



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 1, 2022 – 06:22 PM EDT

PDB ID : 7THI
Title : Annealed structure of oxidized bovine cytochrome c oxidase with reduced metal centers induced by synchrotron X-ray exposure
Authors : Ishigami, I.; Rousseau, D.L.; Yeh, S.-R.; Russi, S.; Cohen, A.
Deposited on : 2022-01-13
Resolution : 2.45 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

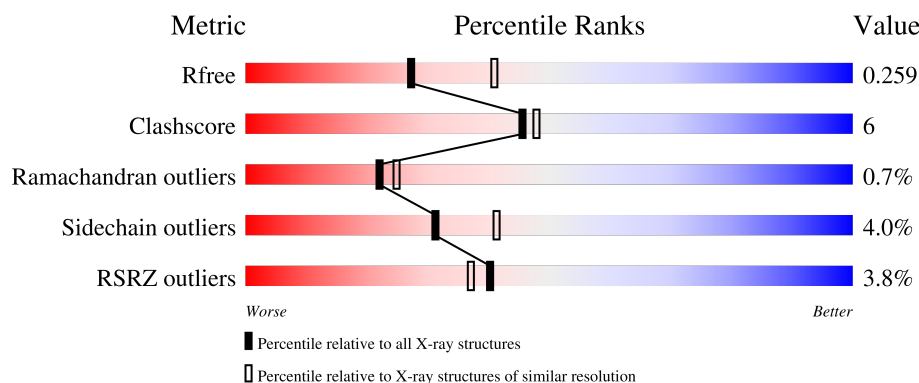
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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.




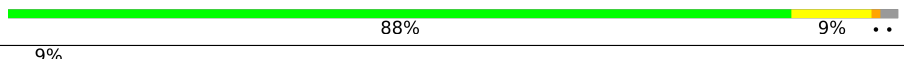
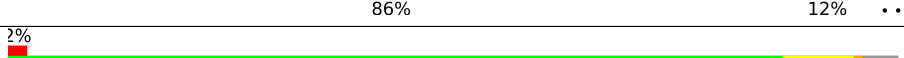
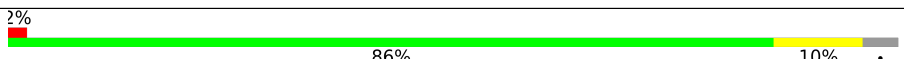
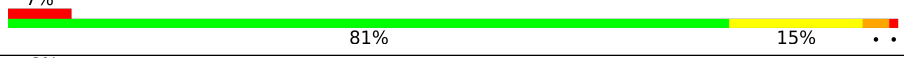

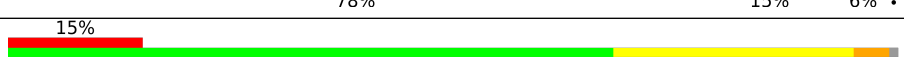

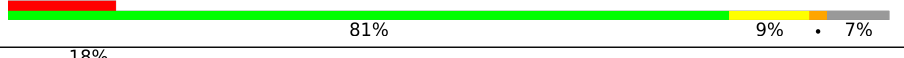
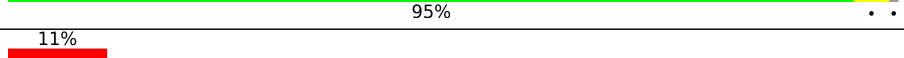
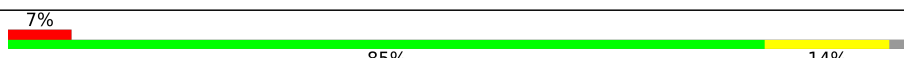


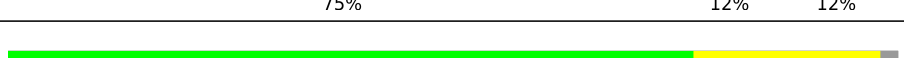
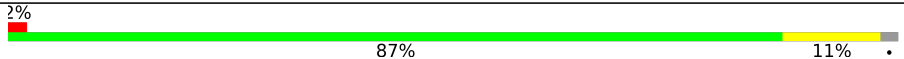

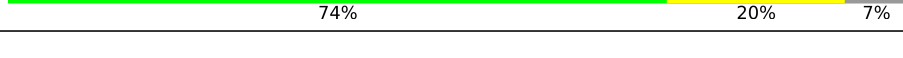
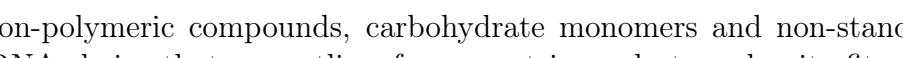

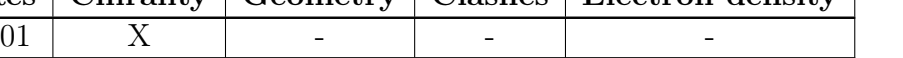
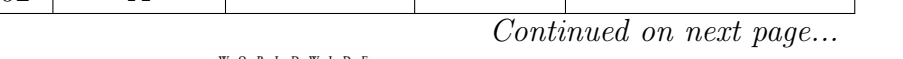
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	<div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	N	514	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>
2	B	227	<div> <div>81%</div> <div>18%</div> <div>.</div> </div>
2	O	227	<div> <div>3%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
3	C	261	<div> <div>88%</div> <div>10%</div> <div>..</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	601	X	-	-	-
14	HEA	A	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	601	X	-	-	-
14	HEA	N	602	X	-	-	-
18	PGV	A	607	X	-	-	-
19	EDO	S	103	-	-	X	-
23	DMU	C	301	-	-	-	X
23	DMU	W	101	-	-	-	X
24	PEK	T	103	-	-	-	X
26	CHD	W	102	X	-	-	-
27	PSC	E	201	-	-	-	X
29	SAC	I	101	-	-	-	X
29	SAC	V	101	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 32401 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
			4181	2791	646	703	41			
1	N	514	Total	C	N	O	S	0	21	0
			4188	2795	647	704	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	6	0
			1874	1216	289	350	19			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	289	348	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	8	0
			2174	1451	345	364	14			
3	P	259	Total	C	N	O	S	0	8	0
			2173	1451	344	363	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	6	0
			1249	814	206	224	5			
4	Q	144	Total	C	N	O	S	0	1	0
			1203	782	197	219	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	1	0
			863	550	148	163	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	5	0
			789	489	142	152	6			
6	S	98	Total	C	N	O	S	0	1	0
			755	468	135	147	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 686	C 440	N 130	O 114	P 1	S 1	0	1	0
7	T	84	Total 706	C 454	N 133	O 117	P 1	S 1	0	3	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	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			
9	V	72	Total	C	N	O	S	0	1	0
			600	390	107	98	5			

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

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

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

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

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

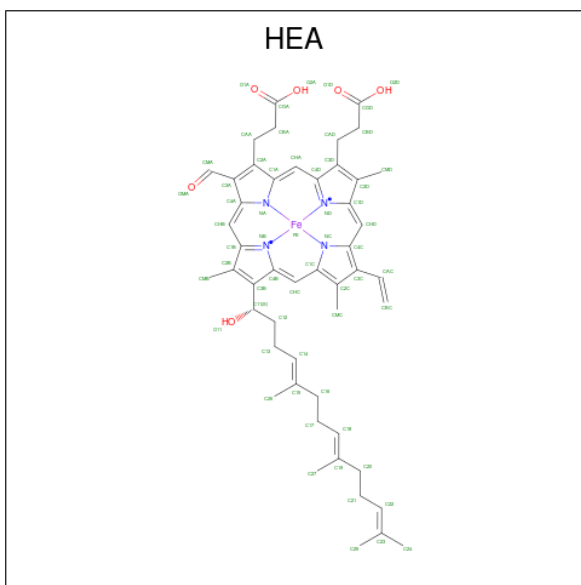
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

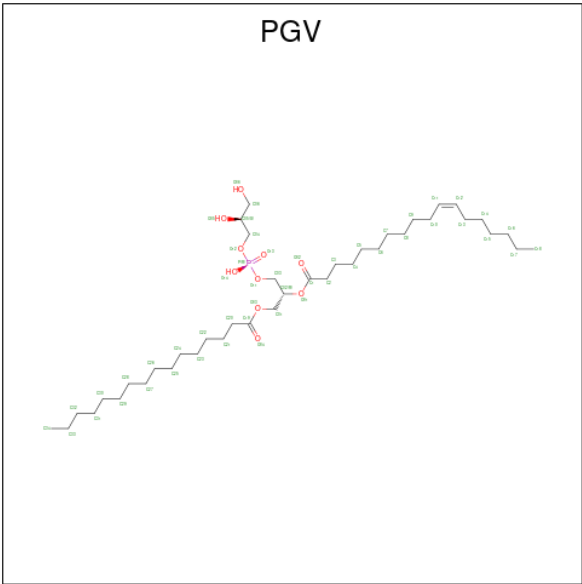
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

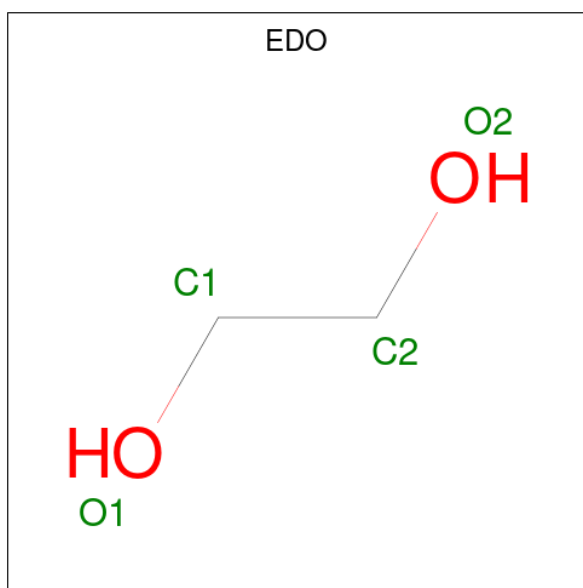
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P) (labeled as "Ligand of Interest" by depositor).



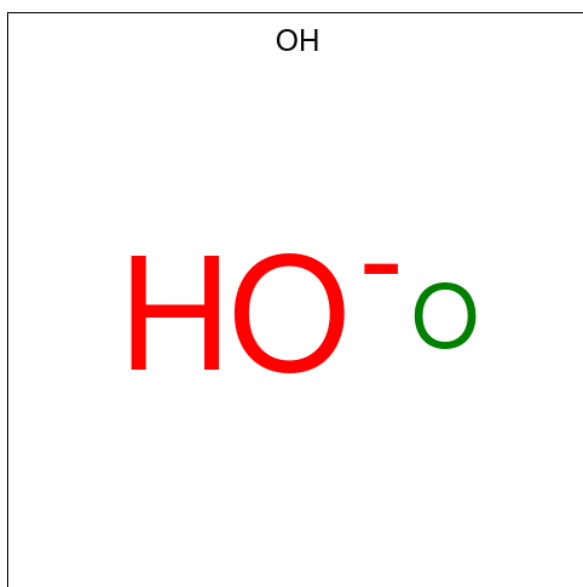
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0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

- Molecule 19 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



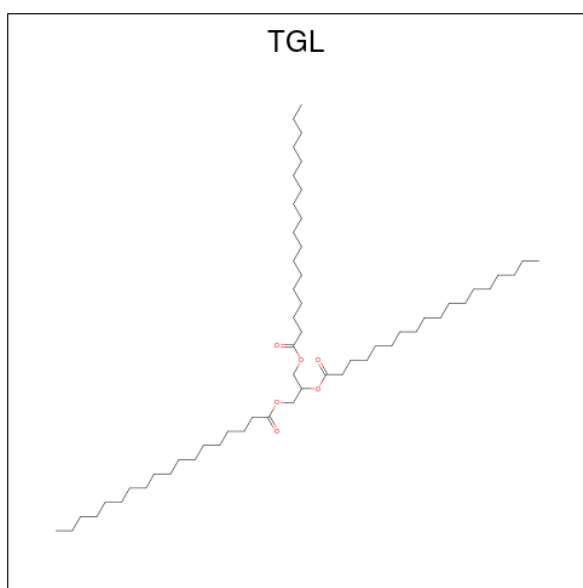
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			4	2	2		
19	A	1	Total	C	O	0	0
			4	2	2		
19	C	1	Total	C	O	0	0
			4	2	2		
19	G	1	Total	C	O	0	0
			4	2	2		
19	N	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	T	1	Total	C	O	0	0
			4	2	2		

- Molecule 20 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



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

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



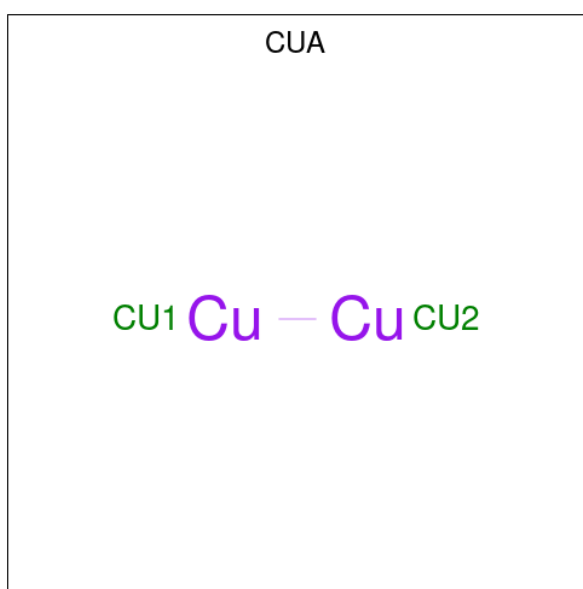
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		

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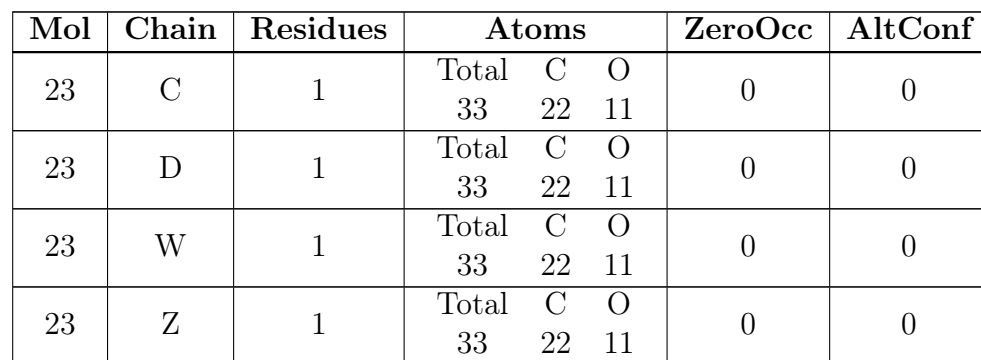
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).

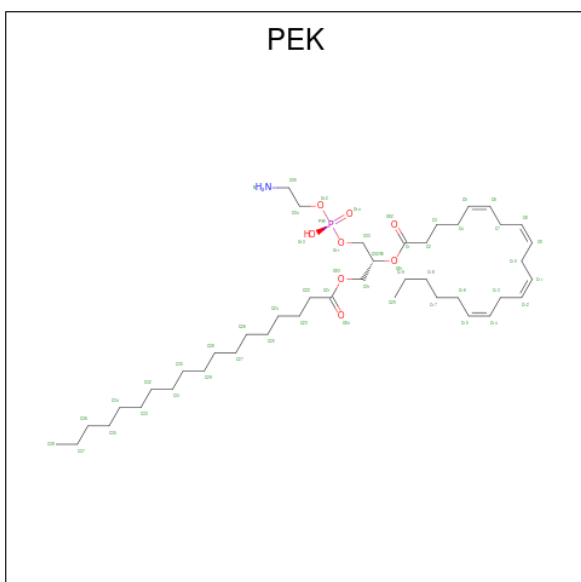


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	B	1	Total	Cu	0	0
			2	2		
22	O	1	Total	Cu	0	0
			2	2		

- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).

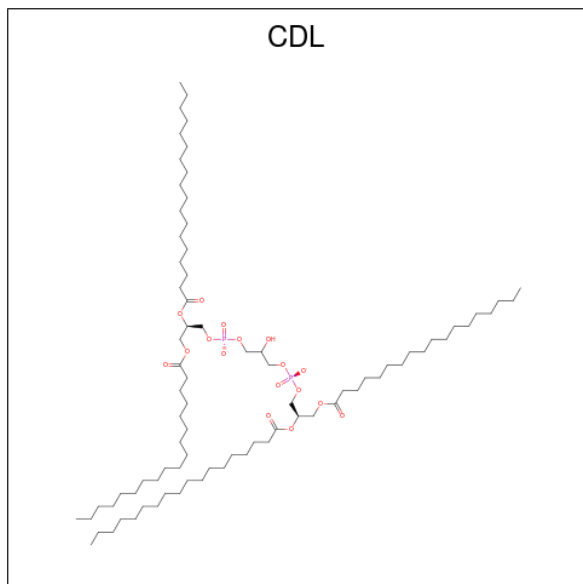


- Molecule 24 is (1S)-2-[[[2-AMINOETHOXY](HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



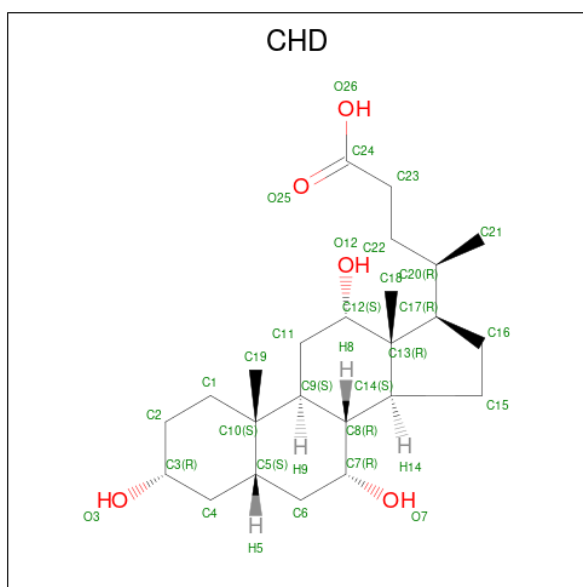
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



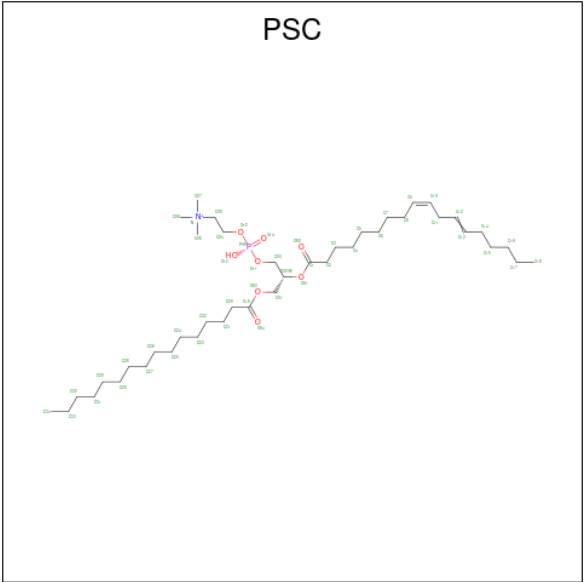
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	G	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 27 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 (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P) (labeled as "Ligand of Interest" by depositor).

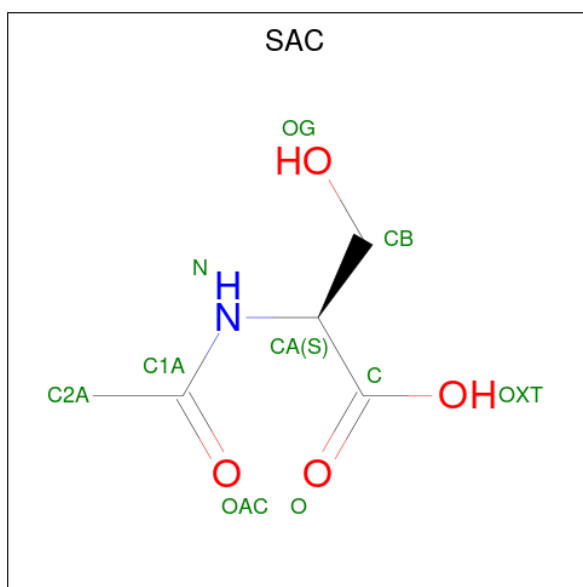


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
27	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 is N-ACETYL-SERINE (three-letter code: SAC) (formula: C₅H₉NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	I	1	Total	C	N	O	0	0
			9	5	1	3		
29	V	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	130	Total	O	0	0
			130	130		
30	B	88	Total	O	0	0
			88	88		
30	C	54	Total	O	0	0
			54	54		
30	D	53	Total	O	0	0
			53	53		
30	E	35	Total	O	0	0
			35	35		
30	F	39	Total	O	0	0
			39	39		
30	G	31	Total	O	0	0
			31	31		
30	H	22	Total	O	0	0
			22	22		
30	I	19	Total	O	0	0
			19	19		
30	J	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	13	Total 13	O 13	0	0
30	L	14	Total 14	O 14	0	0
30	M	14	Total 14	O 14	0	0
30	N	114	Total 114	O 114	0	0
30	O	64	Total 64	O 64	0	0
30	P	54	Total 54	O 54	0	0
30	Q	16	Total 16	O 16	0	0
30	R	19	Total 19	O 19	0	0
30	S	41	Total 41	O 41	0	0
30	T	30	Total 30	O 30	0	0
30	U	18	Total 18	O 18	0	0
30	V	9	Total 9	O 9	0	0
30	W	10	Total 10	O 10	0	0
30	X	1	Total 1	O 1	0	0
30	Y	11	Total 11	O 11	0	0
30	Z	7	Total 7	O 7	0	0

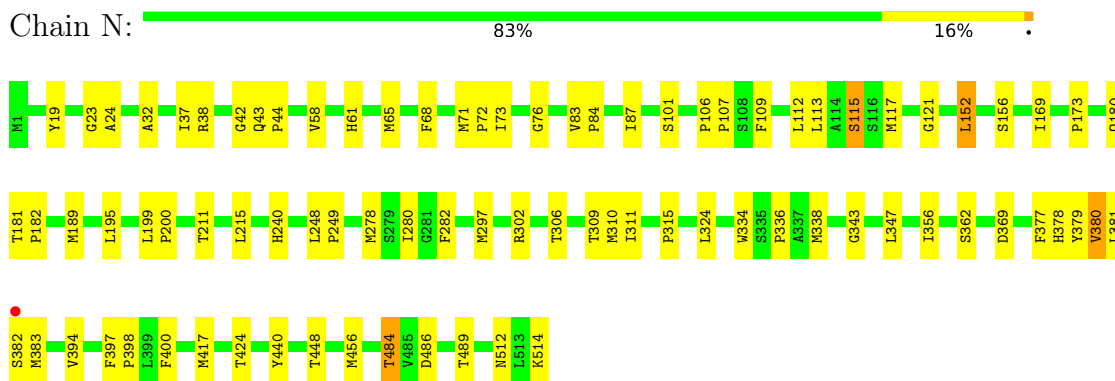
3 Residue-property plots [i](#)

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.

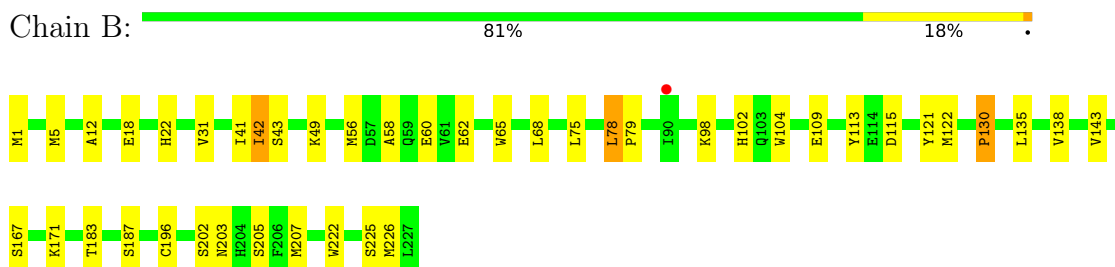
• Molecule 1: Cytochrome c oxidase subunit 1



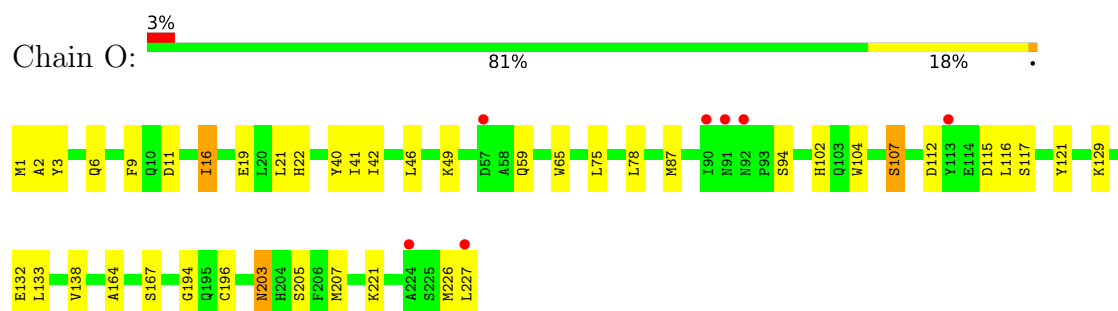
• Molecule 1: Cytochrome c oxidase subunit 1



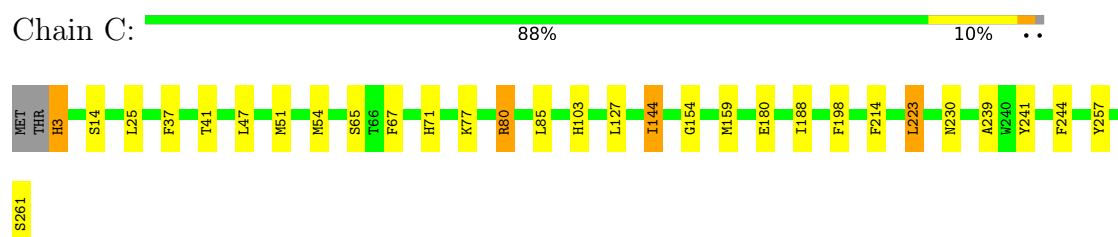
• Molecule 2: Cytochrome c oxidase subunit 2



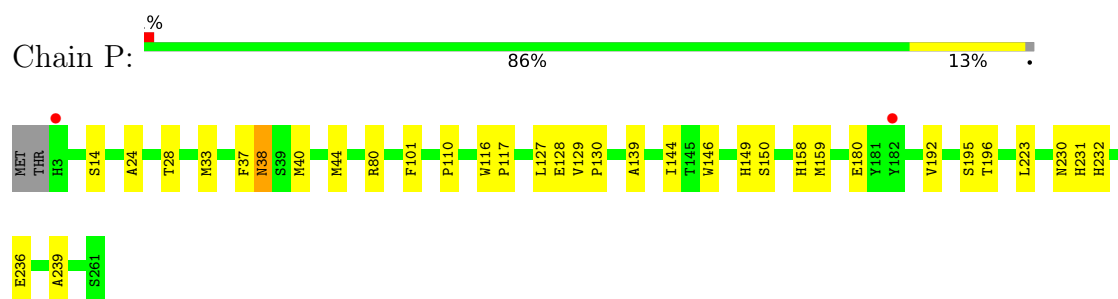
- Molecule 2: Cytochrome c oxidase subunit 2



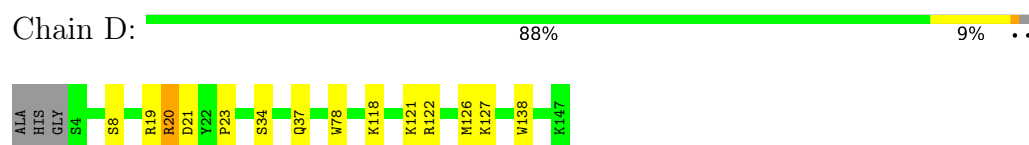
- Molecule 3: Cytochrome c oxidase subunit 3



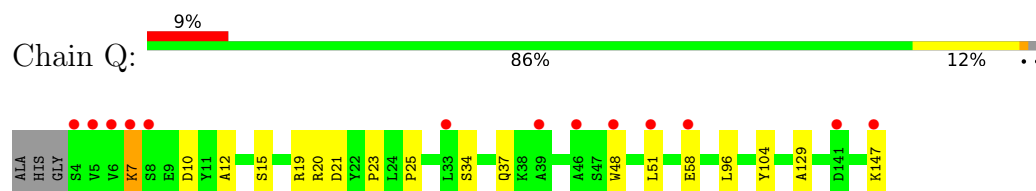
- Molecule 3: Cytochrome c oxidase subunit 3



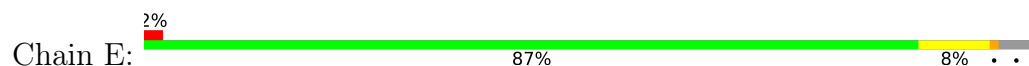
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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

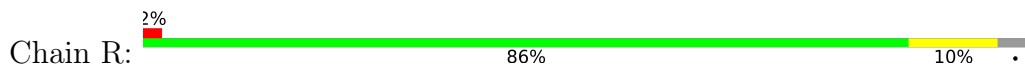


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

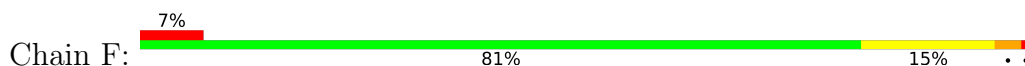




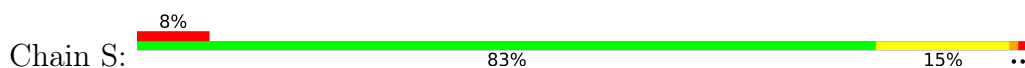
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



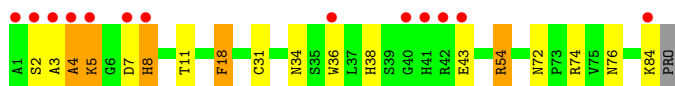
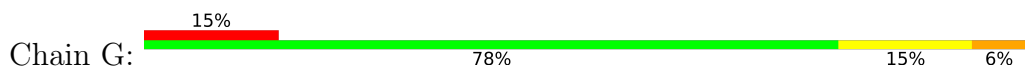
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



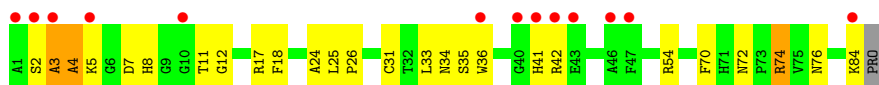
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



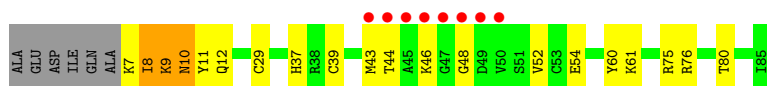
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



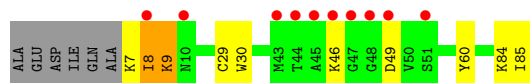
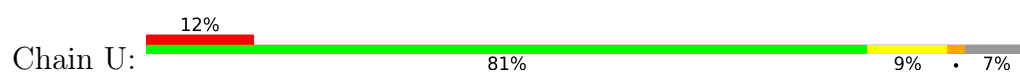
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



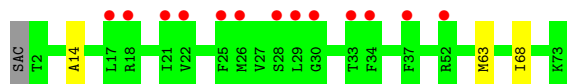
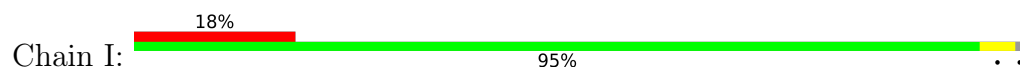
- Molecule 8: Cytochrome c oxidase subunit 6B1



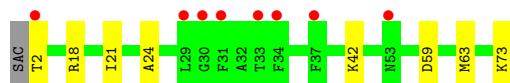
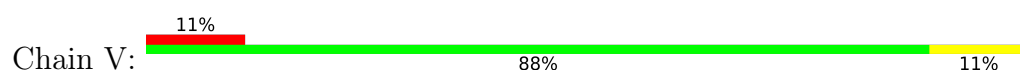
- Molecule 8: Cytochrome c oxidase subunit 6B1



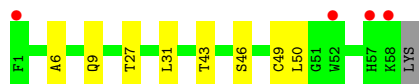
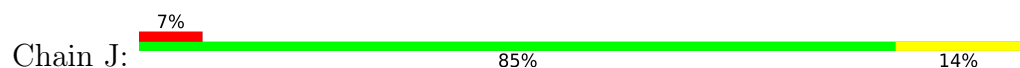
- Molecule 9: Cytochrome c oxidase subunit 6C



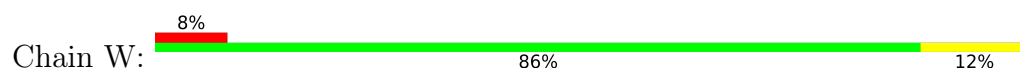
- Molecule 9: Cytochrome c oxidase subunit 6C



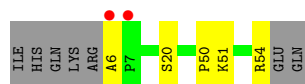
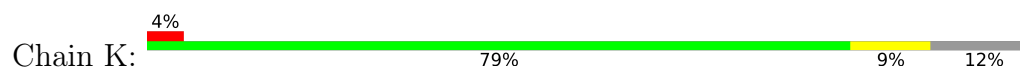
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



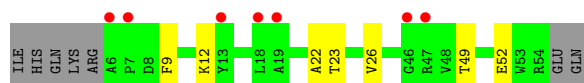
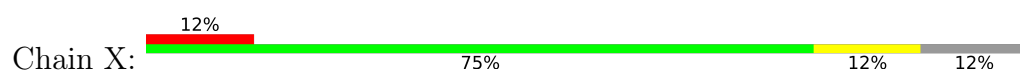
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial




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



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




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

Chain L:  77% 21% .



