



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 12:00 PM JST

PDB ID : 5ZCQ / pdb_00005zcq
Title : Azide-bound cytochrome c oxidase structure determined using the crystals exposed to 10 mM azide solution for 2 days
Authors : Shimada, A.; Hatano, K.; Tadehara, H.; Tsukihara, T.
Deposited on : 2018-02-19
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:

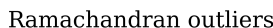
MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

i

X-RAY DIFFRACTION

A.

the following graphic. The table shows the number of entries on which the scores are based.

Ramachandran outliers

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.

			%
1	A	514	72% 24%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	AZI	A	606[B]	-	-	X	-
18	AZI	A	607[B]	-	-	X	-
18	AZI	N	607[B]	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FME	B	1	-	-	X	-
21	EDO	A	611	-	-	X	-
21	EDO	A	621	-	-	X	-
21	EDO	D	202	-	-	X	-
21	EDO	E	202	-	-	X	-
21	EDO	H	101	-	X	X	-
21	EDO	P	312	-	X	-	-
24	PSC	B	303	-	-	X	-
27	CDL	C	305	-	-	X	-
27	CDL	G	102	-	-	X	-
27	CDL	P	305	-	-	X	-
27	CDL	T	103	-	-	X	-
9	SAC	V	1	-	X	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33657 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	22	0
			4193	2793	649	709	42			
1	N	514	Total	C	N	O	S	0	20	0
			4179	2786	647	704	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	10	0
			1907	1238	293	356	20			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	288	347	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	7	0
			2168	1447	347	359	15			
3	P	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			

- 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
			1242	809	206	223	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1224	797	202	221	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	3	0
			771	477	138	150	6			
6	S	98	Total	C	N	O	S	0	2	0
			763	473	136	148	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 686	C 440	N 130	O 114	P 1	S 1	0	1	0
7	T	84	Total 686	C 440	N 130	O 114	P 1	S 1	0	1	0

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	1	0
			469	302	79	85	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			

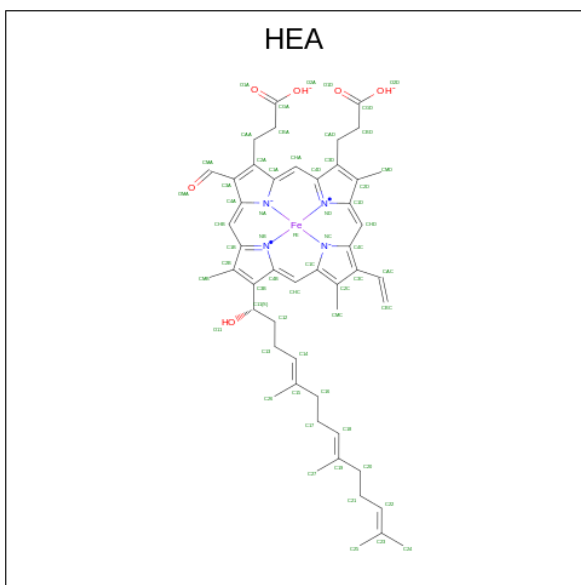
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	1	0
			388	259	65	61	3			

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	A	1	Total 120	C 98	Fe 2	N 8	O 12	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 120	C 98	Fe 2	N 8	O 12	0	1

- 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		

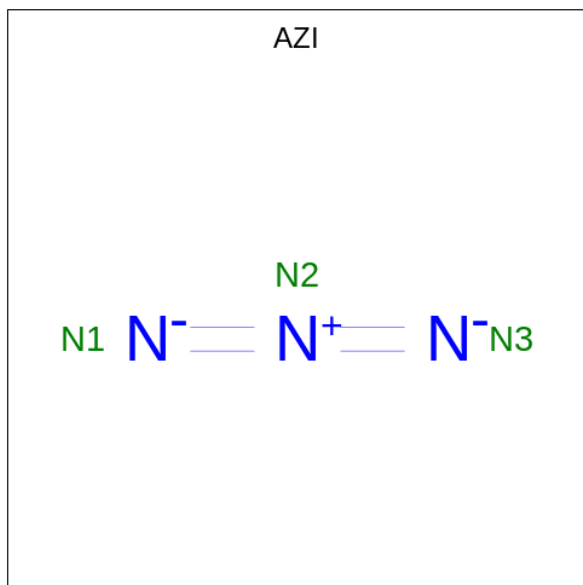
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

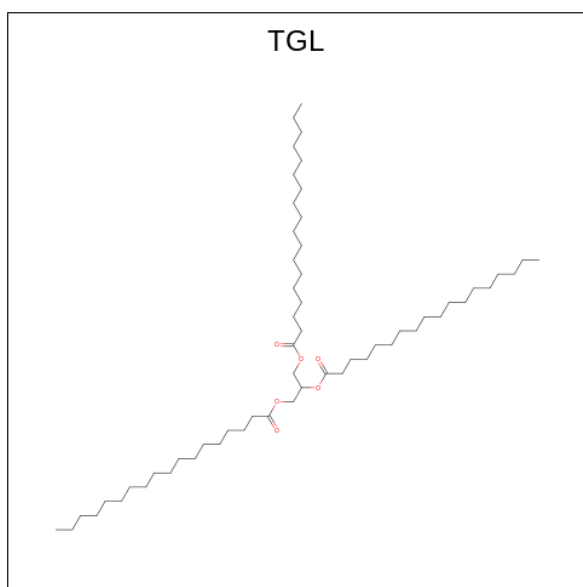
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is AZIDE ION (CCD ID: AZI) (formula: N₃).



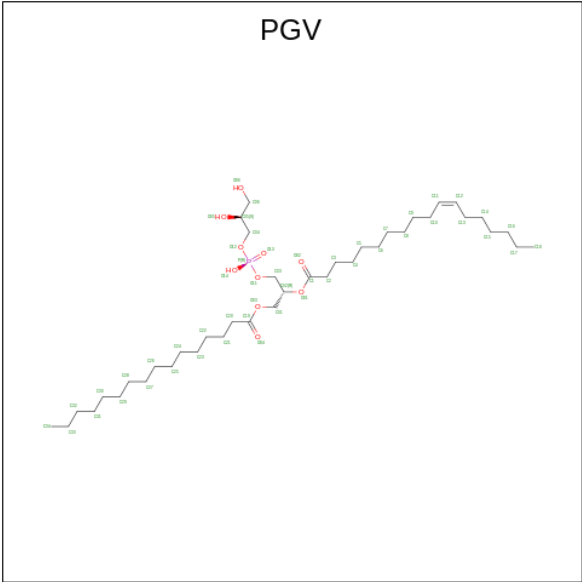
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total N 3 3	0	1
18	A	1	Total N 6 6	0	1
18	N	1	Total N 3 3	0	1
18	N	1	Total N 6 6	0	1

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



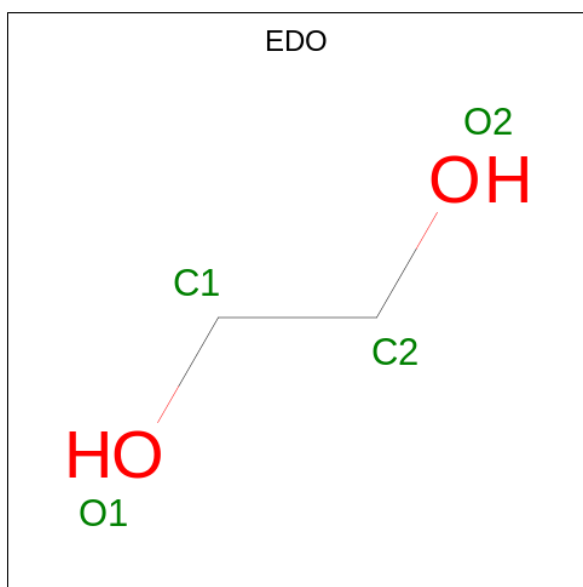
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		
19	Y	1	Total	C	O	0	0
			63	57	6		

- 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
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	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		
20	X	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	B	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		

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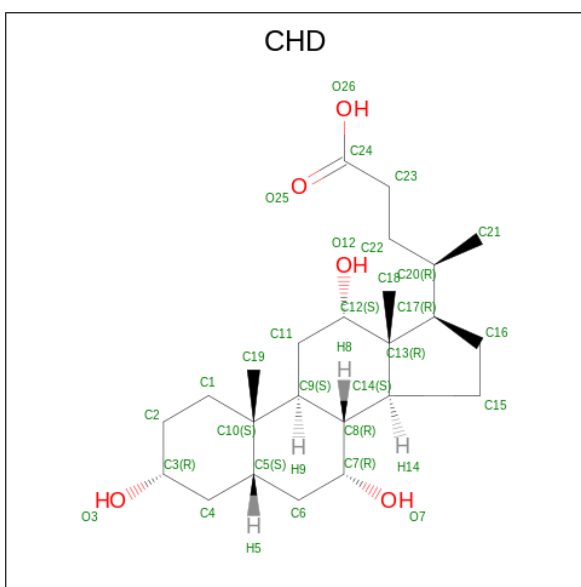
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4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

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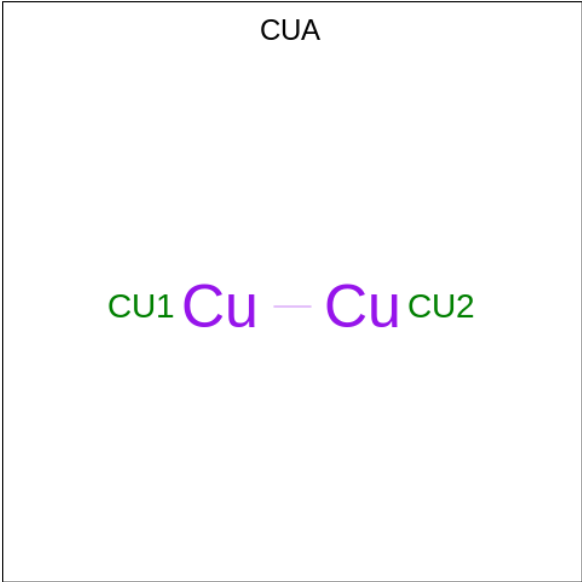
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	O	1	Total	C	O	0	0
			4	2	2		
21	O	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21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

- Molecule 22 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



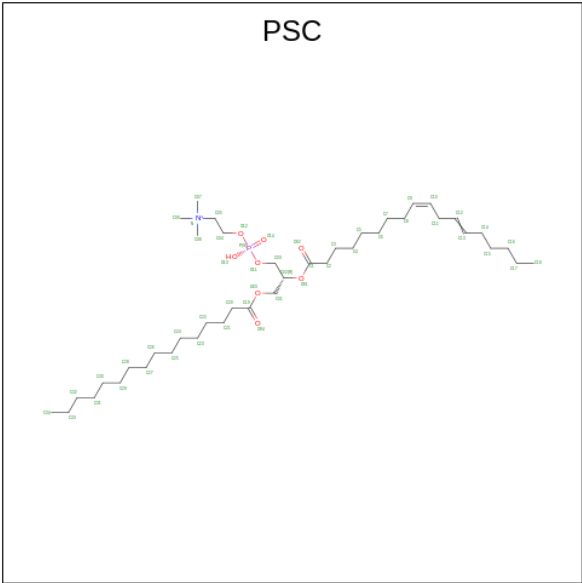
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0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

- Molecule 23 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 24 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).



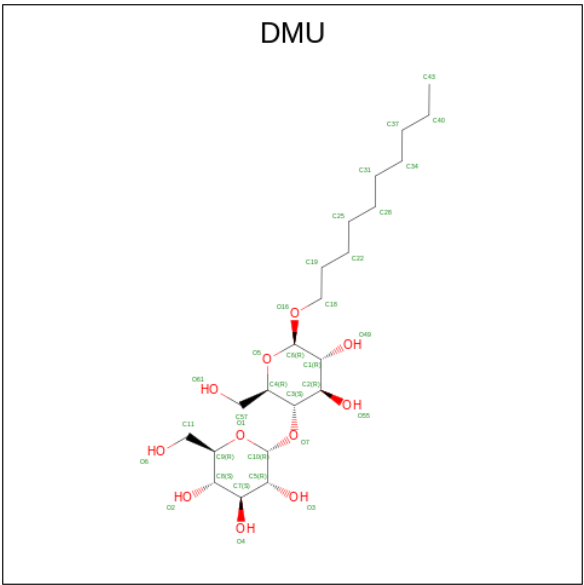
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).

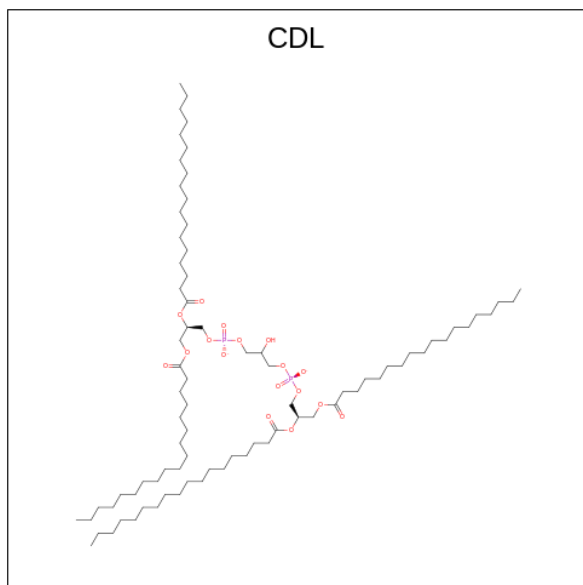


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total	C	O	0	0
			33	22	11		
25	C	1	Total	C	O	0	0
			33	22	11		
25	C	1	Total	C	O	0	0
			33	22	11		
25	L	1	Total	C	O	0	0
			33	22	11		
25	M	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total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

- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

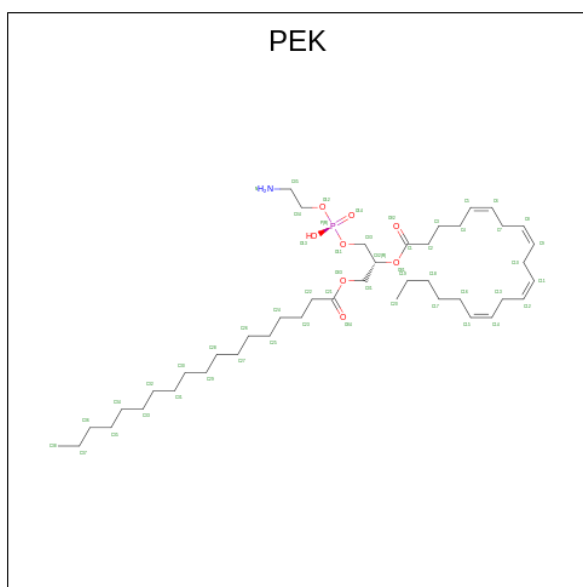
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total X 1 1	0	0
26	P	1	Total X 1 1	0	0

- Molecule 27 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 28 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$).



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

- Molecule 29 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	228	Total	O	0	0
			228	228		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	154	Total O 155 155	0	1
30	C	101	Total O 101 101	0	0
30	D	96	Total O 96 96	0	0
30	E	80	Total O 80 80	0	0
30	F	85	Total O 85 85	0	0
30	G	46	Total O 46 46	0	0
30	H	55	Total O 55 55	0	0
30	I	26	Total O 26 26	0	0
30	J	16	Total O 16 16	0	0
30	K	15	Total O 15 15	0	0
30	L	24	Total O 24 24	0	0
30	M	19	Total O 19 19	0	0
30	N	215	Total O 215 215	0	0
30	O	109	Total O 110 110	0	1
30	P	105	Total O 105 105	0	0
30	Q	37	Total O 37 37	0	0
30	R	49	Total O 49 49	0	0
30	S	79	Total O 79 79	0	0
30	T	36	Total O 36 36	0	0
30	U	38	Total O 38 38	0	0
30	V	14	Total O 14 14	0	0

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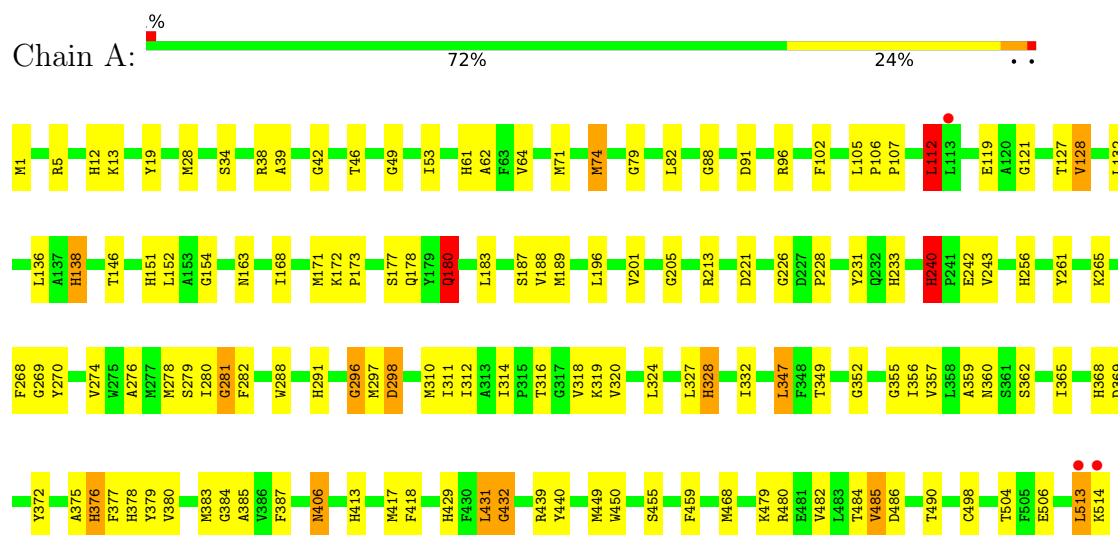
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	W	13	Total 13	O 13	0	0
30	X	11	Total 11	O 11	0	0
30	Y	13	Total 13	O 13	0	0
30	Z	12	Total 12	O 12	0	0

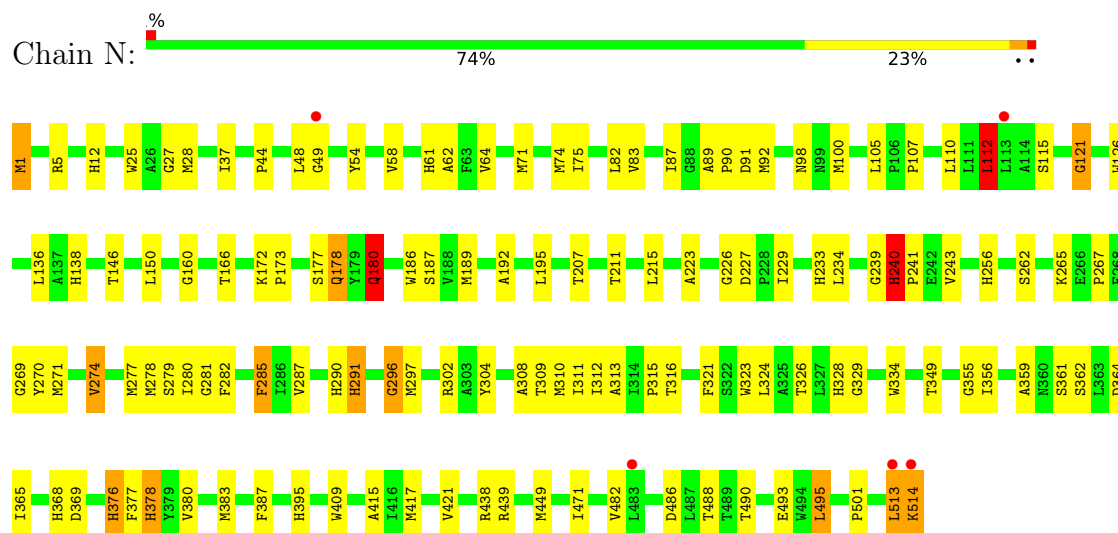
3 Residue-property plots [i](#)

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

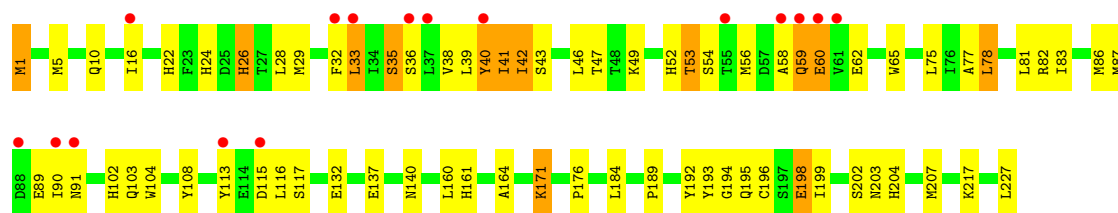


• Molecule 1: Cytochrome c oxidase subunit 1

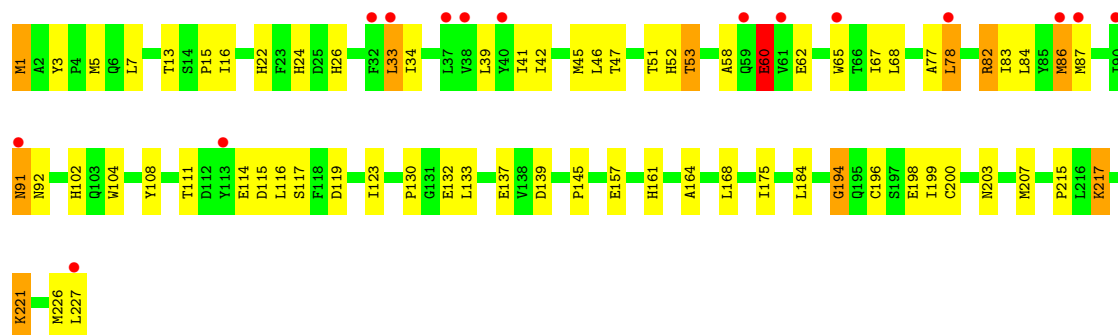


• Molecule 2: Cytochrome c oxidase subunit 2

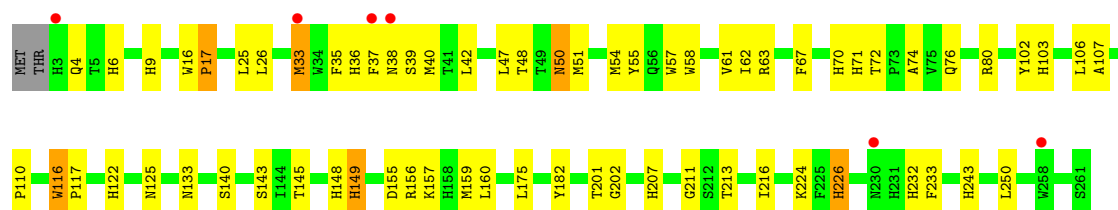
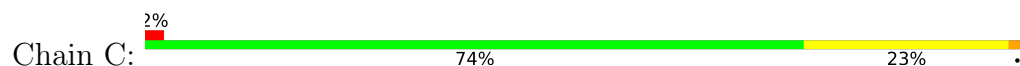




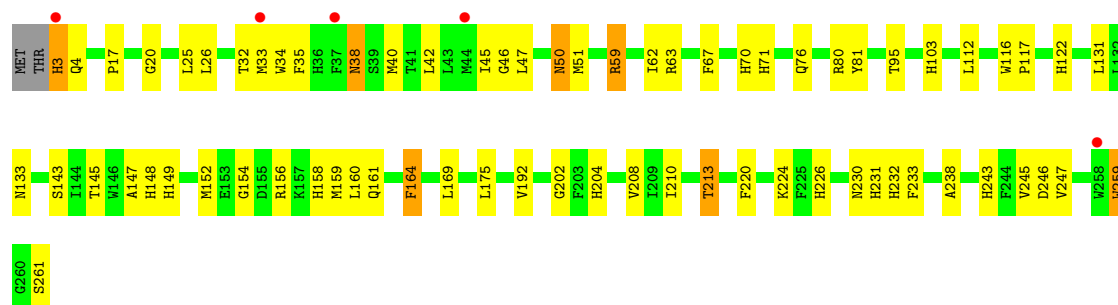
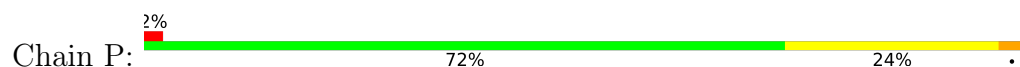
• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 3: Cytochrome c oxidase subunit 3



• Molecule 3: Cytochrome c oxidase subunit 3

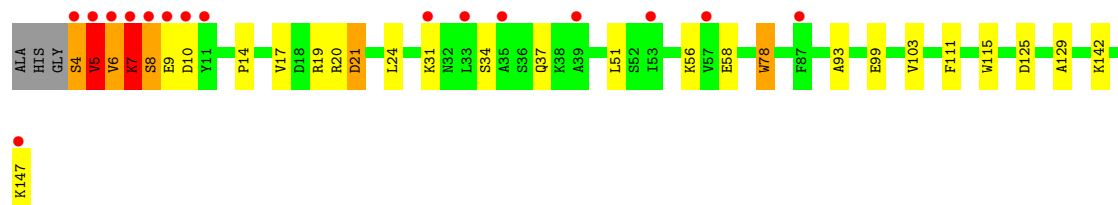
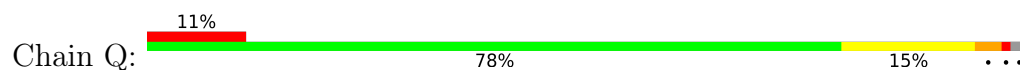


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial





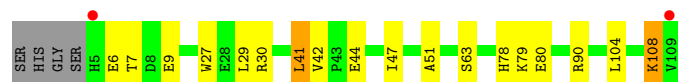
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



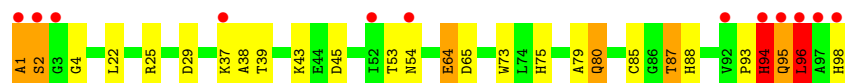
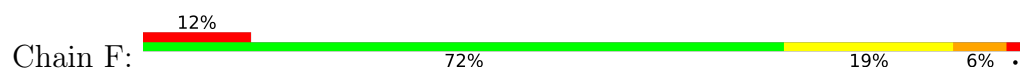
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



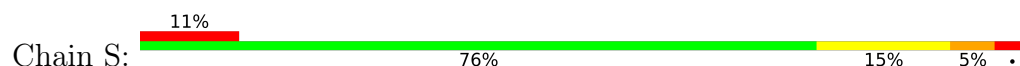
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



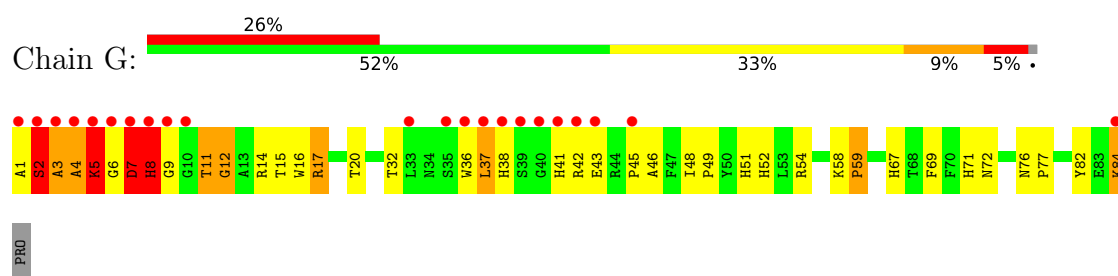
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



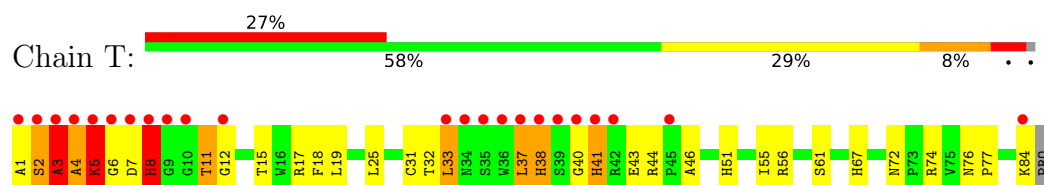
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



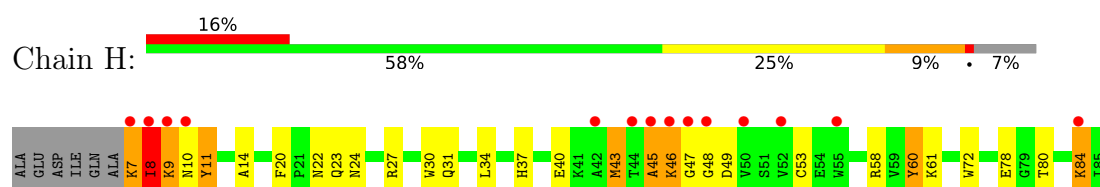
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



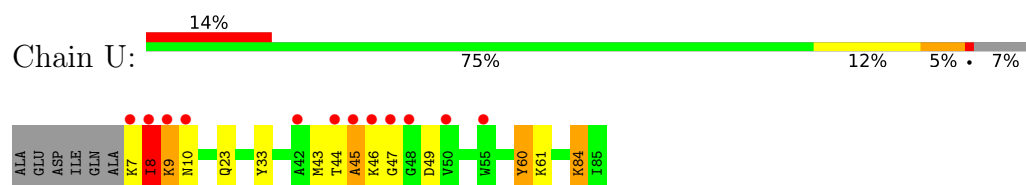
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



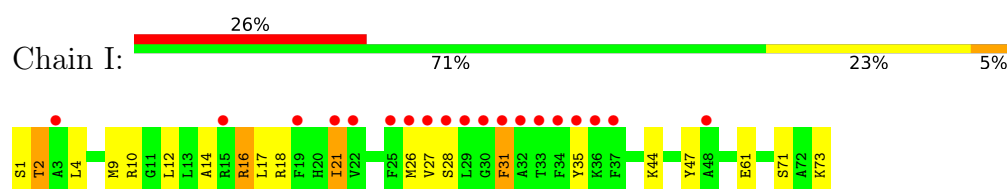
- Molecule 8: Cytochrome c oxidase subunit 6B1



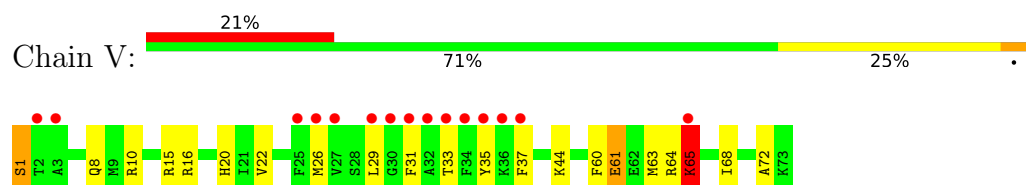
- Molecule 8: Cytochrome c oxidase subunit 6B1



- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 9: Cytochrome c oxidase subunit 6C

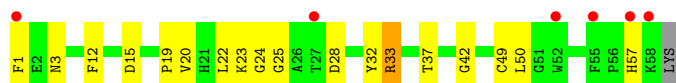


- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

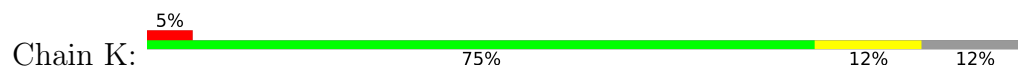




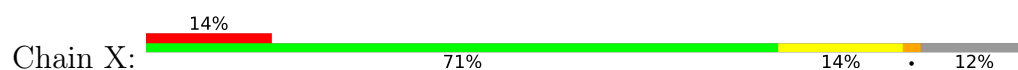
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



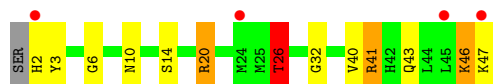
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



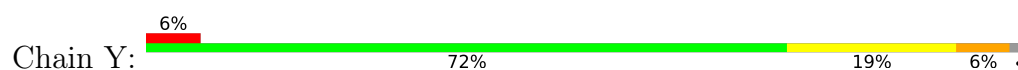
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



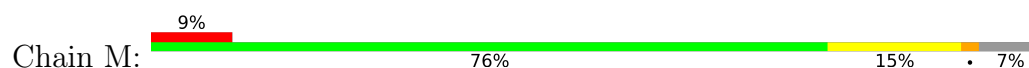
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



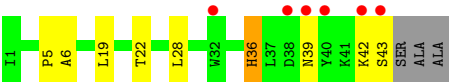
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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	182.33Å 204.83Å 177.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.65 40.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-1.65) 99.9 (40.00-1.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.162 , 0.182 0.164 , 0.183	Depositor DCC
R_{free} test set	39619 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33657	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: ZN, HEA, UNX, NA, MG, TPO, PEK, DMU, CDL, CUA, EDO, PSC, TGL, FME, SAC, CU, AZI, CHD, PGV

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.98	72/4322 (1.7%)	1.70	45/5897 (0.8%)
1	N	1.95	69/4308 (1.6%)	1.58	33/5878 (0.6%)
2	B	1.93	36/1945 (1.9%)	1.62	22/2648 (0.8%)
2	O	1.70	26/1908 (1.4%)	1.40	5/2597 (0.2%)
3	C	1.95	45/2255 (2.0%)	1.52	8/3080 (0.3%)
3	P	1.90	43/2272 (1.9%)	1.49	6/3102 (0.2%)
4	D	1.86	18/1277 (1.4%)	1.52	8/1720 (0.5%)
4	Q	1.54	8/1259 (0.6%)	1.31	9/1698 (0.5%)
5	E	1.92	11/871 (1.3%)	1.63	8/1182 (0.7%)
5	R	1.73	11/871 (1.3%)	1.43	3/1182 (0.3%)
6	F	1.93	13/788 (1.6%)	1.66	8/1069 (0.7%)
6	S	1.82	10/780 (1.3%)	1.53	5/1058 (0.5%)
7	G	2.12	20/702 (2.8%)	1.66	11/953 (1.2%)
7	T	1.99	18/702 (2.6%)	1.55	11/953 (1.2%)
8	H	1.82	10/682 (1.5%)	1.54	5/921 (0.5%)
8	U	1.46	1/682 (0.1%)	1.32	2/921 (0.2%)
9	I	1.80	11/605 (1.8%)	1.53	2/802 (0.2%)
9	V	1.44	3/605 (0.5%)	1.35	0/802
10	J	1.85	9/471 (1.9%)	1.54	3/636 (0.5%)
10	W	1.70	6/480 (1.2%)	1.45	6/648 (0.9%)
11	K	1.85	4/398 (1.0%)	1.47	3/546 (0.5%)
11	X	1.52	5/405 (1.2%)	1.16	0/556
12	L	1.88	4/393 (1.0%)	1.48	5/526 (1.0%)
12	Y	1.63	4/401 (1.0%)	1.33	1/536 (0.2%)
13	M	1.78	2/345 (0.6%)	1.43	0/470
13	Z	1.68	5/345 (1.4%)	1.26	0/470
All	All	1.86	464/30072 (1.5%)	1.53	209/40851 (0.5%)

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	4
1	N	0	3
2	B	0	1
5	R	0	1
6	F	0	2
6	S	0	3
7	T	0	1
8	H	0	1
9	V	0	1
All	All	0	17

The worst 5 of 464 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	83	VAL	CA-CB	11.77	1.60	1.54
7	T	5	LYS	CA-C	10.27	1.66	1.52
1	N	310	MET	SD-CE	-10.16	1.54	1.79
1	A	378	HIS	ND1-CE1	9.98	1.42	1.32
4	D	18	ASP	N-CA	9.86	1.58	1.46

The worst 5 of 209 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	MET	CG-SD-CE	-14.04	70.01	100.90
1	N	71	MET	CG-SD-CE	-13.94	70.24	100.90
4	Q	20	ARG	NE-CZ-NH2	-12.29	108.14	119.20
5	E	90	ARG	NE-CZ-NH1	10.70	132.20	121.50
5	E	90	ARG	NE-CZ-NH2	-10.49	109.75	119.20

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	TYR	Sidechain
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
1	A	38	ARG	Sidechain
2	B	40	TYR	Mainchain

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	4193	0	4162	100	0
1	N	4179	0	4154	109	0
2	B	1907	0	1901	60	0
2	O	1870	0	1868	52	0
3	C	2168	0	2084	53	0
3	P	2185	0	2097	46	0
4	D	1242	0	1235	40	1
4	Q	1224	0	1211	19	0
5	E	852	0	845	16	0
5	R	852	0	845	2	0
6	F	771	0	748	22	0
6	S	763	0	742	32	0
7	G	686	0	650	48	0
7	T	686	0	651	26	0
8	H	662	0	623	26	0
8	U	662	0	623	12	0
9	I	601	0	613	20	0
9	V	601	0	613	16	0
10	J	460	0	459	10	0
10	W	469	0	464	7	0
11	K	384	0	366	2	0
11	X	391	0	374	10	0
12	L	380	0	380	18	0
12	Y	388	0	388	22	0
13	M	335	0	352	5	0
13	Z	335	0	352	4	0
14	A	180	0	162	19	0
14	N	180	0	162	21	0
15	A	1	0	0	1	0
15	N	1	0	0	1	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	9	0	0	8	0
18	N	9	0	0	6	0
19	A	63	0	110	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	63	0	110	12	0
19	L	63	0	110	11	0
19	N	63	0	110	5	0
19	Q	63	0	110	12	0
19	Y	63	0	110	20	0
20	A	102	0	152	11	0
20	C	102	0	152	8	0
20	N	51	0	76	1	0
20	P	102	0	152	14	0
20	X	51	0	76	10	0
21	A	44	0	66	17	0
21	B	12	0	18	0	0
21	C	12	0	18	0	0
21	D	16	0	24	15	0
21	E	12	0	18	9	0
21	F	16	0	24	0	0
21	G	8	0	12	1	0
21	H	4	0	6	5	0
21	L	4	0	6	0	0
21	N	28	0	42	2	0
21	O	8	0	12	0	0
21	P	8	0	12	0	0
21	R	4	0	6	0	0
21	S	20	0	30	0	0
21	T	4	0	6	0	0
21	Y	4	0	6	0	0
22	B	29	0	39	0	0
22	C	58	0	78	6	0
22	G	29	0	39	1	0
22	J	29	0	38	4	0
22	P	58	0	77	4	0
22	W	29	0	39	5	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	52	0	80	21	0
24	O	52	0	80	11	0
25	C	99	0	126	12	0
25	L	33	0	42	4	0
25	M	33	0	42	0	0
25	P	99	0	126	16	0
25	Z	33	0	42	0	0
26	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	P	1	0	0	0	0
27	C	100	0	156	25	0
27	G	100	0	156	24	0
27	P	100	0	156	27	0
27	T	100	0	156	24	0
28	C	53	0	77	13	0
28	G	106	0	154	26	0
28	P	53	0	77	5	0
28	T	106	0	154	2	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	A	228	0	0	23	0
30	B	155	0	0	9	2
30	C	101	0	0	1	0
30	D	96	0	0	11	0
30	E	80	0	0	8	0
30	F	85	0	0	3	0
30	G	46	0	0	7	0
30	H	55	0	0	1	0
30	I	26	0	0	7	0
30	J	16	0	0	1	0
30	K	15	0	0	0	0
30	L	24	0	0	7	1
30	M	19	0	0	1	0
30	N	215	0	0	15	0
30	O	110	0	0	3	0
30	P	105	0	0	6	0
30	Q	37	0	0	1	0
30	R	49	0	0	0	0
30	S	79	0	0	3	0
30	T	36	0	0	0	0
30	U	38	0	0	0	0
30	V	14	0	0	1	0
30	W	13	0	0	0	0
30	X	11	0	0	3	0
30	Y	13	0	0	0	0
30	Z	12	0	0	0	0
All	All	33657	0	32632	851	2

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 13.

