



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 08:36 AM UTC

PDB ID : 5XDX / pdb_00005xdx
Title : Bovine heart cytochrome c oxidase in the reduced state with pH 7.3 at 1.99 angstrom resolution
Authors : Luo, F.J.; Shimada, A.; Hagimoto, N.; Shimada, S.; Shinzawa-Itoh, K.; Yamashita, E.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2017-03-30
Resolution : 1.99 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

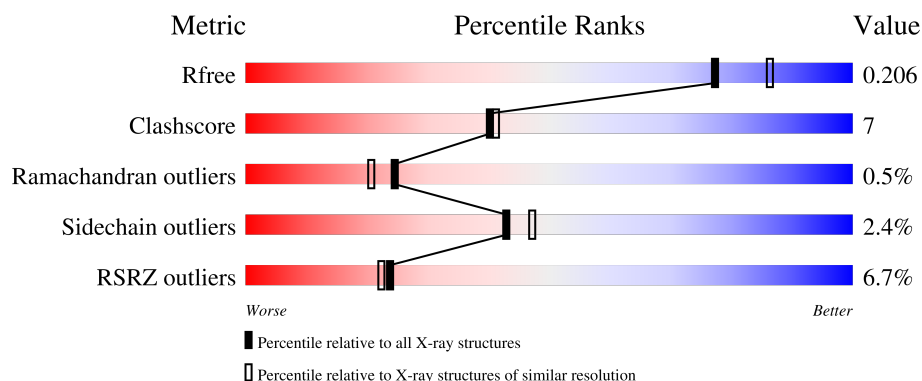
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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% 87% 12%
1	N	514	2% 86% 14%
2	B	227	4% 84% 15% .
2	O	227	7% 84% 15% .

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Mol	Chain	Length	Quality of chain
3	C	260	
3	P	260	
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
20	EDO	N	613	-	-	X	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 33247 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	20	0
			4128	2774	626	685	43			
1	N	514	Total	C	N	O	S	0	21	0
			4132	2773	627	687	45			

- 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	7	0
			1854	1209	281	343	21			
2	O	227	Total	C	N	O	S	0	6	0
			1849	1205	281	343	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	13	0
			2173	1461	338	358	16			
3	P	259	Total	C	N	O	S	0	12	0
			2168	1457	337	357	17			

- 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	0	0
			1195	777	196	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	1	0
			857	548	144	162	3			
5	R	105	Total	C	N	O	S	0	1	0
			857	548	144	162	3			

- 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
			721	448	127	140	6			
6	S	94	Total	C	N	O	S	0	1	0
			721	448	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 675	C 431	N 129	O 113	P 1	S 1	0	0	0
7	T	84	Total 675	C 431	N 129	O 113	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 polypeptide VIc.

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 VIIa-heart.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	2	0
			471	305	78	84	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	2	0
			471	305	78	84	4			

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

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

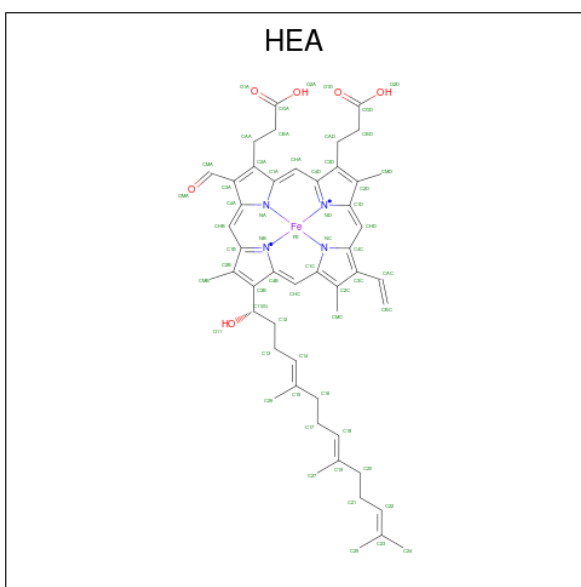
- Molecule 12 is a protein called Cytochrome c oxidase subunit VIIc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	1	0
			385	258	64	60	3			

- Molecule 13 is a protein called Cytochrome c oxidase subunit VIII-heart.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	1	0
			340	228	53	59			
13	Z	43	Total	C	N	O	0	1	0
			340	228	53	59			

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



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

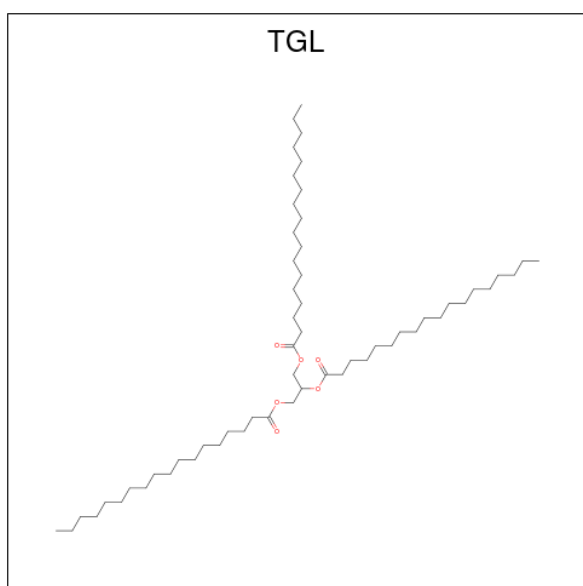
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

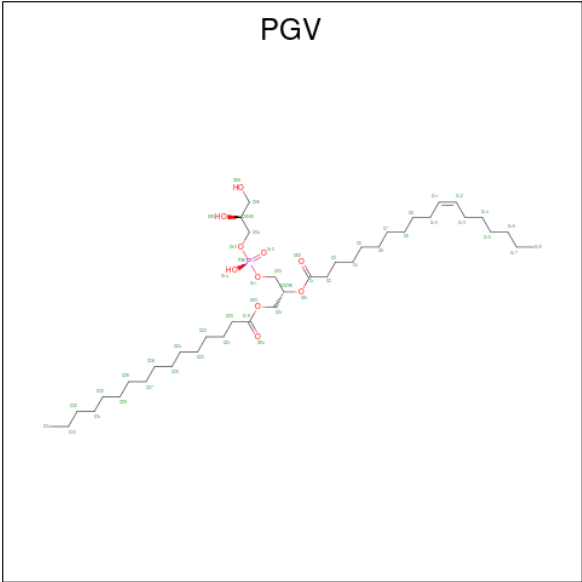
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	C	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		
17	P	1	Total	Na	0	0
			1	1		

- Molecule 18 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



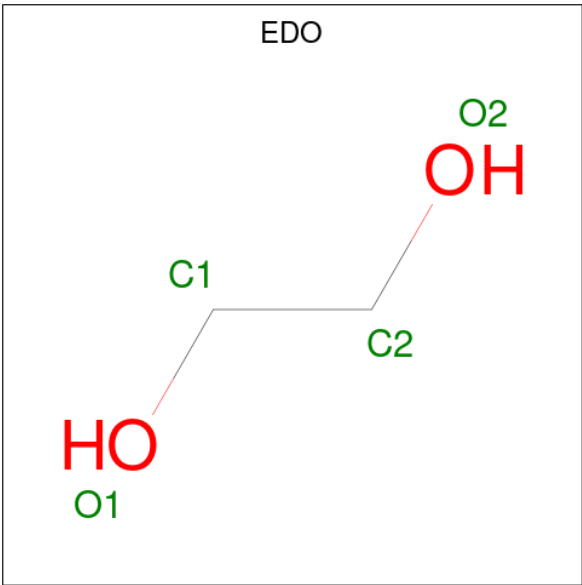
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	D	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	O	1	Total	C	O	0	0
			63	57	6		
18	Q	1	Total	C	O	0	0
			63	57	6		
18	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 19 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



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

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



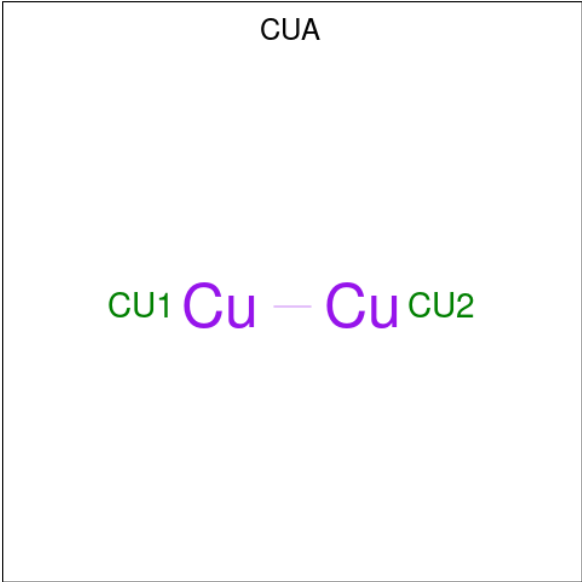
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20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

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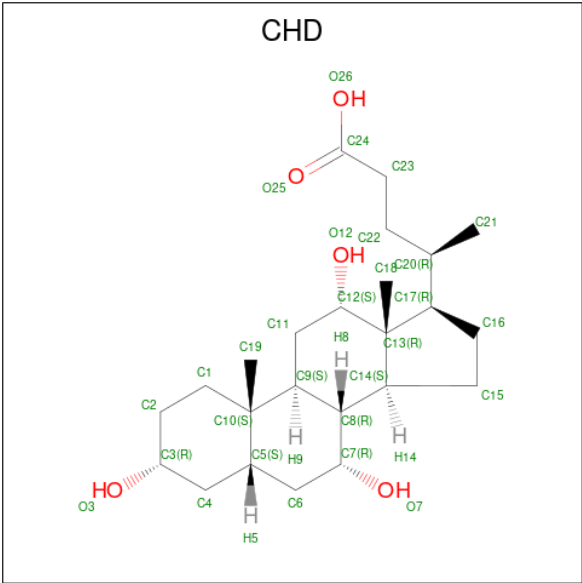
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	D	1	Total C O 4 2 2	0	0
20	E	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0
20	F	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	N	1	Total C O 4 2 2	0	0
20	P	1	Total C O 4 2 2	0	0
20	R	1	Total C O 4 2 2	0	0
20	S	1	Total C O 4 2 2	0	0
20	S	1	Total C O 4 2 2	0	0

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 22 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



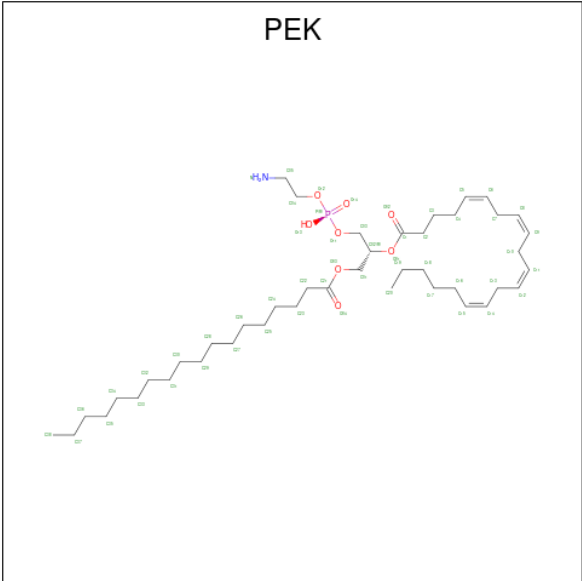
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		

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

- Molecule 23 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



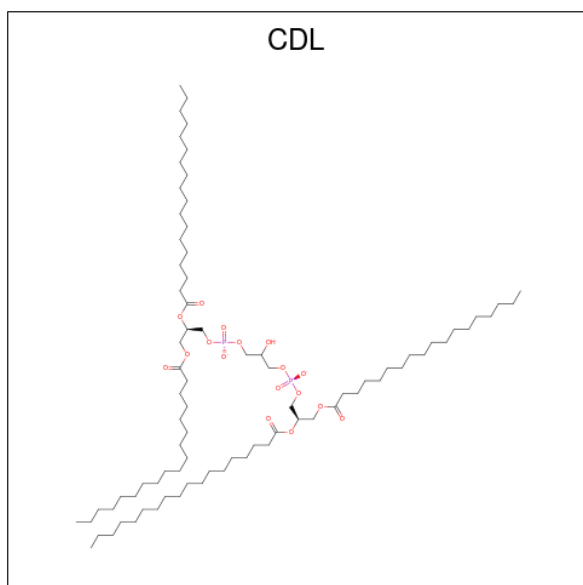
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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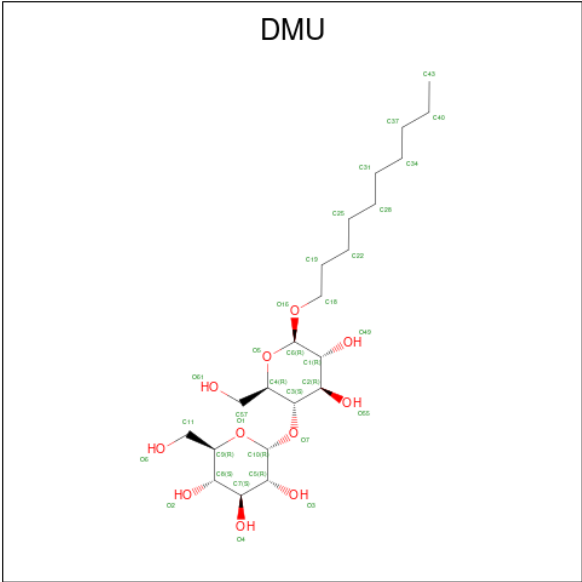
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 24 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



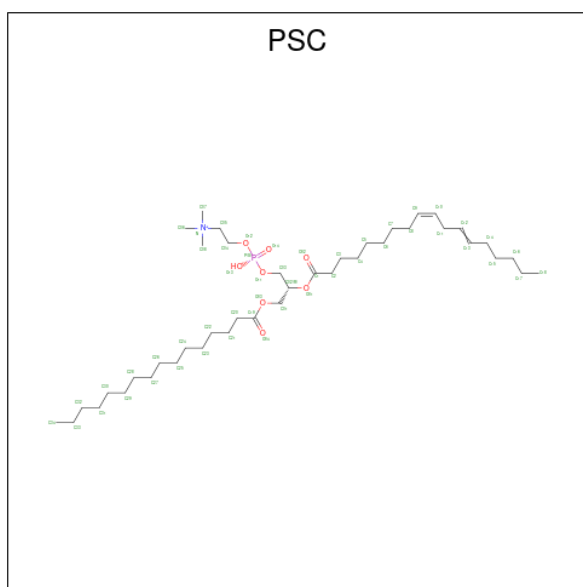
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	O	P		0	0
			100	81	17	2			
24	G	1	Total	C	O	P		0	0
			100	81	17	2			
24	P	1	Total	C	O	P		0	0
			100	81	17	2			
24	T	1	Total	C	O	P		0	0
			100	81	17	2			

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



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

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

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	245	Total	O	0	0
			245	245		
28	B	177	Total	O	0	1
			178	178		
28	C	103	Total	O	0	0
			103	103		
28	D	130	Total	O	0	0
			130	130		
28	E	92	Total	O	0	0
			92	92		

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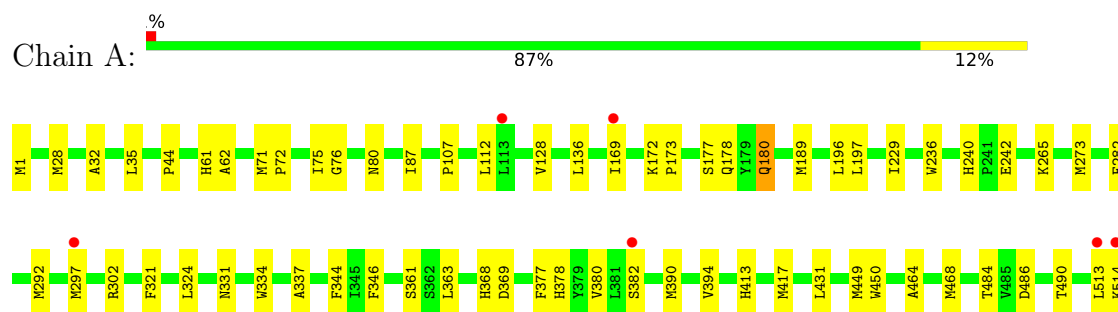
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	F	92	Total 92	O 92	0	0
28	G	58	Total 58	O 58	0	0
28	H	56	Total 56	O 56	0	0
28	I	48	Total 48	O 48	0	0
28	J	28	Total 28	O 28	0	0
28	K	42	Total 42	O 42	0	0
28	L	26	Total 26	O 26	0	0
28	M	27	Total 27	O 27	0	0
28	N	214	Total 214	O 214	0	0
28	O	128	Total 128	O 128	0	0
28	P	99	Total 99	O 99	0	0
28	Q	58	Total 58	O 58	0	0
28	R	62	Total 62	O 62	0	0
28	S	64	Total 64	O 64	0	0
28	T	51	Total 51	O 51	0	0
28	U	45	Total 45	O 45	0	0
28	V	31	Total 31	O 31	0	0
28	W	19	Total 19	O 19	0	0
28	X	11	Total 11	O 11	0	0
28	Y	21	Total 21	O 21	0	0
28	Z	14	Total 14	O 14	0	0

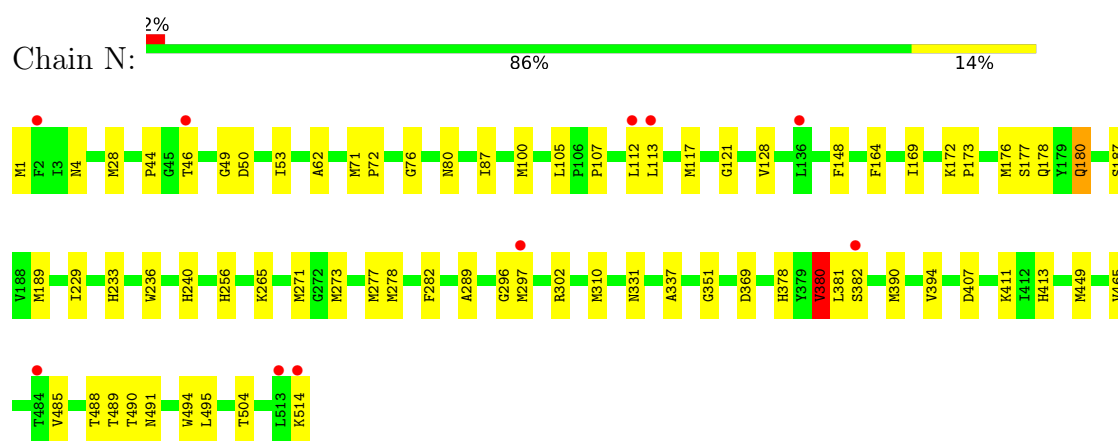
3 Residue-property plots [i](#)

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.

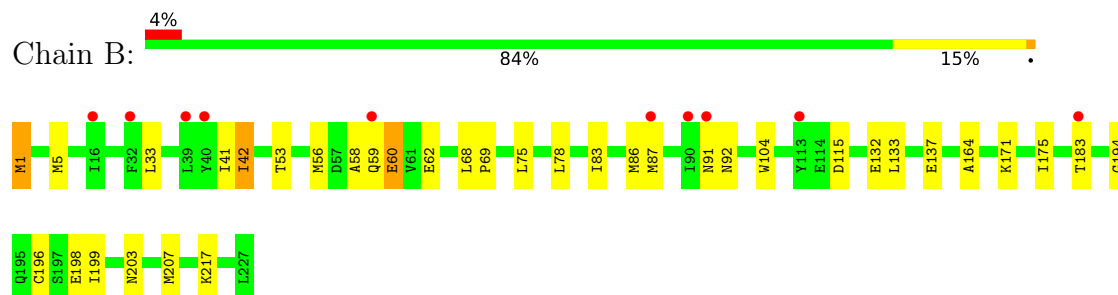
- Molecule 1: Cytochrome c oxidase subunit 1



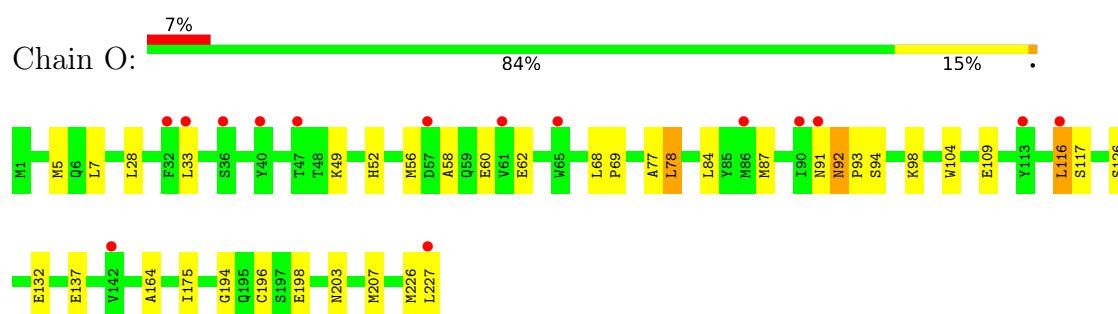
- Molecule 1: Cytochrome c oxidase subunit 1



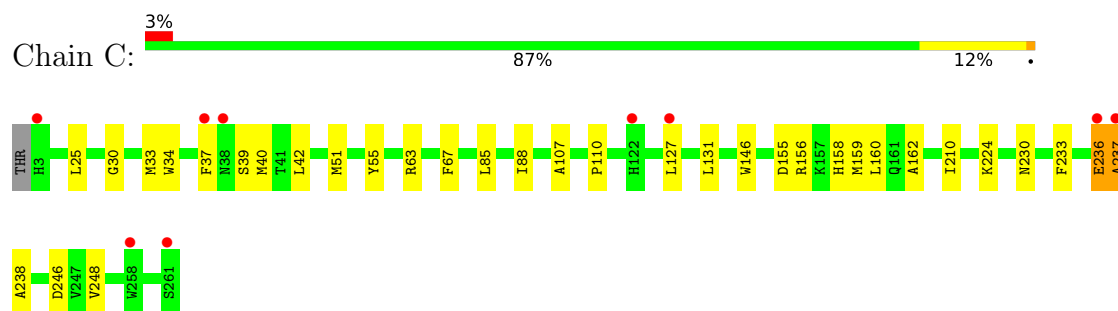
- Molecule 2: Cytochrome c oxidase subunit 2



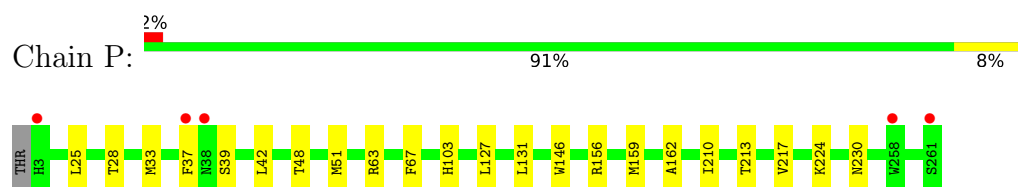
- Molecule 2: Cytochrome c oxidase subunit 2



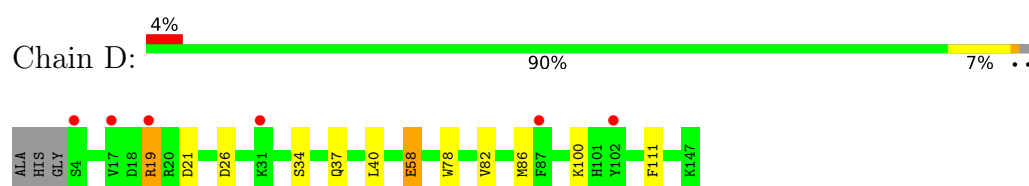
- Molecule 3: Cytochrome c oxidase subunit 3



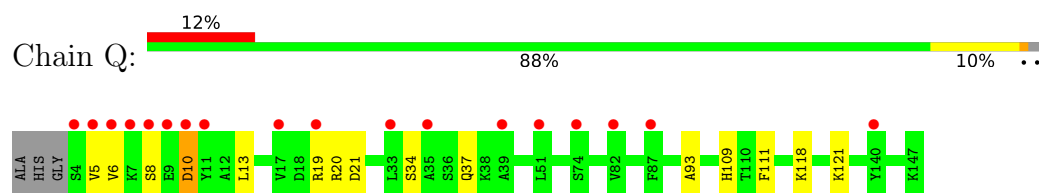
- Molecule 3: Cytochrome c oxidase subunit 3



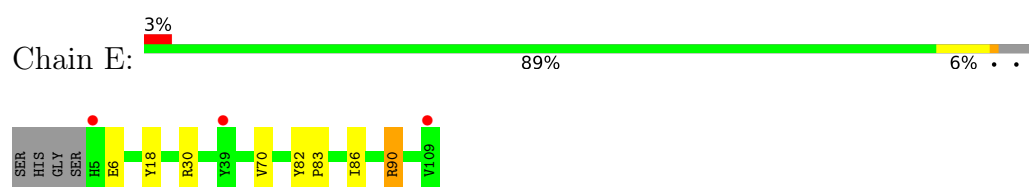
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



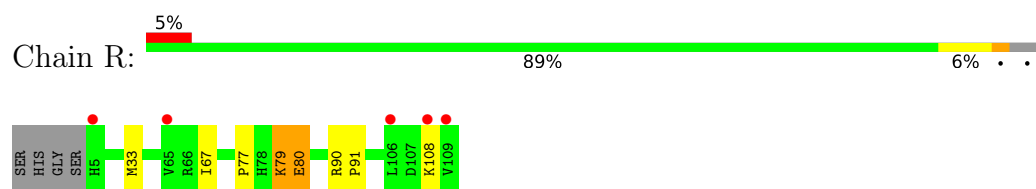
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



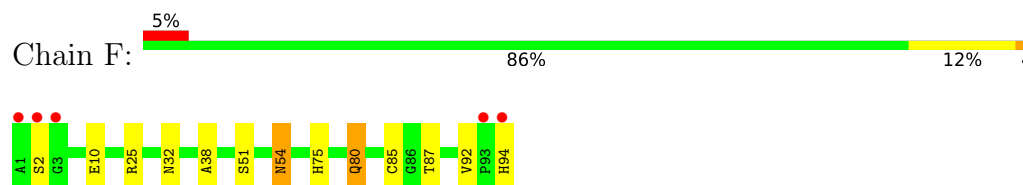
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



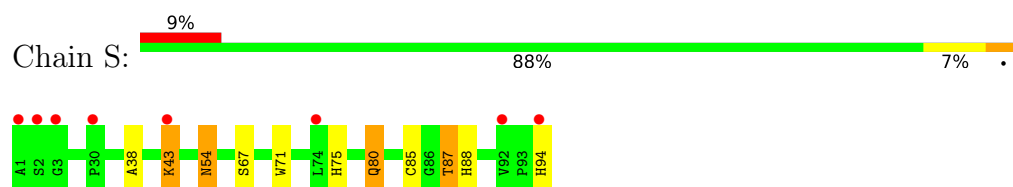
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



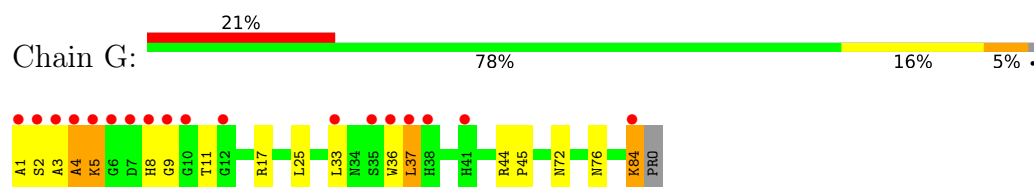
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



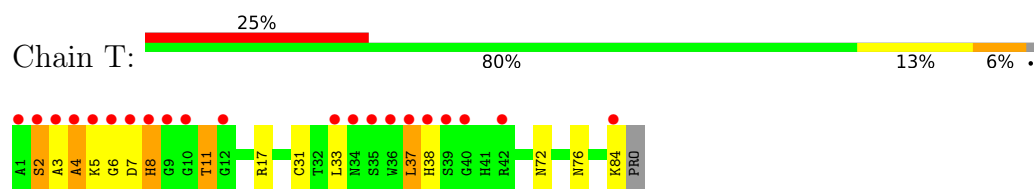
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



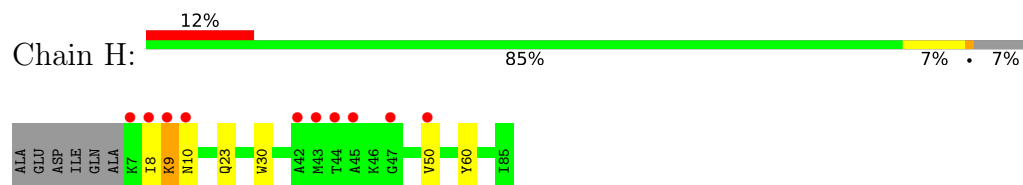
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



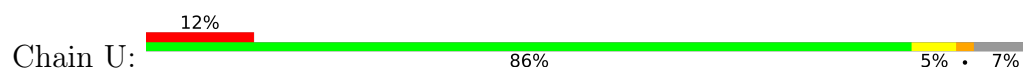
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



- Molecule 8: Cytochrome c oxidase subunit 6B1

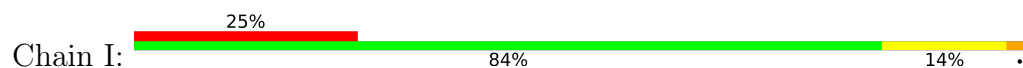


- Molecule 8: Cytochrome c oxidase subunit 6B1

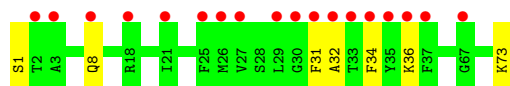
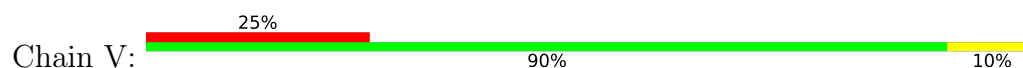




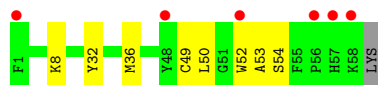
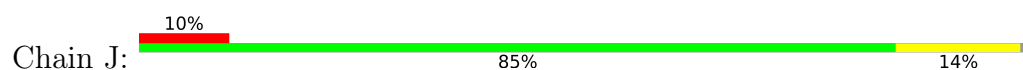
- Molecule 9: Cytochrome c oxidase polypeptide VIc



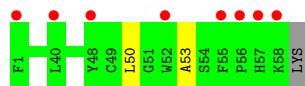
- Molecule 9: Cytochrome c oxidase polypeptide VIc



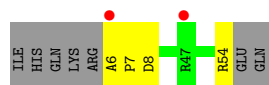
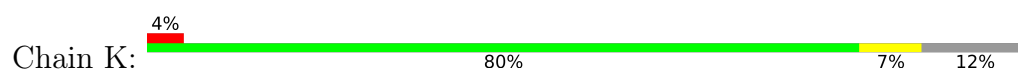
- Molecule 10: Cytochrome c oxidase subunit VIIa-heart



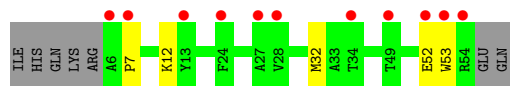
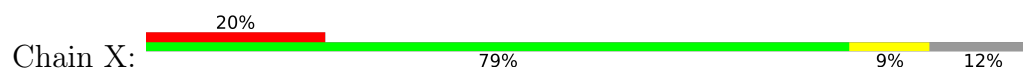
- Molecule 10: Cytochrome c oxidase subunit VIIa-heart



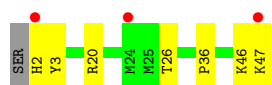
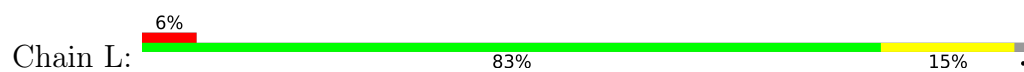
- Molecule 11: Cytochrome c oxidase subunit VIIb



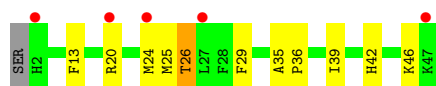
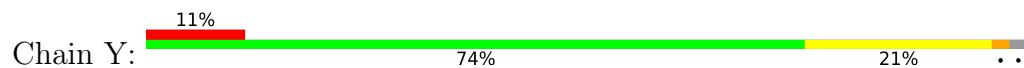
- Molecule 11: Cytochrome c oxidase subunit VIIb



