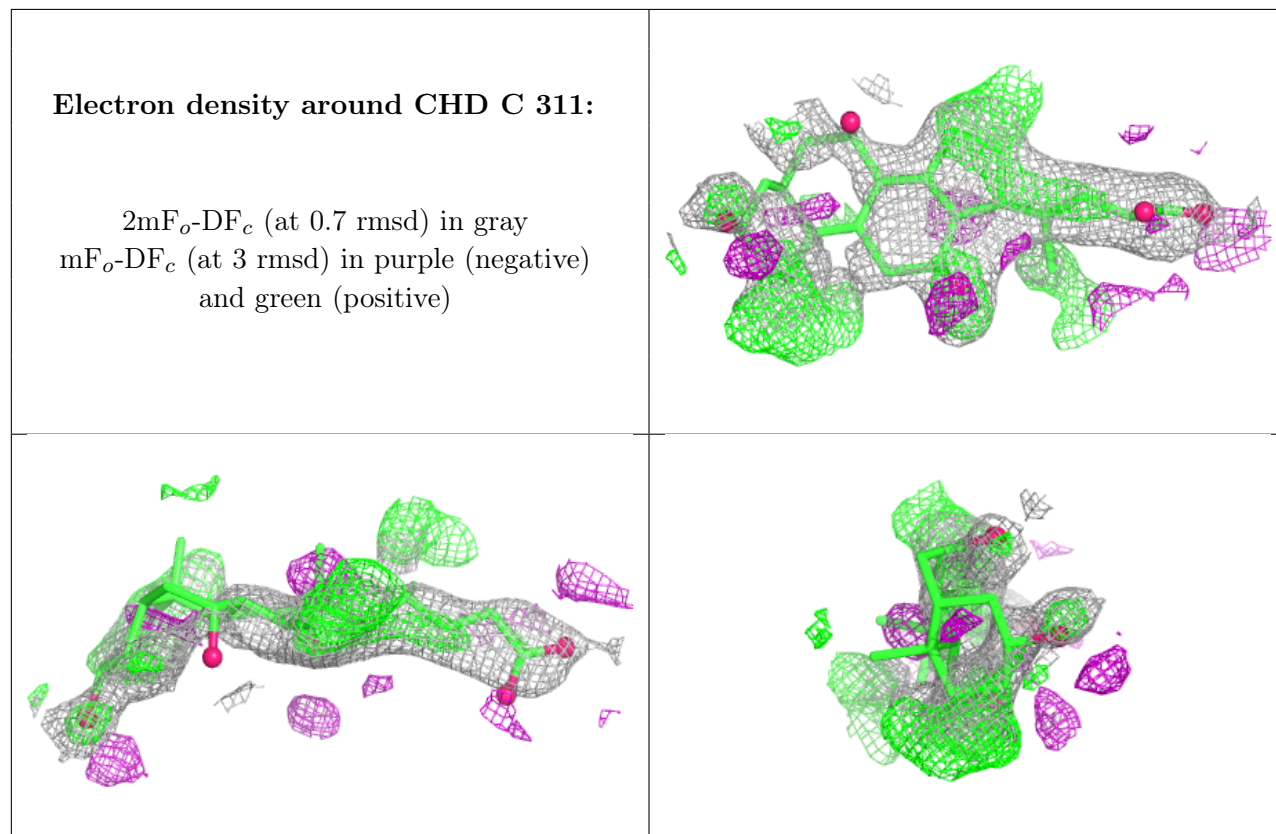
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CHD	B	303	29/29	0.96	0.06	22,25,33,38	0
20	EDO	A	616	4/4	0.96	0.14	28,36,38,38	0
20	EDO	N	610	4/4	0.96	0.11	26,26,26,31	0
20	EDO	S	103	4/4	0.96	0.10	33,34,38,38	0
14	PGV	N	609	51/51	0.96	0.11	22,27,56,61	0
23	CHD	P	301	29/29	0.96	0.07	24,27,32,34	0
20	EDO	S	104	4/4	0.97	0.09	28,29,31,32	0
20	EDO	G	106	4/4	0.97	0.07	28,30,34,36	0
23	CHD	G	102	29/29	0.97	0.06	22,24,28,36	0
14	PGV	P	306	51/51	0.97	0.11	21,30,78,81	0
20	EDO	F	106	4/4	0.97	0.09	29,31,32,35	0
20	EDO	N	622	4/4	0.97	0.12	30,36,38,39	0
14	PGV	A	608	51/51	0.97	0.10	21,26,56,58	0
20	EDO	N	613	4/4	0.97	0.06	22,26,27,30	0
19	CMO	N	607[A]	2/2	0.98	0.13	19,19,19,19	2
19	CMO	N	607[B]	2/2	0.98	0.13	18,18,18,19	2
20	EDO	S	102	4/4	0.98	0.06	22,23,23,23	0
20	EDO	E	203	4/4	0.98	0.06	36,39,40,41	0
20	EDO	B	306	4/4	0.98	0.06	23,23,26,30	0
15	HEA	A	603	60/60	0.98	0.06	18,20,27,30	0
17	MG	A	605	1/1	0.98	0.03	22,22,22,22	0
20	EDO	A	611	4/4	0.98	0.07	21,23,24,27	0
24	CUA	O	302	2/2	0.99	0.04	25,25,25,25	0
15	HEA	A	602[C]	43/60	0.99	0.06	18,20,22,25	1
20	EDO	F	102	4/4	0.99	0.05	22,23,23,25	0
15	HEA	A	602[A]	60/60	0.99	0.06	18,21,28,29	18
19	CMO	A	607[A]	2/2	0.99	0.12	16,16,16,16	2
19	CMO	A	607[B]	2/2	0.99	0.12	16,16,16,16	2
15	HEA	N	602[A]	60/60	0.99	0.06	21,25,30,32	18
15	HEA	N	602[B]	60/60	0.99	0.06	21,25,30,32	18
15	HEA	N	602[C]	43/60	0.99	0.06	21,24,26,27	1
15	HEA	N	603	60/60	0.99	0.05	19,23,28,30	0
28	ZN	F	101	1/1	0.99	0.02	27,27,27,27	0
15	HEA	A	602[B]	60/60	0.99	0.06	18,21,28,30	18
17	MG	N	605	1/1	0.99	0.06	26,26,26,26	0
18	NA	N	606	1/1	1.00	0.02	31,31,31,31	0
16	CU	N	604	1/1	1.00	0.02	23,23,23,23	0
18	NA	A	606	1/1	1.00	0.05	26,26,26,26	0
28	ZN	S	101	1/1	1.00	0.02	27,27,27,27	0
16	CU	A	604	1/1	1.00	0.02	20,20,20,20	0
24	CUA	B	304	2/2	1.00	0.02	21,21,21,21	0

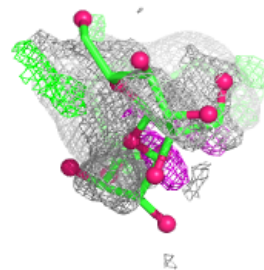
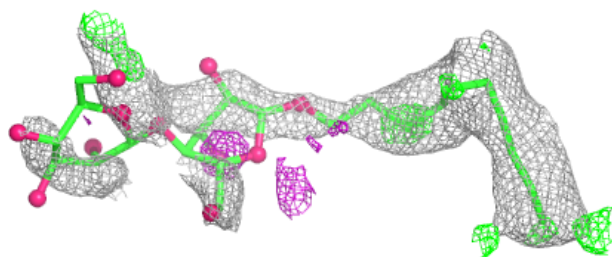
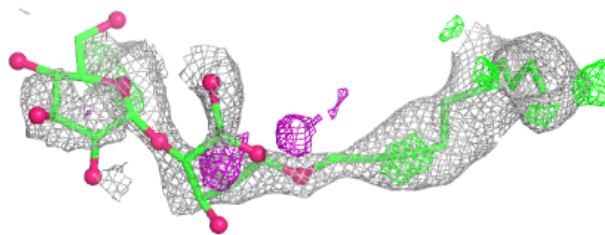
The following is a graphical depiction of the model fit to experimental electron density of all

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

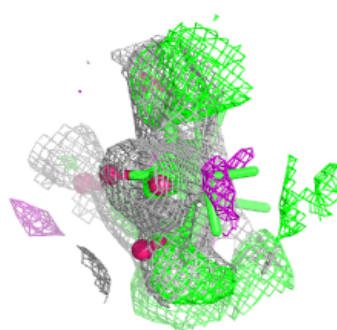
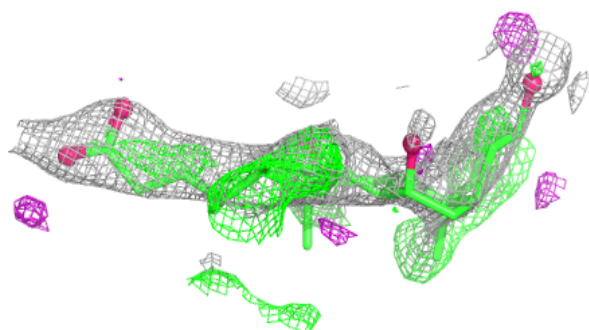
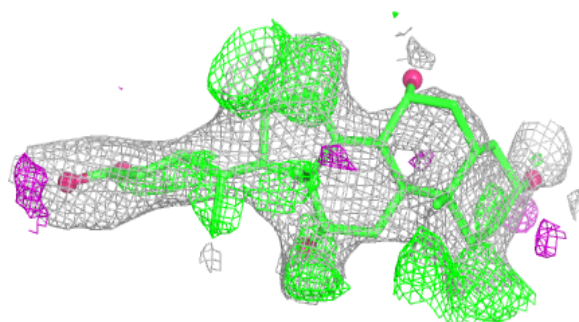


Electron density around DMU V 102:

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

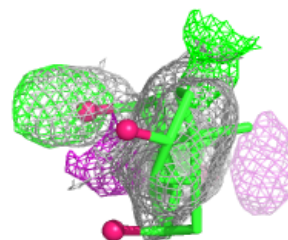
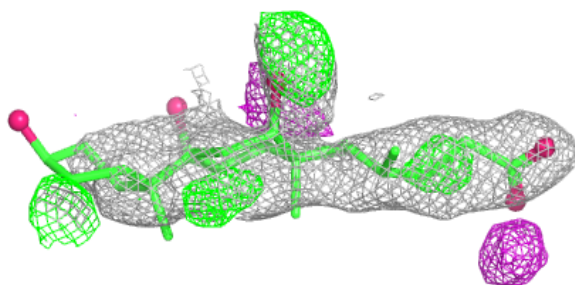
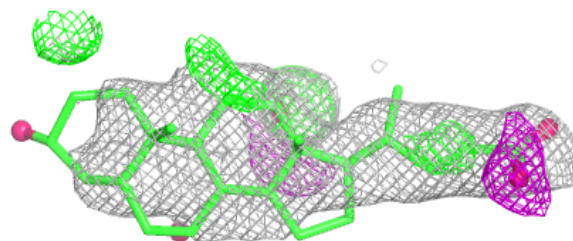
**Electron density around CHD P 310:**

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

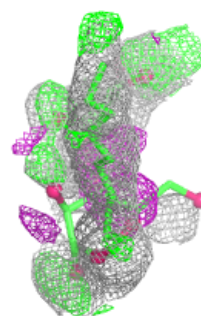
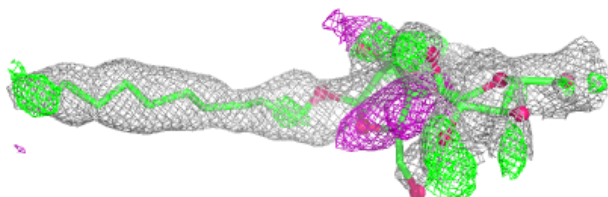
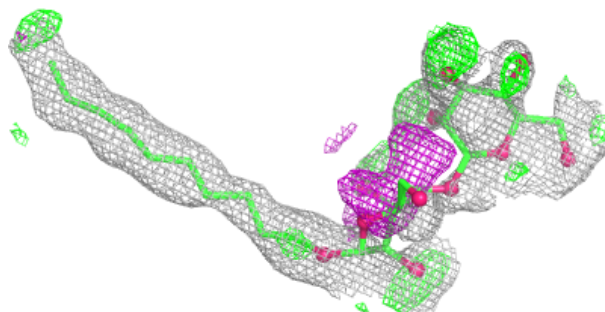


