



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:34 PM UTC

PDB ID : 5XDQ / pdb_00005xdq
Title : Bovine heart cytochrome c oxidase in the fully oxidized state with pH 7.3 at 1.77 angstrom resolution
Authors : Luo, F.J.; Shimada, A.; Hagimoto, N.; Shimada, S.; Shinzawa-Itoh, K.; Yamashita, E.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2017-03-29
Resolution : 1.77 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

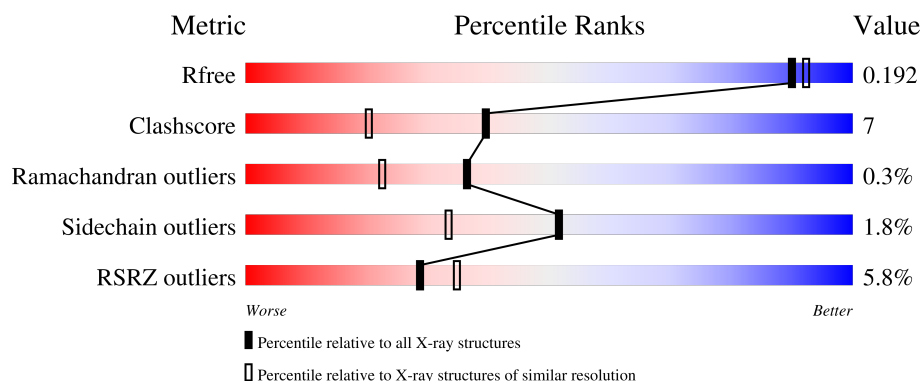
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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

Mol	Chain	Length	Quality of chain
1	A	514	0.1% 86% 13% .
1	N	514	0.1% 89% 10%
2	B	227	2% 88% 11% .
2	O	227	4% 86% 13%

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Mol	Chain	Length	Quality of chain
3	C	261	
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	94	
6	S	94	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	PER	A	607[B]	-	X	-	-
19	PER	N	608[B]	-	X	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 34218 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	33	0
			4118	2757	626	690	45			
1	N	514	Total	C	N	O	S	0	30	0
			4109	2744	627	689	49			

- 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	11	0
			1859	1207	285	345	22			
2	O	227	Total	C	N	O	S	0	10	0
			1851	1200	284	345	22			

- 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	13	0
			2143	1434	336	357	16			
3	P	259	Total	C	N	O	S	0	12	0
			2140	1430	337	357	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	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	1	0
			1200	780	198	218	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	2	0
			858	549	144	162	3			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	94	Total	C	N	O	S	0	1	0
			719	446	127	140	6			
6	S	94	Total	C	N	O	S	0	2	0
			722	449	127	140	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 674	C 431	N 129	O 112	P 1	S 1	0	0	0
7	T	84	Total 674	C 431	N 129	O 112	P 1	S 1	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	2	0
			466	301	78	83	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	1	0
			462	299	78	81	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	1	0
			388	254	65	66	3			
11	X	49	Total	C	N	O	S	0	0	0
			383	250	65	66	2			

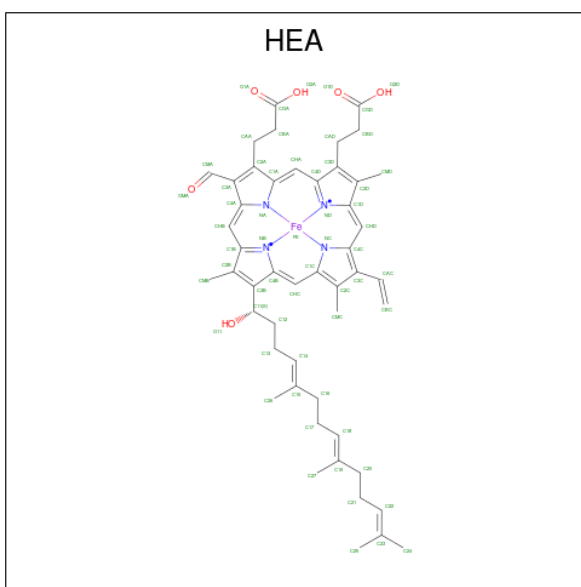
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	4	0
			399	266	66	64	3			
12	Y	46	Total	C	N	O	S	0	1	0
			382	255	64	60	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	1	0
			339	228	53	58			
13	Z	43	Total	C	N	O	0	0	0
			334	223	53	58			

- 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	C	Fe	N	O	
			69	58	1	4	6	1
14	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
14	N	1	Total	C	Fe	N	O	
			69	58	1	4	6	1
14	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	0

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

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

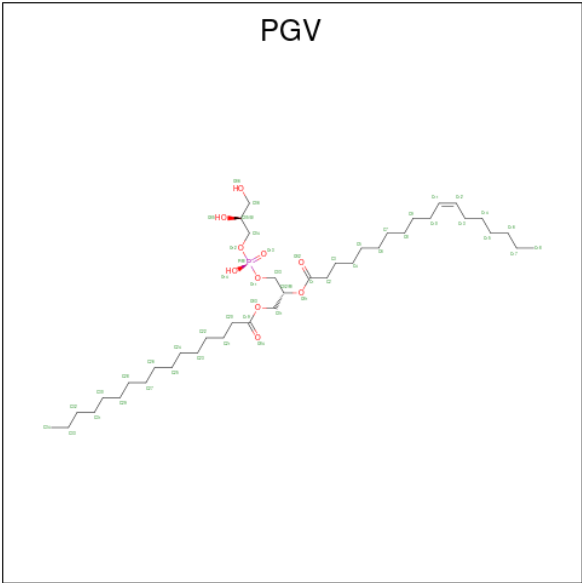
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

- Molecule 18 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



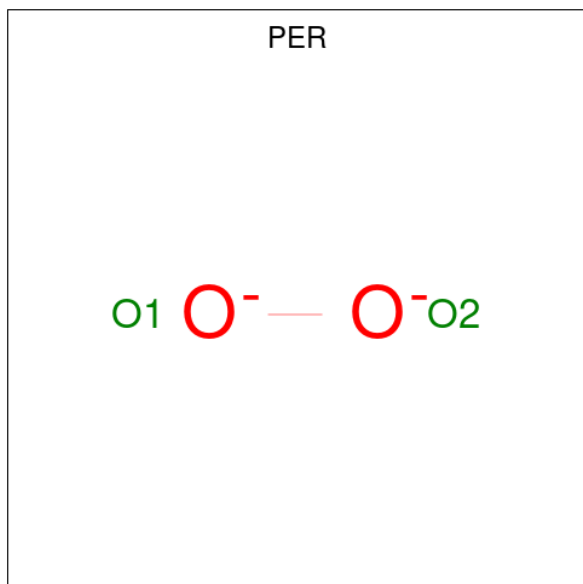
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0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

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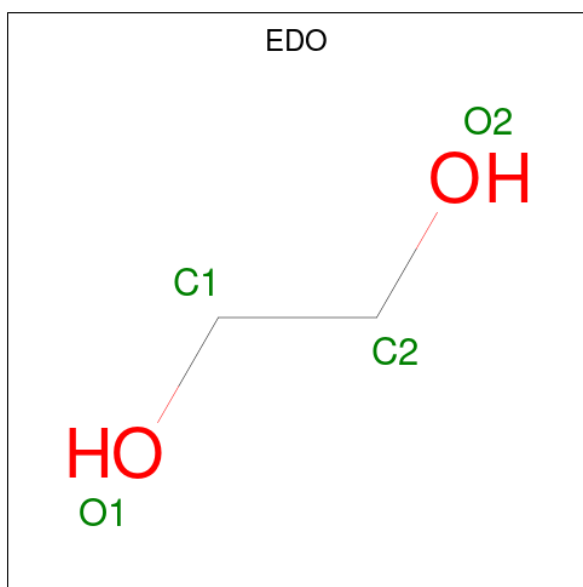
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	U	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 19 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



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

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



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

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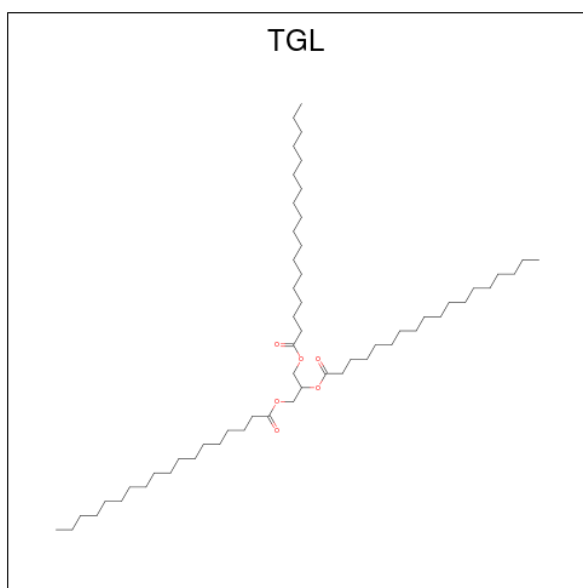
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total 4	C 2	O 2	0	0
20	B	1	Total 4	C 2	O 2	0	0
20	C	1	Total 4	C 2	O 2	0	0
20	C	1	Total 4	C 2	O 2	0	0
20	C	1	Total 4	C 2	O 2	0	0
20	E	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0
20	F	1	Total 4	C 2	O 2	0	0
20	G	1	Total 4	C 2	O 2	0	0
20	H	1	Total 4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

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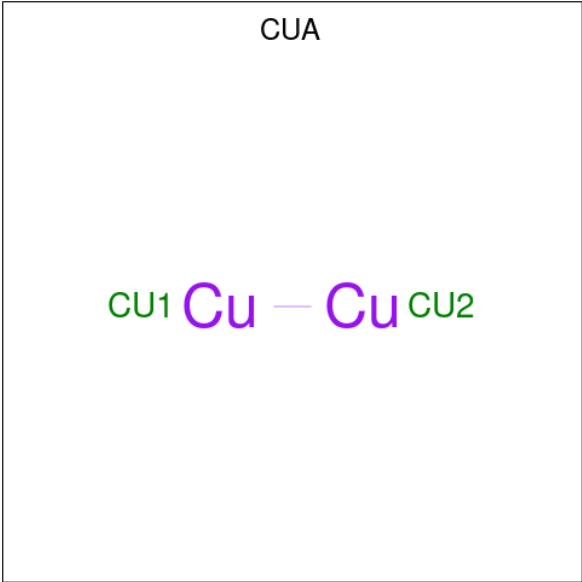
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	N	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	Q	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4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

- Molecule 21 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



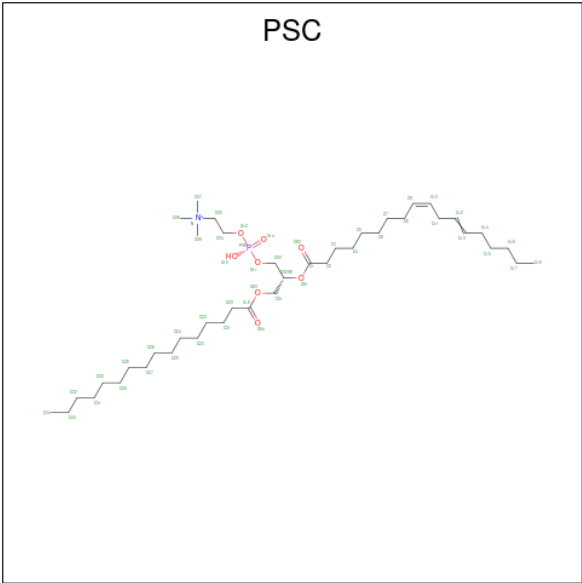
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	O	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



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

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



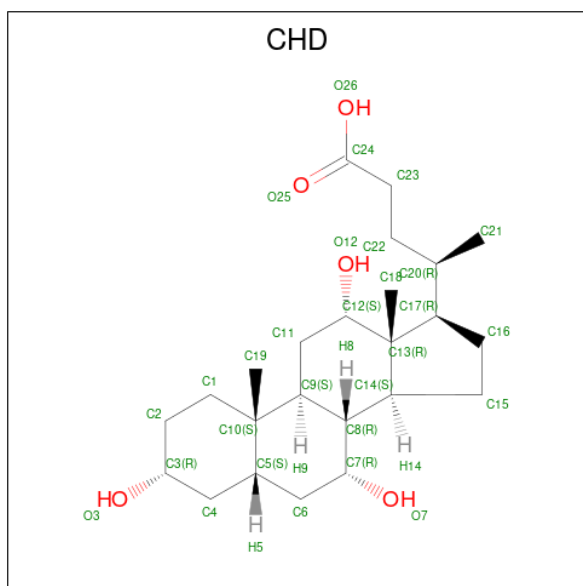
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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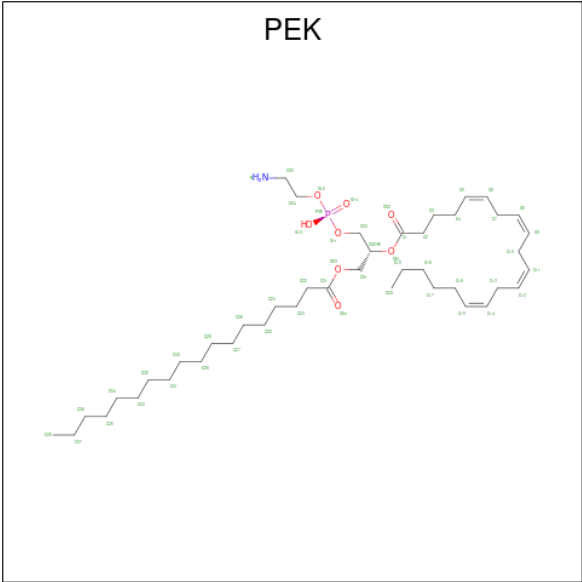
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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



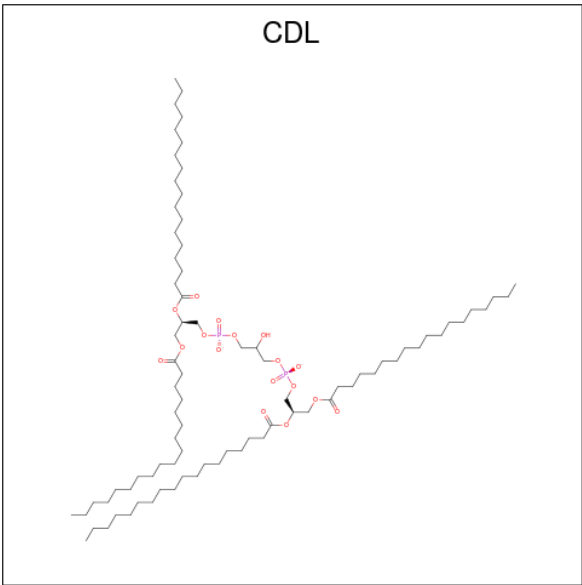
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	O			0	0
			29	24	5				
24	C	1	Total	C	O			0	0
			29	24	5				
24	C	1	Total	C	O			0	0
			29	24	5				
24	G	1	Total	C	O			0	0
			29	24	5				
24	J	1	Total	C	O			0	0
			29	24	5				
24	P	1	Total	C	O			0	0
			29	24	5				
24	P	1	Total	C	O			0	0
			29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

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$).



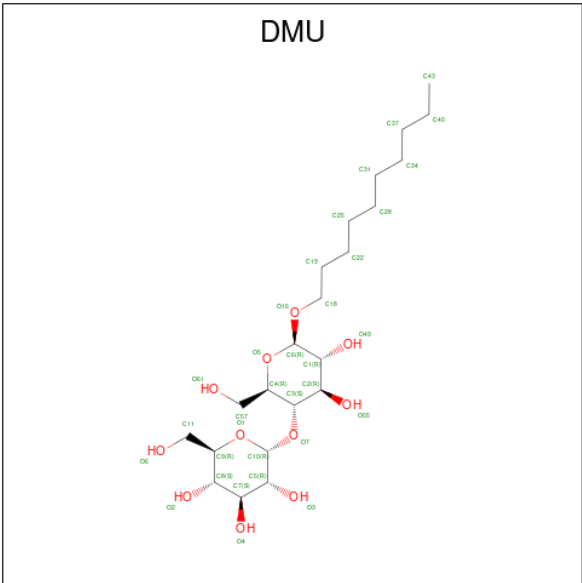
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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



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

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



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

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

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	257	Total O 257 257	0	0
29	B	229	Total O 230 230	0	1
29	C	164	Total O 164 164	0	0
29	D	214	Total O 214 214	0	0
29	E	154	Total O 154 154	0	0
29	F	162	Total O 162 162	0	0
29	G	95	Total O 95 95	0	0
29	H	84	Total O 84 84	0	0
29	I	78	Total O 78 78	0	0
29	J	44	Total O 44 44	0	0

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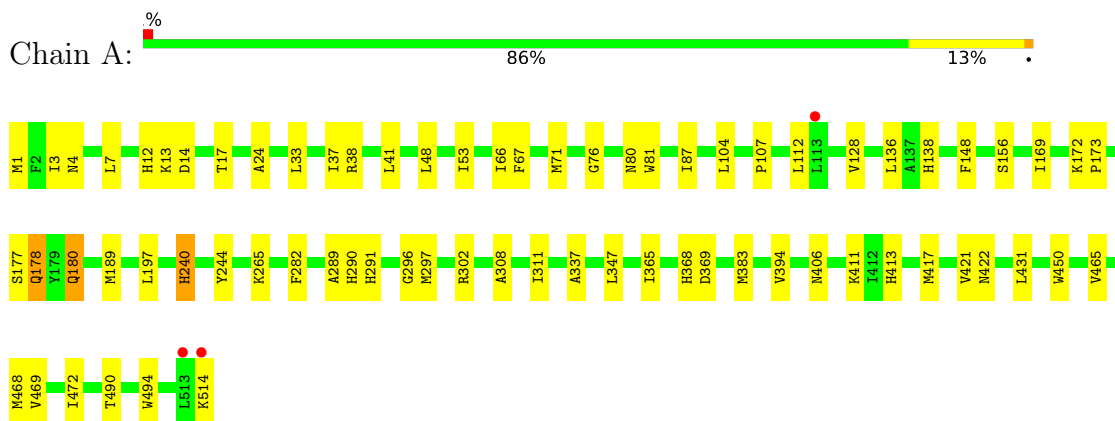
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	K	42	Total 42	O 42	0	0
29	L	57	Total 57	O 57	0	0
29	M	29	Total 29	O 29	0	0
29	N	267	Total 267	O 267	0	0
29	O	186	Total 186	O 186	0	0
29	P	151	Total 151	O 151	0	0
29	Q	98	Total 98	O 98	0	0
29	R	115	Total 115	O 115	0	0
29	S	126	Total 126	O 126	0	0
29	T	87	Total 87	O 87	0	0
29	U	74	Total 74	O 74	0	0
29	V	57	Total 57	O 57	0	0
29	W	32	Total 32	O 32	0	0
29	X	22	Total 22	O 22	0	0
29	Y	37	Total 37	O 37	0	0
29	Z	21	Total 21	O 21	0	0

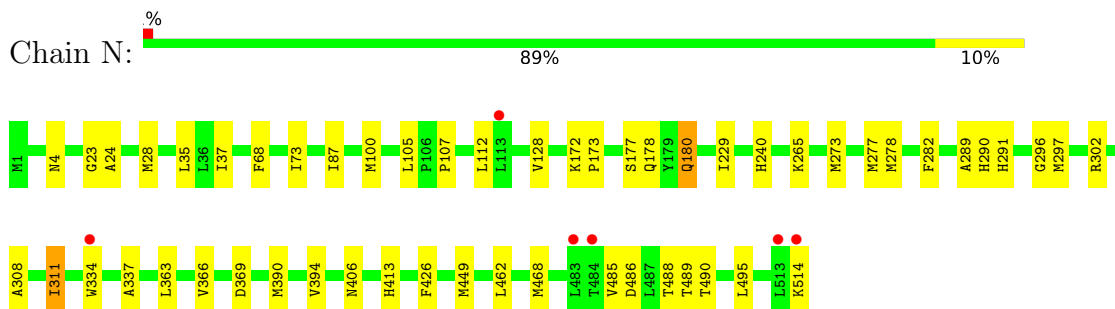
3 Residue-property plots [i](#)

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

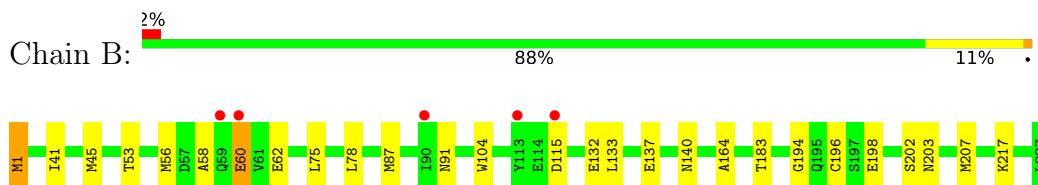
- Molecule 1: Cytochrome c oxidase subunit 1



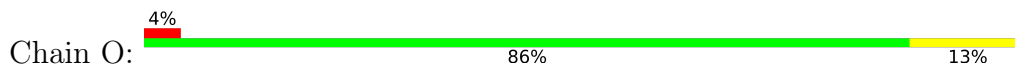
- Molecule 1: Cytochrome c oxidase subunit 1

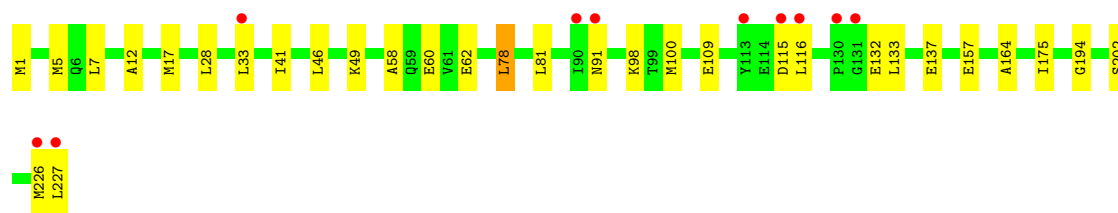


- Molecule 2: Cytochrome c oxidase subunit 2

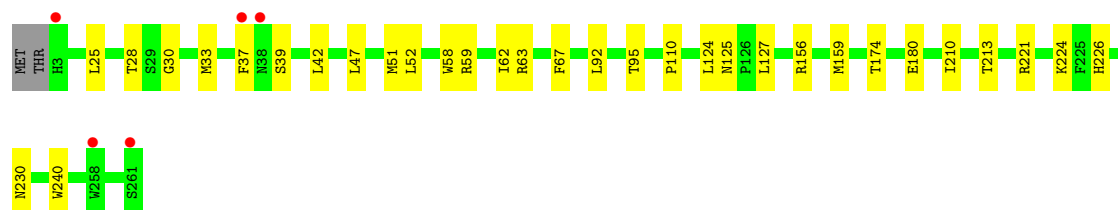
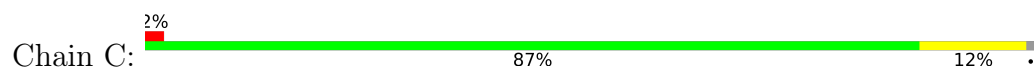


- Molecule 2: Cytochrome c oxidase subunit 2

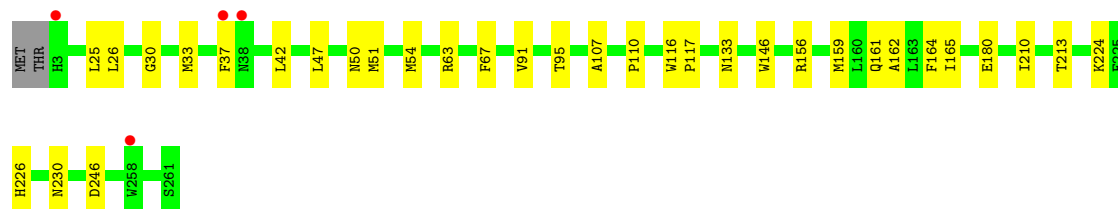
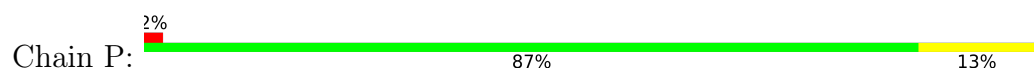




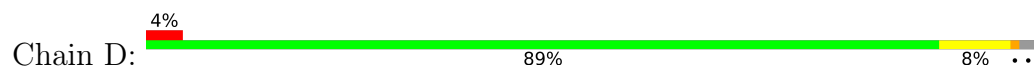
• Molecule 3: Cytochrome c oxidase subunit 3



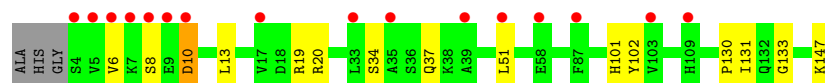
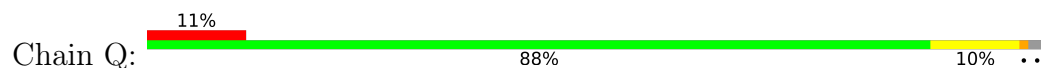
• Molecule 3: Cytochrome c oxidase subunit 3



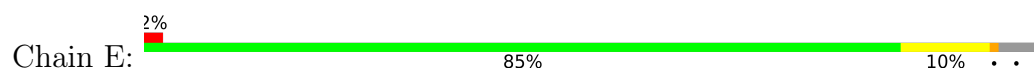
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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

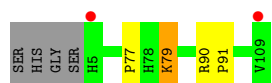


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

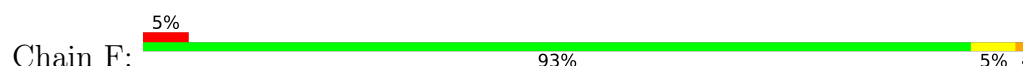




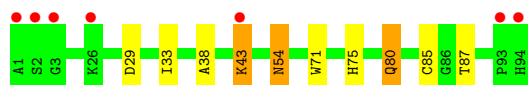
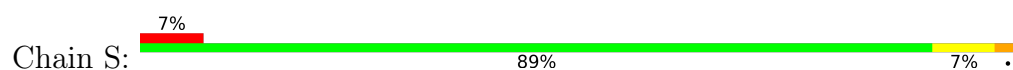
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



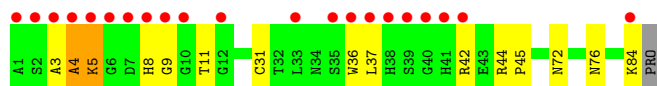
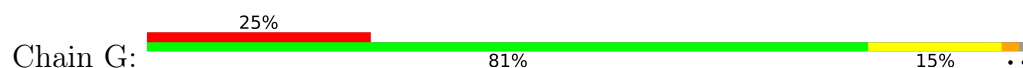
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



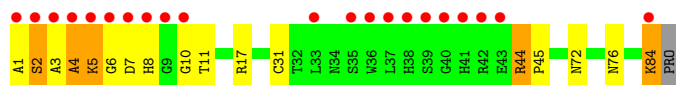
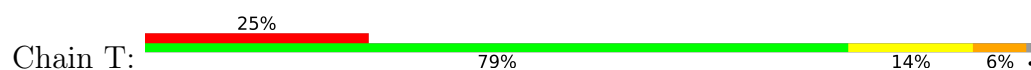
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



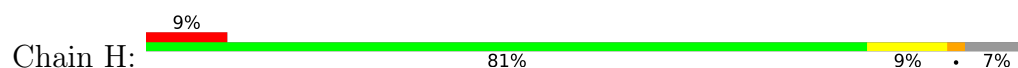
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



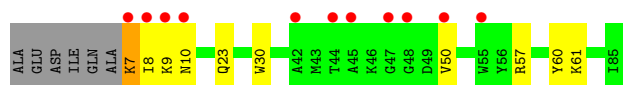
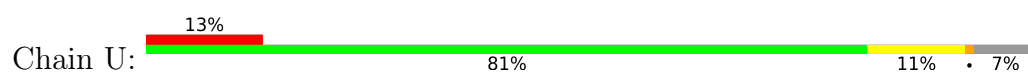
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



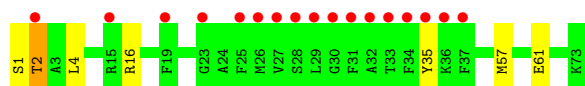
- Molecule 8: Cytochrome c oxidase subunit 6B1



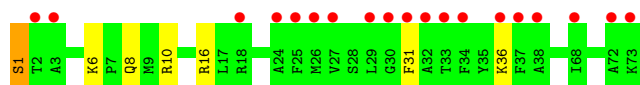
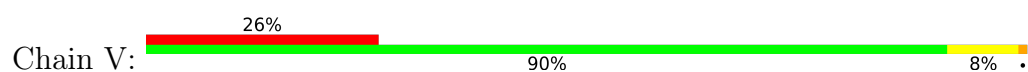
- Molecule 8: Cytochrome c oxidase subunit 6B1



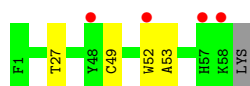
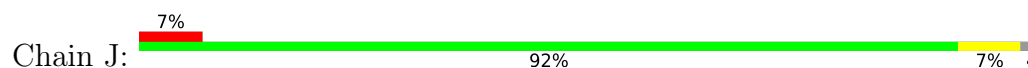
- Molecule 9: Cytochrome c oxidase subunit 6C



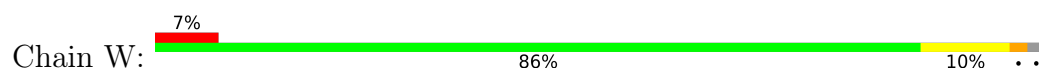
- Molecule 9: Cytochrome c oxidase subunit 6C



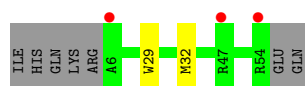
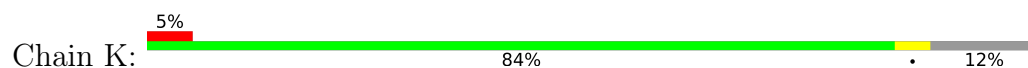
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



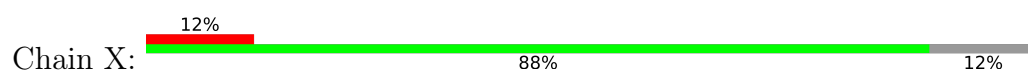
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



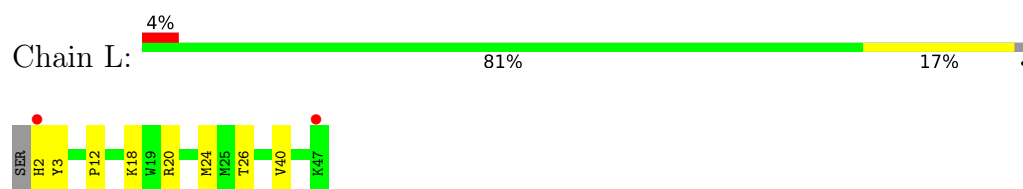
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



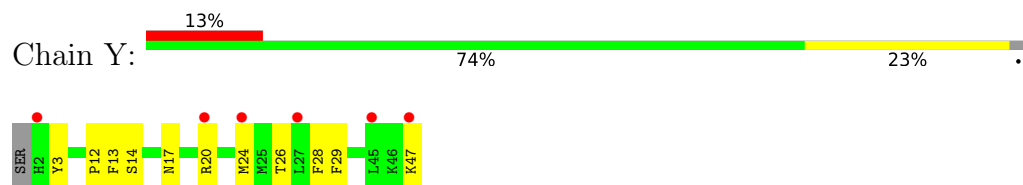
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



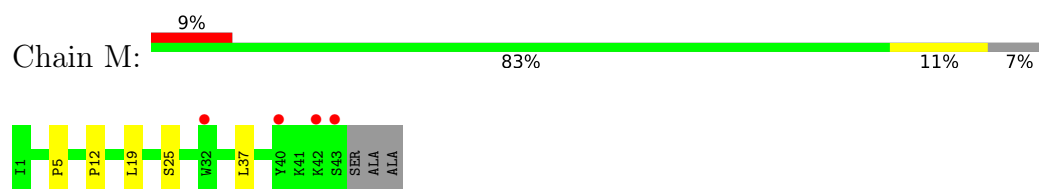
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



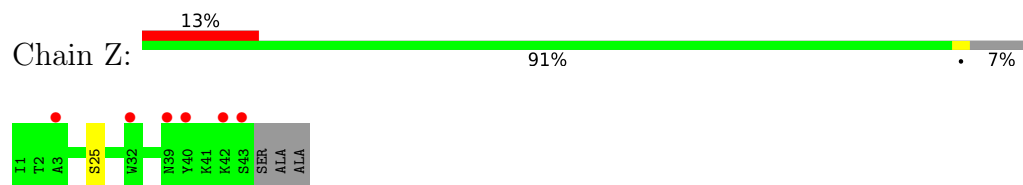
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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	183.31Å 205.90Å 177.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.45 – 1.77 134.45 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.6 (134.45-1.77) 99.6 (134.45-1.77)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.164 , 0.190 0.166 , 0.192	Depositor DCC
R_{free} test set	32362 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 71.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34218	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.77	1/4405 (0.0%)	0.80	1/6009 (0.0%)
1	N	0.74	0/4385	0.81	3/5979 (0.1%)
2	B	0.69	1/1946 (0.1%)	0.78	1/2648 (0.0%)
2	O	0.65	0/1938	0.78	1/2637 (0.0%)
3	C	0.84	0/2298	0.75	0/3139
3	P	0.83	0/2292	0.75	0/3131
4	D	0.66	0/1229	0.73	0/1658
4	Q	0.64	0/1240	0.75	1/1673 (0.1%)
5	E	0.64	0/886	0.73	0/1202
5	R	0.61	0/871	0.78	0/1182
6	F	0.72	0/740	0.76	0/1003
6	S	0.70	0/748	0.76	0/1014
7	G	0.89	0/689	0.78	0/936
7	T	0.89	0/689	0.79	0/936
8	H	0.63	0/682	0.76	0/921
8	U	0.62	0/682	0.76	0/921
9	I	0.52	0/605	0.81	0/802
9	V	0.48	0/605	0.80	0/802
10	J	0.64	0/487	0.70	0/657
10	W	0.65	0/478	0.75	0/645
11	K	0.71	0/405	0.78	0/555
11	X	0.69	0/397	0.77	0/545
12	L	0.76	0/430	0.70	0/575
12	Y	0.69	0/401	0.70	0/536
13	M	0.64	0/352	0.77	0/480
13	Z	0.61	0/344	0.83	0/469
All	All	0.72	2/30224 (0.0%)	0.77	7/41055 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	6.06	1.30	1.23
1	A	368	HIS	ND1-CE1	5.69	1.38	1.32