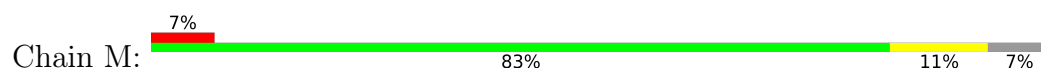
- Molecule 12: Cytochrome c oxidase subunit VIIc



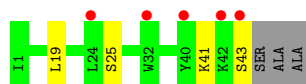
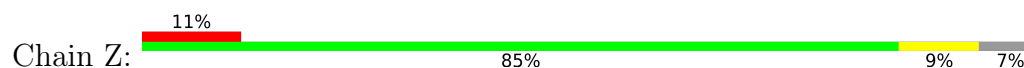
- Molecule 12: Cytochrome c oxidase subunit VIIc



- Molecule 13: Cytochrome c oxidase subunit VIII-heart



- Molecule 13: Cytochrome c oxidase subunit VIII-heart



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.04Å 205.69Å 177.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.99 40.00 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-1.99) 99.9 (40.00-1.99)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.182 , 0.203 0.184 , 0.206	Depositor DCC
R_{free} test set	23139 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33247	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.81	2/4315 (0.0%)	0.81	1/5889 (0.0%)
1	N	0.75	0/4322	0.84	4/5896 (0.1%)
2	B	0.78	1/1911 (0.1%)	0.83	1/2602 (0.0%)
2	O	0.68	1/1903 (0.1%)	0.80	0/2592
3	C	0.88	0/2299	0.78	4/3140 (0.1%)
3	P	0.85	0/2291	0.74	0/3128
4	D	0.69	0/1229	0.73	0/1658
4	Q	0.63	0/1229	0.77	0/1658
5	E	0.66	0/879	0.74	0/1192
5	R	0.62	0/879	0.76	0/1192
6	F	0.73	0/740	0.76	0/1003
6	S	0.72	0/740	0.77	0/1003
7	G	0.90	0/690	0.81	0/937
7	T	0.92	0/690	0.86	1/937 (0.1%)
8	H	0.65	0/682	0.76	0/921
8	U	0.64	0/682	0.80	0/921
9	I	0.58	0/605	0.85	0/802
9	V	0.49	0/605	0.84	0/802
10	J	0.67	0/488	0.76	0/658
10	W	0.68	0/488	0.75	0/658
11	K	0.76	0/398	0.84	0/546
11	X	0.71	0/398	0.82	0/546
12	L	0.72	0/393	0.78	0/526
12	Y	0.69	0/401	0.76	0/536
13	M	0.70	0/353	0.74	0/481
13	Z	0.64	0/353	0.83	0/481
All	All	0.75	4/29963 (0.0%)	0.80	11/40705 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	10.36	1.35	1.23
2	O	198	GLU	C-O	8.21	1.33	1.23
1	A	368	HIS	ND1-CE1	5.43	1.38	1.32
1	A	61	HIS	ND1-CE1	5.03	1.37	1.32

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	236	GLU	CA-C-N	-6.91	108.33	121.54
3	C	236	GLU	C-N-CA	-6.91	108.33	121.54
1	A	240	HIS	N-CA-CB	6.43	118.01	110.42
7	T	37	LEU	N-CA-C	-6.31	105.05	114.64
1	N	240	HIS	N-CA-CB	6.01	117.51	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4128	0	4171	60	0
1	N	4132	0	4169	84	0
2	B	1854	0	1888	26	0
2	O	1849	0	1879	22	0
3	C	2173	0	2130	36	0
3	P	2168	0	2122	24	0
4	D	1195	0	1183	15	0
4	Q	1195	0	1183	11	0
5	E	857	0	854	4	0
5	R	857	0	854	6	0
6	F	721	0	706	13	0
6	S	721	0	706	11	0
7	G	675	0	644	17	0
7	T	675	0	643	15	0
8	H	662	0	623	6	0
8	U	662	0	623	3	0
9	I	601	0	613	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	601	0	613	4	0
10	J	471	0	474	10	0
10	W	471	0	474	3	0
11	K	384	0	366	2	0
11	X	384	0	366	5	0
12	L	380	0	380	9	0
12	Y	385	0	389	12	0
13	M	340	0	363	5	0
13	Z	340	0	363	3	0
14	A	120	0	108	3	0
14	N	120	0	108	3	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	63	0	110	3	0
18	D	63	0	110	4	0
18	L	63	0	110	4	0
18	O	63	0	110	2	0
18	Q	63	0	110	0	0
18	Y	63	0	110	5	0
19	A	51	0	76	2	0
19	C	102	0	152	5	0
19	M	51	0	76	2	0
19	N	102	0	152	6	0
19	P	102	0	152	4	0
20	A	36	0	54	5	0
20	B	4	0	6	0	0
20	C	12	0	18	0	0
20	D	8	0	12	2	0
20	E	4	0	6	1	0
20	F	12	0	18	0	0
20	N	40	0	60	9	0
20	P	4	0	6	0	0
20	R	4	0	6	0	0
20	S	8	0	12	1	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B	29	0	39	0	0
22	C	58	0	78	3	0
22	J	29	0	38	0	0
22	O	29	0	39	1	0
22	P	58	0	78	3	0
22	W	29	0	39	1	0
23	C	106	0	154	5	0
23	G	53	0	77	0	0
23	T	159	0	231	7	0
24	C	100	0	156	10	0
24	G	100	0	156	5	0
24	P	100	0	156	9	0
24	T	100	0	156	13	0
25	C	66	0	84	12	0
25	M	33	0	42	0	0
25	P	66	0	84	9	0
25	Z	33	0	42	0	0
26	E	52	0	80	10	0
26	O	52	0	80	6	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	245	0	0	11	0
28	B	178	0	0	5	0
28	C	103	0	0	2	0
28	D	130	0	0	2	0
28	E	92	0	0	0	0
28	F	92	0	0	1	0
28	G	58	0	0	0	0
28	H	56	0	0	2	0
28	I	48	0	0	0	0
28	J	28	0	0	2	0
28	K	42	0	0	1	0
28	L	26	0	0	0	0
28	M	27	0	0	0	0
28	N	214	0	0	7	0
28	O	128	0	0	1	0
28	P	99	0	0	1	0
28	Q	58	0	0	1	0
28	R	62	0	0	0	0
28	S	64	0	0	0	0
28	T	51	0	0	0	0
28	U	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	V	31	0	0	1	0
28	W	19	0	0	0	0
28	X	11	0	0	3	0
28	Y	21	0	0	0	0
28	Z	14	0	0	0	0
All	All	33247	0	32270	417	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 417 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:113[B]:LEU:CG	1:N:117[B]:MET:HE2	1.65	1.26
3:C:236:GLU:O	3:C:237:ALA:CB	1.79	1.26
1:N:113[B]:LEU:HG	1:N:117[B]:MET:CE	1.69	1.22
20:A:615:EDO:H22	28:A:920:HOH:O	1.42	1.19
3:C:33[B]:MET:SD	25:C:313:DMU:H11	1.83	1.18

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	532/514 (104%)	520 (98%)	12 (2%)	0	100	100
1	N	533/514 (104%)	520 (98%)	13 (2%)	0	100	100
2	B	232/227 (102%)	227 (98%)	4 (2%)	1 (0%)	30	27
2	O	231/227 (102%)	225 (97%)	5 (2%)	1 (0%)	30	27
3	C	270/260 (104%)	263 (97%)	6 (2%)	1 (0%)	30	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	269/260 (104%)	262 (97%)	7 (3%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	136 (96%)	5 (4%)	1 (1%)	18	14
5	E	104/109 (95%)	103 (99%)	0	1 (1%)	12	8
5	R	104/109 (95%)	104 (100%)	0	0	100	100
6	F	93/94 (99%)	91 (98%)	2 (2%)	0	100	100
6	S	93/94 (99%)	91 (98%)	2 (2%)	0	100	100
7	G	81/85 (95%)	71 (88%)	6 (7%)	4 (5%)	1	0
7	T	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	1	0
8	H	77/85 (91%)	74 (96%)	2 (3%)	1 (1%)	9	5
8	U	77/85 (91%)	72 (94%)	5 (6%)	0	100	100
9	I	71/73 (97%)	68 (96%)	2 (3%)	1 (1%)	9	4
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	58/59 (98%)	57 (98%)	1 (2%)	0	100	100
10	W	58/59 (98%)	57 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	5	2
13	M	42/46 (91%)	41 (98%)	1 (2%)	0	100	100
13	Z	42/46 (91%)	41 (98%)	1 (2%)	0	100	100
All	All	3586/3604 (100%)	3478 (97%)	91 (2%)	17 (0%)	24	21

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	237	ALA
7	G	4	ALA
7	G	8	HIS
4	Q	8	SER
7	T	4	ALA

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	446/426 (105%)	440 (99%)	6 (1%)	61	68
1	N	447/426 (105%)	440 (98%)	7 (2%)	55	62
2	B	217/210 (103%)	208 (96%)	9 (4%)	27	26
2	O	216/210 (103%)	209 (97%)	7 (3%)	34	35
3	C	237/225 (105%)	234 (99%)	3 (1%)	61	68
3	P	236/225 (105%)	234 (99%)	2 (1%)	73	80
4	D	128/129 (99%)	126 (98%)	2 (2%)	55	62
4	Q	128/129 (99%)	125 (98%)	3 (2%)	44	49
5	E	93/95 (98%)	91 (98%)	2 (2%)	45	50
5	R	93/95 (98%)	91 (98%)	2 (2%)	45	50
6	F	79/78 (101%)	77 (98%)	2 (2%)	42	45
6	S	79/78 (101%)	74 (94%)	5 (6%)	16	13
7	G	67/68 (98%)	62 (92%)	5 (8%)	12	9
7	T	67/68 (98%)	63 (94%)	4 (6%)	17	14
8	H	71/75 (95%)	68 (96%)	3 (4%)	26	25
8	U	71/75 (95%)	67 (94%)	4 (6%)	19	16
9	I	57/57 (100%)	54 (95%)	3 (5%)	20	18
9	V	57/57 (100%)	56 (98%)	1 (2%)	51	58
10	J	51/50 (102%)	51 (100%)	0	100	100
10	W	51/50 (102%)	50 (98%)	1 (2%)	48	54
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	44
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	39/40 (98%)	39 (100%)	0	100	100
12	Y	40/40 (100%)	39 (98%)	1 (2%)	42	45
13	M	38/38 (100%)	38 (100%)	0	100	100
13	Z	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3124/3074 (102%)	3051 (98%)	73 (2%)	43 49

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	S	43	LYS
10	W	50	LEU
6	S	80	GLN
7	T	84	LYS
7	G	2	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	195	GLN
4	Q	101	HIS
2	O	203	ASN
3	P	68	GLN
4	Q	119	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	N	1	1	8,9,10	0.51	0	8,9,11	1.22	2 (25%)
7	TPO	T	11	7	8,10,11	1.45	1 (12%)	10,14,16	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	A	1	1	8,9,10	0.56	0	8,9,11	1.52	2 (25%)
9	SAC	V	1	9	7,8,9	2.06	2 (28%)	7,9,11	0.99	0
9	SAC	I	1	9	7,8,9	1.99	2 (28%)	7,9,11	0.79	0
2	FME	O	1	2	8,9,10	0.58	0	8,9,11	1.01	0
7	TPO	G	11	7	8,10,11	1.44	1 (12%)	10,14,16	0.87	0
2	FME	B	1	2	8,9,10	0.75	0	8,9,11	1.16	1 (12%)

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

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

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	4.67	1.33	1.23
9	V	1	SAC	OAC-C1A	4.63	1.33	1.23
7	G	11	TPO	P-O1P	2.92	1.59	1.50
7	T	11	TPO	P-O1P	2.88	1.59	1.50
9	V	1	SAC	CA-N	2.69	1.50	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	C-CA-N	3.09	115.47	109.50
1	N	1	FME	C-CA-N	2.20	113.74	109.50
1	N	1	FME	O-C-CA	-2.12	119.32	124.77
2	B	1	FME	O-C-CA	-2.10	119.36	124.77
1	A	1	FME	O-C-CA	-2.07	119.45	124.77

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
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
1	N	1	FME	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0
2	B	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 89 ligands modelled in this entry, 10 are monoatomic - leaving 79 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	$\# Z > 2$
22	CHD	J	101	-	32,32,32	0.59	0	51,51,51	1.59	9 (17%)
19	PGV	P	304	-	50,50,50	0.98	2 (4%)	53,56,56	0.94	2 (3%)
20	EDO	A	613	-	3,3,3	0.47	0	2,2,2	0.50	0
20	EDO	A	614	-	3,3,3	0.33	0	2,2,2	0.44	0
22	CHD	O	301	-	32,32,32	0.69	1 (3%)	51,51,51	1.15	4 (7%)
20	EDO	A	612	-	3,3,3	0.50	0	2,2,2	0.45	0
19	PGV	C	305	-	50,50,50	0.86	2 (4%)	53,56,56	0.82	1 (1%)
20	EDO	S	102	-	3,3,3	0.43	0	2,2,2	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	DMU	C	312	-	34,34,34	0.57	1 (2%)	45,45,45	1.26	5 (11%)
18	TGL	Q	201	-	62,62,62	1.31	6 (9%)	65,65,65	1.12	6 (9%)
19	PGV	N	607	-	50,50,50	0.90	2 (4%)	53,56,56	0.87	2 (3%)
22	CHD	W	101	-	32,32,32	0.57	0	51,51,51	1.50	8 (15%)
22	CHD	P	306	-	32,32,32	0.58	0	51,51,51	1.64	11 (21%)
24	CDL	G	101	-	99,99,99	1.41	12 (12%)	105,111,111	1.08	5 (4%)
20	EDO	P	307	-	3,3,3	0.43	0	2,2,2	0.37	0
20	EDO	A	608	-	3,3,3	0.39	0	2,2,2	0.44	0
20	EDO	F	102	-	3,3,3	0.38	0	2,2,2	0.47	0
23	PEK	T	102	-	52,52,52	0.90	3 (5%)	55,57,57	0.87	3 (5%)
20	EDO	B	303	-	3,3,3	0.38	0	2,2,2	0.43	0
20	EDO	D	202	-	3,3,3	0.47	0	2,2,2	0.29	0
20	EDO	N	613	-	3,3,3	0.32	0	2,2,2	0.62	0
20	EDO	N	614	-	3,3,3	0.44	0	2,2,2	0.18	0
21	CUA	O	303	2	0,1,1	-	-	-	-	-
20	EDO	E	202	-	3,3,3	0.39	0	2,2,2	0.37	0
20	EDO	A	616	-	3,3,3	0.40	0	2,2,2	0.22	0
20	EDO	S	103	-	3,3,3	0.45	0	2,2,2	0.18	0
20	EDO	A	610	-	3,3,3	0.44	0	2,2,2	0.53	0
22	CHD	P	301	-	32,32,32	0.63	0	51,51,51	1.01	2 (3%)
18	TGL	O	302	-	62,62,62	1.31	6 (9%)	65,65,65	1.12	3 (4%)
25	DMU	Z	101	-	34,34,34	0.47	0	45,45,45	0.72	2 (4%)
20	EDO	R	201	-	3,3,3	0.49	0	2,2,2	0.45	0
14	HEA	A	602	1	67,67,67	2.07	27 (40%)	81,103,103	1.28	10 (12%)
20	EDO	F	103	-	3,3,3	0.58	0	2,2,2	0.46	0
19	PGV	P	303	-	50,50,50	0.90	2 (4%)	53,56,56	0.84	3 (5%)
23	PEK	T	101	-	52,52,52	0.95	2 (3%)	55,57,57	0.93	2 (3%)
23	PEK	T	103	-	52,52,52	0.97	2 (3%)	55,57,57	0.88	3 (5%)
24	CDL	T	104	-	99,99,99	1.41	12 (12%)	105,111,111	1.11	6 (5%)
20	EDO	C	309	-	3,3,3	0.43	0	2,2,2	0.36	0
25	DMU	M	102	-	34,34,34	0.47	0	45,45,45	0.70	0
20	EDO	D	203	-	3,3,3	0.46	0	2,2,2	0.43	0
25	DMU	P	309	-	34,34,34	0.59	1 (2%)	45,45,45	0.84	1 (2%)
14	HEA	N	602	1	67,67,67	2.09	24 (35%)	81,103,103	1.24	8 (9%)
19	PGV	N	606	-	50,50,50	0.97	2 (4%)	53,56,56	0.98	2 (3%)
23	PEK	G	102	-	52,52,52	0.94	2 (3%)	55,57,57	0.96	3 (5%)
25	DMU	C	313	-	34,34,34	0.60	1 (2%)	45,45,45	1.05	3 (6%)
20	EDO	N	610	-	3,3,3	0.44	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	N	609	-	3,3,3	0.37	0	2,2,2	0.46	0
20	EDO	F	104	-	3,3,3	0.45	0	2,2,2	0.51	0
14	HEA	N	601	1	67,67,67	2.18	28 (41%)	81,103,103	1.33	11 (13%)
18	TGL	A	606	-	62,62,62	1.31	6 (9%)	65,65,65	1.43	8 (12%)
19	PGV	C	306	-	50,50,50	0.96	2 (4%)	53,56,56	0.97	2 (3%)
19	PGV	M	101	-	50,50,50	0.98	2 (4%)	53,56,56	1.01	3 (5%)
20	EDO	N	617	-	3,3,3	0.38	0	2,2,2	0.46	0
26	PSC	E	201	-	51,51,51	1.11	3 (5%)	57,59,59	1.02	2 (3%)
23	PEK	C	304	-	52,52,52	0.96	2 (3%)	55,57,57	0.94	2 (3%)
22	CHD	C	301	-	32,32,32	0.65	0	51,51,51	1.00	3 (5%)
22	CHD	C	308	-	32,32,32	0.61	0	51,51,51	1.52	11 (21%)
20	EDO	N	611	-	3,3,3	0.39	0	2,2,2	0.30	0
26	PSC	O	304	-	51,51,51	1.12	3 (5%)	57,59,59	1.02	3 (5%)
24	CDL	P	305	-	99,99,99	1.41	12 (12%)	105,111,111	1.12	8 (7%)
24	CDL	C	307	-	99,99,99	1.42	12 (12%)	105,111,111	1.11	4 (3%)
18	TGL	Y	101	-	62,62,62	1.31	6 (9%)	65,65,65	1.03	3 (4%)
18	TGL	D	201	-	62,62,62	1.32	6 (9%)	65,65,65	0.98	3 (4%)
20	EDO	N	615	-	3,3,3	0.35	0	2,2,2	0.45	0
20	EDO	N	616	-	3,3,3	0.43	0	2,2,2	0.37	0
23	PEK	C	303	-	52,52,52	0.84	2 (3%)	55,57,57	0.86	1 (1%)
20	EDO	N	608	-	3,3,3	0.49	0	2,2,2	0.27	0
18	TGL	L	101	-	62,62,62	1.32	6 (9%)	65,65,65	1.07	4 (6%)
25	DMU	P	308	-	34,34,34	0.59	1 (2%)	45,45,45	1.02	2 (4%)
20	EDO	A	611	-	3,3,3	0.39	0	2,2,2	0.34	0
20	EDO	N	612	-	3,3,3	0.55	0	2,2,2	0.23	0
19	PGV	A	607	-	50,50,50	0.89	2 (4%)	53,56,56	0.93	3 (5%)
21	CUA	B	301	2	0,1,1	-	-	-	-	-
22	CHD	B	302	-	32,32,32	0.71	0	51,51,51	1.08	2 (3%)
20	EDO	A	615	-	3,3,3	0.38	0	2,2,2	0.47	0
20	EDO	C	311	-	3,3,3	0.55	0	2,2,2	0.28	0
14	HEA	A	601	1	67,67,67	2.18	26 (38%)	81,103,103	1.31	13 (16%)
20	EDO	A	609	-	3,3,3	0.52	0	2,2,2	0.54	0
20	EDO	C	310	-	3,3,3	0.45	0	2,2,2	0.40	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
22	CHD	J	101	-	-	5/9/74/74	0/4/4/4
19	PGV	P	304	-	-	31/55/55/55	-
20	EDO	A	613	-	-	0/1/1/1	-
20	EDO	A	614	-	-	1/1/1/1	-
22	CHD	O	301	-	-	2/9/74/74	0/4/4/4
20	EDO	A	612	-	-	0/1/1/1	-
19	PGV	C	305	-	-	16/55/55/55	-
20	EDO	S	102	-	-	0/1/1/1	-
25	DMU	C	312	-	-	6/19/59/59	0/2/2/2
18	TGL	Q	201	-	-	35/65/65/65	-
19	PGV	N	607	-	-	11/55/55/55	-
22	CHD	W	101	-	-	5/9/74/74	0/4/4/4
22	CHD	P	306	-	-	8/9/74/74	0/4/4/4
24	CDL	G	101	-	-	61/110/110/110	-
20	EDO	P	307	-	-	0/1/1/1	-
20	EDO	A	608	-	-	0/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
23	PEK	T	102	-	-	20/56/56/56	-
20	EDO	B	303	-	-	1/1/1/1	-
20	EDO	D	202	-	-	1/1/1/1	-
20	EDO	N	613	-	-	1/1/1/1	-
20	EDO	N	614	-	-	0/1/1/1	-
20	EDO	E	202	-	-	0/1/1/1	-
20	EDO	A	616	-	-	1/1/1/1	-
20	EDO	S	103	-	-	0/1/1/1	-
20	EDO	A	610	-	-	0/1/1/1	-
22	CHD	P	301	-	-	2/9/74/74	0/4/4/4
18	TGL	O	302	-	-	33/65/65/65	-
25	DMU	Z	101	-	-	7/19/59/59	0/2/2/2
20	EDO	R	201	-	-	0/1/1/1	-
14	HEA	A	602	1	-	9/36/76/76	-
20	EDO	F	103	-	-	0/1/1/1	-
19	PGV	P	303	-	-	16/55/55/55	-
23	PEK	T	101	-	-	32/56/56/56	-
23	PEK	T	103	-	-	26/56/56/56	-
24	CDL	T	104	-	-	61/110/110/110	-
20	EDO	C	309	-	-	0/1/1/1	-
25	DMU	M	102	-	-	4/19/59/59	0/2/2/2
20	EDO	D	203	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DMU	P	309	-	-	7/19/59/59	0/2/2/2
14	HEA	N	602	1	-	9/36/76/76	-
19	PGV	N	606	-	-	30/55/55/55	-
23	PEK	G	102	-	-	32/56/56/56	-
25	DMU	C	313	-	-	8/19/59/59	0/2/2/2
20	EDO	N	610	-	-	0/1/1/1	-
20	EDO	N	609	-	-	1/1/1/1	-
20	EDO	F	104	-	-	1/1/1/1	-
14	HEA	N	601	1	-	4/36/76/76	-
18	TGL	A	606	-	-	36/65/65/65	-
19	PGV	C	306	-	-	24/55/55/55	-
19	PGV	M	101	-	-	31/55/55/55	-
20	EDO	N	617	-	-	0/1/1/1	-
26	PSC	E	201	-	-	31/55/55/55	-
23	PEK	C	304	-	-	30/56/56/56	-
22	CHD	C	301	-	-	2/9/74/74	0/4/4/4
22	CHD	C	308	-	-	9/9/74/74	0/4/4/4
26	PSC	O	304	-	-	34/55/55/55	-
20	EDO	N	611	-	-	0/1/1/1	-
24	CDL	P	305	-	-	63/110/110/110	-
24	CDL	C	307	-	-	57/110/110/110	-
18	TGL	Y	101	-	-	37/65/65/65	-
18	TGL	D	201	-	-	38/65/65/65	-
20	EDO	N	615	-	-	1/1/1/1	-
20	EDO	N	616	-	-	0/1/1/1	-
23	PEK	C	303	-	-	16/56/56/56	-
20	EDO	N	608	-	-	1/1/1/1	-
18	TGL	L	101	-	-	37/65/65/65	-
25	DMU	P	308	-	-	8/19/59/59	0/2/2/2
20	EDO	A	611	-	-	0/1/1/1	-
20	EDO	N	612	-	-	0/1/1/1	-
19	PGV	A	607	-	-	11/55/55/55	-
22	CHD	B	302	-	-	2/9/74/74	0/4/4/4
20	EDO	A	615	-	-	0/1/1/1	-
20	EDO	C	311	-	-	0/1/1/1	-
14	HEA	A	601	1	-	6/36/76/76	-
20	EDO	A	609	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	C	310	-	-	0/1/1/1	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	FE-ND	5.52	2.11	1.94
14	N	602	HEA	FE-ND	5.18	2.10	1.94
14	A	602	HEA	FE-ND	5.15	2.10	1.94
14	N	602	HEA	FE-NB	5.13	2.10	1.94
14	N	601	HEA	FE-NA	5.02	2.11	1.95

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	101	CHD	C17-C13-C14	-5.02	95.08	100.11
18	A	606	TGL	OG2-CB1-CB2	4.59	121.41	111.48
24	T	104	CDL	OB6-CB5-C51	4.41	121.02	111.48
24	C	307	CDL	OA6-CA5-C11	4.26	120.69	111.48
24	G	101	CDL	OB6-CB5-C51	4.23	120.64	111.48

There are no chirality outliers.

5 of 961 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601	HEA	C2A-C3A-CMA-OMA
14	A	602	HEA	C2A-C3A-CMA-OMA
14	A	602	HEA	C2D-C3D-CAD-CBD
14	A	602	HEA	C4D-C3D-CAD-CBD
14	N	601	HEA	C2A-C3A-CMA-OMA

There are no ring outliers.

49 monomers are involved in 150 short contacts:

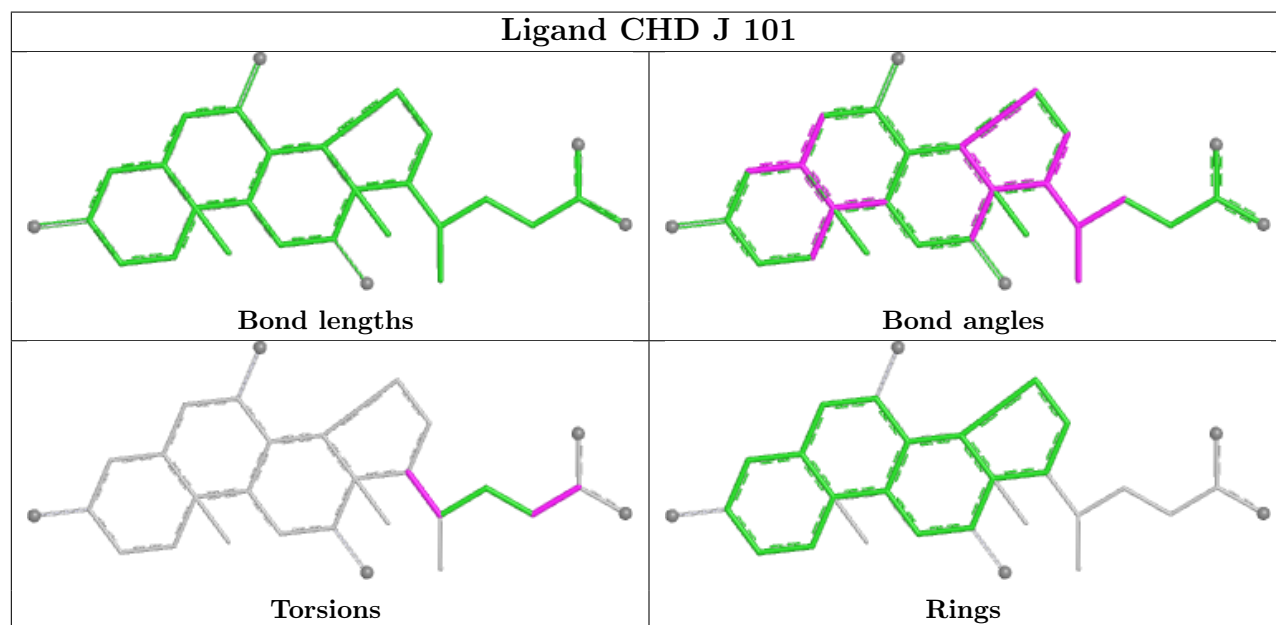
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	P	304	PGV	1	0
22	O	301	CHD	1	0
19	C	305	PGV	4	0
19	N	607	PGV	4	0
22	W	101	CHD	1	0
22	P	306	CHD	1	0
24	G	101	CDL	5	0

