



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 11:56 PM JST

PDB ID : 7VVR / pdb_00007vvr
Title : Bovine cytochrome c oxidase in CN-bound mixed valence state at 50 K
Authors : Shimada, A.; Tsukihara, T.
Deposited on : 2021-11-08
Resolution : 1.65 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

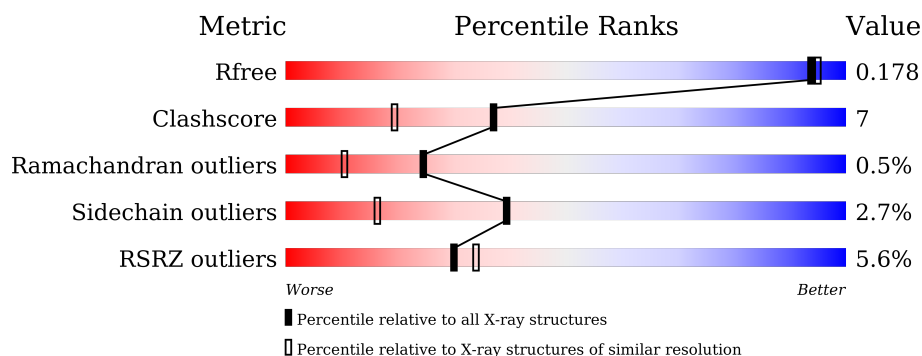
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	89% 11%
1	N	514	87% 12%
2	B	227	7% 81% 17%
2	O	227	5% 77% 22%
3	C	259	2% 92% 8%
3	P	259	92% 8%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	EDO	A	619	-	-	X	-
21	EDO	B	307	-	-	X	-
21	EDO	D	204	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 34984 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	27	0
			4162	2776	642	700	44			
1	N	514	Total	C	N	O	S	0	28	0
			4133	2755	639	696	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	13	0
			1906	1238	294	354	20			
2	O	227	Total	C	N	O	S	0	15	0
			1909	1244	294	351	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	8	0
			2157	1438	343	362	14			
3	P	259	Total	C	N	O	S	0	12	0
			2173	1446	348	364	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	5	0
			1232	801	202	225	4			
4	Q	144	Total	C	N	O	S	0	4	0
			1226	798	199	225	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	1	0
			863	550	148	163	2			
5	R	105	Total	C	N	O	S	0	1	0
			858	547	147	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
			731	452	130	143	6			
6	S	93	Total	C	N	O	S	0	2	0
			716	444	127	140	5			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	5	0
			710	456	134	118	1	1			
7	T	84	Total	C	N	O	P	S	0	3	0
			701	449	134	116	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
			661	417	121	118	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	2	0
			621	401	112	104	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			461	297	78	83	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			461	297	78	83	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	1	0
			392	255	66	69	2			
11	X	49	Total	C	N	O	S	0	1	0
			392	255	66	69	2			

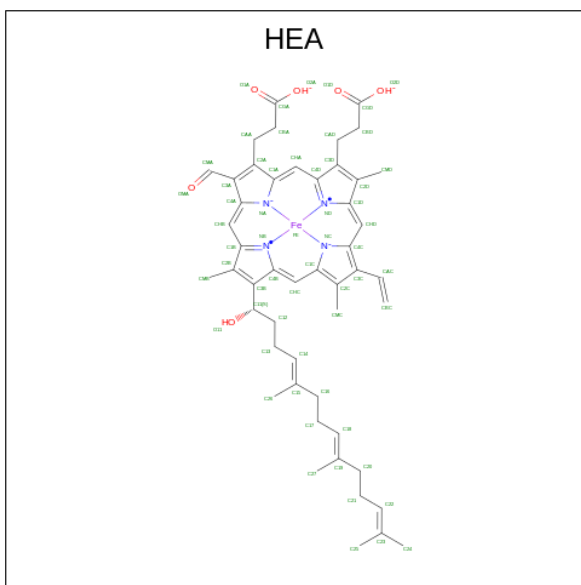
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			384	256	64	62	2			
12	Y	46	Total	C	N	O	S	0	1	0
			382	255	64	60	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	1	0
			338	225	53	60			
13	Z	43	Total	C	N	O	0	1	0
			339	224	53	62			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 79	C 67	Fe 1	N 4	O 7	0	1
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 79	C 67	Fe 1	N 4	O 7	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

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

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

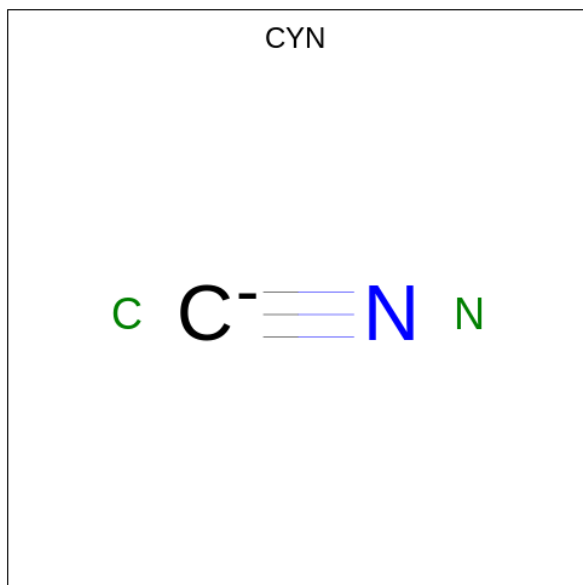
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

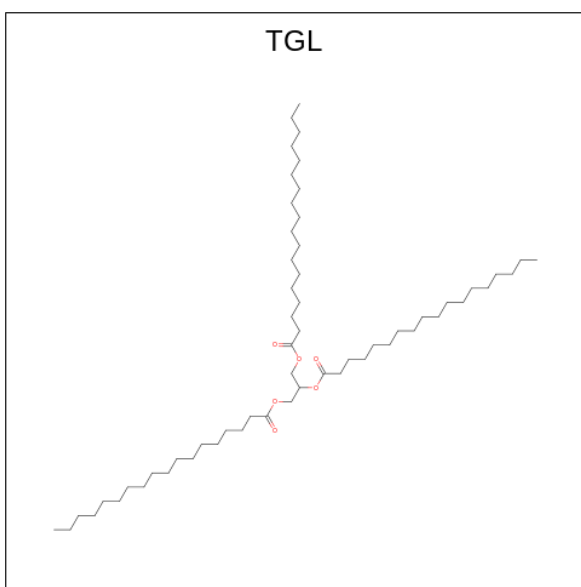
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is CYANIDE ION (CCD ID: CYN) (formula: CN).



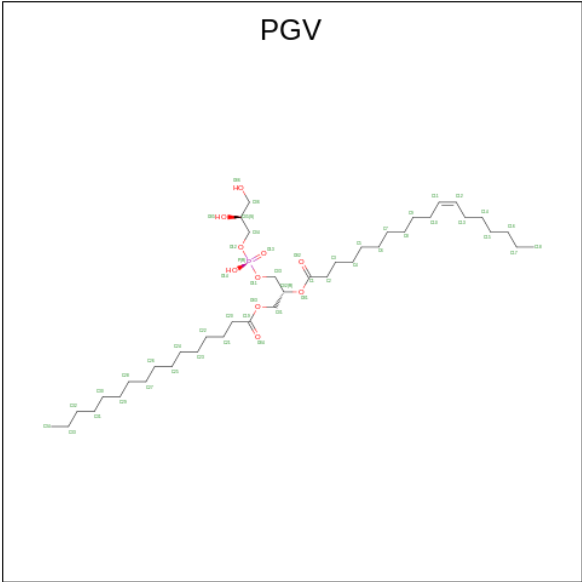
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	N	0	0
			2	1	1		
18	N	1	Total	C	N	0	0
			2	1	1		

- Molecule 19 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



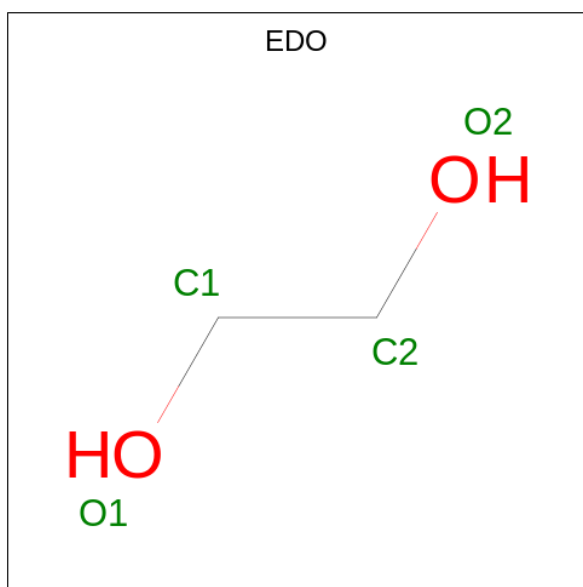
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			60	54	6		
19	B	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			53	47	6		
19	N	1	Total	C	O	0	0
			62	56	6		
19	Q	1	Total	C	O	0	0
			63	57	6		
19	Y	1	Total	C	O	0	0
			56	50	6		

- Molecule 20 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
20	A	1	Total	C	O	P	0	0
			47	36	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			50	39	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			46	35	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

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

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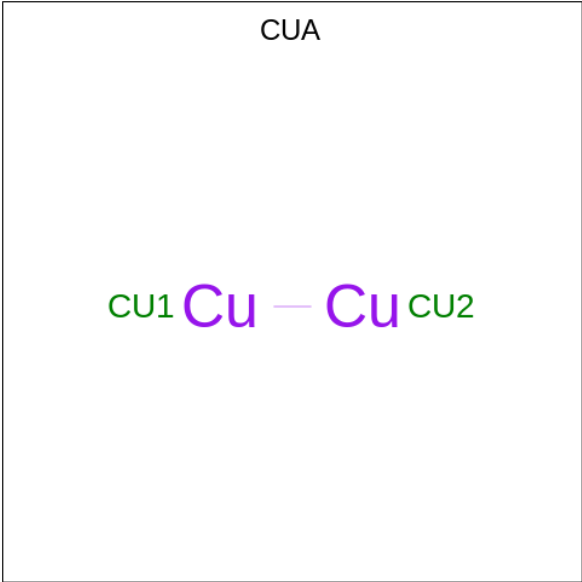
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4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

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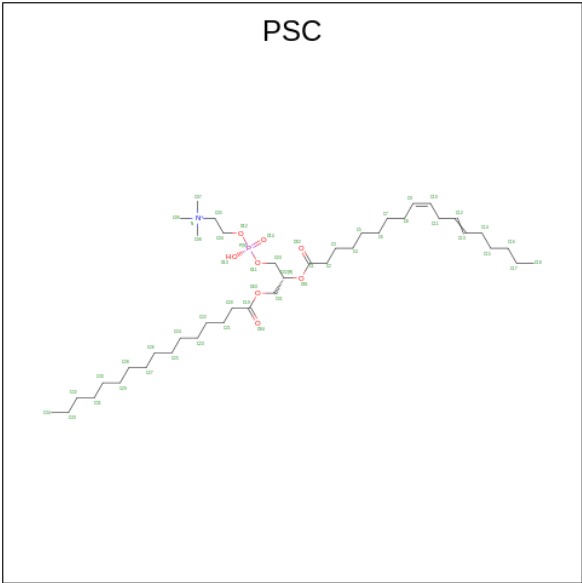
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	R	1	Total	C	O	0	0
			4	2	2		
21	R	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	T	1	Total	C	O	0	0
			4	2	2		
21	T	1	Total	C	O	0	0
			4	2	2		
21	U	1	Total	C	O	0	0
			4	2	2		
21	W	1	Total	C	O	0	0
			4	2	2		
21	Y	1	Total	C	O	0	0
			4	2	2		
21	Y	1	Total	C	O	0	0
			4	2	2		
21	Z	1	Total	C	O	0	0
			4	2	2		

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



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

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



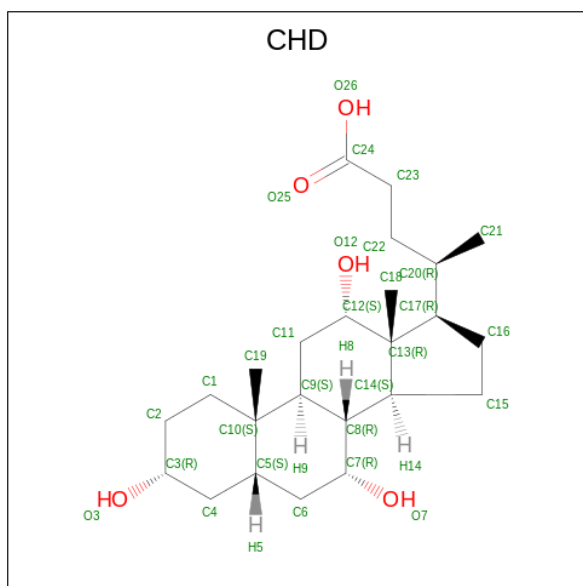
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			48	38	1	8	1		

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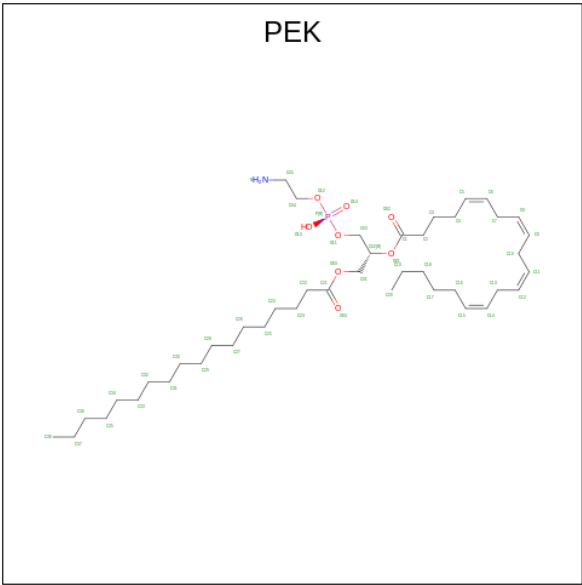
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	R	1	Total	C	N	O	P	
			49	39	1	8	1	
							0	0

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



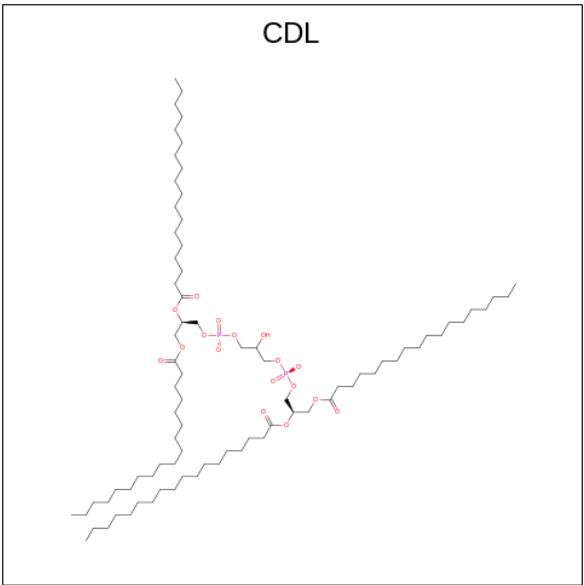
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O		
			29	24	5	0	0
24	C	1	Total	C	O		
			29	24	5	0	0
24	C	1	Total	C	O		
			29	24	5	0	0
24	J	1	Total	C	O		
			29	24	5	0	0
24	L	1	Total	C	O		
			29	24	5	0	0
24	O	1	Total	C	O		
			29	24	5	0	0
24	P	1	Total	C	O		
			29	24	5	0	0
24	P	1	Total	C	O		
			29	24	5	0	0
24	W	1	Total	C	O		
			29	24	5	0	0
24	Y	1	Total	C	O		
			29	24	5	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).



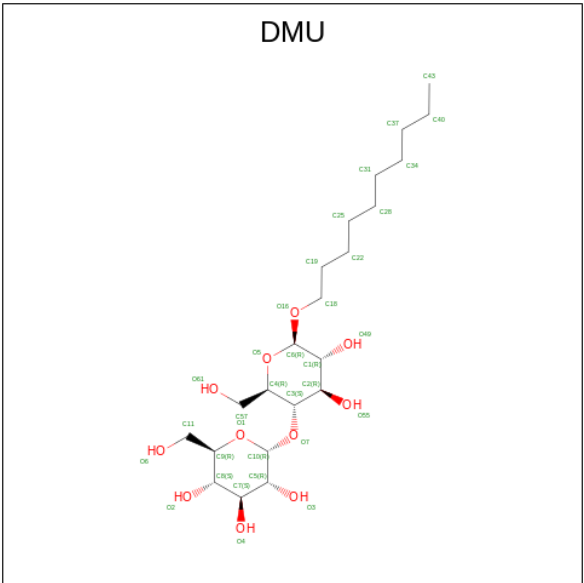
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			37	27	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	O	P		0	0
			50	41	8	1			
25	T	1	Total	C	N	O	P	0	0
			40	32	1	6	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			91	72	17	2		
26	G	1	Total	C	O	P	0	0
			84	66	16	2		
26	P	1	Total	C	O	P	0	0
			84	65	17	2		
26	T	1	Total	C	O	P	0	0
			90	71	17	2		

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

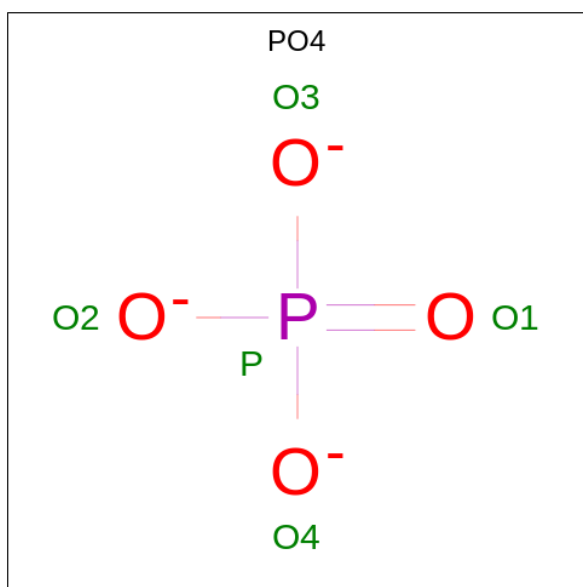


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O 33 22 11	0	0
27	G	1	Total C O 33 22 11	0	0
27	J	1	Total C O 33 22 11	0	0
27	K	1	Total C O 22 16 6	0	0
27	K	1	Total C O 22 16 6	0	0
27	K	1	Total C O 33 22 11	0	0
27	L	1	Total C O 22 16 6	0	0
27	M	1	Total C O 33 22 11	0	0
27	O	1	Total C O 22 16 6	0	0
27	P	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	T	1	Total C O 22 16 6	0	0
27	Z	1	Total C O 33 22 11	0	0

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

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

- Molecule 29 is 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	266	Total	O	0	0
			266	266		
30	B	231	Total	O	0	1
			232	232		
30	C	162	Total	O	0	0
			162	162		
30	D	207	Total	O	0	0
			207	207		
30	E	145	Total	O	0	0
			145	145		
30	F	156	Total	O	0	0
			156	156		
30	G	84	Total	O	0	0
			84	84		
30	H	97	Total	O	0	0
			97	97		
30	I	68	Total	O	0	0
			68	68		
30	J	48	Total	O	0	0
			48	48		

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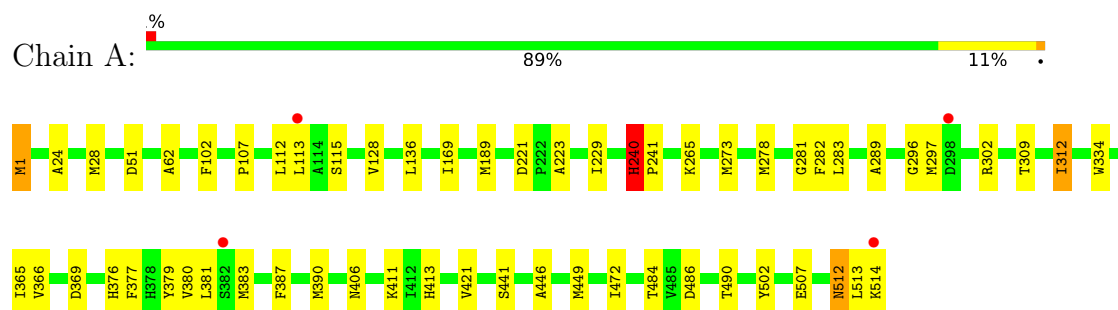
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	45	Total 45	O 45	0	0
30	L	37	Total 37	O 37	0	0
30	M	36	Total 36	O 36	0	0
30	N	278	Total 278	O 278	0	0
30	O	194	Total 195	O 195	0	1
30	P	161	Total 161	O 161	0	1
30	Q	128	Total 128	O 128	0	1
30	R	117	Total 117	O 117	0	0
30	S	141	Total 141	O 141	0	0
30	T	83	Total 83	O 83	0	0
30	U	96	Total 96	O 96	0	0
30	V	68	Total 68	O 68	0	0
30	W	44	Total 44	O 44	0	0
30	X	43	Total 43	O 43	0	0
30	Y	36	Total 36	O 36	0	0
30	Z	27	Total 27	O 27	0	0

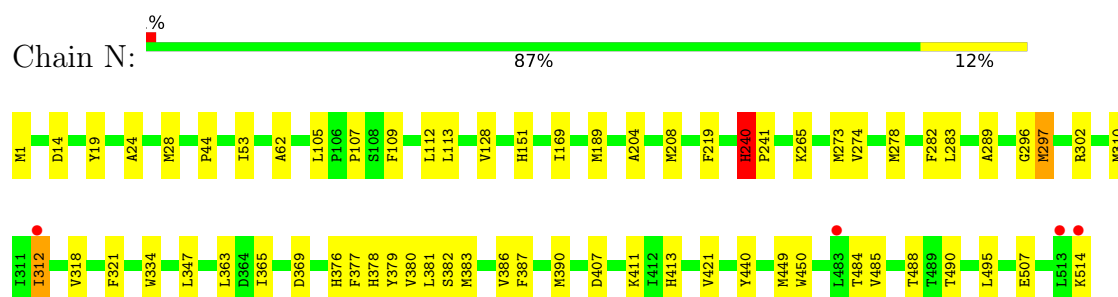
3 Residue-property plots [i](#)

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

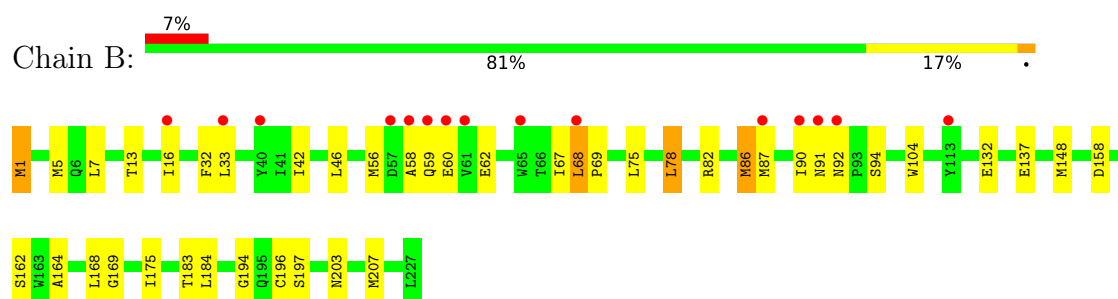
- Molecule 1: Cytochrome c oxidase subunit 1



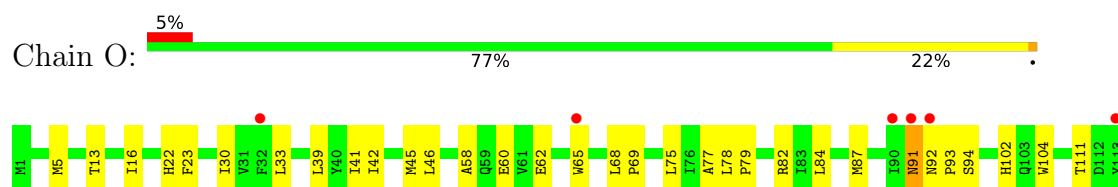
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2





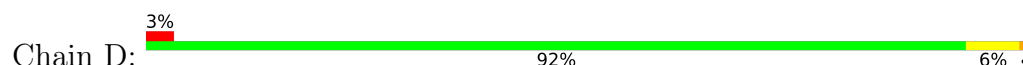
- Molecule 3: Cytochrome c oxidase subunit 3



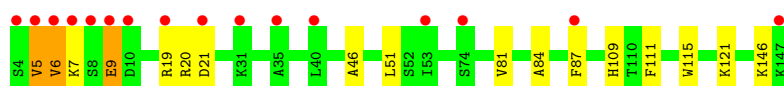
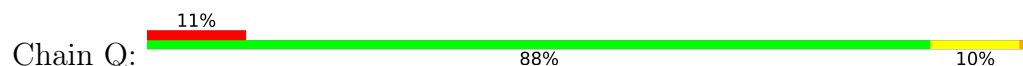
- Molecule 3: Cytochrome c oxidase subunit 3



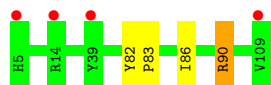
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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



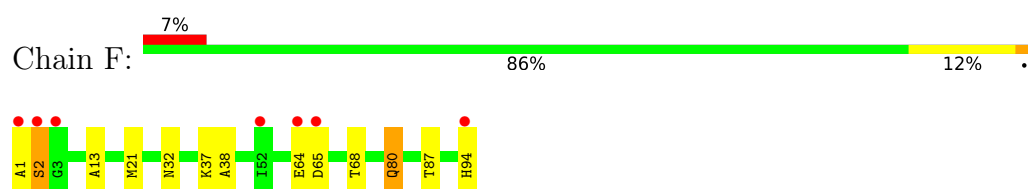
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



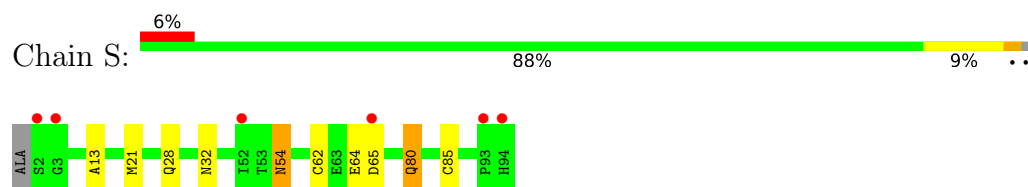
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



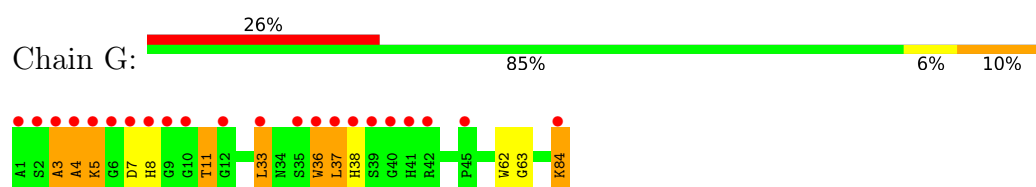
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



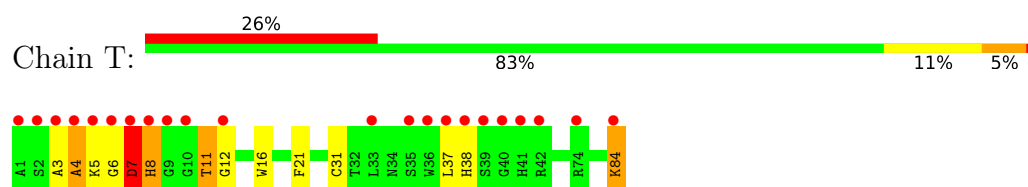
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



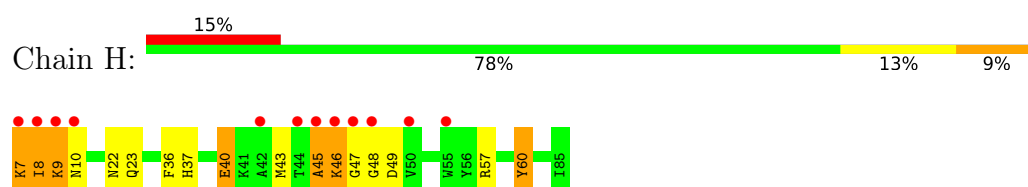
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



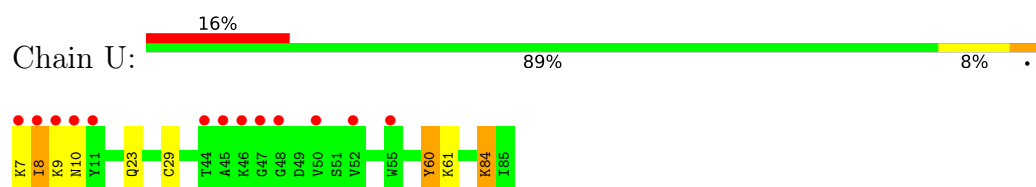
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



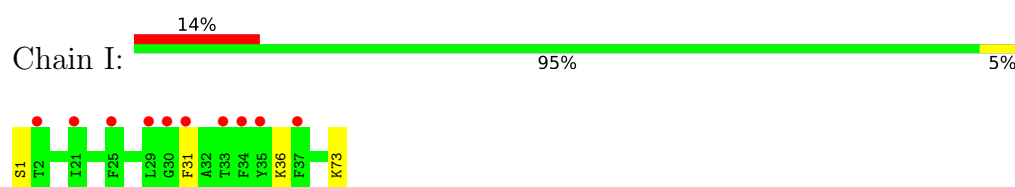
- Molecule 8: Cytochrome c oxidase subunit 6B1



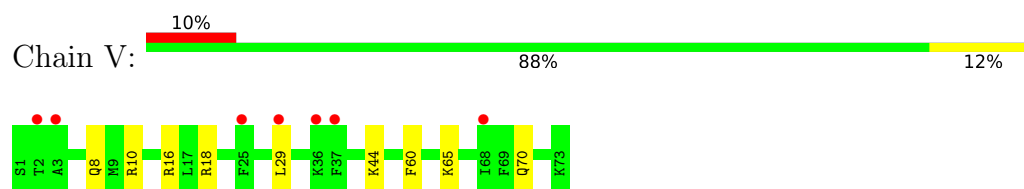
- Molecule 8: Cytochrome c oxidase subunit 6B1



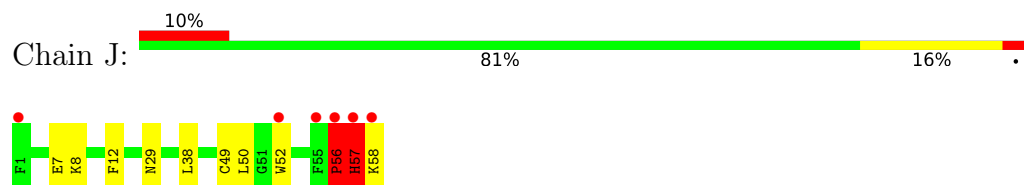
- Molecule 9: Cytochrome c oxidase subunit 6C



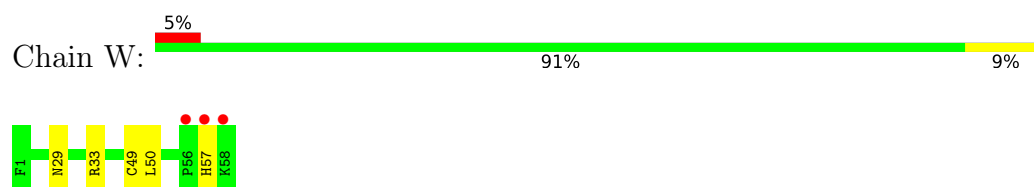
- Molecule 9: Cytochrome c oxidase subunit 6C



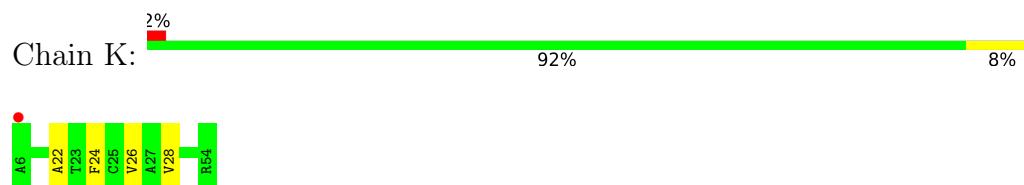
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



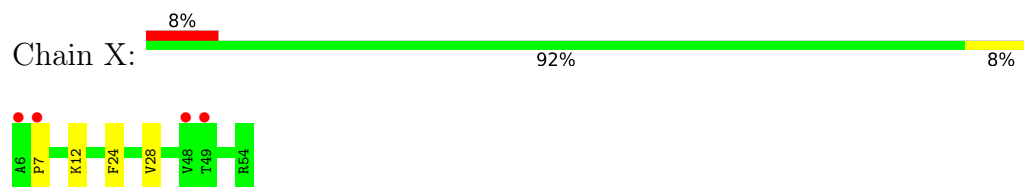
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



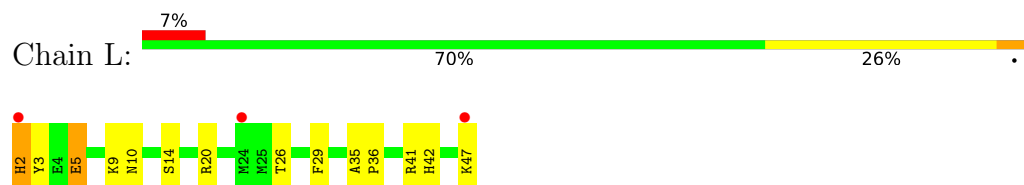
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



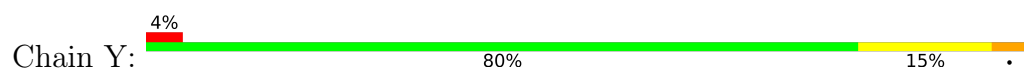
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

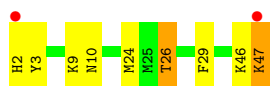


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

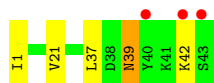
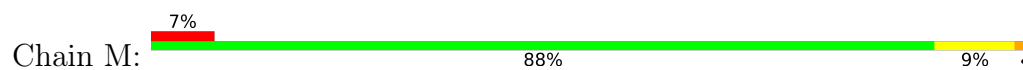


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

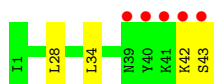
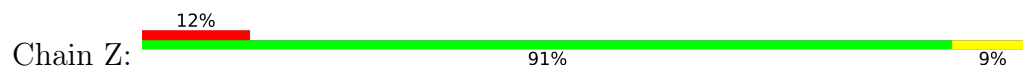




- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.31Å 204.71Å 177.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.95 – 1.65 39.95 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.95-1.65) 100.0 (39.95-1.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.152 , 0.176 0.154 , 0.178	Depositor DCC
R_{free} test set	43326 reflections (3.41%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34984	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.94	0/4369	0.95	2/5961 (0.0%)
1	N	0.86	0/4377	0.86	1/5972 (0.0%)
2	B	0.85	0/1968	0.95	0/2678
2	O	0.74	0/1994	0.86	0/2715
3	C	0.81	1/2261 (0.0%)	0.80	0/3090
3	P	0.77	0/2295	0.78	0/3134
4	D	0.78	1/1277 (0.1%)	0.85	1/1722 (0.1%)
4	Q	0.57	0/1266	0.72	2/1708 (0.1%)
5	E	0.73	0/882	0.74	0/1196
5	R	0.63	0/882	0.71	0/1196
6	F	0.80	1/757 (0.1%)	0.90	0/1026
6	S	0.81	0/744	0.88	0/1008
7	G	0.76	0/742	0.84	0/1005
7	T	0.67	0/722	0.87	0/978
8	H	0.78	0/682	0.87	2/921 (0.2%)
8	U	0.66	0/681	0.81	0/919
9	I	0.65	0/625	0.70	0/828
9	V	0.56	0/605	0.73	0/802
10	J	0.64	0/472	1.02	5/636 (0.8%)
10	W	0.61	0/472	0.75	0/636
11	K	0.69	0/406	0.72	0/556
11	X	0.53	0/406	0.66	0/556
12	L	0.83	0/402	0.85	0/538
12	Y	0.65	0/401	0.73	0/536
13	M	0.79	0/354	0.79	0/481
13	Z	0.62	0/354	0.71	0/481
All	All	0.79	3/30396 (0.0%)	0.84	13/41279 (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
10	J	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	21	ASP	CG-OD2	5.84	1.36	1.25
3	C	76	GLN	CD-OE1	5.83	1.34	1.23
6	F	87	THR	CB-CG2	-5.12	1.35	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	56	PRO	CA-C-N	-8.90	104.53	121.54
10	J	56	PRO	C-N-CA	-8.90	104.53	121.54
10	J	57	HIS	CA-CB-CG	-8.69	105.11	113.80
1	A	240	HIS	CA-CB-CG	-7.82	105.98	113.80
1	N	240	HIS	CA-CB-CG	-7.34	106.46	113.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
10	J	56	PRO	Peptide
10	J	57	HIS	Sidechain
1	N	240	HIS	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4162	0	4153	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4133	0	4127	65	0
2	B	1906	0	1920	37	0
2	O	1909	0	1926	39	0
3	C	2157	0	2064	23	0
3	P	2173	0	2087	20	0
4	D	1232	0	1215	13	0
4	Q	1226	0	1206	13	0
5	E	863	0	857	3	0
5	R	858	0	854	6	0
6	F	731	0	711	9	0
6	S	716	0	693	8	0
7	G	710	0	675	16	0
7	T	701	0	671	12	0
8	H	662	0	623	14	0
8	U	661	0	621	4	0
9	I	621	0	630	3	0
9	V	601	0	613	8	0
10	J	461	0	459	11	0
10	W	461	0	459	2	0
11	K	392	0	374	3	0
11	X	392	0	374	2	0
12	L	384	0	382	12	0
12	Y	382	0	381	7	0
13	M	338	0	355	6	0
13	Z	339	0	352	2	0
14	A	139	0	112	7	0
14	N	139	0	112	6	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	0	0
18	N	2	0	0	0	0
19	A	60	0	101	5	0
19	B	63	0	110	5	0
19	D	53	0	87	9	0
19	N	62	0	105	2	0
19	Q	63	0	110	5	0
19	Y	56	0	89	4	0
20	A	98	0	141	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	C	101	0	147	9	0
20	N	97	0	139	4	0
20	P	102	0	152	2	0
21	A	68	0	102	25	0
21	B	24	0	36	10	0
21	C	32	0	48	1	0
21	D	12	0	18	8	0
21	E	8	0	12	0	0
21	F	16	0	24	1	0
21	G	8	0	12	1	0
21	H	4	0	6	0	0
21	J	4	0	6	0	0
21	L	8	0	12	0	0
21	M	8	0	12	1	0
21	N	60	0	90	9	0
21	O	20	0	30	1	0
21	P	24	0	36	1	0
21	Q	12	0	18	2	0
21	R	8	0	12	0	0
21	S	16	0	24	0	0
21	T	8	0	12	0	0
21	U	4	0	6	0	0
21	W	4	0	6	0	0
21	Y	8	0	12	0	0
21	Z	4	0	6	0	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	48	0	66	5	0
23	R	49	0	69	7	0
24	B	29	0	39	0	0
24	C	58	0	78	3	0
24	J	29	0	39	1	0
24	L	29	0	39	2	0
24	O	29	0	39	1	0
24	P	58	0	78	3	0
24	W	29	0	39	0	0
24	Y	29	0	39	2	0
25	C	53	0	77	1	0
25	G	51	0	70	1	0
25	P	140	0	190	7	0
25	T	40	0	51	1	0
26	C	91	0	131	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	G	84	0	114	4	0
26	P	84	0	114	9	0
26	T	90	0	119	11	0
27	C	33	0	42	2	0
27	G	33	0	42	5	0
27	J	33	0	42	4	0
27	K	77	0	104	2	0
27	L	22	0	31	4	0
27	M	33	0	42	0	0
27	O	22	0	31	1	0
27	P	66	0	84	3	0
27	T	22	0	31	0	0
27	Z	33	0	42	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	266	0	0	16	0
30	B	232	0	0	7	0
30	C	162	0	0	3	0
30	D	207	0	0	4	0
30	E	145	0	0	1	0
30	F	156	0	0	4	0
30	G	84	0	0	5	0
30	H	97	0	0	1	0
30	I	68	0	0	4	0
30	J	48	0	0	1	0
30	K	45	0	0	0	0
30	L	37	0	0	3	0
30	M	36	0	0	1	0
30	N	278	0	0	11	0
30	O	195	0	0	2	0
30	P	161	0	0	4	0
30	Q	128	0	0	3	0
30	R	117	0	0	0	0
30	S	141	0	0	3	0
30	T	83	0	0	1	0
30	U	96	0	0	1	0
30	V	68	0	0	5	0
30	W	44	0	0	0	0
30	X	43	0	0	0	0
30	Y	36	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	Z	27	0	0	0	0
All	All	34984	0	32609	458	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 458 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:105:LEU:HD11	21:N:610:EDO:H22	1.54	0.90
7:G:11:TPO:HA	7:G:11:TPO:O2P	1.77	0.83
19:A:607:TGL:HC32	12:L:20:ARG:HH12	1.42	0.82
1:A:446:ALA:HB2	21:A:617:EDO:H11	1.62	0.81
21:A:618:EDO:H12	21:B:307:EDO:H22	1.62	0.80