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	240	HIS	N-CA-CB	7.95	117.94	110.39
1	A	240	HIS	N-CA-CB	6.58	118.18	110.42
4	Q	133	GLY	N-CA-C	6.12	119.89	112.49
1	N	105	LEU	CA-C-N	-5.27	114.95	120.38
1	N	105	LEU	C-N-CA	-5.27	114.95	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4118	0	4147	75	0
1	N	4109	0	4118	60	0
2	B	1859	0	1889	20	0
2	O	1851	0	1866	23	0
3	C	2143	0	2072	40	0
3	P	2140	0	2058	34	0
4	D	1195	0	1183	16	0
4	Q	1200	0	1186	7	0
5	E	858	0	855	21	0
5	R	852	0	845	2	0
6	F	719	0	702	6	0
6	S	722	0	709	10	0
7	G	674	0	644	15	0
7	T	674	0	644	15	0
8	H	662	0	623	8	0
8	U	662	0	623	5	0
9	I	601	0	613	5	0
9	V	601	0	613	7	0
10	J	466	0	466	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	W	462	0	464	8	0
11	K	388	0	375	2	0
11	X	383	0	366	0	0
12	L	399	0	395	10	0
12	Y	382	0	381	12	0
13	M	339	0	363	6	0
13	Z	334	0	352	2	0
14	A	129	0	88	7	0
14	N	129	0	88	13	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	102	0	152	8	0
18	C	102	0	152	7	0
18	N	102	0	152	3	0
18	P	51	0	76	2	0
18	U	51	0	76	2	0
19	A	4	0	0	0	0
19	N	4	0	0	0	0
20	A	44	0	66	5	0
20	B	20	0	30	2	0
20	C	12	0	18	0	0
20	E	4	0	6	0	0
20	F	8	0	12	0	0
20	G	4	0	6	0	0
20	H	4	0	6	1	0
20	J	4	0	6	2	0
20	L	16	0	24	2	0
20	M	8	0	12	0	0
20	N	20	0	30	1	0
20	O	4	0	6	0	0
20	P	24	0	36	0	0
20	Q	4	0	6	0	0
20	R	16	0	24	0	0
20	S	12	0	18	0	0
20	T	8	0	12	0	0
20	W	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	Y	4	0	6	0	0
21	B	63	0	110	3	0
21	D	63	0	110	6	0
21	L	63	0	110	5	0
21	N	63	0	110	4	0
21	O	63	0	110	4	0
21	Q	63	0	110	2	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	52	0	80	6	0
23	O	52	0	80	5	0
24	B	29	0	39	1	0
24	C	58	0	78	2	0
24	G	29	0	39	0	0
24	J	29	0	39	2	0
24	P	58	0	78	5	0
24	W	29	0	39	2	0
25	C	106	0	154	6	0
25	G	53	0	77	1	0
25	P	53	0	77	2	0
25	T	106	0	154	7	0
26	C	100	0	156	16	0
26	G	100	0	156	12	0
26	P	100	0	156	9	0
26	T	100	0	156	7	0
27	C	66	0	84	10	0
27	M	33	0	42	0	0
27	P	33	0	42	0	0
27	W	33	0	42	11	0
27	Z	33	0	42	1	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	257	0	0	4	0
29	B	230	0	0	5	0
29	C	164	0	0	1	0
29	D	214	0	0	6	0
29	E	154	0	0	3	0
29	F	162	0	0	0	0
29	G	95	0	0	0	0
29	H	84	0	0	1	0
29	I	78	0	0	1	0
29	J	44	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	K	42	0	0	1	0
29	L	57	0	0	4	0
29	M	29	0	0	0	0
29	N	267	0	0	3	0
29	O	186	0	0	0	0
29	P	151	0	0	2	0
29	Q	98	0	0	0	0
29	R	115	0	0	0	0
29	S	126	0	0	1	0
29	T	87	0	0	1	0
29	U	74	0	0	0	0
29	V	57	0	0	2	0
29	W	32	0	0	1	0
29	X	22	0	0	0	0
29	Y	37	0	0	0	0
29	Z	21	0	0	0	0
All	All	34218	0	32142	424	0

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

The worst 5 of 424 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:468[B]:MET:HE1	14:N:601[B]:HEA:C23	1.54	1.38
3:C:33[A]:MET:SD	27:C:313:DMU:H11	1.64	1.36
27:C:313:DMU:H8	10:J:53:ALA:HB2	1.25	1.18
1:A:468[B]:MET:HE1	14:A:601[B]:HEA:H212	1.28	1.15
1:N:468[B]:MET:HE1	14:N:601[B]:HEA:C22	1.77	1.14

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	545/514 (106%)	532 (98%)	13 (2%)	0	100	100
1	N	542/514 (105%)	528 (97%)	14 (3%)	0	100	100
2	B	236/227 (104%)	230 (98%)	6 (2%)	0	100	100
2	O	235/227 (104%)	231 (98%)	4 (2%)	0	100	100
3	C	270/261 (103%)	266 (98%)	4 (2%)	0	100	100
3	P	269/261 (103%)	265 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	143/147 (97%)	136 (95%)	5 (4%)	2 (1%)	9	2
5	E	105/109 (96%)	105 (100%)	0	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	93/94 (99%)	91 (98%)	2 (2%)	0	100	100
6	S	94/94 (100%)	93 (99%)	1 (1%)	0	100	100
7	G	81/85 (95%)	71 (88%)	8 (10%)	2 (2%)	4	0
7	T	81/85 (95%)	72 (89%)	4 (5%)	5 (6%)	1	0
8	H	77/85 (91%)	74 (96%)	3 (4%)	0	100	100
8	U	77/85 (91%)	75 (97%)	1 (1%)	1 (1%)	9	2
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	71 (100%)	0	0	100	100
10	J	58/59 (98%)	57 (98%)	1 (2%)	0	100	100
10	W	57/59 (97%)	57 (100%)	0	0	100	100
11	K	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	47/47 (100%)	44 (94%)	3 (6%)	0	100	100
12	Y	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
13	M	42/46 (91%)	42 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3620/3606 (100%)	3528 (98%)	82 (2%)	10 (0%)	36	22

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	T	4	ALA
7	T	5	LYS
7	G	5	LYS
4	Q	8	SER

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	459/426 (108%)	453 (99%)	6 (1%)	61	46
1	N	456/426 (107%)	449 (98%)	7 (2%)	57	41
2	B	221/210 (105%)	214 (97%)	7 (3%)	34	13
2	O	220/210 (105%)	214 (97%)	6 (3%)	39	19
3	C	237/226 (105%)	234 (99%)	3 (1%)	61	46
3	P	236/226 (104%)	232 (98%)	4 (2%)	53	36
4	D	128/129 (99%)	126 (98%)	2 (2%)	55	38
4	Q	129/129 (100%)	126 (98%)	3 (2%)	44	25
5	E	94/95 (99%)	93 (99%)	1 (1%)	65	51
5	R	92/95 (97%)	91 (99%)	1 (1%)	65	51
6	F	79/78 (101%)	77 (98%)	2 (2%)	42	22
6	S	80/78 (103%)	77 (96%)	3 (4%)	29	9
7	G	67/68 (98%)	64 (96%)	3 (4%)	24	6
7	T	67/68 (98%)	64 (96%)	3 (4%)	24	6
8	H	71/75 (95%)	69 (97%)	2 (3%)	38	17
8	U	71/75 (95%)	68 (96%)	3 (4%)	26	7
9	I	57/57 (100%)	56 (98%)	1 (2%)	51	33
9	V	57/57 (100%)	56 (98%)	1 (2%)	51	33
10	J	51/50 (102%)	51 (100%)	0	100	100
10	W	50/50 (100%)	48 (96%)	2 (4%)	28	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	40/46 (87%)	40 (100%)	0	100	100
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	43/40 (108%)	43 (100%)	0	100	100
12	Y	40/40 (100%)	39 (98%)	1 (2%)	42	22
13	M	38/38 (100%)	38 (100%)	0	100	100
13	Z	37/38 (97%)	37 (100%)	0	100	100
All	All	3159/3076 (103%)	3098 (98%)	61 (2%)	51	32

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	180	GLN
8	U	50	VAL
2	O	78	LEU
8	U	7	LYS
10	W	58	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	55	ASN
2	O	181	GLN
8	U	37	HIS
1	N	80	ASN
1	N	422	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	TPO	G	11	7	8,10,11	1.39	1 (12%)	10,14,16	0.81	0
9	SAC	V	1	9	7,8,9	2.01	2 (28%)	7,9,11	1.10	0
2	FME	B	1	2	8,9,10	0.74	0	8,9,11	2.91	3 (37%)
2	FME	O	1	2	8,9,10	0.59	0	8,9,11	1.07	0
7	TPO	T	11	7	8,10,11	1.35	1 (12%)	10,14,16	0.87	0
9	SAC	I	1	9	7,8,9	2.02	2 (28%)	7,9,11	0.82	0
1	FME	N	1	1	8,9,10	0.56	0	8,9,11	1.19	0
1	FME	A	1	1	8,9,10	0.56	0	8,9,11	1.42	2 (25%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	4.70	1.33	1.23
9	V	1	SAC	OAC-C1A	4.54	1.33	1.23
7	G	11	TPO	P-O1P	2.94	1.59	1.50
7	T	11	TPO	P-O1P	2.92	1.59	1.50
9	V	1	SAC	CA-N	2.56	1.50	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-6.99	112.07	122.82
1	A	1	FME	C-CA-N	2.97	115.23	109.50
2	B	1	FME	C-CA-N	2.87	115.03	109.50
1	A	1	FME	O-C-CA	-2.06	119.46	124.77
2	B	1	FME	O1-CN-N	-2.06	120.00	125.32

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	V	1	SAC	1	0
2	B	1	FME	2	0
2	O	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 118 ligands modelled in this entry, 10 are monoatomic - 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
20	EDO	N	610	-	3,3,3	0.46	0	2,2,2	0.32	0
20	EDO	B	307	-	3,3,3	0.47	0	2,2,2	0.33	0
20	EDO	L	102	-	3,3,3	0.38	0	2,2,2	0.48	0
20	EDO	B	309	-	3,3,3	0.53	0	2,2,2	0.27	0
23	PSC	B	303	-	51,51,51	1.13	3 (5%)	57,59,59	0.98	2 (3%)
19	PER	N	608[A]	14,15	1,1,1	0.54	0	-		
20	EDO	S	104	-	3,3,3	0.37	0	2,2,2	0.52	0
20	EDO	E	201	-	3,3,3	0.41	0	2,2,2	0.44	0
25	PEK	T	101	-	52,52,52	0.95	2 (3%)	55,57,57	0.96	3 (5%)
27	DMU	C	313	-	34,34,34	0.54	1 (2%)	45,45,45	0.92	2 (4%)
20	EDO	R	202	-	3,3,3	0.39	0	2,2,2	0.45	0
20	EDO	A	618	-	3,3,3	0.44	0	2,2,2	0.32	0
20	EDO	B	306	-	3,3,3	0.32	0	2,2,2	0.34	0
20	EDO	C	311	-	3,3,3	0.49	0	2,2,2	0.29	0
20	EDO	F	102	-	3,3,3	0.47	0	2,2,2	0.19	0
24	CHD	P	306	-	32,32,32	0.59	0	51,51,51	1.35	7 (13%)
20	EDO	W	102	-	3,3,3	0.43	0	2,2,2	0.37	0
27	DMU	C	312	-	34,34,34	0.49	0	45,45,45	0.87	2 (4%)
20	EDO	P	312	-	3,3,3	0.46	0	2,2,2	0.33	0
18	PGV	U	101	-	50,50,50	0.97	2 (4%)	53,56,56	1.03	3 (5%)
20	EDO	N	612	-	3,3,3	0.42	0	2,2,2	0.32	0
18	PGV	N	609	-	50,50,50	0.87	2 (4%)	53,56,56	0.93	2 (3%)
20	EDO	L	103	-	3,3,3	0.44	0	2,2,2	0.29	0
20	EDO	O	304	-	3,3,3	0.42	0	2,2,2	0.40	0
27	DMU	Z	101	-	34,34,34	0.45	0	45,45,45	0.78	1 (2%)
21	TGL	N	606	-	62,62,62	1.32	6 (9%)	65,65,65	1.12	3 (4%)
14	HEA	N	602	1,19	67,67,67	2.15	26 (38%)	81,103,103	1.15	6 (7%)
18	PGV	A	608	-	50,50,50	0.95	2 (4%)	53,56,56	0.87	3 (5%)
19	PER	A	607[A]	14,15	1,1,1	0.55	0	-		
20	EDO	W	103	-	3,3,3	0.38	0	2,2,2	0.46	0
20	EDO	C	309	-	3,3,3	0.35	0	2,2,2	0.61	0
20	EDO	G	104	-	3,3,3	0.45	0	2,2,2	0.28	0
20	EDO	T	104	-	3,3,3	0.40	0	2,2,2	0.42	0
25	PEK	P	303	-	52,52,52	0.91	3 (5%)	55,57,57	0.90	2 (3%)
20	EDO	S	103	-	3,3,3	0.47	0	2,2,2	0.33	0
20	EDO	A	617	-	3,3,3	0.45	0	2,2,2	0.23	0
20	EDO	J	102	-	3,3,3	0.39	0	2,2,2	0.50	0
24	CHD	C	301	-	32,32,32	0.65	0	51,51,51	1.06	2 (3%)
26	CDL	T	103	-	99,99,99	1.41	12 (12%)	105,111,111	1.10	5 (4%)
20	EDO	S	102	-	3,3,3	0.44	0	2,2,2	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	DMU	P	313	-	34,34,34	0.54	0	45,45,45	1.18	5 (11%)
20	EDO	N	613	-	3,3,3	0.41	0	2,2,2	0.23	0
27	DMU	W	104	-	34,34,34	0.56	1 (2%)	45,45,45	0.77	1 (2%)
18	PGV	N	607	-	50,50,50	0.95	2 (4%)	53,56,56	0.98	5 (9%)
20	EDO	P	308	-	3,3,3	0.40	0	2,2,2	0.43	0
20	EDO	A	615	-	3,3,3	0.34	0	2,2,2	0.54	0
22	CUA	B	302	2	0,1,1	-	-	-	-	-
14	HEA	N	601[B]	-	67,67,67	2.16	27 (40%)	81,103,103	1.14	6 (7%)
20	EDO	F	103	-	3,3,3	0.40	0	2,2,2	0.38	0
20	EDO	N	614	-	3,3,3	0.47	0	2,2,2	0.37	0
24	CHD	P	301	-	32,32,32	0.61	0	51,51,51	1.06	4 (7%)
14	HEA	A	601[B]	-	67,67,67	2.17	27 (40%)	81,103,103	1.16	8 (9%)
20	EDO	A	619	-	3,3,3	0.41	0	2,2,2	0.30	0
18	PGV	C	305	-	50,50,50	0.88	2 (4%)	53,56,56	0.82	2 (3%)
20	EDO	P	311	-	3,3,3	0.50	0	2,2,2	0.25	0
21	TGL	O	301	-	62,62,62	1.31	6 (9%)	65,65,65	1.09	3 (4%)
21	TGL	Q	201	-	62,62,62	1.32	6 (9%)	65,65,65	1.10	4 (6%)
24	CHD	C	308	-	32,32,32	0.68	0	51,51,51	1.72	10 (19%)
18	PGV	A	606	-	50,50,50	0.97	2 (4%)	53,56,56	1.02	3 (5%)
20	EDO	B	308	-	3,3,3	0.39	0	2,2,2	0.45	0
24	CHD	B	304	-	32,32,32	0.66	0	51,51,51	1.01	2 (3%)
25	PEK	T	102	-	52,52,52	0.97	2 (3%)	55,57,57	0.89	3 (5%)
25	PEK	C	303	-	52,52,52	0.88	2 (3%)	55,57,57	0.80	2 (3%)
20	EDO	L	105	-	3,3,3	0.40	0	2,2,2	0.37	0
20	EDO	R	204	-	3,3,3	0.45	0	2,2,2	0.35	0
20	EDO	P	309	-	3,3,3	0.42	0	2,2,2	0.33	0
20	EDO	T	105	-	3,3,3	0.42	0	2,2,2	0.40	0
21	TGL	B	301	-	62,62,62	1.27	6 (9%)	65,65,65	1.12	5 (7%)
20	EDO	B	305	-	3,3,3	0.46	0	2,2,2	0.26	0
24	CHD	W	101	-	32,32,32	0.60	0	51,51,51	1.45	7 (13%)
19	PER	N	608[B]	14,15	1,1,1	8.76	1 (100%)	-	-	-
20	EDO	N	611	-	3,3,3	0.45	0	2,2,2	0.39	0
20	EDO	A	613	-	3,3,3	0.53	0	2,2,2	0.52	0
20	EDO	R	203	-	3,3,3	0.39	0	2,2,2	0.41	0
21	TGL	L	101	-	62,62,62	1.34	6 (9%)	65,65,65	1.13	3 (4%)
26	CDL	G	101	-	99,99,99	1.41	12 (12%)	105,111,111	1.11	6 (5%)
20	EDO	Y	101	-	3,3,3	0.43	0	2,2,2	0.37	0
20	EDO	L	104	-	3,3,3	0.41	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	Q	202	-	3,3,3	0.43	0	2,2,2	0.28	0
26	CDL	P	305	-	99,99,99	1.42	12 (12%)	105,111,111	1.08	5 (4%)
14	HEA	A	602	1,19	67,67,67	2.10	26 (38%)	81,103,103	1.17	9 (11%)
24	CHD	G	102	-	32,32,32	0.68	0	51,51,51	1.07	3 (5%)
24	CHD	J	101	-	32,32,32	0.60	0	51,51,51	1.41	7 (13%)
25	PEK	G	103	-	52,52,52	0.91	2 (3%)	55,57,57	0.98	4 (7%)
20	EDO	C	310	-	3,3,3	0.50	0	2,2,2	0.29	0
20	EDO	A	611	-	3,3,3	0.43	0	2,2,2	0.40	0
20	EDO	A	609	-	3,3,3	0.41	0	2,2,2	0.47	0
20	EDO	A	614	-	3,3,3	0.36	0	2,2,2	0.45	0
21	TGL	D	201	-	62,62,62	1.31	6 (9%)	65,65,65	1.01	5 (7%)
23	PSC	O	303	-	51,51,51	1.11	3 (5%)	57,59,59	1.09	3 (5%)
20	EDO	A	616	-	3,3,3	0.38	0	2,2,2	0.47	0
22	CUA	O	302	2	0,1,1	-	-	-	-	-
19	PER	A	607[B]	14,15	1,1,1	8.90	1 (100%)	-	-	-
20	EDO	A	612	-	3,3,3	0.36	0	2,2,2	0.29	0
18	PGV	C	306	-	50,50,50	0.99	2 (4%)	53,56,56	1.00	3 (5%)
25	PEK	C	304	-	52,52,52	0.94	2 (3%)	55,57,57	0.99	2 (3%)
14	HEA	N	601[A]	-	67,67,67	2.16	27 (40%)	81,103,103	1.17	7 (8%)
20	EDO	P	307	-	3,3,3	0.40	0	2,2,2	0.47	0
14	HEA	A	601[A]	-	67,67,67	2.17	27 (40%)	81,103,103	1.19	9 (11%)
27	DMU	M	101	-	34,34,34	0.44	0	45,45,45	0.88	1 (2%)
20	EDO	A	610	-	3,3,3	0.47	0	2,2,2	0.38	0
20	EDO	H	101	-	3,3,3	0.38	0	2,2,2	0.45	0
20	EDO	P	310	-	3,3,3	0.40	0	2,2,2	0.39	0
26	CDL	C	307	-	99,99,99	1.42	12 (12%)	105,111,111	1.08	4 (3%)
20	EDO	R	201	-	3,3,3	0.43	0	2,2,2	0.38	0
20	EDO	M	102	-	3,3,3	0.39	0	2,2,2	0.41	0
18	PGV	P	304	-	50,50,50	0.89	2 (4%)	53,56,56	0.79	1 (1%)
20	EDO	M	103	-	3,3,3	0.42	0	2,2,2	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	610	-	-	0/1/1/1	-
20	EDO	B	307	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	L	102	-	-	0/1/1/1	-
20	EDO	B	309	-	-	0/1/1/1	-
23	PSC	B	303	-	-	27/55/55/55	-
20	EDO	S	104	-	-	1/1/1/1	-
20	EDO	E	201	-	-	0/1/1/1	-
25	PEK	T	101	-	-	25/56/56/56	-
27	DMU	C	313	-	-	10/19/59/59	0/2/2/2
20	EDO	R	202	-	-	0/1/1/1	-
20	EDO	A	618	-	-	0/1/1/1	-
20	EDO	B	306	-	-	1/1/1/1	-
20	EDO	C	311	-	-	0/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
24	CHD	P	306	-	-	9/9/74/74	0/4/4/4
20	EDO	W	102	-	-	0/1/1/1	-
27	DMU	C	312	-	-	10/19/59/59	0/2/2/2
20	EDO	P	312	-	-	0/1/1/1	-
18	PGV	U	101	-	-	27/55/55/55	-
20	EDO	N	612	-	-	0/1/1/1	-
18	PGV	N	609	-	-	13/55/55/55	-
20	EDO	L	103	-	-	0/1/1/1	-
20	EDO	O	304	-	-	0/1/1/1	-
27	DMU	Z	101	-	-	7/19/59/59	0/2/2/2
21	TGL	N	606	-	-	31/65/65/65	-
14	HEA	N	602	1,19	-	6/36/76/76	-
18	PGV	A	608	-	-	11/55/55/55	-
20	EDO	W	103	-	-	1/1/1/1	-
20	EDO	C	309	-	-	0/1/1/1	-
20	EDO	G	104	-	-	0/1/1/1	-
20	EDO	T	104	-	-	0/1/1/1	-
25	PEK	P	303	-	-	16/56/56/56	-
20	EDO	S	103	-	-	0/1/1/1	-
20	EDO	A	617	-	-	1/1/1/1	-
20	EDO	J	102	-	-	0/1/1/1	-
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
26	CDL	T	103	-	-	59/110/110/110	-
20	EDO	S	102	-	-	0/1/1/1	-
27	DMU	P	313	-	-	8/19/59/59	0/2/2/2
20	EDO	N	613	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DMU	W	104	-	-	9/19/59/59	0/2/2/2
18	PGV	N	607	-	-	28/55/55/55	-
20	EDO	P	308	-	-	1/1/1/1	-
20	EDO	A	615	-	-	1/1/1/1	-
14	HEA	N	601[B]	-	-	9/36/76/76	-
20	EDO	F	103	-	-	0/1/1/1	-
20	EDO	N	614	-	-	0/1/1/1	-
24	CHD	P	301	-	-	2/9/74/74	0/4/4/4
14	HEA	A	601[B]	-	-	8/36/76/76	-
20	EDO	A	619	-	-	1/1/1/1	-
18	PGV	C	305	-	-	19/55/55/55	-
20	EDO	P	311	-	-	0/1/1/1	-
21	TGL	O	301	-	-	34/65/65/65	-
21	TGL	Q	201	-	-	35/65/65/65	-
24	CHD	C	308	-	-	8/9/74/74	0/4/4/4
18	PGV	A	606	-	-	25/55/55/55	-
20	EDO	B	308	-	-	1/1/1/1	-
24	CHD	B	304	-	-	2/9/74/74	0/4/4/4
25	PEK	T	102	-	-	30/56/56/56	-
25	PEK	C	303	-	-	17/56/56/56	-
20	EDO	L	105	-	-	1/1/1/1	-
20	EDO	R	204	-	-	0/1/1/1	-
20	EDO	P	309	-	-	1/1/1/1	-
20	EDO	T	105	-	-	1/1/1/1	-
21	TGL	B	301	-	-	42/65/65/65	-
20	EDO	B	305	-	-	0/1/1/1	-
24	CHD	W	101	-	-	5/9/74/74	0/4/4/4
20	EDO	N	611	-	-	0/1/1/1	-
20	EDO	A	613	-	-	0/1/1/1	-
20	EDO	R	203	-	-	0/1/1/1	-
21	TGL	L	101	-	-	33/65/65/65	-
26	CDL	G	101	-	-	64/110/110/110	-
20	EDO	Y	101	-	-	0/1/1/1	-
20	EDO	L	104	-	-	0/1/1/1	-
20	EDO	Q	202	-	-	1/1/1/1	-
26	CDL	P	305	-	-	67/110/110/110	-
14	HEA	A	602	1,19	-	6/36/76/76	-
24	CHD	G	102	-	-	2/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHD	J	101	-	-	5/9/74/74	0/4/4/4
25	PEK	G	103	-	-	31/56/56/56	-
20	EDO	C	310	-	-	0/1/1/1	-
20	EDO	A	611	-	-	0/1/1/1	-
20	EDO	A	609	-	-	1/1/1/1	-
20	EDO	A	614	-	-	0/1/1/1	-
21	TGL	D	201	-	-	39/65/65/65	-
23	PSC	O	303	-	-	31/55/55/55	-
20	EDO	A	616	-	-	0/1/1/1	-
20	EDO	A	612	-	-	0/1/1/1	-
18	PGV	C	306	-	-	25/55/55/55	-
25	PEK	C	304	-	-	25/56/56/56	-
14	HEA	N	601[A]	-	-	7/36/76/76	-
20	EDO	P	307	-	-	1/1/1/1	-
14	HEA	A	601[A]	-	-	8/36/76/76	-
27	DMU	M	101	-	-	8/19/59/59	0/2/2/2
20	EDO	A	610	-	-	0/1/1/1	-
20	EDO	H	101	-	-	1/1/1/1	-
20	EDO	P	310	-	-	1/1/1/1	-
26	CDL	C	307	-	-	66/110/110/110	-
20	EDO	R	201	-	-	0/1/1/1	-
20	EDO	M	102	-	-	0/1/1/1	-
18	PGV	P	304	-	-	18/55/55/55	-
20	EDO	M	103	-	-	1/1/1/1	-

The worst 5 of 283 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	607[B]	PER	O2-O1	8.90	2.67	1.42
19	N	608[B]	PER	O2-O1	8.76	2.65	1.42
14	N	602	HEA	FE-NB	5.64	2.12	1.94
14	A	601[A]	HEA	FE-ND	5.58	2.12	1.94
14	A	601[B]	HEA	FE-ND	5.58	2.12	1.94

The worst 5 of 185 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	308	CHD	C17-C13-C12	-4.66	113.47	117.67
21	L	101	TGL	OG2-CB1-CB2	4.58	121.39	111.48
26	G	101	CDL	OA6-CA5-C11	4.57	121.37	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	308	CHD	C16-C17-C20	4.49	118.97	112.18
23	O	303	PSC	O01-C1-C2	4.42	121.05	111.48

There are no chirality outliers.

5 of 987 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C2A-C3A-CMA-OMA
14	A	601[B]	HEA	C2A-C3A-CMA-OMA
14	A	602	HEA	C2A-C3A-CMA-OMA
14	A	602	HEA	C4A-C3A-CMA-OMA
14	N	601[A]	HEA	C2A-C3A-CMA-OMA

There are no ring outliers.

48 monomers are involved in 175 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	303	PSC	6	0
25	T	101	PEK	3	0
27	C	313	DMU	10	0
20	B	306	EDO	2	0
24	P	306	CHD	4	0
18	U	101	PGV	2	0
20	L	103	EDO	2	0
27	Z	101	DMU	1	0
21	N	606	TGL	4	0
14	N	602	HEA	2	0
18	A	608	PGV	2	0
25	P	303	PEK	2	0
20	J	102	EDO	2	0
26	T	103	CDL	7	0
20	N	613	EDO	1	0
27	W	104	DMU	11	0
18	N	607	PGV	3	0
20	A	615	EDO	1	0
14	N	601[B]	HEA	10	0
24	P	301	CHD	1	0
14	A	601[B]	HEA	4	0
20	A	619	EDO	3	0
18	C	305	PGV	6	0
21	O	301	TGL	4	0

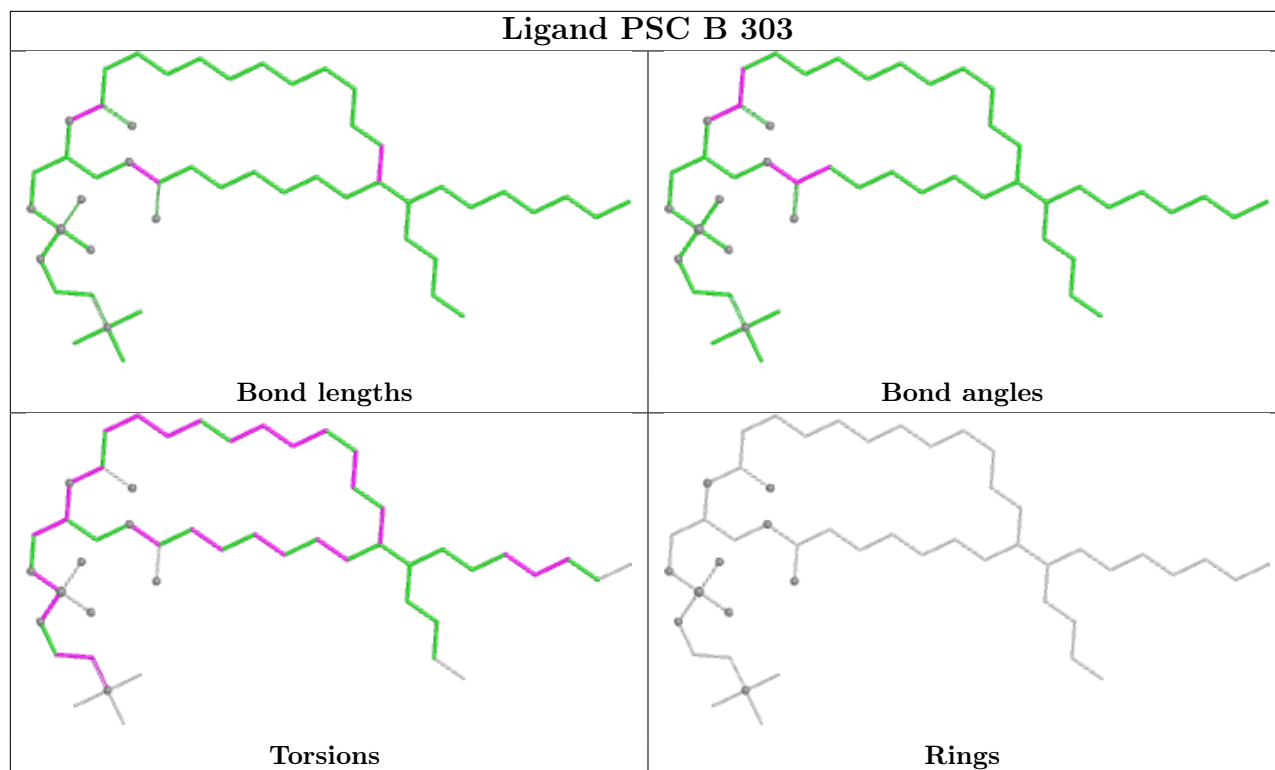
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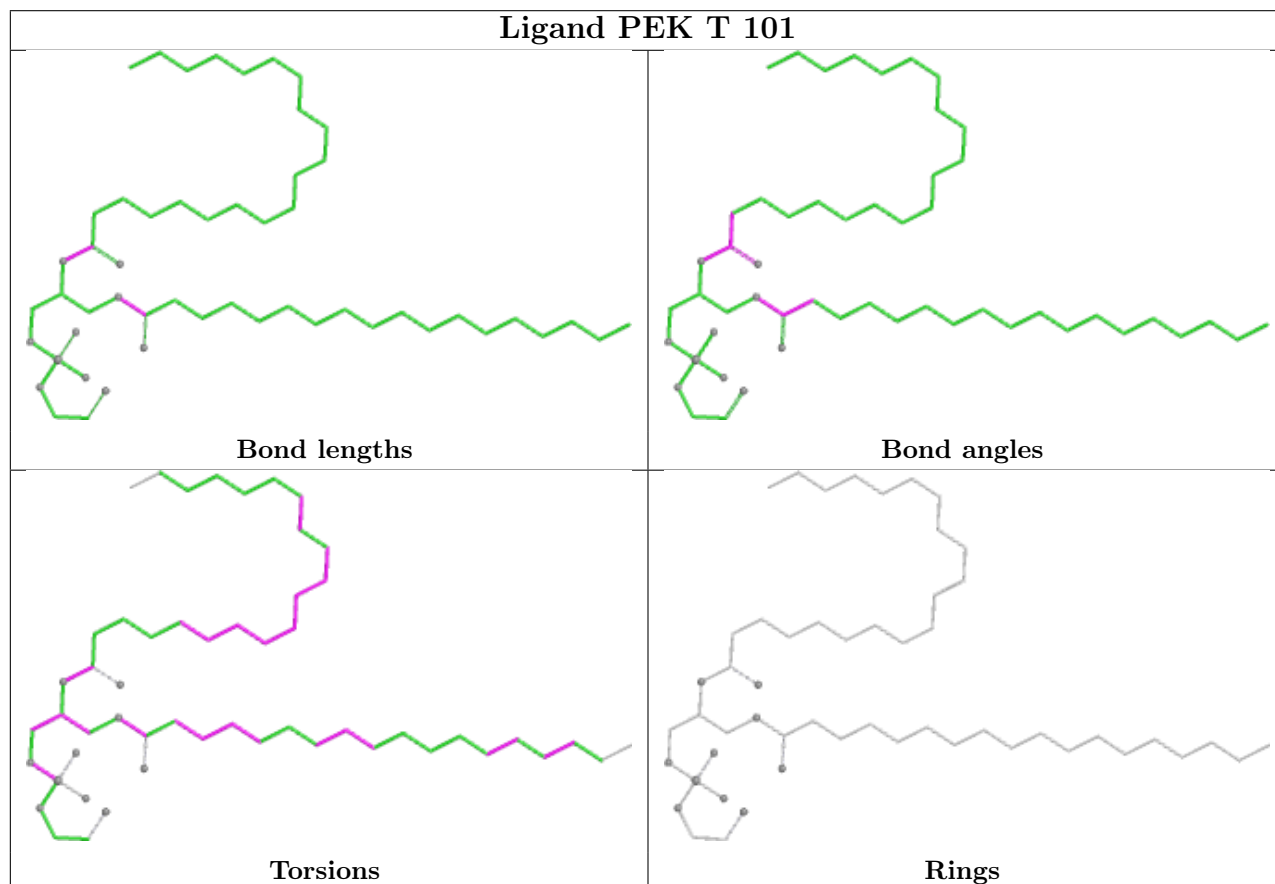
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	Q	201	TGL	2	0
24	C	308	CHD	2	0
18	A	606	PGV	6	0
24	B	304	CHD	1	0
25	T	102	PEK	4	0
25	C	303	PEK	3	0
21	B	301	TGL	3	0
24	W	101	CHD	2	0
21	L	101	TGL	5	0
26	G	101	CDL	12	0
26	P	305	CDL	9	0
14	A	602	HEA	2	0
24	J	101	CHD	2	0
25	G	103	PEK	1	0
21	D	201	TGL	6	0
23	O	303	PSC	5	0
20	A	612	EDO	1	0
18	C	306	PGV	1	0
25	C	304	PEK	3	0
14	N	601[A]	HEA	1	0
14	A	601[A]	HEA	1	0
20	H	101	EDO	1	0
26	C	307	CDL	16	0
18	P	304	PGV	2	0