Electron density around CHD Y 104:

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

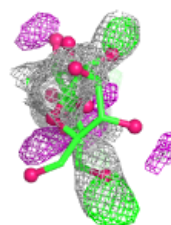
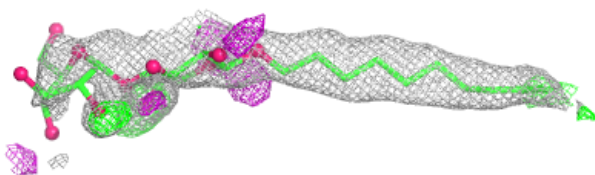
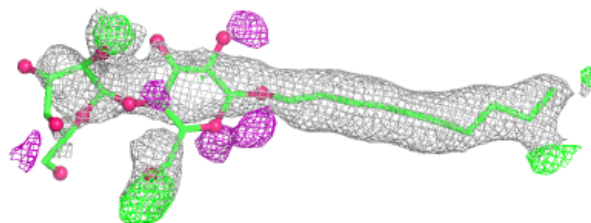
**Electron density around DMU P 324:**

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

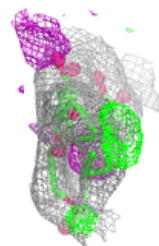
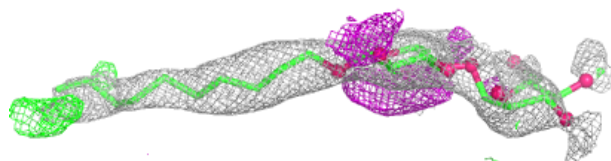
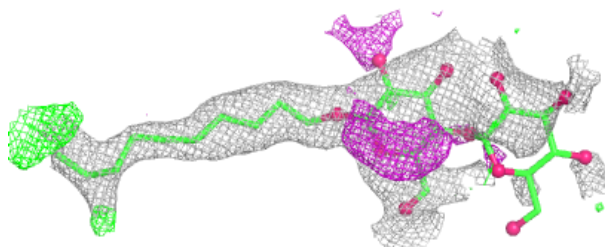


Electron density around DMU G 108:

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

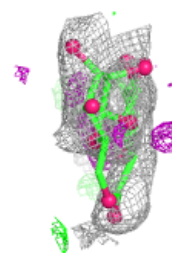
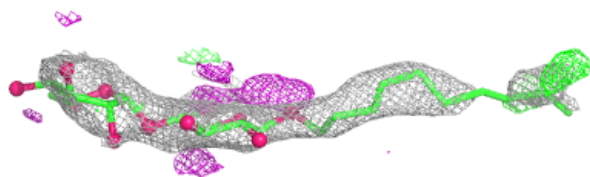
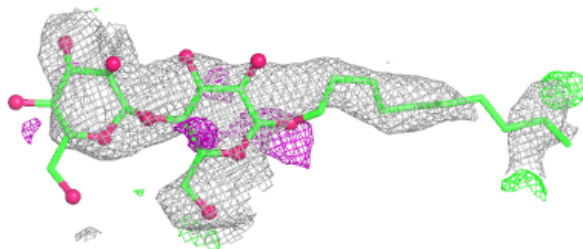
**Electron density around DMU M 106:**

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

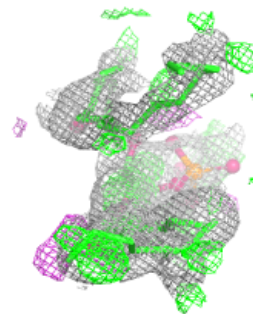
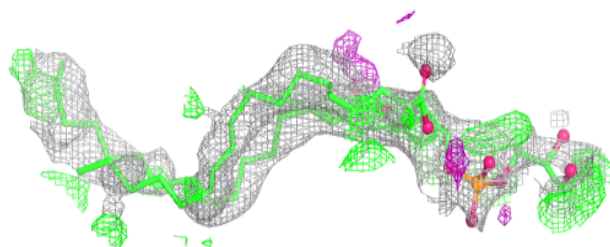
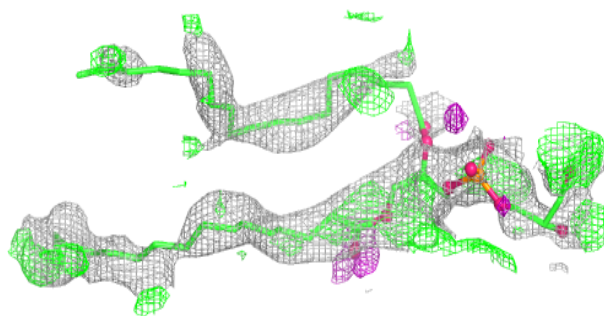


Electron density around DMU Z 102:

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

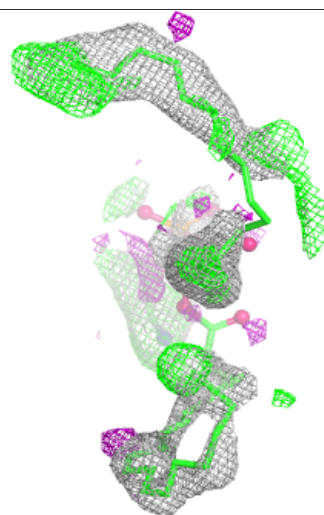
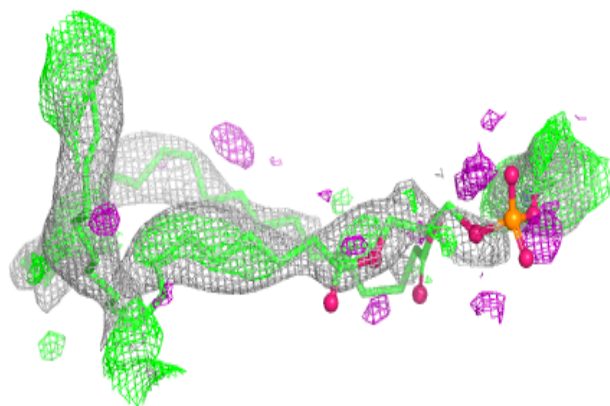
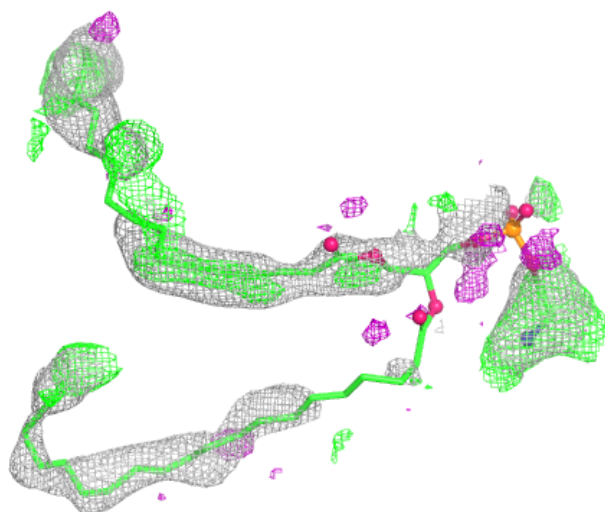
**Electron density around PGV P 307:**

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



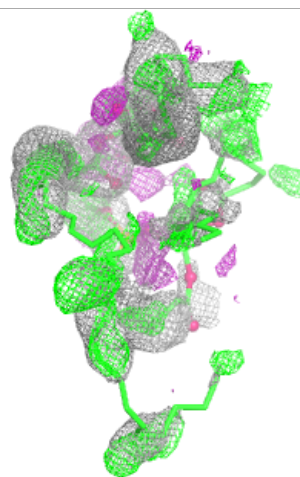
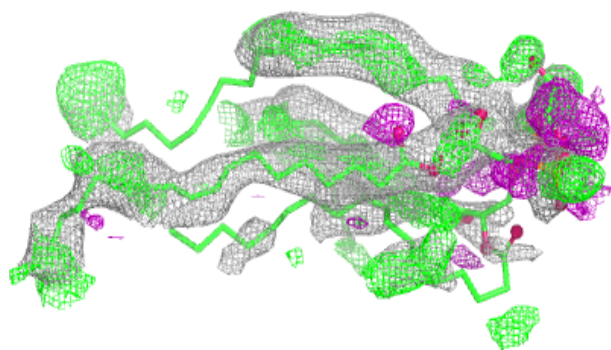
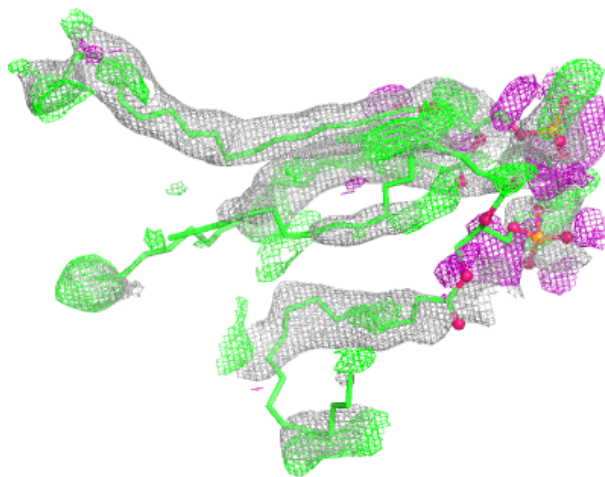
Electron density around PEK P 305:

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



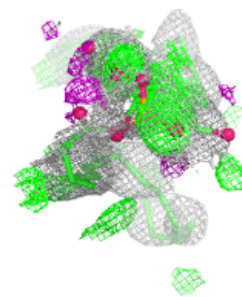
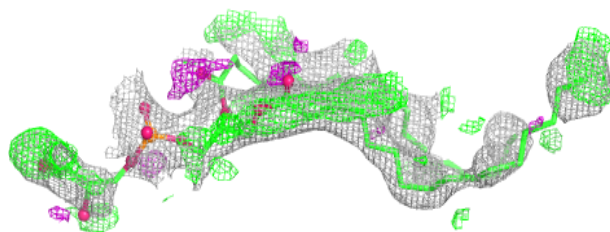
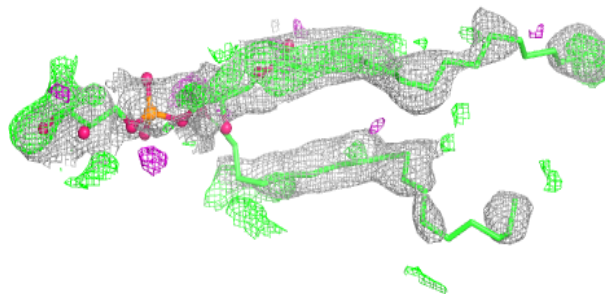
Electron density around CDL P 308:

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

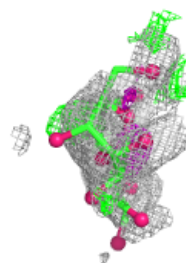
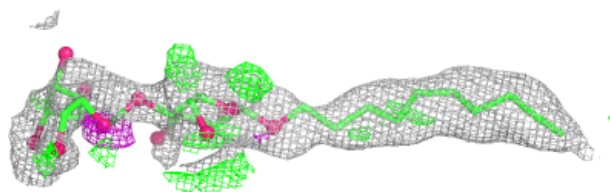
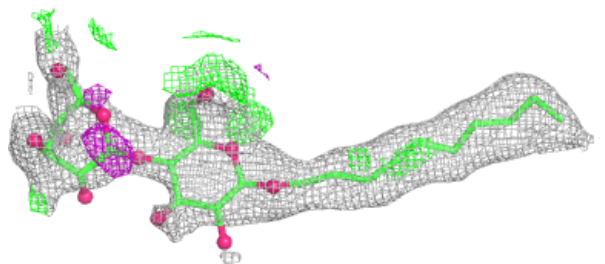


Electron density around PGV C 307:

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

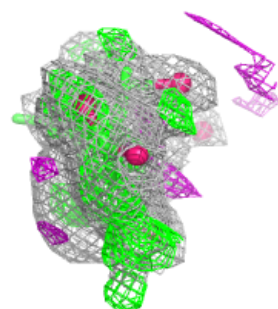
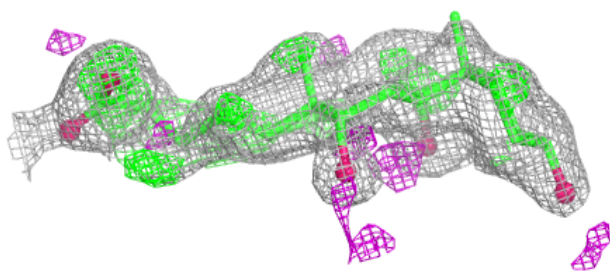
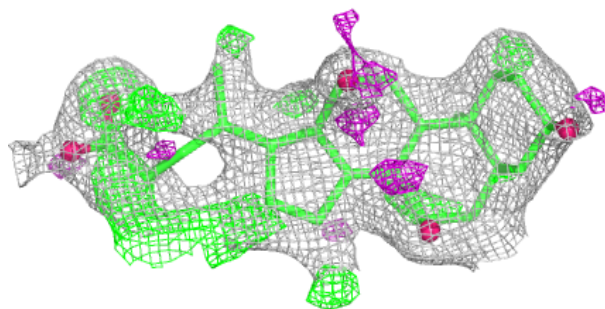
**Electron density around DMU C 319:**

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

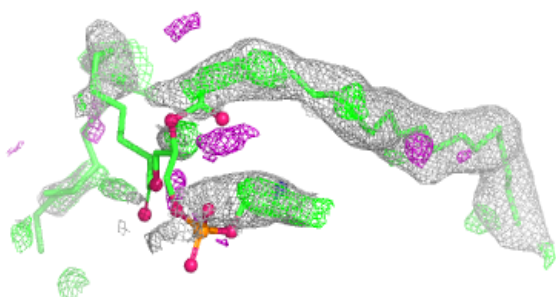
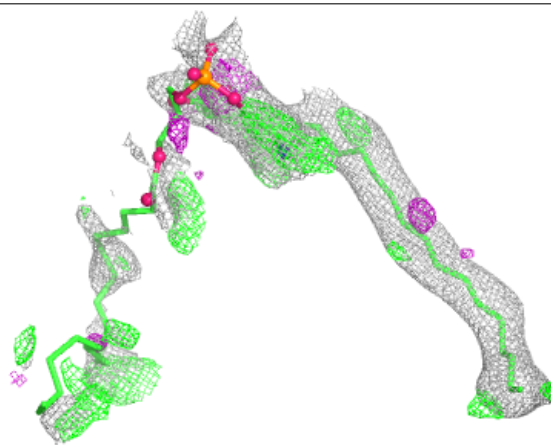


Electron density around CHD P 311:

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

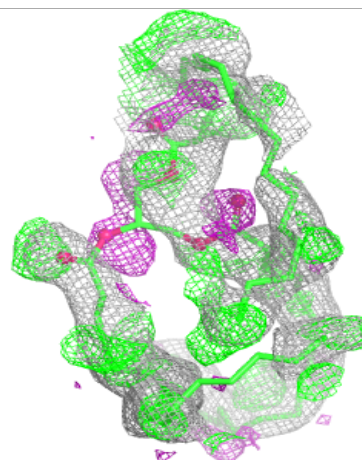
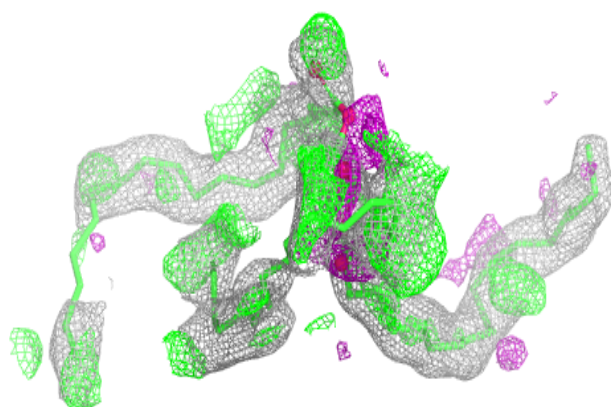
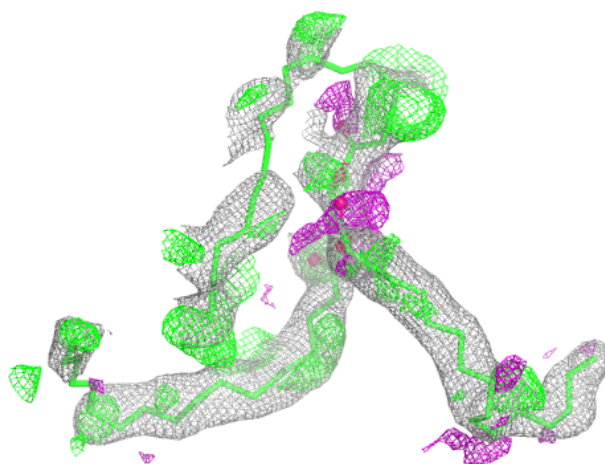
**Electron density around PEK C 303:**

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



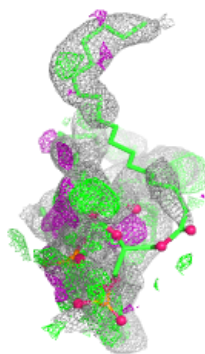
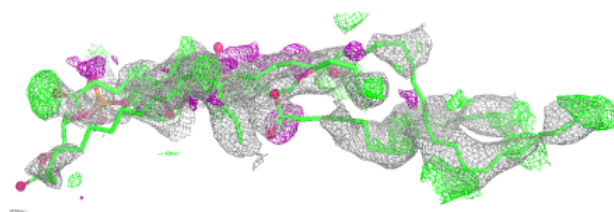
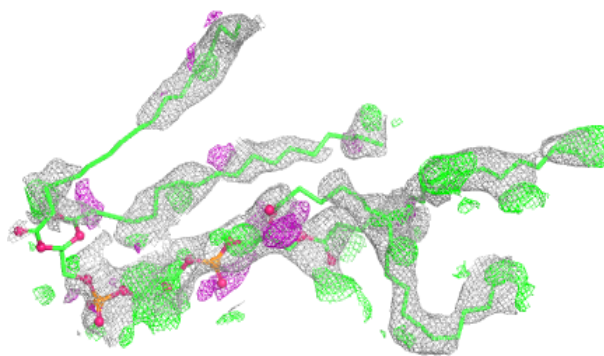
Electron density around TGL L 101:

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

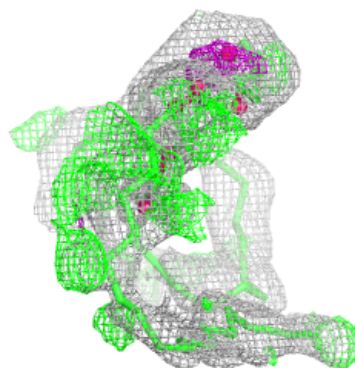
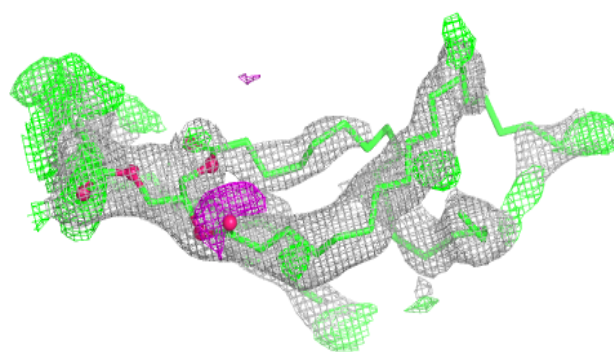
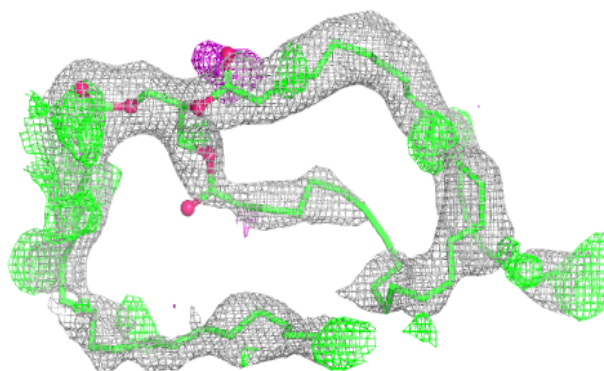


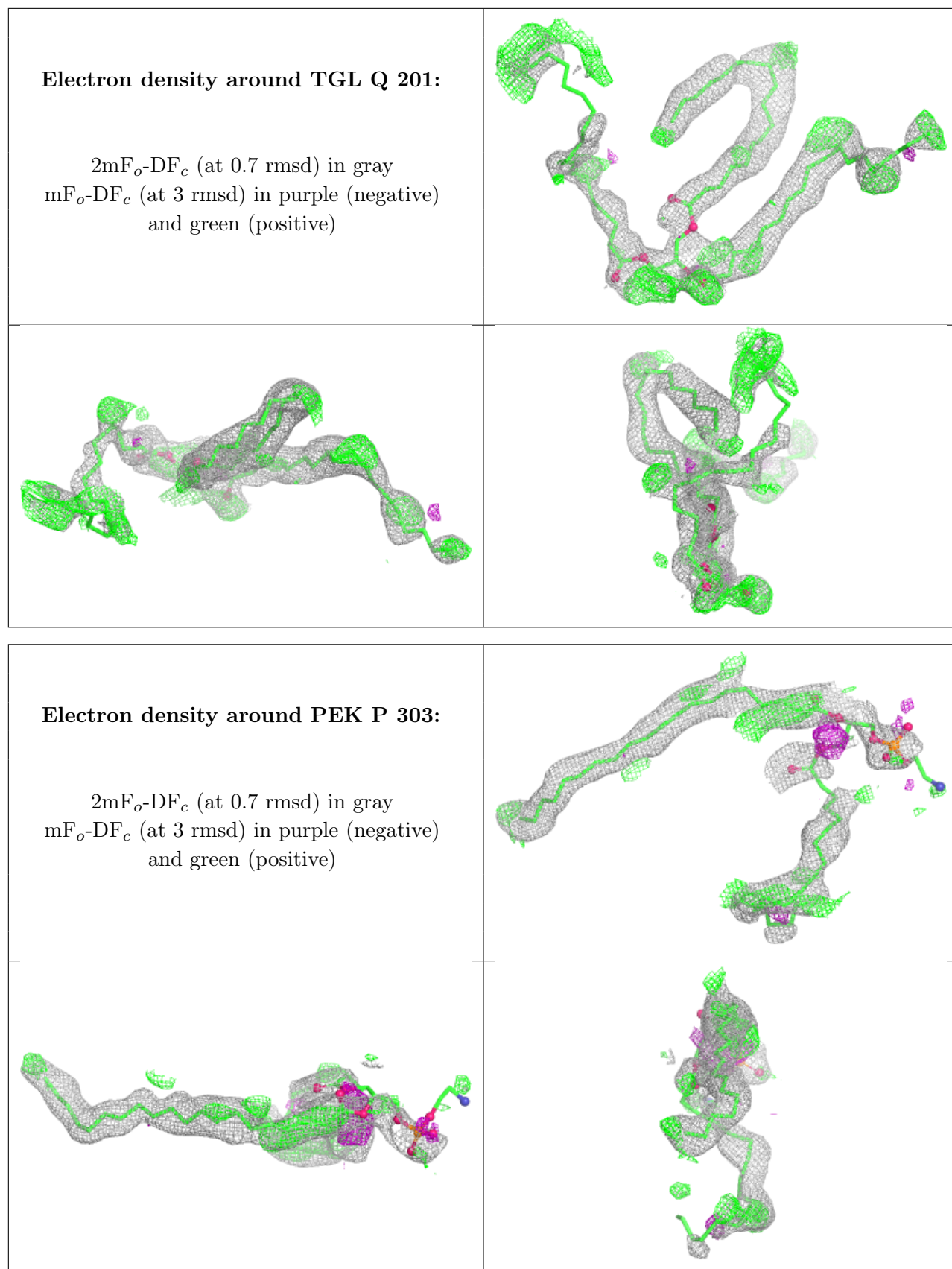
Electron density around CDL T 101:

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

**Electron density around TGL N 608:**

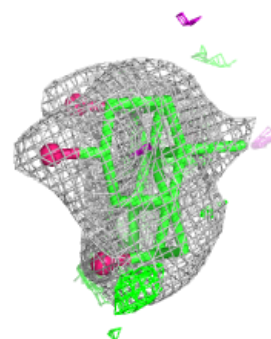
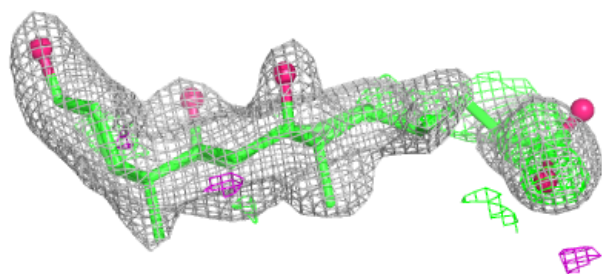
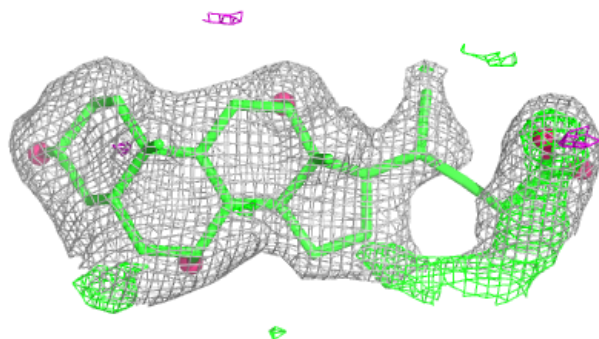
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



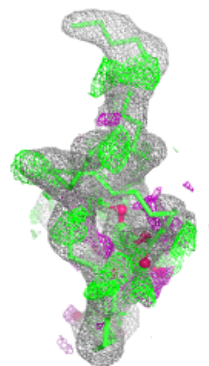
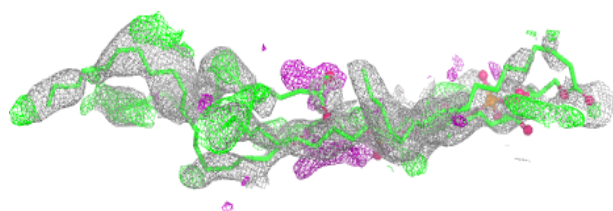
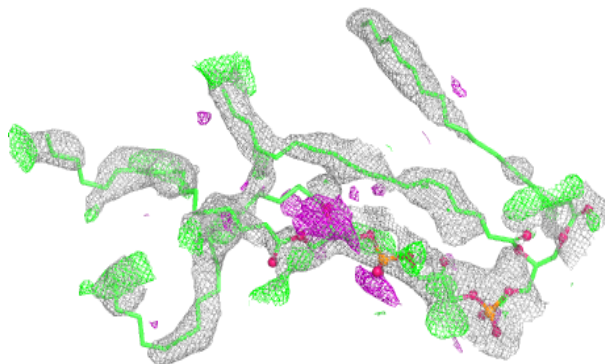


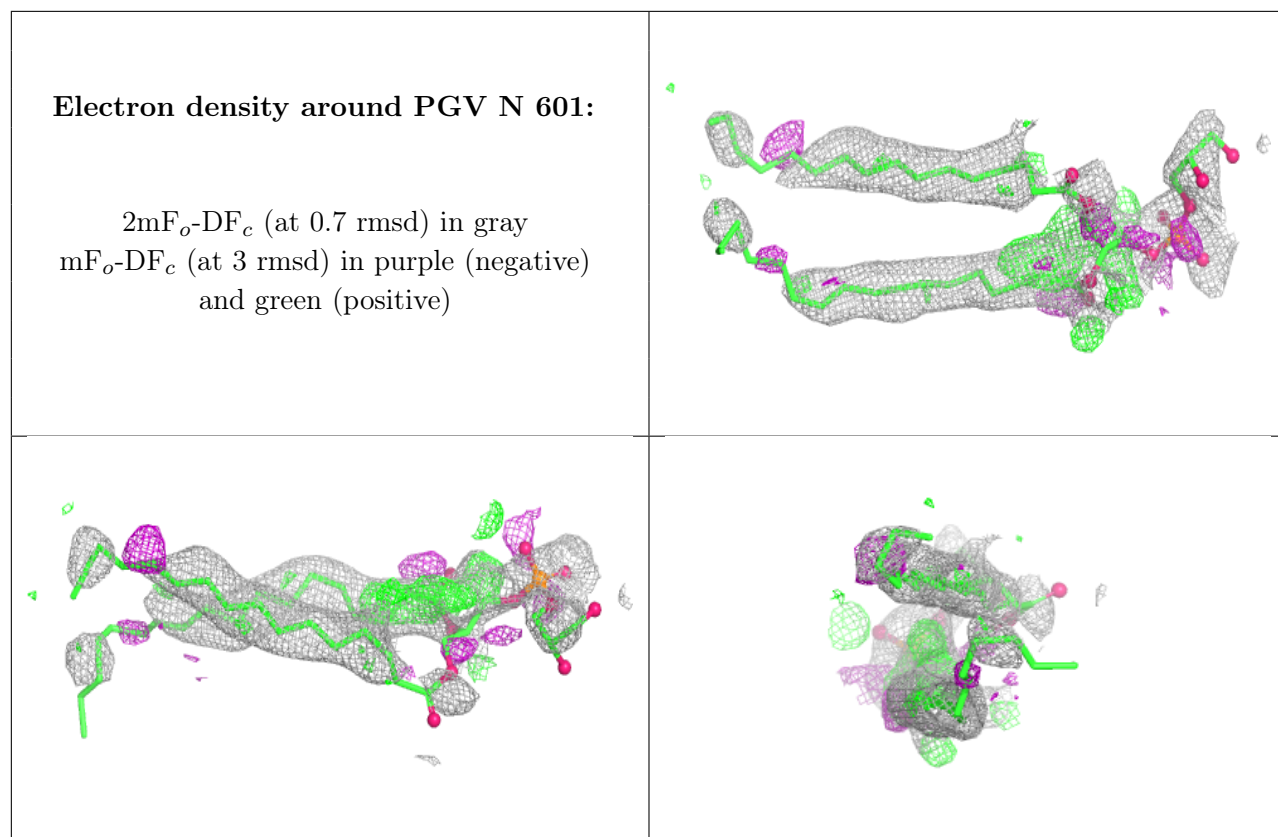
Electron density around CHD C 309:

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

**Electron density around CDL G 101:**

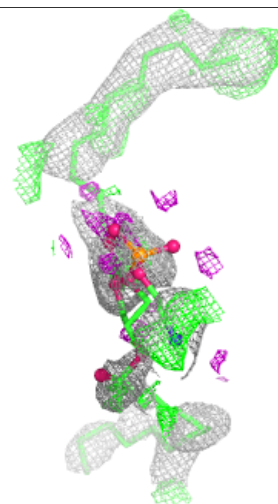
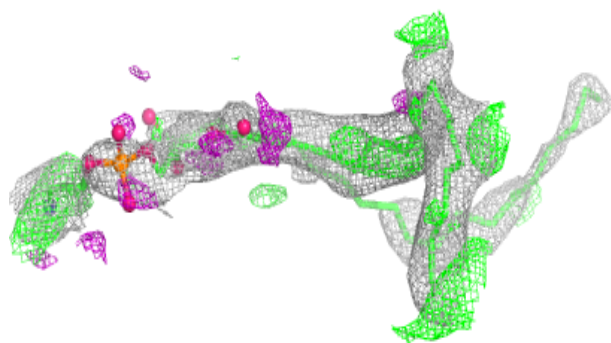
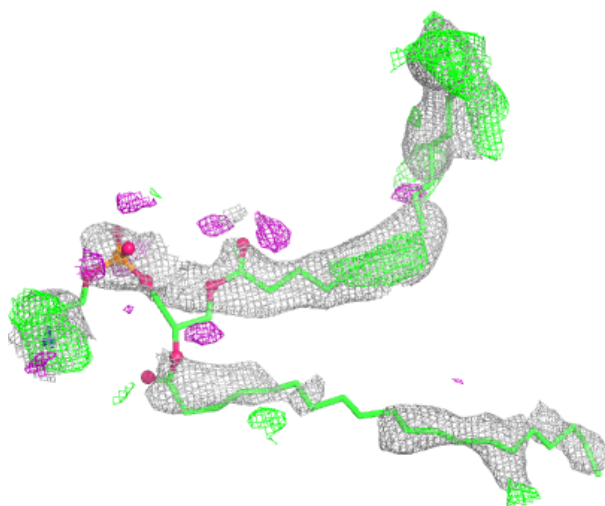
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





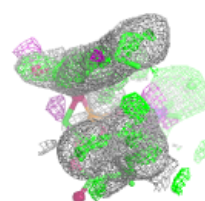
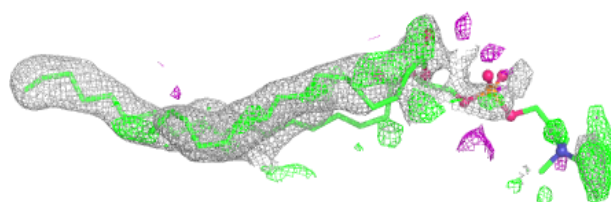
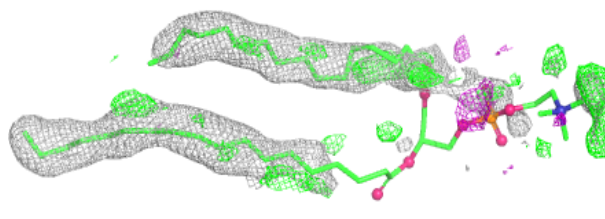
Electron density around PEK C 305:

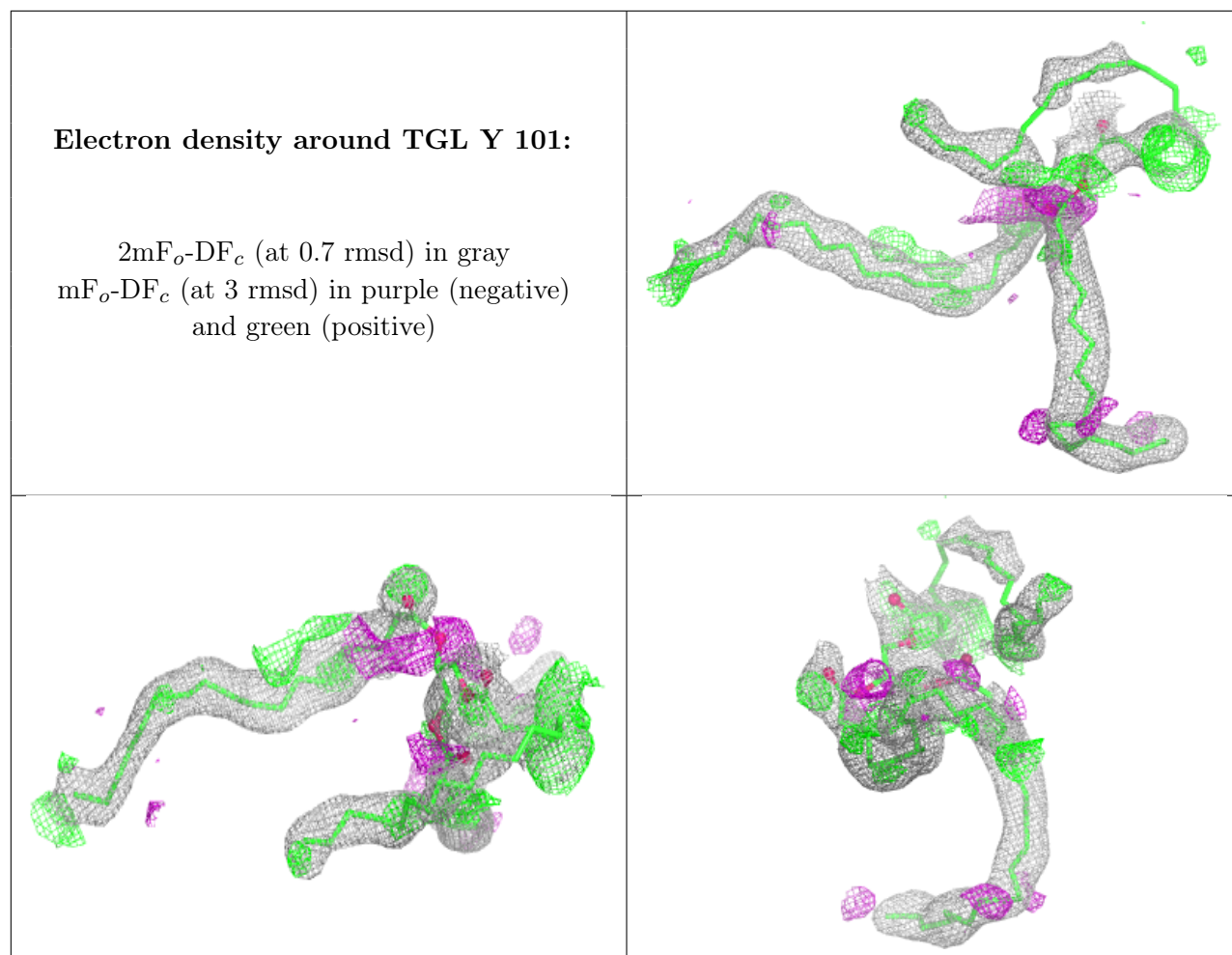
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PSC O 301:

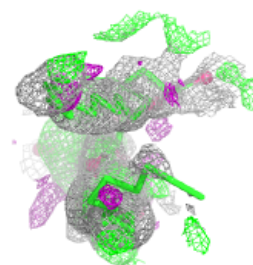
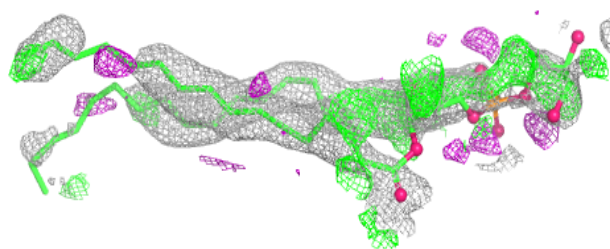
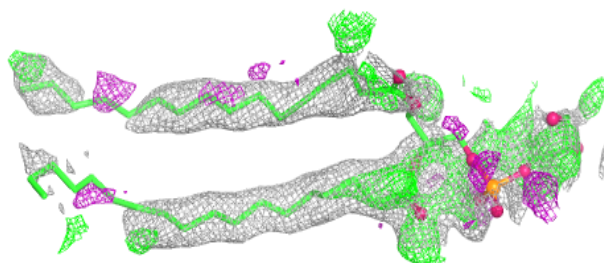
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



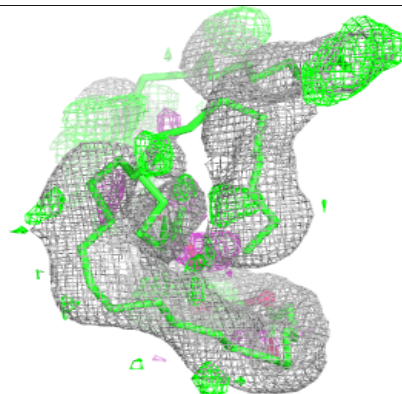
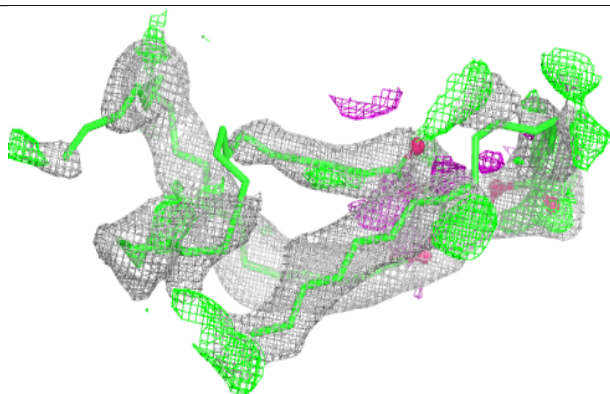
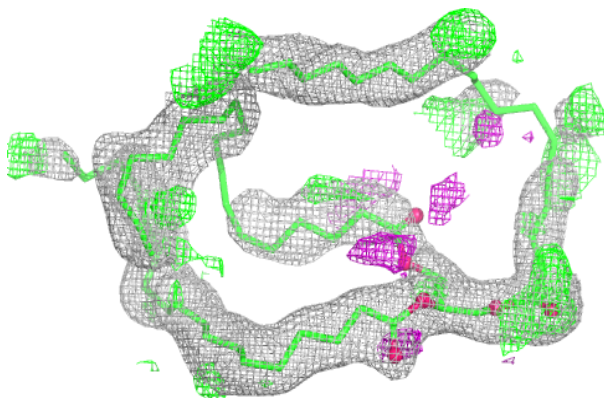


Electron density around PGV A 601:

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

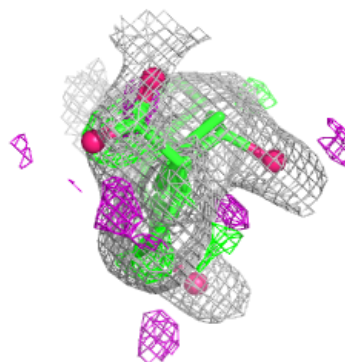
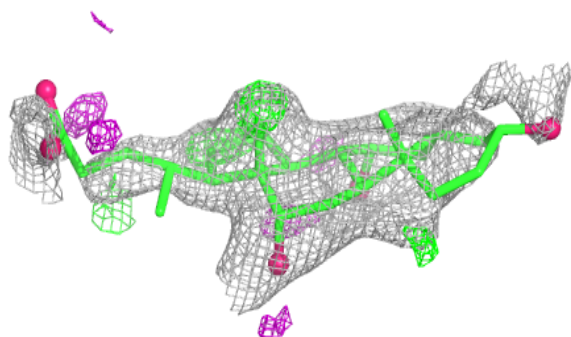
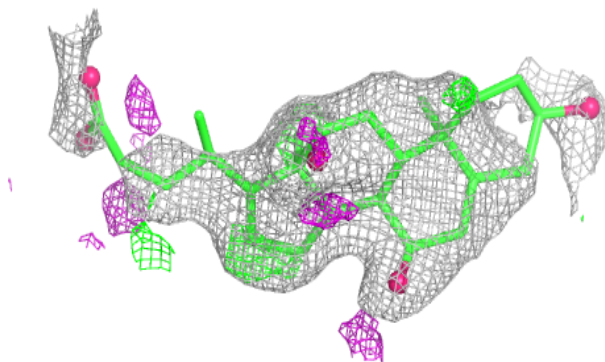
**Electron density around TGL B 301:**

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

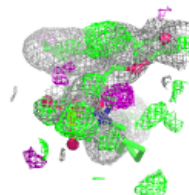
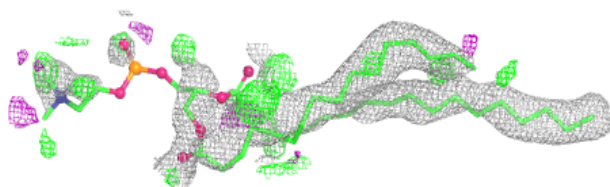
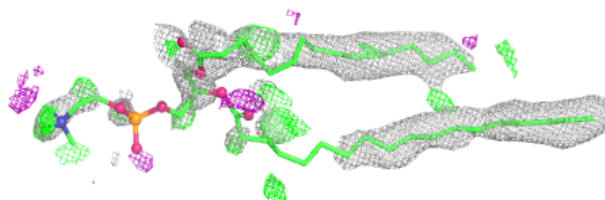


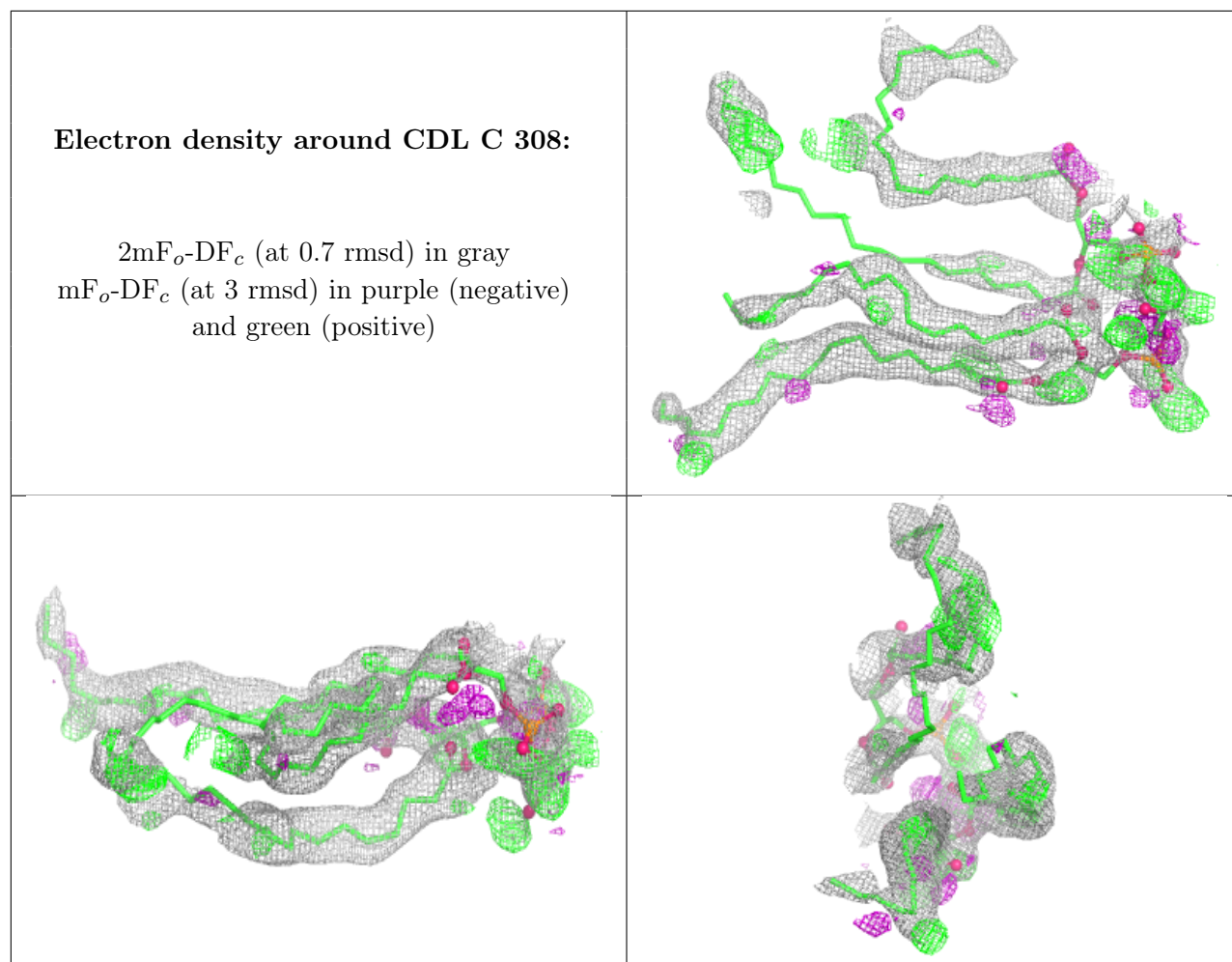
Electron density around CHD J 101:

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

**Electron density around PSC B 302:**

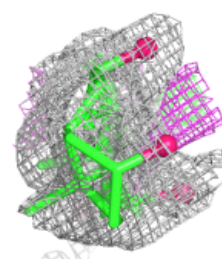
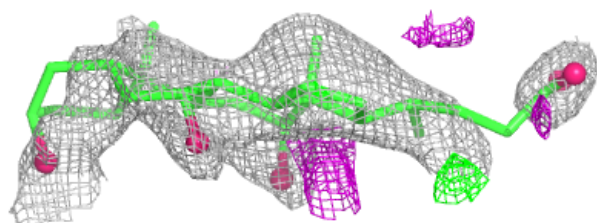
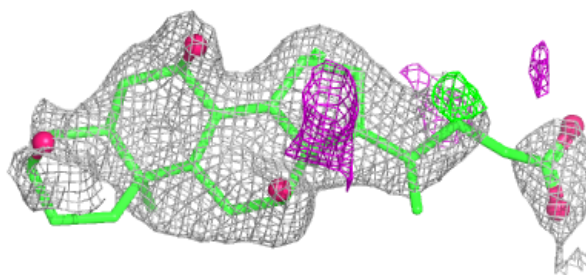
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



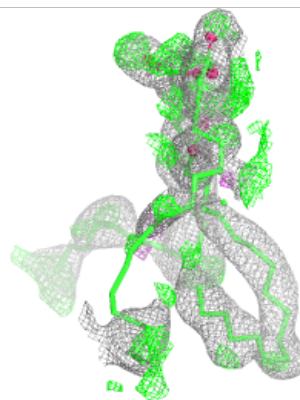
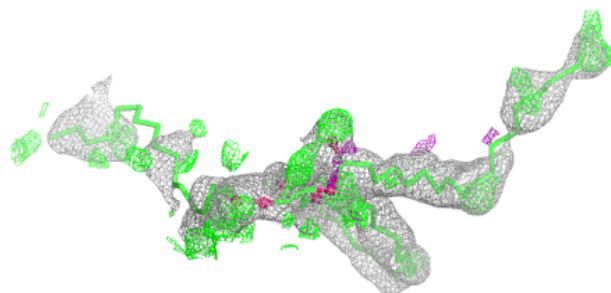
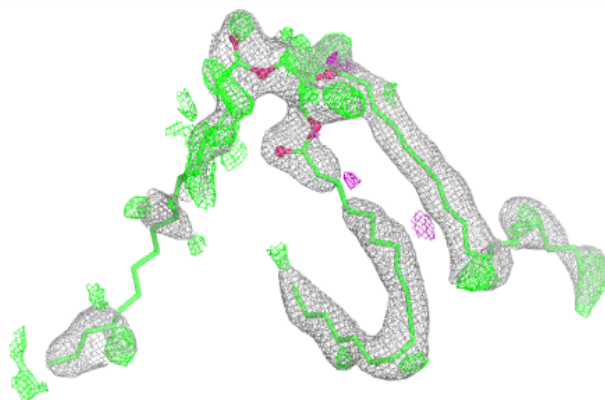


Electron density around CHD W 101:

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

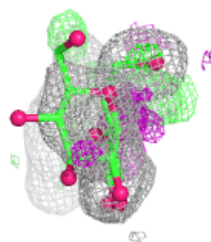
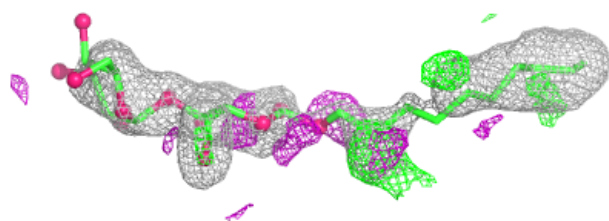
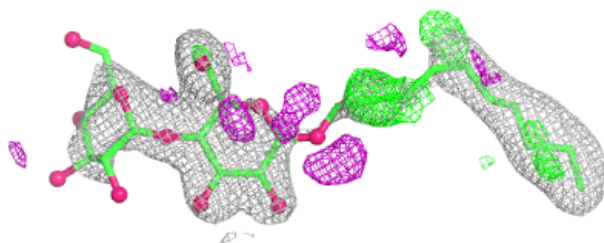
**Electron density around TGL D 201:**

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

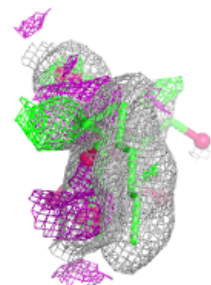
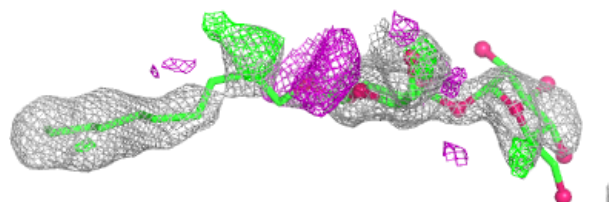
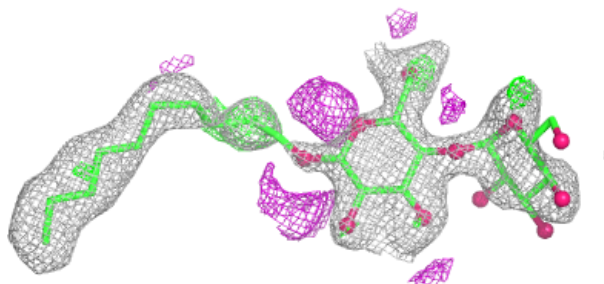


Electron density around DMU C 310:

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

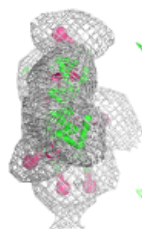
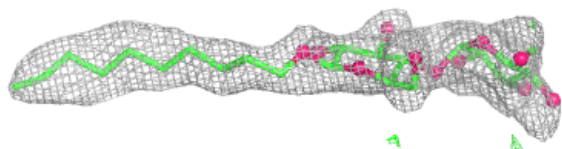
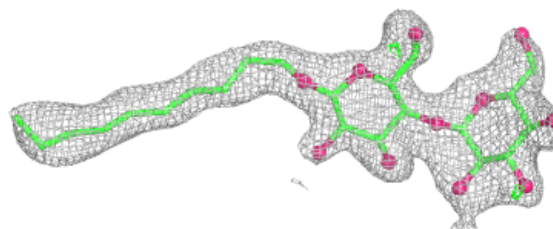
**Electron density around DMU P 309:**

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

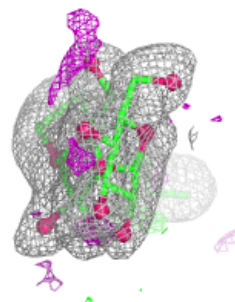
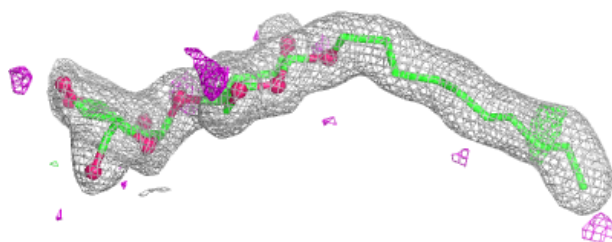
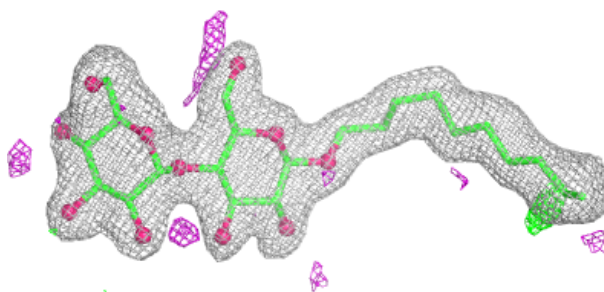


Electron density around DMU P 323:

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

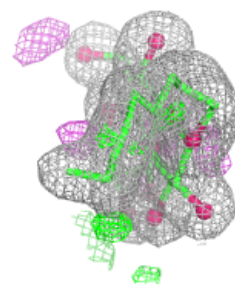
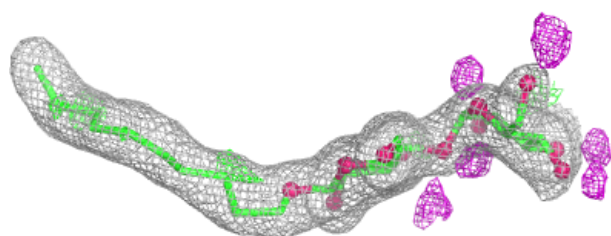
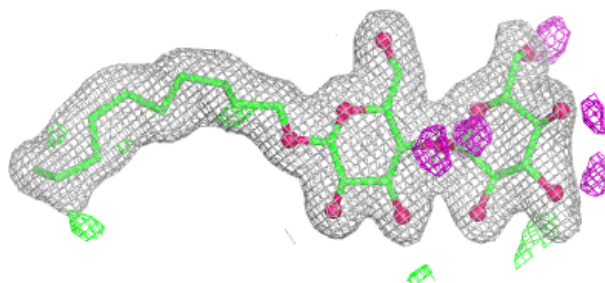
**Electron density around DMU Z 101:**

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

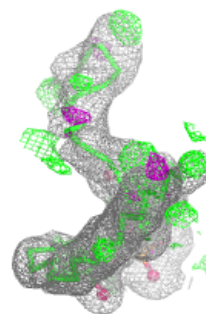
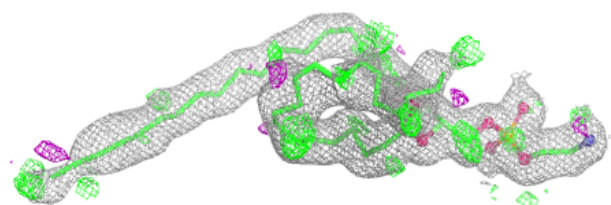
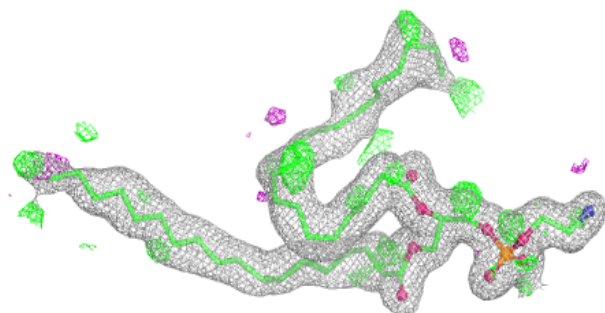


Electron density around DMU M 101:

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

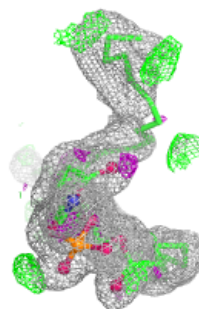
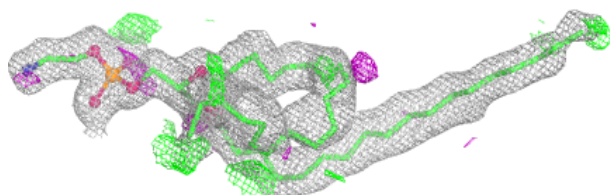
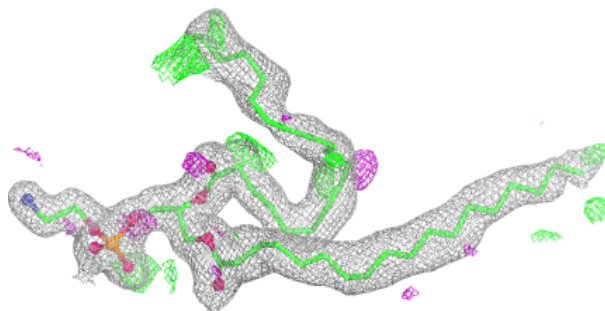
**Electron density around PEK C 304:**

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

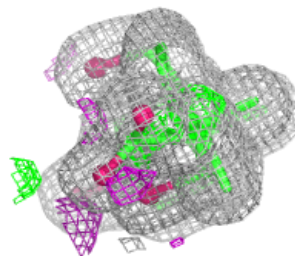
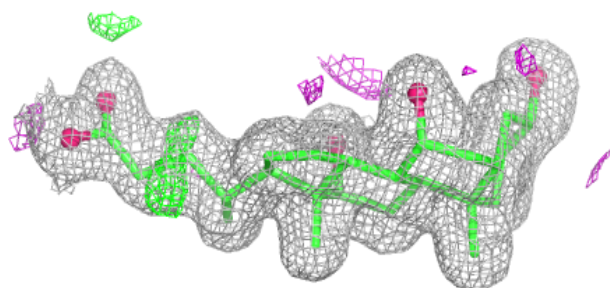
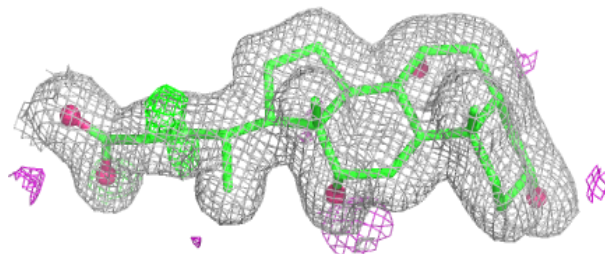