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	540/514 (105%)	526 (97%)	14 (3%)	0	100	100
1	N	541/514 (105%)	527 (97%)	14 (3%)	0	100	100
2	B	238/227 (105%)	232 (98%)	5 (2%)	1 (0%)	30	15
2	O	240/227 (106%)	234 (98%)	5 (2%)	1 (0%)	30	15
3	C	265/259 (102%)	259 (98%)	6 (2%)	0	100	100
3	P	269/259 (104%)	264 (98%)	5 (2%)	0	100	100
4	D	147/144 (102%)	143 (97%)	4 (3%)	0	100	100
4	Q	146/144 (101%)	141 (97%)	4 (3%)	1 (1%)	18	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	104/105 (99%)	104 (100%)	0	0	100	100
5	R	104/105 (99%)	104 (100%)	0	0	100	100
6	F	95/94 (101%)	93 (98%)	1 (1%)	1 (1%)	11	2
6	S	93/94 (99%)	91 (98%)	2 (2%)	0	100	100
7	G	86/84 (102%)	79 (92%)	3 (4%)	4 (5%)	2	0
7	T	84/84 (100%)	75 (89%)	3 (4%)	6 (7%)	1	0
8	H	77/79 (98%)	71 (92%)	3 (4%)	3 (4%)	2	0
8	U	77/79 (98%)	73 (95%)	3 (4%)	1 (1%)	9	1
9	I	73/73 (100%)	72 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
10	W	56/58 (97%)	56 (100%)	0	0	100	100
11	K	48/49 (98%)	47 (98%)	1 (2%)	0	100	100
11	X	48/49 (98%)	47 (98%)	1 (2%)	0	100	100
12	L	45/46 (98%)	43 (96%)	2 (4%)	0	100	100
12	Y	45/46 (98%)	44 (98%)	1 (2%)	0	100	100
13	M	42/43 (98%)	41 (98%)	1 (2%)	0	100	100
13	Z	42/43 (98%)	42 (100%)	0	0	100	100
All	All	3632/3550 (102%)	3532 (97%)	82 (2%)	18 (0%)	24	10

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	92	ASN
6	F	2	SER
7	G	4	ALA
7	G	8	HIS
8	H	8	ILE

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	453/426 (106%)	445 (98%)	8 (2%)	51	30
1	N	454/426 (107%)	447 (98%)	7 (2%)	57	37
2	B	223/210 (106%)	213 (96%)	10 (4%)	24	5
2	O	225/210 (107%)	214 (95%)	11 (5%)	22	5
3	C	232/224 (104%)	231 (100%)	1 (0%)	84	77
3	P	236/224 (105%)	235 (100%)	1 (0%)	84	77
4	D	133/128 (104%)	130 (98%)	3 (2%)	44	21
4	Q	132/128 (103%)	127 (96%)	5 (4%)	29	7
5	E	93/92 (101%)	92 (99%)	1 (1%)	65	48
5	R	93/92 (101%)	92 (99%)	1 (1%)	65	48
6	F	81/78 (104%)	79 (98%)	2 (2%)	42	18
6	S	80/78 (103%)	77 (96%)	3 (4%)	29	7
7	G	72/67 (108%)	65 (90%)	7 (10%)	8	1
7	T	70/67 (104%)	66 (94%)	4 (6%)	18	3
8	H	71/71 (100%)	67 (94%)	4 (6%)	19	3
8	U	70/71 (99%)	64 (91%)	6 (9%)	10	1
9	I	59/57 (104%)	58 (98%)	1 (2%)	53	32
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	4
10	J	49/49 (100%)	47 (96%)	2 (4%)	27	6
10	W	49/49 (100%)	46 (94%)	3 (6%)	17	3
11	K	40/39 (103%)	40 (100%)	0	100	100
11	X	40/39 (103%)	40 (100%)	0	100	100
12	L	40/39 (103%)	35 (88%)	5 (12%)	4	0
12	Y	40/39 (103%)	37 (92%)	3 (8%)	12	2
13	M	38/37 (103%)	36 (95%)	2 (5%)	20	4
13	Z	38/37 (103%)	36 (95%)	2 (5%)	20	4
All	All	3168/3034 (104%)	3073 (97%)	95 (3%)	39	13

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	91	ASN

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Mol	Chain	Res	Type
6	S	54	ASN
2	O	115	ASP
4	Q	5	VAL
7	T	37	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	68	GLN
8	U	25	GLN
4	Q	32	ASN
5	R	94	ASN
8	U	31	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	TPO	T	11	7	8,10,11	1.47	1 (12%)	10,14,16	0.74	0
2	FME	O	1	2	8,9,10	0.72	0	7,9,11	1.03	0
7	TPO	G	11	7	8,10,11	1.32	1 (12%)	10,14,16	1.29	2 (20%)
2	FME	B	1	2	8,9,10	0.96	0	7,9,11	1.60	1 (14%)
1	FME	N	1	1	8,9,10	0.56	0	7,9,11	1.61	2 (28%)
9	SAC	I	1	9	7,8,9	0.62	0	8,9,11	0.96	0
1	FME	A	1	1	8,9,10	0.63	0	7,9,11	1.22	1 (14%)
9	SAC	V	1	9	7,8,9	0.58	0	8,9,11	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TPO	T	11	7	-	5/9/11/13	-
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	G	11	7	-	6/9/11/13	-
2	FME	B	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-
9	SAC	I	1	9	-	0/7/8/10	-
1	FME	A	1	1	-	3/7/9/11	-
9	SAC	V	1	9	-	5/7/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	3.20	1.60	1.50
7	G	11	TPO	P-O1P	2.48	1.58	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	O-C-CA	-2.93	117.09	124.78
1	N	1	FME	CE-SD-CG	2.72	109.75	100.40
1	A	1	FME	O-C-CA	-2.61	117.94	124.78
7	G	11	TPO	O2P-P-OG1	2.36	116.55	105.99
7	G	11	TPO	CG2-CB-CA	2.25	117.61	113.16

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	2	0
7	G	11	TPO	1	0
2	B	1	FME	3	0
9	I	1	SAC	1	0
1	A	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 161 ligands modelled in this entry, 8 are monoatomic - leaving 153 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PEK	P	303	-	52,52,52	0.69	2 (3%)	55,57,57	1.14	5 (9%)
21	EDO	D	202	-	3,3,3	0.39	0	2,2,2	0.79	0
26	CDL	T	102	-	87,87,99	1.43	11 (12%)	91,97,111	1.50	12 (13%)
21	EDO	A	620	-	3,3,3	0.61	0	2,2,2	0.81	0
21	EDO	B	310	-	3,3,3	0.66	0	2,2,2	0.25	0
18	CYN	N	606	15	0,1,1	-	-	-	-	-
14	HEA	N	601[A]	-	66,67,67	1.70	14 (21%)	78,103,103	1.95	23 (29%)
19	TGL	Y	101	-	54,54,62	1.31	4 (7%)	56,56,65	1.70	12 (21%)
21	EDO	N	610	-	3,3,3	0.75	0	2,2,2	2.43	1 (50%)
19	TGL	D	201	-	52,52,62	1.13	3 (5%)	55,55,65	1.31	6 (10%)
14	HEA	N	602	1	66,67,67	1.92	23 (34%)	78,103,103	2.25	24 (30%)
21	EDO	N	620	-	3,3,3	0.60	0	2,2,2	0.58	0
21	EDO	C	312	-	3,3,3	0.60	0	2,2,2	0.18	0
21	EDO	G	103	-	3,3,3	0.75	0	2,2,2	0.83	0
21	EDO	C	310	-	3,3,3	0.40	0	2,2,2	1.35	0
21	EDO	A	625	-	3,3,3	0.57	0	2,2,2	0.26	0
21	EDO	H	101	-	3,3,3	0.50	0	2,2,2	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHD	P	308	-	32,32,32	0.67	0	51,51,51	1.69	13 (25%)
26	CDL	C	305	-	89,89,99	1.43	13 (14%)	95,99,111	1.97	22 (23%)
21	EDO	N	611	-	3,3,3	0.61	0	2,2,2	0.62	0
21	EDO	F	103	-	3,3,3	0.78	0	2,2,2	0.57	0
21	EDO	N	621	-	3,3,3	0.61	0	2,2,2	0.35	0
21	EDO	O	307	-	3,3,3	0.78	0	2,2,2	0.46	0
21	EDO	T	104	-	3,3,3	0.67	0	2,2,2	0.86	0
27	DMU	K	101	-	22,22,34	1.27	2 (9%)	27,27,45	1.61	7 (25%)
21	EDO	Q	204	-	3,3,3	0.49	0	2,2,2	0.10	0
21	EDO	F	102	-	3,3,3	1.04	0	2,2,2	0.66	0
27	DMU	L	104	-	22,22,34	0.81	1 (4%)	27,27,45	1.39	5 (18%)
27	DMU	O	308	-	22,22,34	1.04	1 (4%)	27,27,45	1.49	3 (11%)
21	EDO	A	623	-	3,3,3	0.38	0	2,2,2	0.56	0
21	EDO	Z	102	-	3,3,3	0.51	0	2,2,2	0.20	0
20	PGV	P	305	-	50,50,50	0.74	2 (4%)	53,56,56	1.11	4 (7%)
27	DMU	K	102	-	22,22,34	1.30	3 (13%)	27,27,45	1.69	9 (33%)
21	EDO	O	306	-	3,3,3	0.65	0	2,2,2	0.44	0
19	TGL	N	607	-	61,61,62	1.17	3 (4%)	64,64,65	1.29	6 (9%)
21	EDO	N	615	-	3,3,3	1.03	0	2,2,2	0.64	0
21	EDO	A	616	-	3,3,3	0.73	0	2,2,2	0.42	0
14	HEA	N	601[B]	-	66,67,67	1.73	15 (22%)	78,103,103	1.94	24 (30%)
21	EDO	E	202	-	3,3,3	0.60	0	2,2,2	0.28	0
21	EDO	A	626	-	3,3,3	0.49	0	2,2,2	0.62	0
21	EDO	F	105	-	3,3,3	0.64	0	2,2,2	0.63	0
21	EDO	A	611	-	3,3,3	0.37	0	2,2,2	0.60	0
25	PEK	P	302	-	36,36,52	1.14	2 (5%)	39,41,57	1.92	9 (23%)
21	EDO	R	203	-	3,3,3	0.73	0	2,2,2	0.13	0
21	EDO	L	102	-	3,3,3	0.52	0	2,2,2	0.12	0
21	EDO	M	102	-	3,3,3	0.49	0	2,2,2	0.14	0
21	EDO	F	104	-	3,3,3	0.66	0	2,2,2	0.64	0
21	EDO	N	622	-	3,3,3	0.73	0	2,2,2	0.39	0
24	CHD	B	304	-	32,32,32	0.95	1 (3%)	51,51,51	1.60	12 (23%)
24	CHD	J	102	-	32,32,32	0.83	0	51,51,51	2.14	17 (33%)
21	EDO	A	622	-	3,3,3	0.62	0	2,2,2	0.72	0
20	PGV	N	609	-	50,50,50	1.02	3 (6%)	53,56,56	1.17	3 (5%)
21	EDO	W	102	-	3,3,3	0.80	0	2,2,2	0.54	0
21	EDO	N	614	-	3,3,3	0.60	0	2,2,2	0.81	0
21	EDO	B	305	-	3,3,3	0.42	0	2,2,2	0.16	0
21	EDO	P	315	-	3,3,3	0.42	0	2,2,2	0.57	0
21	EDO	E	201	-	3,3,3	0.61	0	2,2,2	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	C	311	-	3,3,3	0.35	0	2,2,2	0.96	0
27	DMU	M	101	-	34,34,34	0.55	1 (2%)	45,45,45	1.15	3 (6%)
20	PGV	N	608	-	45,45,50	1.07	3 (6%)	48,51,56	1.40	6 (12%)
21	EDO	A	617	-	3,3,3	0.46	0	2,2,2	0.17	0
21	EDO	N	612	-	3,3,3	0.50	0	2,2,2	0.55	0
27	DMU	Z	101	-	34,34,34	0.55	1 (2%)	45,45,45	1.11	2 (4%)
21	EDO	P	310	-	3,3,3	0.61	0	2,2,2	0.19	0
25	PEK	C	302	-	52,52,52	1.11	2 (3%)	55,57,57	1.42	5 (9%)
21	EDO	U	101	-	3,3,3	0.63	0	2,2,2	0.30	0
21	EDO	A	618	-	3,3,3	0.58	0	2,2,2	0.33	0
27	DMU	P	316	-	34,34,34	0.59	1 (2%)	45,45,45	1.76	10 (22%)
21	EDO	N	618	-	3,3,3	0.76	0	2,2,2	0.41	0
21	EDO	A	610	-	3,3,3	0.43	0	2,2,2	1.18	0
19	TGL	Q	201	-	62,62,62	1.03	3 (4%)	65,65,65	1.35	8 (12%)
21	EDO	N	624	-	3,3,3	0.52	0	2,2,2	0.20	0
21	EDO	C	307	-	3,3,3	0.83	0	2,2,2	0.11	0
20	PGV	C	304	-	50,50,50	1.13	2 (4%)	53,56,56	1.79	12 (22%)
21	EDO	A	619	-	3,3,3	0.25	0	2,2,2	0.18	0
21	EDO	B	308	-	3,3,3	0.93	0	2,2,2	0.14	0
21	EDO	Y	103	-	3,3,3	0.64	0	2,2,2	0.07	0
21	EDO	P	313	-	3,3,3	0.53	0	2,2,2	0.72	0
27	DMU	J	101	-	34,34,34	0.77	1 (2%)	45,45,45	2.53	16 (35%)
27	DMU	K	103	-	34,34,34	1.23	3 (8%)	45,45,45	2.05	16 (35%)
14	HEA	A	601[A]	-	66,67,67	1.78	16 (24%)	78,103,103	2.00	23 (29%)
29	PO4	H	102	-	4,4,4	0.77	0	6,6,6	0.45	0
21	EDO	Y	102	-	3,3,3	0.61	0	2,2,2	0.08	0
25	PEK	T	101	-	38,38,52	1.06	1 (2%)	39,40,57	1.34	4 (10%)
14	HEA	A	602	1	66,67,67	1.86	17 (25%)	78,103,103	2.91	32 (41%)
21	EDO	T	103	-	3,3,3	0.41	0	2,2,2	0.71	0
18	CYN	A	606	15	0,1,1	-	-	-	-	-
21	EDO	L	101	-	3,3,3	0.55	0	2,2,2	0.18	0
21	EDO	S	102	-	3,3,3	0.71	0	2,2,2	0.08	0
19	TGL	B	301	-	62,62,62	1.19	3 (4%)	65,65,65	1.63	6 (9%)
20	PGV	A	609	-	50,50,50	0.88	2 (4%)	53,56,56	1.01	1 (1%)
21	EDO	D	203	-	3,3,3	0.67	0	2,2,2	0.26	0
23	PSC	R	201	-	47,47,51	1.67	5 (10%)	50,53,59	1.51	6 (12%)
21	EDO	A	614	-	3,3,3	0.62	0	2,2,2	0.08	0
21	EDO	P	314	-	3,3,3	0.93	0	2,2,2	1.01	0
21	EDO	N	623	-	3,3,3	1.16	0	2,2,2	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	O	303	-	3,3,3	0.63	0	2,2,2	0.26	0
21	EDO	A	624	-	3,3,3	0.47	0	2,2,2	0.99	0
21	EDO	N	613	-	3,3,3	1.00	0	2,2,2	0.07	0
21	EDO	A	613	-	3,3,3	0.73	0	2,2,2	0.71	0
22	CUA	B	302	2	0,1,1	-	-	-	-	-
21	EDO	C	313	-	3,3,3	0.43	0	2,2,2	0.41	0
21	EDO	P	312	-	3,3,3	0.88	0	2,2,2	0.25	0
21	EDO	N	616	-	3,3,3	0.31	0	2,2,2	0.39	0
21	EDO	D	204	-	3,3,3	0.47	0	2,2,2	0.12	0
25	PEK	P	304	-	49,49,52	1.20	3 (6%)	53,54,57	1.71	7 (13%)
22	CUA	O	302	2	0,1,1	-	-	-	-	-
19	TGL	A	607	1	59,59,62	1.25	4 (6%)	62,62,65	1.89	15 (24%)
21	EDO	B	309	-	3,3,3	0.59	0	2,2,2	0.59	0
21	EDO	A	615	-	3,3,3	0.69	0	2,2,2	1.09	0
21	EDO	C	314	-	3,3,3	0.64	0	2,2,2	0.79	0
14	HEA	A	601[B]	-	66,67,67	1.84	16 (24%)	78,103,103	1.93	23 (29%)
27	DMU	C	315	-	34,34,34	0.91	1 (2%)	45,45,45	2.53	18 (40%)
21	EDO	S	104	-	3,3,3	0.89	0	2,2,2	0.51	0
27	DMU	G	105	-	34,34,34	1.05	1 (2%)	45,45,45	2.49	15 (33%)
24	CHD	W	101	-	32,32,32	0.82	0	51,51,51	1.99	12 (23%)
21	EDO	C	309	-	3,3,3	0.81	0	2,2,2	1.05	0
21	EDO	J	103	-	3,3,3	0.67	0	2,2,2	0.50	0
24	CHD	O	301	-	32,32,32	1.06	0	51,51,51	1.25	4 (7%)
20	PGV	P	306	-	50,50,50	1.09	2 (4%)	53,56,56	1.39	8 (15%)
29	PO4	U	102	-	4,4,4	0.77	0	6,6,6	0.45	0
26	CDL	P	307	-	82,82,99	1.44	11 (13%)	88,92,111	2.23	17 (19%)
20	PGV	A	608	-	46,46,50	1.19	2 (4%)	49,52,56	1.40	10 (20%)
21	EDO	G	104	-	3,3,3	0.52	0	2,2,2	0.34	0
27	DMU	T	105	-	22,22,34	1.39	3 (13%)	27,27,45	1.85	8 (29%)
23	PSC	B	303	-	47,47,51	1.31	3 (6%)	50,52,59	1.44	5 (10%)
20	PGV	C	303	-	49,49,50	0.76	1 (2%)	52,55,56	0.98	1 (1%)
21	EDO	P	311	-	3,3,3	0.69	0	2,2,2	0.37	0
21	EDO	Q	203	-	3,3,3	0.69	0	2,2,2	0.60	0
21	EDO	S	105	-	3,3,3	0.71	0	2,2,2	0.62	0
21	EDO	S	103	-	3,3,3	0.81	0	2,2,2	0.63	0
21	EDO	O	305	-	3,3,3	0.76	0	2,2,2	0.48	0
21	EDO	M	103	-	3,3,3	0.53	0	2,2,2	0.23	0
24	CHD	C	306	-	32,32,32	1.00	2 (6%)	51,51,51	2.80	22 (43%)
21	EDO	A	621	-	3,3,3	0.74	0	2,2,2	2.40	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	O	304	-	3,3,3	0.61	0	2,2,2	0.31	0
24	CHD	P	301	-	32,32,32	1.03	1 (3%)	51,51,51	1.50	10 (19%)
21	EDO	N	617	-	3,3,3	0.61	0	2,2,2	0.25	0
21	EDO	Q	202	-	3,3,3	0.43	0	2,2,2	0.78	0
21	EDO	C	308	-	3,3,3	0.75	0	2,2,2	0.52	0
21	EDO	A	612	-	3,3,3	0.87	0	2,2,2	0.42	0
24	CHD	L	103	-	32,32,32	0.90	0	51,51,51	3.10	28 (54%)
24	CHD	C	301	-	32,32,32	1.00	2 (6%)	51,51,51	1.29	9 (17%)
21	EDO	B	306	-	3,3,3	0.68	0	2,2,2	0.35	0
24	CHD	Y	104	-	32,32,32	0.82	0	51,51,51	2.49	19 (37%)
21	EDO	N	619	-	3,3,3	0.42	0	2,2,2	0.64	0
21	EDO	B	307	-	3,3,3	0.37	0	2,2,2	1.69	0
26	CDL	G	102	-	80,80,99	1.49	11 (13%)	80,86,111	1.59	12 (15%)
25	PEK	G	101	-	50,50,52	0.87	2 (4%)	53,55,57	1.05	3 (5%)
27	DMU	P	309	-	34,34,34	0.88	1 (2%)	45,45,45	1.18	5 (11%)
21	EDO	R	202	-	3,3,3	0.55	0	2,2,2	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEK	P	303	-	-	10/56/56/56	-
21	EDO	D	202	-	-	1/1/1/1	-
26	CDL	T	102	-	-	41/94/94/110	-
21	EDO	A	620	-	-	0/1/1/1	-
21	EDO	B	310	-	-	0/1/1/1	-
14	HEA	N	601[A]	-	-	6/36/76/76	-
19	TGL	Y	101	-	-	33/54/54/65	-
21	EDO	N	610	-	-	0/1/1/1	-
19	TGL	D	201	-	-	29/55/55/65	-
14	HEA	N	602	1	-	7/36/76/76	-
21	EDO	N	620	-	-	0/1/1/1	-
21	EDO	C	312	-	-	1/1/1/1	-
21	EDO	G	103	-	-	0/1/1/1	-
21	EDO	C	310	-	-	0/1/1/1	-
21	EDO	A	625	-	-	1/1/1/1	-
21	EDO	H	101	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHD	P	308	-	-	5/9/74/74	0/4/4/4
26	CDL	C	305	-	-	46/94/94/110	-
21	EDO	N	611	-	-	0/1/1/1	-
21	EDO	F	103	-	-	0/1/1/1	-
21	EDO	N	621	-	-	1/1/1/1	-
21	EDO	O	307	-	-	0/1/1/1	-
21	EDO	T	104	-	-	0/1/1/1	-
27	DMU	K	101	-	-	7/13/33/59	0/1/1/2
21	EDO	Q	204	-	-	0/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
27	DMU	L	104	-	-	8/13/33/59	0/1/1/2
27	DMU	O	308	-	-	3/13/33/59	0/1/1/2
21	EDO	A	623	-	-	0/1/1/1	-
21	EDO	Z	102	-	-	1/1/1/1	-
20	PGV	P	305	-	-	9/55/55/55	-
27	DMU	K	102	-	-	9/13/33/59	0/1/1/2
21	EDO	O	306	-	-	0/1/1/1	-
19	TGL	N	607	-	-	33/64/64/65	-
21	EDO	N	615	-	-	0/1/1/1	-
21	EDO	A	616	-	-	0/1/1/1	-
14	HEA	N	601[B]	-	-	7/36/76/76	-
21	EDO	E	202	-	-	1/1/1/1	-
21	EDO	A	626	-	-	0/1/1/1	-
21	EDO	F	105	-	-	0/1/1/1	-
21	EDO	A	611	-	-	0/1/1/1	-
25	PEK	P	302	-	-	17/39/39/56	-
21	EDO	R	203	-	-	1/1/1/1	-
21	EDO	L	102	-	-	0/1/1/1	-
21	EDO	M	102	-	-	0/1/1/1	-
21	EDO	F	104	-	-	1/1/1/1	-
21	EDO	N	622	-	-	0/1/1/1	-
24	CHD	B	304	-	-	2/9/74/74	0/4/4/4
24	CHD	J	102	-	-	5/9/74/74	0/4/4/4
21	EDO	A	622	-	-	1/1/1/1	-
20	PGV	N	609	-	-	7/55/55/55	-
21	EDO	W	102	-	-	0/1/1/1	-
21	EDO	N	614	-	-	1/1/1/1	-
21	EDO	B	305	-	-	0/1/1/1	-
21	EDO	P	315	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	E	201	-	-	0/1/1/1	-
21	EDO	C	311	-	-	0/1/1/1	-
27	DMU	M	101	-	-	2/19/59/59	0/2/2/2
20	PGV	N	608	-	-	18/50/50/55	-
21	EDO	A	617	-	-	1/1/1/1	-
21	EDO	N	612	-	-	0/1/1/1	-
27	DMU	Z	101	-	-	2/19/59/59	0/2/2/2
21	EDO	P	310	-	-	0/1/1/1	-
25	PEK	C	302	-	-	24/56/56/56	-
21	EDO	U	101	-	-	0/1/1/1	-
21	EDO	A	618	-	-	1/1/1/1	-
27	DMU	P	316	-	-	8/19/59/59	0/2/2/2
21	EDO	N	618	-	-	0/1/1/1	-
21	EDO	A	610	-	-	0/1/1/1	-
19	TGL	Q	201	-	-	35/65/65/65	-
21	EDO	N	624	-	-	0/1/1/1	-
21	EDO	C	307	-	-	0/1/1/1	-
20	PGV	C	304	-	-	21/55/55/55	-
21	EDO	A	619	-	-	1/1/1/1	-
21	EDO	B	308	-	-	1/1/1/1	-
21	EDO	Y	103	-	-	0/1/1/1	-
21	EDO	P	313	-	-	0/1/1/1	-
27	DMU	J	101	-	-	8/19/59/59	0/2/2/2
27	DMU	K	103	-	-	9/19/59/59	0/2/2/2
14	HEA	A	601[A]	-	-	8/36/76/76	-
21	EDO	Y	102	-	-	0/1/1/1	-
25	PEK	T	101	-	-	14/37/37/56	-
14	HEA	A	602	1	-	6/36/76/76	-
21	EDO	T	103	-	-	0/1/1/1	-
21	EDO	L	101	-	-	0/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
19	TGL	B	301	-	-	22/65/65/65	-
20	PGV	A	609	-	-	6/55/55/55	-
21	EDO	D	203	-	-	1/1/1/1	-
23	PSC	R	201	-	-	24/48/48/55	-
21	EDO	A	614	-	-	1/1/1/1	-
21	EDO	P	314	-	-	1/1/1/1	-
21	EDO	N	623	-	-	1/1/1/1	-
21	EDO	O	303	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	A	624	-	-	0/1/1/1	-
21	EDO	N	613	-	-	0/1/1/1	-
21	EDO	A	613	-	-	0/1/1/1	-
21	EDO	C	313	-	-	0/1/1/1	-
21	EDO	P	312	-	-	0/1/1/1	-
21	EDO	N	616	-	-	0/1/1/1	-
21	EDO	D	204	-	-	1/1/1/1	-
25	PEK	P	304	-	-	26/51/51/56	-
19	TGL	A	607	1	-	34/62/62/65	-
21	EDO	B	309	-	-	1/1/1/1	-
21	EDO	A	615	-	-	0/1/1/1	-
21	EDO	C	314	-	-	0/1/1/1	-
14	HEA	A	601[B]	-	-	6/36/76/76	-
27	DMU	C	315	-	-	7/19/59/59	0/2/2/2
21	EDO	S	104	-	-	0/1/1/1	-
27	DMU	G	105	-	-	9/19/59/59	0/2/2/2
24	CHD	W	101	-	-	6/9/74/74	0/4/4/4
21	EDO	C	309	-	-	0/1/1/1	-
21	EDO	J	103	-	-	0/1/1/1	-
24	CHD	O	301	-	-	2/9/74/74	0/4/4/4
20	PGV	P	306	-	-	15/55/55/55	-
26	CDL	P	307	-	-	48/87/87/110	-
20	PGV	A	608	-	-	24/51/51/55	-
21	EDO	G	104	-	-	0/1/1/1	-
27	DMU	T	105	-	-	5/13/33/59	0/1/1/2
23	PSC	B	303	-	-	20/51/51/55	-
20	PGV	C	303	-	-	12/54/54/55	-
21	EDO	P	311	-	-	0/1/1/1	-
21	EDO	Q	203	-	-	0/1/1/1	-
21	EDO	S	105	-	-	0/1/1/1	-
21	EDO	S	103	-	-	0/1/1/1	-
21	EDO	O	305	-	-	0/1/1/1	-
21	EDO	M	103	-	-	1/1/1/1	-
24	CHD	C	306	-	-	7/9/74/74	0/4/4/4
21	EDO	A	621	-	-	0/1/1/1	-
21	EDO	O	304	-	-	0/1/1/1	-
24	CHD	P	301	-	-	2/9/74/74	0/4/4/4
21	EDO	N	617	-	-	0/1/1/1	-
21	EDO	Q	202	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	C	308	-	-	0/1/1/1	-
21	EDO	A	612	-	-	0/1/1/1	-
24	CHD	L	103	-	-	5/9/74/74	0/4/4/4
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
21	EDO	B	306	-	-	0/1/1/1	-
24	CHD	Y	104	-	-	4/9/74/74	0/4/4/4
21	EDO	N	619	-	-	0/1/1/1	-
21	EDO	B	307	-	-	1/1/1/1	-
26	CDL	G	102	-	-	45/80/80/110	-
25	PEK	G	101	-	-	10/54/54/56	-
27	DMU	P	309	-	-	4/19/59/59	0/2/2/2
21	EDO	R	202	-	-	0/1/1/1	-

The worst 5 of 230 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	R	201	PSC	O01-C1	7.13	1.48	1.33
19	Y	101	TGL	OG2-CB1	6.10	1.51	1.34
23	B	303	PSC	O01-C1	5.82	1.50	1.34
25	T	101	PEK	O01-C1	5.68	1.50	1.33
26	G	102	CDL	OB6-CB5	5.68	1.45	1.33

The worst 5 of 619 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	306	CHD	C23-C22-C20	-10.79	94.81	114.52
26	P	307	CDL	OB5-PB2-OB2	-10.36	79.17	106.73
14	A	602	HEA	CHB-C4A-NA	9.65	134.88	124.44
26	G	102	CDL	OB6-CB5-OB7	-9.01	114.10	125.57
26	C	305	CDL	OB5-PB2-OB2	-8.97	82.87	106.73

There are no chirality outliers.

5 of 808 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[B]	HEA	C14-C15-C16-C17
14	A	601[B]	HEA	C26-C15-C16-C17
14	A	602	HEA	C2A-C3A-CMA-OMA
14	N	601[A]	HEA	C2A-C3A-CMA-OMA
14	N	601[B]	HEA	C2A-C3A-CMA-OMA

There are no ring outliers.

78 monomers are involved in 209 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	303	PEK	4	0
26	T	102	CDL	11	0
21	B	310	EDO	2	0
14	N	601[A]	HEA	3	0
19	Y	101	TGL	4	0
21	N	610	EDO	2	0
19	D	201	TGL	9	0
14	N	602	HEA	2	0
21	N	620	EDO	1	0
21	A	625	EDO	1	0
24	P	308	CHD	2	0
26	C	305	CDL	15	0
27	K	101	DMU	1	0
27	L	104	DMU	4	0
27	O	308	DMU	1	0
21	A	623	EDO	2	0
20	P	305	PGV	1	0
21	O	306	EDO	1	0
19	N	607	TGL	2	0
14	N	601[B]	HEA	1	0
21	A	626	EDO	1	0
21	F	104	EDO	1	0
24	J	102	CHD	1	0
21	A	622	EDO	3	0
20	N	609	PGV	1	0
21	N	614	EDO	2	0
20	N	608	PGV	3	0
21	A	617	EDO	3	0
27	Z	101	DMU	1	0
25	C	302	PEK	1	0
21	A	618	EDO	1	0
21	A	610	EDO	1	0
19	Q	201	TGL	5	0
20	C	304	PGV	6	0
21	A	619	EDO	5	0
27	J	101	DMU	4	0
27	K	103	DMU	1	0
14	A	601[A]	HEA	2	0
25	T	101	PEK	1	0
14	A	602	HEA	5	0