The worst 5 of 851 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:MET:CG	1:A:74:MET:CB	1.77	1.58
2:B:1:FME:CN	2:B:1:FME:N	1.71	1.50
4:D:38:LYS:HE2	30:D:303:HOH:O	1.16	1.31
24:B:303:PSC:O02	9:I:14:ALA:CB	1.80	1.28
2:B:1:FME:N	2:B:1:FME:O1	1.65	1.26

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:541:HOH:O	30:L:219:HOH:O[2_584]	2.09	0.11
4:D:7:LYS:CD	30:B:405:HOH:O[2_585]	2.11	0.09

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	534/514 (104%)	518 (97%)	16 (3%)	0	100	100
1	N	532/514 (104%)	515 (97%)	17 (3%)	0	100	100
2	B	235/227 (104%)	224 (95%)	11 (5%)	0	100	100
2	O	230/227 (101%)	224 (97%)	6 (3%)	0	100	100
3	C	264/261 (101%)	259 (98%)	5 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	147/147 (100%)	144 (98%)	3 (2%)	0	100	100
4	Q	145/147 (99%)	137 (94%)	4 (3%)	4 (3%)	4	0
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	0	1 (1%)	12	2
6	F	99/98 (101%)	93 (94%)	3 (3%)	3 (3%)	3	0
6	S	98/98 (100%)	93 (95%)	3 (3%)	2 (2%)	6	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	82/85 (96%)	69 (84%)	9 (11%)	4 (5%)	1	0
7	T	82/85 (96%)	72 (88%)	6 (7%)	4 (5%)	1	0
8	H	77/85 (91%)	70 (91%)	3 (4%)	4 (5%)	1	0
8	U	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	2	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	57 (100%)	0	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	45/47 (96%)	45 (100%)	0	0	100	100
13	M	41/46 (89%)	38 (93%)	1 (2%)	2 (5%)	1	0
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3595/3614 (100%)	3465 (96%)	103 (3%)	27 (1%)	16	4

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	95	GLN
6	F	96	LEU
7	G	4	ALA
7	G	8	HIS

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	447/426 (105%)	441 (99%)	6 (1%)	61	42
1	N	445/426 (104%)	438 (98%)	7 (2%)	55	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	220/210 (105%)	209 (95%)	11 (5%)	22	5
2	O	215/210 (102%)	206 (96%)	9 (4%)	26	6
3	C	231/226 (102%)	227 (98%)	4 (2%)	53	32
3	P	233/226 (103%)	228 (98%)	5 (2%)	47	24
4	D	133/129 (103%)	128 (96%)	5 (4%)	29	7
4	Q	131/129 (102%)	123 (94%)	8 (6%)	17	3
5	E	92/95 (97%)	87 (95%)	5 (5%)	20	4
5	R	92/95 (97%)	89 (97%)	3 (3%)	33	11
6	F	84/81 (104%)	81 (96%)	3 (4%)	31	9
6	S	83/81 (102%)	76 (92%)	7 (8%)	10	1
7	G	68/68 (100%)	61 (90%)	7 (10%)	7	1
7	T	68/68 (100%)	63 (93%)	5 (7%)	13	2
8	H	71/75 (95%)	66 (93%)	5 (7%)	14	2
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	1
9	I	57/57 (100%)	54 (95%)	3 (5%)	20	4
9	V	57/57 (100%)	53 (93%)	4 (7%)	14	2
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	26
10	W	50/50 (100%)	48 (96%)	2 (4%)	28	7
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	40/46 (87%)	39 (98%)	1 (2%)	42	18
12	L	39/40 (98%)	37 (95%)	2 (5%)	21	4
12	Y	40/40 (100%)	39 (98%)	1 (2%)	42	18
13	M	37/38 (97%)	36 (97%)	1 (3%)	39	16
13	Z	37/38 (97%)	35 (95%)	2 (5%)	20	4
All	All	3129/3082 (102%)	3016 (96%)	113 (4%)	31	9

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	369	ASP
12	Y	26	THR
3	P	76	GLN
11	X	47	ARG
8	U	9	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	170	ASN
3	P	68	GLN
8	U	37	HIS
1	N	180	GLN
2	O	181	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
2	FME	O	1	2	8,9,10	1.45	2 (25%)	7,9,11	1.59	1 (14%)
7	TPO	T	11	7	8,10,11	2.06	2 (25%)	10,14,16	1.88	4 (40%)
1	FME	A	1	1	8,9,10	0.94	1 (12%)	7,9,11	2.16	5 (71%)
2	FME	B	1	2	8,9,10	5.13	6 (75%)	7,9,11	9.46	3 (42%)
9	SAC	V	1	9	7,8,9	2.00	1 (14%)	8,9,11	2.36	3 (37%)
1	FME	N	1	1	8,9,10	1.22	1 (12%)	7,9,11	1.27	1 (14%)
7	TPO	G	11	7	8,10,11	1.98	2 (25%)	10,14,16	1.70	2 (20%)
9	SAC	I	1	9	7,8,9	1.11	1 (14%)	8,9,11	2.33	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	0/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-
1	FME	A	1	1	-	3/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
9	SAC	V	1	9	-	7/7/8/10	-
1	FME	N	1	1	-	2/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
9	SAC	I	1	9	-	4/7/8/10	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CN-N	11.20	1.71	1.33
2	B	1	FME	CA-N	5.36	1.53	1.46
9	V	1	SAC	CA-N	5.06	1.53	1.46
2	B	1	FME	CB-CG	4.89	1.70	1.51
2	B	1	FME	CG-SD	-3.59	1.62	1.81

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	O1-CN-N	-22.22	66.76	125.27
2	B	1	FME	CA-N-CN	-10.90	106.06	122.82
9	I	1	SAC	OG-CB-CA	-5.84	96.06	110.97
9	V	1	SAC	CA-N-C1A	4.86	132.10	123.15
7	T	11	TPO	CG2-CB-CA	3.82	120.71	113.16

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	CA-CB-OG1-P
7	G	11	TPO	CB-OG1-P-O1P

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	FME	3	0
7	T	11	TPO	1	0
2	B	1	FME	6	0
1	N	1	FME	1	0
7	G	11	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 118 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 108 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	$\# Z > 2$
21	EDO	D	203	-	3,3,3	0.41	0	2,2,2	0.88	0
21	EDO	A	616	-	3,3,3	1.06	0	2,2,2	2.70	2 (100%)
25	DMU	Z	101	-	34,34,34	0.85	3 (8%)	45,45,45	1.43	5 (11%)
19	TGL	L	101	-	62,62,62	1.61	7 (11%)	65,65,65	2.71	21 (32%)
20	PGV	P	302	-	50,50,50	1.22	2 (4%)	53,56,56	1.34	4 (7%)
24	PSC	B	303	-	51,51,51	1.54	7 (13%)	57,59,59	2.16	12 (21%)
22	CHD	J	101	-	32,32,32	1.23	3 (9%)	51,51,51	3.23	24 (47%)
22	CHD	P	306	-	32,32,32	1.63	7 (21%)	51,51,51	2.88	20 (39%)
21	EDO	G	106	-	3,3,3	0.53	0	2,2,2	0.94	0
21	EDO	C	312	-	3,3,3	0.44	0	2,2,2	0.79	0
21	EDO	B	304	-	3,3,3	0.88	0	2,2,2	0.78	0
23	CUA	O	301	2	0,1,1	-	-	-		
19	TGL	Q	201	-	62,62,62	1.60	4 (6%)	65,65,65	1.44	9 (13%)
14	HEA	A	602[A]	1,18	66,67,67	1.77	17 (25%)	78,103,103	2.02	24 (30%)
21	EDO	A	619	-	3,3,3	0.39	0	2,2,2	0.70	0
21	EDO	E	201	-	3,3,3	0.84	0	2,2,2	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	A	621	-	3,3,3	0.38	0	2,2,2	1.22	0
14	HEA	N	602[A]	1,18	66,67,67	1.88	18 (27%)	78,103,103	2.05	22 (28%)
19	TGL	D	201	-	62,62,62	2.27	6 (9%)	65,65,65	2.97	16 (24%)
21	EDO	O	304	-	3,3,3	0.82	0	2,2,2	0.54	0
21	EDO	N	612	-	3,3,3	0.68	0	2,2,2	0.77	0
21	EDO	A	615	-	3,3,3	0.93	0	2,2,2	0.72	0
21	EDO	P	312	-	3,3,3	1.12	0	2,2,2	2.42	2 (100%)
21	EDO	Y	102	-	3,3,3	0.63	0	2,2,2	0.15	0
22	CHD	C	306	-	32,32,32	1.26	4 (12%)	51,51,51	3.31	21 (41%)
19	TGL	N	609	-	62,62,62	1.10	4 (6%)	65,65,65	1.91	10 (15%)
21	EDO	C	313	-	3,3,3	1.05	0	2,2,2	0.80	0
21	EDO	N	611	-	3,3,3	0.70	0	2,2,2	1.02	0
21	EDO	S	104	-	3,3,3	1.36	0	2,2,2	0.40	0
20	PGV	P	304	-	50,50,50	0.93	1 (2%)	53,56,56	1.32	5 (9%)
25	DMU	P	307	-	34,34,34	1.20	1 (2%)	45,45,45	1.38	6 (13%)
21	EDO	N	613	-	3,3,3	0.73	0	2,2,2	0.24	0
21	EDO	A	614	-	3,3,3	1.10	0	2,2,2	0.75	0
14	HEA	A	601	1	66,67,67	1.94	24 (36%)	78,103,103	2.61	32 (41%)
21	EDO	S	105	-	3,3,3	1.04	0	2,2,2	1.61	1 (50%)
21	EDO	N	610	-	3,3,3	1.33	1 (33%)	2,2,2	0.34	0
18	AZI	A	607[B]	15	0,2,2	-	-	0,1,1	-	-
19	TGL	Y	101	-	62,62,62	1.64	7 (11%)	65,65,65	2.16	19 (29%)
21	EDO	S	103	-	3,3,3	0.47	0	2,2,2	0.27	0
25	DMU	C	309	-	34,34,34	0.80	1 (2%)	45,45,45	2.56	12 (26%)
21	EDO	T	104	-	3,3,3	1.14	0	2,2,2	0.72	0
14	HEA	N	602[B]	1,18	66,67,67	1.92	18 (27%)	78,103,103	2.03	22 (28%)
28	PEK	T	102	-	52,52,52	0.95	3 (5%)	55,57,57	1.27	5 (9%)
20	PGV	A	610	-	50,50,50	1.86	4 (8%)	53,56,56	2.74	10 (18%)
22	CHD	B	301	-	32,32,32	1.98	14 (43%)	51,51,51	2.64	26 (50%)
21	EDO	F	105	-	3,3,3	1.15	0	2,2,2	0.70	0
20	PGV	C	308	-	50,50,50	1.40	3 (6%)	53,56,56	1.62	7 (13%)
21	EDO	C	311	-	3,3,3	1.03	0	2,2,2	0.27	0
21	EDO	D	204	-	3,3,3	0.58	0	2,2,2	0.60	0
20	PGV	X	101	-	50,50,50	1.35	3 (6%)	53,56,56	1.59	8 (15%)
21	EDO	A	612	-	3,3,3	1.74	1 (33%)	2,2,2	0.97	0
22	CHD	G	103	-	32,32,32	2.05	13 (40%)	51,51,51	2.38	22 (43%)
21	EDO	A	618	-	3,3,3	1.10	0	2,2,2	1.10	0
21	EDO	L	103	-	3,3,3	0.59	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	N	608	-	50,50,50	1.15	5 (10%)	53,56,56	1.53	8 (15%)
27	CDL	G	102	-	99,99,99	1.57	16 (16%)	105,111,111	1.72	22 (20%)
21	EDO	B	305	-	3,3,3	0.55	0	2,2,2	0.77	0
25	DMU	P	310	-	34,34,34	1.06	1 (2%)	45,45,45	1.49	5 (11%)
28	PEK	C	307	-	52,52,52	1.37	5 (9%)	55,57,57	1.54	7 (12%)
21	EDO	N	614	-	3,3,3	1.34	0	2,2,2	0.57	0
21	EDO	S	102	-	3,3,3	0.86	0	2,2,2	0.43	0
18	AZI	N	606[B]	14	0,2,2	-	-	0,1,1	-	-
21	EDO	A	611	-	3,3,3	0.47	0	2,2,2	0.21	0
22	CHD	W	101	-	32,32,32	1.18	2 (6%)	51,51,51	3.62	24 (47%)
27	CDL	C	305	-	99,99,99	1.64	18 (18%)	105,111,111	1.64	21 (20%)
24	PSC	O	302	-	51,51,51	1.29	3 (5%)	57,59,59	1.56	9 (15%)
21	EDO	A	613	-	3,3,3	0.80	0	2,2,2	0.71	0
14	HEA	A	602[B]	1,18	66,67,67	1.78	17 (25%)	78,103,103	2.22	26 (33%)
21	EDO	A	620	-	3,3,3	0.62	0	2,2,2	0.41	0
21	EDO	E	202	-	3,3,3	0.91	0	2,2,2	0.57	0
28	PEK	G	101	-	52,52,52	1.02	3 (5%)	55,57,57	1.34	8 (14%)
20	PGV	A	609	-	50,50,50	1.11	4 (8%)	53,56,56	1.28	5 (9%)
28	PEK	T	101	-	52,52,52	1.34	2 (3%)	55,57,57	1.62	9 (16%)
21	EDO	F	103	-	3,3,3	0.79	0	2,2,2	0.19	0
28	PEK	G	104	-	52,52,52	1.32	3 (5%)	55,57,57	1.47	8 (14%)
21	EDO	D	202	-	3,3,3	0.76	0	2,2,2	1.03	0
22	CHD	C	301	-	32,32,32	1.88	8 (25%)	51,51,51	2.37	17 (33%)
21	EDO	B	306	-	3,3,3	0.56	0	2,2,2	0.03	0
21	EDO	D	205	-	3,3,3	0.26	0	2,2,2	1.60	1 (50%)
19	TGL	A	608	-	62,62,62	1.36	5 (8%)	65,65,65	1.87	11 (16%)
28	PEK	P	308	-	52,52,52	1.31	3 (5%)	55,57,57	1.42	8 (14%)
20	PGV	C	304	-	50,50,50	0.82	0	53,56,56	1.31	6 (11%)
21	EDO	H	101	-	3,3,3	0.30	0	2,2,2	2.28	2 (100%)
21	EDO	F	104	-	3,3,3	1.59	0	2,2,2	0.63	0
18	AZI	A	606[B]	14	0,2,2	-	-	0,1,1	-	-
21	EDO	A	617	-	3,3,3	1.23	0	2,2,2	0.34	0
25	DMU	C	302	-	34,34,34	0.98	1 (2%)	45,45,45	1.57	5 (11%)
21	EDO	S	106	-	3,3,3	1.15	0	2,2,2	0.83	0
21	EDO	O	303	-	3,3,3	0.59	0	2,2,2	0.60	0
22	CHD	P	301	-	32,32,32	1.76	9 (28%)	51,51,51	2.35	16 (31%)
21	EDO	G	105	-	3,3,3	0.97	0	2,2,2	0.58	0
25	DMU	C	310	-	34,34,34	1.76	8 (23%)	45,45,45	3.10	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	AZI	N	607[A]	15,14	0,2,2	-	-	0,1,1	-	-
18	AZI	A	607[A]	15,14	0,2,2	-	-	0,1,1	-	-
21	EDO	F	102	-	3,3,3	0.99	0	2,2,2	0.31	0
27	CDL	P	305	-	99,99,99	1.73	21 (21%)	105,111,111	1.57	18 (17%)
25	DMU	P	309	-	34,34,34	0.84	2 (5%)	45,45,45	2.27	12 (26%)
21	EDO	N	615	-	3,3,3	0.45	0	2,2,2	1.04	0
21	EDO	E	203	-	3,3,3	0.50	0	2,2,2	0.93	0
21	EDO	P	311	-	3,3,3	0.99	0	2,2,2	0.39	0
21	EDO	R	201	-	3,3,3	0.66	0	2,2,2	0.81	0
23	CUA	B	302	2	0,1,1	-	-	-	-	-
21	EDO	N	616	-	3,3,3	1.35	1 (33%)	2,2,2	1.66	0
25	DMU	M	101	-	34,34,34	0.97	2 (5%)	45,45,45	1.36	7 (15%)
14	HEA	N	601	1	66,67,67	1.75	22 (33%)	78,103,103	2.47	23 (29%)
27	CDL	T	103	-	99,99,99	1.58	15 (15%)	105,111,111	1.62	17 (16%)
18	AZI	N	607[B]	15	0,2,2	-	-	0,1,1	-	-
25	DMU	L	102	-	34,34,34	1.11	4 (11%)	45,45,45	1.75	12 (26%)

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
21	EDO	D	203	-	-	1/1/1/1	-
21	EDO	A	616	-	-	0/1/1/1	-
25	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
19	TGL	L	101	-	-	39/65/65/65	-
20	PGV	P	302	-	-	27/55/55/55	-
24	PSC	B	303	-	-	21/55/55/55	-
22	CHD	J	101	-	-	6/9/74/74	0/4/4/4
22	CHD	P	306	-	-	3/9/74/74	0/4/4/4
21	EDO	G	106	-	-	1/1/1/1	-
21	EDO	C	312	-	-	0/1/1/1	-
21	EDO	B	304	-	-	1/1/1/1	-
19	TGL	Q	201	-	-	34/65/65/65	-
14	HEA	A	602[A]	1,18	-	5/36/76/76	-
21	EDO	A	619	-	-	0/1/1/1	-
21	EDO	E	201	-	-	0/1/1/1	-
21	EDO	A	621	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	N	602[A]	1,18	-	6/36/76/76	-
19	TGL	D	201	-	-	39/65/65/65	-
21	EDO	O	304	-	-	0/1/1/1	-
21	EDO	N	612	-	-	0/1/1/1	-
21	EDO	A	615	-	-	1/1/1/1	-
21	EDO	P	312	-	-	1/1/1/1	-
21	EDO	Y	102	-	-	1/1/1/1	-
22	CHD	C	306	-	-	7/9/74/74	0/4/4/4
19	TGL	N	609	-	-	33/65/65/65	-
21	EDO	C	313	-	-	1/1/1/1	-
21	EDO	N	611	-	-	0/1/1/1	-
21	EDO	S	104	-	-	0/1/1/1	-
20	PGV	P	304	-	-	11/55/55/55	-
25	DMU	P	307	-	-	5/19/59/59	0/2/2/2
21	EDO	N	613	-	-	1/1/1/1	-
21	EDO	A	614	-	-	0/1/1/1	-
14	HEA	A	601	1	-	5/36/76/76	-
21	EDO	S	105	-	-	0/1/1/1	-
21	EDO	N	610	-	-	0/1/1/1	-
19	TGL	Y	101	-	-	40/65/65/65	-
21	EDO	S	103	-	-	1/1/1/1	-
25	DMU	C	309	-	-	6/19/59/59	0/2/2/2
21	EDO	T	104	-	-	0/1/1/1	-
14	HEA	N	602[B]	1,18	-	7/36/76/76	-
28	PEK	T	102	-	-	16/56/56/56	-
20	PGV	A	610	-	-	26/55/55/55	-
22	CHD	B	301	-	-	2/9/74/74	0/4/4/4
21	EDO	F	105	-	-	0/1/1/1	-
20	PGV	C	308	-	-	37/55/55/55	-
21	EDO	C	311	-	-	0/1/1/1	-
21	EDO	D	204	-	-	0/1/1/1	-
20	PGV	X	101	-	-	31/55/55/55	-
22	CHD	G	103	-	-	2/9/74/74	0/4/4/4
21	EDO	A	612	-	-	0/1/1/1	-
21	EDO	A	618	-	-	1/1/1/1	-
21	EDO	L	103	-	-	0/1/1/1	-
20	PGV	N	608	-	-	7/55/55/55	-
27	CDL	G	102	-	-	71/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	B	305	-	-	0/1/1/1	-
25	DMU	P	310	-	-	7/19/59/59	0/2/2/2
28	PEK	C	307	-	-	23/56/56/56	-
21	EDO	N	614	-	-	0/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
21	EDO	A	611	-	-	0/1/1/1	-
22	CHD	W	101	-	-	8/9/74/74	0/4/4/4
27	CDL	C	305	-	-	58/110/110/110	-
24	PSC	O	302	-	-	28/55/55/55	-
21	EDO	A	613	-	-	0/1/1/1	-
14	HEA	A	602[B]	1,18	-	7/36/76/76	-
21	EDO	A	620	-	-	1/1/1/1	-
21	EDO	E	202	-	-	1/1/1/1	-
28	PEK	G	101	-	-	17/56/56/56	-
20	PGV	A	609	-	-	7/55/55/55	-
28	PEK	T	101	-	-	31/56/56/56	-
21	EDO	F	103	-	-	1/1/1/1	-
28	PEK	G	104	-	-	27/56/56/56	-
21	EDO	D	202	-	-	0/1/1/1	-
22	CHD	C	301	-	-	2/9/74/74	0/4/4/4
21	EDO	B	306	-	-	0/1/1/1	-
21	EDO	D	205	-	-	1/1/1/1	-
19	TGL	A	608	-	-	36/65/65/65	-
28	PEK	P	308	-	-	32/56/56/56	-
20	PGV	C	304	-	-	15/55/55/55	-
21	EDO	H	101	-	-	1/1/1/1	-
21	EDO	F	104	-	-	0/1/1/1	-
21	EDO	A	617	-	-	1/1/1/1	-
25	DMU	C	302	-	-	5/19/59/59	0/2/2/2
21	EDO	S	106	-	-	0/1/1/1	-
21	EDO	O	303	-	-	0/1/1/1	-
22	CHD	P	301	-	-	3/9/74/74	0/4/4/4
21	EDO	G	105	-	-	0/1/1/1	-
25	DMU	C	310	-	-	11/19/59/59	0/2/2/2
21	EDO	F	102	-	-	0/1/1/1	-
27	CDL	P	305	-	-	59/110/110/110	-
25	DMU	P	309	-	-	6/19/59/59	0/2/2/2
21	EDO	N	615	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	E	203	-	-	1/1/1/1	-
21	EDO	P	311	-	-	1/1/1/1	-
21	EDO	R	201	-	-	0/1/1/1	-
21	EDO	N	616	-	-	1/1/1/1	-
25	DMU	M	101	-	-	2/19/59/59	0/2/2/2
14	HEA	N	601	1	-	4/36/76/76	-
27	CDL	T	103	-	-	51/110/110/110	-
25	DMU	L	102	-	-	14/19/59/59	0/2/2/2

The worst 5 of 356 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	201	TGL	OB1-CB1	11.00	1.55	1.22
19	D	201	TGL	OG2-CB1	8.23	1.57	1.34
20	A	610	PGV	O02-C1	8.05	1.46	1.22
19	L	101	TGL	OG2-CB1	7.02	1.54	1.34
20	A	610	PGV	O01-C1	6.83	1.53	1.34

The worst 5 of 692 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	201	TGL	OG2-CB1-CB2	-13.46	82.48	111.50
19	D	201	TGL	OG2-CB1-OB1	12.52	153.95	123.70
22	C	306	CHD	C23-C22-C20	-12.09	92.43	114.52
22	W	101	CHD	C17-C13-C12	11.12	127.81	117.67
20	A	610	PGV	O01-C1-O02	10.68	149.52	123.70

There are no chirality outliers.

5 of 964 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602[B]	HEA	C2A-C3A-CMA-OMA
14	A	602[B]	HEA	C4D-C3D-CAD-CBD
14	N	602[B]	HEA	C2A-C3A-CMA-OMA
14	N	602[B]	HEA	C2D-C3D-CAD-CBD
19	D	201	TGL	CG2-CG1-OG1-CA1

There are no ring outliers.

61 monomers are involved in 411 short contacts:

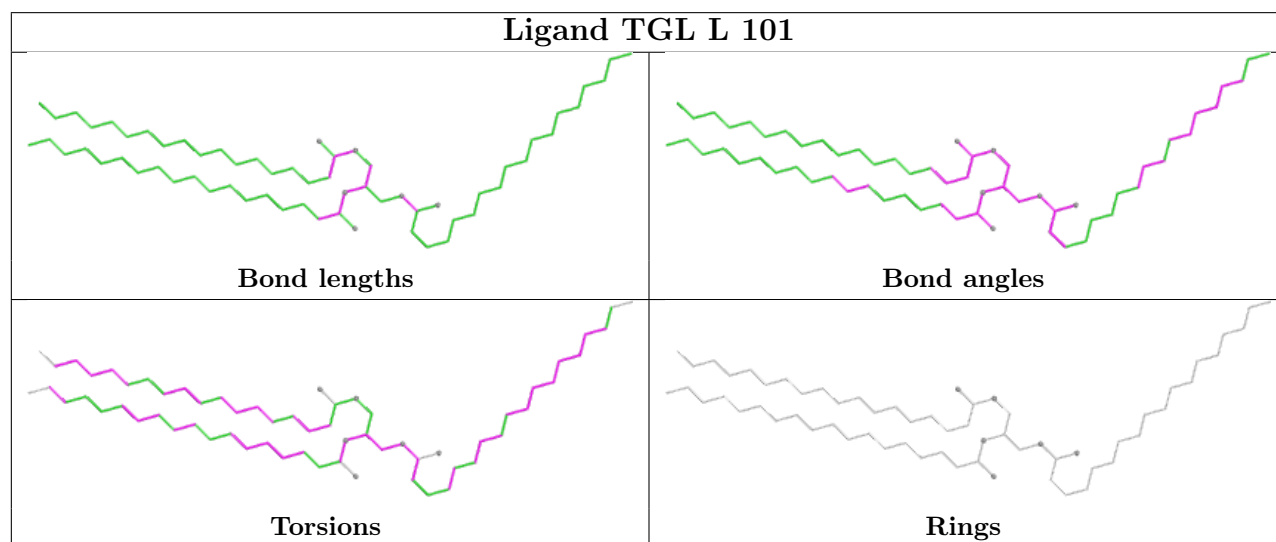
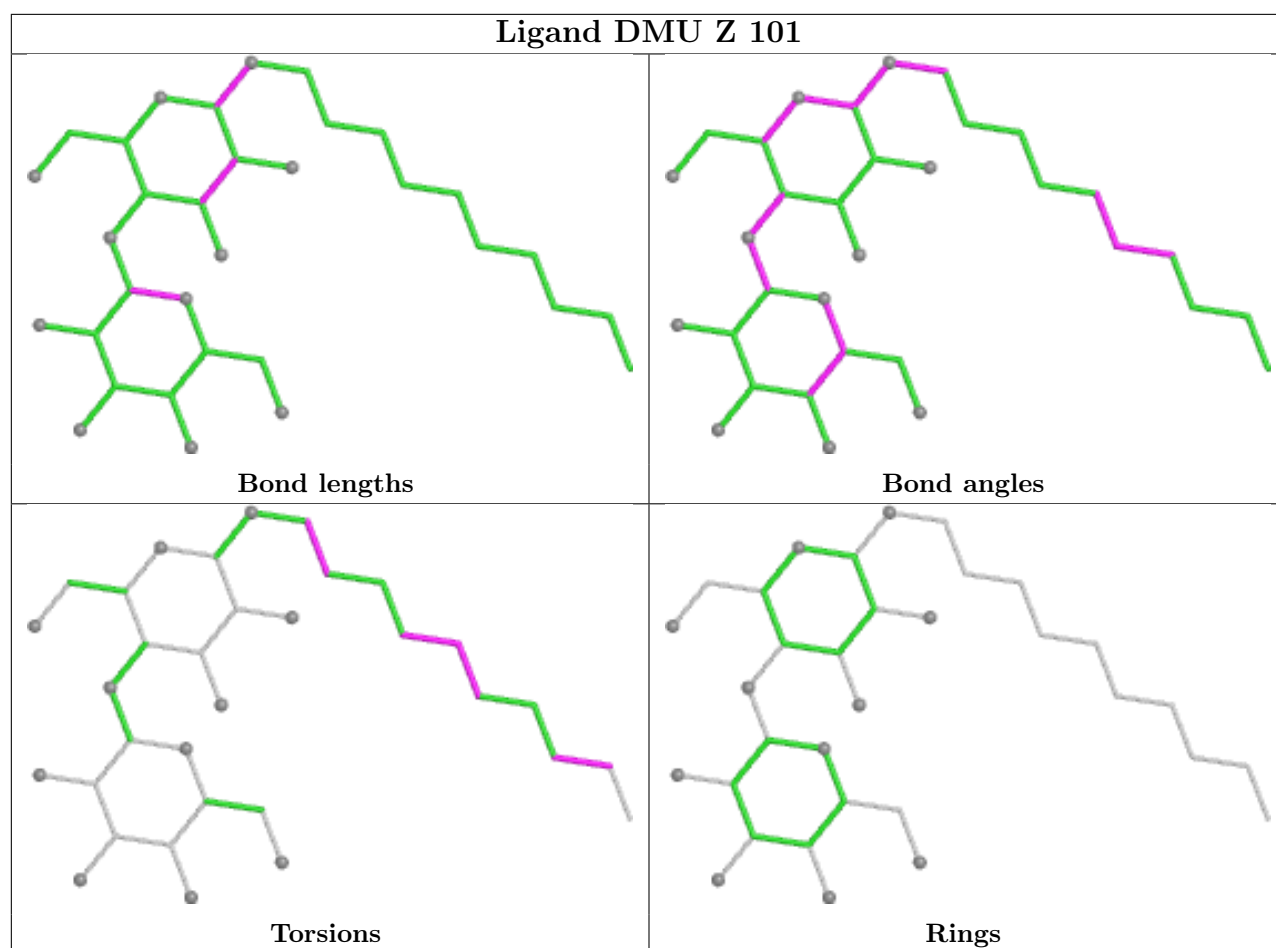
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	D	203	EDO	2	0
21	A	616	EDO	3	0
19	L	101	TGL	11	0
20	P	302	PGV	4	0
24	B	303	PSC	21	0
22	J	101	CHD	4	0
22	P	306	CHD	2	0
21	G	106	EDO	1	0
19	Q	201	TGL	12	0
14	A	602[A]	HEA	2	0
21	A	619	EDO	2	0
21	A	621	EDO	10	0
14	N	602[A]	HEA	1	0
19	D	201	TGL	12	0
22	C	306	CHD	5	0
19	N	609	TGL	5	0
20	P	304	PGV	10	0
25	P	307	DMU	13	0
21	A	614	EDO	2	0
14	A	601	HEA	11	0
18	A	607[B]	AZI	6	0
19	Y	101	TGL	20	0
25	C	309	DMU	1	0
14	N	602[B]	HEA	9	0
28	T	102	PEK	2	0
20	A	610	PGV	5	0
20	C	308	PGV	6	0
20	X	101	PGV	10	0
22	G	103	CHD	1	0
20	N	608	PGV	1	0
27	G	102	CDL	24	0
25	P	310	DMU	1	0
28	C	307	PEK	13	0
21	A	611	EDO	5	0
22	W	101	CHD	5	0
27	C	305	CDL	25	0
24	O	302	PSC	11	0
14	A	602[B]	HEA	6	0
21	E	202	EDO	9	0
28	G	101	PEK	7	0
20	A	609	PGV	6	0
28	G	104	PEK	19	0
21	D	202	EDO	11	0