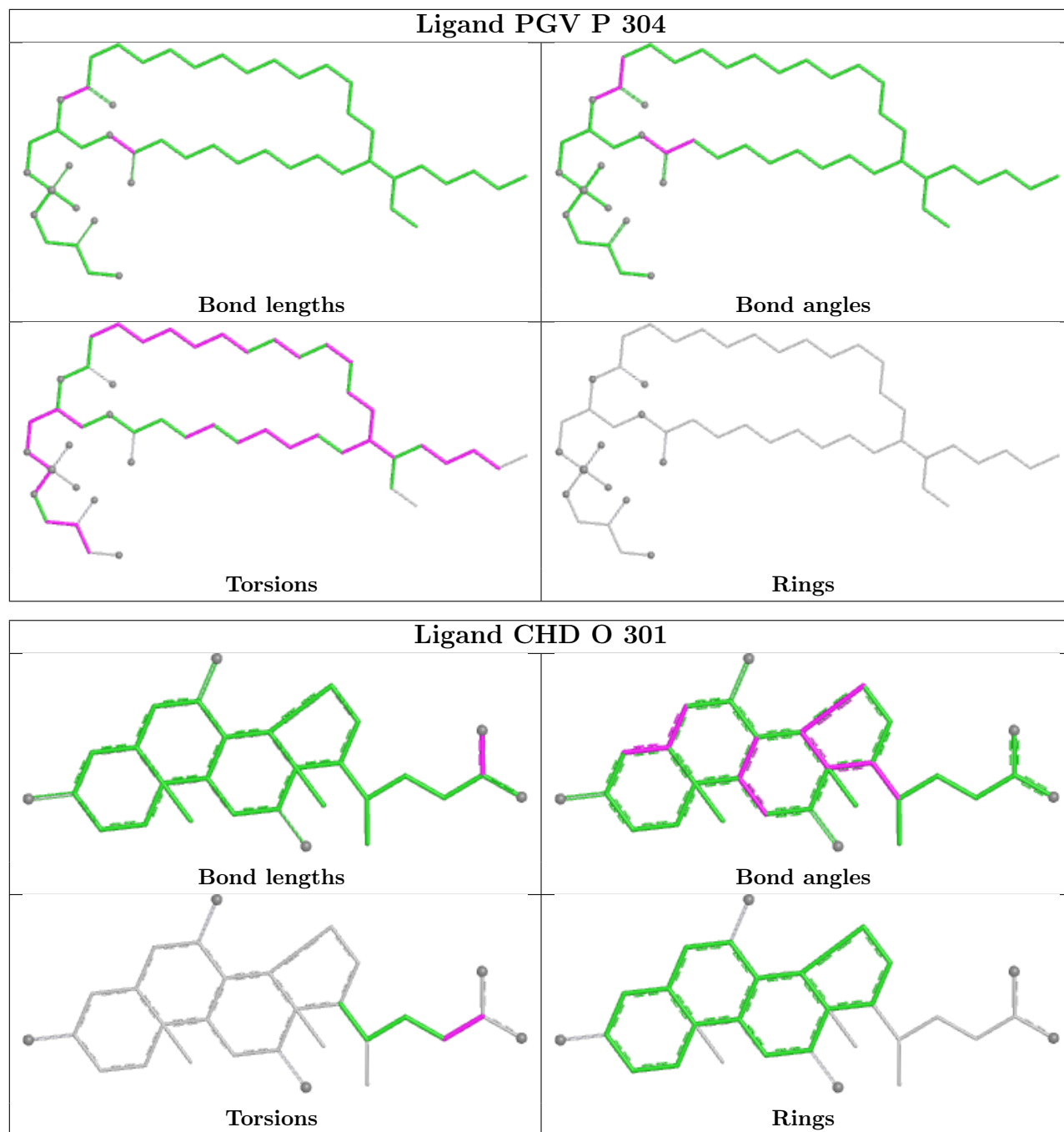
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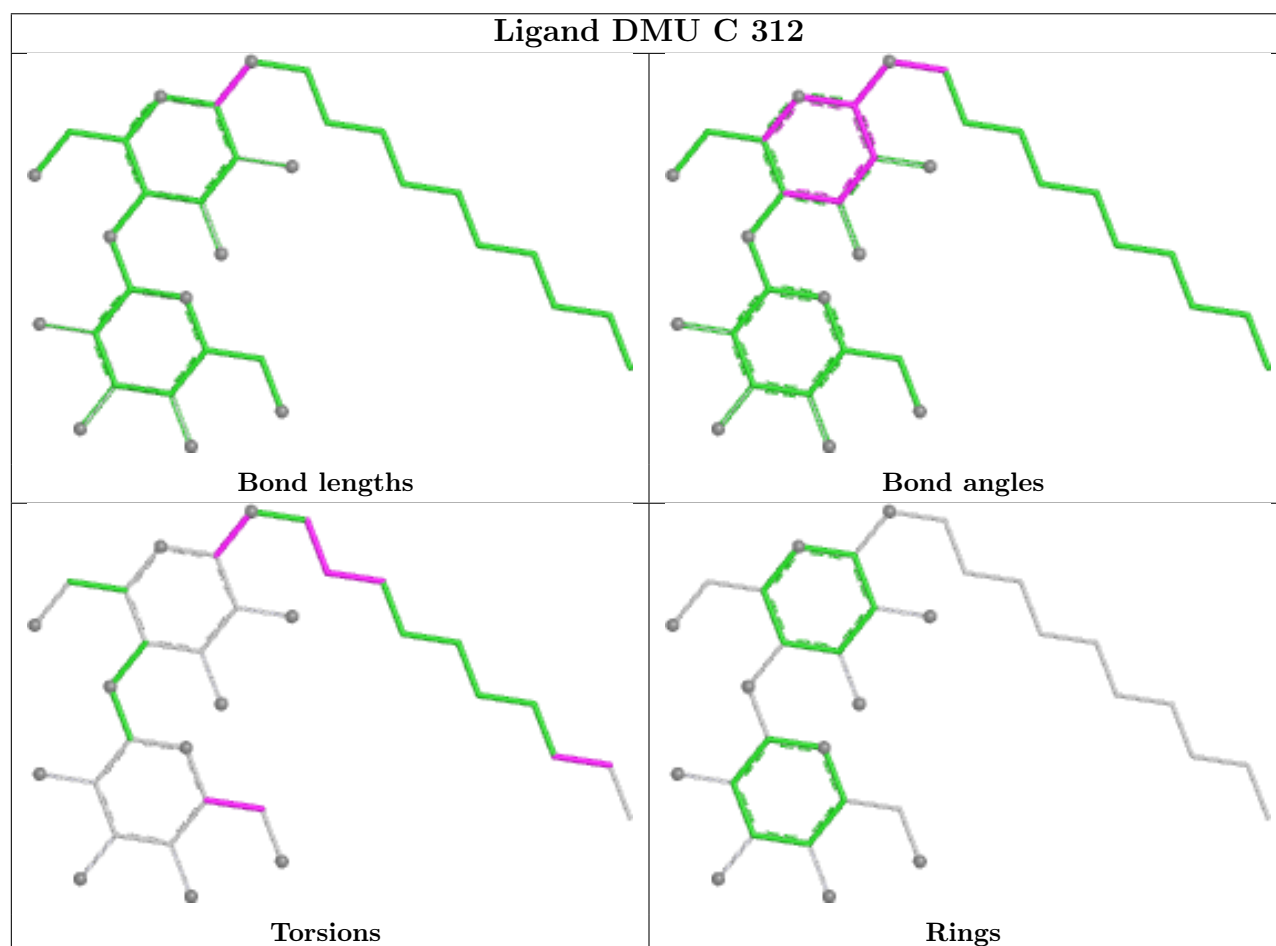
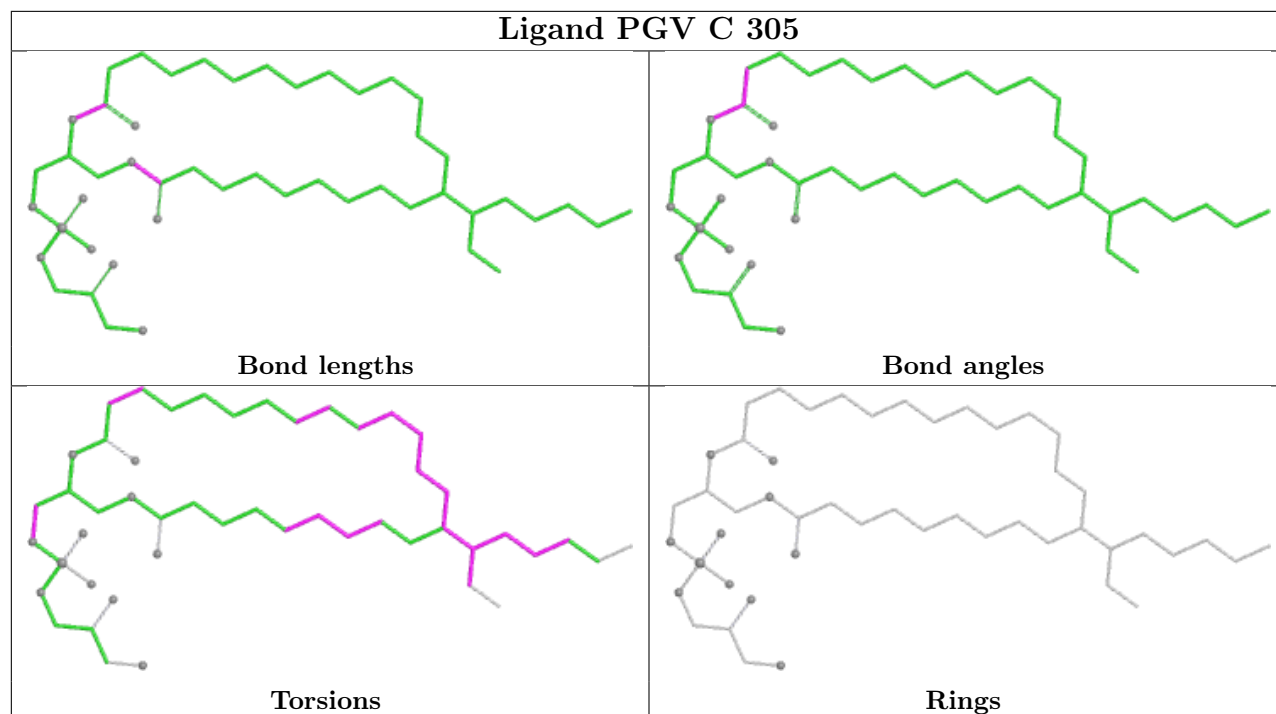
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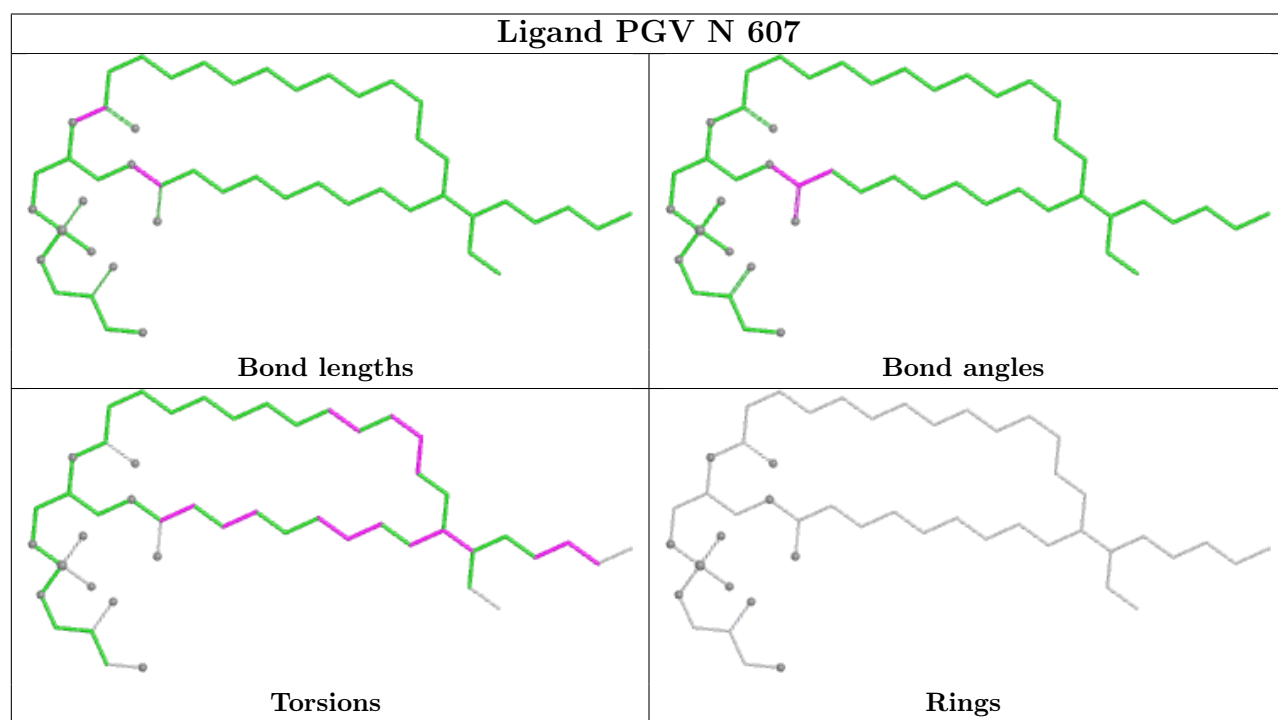
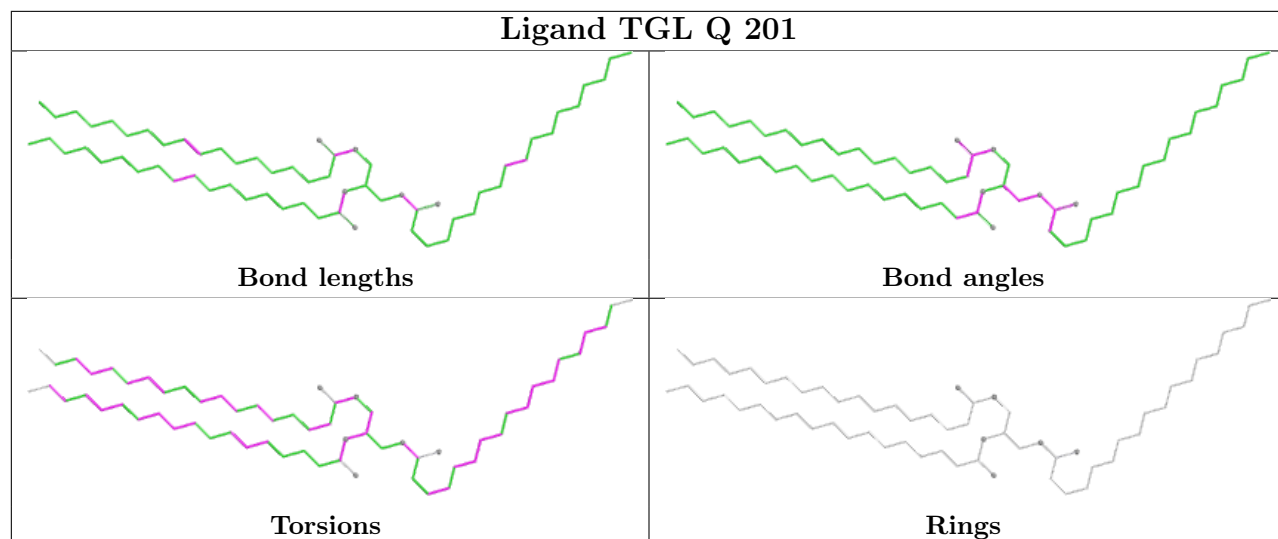
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	608	EDO	1	0
23	T	102	PEK	3	0
20	D	202	EDO	2	0
20	N	613	EDO	4	0
20	N	614	EDO	1	0
20	E	202	EDO	1	0
20	A	616	EDO	1	0
20	S	103	EDO	1	0
22	P	301	CHD	2	0
18	O	302	TGL	2	0
14	A	602	HEA	1	0
19	P	303	PGV	3	0
23	T	101	PEK	2	0
23	T	103	PEK	2	0
24	T	104	CDL	13	0
25	P	309	DMU	8	0
14	N	602	HEA	2	0
19	N	606	PGV	2	0
25	C	313	DMU	12	0
14	N	601	HEA	1	0
18	A	606	TGL	3	0
19	C	306	PGV	1	0
19	M	101	PGV	2	0
20	N	617	EDO	1	0
26	E	201	PSC	10	0
23	C	304	PEK	2	0
22	C	308	CHD	3	0
26	O	304	PSC	6	0
24	P	305	CDL	9	0
24	C	307	CDL	10	0
18	Y	101	TGL	5	0
18	D	201	TGL	4	0
20	N	615	EDO	2	0
23	C	303	PEK	3	0
20	N	608	EDO	1	0
18	L	101	TGL	4	0
25	P	308	DMU	1	0
20	A	611	EDO	2	0
20	N	612	EDO	1	0
19	A	607	PGV	2	0
20	A	615	EDO	1	0
14	A	601	HEA	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.

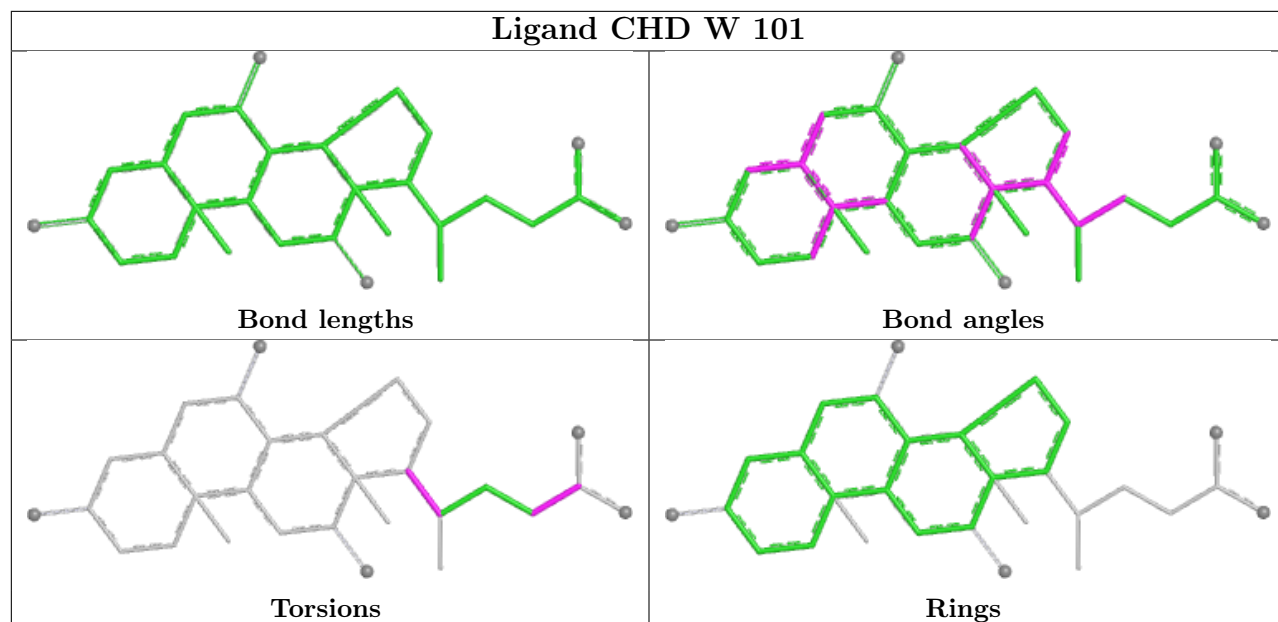




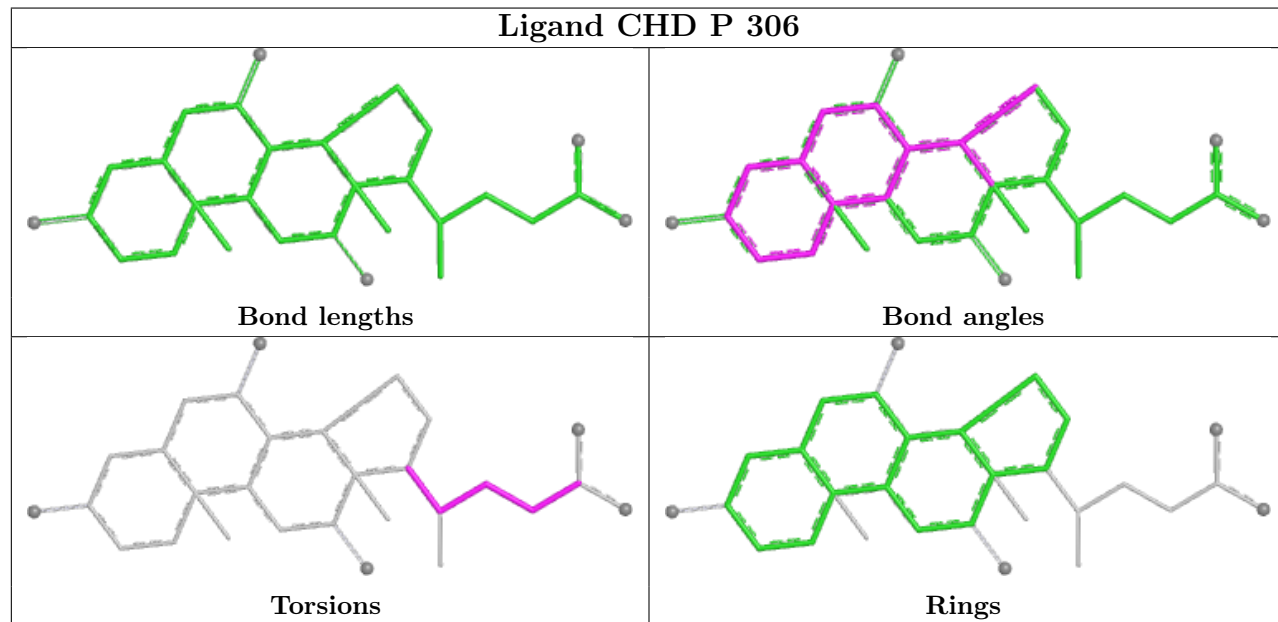


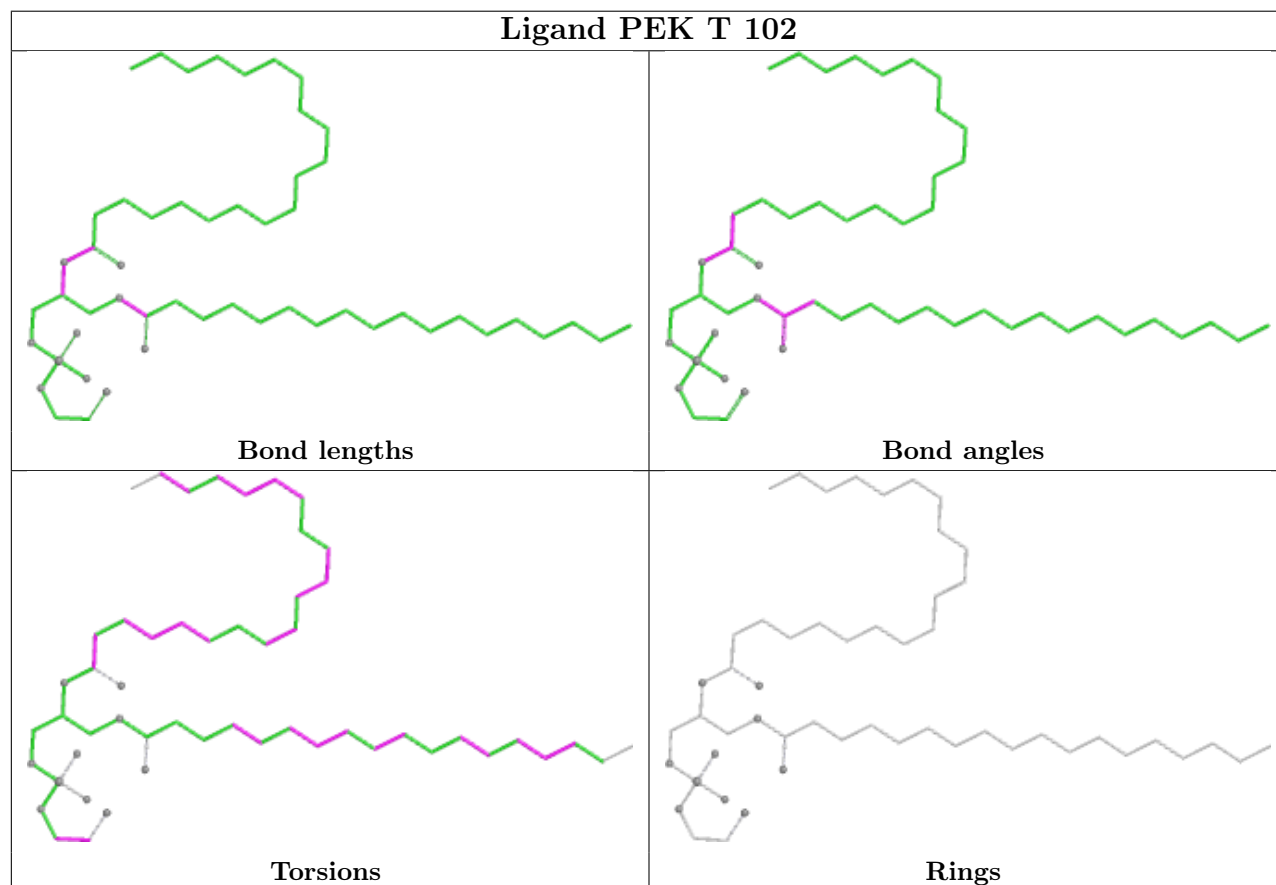
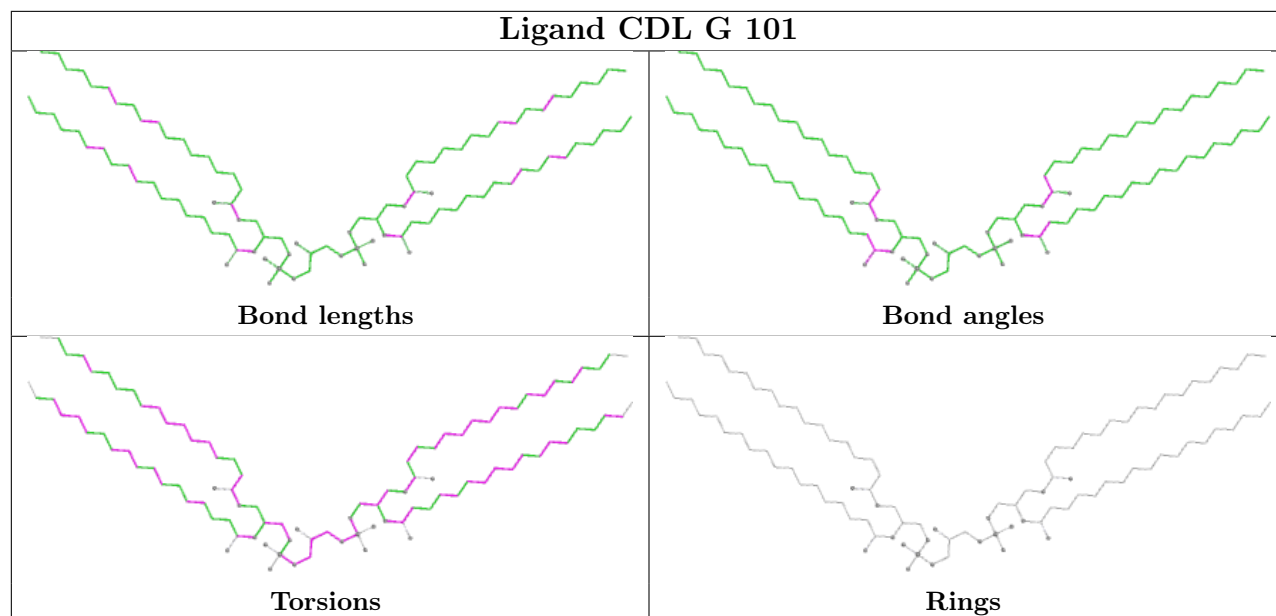


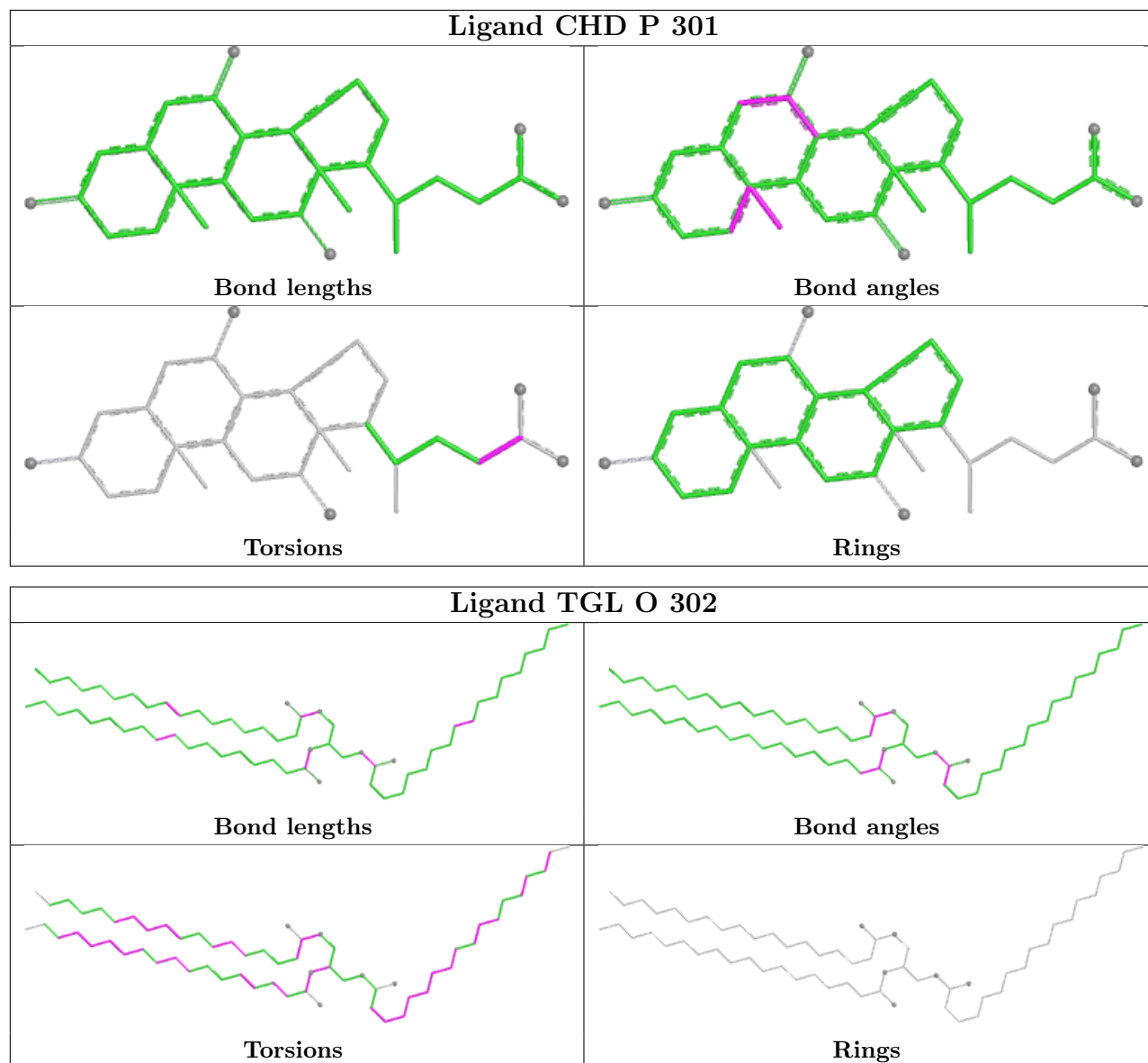
Ligand CHD W 101

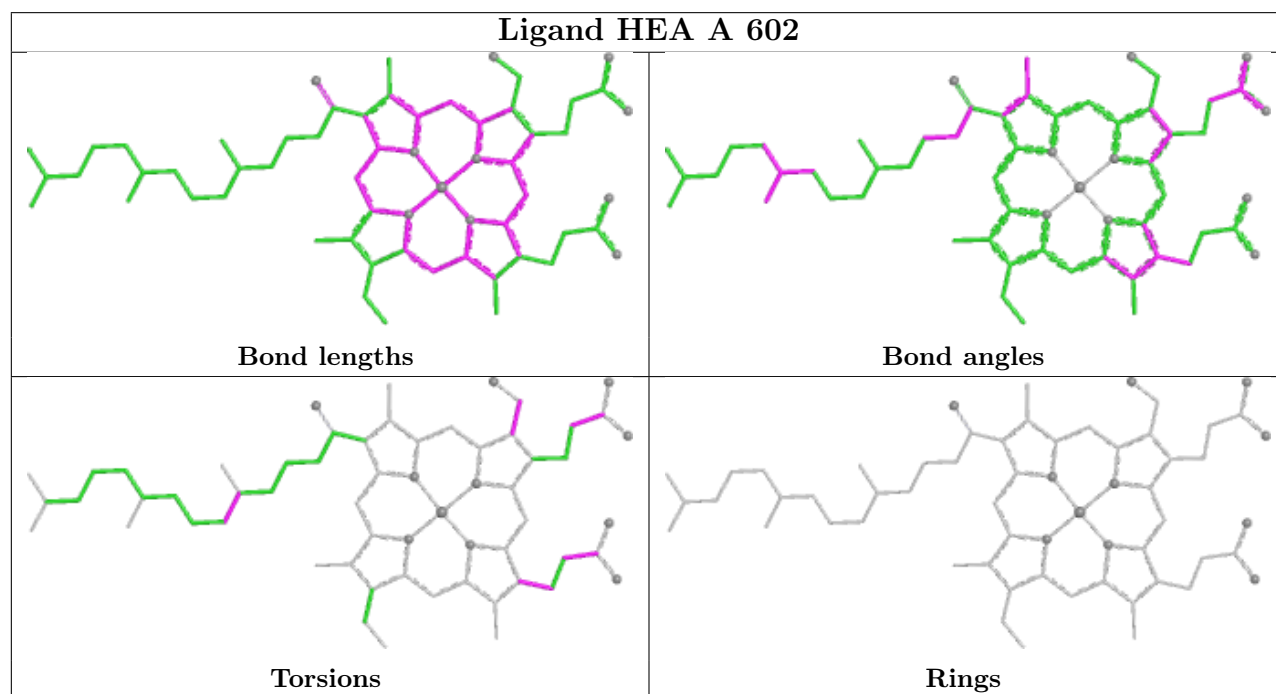
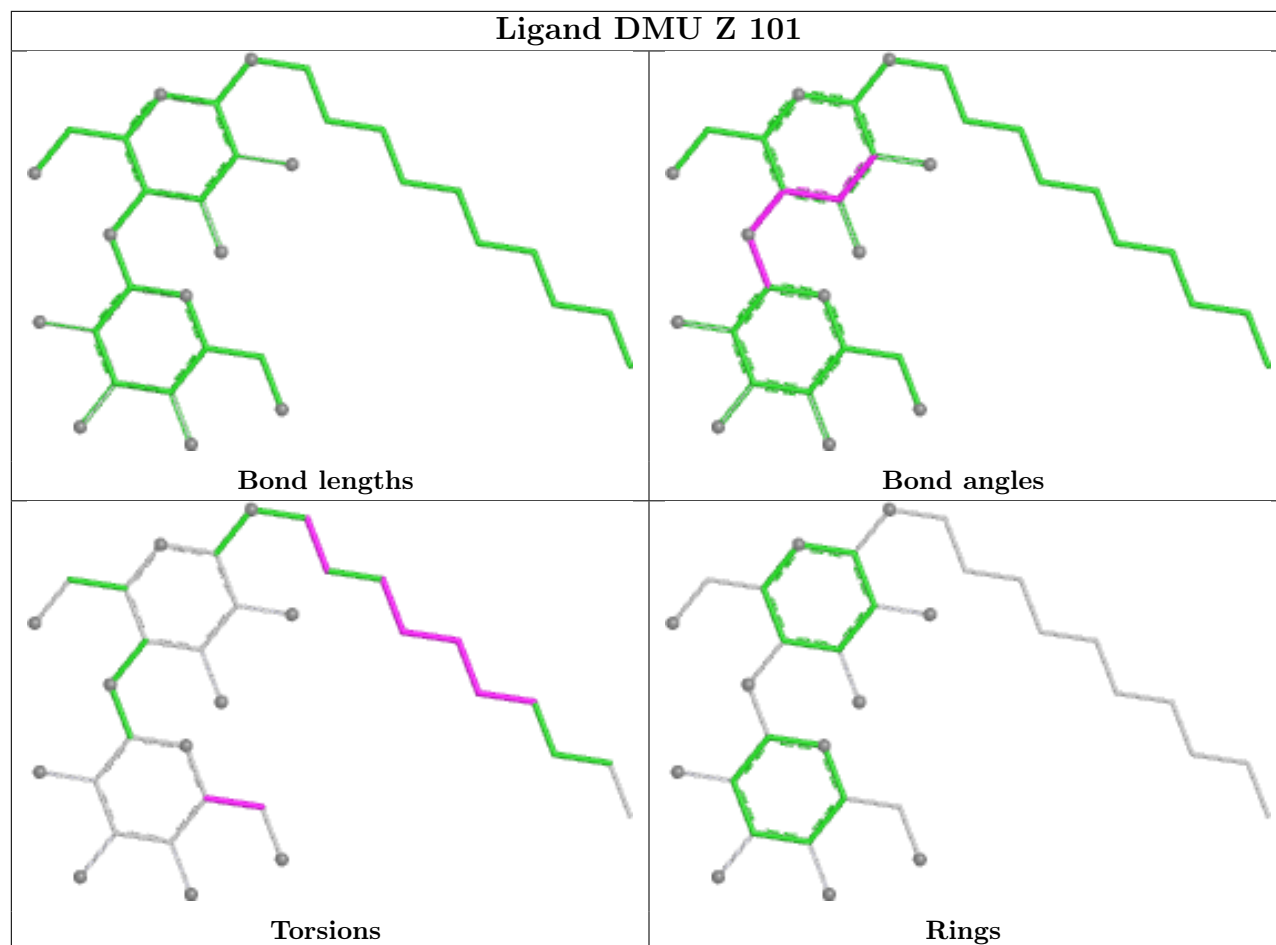