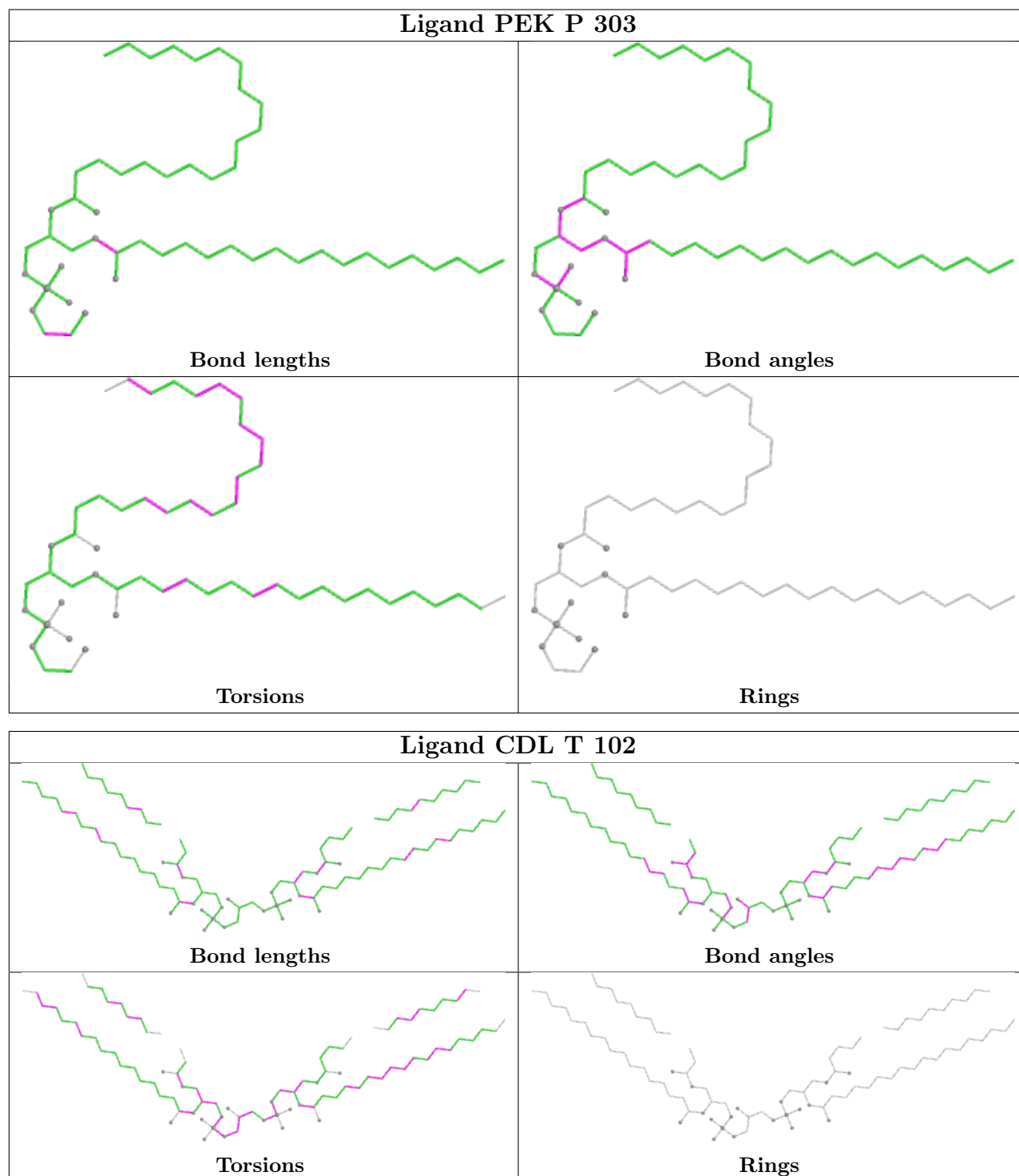
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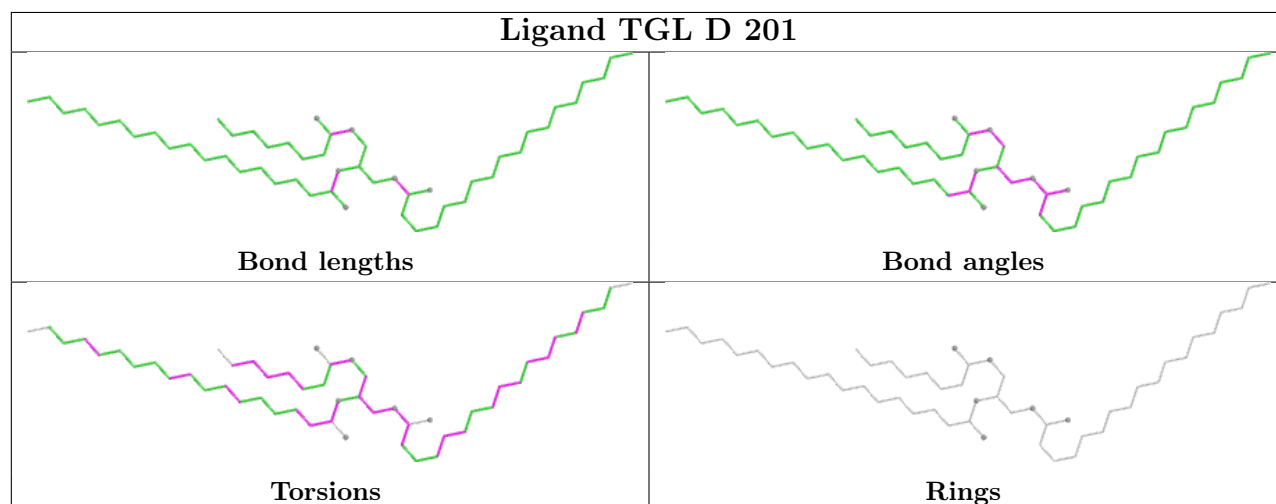
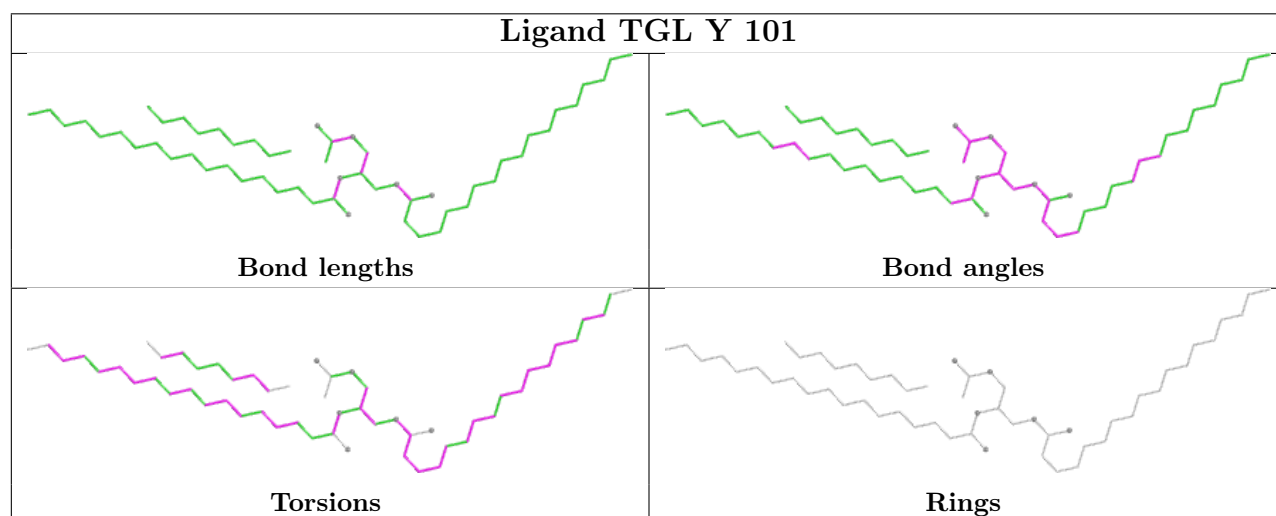
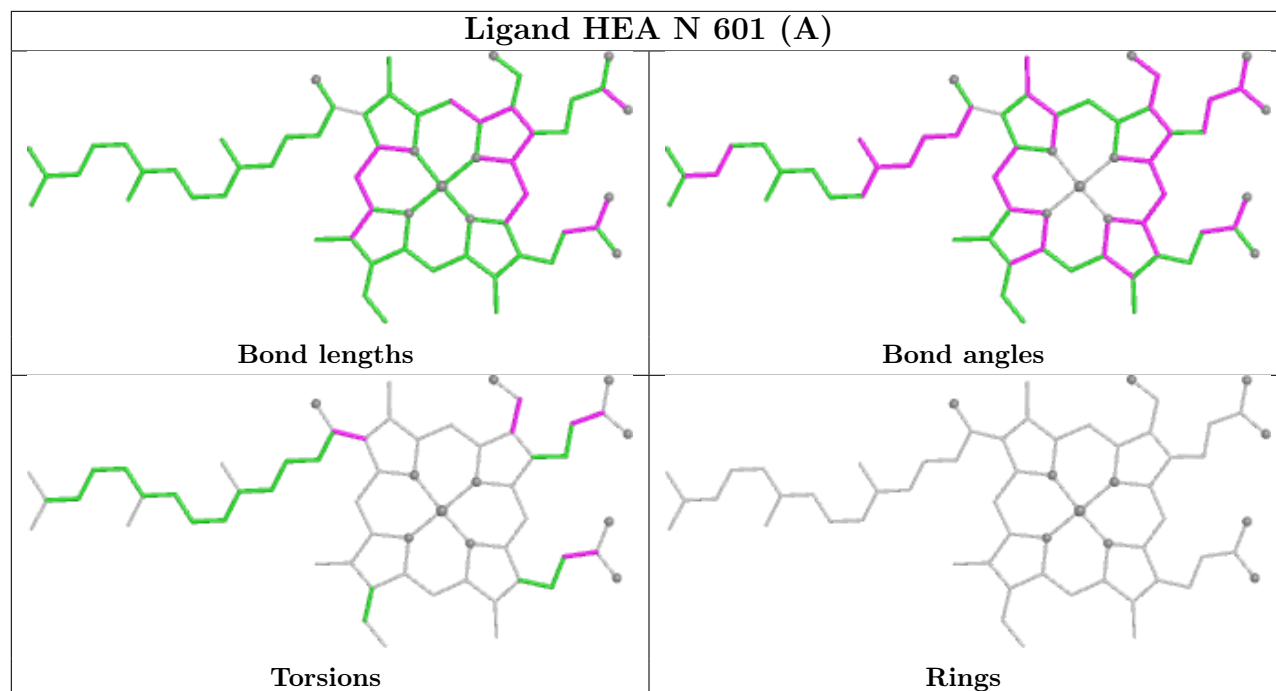
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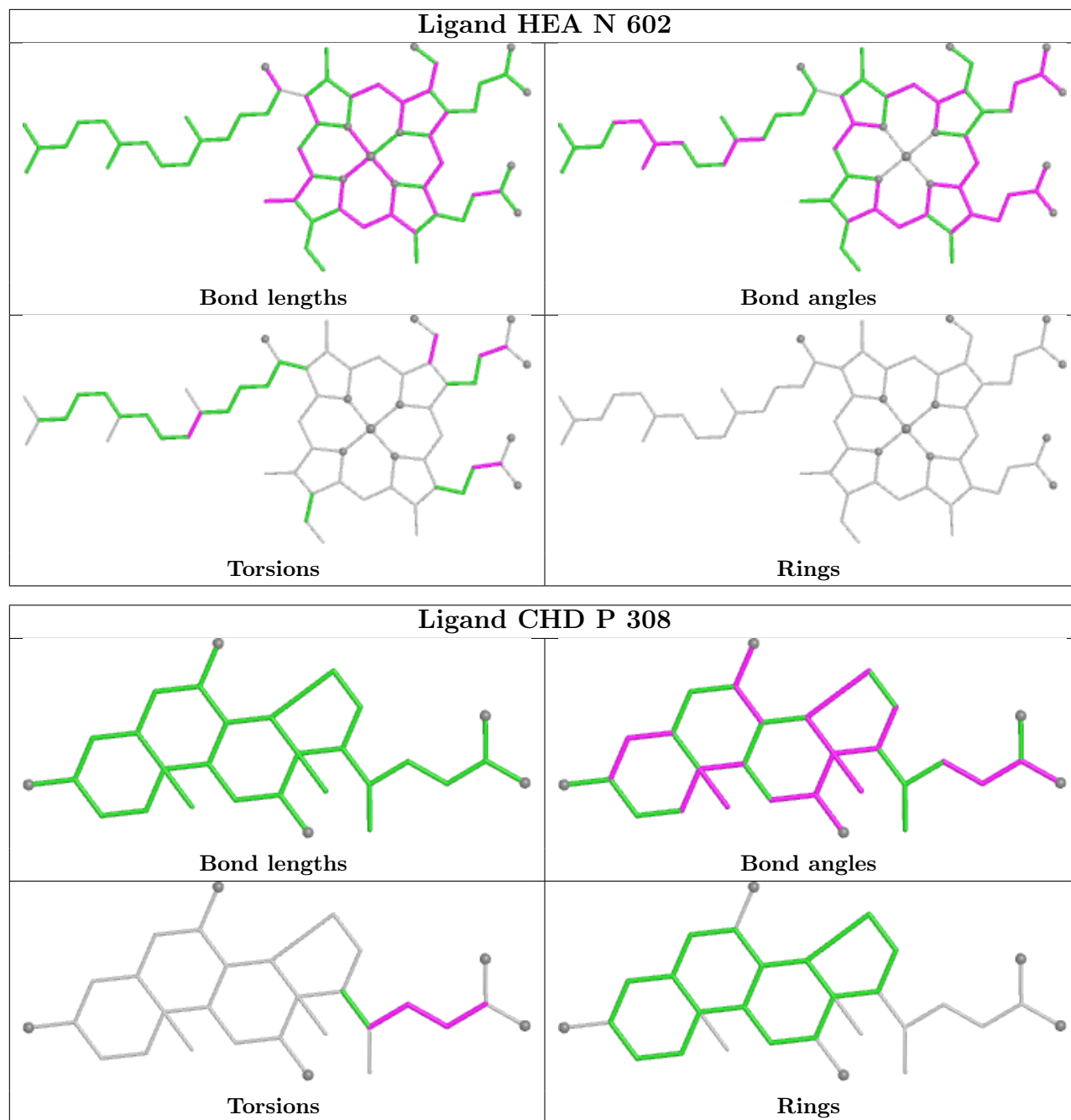
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	301	TGL	5	0
21	D	203	EDO	2	0
23	R	201	PSC	7	0
21	A	614	EDO	3	0
21	N	623	EDO	1	0
21	A	624	EDO	2	0
21	N	616	EDO	2	0
21	D	204	EDO	6	0
25	P	304	PEK	3	0
19	A	607	TGL	5	0
21	B	309	EDO	2	0
21	A	615	EDO	2	0
21	C	314	EDO	1	0
27	C	315	DMU	2	0
27	G	105	DMU	5	0
24	O	301	CHD	1	0
20	P	306	PGV	1	0
26	P	307	CDL	9	0
20	A	608	PGV	5	0
21	G	104	EDO	1	0
23	B	303	PSC	5	0
20	C	303	PGV	3	0
21	P	311	EDO	1	0
21	Q	203	EDO	1	0
21	M	103	EDO	1	0
24	C	306	CHD	3	0
21	A	621	EDO	1	0
24	P	301	CHD	1	0
21	N	617	EDO	1	0
21	Q	202	EDO	1	0
21	C	308	EDO	1	0
24	L	103	CHD	2	0
21	B	306	EDO	1	0
24	Y	104	CHD	2	0
21	B	307	EDO	5	0
26	G	102	CDL	4	0
25	G	101	PEK	1	0
27	P	309	DMU	3	0

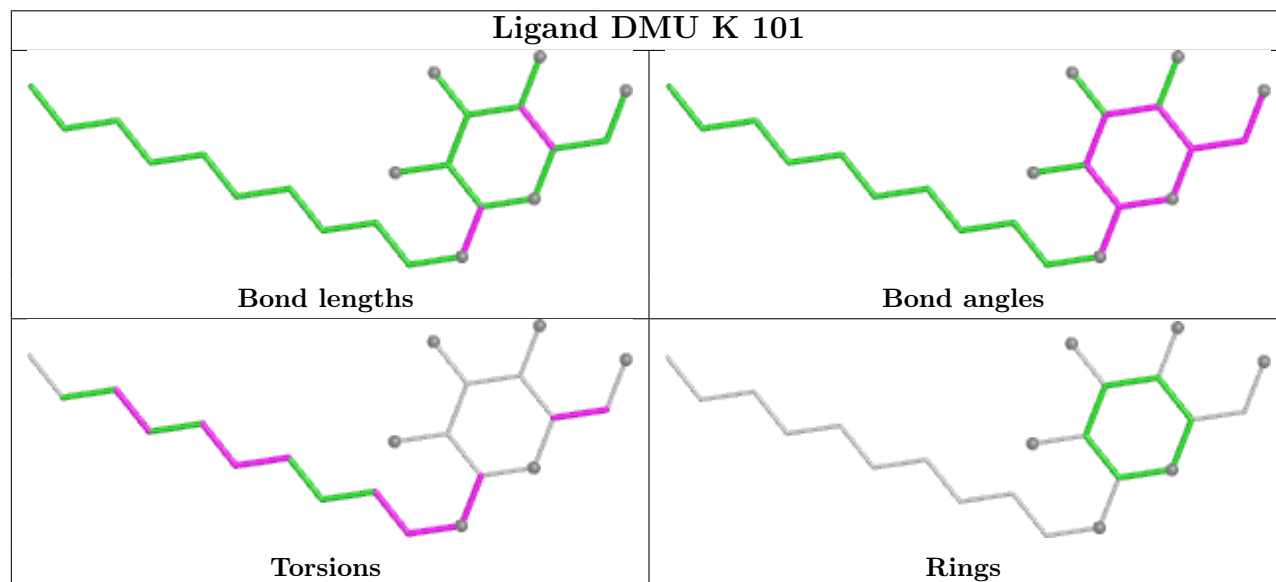
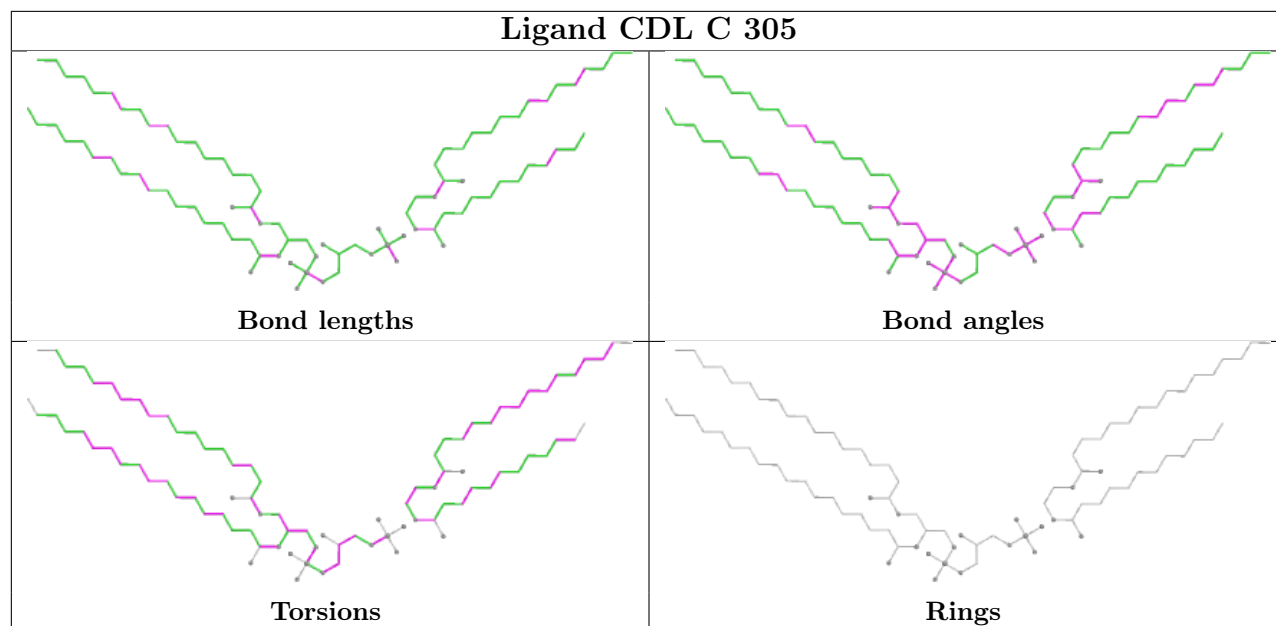
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

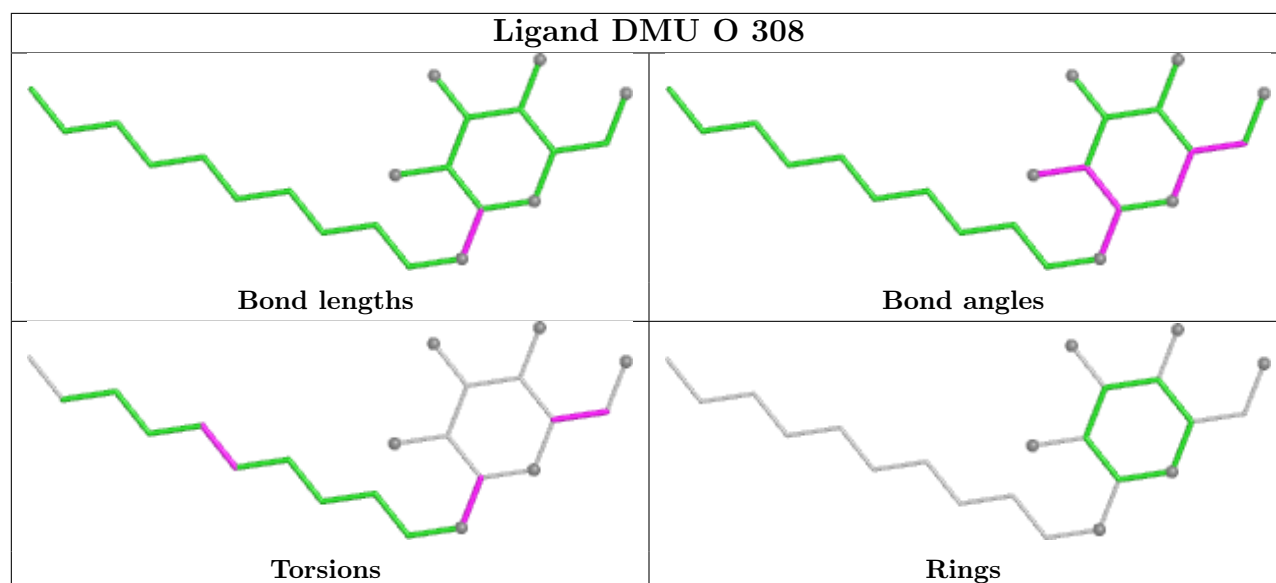
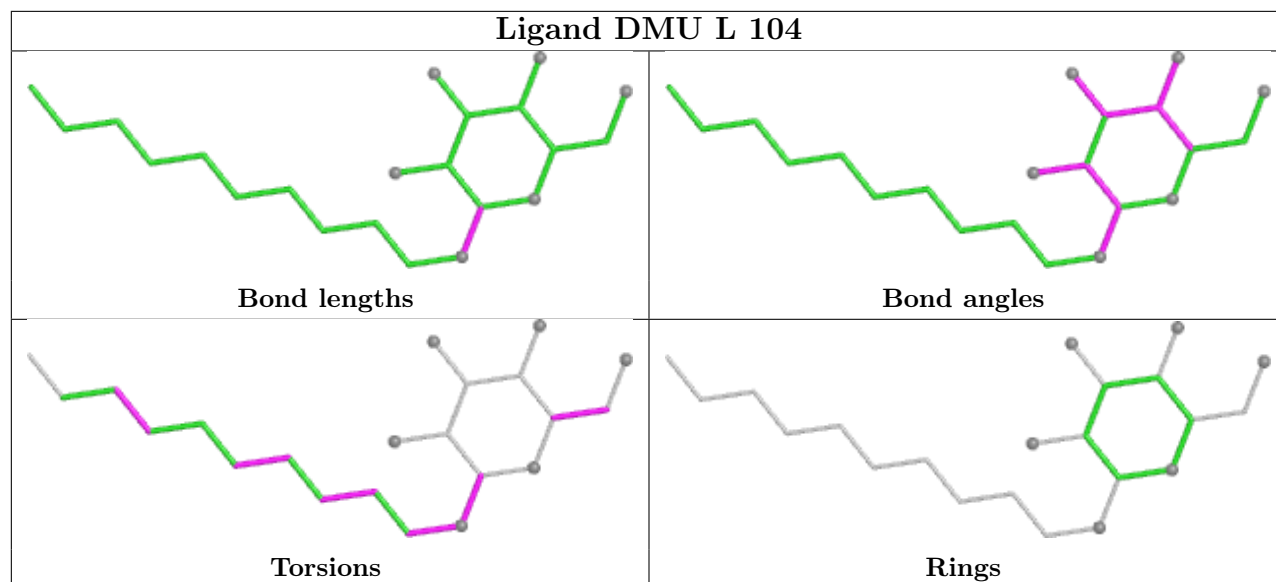
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question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

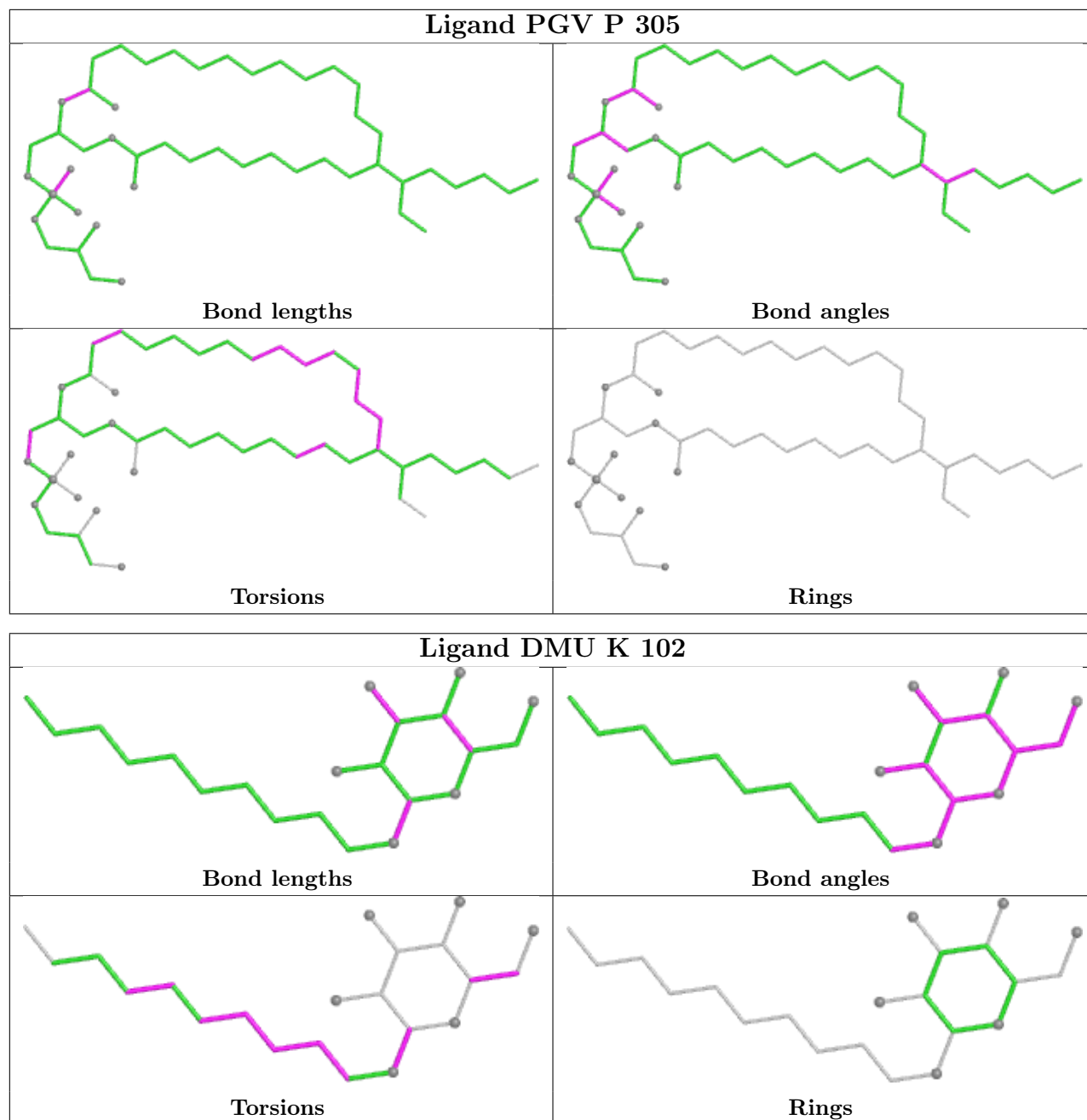


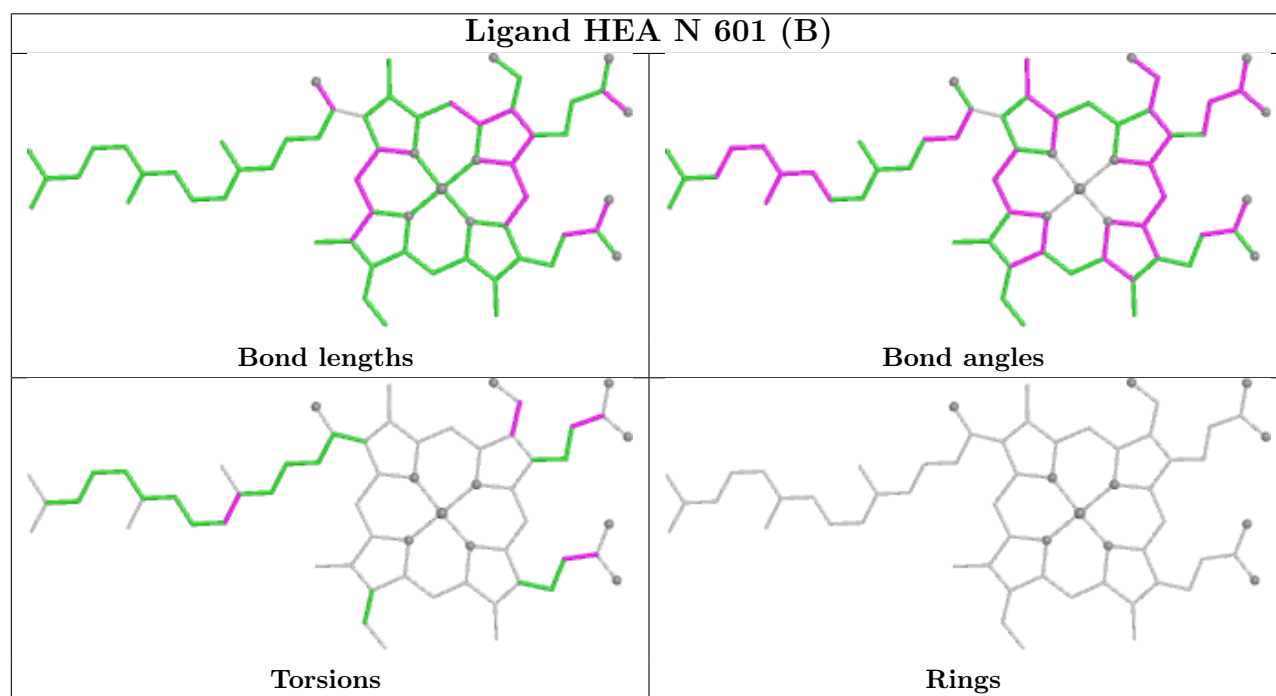
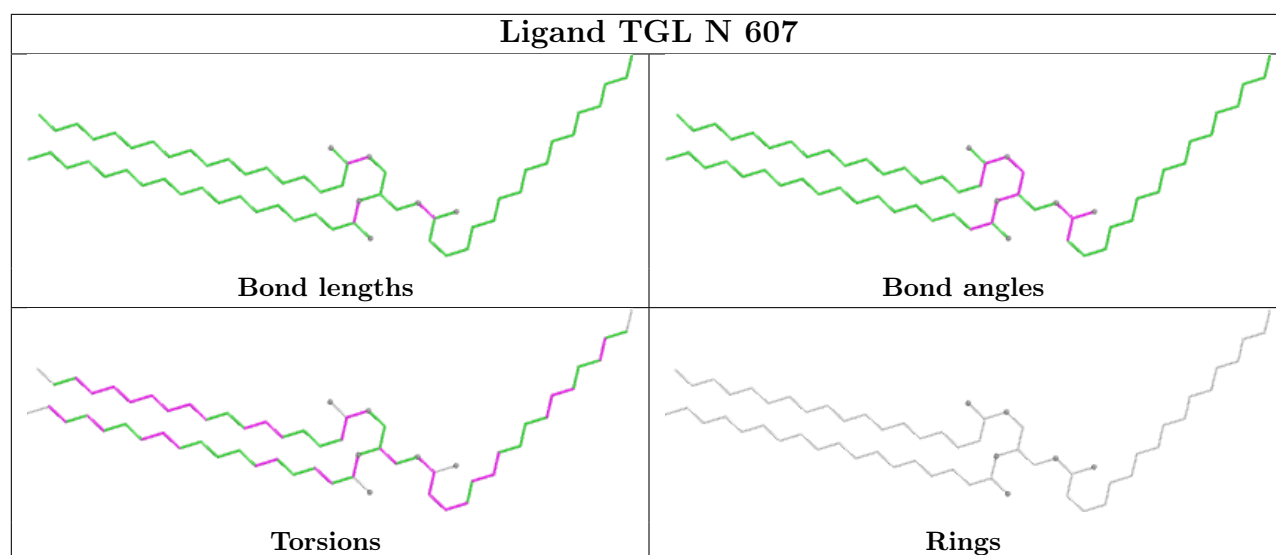


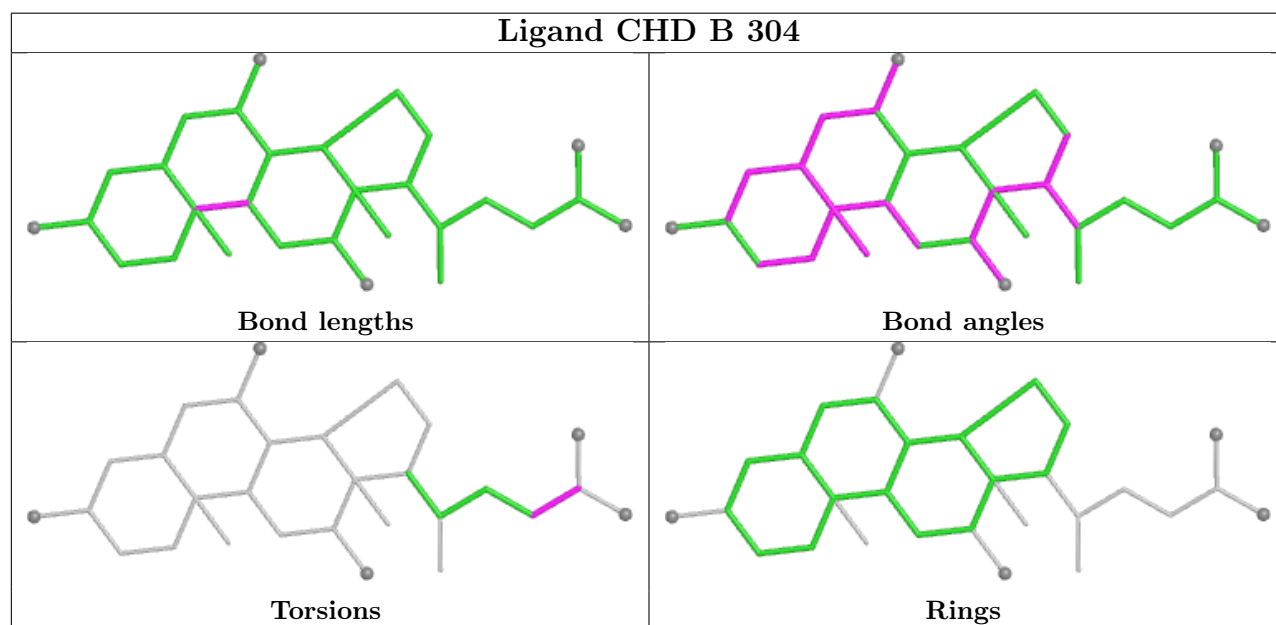
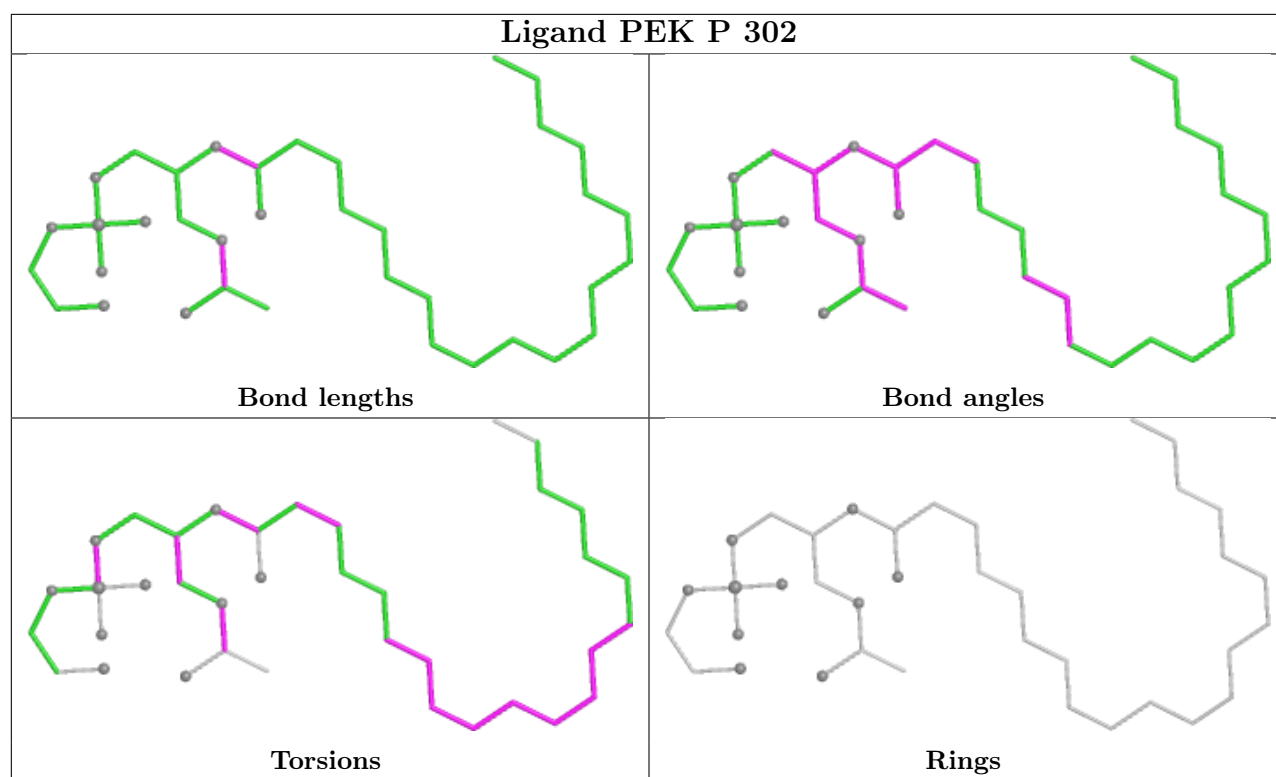


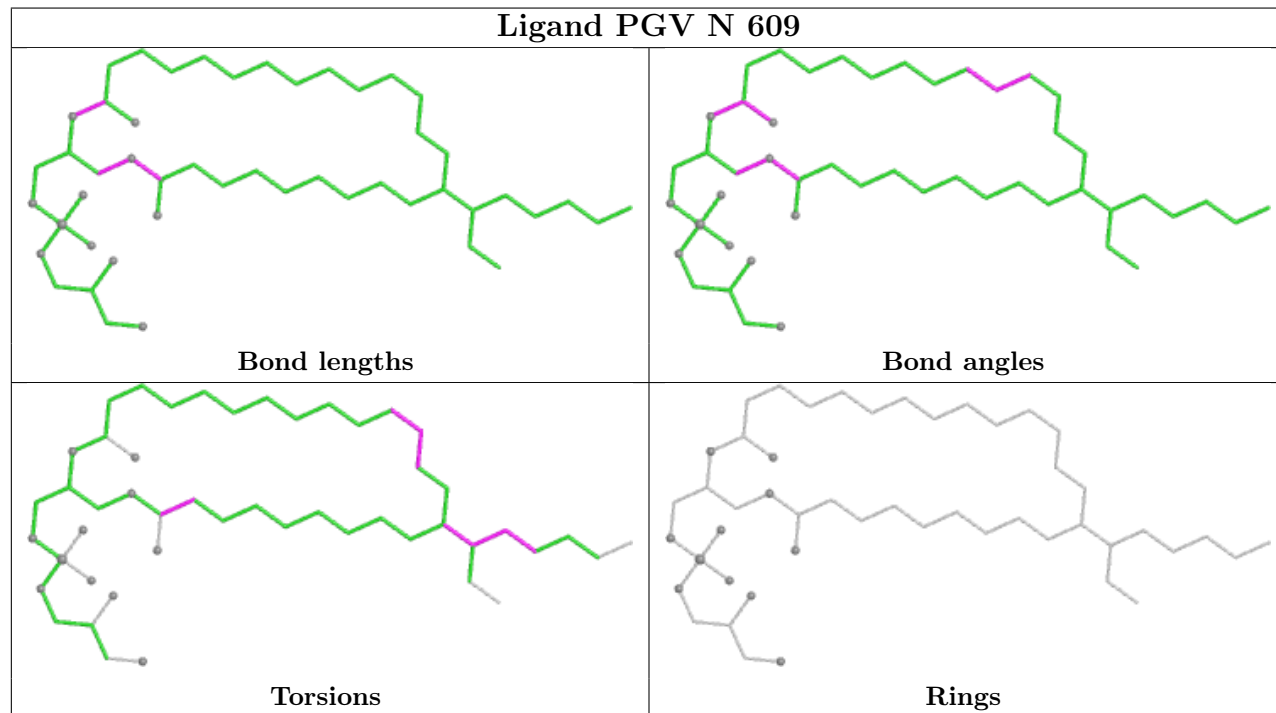
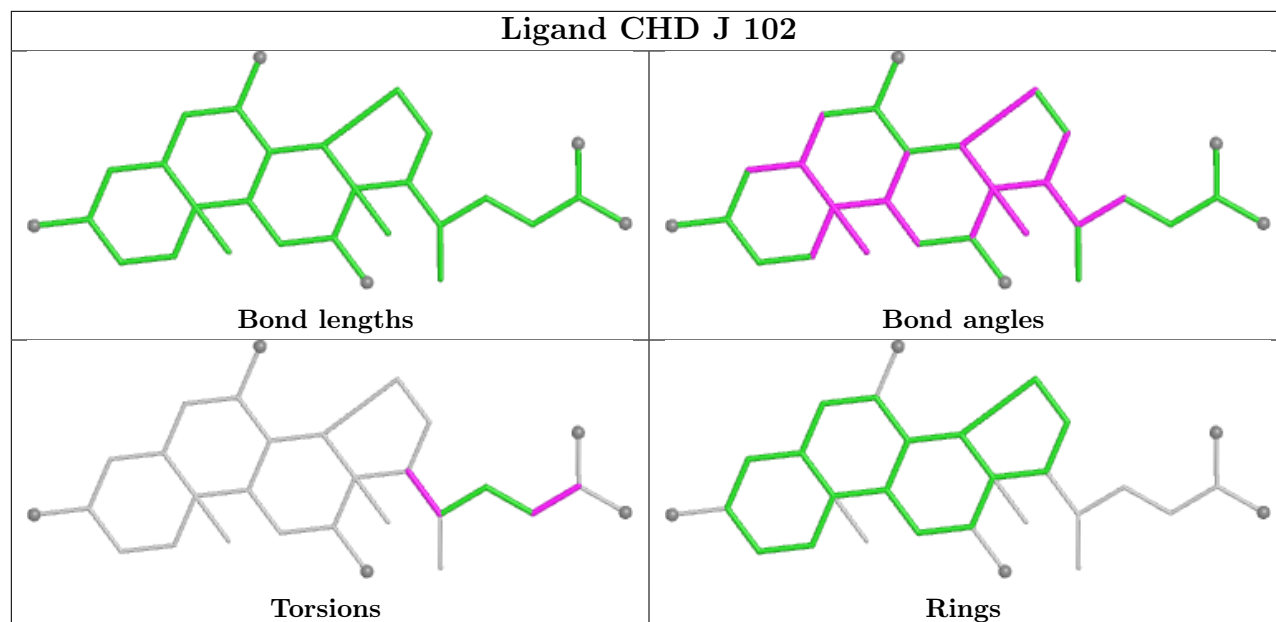