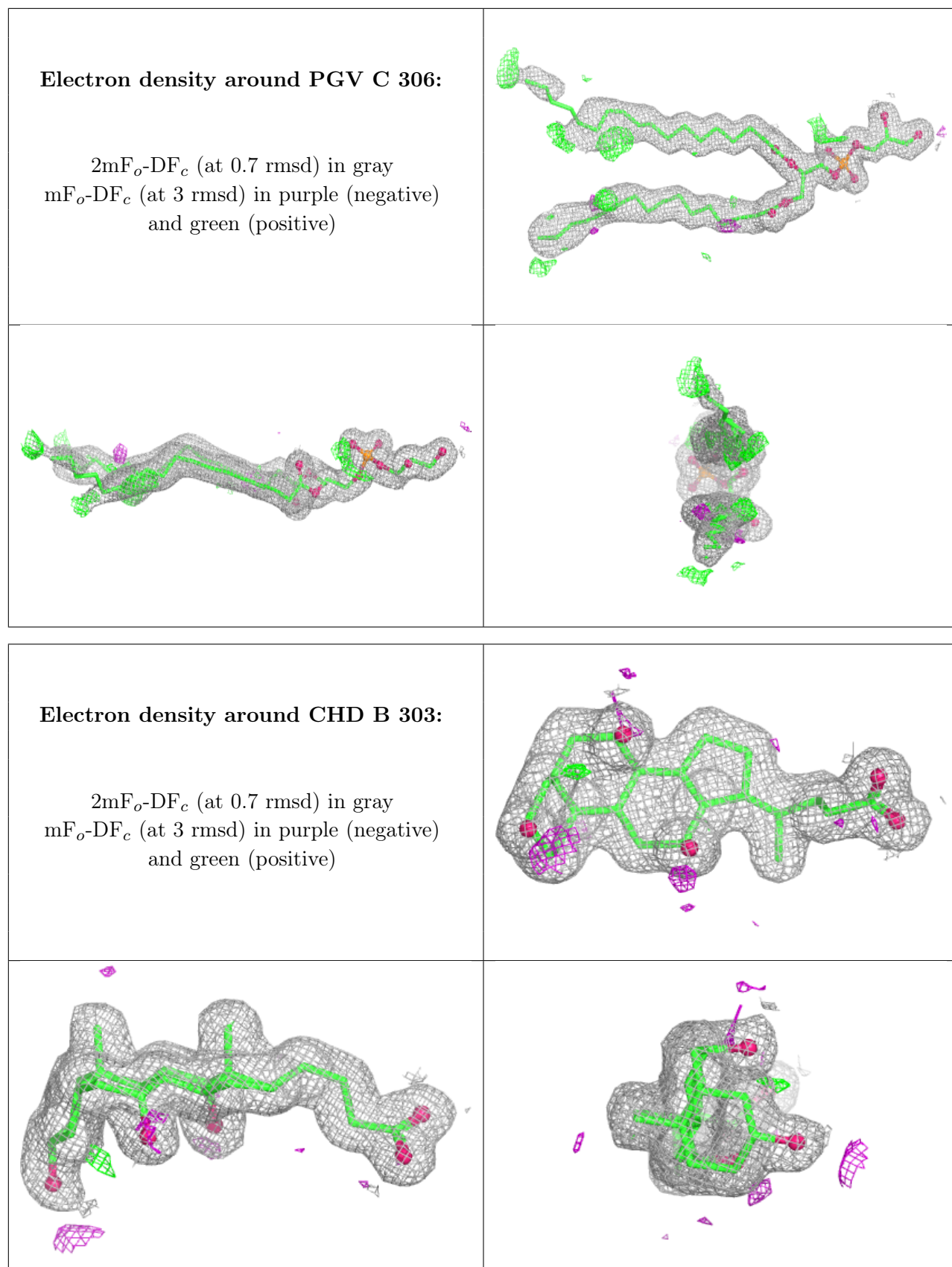
Electron density around PEK P 304:

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

**Electron density around CHD C 301:**

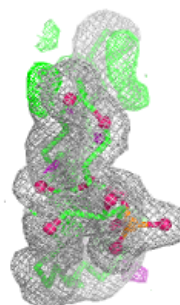
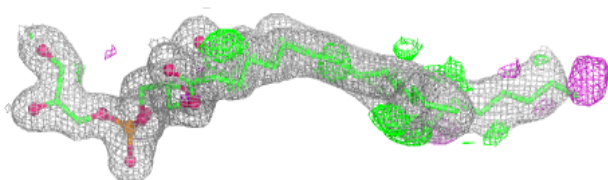
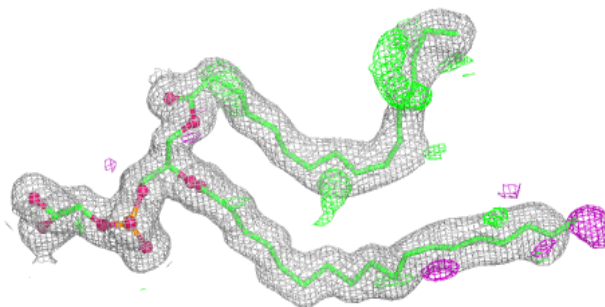
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



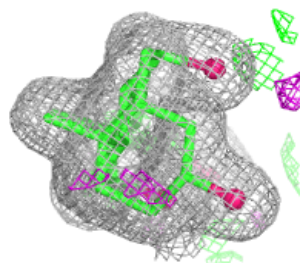
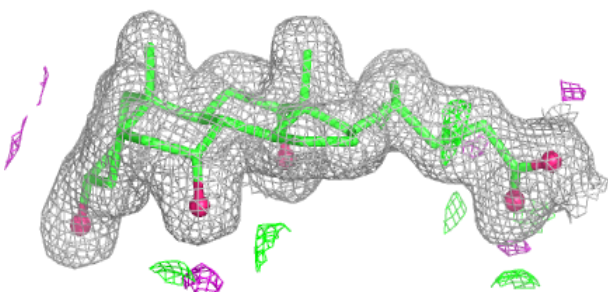
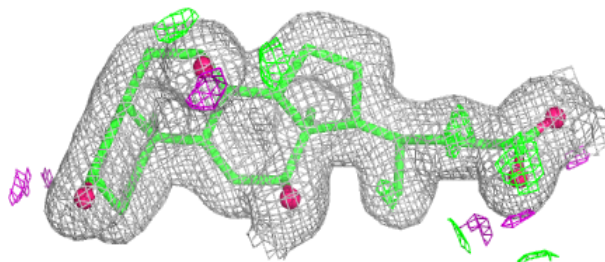


Electron density around PGV N 609:

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

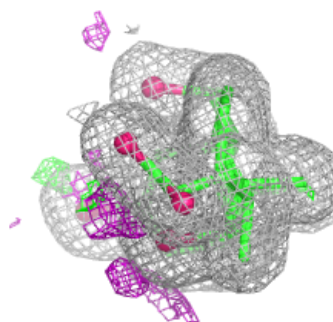
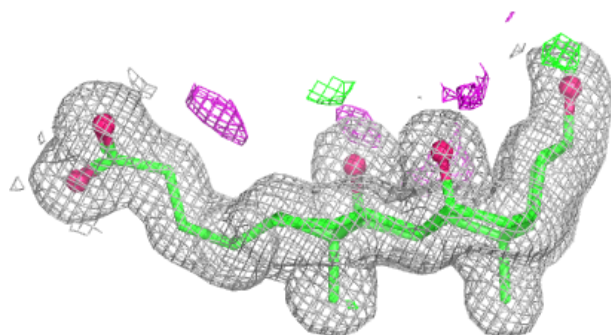
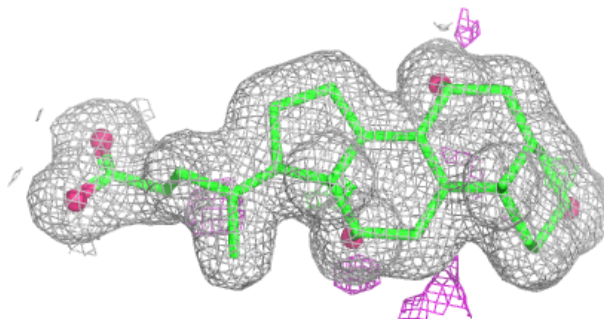
**Electron density around CHD P 301:**

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

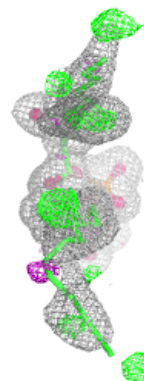
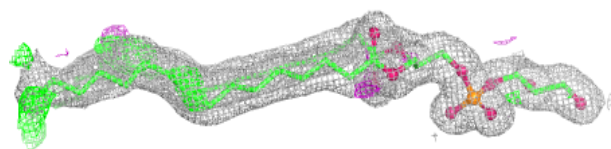
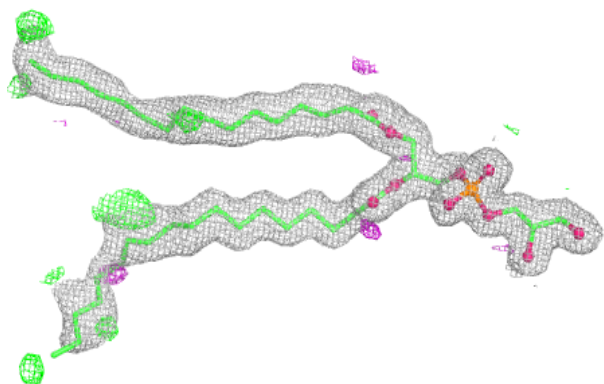


Electron density around CHD G 102:

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

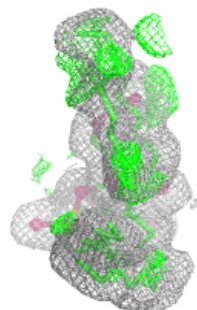
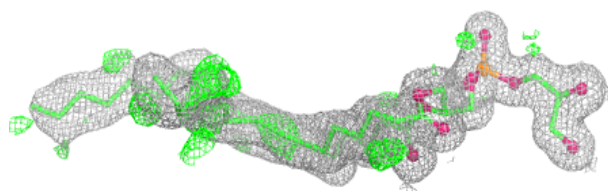
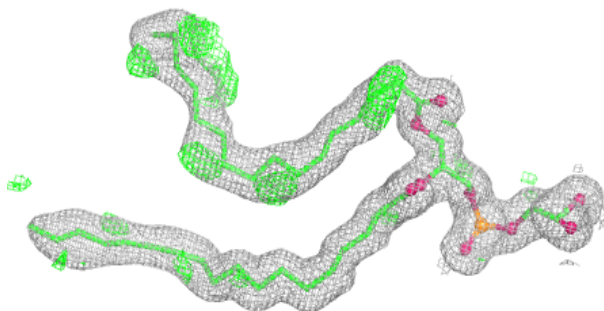
**Electron density around PGV P 306:**