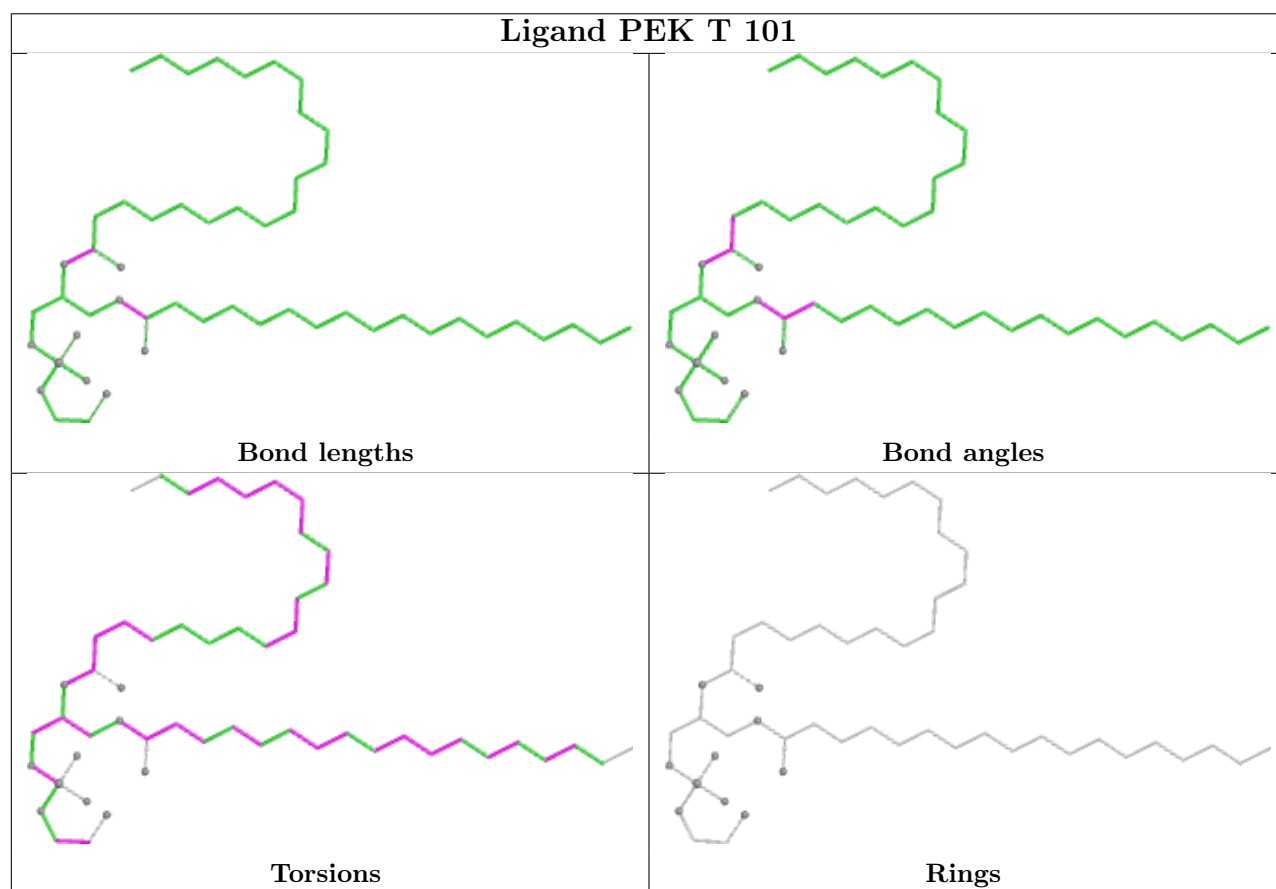
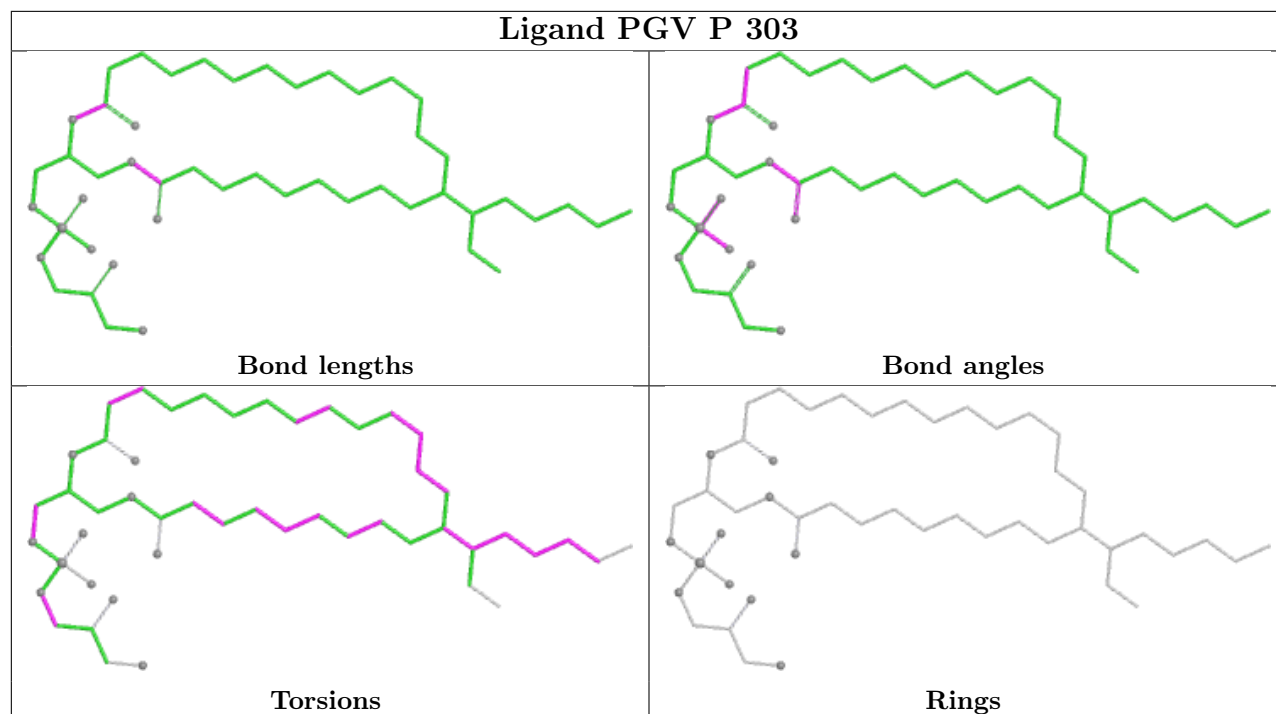
Ligand CHD P 306

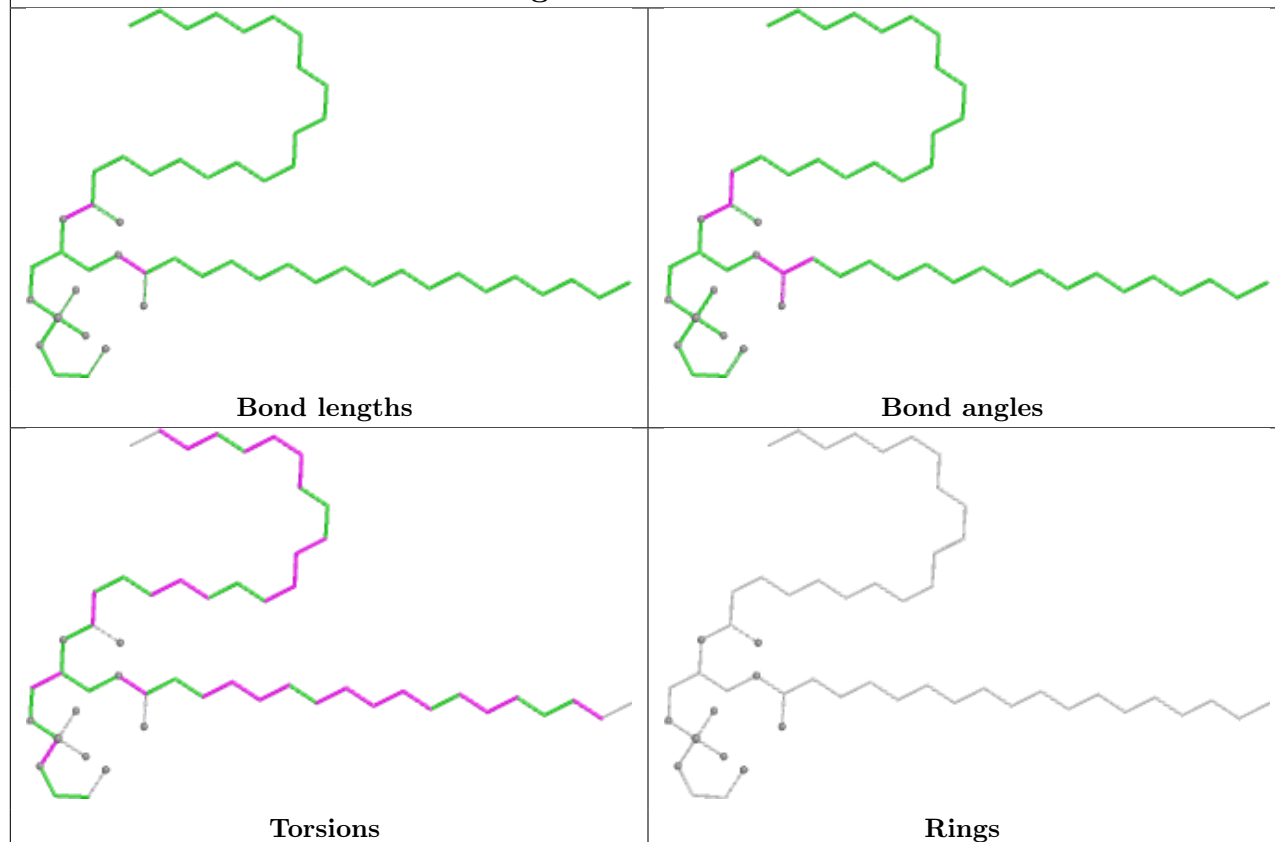
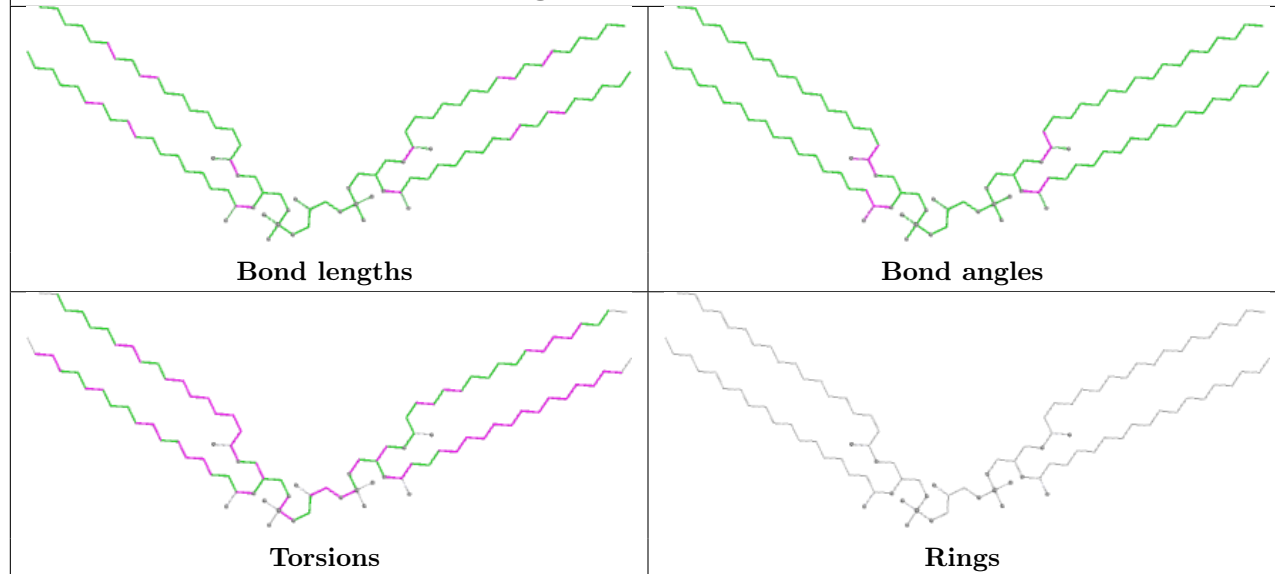


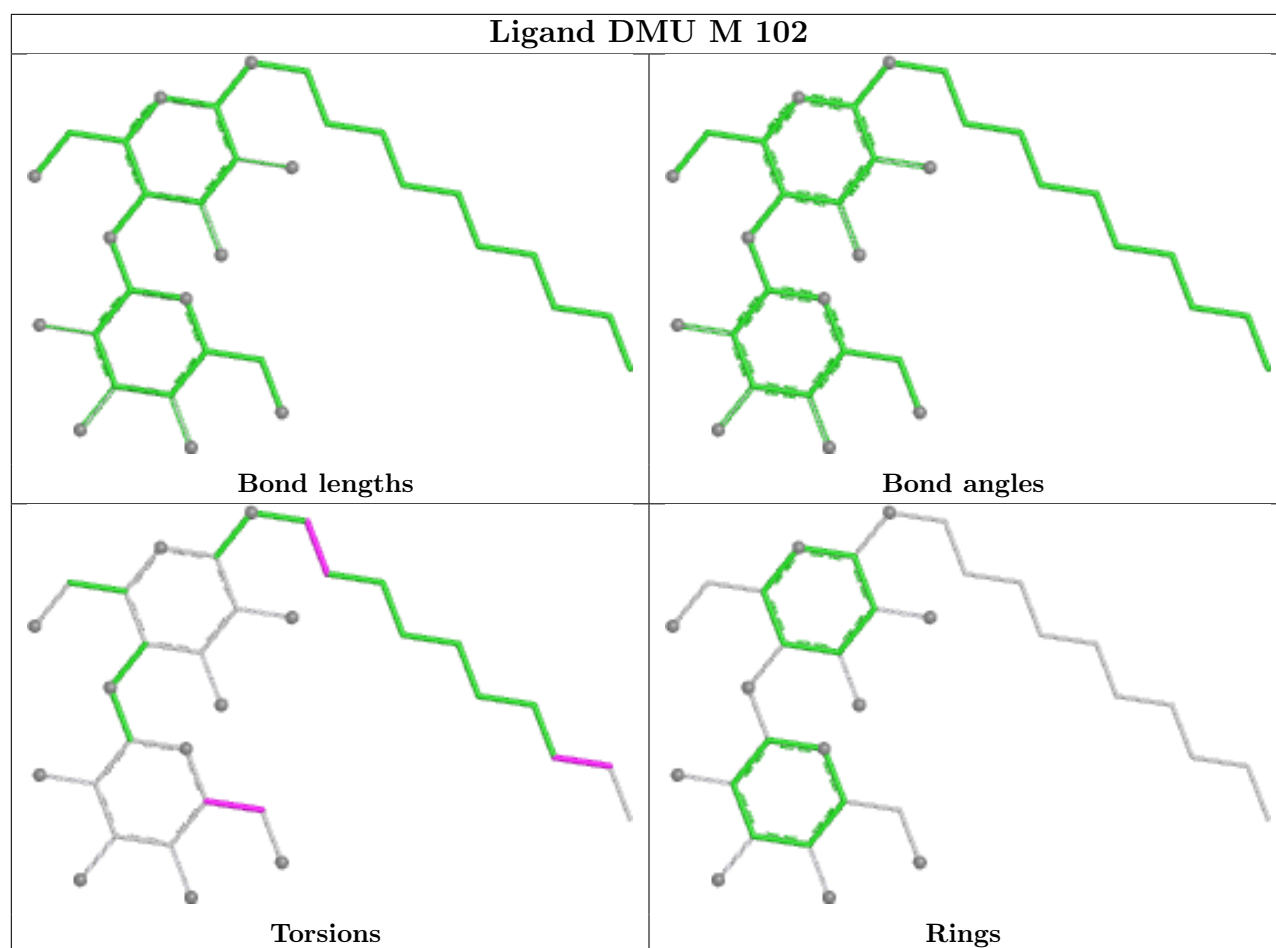


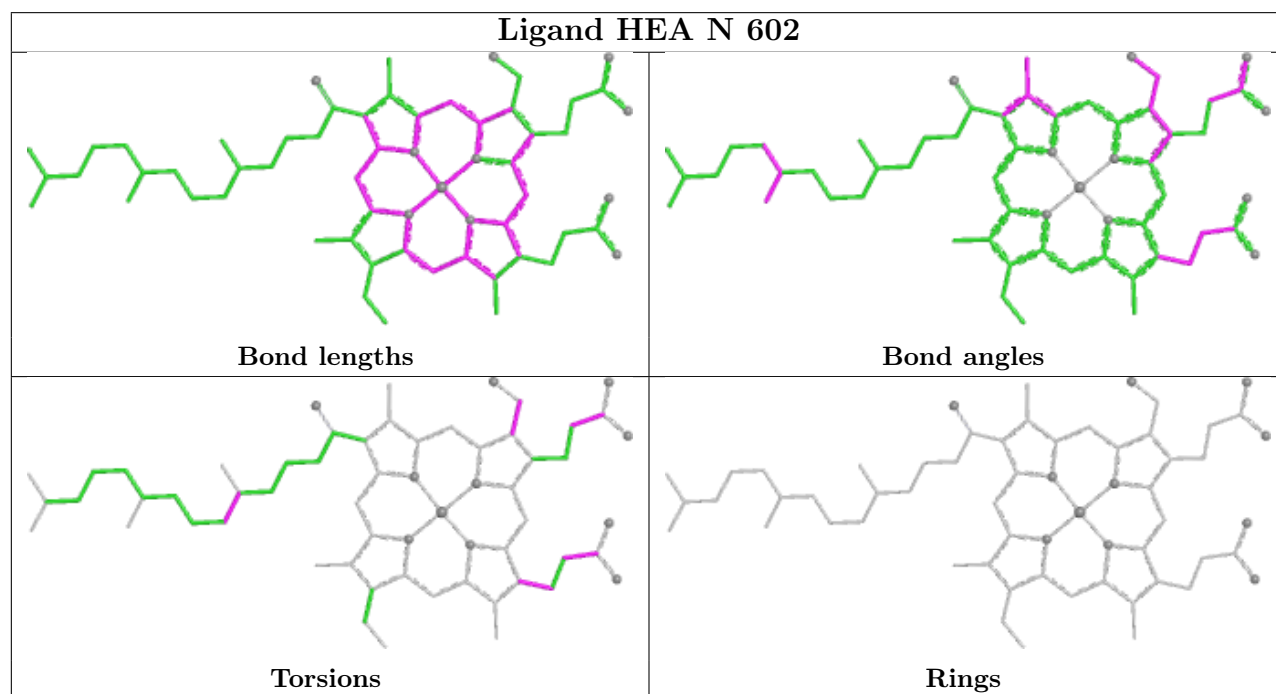
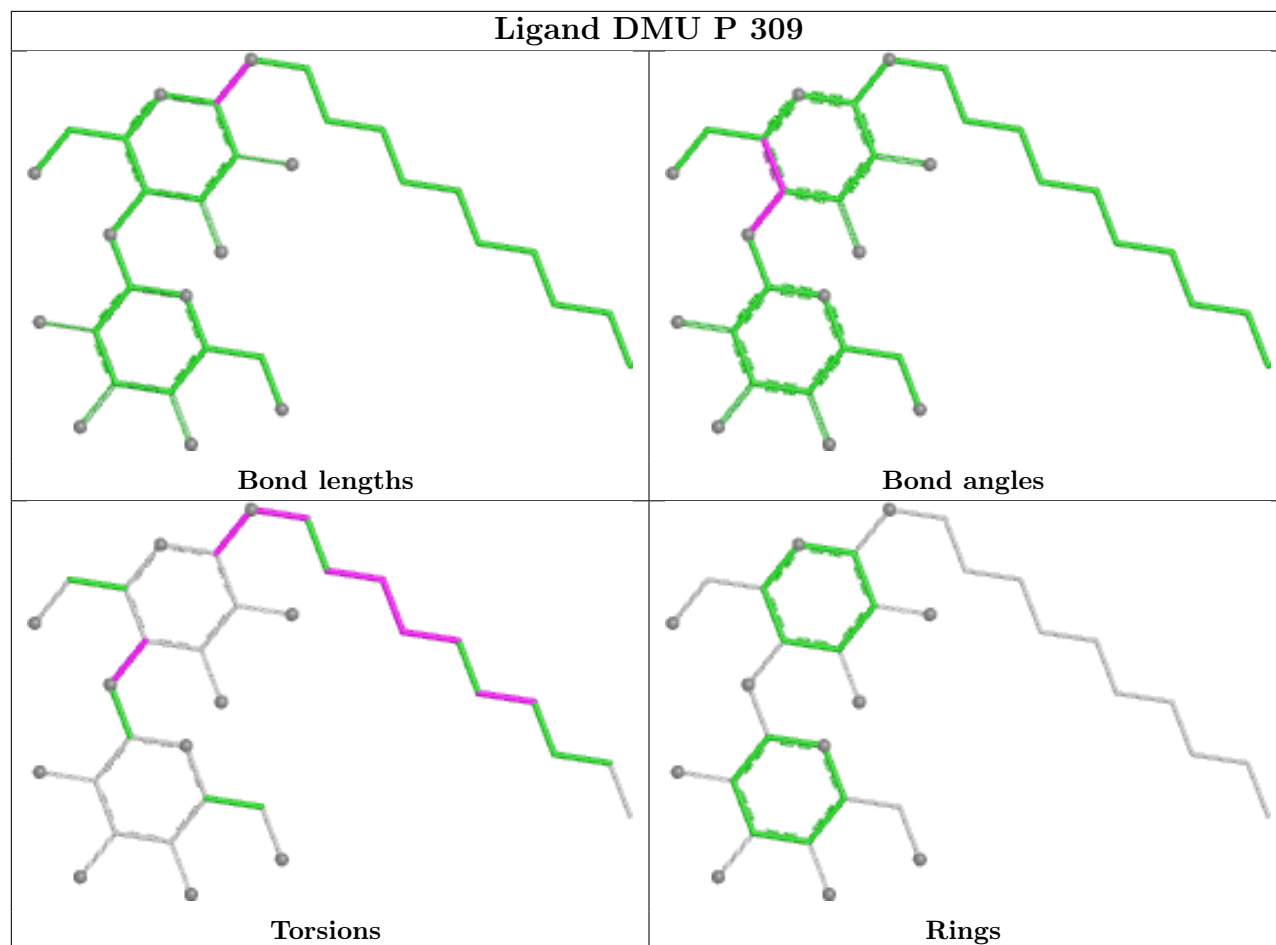


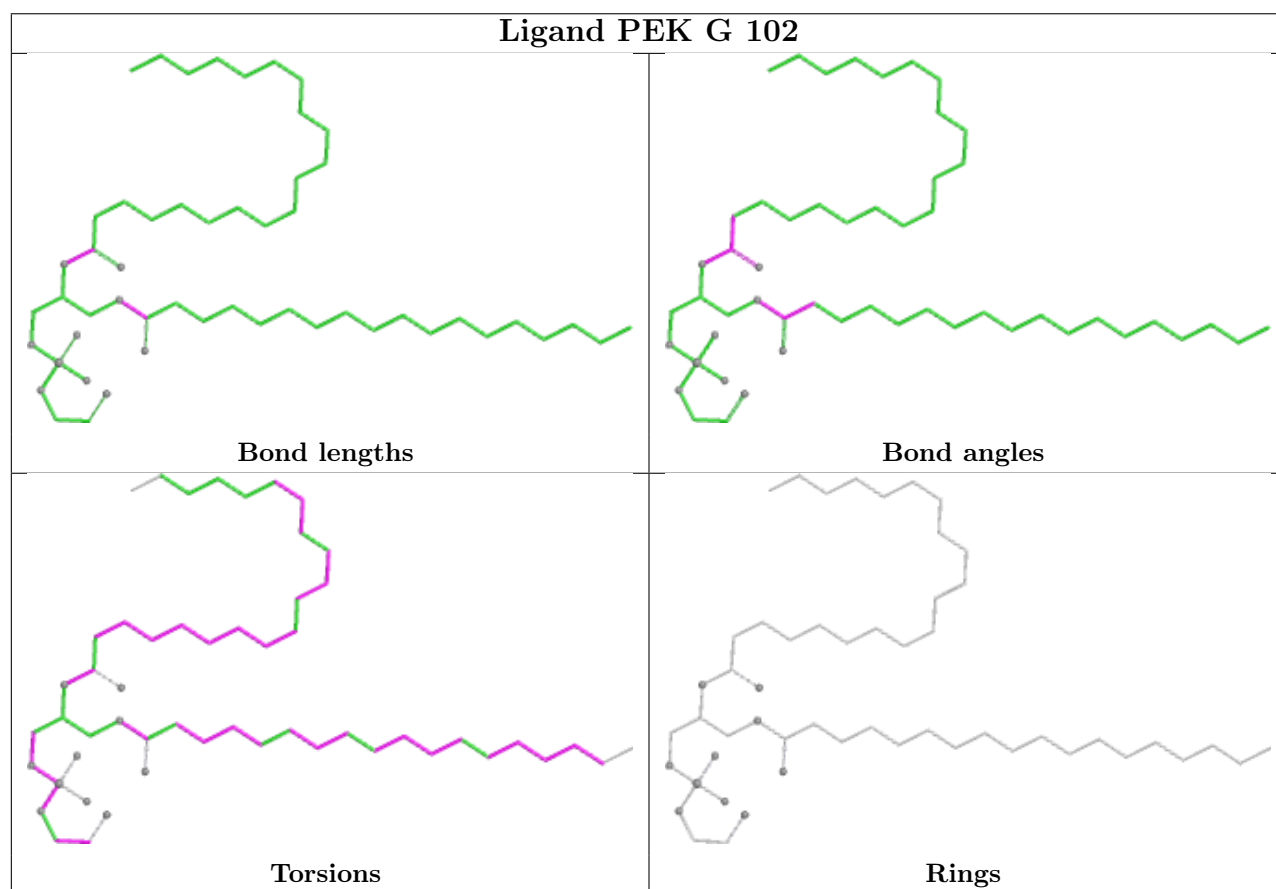
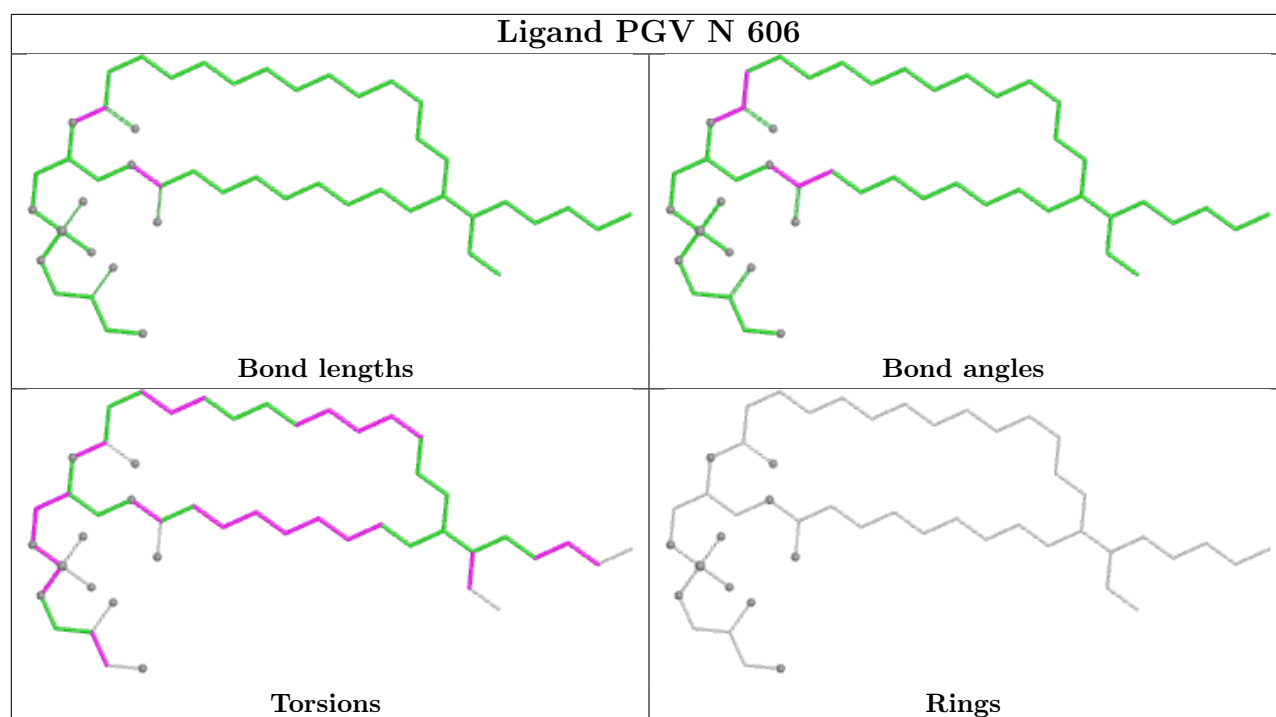