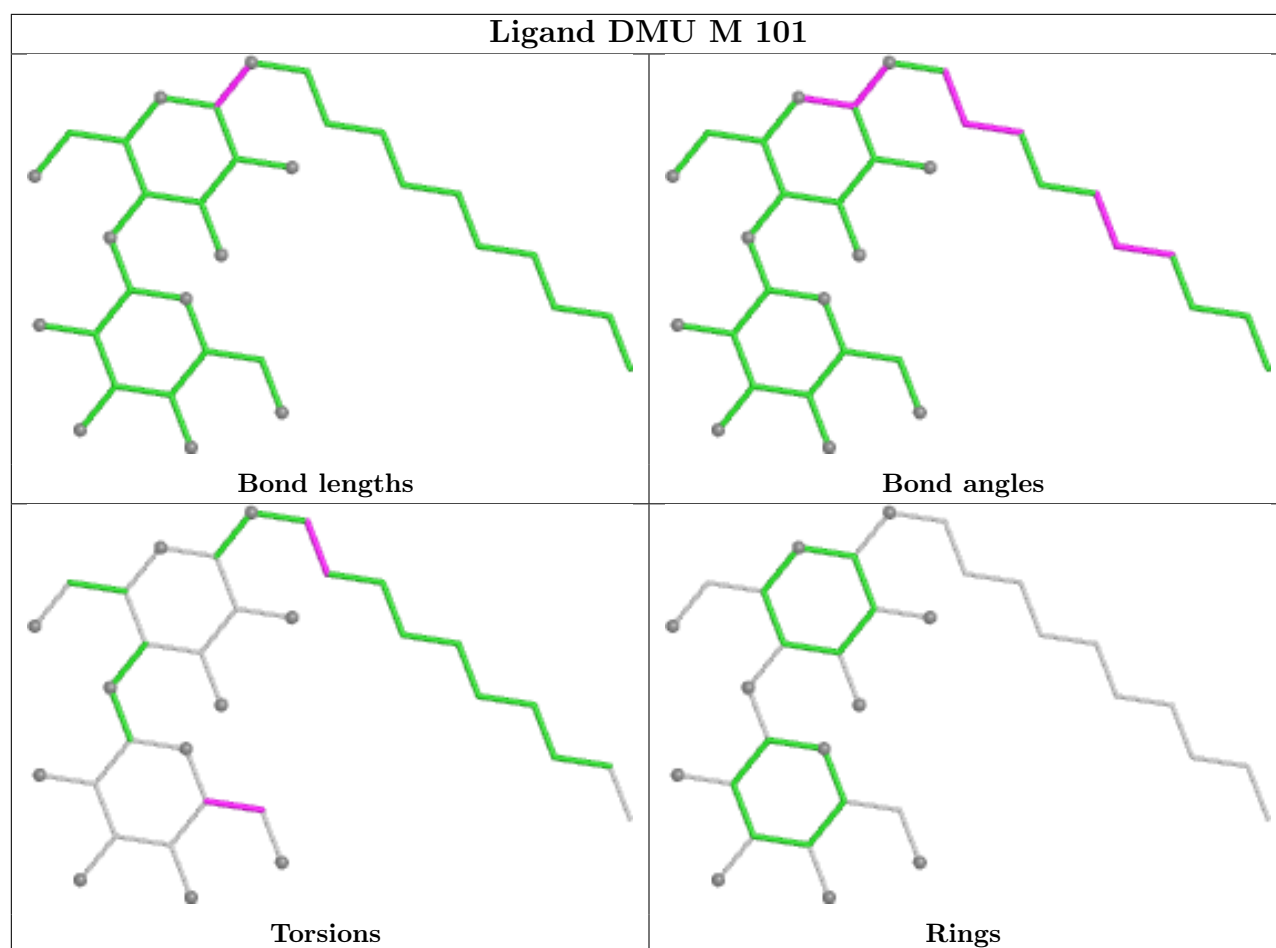


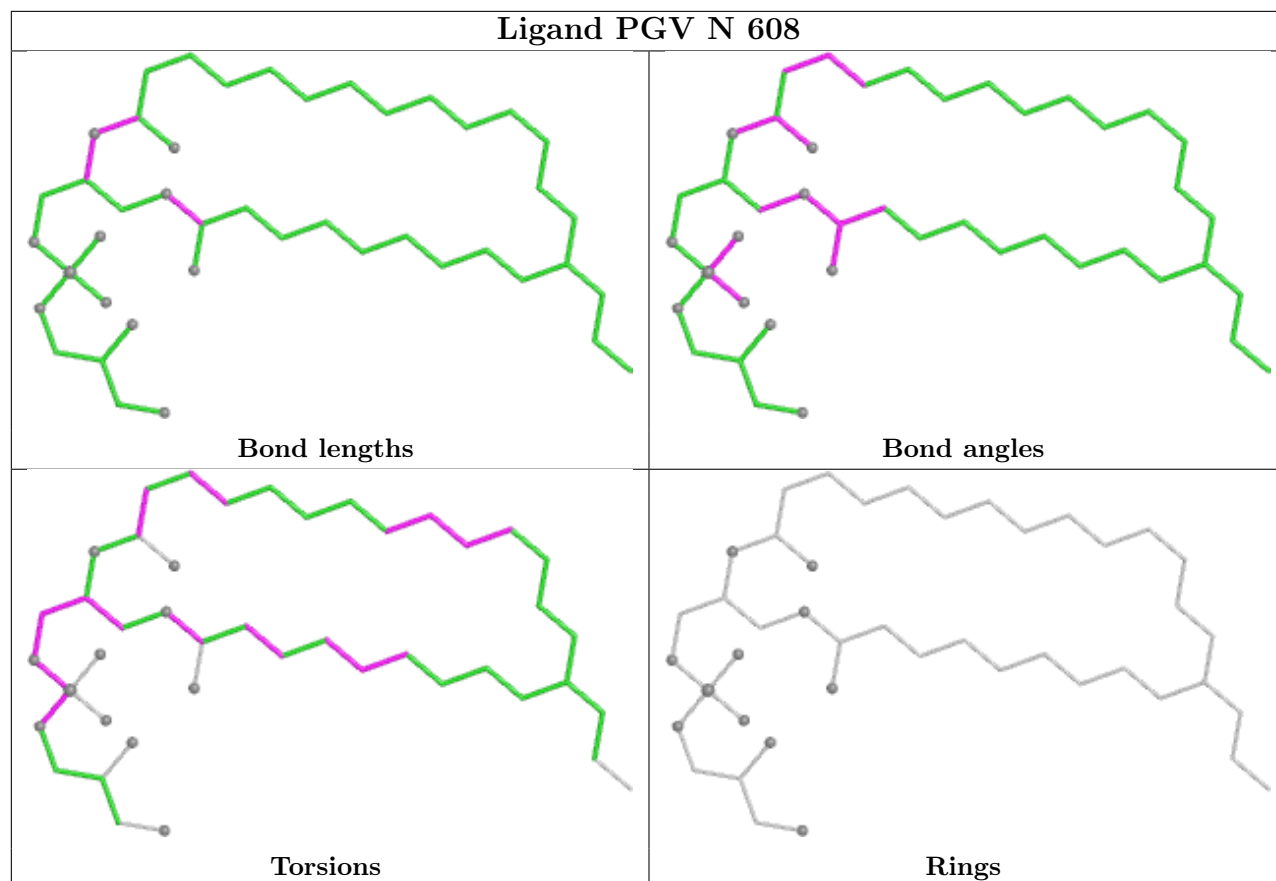


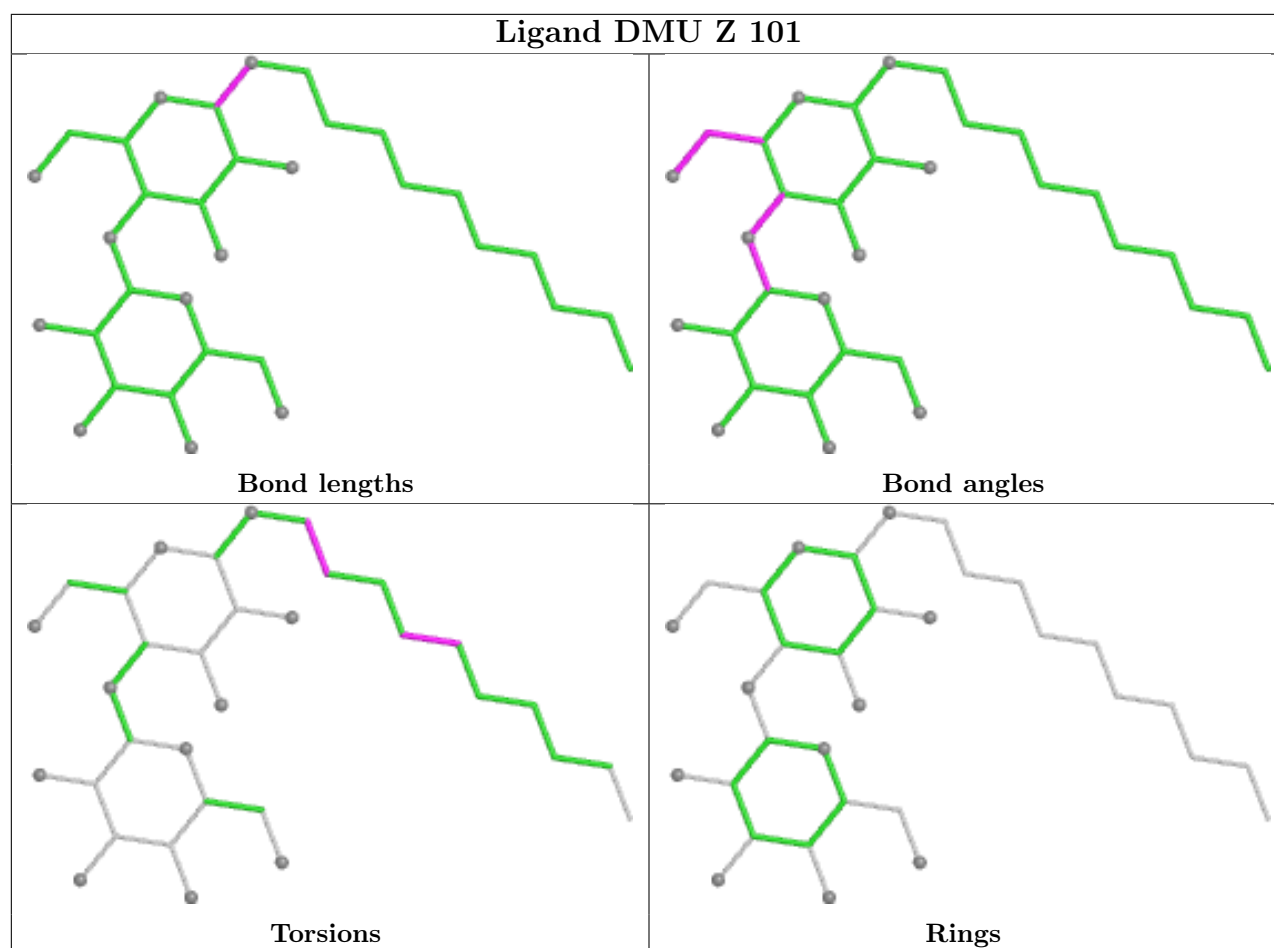


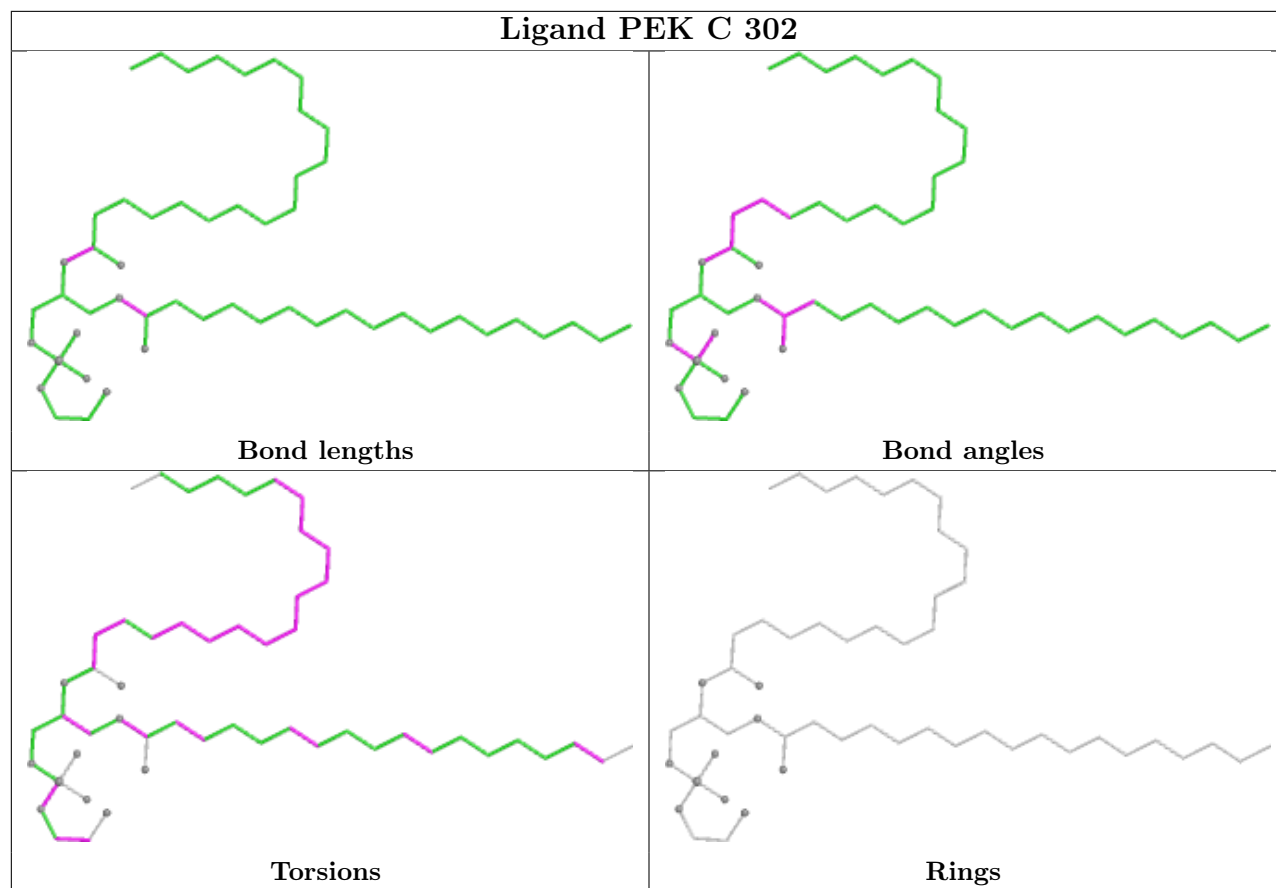


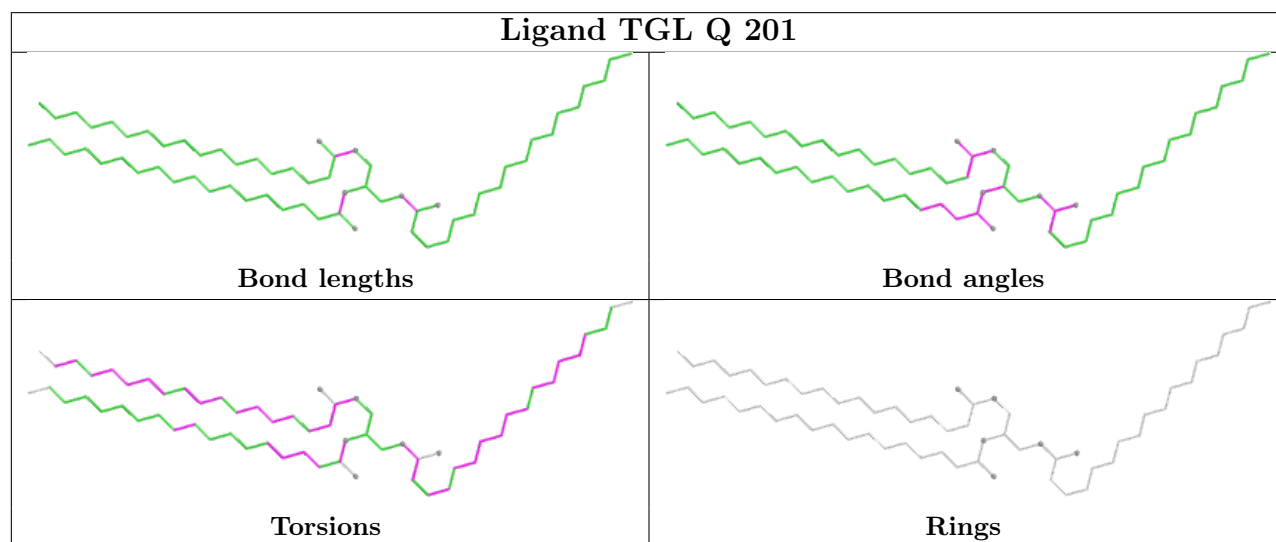
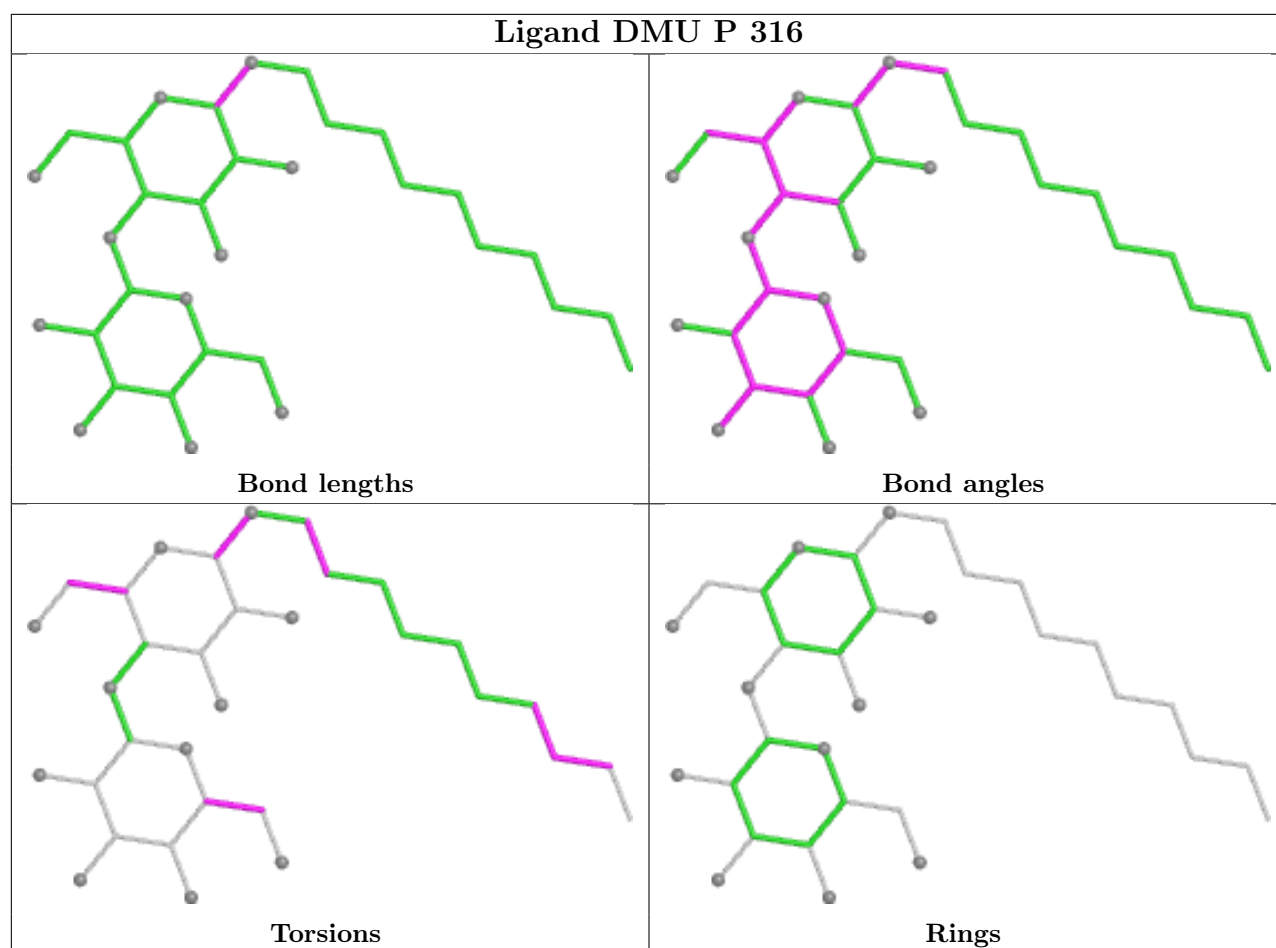


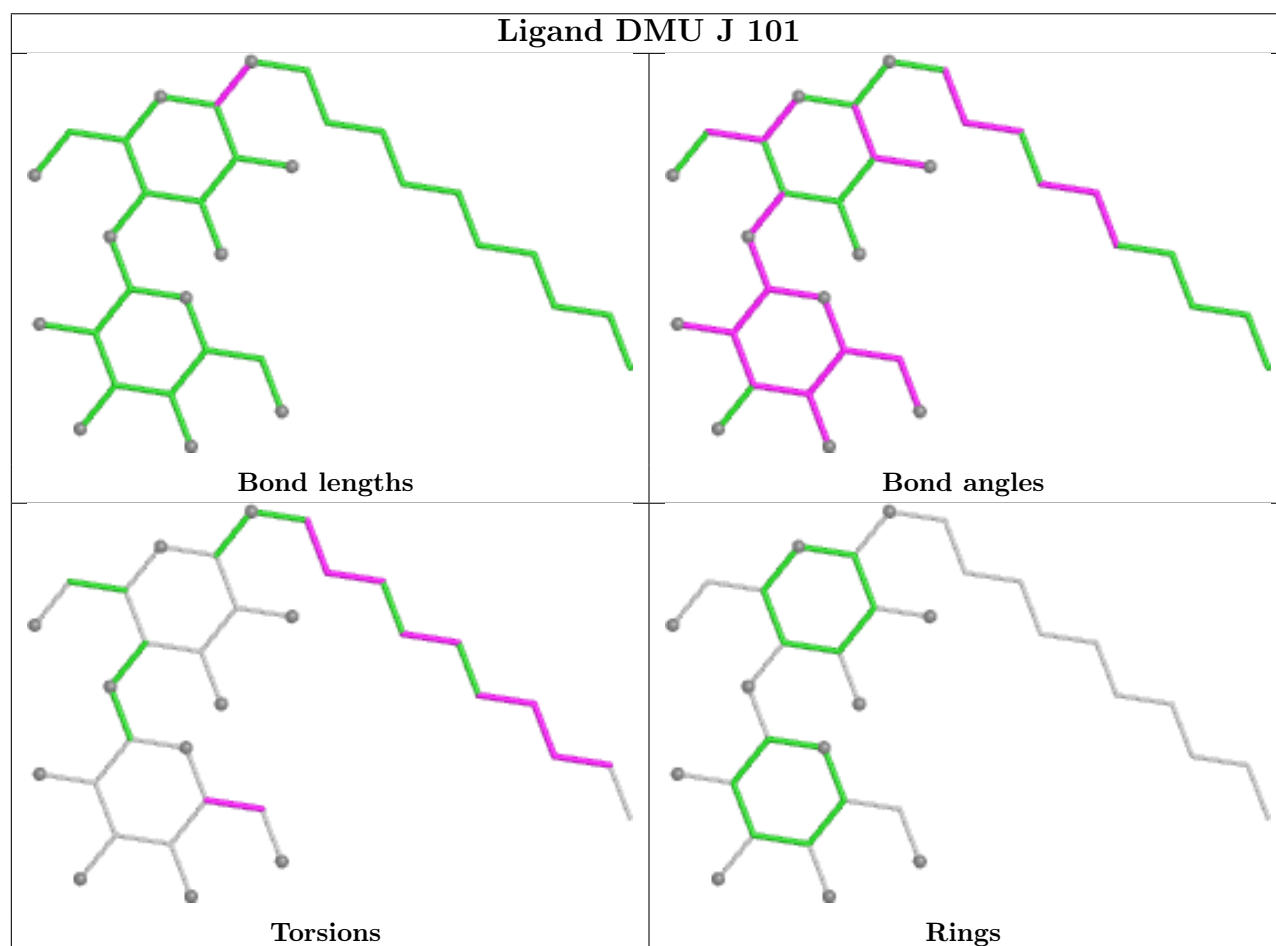
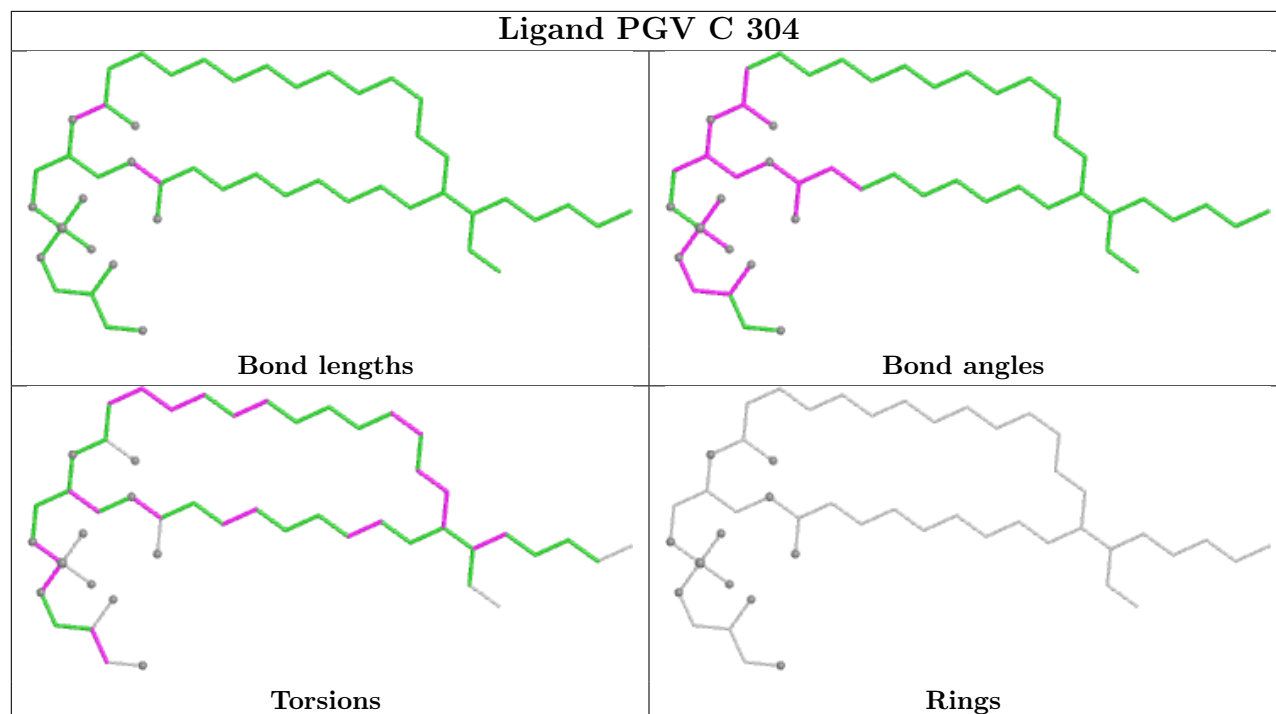


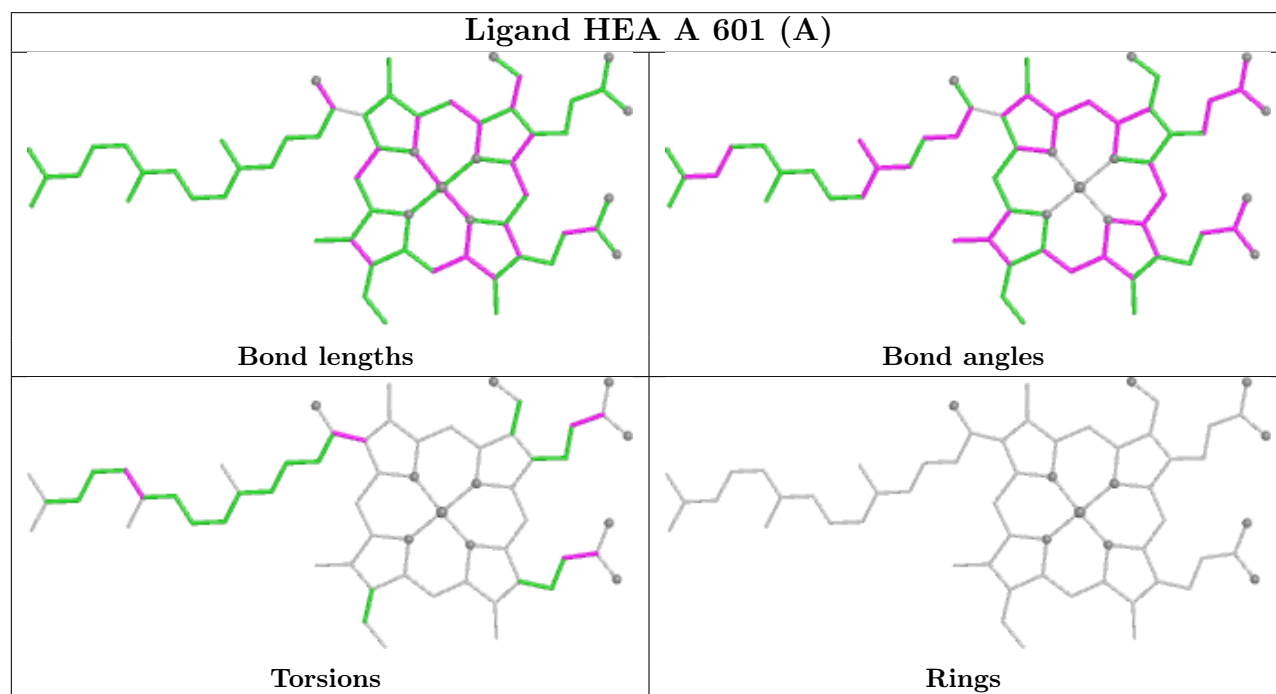
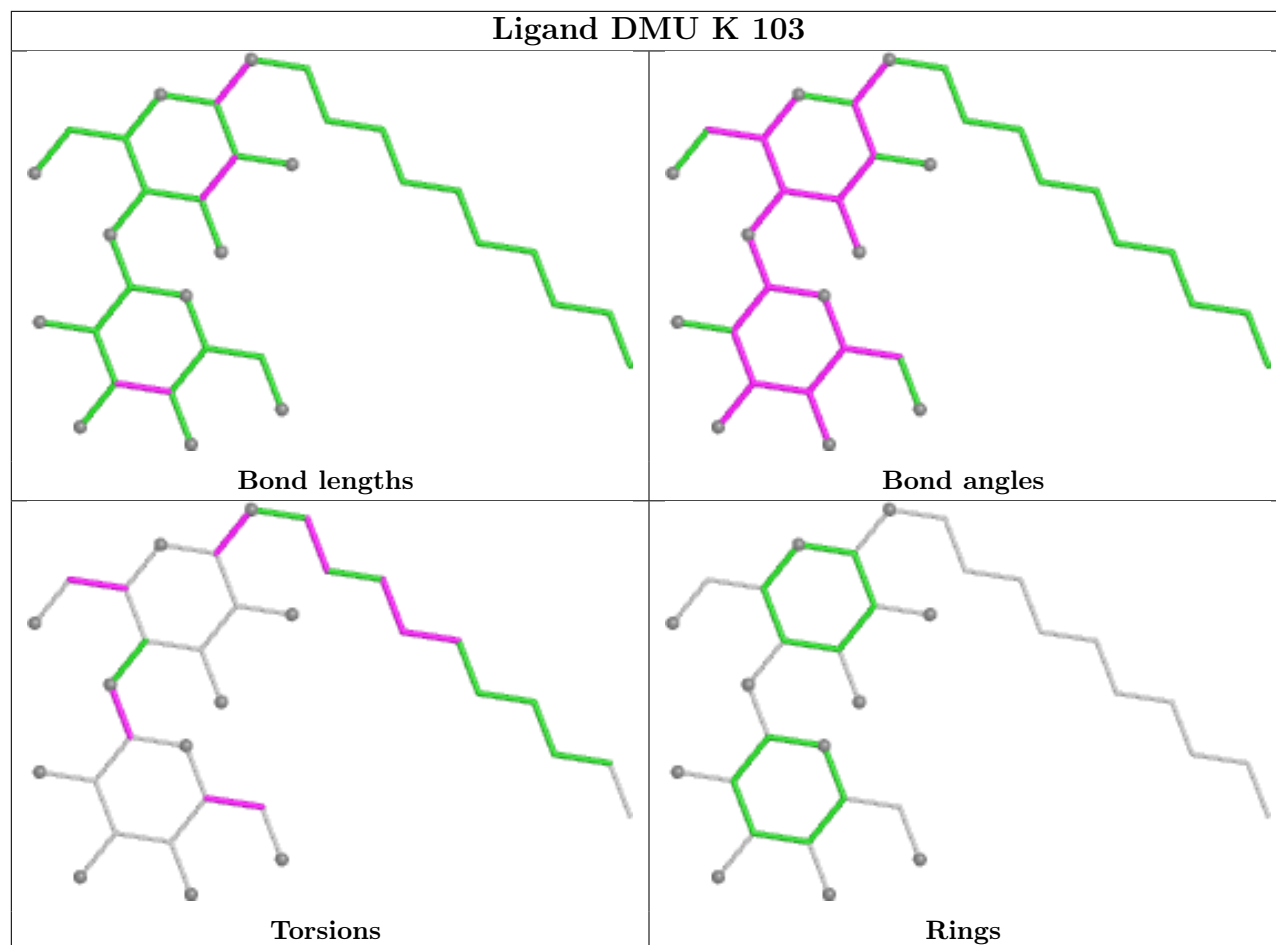


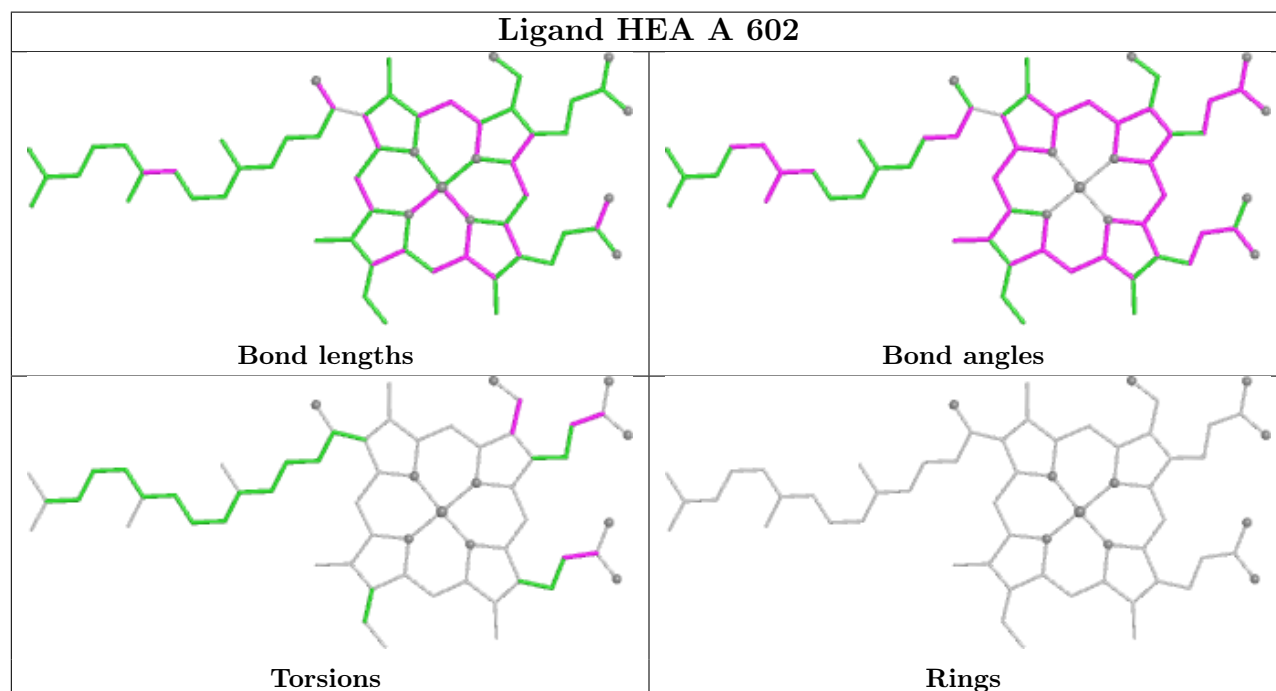
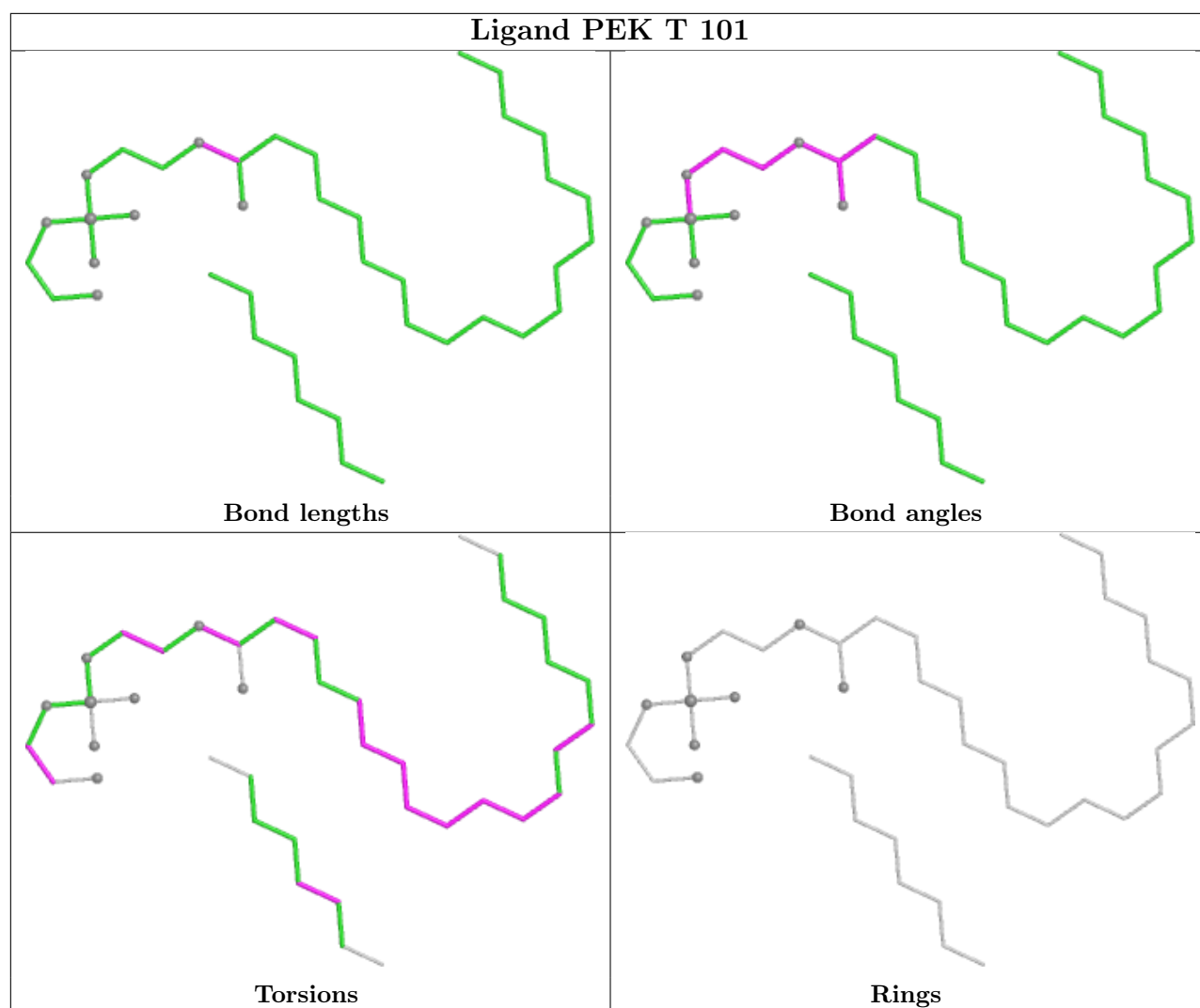