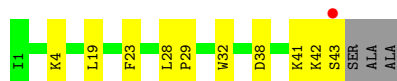
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:  2% 87% 11% .




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

Chain M:  2% 72% 22% 7%



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

Chain Z:  7% 74% 20% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	178.04Å 182.63Å 205.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.30 – 2.45 39.27 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.30-2.45) 99.9 (39.27-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.206 , 0.253 0.215 , 0.259	Depositor DCC
R_{free} test set	12054 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32401	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 4.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.67	0/4311	0.79	2/5884 (0.0%)
1	N	0.68	0/4318	0.77	1/5893 (0.0%)
2	B	0.70	0/1912	0.85	0/2603
2	O	0.68	0/1908	0.83	0/2599
3	C	0.65	0/2261	0.76	1/3090 (0.0%)
3	P	0.65	0/2260	0.77	0/3088
4	D	0.69	0/1284	0.80	0/1730
4	Q	0.67	0/1237	0.82	0/1668
5	E	0.68	0/882	0.78	0/1196
5	R	0.66	0/871	0.77	0/1182
6	F	0.73	0/806	0.90	0/1093
6	S	0.72	0/772	0.86	0/1048
7	G	0.66	0/702	0.82	0/953
7	T	0.65	0/724	0.83	0/984
8	H	0.66	0/682	0.85	0/921
8	U	0.69	0/682	0.83	0/921
9	I	0.67	0/605	0.83	0/802
9	V	0.67	0/613	0.81	0/812
10	J	0.67	0/471	0.79	0/636
10	W	0.68	0/471	0.76	0/636
11	K	0.68	0/405	0.80	0/556
11	X	0.67	0/405	0.76	0/556
12	L	0.62	0/393	0.81	0/526
12	Y	0.64	0/393	0.75	0/526
13	M	0.66	0/345	0.77	0/470
13	Z	0.66	0/345	0.78	0/470
All	All	0.67	0/30058	0.80	4/40843 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	ASN	CB-CA-C	-5.92	98.55	110.40
1	N	512	ASN	CB-CA-C	-5.73	98.93	110.40
3	C	80	ARG	CG-CD-NE	-5.58	100.08	111.80
1	A	439	ARG	CB-CA-C	5.54	121.48	110.40

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	4181	0	4161	69	0
1	N	4188	0	4166	76	0
2	B	1874	0	1869	22	0
2	O	1870	0	1867	33	0
3	C	2174	0	2082	23	0
3	P	2173	0	2083	25	0
4	D	1249	0	1242	12	0
4	Q	1203	0	1191	13	0
5	E	863	0	857	8	0
5	R	852	0	845	5	0
6	F	789	0	769	14	0
6	S	755	0	734	14	0
7	G	686	0	651	11	0
7	T	706	0	664	18	0
8	H	662	0	623	14	0
8	U	662	0	623	4	0
9	I	592	0	604	2	0
9	V	600	0	612	6	0
10	J	460	0	459	5	0
10	W	460	0	459	3	0
11	K	391	0	374	4	0
11	X	391	0	374	2	0
12	L	380	0	380	8	0
12	Y	380	0	380	3	0
13	M	335	0	352	7	0
13	Z	335	0	352	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	120	0	108	11	0
14	N	120	0	108	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	N	1	0	0	0	0
18	A	102	0	152	5	0
18	C	102	0	152	0	0
18	P	153	0	228	6	0
18	Z	51	0	76	2	0
19	A	8	0	12	0	0
19	C	4	0	6	1	0
19	G	4	0	6	1	0
19	N	4	0	6	0	0
19	S	8	0	12	5	0
19	T	4	0	6	0	0
20	A	1	0	0	1	0
20	N	1	0	0	1	0
21	B	63	0	110	0	0
21	D	63	0	110	4	0
21	L	63	0	110	4	0
21	N	63	0	110	0	0
21	Q	63	0	110	0	0
21	Y	63	0	110	2	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	C	33	0	42	6	0
23	D	33	0	42	0	0
23	W	33	0	42	7	0
23	Z	33	0	42	0	0
24	C	106	0	154	1	0
24	G	53	0	77	3	0
24	T	159	0	231	6	0
25	C	100	0	156	2	0
25	G	100	0	156	4	0
25	P	100	0	156	2	0
25	T	100	0	156	7	0
26	C	58	0	78	2	0
26	G	29	0	39	0	0
26	J	29	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	P	58	0	78	1	0
26	T	29	0	39	1	0
26	W	29	0	39	1	0
27	E	52	0	80	6	0
27	O	52	0	80	2	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	I	9	0	8	0	0
29	V	9	0	8	1	0
30	A	130	0	0	4	0
30	B	88	0	0	0	0
30	C	54	0	0	2	0
30	D	53	0	0	1	0
30	E	35	0	0	2	0
30	F	39	0	0	1	0
30	G	31	0	0	3	0
30	H	22	0	0	2	0
30	I	19	0	0	2	0
30	J	8	0	0	0	0
30	K	13	0	0	1	0
30	L	14	0	0	2	0
30	M	14	0	0	2	0
30	N	114	0	0	3	0
30	O	64	0	0	2	0
30	P	54	0	0	4	0
30	Q	16	0	0	0	0
30	R	19	0	0	0	0
30	S	41	0	0	1	0
30	T	30	0	0	5	0
30	U	18	0	0	0	0
30	V	9	0	0	0	0
30	W	10	0	0	0	0
30	X	1	0	0	0	0
30	Y	11	0	0	0	0
30	Z	7	0	0	0	0
All	All	32401	0	32047	404	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 6.

The worst 5 of 404 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:297[B]:MET:SD	1:N:302[B]:ARG:HG2	1.77	1.22
20:A:610:OH:O	30:A:701:HOH:O	1.67	1.12
3:P:40[B]:MET:O	3:P:44[B]:MET:HG3	1.57	1.03
1:A:51:ASP:OD2	1:A:441:SER:OG	1.78	0.99
8:H:9:LYS:HB3	30:H:121:HOH:O	1.65	0.95

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%)	507 (95%)	24 (4%)	1 (0%)	47	57
1	N	533/514 (104%)	514 (96%)	19 (4%)	0	100	100
2	B	231/227 (102%)	218 (94%)	12 (5%)	1 (0%)	34	41
2	O	230/227 (101%)	213 (93%)	16 (7%)	1 (0%)	34	41
3	C	265/261 (102%)	258 (97%)	7 (3%)	0	100	100
3	P	265/261 (102%)	256 (97%)	7 (3%)	2 (1%)	19	22
4	D	148/147 (101%)	142 (96%)	6 (4%)	0	100	100
4	Q	143/147 (97%)	132 (92%)	11 (8%)	0	100	100
5	E	104/109 (95%)	103 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	101/98 (103%)	92 (91%)	4 (4%)	5 (5%)	2	0
6	S	97/98 (99%)	88 (91%)	8 (8%)	1 (1%)	15	16
7	G	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	2	1
7	T	84/85 (99%)	71 (84%)	9 (11%)	4 (5%)	2	1
8	H	77/85 (91%)	66 (86%)	9 (12%)	2 (3%)	5	3
8	U	77/85 (91%)	69 (90%)	7 (9%)	1 (1%)	12	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	70/73 (96%)	67 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
11	K	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
11	X	48/56 (86%)	45 (94%)	2 (4%)	1 (2%)	7	5
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6	3
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3591/3614 (99%)	3393 (94%)	174 (5%)	24 (1%)	22	25

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
6	F	96	LEU
6	F	97	ALA
7	G	4	ALA
7	G	8	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	444/426 (104%)	435 (98%)	9 (2%)	55	67
1	N	445/426 (104%)	432 (97%)	13 (3%)	42	53
2	B	216/210 (103%)	202 (94%)	14 (6%)	17	21
2	O	215/210 (102%)	202 (94%)	13 (6%)	19	24
3	C	232/226 (103%)	220 (95%)	12 (5%)	23	30
3	P	232/226 (103%)	225 (97%)	7 (3%)	41	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	134/129 (104%)	131 (98%)	3 (2%)	52	64
4	Q	129/129 (100%)	125 (97%)	4 (3%)	40	52
5	E	93/95 (98%)	92 (99%)	1 (1%)	73	82
5	R	92/95 (97%)	90 (98%)	2 (2%)	52	64
6	F	86/81 (106%)	83 (96%)	3 (4%)	36	47
6	S	82/81 (101%)	78 (95%)	4 (5%)	25	32
7	G	68/68 (100%)	59 (87%)	9 (13%)	4	3
7	T	70/68 (103%)	62 (89%)	8 (11%)	5	5
8	H	71/75 (95%)	64 (90%)	7 (10%)	8	7
8	U	71/75 (95%)	64 (90%)	7 (10%)	8	7
9	I	57/57 (100%)	57 (100%)	0	100	100
9	V	58/57 (102%)	56 (97%)	2 (3%)	37	48
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	67
10	W	49/50 (98%)	46 (94%)	3 (6%)	18	24
11	K	40/46 (87%)	39 (98%)	1 (2%)	47	60
11	X	40/46 (87%)	37 (92%)	3 (8%)	13	16
12	L	39/40 (98%)	37 (95%)	2 (5%)	24	31
12	Y	39/40 (98%)	38 (97%)	1 (3%)	46	58
13	M	37/38 (97%)	36 (97%)	1 (3%)	44	57
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	13
All	All	3125/3082 (101%)	2992 (96%)	133 (4%)	31	38

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	U	8	ILE
8	U	60	TYR
13	Z	13	LYS
7	G	54	ARG
7	G	36	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	91	ASN
6	S	80	GLN
2	O	92	ASN
4	Q	37	GLN
6	S	95	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	A	1	1	8,9,10	0.53	0	7,9,11	0.82	0
7	TPO	T	11	7	8,10,11	0.78	0	10,14,16	1.01	0
7	TPO	G	11	7	8,10,11	1.28	1 (12%)	10,14,16	0.85	0
2	FME	O	1	2	8,9,10	0.50	0	7,9,11	0.79	0
1	FME	N	1	1	8,9,10	0.45	0	7,9,11	0.84	0
2	FME	B	1	2	8,9,10	0.56	0	7,9,11	1.37	2 (28%)

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	A	1	1	-	4/7/9/11	-
7	TPO	T	11	7	-	4/9/11/13	-
7	TPO	G	11	7	-	6/9/11/13	-
2	FME	O	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	B	1	2	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	3.15	1.65	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-2.70	118.68	122.82
2	B	1	FME	C-CA-N	2.15	113.62	109.73

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 8 are monoatomic and 2 are modelled with single atom - leaving 54 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	$\# Z > 2$
19	EDO	G	104	-	3,3,3	0.16	0	2,2,2	0.12	0
25	CDL	G	101	-	99,99,99	0.40	0	105,111,111	0.51	1 (0%)
23	DMU	C	301	-	34,34,34	1.62	6 (17%)	45,45,45	1.49	7 (15%)
26	CHD	C	305	-	32,32,32	0.57	0	51,51,51	0.80	0
21	TGL	Y	101	-	62,62,62	0.33	0	65,65,65	0.30	0
23	DMU	D	202	-	34,34,34	1.00	1 (2%)	45,45,45	1.51	5 (11%)
26	CHD	T	101	-	32,32,32	0.57	0	51,51,51	0.93	0
25	CDL	T	105	-	99,99,99	0.33	0	105,111,111	0.41	0
19	EDO	S	103	-	3,3,3	0.18	0	2,2,2	0.15	0
26	CHD	J	101	-	32,32,32	0.71	0	51,51,51	1.10	3 (5%)
24	PEK	C	302	-	52,52,52	0.29	0	55,57,57	0.60	0
21	TGL	B	301	-	62,62,62	0.36	0	65,65,65	0.46	1 (1%)
24	PEK	G	102	-	52,52,52	0.33	0	55,57,57	0.46	0
14	HEA	A	601	1	57,67,67	2.15	17 (29%)	61,103,103	2.47	22 (36%)
18	PGV	P	303	-	50,50,50	0.31	0	53,56,56	0.49	0
26	CHD	P	306	-	32,32,32	0.64	0	51,51,51	1.03	5 (9%)
24	PEK	T	103	-	52,52,52	0.36	0	55,57,57	0.50	0
22	CUA	B	302	2	0,1,1	-	-	-	-	-
18	PGV	A	606	-	50,50,50	0.38	0	53,56,56	0.51	0
25	CDL	P	304	-	99,99,99	0.37	0	105,111,111	0.45	1 (0%)
19	EDO	C	309	-	3,3,3	0.13	0	2,2,2	0.16	0
19	EDO	N	607	-	3,3,3	0.17	0	2,2,2	0.28	0
19	EDO	T	106	-	3,3,3	0.35	0	2,2,2	0.40	0
18	PGV	C	308	-	50,50,50	0.47	0	53,56,56	0.52	0
18	PGV	C	303	-	50,50,50	0.35	0	53,56,56	0.62	1 (1%)
21	TGL	N	606	-	62,62,62	0.34	0	65,65,65	0.42	0
22	CUA	O	301	2	0,1,1	-	-	-	-	-
27	PSC	E	201	-	51,51,51	0.33	0	57,59,59	0.42	0
14	HEA	N	602	1	57,67,67	1.96	13 (22%)	61,103,103	2.48	24 (39%)
21	TGL	L	101	-	62,62,62	0.36	0	65,65,65	0.47	0
21	TGL	Q	201	-	62,62,62	0.38	0	65,65,65	0.49	2 (3%)
14	HEA	A	602	1	57,67,67	1.95	16 (28%)	61,103,103	2.56	26 (42%)
18	PGV	A	607	-	50,50,50	0.36	0	53,56,56	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	PEK	T	102	-	52,52,52	0.27	0	55,57,57	0.62	2 (3%)
25	CDL	C	304	-	99,99,99	0.38	0	105,111,111	0.39	0
19	EDO	S	102	-	3,3,3	0.18	0	2,2,2	0.14	0
18	PGV	Z	101	-	50,50,50	0.39	0	53,56,56	0.77	1 (1%)
27	PSC	O	302	-	51,51,51	0.34	0	57,59,59	0.50	1 (1%)
19	EDO	A	608	-	3,3,3	0.23	0	2,2,2	0.20	0
18	PGV	P	301	-	50,50,50	0.32	0	53,56,56	0.52	0
14	HEA	N	601	1	57,67,67	1.96	14 (24%)	61,103,103	2.31	22 (36%)
19	EDO	A	609	-	3,3,3	0.08	0	2,2,2	0.34	0
18	PGV	P	302	-	50,50,50	0.39	0	53,56,56	0.44	0
26	CHD	C	306	-	32,32,32	0.50	0	51,51,51	0.64	0
24	PEK	T	104	-	52,52,52	0.41	0	55,57,57	0.56	1 (1%)
26	CHD	W	102	-	32,32,32	0.67	0	51,51,51	0.85	2 (3%)
29	SAC	V	101	-	7,8,9	0.52	0	8,9,11	0.92	1 (12%)
29	SAC	I	101	-	7,8,9	0.53	0	8,9,11	1.21	1 (12%)
21	TGL	D	201	-	62,62,62	0.37	0	65,65,65	0.64	2 (3%)
23	DMU	W	101	-	34,34,34	2.02	9 (26%)	45,45,45	1.78	12 (26%)
26	CHD	P	305	-	32,32,32	0.61	0	51,51,51	0.75	0
26	CHD	G	103	-	32,32,32	0.58	0	51,51,51	0.73	0
24	PEK	C	307	-	52,52,52	0.43	0	55,57,57	0.49	0
23	DMU	Z	102	-	34,34,34	1.09	3 (8%)	45,45,45	1.14	3 (6%)

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
19	EDO	G	104	-	-	1/1/1/1	-
25	CDL	G	101	-	-	60/110/110/110	-
23	DMU	C	301	-	-	12/19/59/59	0/2/2/2
26	CHD	C	305	-	-	5/9/74/74	0/4/4/4
21	TGL	Y	101	-	-	37/65/65/65	-
23	DMU	D	202	-	-	10/19/59/59	0/2/2/2
26	CHD	T	101	-	-	2/9/74/74	0/4/4/4
25	CDL	T	105	-	-	56/110/110/110	-
19	EDO	S	103	-	-	0/1/1/1	-
26	CHD	J	101	-	-	4/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PEK	C	302	-	-	13/56/56/56	-
21	TGL	B	301	-	-	31/65/65/65	-
24	PEK	G	102	-	-	28/56/56/56	-
14	HEA	A	601	1	3/3/7/16	6/32/76/76	-
18	PGV	P	303	-	-	12/55/55/55	-
26	CHD	P	306	-	-	1/9/74/74	0/4/4/4
24	PEK	T	103	-	-	29/56/56/56	-
18	PGV	A	606	-	-	11/55/55/55	-
25	CDL	P	304	-	-	59/110/110/110	-
19	EDO	C	309	-	-	1/1/1/1	-
19	EDO	N	607	-	-	0/1/1/1	-
19	EDO	T	106	-	-	0/1/1/1	-
18	PGV	C	308	-	-	37/55/55/55	-
18	PGV	C	303	-	-	13/55/55/55	-
21	TGL	N	606	-	-	34/65/65/65	-
27	PSC	E	201	-	-	25/55/55/55	-
14	HEA	N	602	1	3/3/7/16	6/32/76/76	-
21	TGL	L	101	-	-	38/65/65/65	-
21	TGL	Q	201	-	-	33/65/65/65	-
18	PGV	A	607	-	1/1/5/7	34/55/55/55	-
14	HEA	A	602	1	3/3/7/16	4/32/76/76	-
24	PEK	T	102	-	-	17/56/56/56	-
25	CDL	C	304	-	-	69/110/110/110	-
19	EDO	S	102	-	-	0/1/1/1	-
18	PGV	Z	101	-	-	31/55/55/55	-
27	PSC	O	302	-	-	23/55/55/55	-
19	EDO	A	608	-	-	1/1/1/1	-
18	PGV	P	301	-	-	13/55/55/55	-
14	HEA	N	601	1	3/3/7/16	8/32/76/76	-
19	EDO	A	609	-	-	0/1/1/1	-
18	PGV	P	302	-	-	22/55/55/55	-
26	CHD	C	306	-	-	0/9/74/74	0/4/4/4
26	CHD	W	102	-	1/1/12/12	4/9/74/74	0/4/4/4
24	PEK	T	104	-	-	23/56/56/56	-
29	SAC	V	101	-	-	3/7/8/10	-
29	SAC	I	101	-	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	TGL	D	201	-	-	36/65/65/65	-
23	DMU	W	101	-	-	4/19/59/59	0/2/2/2
26	CHD	P	305	-	-	6/9/74/74	0/4/4/4
26	CHD	G	103	-	-	4/9/74/74	0/4/4/4
24	PEK	C	307	-	-	24/56/56/56	-
23	DMU	Z	102	-	-	5/19/59/59	0/2/2/2

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	101	DMU	O16-C6	6.96	1.52	1.40
23	C	301	DMU	O16-C6	6.15	1.50	1.40
14	N	601	HEA	C3B-C2B	5.57	1.47	1.34
14	A	601	HEA	C3D-C2D	5.40	1.48	1.36
14	A	601	HEA	CHD-C1D	5.20	1.48	1.35

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	C13-C12-C11	-7.67	102.82	114.35
14	N	602	HEA	C3D-C4D-ND	7.05	117.18	110.36
14	A	602	HEA	C2B-C1B-NB	6.64	117.83	109.88
23	D	202	DMU	C18-O16-C6	5.83	123.51	113.84
14	N	602	HEA	C3B-C4B-NB	5.81	116.73	109.84

5 of 14 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	601	HEA	NB
14	A	601	HEA	ND
14	A	601	HEA	NA
14	A	602	HEA	NB
14	A	602	HEA	ND

5 of 899 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601	HEA	C26-C15-C16-C17
14	A	602	HEA	C2D-C3D-CAD-CBD
14	N	602	HEA	C4D-C3D-CAD-CBD

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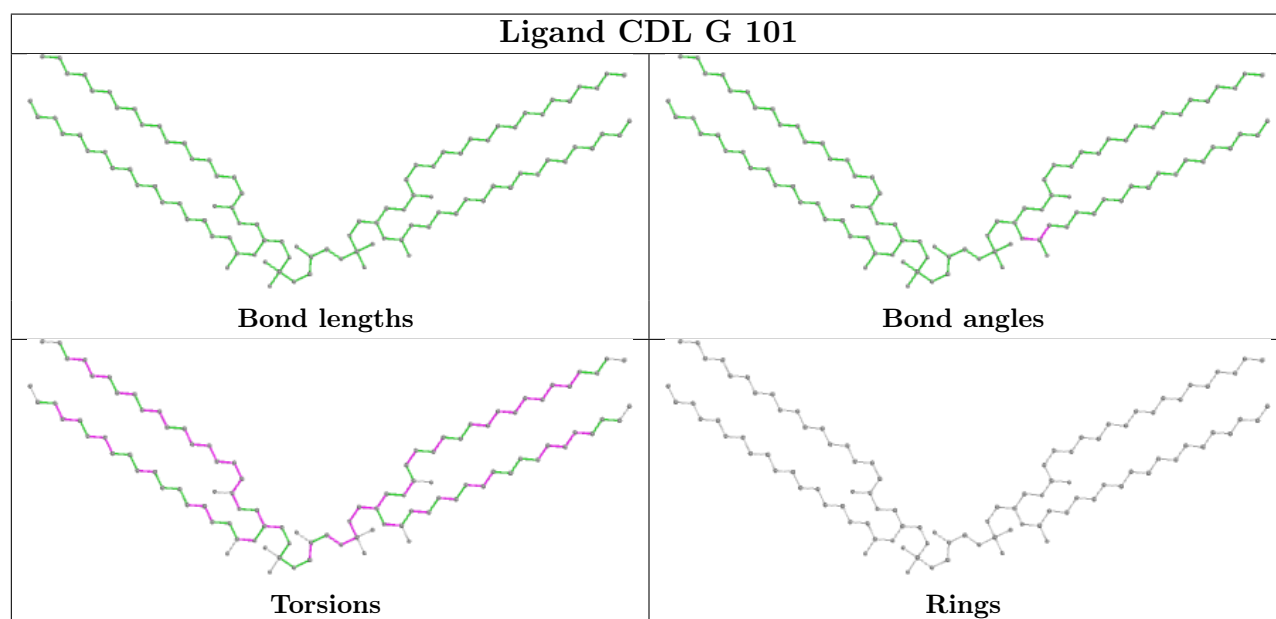
Mol	Chain	Res	Type	Atoms
18	A	607	PGV	C04-O12-P-O13
18	A	607	PGV	C04-O12-P-O14

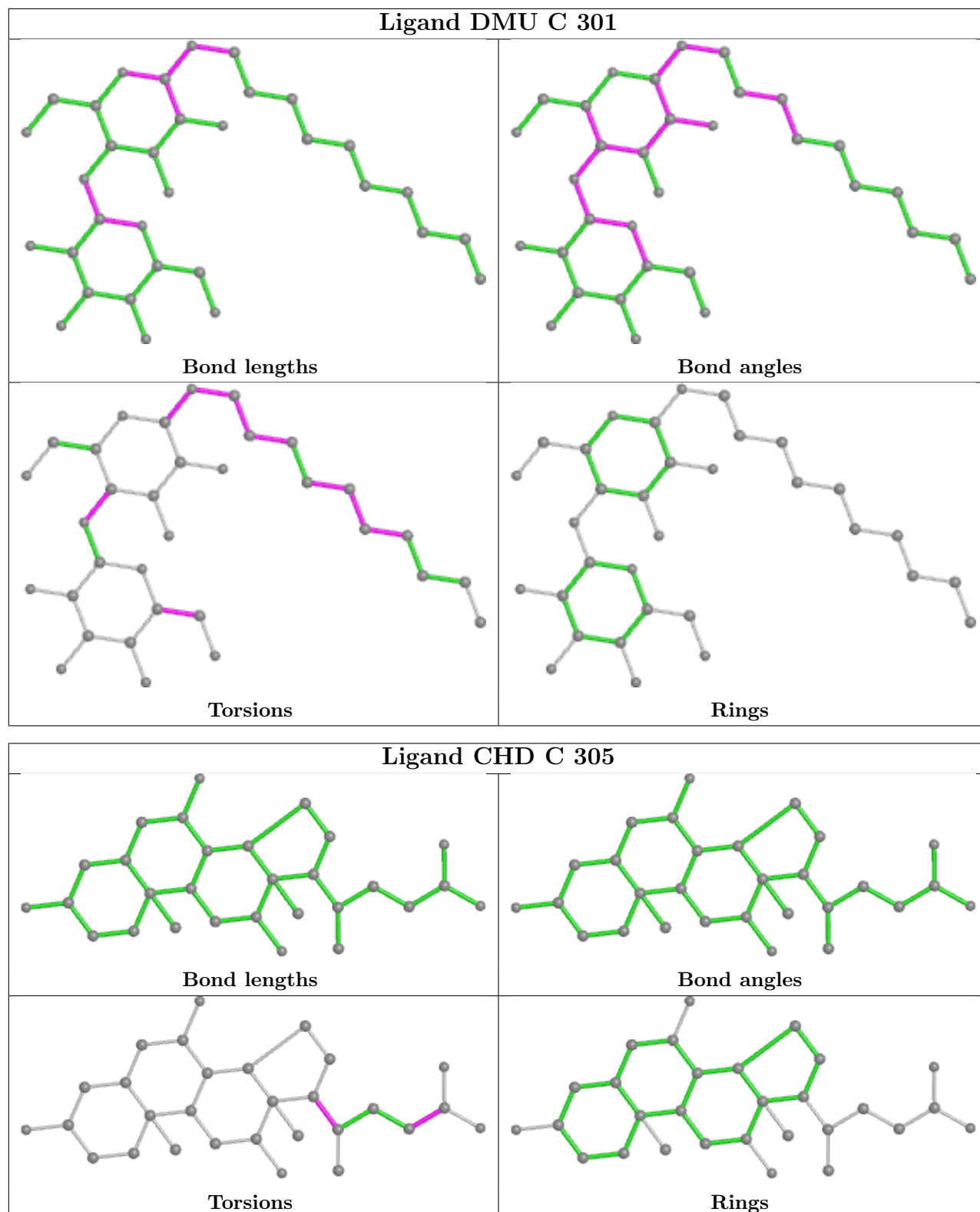
There are no ring outliers.