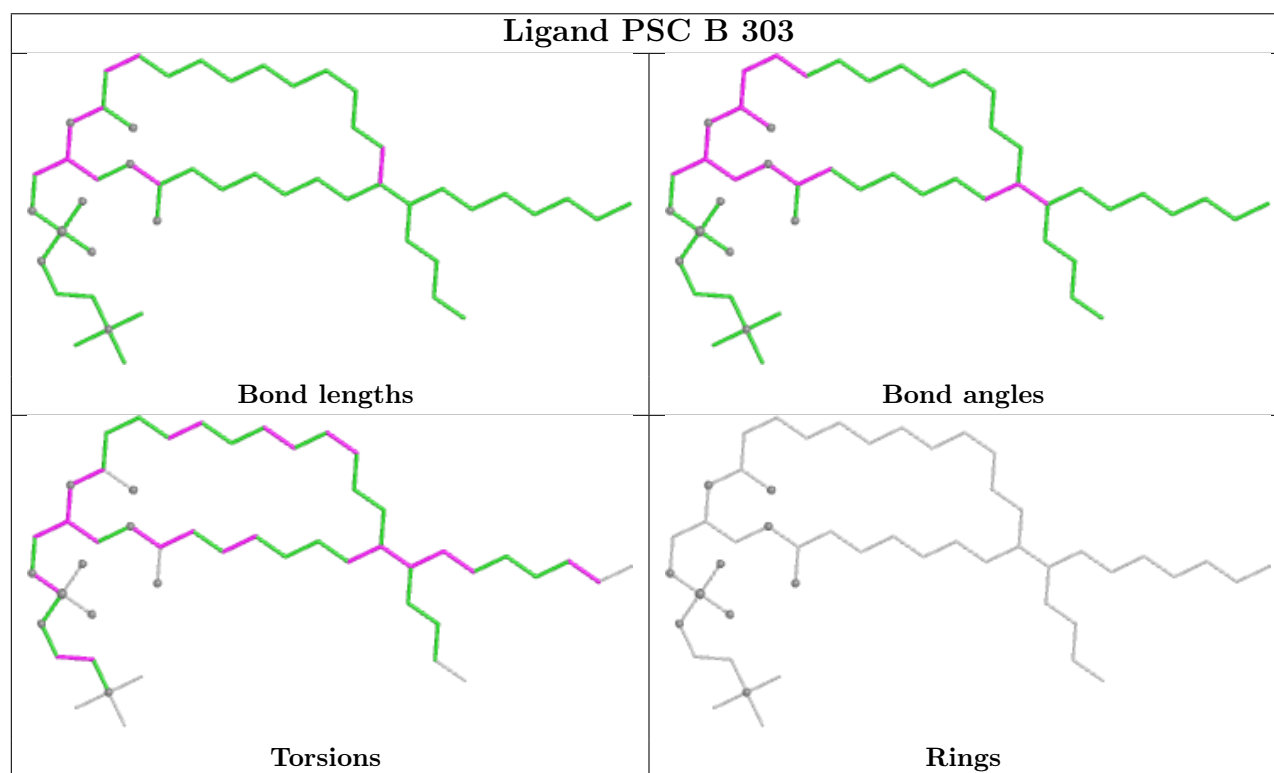
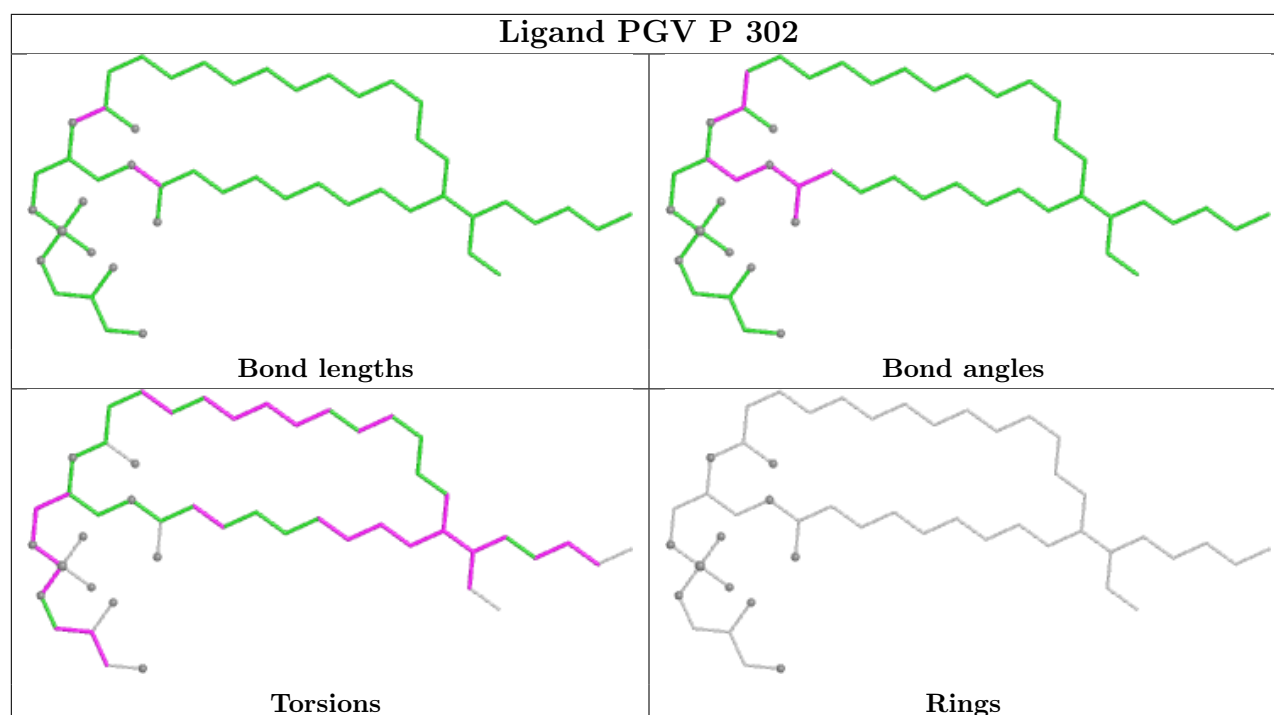
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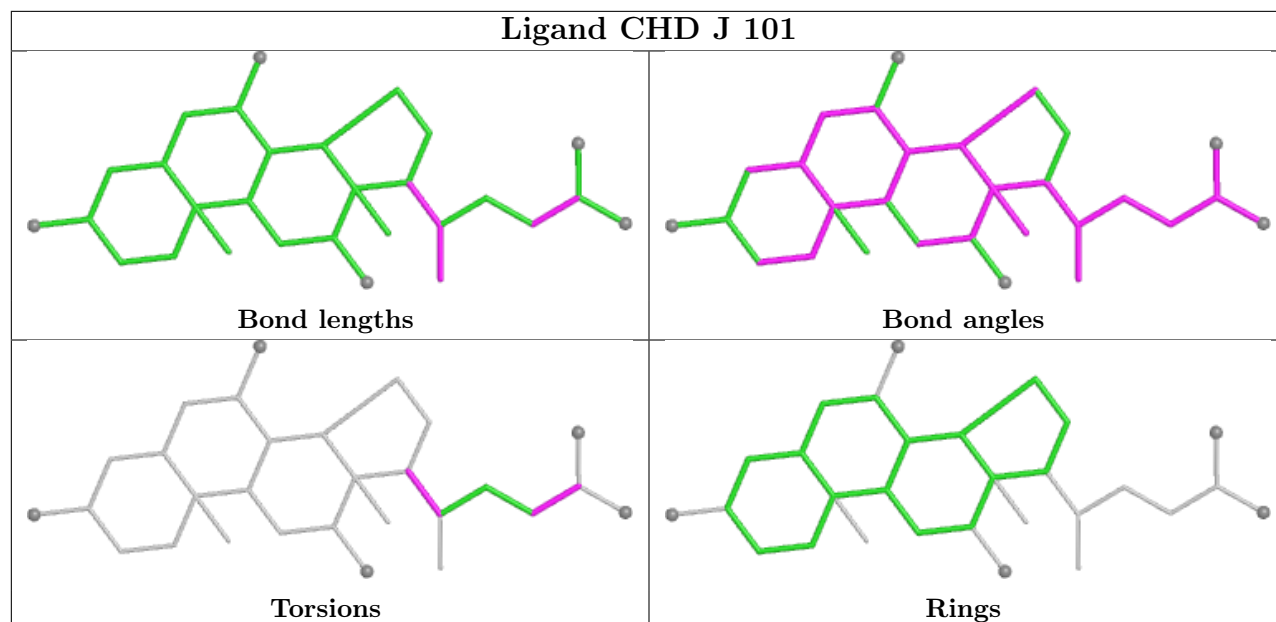
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	301	CHD	1	0
21	D	205	EDO	2	0
19	A	608	TGL	1	0
28	P	308	PEK	5	0
20	C	304	PGV	2	0
21	H	101	EDO	5	0
18	A	606[B]	AZI	3	0
25	C	302	DMU	9	0
22	P	301	CHD	2	0
25	C	310	DMU	3	0
18	N	607[A]	AZI	1	0
27	P	305	CDL	27	0
25	P	309	DMU	2	0
21	N	616	EDO	2	0
14	N	601	HEA	11	0
27	T	103	CDL	24	0
18	N	607[B]	AZI	5	0
25	L	102	DMU	4	0

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

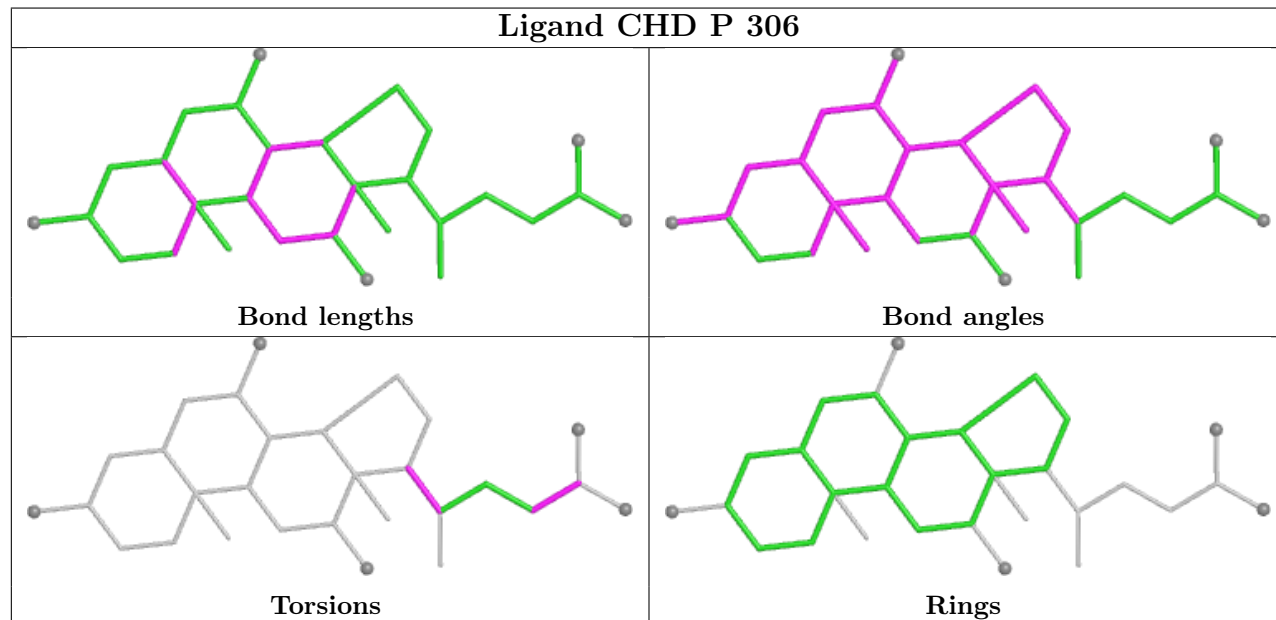


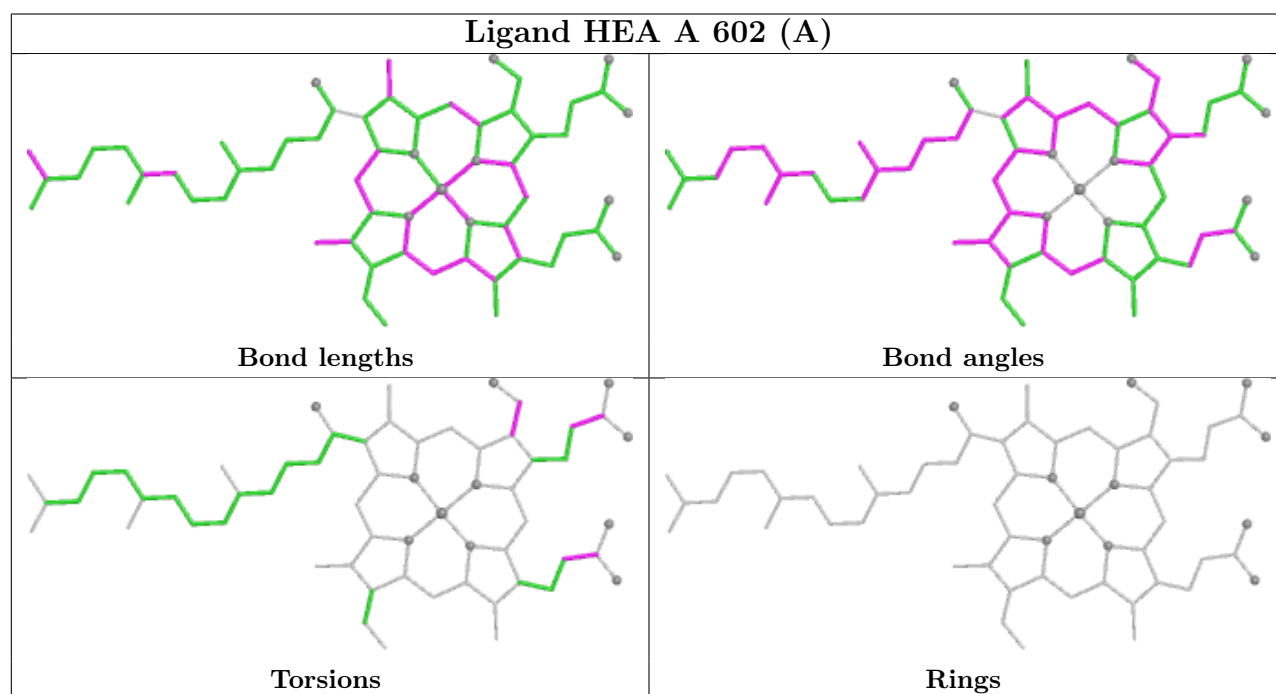
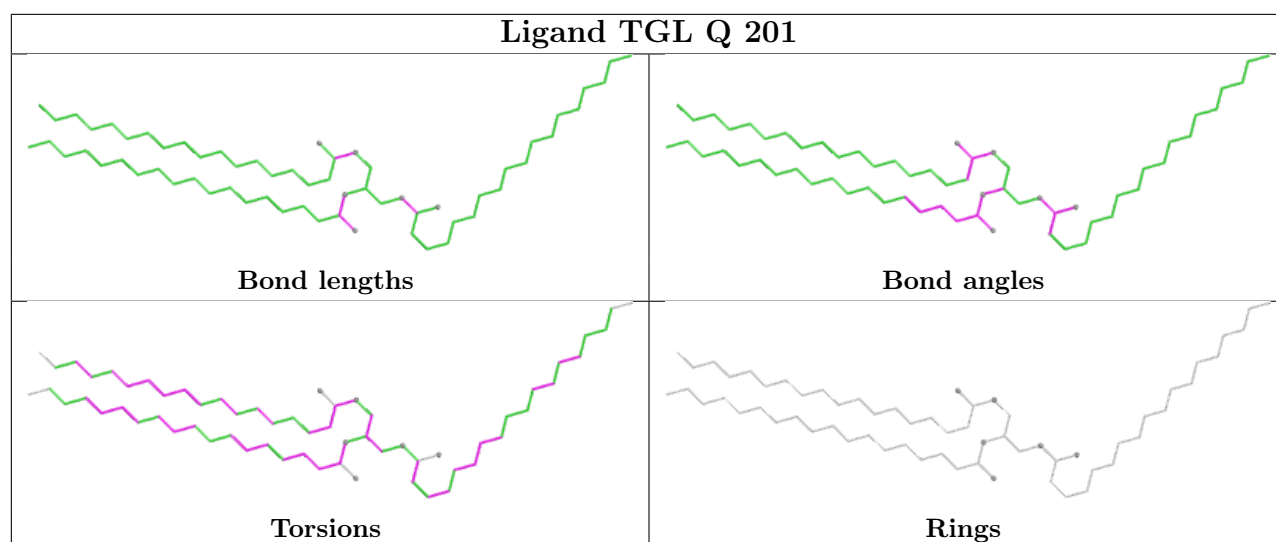


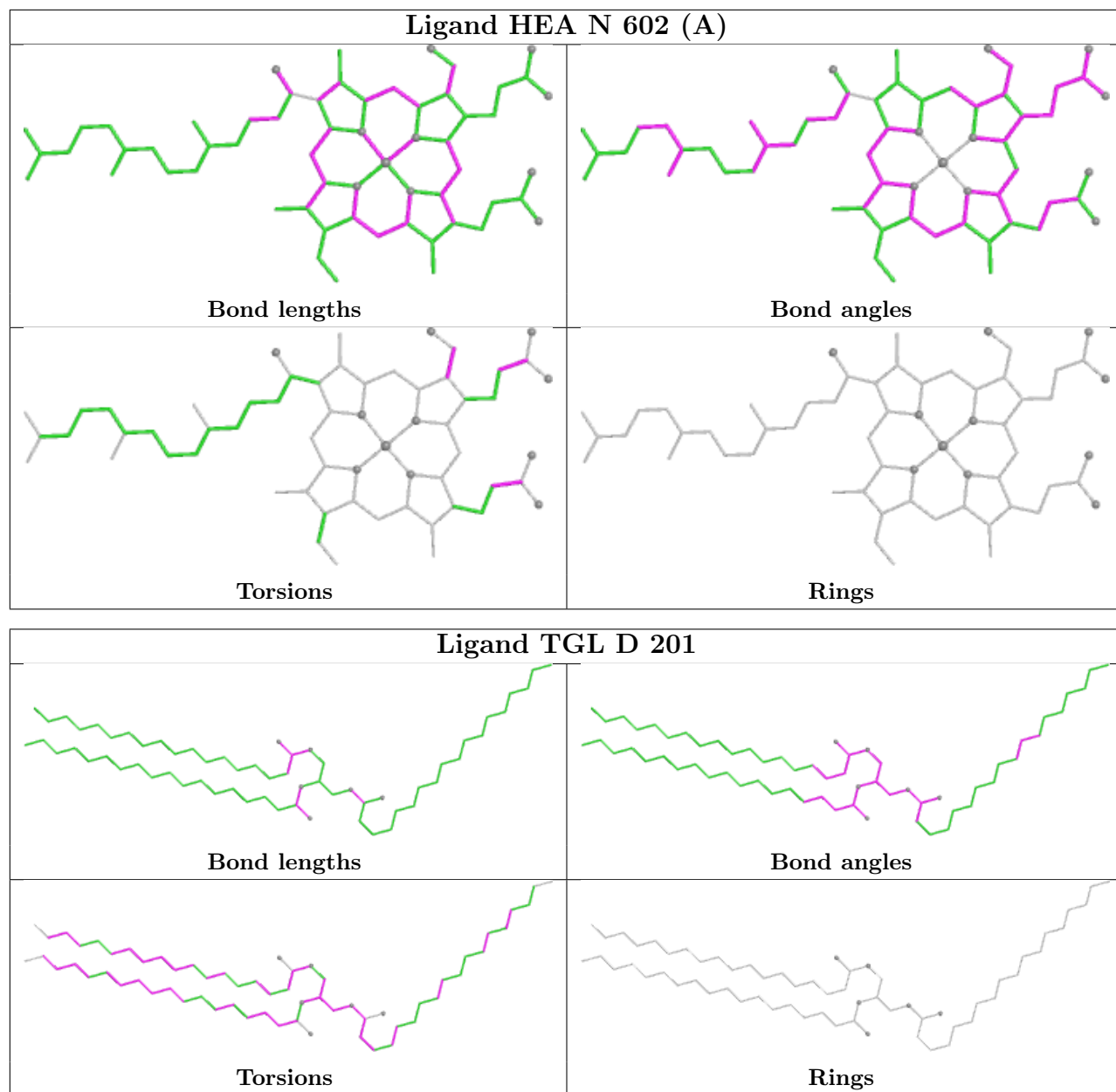
Ligand CHD J 101

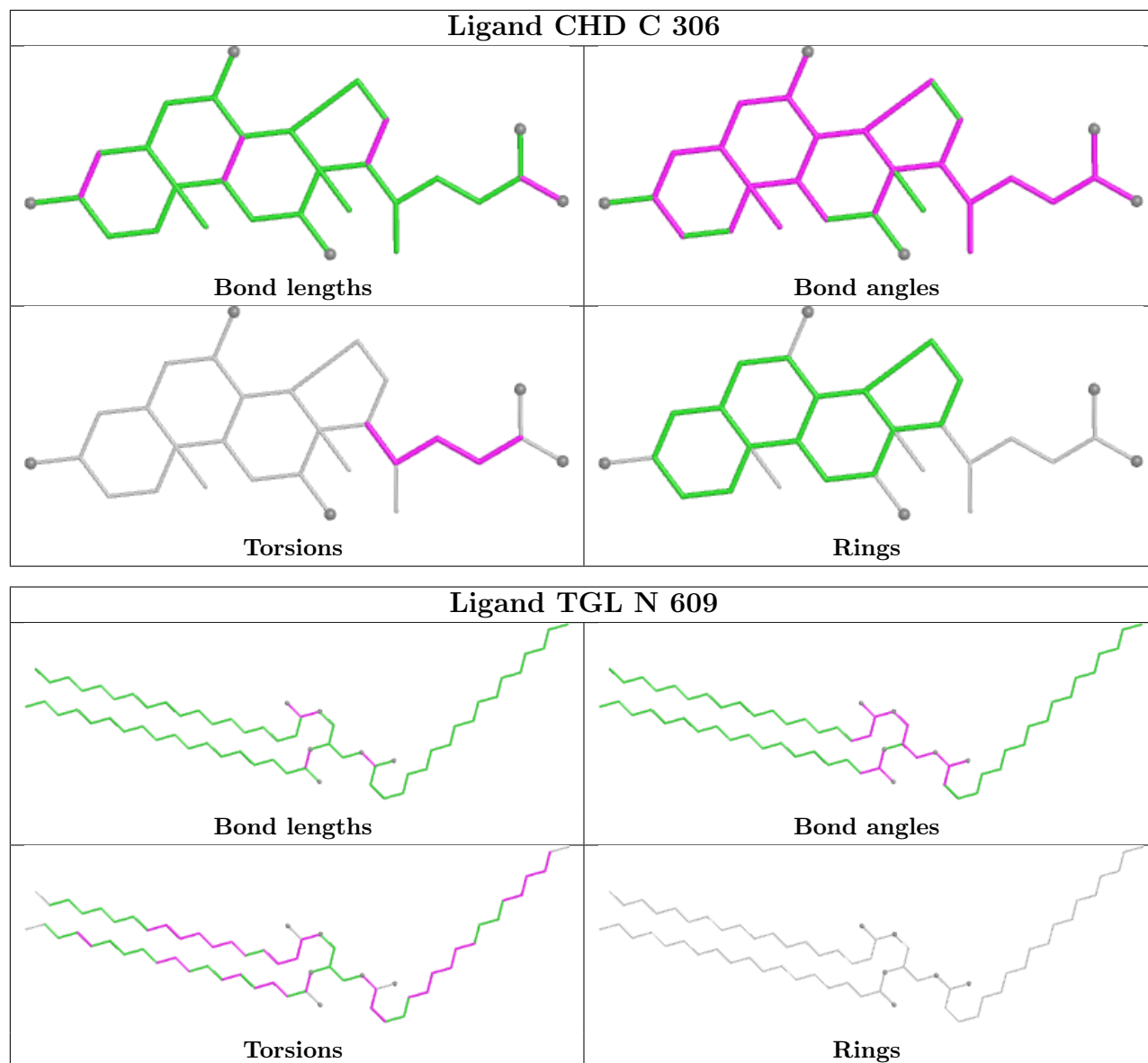


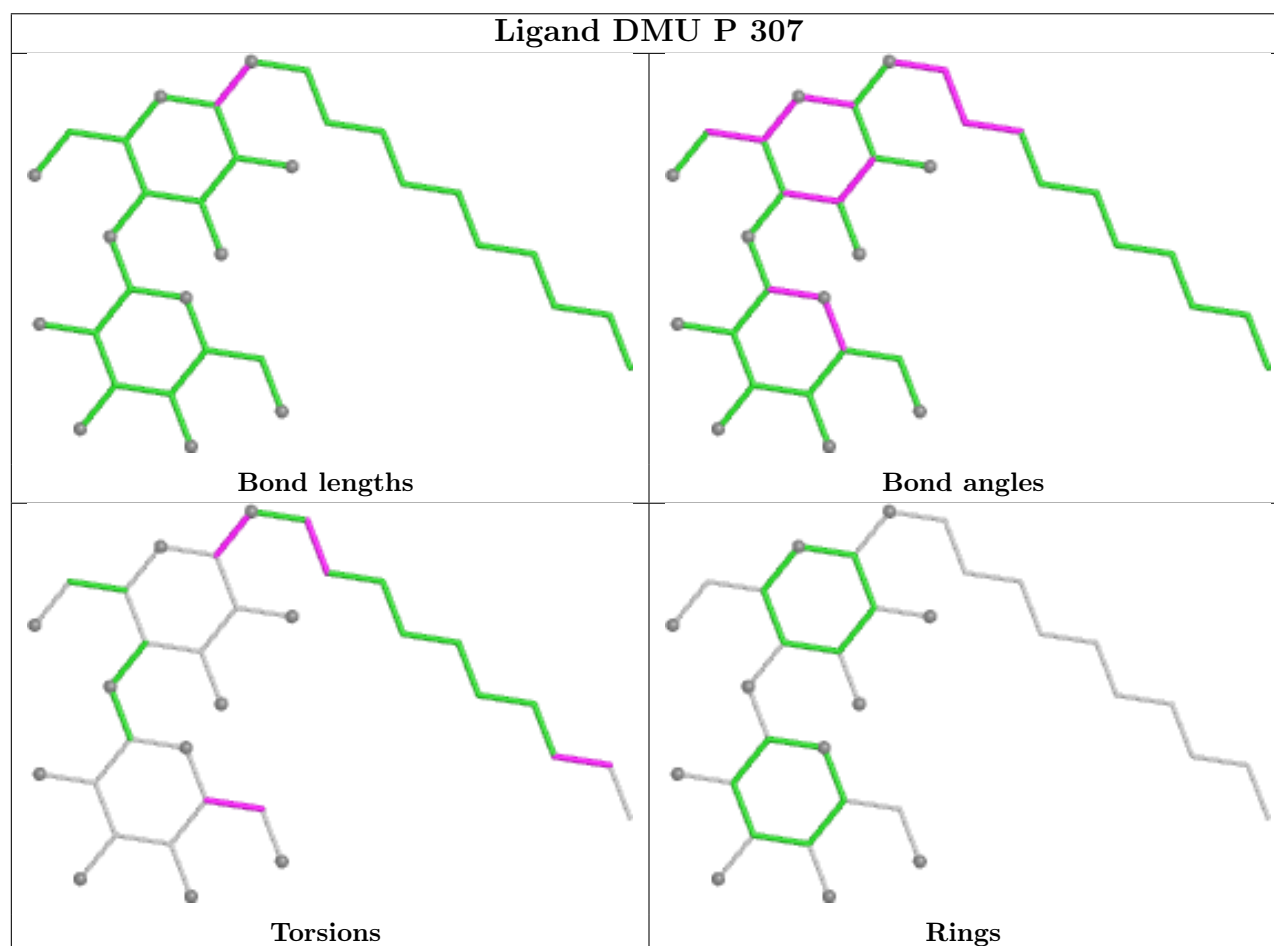
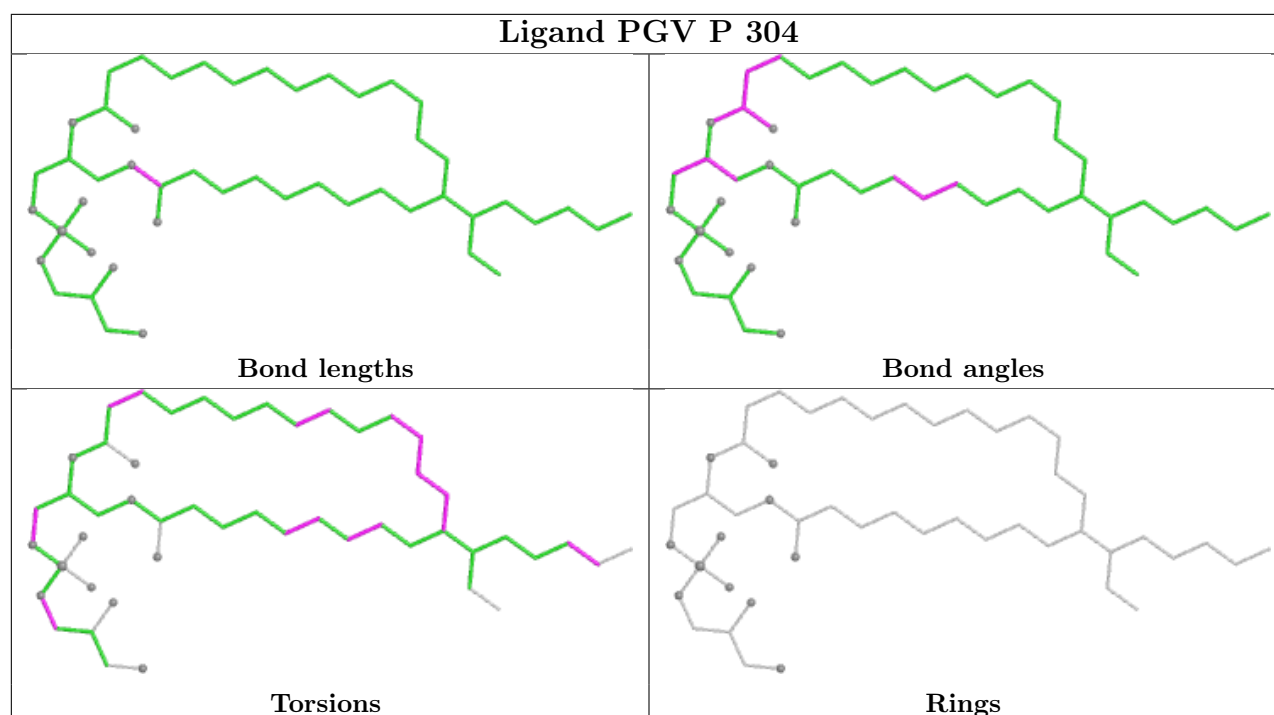
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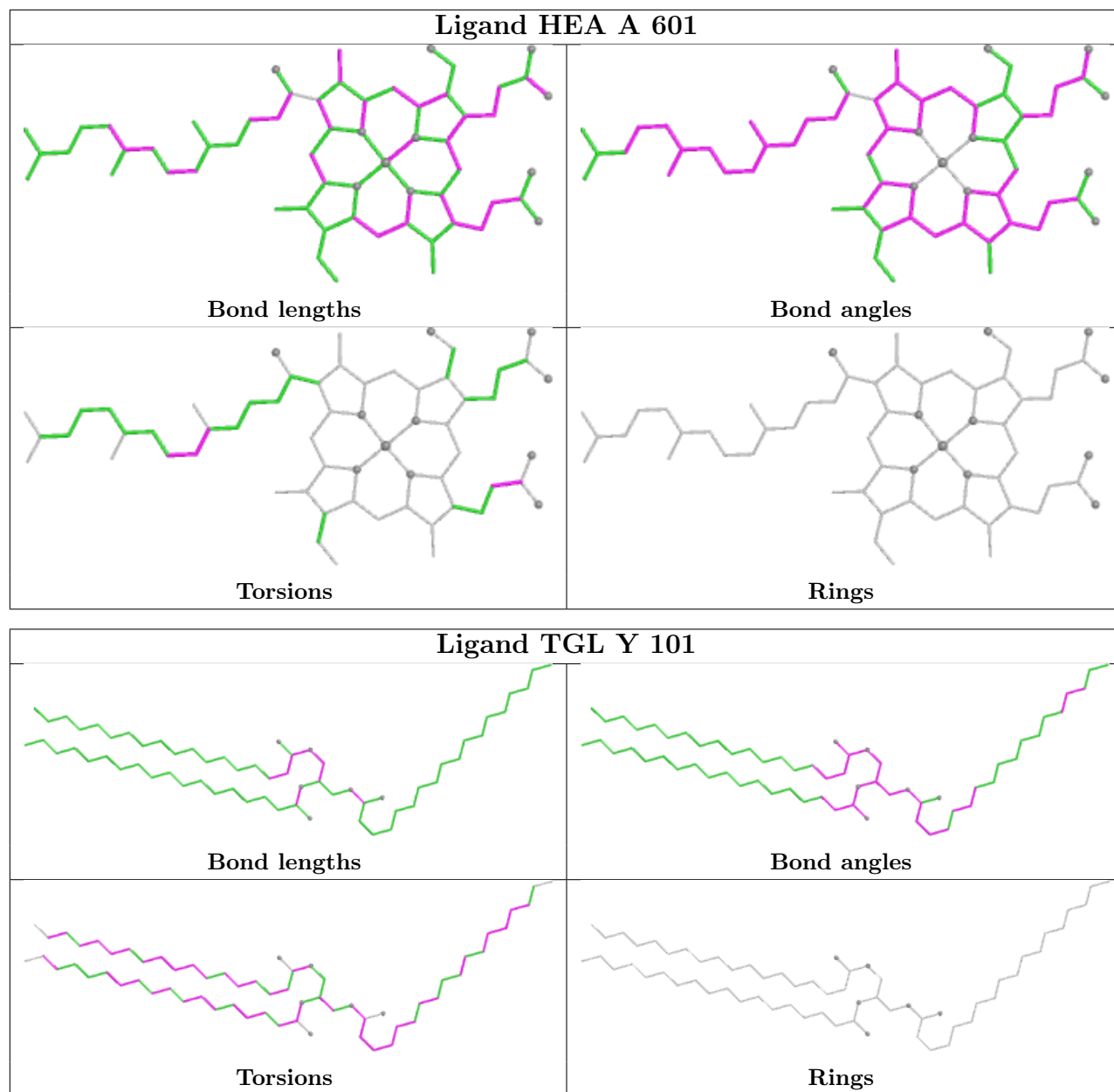