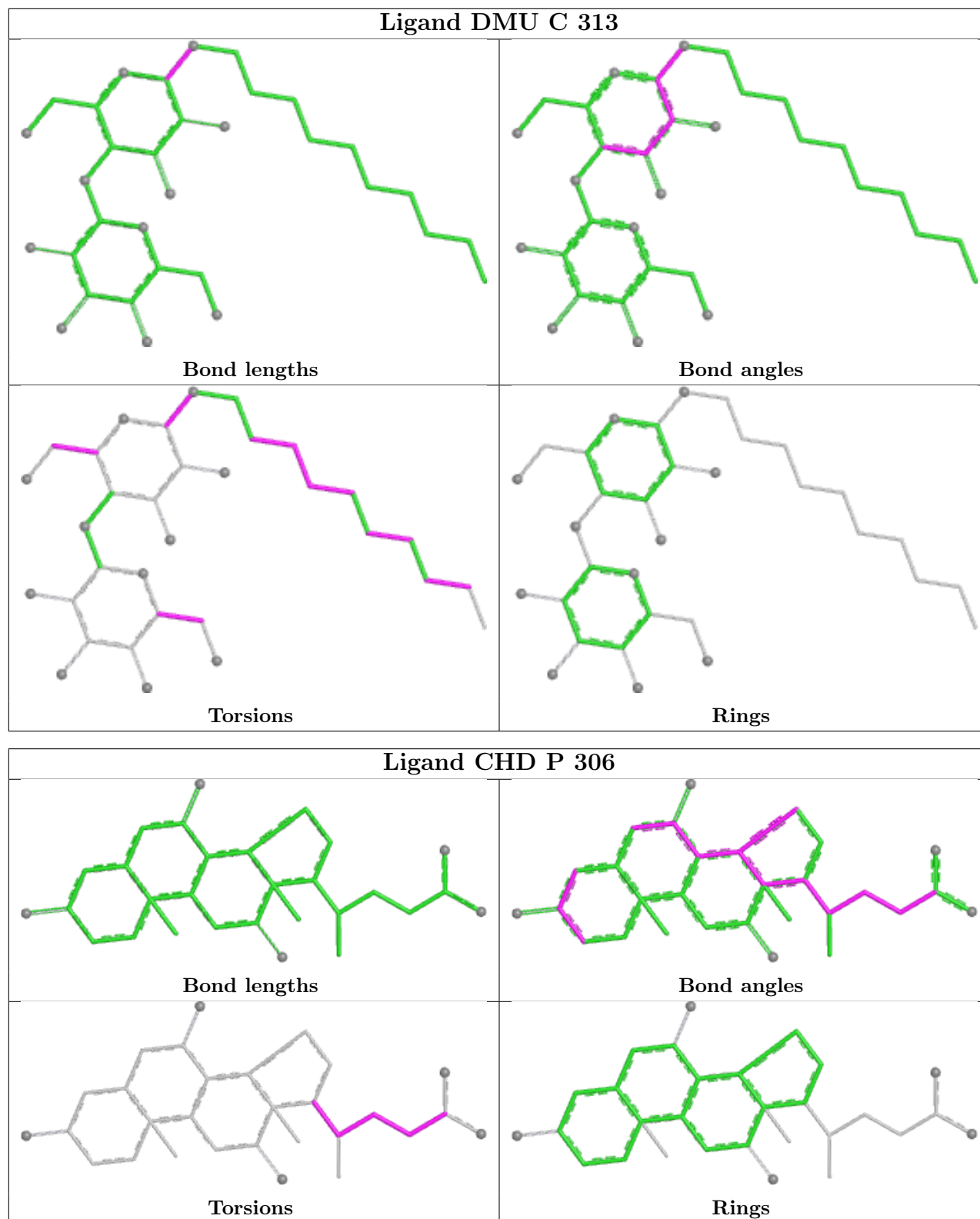
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

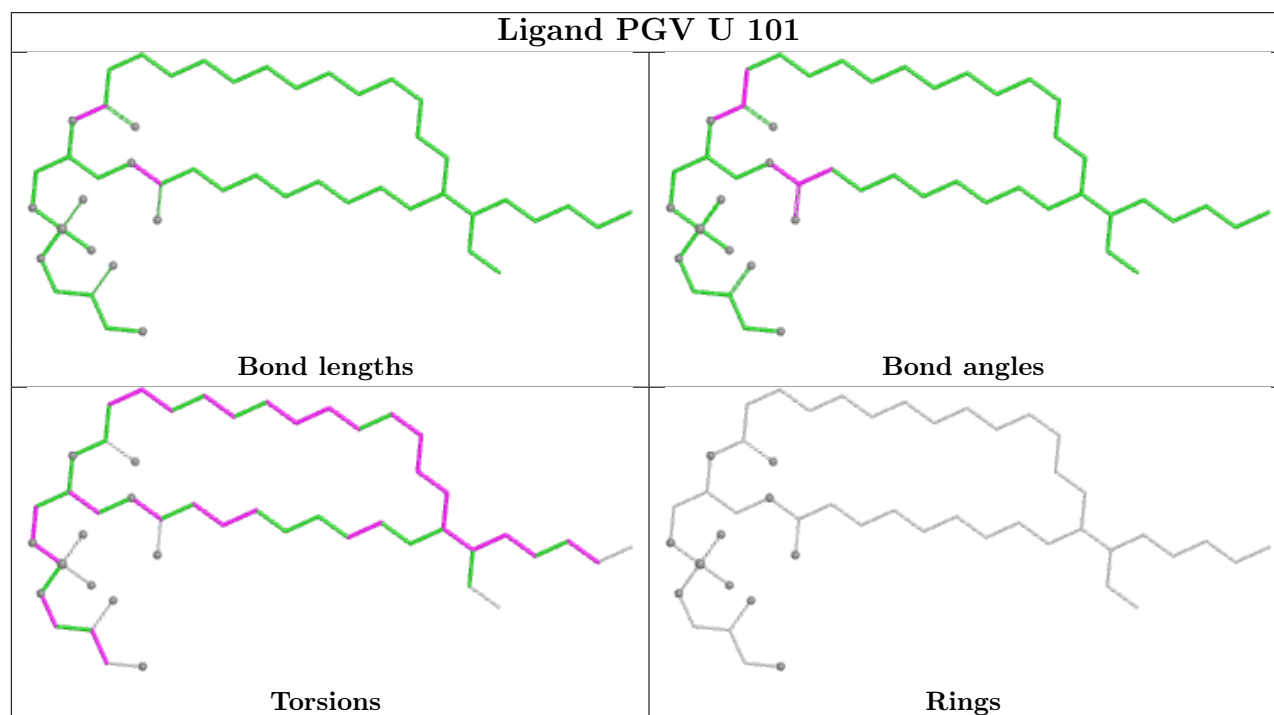
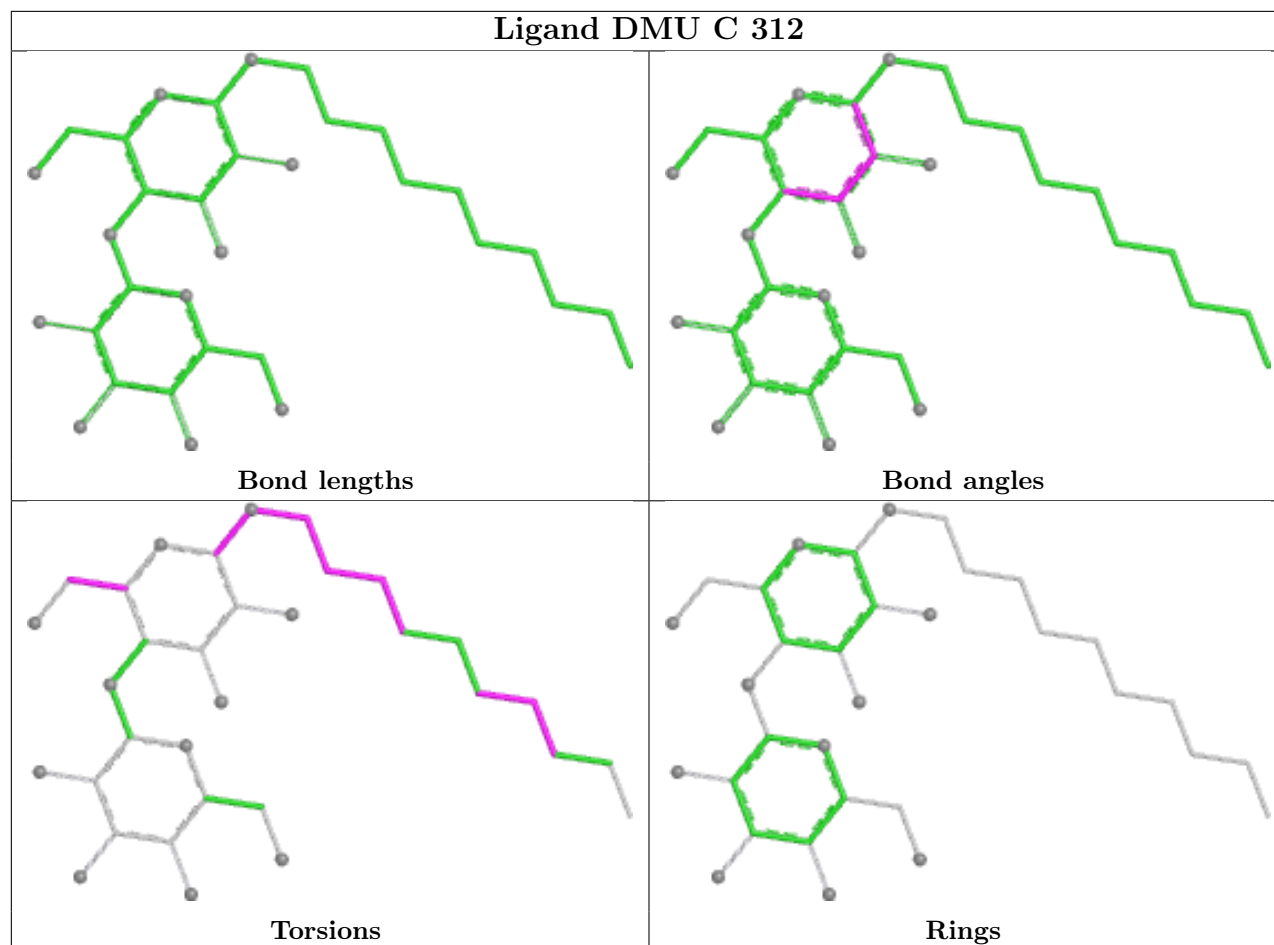
Ligand PSC B 303

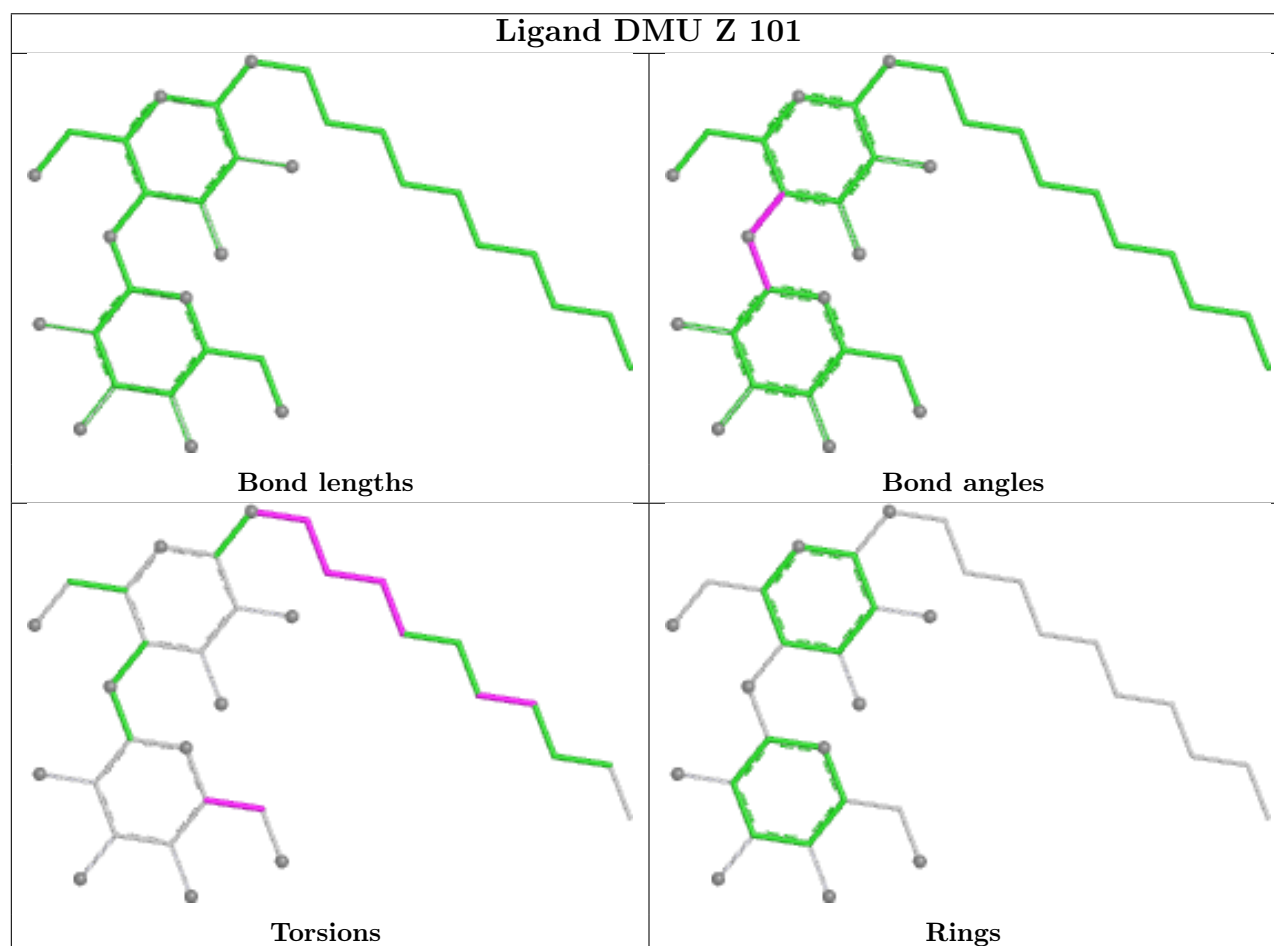
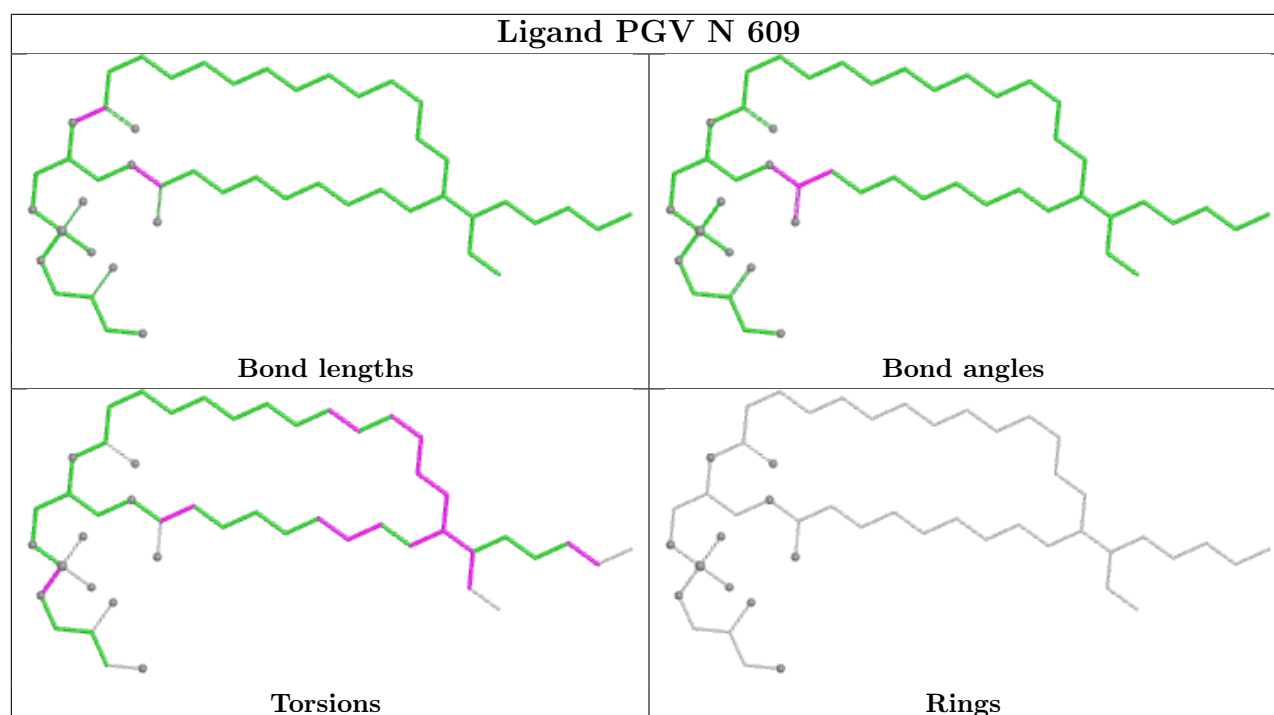


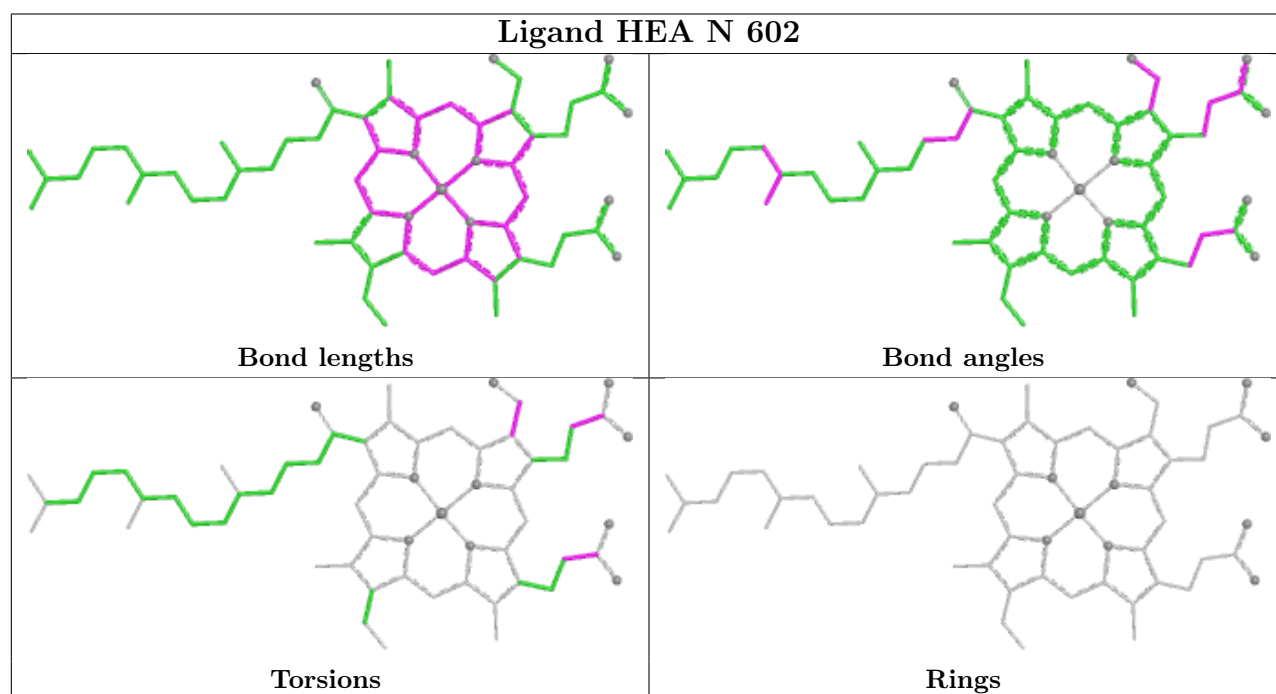
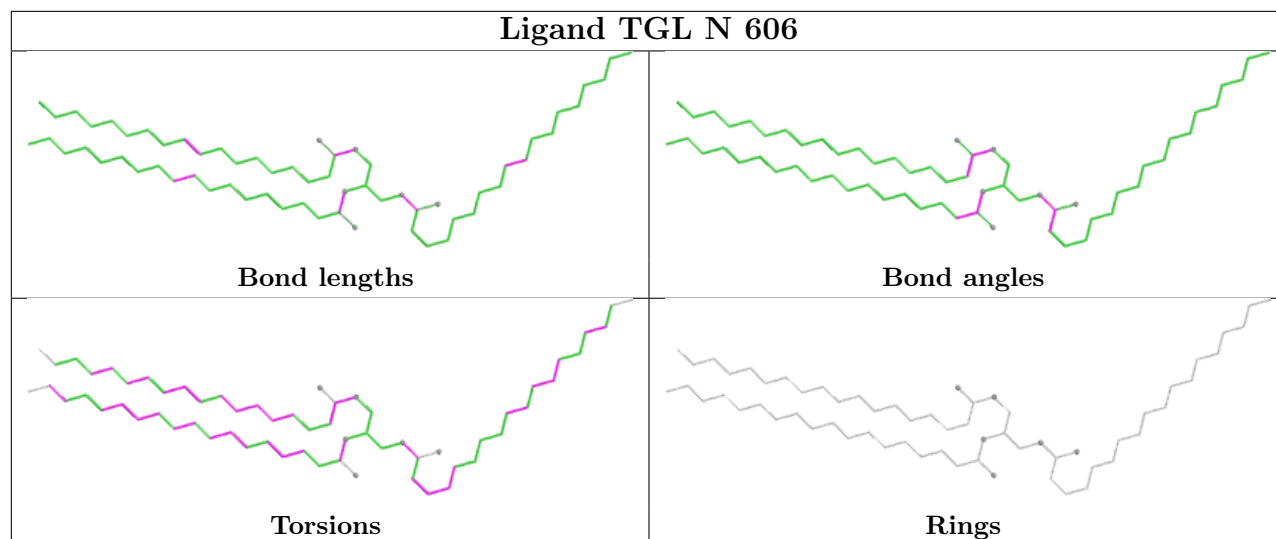
Ligand PEK T 101

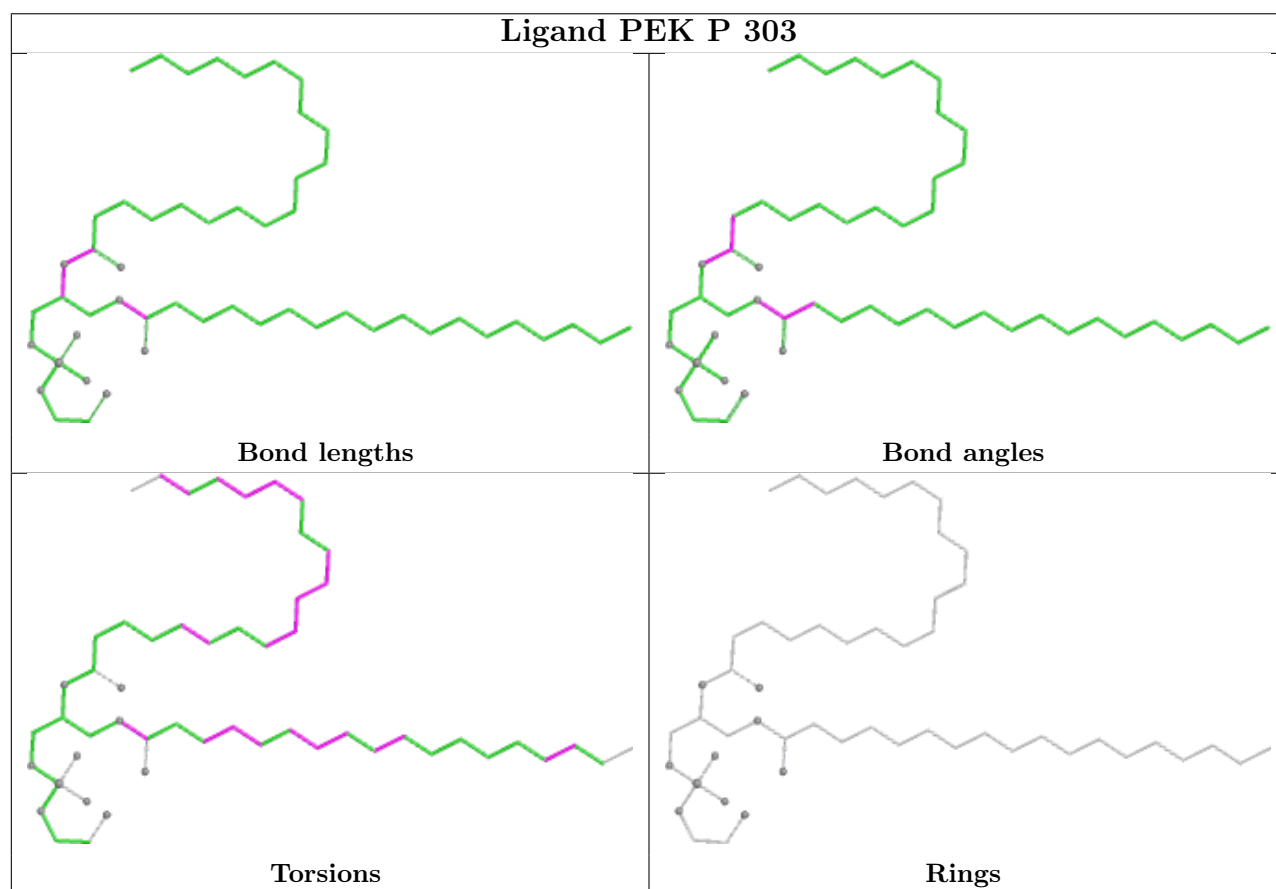
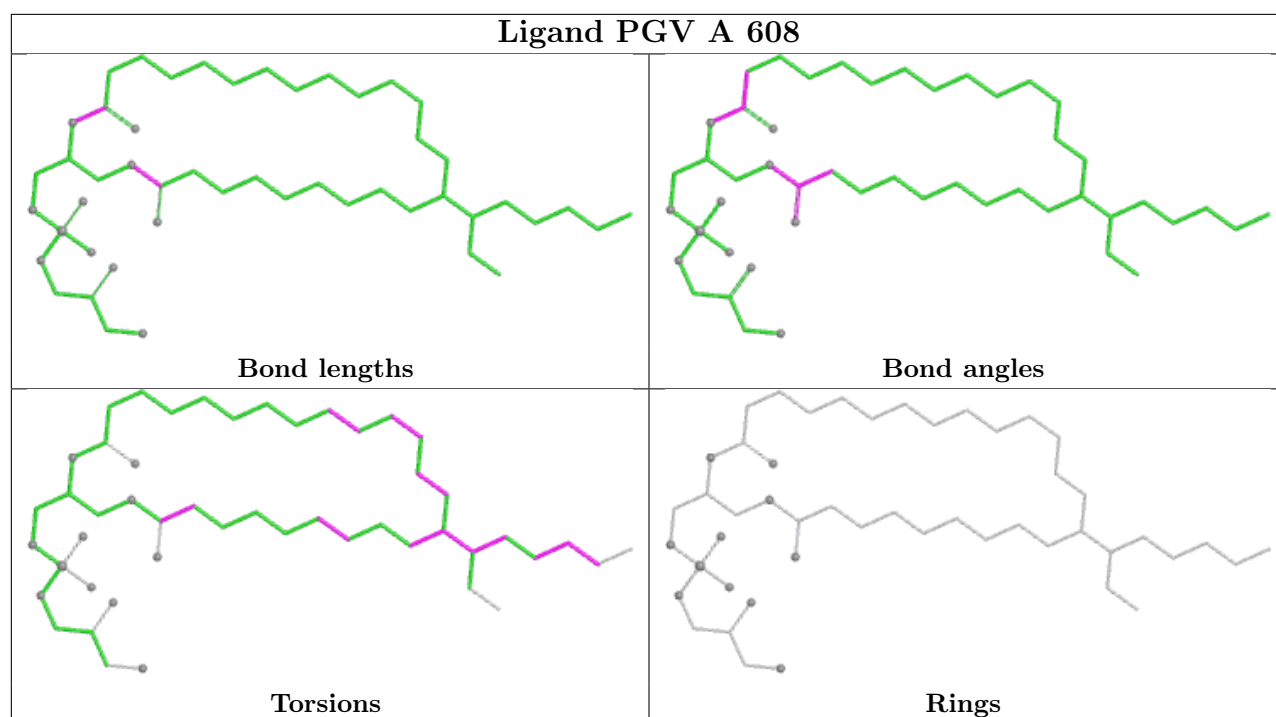


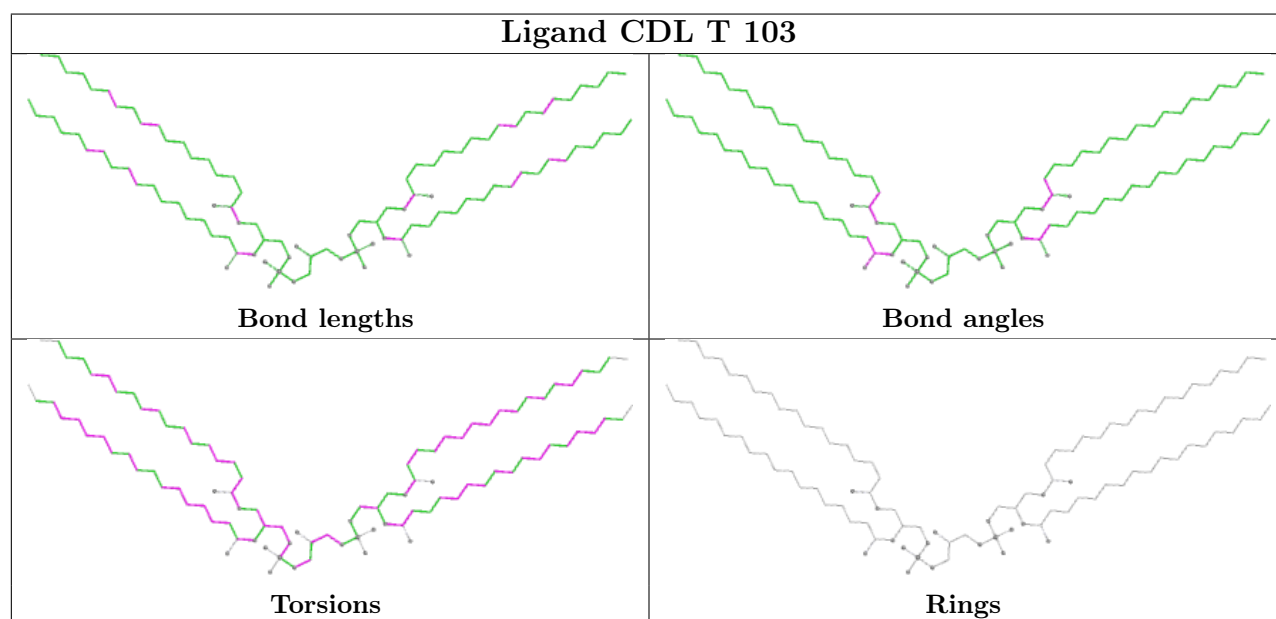
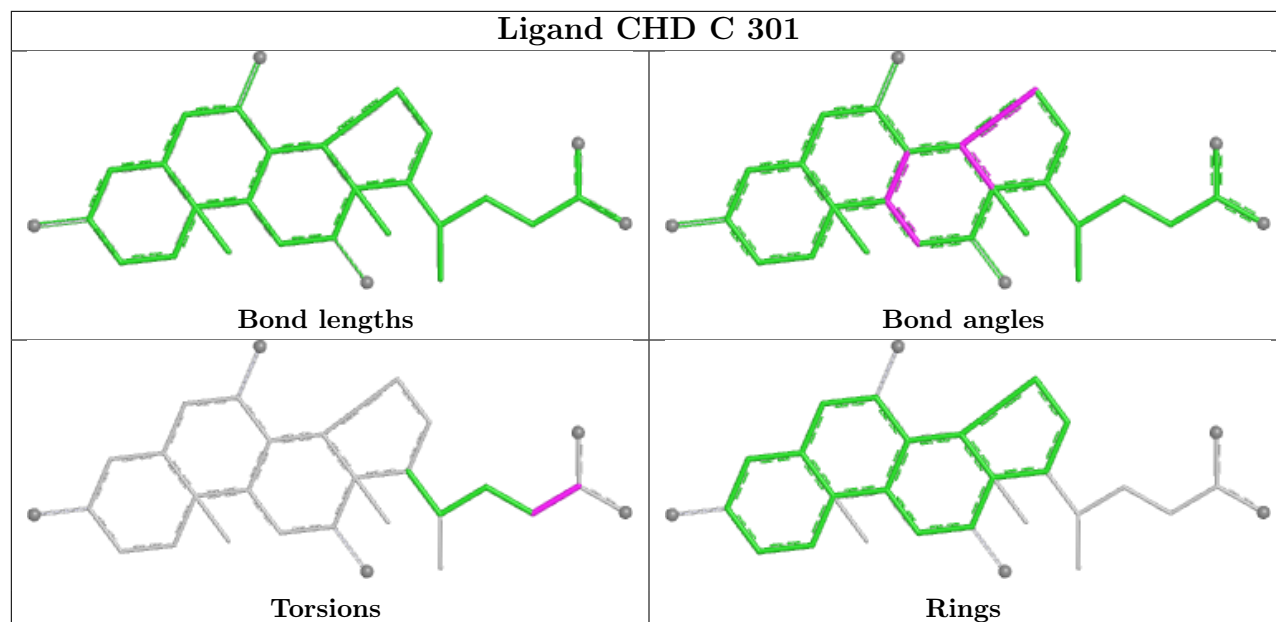