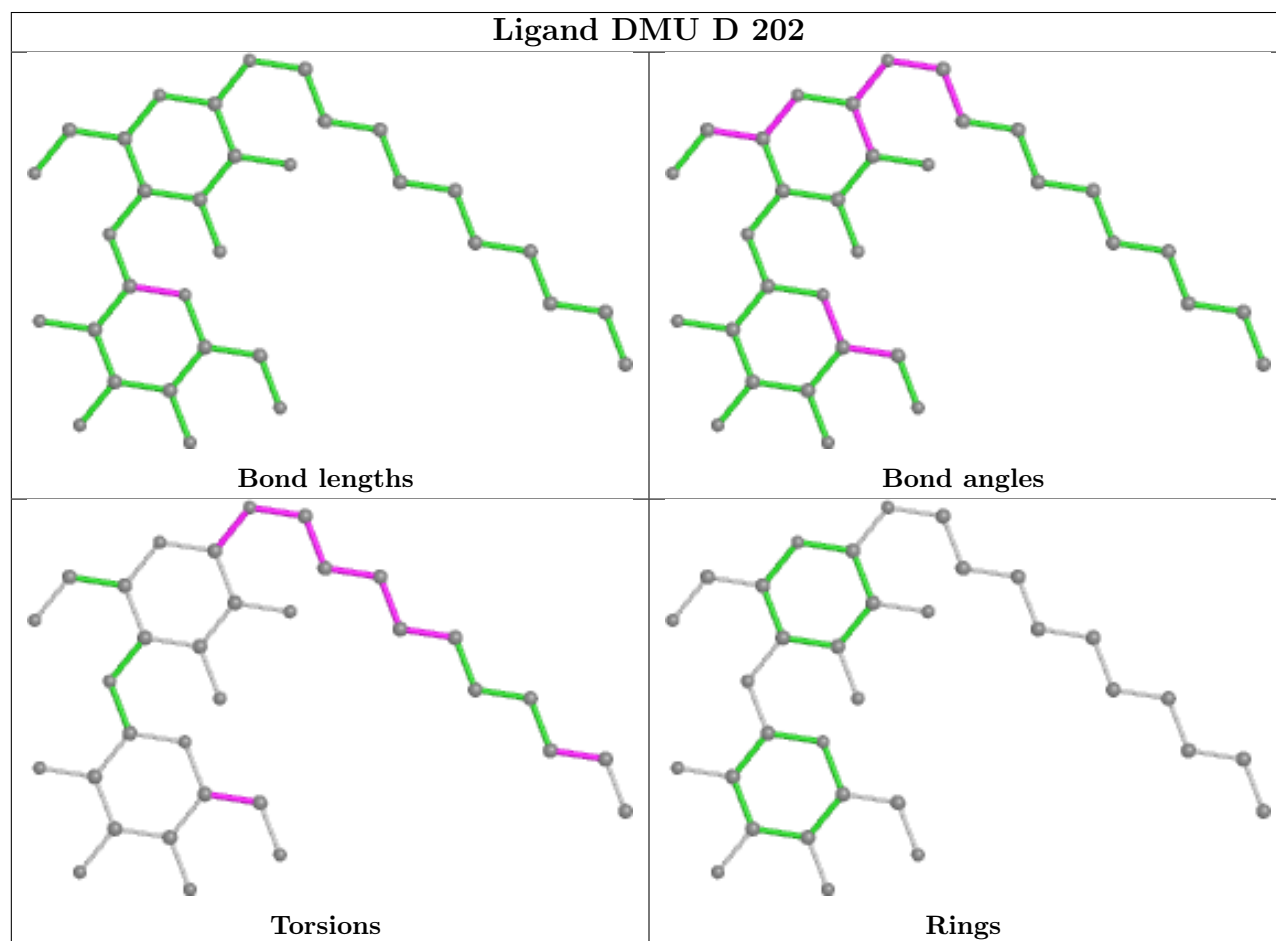
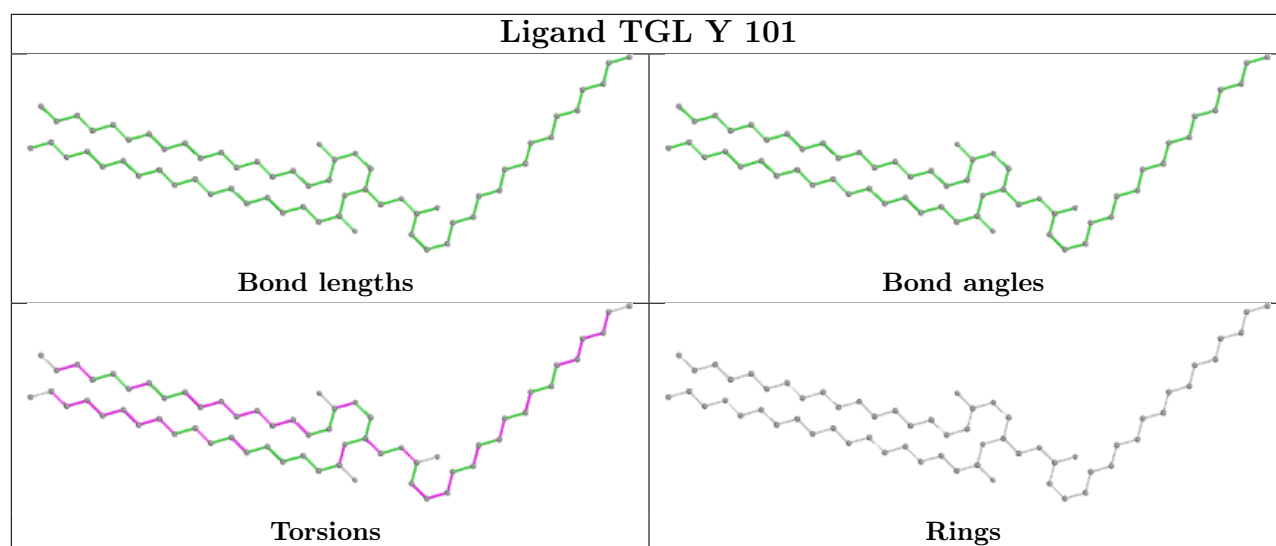
34 monomers are involved in 103 short contacts:

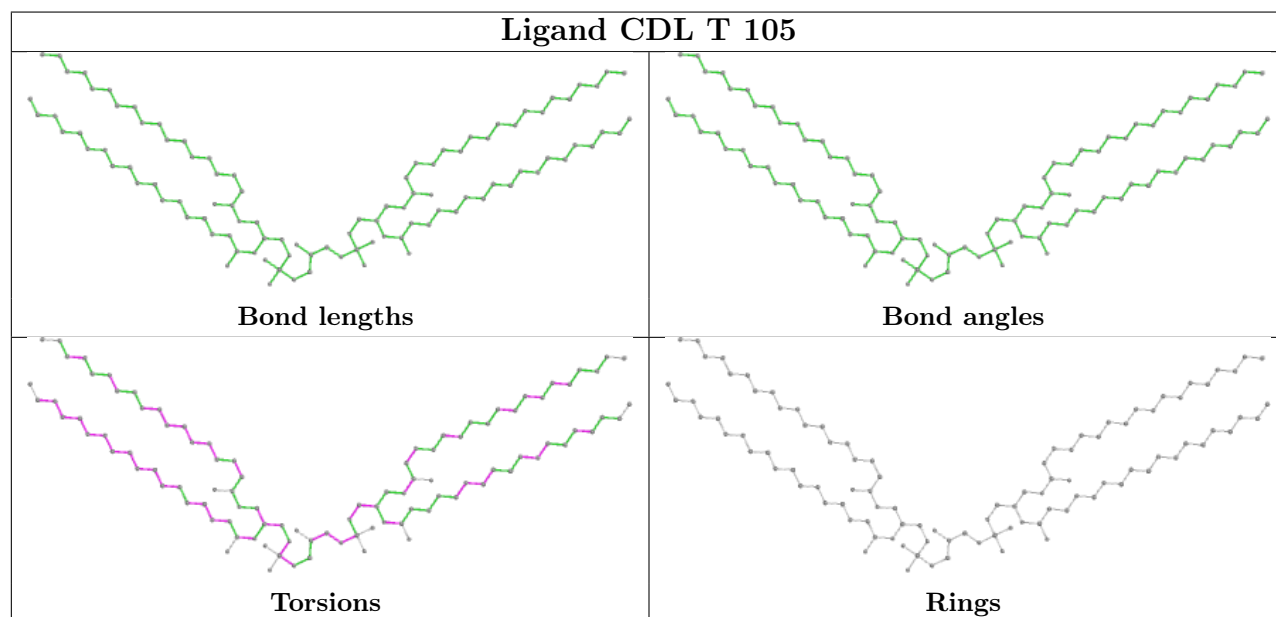
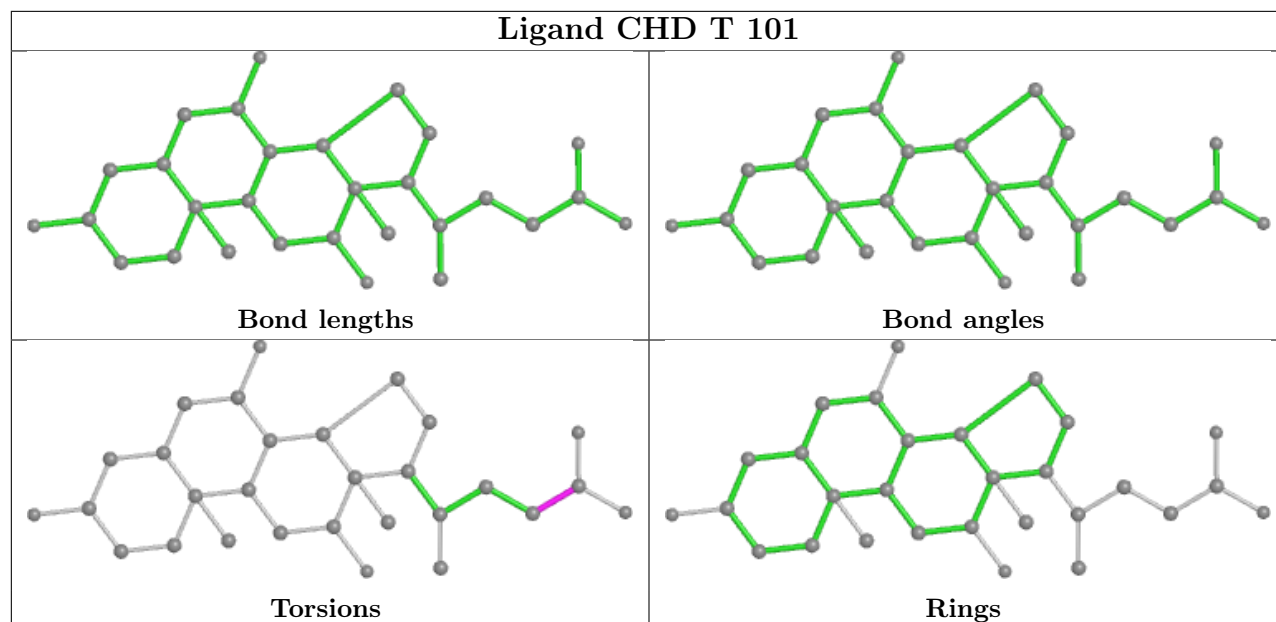
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	G	104	EDO	1	0
25	G	101	CDL	4	0
23	C	301	DMU	6	0
26	C	305	CHD	1	0
21	Y	101	TGL	2	0
26	T	101	CHD	1	0
25	T	105	CDL	7	0
19	S	103	EDO	4	0
24	C	302	PEK	1	0
24	G	102	PEK	3	0
14	A	601	HEA	5	0
18	P	303	PGV	1	0
25	P	304	CDL	2	0
19	C	309	EDO	1	0
27	E	201	PSC	6	0
14	N	602	HEA	8	0
21	L	101	TGL	4	0
14	A	602	HEA	6	0
18	A	607	PGV	5	0
24	T	102	PEK	4	0
25	C	304	CDL	2	0
19	S	102	EDO	1	0
18	Z	101	PGV	2	0
27	O	302	PSC	2	0
18	P	301	PGV	4	0
14	N	601	HEA	5	0
18	P	302	PGV	1	0
26	C	306	CHD	1	0
24	T	104	PEK	2	0
26	W	102	CHD	1	0
29	V	101	SAC	1	0
21	D	201	TGL	4	0
23	W	101	DMU	7	0
26	P	305	CHD	1	0

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

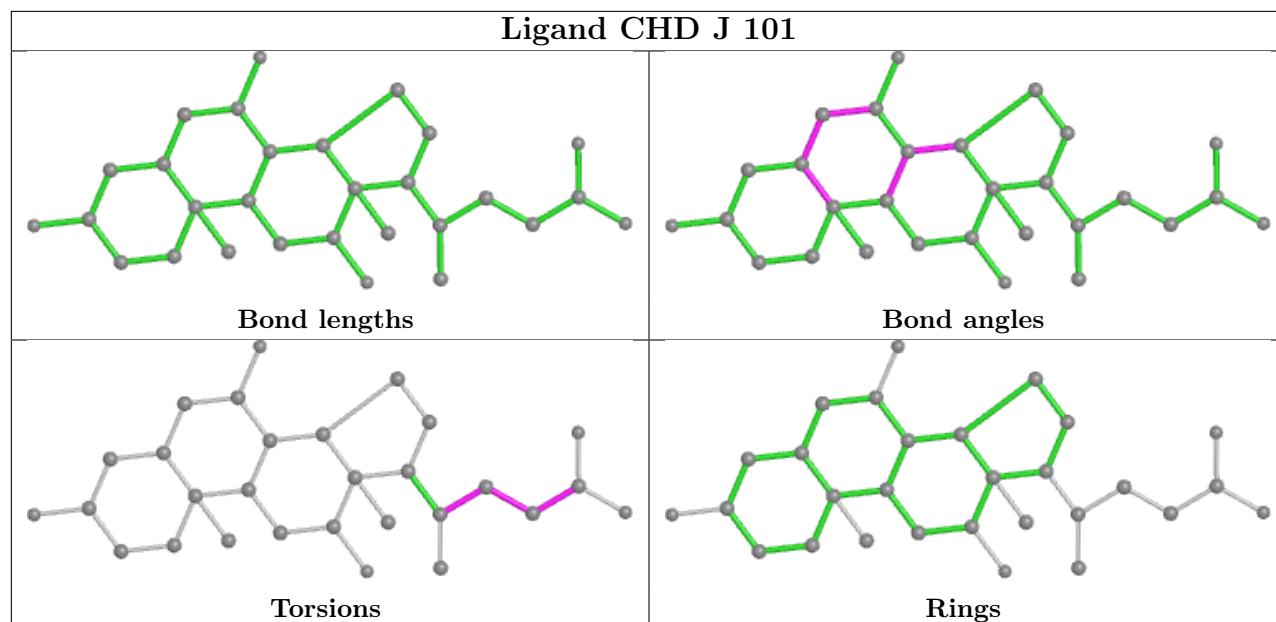




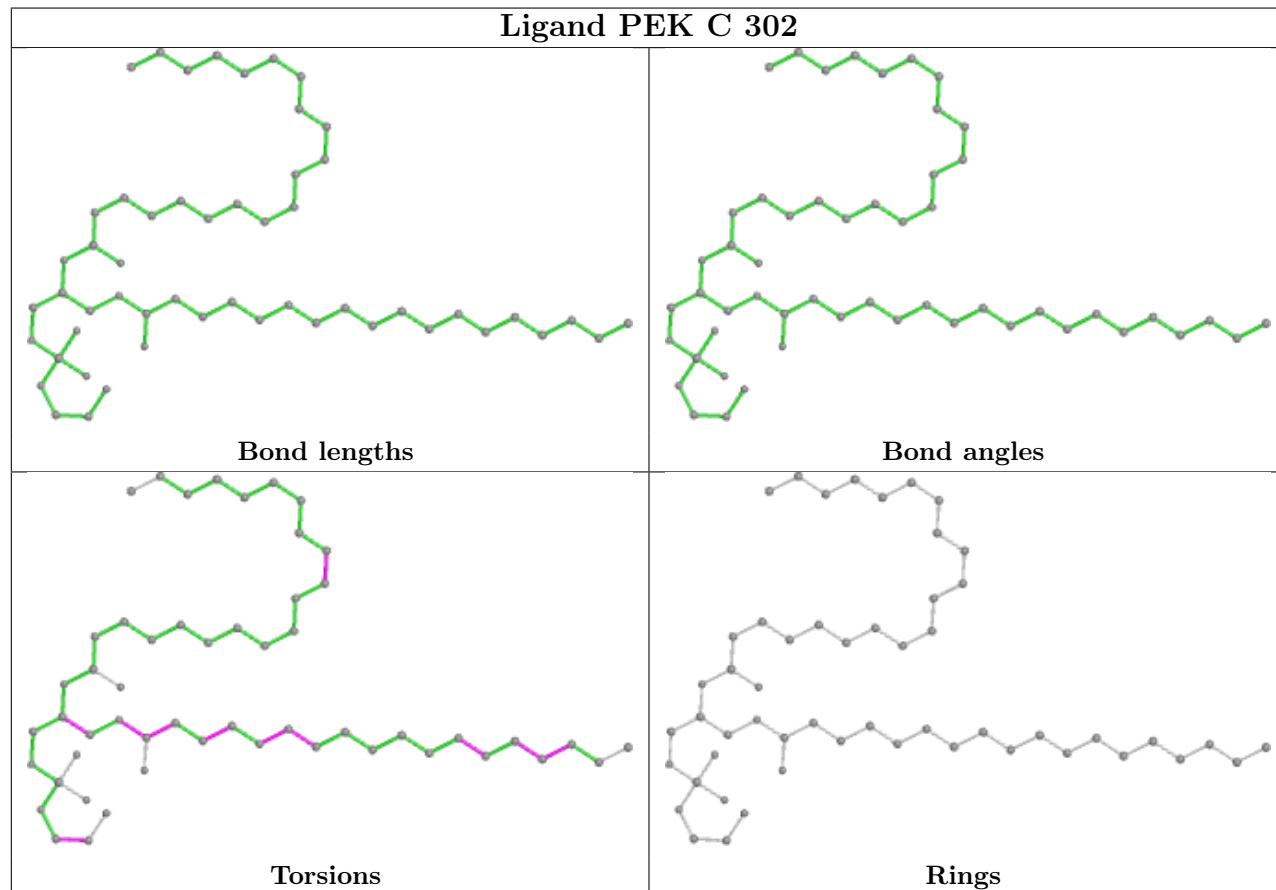


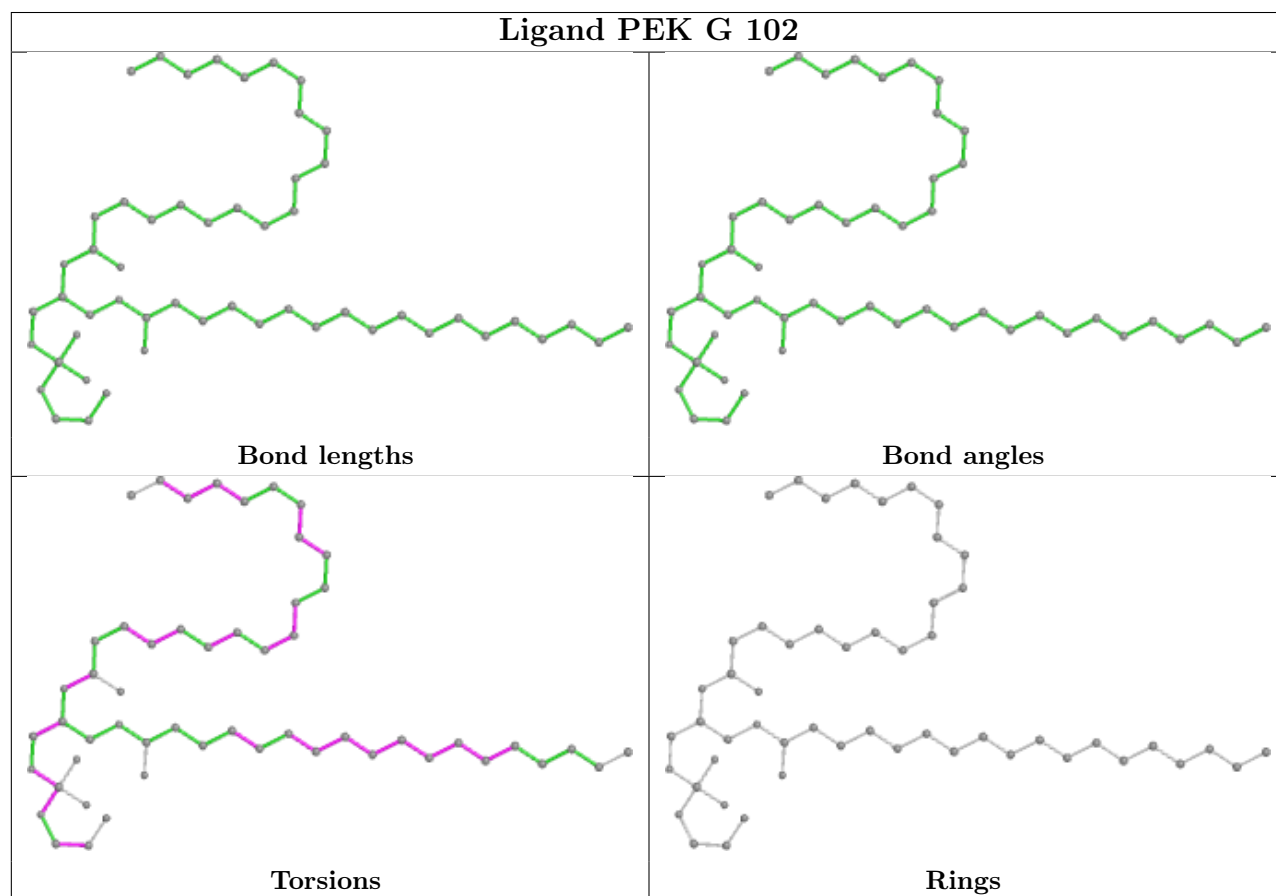
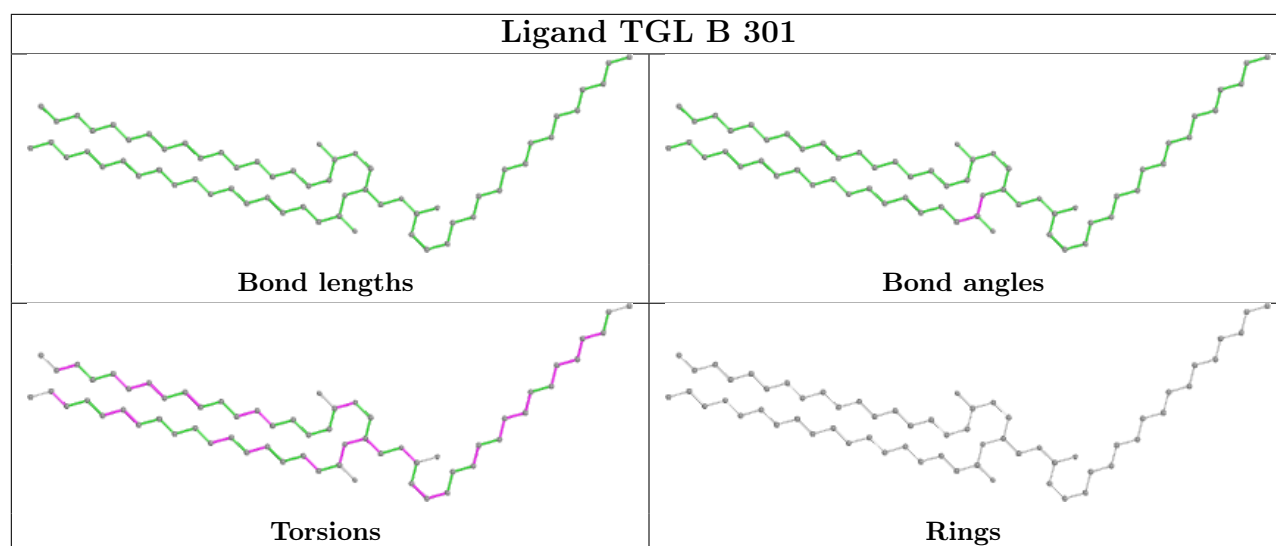


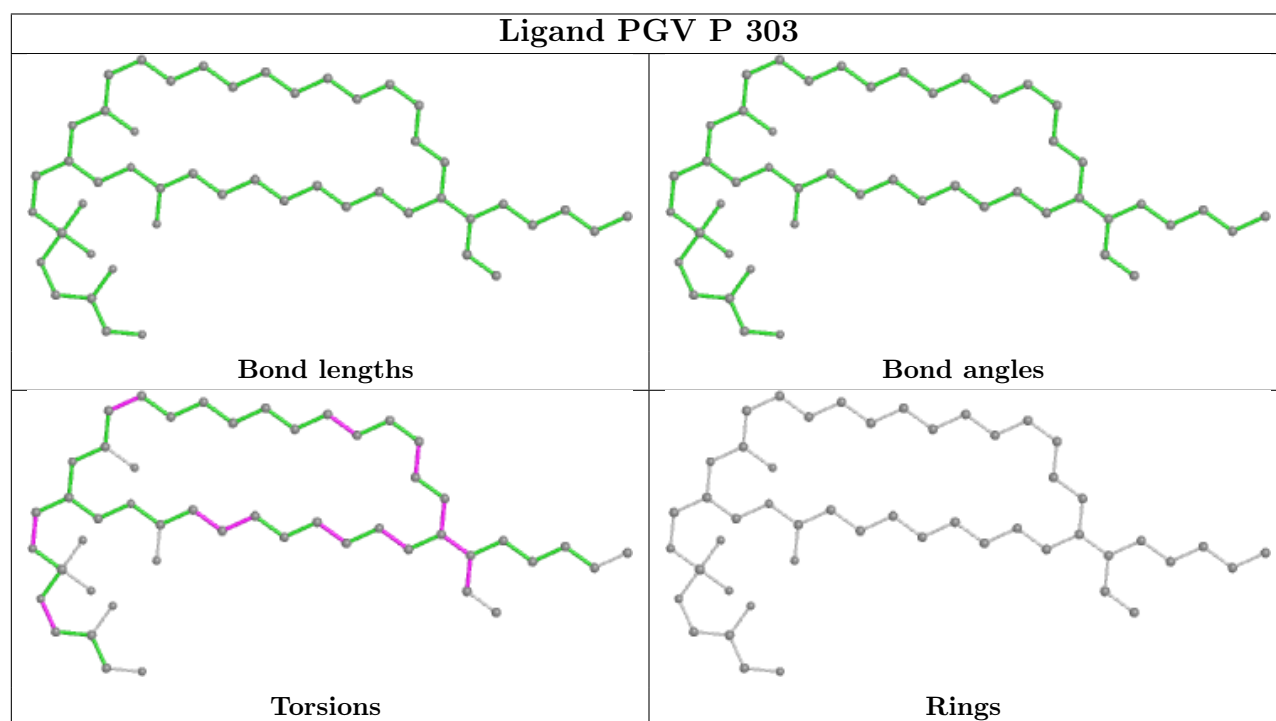
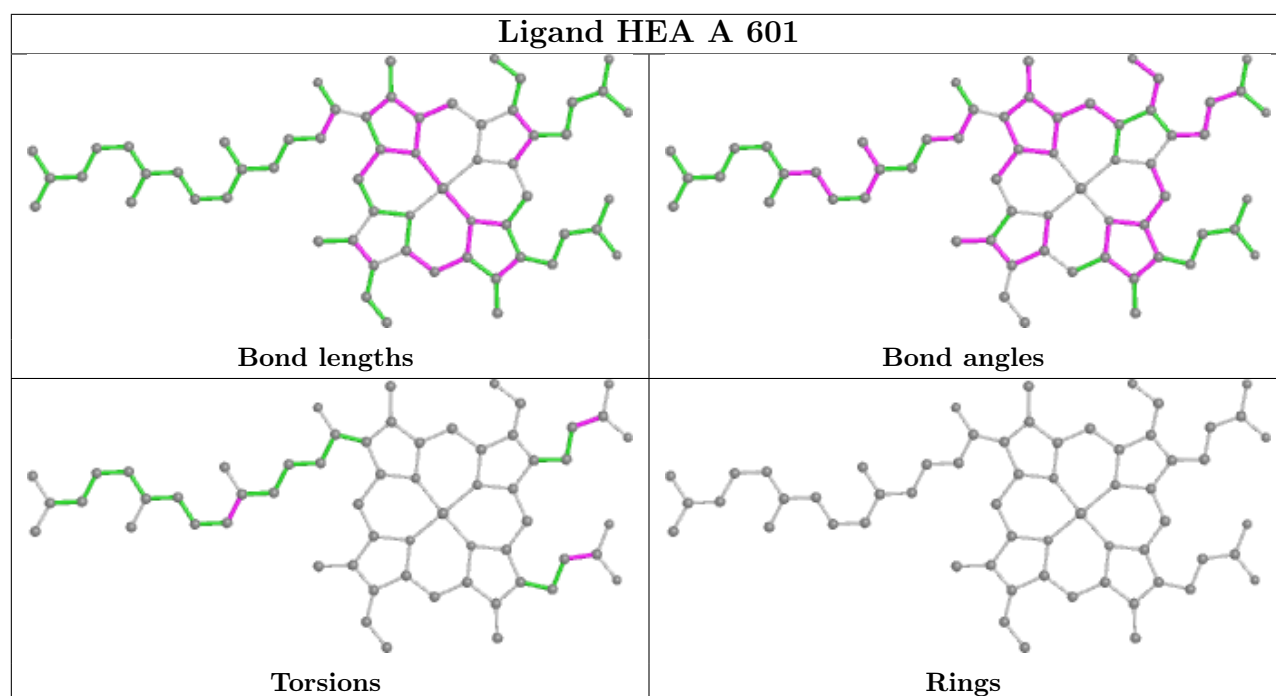
Ligand CHD J 101