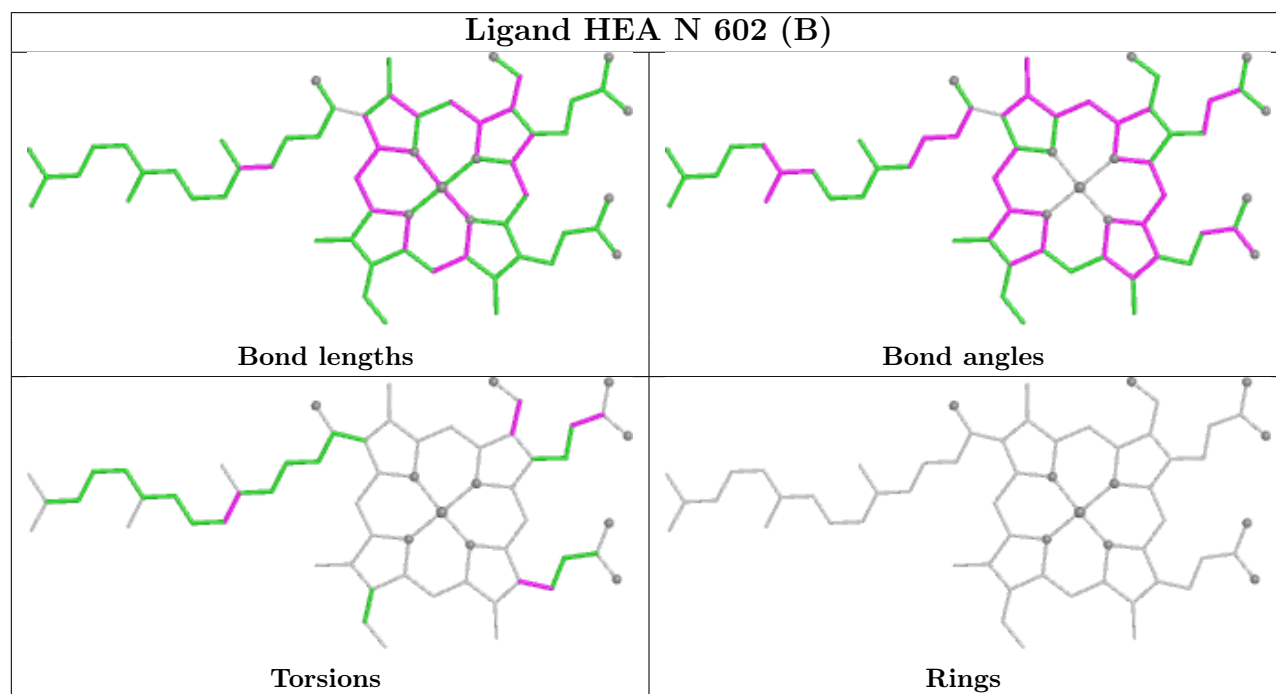
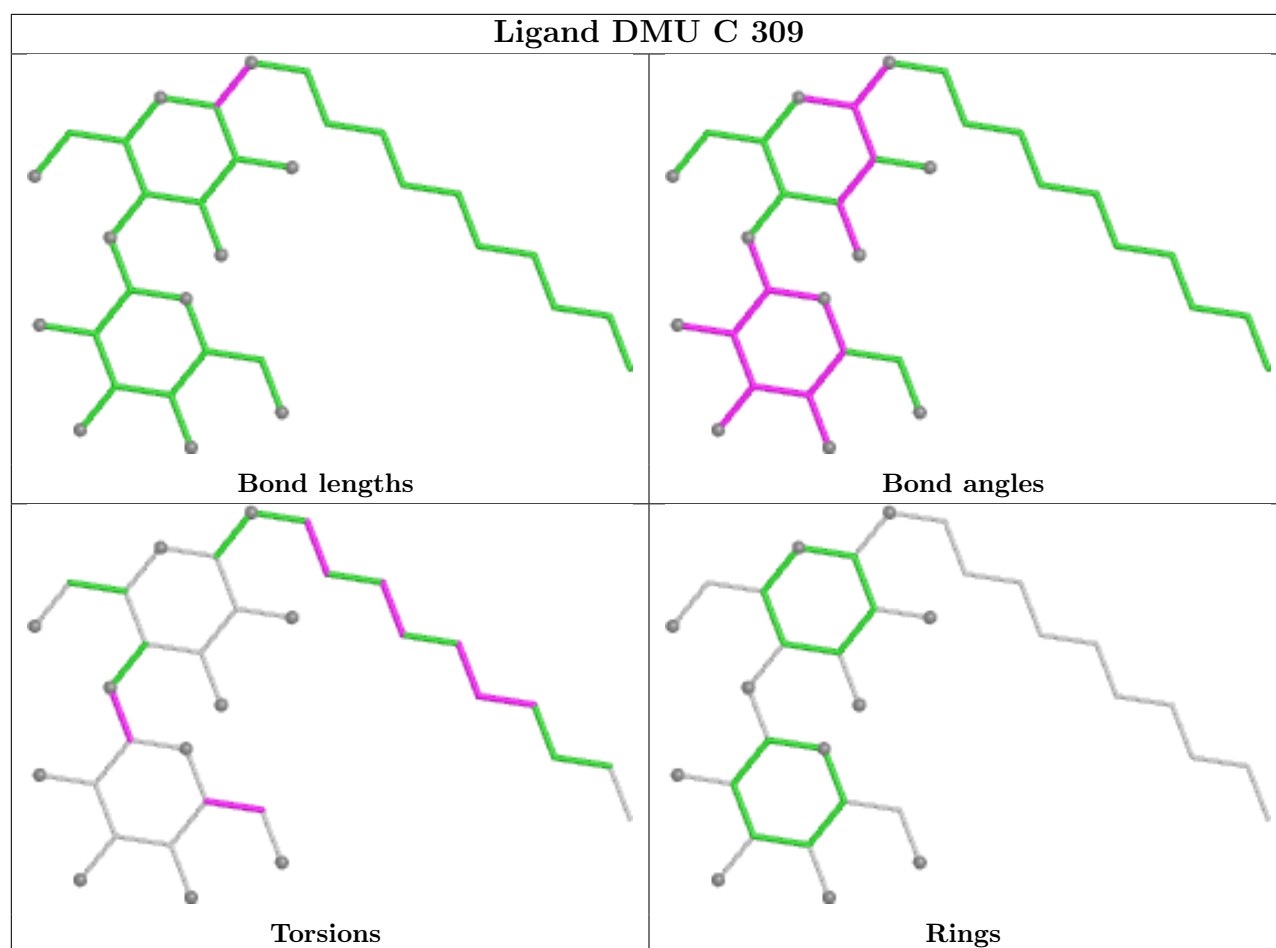




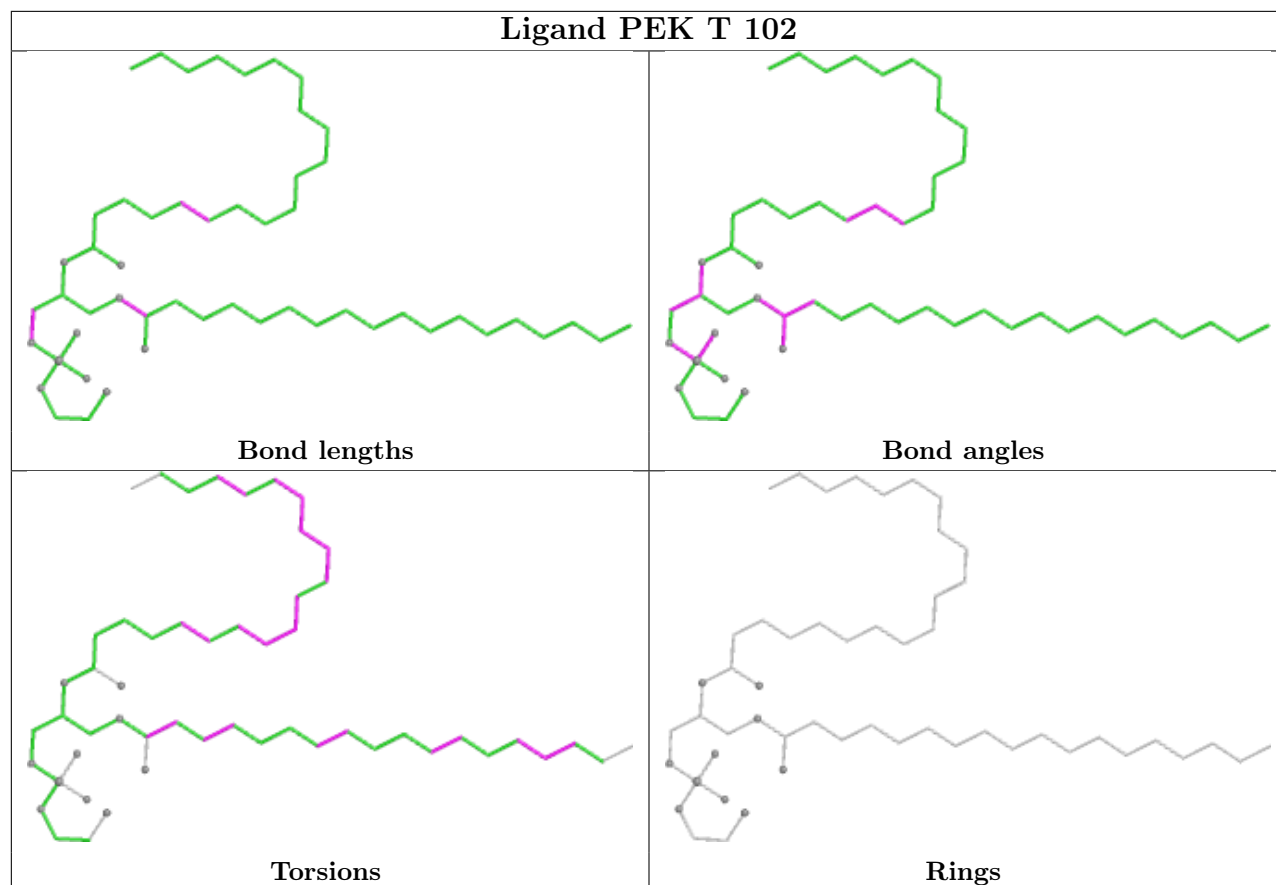




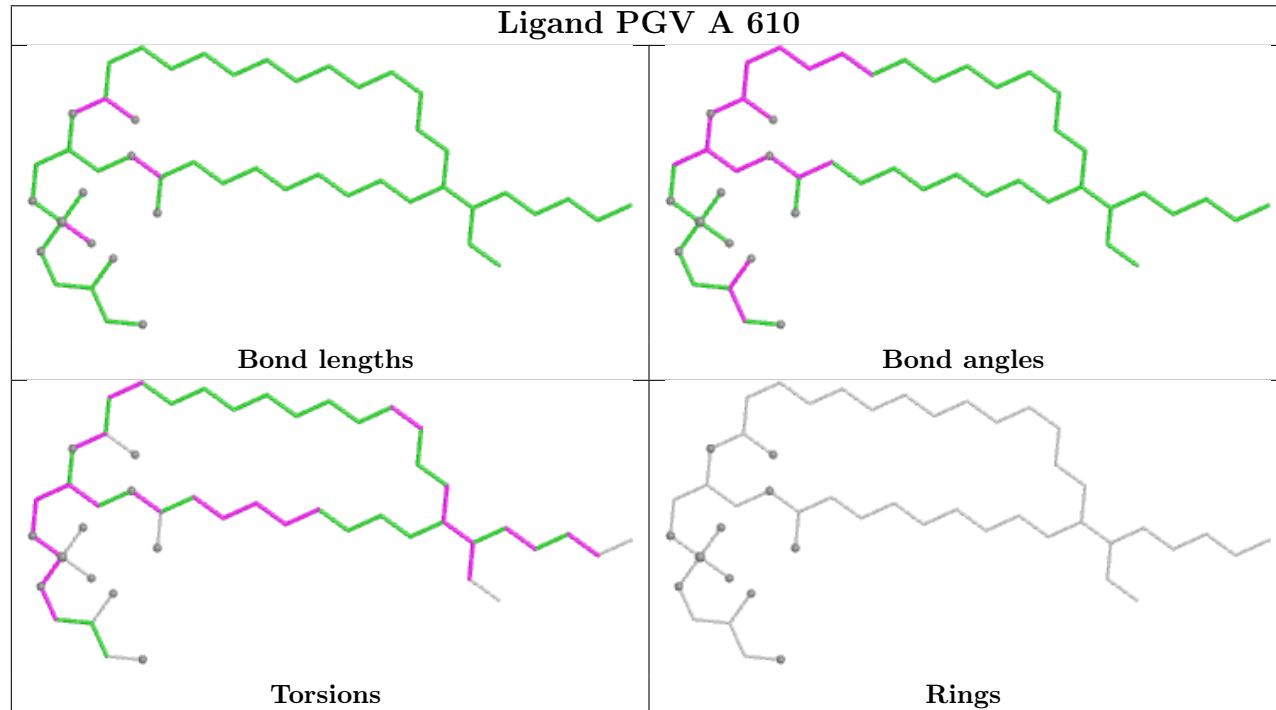


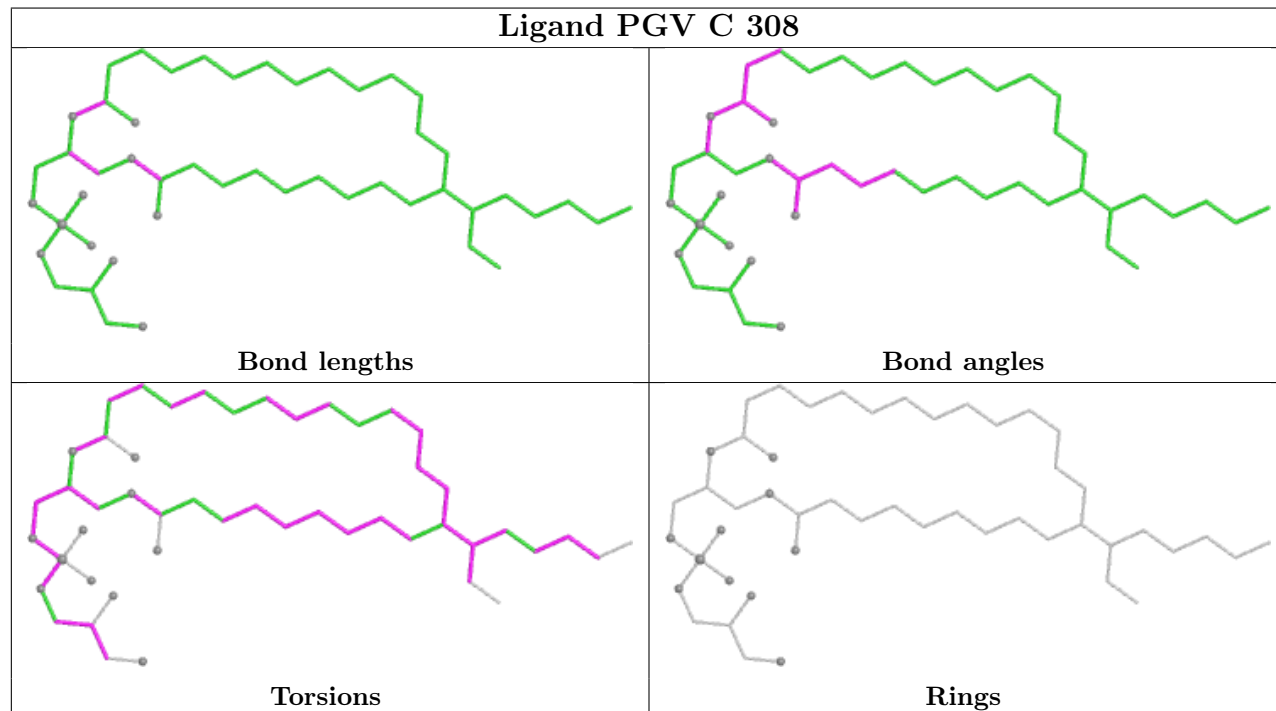
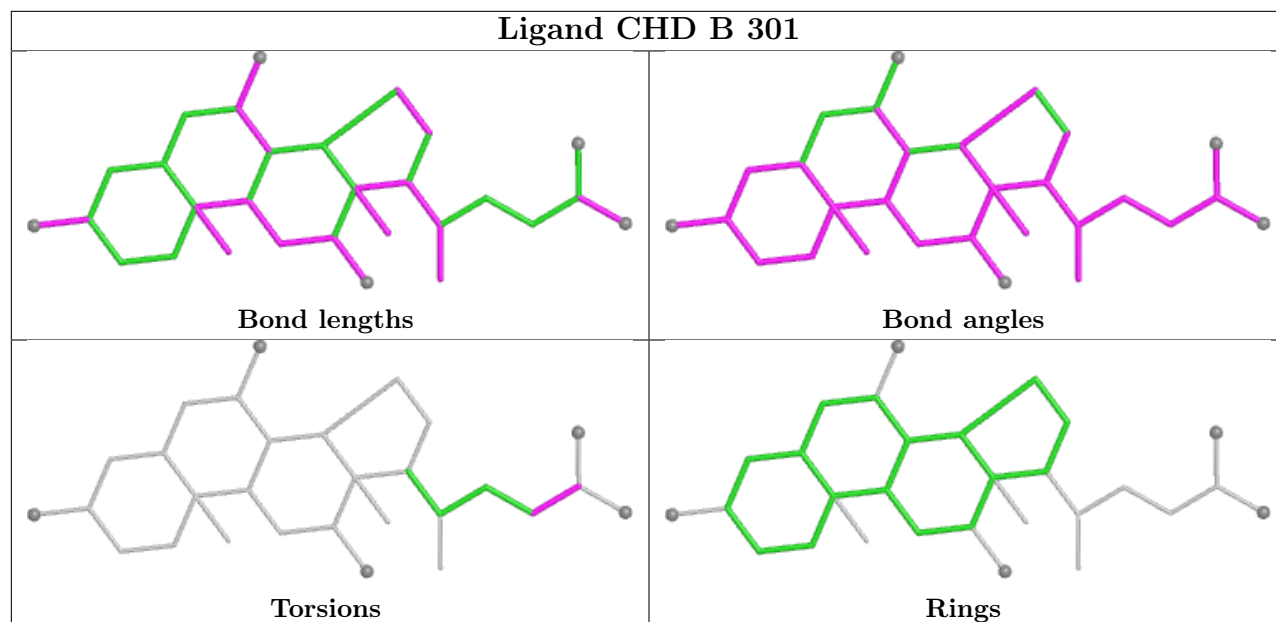


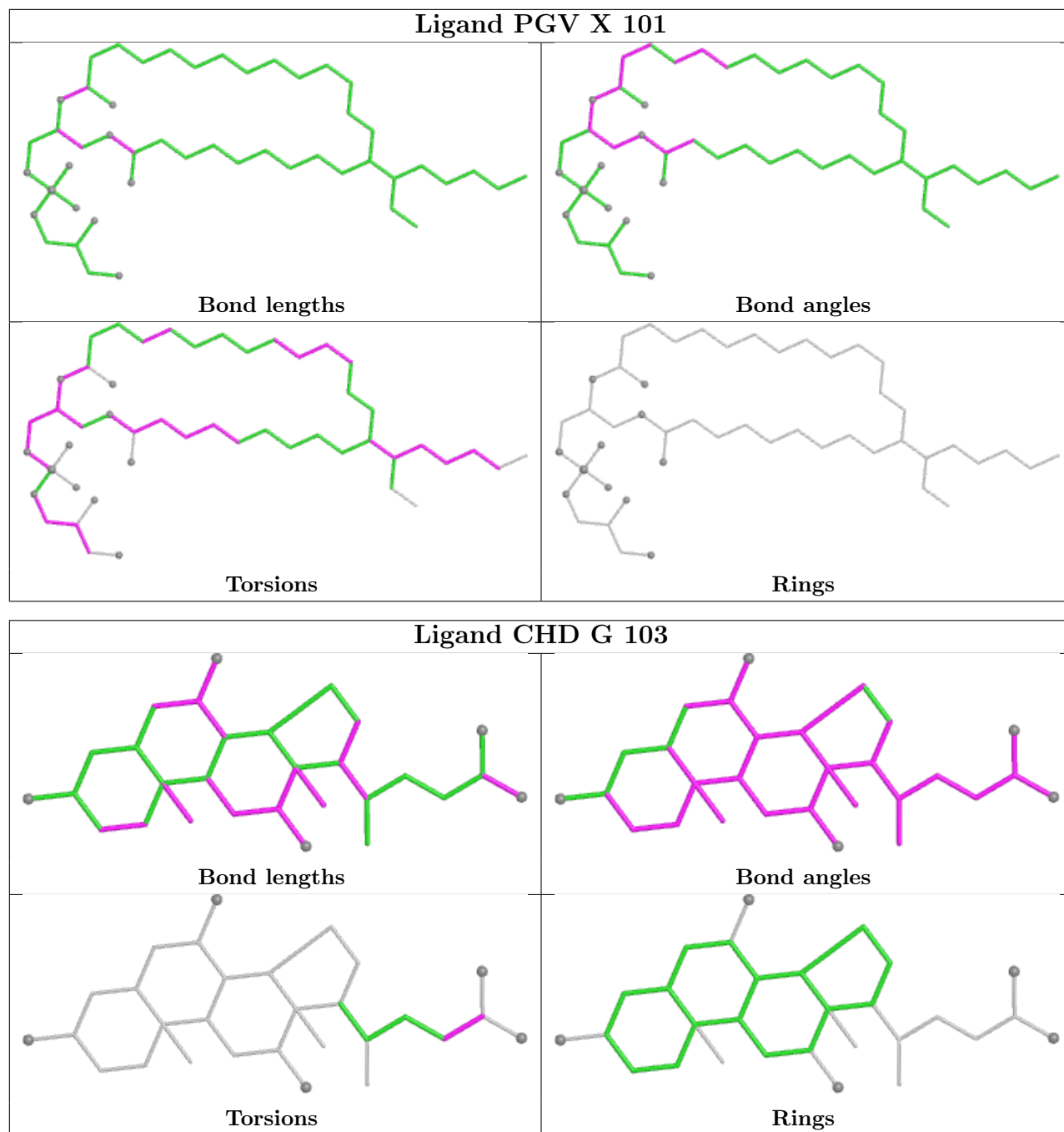
Ligand PEK T 102

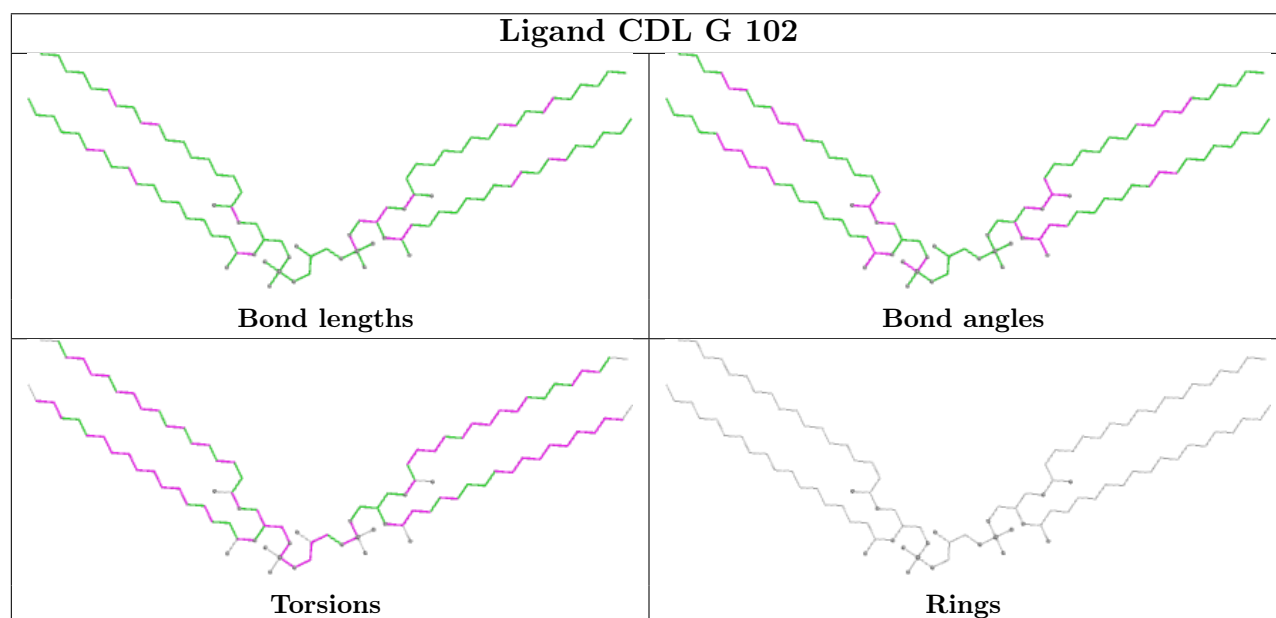
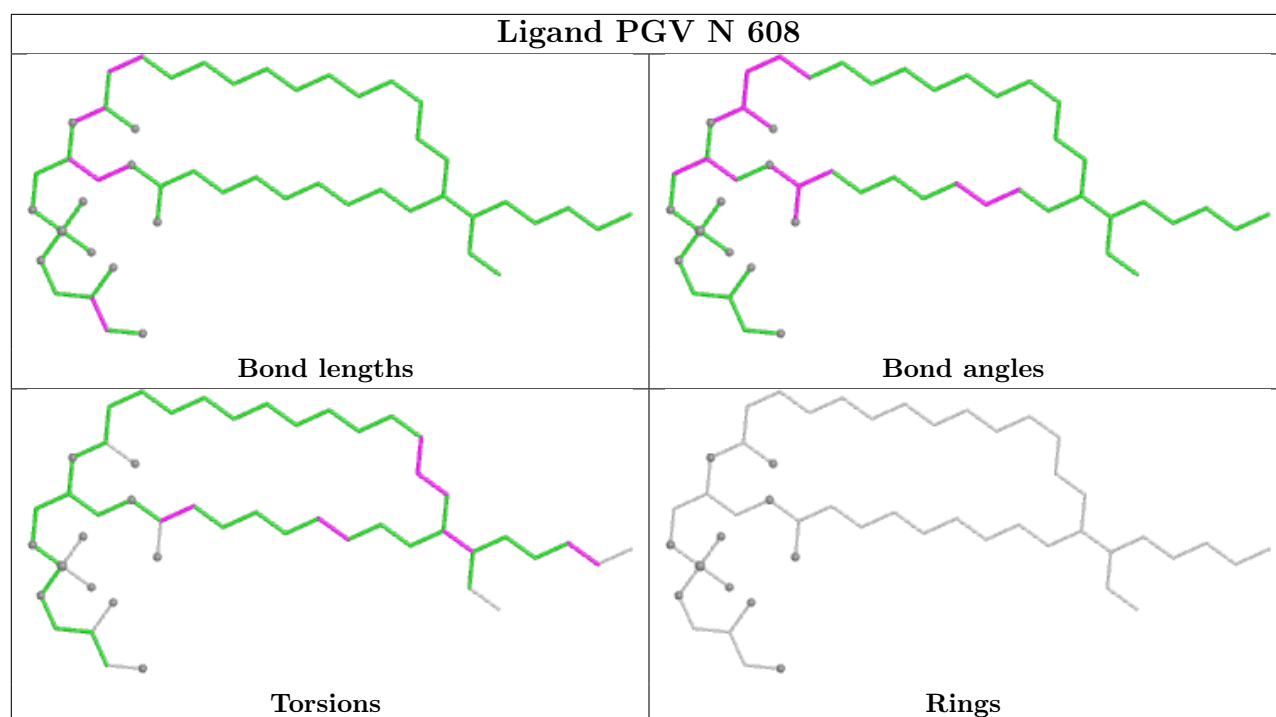


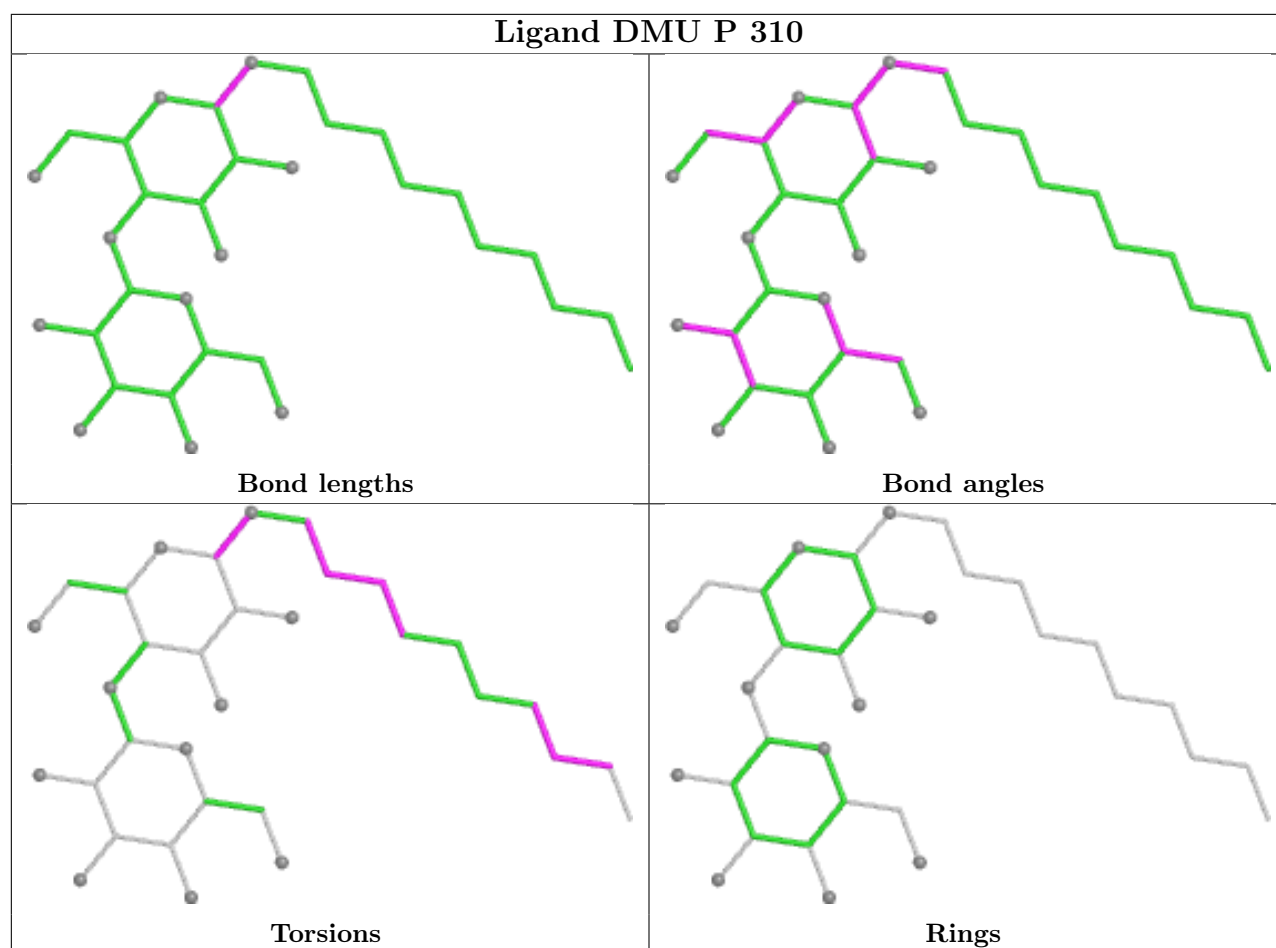
Ligand PGV A 610



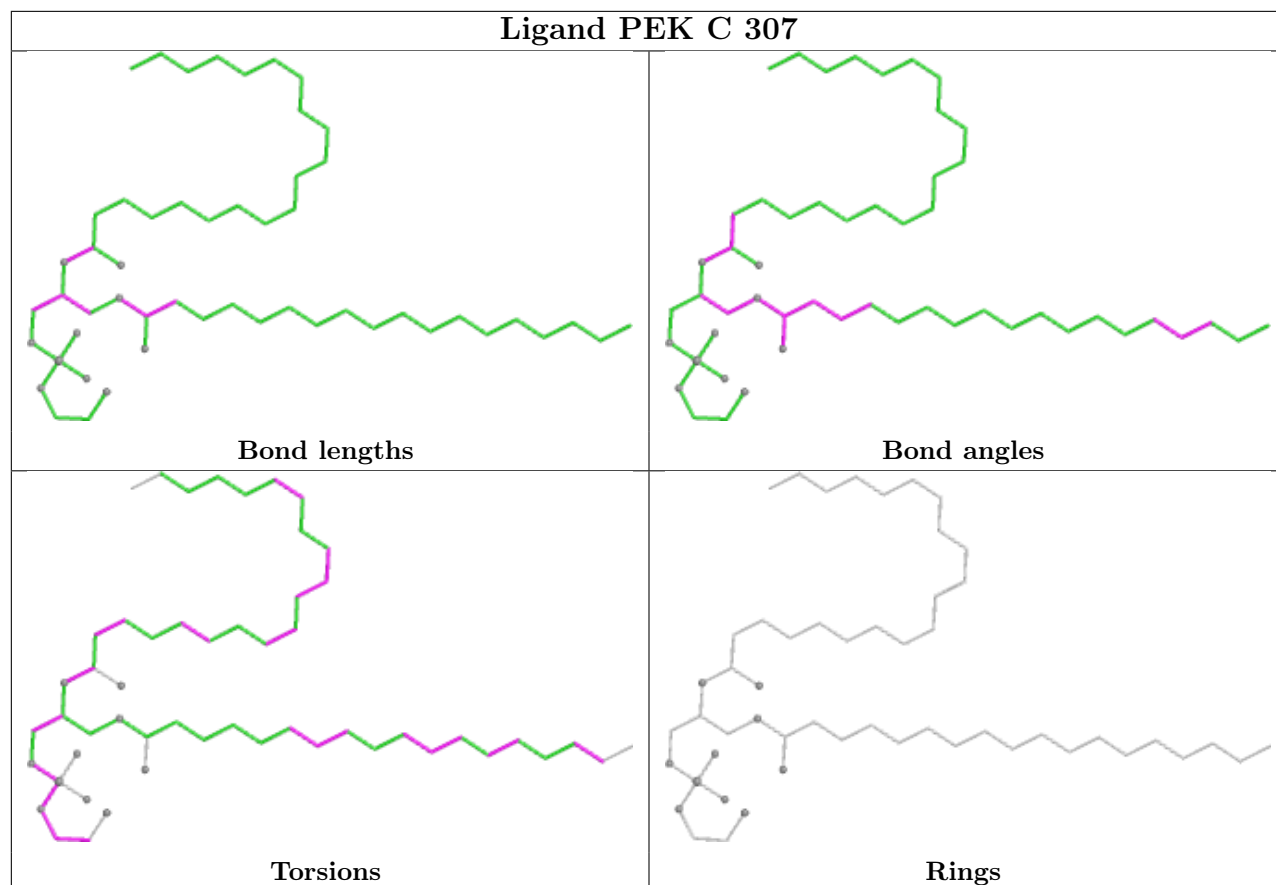




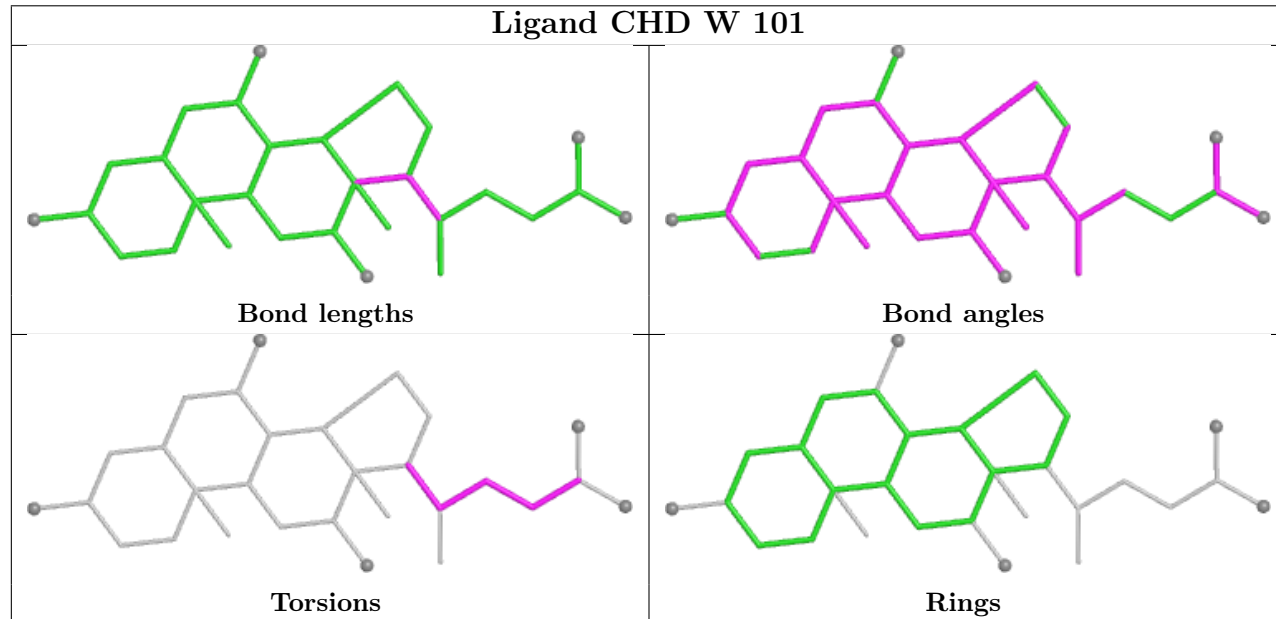


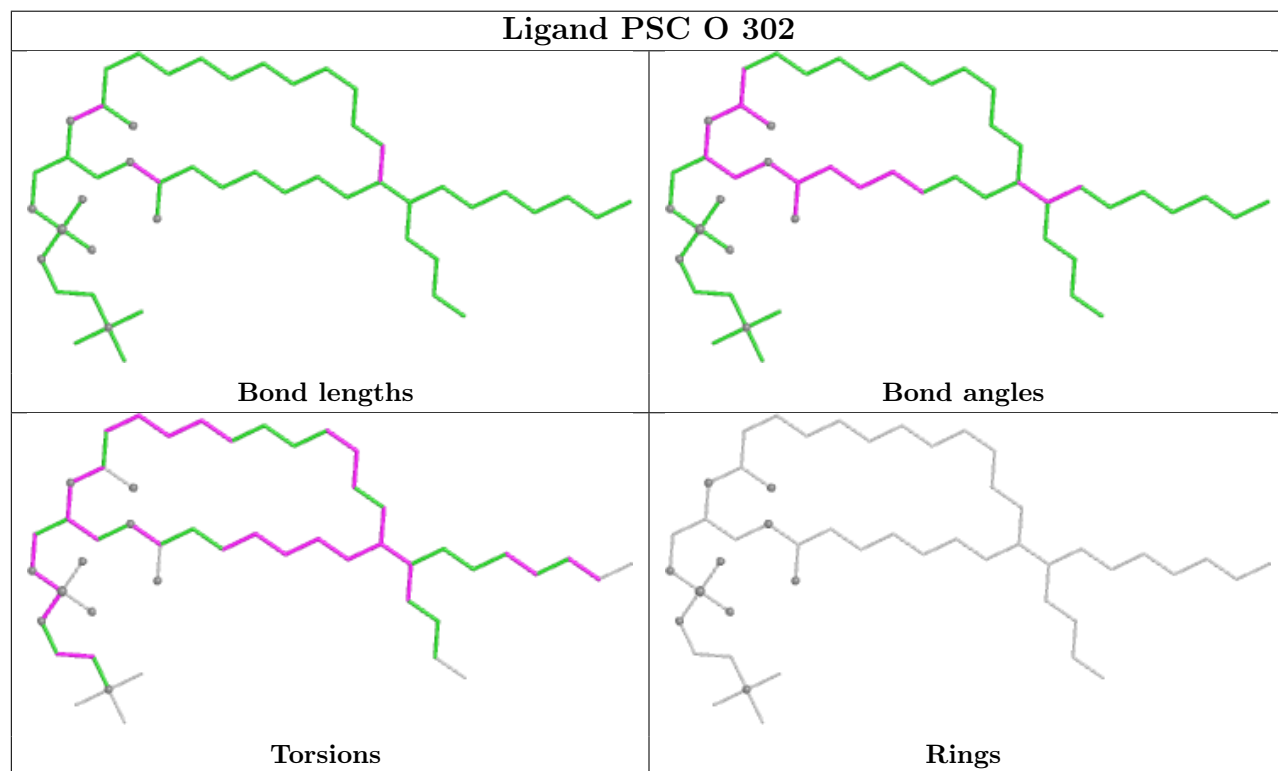
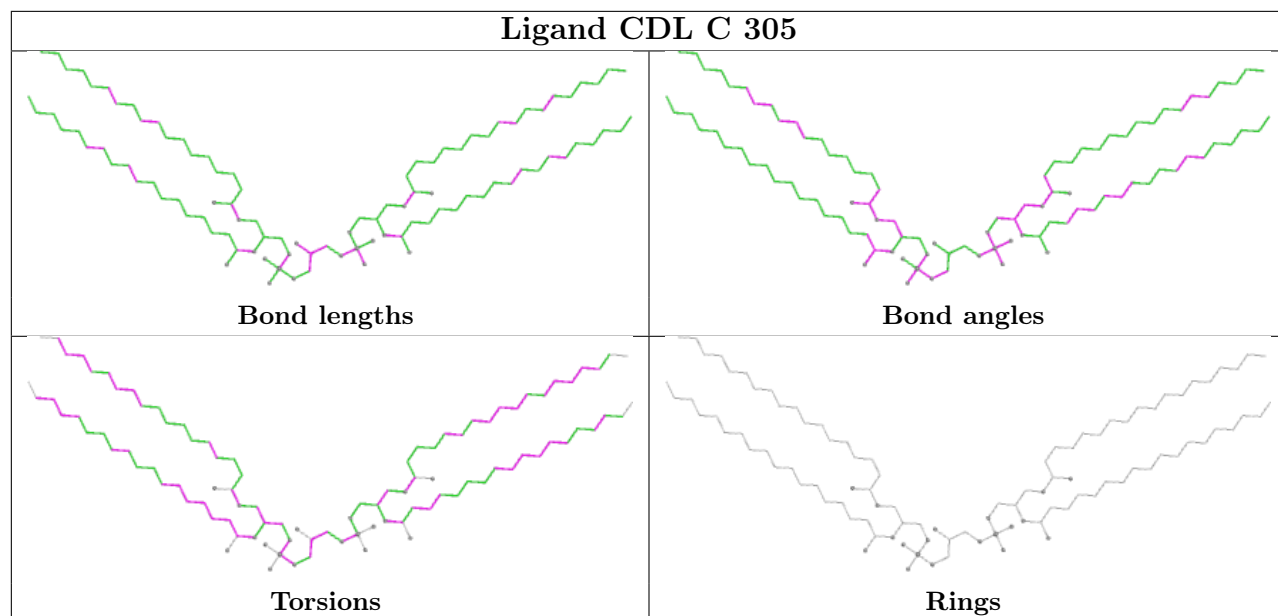