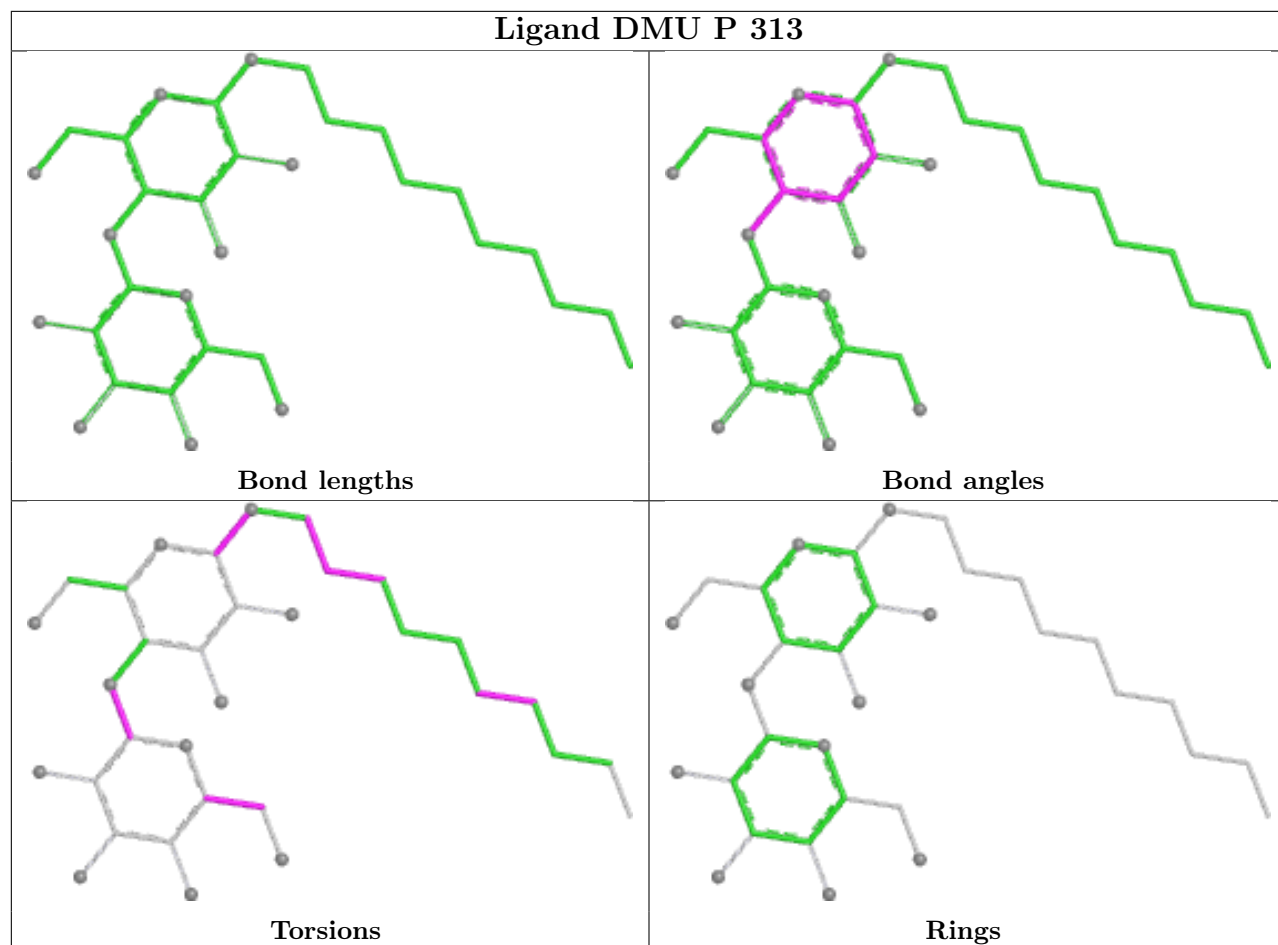




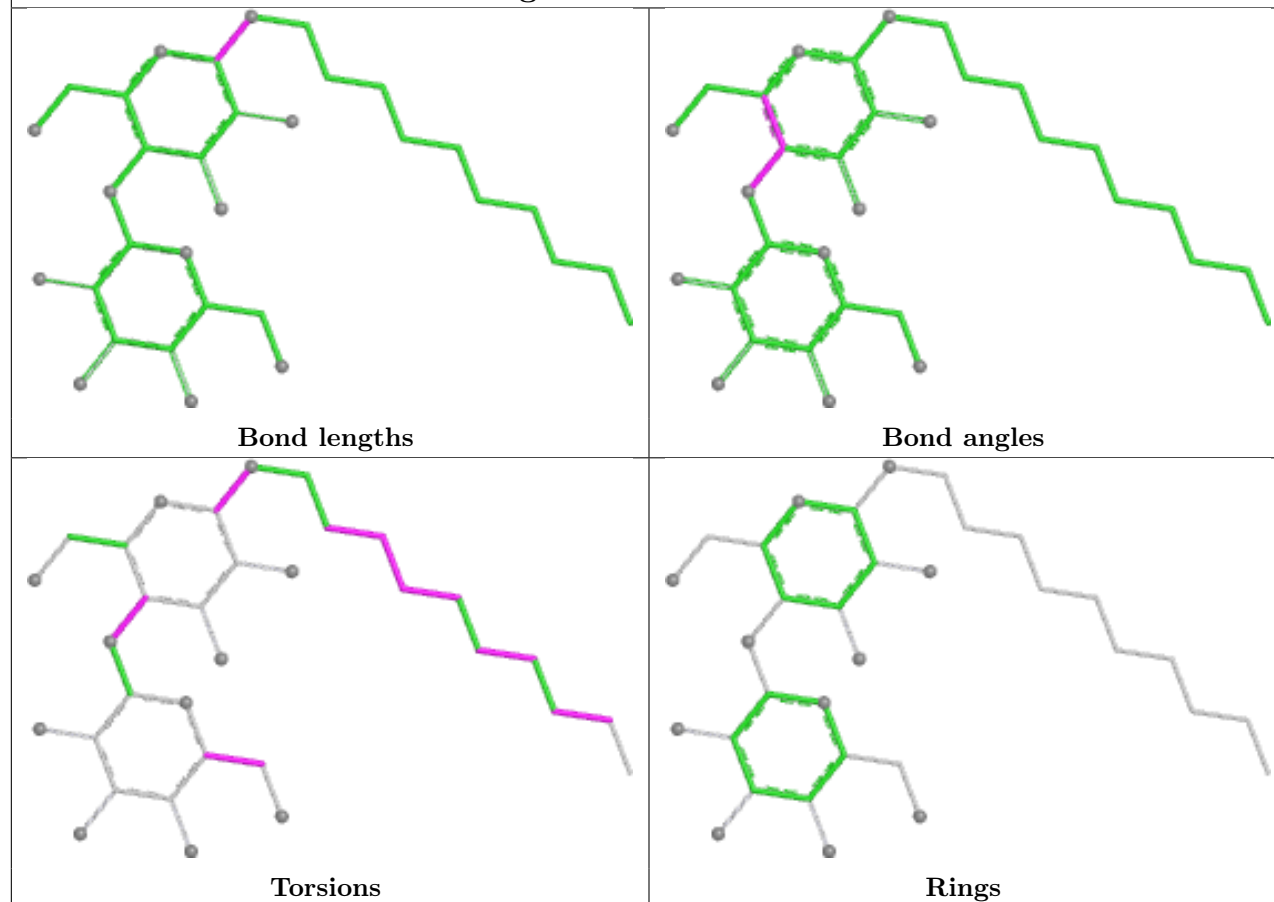




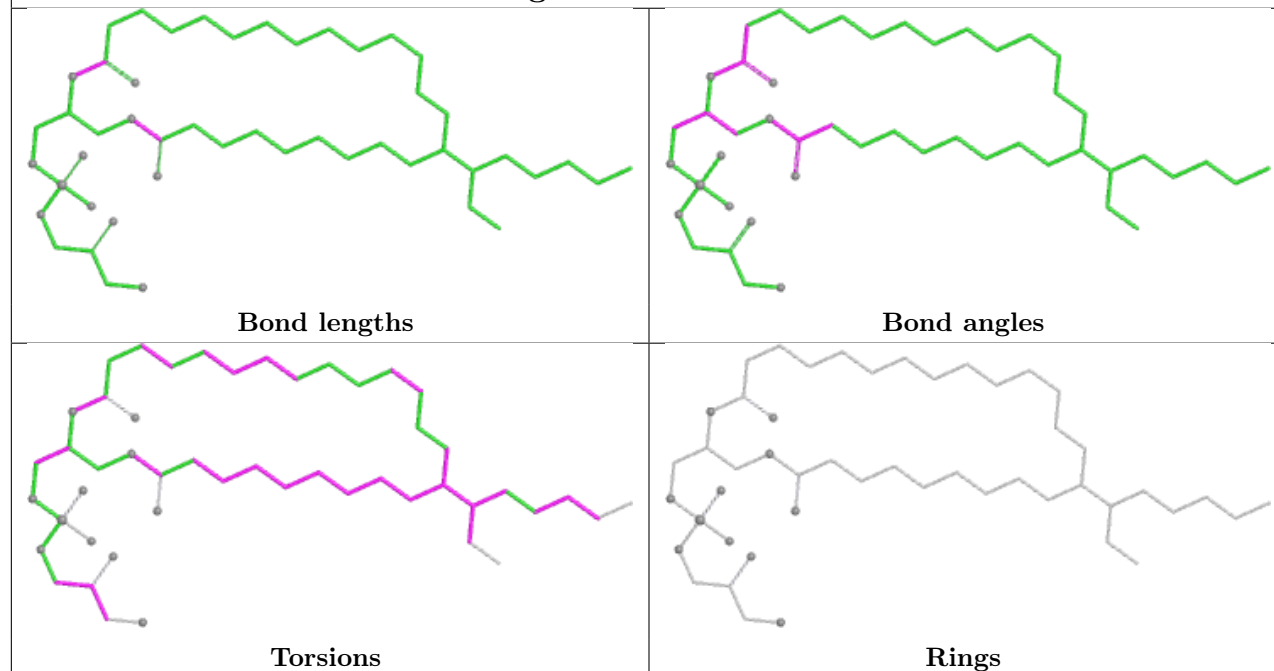




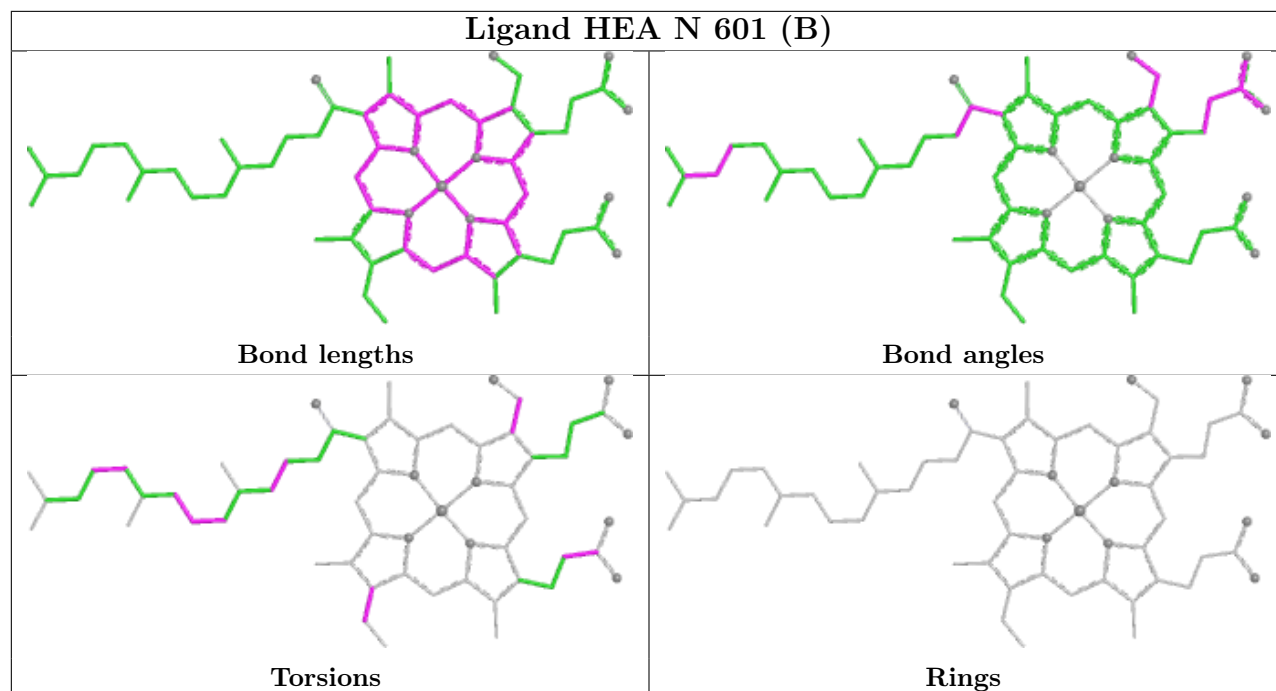
Ligand DMU W 104



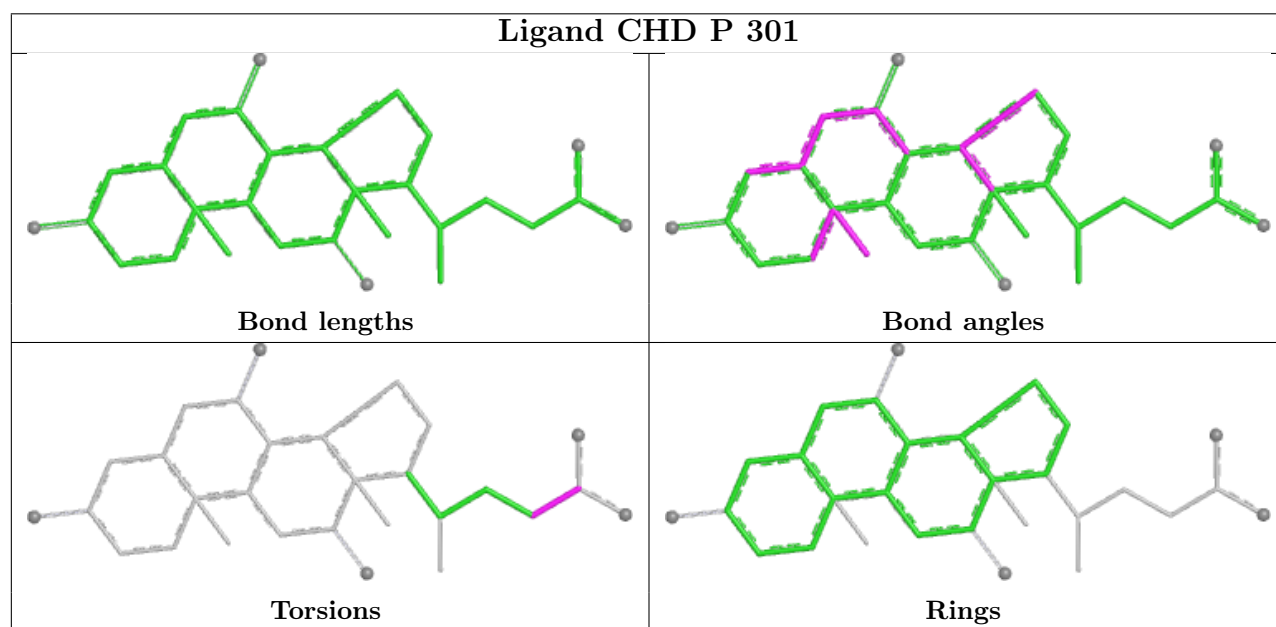
Ligand PGV N 607

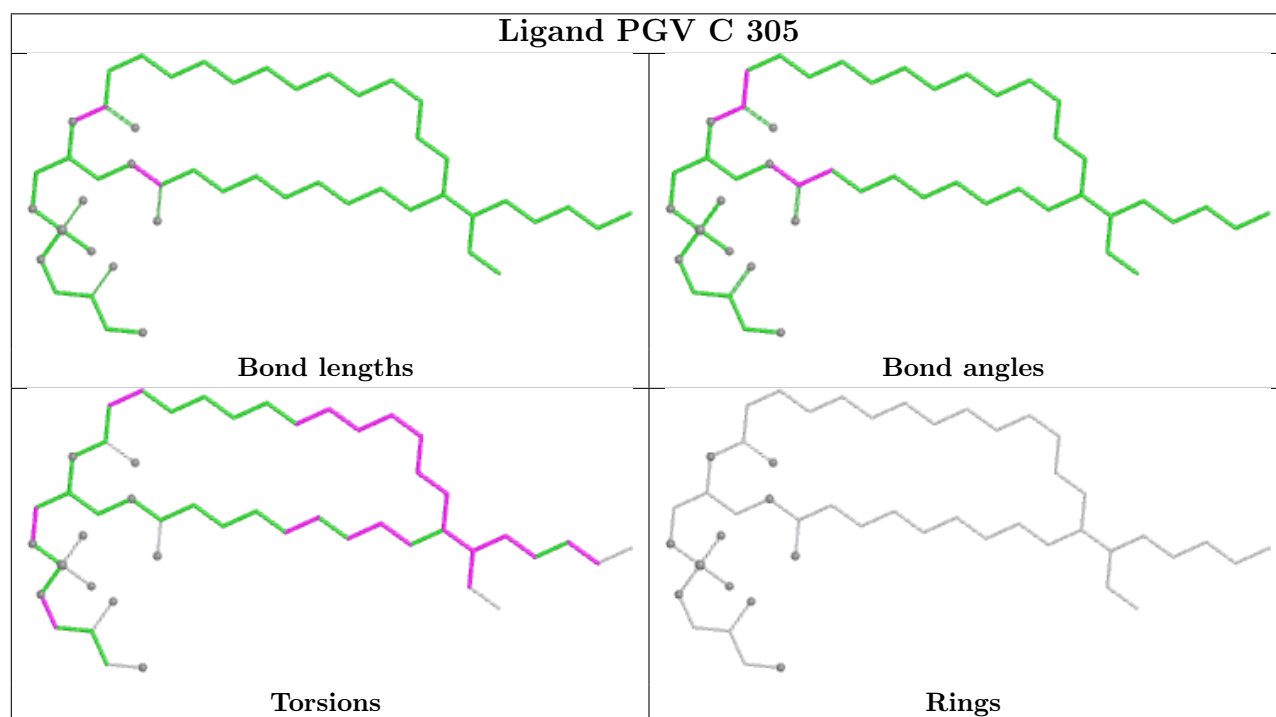
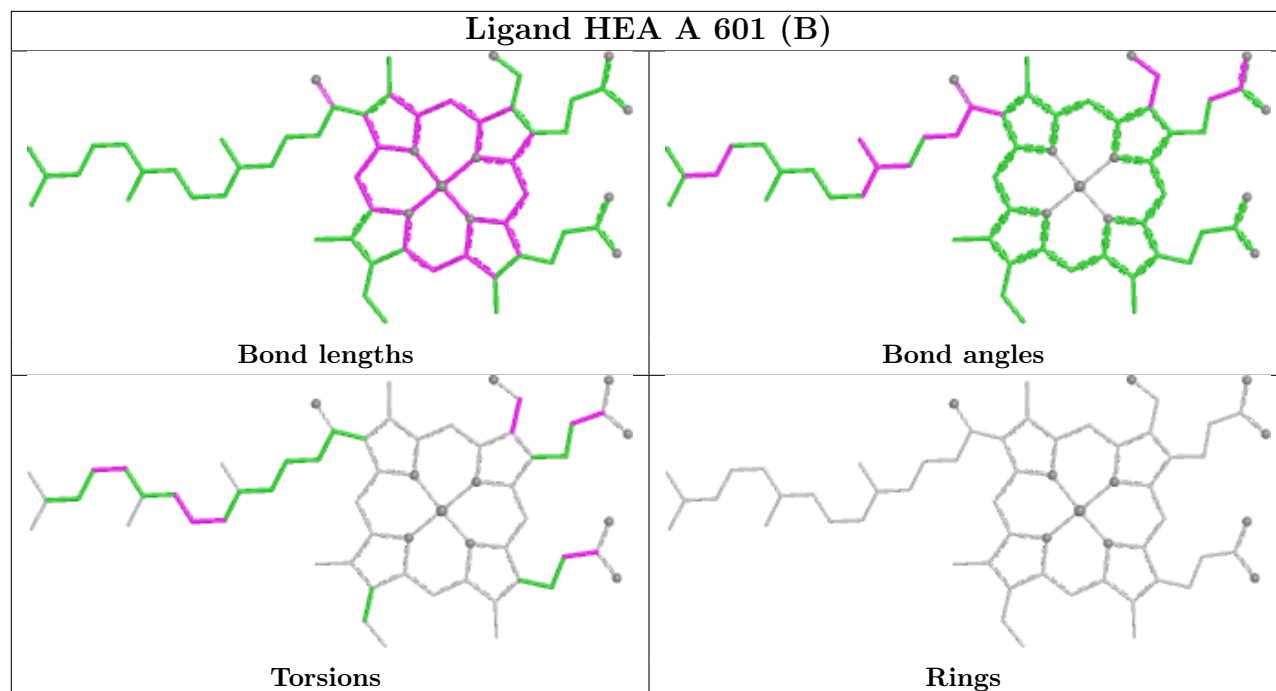


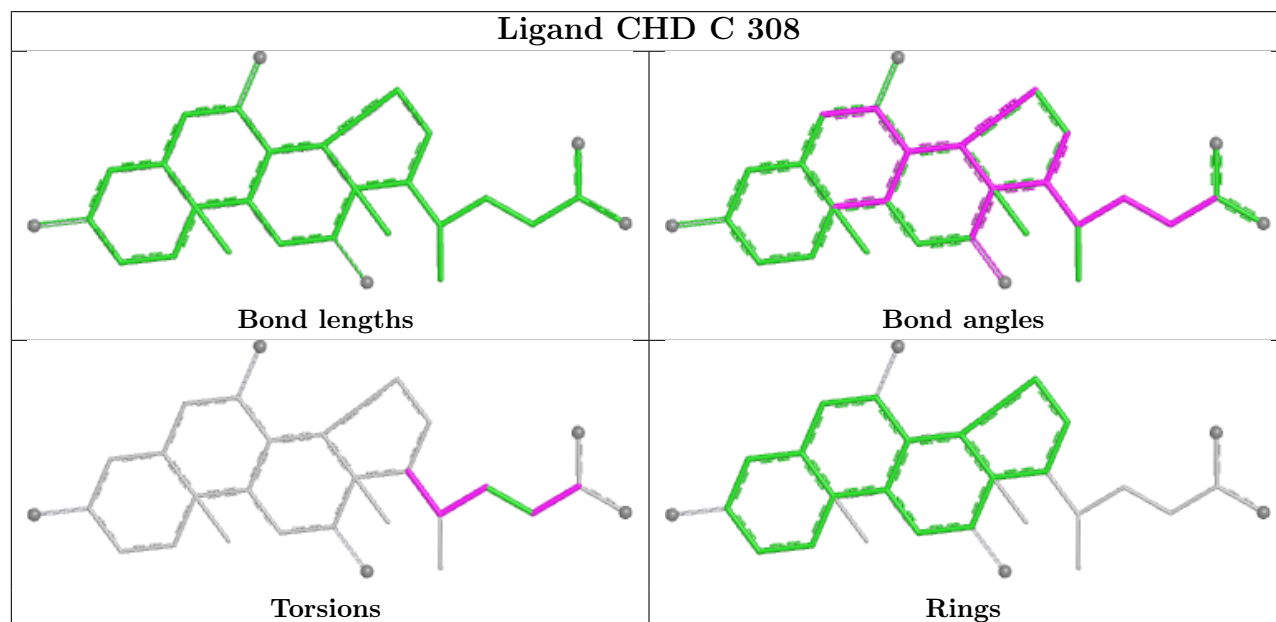
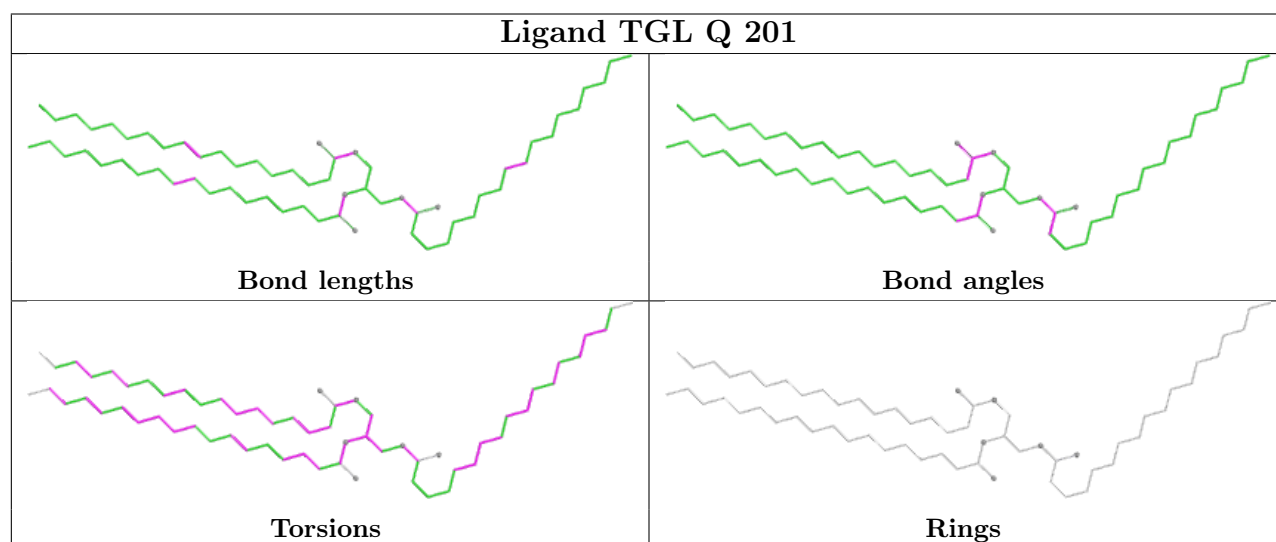
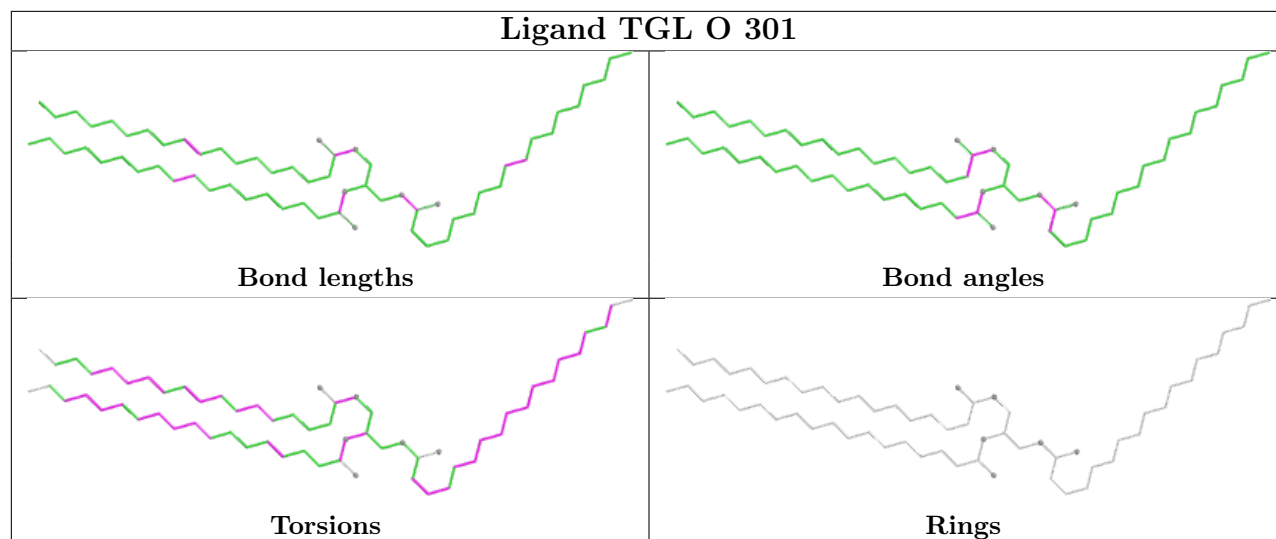
Ligand HEA N 601 (B)