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

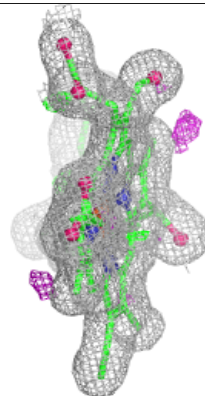
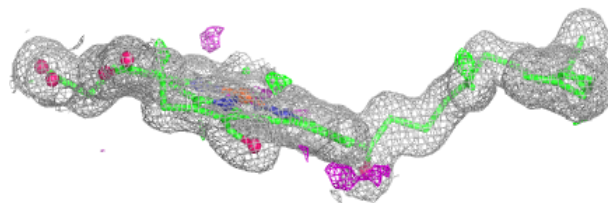
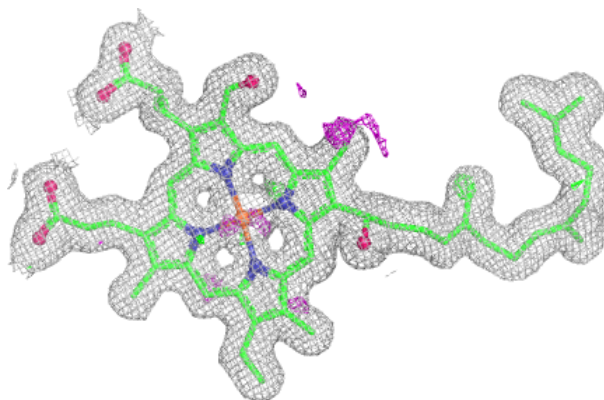


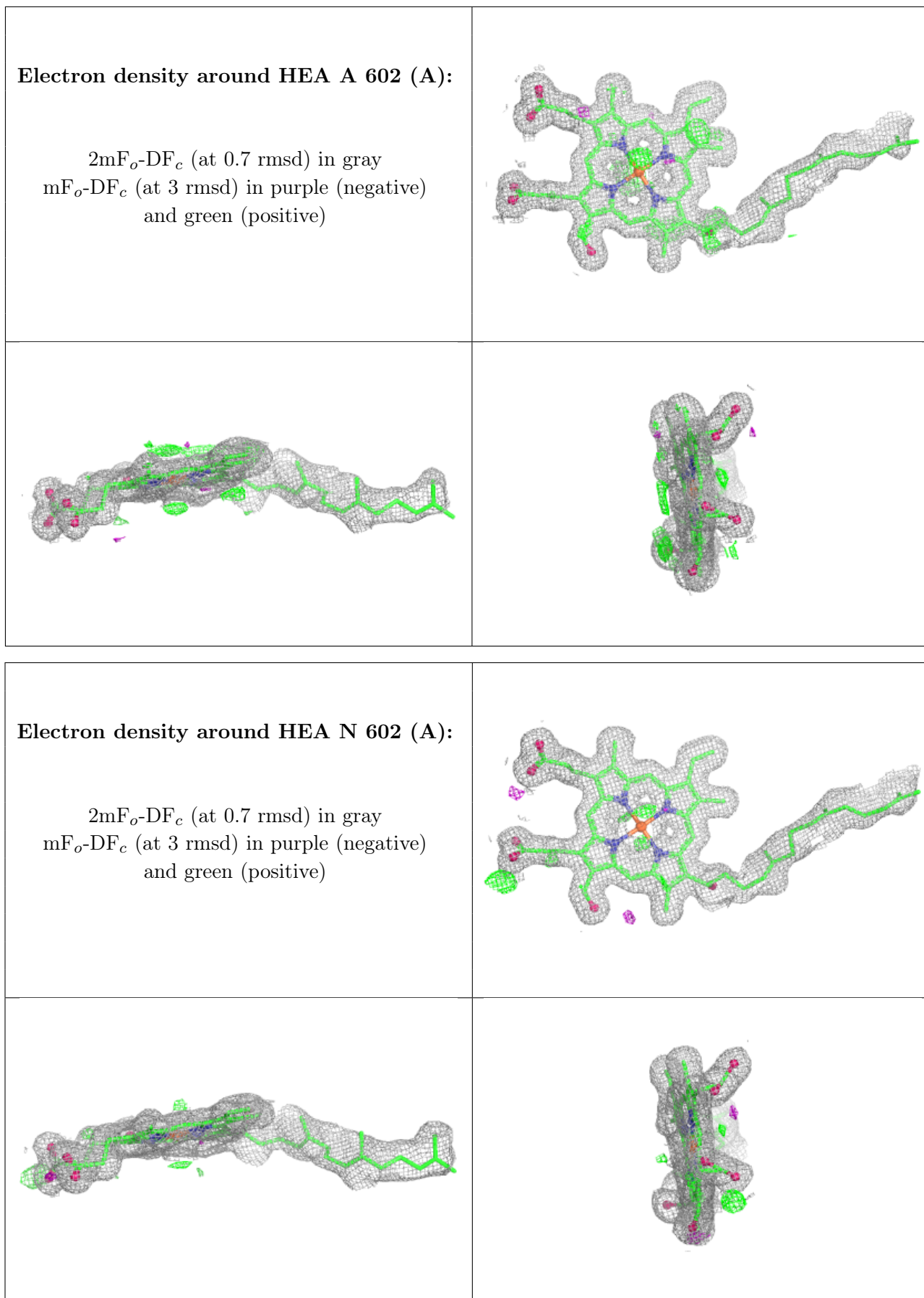
Electron density around PGV A 608:

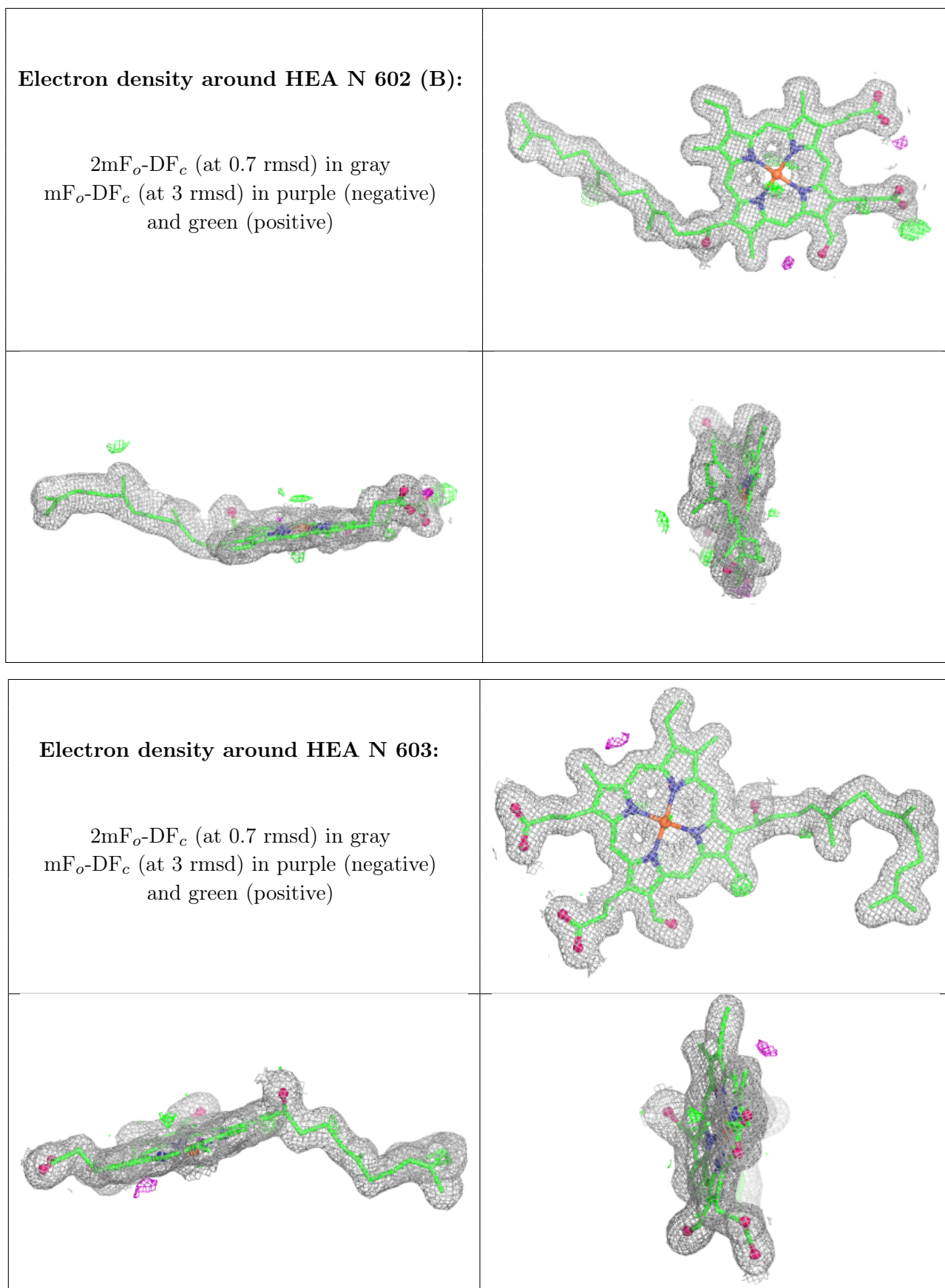
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

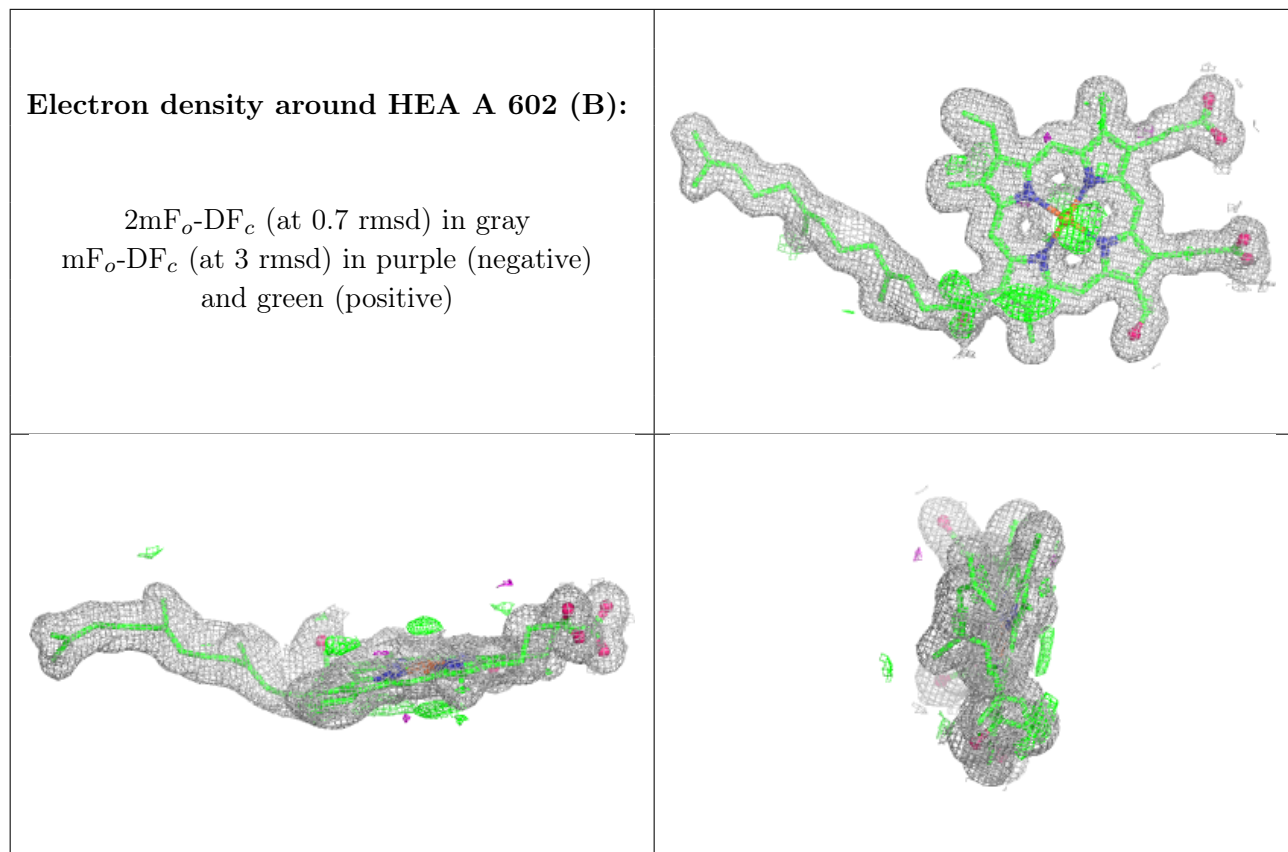
**Electron density around HEA A 603:**

$2mF_o-DF_c$ (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.