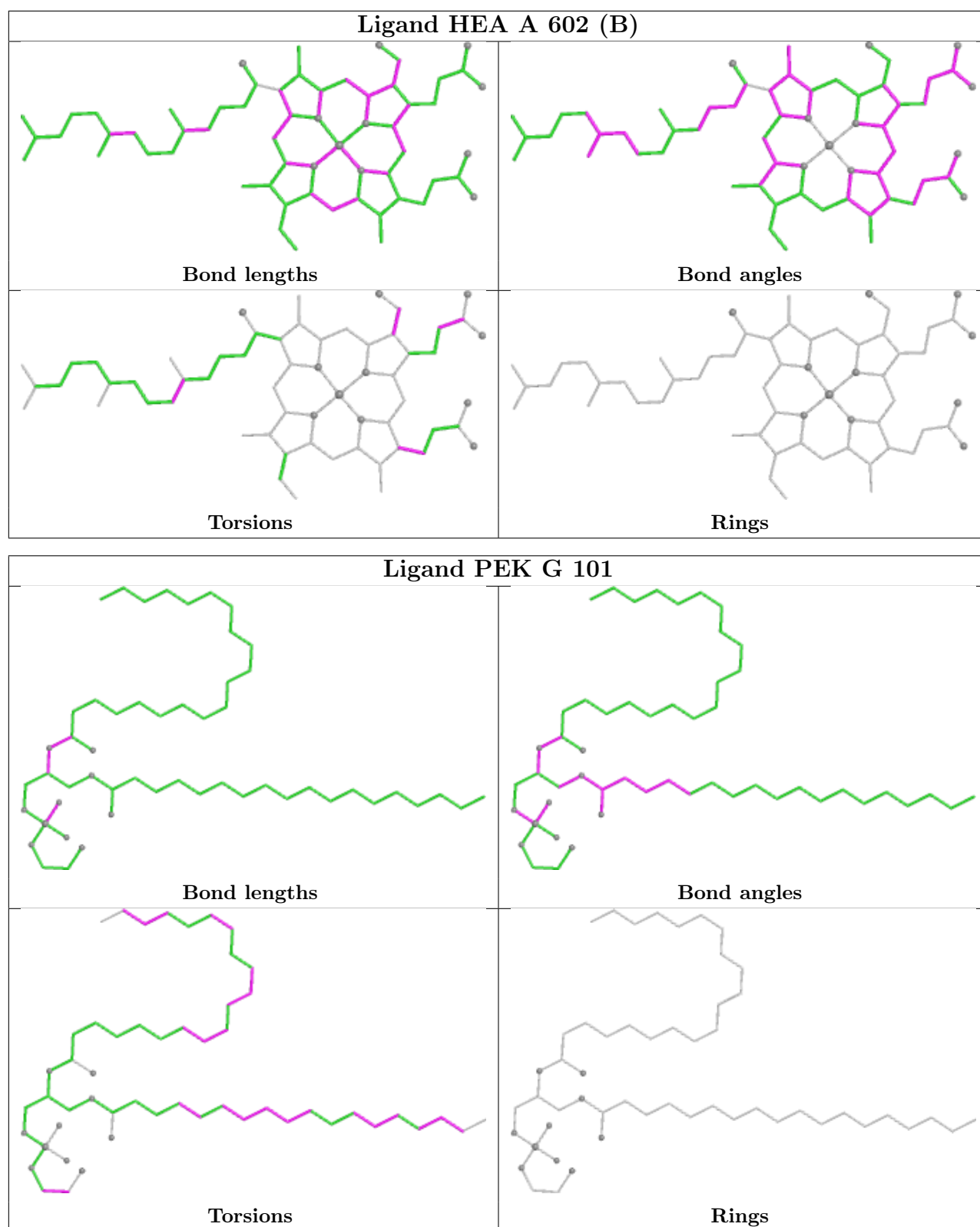
Ligand PEK C 307

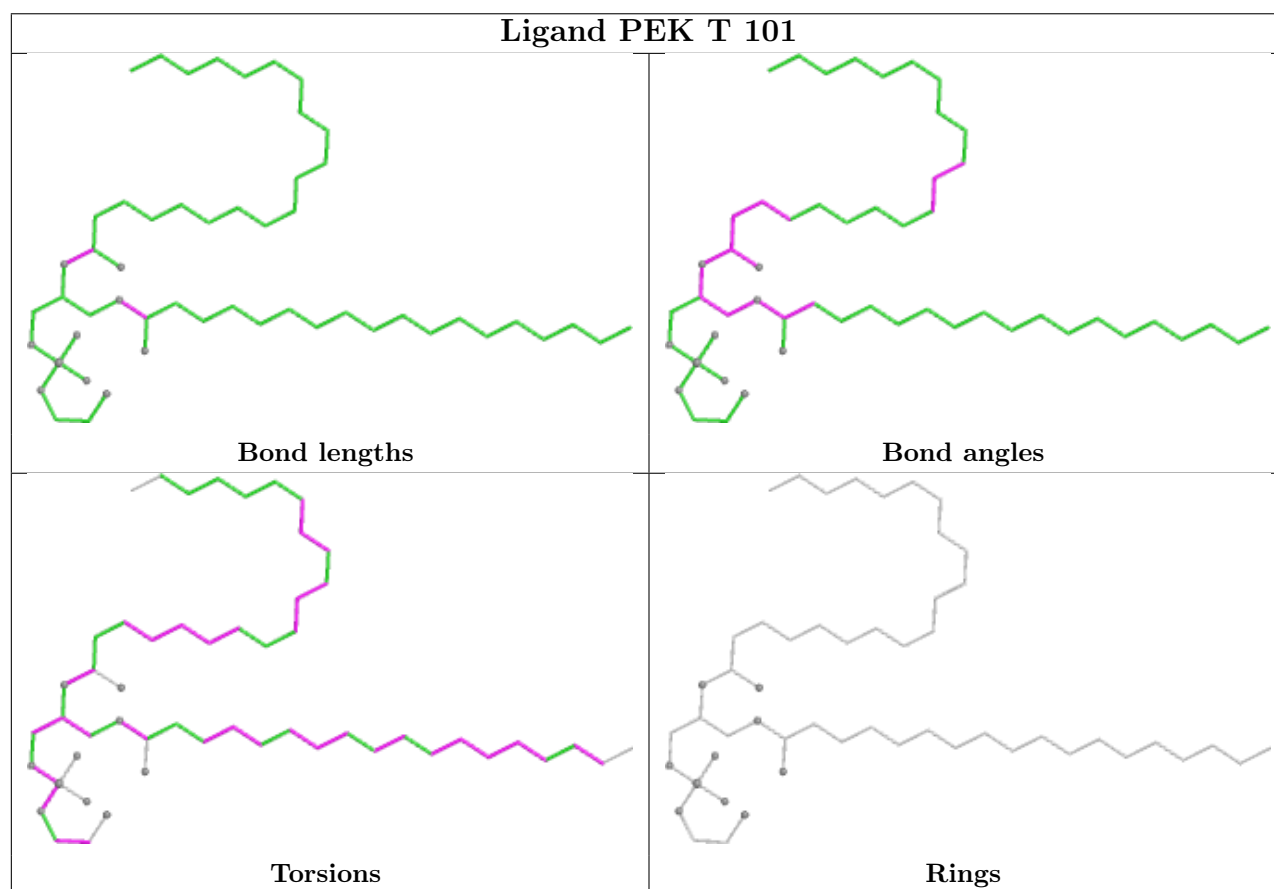
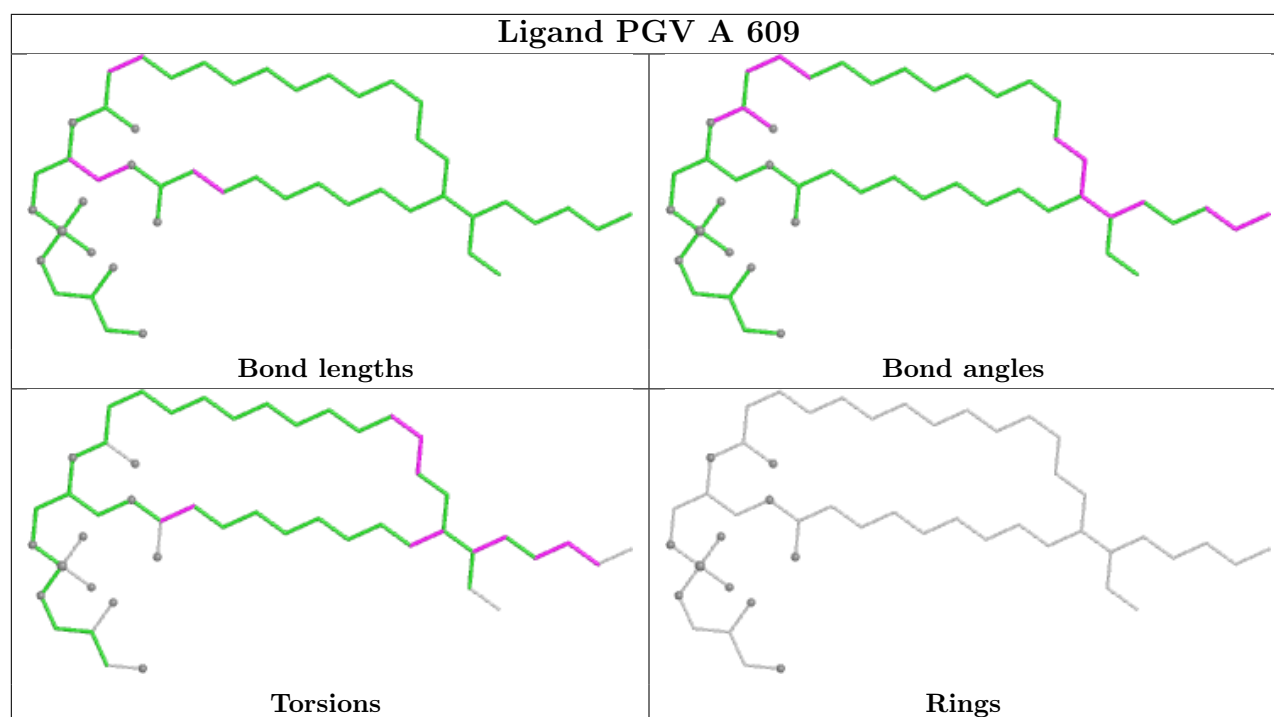


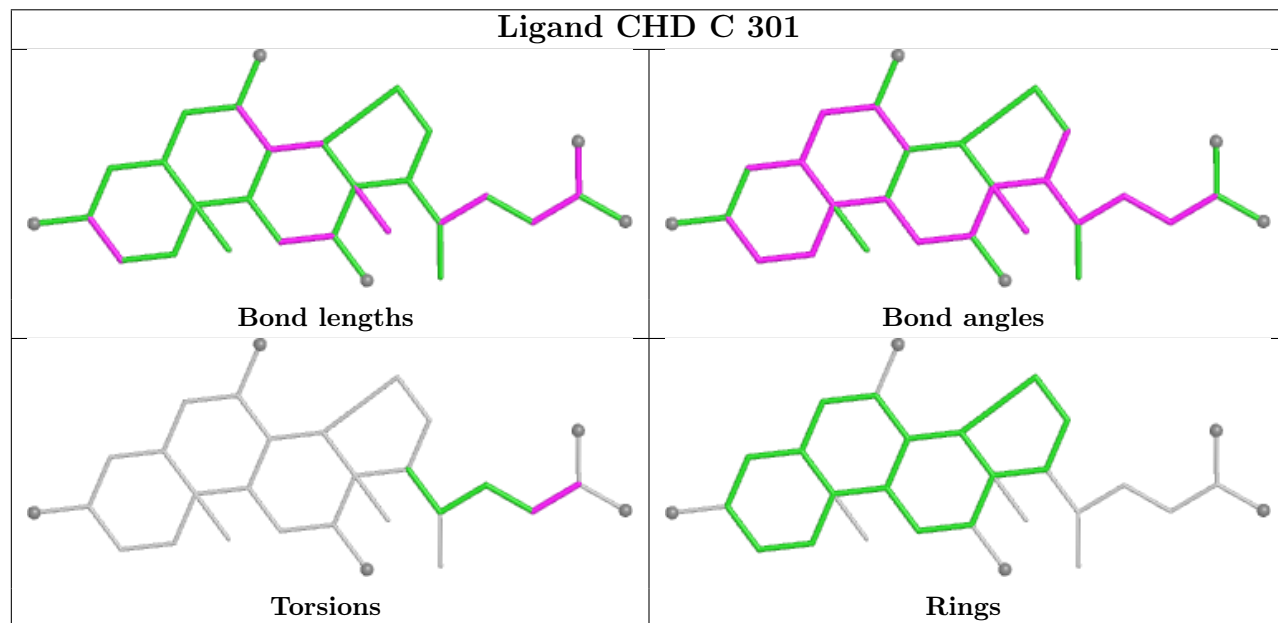
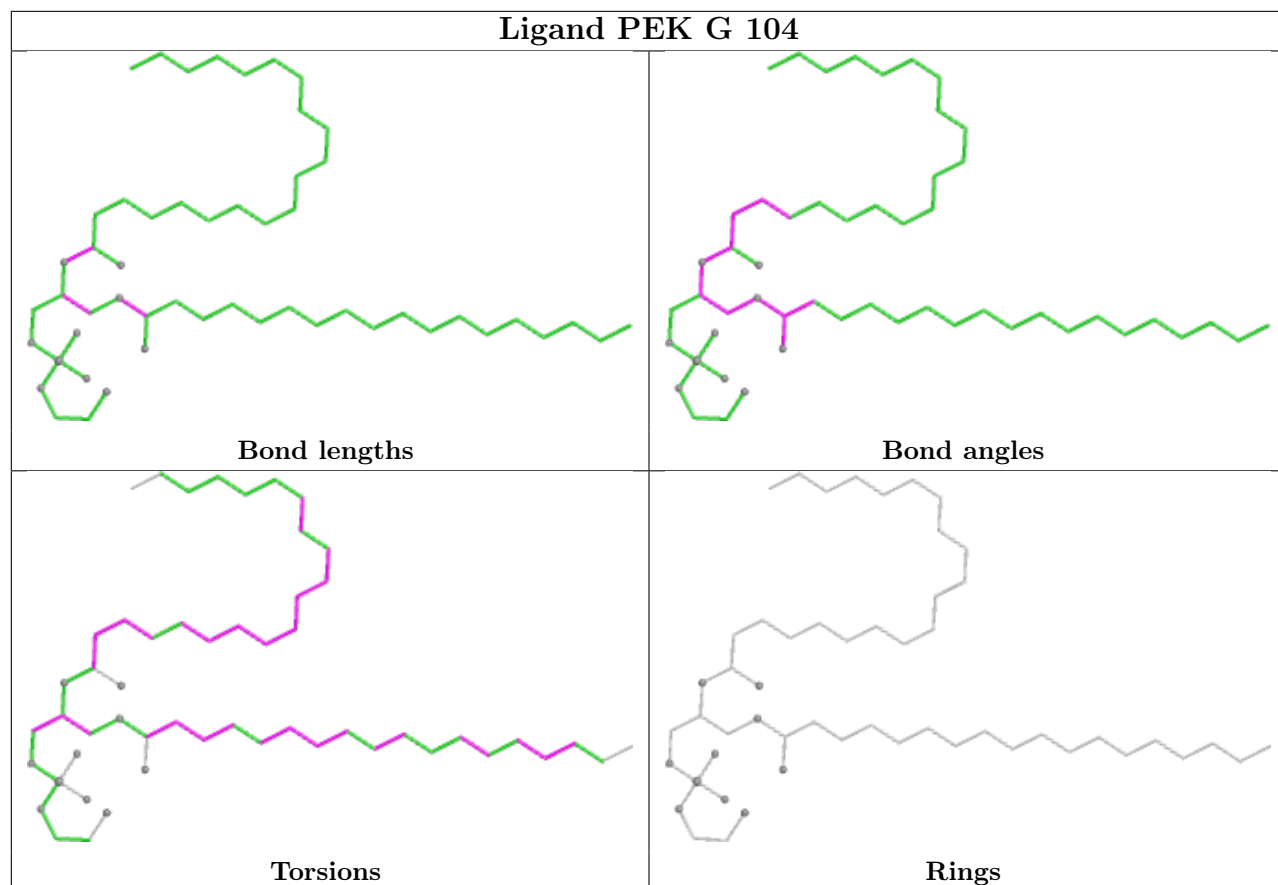
Ligand CHD W 101

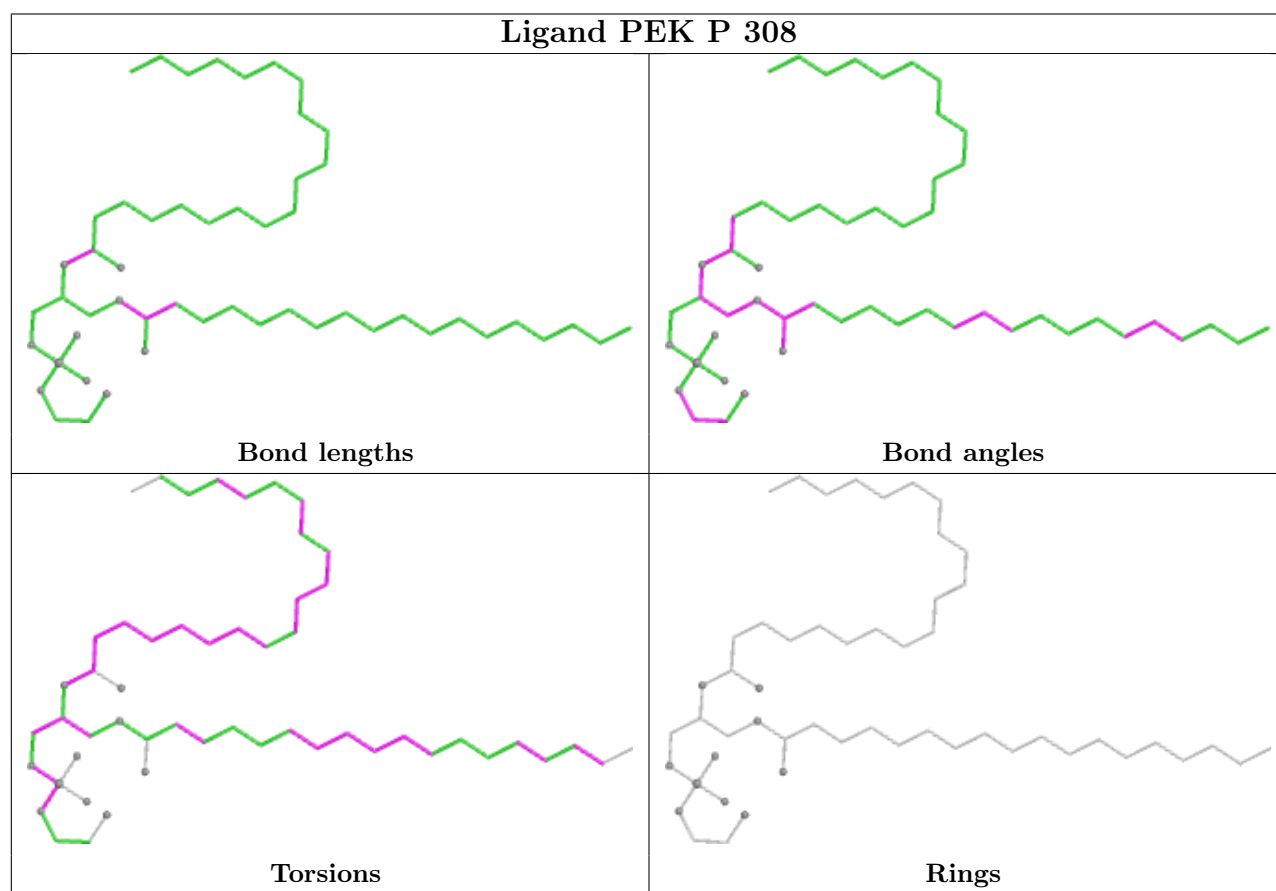
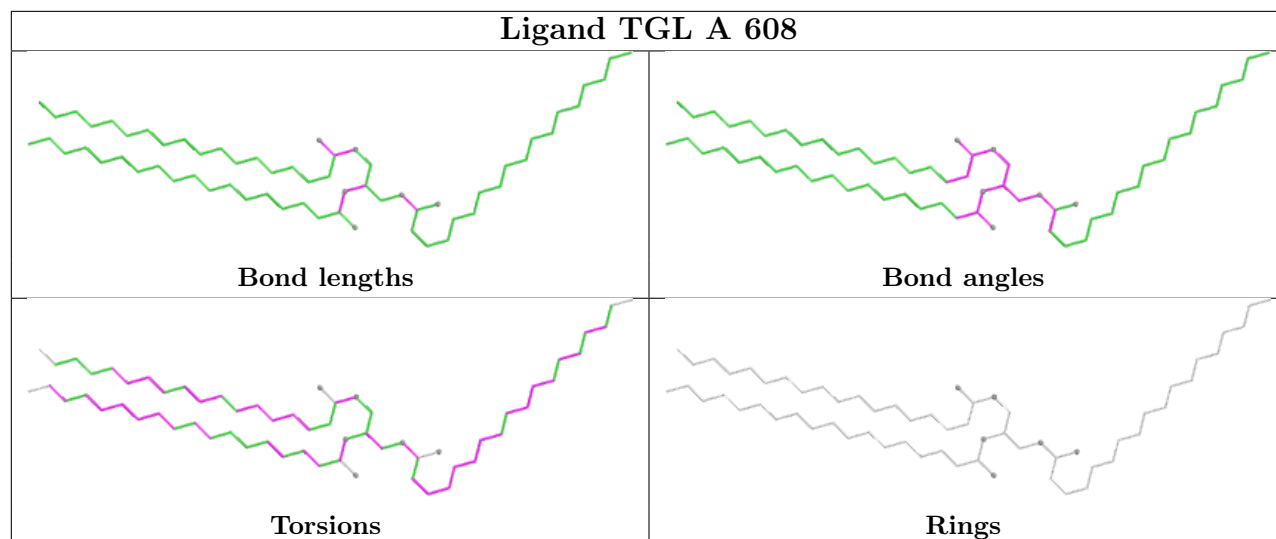


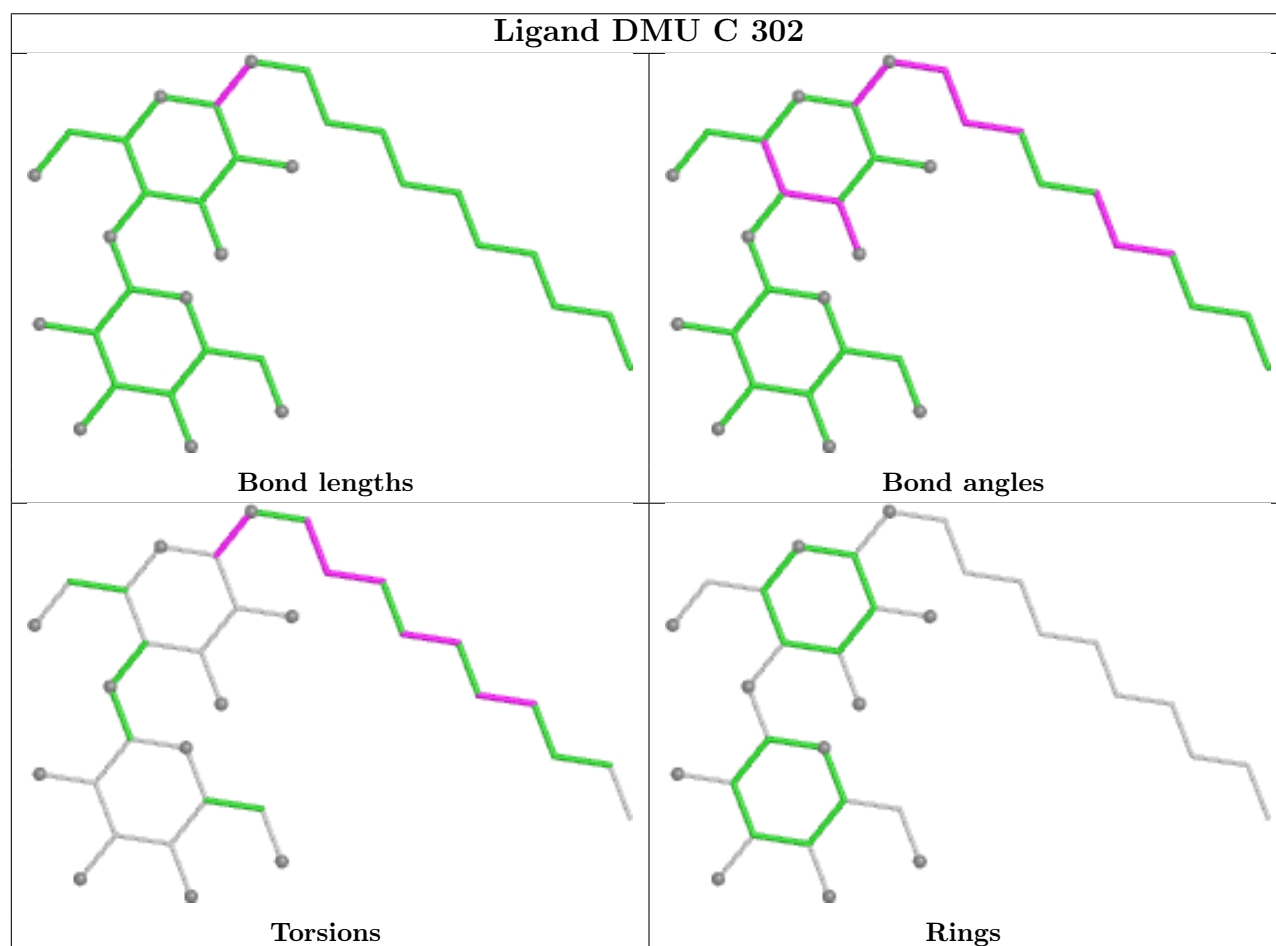
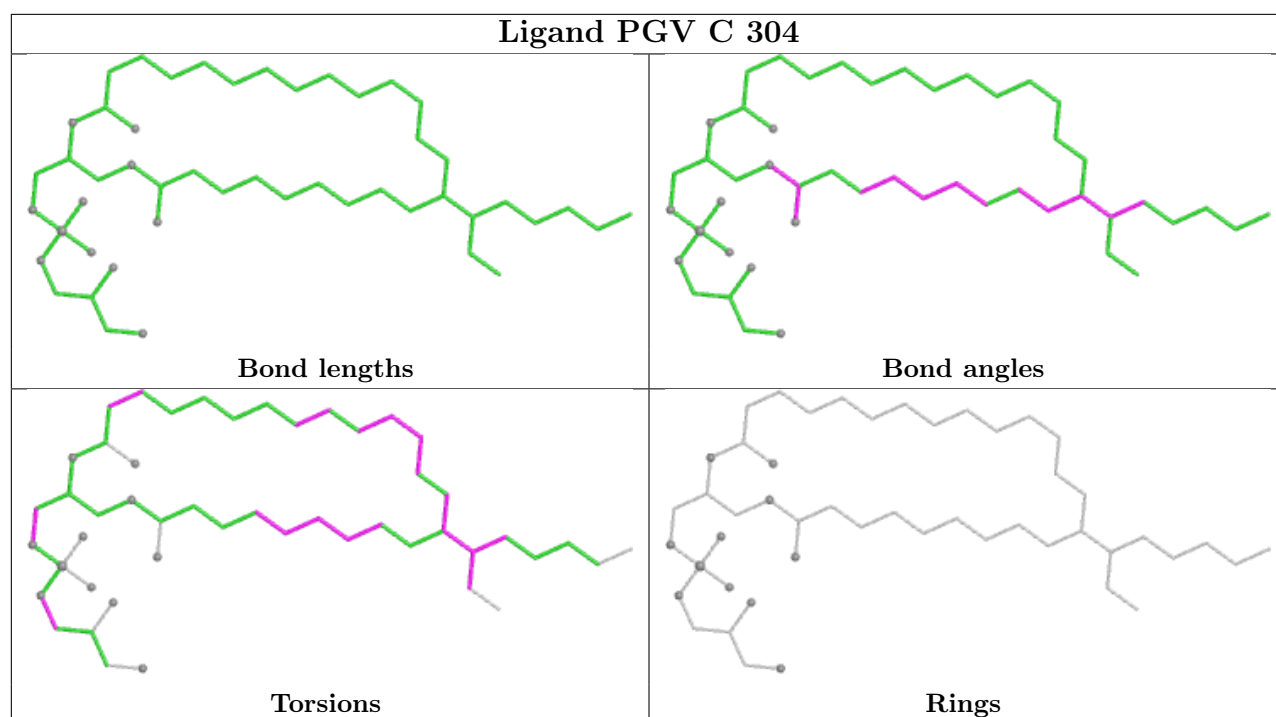


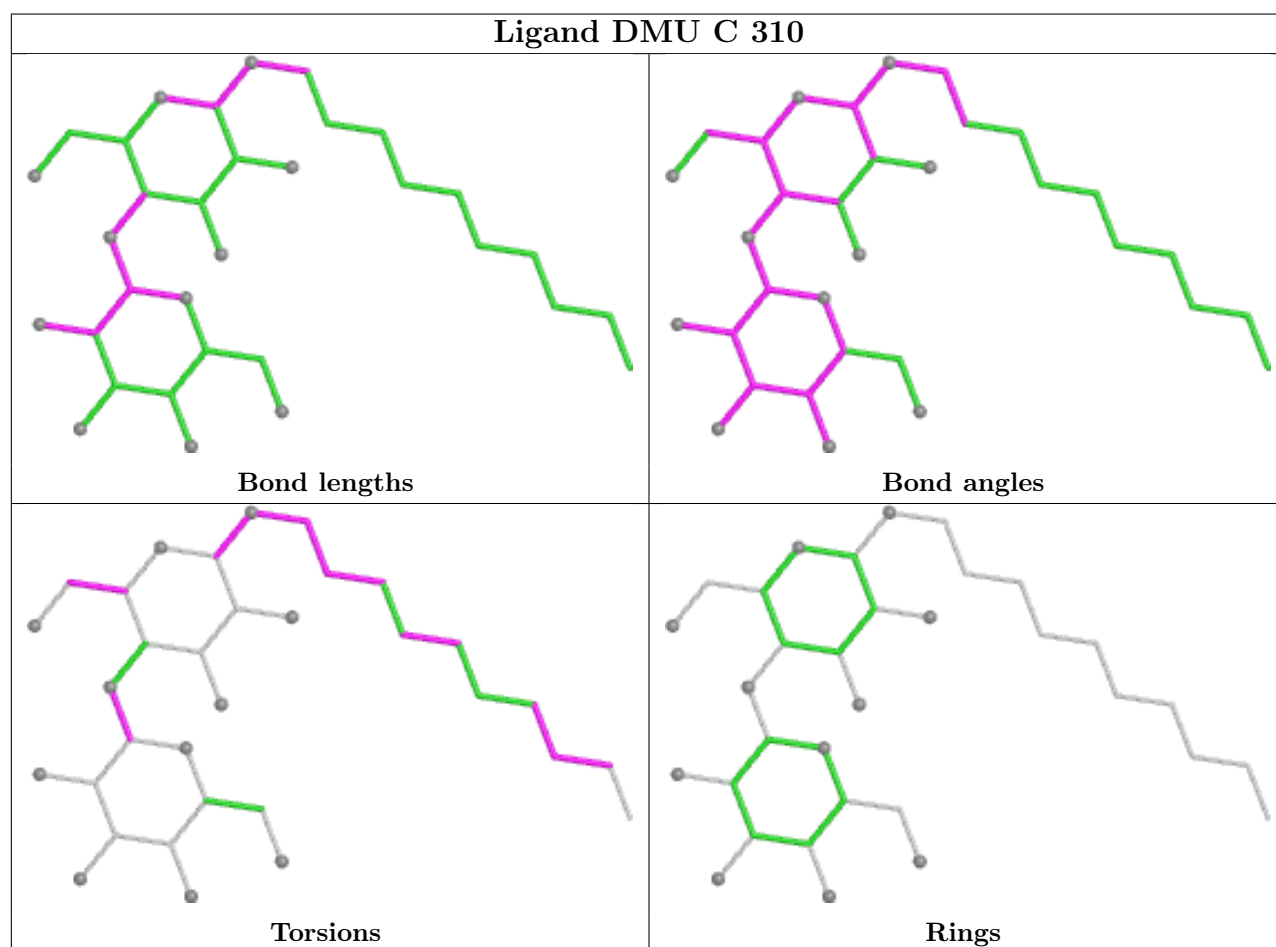
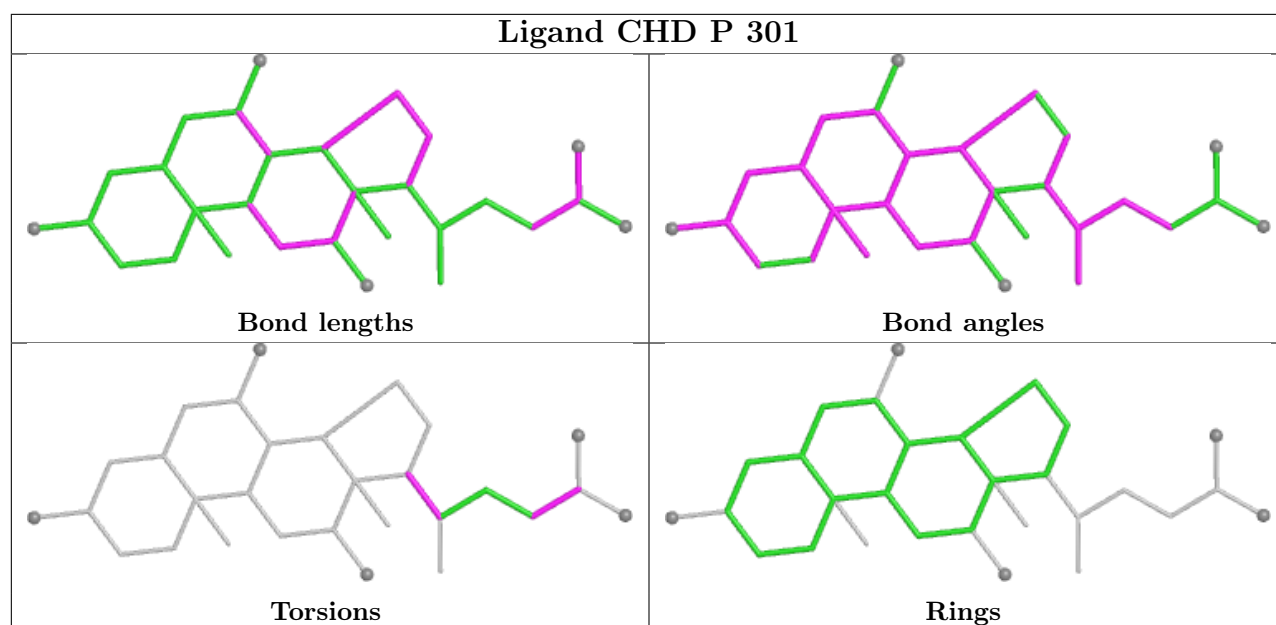