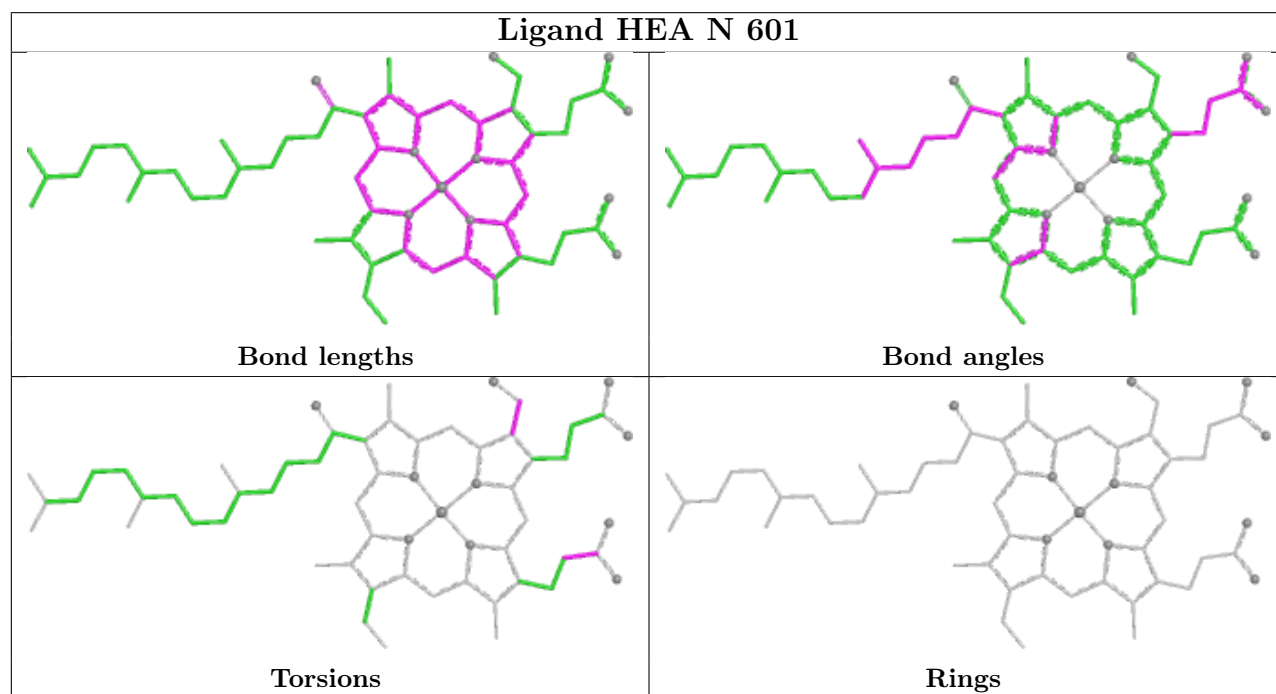
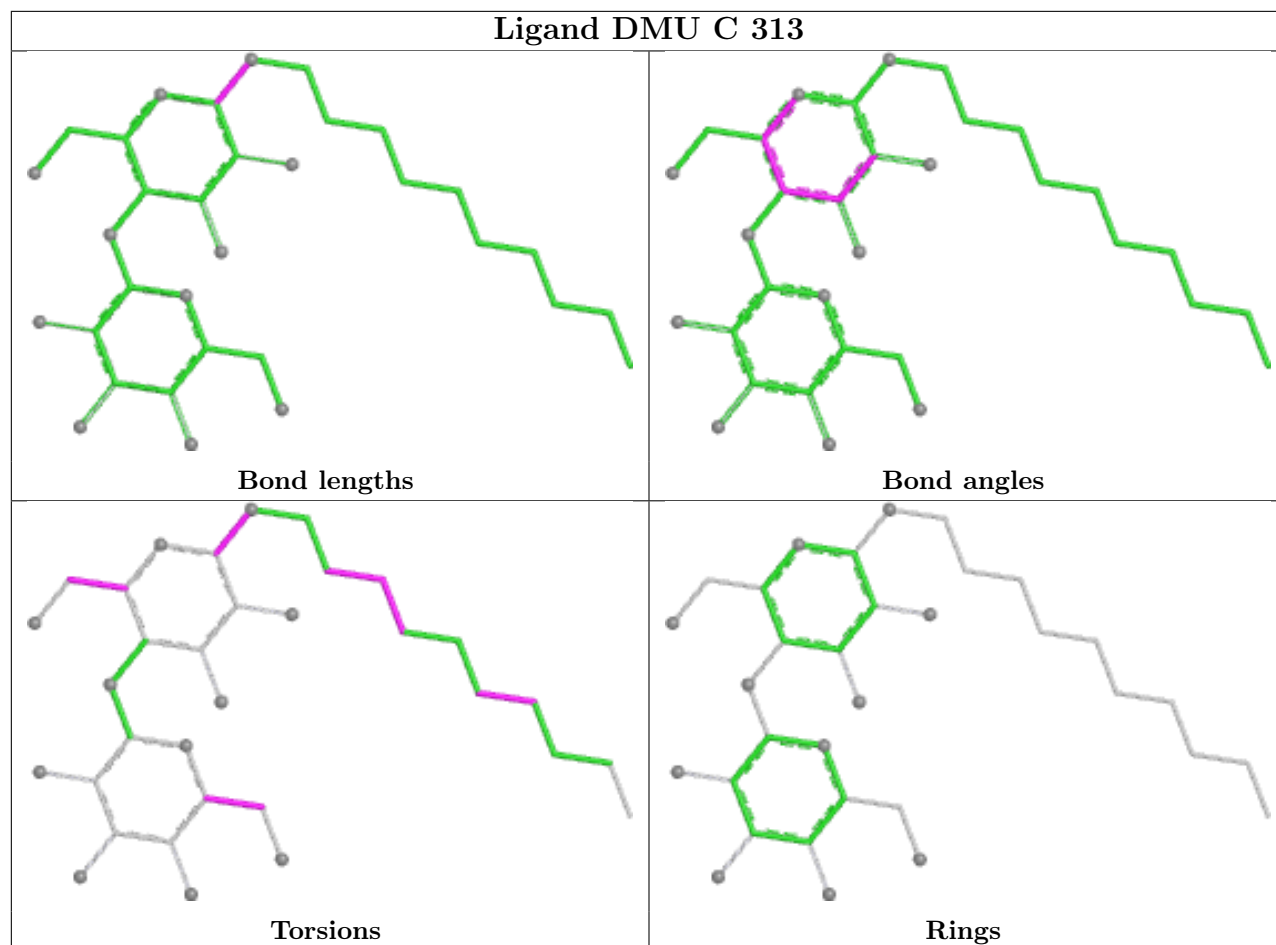


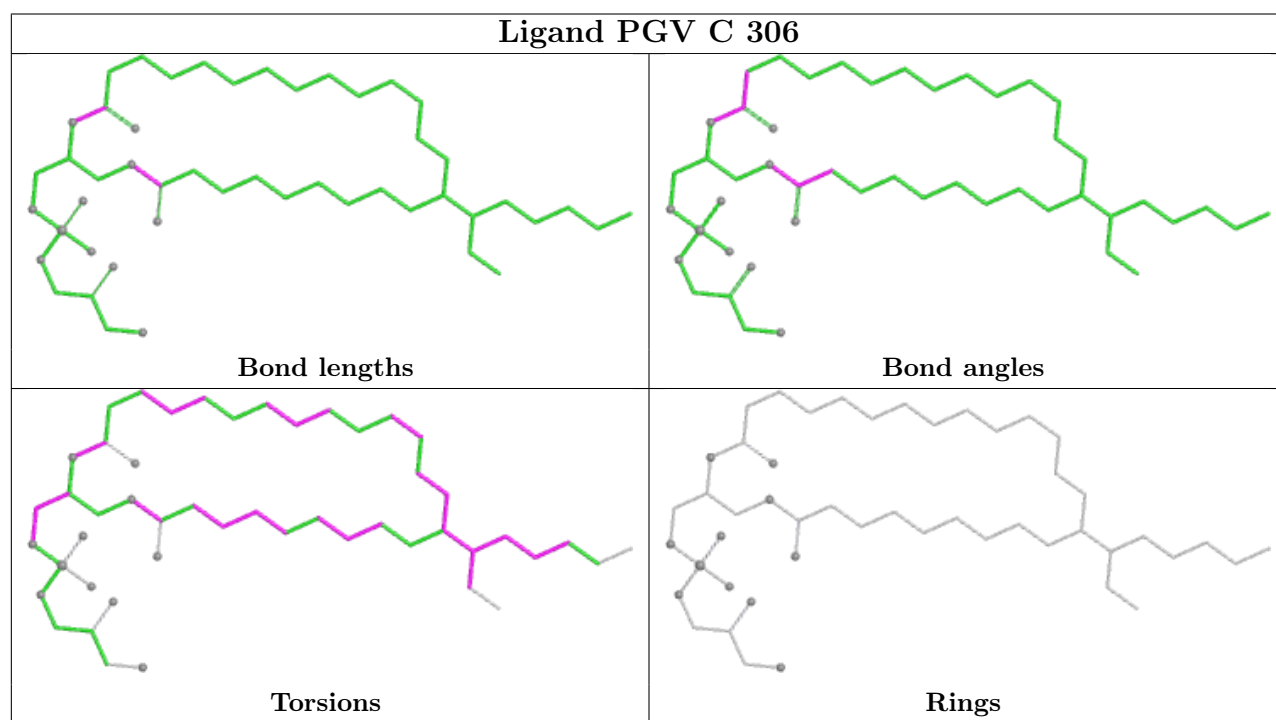
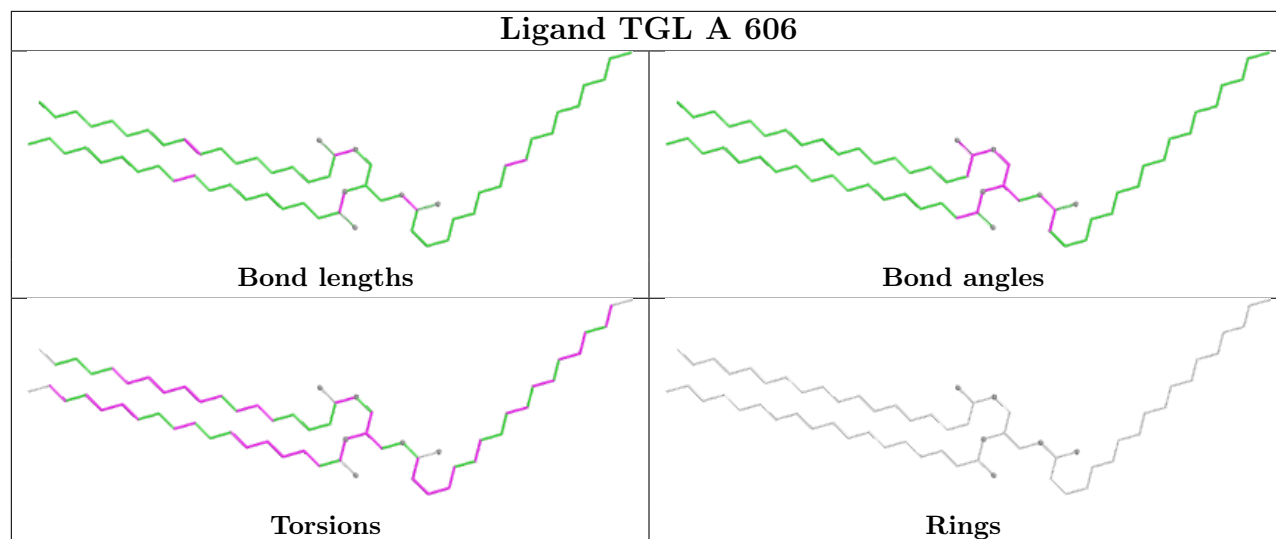
Ligand PEK T 103**Ligand CDL T 104**

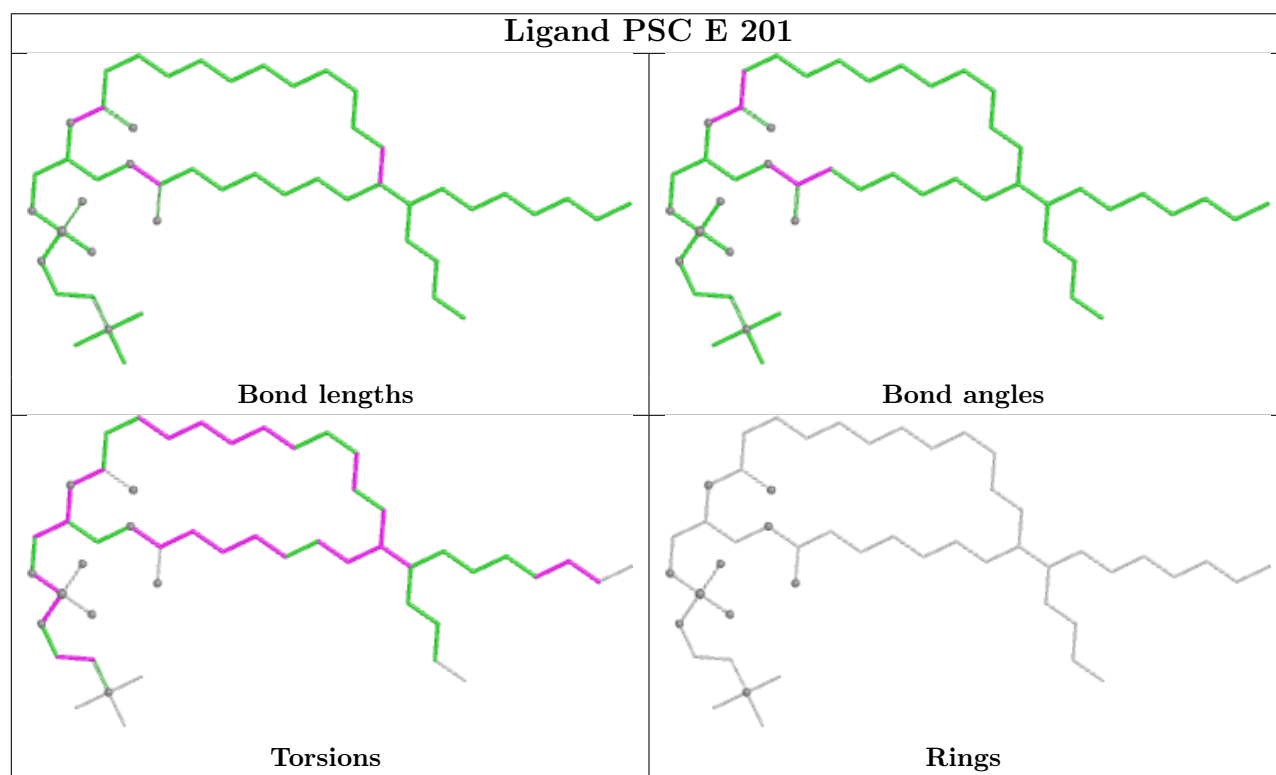
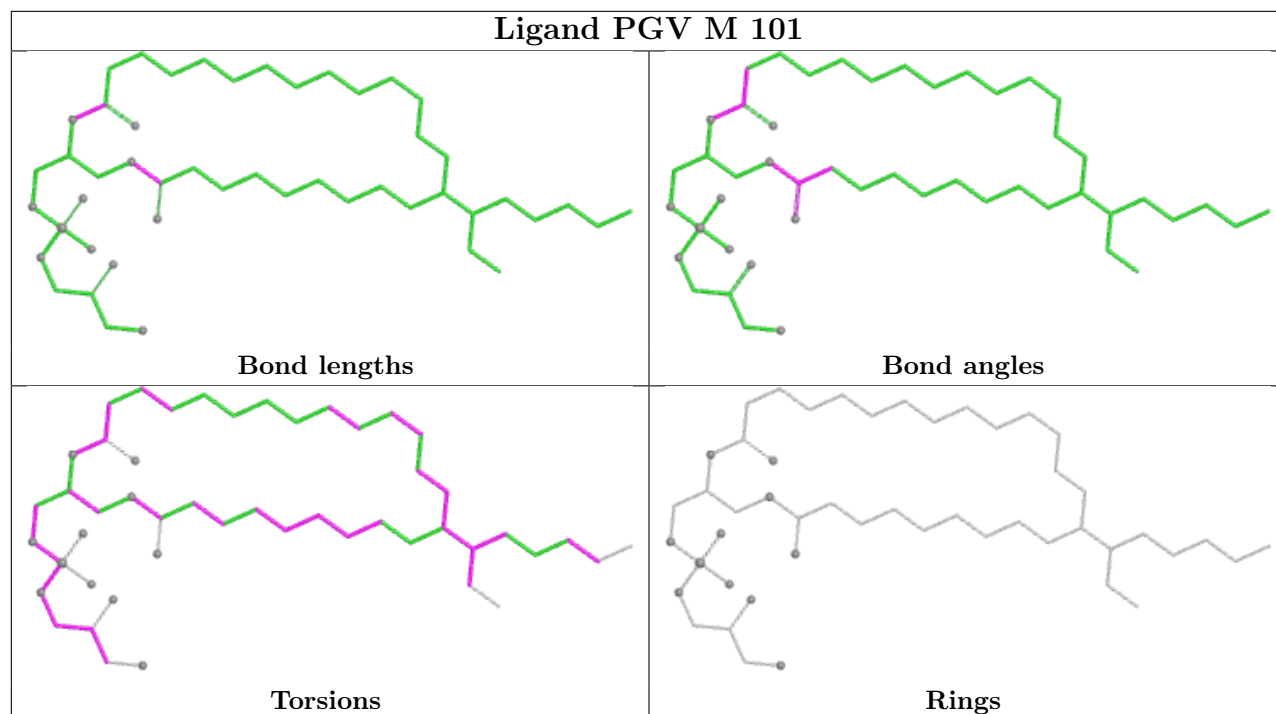




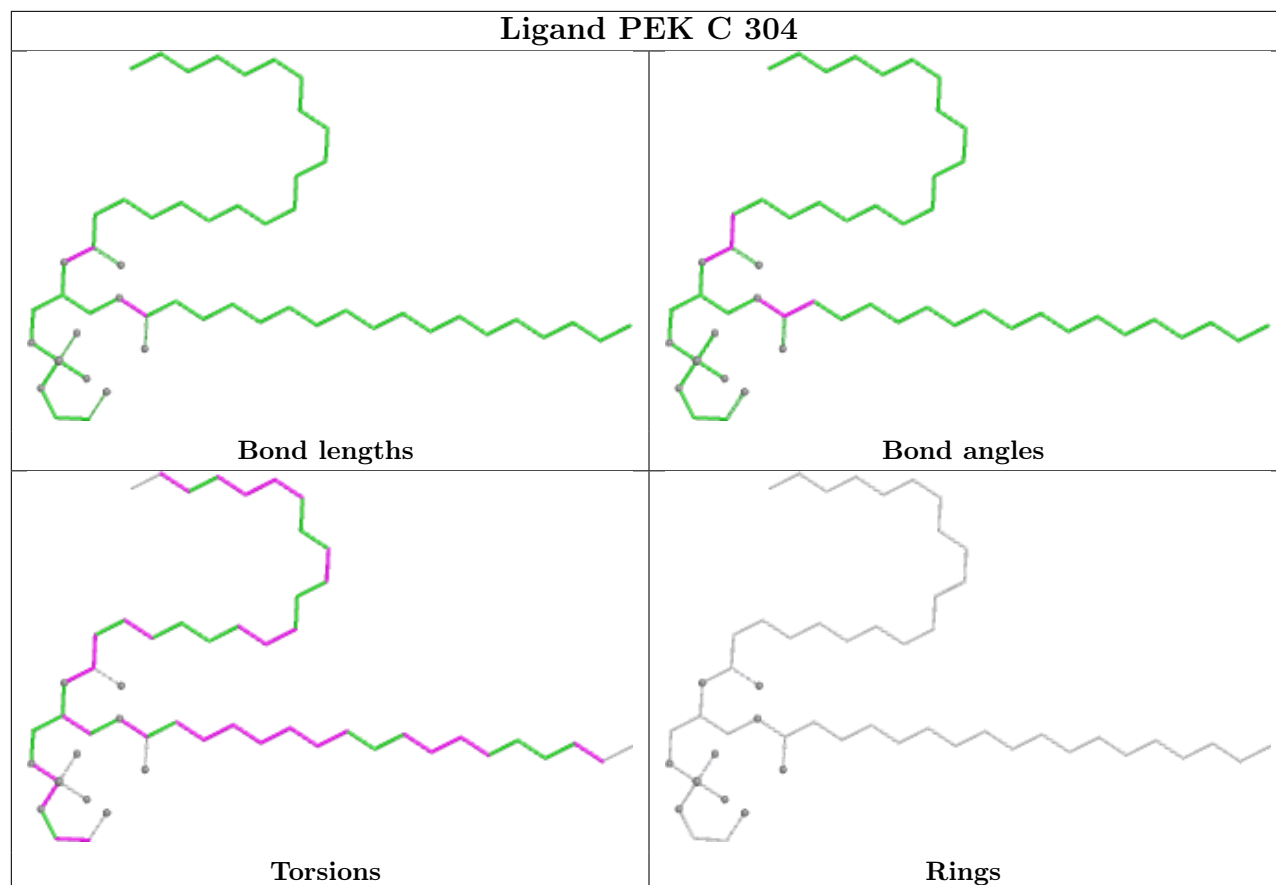




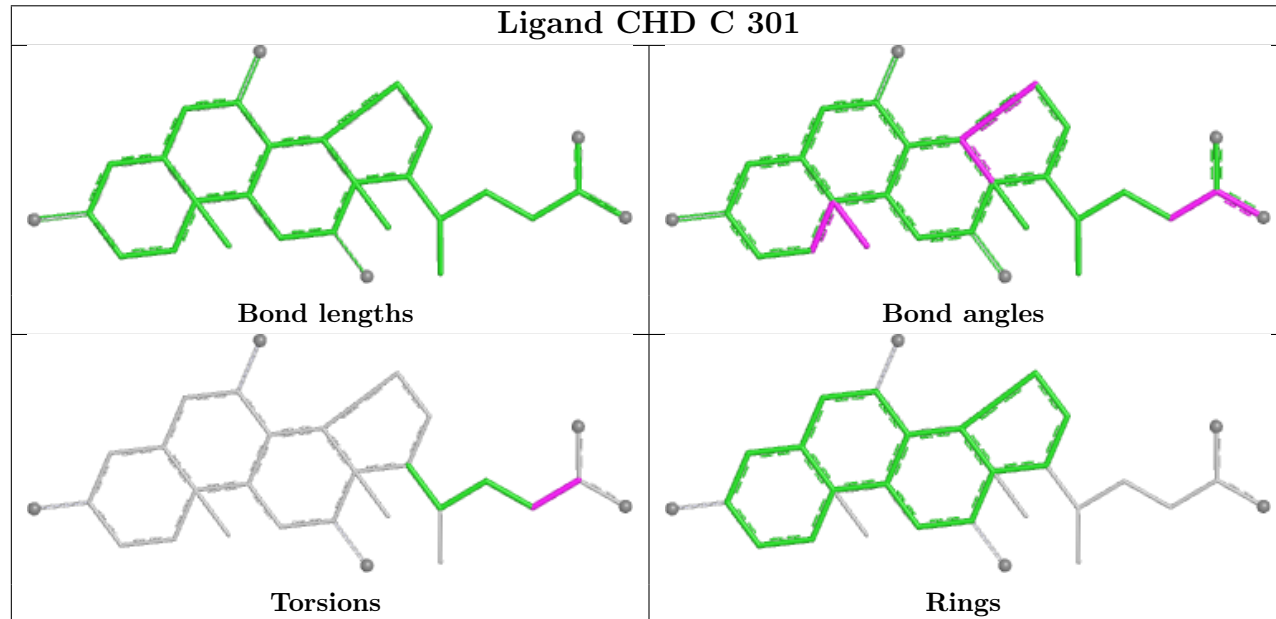


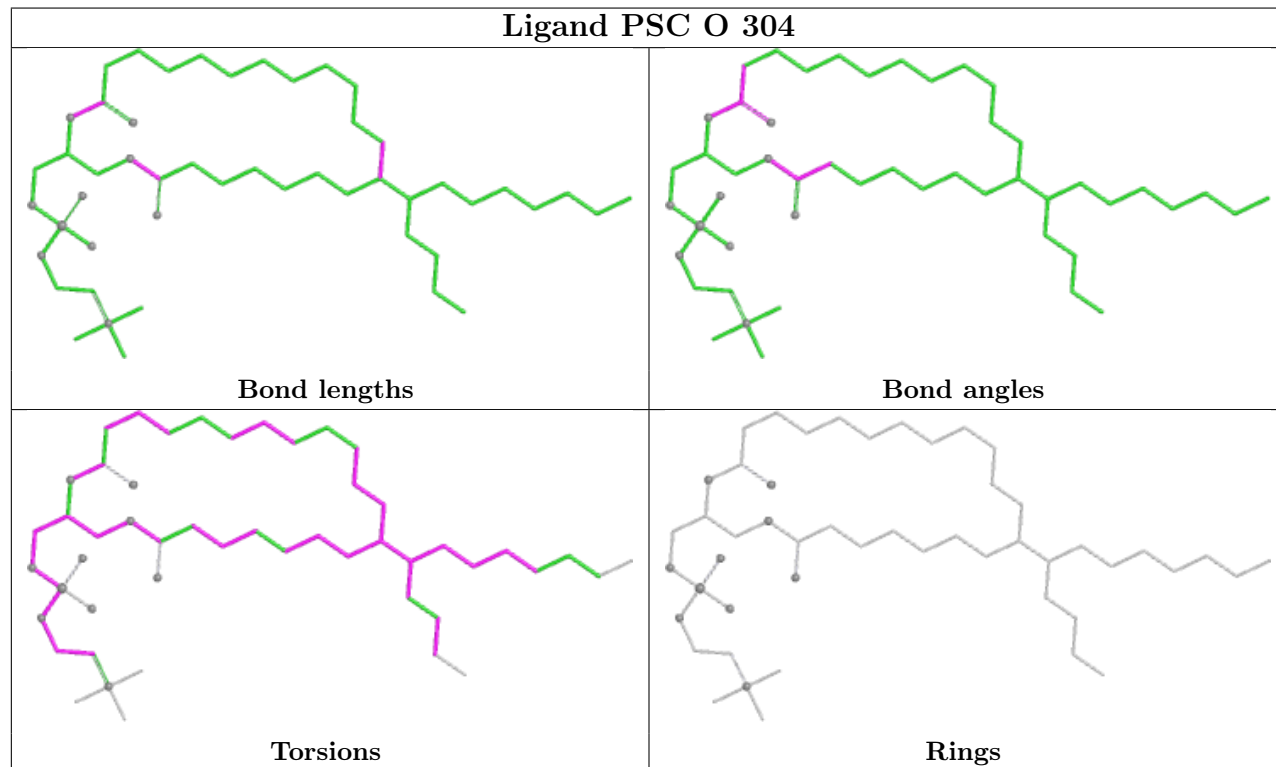
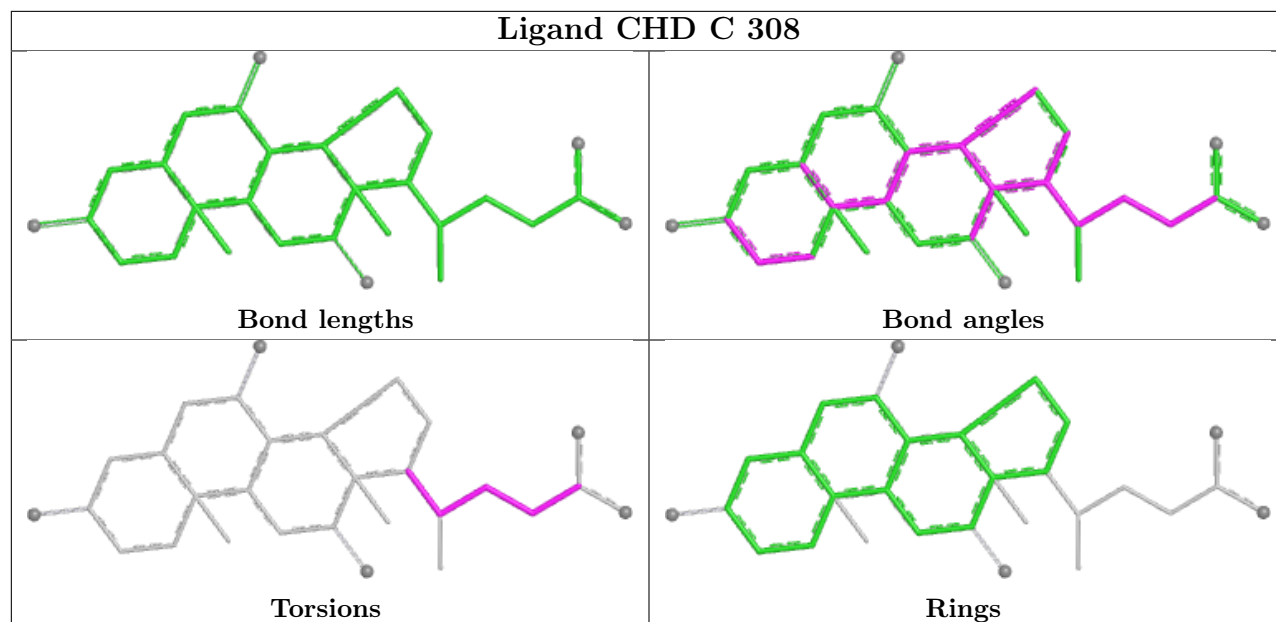


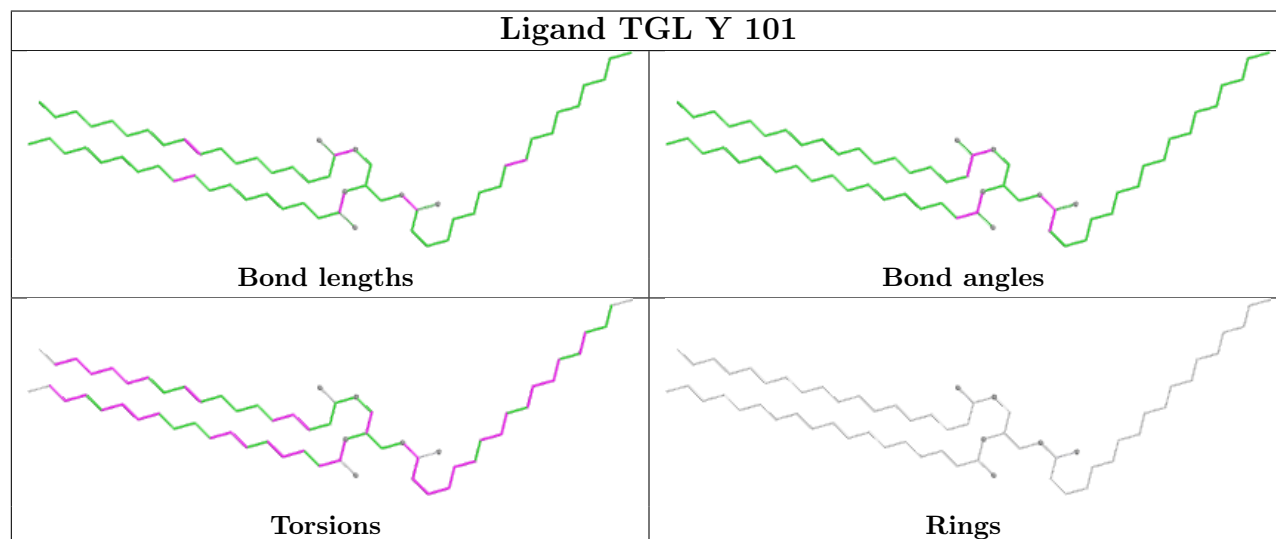
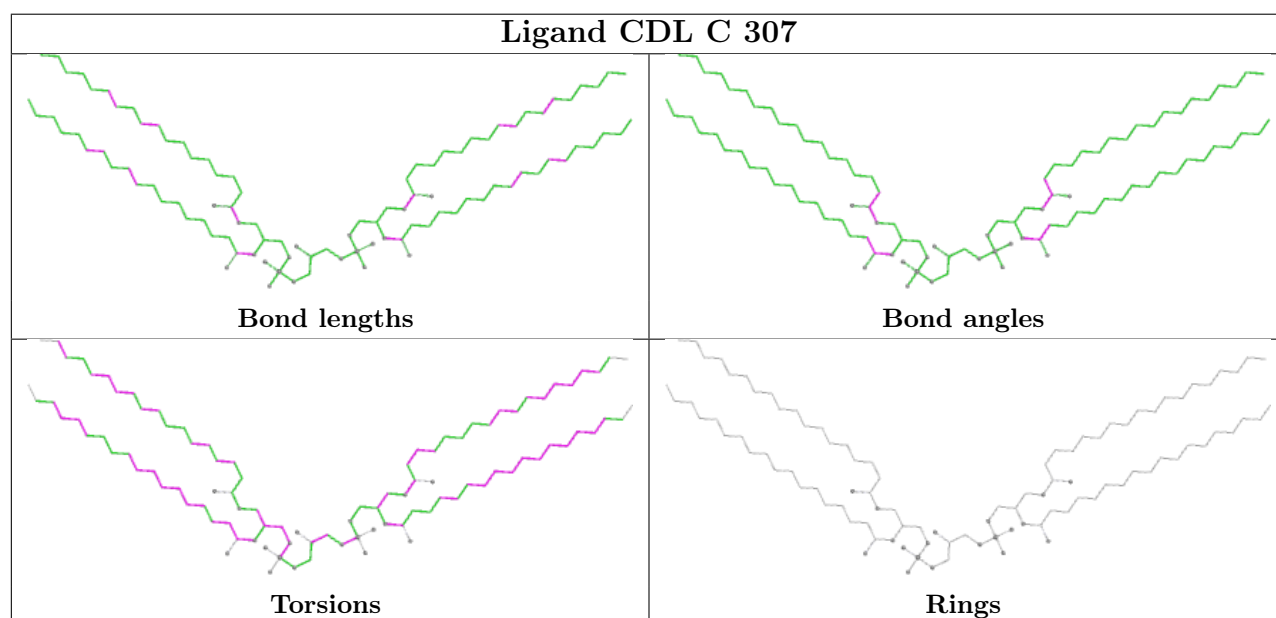
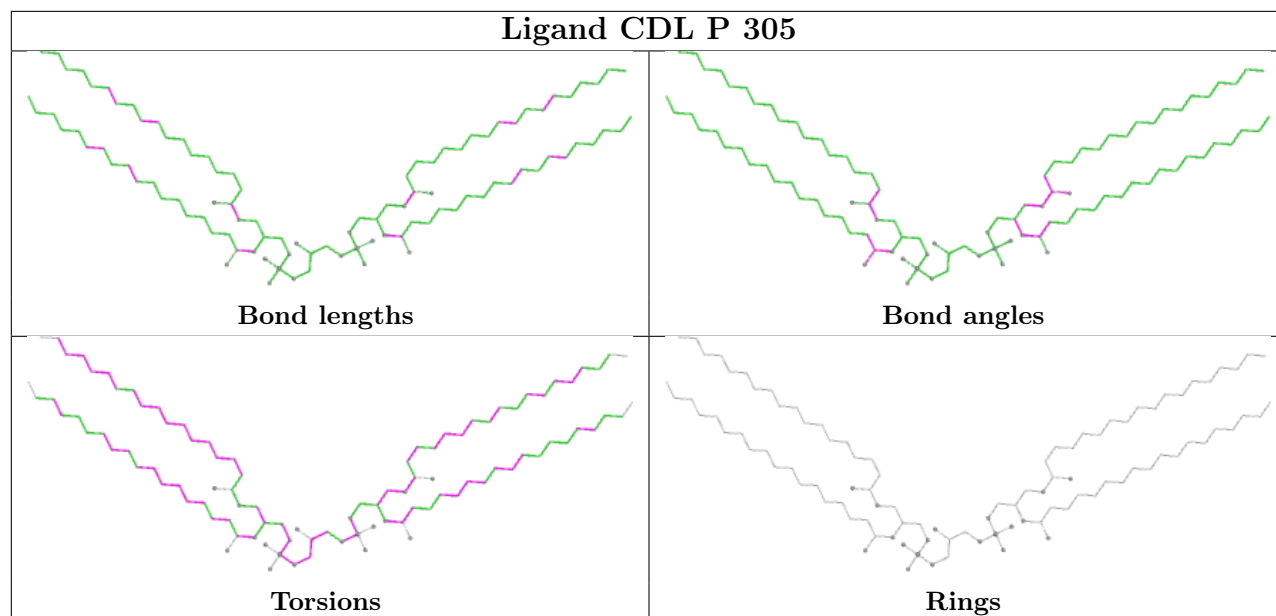
Ligand PEK C 304