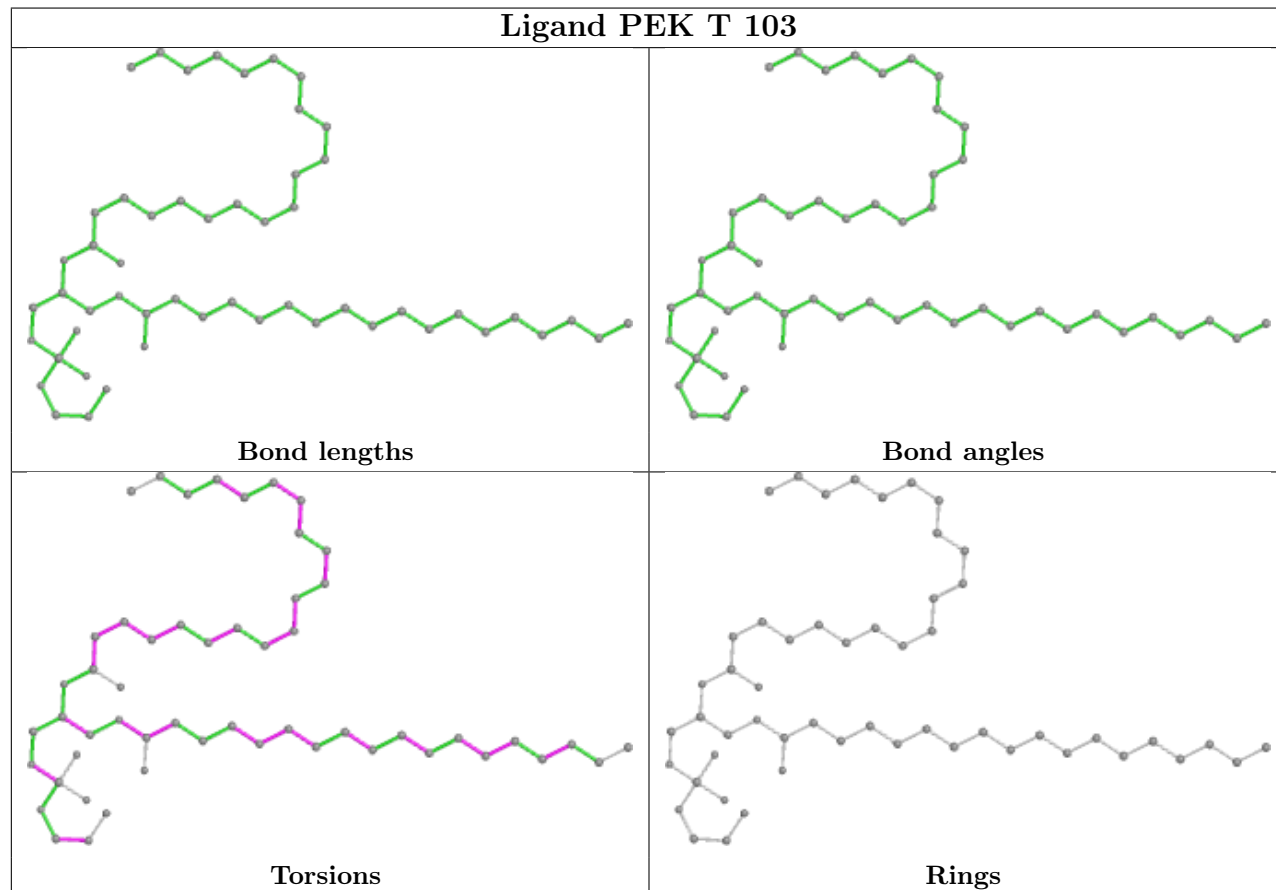
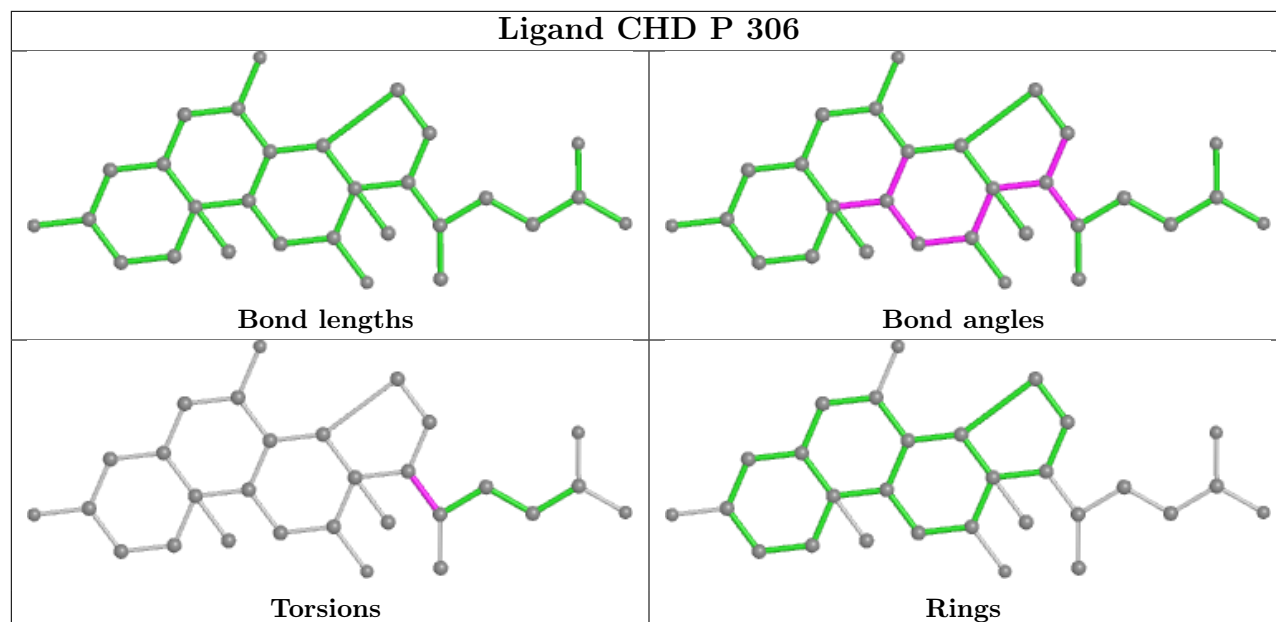


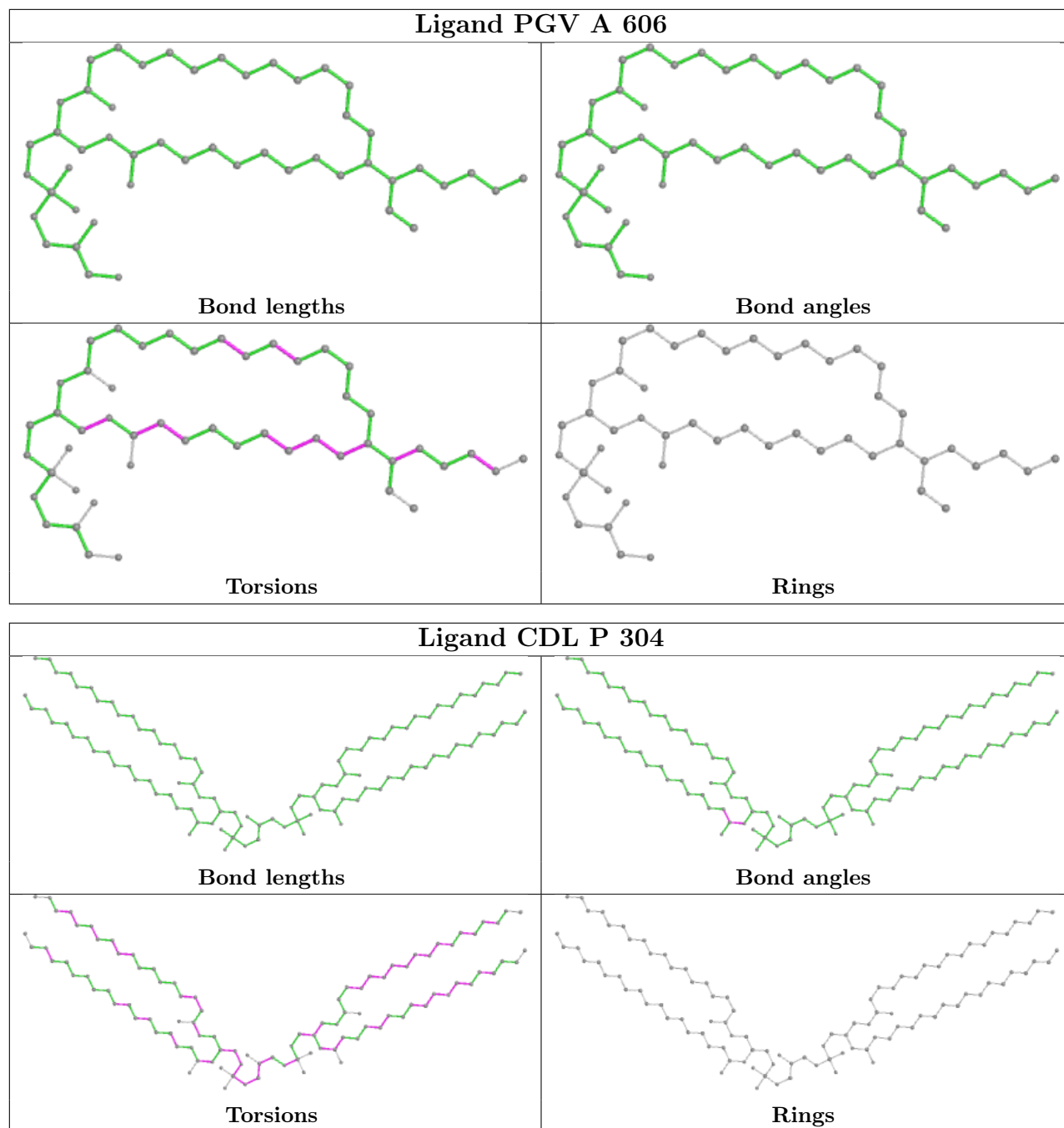
Ligand PEK C 302

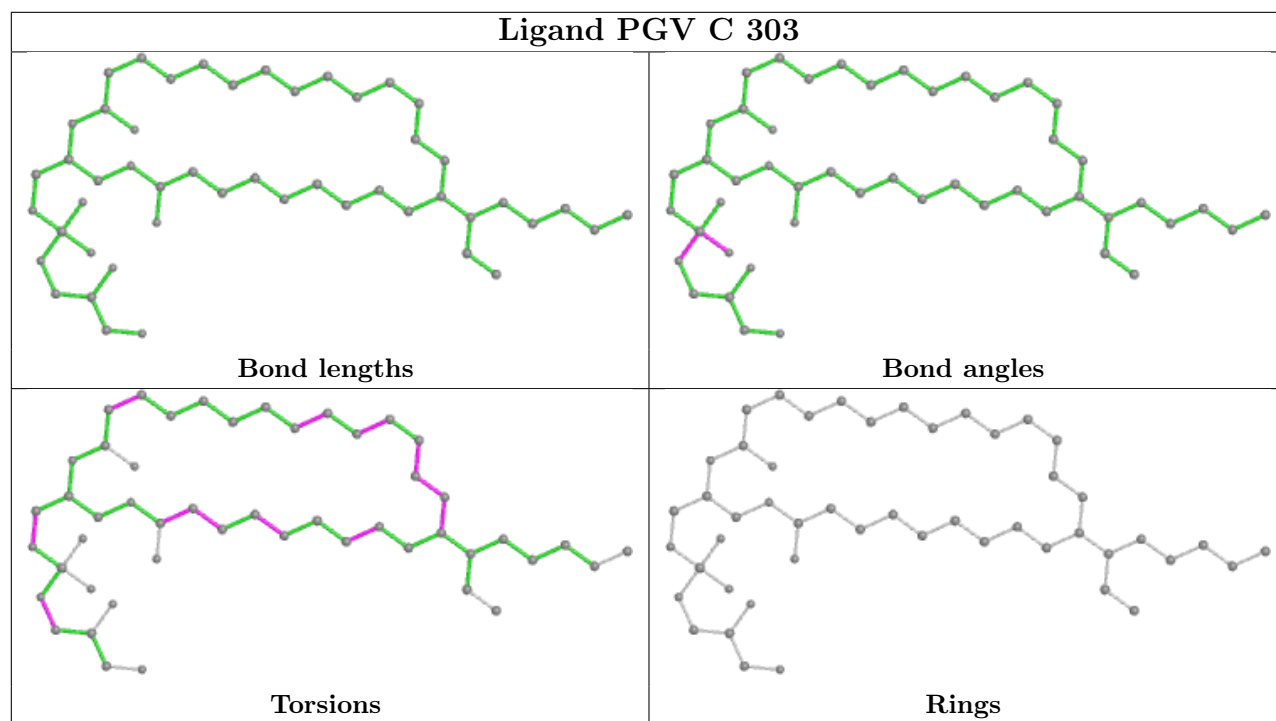
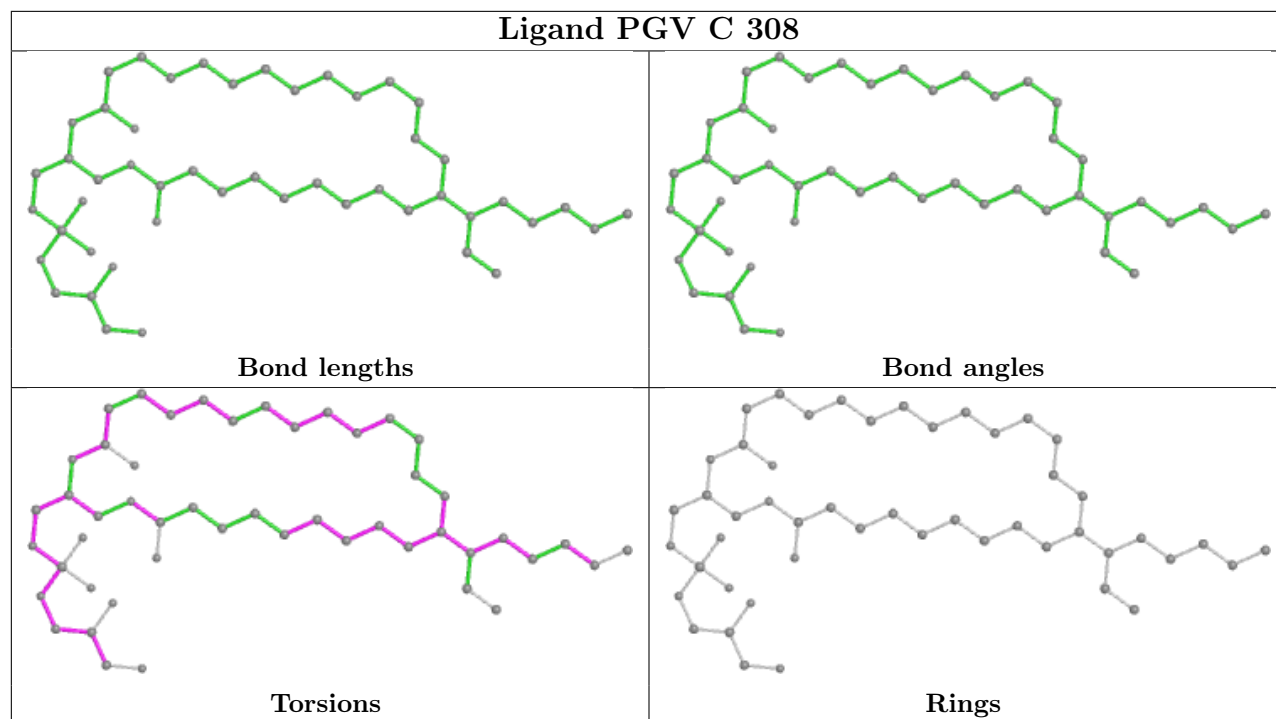


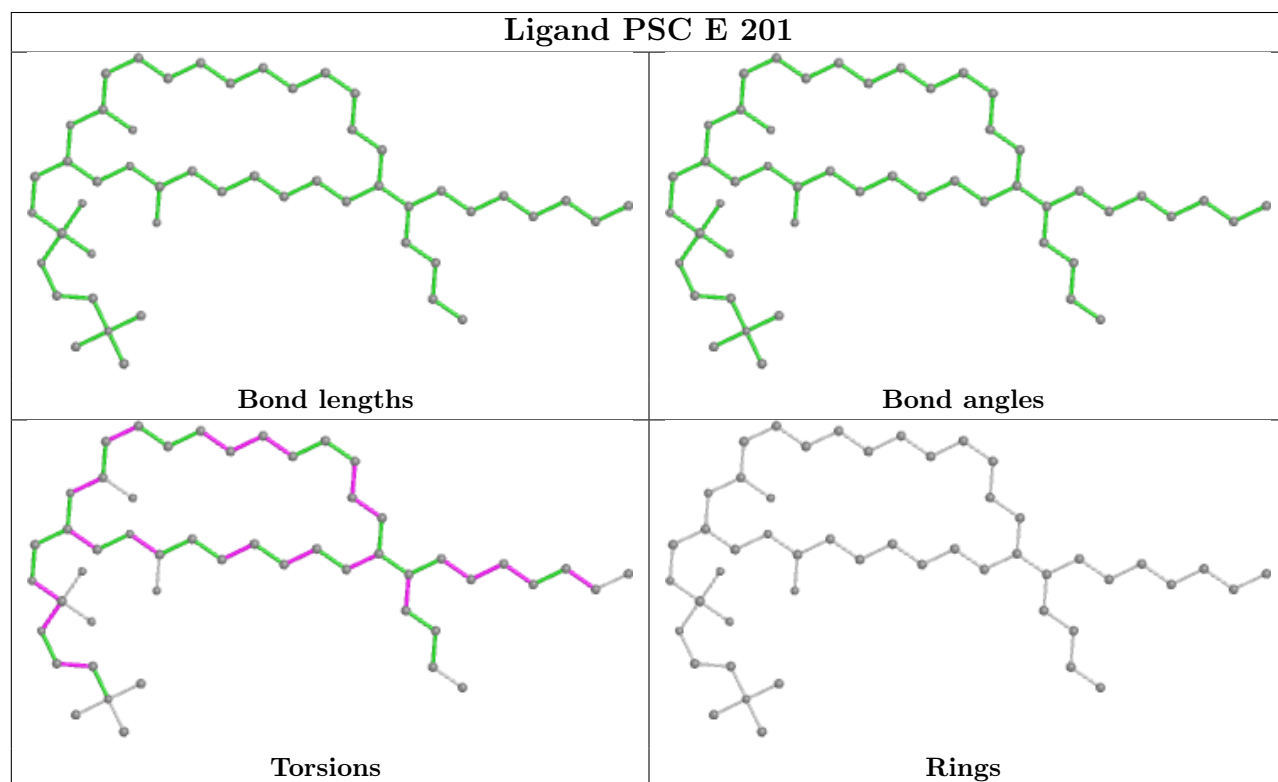
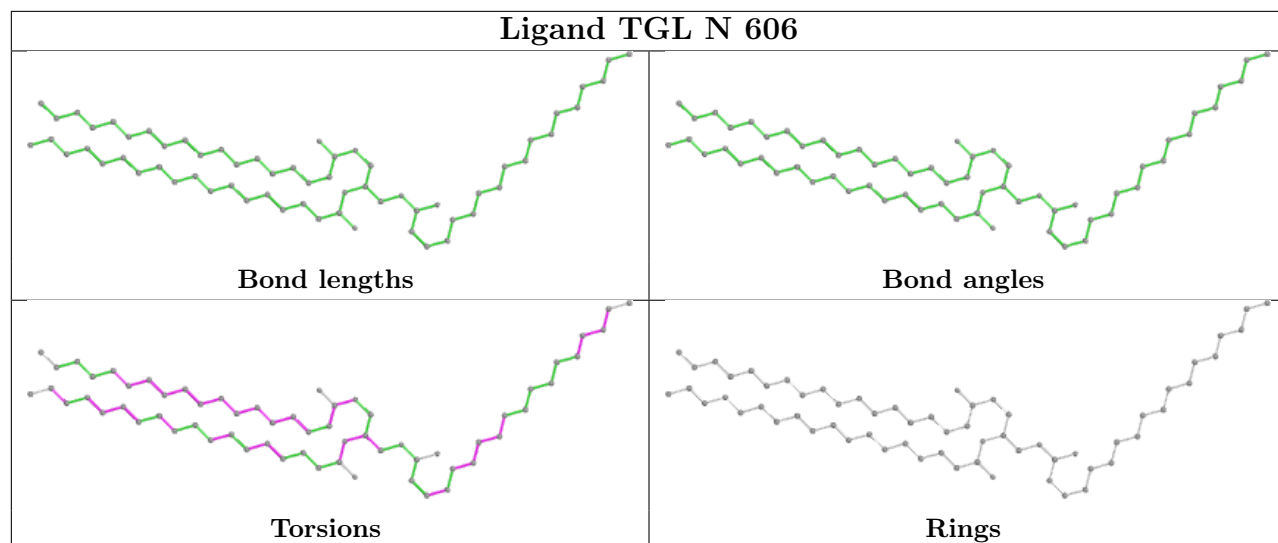


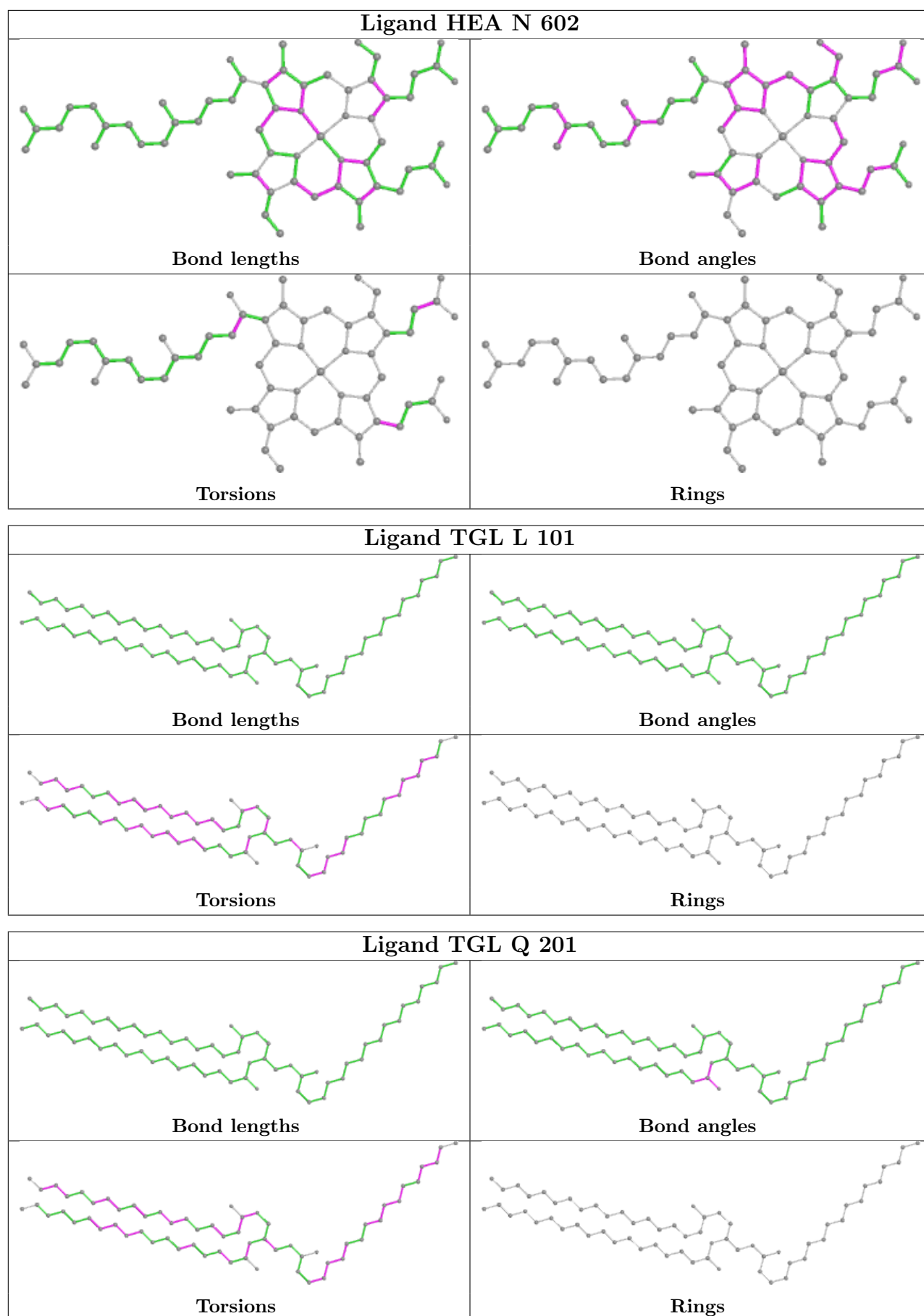


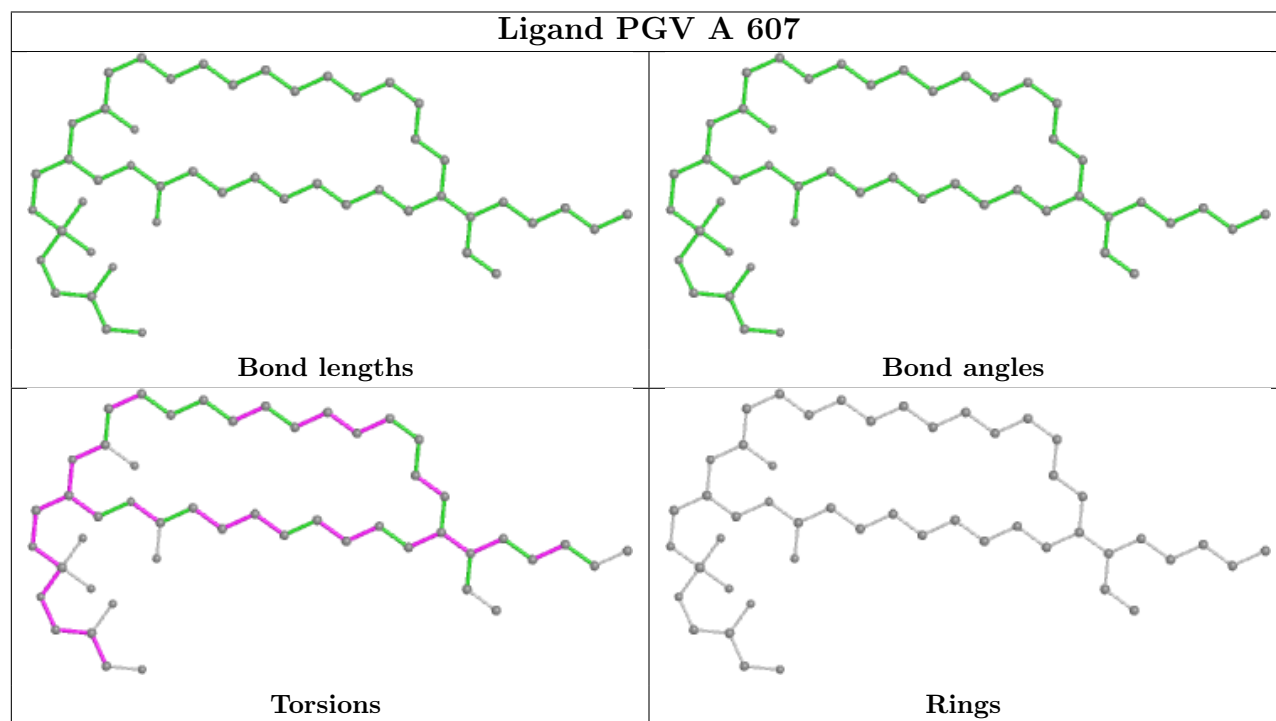
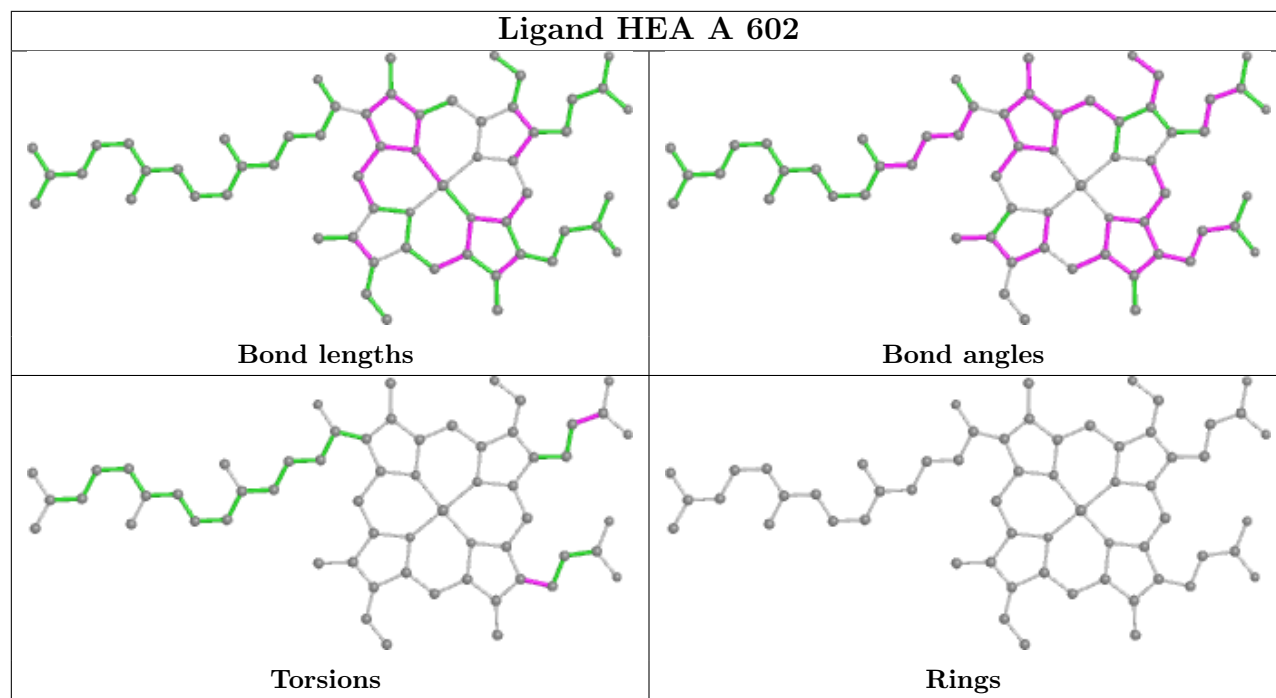