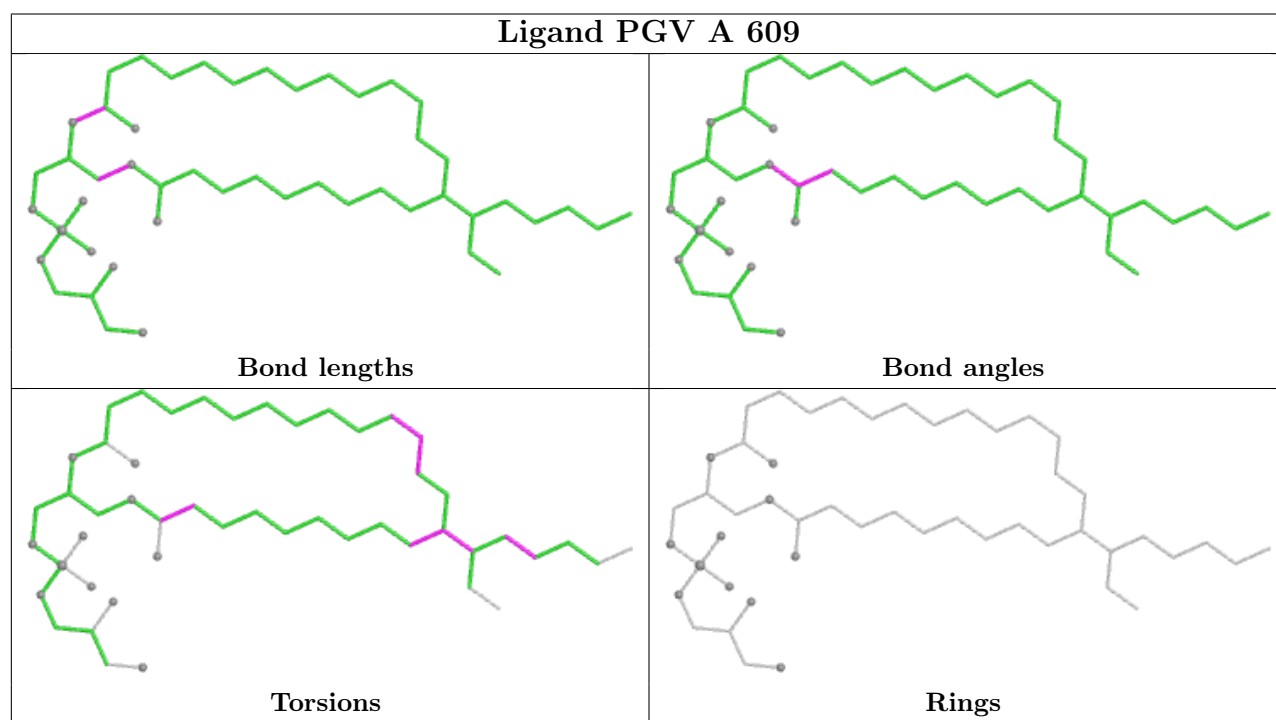
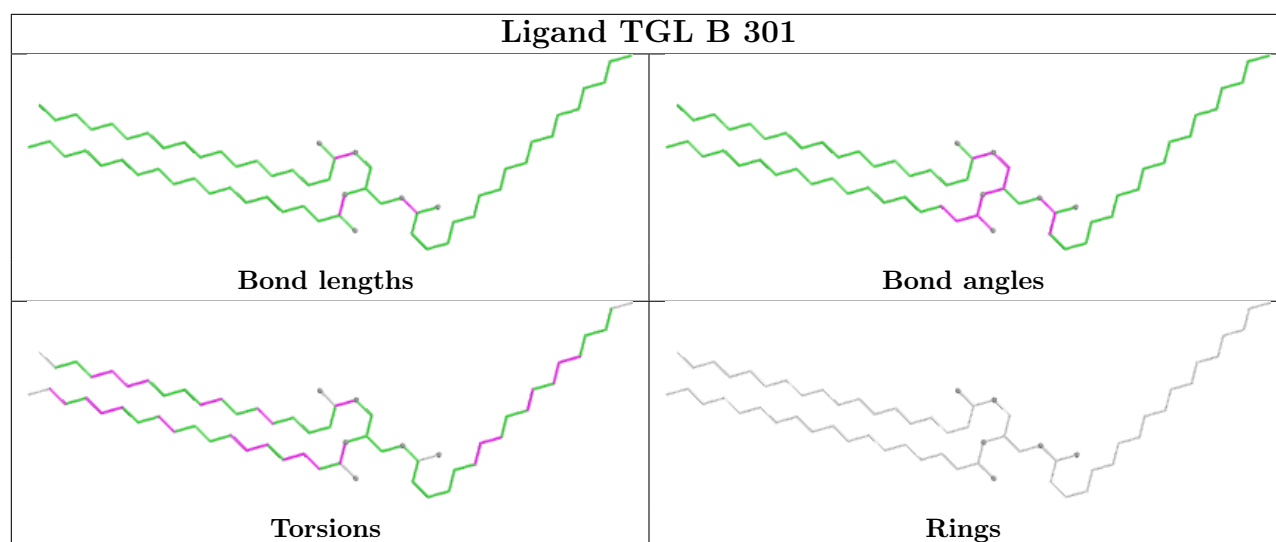


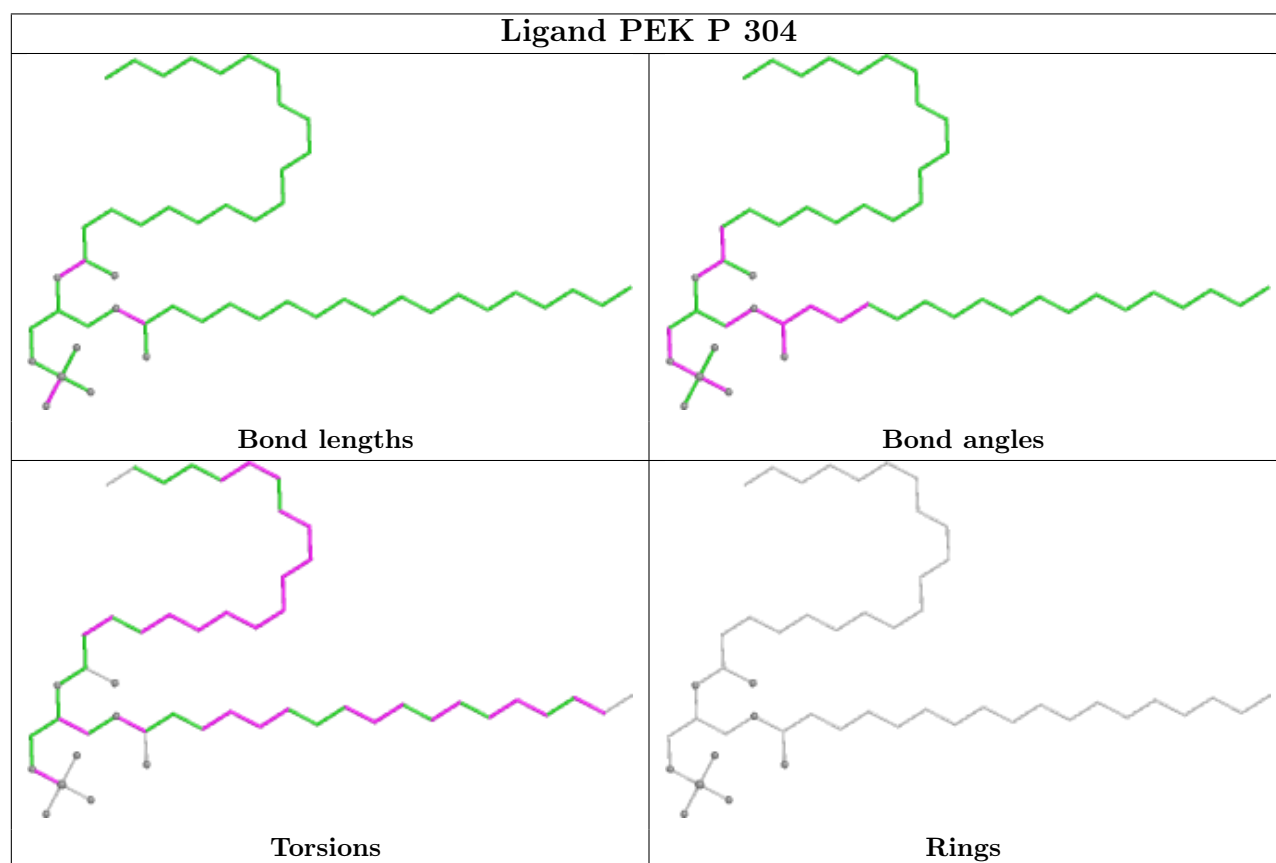
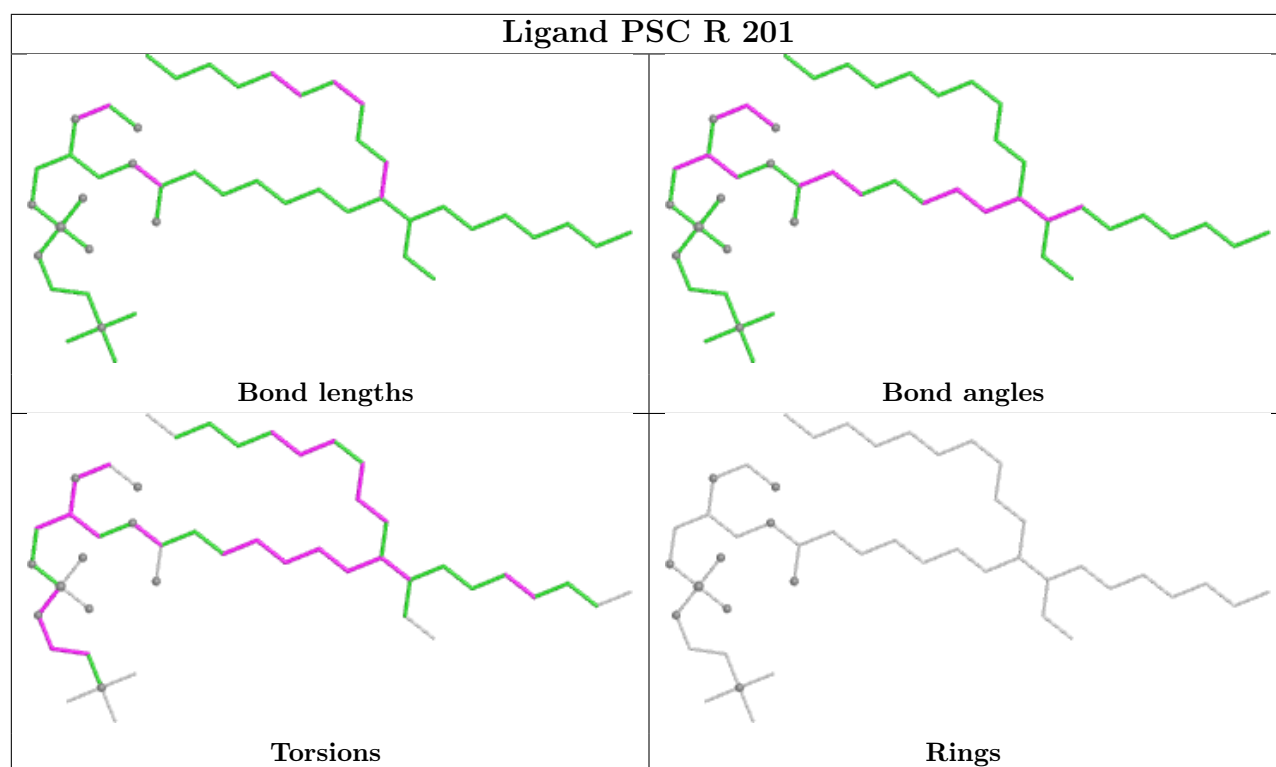


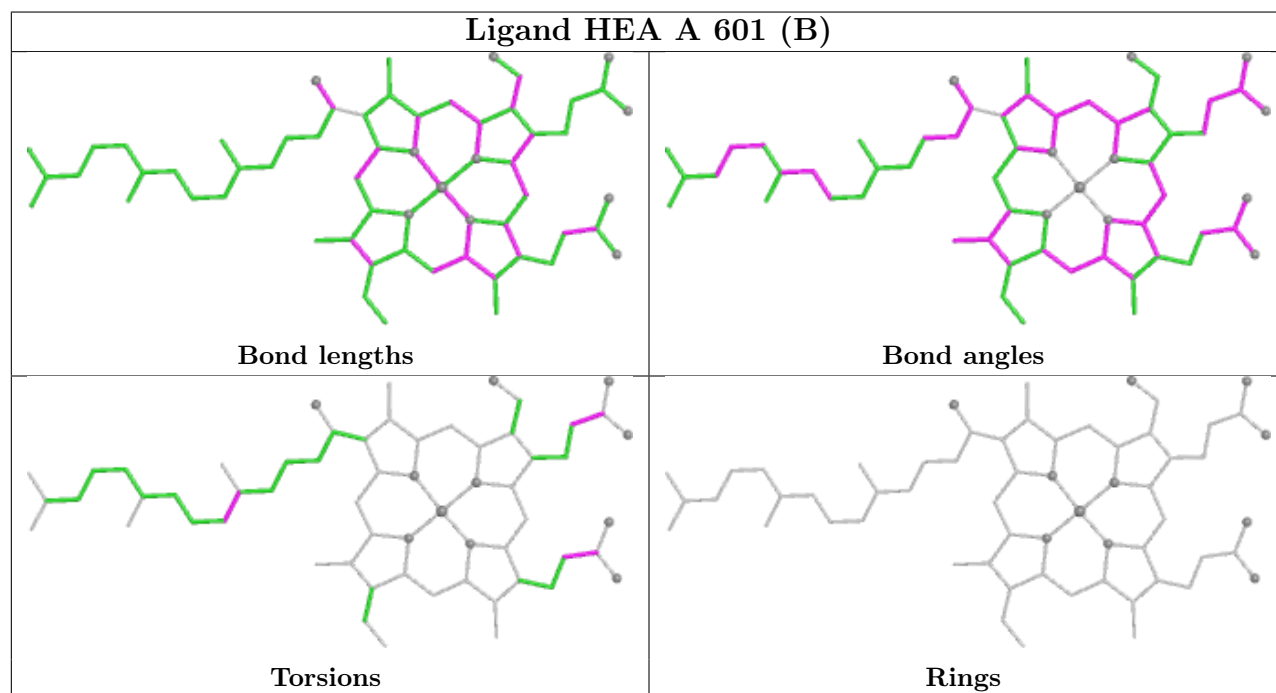
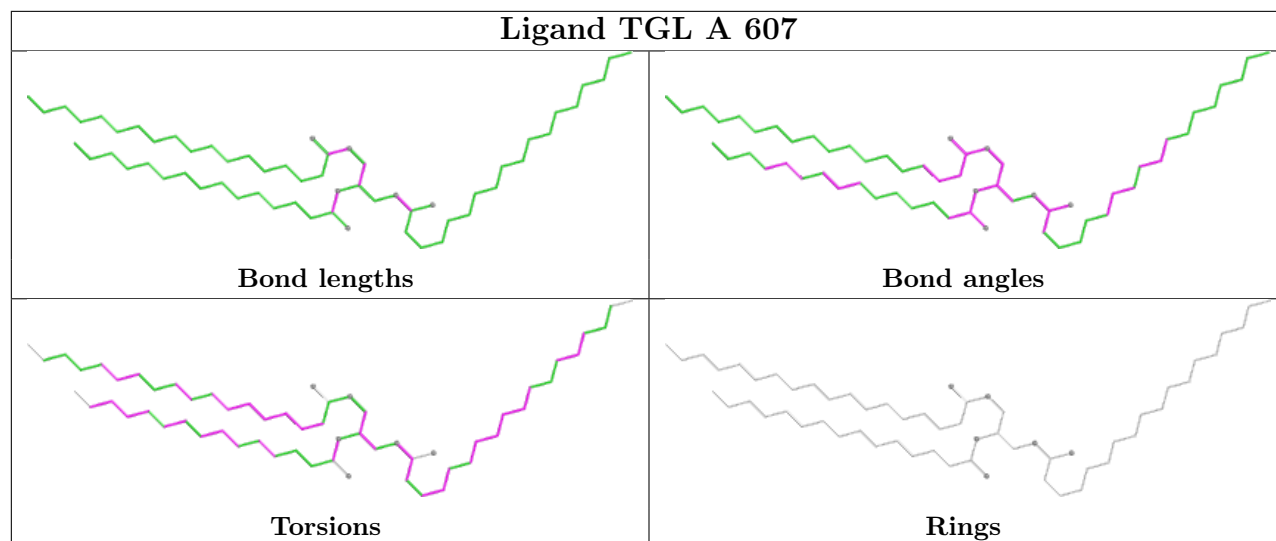


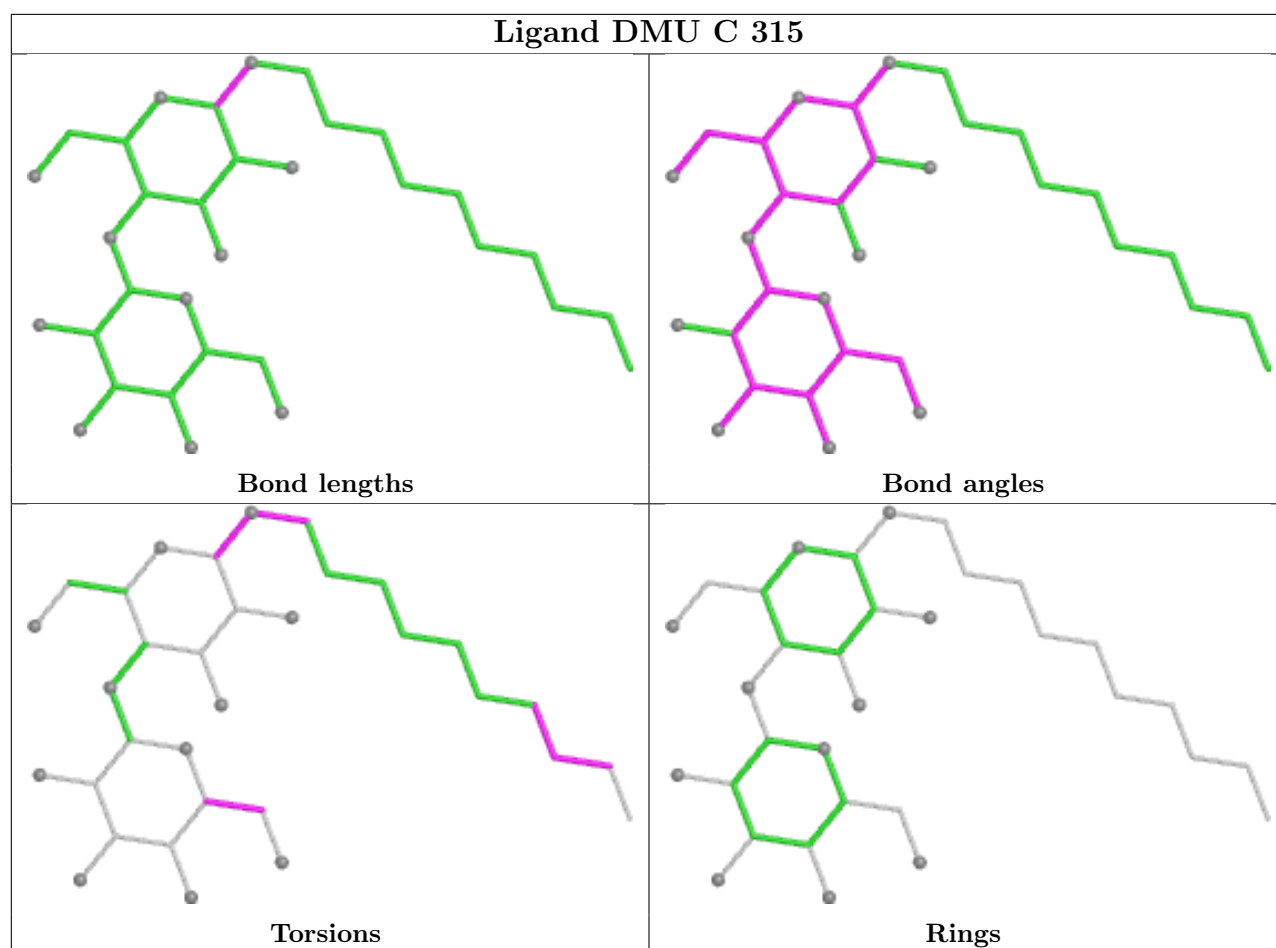


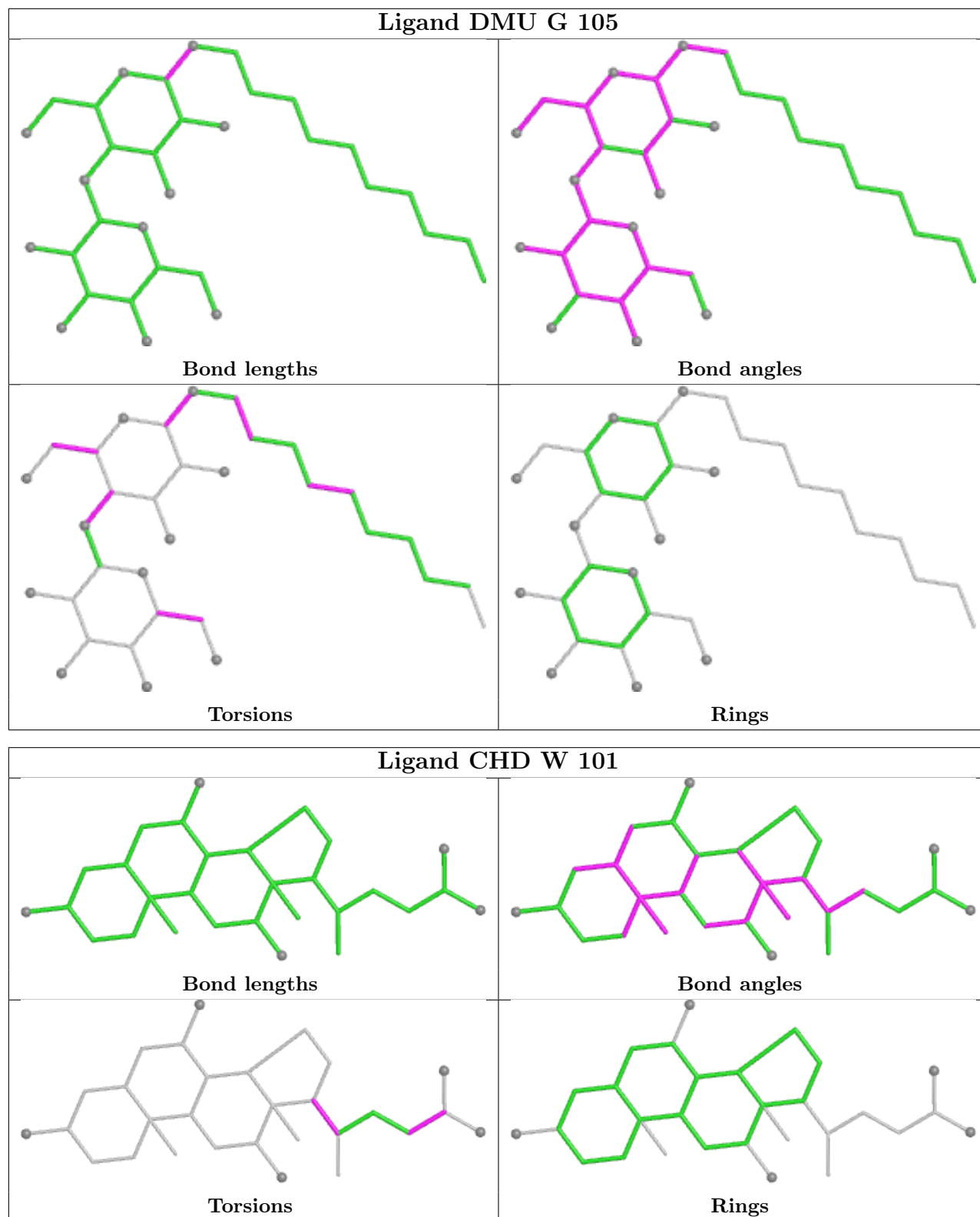


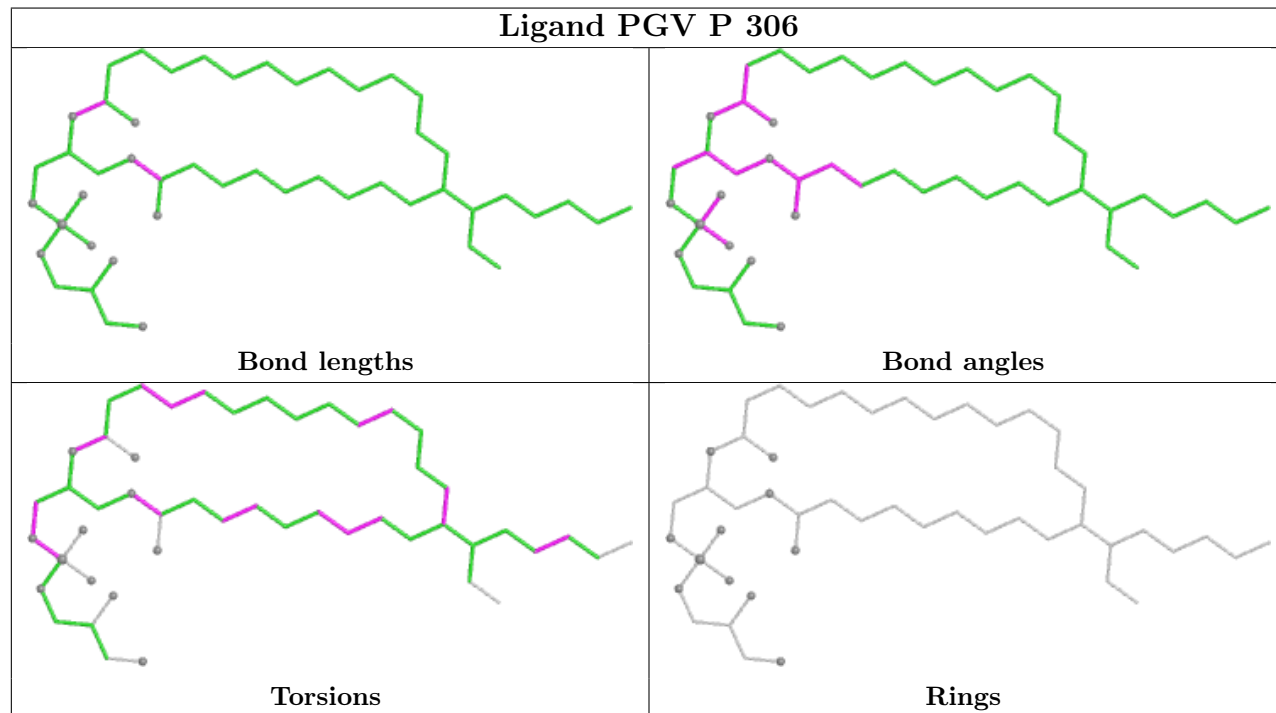
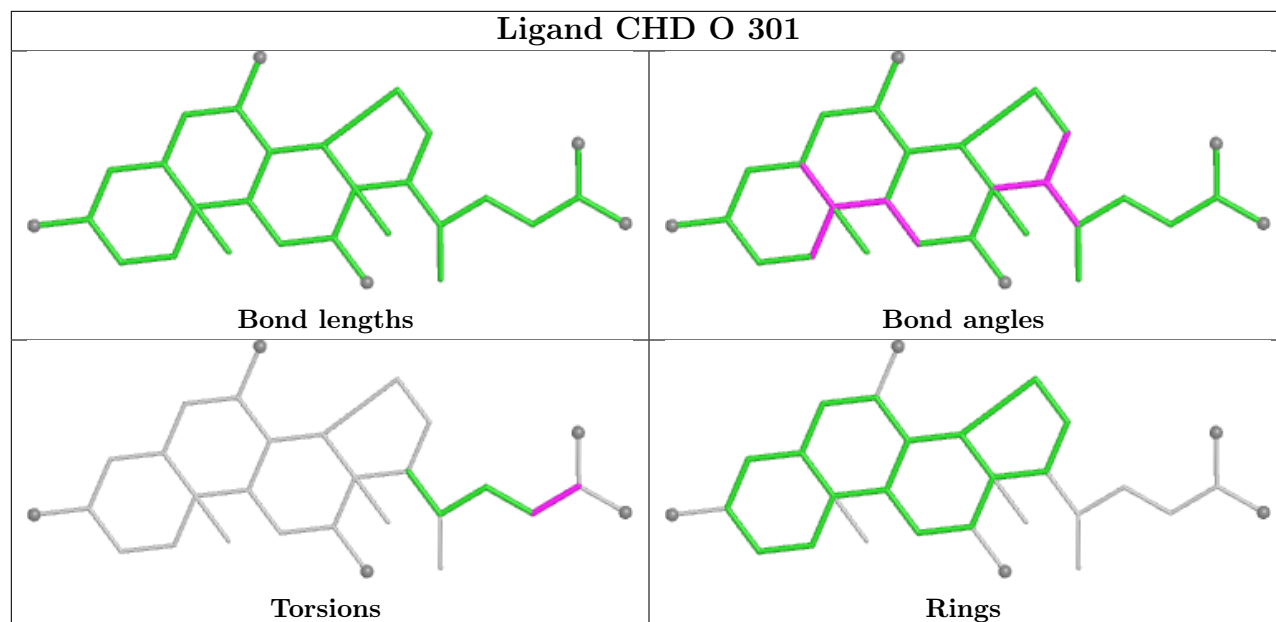


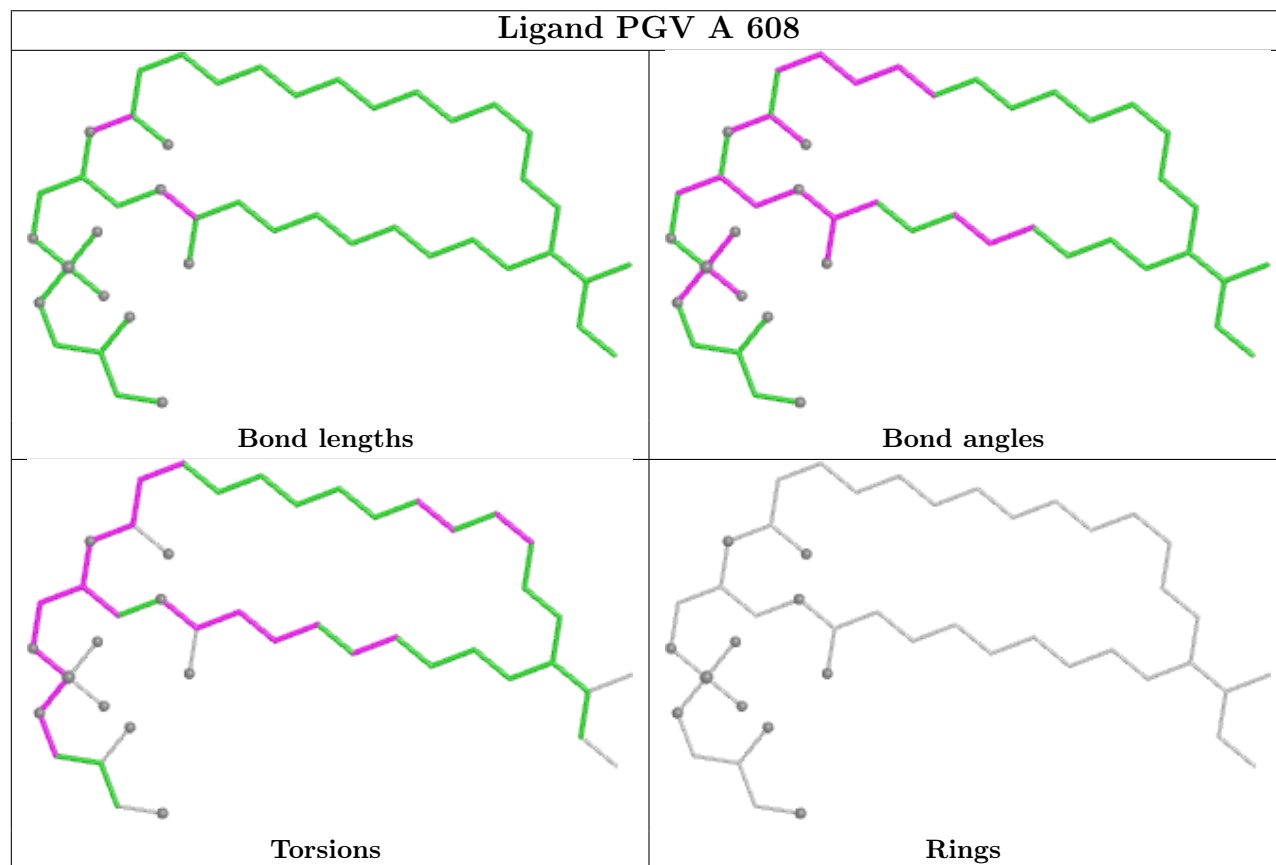
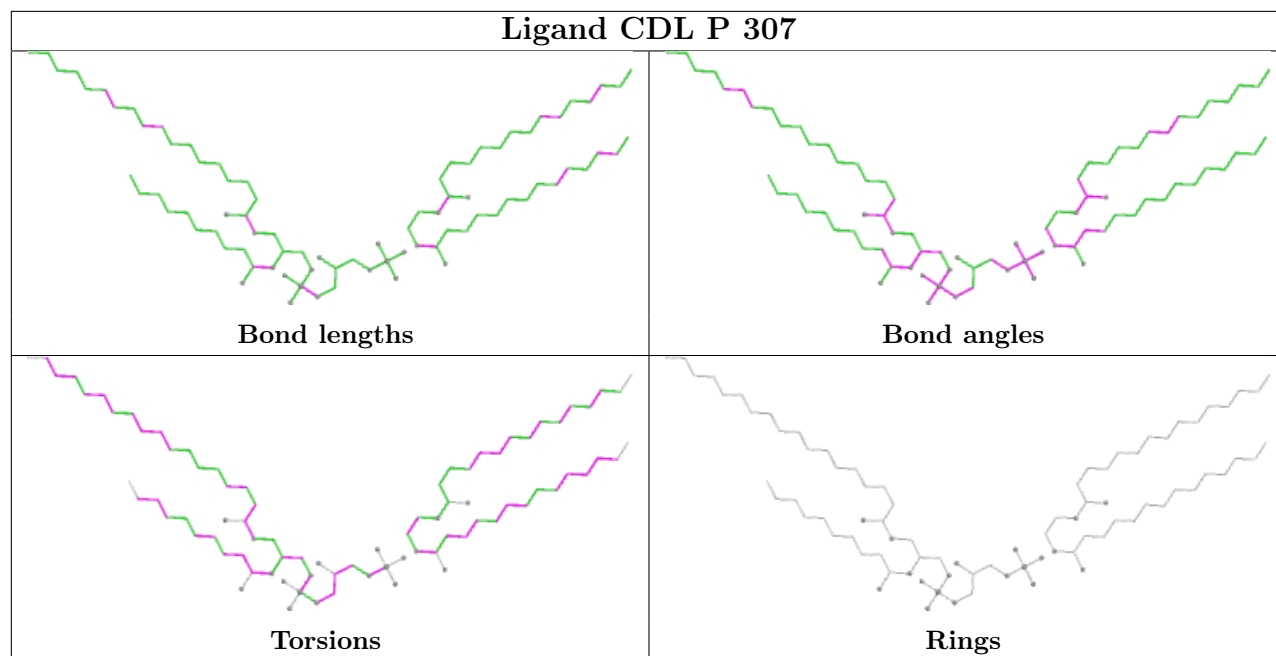


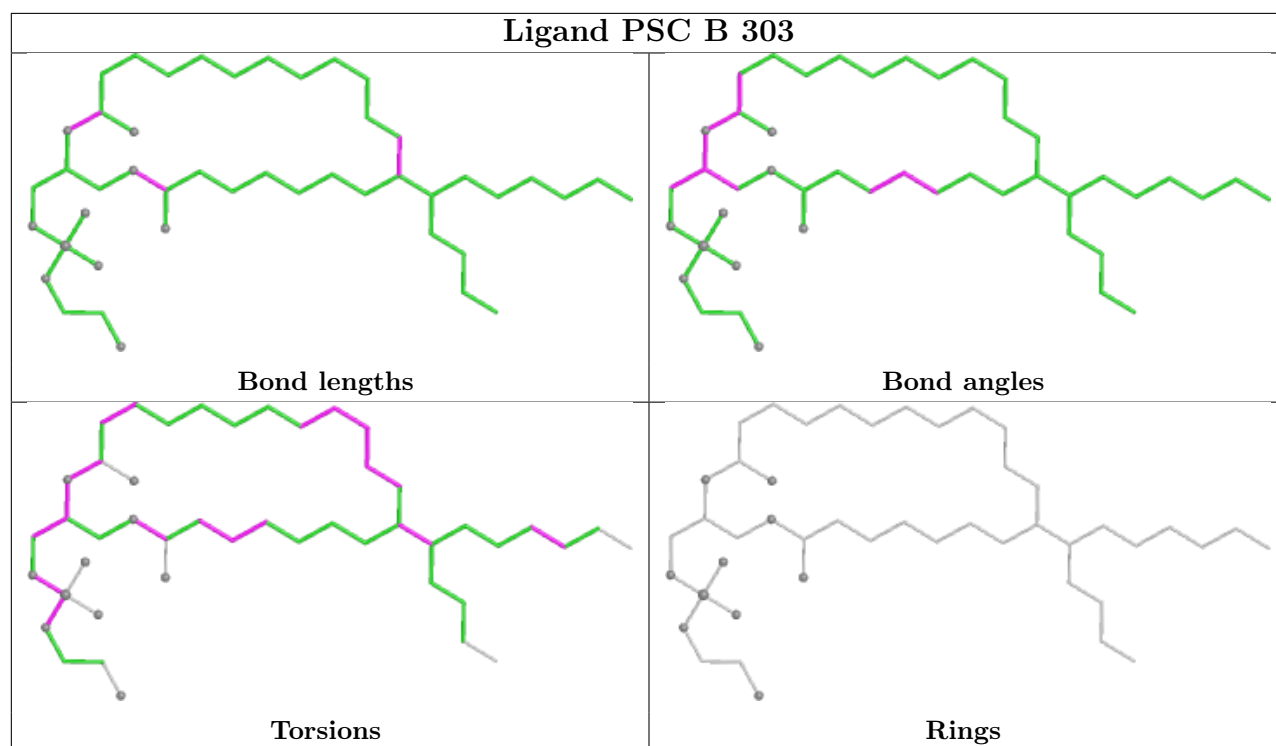
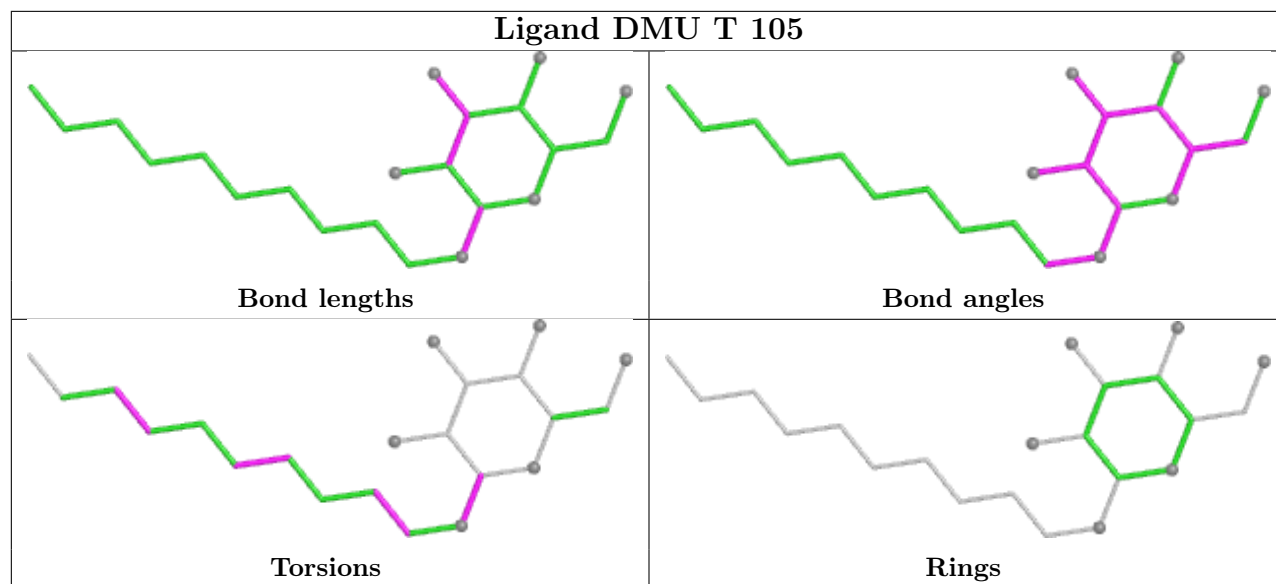