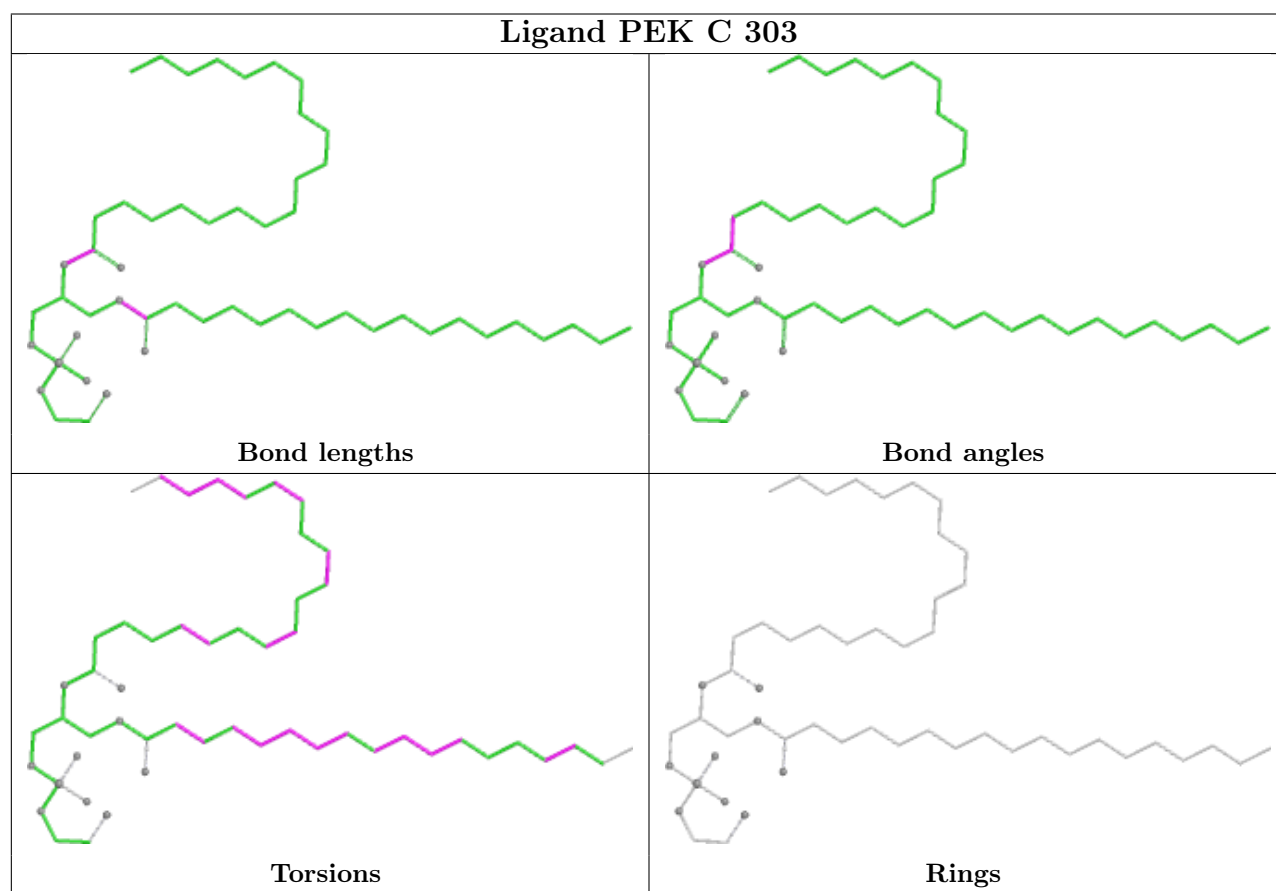
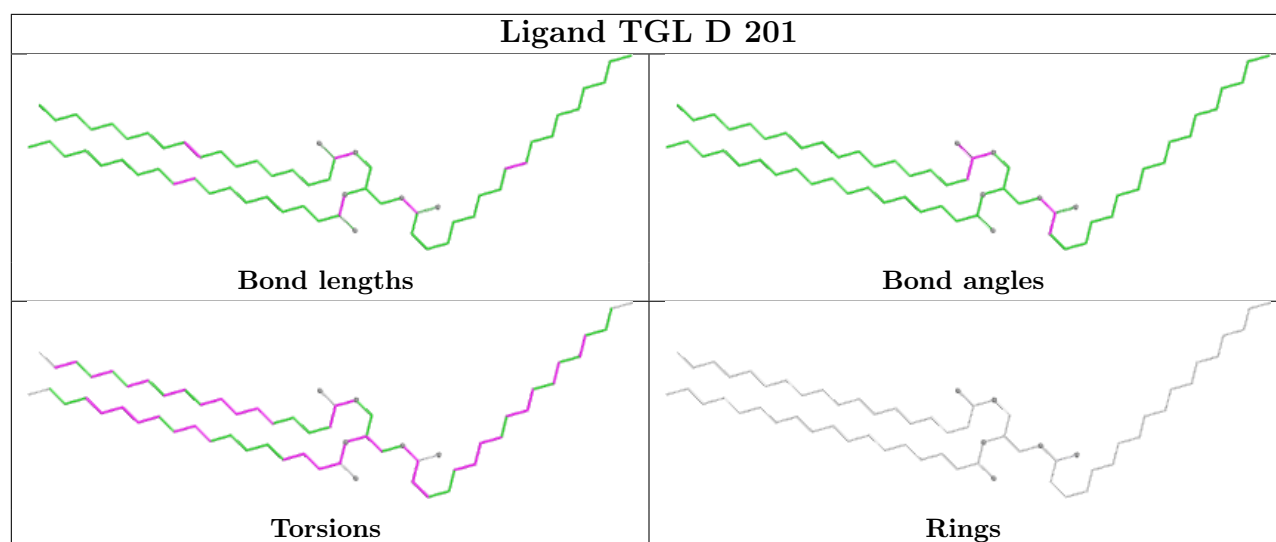


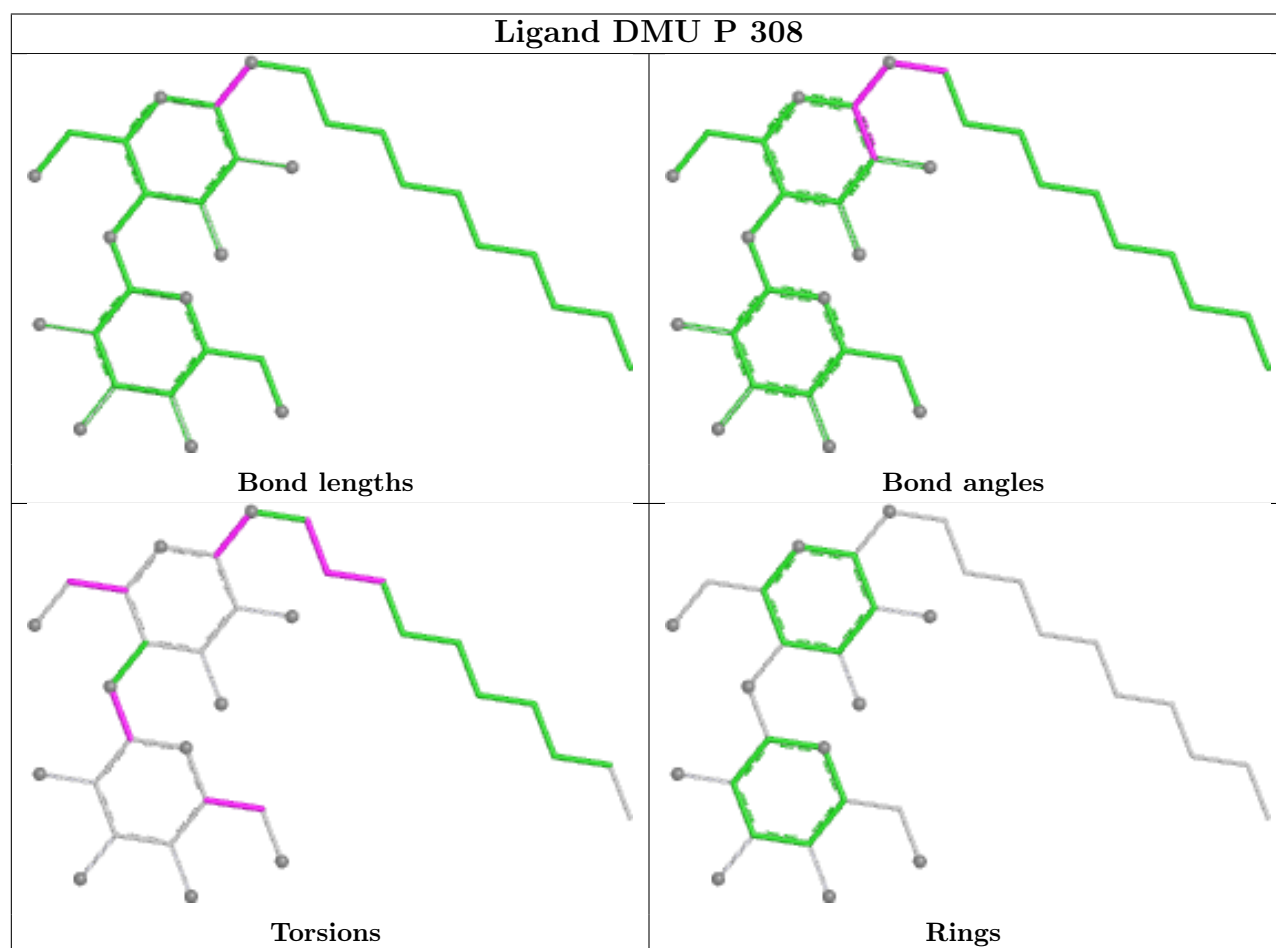
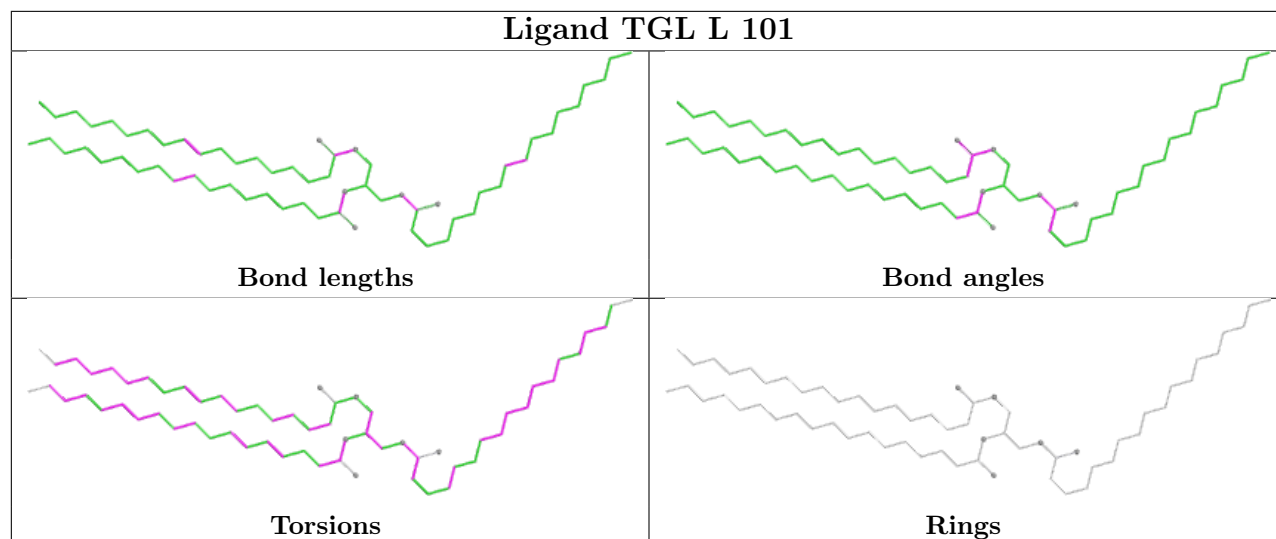
Ligand CHD C 301

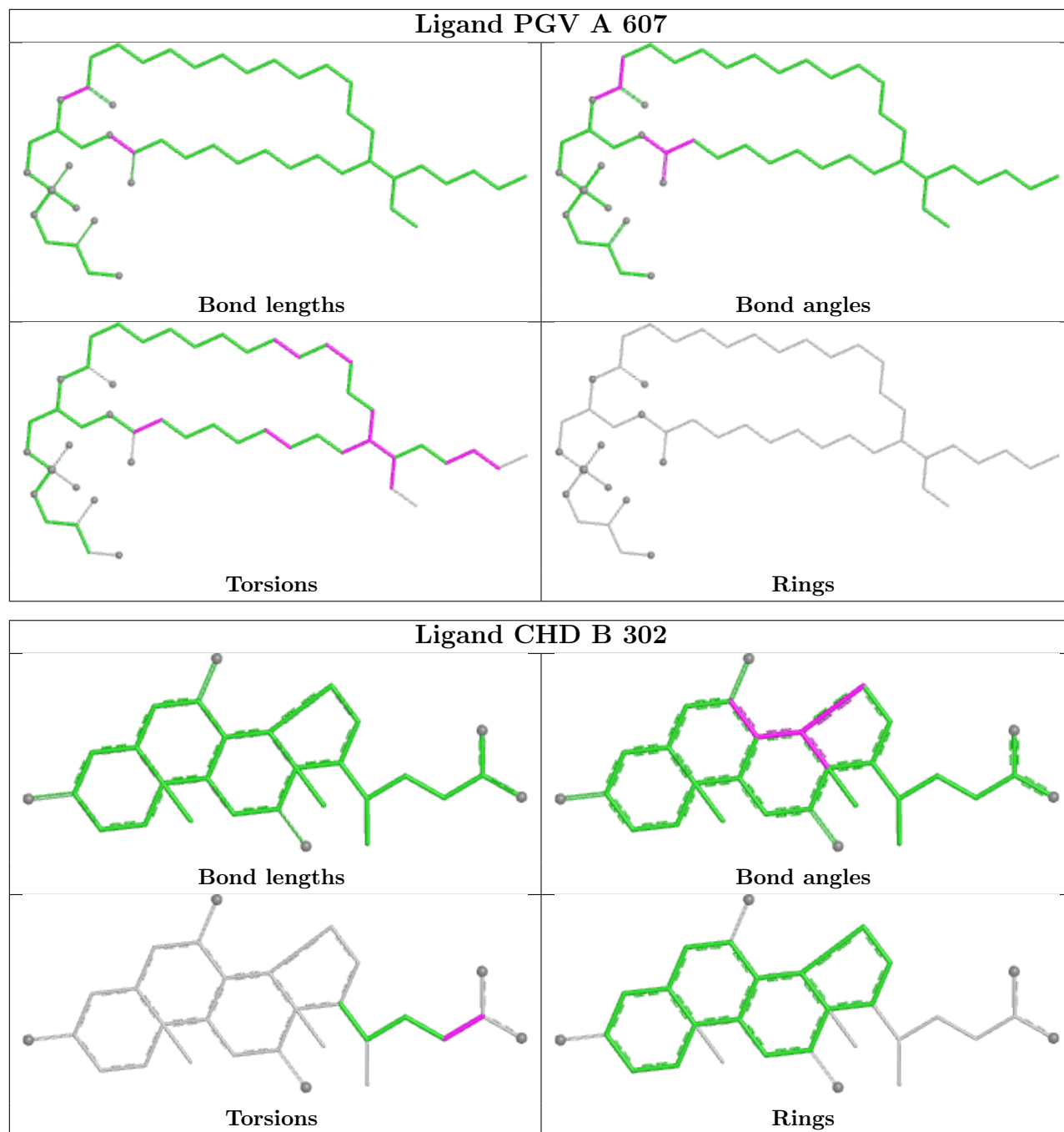


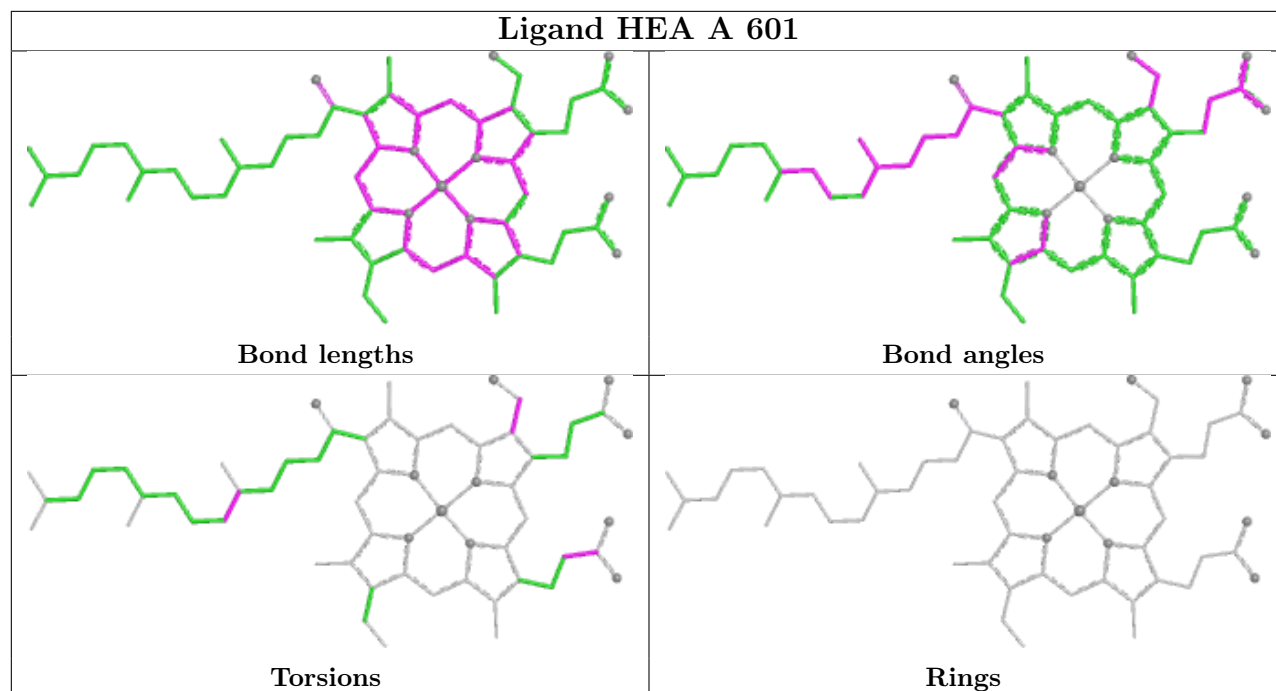












5.7 Other polymers [i](#)

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%)	-0.26	6 (1%) 76 76	19, 31, 39, 76	20 (3%)
1	N	513/514 (99%)	0.18	10 (1%) 66 66	20, 40, 53, 77	21 (4%)
2	B	226/227 (99%)	0.16	10 (4%) 39 38	22, 38, 57, 75	7 (3%)
2	O	226/227 (99%)	0.66	15 (6%) 24 23	29, 52, 72, 99	6 (2%)
3	C	259/260 (99%)	0.03	9 (3%) 47 46	17, 36, 48, 82	13 (5%)
3	P	259/260 (99%)	0.16	5 (1%) 66 66	20, 40, 50, 77	12 (4%)
4	D	144/147 (97%)	0.32	6 (4%) 40 39	34, 43, 55, 75	0
4	Q	144/147 (97%)	1.16	18 (12%) 8 7	48, 63, 88, 137	0
5	E	105/109 (96%)	0.20	3 (2%) 53 52	23, 44, 63, 109	1 (0%)
5	R	105/109 (96%)	0.58	5 (4%) 35 34	29, 55, 71, 115	1 (0%)
6	F	94/94 (100%)	0.62	5 (5%) 32 31	27, 46, 64, 119	1 (1%)
6	S	94/94 (100%)	0.88	8 (8%) 16 15	32, 51, 75, 117	1 (1%)
7	G	83/85 (97%)	1.51	18 (21%) 2 2	34, 44, 114, 145	0
7	T	83/85 (97%)	1.54	21 (25%) 1 1	35, 48, 108, 150	0
8	H	79/85 (92%)	0.72	10 (12%) 8 7	36, 47, 80, 99	0
8	U	79/85 (92%)	0.98	10 (12%) 8 7	43, 54, 93, 109	0
9	I	72/73 (98%)	1.26	18 (25%) 2 1	36, 50, 82, 91	0
9	V	72/73 (98%)	1.69	18 (25%) 2 1	42, 67, 95, 103	0
10	J	58/59 (98%)	0.71	6 (10%) 12 11	25, 47, 73, 117	2 (3%)
10	W	58/59 (98%)	1.00	8 (13%) 6 6	31, 54, 81, 128	2 (3%)
11	K	49/56 (87%)	0.46	2 (4%) 41 40	38, 45, 58, 66	0
11	X	49/56 (87%)	1.17	11 (22%) 2 2	56, 66, 83, 90	0
12	L	46/47 (97%)	0.21	3 (6%) 25 23	31, 38, 53, 84	0
12	Y	46/47 (97%)	1.08	5 (10%) 10 9	36, 54, 70, 108	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.29	3 (6%) 22 21	30, 38, 66, 104	1 (2%)
13	Z	43/46 (93%)	1.06	5 (11%) 9 8	43, 58, 85, 118	1 (2%)
All	All	3542/3604 (98%)	0.43	238 (6%) 24 22	17, 43, 75, 150	90 (2%)

The worst 5 of 238 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	1	ALA	12.8
6	S	1	ALA	12.2
4	Q	6	VAL	11.8
4	Q	5	VAL	9.8
7	G	3	ALA	9.6

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	0.33	0.23	118,123,127,131	0
7	TPO	T	11	11/12	0.61	0.26	93,108,122,125	0
7	TPO	G	11	11/12	0.64	0.28	88,102,120,124	0
9	SAC	I	1	9/10	0.80	0.16	74,75,78,79	0
1	FME	N	1	10/11	0.88	0.15	58,63,83,86	0
1	FME	A	1	10/11	0.90	0.16	46,53,70,78	0
2	FME	O	1	10/11	0.95	0.12	52,53,59,60	0
2	FME	B	1	10/11	0.96	0.09	35,36,44,47	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	DMU	P	308	33/33	0.61	0.25	71,126,142,143	0
22	CHD	W	101	29/29	0.72	0.21	89,96,106,107	0
22	CHD	J	101	29/29	0.73	0.20	73,78,100,104	0
24	CDL	P	305	100/100	0.74	0.30	65,90,111,114	0
25	DMU	C	312	33/33	0.75	0.20	65,100,138,139	0
19	PGV	P	304	51/51	0.75	0.27	66,92,122,129	0
23	PEK	G	102	53/53	0.76	0.24	55,101,139,150	0
24	CDL	G	101	100/100	0.77	0.29	65,97,136,145	0
23	PEK	C	304	53/53	0.77	0.28	60,91,135,141	0
19	PGV	C	306	51/51	0.77	0.24	62,82,121,124	0
23	PEK	T	101	53/53	0.77	0.27	56,94,139,144	0
18	TGL	Q	201	63/63	0.78	0.27	67,86,96,100	0
24	CDL	T	104	100/100	0.78	0.27	63,92,121,138	0
24	CDL	C	307	100/100	0.78	0.26	56,85,110,116	0
25	DMU	C	313	33/33	0.78	0.22	49,130,146,147	0
18	TGL	Y	101	63/63	0.78	0.28	63,83,104,107	0
18	TGL	D	201	63/63	0.79	0.27	56,71,89,92	0
18	TGL	L	101	63/63	0.79	0.28	46,71,85,86	0
20	EDO	S	103	4/4	0.79	0.24	57,66,69,72	0
26	PSC	E	201	52/52	0.79	0.26	56,87,141,150	0
23	PEK	T	103	53/53	0.80	0.25	59,85,124,134	0
19	PGV	N	606	51/51	0.80	0.26	70,87,126,128	0
18	TGL	A	606	63/63	0.80	0.28	53,78,95,98	0
26	PSC	O	304	52/52	0.80	0.25	60,92,142,154	0
22	CHD	P	306	29/29	0.81	0.18	71,76,81,81	0
20	EDO	B	303	4/4	0.81	0.25	62,72,75,79	0
20	EDO	P	307	4/4	0.81	0.30	82,88,90,97	0
18	TGL	O	302	63/63	0.81	0.30	64,87,99,105	0
19	PGV	M	101	51/51	0.81	0.23	49,77,115,124	0
25	DMU	P	309	33/33	0.82	0.20	64,128,146,149	0
17	NA	C	302	1/1	0.82	0.23	51,51,51,51	0
22	CHD	C	308	29/29	0.82	0.18	72,74,79,80	0
17	NA	P	302	1/1	0.83	0.19	51,51,51,51	0
25	DMU	Z	101	33/33	0.86	0.14	57,80,91,94	0
20	EDO	C	310	4/4	0.87	0.16	71,76,80,84	0
20	EDO	D	202	4/4	0.87	0.19	54,63,65,68	0
20	EDO	D	203	4/4	0.87	0.23	61,65,70,71	0
25	DMU	M	102	33/33	0.88	0.12	48,58,74,77	0
20	EDO	A	612	4/4	0.88	0.15	38,39,43,43	0
20	EDO	F	104	4/4	0.88	0.16	56,58,60,62	0
20	EDO	C	309	4/4	0.89	0.24	82,86,90,92	0
20	EDO	N	616	4/4	0.89	0.18	59,59,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	EDO	A	615	4/4	0.89	0.34	49,50,56,58	0
20	EDO	N	611	4/4	0.90	0.18	60,62,64,66	0
20	EDO	A	611	4/4	0.90	0.19	62,67,67,69	0
20	EDO	N	608	4/4	0.91	0.12	37,39,40,40	0
20	EDO	A	613	4/4	0.92	0.14	46,49,51,52	0
20	EDO	N	617	4/4	0.92	0.17	58,70,75,86	0
20	EDO	N	609	4/4	0.92	0.16	63,69,69,74	0
20	EDO	A	608	4/4	0.92	0.14	55,59,59,65	0
20	EDO	N	613	4/4	0.92	0.24	49,51,53,55	0
20	EDO	N	615	4/4	0.92	0.26	54,58,59,65	0
20	EDO	N	610	4/4	0.93	0.12	62,64,65,66	0
20	EDO	A	614	4/4	0.93	0.14	50,53,54,59	0
20	EDO	A	610	4/4	0.94	0.13	54,56,56,57	0
16	MG	N	604	1/1	0.94	0.12	44,44,44,44	0
23	PEK	T	102	53/53	0.94	0.15	40,58,95,98	0
16	MG	A	604	1/1	0.94	0.08	30,30,30,30	0
19	PGV	N	607	51/51	0.95	0.11	38,46,68,70	0
22	CHD	B	302	29/29	0.95	0.08	36,38,40,44	0
22	CHD	C	301	29/29	0.95	0.08	34,37,39,42	0
20	EDO	N	612	4/4	0.95	0.14	45,46,46,47	0
20	EDO	F	102	4/4	0.95	0.13	41,44,45,47	0
22	CHD	P	301	29/29	0.95	0.08	37,40,42,45	0
20	EDO	N	614	4/4	0.95	0.15	46,48,49,50	0
19	PGV	C	305	51/51	0.95	0.13	35,41,90,101	0
23	PEK	C	303	53/53	0.95	0.14	35,52,84,86	0
19	PGV	A	607	51/51	0.95	0.11	33,40,61,66	0
20	EDO	C	311	4/4	0.95	0.10	40,43,45,48	0
20	EDO	A	616	4/4	0.95	0.17	43,45,49,49	0
20	EDO	R	201	4/4	0.95	0.19	52,53,53,53	0
22	CHD	O	301	29/29	0.96	0.07	40,42,44,47	0
19	PGV	P	303	51/51	0.96	0.12	38,46,76,79	0
20	EDO	S	102	4/4	0.97	0.10	37,39,40,42	0
20	EDO	E	202	4/4	0.97	0.09	51,52,52,53	0
20	EDO	A	609	4/4	0.97	0.07	30,32,32,33	0
14	HEA	N	602	60/60	0.97	0.08	35,37,42,44	0
17	NA	A	605	1/1	0.98	0.05	30,30,30,30	0
14	HEA	A	601	60/60	0.98	0.07	25,28,38,40	0
20	EDO	F	103	4/4	0.98	0.06	31,33,33,33	0
21	CUA	B	301	2/2	0.98	0.03	30,30,30,30	0
14	HEA	A	602	60/60	0.98	0.06	26,28,34,38	0
14	HEA	N	601	60/60	0.98	0.08	36,42,49,51	0
17	NA	N	605	1/1	0.99	0.04	49,49,49,49	0

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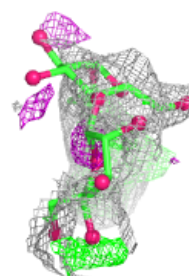
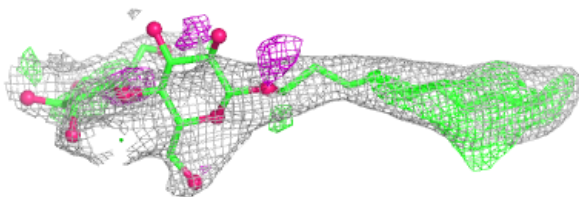
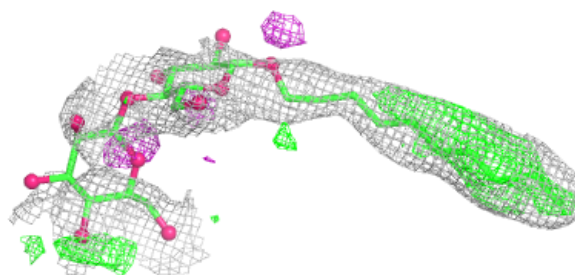
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	CUA	O	303	2/2	0.99	0.03	42,42,42,43	0
27	ZN	S	101	1/1	0.99	0.03	46,46,46,46	0
15	CU	A	603	1/1	1.00	0.01	28,28,28,28	0
27	ZN	F	101	1/1	1.00	0.02	39,39,39,39	0
15	CU	N	603	1/1	1.00	0.01	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.