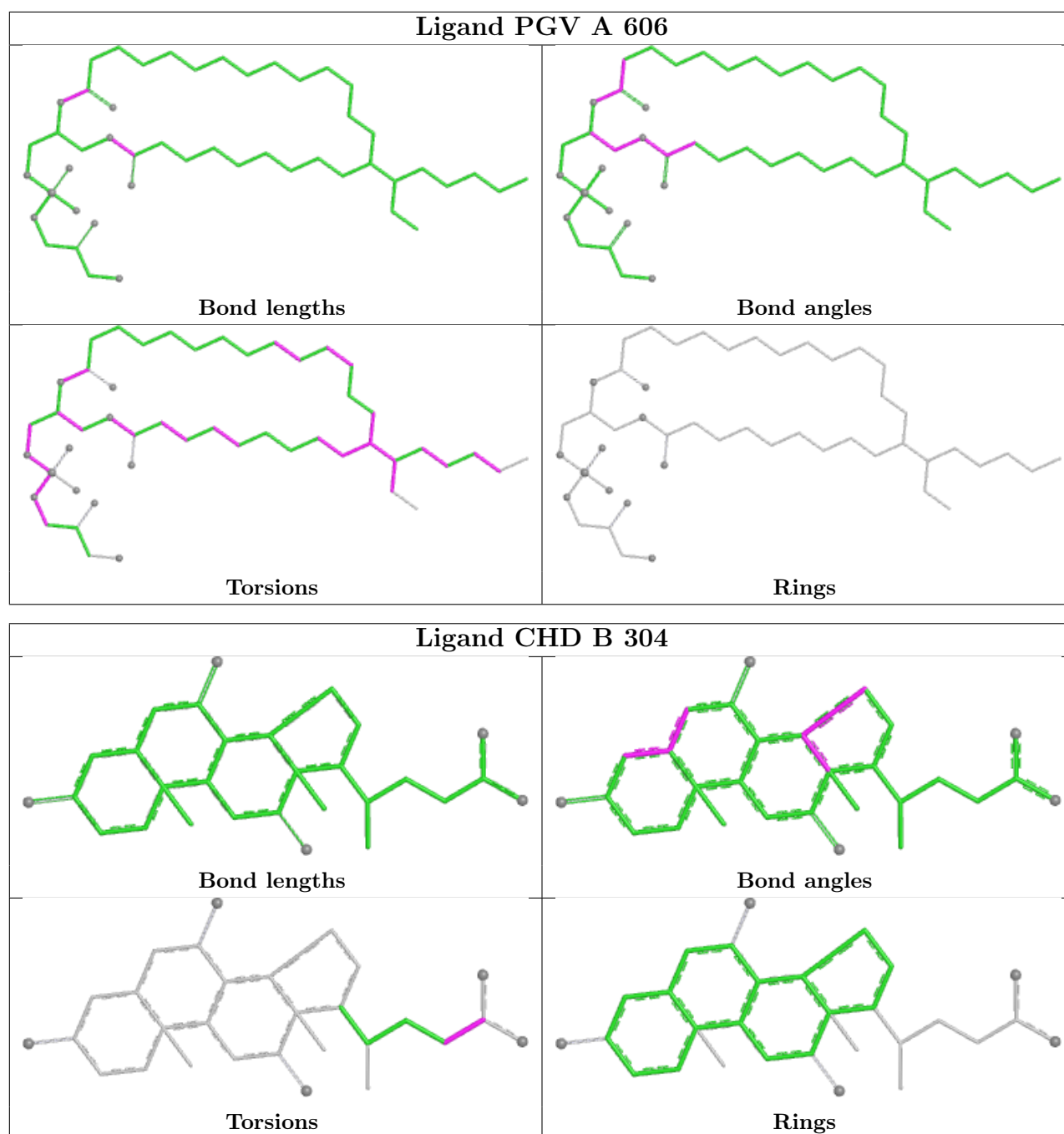


Ligand CHD P 301

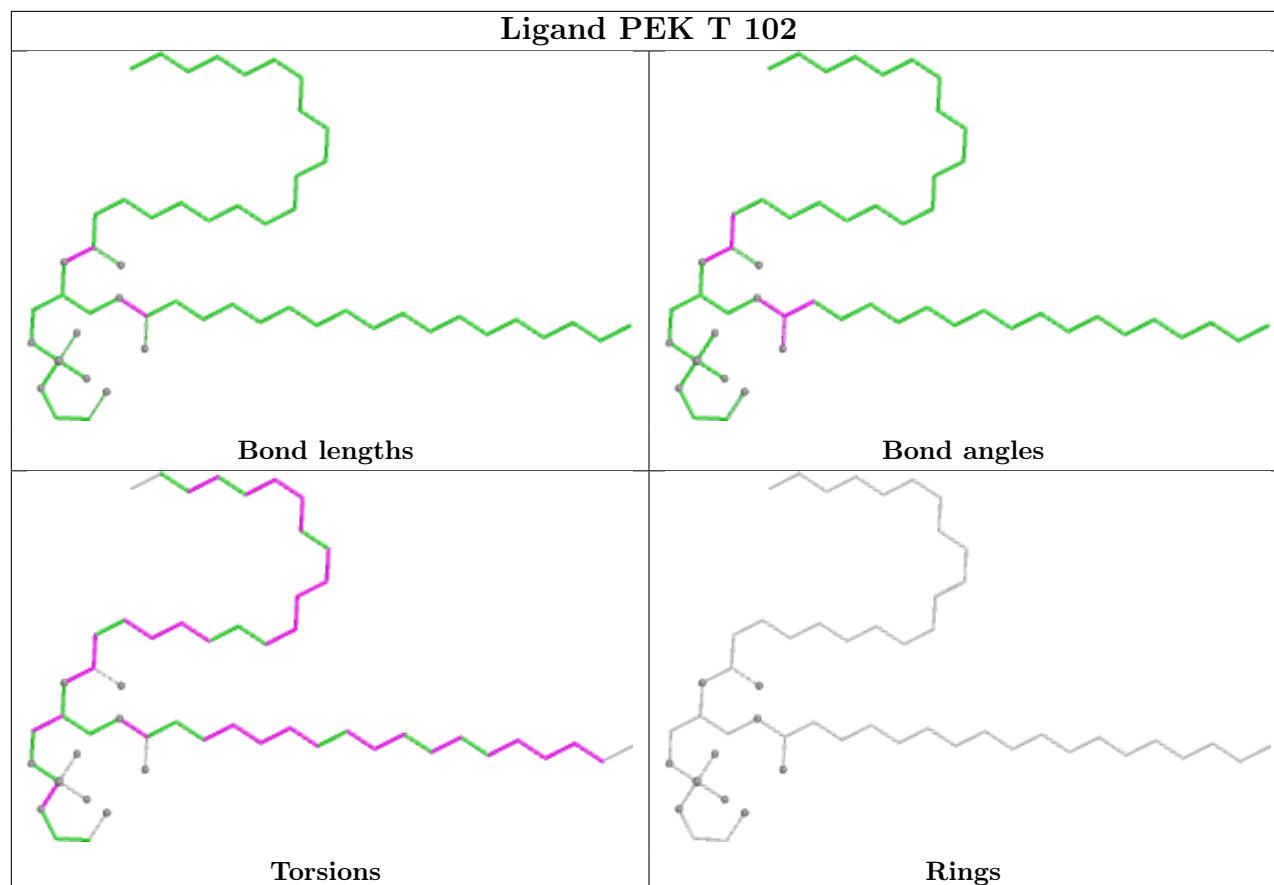




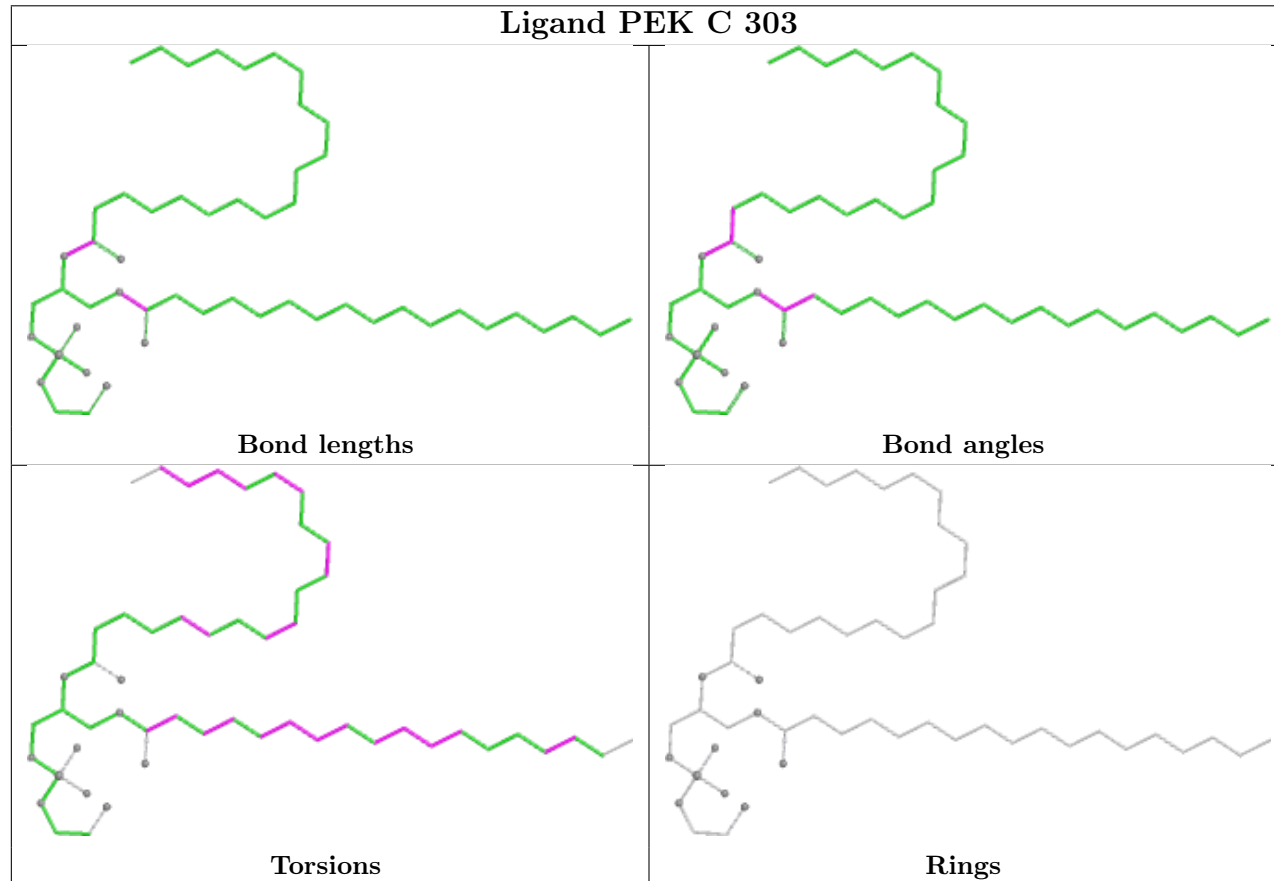


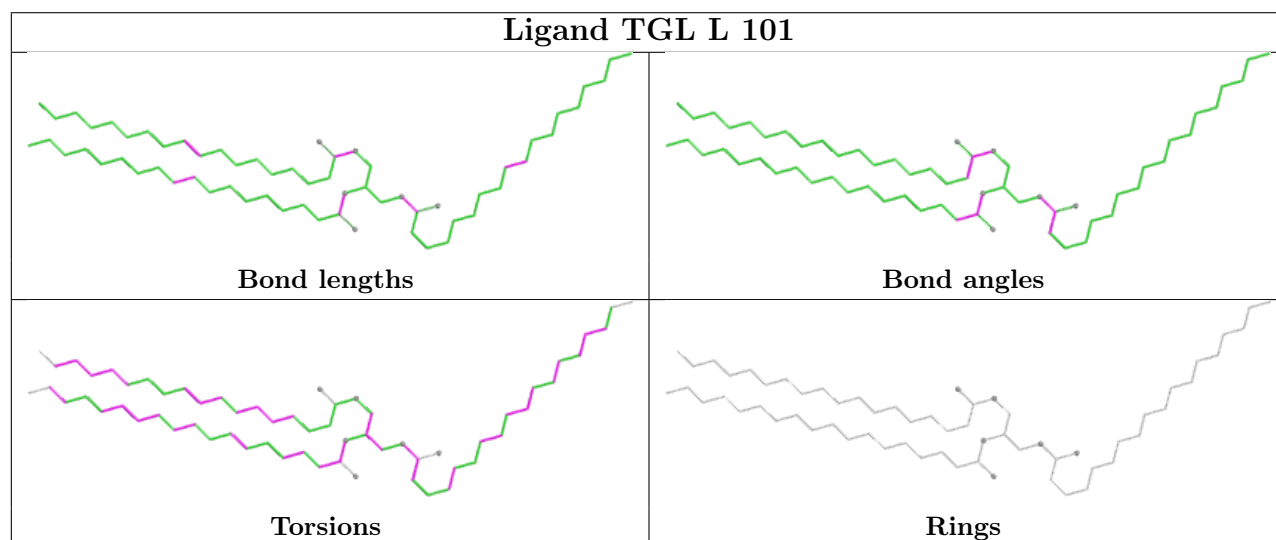
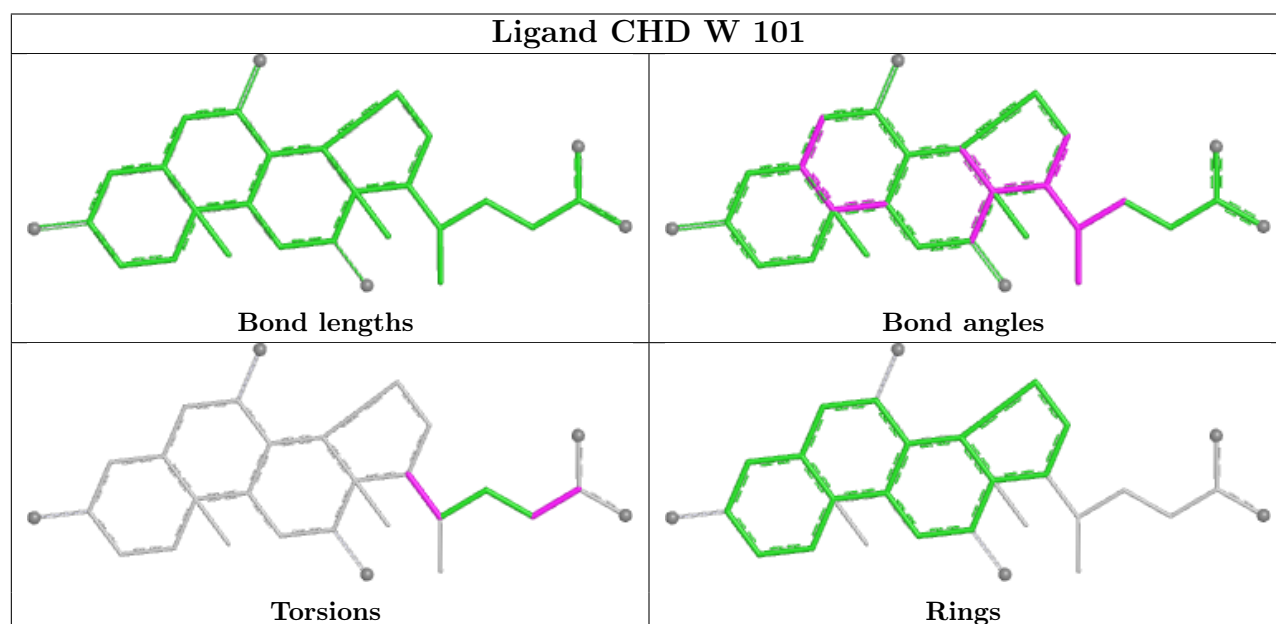
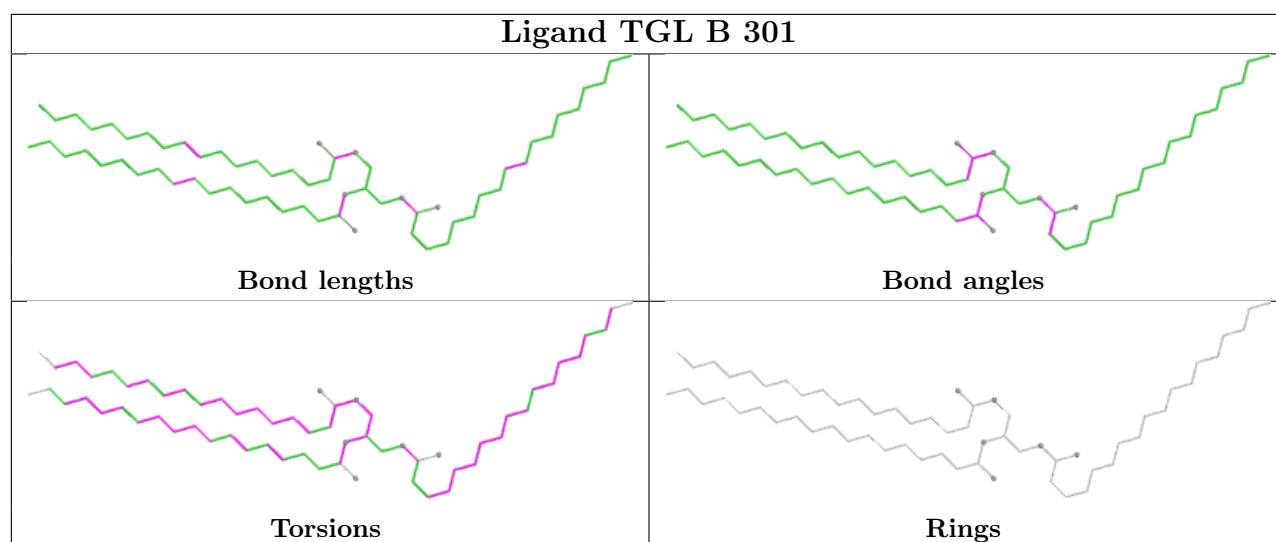


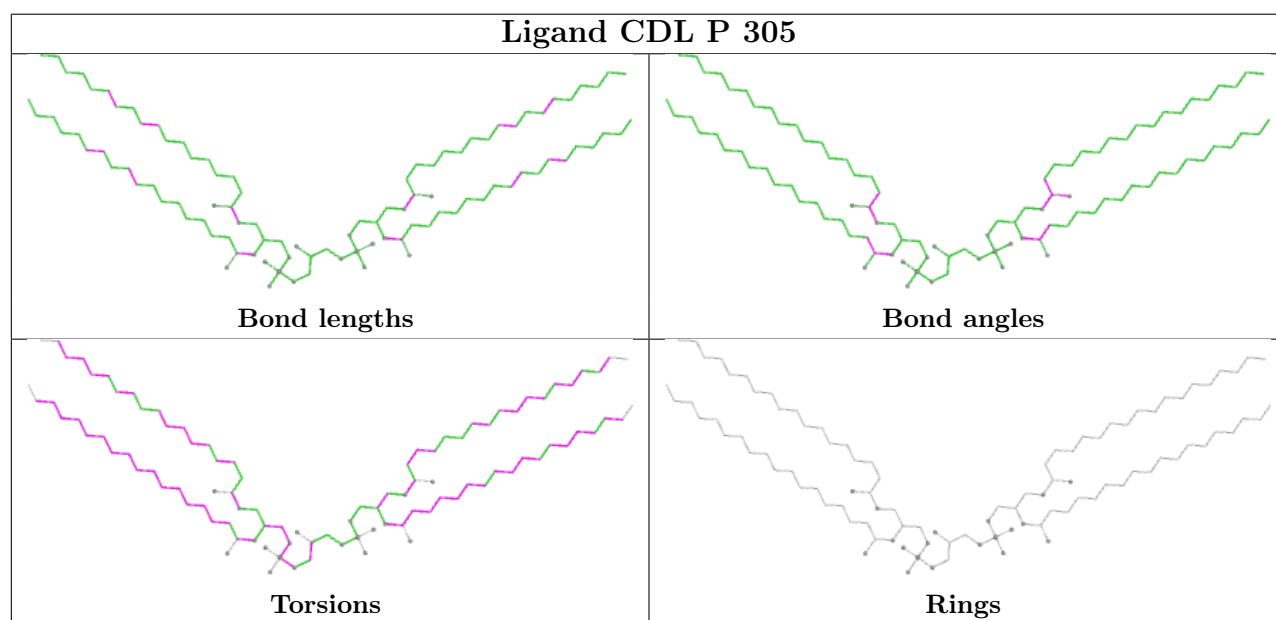
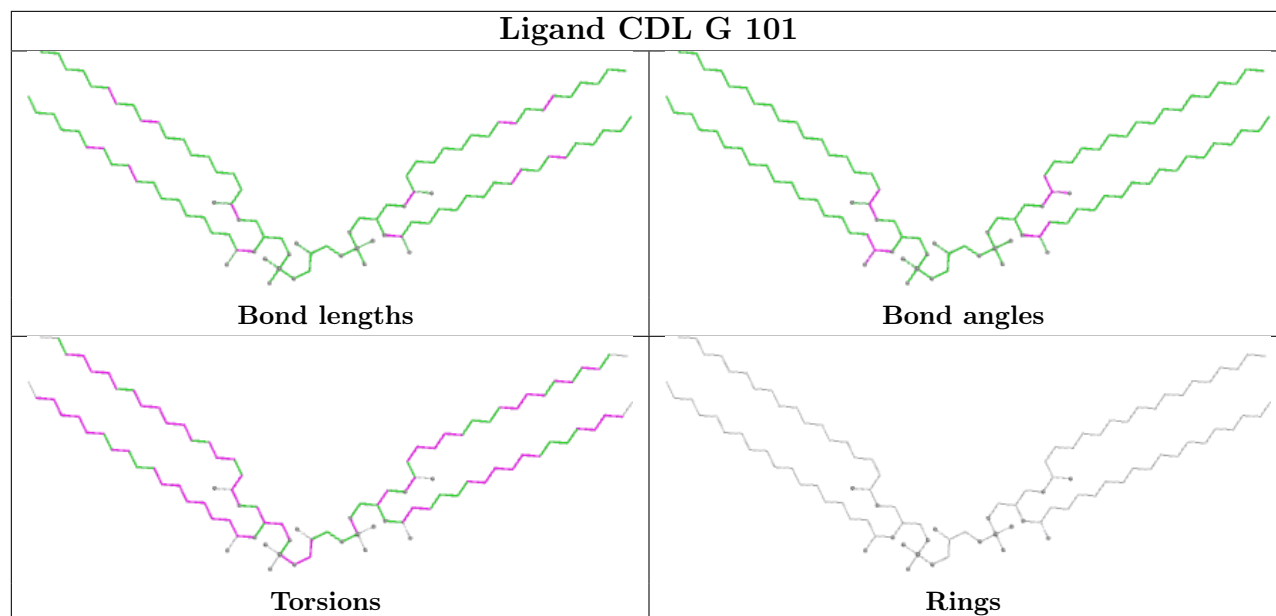
Ligand PEK T 102

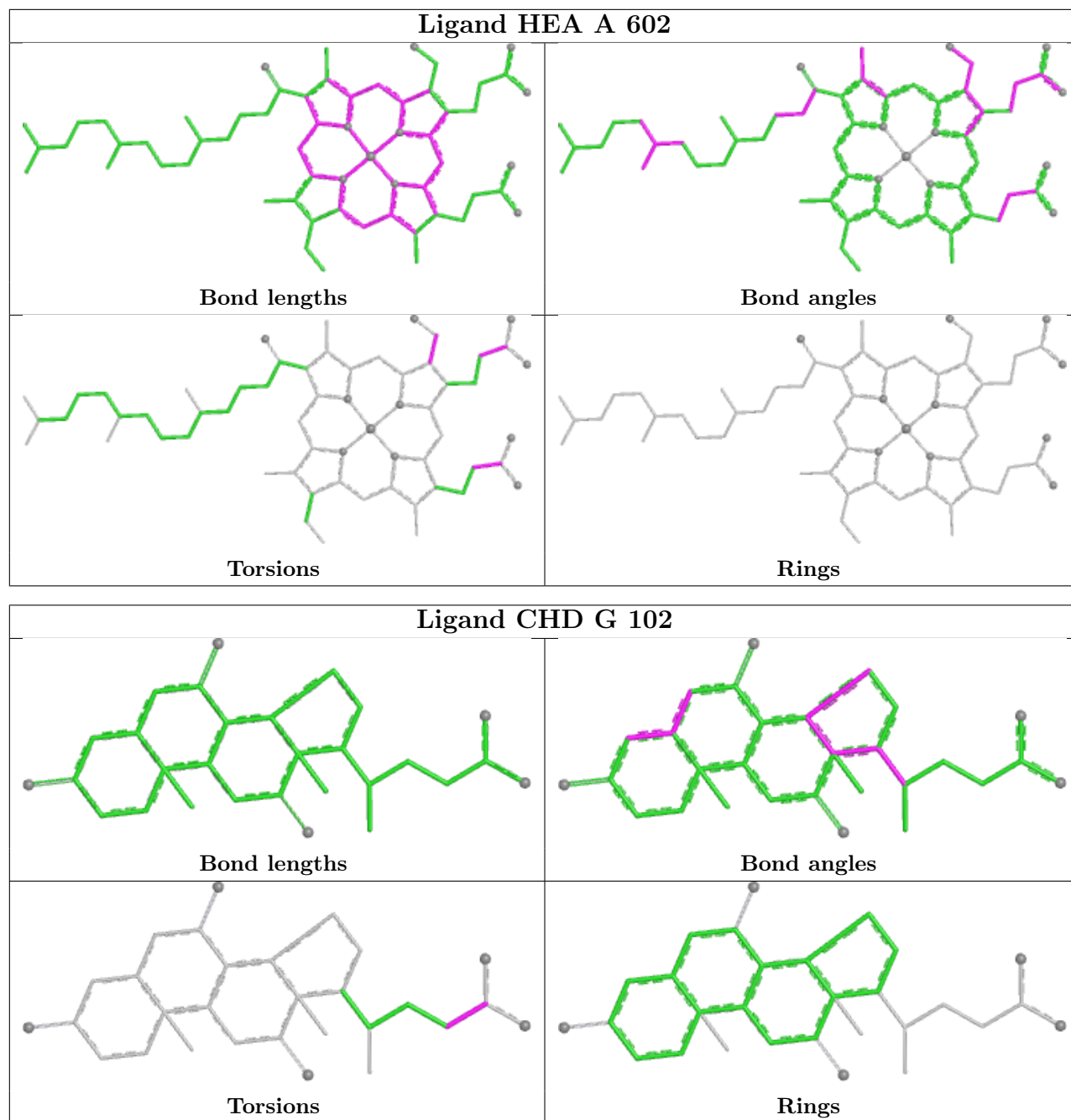


Ligand PEK C 303

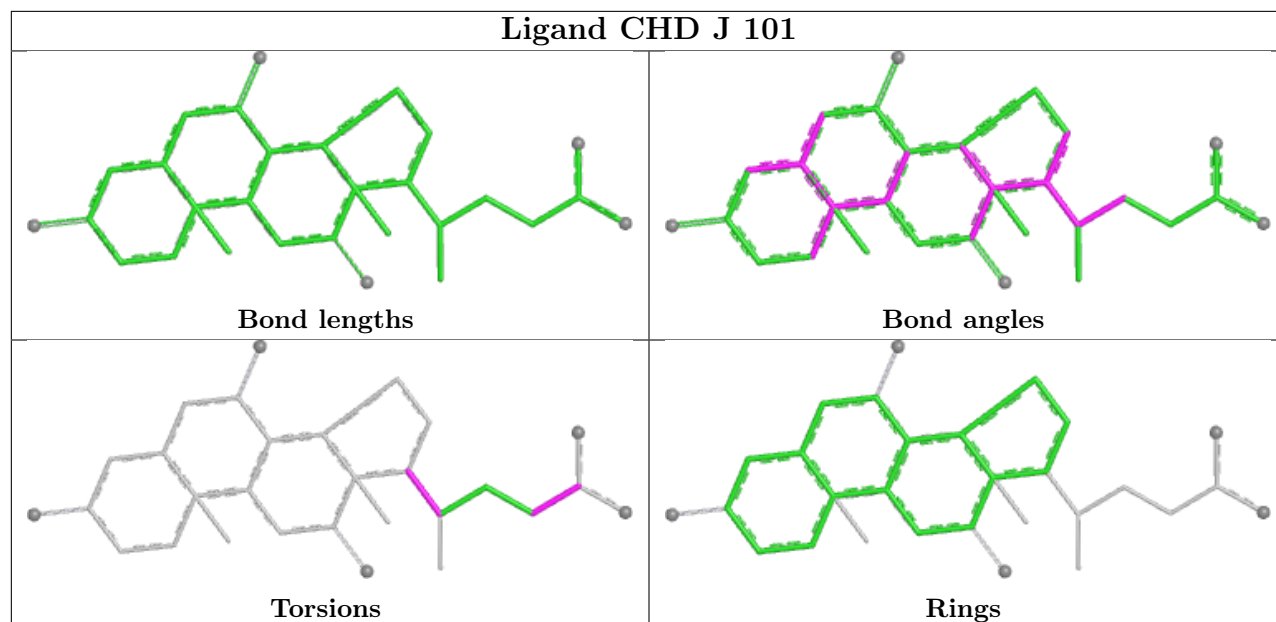




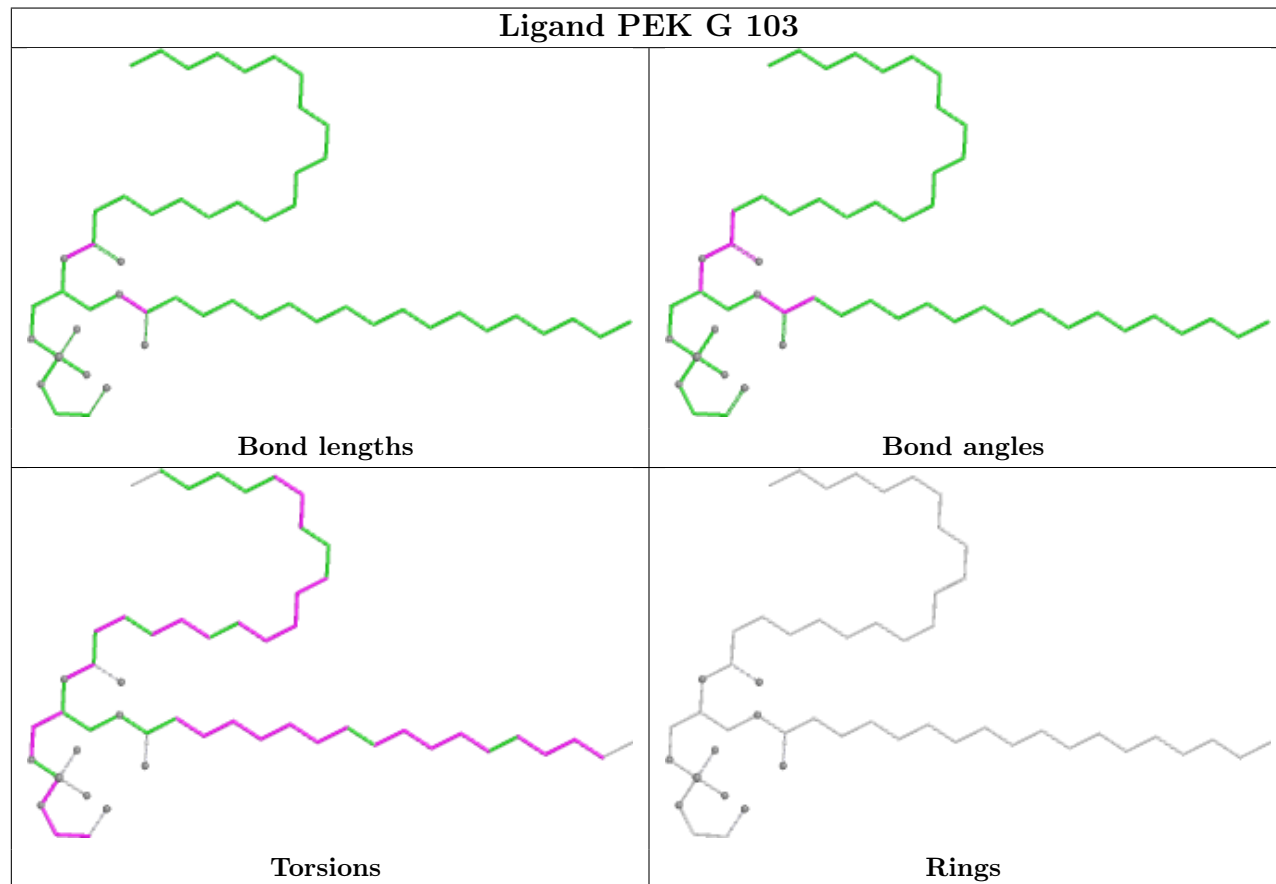


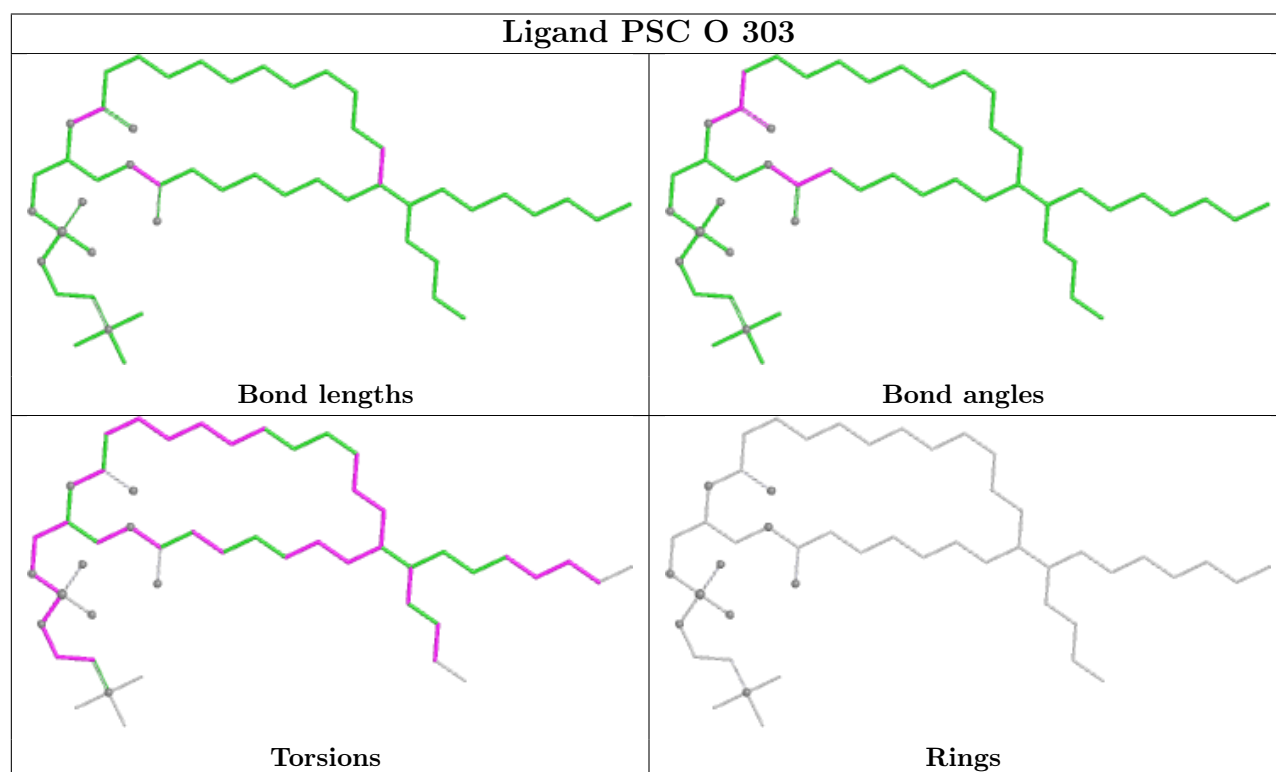
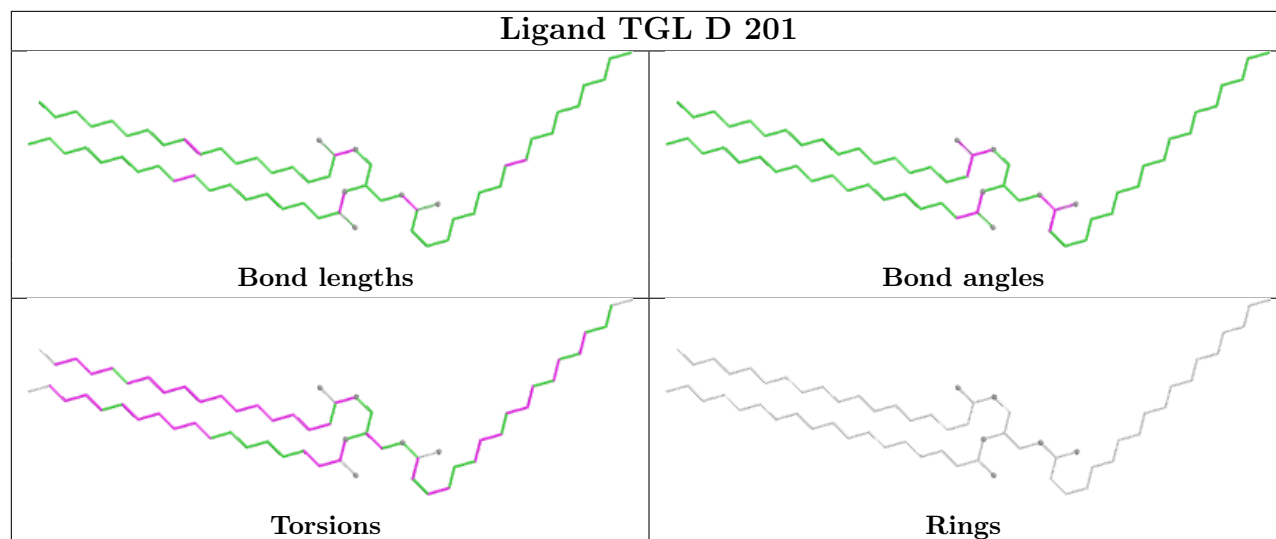