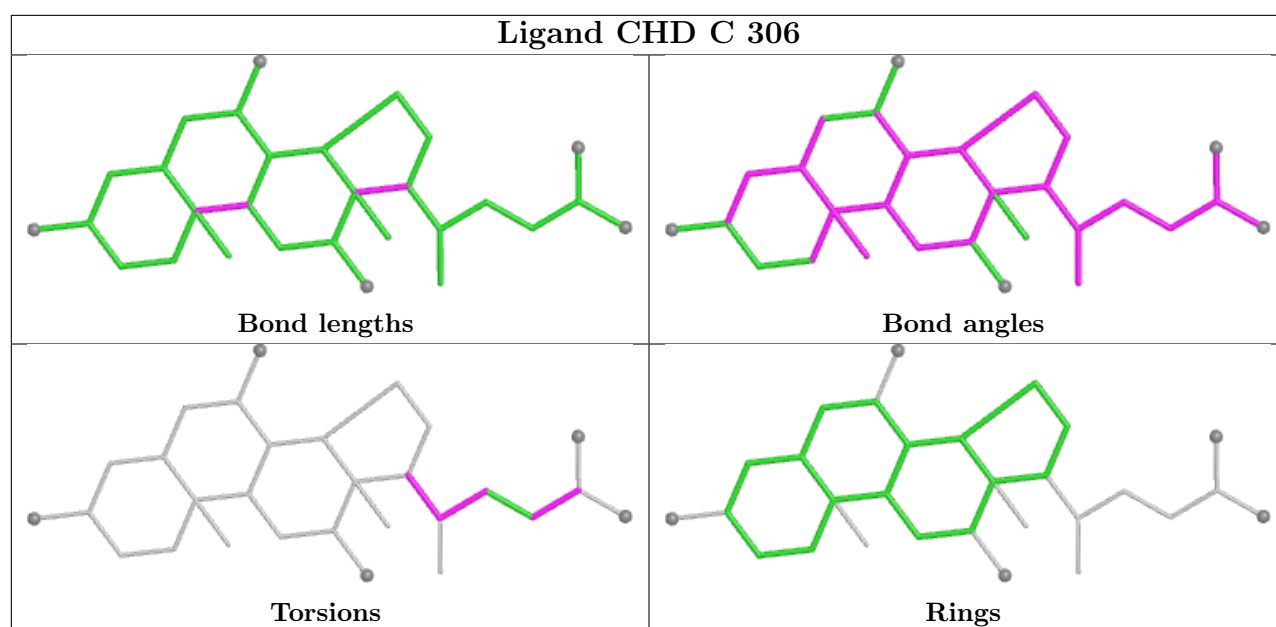
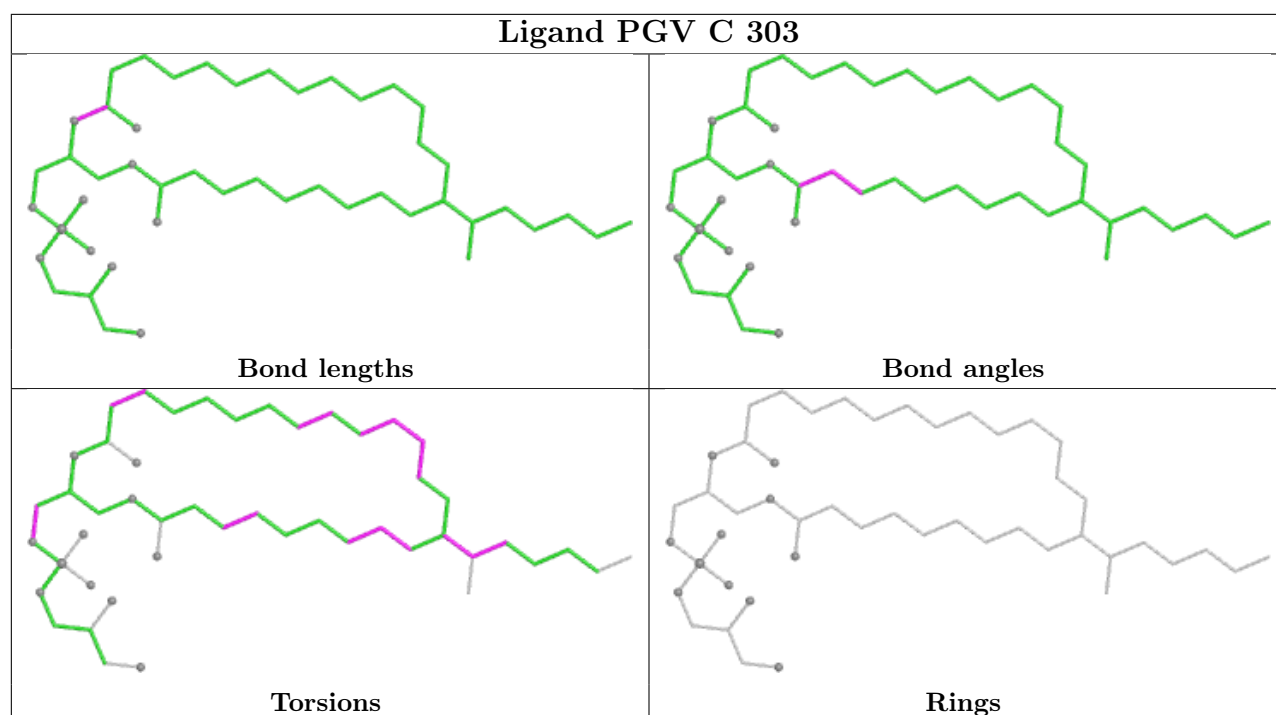


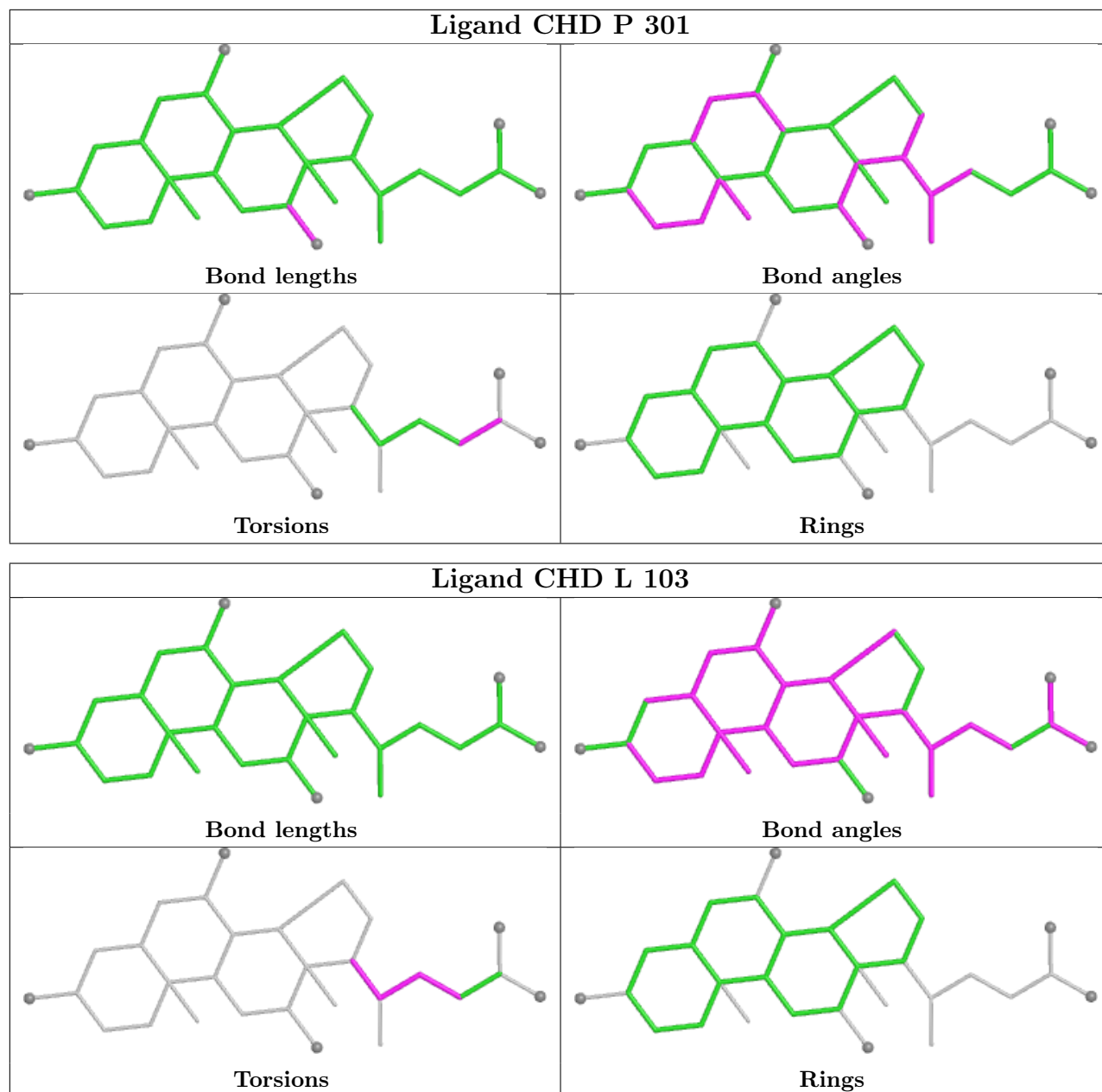


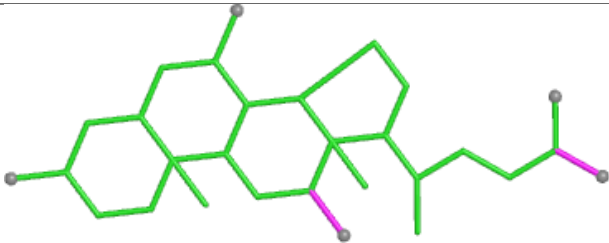
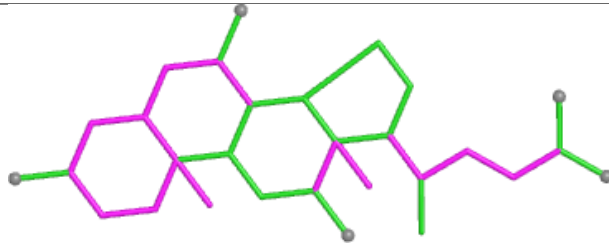
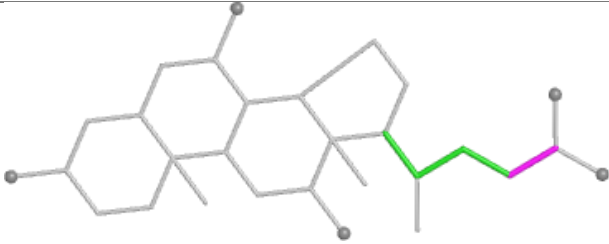
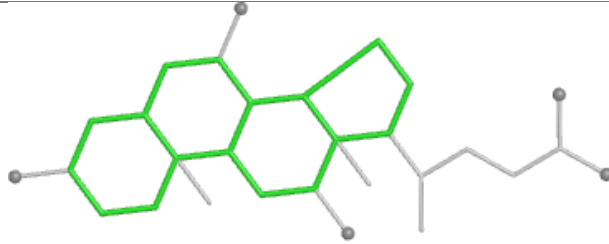


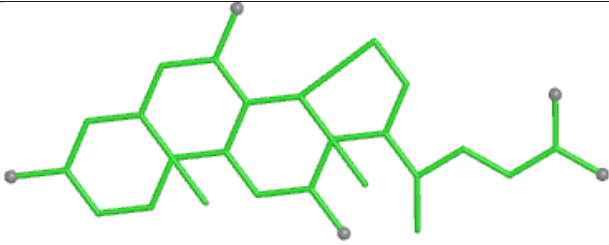
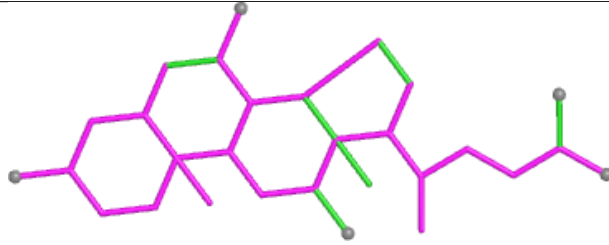
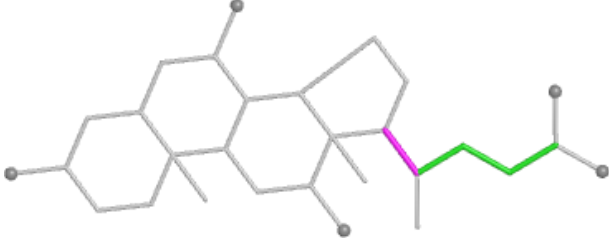
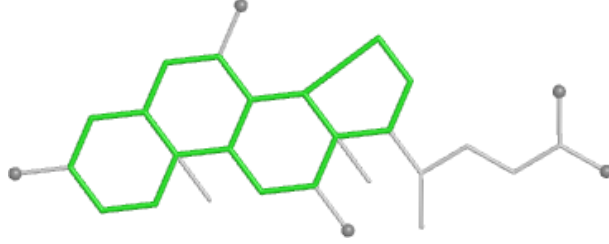


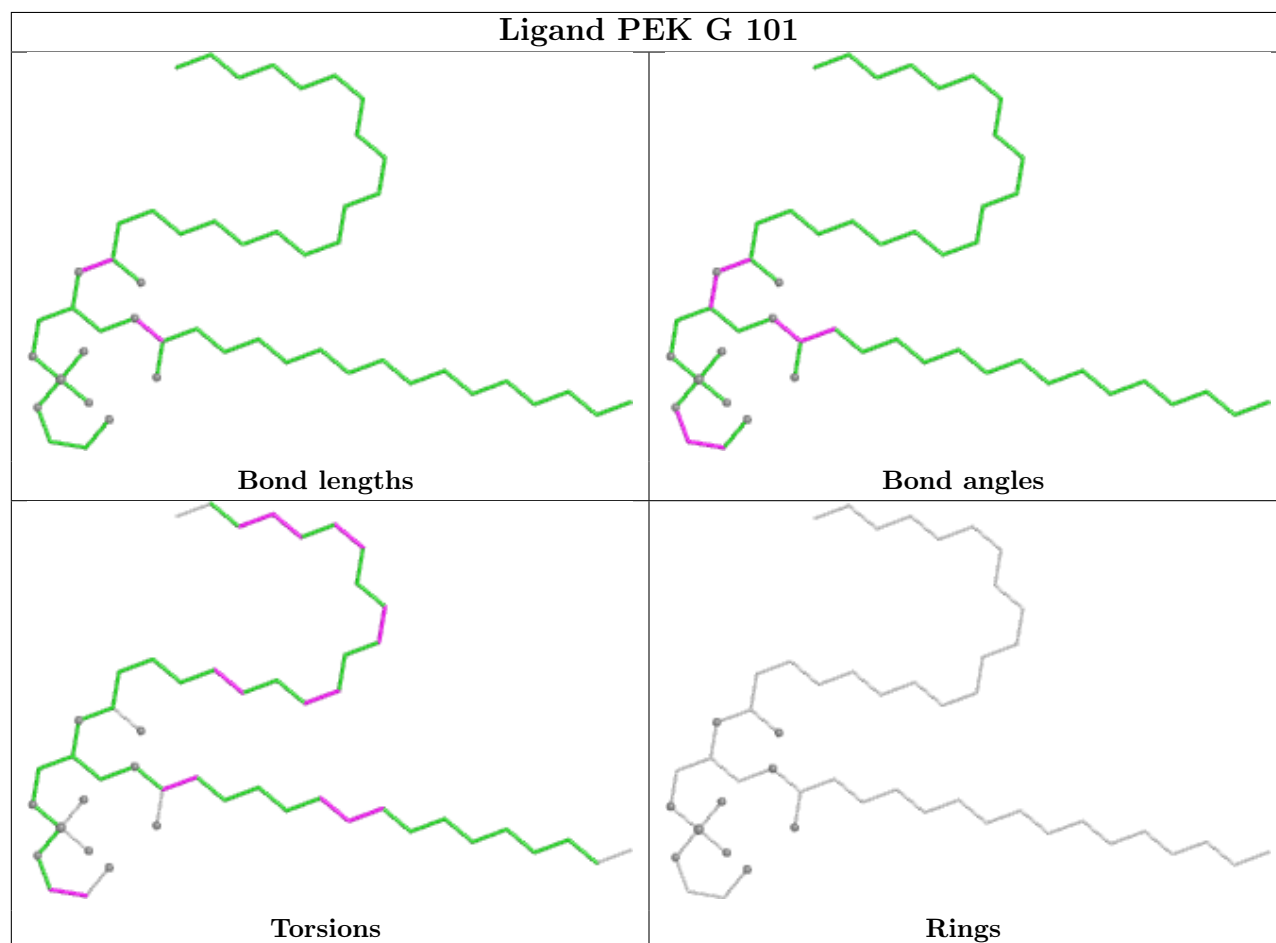
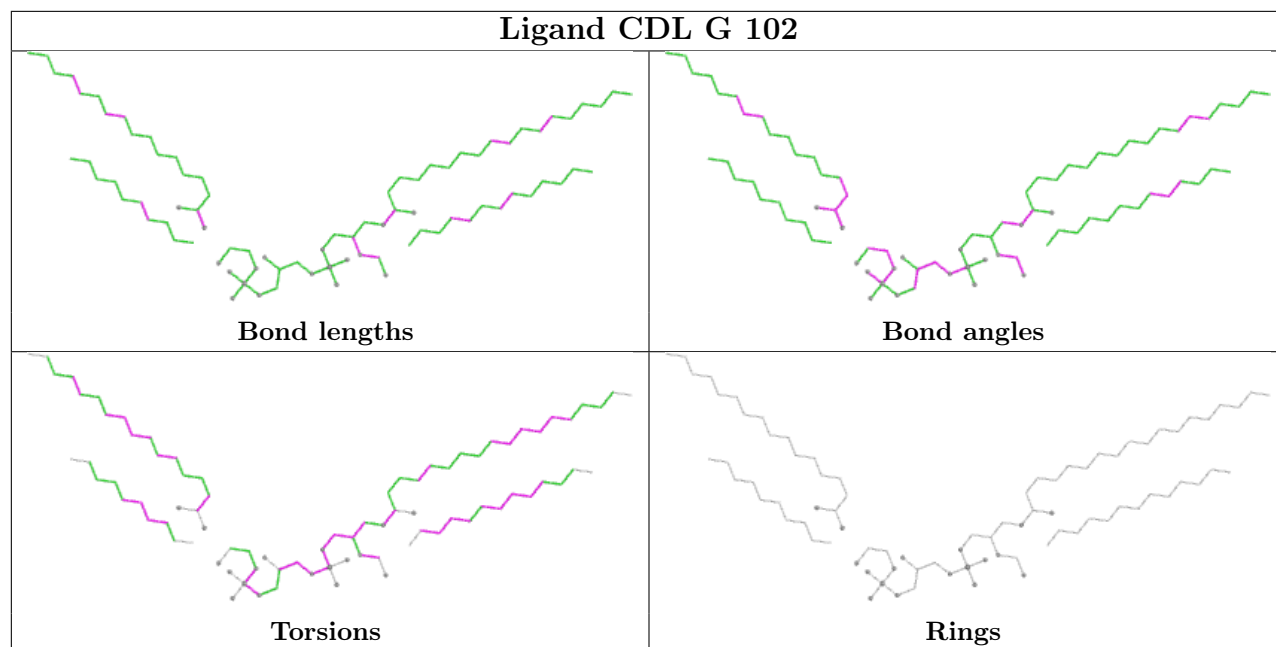


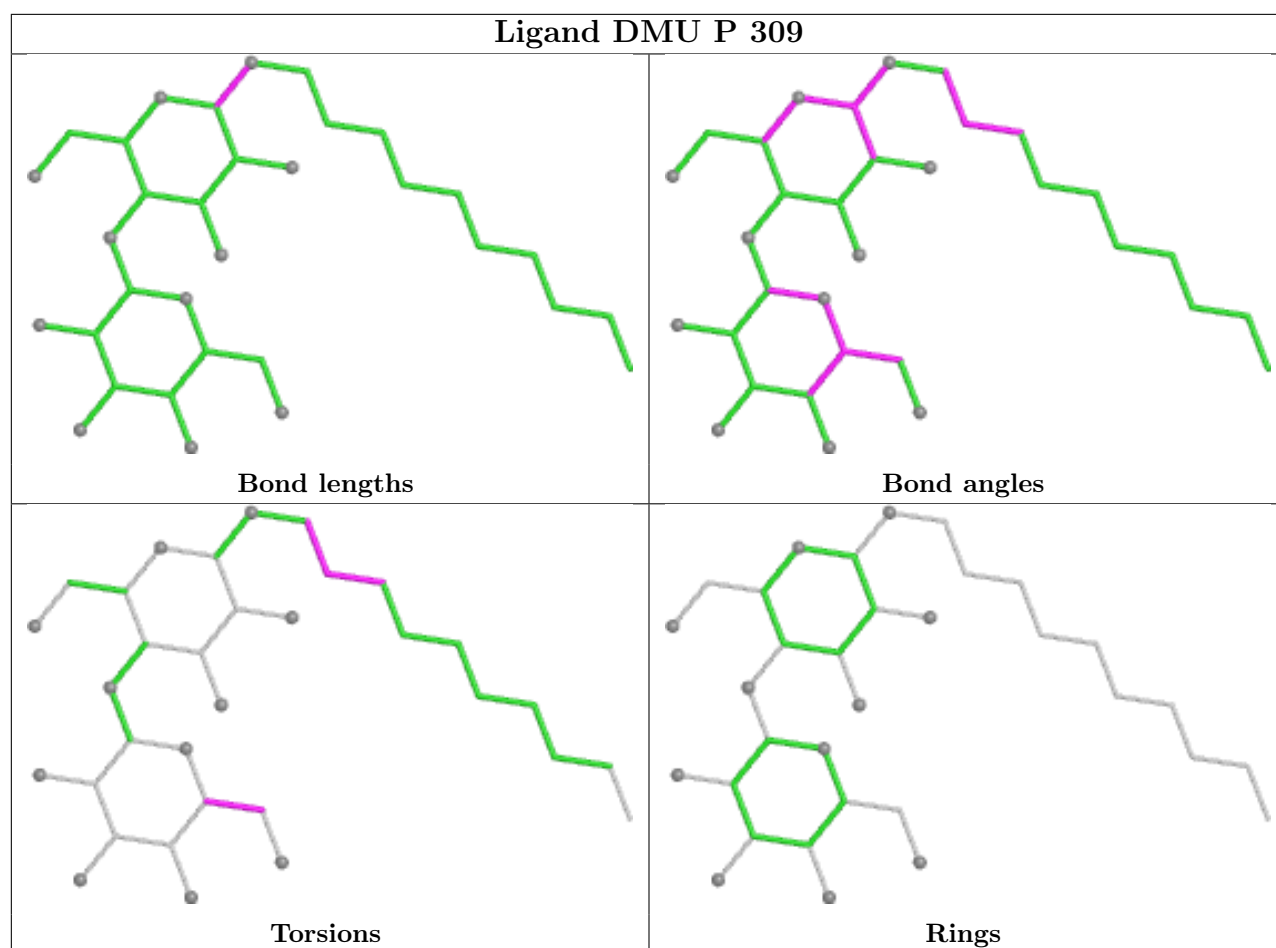




Ligand CHD C 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHD Y 104	
	
Bond lengths	Bond angles
	
Torsions	Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.45	4 (0%) 82 87	11, 24, 31, 87	27 (5%)
1	N	513/514 (99%)	-0.37	4 (0%) 82 87	12, 26, 35, 84	28 (5%)
2	B	226/227 (99%)	0.14	15 (6%) 24 27	15, 30, 47, 116	13 (5%)
2	O	226/227 (99%)	0.16	11 (4%) 35 39	16, 35, 60, 130	15 (6%)
3	C	259/259 (100%)	-0.23	6 (2%) 61 66	12, 27, 39, 74	8 (3%)
3	P	259/259 (100%)	-0.26	3 (1%) 76 81	12, 27, 40, 93	12 (4%)
4	D	144/144 (100%)	0.05	5 (3%) 47 51	16, 32, 56, 87	5 (3%)
4	Q	144/144 (100%)	0.78	16 (11%) 10 11	20, 44, 83, 183	4 (2%)
5	E	105/105 (100%)	0.02	4 (3%) 44 48	22, 32, 60, 149	1 (0%)
5	R	105/105 (100%)	0.06	3 (2%) 53 58	27, 38, 64, 156	1 (0%)
6	F	94/94 (100%)	0.26	7 (7%) 20 23	16, 33, 59, 158	3 (3%)
6	S	93/94 (98%)	0.31	6 (6%) 25 28	21, 31, 58, 178	2 (2%)
7	G	83/84 (98%)	1.18	22 (26%) 1 1	16, 35, 123, 171	5 (6%)
7	T	83/84 (98%)	1.12	22 (26%) 1 1	22, 36, 120, 191	3 (3%)
8	H	79/79 (100%)	0.67	12 (15%) 5 5	28, 38, 104, 125	0
8	U	79/79 (100%)	0.78	13 (16%) 4 4	32, 42, 120, 165	0
9	I	72/73 (98%)	0.78	10 (13%) 6 7	19, 42, 80, 95	2 (2%)
9	V	72/73 (98%)	0.91	7 (9%) 13 14	29, 51, 76, 179	0
10	J	58/58 (100%)	0.54	6 (10%) 12 12	26, 37, 71, 114	0
10	W	58/58 (100%)	0.36	3 (5%) 33 36	28, 40, 74, 185	0
11	K	49/49 (100%)	0.32	1 (2%) 65 70	16, 37, 54, 58	1 (2%)
11	X	49/49 (100%)	0.77	4 (8%) 17 19	21, 46, 68, 89	1 (2%)
12	L	46/46 (100%)	0.13	3 (6%) 25 28	24, 29, 51, 112	1 (2%)
12	Y	46/46 (100%)	0.15	2 (4%) 40 43	29, 35, 61, 126	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/43 (100%)	0.15	3 (6%) 22 25	24, 29, 70, 146	1 (2%)
13	Z	43/43 (100%)	0.59	5 (11%) 9 10	33, 39, 91, 169	1 (2%)
All	All	3541/3550 (99%)	0.08	197 (5%) 30 34	11, 30, 66, 191	135 (3%)

The worst 5 of 197 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	1	ALA	16.6
4	Q	6	VAL	13.0
4	Q	5	VAL	10.8
7	T	3	ALA	9.2
7	G	6	GLY	8.2

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	0.12	0.23	199,206,224,225	0
7	TPO	G	11	11/12	0.54	0.32	98,131,187,273	0
9	SAC	I	1	9/10	0.64	0.20	106,117,130,136	0
7	TPO	T	11	11/12	0.78	0.23	59,104,147,283	0
1	FME	A	1	10/11	0.90	0.18	34,43,78,247	0
1	FME	N	1	10/11	0.93	0.15	34,44,87,91	0
2	FME	O	1	10/11	0.97	0.08	34,36,40,71	0
2	FME	B	1	10/11	0.98	0.07	27,30,36,67	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($\text{\AA}^2$)	Q<0.9
27	DMU	K	103	33/33	0.34	0.20	63,75,85,88	0
24	CHD	Y	104	29/29	0.58	0.26	68,85,91,98	0
27	DMU	K	101	22/33	0.62	0.21	44,71,84,86	0
24	CHD	W	101	29/29	0.66	0.20	56,73,83,84	0
24	CHD	L	103	29/29	0.67	0.26	59,82,95,106	0
27	DMU	K	102	22/33	0.68	0.20	46,74,82,88	0
21	EDO	W	102	4/4	0.68	0.29	48,55,71,72	0
27	DMU	O	308	22/33	0.69	0.17	49,70,85,86	0
24	CHD	J	102	29/29	0.70	0.17	49,68,93,104	0
25	PEK	T	101	40/53	0.70	0.23	48,67,116,204	0
21	EDO	P	314	4/4	0.71	0.29	52,57,70,76	0
27	DMU	G	105	33/33	0.71	0.19	56,76,98,99	0
26	CDL	G	102	84/100	0.72	0.24	46,74,103,186	0
21	EDO	C	314	4/4	0.72	0.24	59,61,65,82	0
27	DMU	C	315	33/33	0.74	0.17	56,78,92,94	0
25	PEK	C	302	53/53	0.74	0.23	41,68,111,197	0
26	CDL	T	102	90/100	0.74	0.24	46,73,102,173	0
21	EDO	Y	103	4/4	0.75	0.22	58,67,76,85	0
27	DMU	J	101	33/33	0.75	0.17	47,72,87,95	0
27	DMU	L	104	22/33	0.75	0.18	46,69,80,82	0
25	PEK	P	304	50/53	0.75	0.23	36,72,108,183	0
19	TGL	Q	201	63/63	0.76	0.22	45,69,87,103	0
27	DMU	T	105	22/33	0.76	0.19	54,68,79,88	0
19	TGL	Y	101	56/63	0.77	0.24	40,62,94,105	0
20	PGV	P	306	51/51	0.77	0.22	43,74,99,167	0
21	EDO	D	204	4/4	0.78	0.33	72,85,85,92	0
20	PGV	C	304	51/51	0.78	0.21	38,68,102,170	0
21	EDO	D	203	4/4	0.79	0.19	48,60,70,71	0
25	PEK	P	302	37/53	0.79	0.18	45,69,106,186	0
21	EDO	A	622	4/4	0.79	0.21	50,58,63,73	0
21	EDO	J	103	4/4	0.79	0.24	46,49,68,77	0
23	PSC	B	303	48/52	0.79	0.21	43,71,103,194	0
23	PSC	R	201	49/52	0.80	0.22	36,68,104,175	0
20	PGV	N	608	46/51	0.80	0.21	42,71,109,162	0
19	TGL	N	607	62/63	0.80	0.22	45,69,83,90	0
21	EDO	A	614	4/4	0.80	0.24	49,63,65,67	0
19	TGL	B	301	63/63	0.80	0.21	31,64,87,93	0
24	CHD	P	308	29/29	0.81	0.15	46,56,80,93	0
27	DMU	P	309	33/33	0.81	0.15	45,73,86,92	0
19	TGL	D	201	53/63	0.81	0.21	36,60,83,94	0
26	CDL	P	307	84/100	0.82	0.22	37,71,98,148	0
27	DMU	P	316	33/33	0.82	0.14	54,64,77,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	N	623	4/4	0.82	0.22	34,42,44,60	0
21	EDO	P	311	4/4	0.83	0.17	36,53,56,62	0
29	PO4	U	102	5/5	0.83	0.12	54,57,73,89	0
21	EDO	G	104	4/4	0.84	0.18	46,70,74,76	0
21	EDO	B	309	4/4	0.84	0.24	37,68,75,84	0
21	EDO	S	105	4/4	0.84	0.18	43,46,63,66	0
19	TGL	A	607	60/63	0.84	0.22	30,61,95,112	0
26	CDL	C	305	91/100	0.84	0.18	40,68,97,127	0
21	EDO	Q	202	4/4	0.85	0.18	45,56,64,74	0
21	EDO	A	619	4/4	0.85	0.19	31,40,56,77	0
21	EDO	C	309	4/4	0.85	0.16	33,37,39,43	0
21	EDO	N	620	4/4	0.85	0.18	37,64,65,74	0
20	PGV	A	608	47/51	0.85	0.19	36,61,99,182	0
21	EDO	A	624	4/4	0.85	0.20	40,69,78,86	0
24	CHD	C	306	29/29	0.85	0.12	48,55,71,75	0
21	EDO	A	625	4/4	0.85	0.20	34,43,77,84	0
21	EDO	T	103	4/4	0.86	0.17	55,73,79,83	0
21	EDO	Q	203	4/4	0.86	0.20	52,53,53,56	0
21	EDO	B	310	4/4	0.86	0.18	69,69,79,88	0
29	PO4	H	102	5/5	0.86	0.12	57,68,74,78	0
21	EDO	Z	102	4/4	0.86	0.15	63,71,78,78	0
21	EDO	N	617	4/4	0.87	0.13	56,58,59,72	0
21	EDO	U	101	4/4	0.87	0.21	63,69,78,79	0
21	EDO	Q	204	4/4	0.88	0.17	44,50,54,55	0
21	EDO	F	104	4/4	0.88	0.20	46,48,57,65	0
21	EDO	A	610	4/4	0.88	0.20	25,31,68,79	0
27	DMU	Z	101	33/33	0.89	0.13	37,49,66,74	0
21	EDO	C	308	4/4	0.89	0.14	59,59,60,68	0
21	EDO	H	101	4/4	0.89	0.16	52,62,65,74	0
21	EDO	A	626	4/4	0.90	0.17	45,58,63,63	0
21	EDO	A	616	4/4	0.90	0.16	38,41,41,60	0
21	EDO	C	313	4/4	0.90	0.14	55,62,63,79	0
21	EDO	A	617	4/4	0.90	0.18	27,43,53,68	0
21	EDO	D	202	4/4	0.90	0.13	42,50,57,62	0
21	EDO	L	101	4/4	0.91	0.13	45,50,59,64	0
21	EDO	L	102	4/4	0.91	0.17	38,68,75,77	0
21	EDO	N	624	4/4	0.91	0.11	51,53,64,76	0
21	EDO	C	312	4/4	0.91	0.14	57,68,76,76	0
27	DMU	M	101	33/33	0.92	0.10	35,41,52,73	0
21	EDO	P	313	4/4	0.92	0.15	38,55,67,72	0
21	EDO	F	103	4/4	0.92	0.10	35,38,40,47	0
21	EDO	N	610	4/4	0.92	0.14	30,34,48,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	N	611	4/4	0.92	0.12	41,42,48,50	0
21	EDO	O	304	4/4	0.92	0.13	39,51,53,57	0
21	EDO	R	203	4/4	0.92	0.12	39,42,53,54	0
21	EDO	B	308	4/4	0.92	0.14	30,44,53,64	0
21	EDO	N	618	4/4	0.93	0.11	36,38,42,42	0
21	EDO	M	102	4/4	0.93	0.12	54,61,72,72	0
21	EDO	A	623	4/4	0.93	0.14	41,50,61,65	0
21	EDO	P	315	4/4	0.93	0.15	31,37,44,54	0
21	EDO	C	311	4/4	0.93	0.12	45,56,59,62	0
21	EDO	A	620	4/4	0.93	0.13	36,40,41,45	0
21	EDO	O	306	4/4	0.93	0.14	34,42,49,60	0
21	EDO	O	307	4/4	0.93	0.14	35,43,53,55	0
21	EDO	P	310	4/4	0.93	0.14	50,58,64,67	0
21	EDO	O	303	4/4	0.94	0.10	38,43,44,47	0
21	EDO	Y	102	4/4	0.94	0.13	59,62,65,73	0
21	EDO	N	613	4/4	0.94	0.11	37,37,44,47	0
21	EDO	A	615	4/4	0.94	0.09	29,30,31,34	0
21	EDO	M	103	4/4	0.94	0.12	47,52,55,60	0
21	EDO	N	622	4/4	0.95	0.10	40,40,43,44	0
21	EDO	N	614	4/4	0.95	0.12	32,43,49,67	0
21	EDO	N	616	4/4	0.95	0.14	34,52,57,70	0
21	EDO	A	612	4/4	0.95	0.11	37,38,41,46	0
21	EDO	C	310	4/4	0.95	0.11	30,36,48,50	0
25	PEK	P	303	53/53	0.95	0.13	26,44,80,86	0
21	EDO	T	104	4/4	0.95	0.10	30,32,39,44	0
21	EDO	O	305	4/4	0.95	0.08	29,30,32,32	0
21	EDO	B	306	4/4	0.95	0.13	36,41,48,59	0
21	EDO	A	621	4/4	0.96	0.12	29,36,38,65	0
21	EDO	B	307	4/4	0.96	0.11	39,41,61,72	0
25	PEK	G	101	51/53	0.96	0.12	27,42,75,92	0
21	EDO	A	611	4/4	0.96	0.14	30,41,61,85	0
21	EDO	N	615	4/4	0.96	0.09	28,29,29,34	0
20	PGV	N	609	51/51	0.96	0.11	22,29,65,72	0
21	EDO	E	202	4/4	0.96	0.07	37,38,41,44	0
24	CHD	C	301	29/29	0.96	0.07	23,28,33,35	0
21	EDO	S	102	4/4	0.96	0.09	34,36,37,46	0
21	EDO	B	305	4/4	0.96	0.10	26,26,29,30	0
21	EDO	N	619	4/4	0.96	0.12	30,42,62,74	0
21	EDO	C	307	4/4	0.96	0.08	32,33,33,35	0
21	EDO	G	103	4/4	0.96	0.08	31,32,37,38	0
20	PGV	C	303	50/51	0.97	0.10	22,29,76,79	0
20	PGV	P	305	51/51	0.97	0.10	23,30,70,84	0

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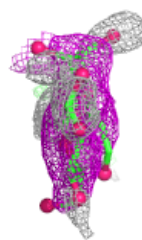
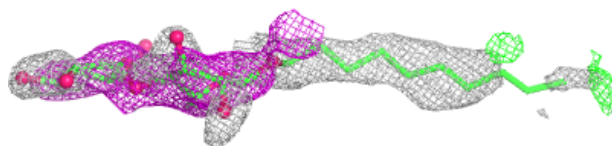
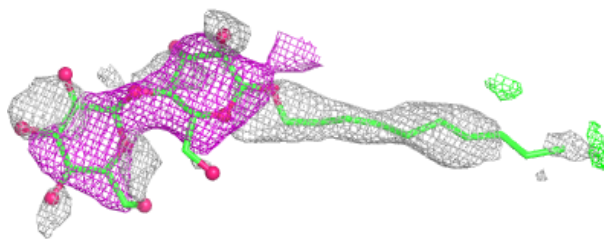
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CHD	B	304	29/29	0.97	0.06	24,27,34,45	0
21	EDO	P	312	4/4	0.97	0.08	35,37,38,42	0
21	EDO	A	618	4/4	0.97	0.08	30,36,39,43	0
21	EDO	E	201	4/4	0.97	0.08	37,37,39,44	0
17	NA	N	605	1/1	0.97	0.06	30,30,30,30	0
24	CHD	P	301	29/29	0.97	0.06	24,29,34,34	0
21	EDO	N	612	4/4	0.97	0.08	25,28,29,32	0
20	PGV	A	609	51/51	0.97	0.10	21,27,66,71	0
21	EDO	N	621	4/4	0.97	0.09	31,38,42,48	0
21	EDO	R	202	4/4	0.97	0.07	37,40,41,42	0
21	EDO	S	104	4/4	0.98	0.06	25,25,25,25	0
14	HEA	A	602	60/60	0.98	0.06	20,23,28,31	0
24	CHD	O	301	29/29	0.98	0.05	23,27,31,38	0
21	EDO	A	613	4/4	0.98	0.06	21,24,24,26	0
18	CYN	A	606	2/2	0.98	0.08	21,21,21,21	0
14	HEA	N	602	60/60	0.98	0.06	21,24,29,35	0
21	EDO	F	105	4/4	0.98	0.07	30,31,33,34	0
21	EDO	S	103	4/4	0.98	0.08	29,30,31,34	0
17	NA	A	605	1/1	0.99	0.05	25,25,25,25	0
14	HEA	A	601[C]	43/60	0.99	0.05	18,21,23,24	1
14	HEA	A	601[A]	60/60	0.99	0.05	18,21,31,32	18
18	CYN	N	606	2/2	0.99	0.04	25,25,25,26	0
14	HEA	N	601[A]	60/60	0.99	0.06	19,25,32,35	18
14	HEA	N	601[B]	60/60	0.99	0.06	21,25,33,41	18
14	HEA	N	601[C]	43/60	0.99	0.06	21,24,28,29	1
14	HEA	A	601[B]	60/60	0.99	0.05	18,21,30,39	18
16	MG	N	604	1/1	0.99	0.05	23,23,23,23	0
21	EDO	F	102	4/4	0.99	0.04	24,24,26,26	0
15	CU	A	603	1/1	1.00	0.01	21,21,21,21	0
22	CUA	B	302	2/2	1.00	0.01	23,23,23,24	0
22	CUA	O	302	2/2	1.00	0.02	27,27,27,28	0
28	ZN	F	101	1/1	1.00	0.03	26,26,26,26	0
28	ZN	S	101	1/1	1.00	0.02	28,28,28,28	0
15	CU	N	603	1/1	1.00	0.01	23,23,23,23	0
16	MG	A	604	1/1	1.00	0.07	19,19,19,19	0