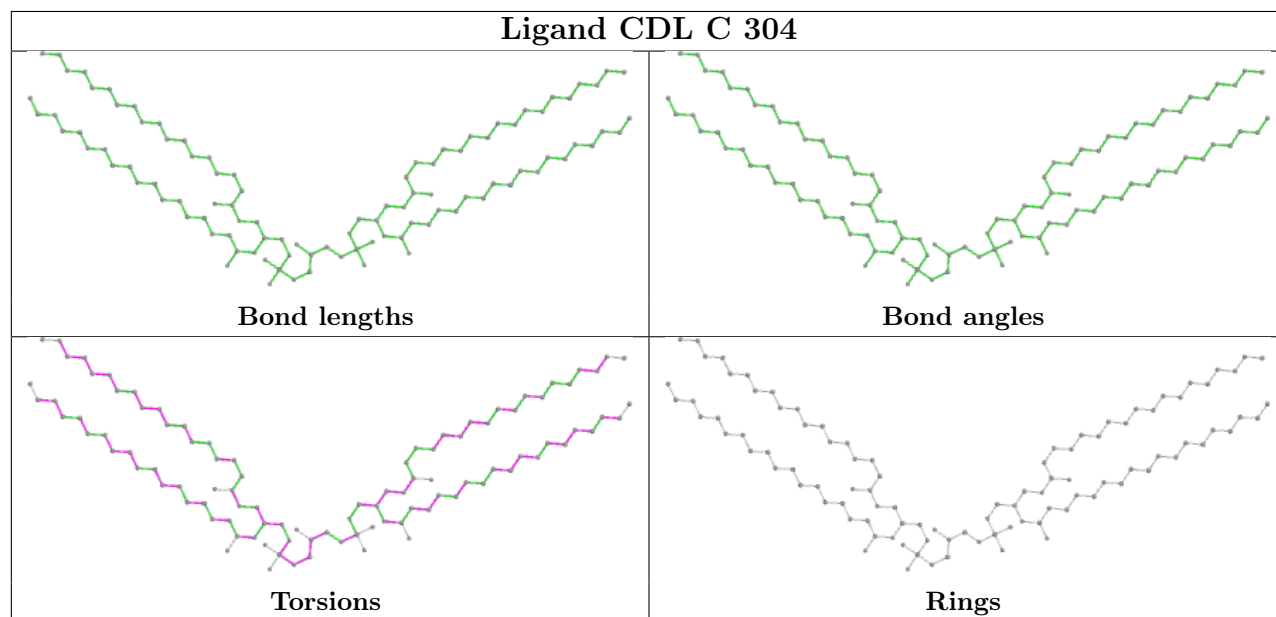
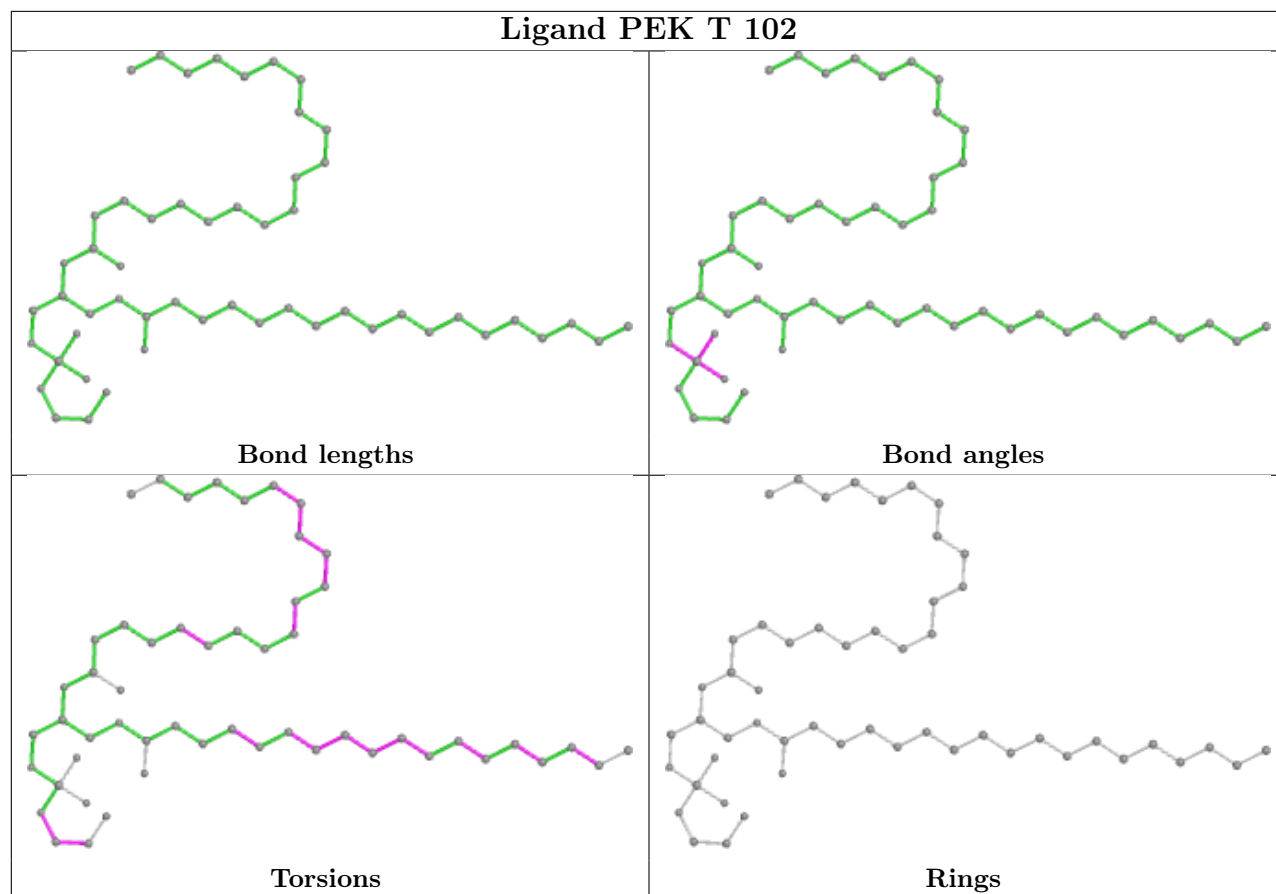


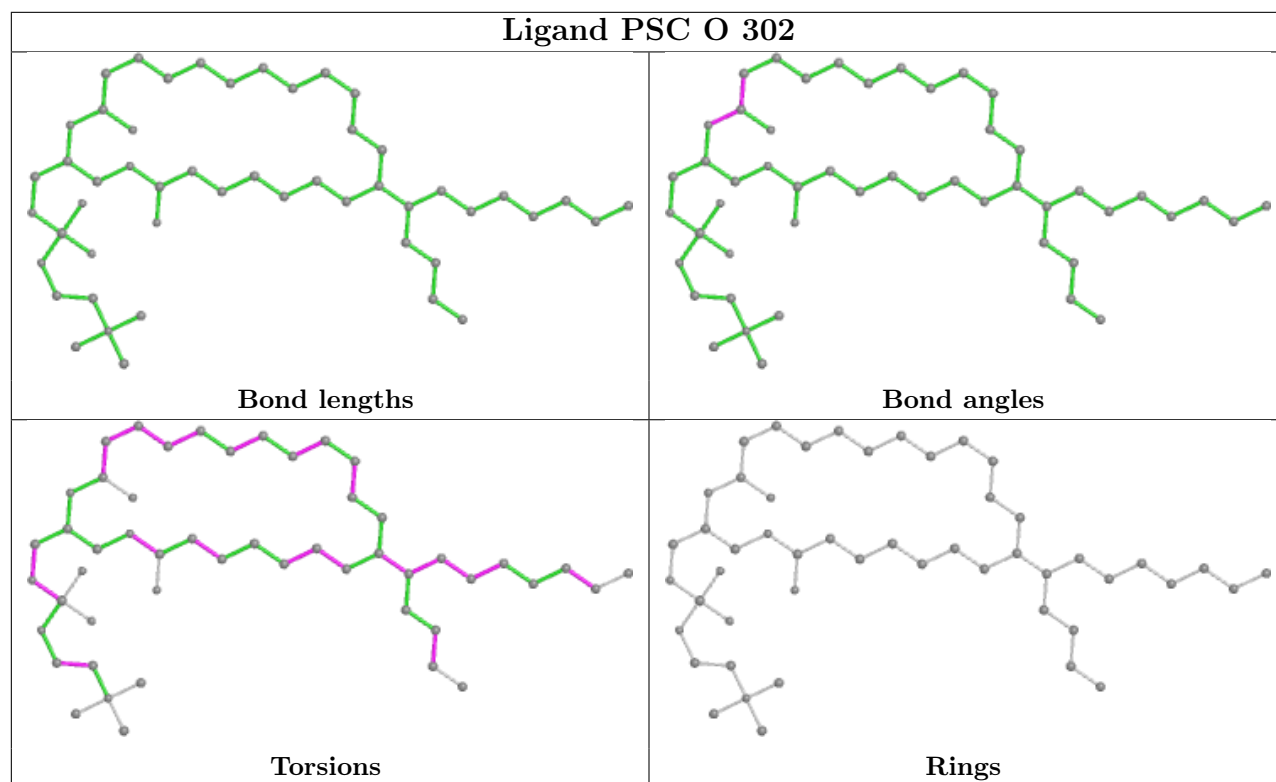
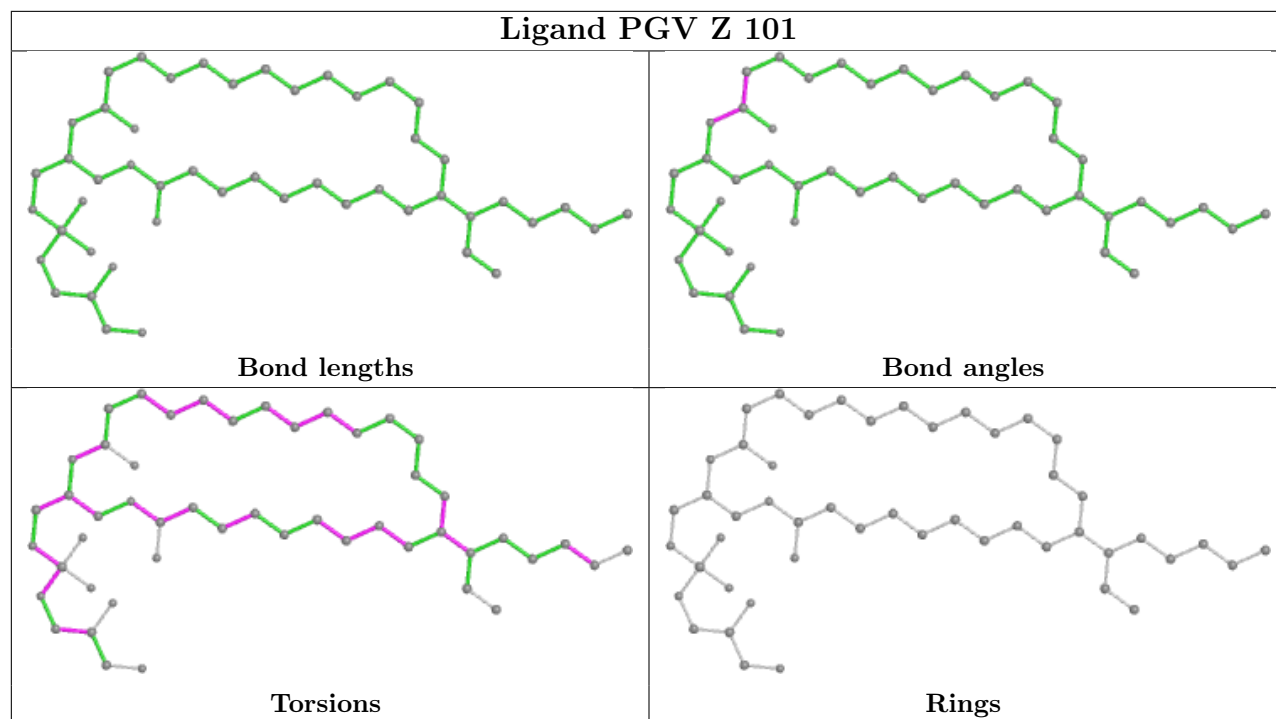


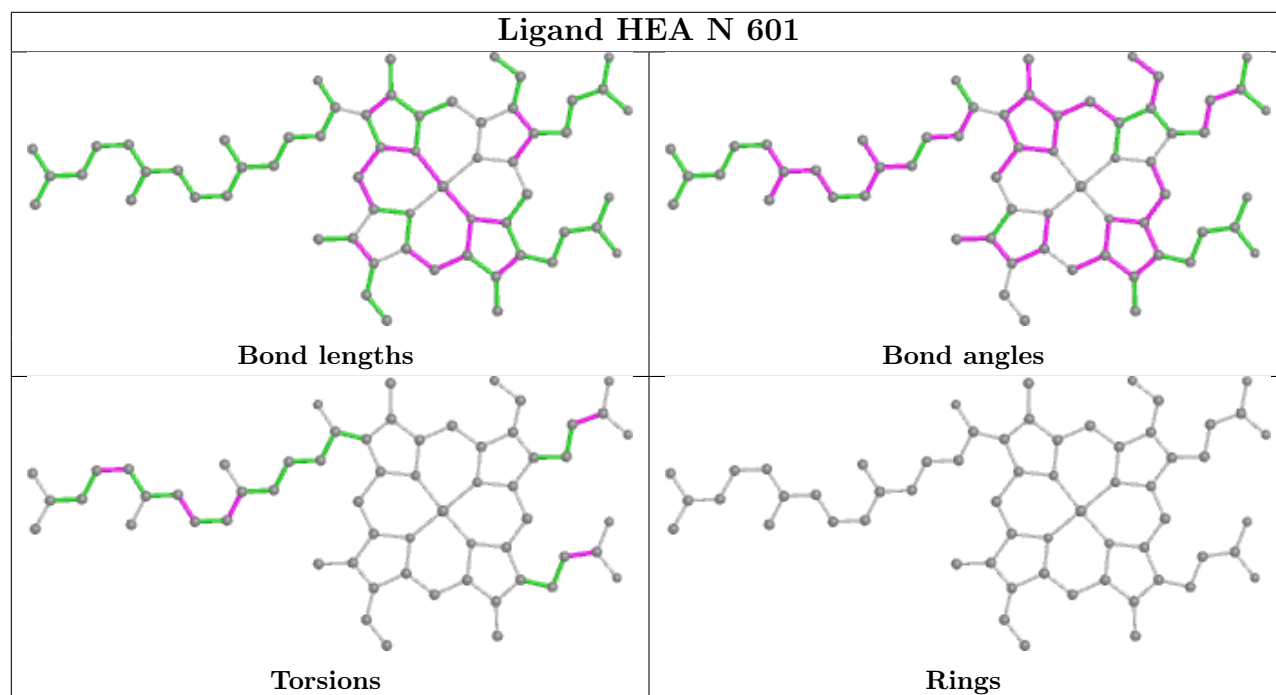
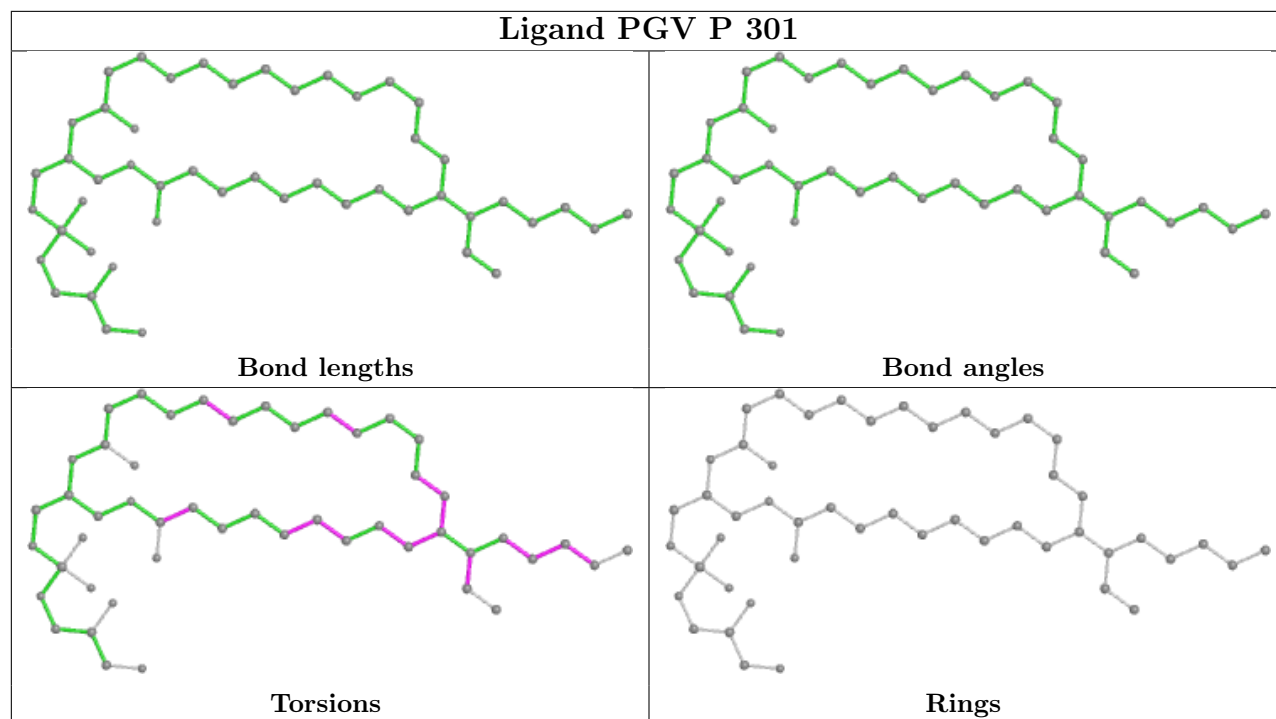


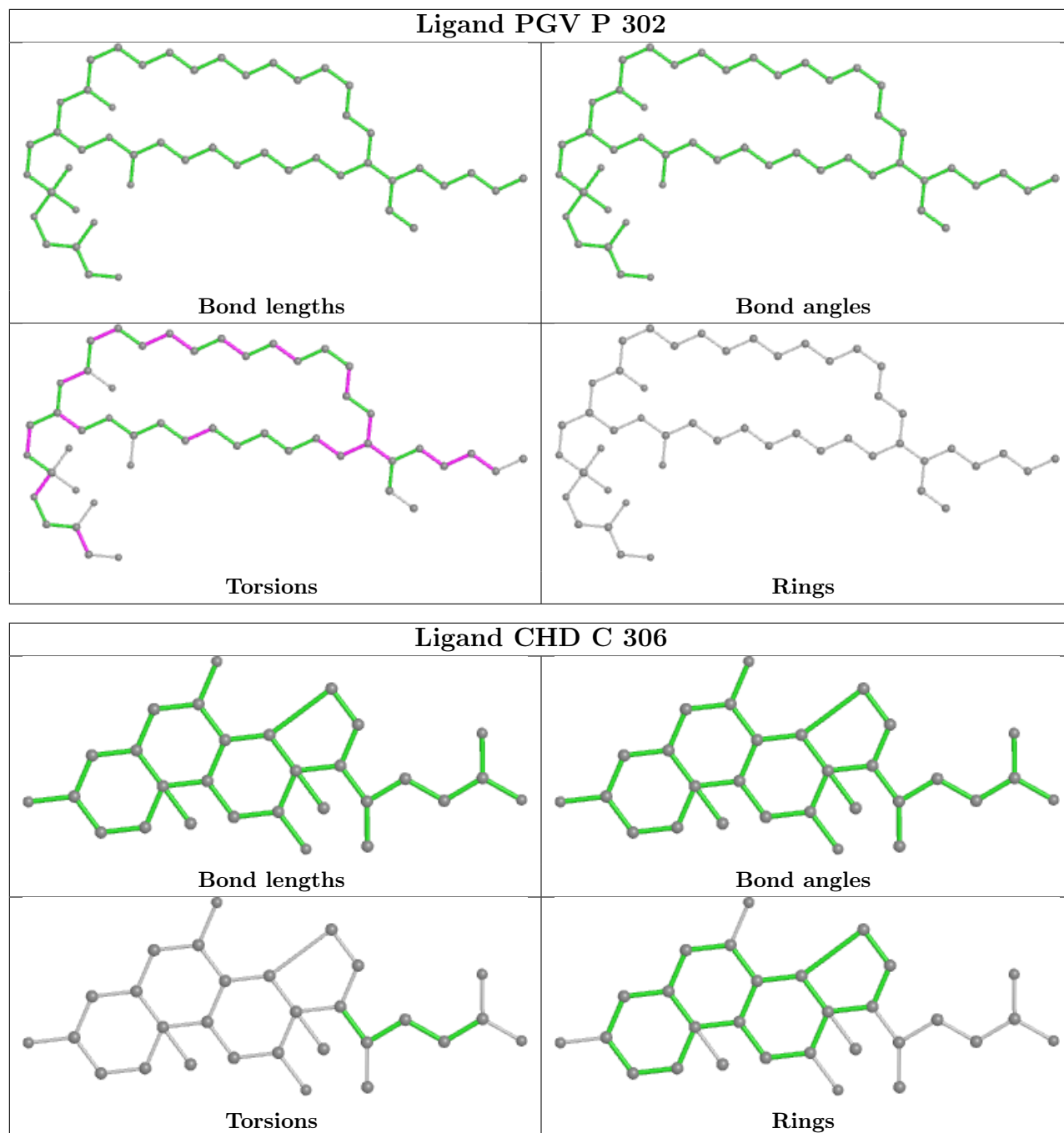


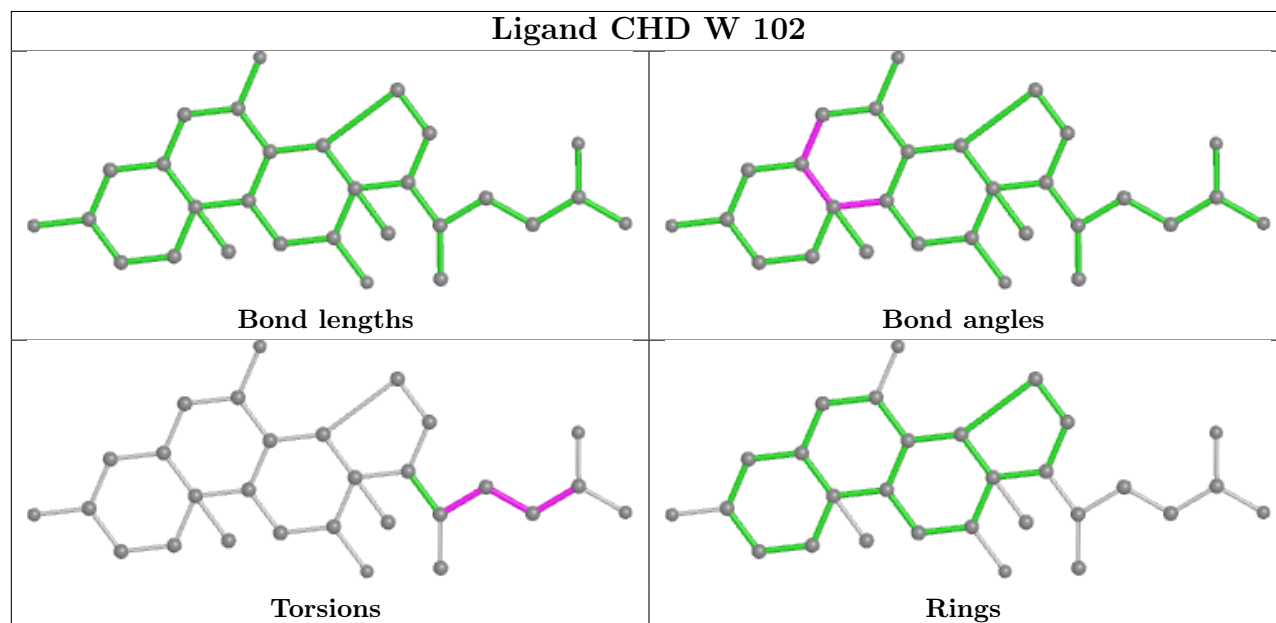
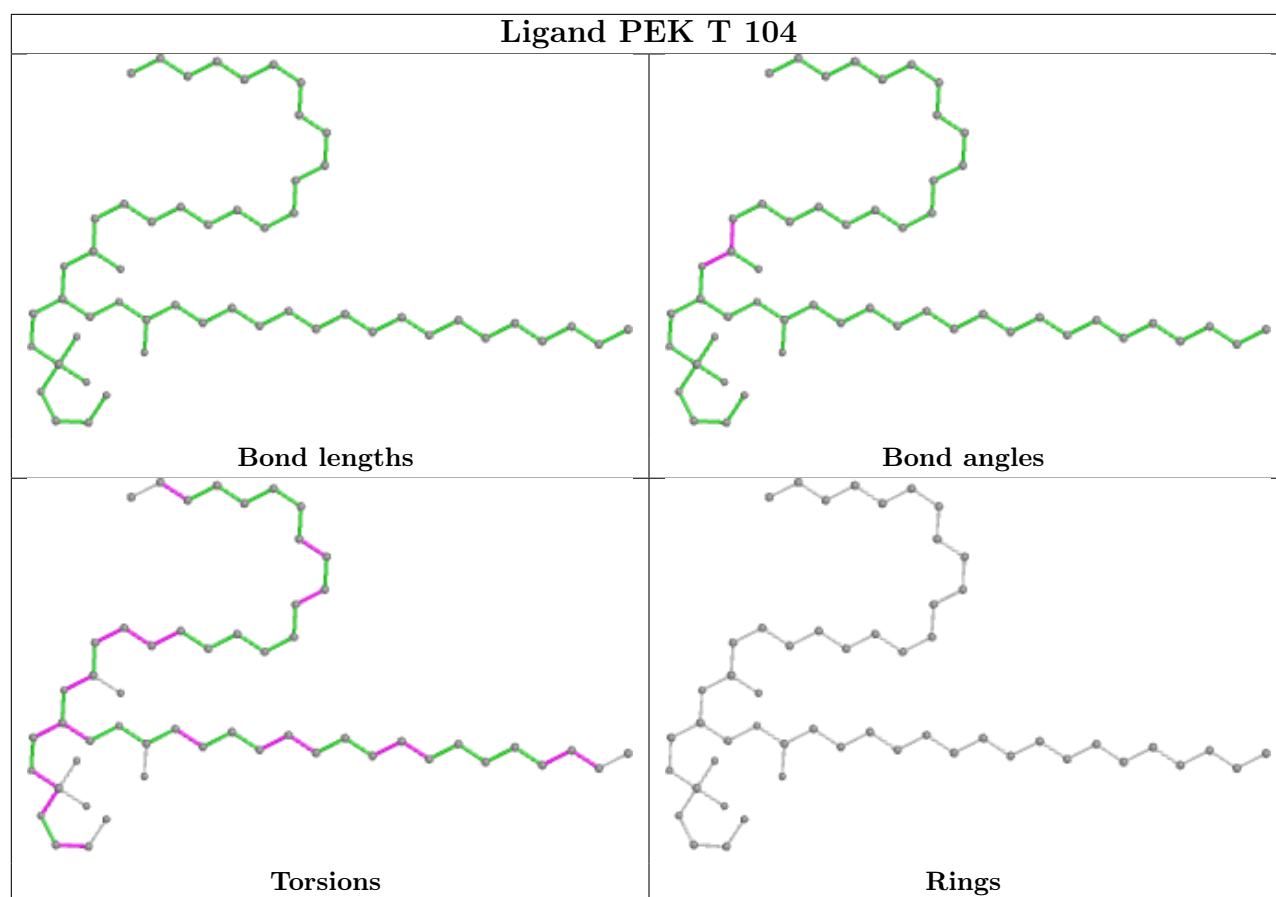