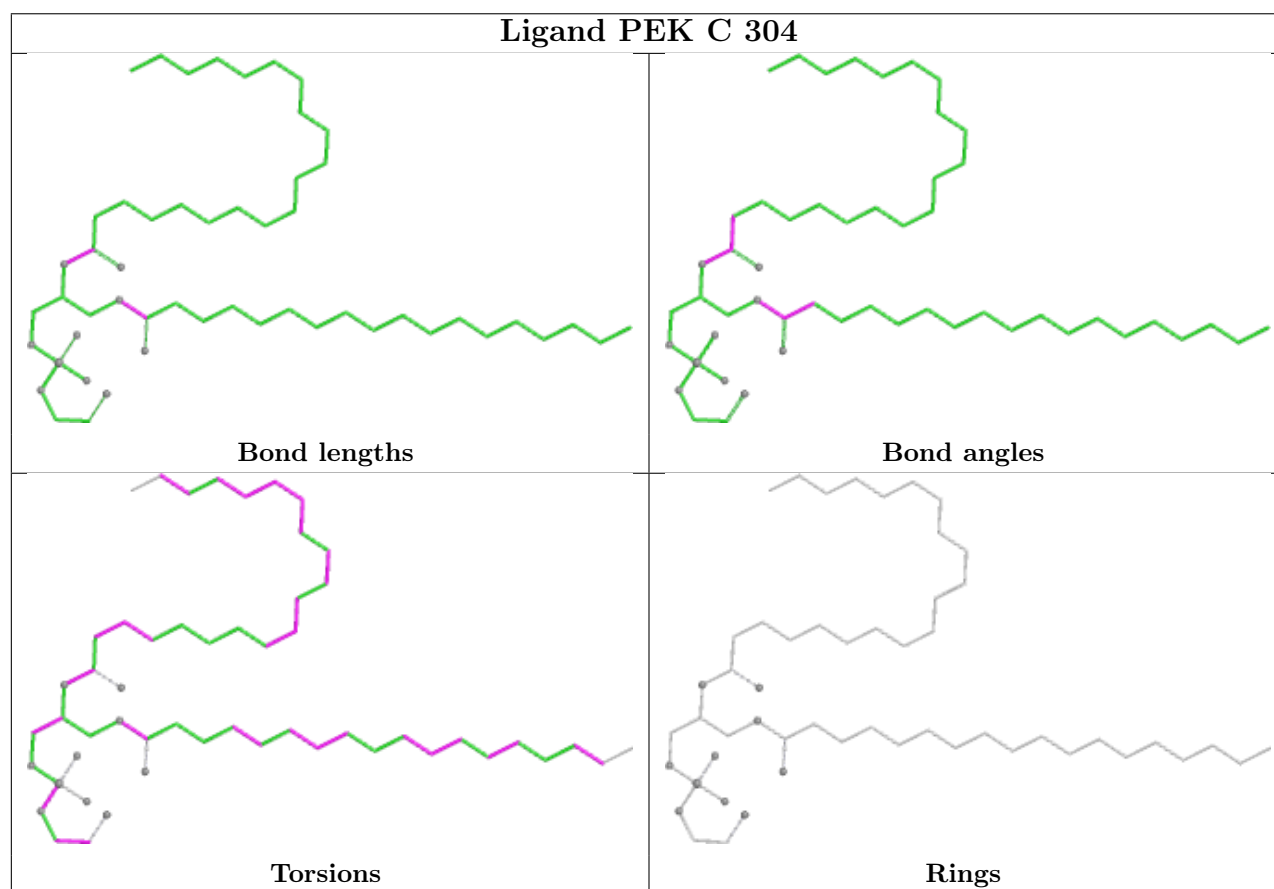
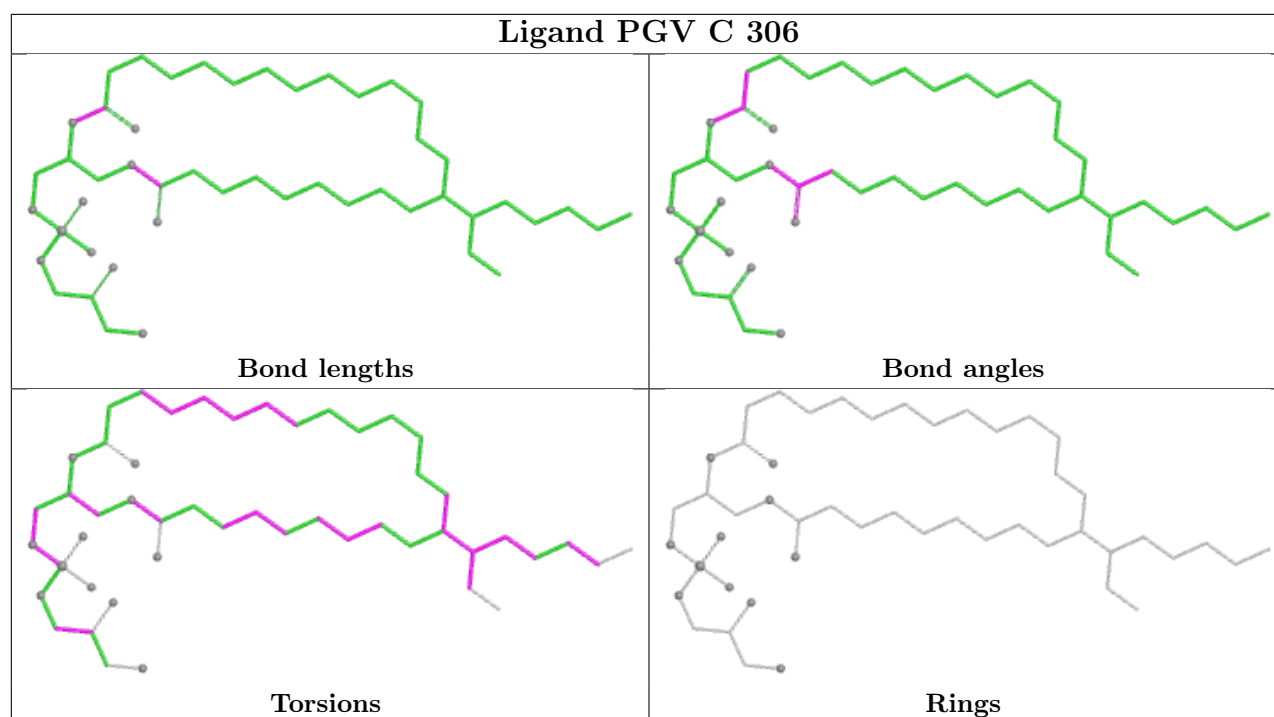
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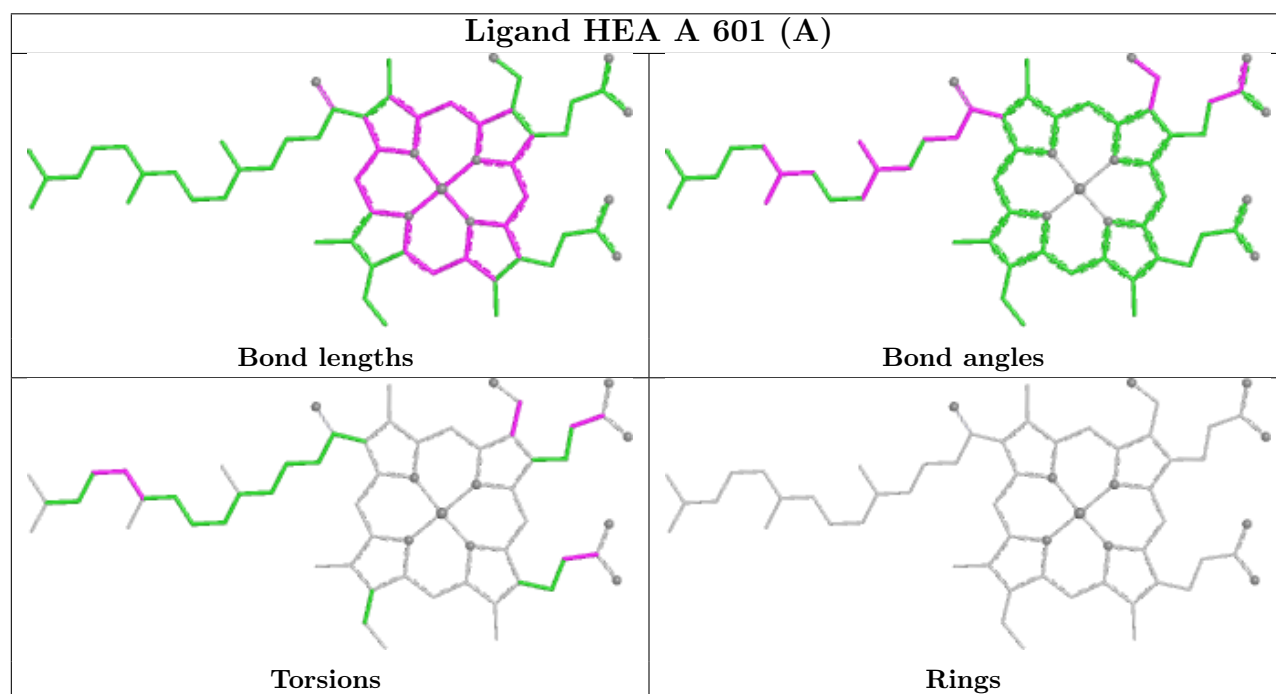
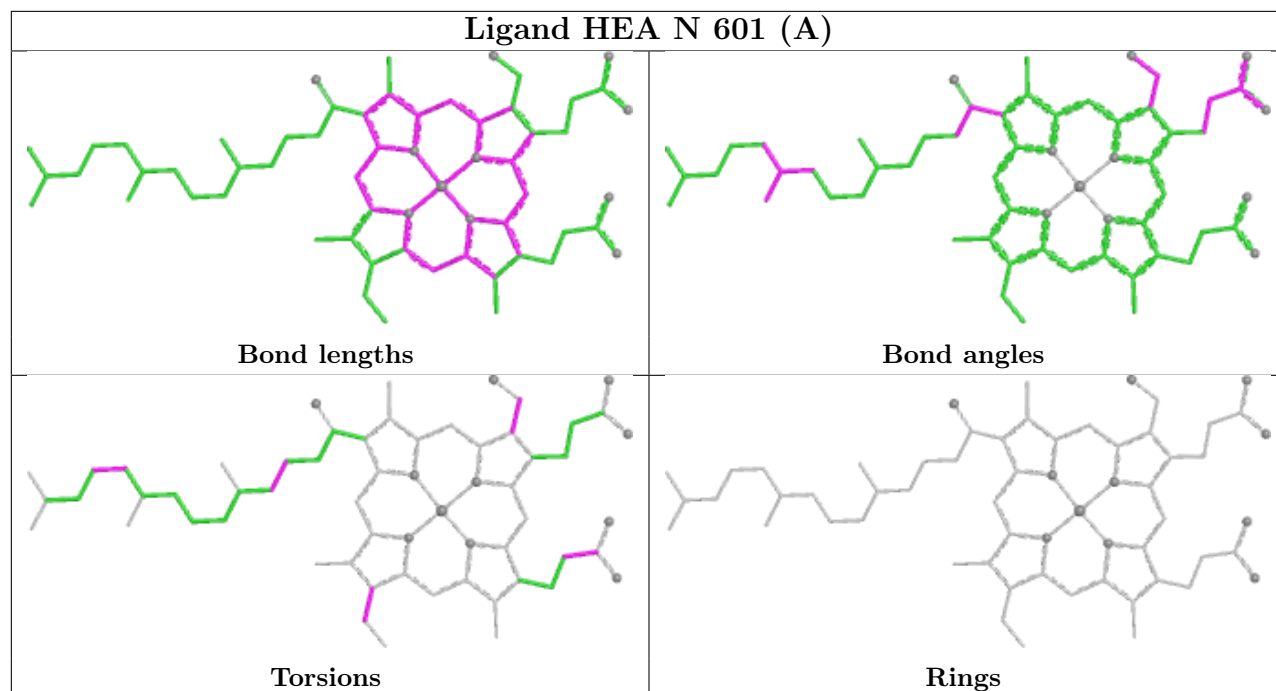


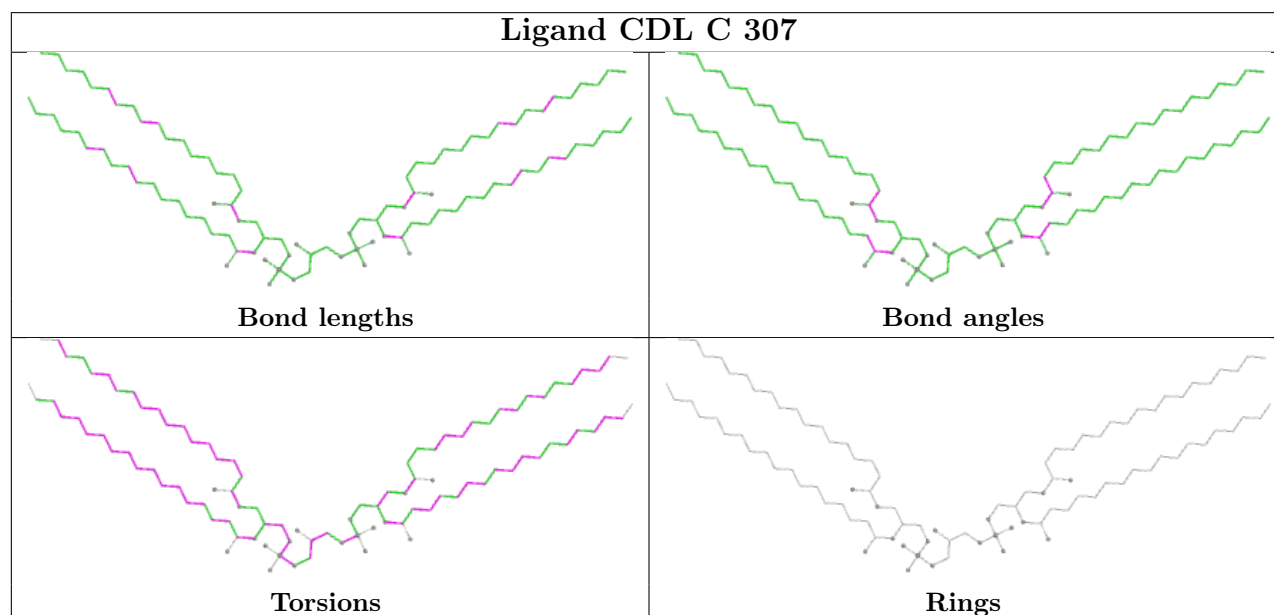
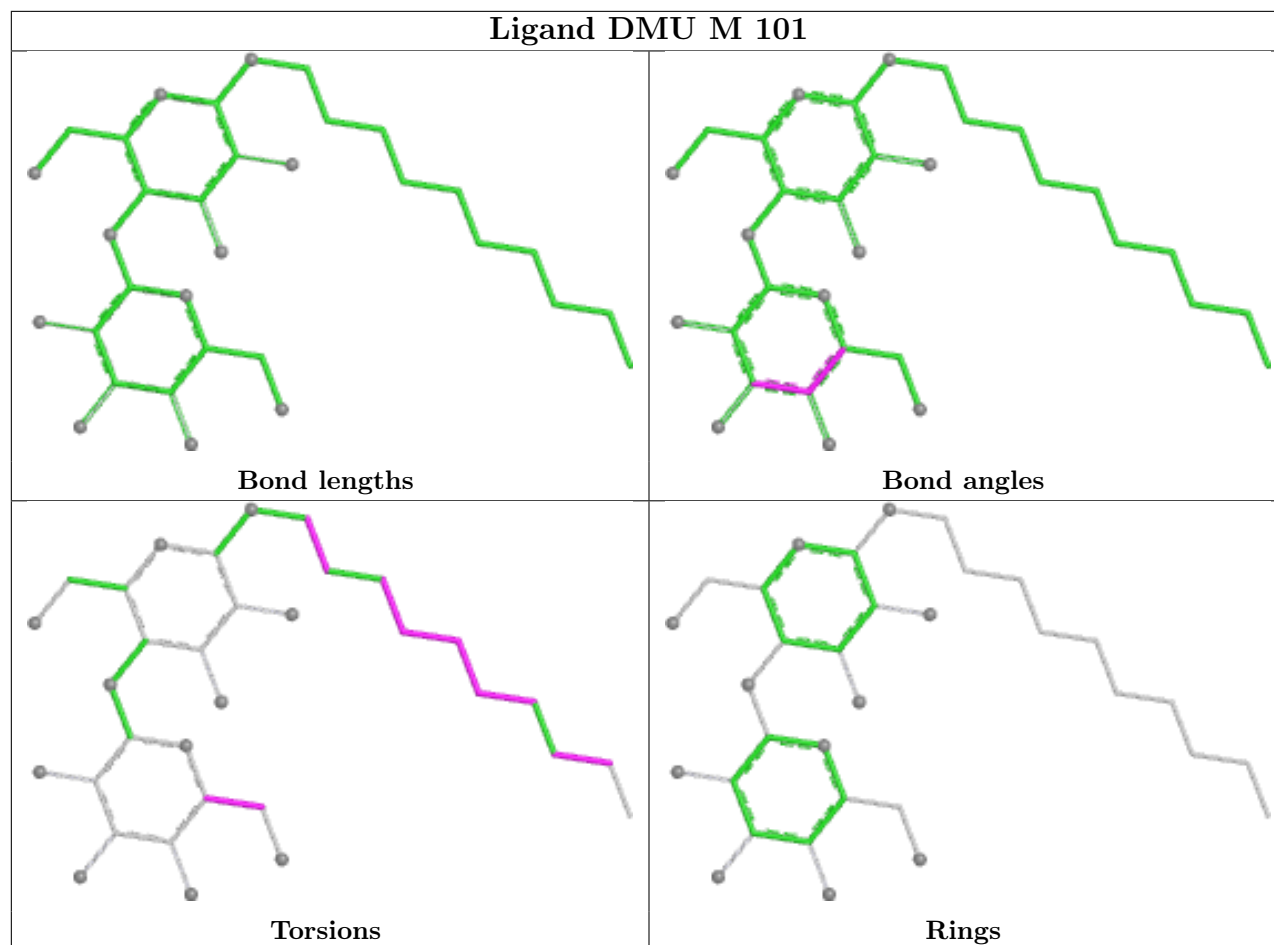
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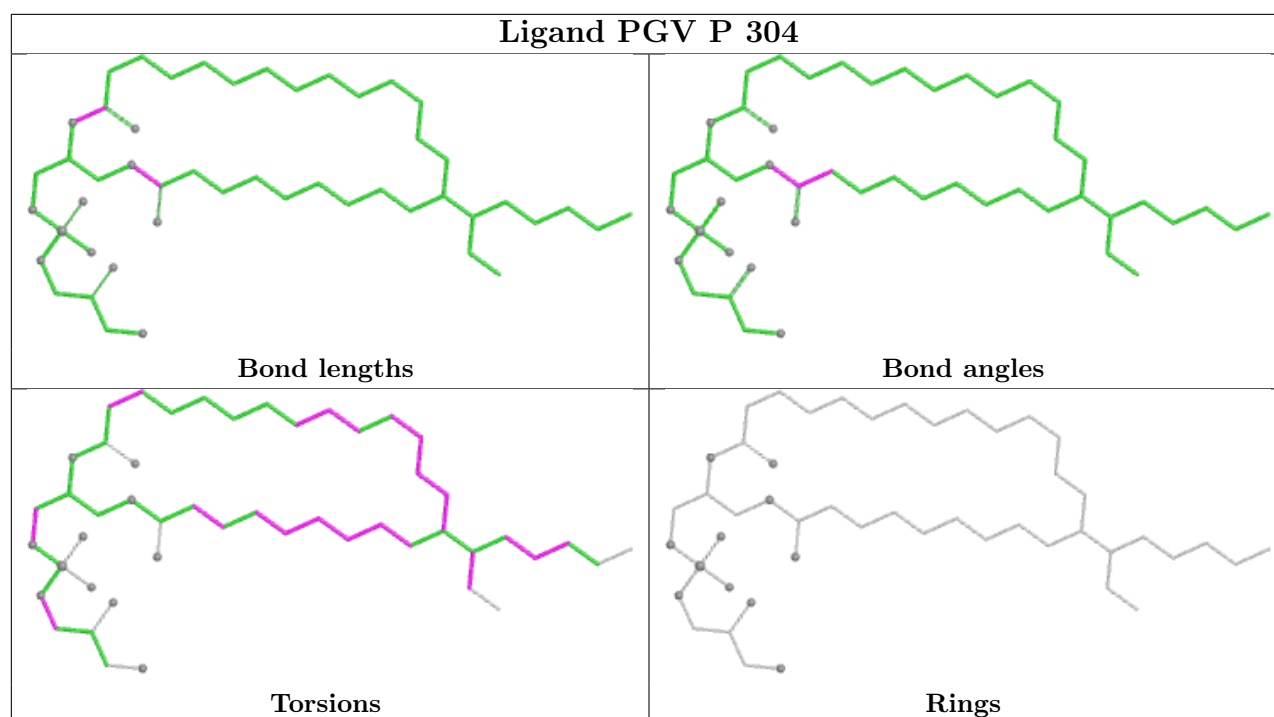












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.35	3 (0%) 85 89	16, 28, 35, 78	33 (6%)
1	N	513/514 (99%)	-0.14	6 (1%) 76 82	19, 33, 44, 76	30 (5%)
2	B	226/227 (99%)	0.06	5 (2%) 62 70	25, 34, 49, 70	11 (4%)
2	O	226/227 (99%)	0.42	10 (4%) 39 44	26, 44, 67, 98	10 (4%)
3	C	259/261 (99%)	-0.16	5 (1%) 66 74	19, 31, 42, 77	13 (5%)
3	P	259/261 (99%)	-0.12	4 (1%) 72 78	23, 34, 44, 70	12 (4%)
4	D	144/147 (97%)	0.17	6 (4%) 40 47	29, 37, 55, 75	0
4	Q	144/147 (97%)	0.98	16 (11%) 10 11	36, 54, 80, 139	1 (0%)
5	E	105/109 (96%)	-0.17	2 (1%) 66 74	22, 35, 56, 108	2 (1%)
5	R	105/109 (96%)	0.19	2 (1%) 66 74	34, 43, 60, 131	0
6	F	94/94 (100%)	0.46	5 (5%) 32 38	26, 39, 59, 116	1 (1%)
6	S	94/94 (100%)	0.53	7 (7%) 20 24	27, 39, 71, 116	2 (2%)
7	G	83/85 (97%)	1.30	21 (25%) 1 1	30, 39, 106, 139	0
7	T	83/85 (97%)	1.31	21 (25%) 1 1	30, 43, 98, 139	0
8	H	79/85 (92%)	0.66	8 (10%) 12 14	32, 42, 87, 103	0
8	U	79/85 (92%)	0.85	11 (13%) 6 7	39, 49, 95, 120	0
9	I	72/73 (98%)	1.04	17 (23%) 2 2	32, 44, 78, 97	0
9	V	72/73 (98%)	1.39	19 (26%) 1 1	33, 59, 86, 93	0
10	J	58/59 (98%)	0.39	4 (6%) 23 27	27, 41, 64, 106	2 (3%)
10	W	58/59 (98%)	0.58	4 (6%) 23 27	32, 48, 72, 120	1 (1%)
11	K	49/56 (87%)	0.55	3 (6%) 27 33	23, 42, 55, 61	1 (2%)
11	X	49/56 (87%)	1.01	7 (14%) 6 6	47, 57, 74, 79	0
12	L	46/47 (97%)	0.17	2 (4%) 40 45	23, 33, 48, 94	4 (8%)
12	Y	46/47 (97%)	0.73	6 (13%) 7 8	37, 44, 64, 110	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.48	4 (9%) 14 16	26, 34, 72, 105	1 (2%)
13	Z	43/46 (93%)	1.07	6 (13%) 6 7	42, 49, 81, 124	0
All	All	3542/3606 (98%)	0.22	204 (5%) 29 35	16, 36, 67, 139	125 (3%)

The worst 5 of 204 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	1	ALA	14.3
6	F	1	ALA	11.8
4	Q	6	VAL	10.9
4	Q	5	VAL	9.9
7	G	36	TRP	8.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.48	0.17	109,117,122,124	0
7	TPO	T	11	11/12	0.56	0.28	107,125,143,144	0
7	TPO	G	11	11/12	0.67	0.25	74,90,145,146	0
9	SAC	I	1	9/10	0.72	0.19	62,71,77,78	0
1	FME	A	1	10/11	0.90	0.19	40,47,73,88	0
1	FME	N	1	10/11	0.92	0.14	47,55,88,93	0
2	FME	B	1	10/11	0.93	0.12	32,35,51,58	0
2	FME	O	1	10/11	0.96	0.10	43,46,57,65	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	EDO	P	309	4/4	0.67	0.31	88,91,92,95	0
27	DMU	P	313	33/33	0.71	0.32	84,143,147,148	0
24	CHD	W	101	29/29	0.76	0.18	62,72,98,102	0
18	PGV	U	101	51/51	0.76	0.27	48,83,126,143	0
24	CHD	J	101	29/29	0.77	0.20	53,65,103,108	0
27	DMU	C	313	33/33	0.78	0.29	76,136,146,147	0
26	CDL	T	103	100/100	0.78	0.25	56,83,115,139	0
20	EDO	M	103	4/4	0.79	0.40	113,116,116,117	0
20	EDO	W	102	4/4	0.79	0.33	103,107,108,109	0
25	PEK	C	304	53/53	0.79	0.26	45,80,138,146	0
26	CDL	P	305	100/100	0.80	0.26	45,82,111,117	0
23	PSC	B	303	52/52	0.80	0.27	45,83,142,149	0
18	PGV	C	306	51/51	0.80	0.25	45,73,111,133	0
25	PEK	T	101	53/53	0.80	0.24	51,87,142,148	0
26	CDL	G	101	100/100	0.81	0.25	58,89,138,147	0
21	TGL	Q	201	63/63	0.81	0.26	56,76,92,95	0
21	TGL	N	606	63/63	0.81	0.26	49,73,104,120	0
27	DMU	C	312	33/33	0.81	0.28	83,116,143,145	0
25	PEK	T	102	53/53	0.81	0.24	39,77,126,137	0
26	CDL	C	307	100/100	0.81	0.23	41,74,102,117	0
25	PEK	G	103	53/53	0.82	0.25	52,87,125,139	0
23	PSC	O	303	52/52	0.82	0.24	40,76,138,147	0
18	PGV	N	607	51/51	0.82	0.23	49,81,128,140	0
17	NA	C	302	1/1	0.82	0.28	53,53,53,53	0
20	EDO	C	311	4/4	0.82	0.22	48,56,58,61	0
27	DMU	W	104	33/33	0.82	0.27	78,131,146,146	0
21	TGL	B	301	63/63	0.83	0.24	36,69,89,100	0
21	TGL	D	201	63/63	0.83	0.25	46,68,87,89	0
21	TGL	L	101	63/63	0.83	0.25	37,59,92,99	0
20	EDO	A	618	4/4	0.83	0.26	55,58,59,61	0
20	EDO	P	307	4/4	0.83	0.35	89,96,96,98	0
20	EDO	A	616	4/4	0.83	0.32	85,86,89,93	0
20	EDO	L	102	4/4	0.83	0.29	86,90,91,91	0
21	TGL	O	301	63/63	0.84	0.24	50,76,98,105	0
17	NA	P	302	1/1	0.84	0.20	49,49,49,49	0
20	EDO	Y	101	4/4	0.84	0.32	96,97,99,100	0
18	PGV	A	606	51/51	0.85	0.22	35,74,106,132	0
20	EDO	S	104	4/4	0.85	0.32	74,75,77,80	0
20	EDO	B	308	4/4	0.86	0.30	88,89,93,97	0
20	EDO	N	614	4/4	0.87	0.19	52,53,56,57	0
20	EDO	Q	202	4/4	0.87	0.22	43,54,59,68	0
20	EDO	A	610	4/4	0.87	0.18	36,39,39,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	DMU	Z	101	33/33	0.87	0.14	55,66,92,94	0
20	EDO	A	619	4/4	0.88	0.34	81,83,87,89	4
20	EDO	L	103	4/4	0.88	0.19	45,61,62,66	0
20	EDO	A	609	4/4	0.88	0.19	45,51,52,53	0
20	EDO	R	204	4/4	0.88	0.20	55,63,67,67	0
20	EDO	A	611	4/4	0.88	0.31	70,77,78,81	0
20	EDO	B	309	4/4	0.89	0.18	42,52,53,55	0
20	EDO	B	306	4/4	0.89	0.21	47,52,54,55	0
20	EDO	H	101	4/4	0.89	0.26	75,75,77,78	0
20	EDO	P	310	4/4	0.89	0.38	86,90,94,97	0
24	CHD	C	308	29/29	0.89	0.12	48,54,65,67	0
20	EDO	W	103	4/4	0.89	0.31	72,78,78,81	0
24	CHD	P	306	29/29	0.89	0.13	45,55,61,76	0
20	EDO	R	203	4/4	0.90	0.27	90,92,93,95	0
20	EDO	N	613	4/4	0.90	0.29	85,92,94,99	0
20	EDO	C	309	4/4	0.90	0.21	41,47,51,54	0
20	EDO	T	105	4/4	0.90	0.45	144,145,145,145	4
27	DMU	M	101	33/33	0.91	0.13	44,51,71,86	0
20	EDO	B	307	4/4	0.91	0.16	50,54,56,58	0
20	EDO	L	105	4/4	0.91	0.27	85,86,87,87	0
20	EDO	P	312	4/4	0.91	0.18	57,65,67,67	0
20	EDO	P	308	4/4	0.92	0.32	97,100,100,102	0
20	EDO	N	612	4/4	0.92	0.18	58,62,66,66	0
20	EDO	R	202	4/4	0.92	0.22	88,90,90,94	0
20	EDO	A	615	4/4	0.92	0.22	64,67,70,72	0
20	EDO	N	611	4/4	0.93	0.12	34,35,38,39	0
20	EDO	A	617	4/4	0.93	0.14	38,44,48,49	0
20	EDO	S	103	4/4	0.94	0.13	44,44,46,46	0
20	EDO	A	614	4/4	0.94	0.19	73,73,76,77	0
20	EDO	T	104	4/4	0.94	0.34	98,101,103,104	0
20	EDO	P	311	4/4	0.94	0.12	48,49,51,52	0
20	EDO	C	310	4/4	0.94	0.12	39,43,43,43	0
20	EDO	O	304	4/4	0.94	0.12	44,46,48,48	0
20	EDO	R	201	4/4	0.94	0.12	49,49,49,52	0
20	EDO	N	610	4/4	0.94	0.12	40,40,42,42	0
20	EDO	A	612	4/4	0.94	0.16	54,63,64,64	0
20	EDO	L	104	4/4	0.94	0.32	97,97,98,99	0
20	EDO	S	102	4/4	0.94	0.12	31,33,33,34	0
24	CHD	B	304	29/29	0.95	0.08	29,32,35,41	0
25	PEK	P	303	53/53	0.95	0.14	30,49,94,97	0
20	EDO	M	102	4/4	0.95	0.25	83,84,85,85	0
20	EDO	F	102	4/4	0.95	0.12	29,30,30,32	0

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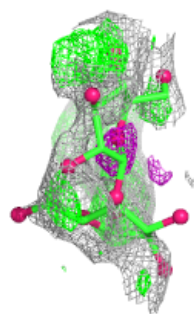
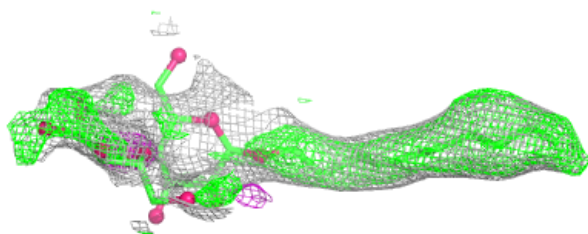
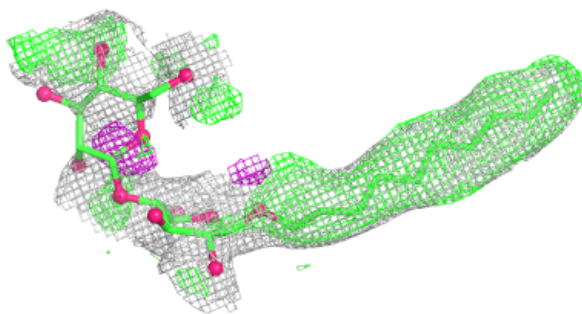
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	EDO	F	103	4/4	0.95	0.12	43,45,45,46	0
20	EDO	A	613	4/4	0.95	0.11	28,28,32,32	0
20	EDO	J	102	4/4	0.95	0.15	55,65,65,67	0
16	MG	A	604	1/1	0.96	0.07	30,30,30,30	0
20	EDO	E	201	4/4	0.96	0.10	48,49,51,51	0
20	EDO	G	104	4/4	0.96	0.10	37,39,40,40	0
24	CHD	C	301	29/29	0.96	0.07	28,31,35,36	0
25	PEK	C	303	53/53	0.96	0.14	30,47,86,95	0
24	CHD	G	102	29/29	0.97	0.06	29,32,34,42	0
18	PGV	C	305	51/51	0.97	0.11	29,34,81,94	0
24	CHD	P	301	29/29	0.97	0.07	30,33,36,39	0
16	MG	N	604	1/1	0.97	0.12	39,39,39,39	0
18	PGV	A	608	51/51	0.97	0.10	27,38,61,65	0
18	PGV	N	609	51/51	0.97	0.10	30,43,65,70	0
20	EDO	B	305	4/4	0.97	0.08	34,36,36,37	0
19	PER	N	608[A]	2/2	0.98	0.11	28,28,28,31	0
19	PER	N	608[B]	2/2	0.98	0.11	15,15,15,16	2
18	PGV	P	304	51/51	0.98	0.09	31,40,70,78	0
14	HEA	N	602	60/60	0.98	0.07	25,29,34,37	0
19	PER	A	607[A]	2/2	0.98	0.11	24,24,24,25	0
19	PER	A	607[B]	2/2	0.98	0.11	6,6,6,6	2
22	CUA	O	302	2/2	0.99	0.04	39,39,39,39	0
14	HEA	N	601[A]	60/60	0.99	0.06	28,34,43,49	9
17	NA	N	605	1/1	0.99	0.07	41,41,41,41	0
14	HEA	N	601[B]	60/60	0.99	0.06	28,33,39,41	9
14	HEA	A	601[A]	60/60	0.99	0.06	22,26,38,41	9
14	HEA	A	601[B]	60/60	0.99	0.06	22,26,33,38	9
14	HEA	A	602	60/60	0.99	0.05	21,25,30,34	0
17	NA	A	605	1/1	0.99	0.08	30,30,30,30	0
22	CUA	B	302	2/2	0.99	0.03	29,29,29,30	0
15	CU	A	603	1/1	1.00	0.01	27,27,27,27	0
15	CU	N	603	1/1	1.00	0.02	31,31,31,31	0
28	ZN	F	101	1/1	1.00	0.02	35,35,35,35	0
28	ZN	S	101	1/1	1.00	0.03	37,37,37,37	0