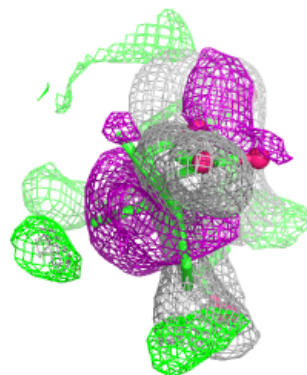
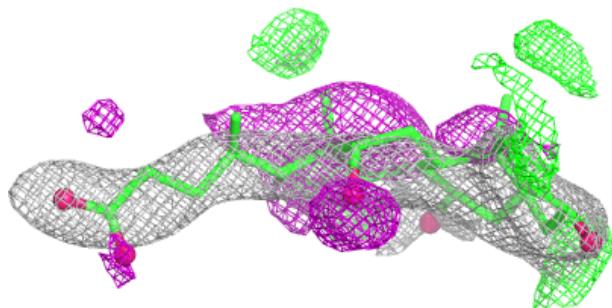
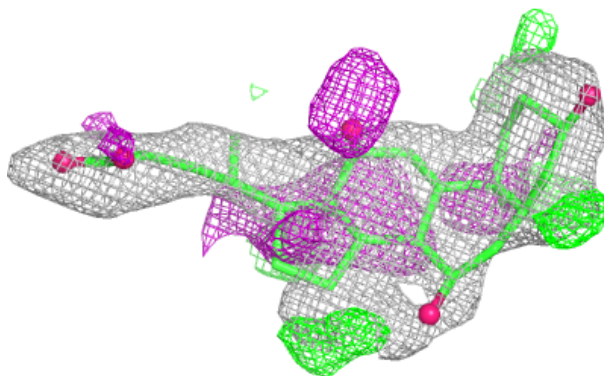
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU K 103:

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

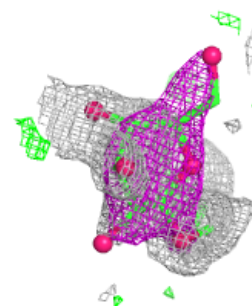
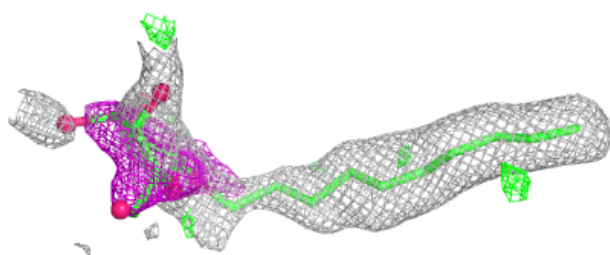
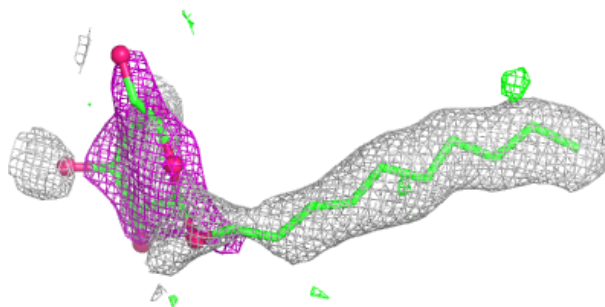
**Electron density around CHD Y 104:**

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

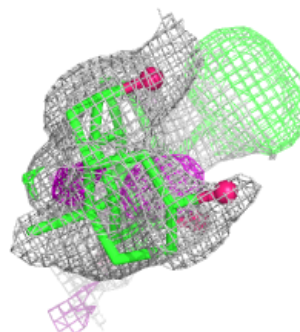
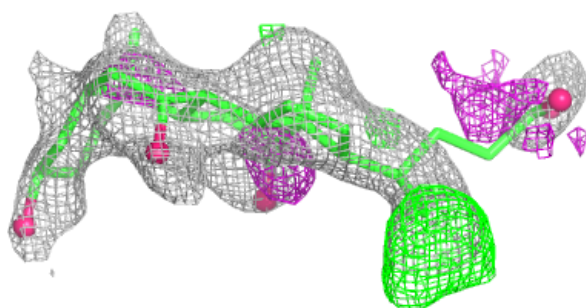
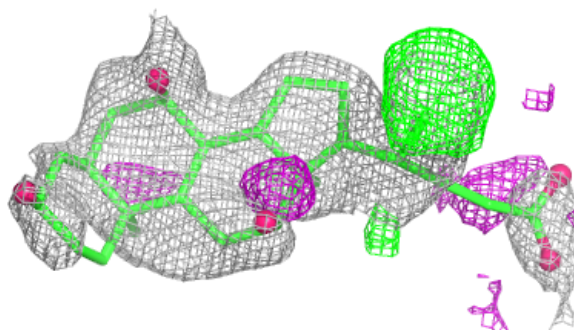


Electron density around DMU K 101:

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

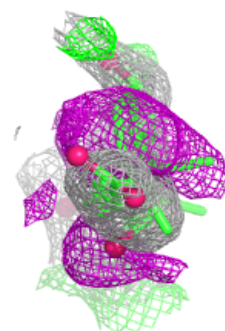
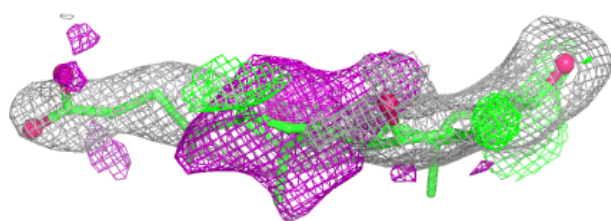
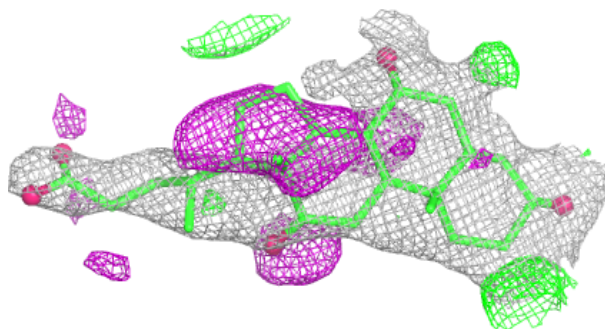
**Electron density around CHD W 101:**

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

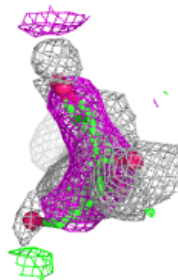
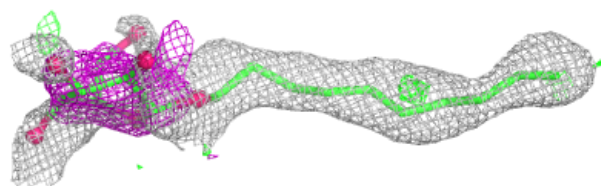
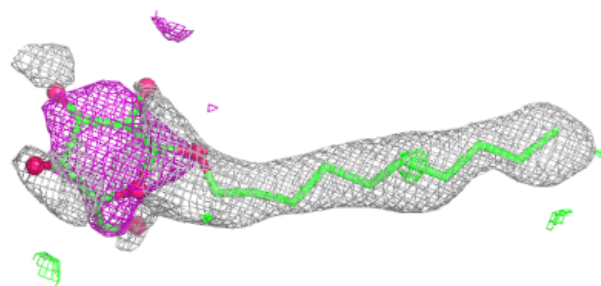


Electron density around CHD L 103:

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

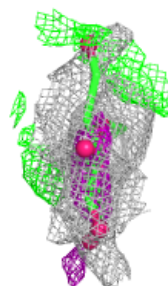
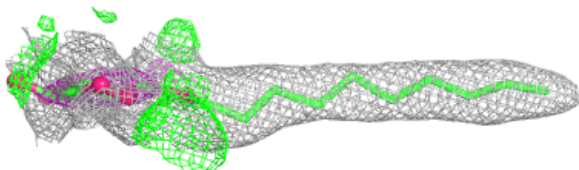
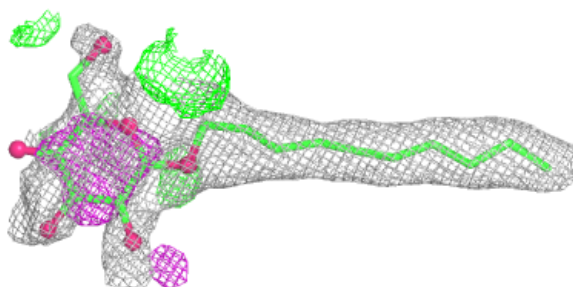
**Electron density around DMU K 102:**

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

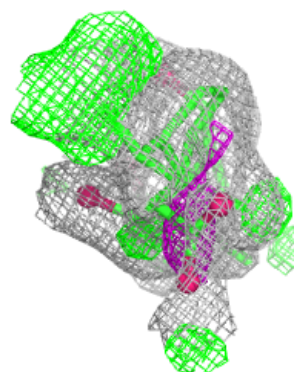
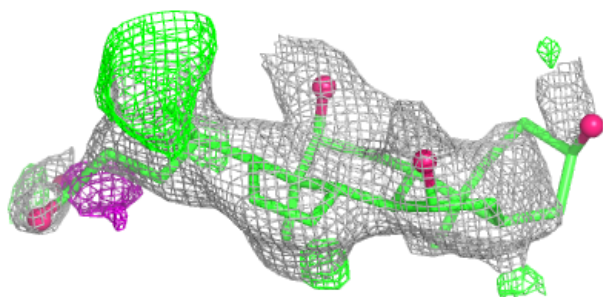
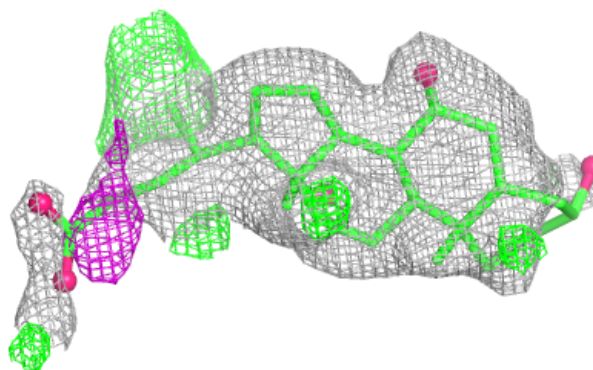


Electron density around DMU O 308:

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

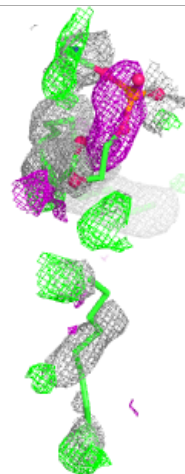
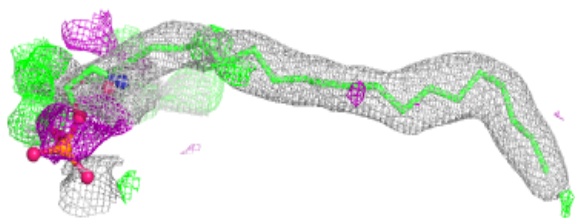
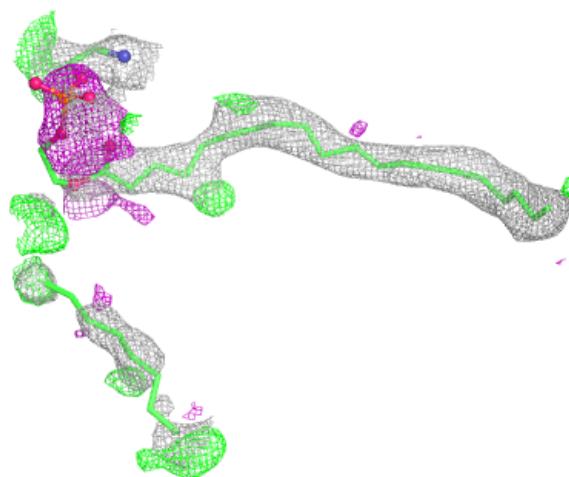
**Electron density around CHD J 102:**

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



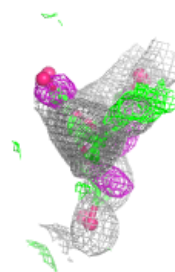
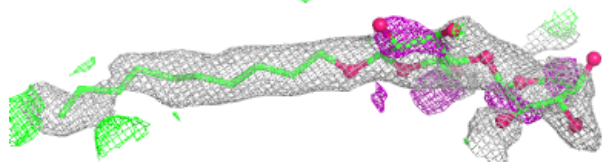
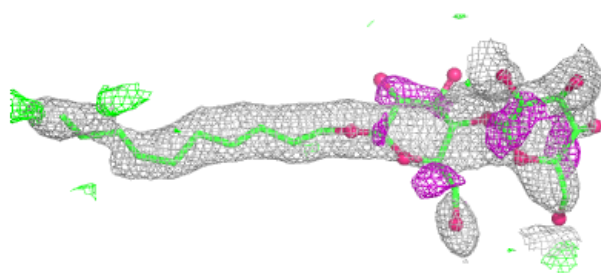
Electron density around PEK T 101:

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

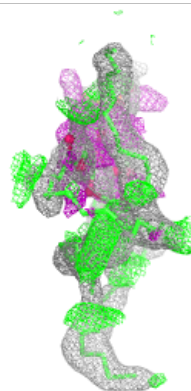
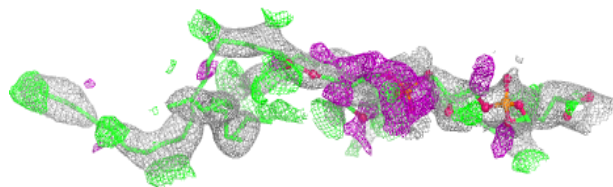
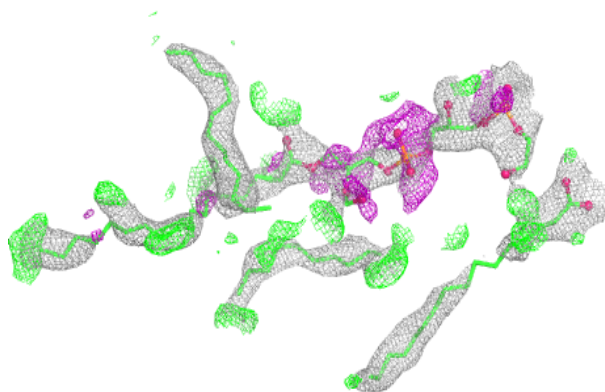


Electron density around DMU G 105:

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

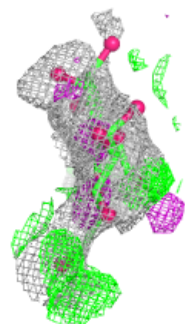
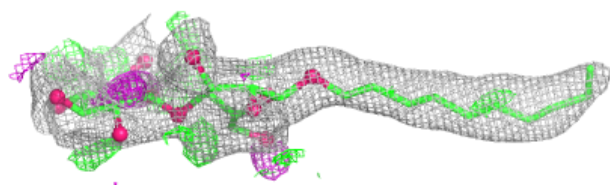
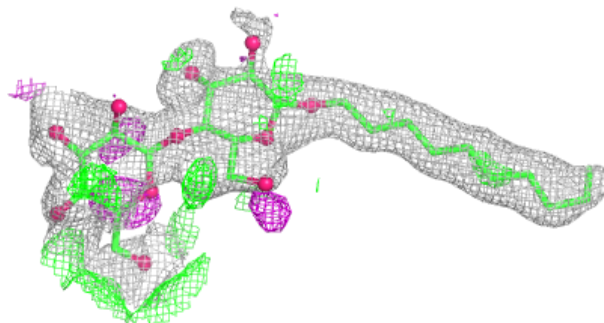
**Electron density around CDL G 102:**

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



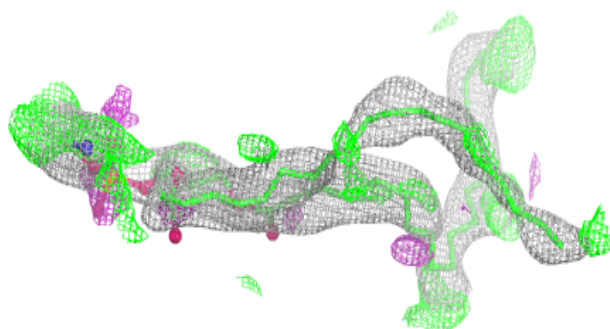
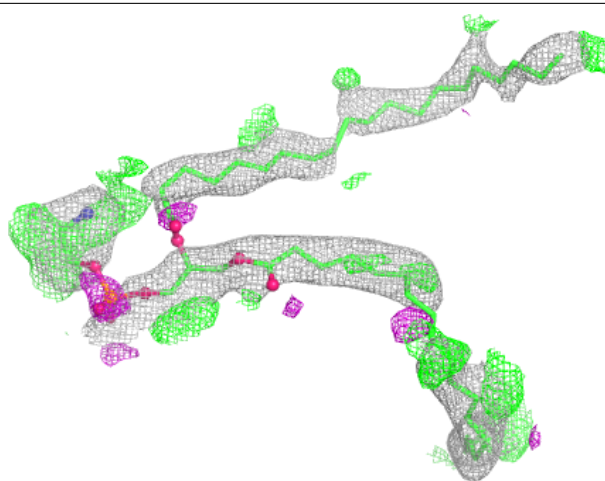
Electron density around DMU C 315:

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



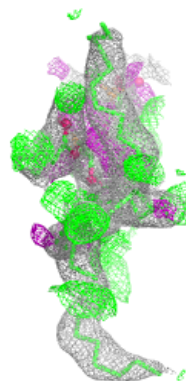
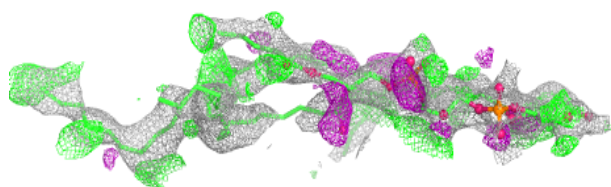
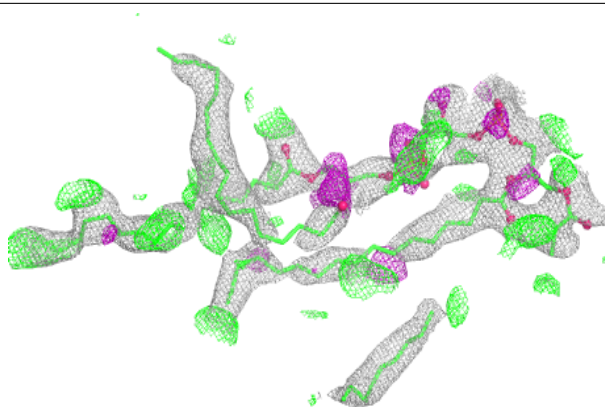
Electron density around PEK C 302:

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

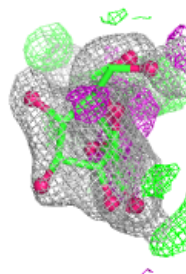
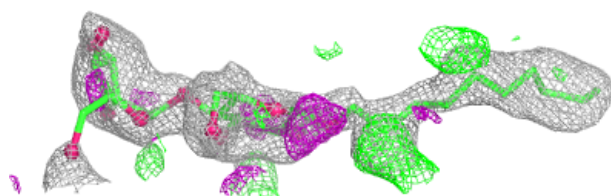
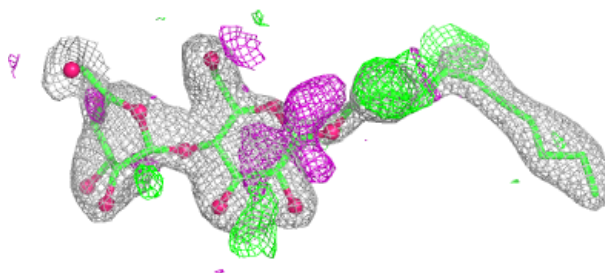


Electron density around CDL T 102:

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

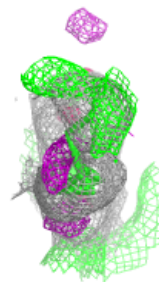
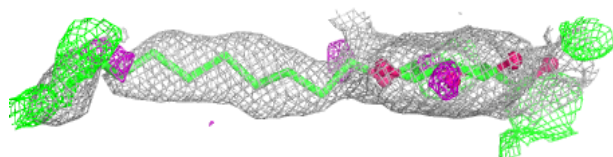
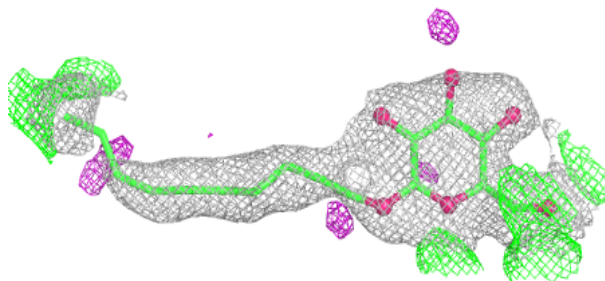
**Electron density around DMU J 101:**

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



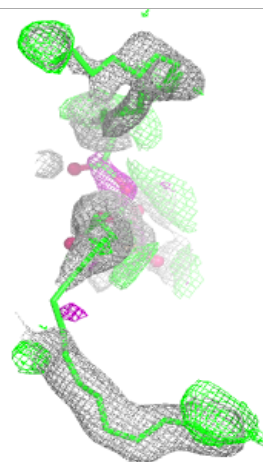
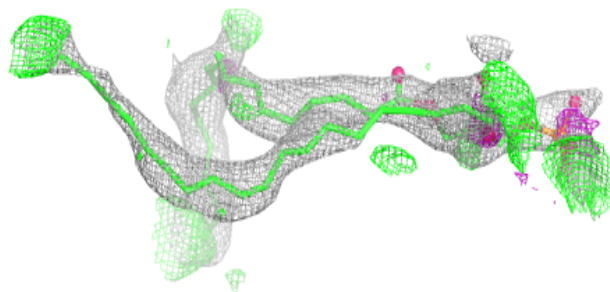
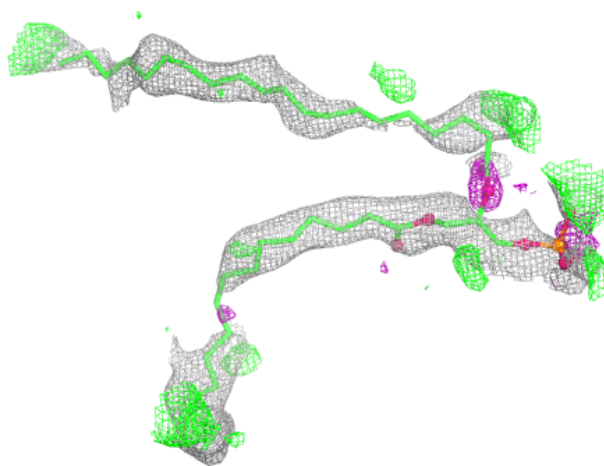
Electron density around DMU L 104:

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



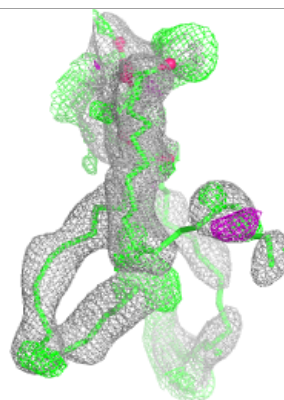
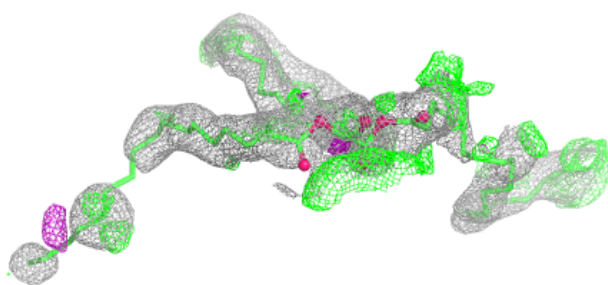
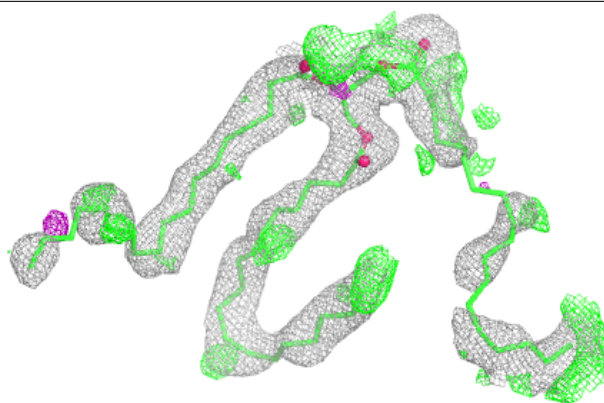
Electron density around PEK P 304:

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

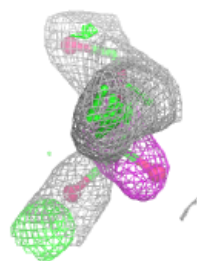
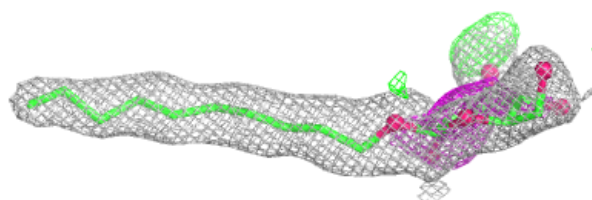
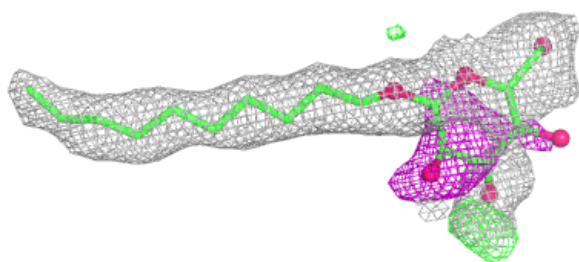


Electron density around TGL Q 201:

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

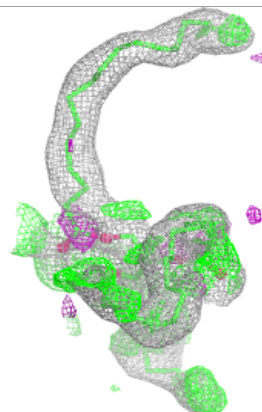
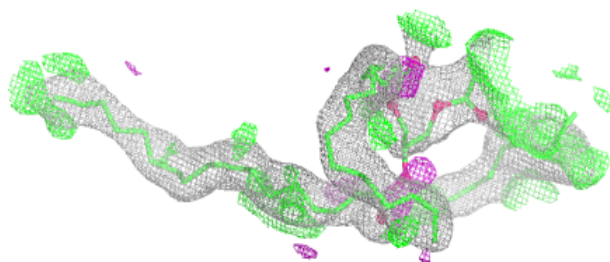
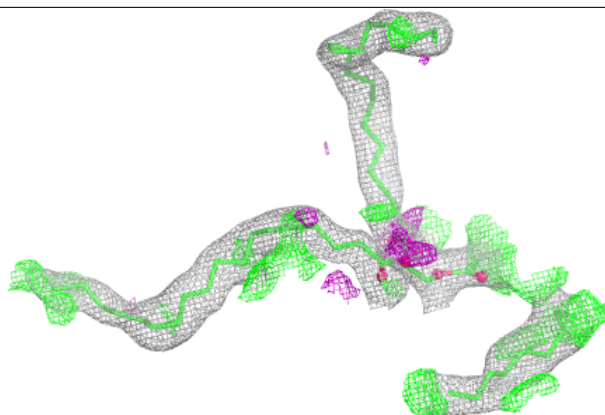
**Electron density around DMU T 105:**

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

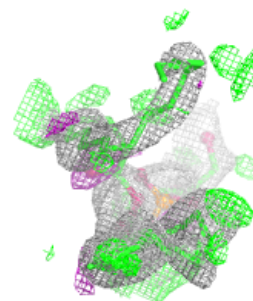
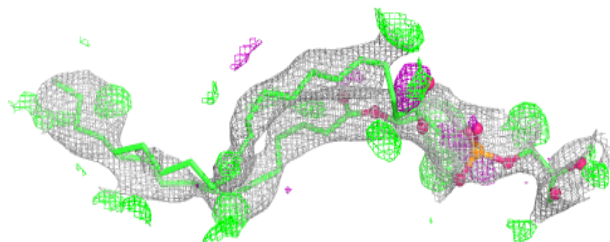
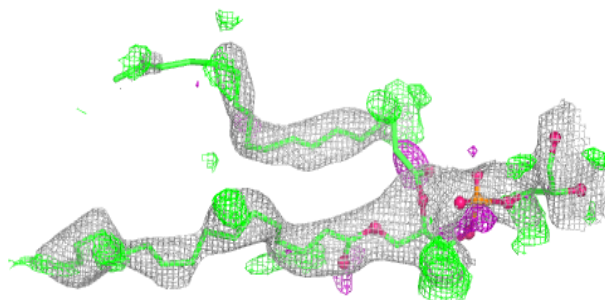


Electron density around TGL Y 101:

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

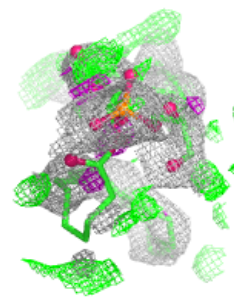
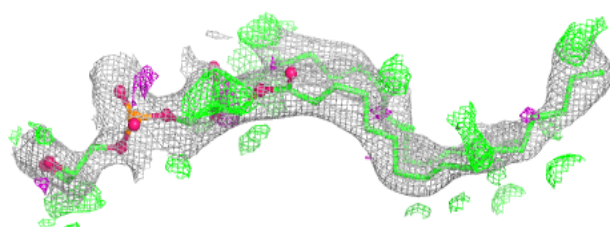
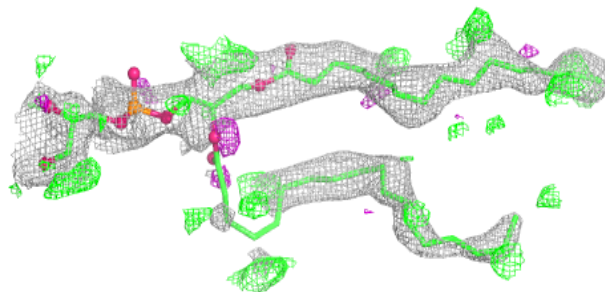
**Electron density around PGV P 306:**

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

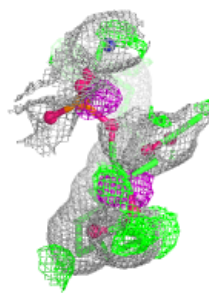
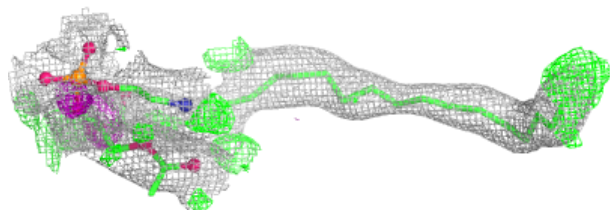
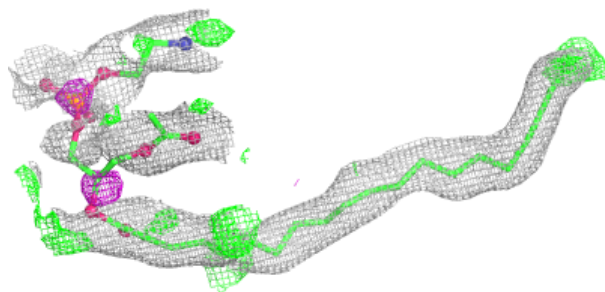


Electron density around PGV C 304:

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

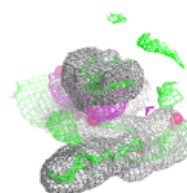
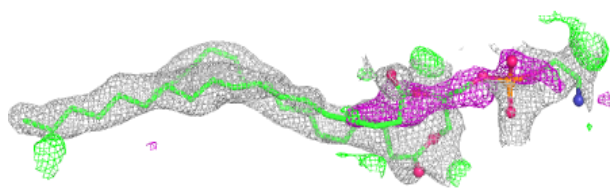
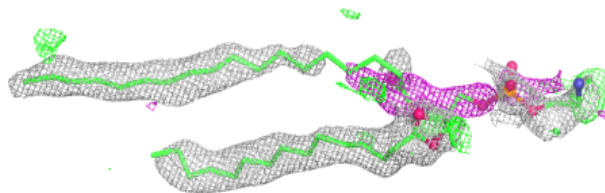
**Electron density around PEK P 302:**

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

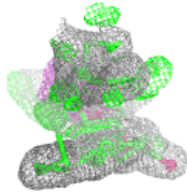
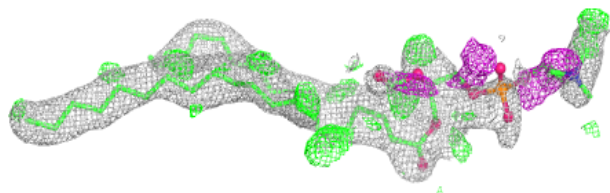
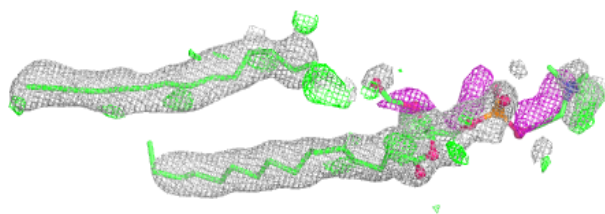


Electron density around PSC B 303:

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

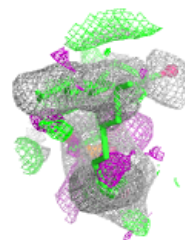
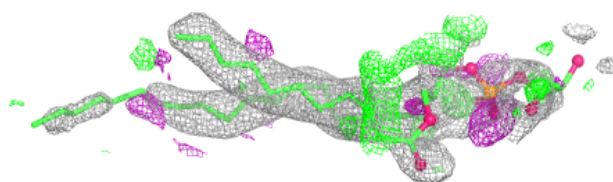
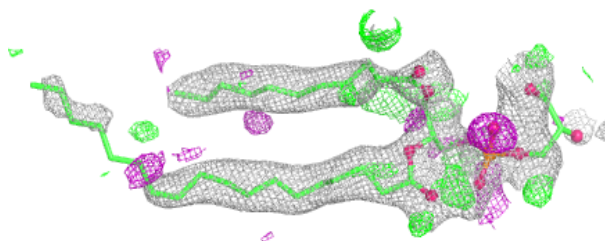
**Electron density around PSC R 201:**

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

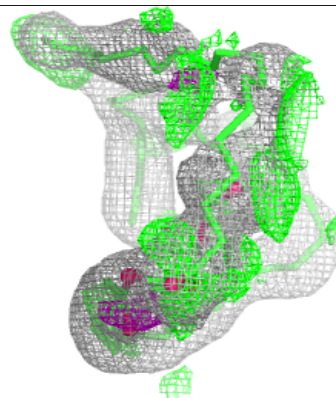
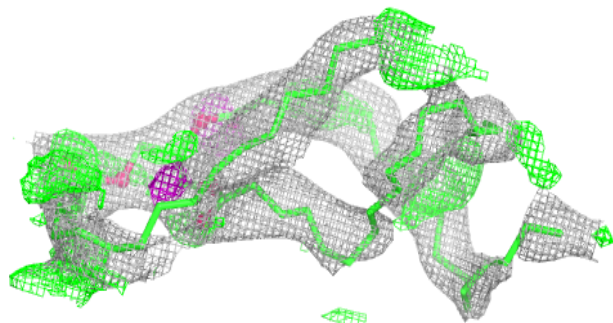
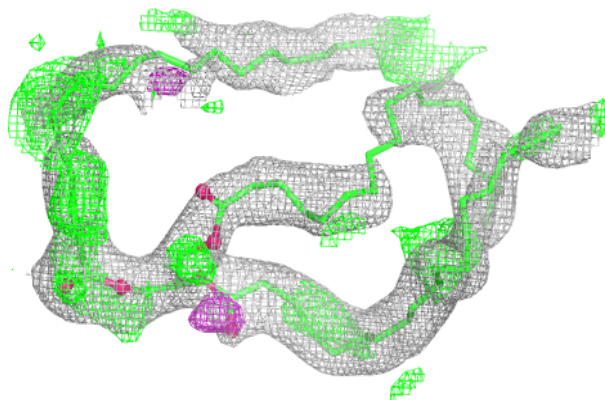


Electron density around PGV N 608:

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

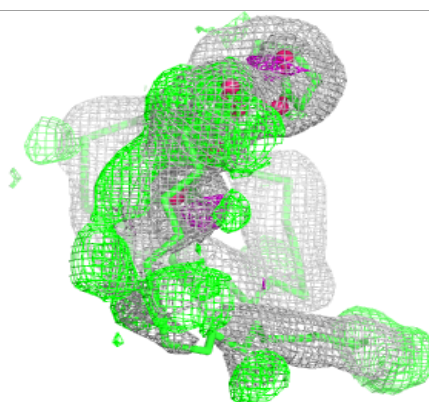
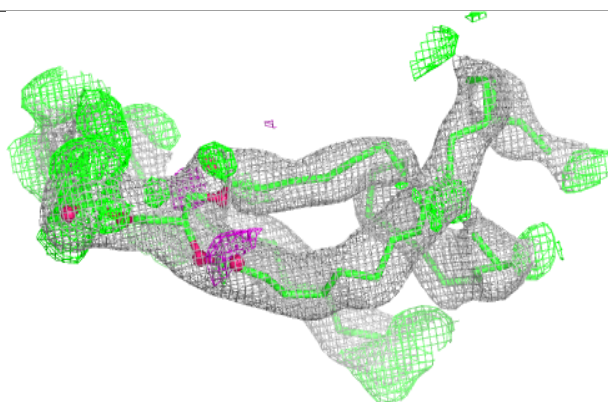
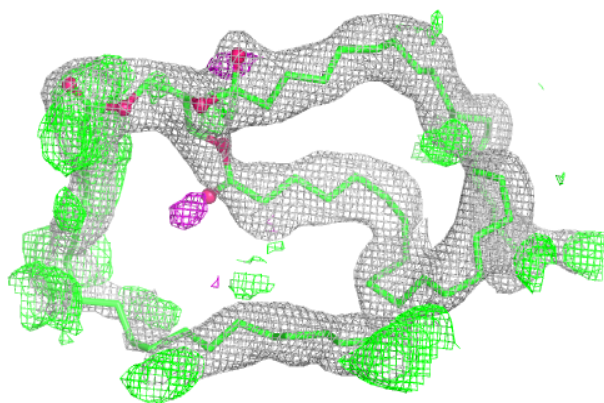
**Electron density around TGL N 607:**