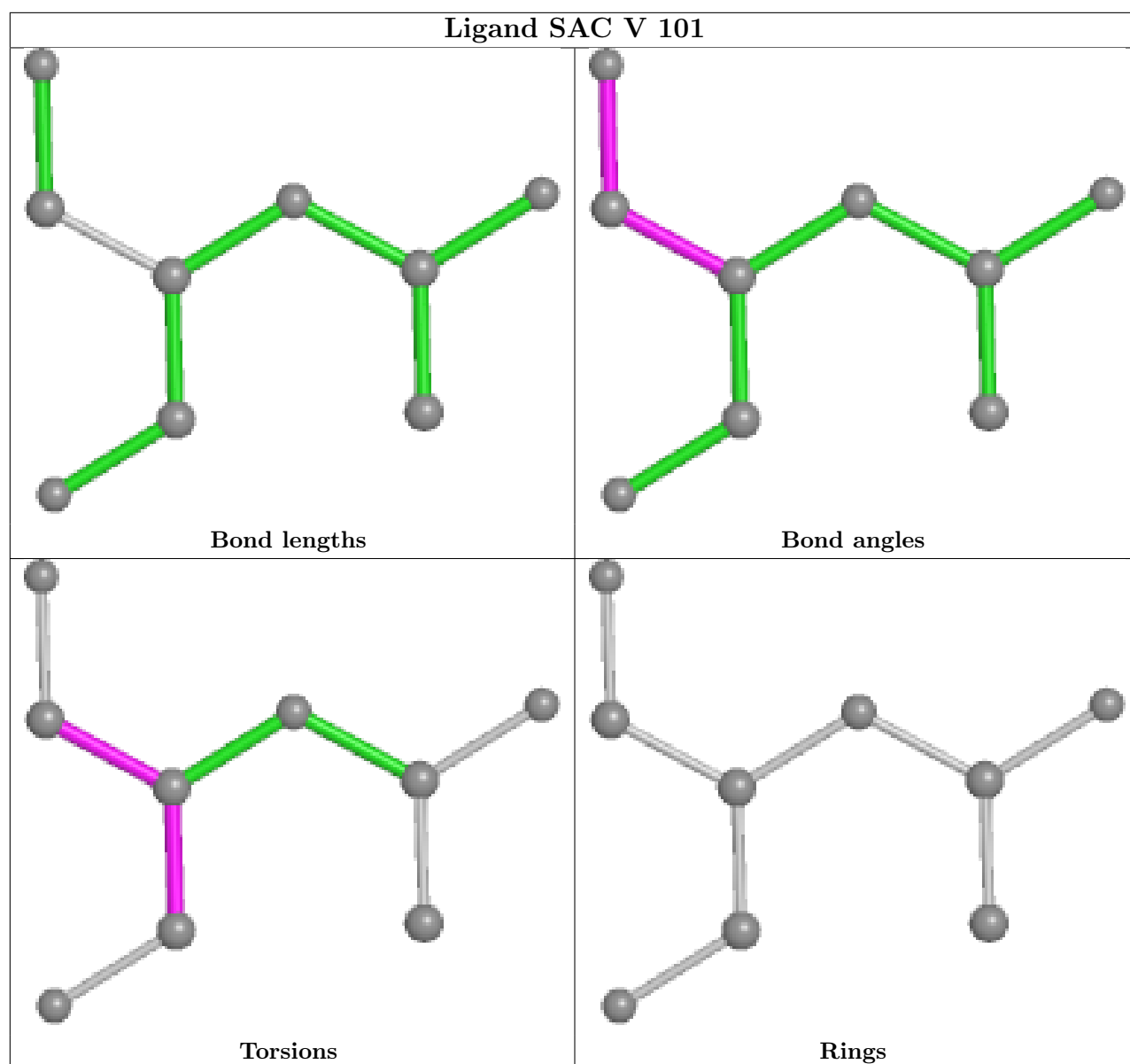


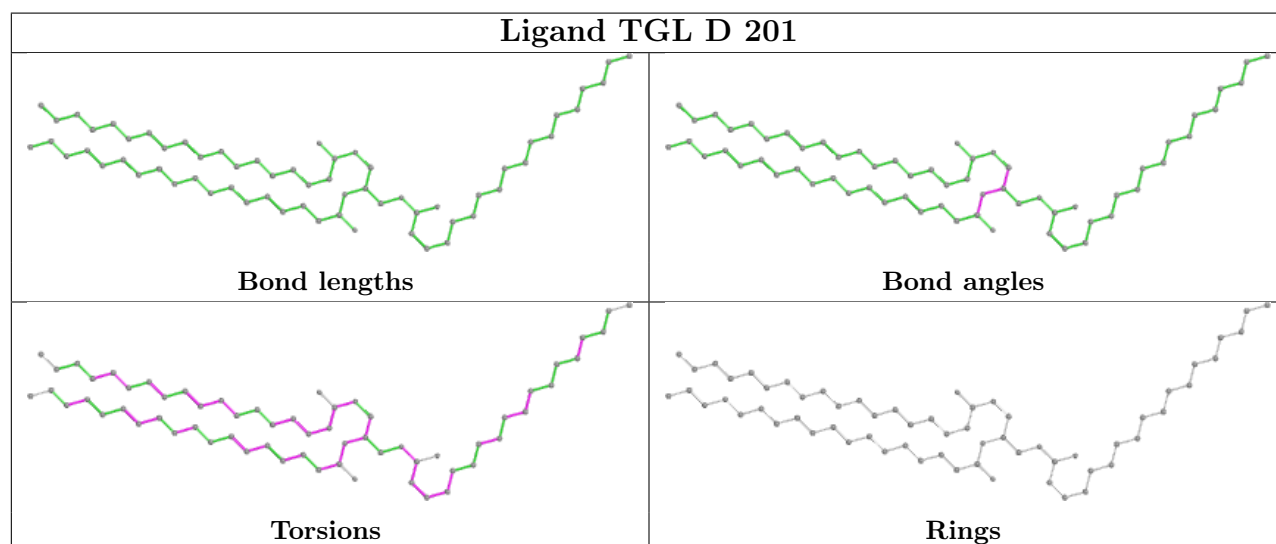
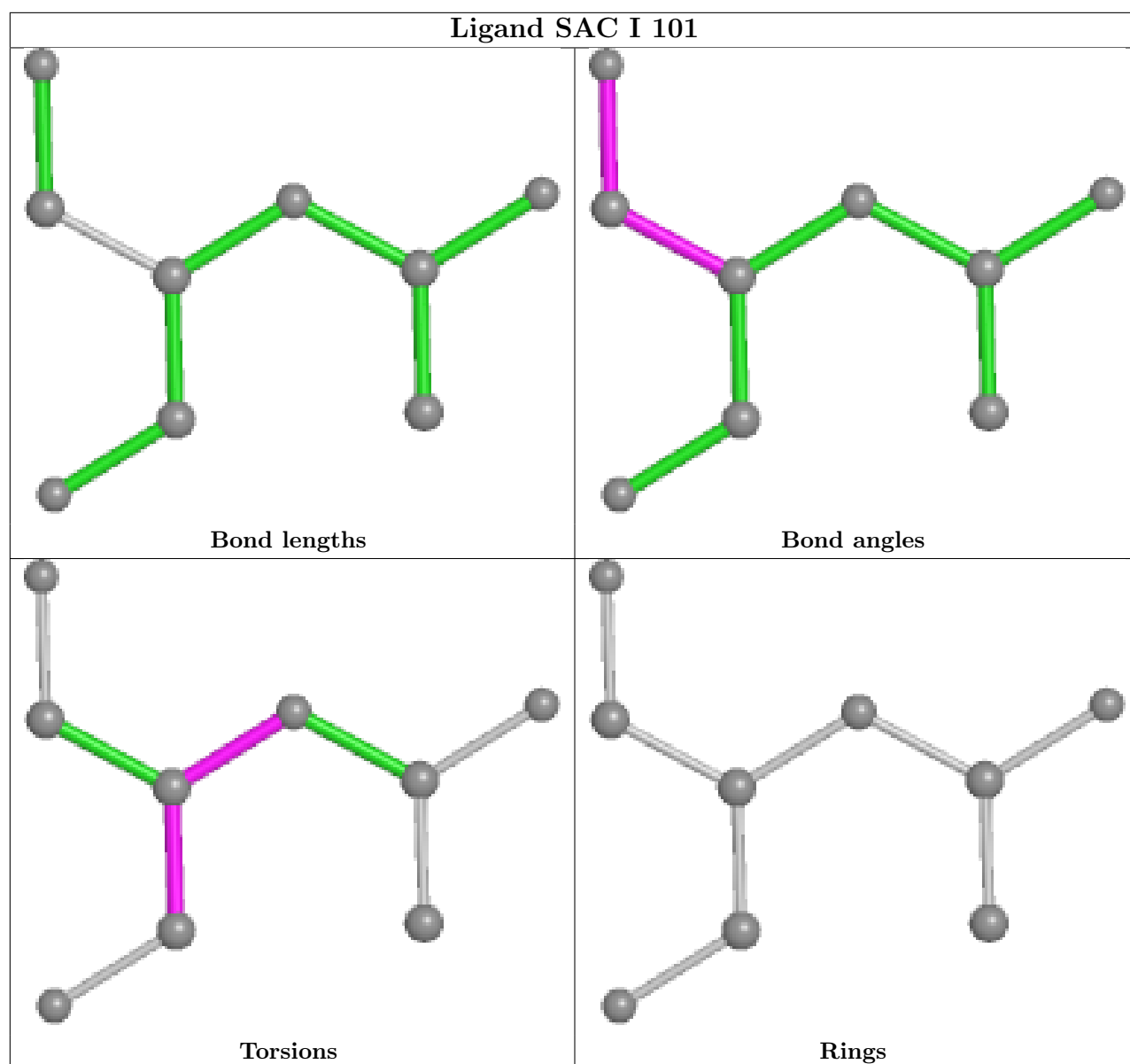




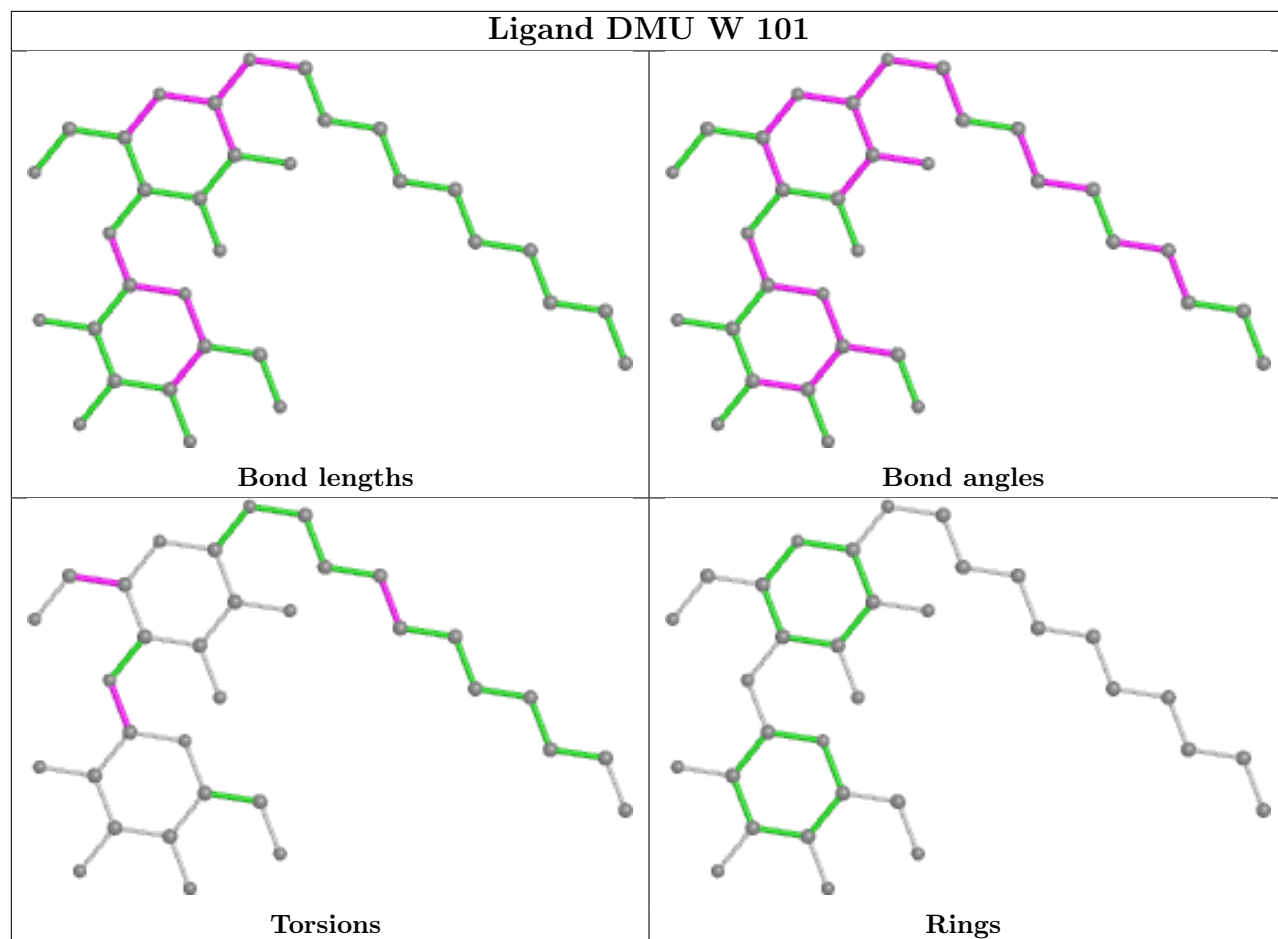




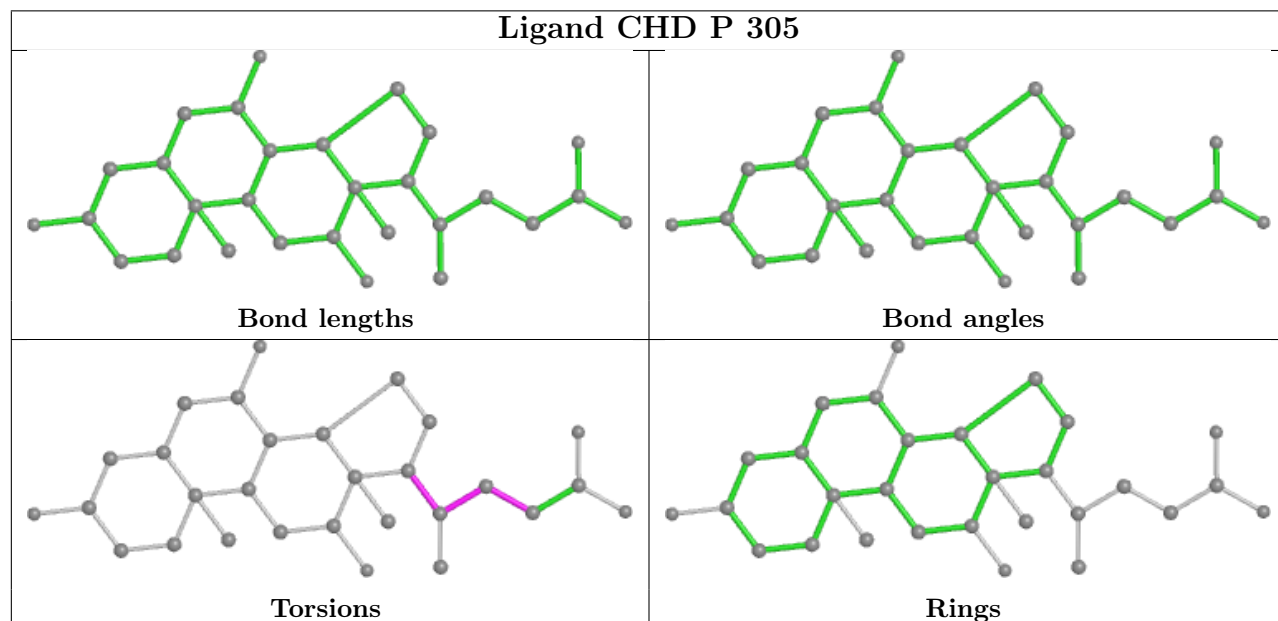


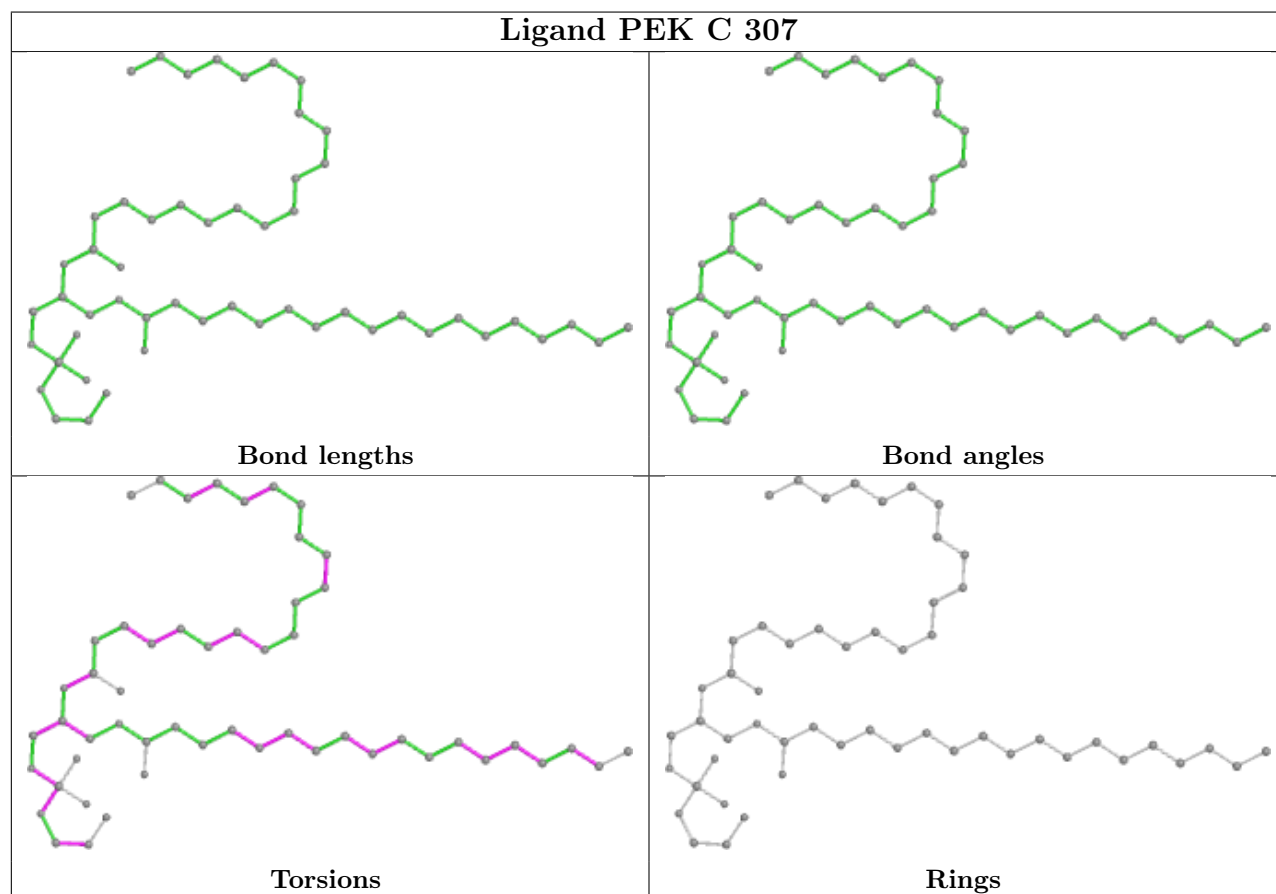
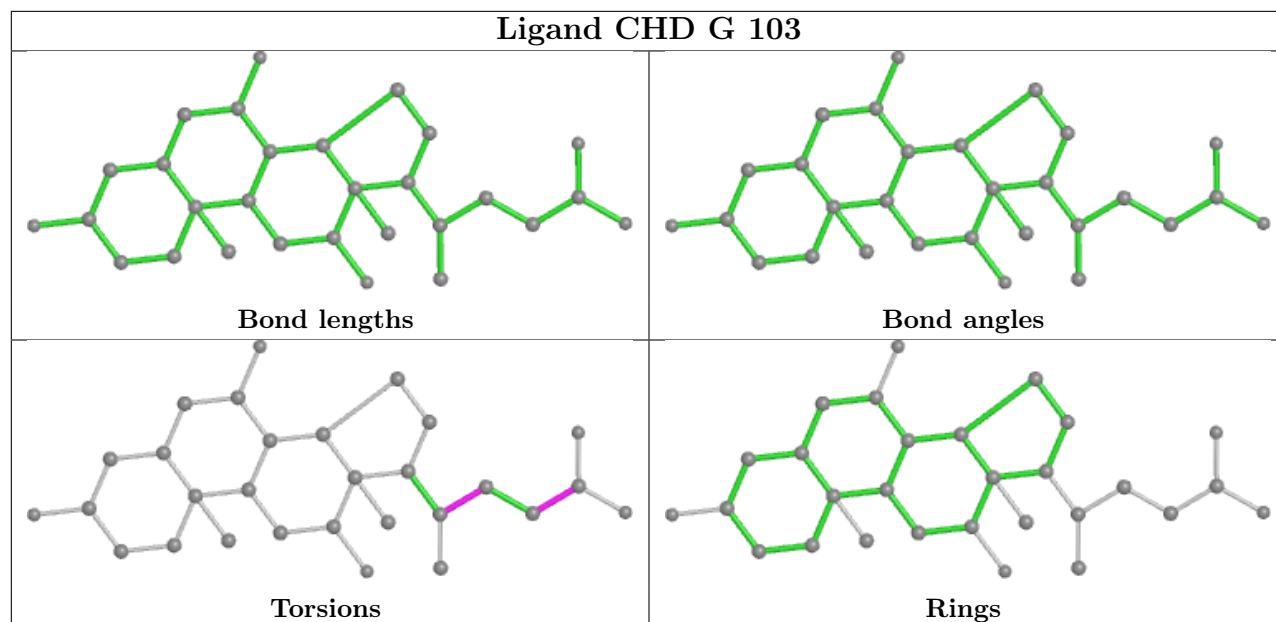


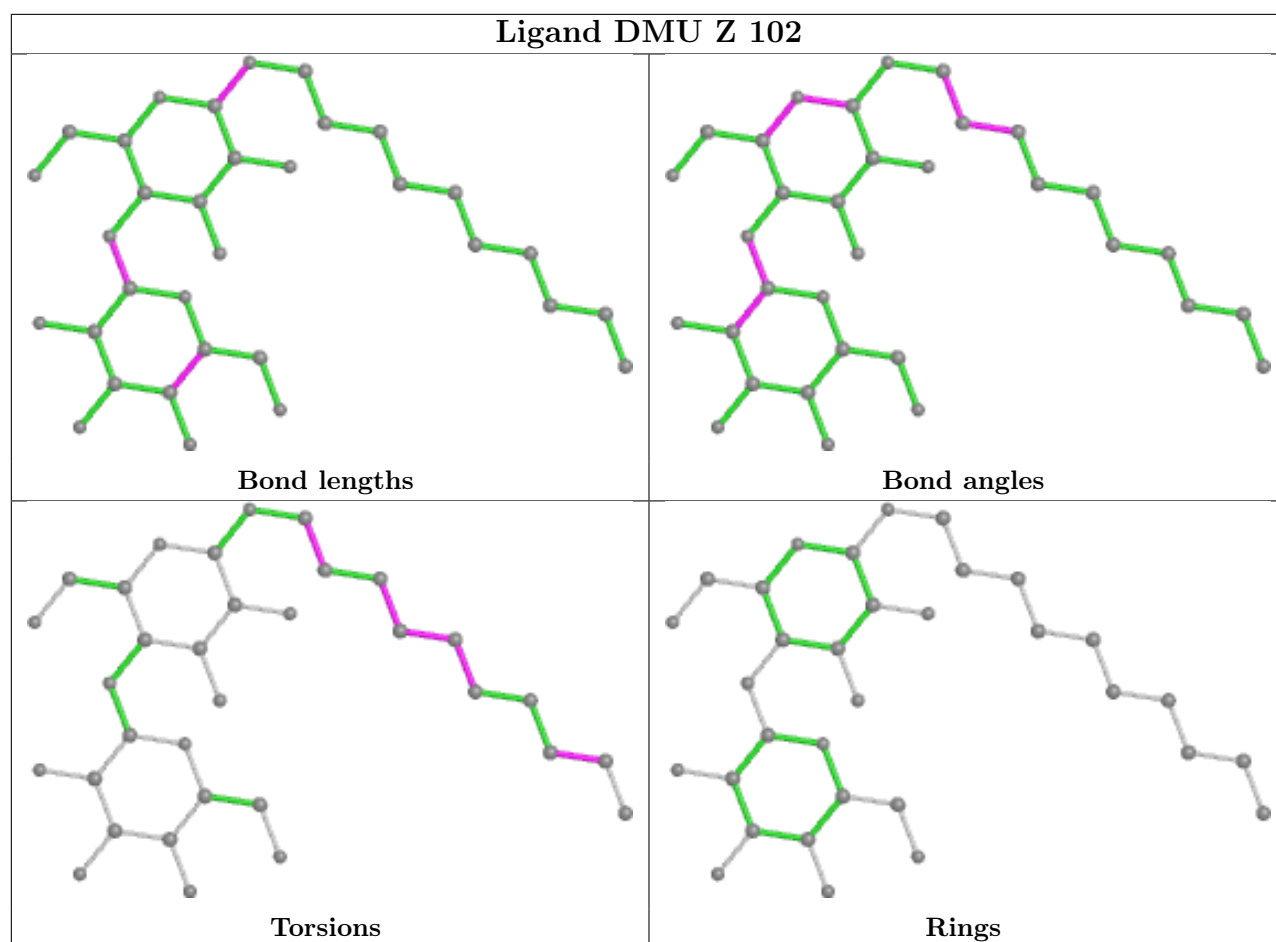
Ligand DMU W 101



Ligand CHD P 305







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%)	-0.30	4 (0%) 86 86	24, 33, 42, 77	0
1	N	513/514 (99%)	-0.31	1 (0%) 95 95	28, 37, 48, 84	0
2	B	226/227 (99%)	-0.50	1 (0%) 92 93	26, 42, 77, 117	0
2	O	226/227 (99%)	-0.36	7 (3%) 49 45	31, 48, 79, 118	0
3	C	259/261 (99%)	-0.70	0 100 100	26, 37, 52, 96	0
3	P	259/261 (99%)	-0.62	2 (0%) 86 86	29, 38, 55, 94	0
4	D	144/147 (97%)	-0.53	0 100 100	32, 43, 63, 83	0
4	Q	144/147 (97%)	0.42	13 (9%) 9 6	41, 59, 90, 149	0
5	E	105/109 (96%)	-0.44	2 (1%) 66 64	33, 45, 75, 122	0
5	R	105/109 (96%)	-0.28	2 (1%) 66 64	41, 52, 74, 119	0
6	F	98/98 (100%)	0.15	7 (7%) 16 12	30, 43, 111, 165	0
6	S	98/98 (100%)	0.18	8 (8%) 11 8	33, 44, 133, 189	0
7	G	83/85 (97%)	0.34	13 (15%) 2 1	31, 47, 124, 150	0
7	T	83/85 (97%)	0.42	13 (15%) 2 1	34, 49, 111, 135	0
8	H	79/85 (92%)	0.32	8 (10%) 7 4	35, 47, 114, 130	0
8	U	79/85 (92%)	0.39	10 (12%) 3 2	35, 52, 116, 152	0
9	I	72/73 (98%)	0.45	13 (18%) 1 0	36, 53, 92, 107	0
9	V	72/73 (98%)	0.29	8 (11%) 5 3	40, 62, 93, 107	0
10	J	58/59 (98%)	-0.11	4 (6%) 16 13	36, 47, 82, 128	0
10	W	58/59 (98%)	-0.04	5 (8%) 10 7	38, 52, 84, 138	0
11	K	49/56 (87%)	-0.33	2 (4%) 37 34	33, 48, 62, 76	0
11	X	49/56 (87%)	0.37	7 (14%) 2 1	43, 57, 82, 100	0
12	L	46/47 (97%)	-0.66	0 100 100	33, 39, 56, 106	0
12	Y	46/47 (97%)	-0.47	1 (2%) 62 58	36, 49, 71, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.36	1 (2%) 60 56	30, 39, 69, 97	0
13	Z	43/46 (93%)	0.08	3 (6%) 16 13	43, 51, 95, 138	0
All	All	3550/3614 (98%)	-0.23	135 (3%) 40 37	24, 42, 82, 189	0

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	16.3
4	Q	6	VAL	13.2
4	Q	4	SER	11.9
8	U	45	ALA	11.3
4	Q	5	VAL	11.0

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
7	TPO	G	11	11/12	0.68	0.30	110,125,150,150	0
7	TPO	T	11	11/12	0.79	0.24	116,120,142,143	0
1	FME	N	1	10/11	0.95	0.25	51,63,84,88	0
1	FME	A	1	10/11	0.95	0.21	55,60,85,92	0
2	FME	O	1	10/11	0.96	0.14	41,48,54,55	0
2	FME	B	1	10/11	0.97	0.14	33,40,47,61	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
29	SAC	I	101	9/10	0.22	0.59	80,104,115,123	0
29	SAC	V	101	9/10	0.32	0.49	118,130,141,147	0
27	PSC	E	201	52/52	0.58	0.46	66,112,177,181	0
21	TGL	Q	201	63/63	0.59	0.28	69,98,120,131	0
24	PEK	C	307	53/53	0.60	0.30	57,90,174,186	0
21	TGL	Y	101	63/63	0.61	0.38	55,84,128,139	0
24	PEK	T	103	53/53	0.64	0.41	54,124,165,170	0
24	PEK	G	102	53/53	0.66	0.32	56,120,164,170	0
27	PSC	O	302	52/52	0.68	0.37	54,111,177,203	0
25	CDL	G	101	100/100	0.68	0.33	70,109,164,179	0
23	DMU	W	101	33/33	0.68	0.50	59,104,124,144	0
25	CDL	P	304	100/100	0.70	0.32	58,109,142,159	0
18	PGV	P	302	51/51	0.71	0.33	69,104,137,150	0
24	PEK	T	104	53/53	0.71	0.34	51,98,170,183	0
23	DMU	C	301	33/33	0.72	0.50	60,111,136,138	0
21	TGL	N	606	63/63	0.73	0.32	61,94,161,172	0
25	CDL	T	105	100/100	0.73	0.29	76,115,154,202	0
25	CDL	C	304	100/100	0.74	0.33	52,101,131,139	0
18	PGV	C	308	51/51	0.74	0.28	60,93,116,126	0
18	PGV	Z	101	51/51	0.75	0.34	51,98,124,137	0
21	TGL	B	301	63/63	0.79	0.29	61,88,159,165	0
21	TGL	L	101	63/63	0.80	0.25	47,73,104,111	0
18	PGV	A	607	51/51	0.82	0.26	52,87,123,134	0
21	TGL	D	201	63/63	0.82	0.22	52,80,107,110	0
23	DMU	Z	102	33/33	0.85	0.24	55,63,88,90	0
26	CHD	W	102	29/29	0.85	0.24	64,77,91,94	0
26	CHD	J	101	29/29	0.86	0.30	59,70,95,96	0
23	DMU	D	202	33/33	0.88	0.18	44,50,69,72	0
19	EDO	T	106	4/4	0.91	0.28	42,51,51,56	0
24	PEK	T	102	53/53	0.91	0.21	34,56,92,98	0
19	EDO	A	608	4/4	0.92	0.21	31,37,38,43	0
19	EDO	C	309	4/4	0.92	0.14	54,54,57,61	0
26	CHD	C	305	29/29	0.93	0.26	52,63,72,74	0
19	EDO	G	104	4/4	0.94	0.20	51,58,59,59	0
26	CHD	P	305	29/29	0.95	0.24	53,61,66,72	0
16	MG	N	604	1/1	0.95	0.10	34,34,34,34	0
19	EDO	A	609	4/4	0.95	0.17	54,57,57,58	0
16	MG	A	604	1/1	0.95	0.13	29,29,29,29	0
24	PEK	C	302	53/53	0.95	0.19	38,57,85,94	0
18	PGV	C	303	51/51	0.95	0.21	31,45,80,81	0
26	CHD	P	306	29/29	0.96	0.10	32,38,42,43	0
18	PGV	P	303	51/51	0.96	0.18	29,47,84,86	0
19	EDO	S	102	4/4	0.96	0.20	59,59,60,61	0

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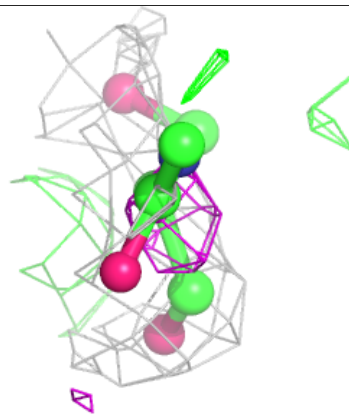
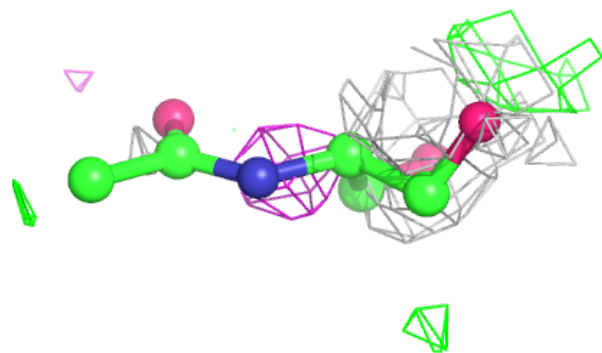
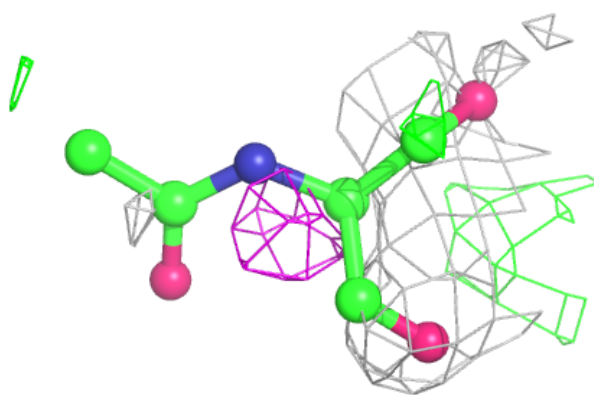
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	HEA	N	602	60/60	0.97	0.15	30,34,47,52	0
26	CHD	C	306	29/29	0.97	0.10	31,37,41,41	0
26	CHD	G	103	29/29	0.97	0.09	34,36,39,41	0
14	HEA	A	601	60/60	0.97	0.19	29,35,47,50	0
18	PGV	P	301	51/51	0.97	0.22	30,50,72,75	0
19	EDO	N	607	4/4	0.97	0.15	37,37,37,38	0
26	CHD	T	101	29/29	0.97	0.10	32,36,40,49	0
14	HEA	A	602	60/60	0.97	0.17	25,32,40,42	0
19	EDO	S	103	4/4	0.97	0.14	45,49,49,51	0
17	NA	A	605	1/1	0.97	0.07	32,32,32,32	0
18	PGV	A	606	51/51	0.97	0.22	27,41,71,81	0
14	HEA	N	601	60/60	0.97	0.19	31,39,53,57	0
22	CUA	B	302	2/2	0.98	0.07	29,29,29,31	0
22	CUA	O	301	2/2	0.98	0.06	36,36,36,38	0
17	NA	N	605	1/1	0.99	0.04	35,35,35,35	0
20	OH	A	610	1/1	0.99	0.24	26,26,26,26	1
15	CU	A	603	1/1	1.00	0.12	32,32,32,32	0
28	ZN	F	101	1/1	1.00	0.07	36,36,36,36	0
28	ZN	S	101	1/1	1.00	0.05	40,40,40,40	0
20	OH	N	608	1/1	1.00	0.26	27,27,27,27	1
15	CU	N	603	1/1	1.00	0.13	36,36,36,36	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.