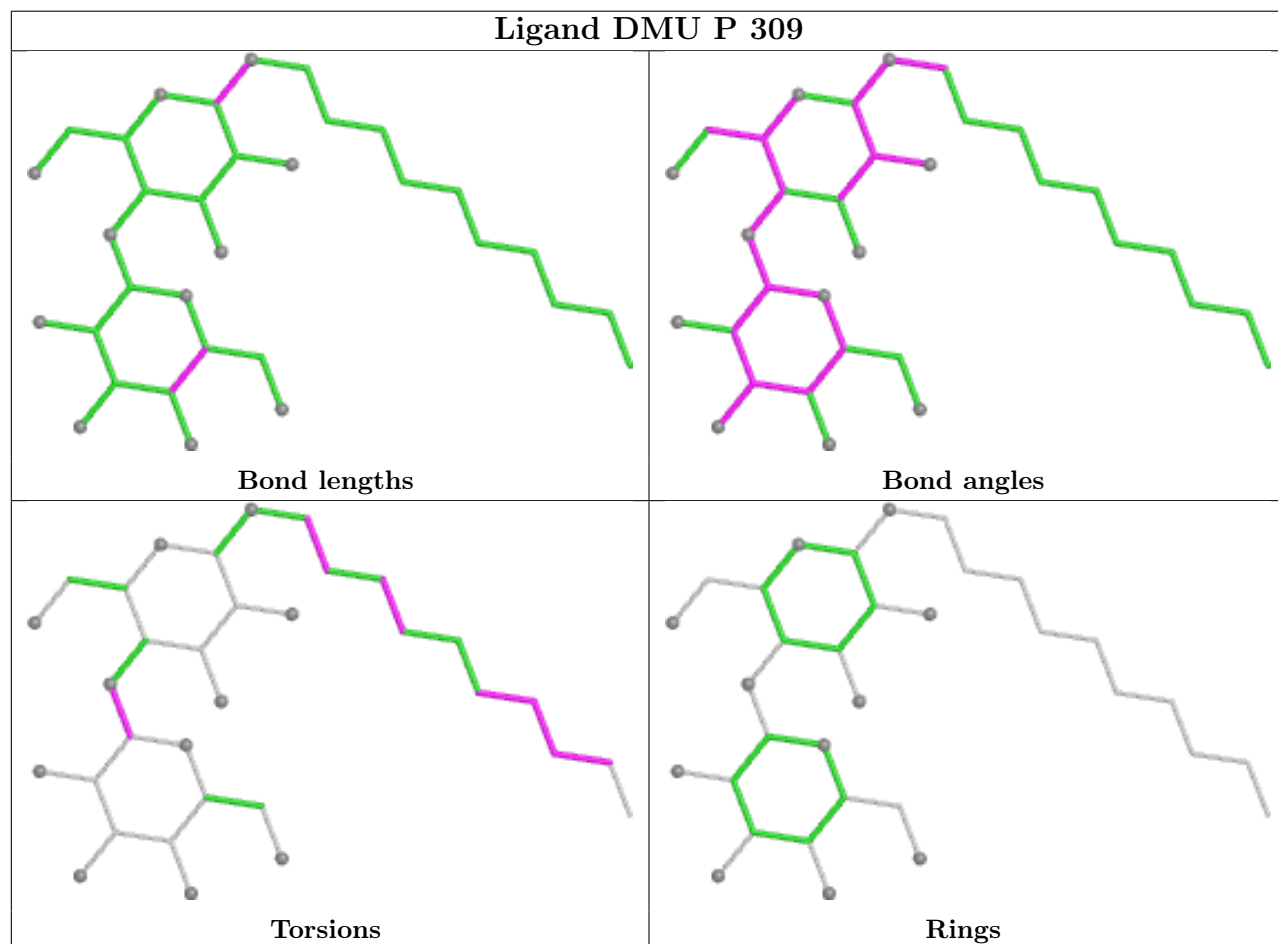
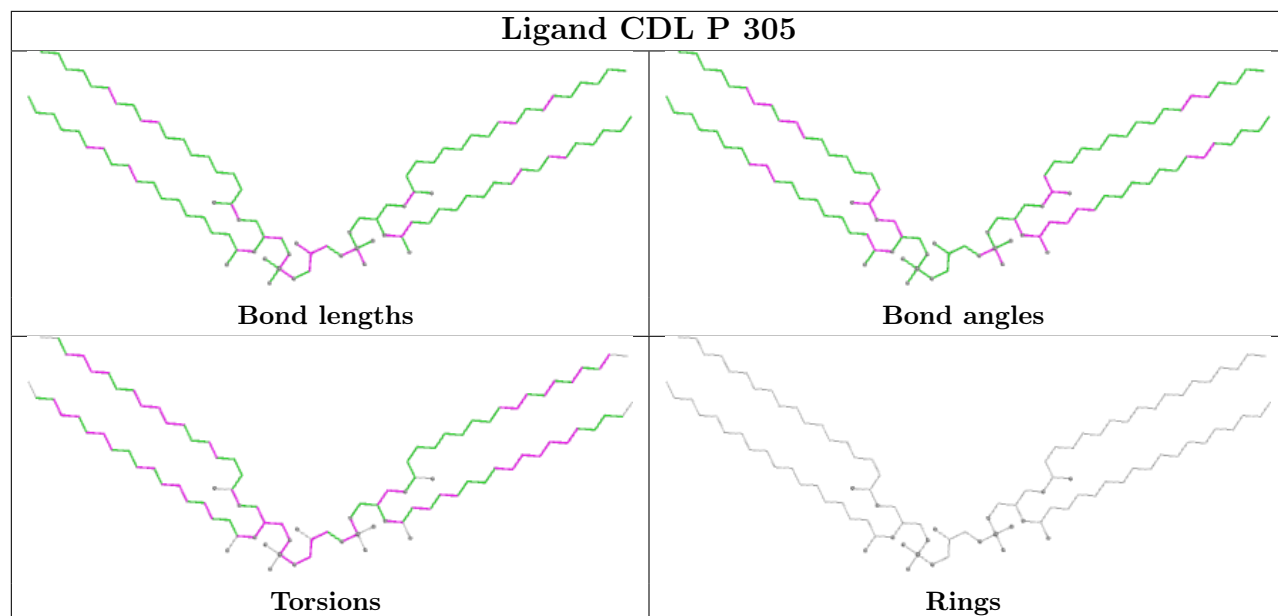


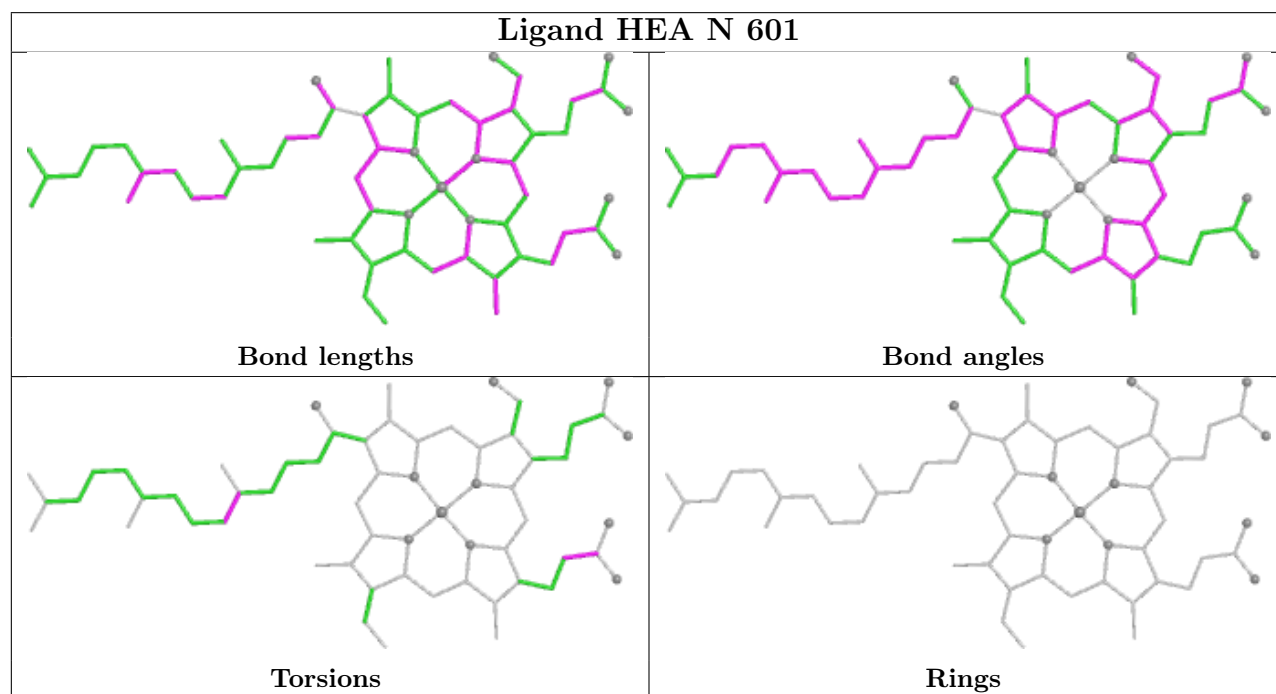
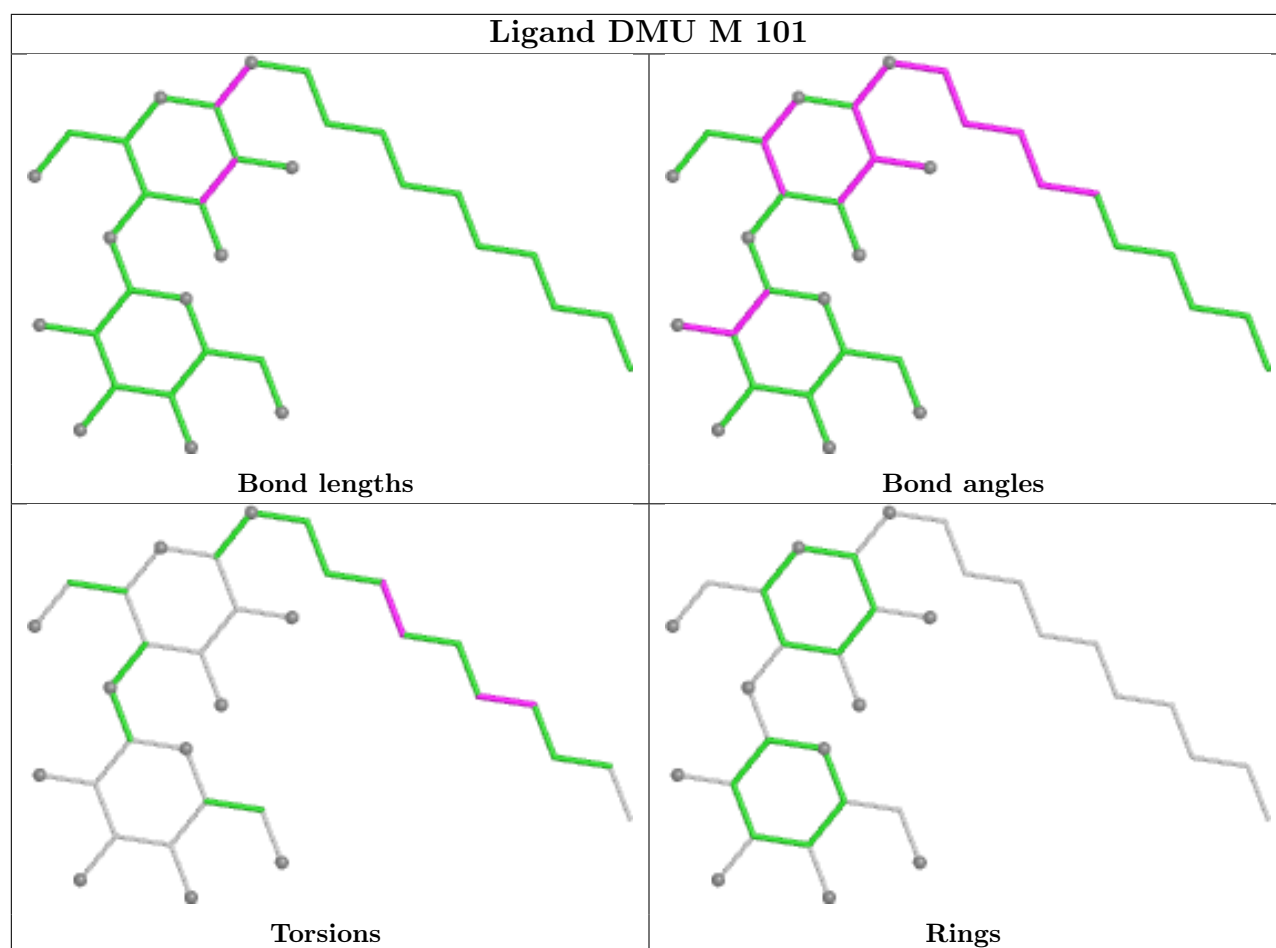


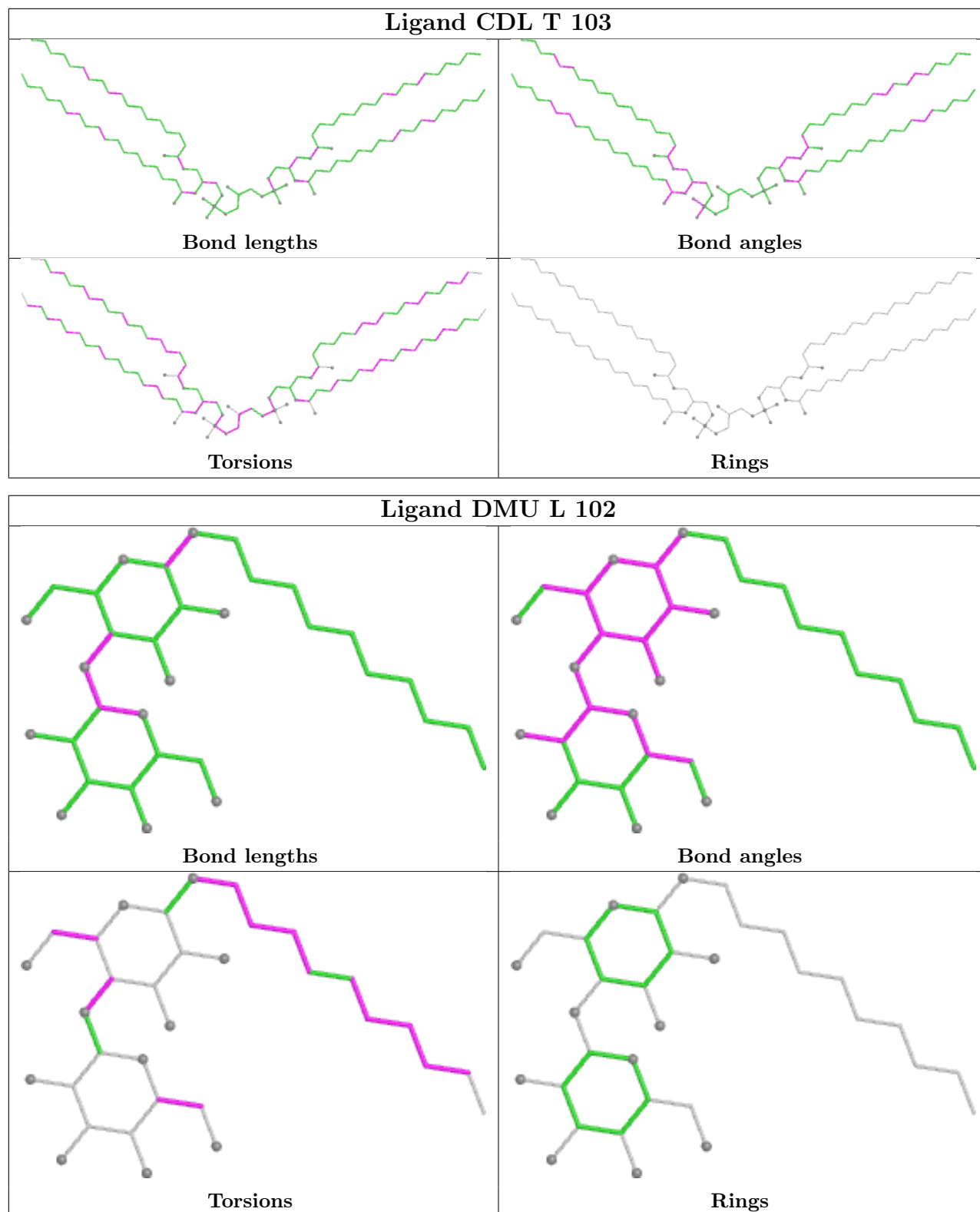












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.47	3 (0%) 85 90	11, 23, 30, 69	22 (4%)
1	N	513/514 (99%)	-0.25	5 (0%) 79 84	12, 27, 36, 68	20 (3%)
2	B	226/227 (99%)	0.21	16 (7%) 22 25	16, 29, 48, 64	10 (4%)
2	O	226/227 (99%)	0.44	15 (6%) 24 27	19, 37, 59, 78	5 (2%)
3	C	259/261 (99%)	-0.18	6 (2%) 61 66	11, 26, 38, 74	7 (2%)
3	P	259/261 (99%)	-0.11	5 (1%) 66 71	11, 28, 38, 57	9 (3%)
4	D	144/147 (97%)	0.11	6 (4%) 40 44	14, 31, 46, 73	5 (3%)
4	Q	144/147 (97%)	0.87	16 (11%) 10 11	18, 44, 69, 141	3 (2%)
5	E	105/109 (96%)	0.04	3 (2%) 53 58	24, 31, 53, 103	0
5	R	105/109 (96%)	0.29	2 (1%) 66 71	28, 38, 57, 103	0
6	F	98/98 (100%)	0.72	12 (12%) 8 9	15, 33, 88, 139	3 (3%)
6	S	98/98 (100%)	0.78	11 (11%) 10 11	16, 33, 84, 114	2 (2%)
7	G	83/85 (97%)	1.28	22 (26%) 1 1	15, 34, 100, 127	1 (1%)
7	T	83/85 (97%)	1.40	23 (27%) 1 1	17, 37, 93, 135	1 (1%)
8	H	79/85 (92%)	0.83	14 (17%) 4 4	27, 37, 83, 101	0
8	U	79/85 (92%)	0.94	12 (15%) 5 5	34, 42, 93, 103	0
9	I	72/73 (98%)	1.29	19 (26%) 1 1	28, 40, 75, 85	0
9	V	72/73 (98%)	1.26	15 (20%) 2 3	28, 51, 74, 90	0
10	J	58/59 (98%)	0.67	5 (8%) 16 18	26, 36, 63, 99	0
10	W	58/59 (98%)	0.94	6 (10%) 12 12	20, 39, 68, 115	1 (1%)
11	K	49/56 (87%)	0.58	3 (6%) 27 30	30, 37, 50, 57	0
11	X	49/56 (87%)	1.06	8 (16%) 4 5	21, 46, 65, 76	1 (2%)
12	L	46/47 (97%)	0.29	4 (8%) 16 17	24, 29, 47, 83	0
12	Y	46/47 (97%)	0.55	3 (6%) 25 28	20, 36, 55, 104	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.47	4 (9%) 14 15	26, 29, 61, 107	0
13	Z	43/46 (93%)	0.86	6 (13%) 6 7	33, 40, 75, 116	0
All	All	3550/3614 (98%)	0.24	244 (6%) 23 26	11, 31, 61, 141	91 (2%)

The worst 5 of 244 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	1	ALA	14.4
6	S	97	ALA	10.7
6	S	96	LEU	10.3
6	S	94	HIS	9.5
8	U	8	ILE	8.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.38	0.27	107,118,124,126	0
7	TPO	G	11	11/12	0.58	0.28	84,110,125,127	0
7	TPO	T	11	11/12	0.63	0.23	76,101,117,121	0
9	SAC	I	1	9/10	0.75	0.20	59,70,74,74	0
1	FME	A	1	10/11	0.92	0.13	33,43,67,83	0
1	FME	N	1	10/11	0.94	0.12	36,44,71,76	0
2	FME	B	1	10/11	0.95	0.12	20,28,45,61	0
2	FME	O	1	10/11	0.97	0.08	36,36,43,57	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	F	103	4/4	0.65	0.33	52,76,77,81	0
22	CHD	J	101	29/29	0.66	0.30	50,112,133,141	0
22	CHD	W	101	29/29	0.68	0.26	58,114,135,143	0
20	PGV	C	308	51/51	0.71	0.25	42,72,109,132	0
28	PEK	T	101	53/53	0.73	0.23	43,93,153,154	0
25	DMU	P	309	33/33	0.74	0.18	53,72,93,94	0
28	PEK	G	104	53/53	0.74	0.26	44,88,153,155	0
24	PSC	B	303	52/52	0.74	0.28	31,74,150,157	0
19	TGL	Q	201	63/63	0.75	0.27	47,72,92,103	0
27	CDL	T	103	100/100	0.76	0.23	51,84,123,146	0
25	DMU	C	310	33/33	0.76	0.21	46,72,105,111	0
27	CDL	P	305	100/100	0.76	0.26	35,80,118,122	0
25	DMU	C	309	33/33	0.77	0.18	51,70,95,98	0
28	PEK	C	307	53/53	0.77	0.23	39,79,139,146	0
27	CDL	G	102	100/100	0.77	0.25	49,86,117,152	0
28	PEK	P	308	53/53	0.77	0.23	37,69,131,149	0
20	PGV	P	302	51/51	0.77	0.21	50,77,127,132	0
21	EDO	E	202	4/4	0.78	0.18	39,41,54,60	0
22	CHD	P	306	29/29	0.78	0.18	48,58,64,66	0
20	PGV	X	101	51/51	0.78	0.22	42,70,129,151	0
25	DMU	L	102	33/33	0.78	0.20	47,83,107,120	0
25	DMU	P	310	33/33	0.79	0.18	61,74,92,94	0
19	TGL	N	609	63/63	0.79	0.22	44,70,96,112	0
20	PGV	A	610	51/51	0.80	0.23	30,59,101,112	0
27	CDL	C	305	100/100	0.80	0.22	30,70,103,110	0
19	TGL	Y	101	63/63	0.80	0.25	39,66,108,129	0
22	CHD	C	306	29/29	0.81	0.17	50,61,66,68	0
24	PSC	O	302	52/52	0.81	0.25	39,78,148,161	0
25	DMU	C	302	33/33	0.81	0.19	30,61,103,109	0
19	TGL	L	101	63/63	0.81	0.24	30,58,91,103	0
19	TGL	A	608	63/63	0.82	0.20	33,66,93,101	0
19	TGL	D	201	63/63	0.82	0.21	27,58,80,93	0
21	EDO	C	313	4/4	0.82	0.19	46,58,62,63	0
21	EDO	D	203	4/4	0.82	0.22	45,50,64,66	0
25	DMU	P	307	33/33	0.82	0.16	38,61,96,102	0
21	EDO	D	205	4/4	0.83	0.17	44,47,49,58	0
21	EDO	G	106	4/4	0.85	0.19	47,58,62,69	0
21	EDO	A	618	4/4	0.86	0.18	41,47,51,58	0
21	EDO	A	615	4/4	0.86	0.23	43,43,47,61	0
21	EDO	S	105	4/4	0.87	0.15	41,47,48,57	0
21	EDO	B	305	4/4	0.87	0.21	45,50,51,54	0
21	EDO	L	103	4/4	0.88	0.17	43,56,67,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	A	621	4/4	0.89	0.11	41,45,46,59	0
21	EDO	N	615	4/4	0.89	0.17	66,67,67,72	0
21	EDO	A	620	4/4	0.89	0.15	54,57,62,64	0
21	EDO	H	101	4/4	0.89	0.15	54,54,59,66	0
21	EDO	O	303	4/4	0.90	0.14	49,51,51,57	0
21	EDO	N	612	4/4	0.90	0.15	51,51,59,60	0
21	EDO	C	312	4/4	0.90	0.14	54,56,58,68	0
25	DMU	Z	101	33/33	0.90	0.12	44,50,65,65	0
21	EDO	A	619	4/4	0.91	0.14	34,48,49,55	0
21	EDO	A	617	4/4	0.91	0.14	39,42,42,45	0
21	EDO	A	614	4/4	0.91	0.17	45,49,54,83	0
26	UNX	P	303	1/1	0.91	0.17	24,24,24,24	0
21	EDO	Y	102	4/4	0.91	0.16	59,62,66,70	0
21	EDO	D	202	4/4	0.91	0.18	31,40,46,85	0
21	EDO	N	613	4/4	0.92	0.11	34,42,44,45	0
21	EDO	P	312	4/4	0.92	0.13	29,34,43,47	0
25	DMU	M	101	33/33	0.92	0.10	36,40,53,57	0
21	EDO	F	104	4/4	0.92	0.13	35,39,40,45	0
21	EDO	N	616	4/4	0.93	0.12	26,33,42,59	0
21	EDO	B	304	4/4	0.93	0.12	36,42,48,49	0
26	UNX	C	303	1/1	0.93	0.11	24,24,24,24	0
21	EDO	P	311	4/4	0.94	0.12	39,40,40,43	0
22	CHD	C	301	29/29	0.94	0.08	24,29,33,35	0
21	EDO	T	104	4/4	0.94	0.11	33,33,41,43	0
28	PEK	T	102	53/53	0.94	0.13	27,43,78,91	0
21	EDO	D	204	4/4	0.95	0.09	35,35,50,57	0
28	PEK	G	101	53/53	0.95	0.12	25,43,71,86	0
21	EDO	A	612	4/4	0.95	0.12	28,28,30,35	0
21	EDO	O	304	4/4	0.95	0.09	34,35,35,35	0
21	EDO	N	614	4/4	0.95	0.09	36,37,42,45	0
21	EDO	N	611	4/4	0.95	0.08	24,27,31,32	0
21	EDO	N	610	4/4	0.96	0.12	29,30,32,38	0
20	PGV	N	608	51/51	0.96	0.09	23,32,61,63	0
21	EDO	A	611	4/4	0.96	0.09	31,40,44,46	0
21	EDO	S	103	4/4	0.96	0.12	35,58,59,60	0
21	EDO	S	104	4/4	0.96	0.10	35,38,42,44	0
20	PGV	C	304	51/51	0.96	0.11	24,32,80,88	0
22	CHD	B	301	29/29	0.97	0.06	23,26,30,37	0
18	AZI	N	606[B]	3/3	0.97	0.13	21,21,23,24	3
21	EDO	F	105	4/4	0.97	0.09	32,33,36,36	0
21	EDO	G	105	4/4	0.97	0.08	29,30,37,39	0
22	CHD	P	301	29/29	0.97	0.06	26,30,34,38	0

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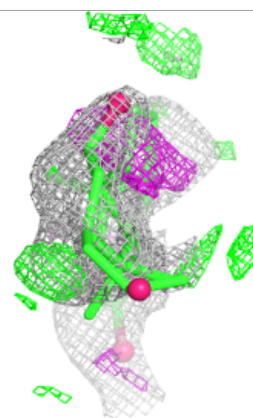
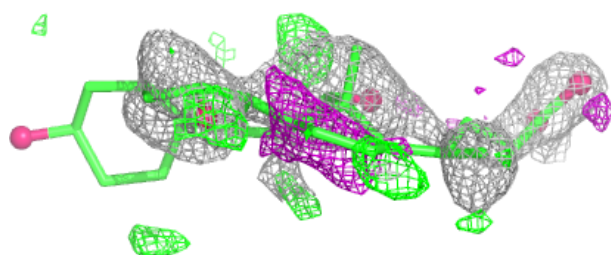
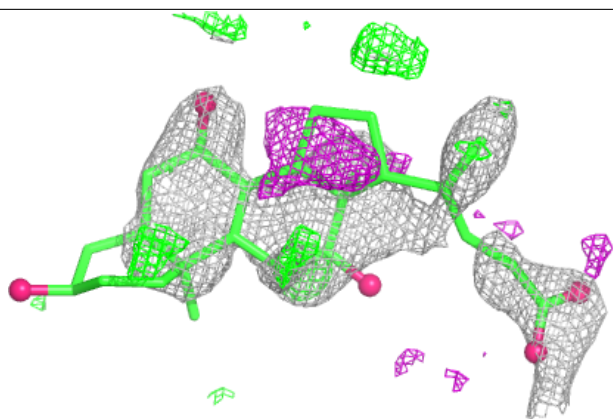
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	PGV	P	304	51/51	0.97	0.10	24,33,75,82	0
18	AZI	N	607[A]	3/3	0.97	0.10	25,25,26,29	3
18	AZI	N	607[B]	3/3	0.97	0.10	19,19,20,27	3
21	EDO	R	201	4/4	0.97	0.07	38,40,42,43	0
21	EDO	B	306	4/4	0.97	0.07	25,26,31,31	0
21	EDO	E	201	4/4	0.97	0.08	36,37,39,41	0
21	EDO	C	311	4/4	0.97	0.08	34,35,36,37	0
21	EDO	S	106	4/4	0.97	0.08	32,33,33,34	0
21	EDO	E	203	4/4	0.97	0.07	34,37,43,45	0
20	PGV	A	609	51/51	0.97	0.09	21,29,60,64	0
21	EDO	A	613	4/4	0.98	0.08	23,24,25,26	0
18	AZI	A	607[A]	3/3	0.98	0.06	20,20,21,24	3
18	AZI	A	607[B]	3/3	0.98	0.06	16,16,17,26	3
21	EDO	A	616	4/4	0.98	0.07	32,36,40,45	0
14	HEA	N	601	60/60	0.98	0.07	23,26,45,50	0
22	CHD	G	103	29/29	0.98	0.05	24,27,30,34	0
21	EDO	S	102	4/4	0.98	0.06	25,25,25,26	0
14	HEA	N	602[A]	60/60	0.98	0.06	19,23,26,27	60
14	HEA	N	602[B]	60/60	0.98	0.06	22,25,38,39	60
16	MG	N	604	1/1	0.98	0.04	28,28,28,28	0
18	AZI	A	606[B]	3/3	0.98	0.07	20,20,20,21	3
16	MG	A	604	1/1	0.99	0.03	23,23,23,23	0
14	HEA	A	601	60/60	0.99	0.06	19,21,43,47	0
21	EDO	F	102	4/4	0.99	0.04	23,24,26,26	0
14	HEA	A	602[A]	60/60	0.99	0.06	17,20,25,28	60
14	HEA	A	602[B]	60/60	0.99	0.06	17,21,28,31	60
23	CUA	O	301	2/2	1.00	0.01	29,29,29,30	0
17	NA	N	605	1/1	1.00	0.04	33,33,33,33	0
15	CU	A	603	1/1	1.00	0.02	23,23,23,23	0
15	CU	N	603	1/1	1.00	0.01	26,26,26,26	0
17	NA	A	605	1/1	1.00	0.03	25,25,25,25	0
23	CUA	B	302	2/2	1.00	0.01	23,23,23,23	0
29	ZN	F	101	1/1	1.00	0.03	28,28,28,28	0
29	ZN	S	101	1/1	1.00	0.03	29,29,29,29	0

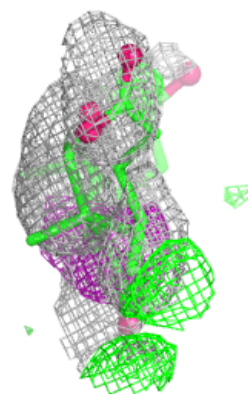
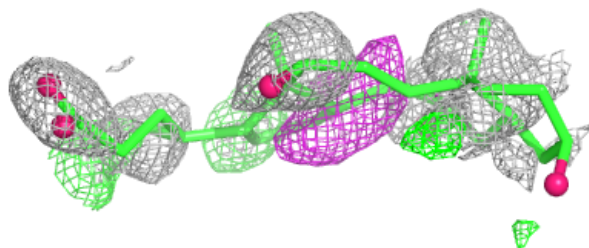
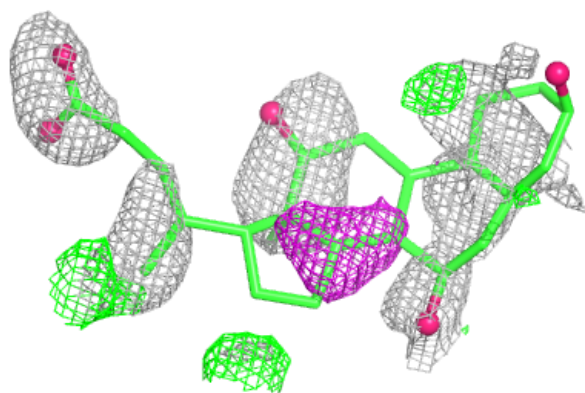
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD J 101:

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

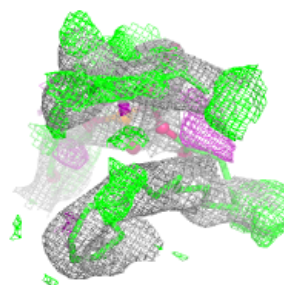
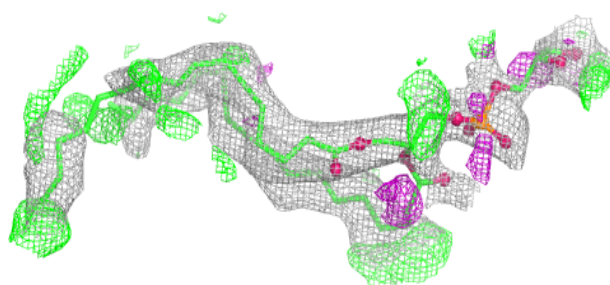
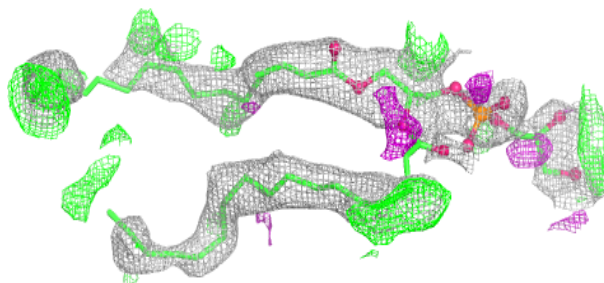
**Electron density around CHD W 101:**