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

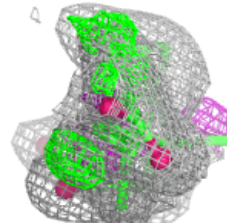
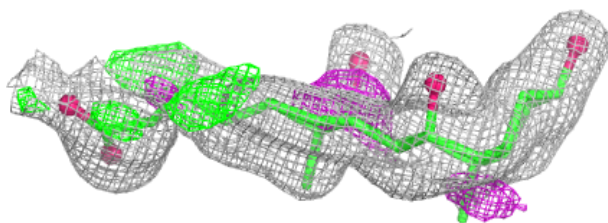
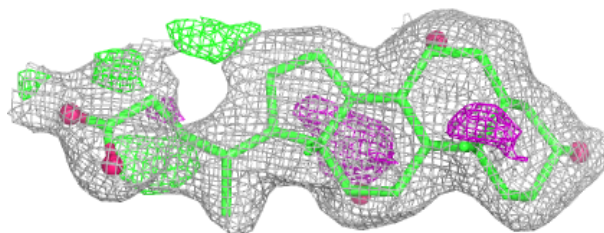


Electron density around TGL B 301:

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

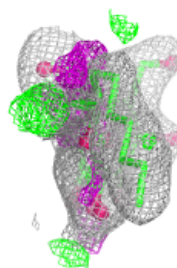
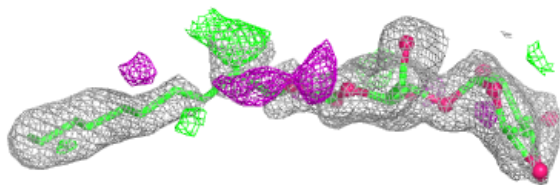
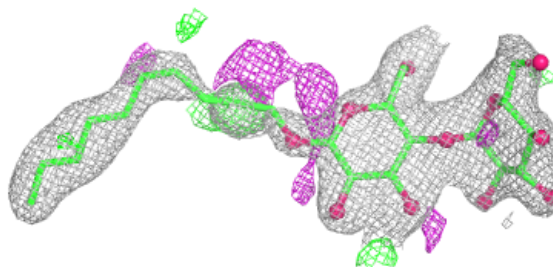
**Electron density around CHD P 308:**

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

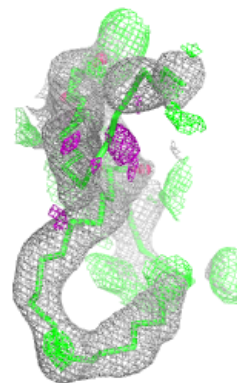
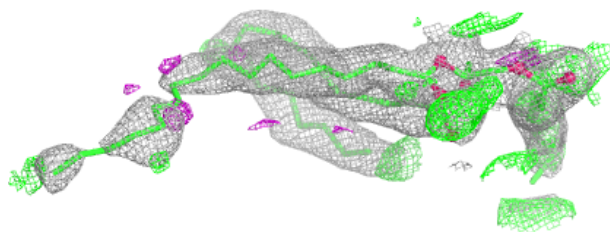
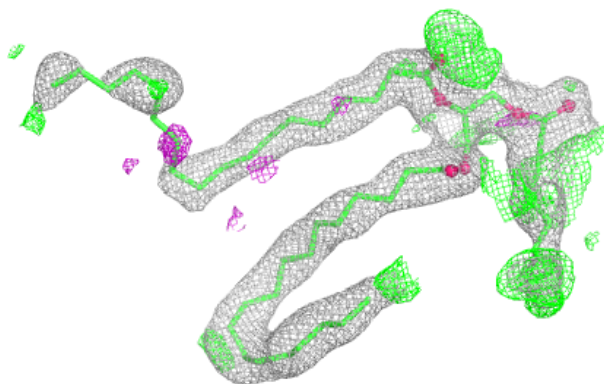


Electron density around DMU P 309:

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

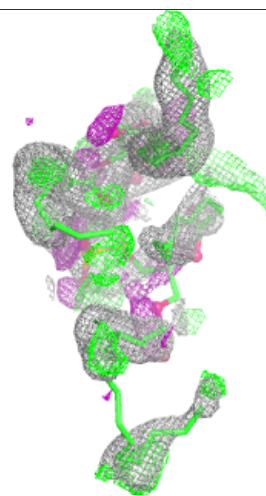
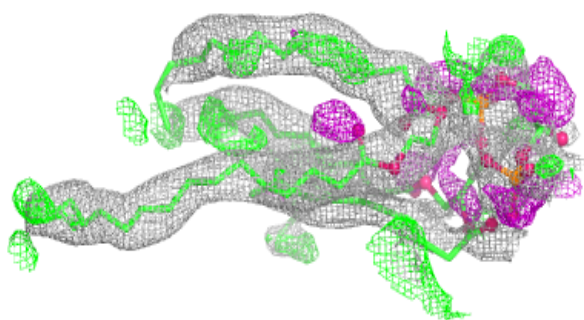
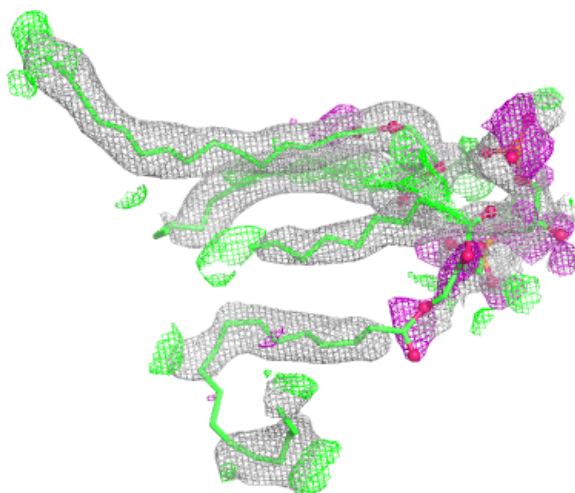
**Electron density around TGL D 201:**

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



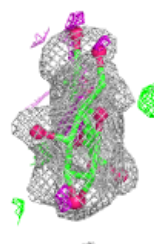
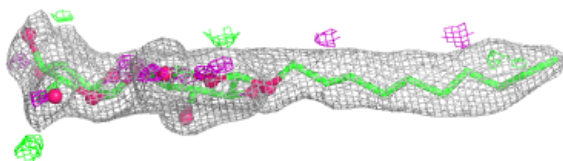
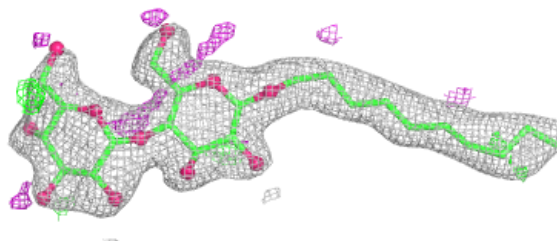
Electron density around CDL P 307:

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



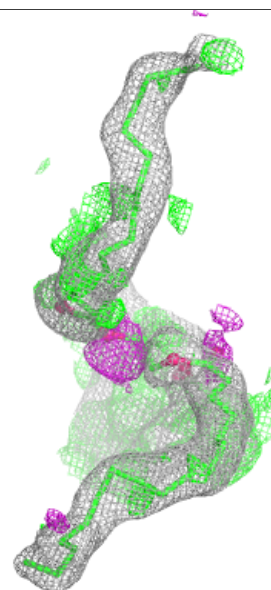
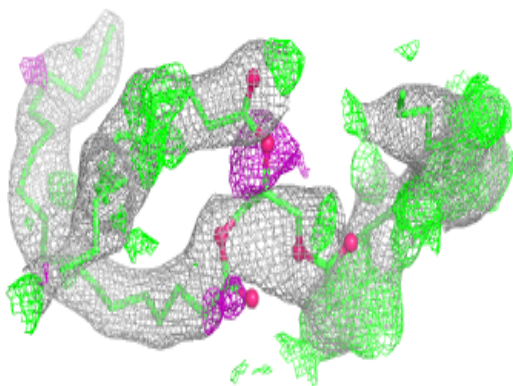
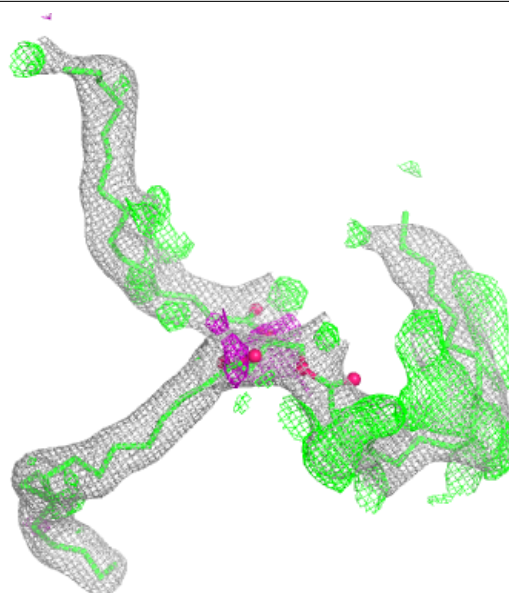
Electron density around DMU P 316:

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



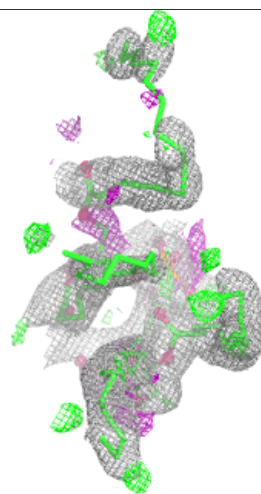
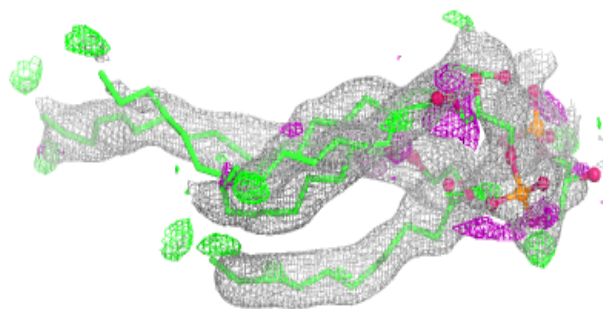
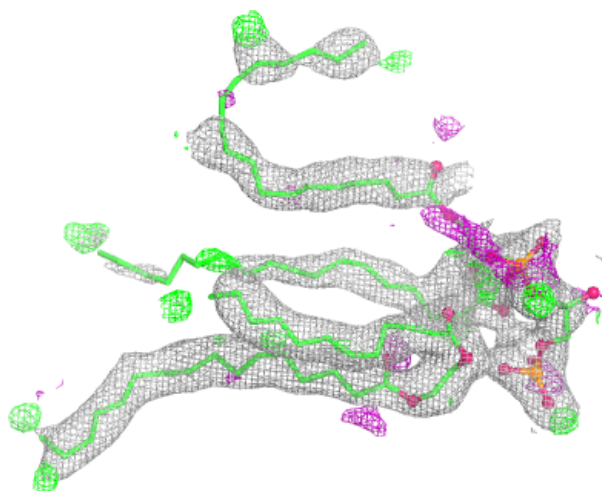
Electron density around TGL A 607:

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



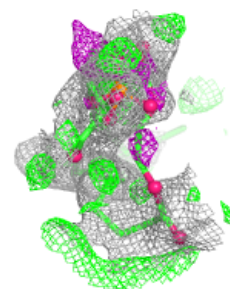
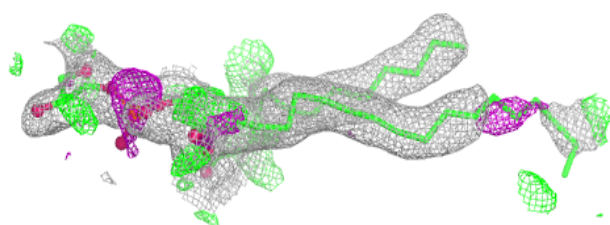
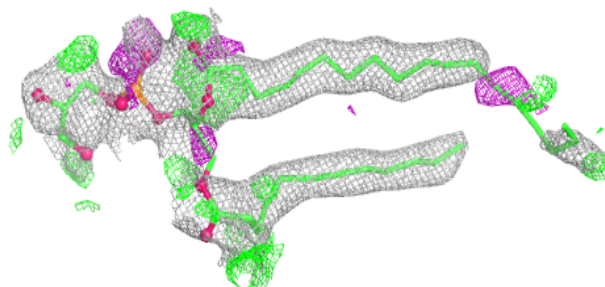
Electron density around CDL C 305:

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

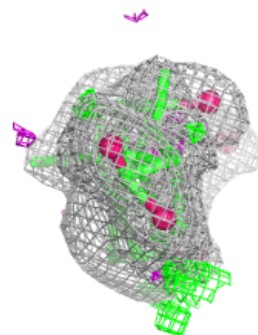
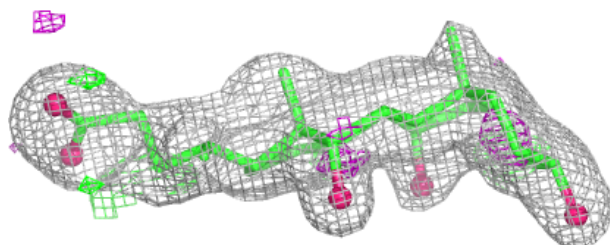
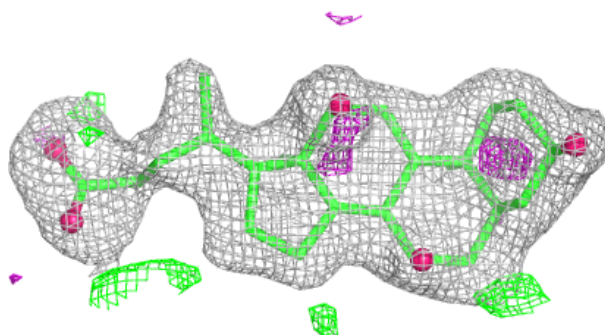


Electron density around PGV A 608:

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

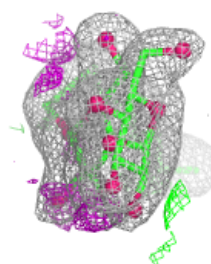
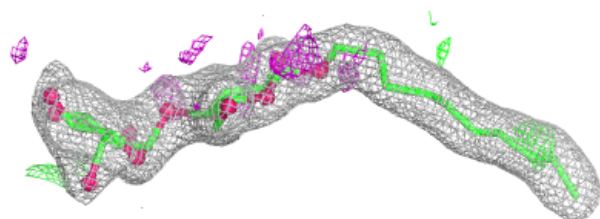
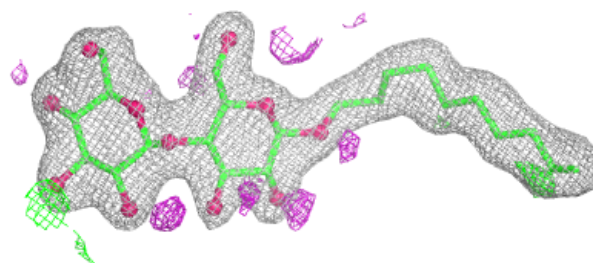
**Electron density around CHD C 306:**

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

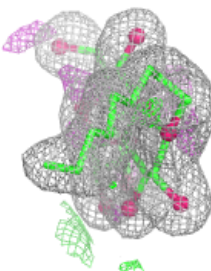
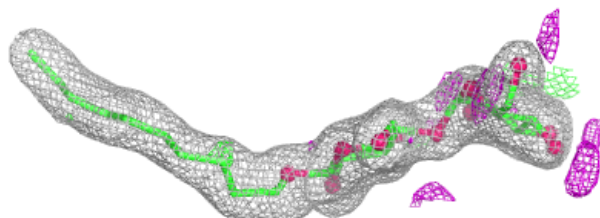
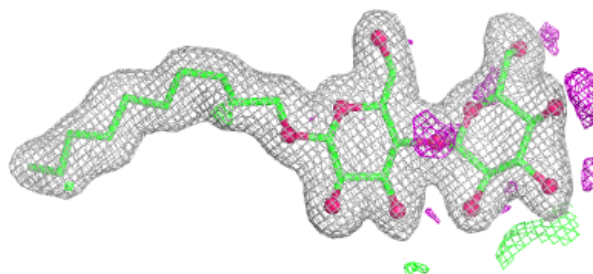


Electron density around DMU Z 101:

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

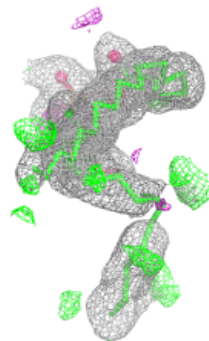
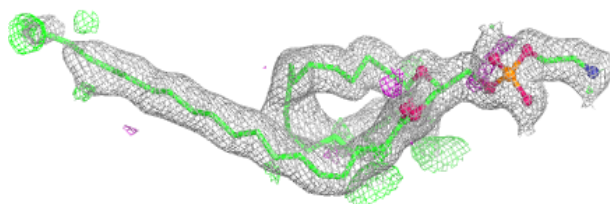
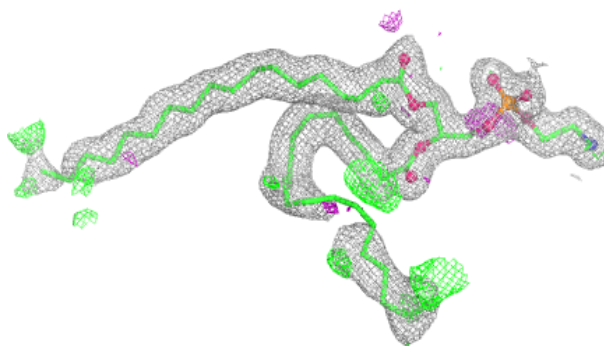
**Electron density around DMU M 101:**

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

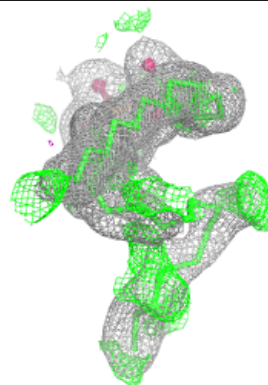
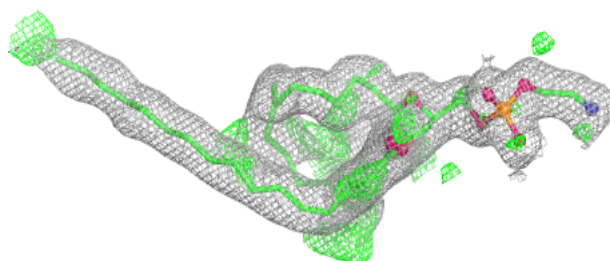
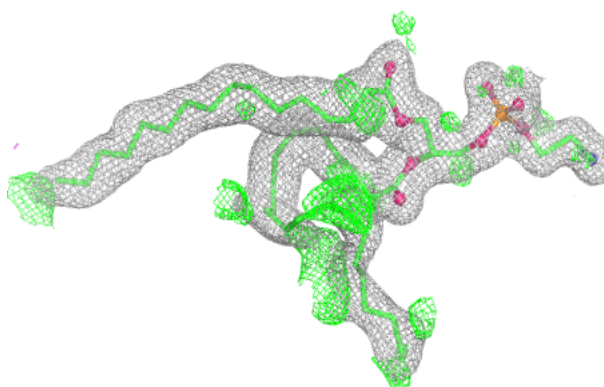


Electron density around PEK P 303:

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

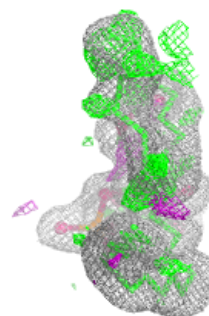
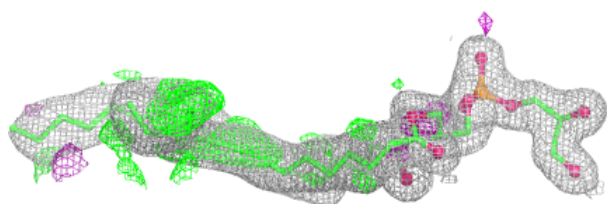
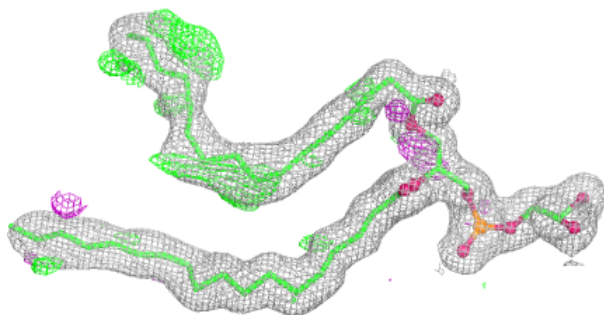
**Electron density around PEK G 101:**

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

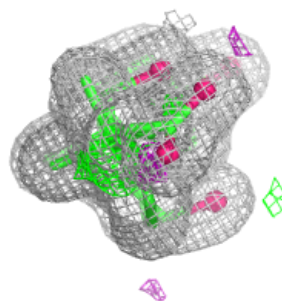
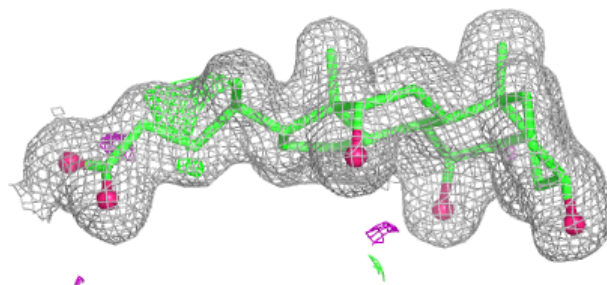
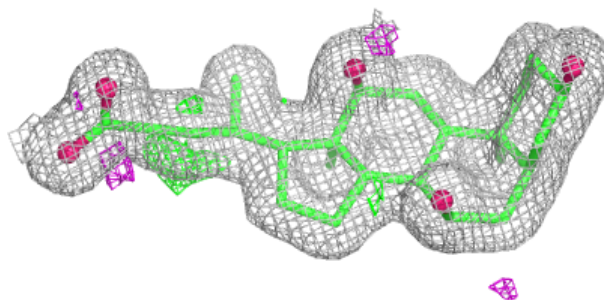


Electron density around PGV N 609:

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

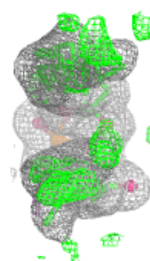
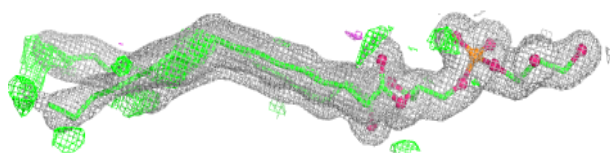
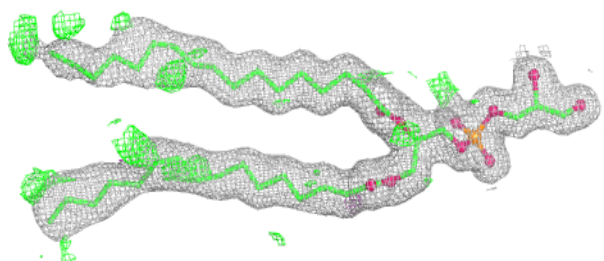
**Electron density around CHD C 301:**

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

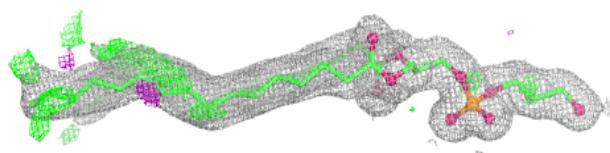
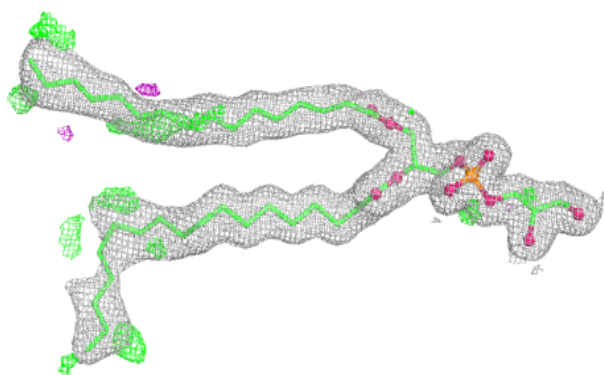


Electron density around PGV C 303:

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

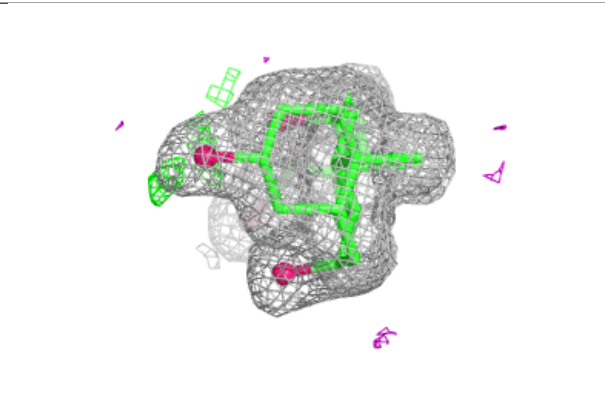
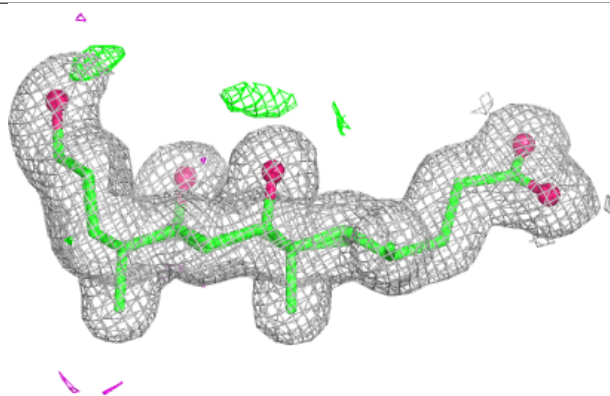
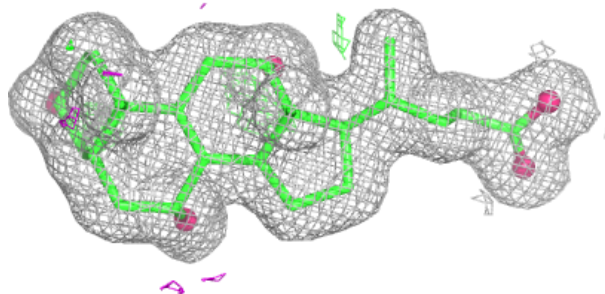
**Electron density around PGV P 305:**

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

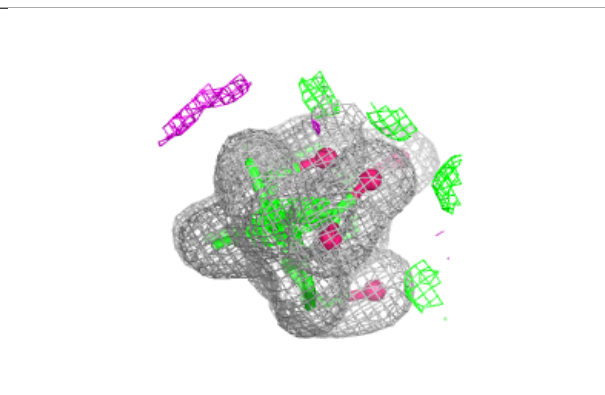
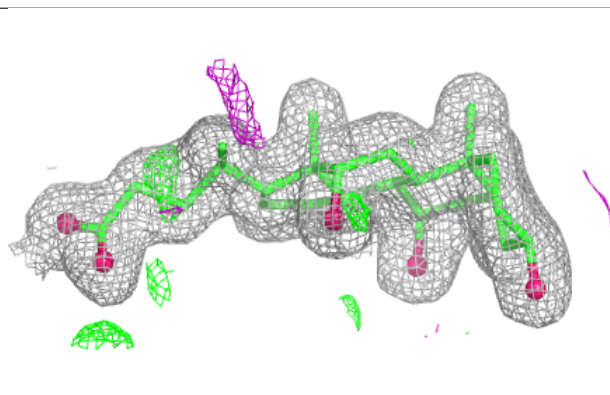
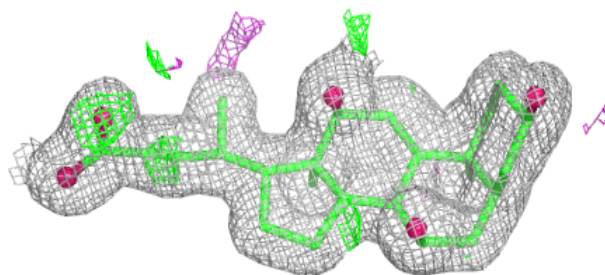


Electron density around CHD B 304:

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

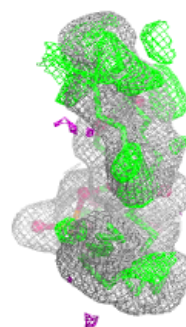
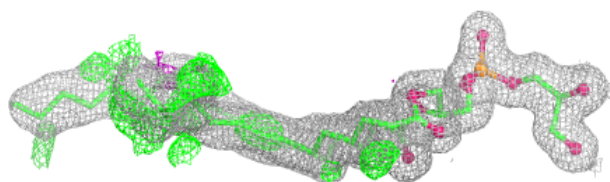
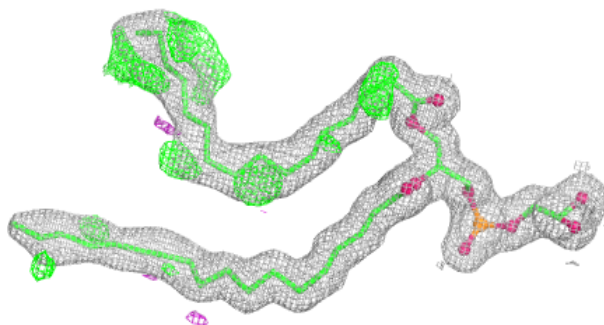
**Electron density around CHD P 301:**

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

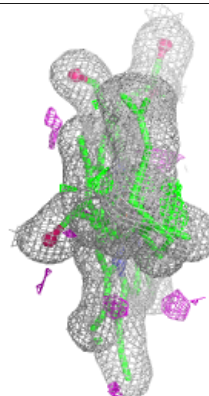
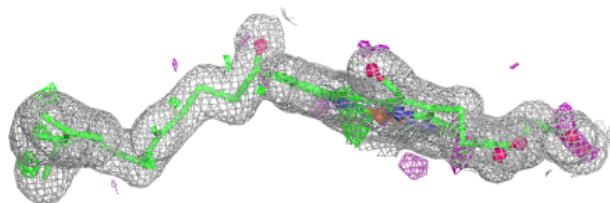
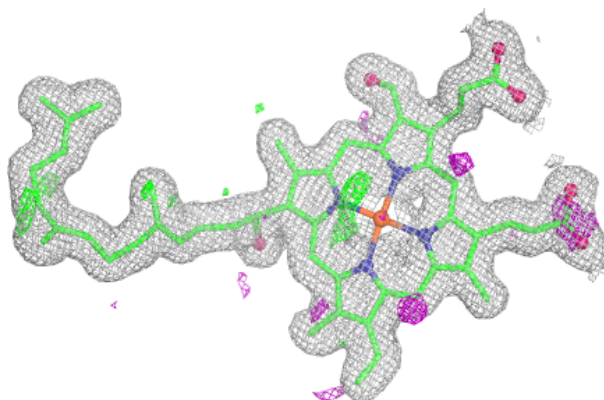


Electron density around PGV A 609:

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

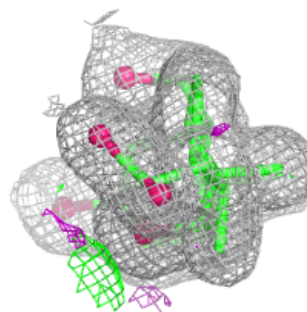
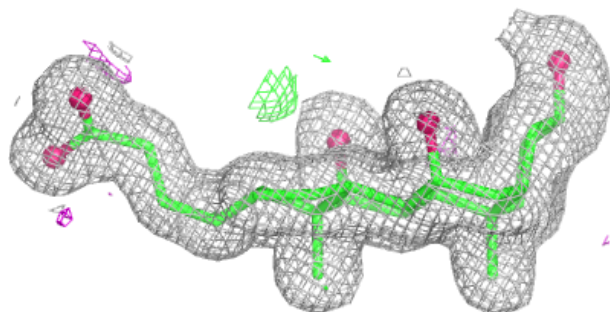
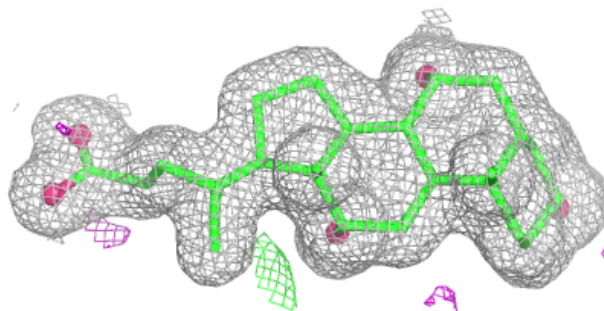
**Electron density around HEA A 602:**

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

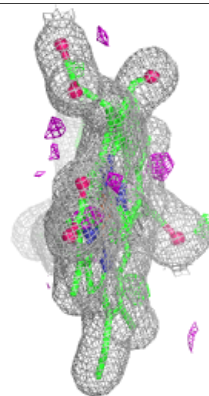
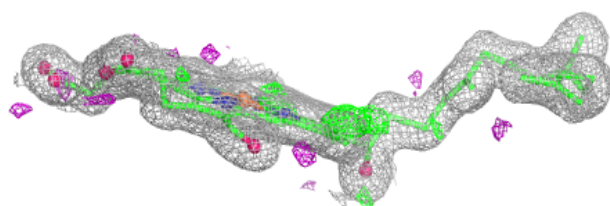
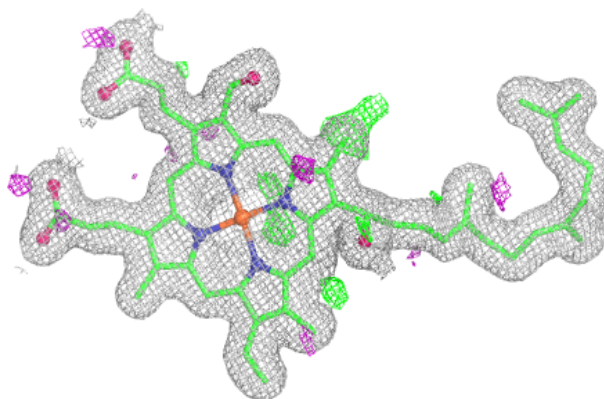


Electron density around CHD O 301:

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

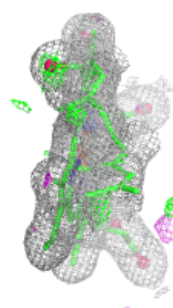
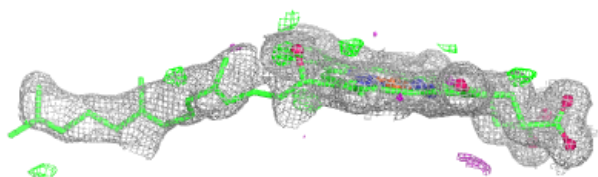
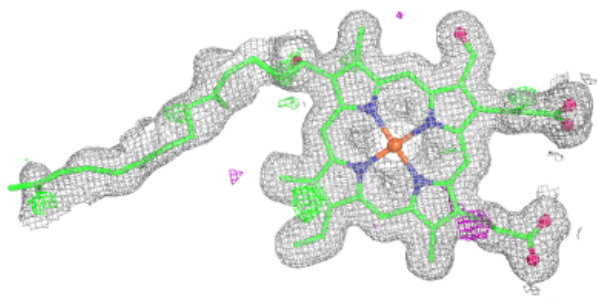
**Electron density around HEA N 602:**

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

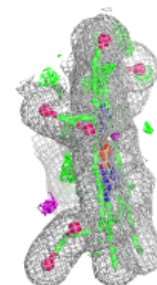
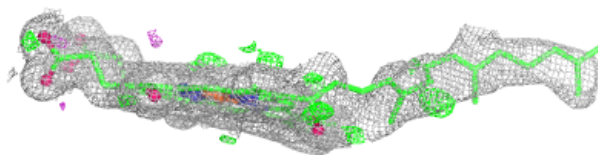
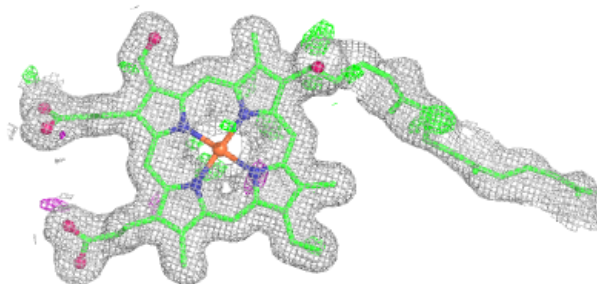


Electron density around HEA A 601 (A):

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

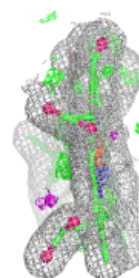
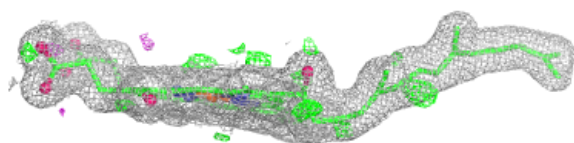
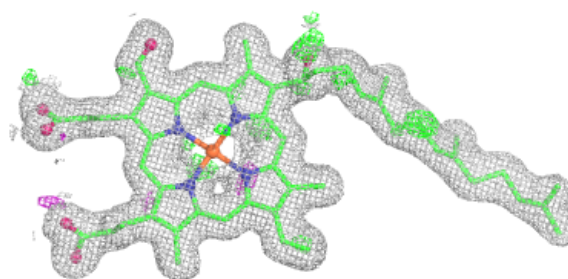
**Electron density around HEA N 601 (A):**

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

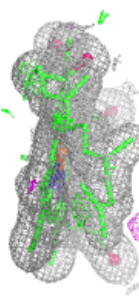
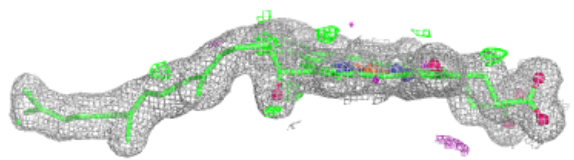
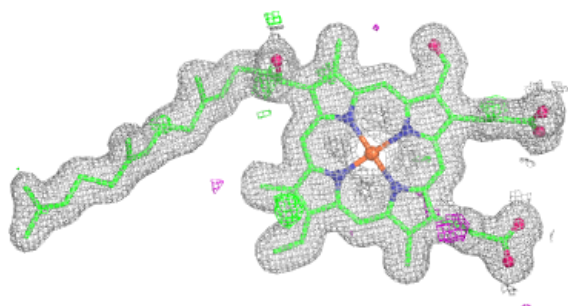


Electron density around HEA N 601 (B):

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

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

$2mF_o-DF_c$ (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.