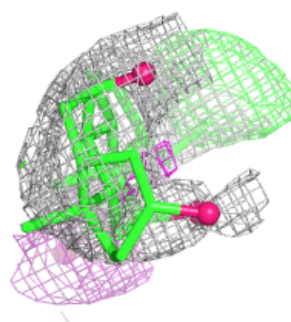
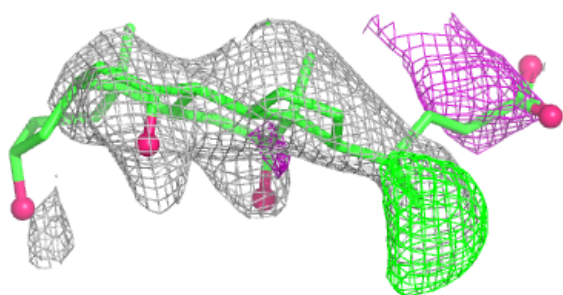
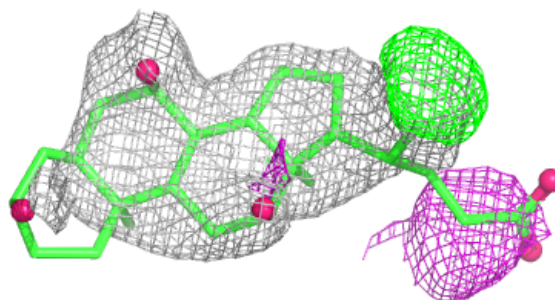
Electron density around DMU P 308:

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

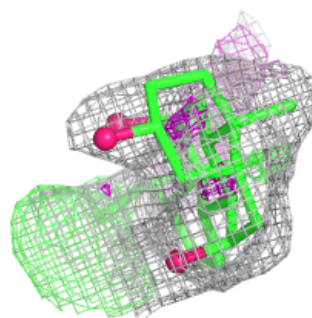
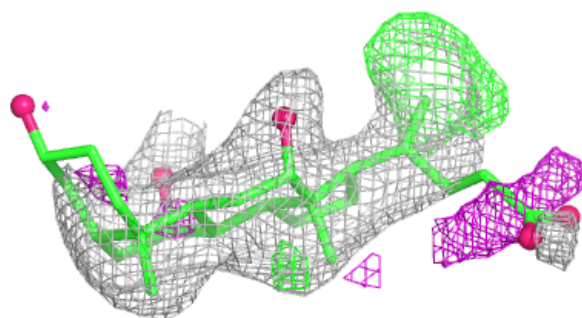
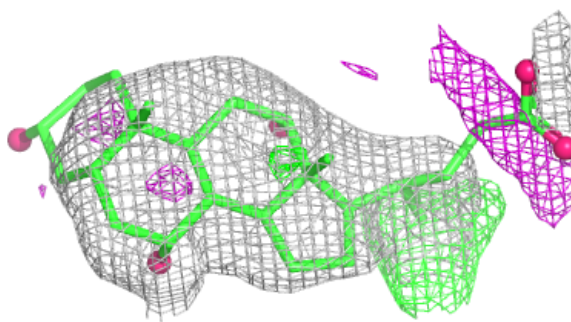


Electron density around CHD W 101:

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

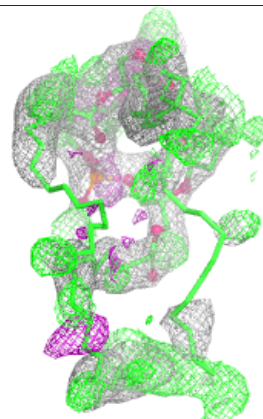
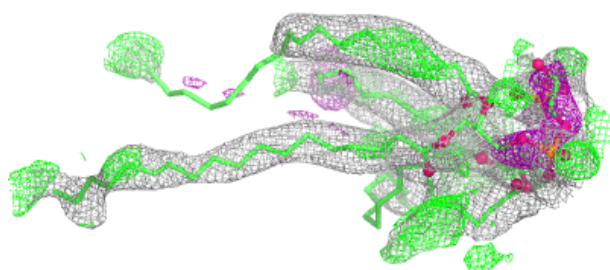
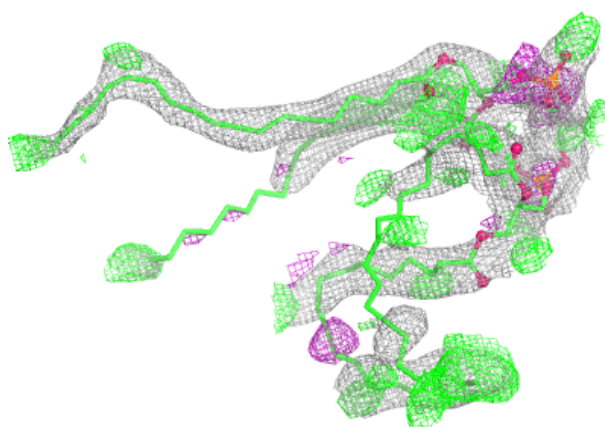
**Electron density around CHD J 101:**

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

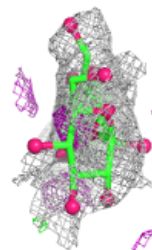
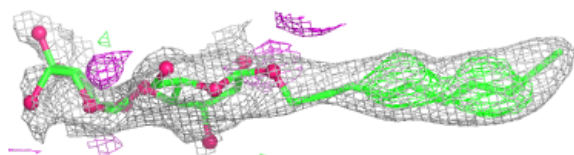
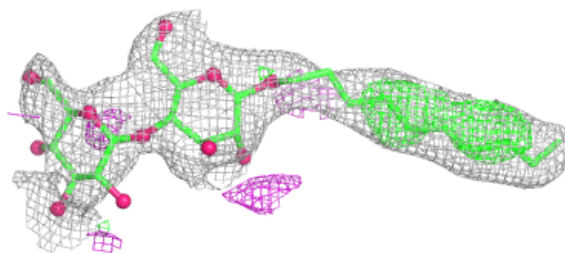


Electron density around CDL P 305:

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

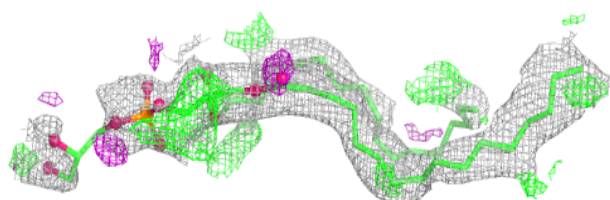
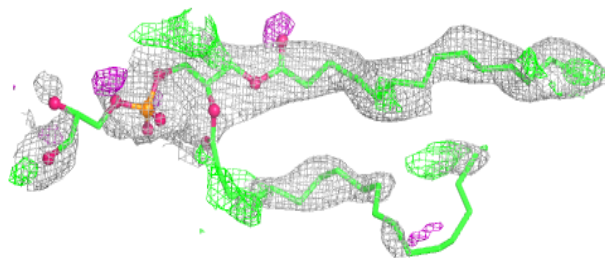
**Electron density around DMU C 312:**

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

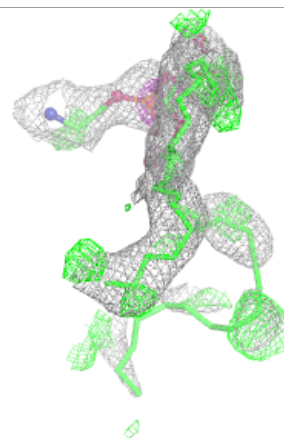
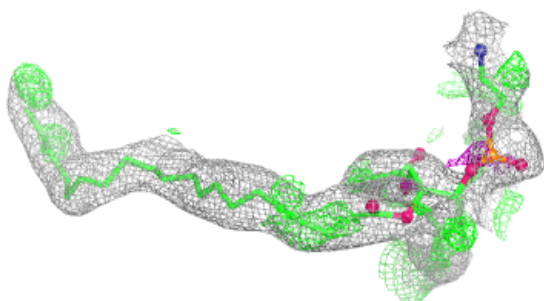
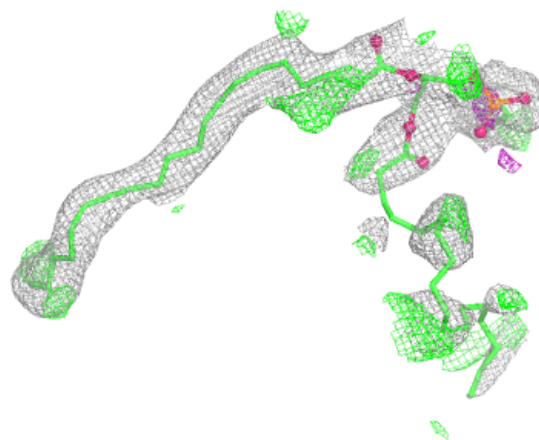


Electron density around PGV P 304:

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

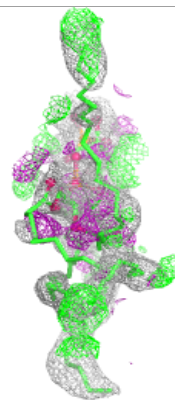
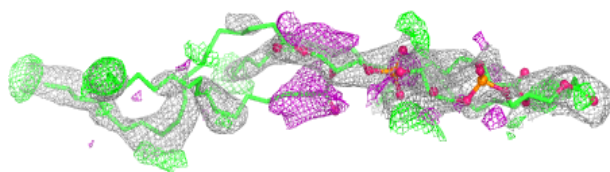
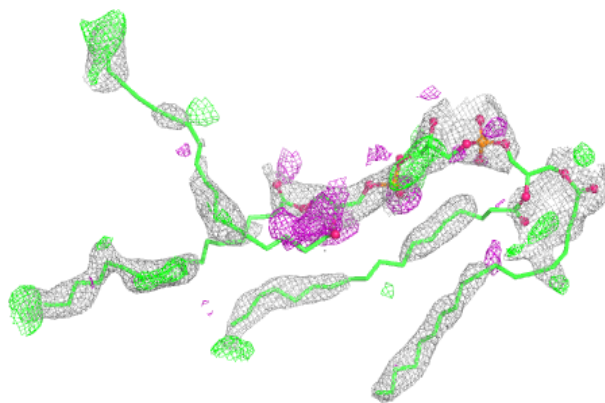
**Electron density around PEK G 102:**

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



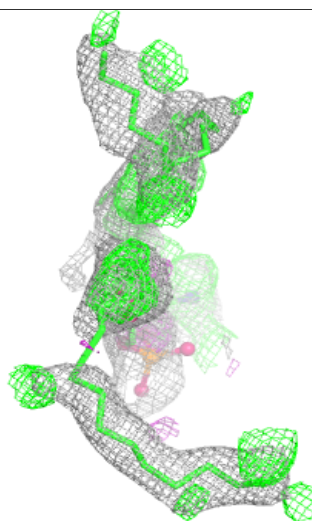
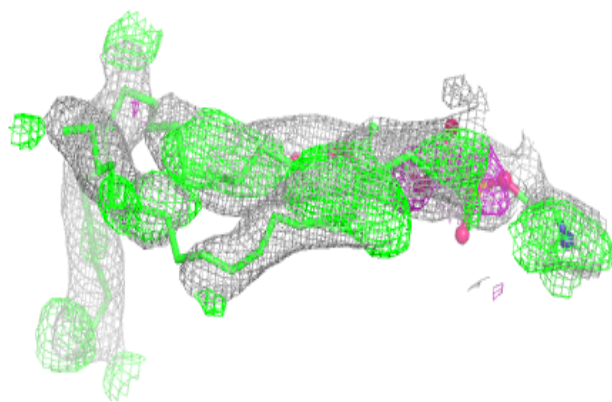
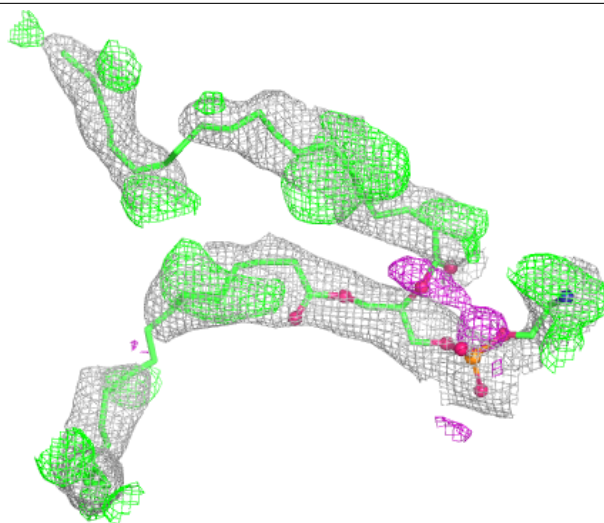
Electron density around CDL G 101:

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



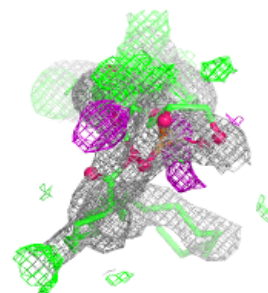
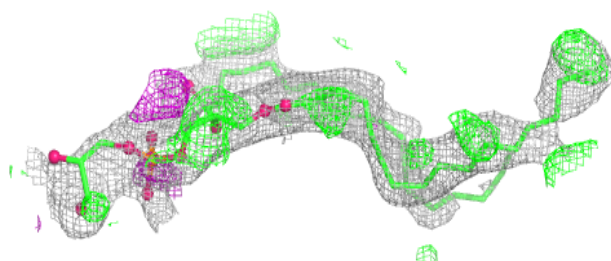
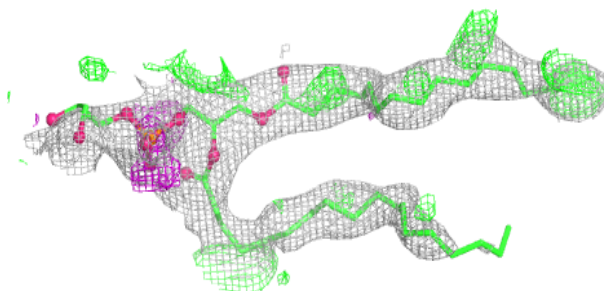
Electron density around PEK C 304:

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

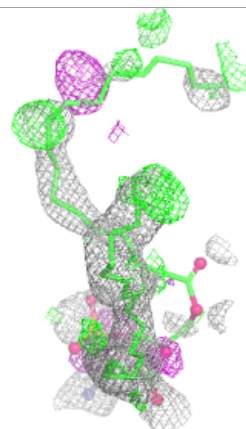
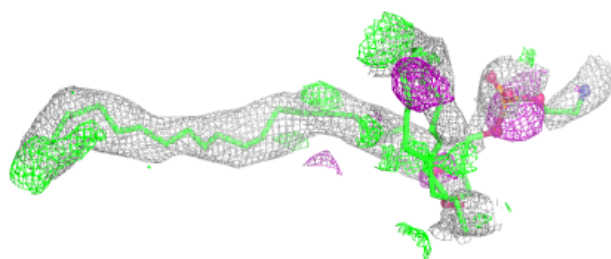
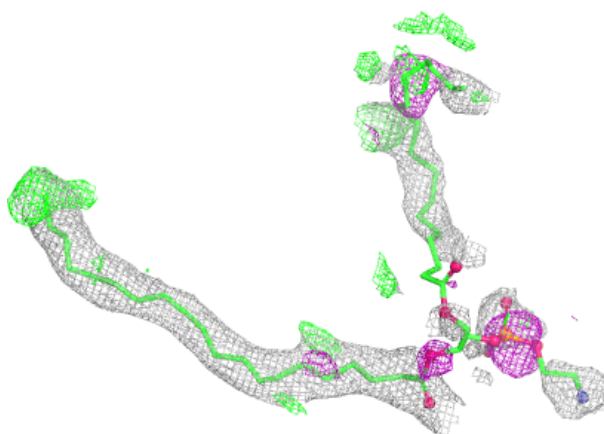


Electron density around PGV C 306:

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

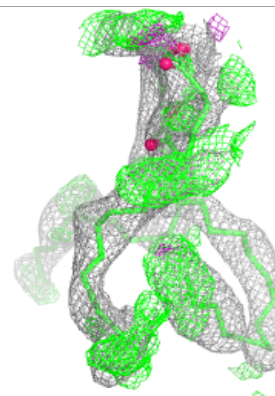
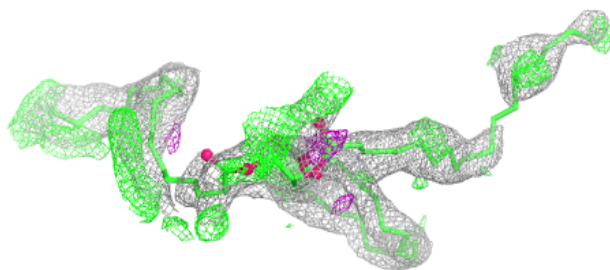
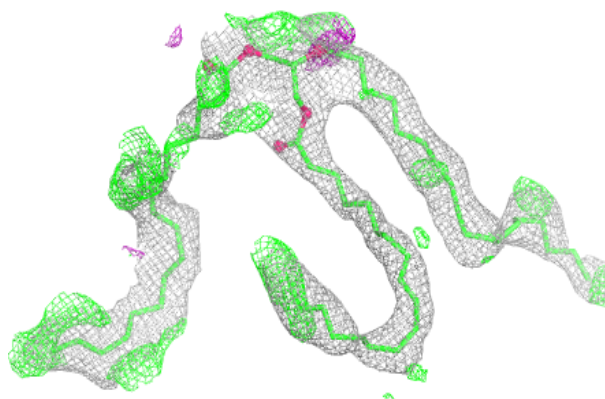
**Electron density around PEK T 101:**

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

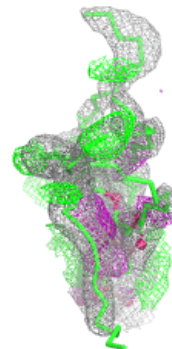
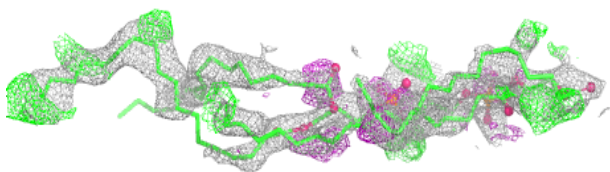
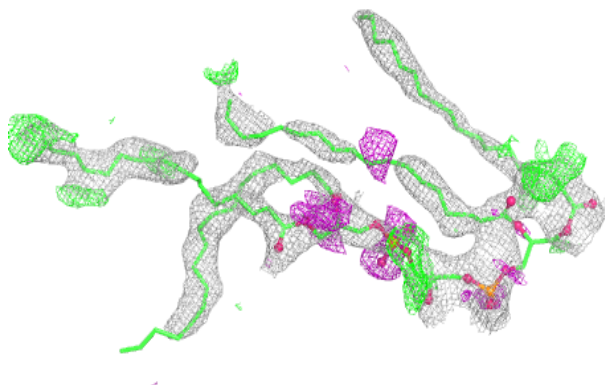


Electron density around TGL Q 201:

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

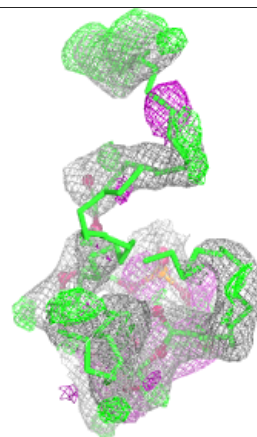
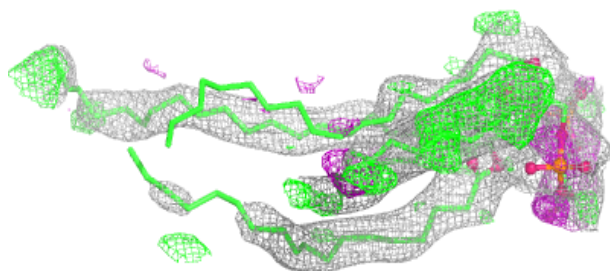
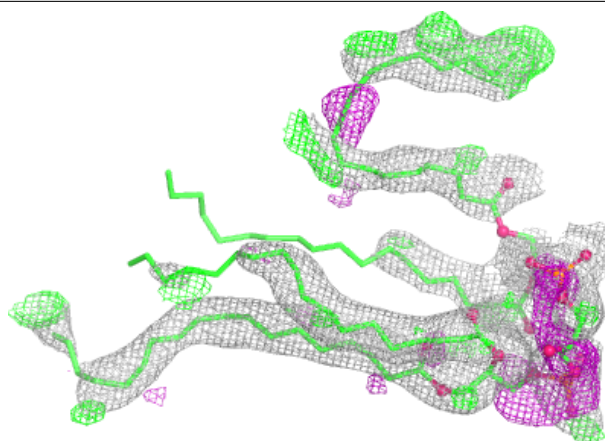
**Electron density around CDL T 104:**

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and green (positive)



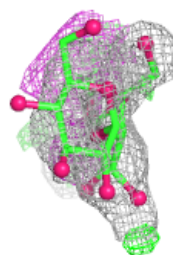
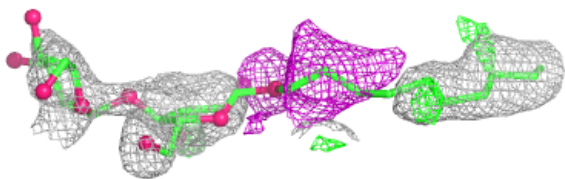
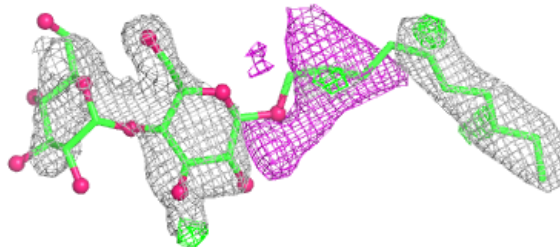
Electron density around CDL C 307:

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



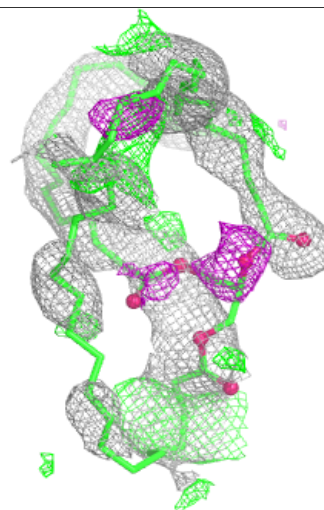
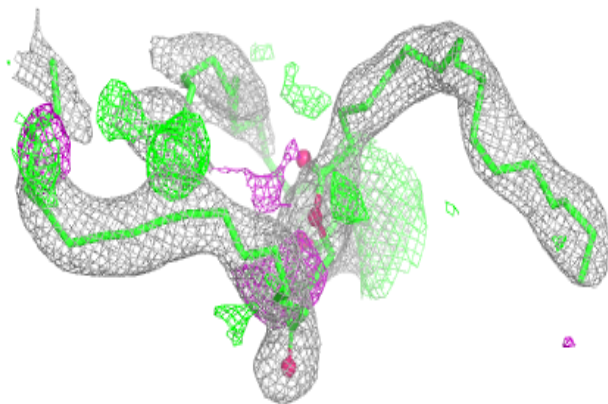
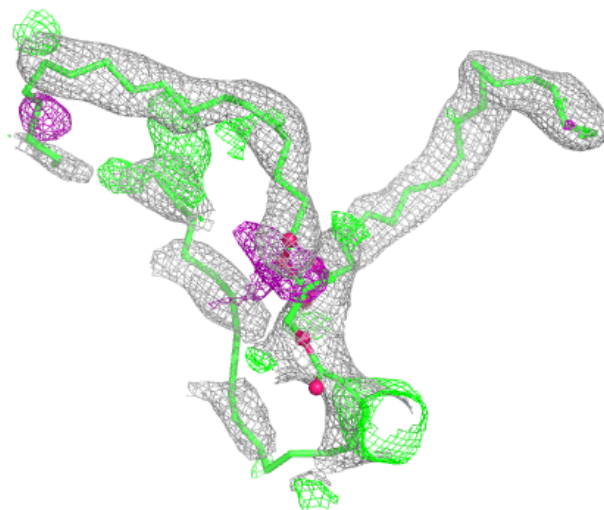
Electron density around DMU C 313:

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



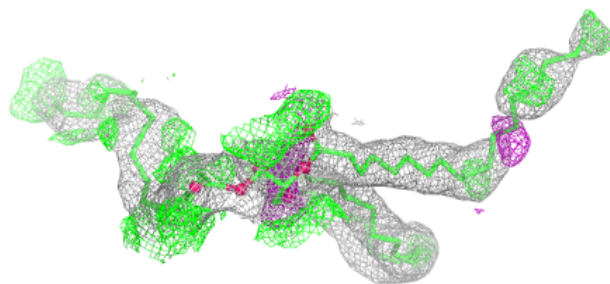
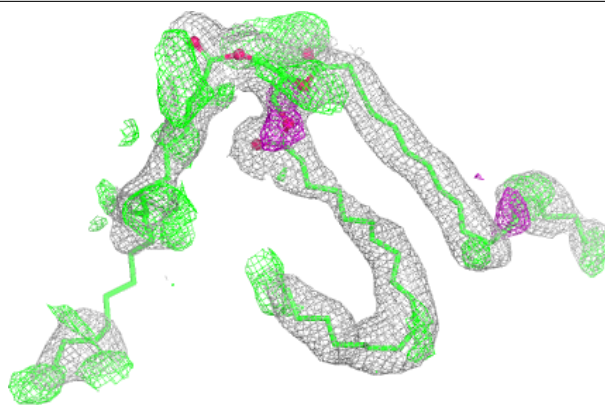
Electron density around TGL Y 101:

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and green (positive)



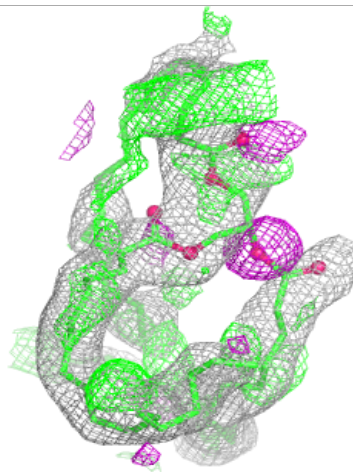
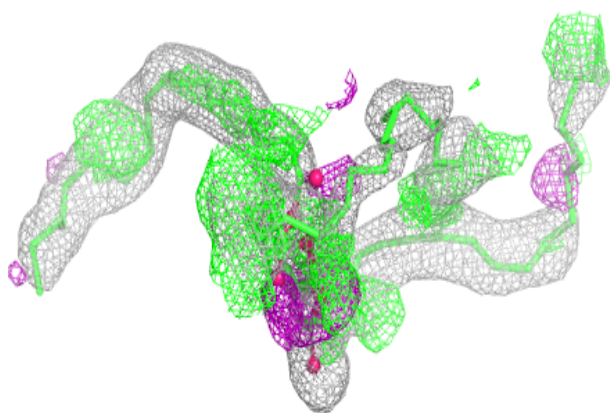
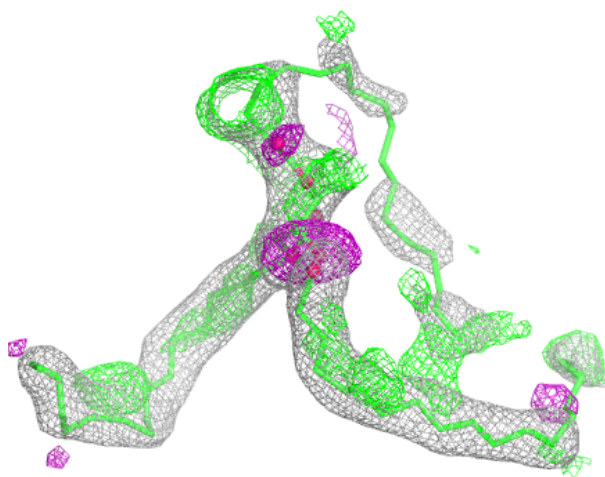
Electron density around TGL D 201:

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and green (positive)



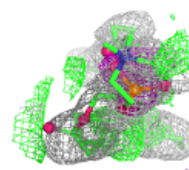
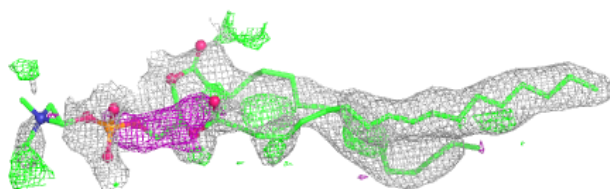
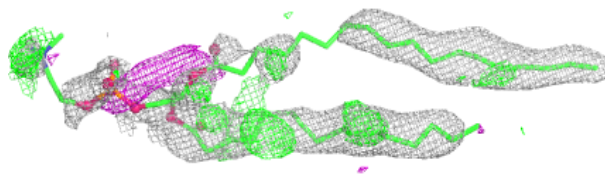
Electron density around TGL L 101:

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and green (positive)



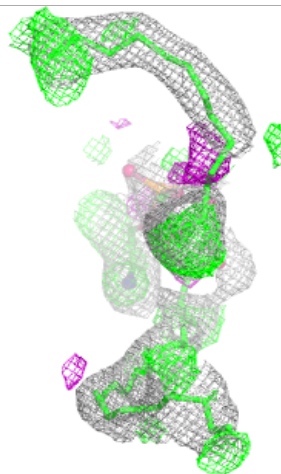
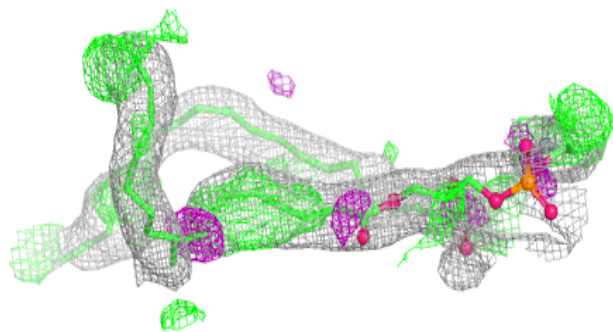
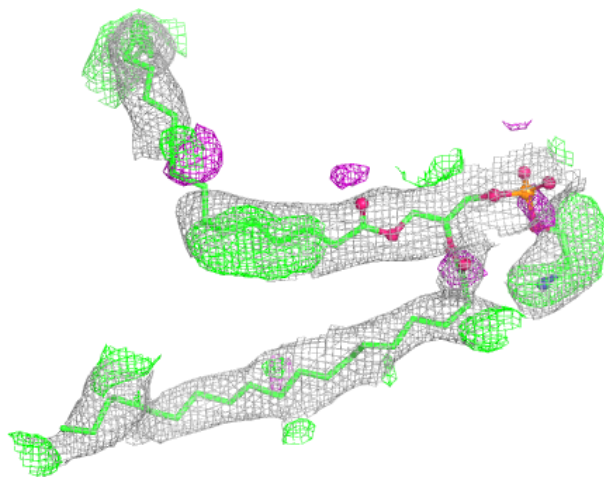
Electron density around PSC E 201:

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and green (positive)



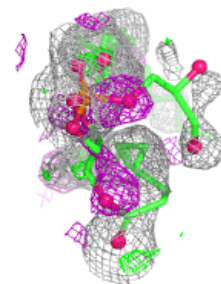
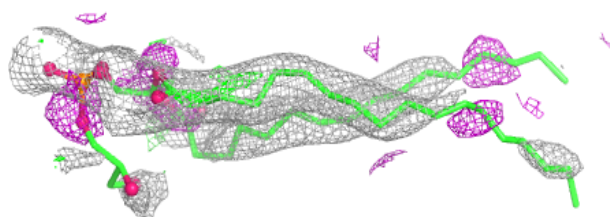
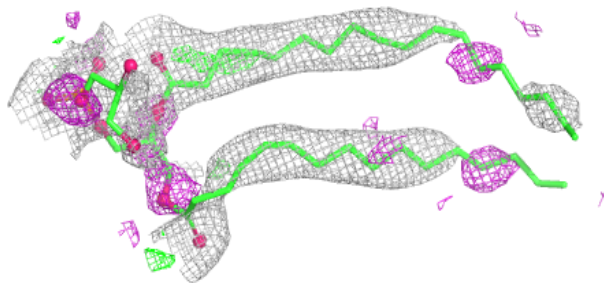
Electron density around PEK T 103:

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and green (positive)

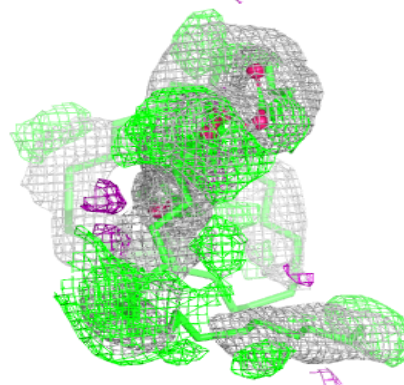
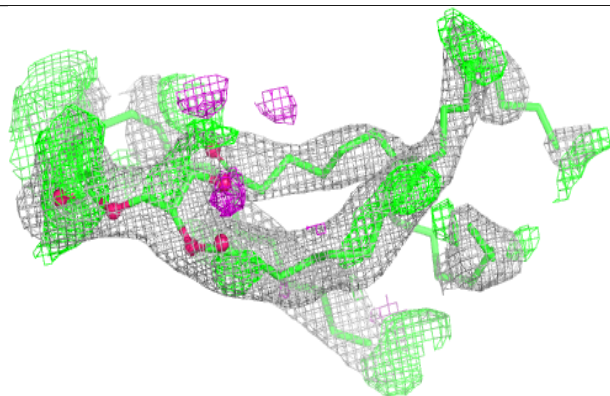
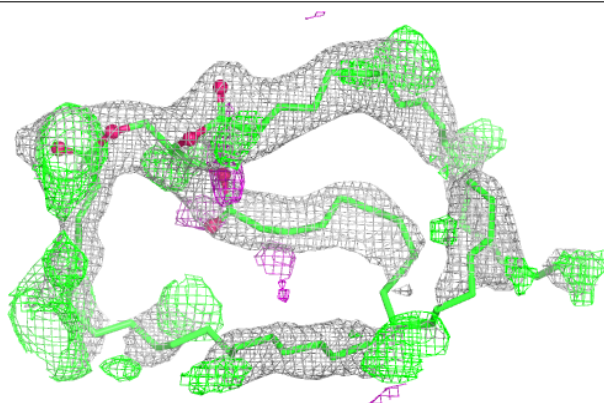


Electron density around PGV N 606:

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and green (positive)

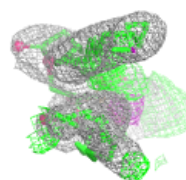
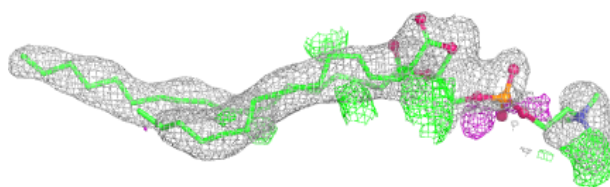
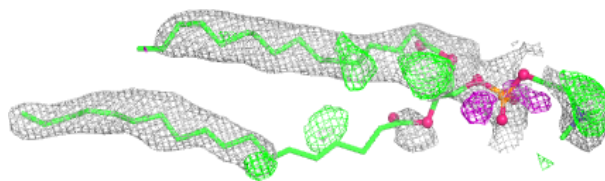
**Electron density around TGL A 606:**

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

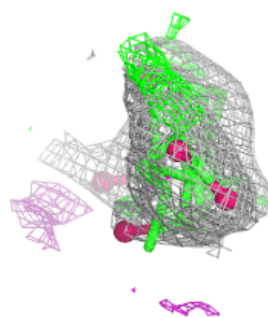
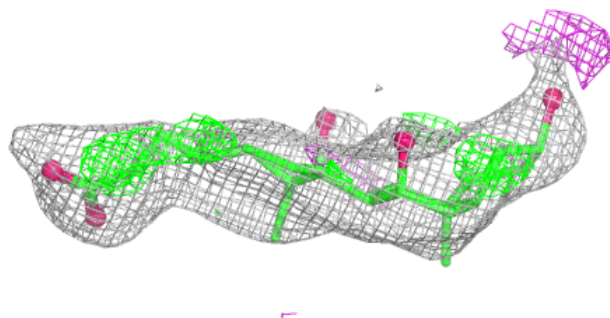
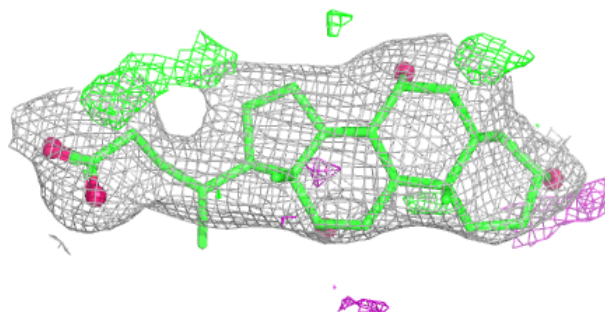


Electron density around PSC O 304:

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

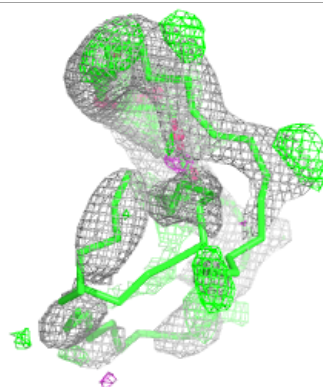
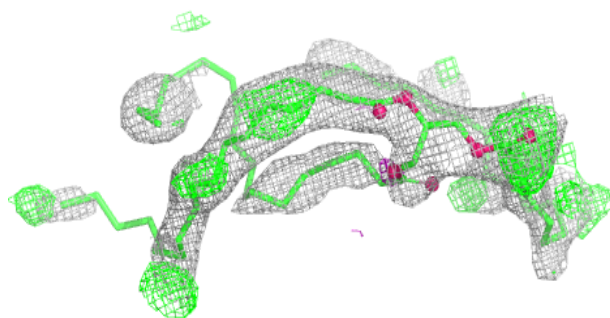
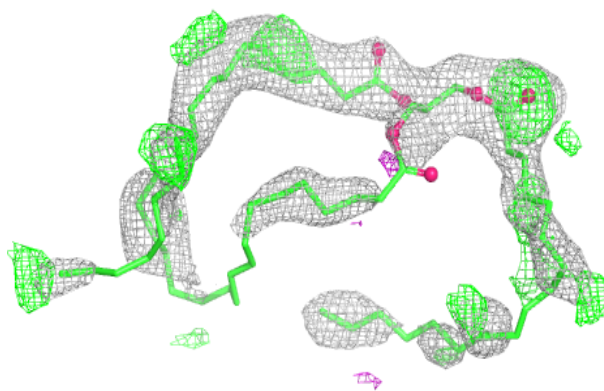
**Electron density around CHD P 306:**

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

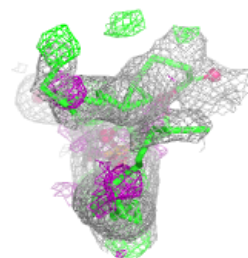
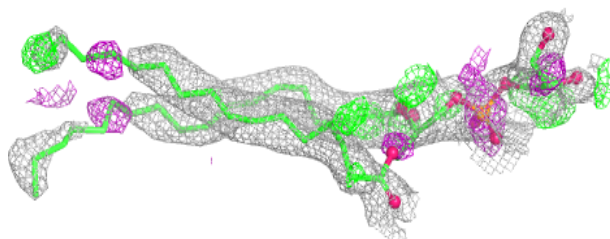
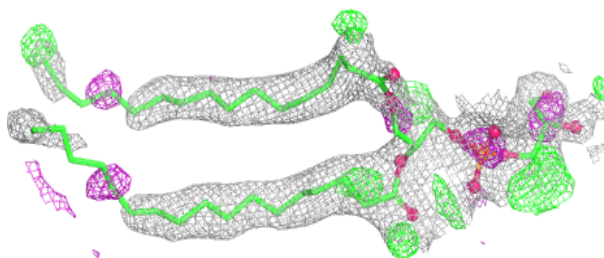


Electron density around TGL O 302:

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

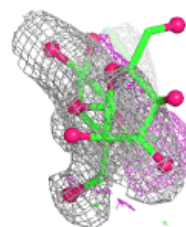
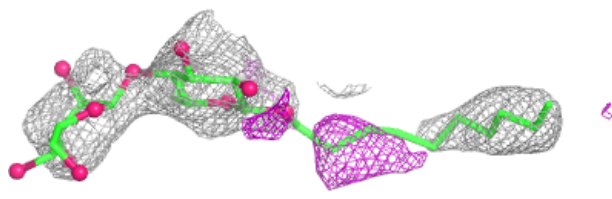
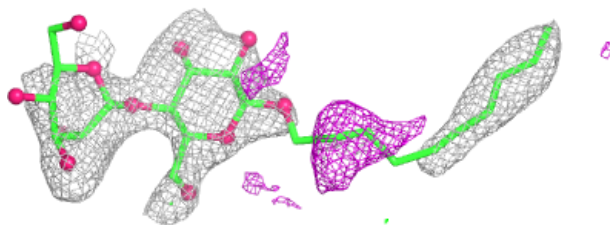
**Electron density around PGV M 101:**

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

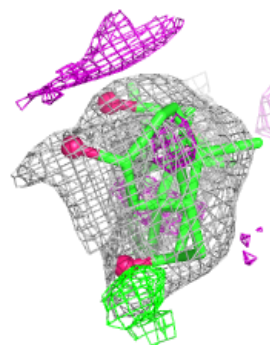
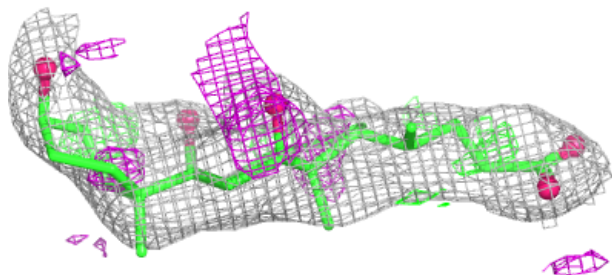
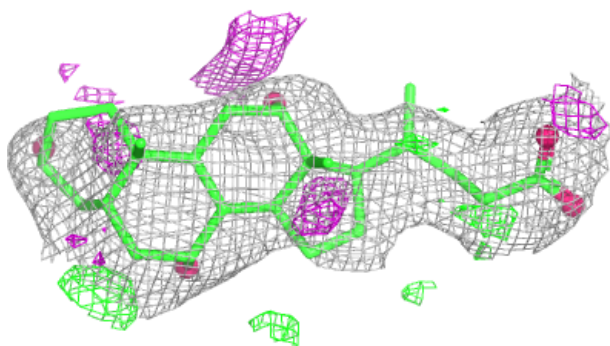


Electron density around DMU P 309:

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

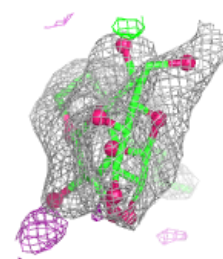
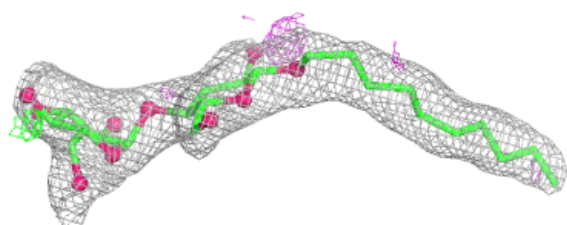
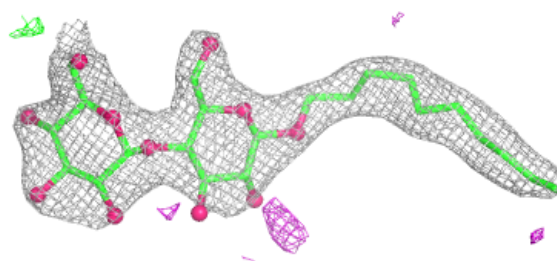
**Electron density around CHD C 308:**

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

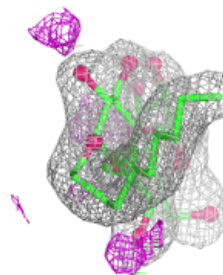
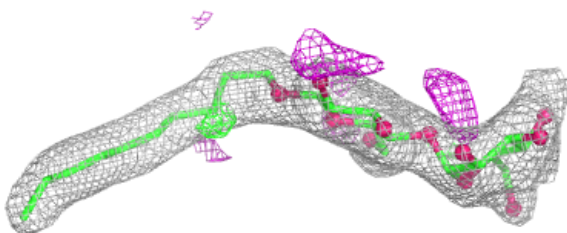
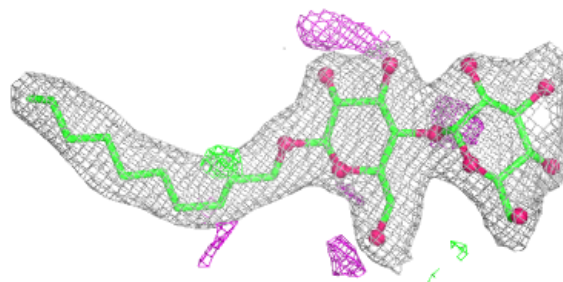


Electron density around DMU Z 101:

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

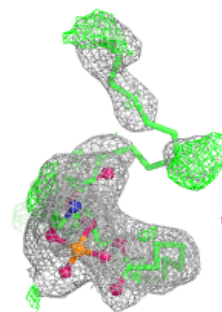
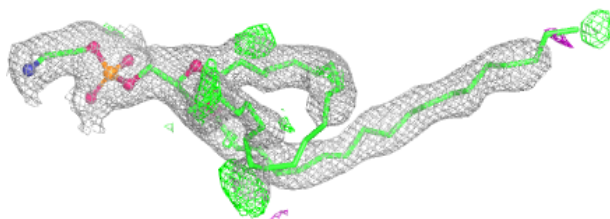
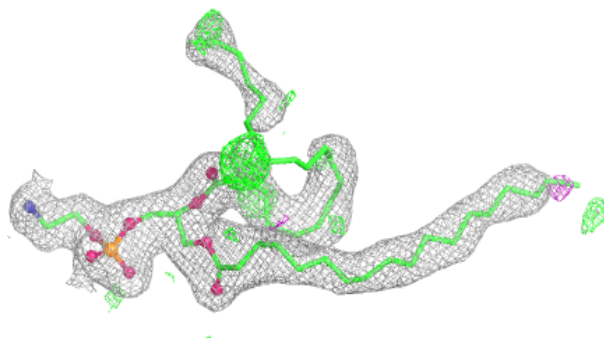
**Electron density around DMU M 102:**

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

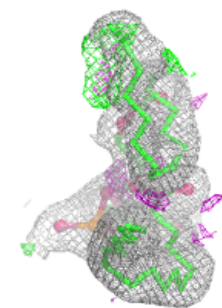
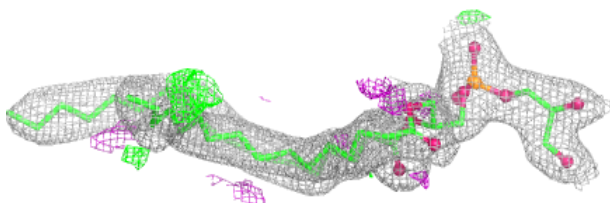
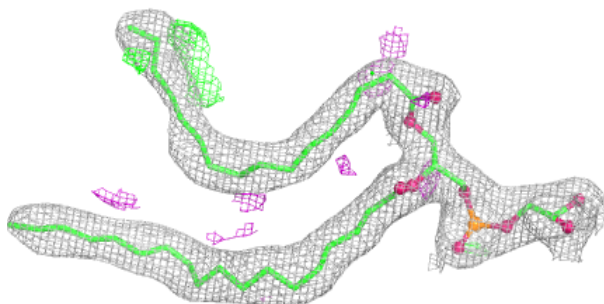


Electron density around PEK T 102:

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

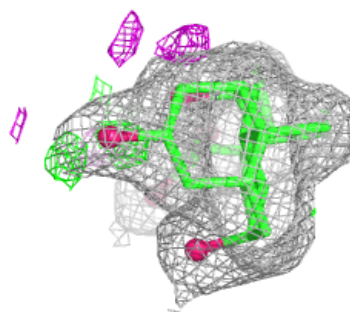
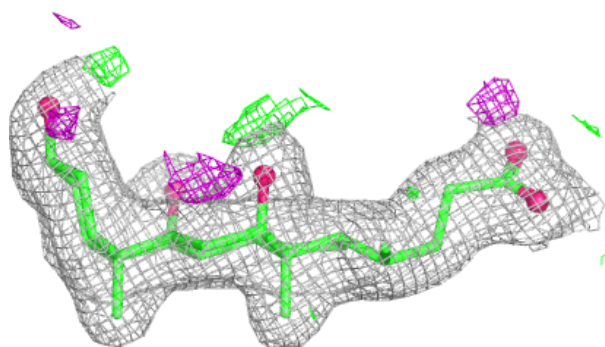
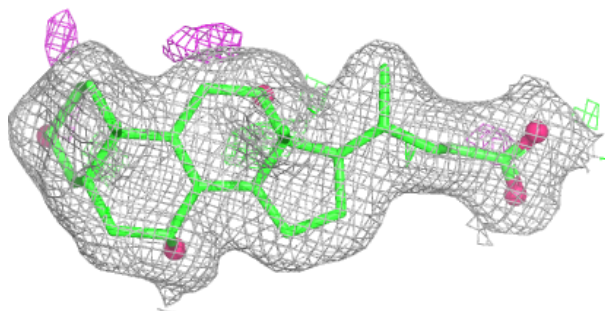
**Electron density around PGV N 607:**

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

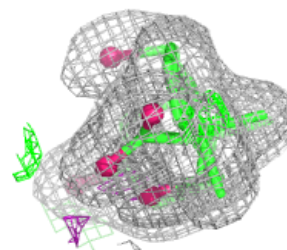
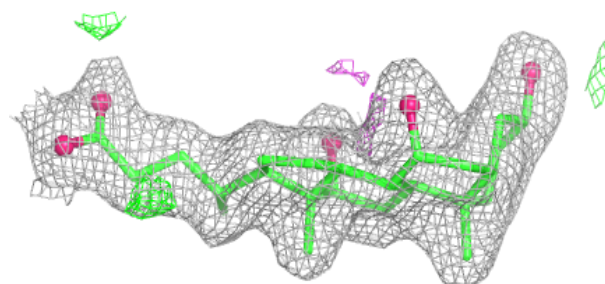
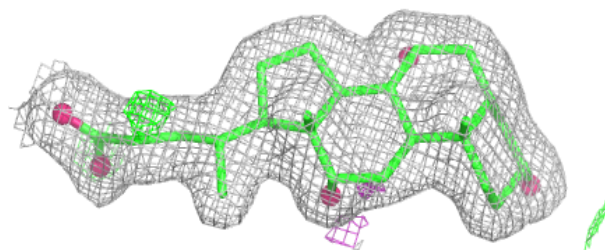


Electron density around CHD B 302:

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

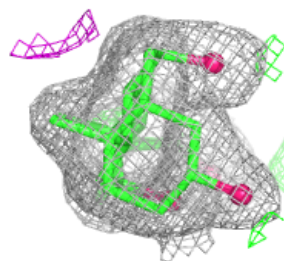
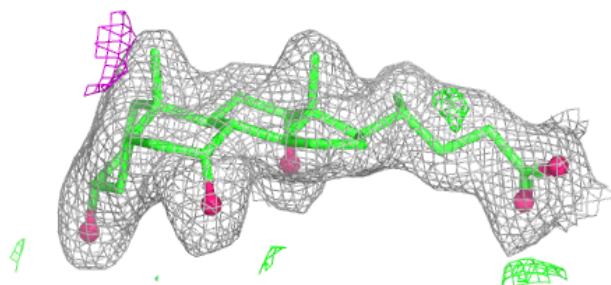
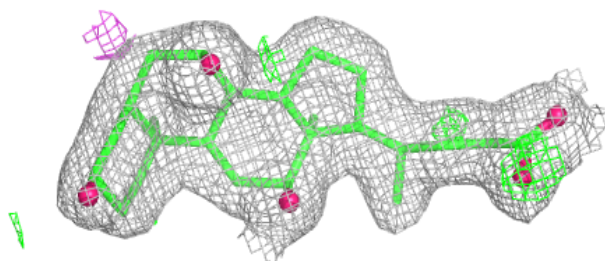
**Electron density around CHD C 301:**

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

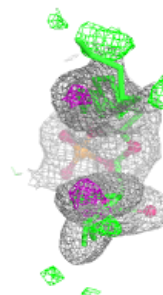
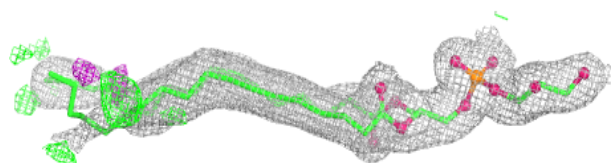
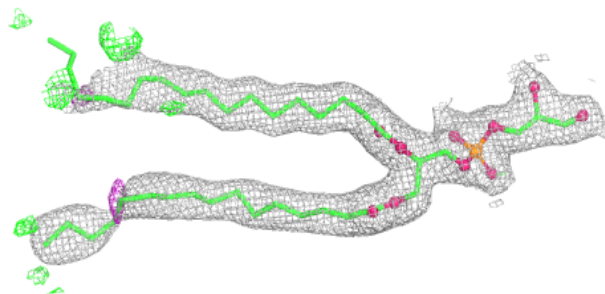


Electron density around CHD P 301:

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

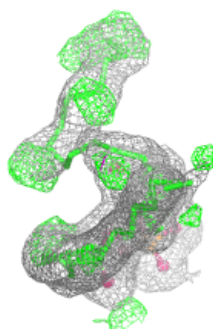
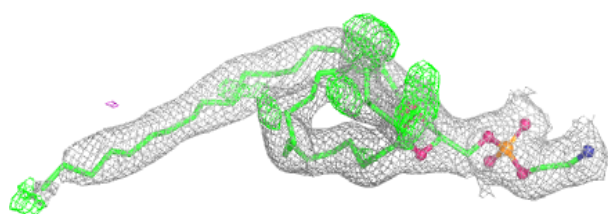
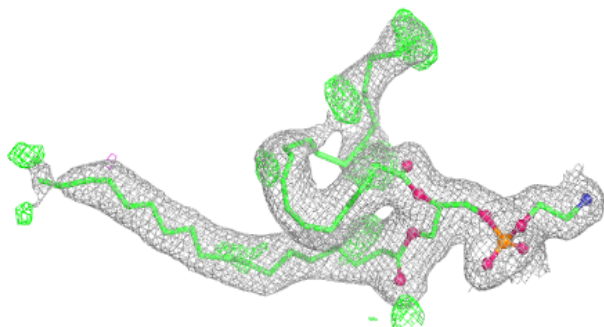
**Electron density around PGV C 305:**

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

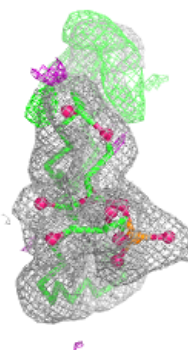
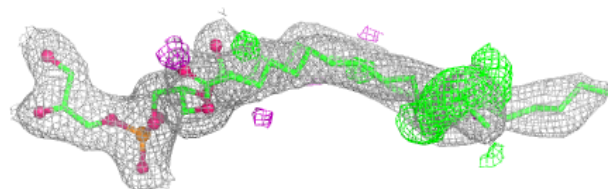
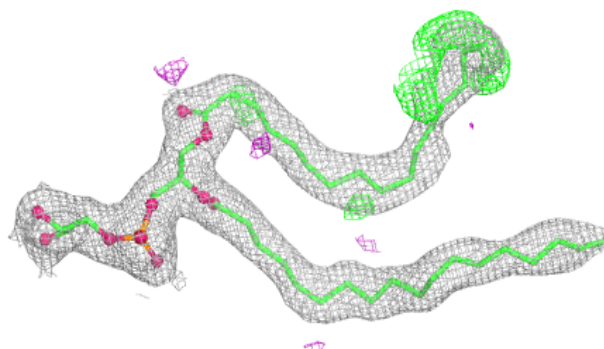


Electron density around PEK C 303:

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

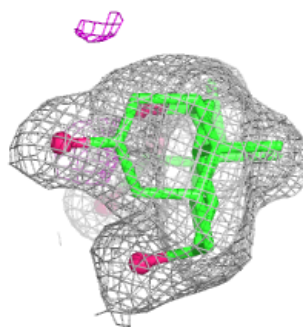
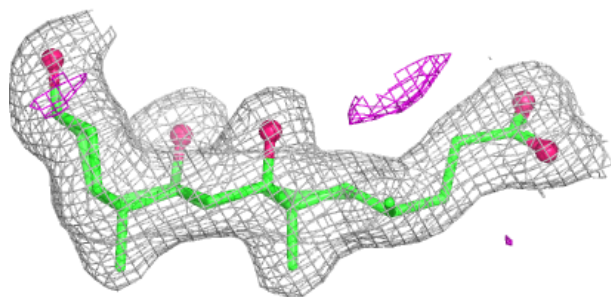
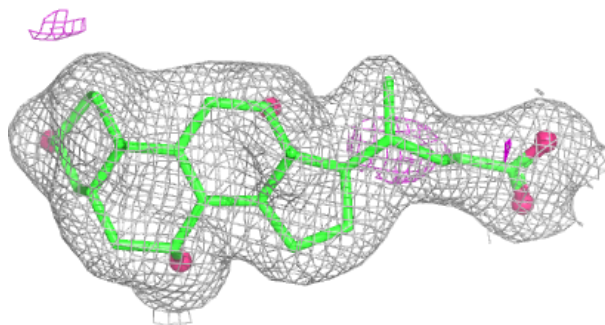
**Electron density around PGV A 607:**

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

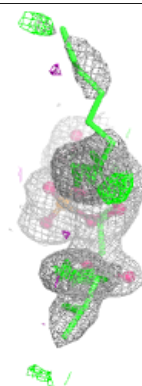
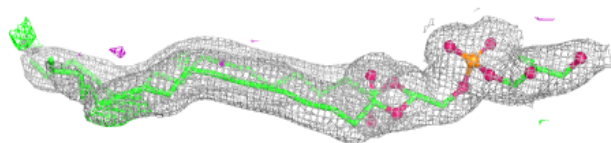
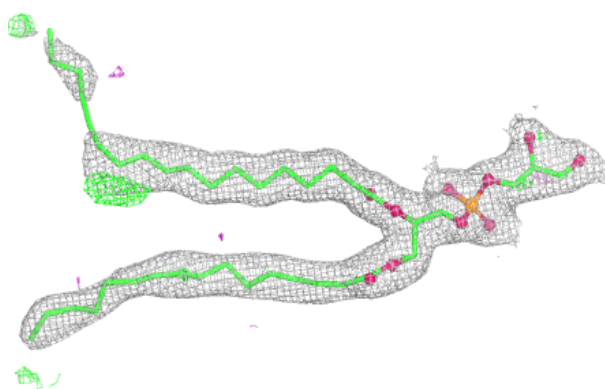


Electron density around CHD O 301:

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

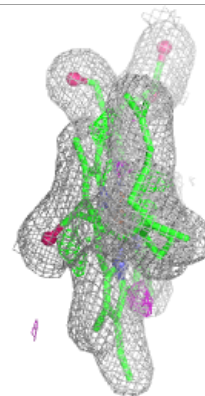
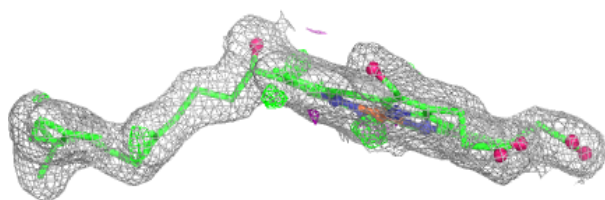
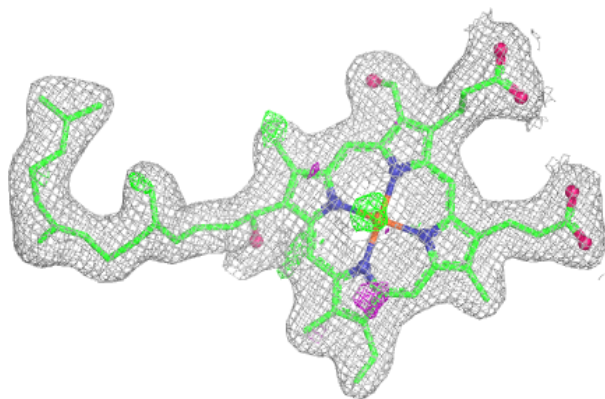
**Electron density around PGV P 303:**

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

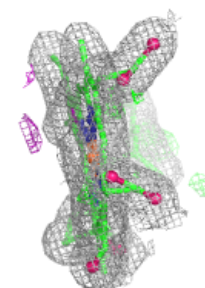
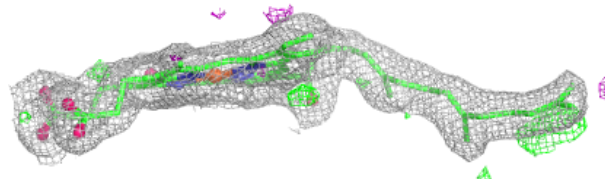
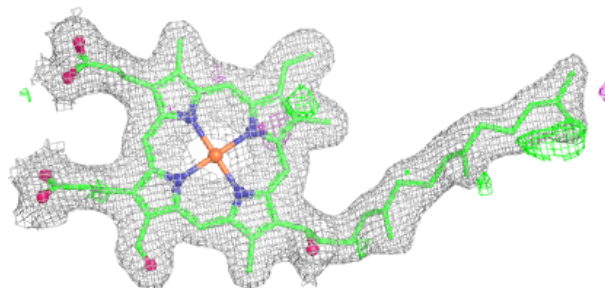


Electron density around HEA N 602:

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

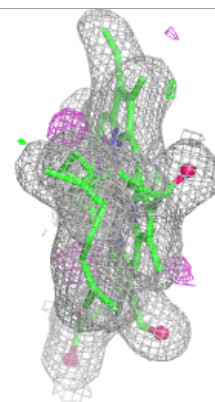
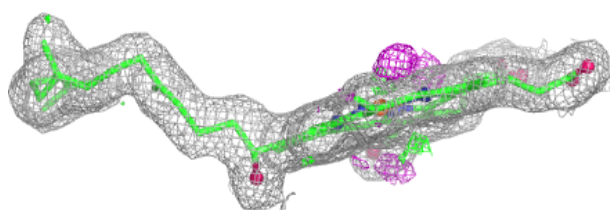
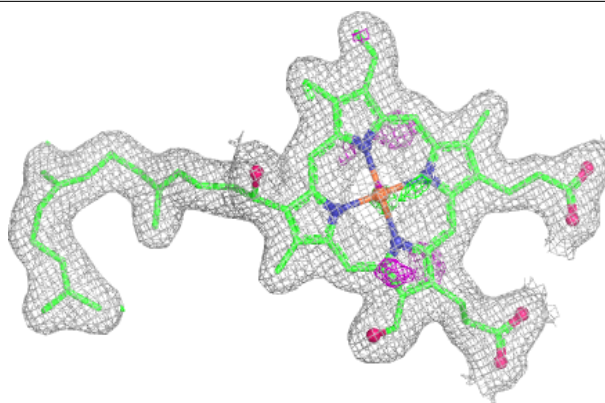
**Electron density around HEA A 601:**

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

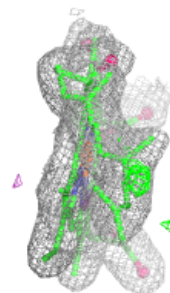
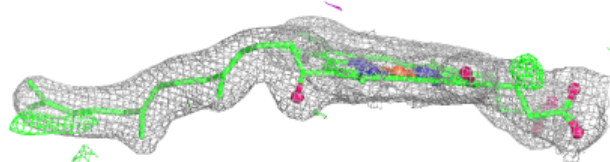
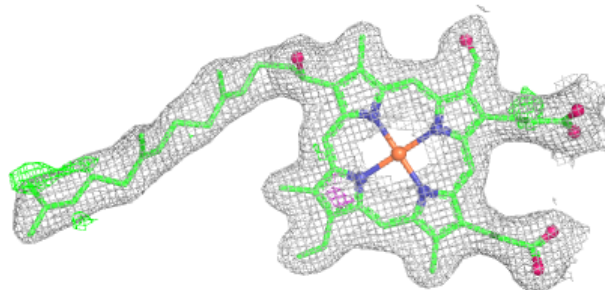


Electron density around HEA A 602:

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

**Electron density around HEA N 601:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.