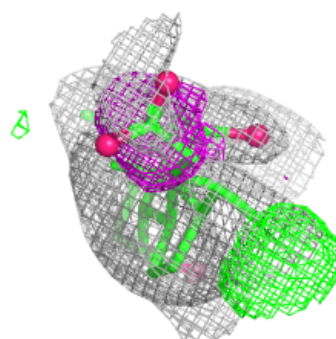
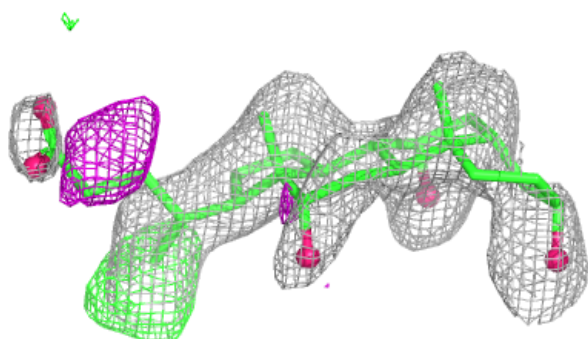
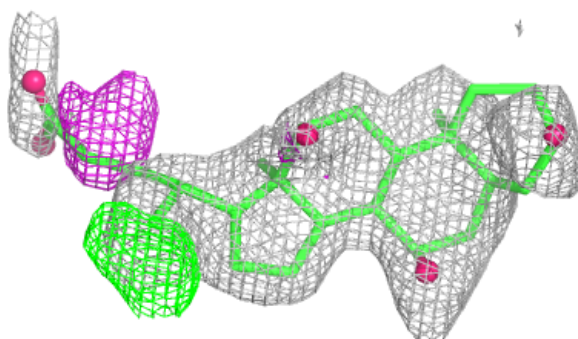
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU P 313:

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

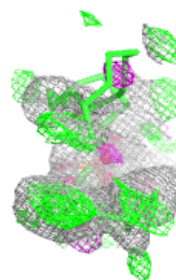
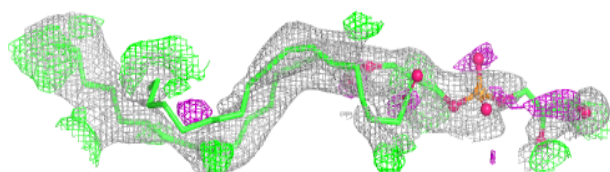
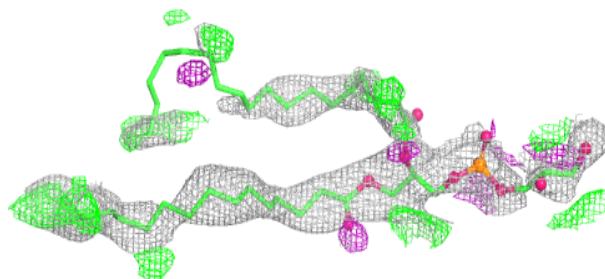
**Electron density around CHD W 101:**

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

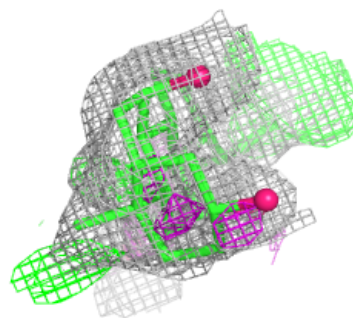
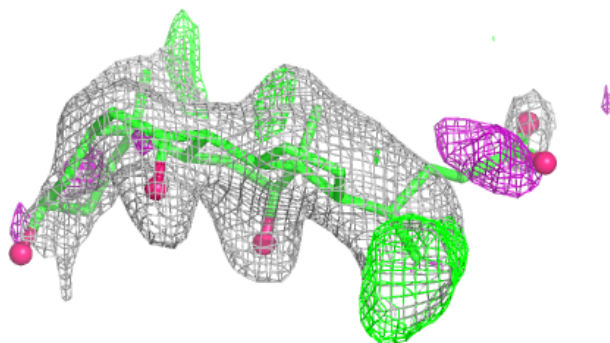
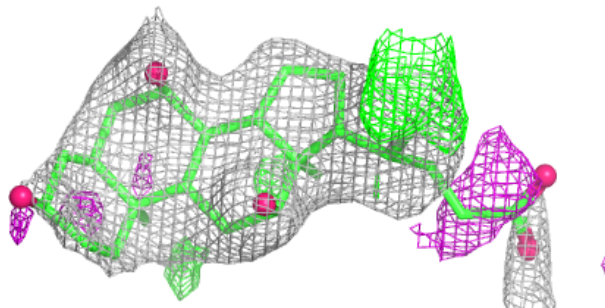


Electron density around PGV U 101:

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

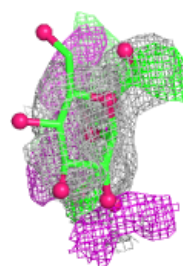
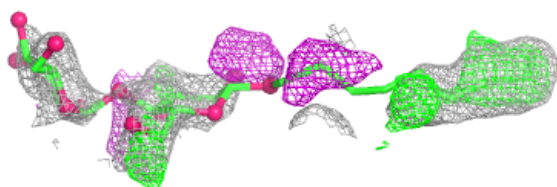
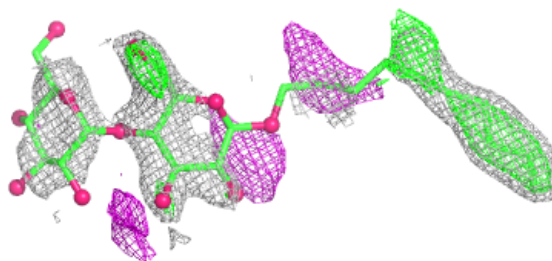
**Electron density around CHD J 101:**

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

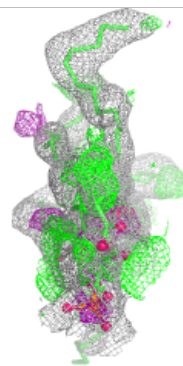
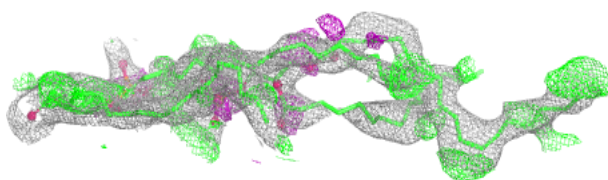
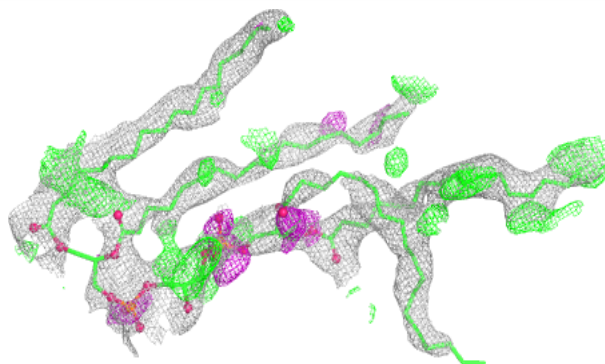


Electron density around DMU C 313:

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

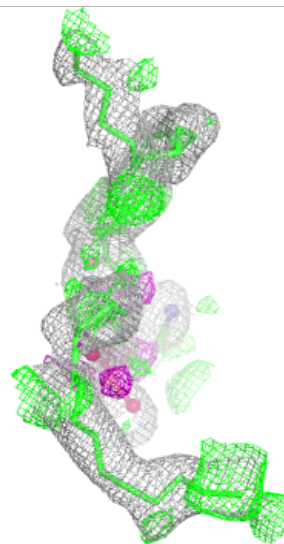
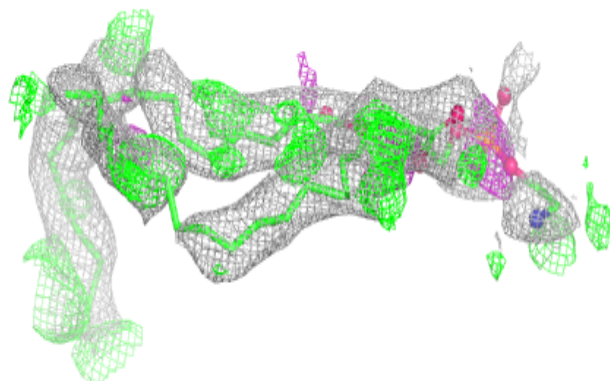
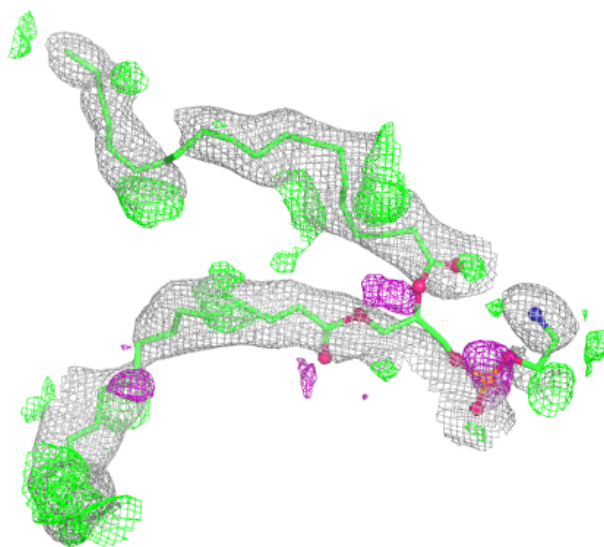
**Electron density around CDL T 103:**

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



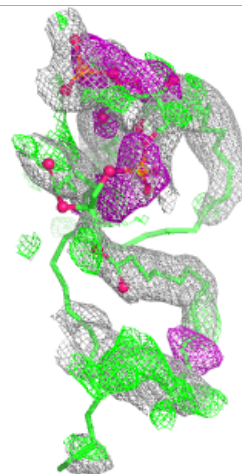
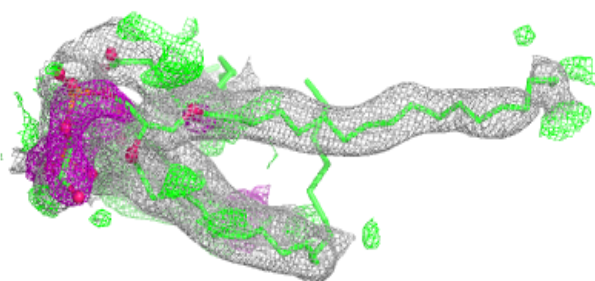
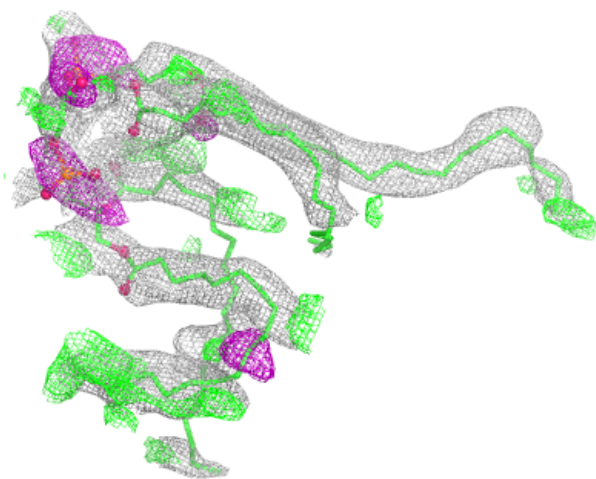
Electron density around PEK C 304:

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and green (positive)



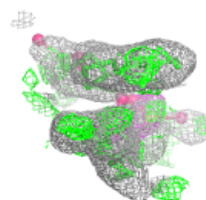
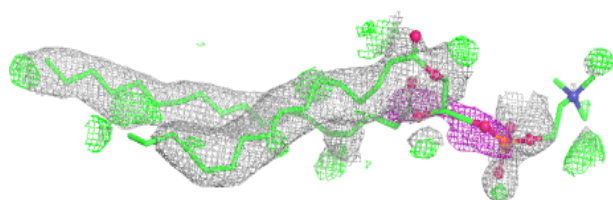
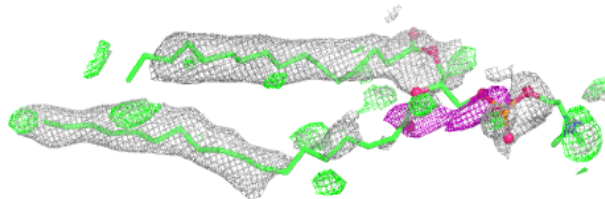
Electron density around CDL P 305:

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and green (positive)

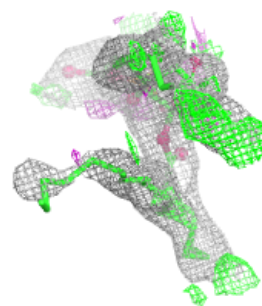
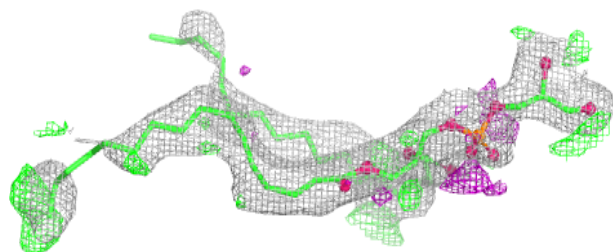
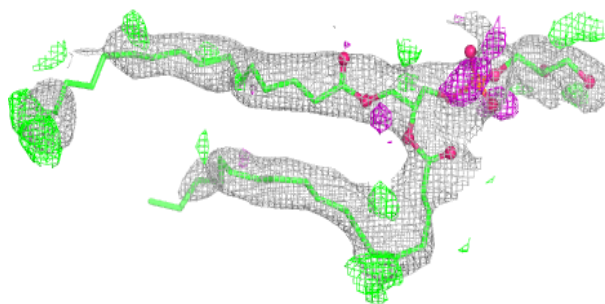


Electron density around PSC B 303:

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

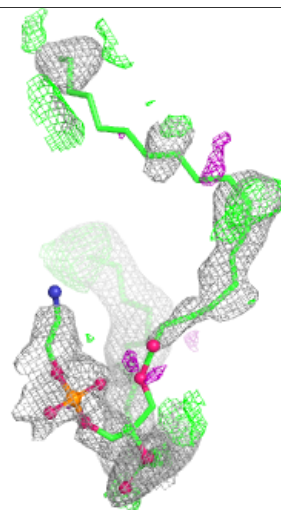
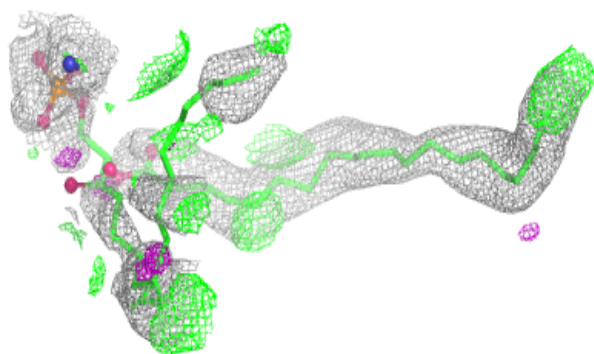
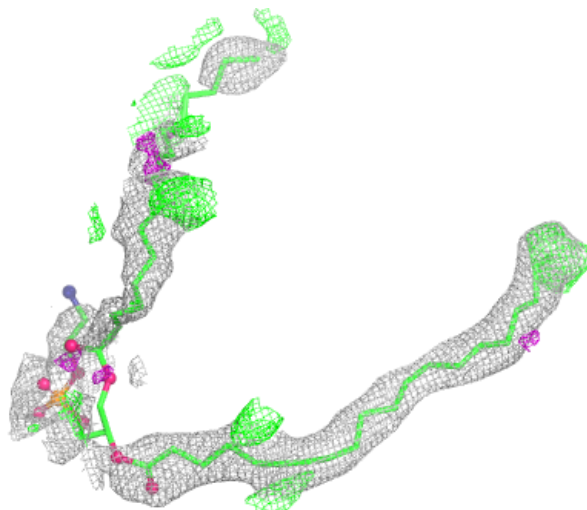
**Electron density around PGV C 306:**

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



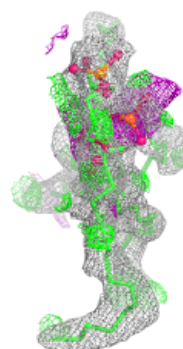
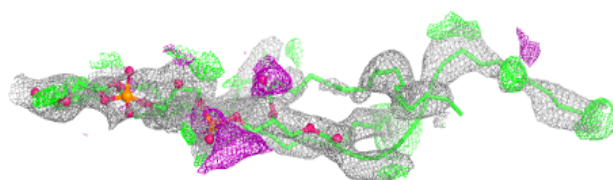
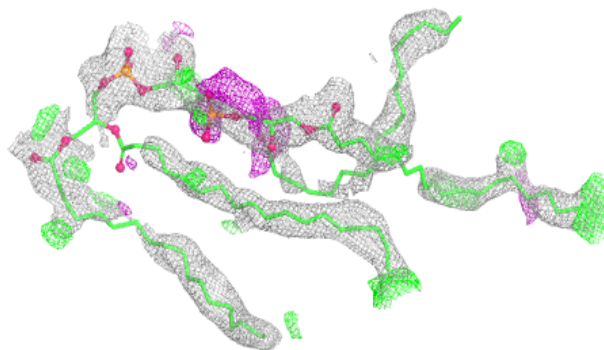
Electron density around PEK T 101:

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

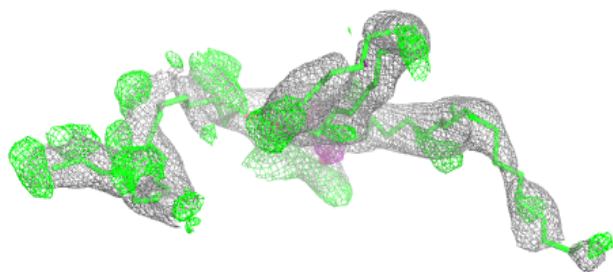
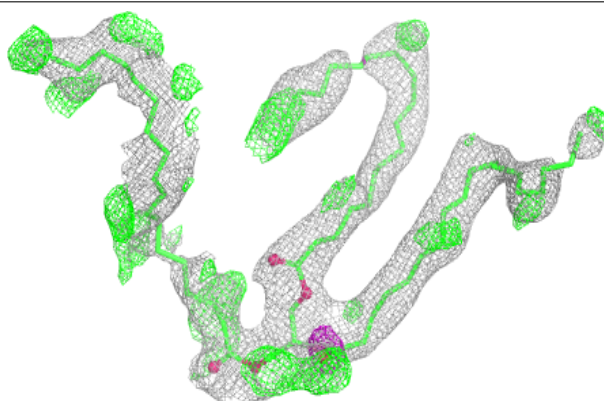


Electron density around CDL G 101:

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

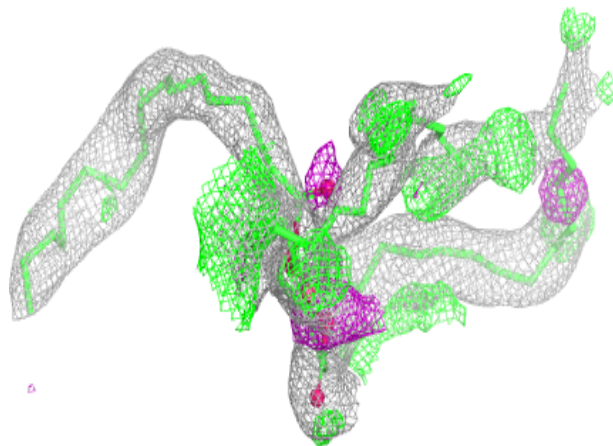
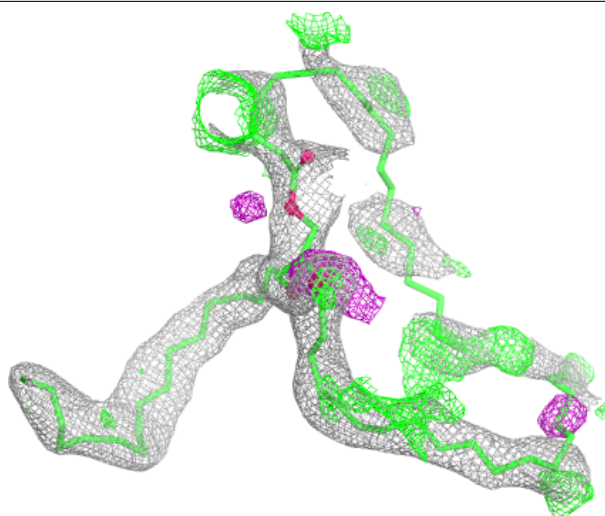
**Electron density around TGL Q 201:**

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



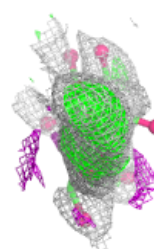
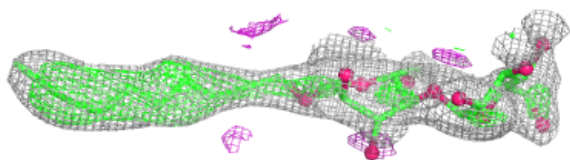
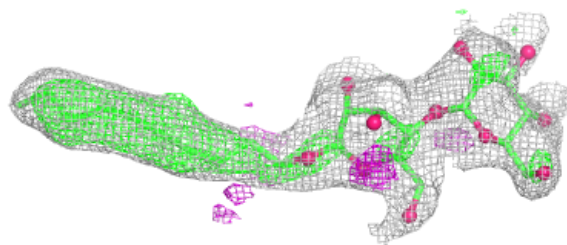
Electron density around TGL N 606:

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



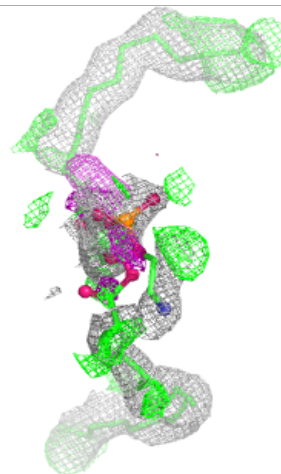
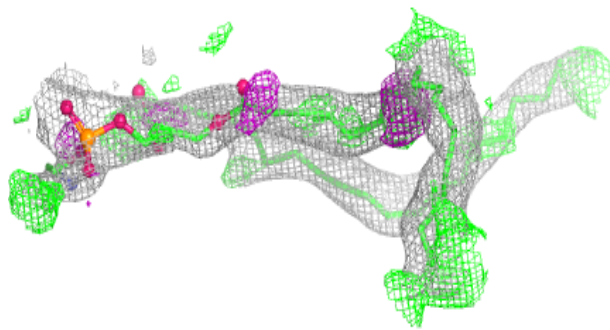
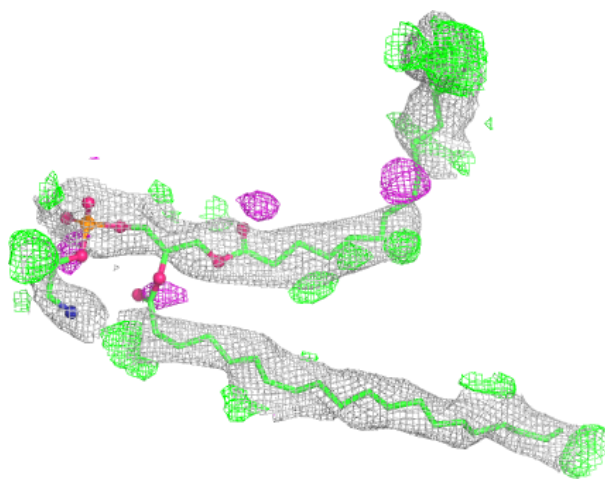
Electron density around DMU C 312:

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



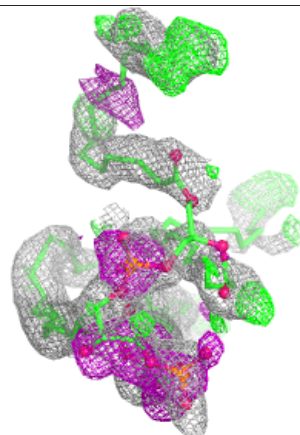
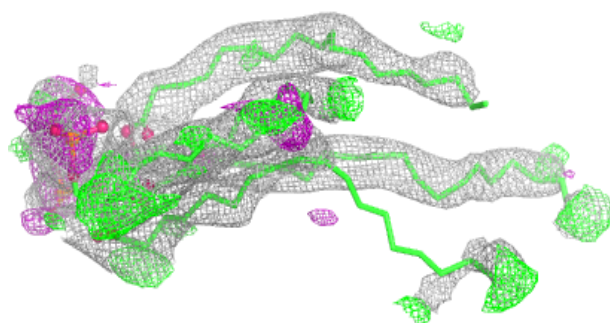
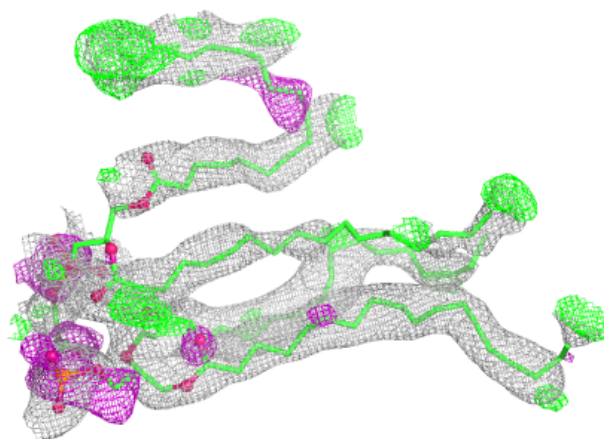
Electron density around PEK T 102:

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



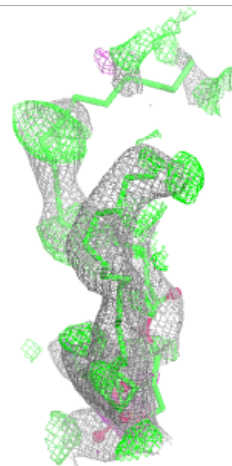
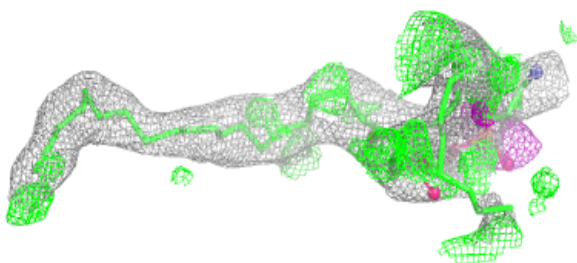
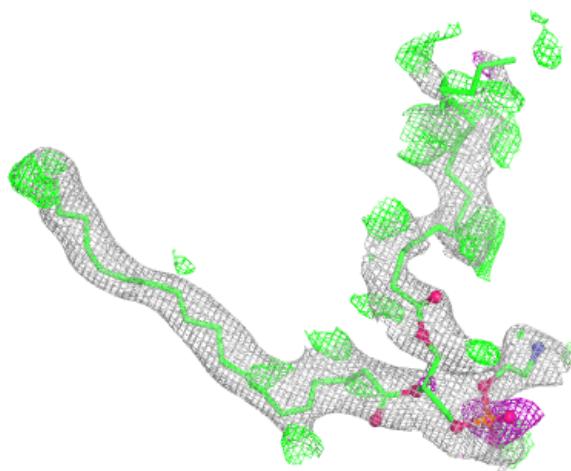
Electron density around CDL C 307:

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



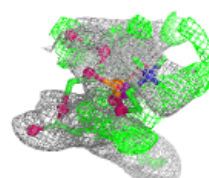
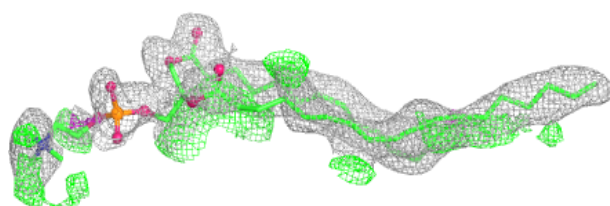
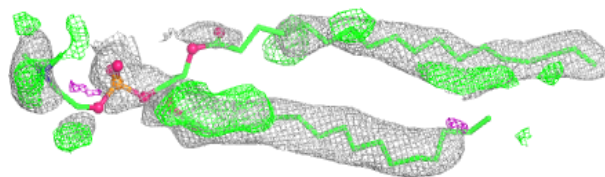
Electron density around PEK G 103:

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

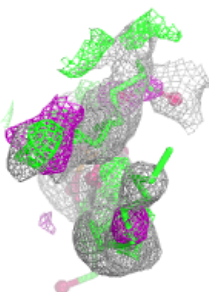
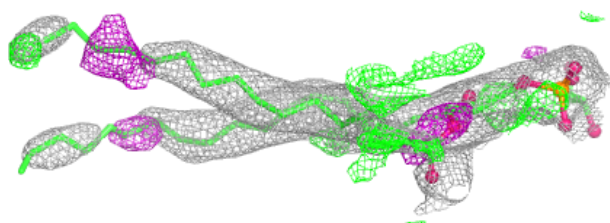
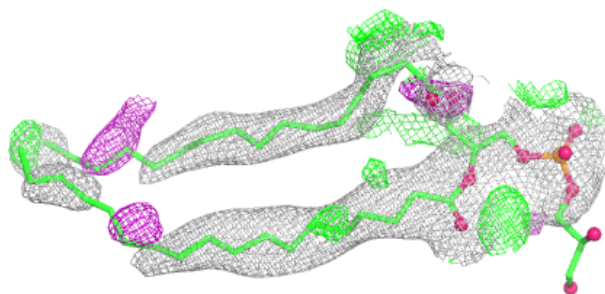


Electron density around PSC O 303:

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

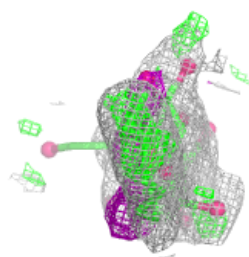
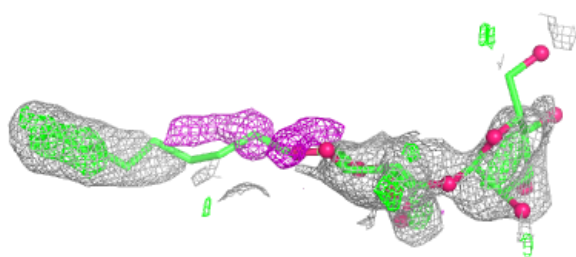
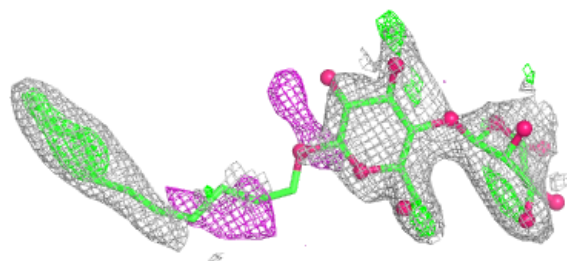
**Electron density around PGV N 607:**

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

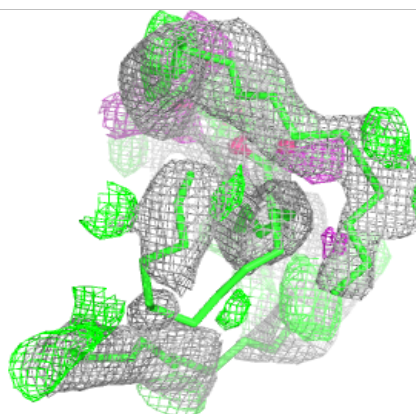
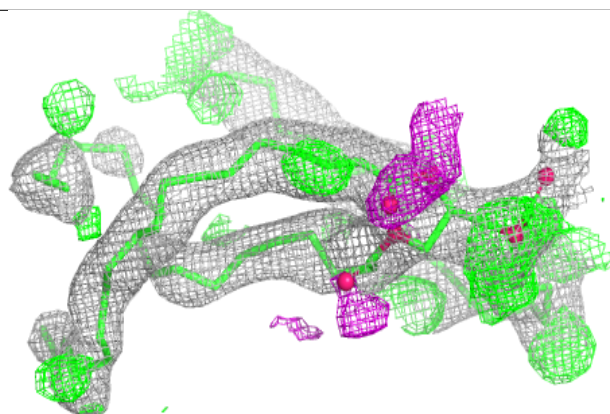
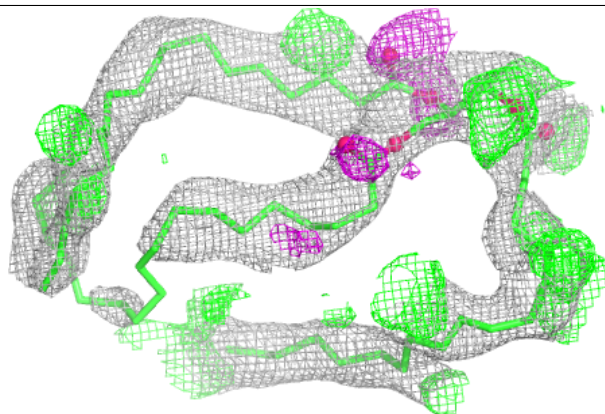