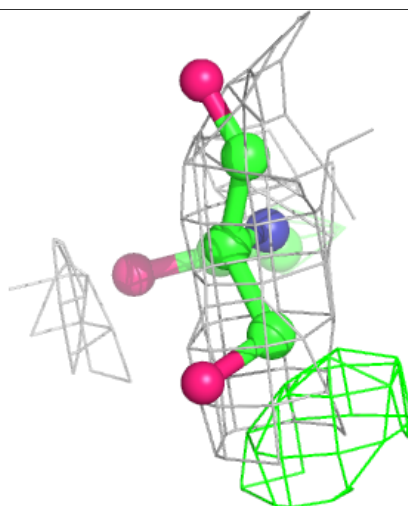
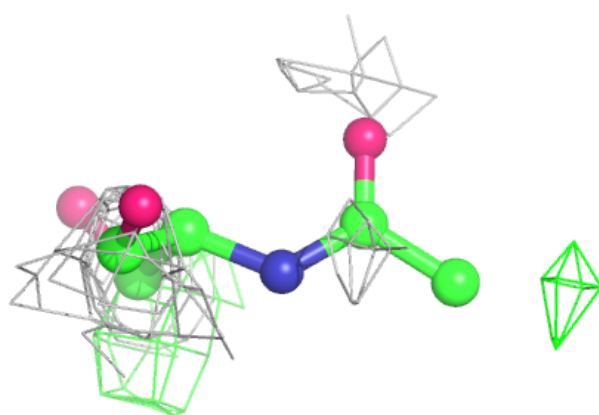
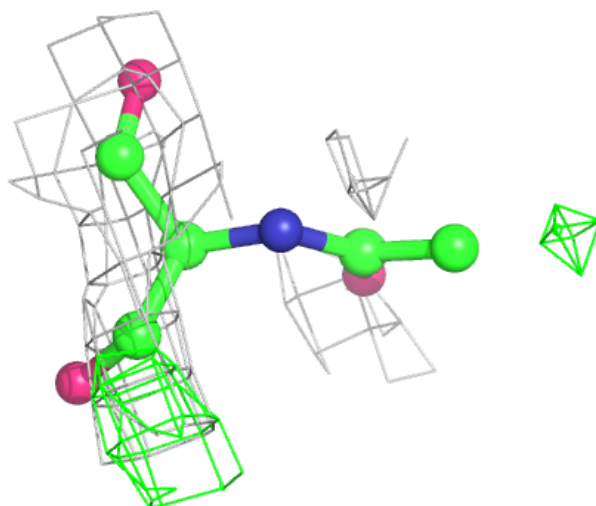
Electron density around SAC I 101:

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



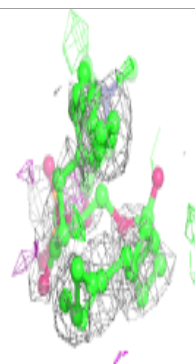
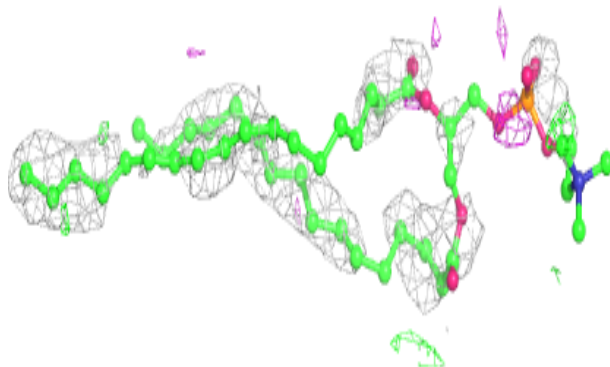
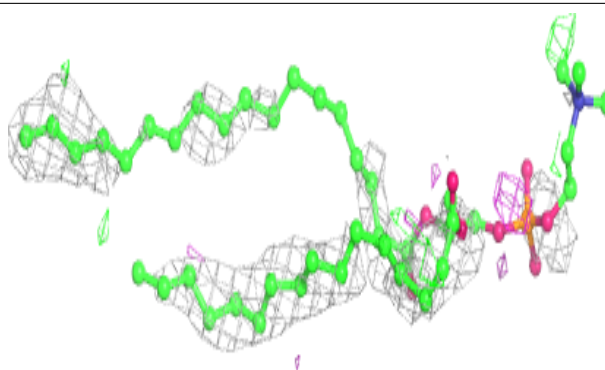
Electron density around SAC V 101:

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

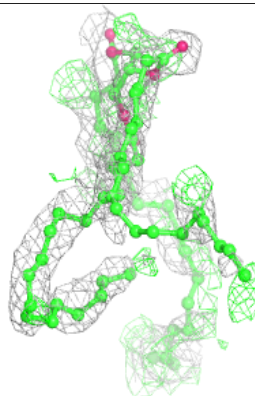
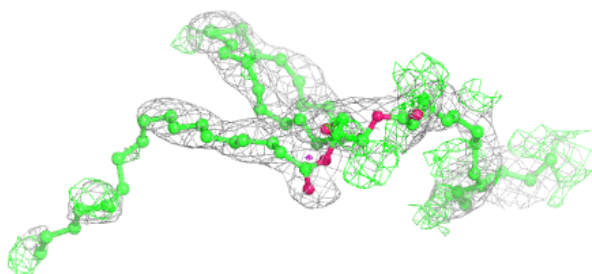
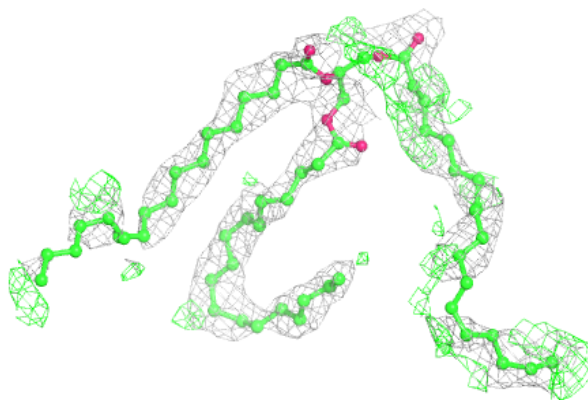


Electron density around PSC E 201:

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

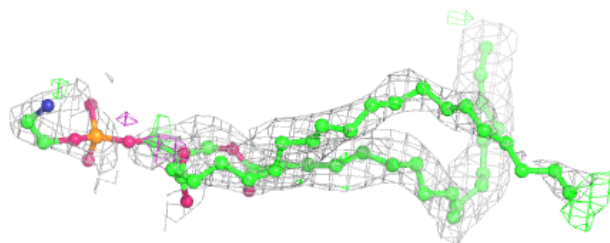
**Electron density around TGL Q 201:**

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



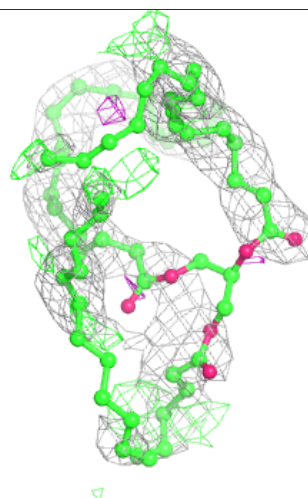
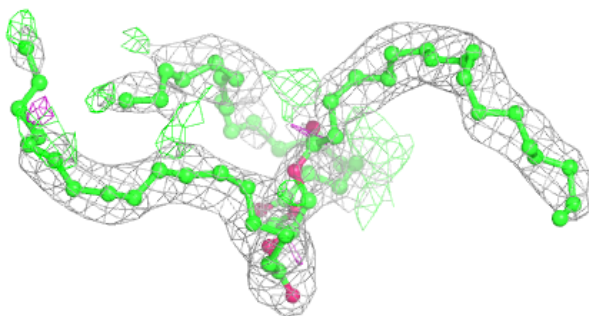
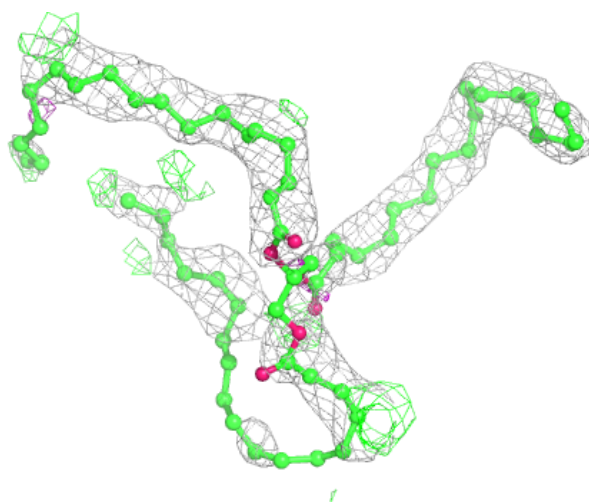
Electron density around PEK C 307:

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



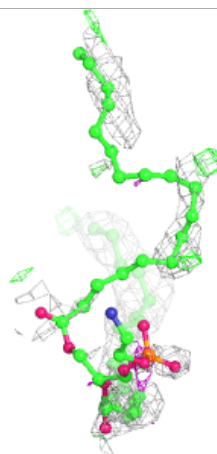
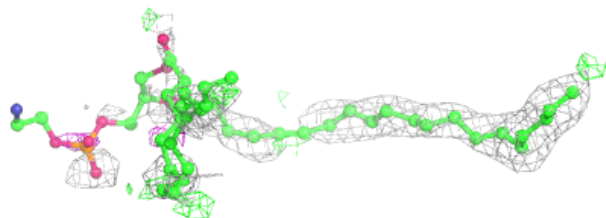
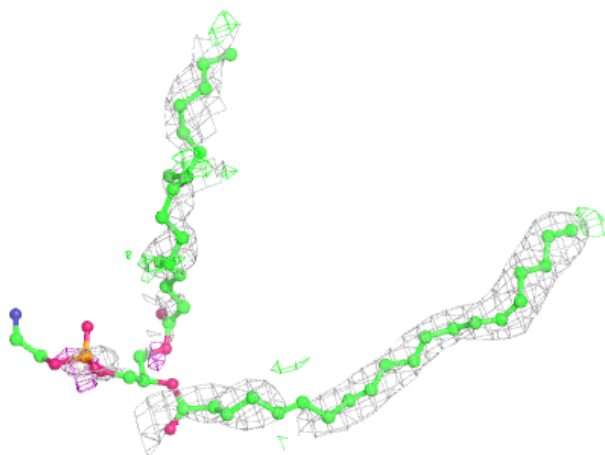
Electron density around TGL Y 101:

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



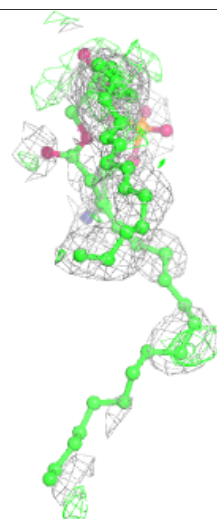
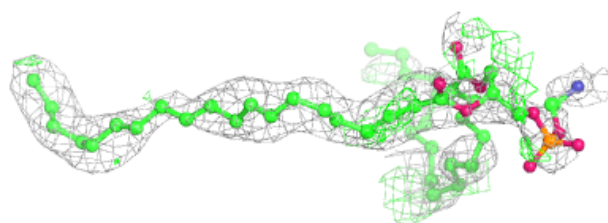
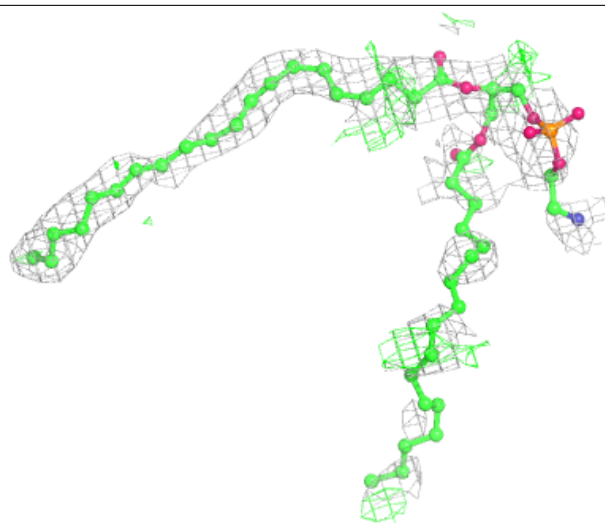
Electron density around PEK T 103:

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



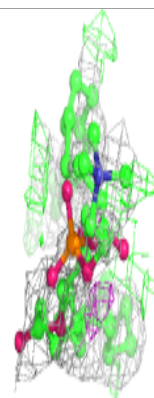
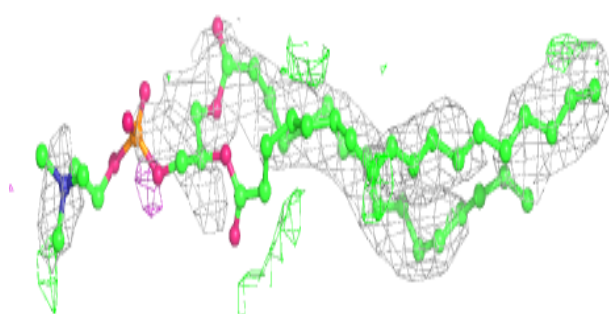
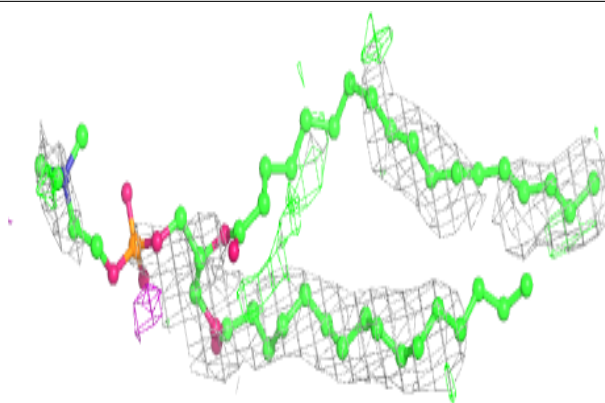
Electron density around PEK G 102:

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

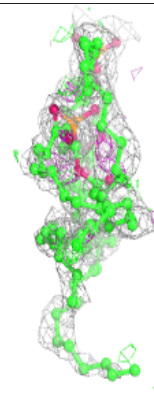
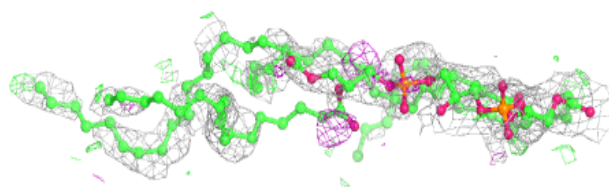
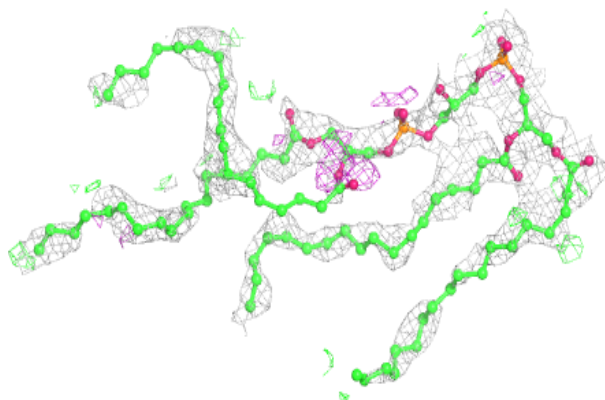


Electron density around PSC O 302:

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

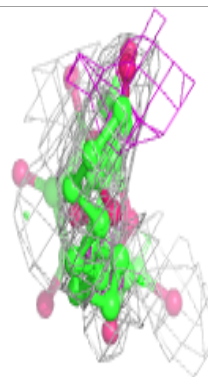
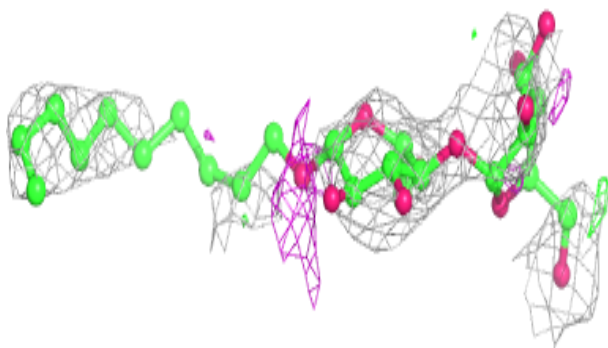
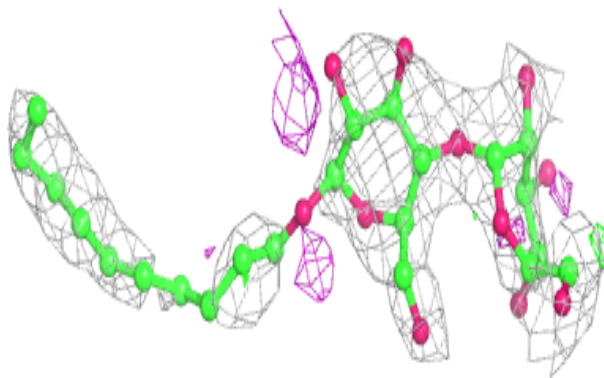
**Electron density around CDL G 101:**

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



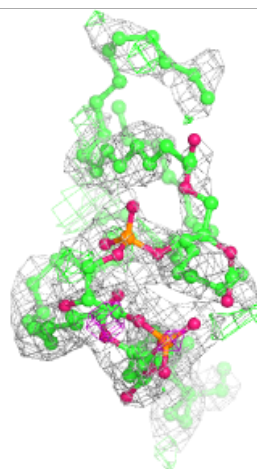
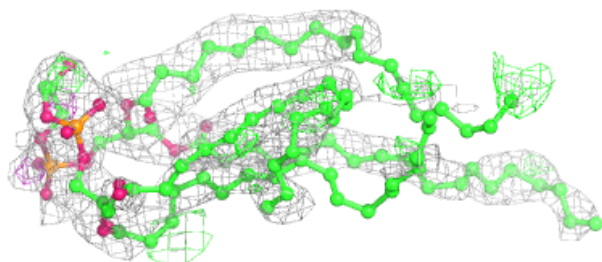
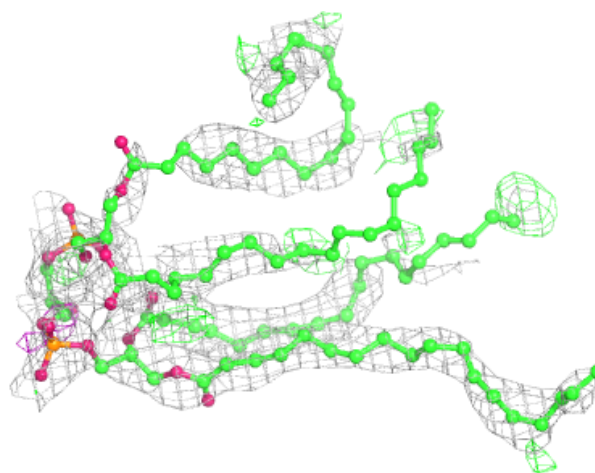
Electron density around DMU W 101:

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



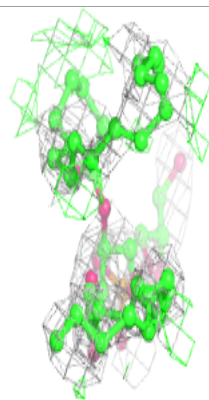
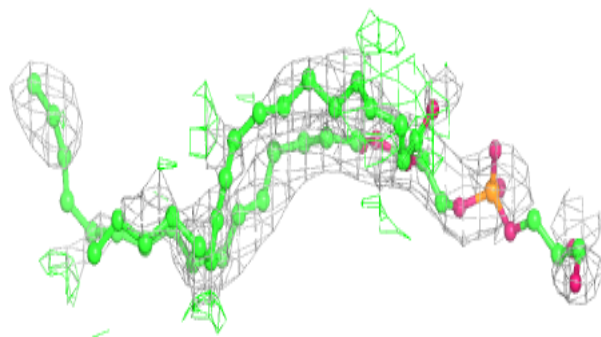
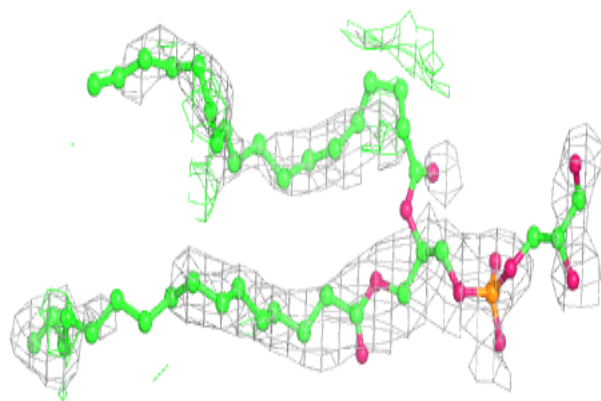
Electron density around CDL P 304:

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



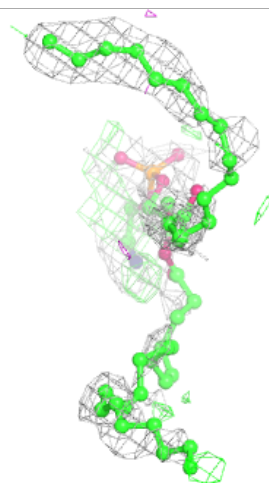
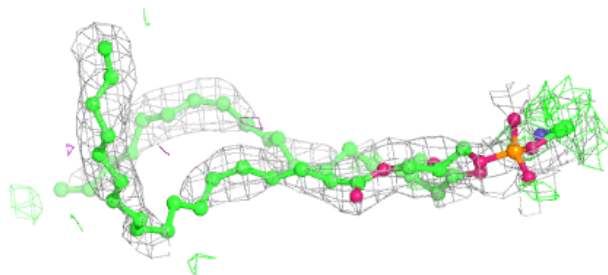
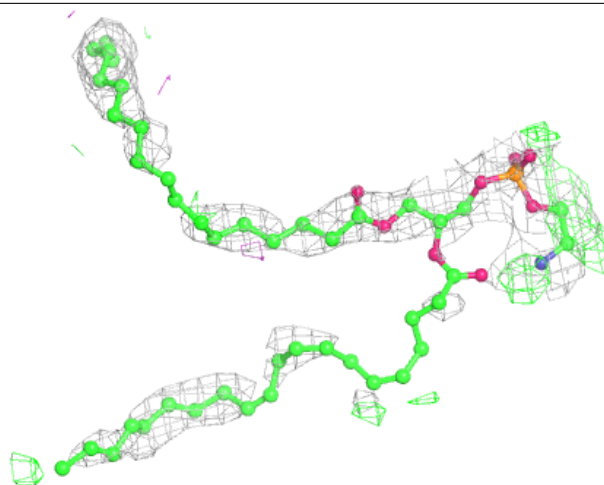
Electron density around PGV P 302:

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



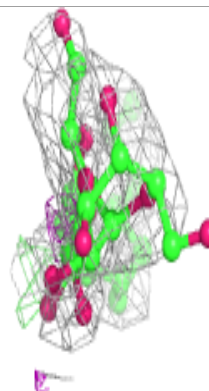
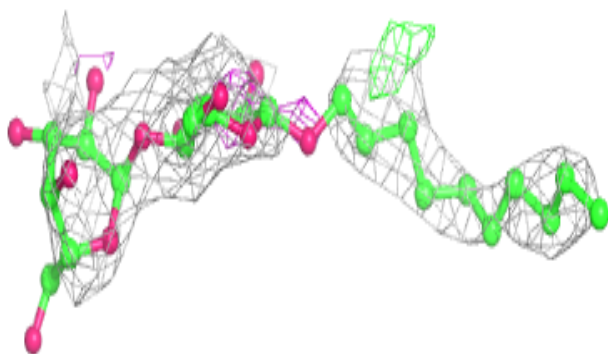
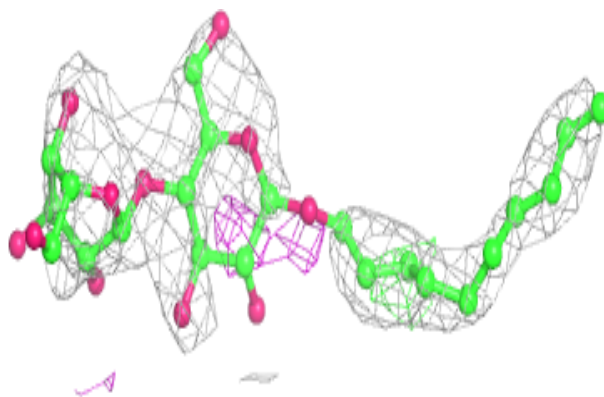
Electron density around PEK T 104:

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

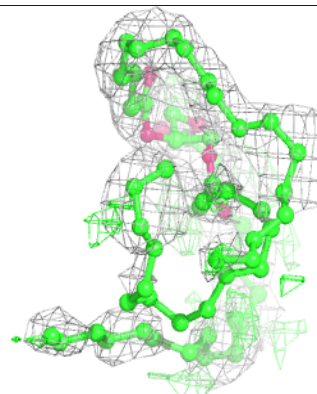
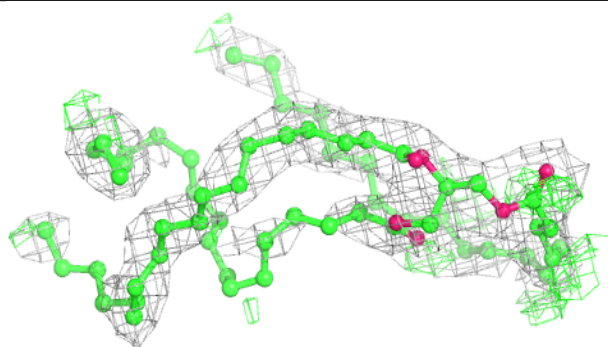
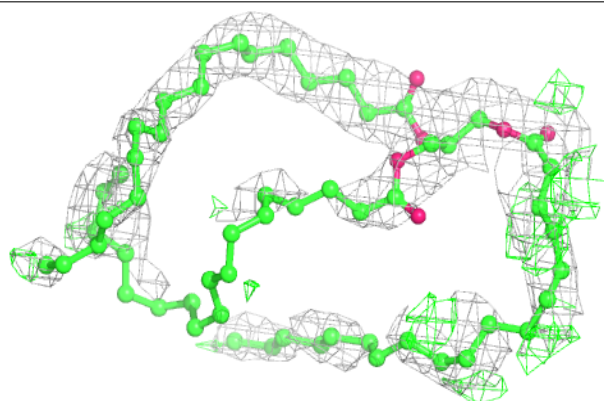