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



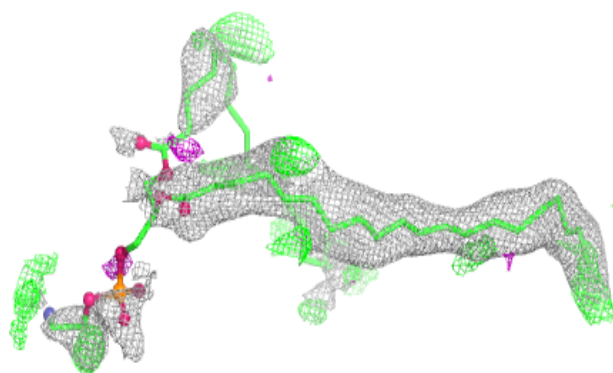
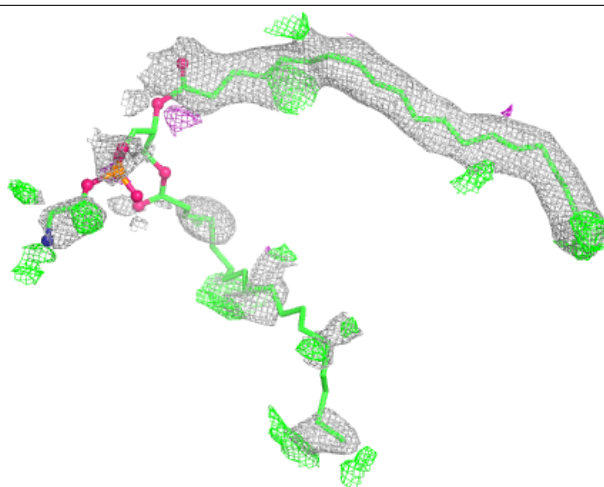
Electron density around PGV C 308:

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



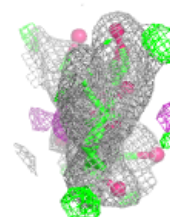
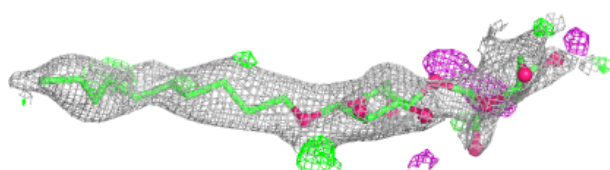
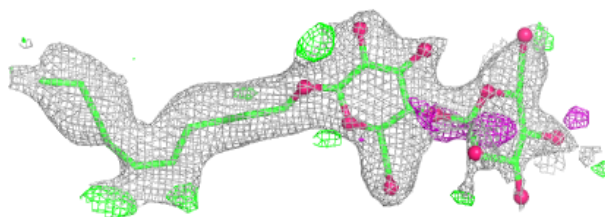
Electron density around PEK T 101:

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

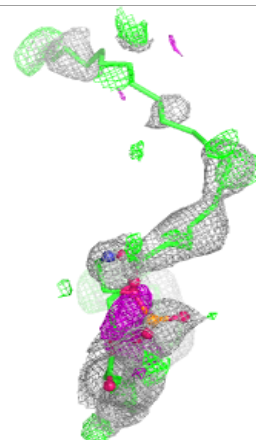
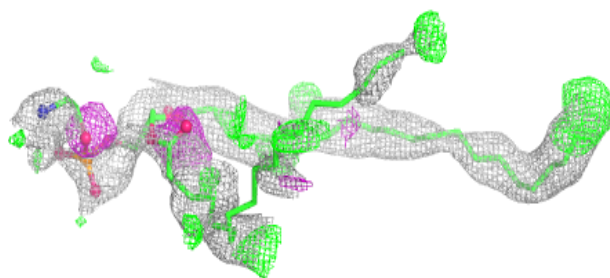
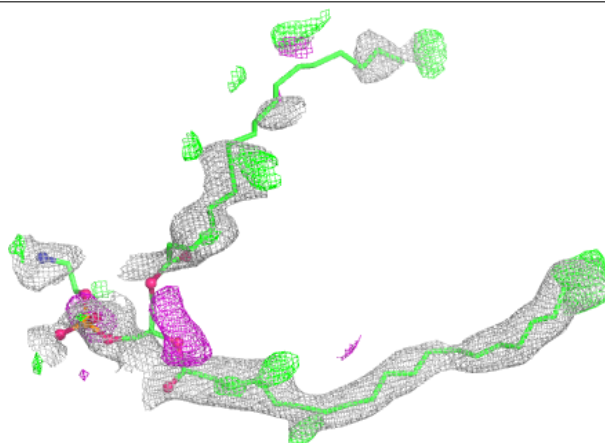


Electron density around DMU P 309:

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

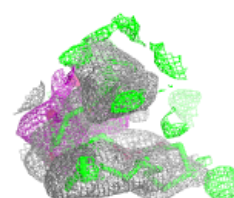
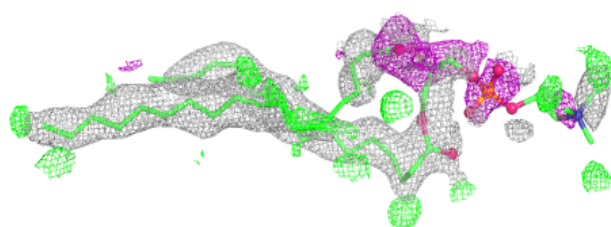
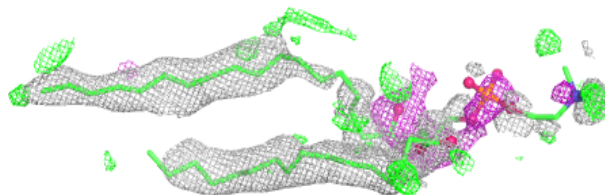
**Electron density around PEK G 104:**

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

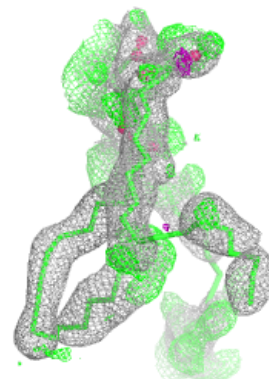
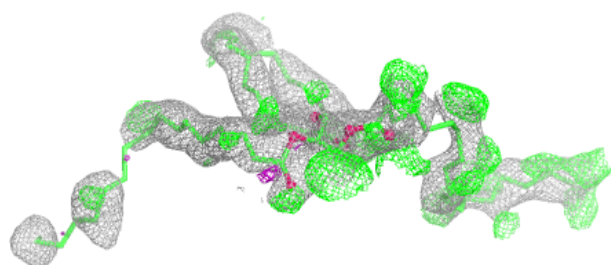
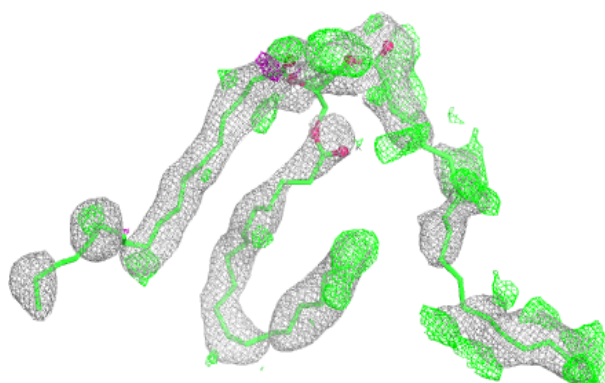


Electron density around PSC B 303:

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

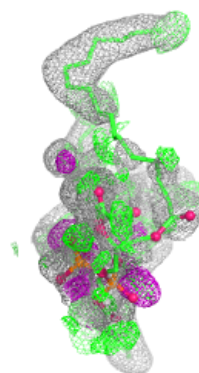
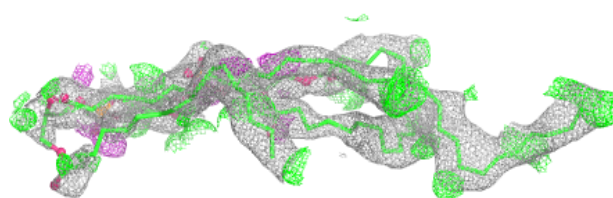
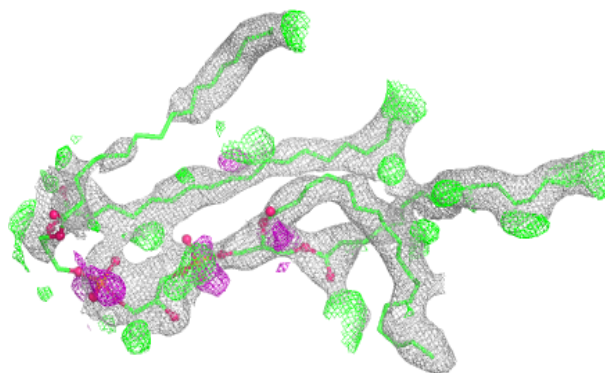
**Electron density around TGL Q 201:**

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

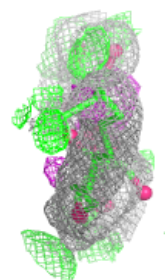
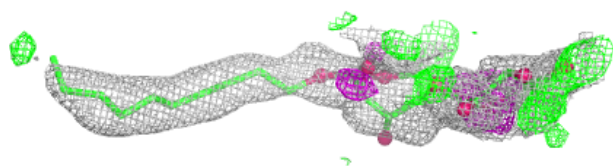
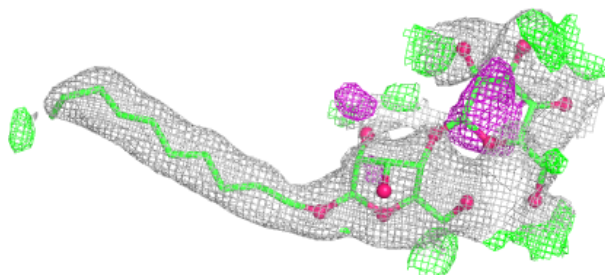


Electron density around CDL T 103:

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

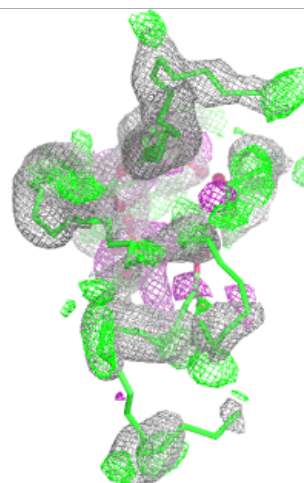
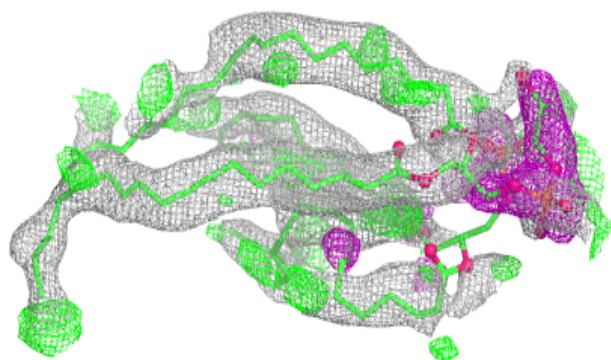
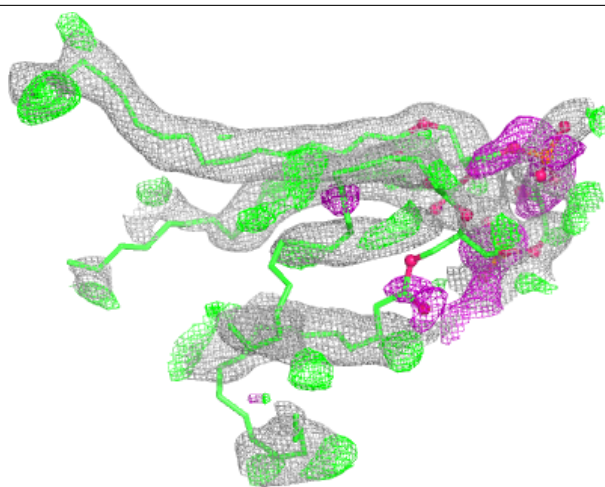
**Electron density around DMU C 310:**

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



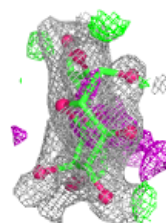
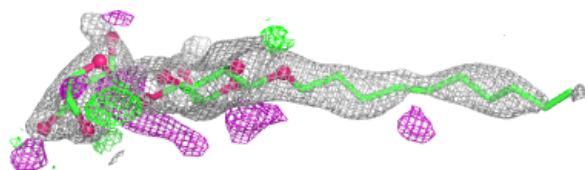
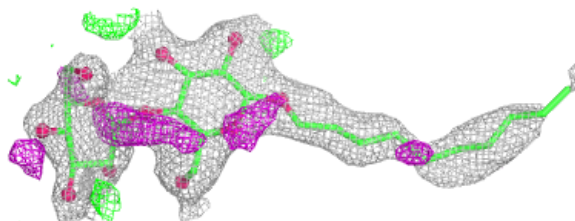
Electron density around CDL P 305:

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



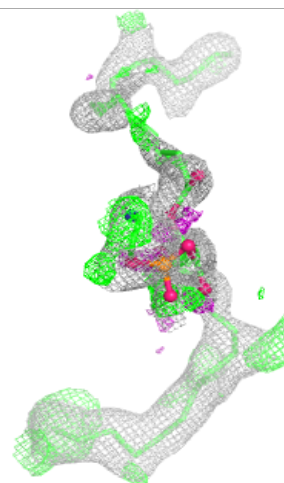
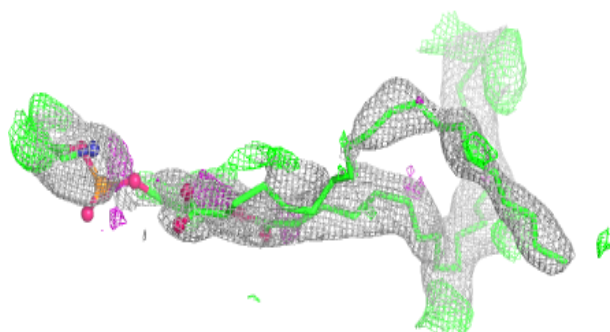
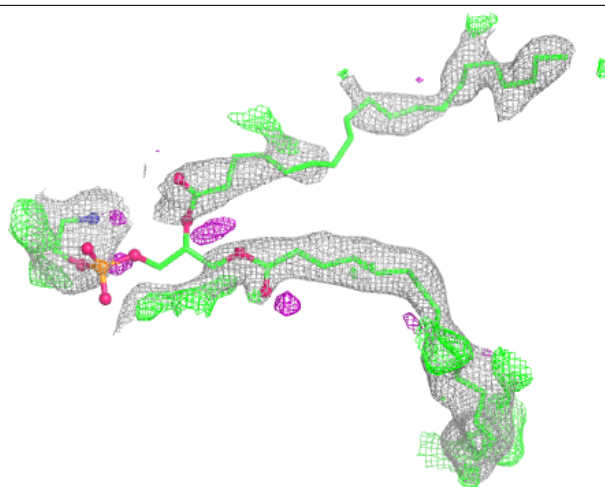
Electron density around DMU C 309:

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



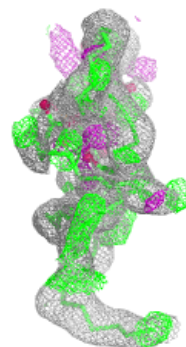
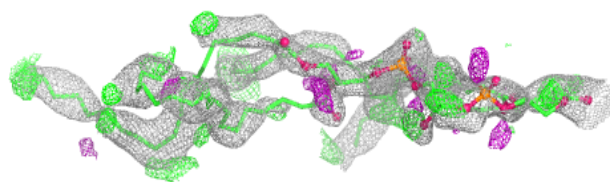
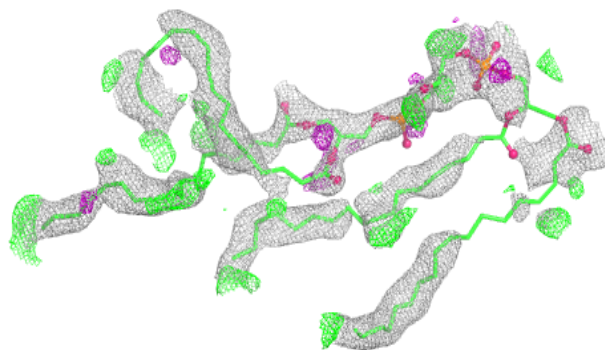
Electron density around PEK C 307:

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



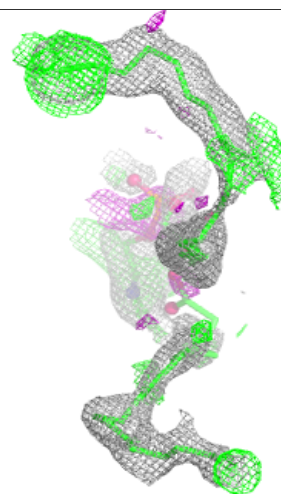
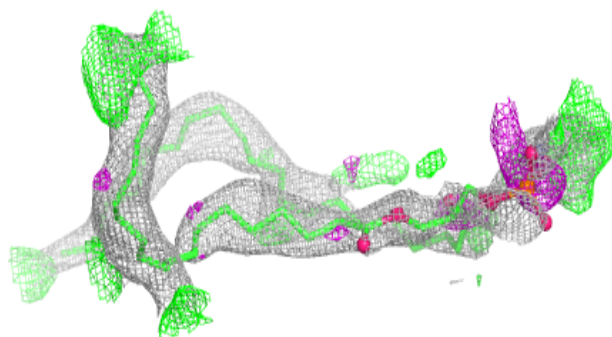
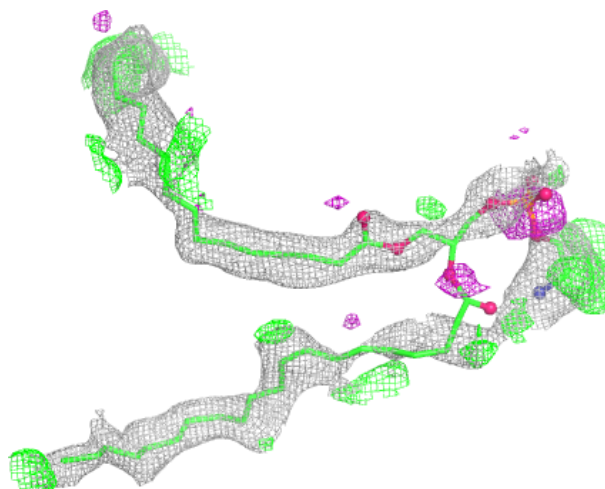
Electron density around CDL G 102:

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



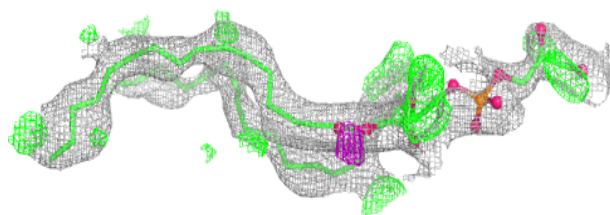
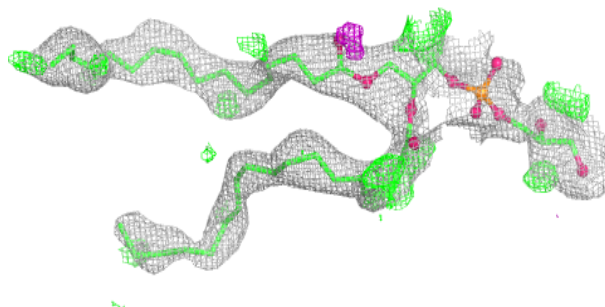
Electron density around PEK P 308:

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

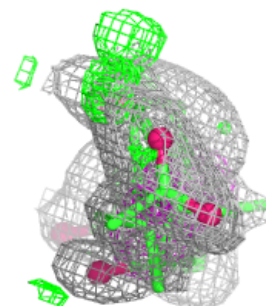
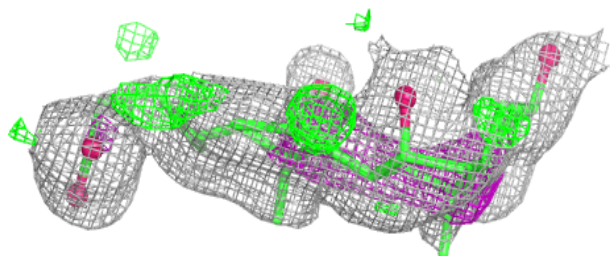
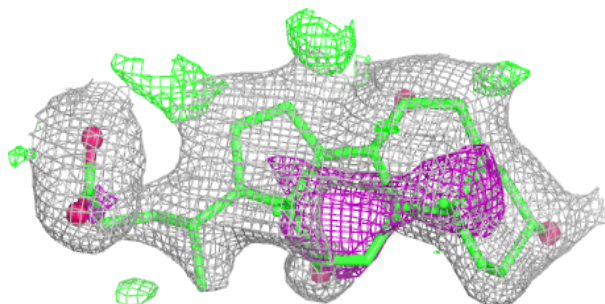


Electron density around PGV P 302:

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

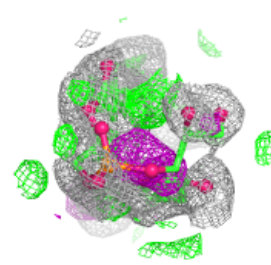
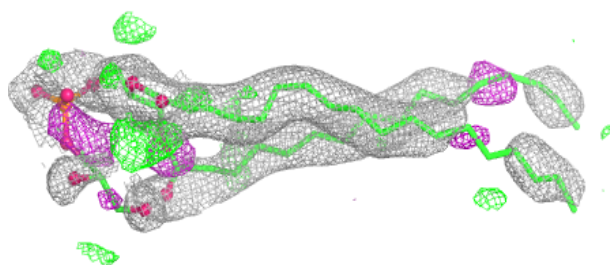
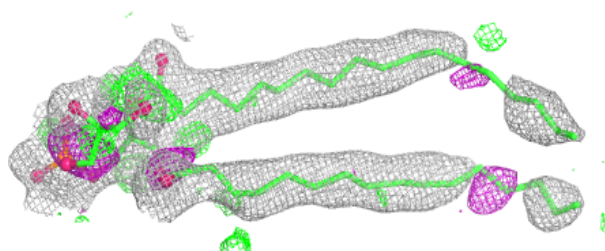
**Electron density around CHD P 306:**

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

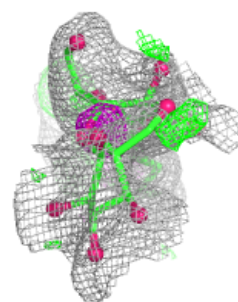
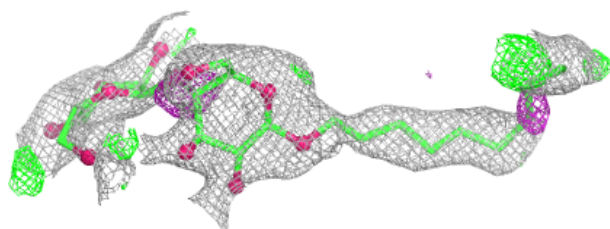
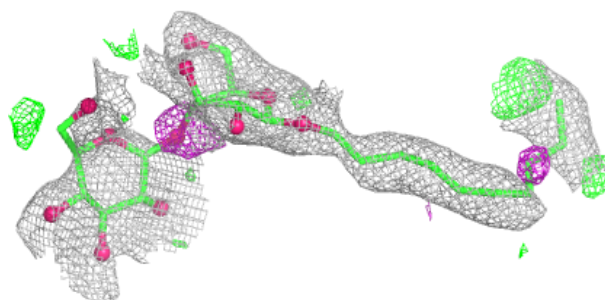


Electron density around PGV X 101:

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

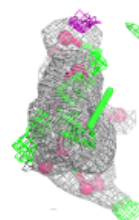
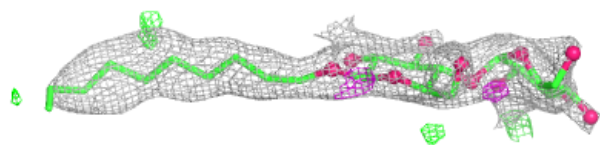
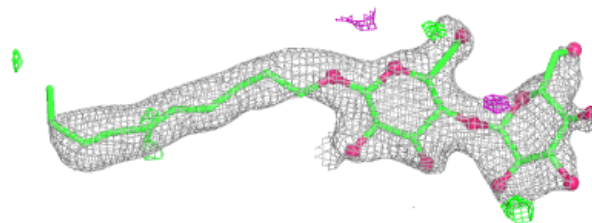
**Electron density around DMU L 102:**

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

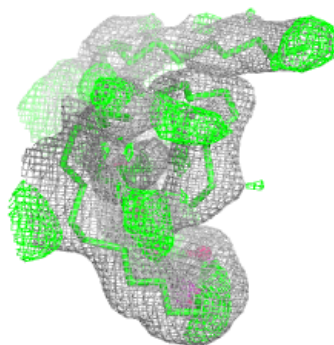
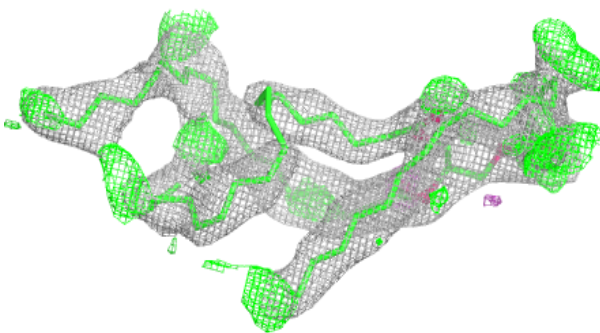
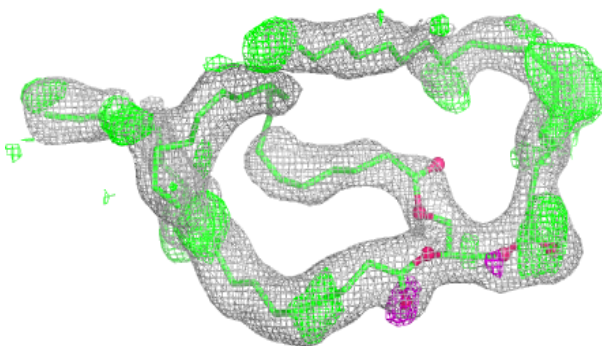


Electron density around DMU P 310:

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

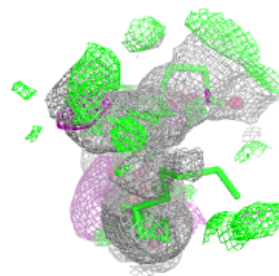
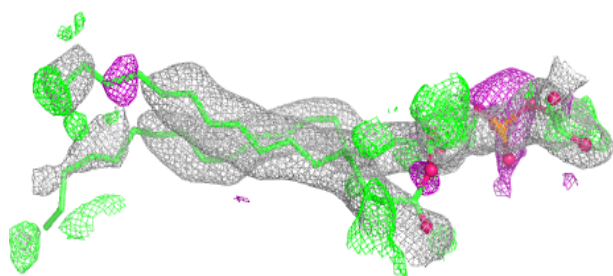
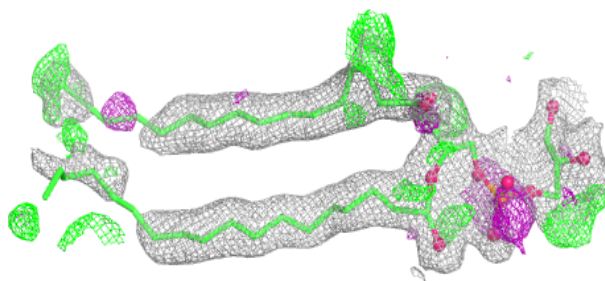
**Electron density around TGL N 609:**

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

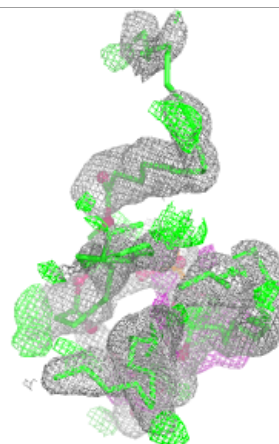
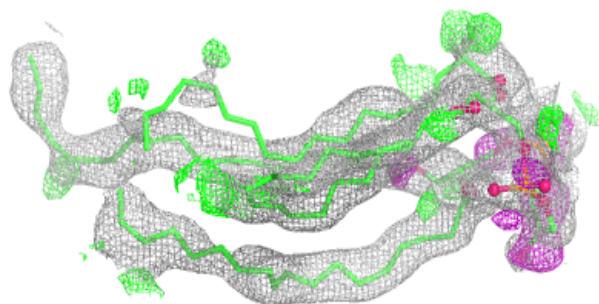
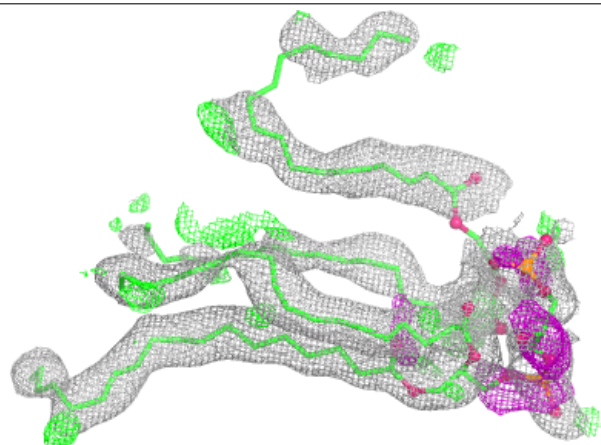


Electron density around PGV A 610:

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

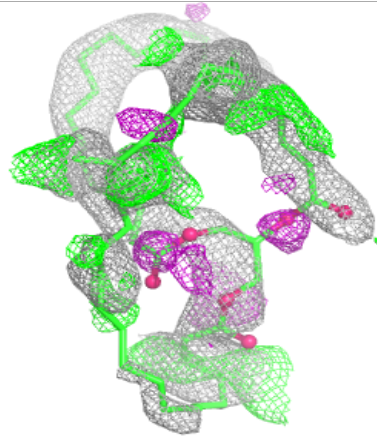
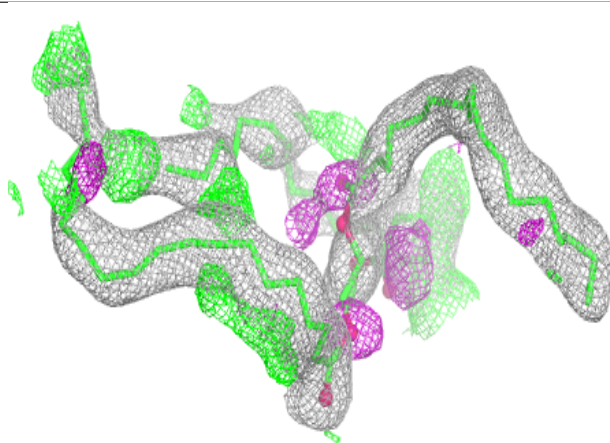
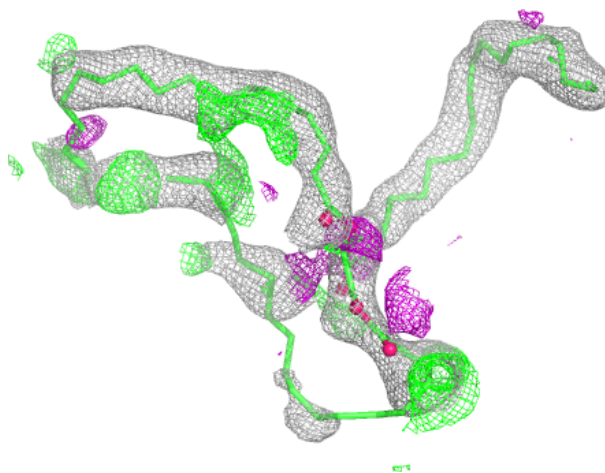
**Electron density around CDL C 305:**

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



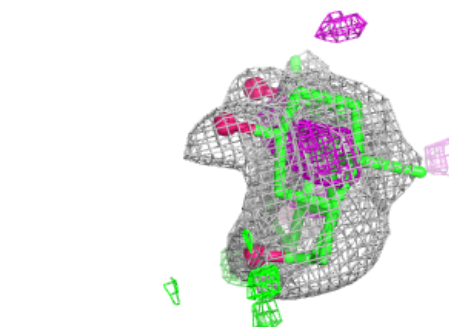
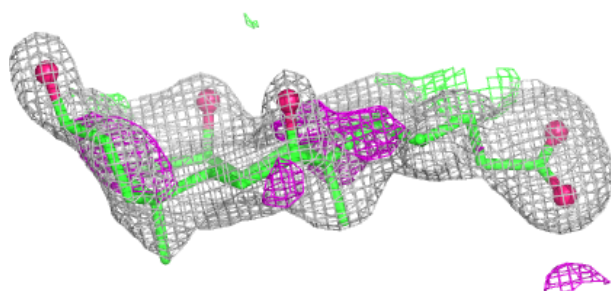
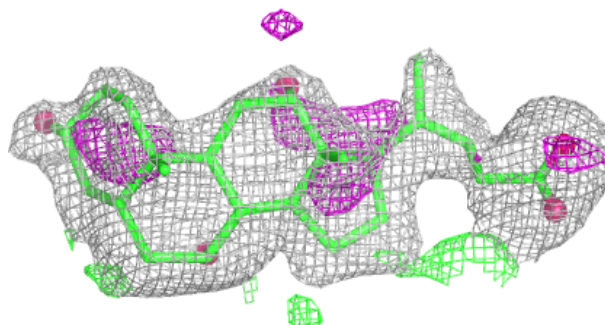
Electron density around TGL Y 101:

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

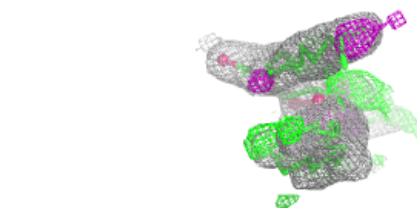
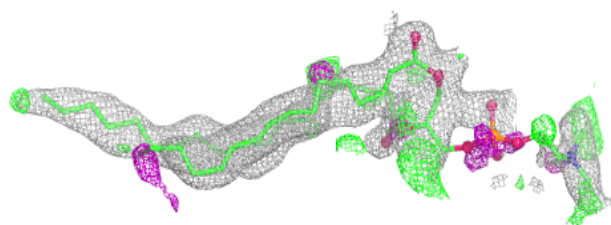
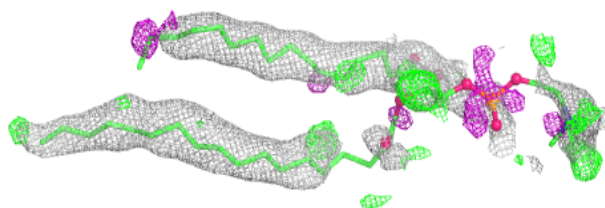


Electron density around CHD C 306:

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

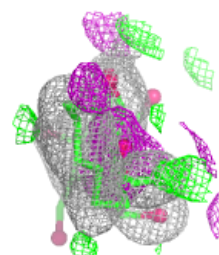
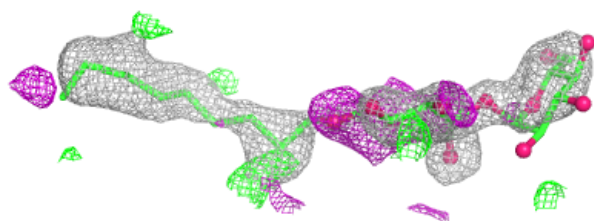
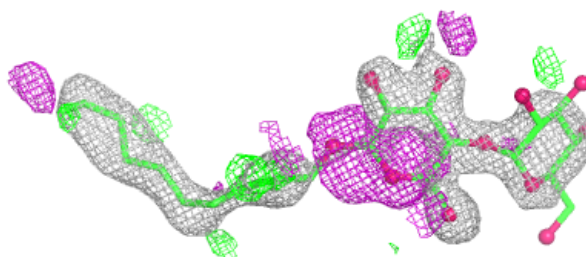
**Electron density around PSC O 302:**

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



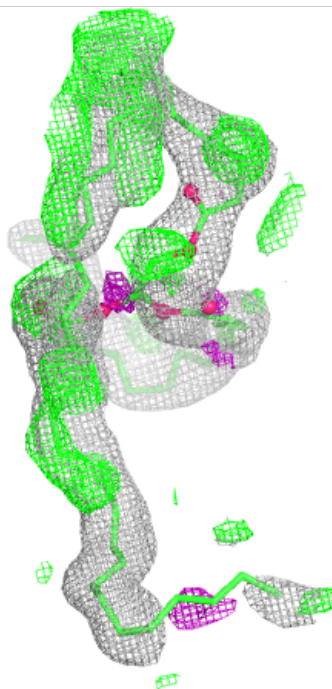
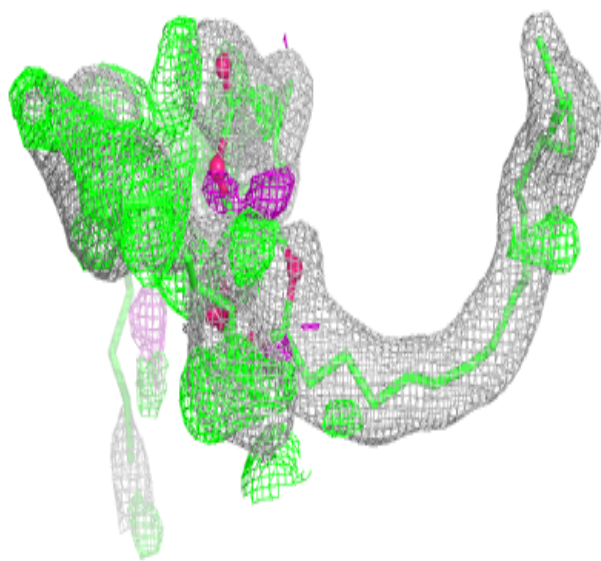
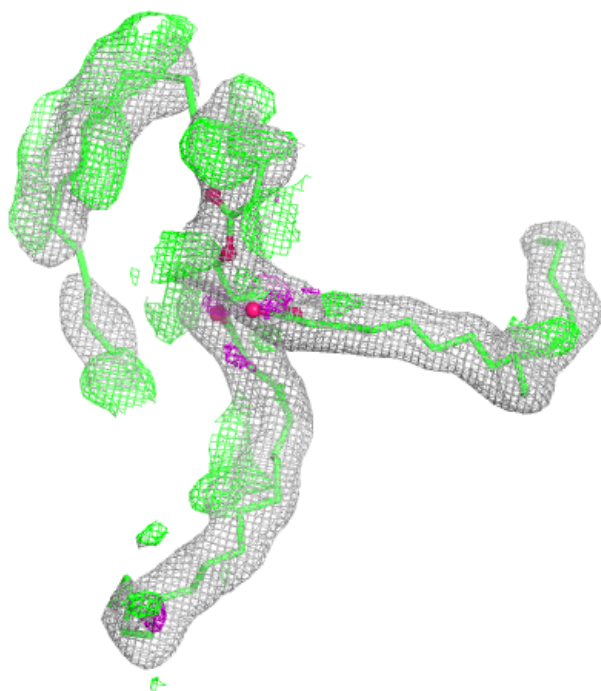
Electron density around DMU C 302:

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



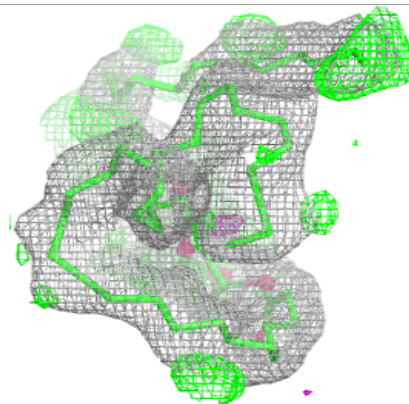
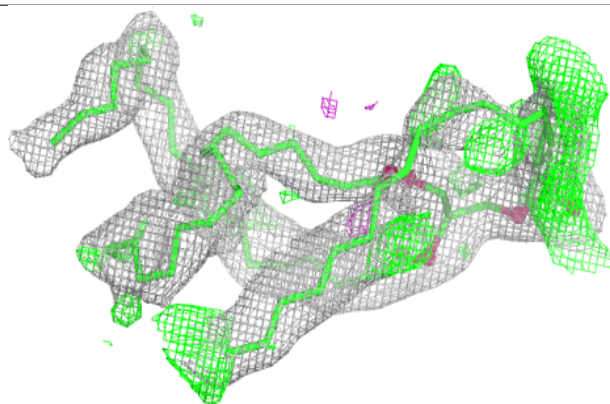
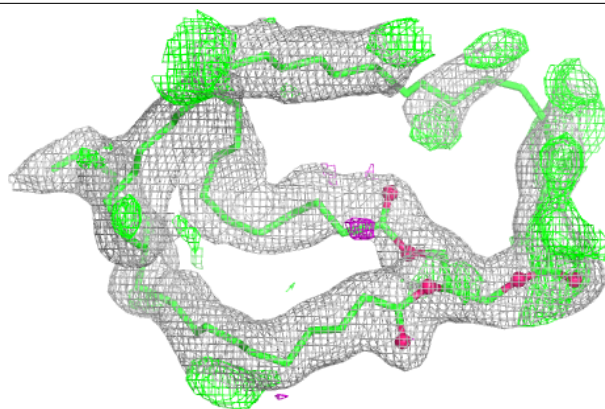
Electron density around TGL L 101:

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

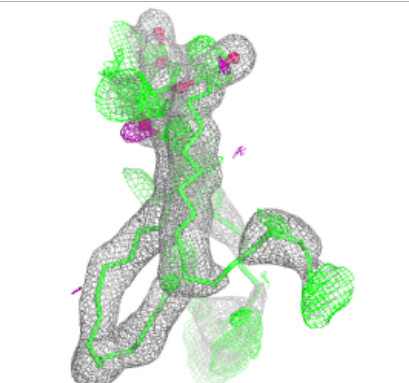
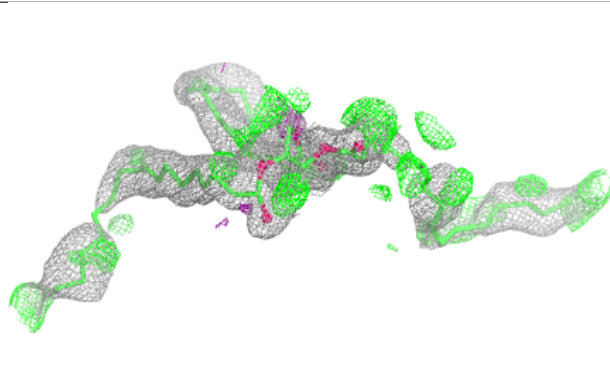
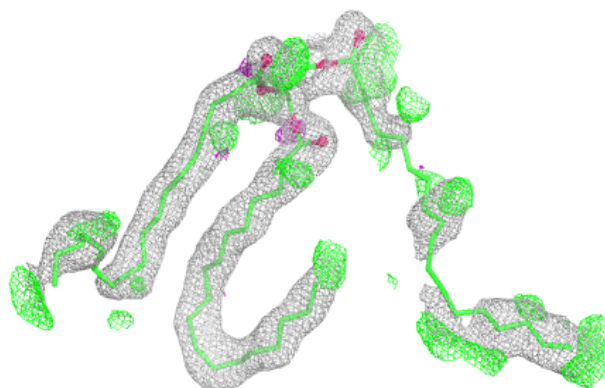


Electron density around TGL A 608:

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

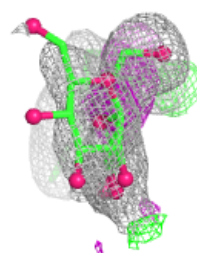
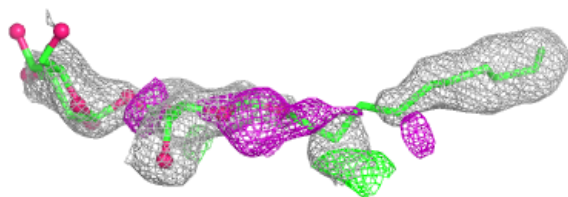
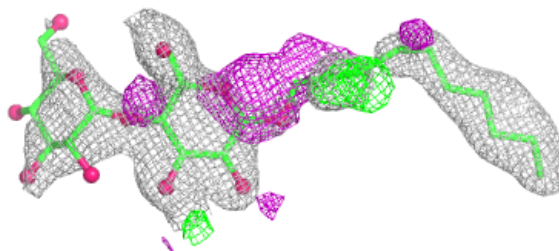
**Electron density around TGL D 201:**

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

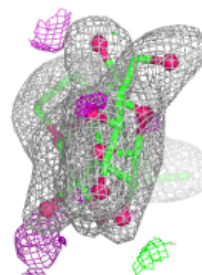
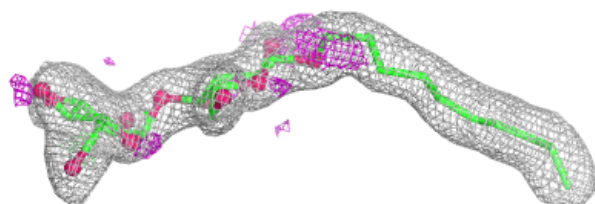
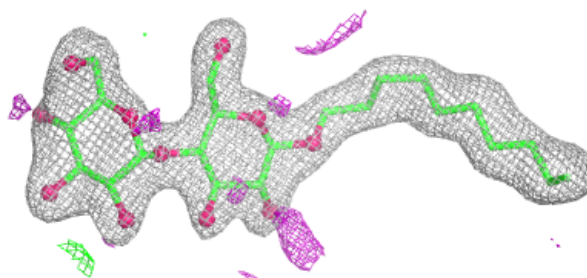


Electron density around DMU P 307:

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

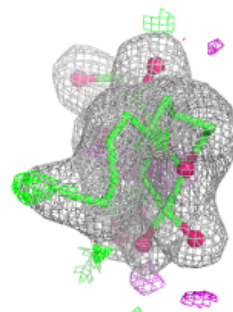
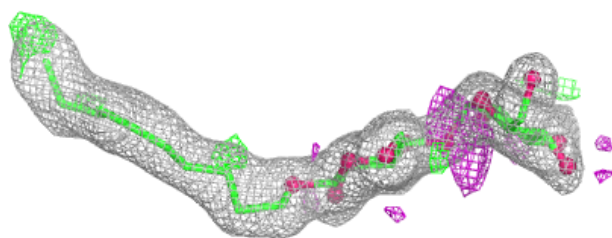
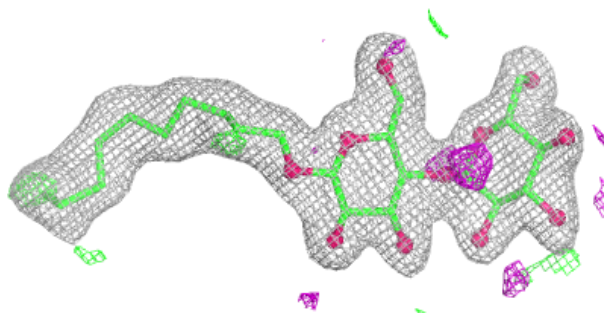
**Electron density around DMU Z 101:**

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

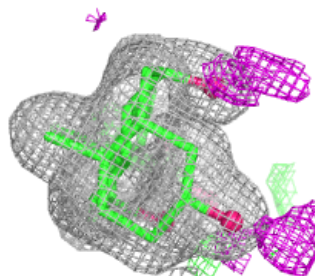
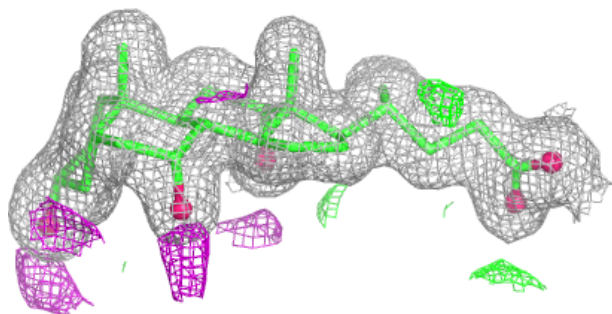
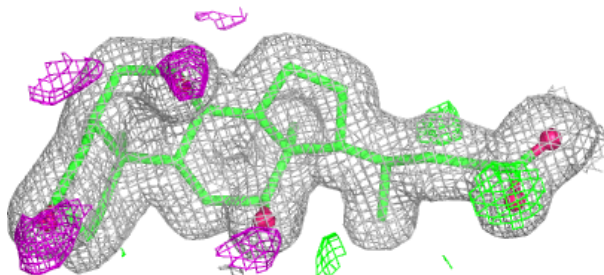


Electron density around DMU M 101:

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

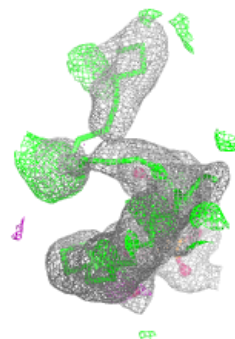
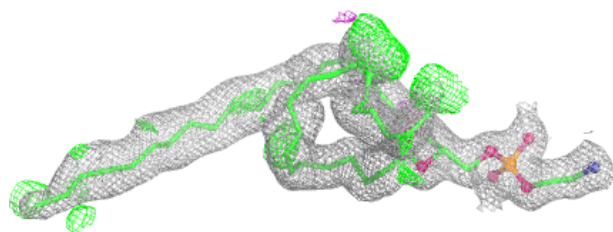
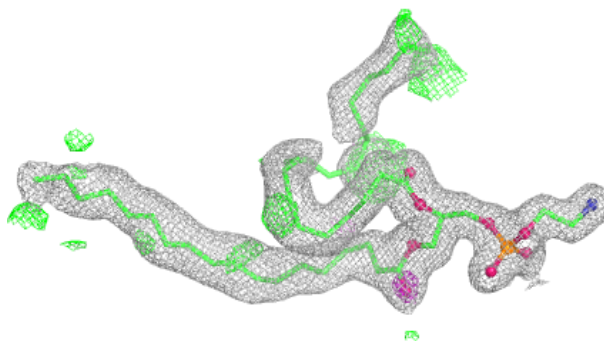
**Electron density around CHD C 301:**

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

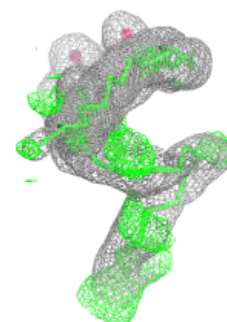
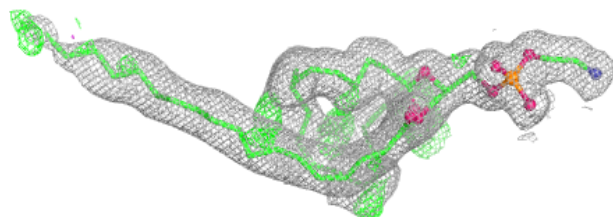
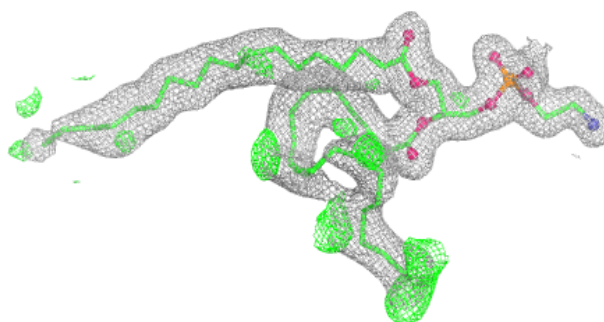


Electron density around PEK T 102:

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

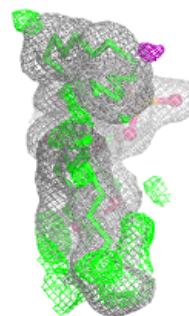
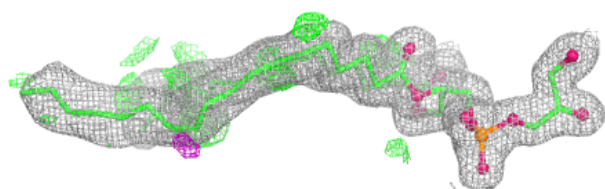
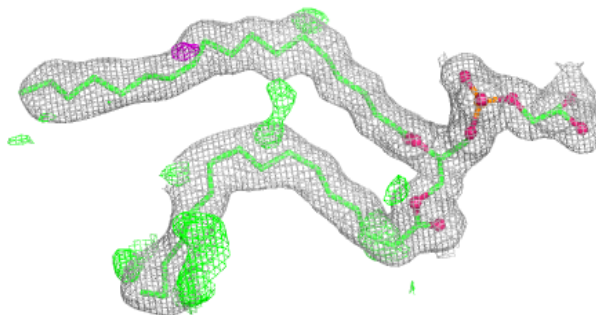
**Electron density around PEK G 101:**

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

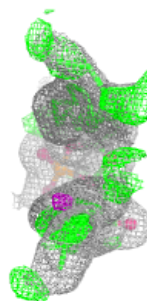
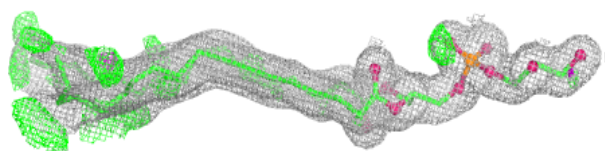
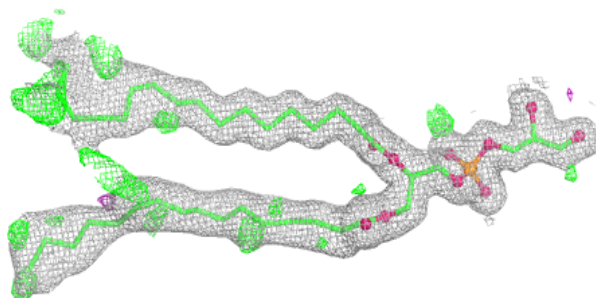


Electron density around PGV N 608:

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

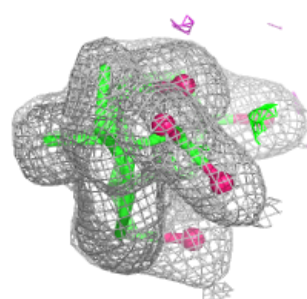
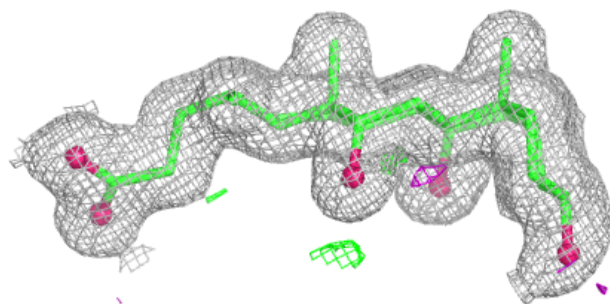
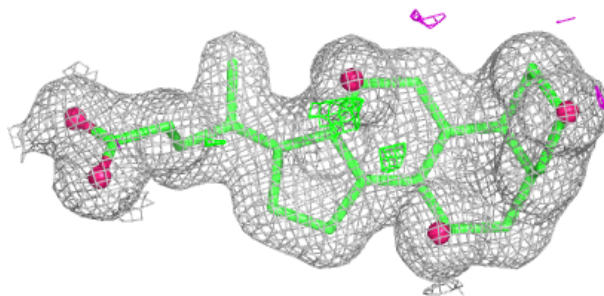
**Electron density around PGV C 304:**

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

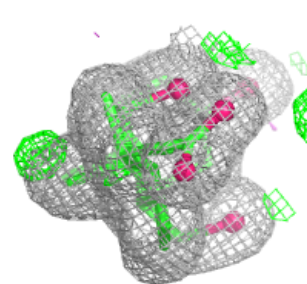
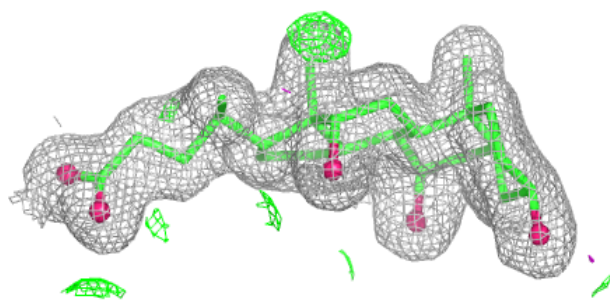
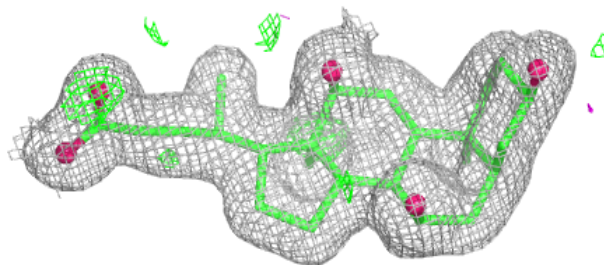


Electron density around CHD B 301:

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

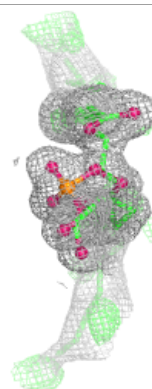
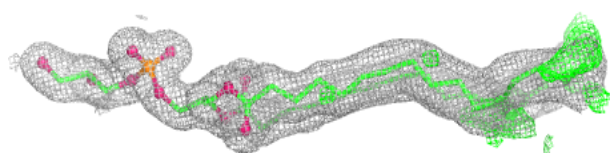
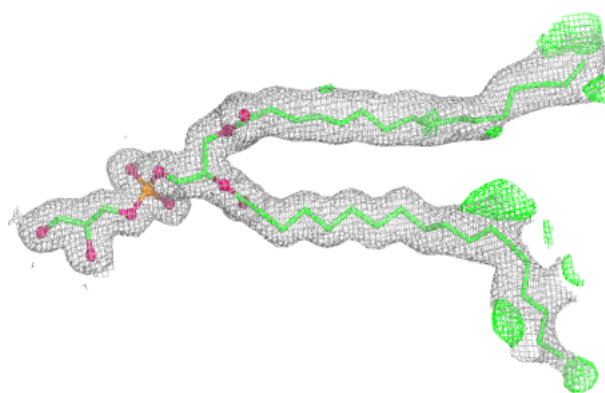
**Electron density around CHD P 301:**

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

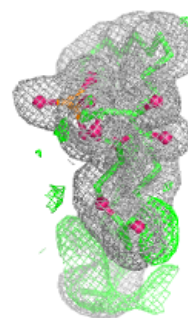
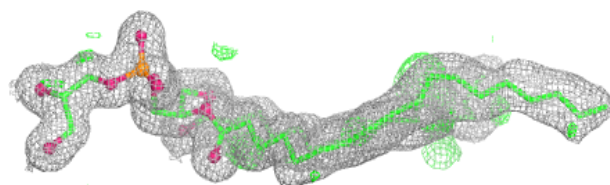
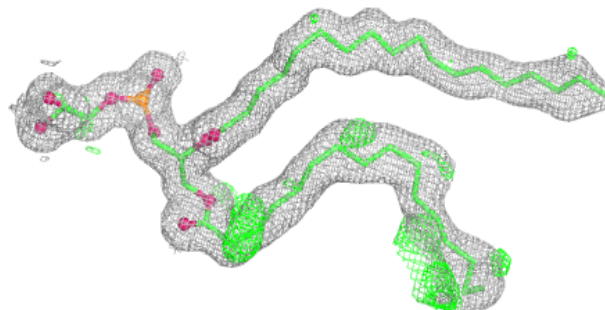


Electron density around PGV P 304:

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

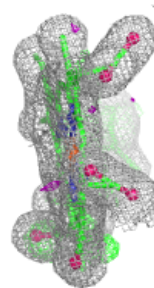
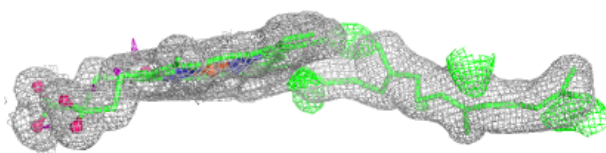
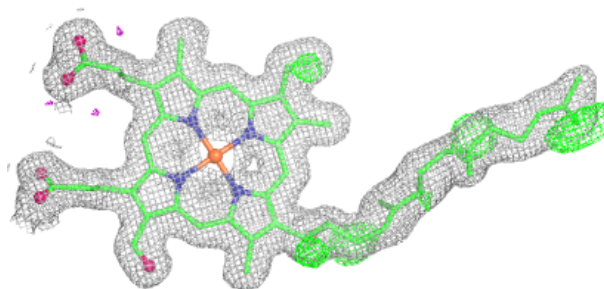
**Electron density around PGV A 609:**

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

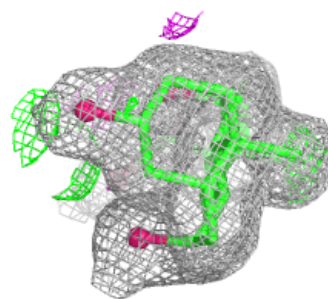
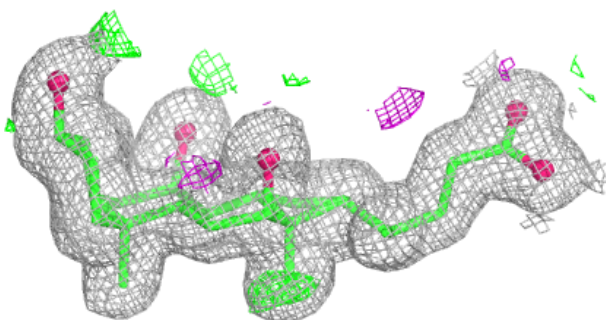
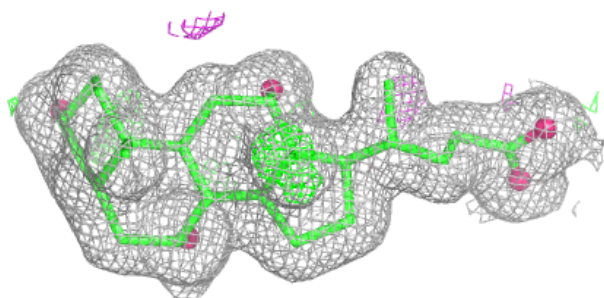


Electron density around HEA N 601:

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

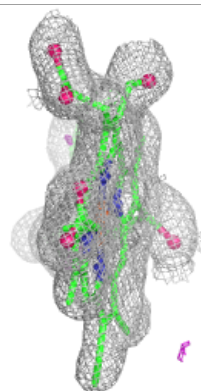
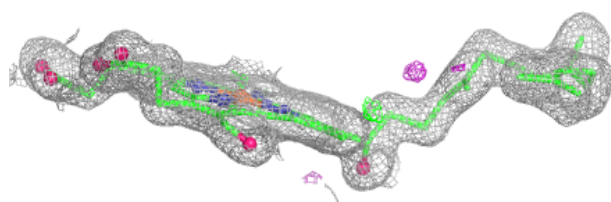
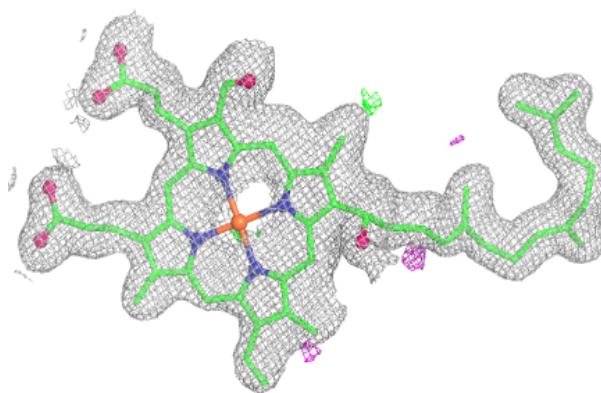
**Electron density around CHD G 103:**

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

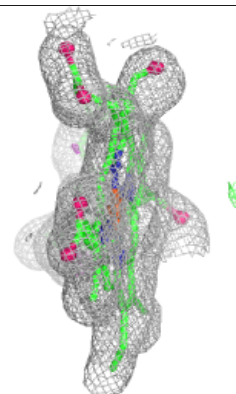
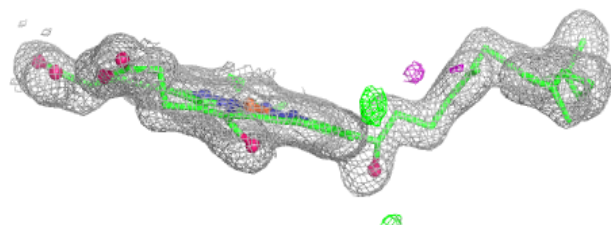
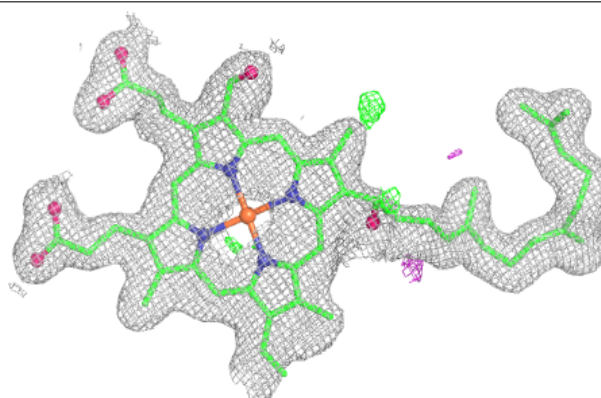


Electron density around HEA N 602 (A):

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

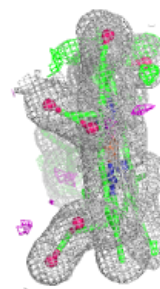
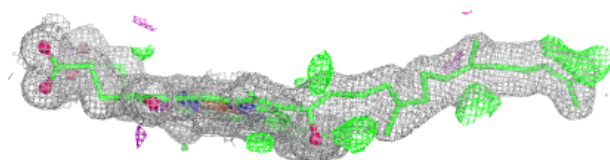
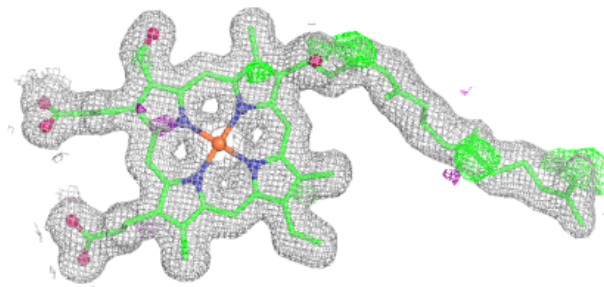
**Electron density around HEA N 602 (B):**

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

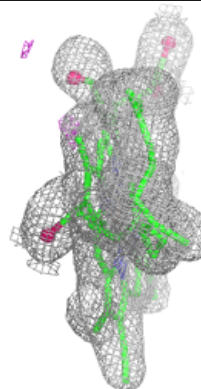
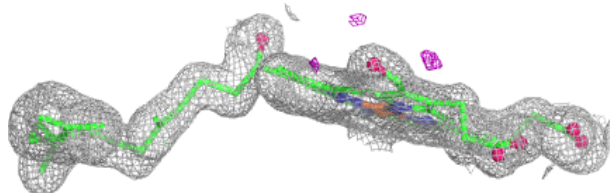
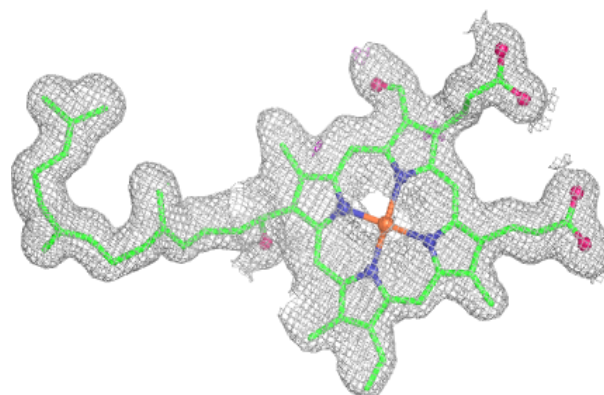


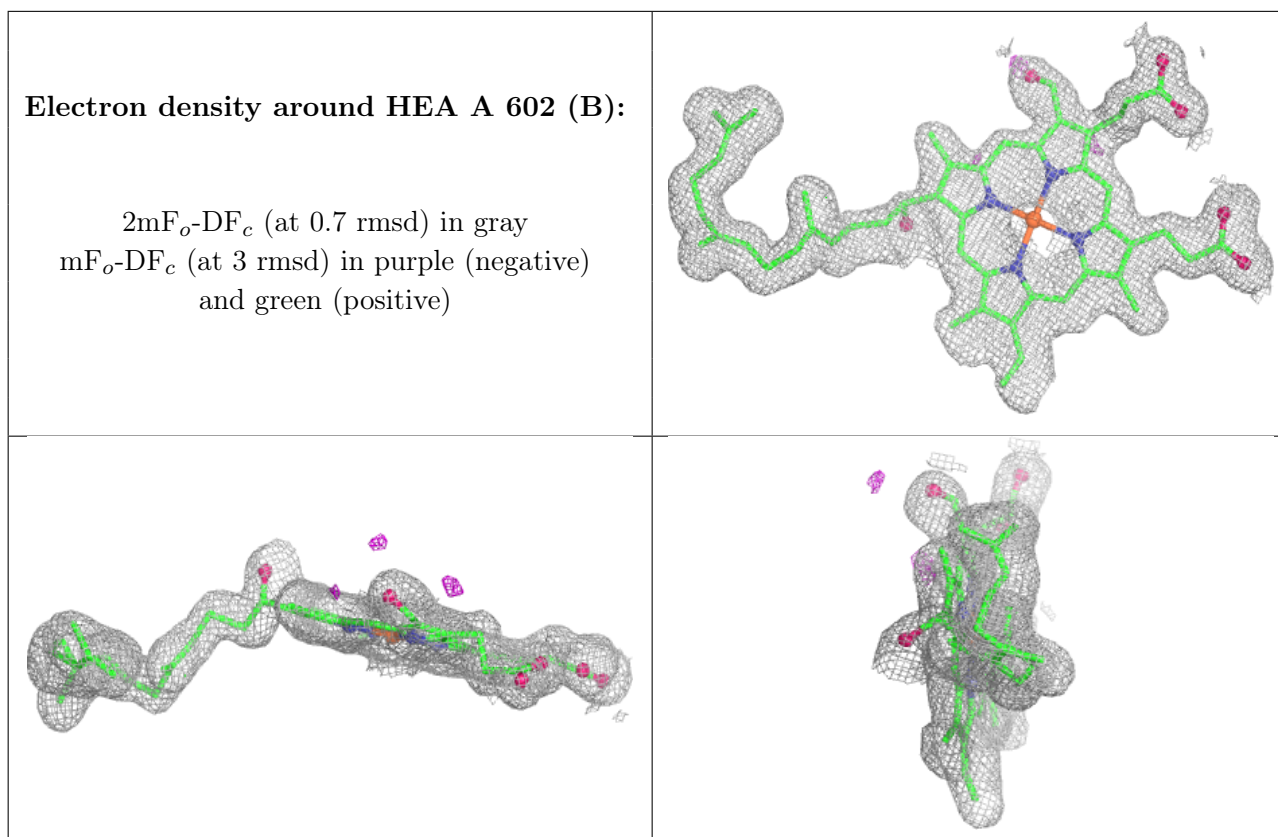
Electron density around HEA A 601:

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

$2mF_o-DF_c$ (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.