Electron density around DMU W 104:

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

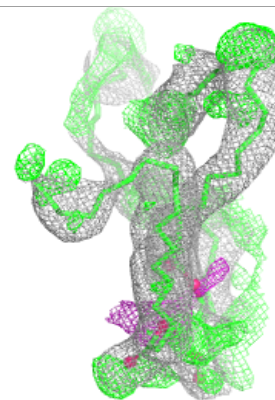
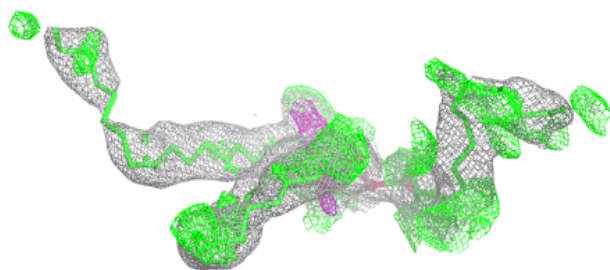
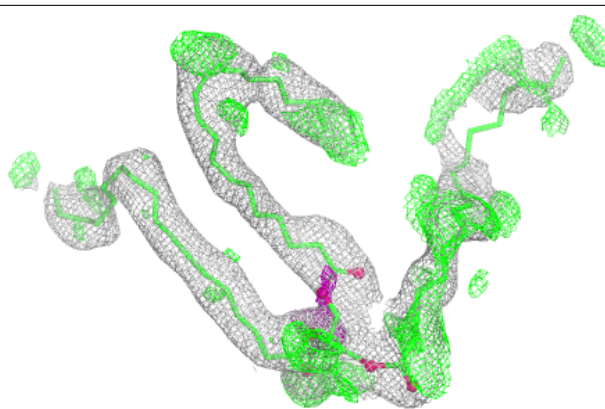
**Electron density around TGL B 301:**

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



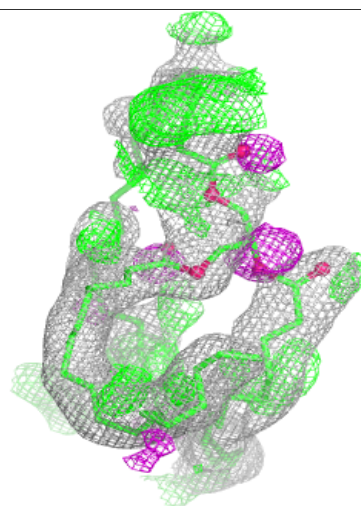
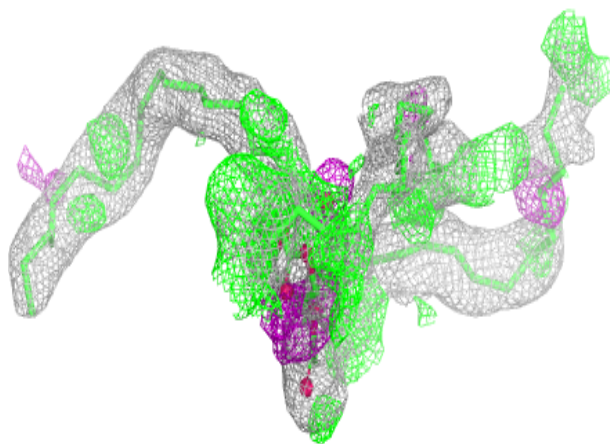
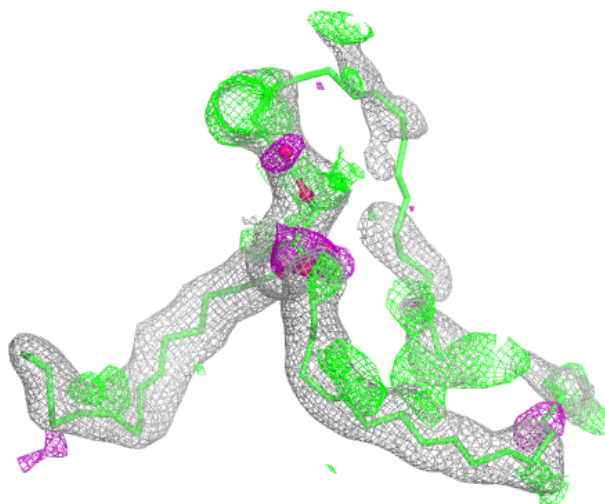
Electron density around TGL D 201:

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



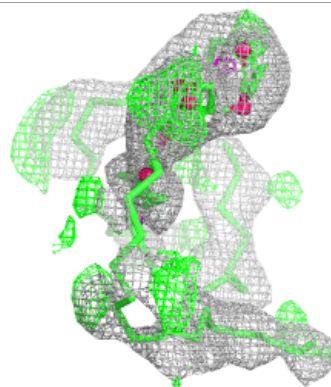
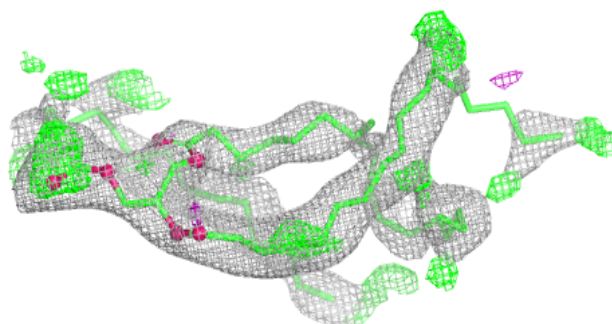
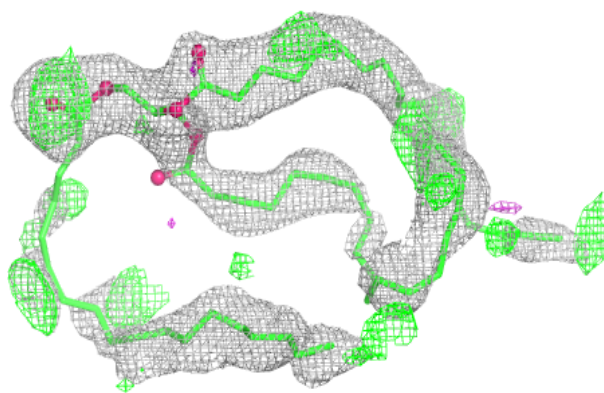
Electron density around TGL L 101:

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

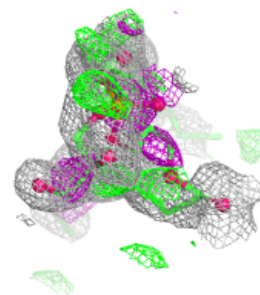
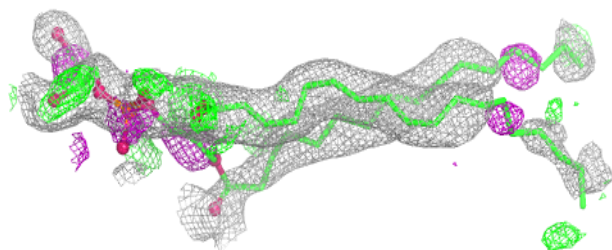
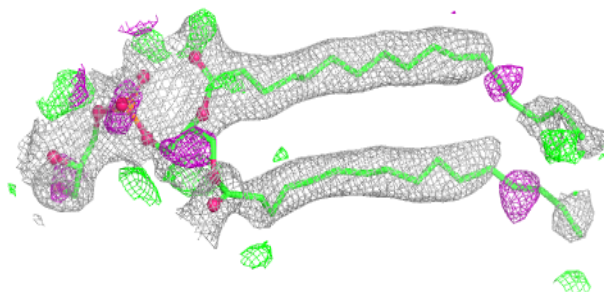


Electron density around TGL O 301:

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

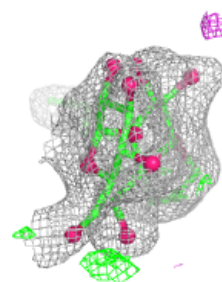
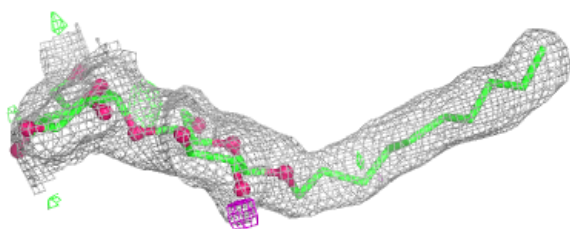
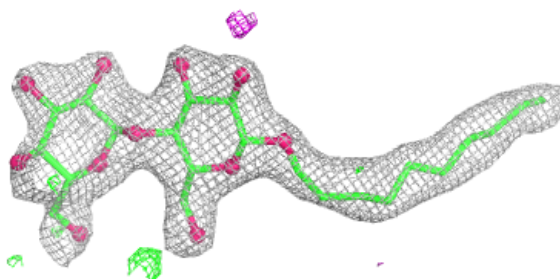
**Electron density around PGV A 606:**

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

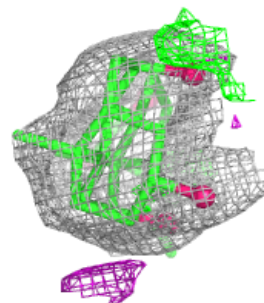
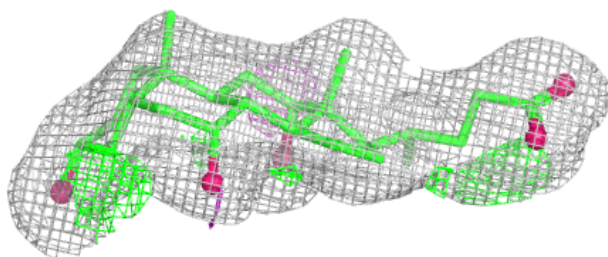
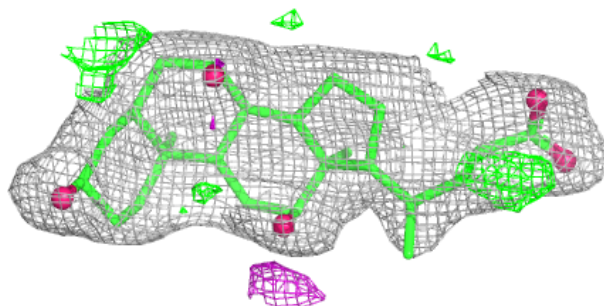


Electron density around DMU Z 101:

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

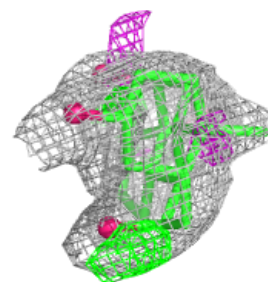
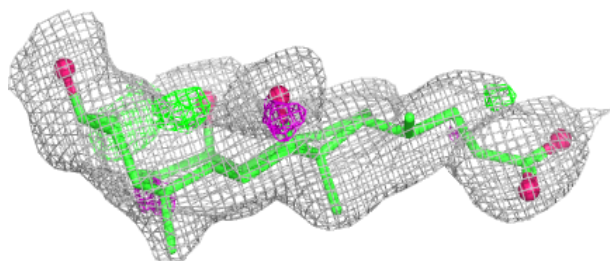
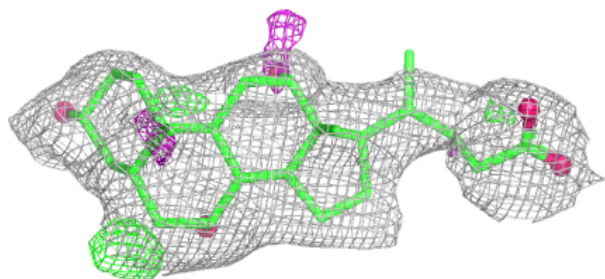
**Electron density around CHD C 308:**

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

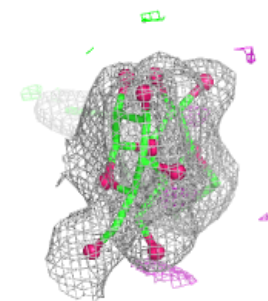
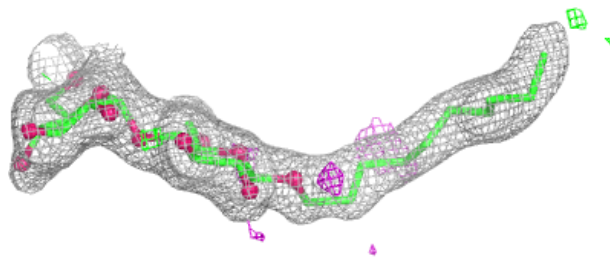
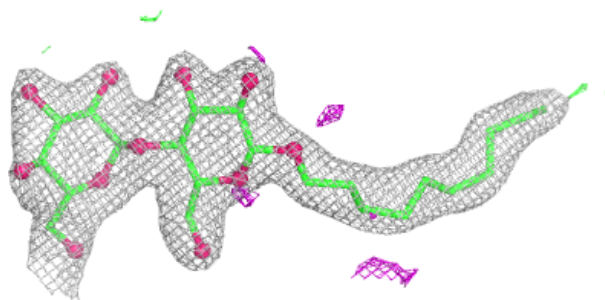


Electron density around CHD P 306:

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

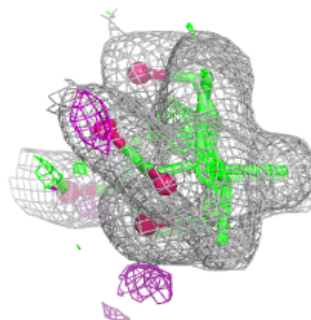
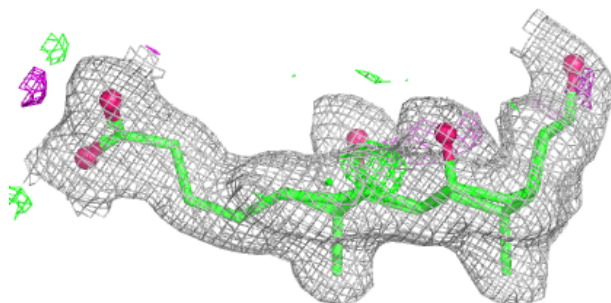
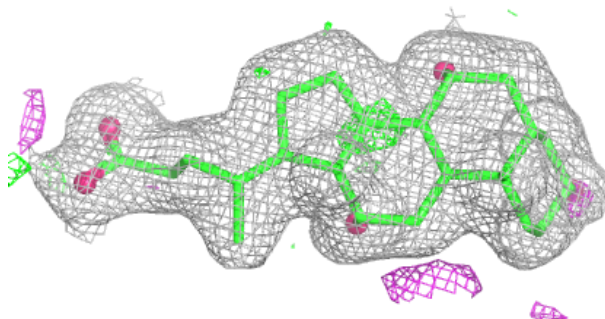
**Electron density around DMU M 101:**

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

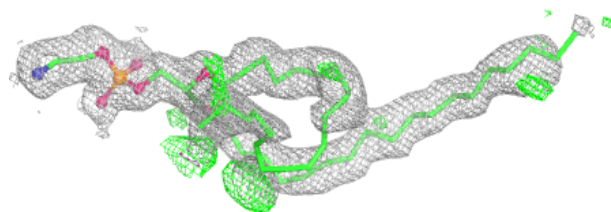
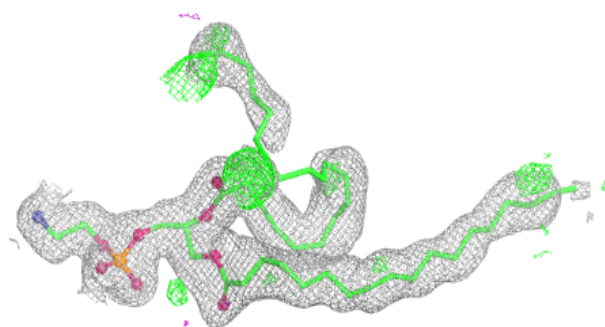


Electron density around CHD B 304:

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

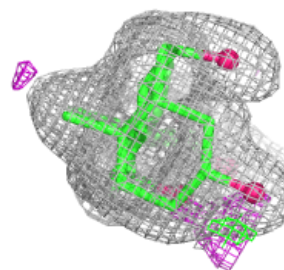
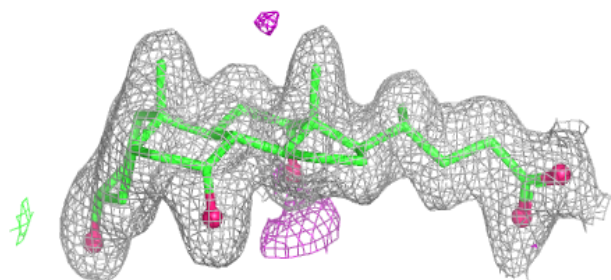
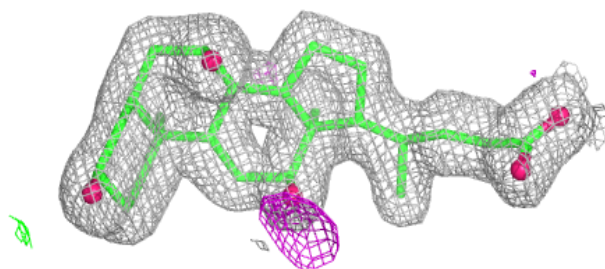
**Electron density around PEK P 303:**

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

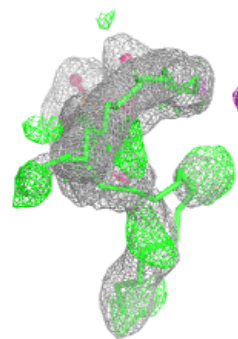
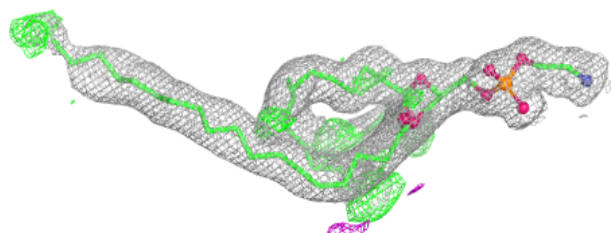
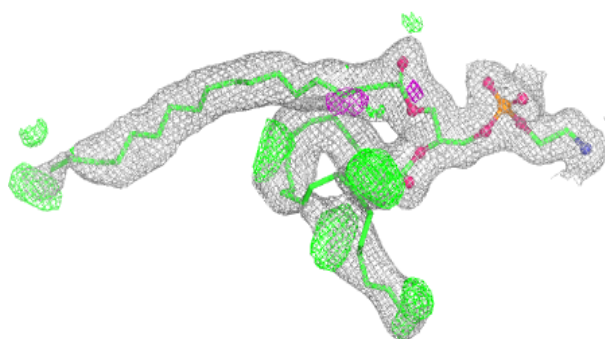


Electron density around CHD C 301:

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

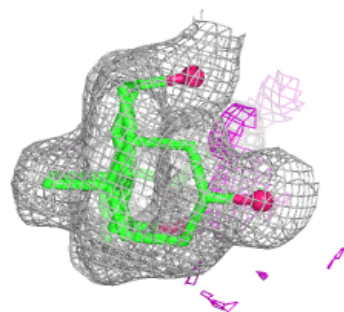
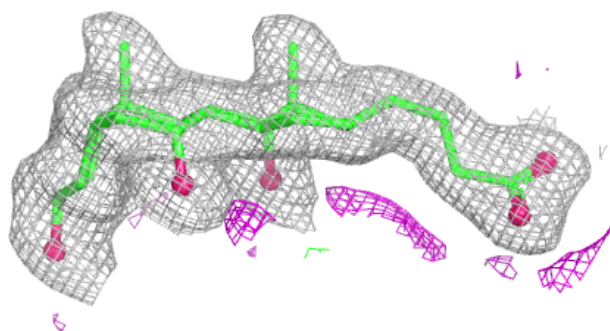
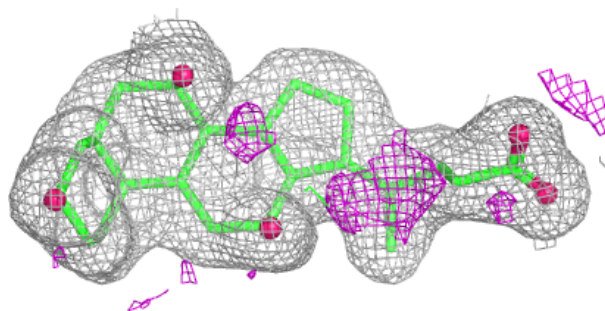
**Electron density around PEK C 303:**

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

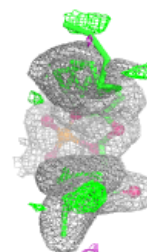
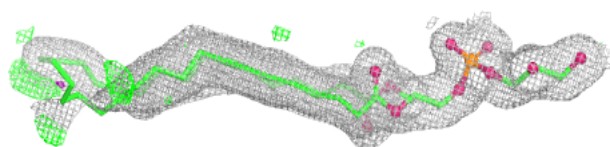
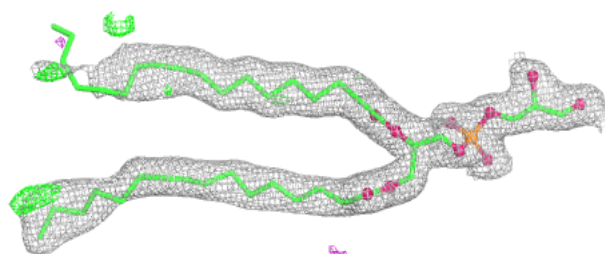


Electron density around CHD G 102:

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

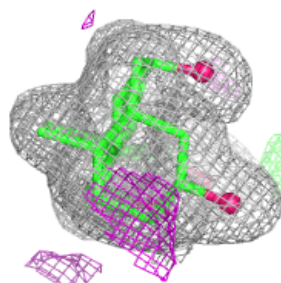
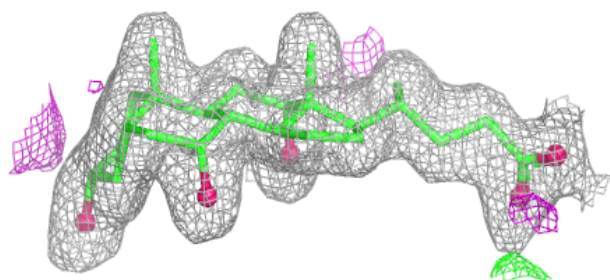
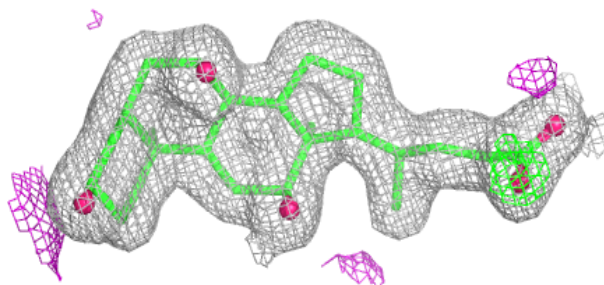
**Electron density around PGV C 305:**

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

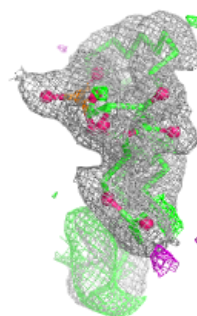
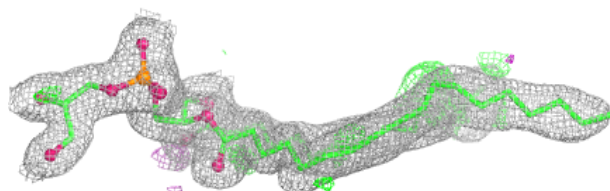
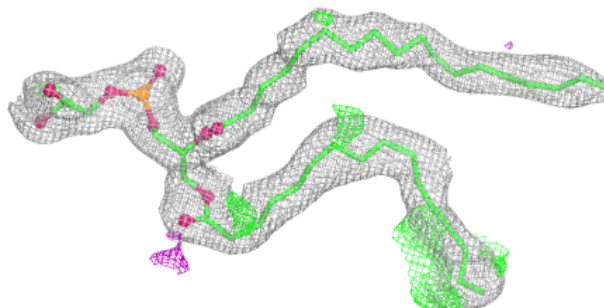


Electron density around CHD P 301:

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

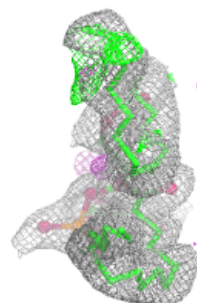
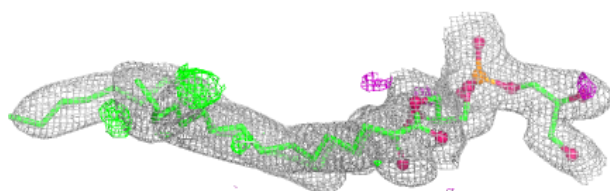
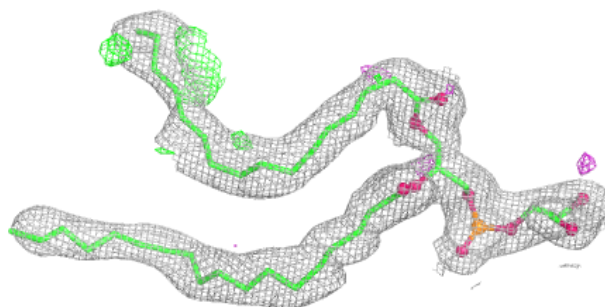
**Electron density around PGV A 608:**

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

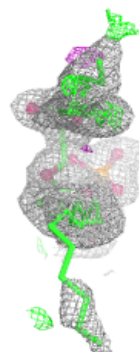
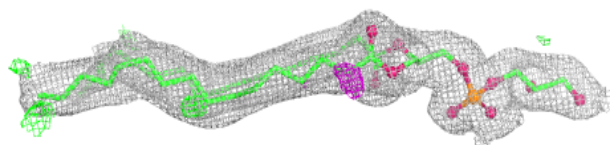
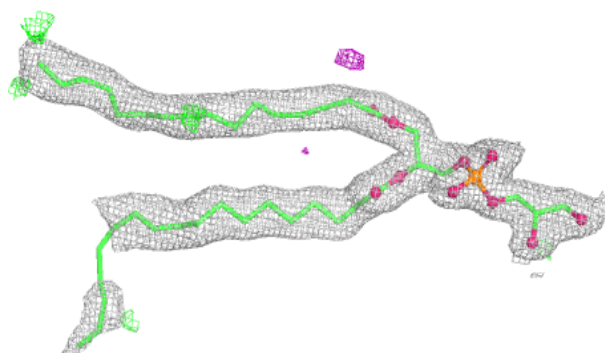


Electron density around PGV N 609:

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

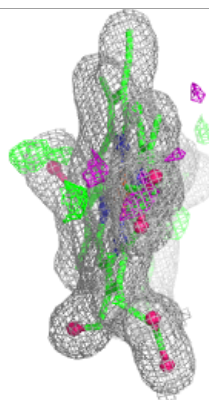
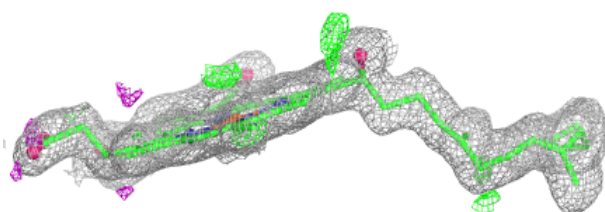
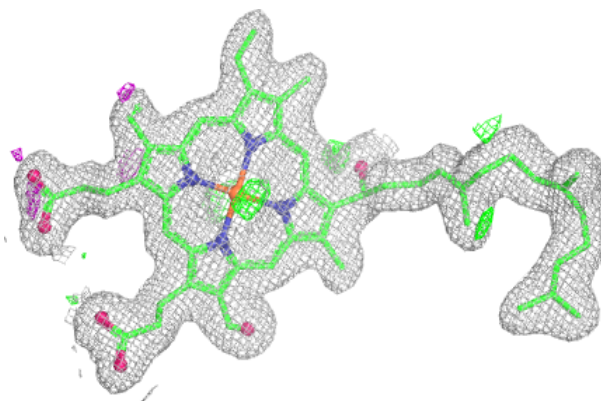
**Electron density around PGV P 304:**

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

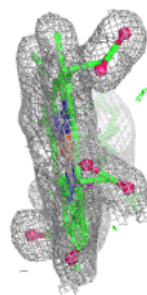
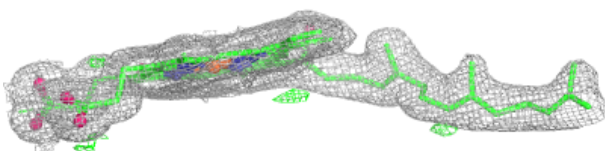
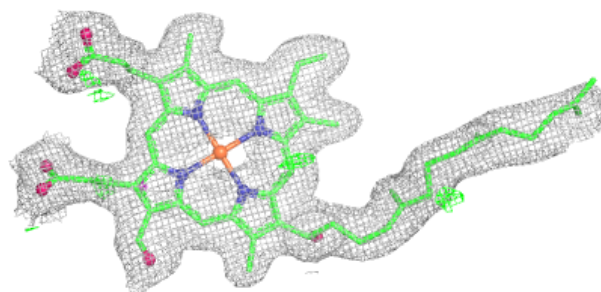


Electron density around HEA N 602:

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

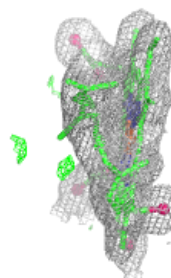
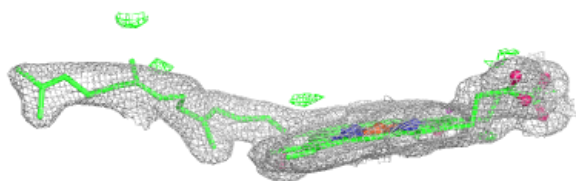
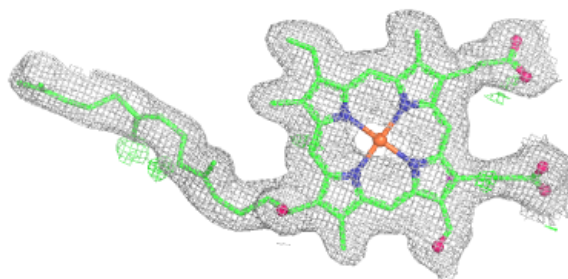
**Electron density around HEA N 601 (A):**

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

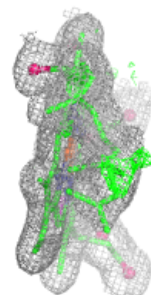
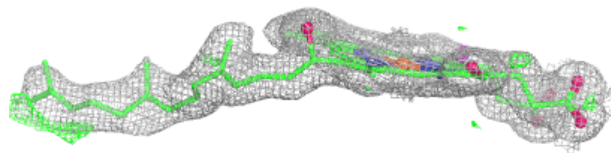
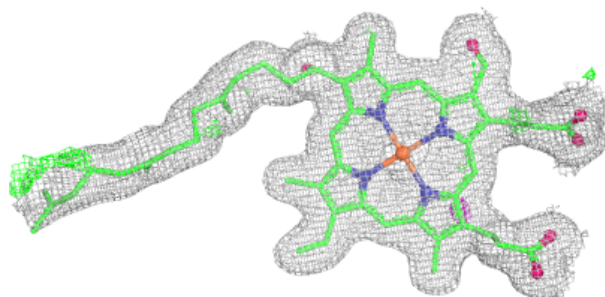


Electron density around HEA N 601 (B):

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

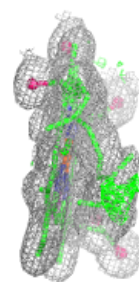
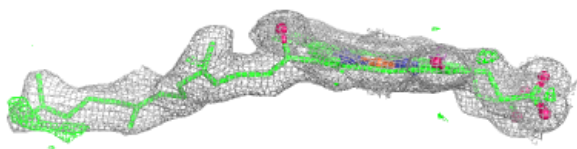
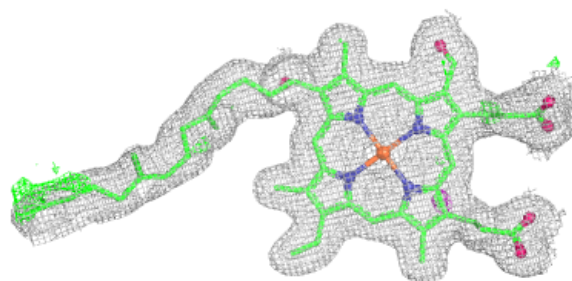
**Electron density around HEA A 601 (A):**

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

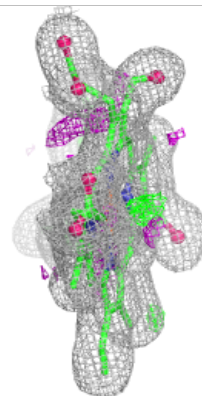
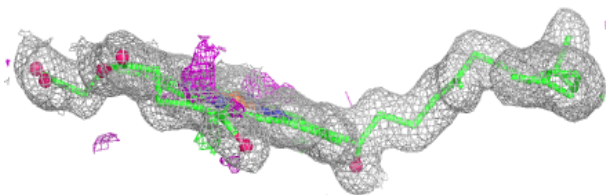
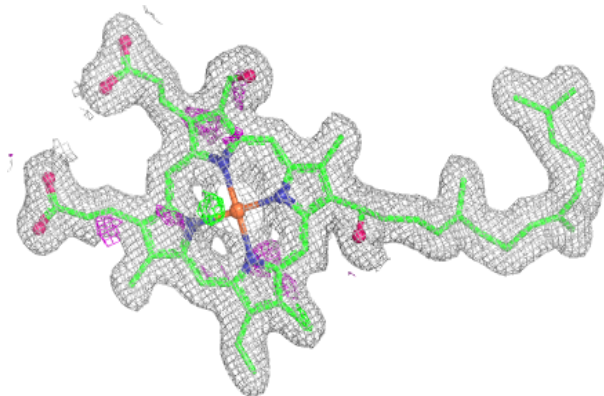


Electron density around HEA A 601 (B):

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

**Electron density around HEA A 602:**

$2mF_o-DF_c$ (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.