Electron density around DMU C 301:

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

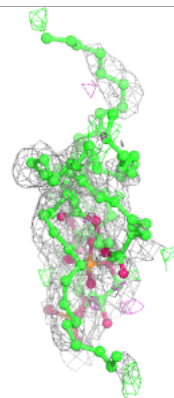
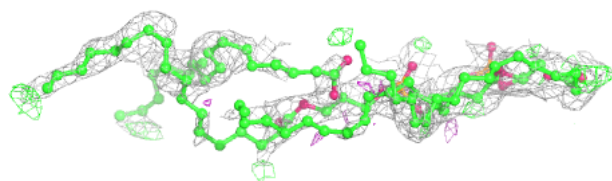
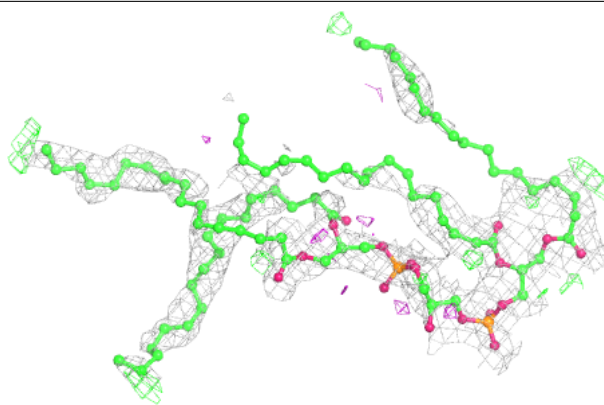
**Electron density around TGL N 606:**

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



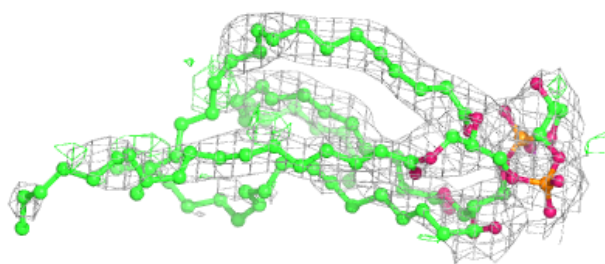
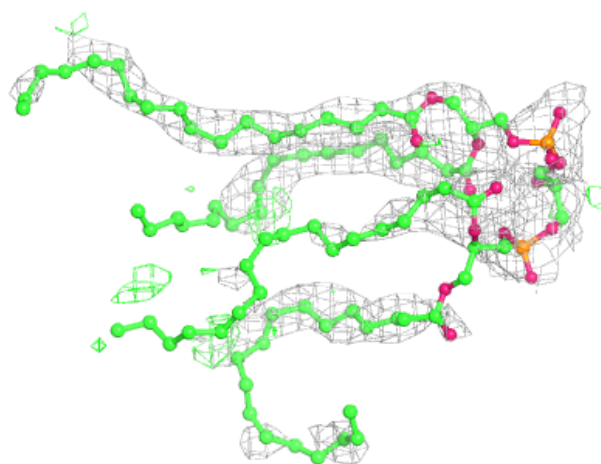
Electron density around CDL T 105:

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



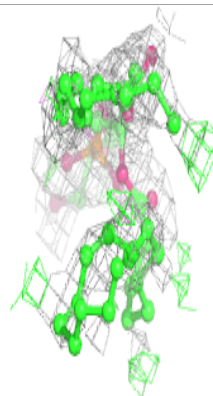
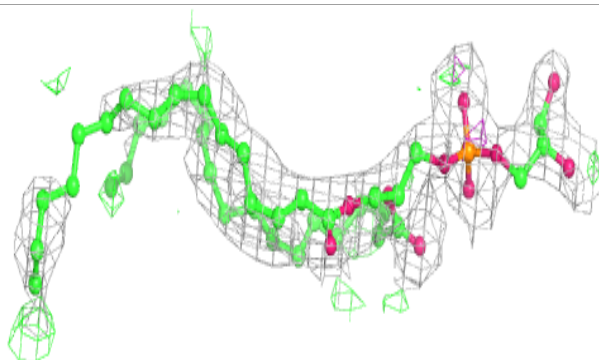
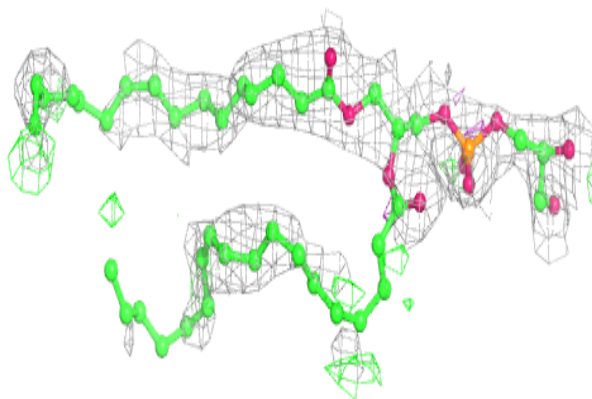
Electron density around CDL C 304:

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

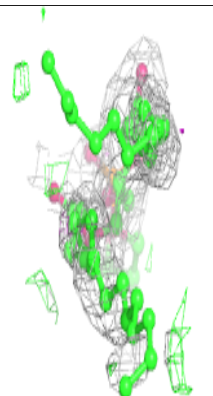
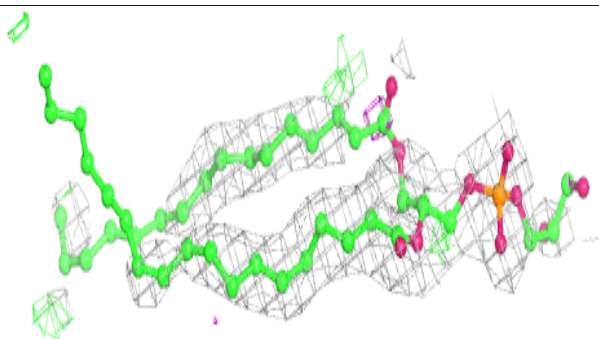
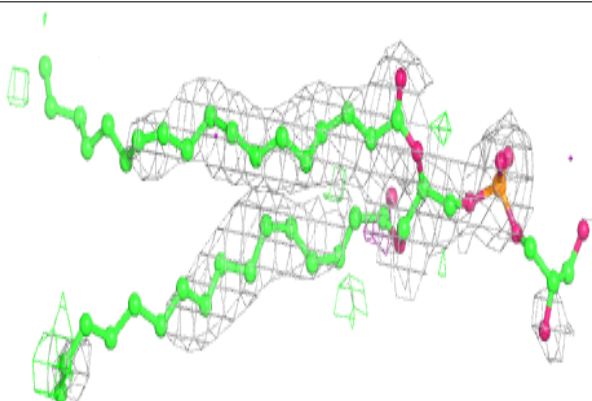


Electron density around PGV C 308:

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

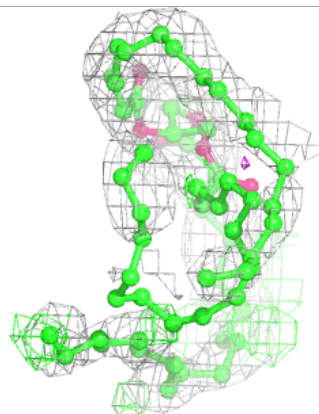
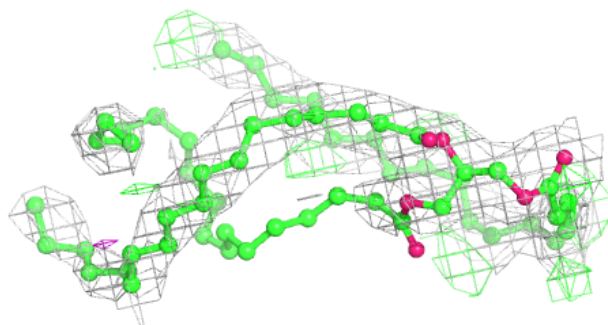
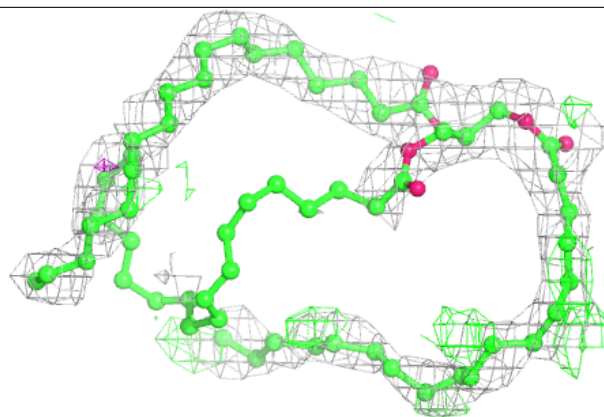
**Electron density around PGV Z 101:**

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



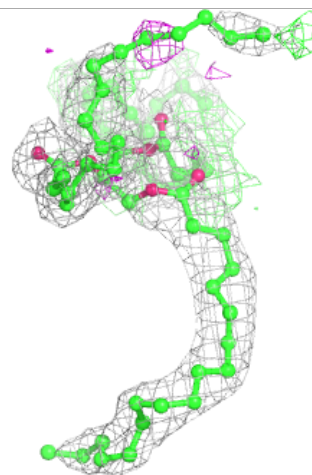
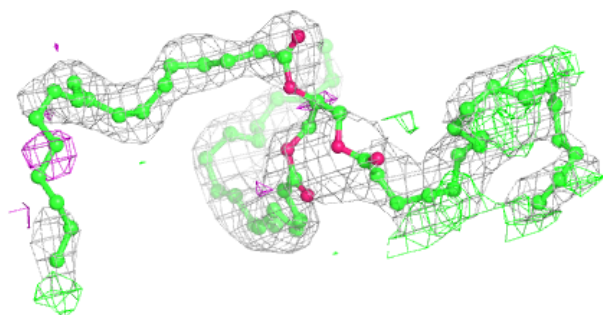
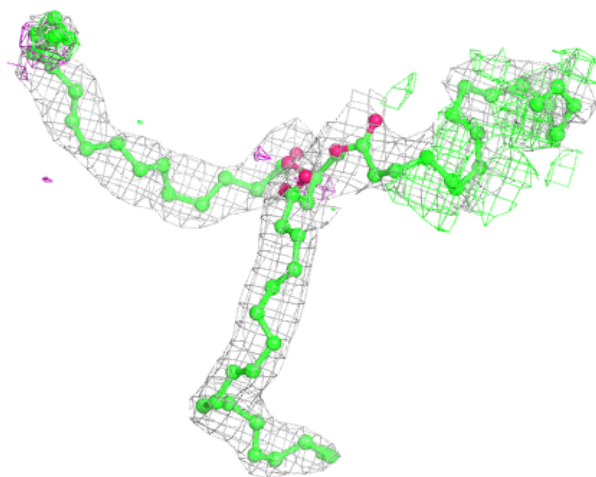
Electron density around TGL B 301:

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



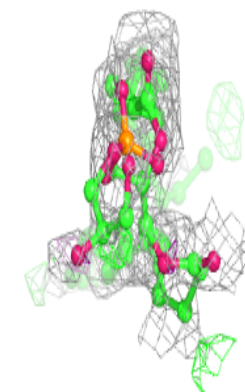
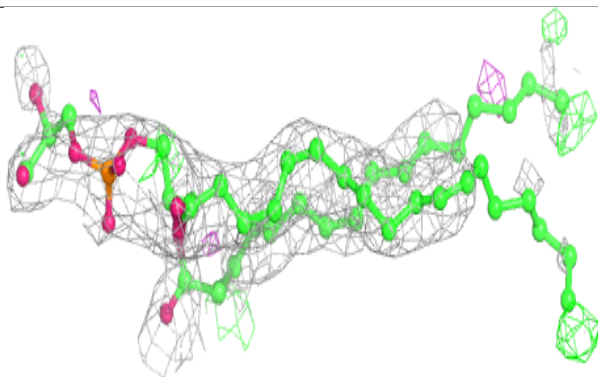
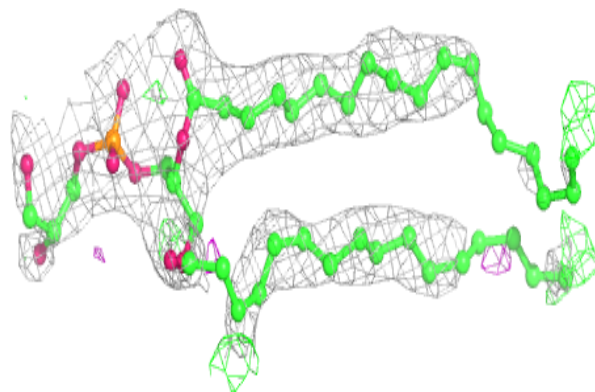
Electron density around TGL L 101:

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

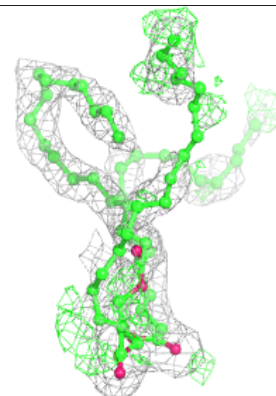
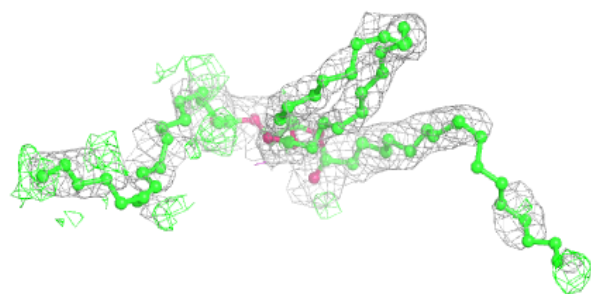
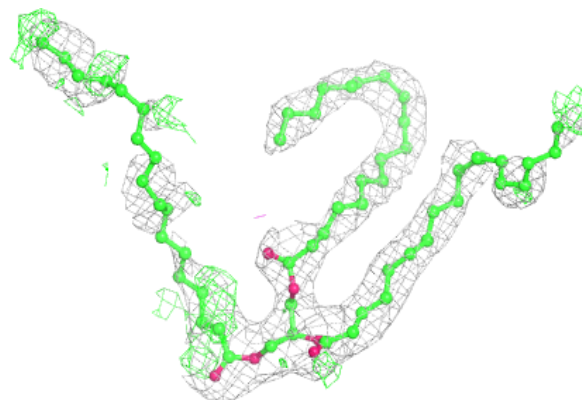


Electron density around PGV A 607:

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

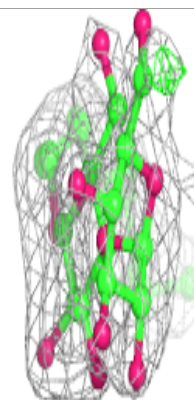
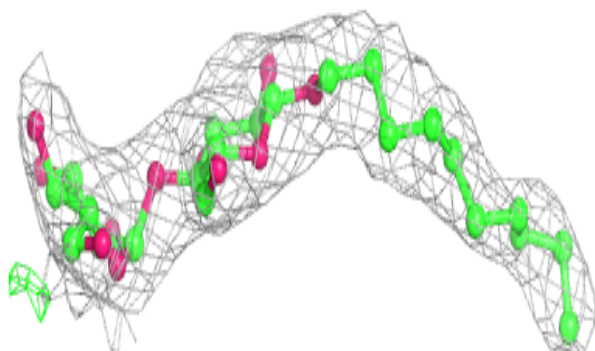
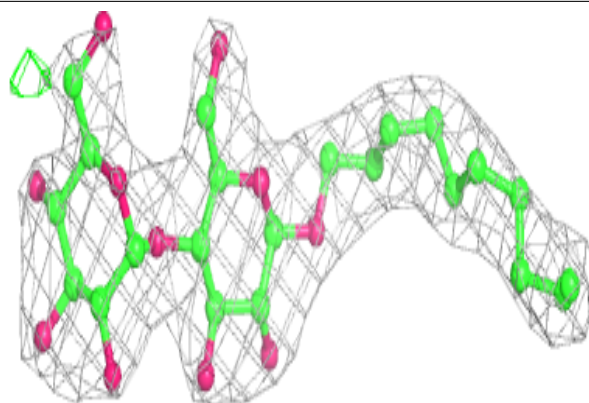
**Electron density around TGL D 201:**

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

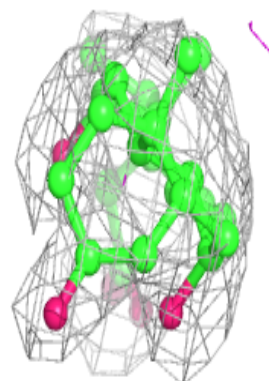
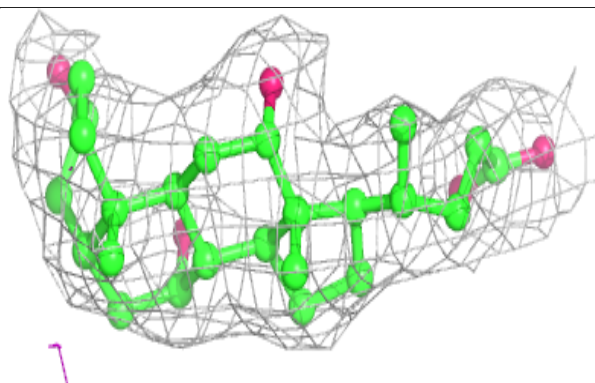
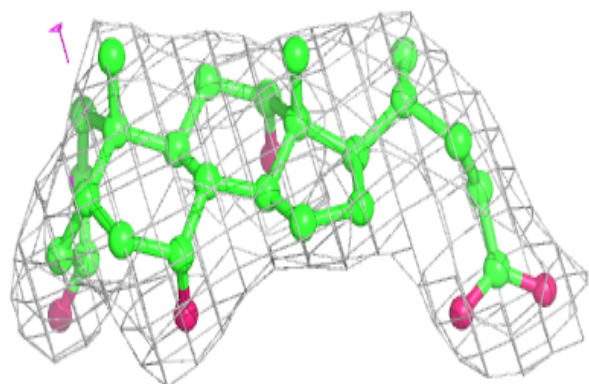


Electron density around DMU Z 102:

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

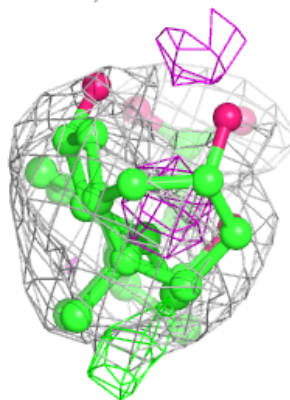
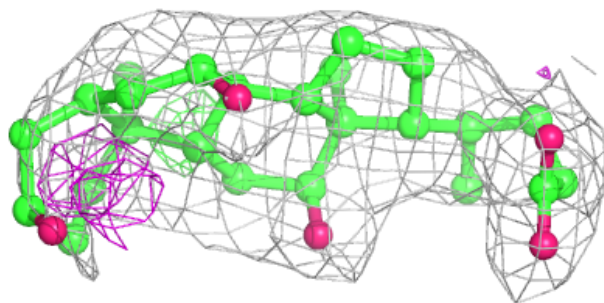
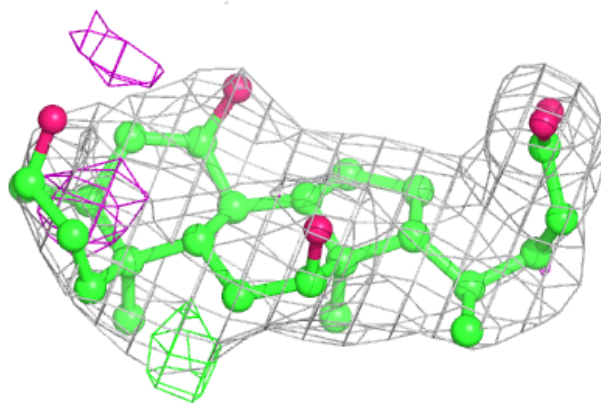
**Electron density around CHD W 102:**

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

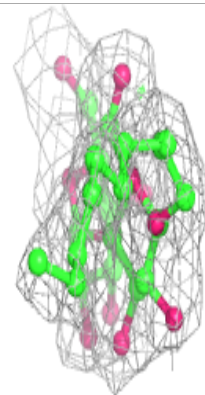
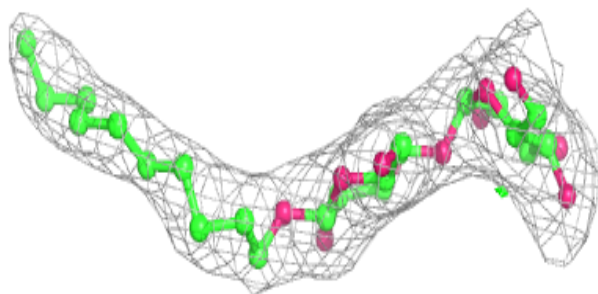
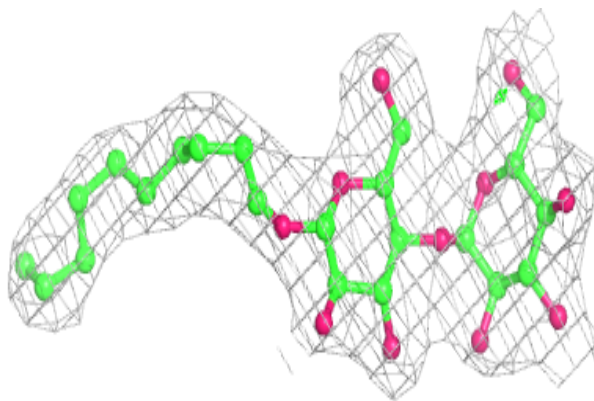


Electron density around CHD J 101:

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

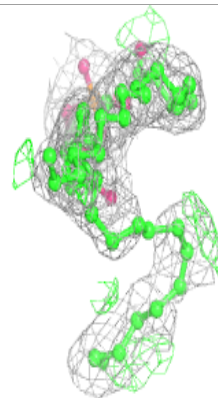
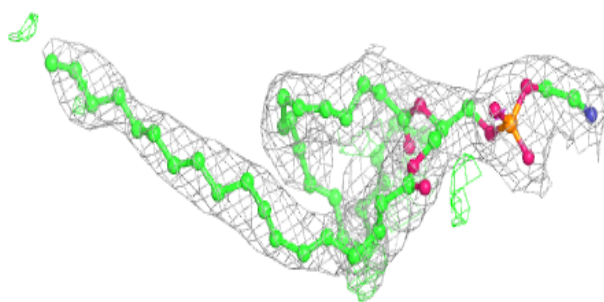
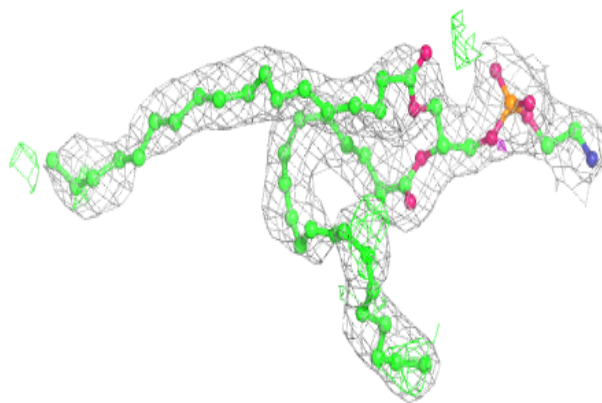
**Electron density around DMU D 202:**

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

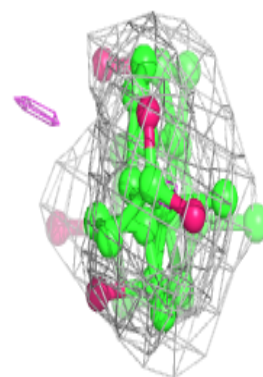
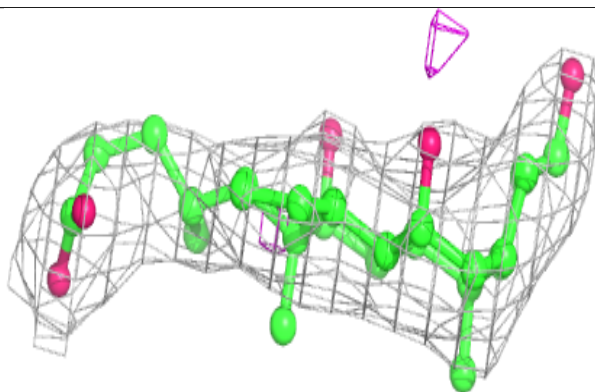
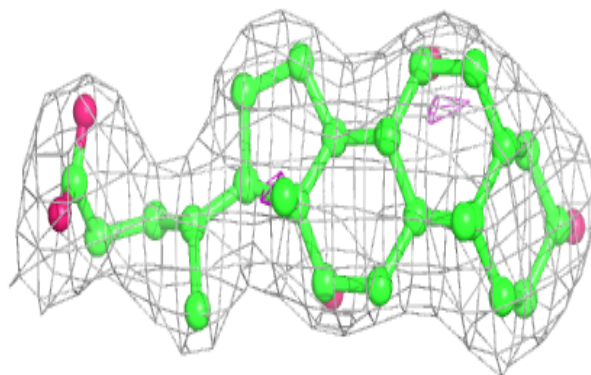


Electron density around PEK T 102:

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

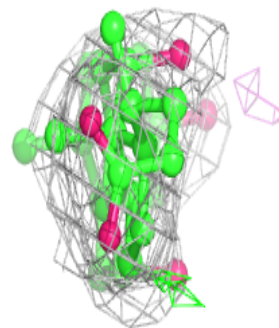
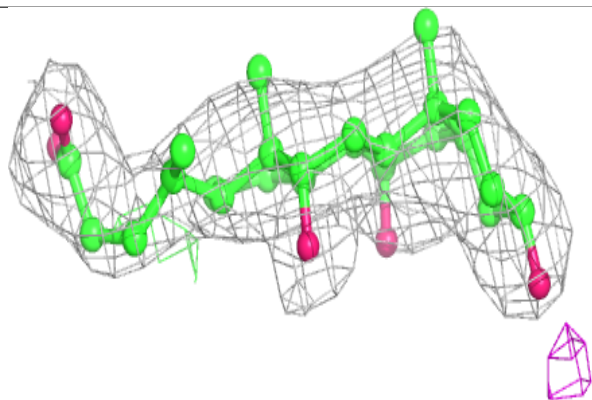
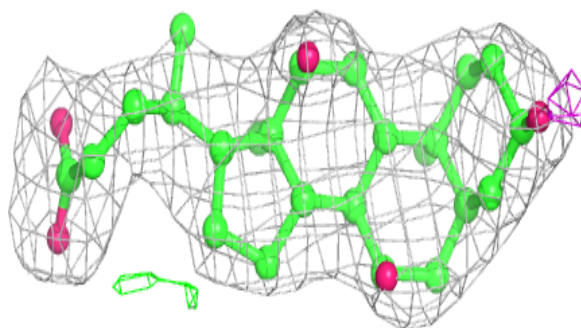
**Electron density around CHD C 305:**

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

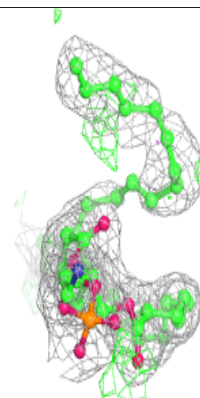
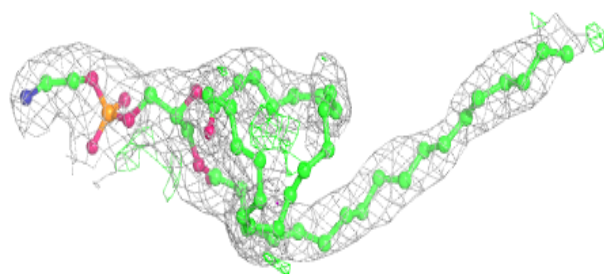
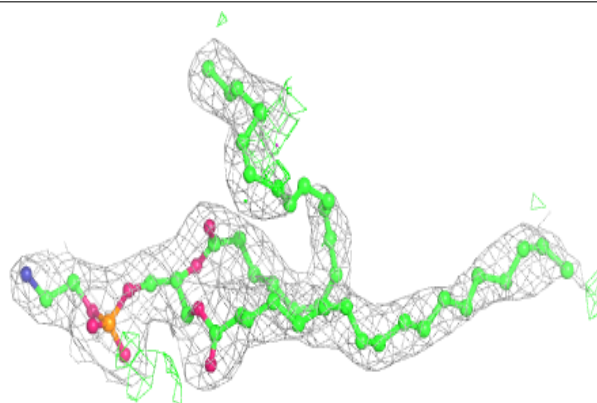


Electron density around CHD P 305:

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

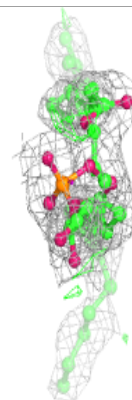
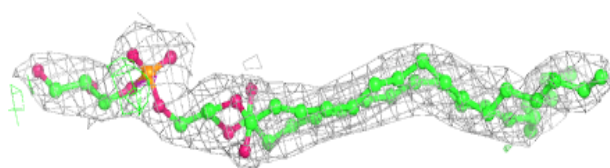
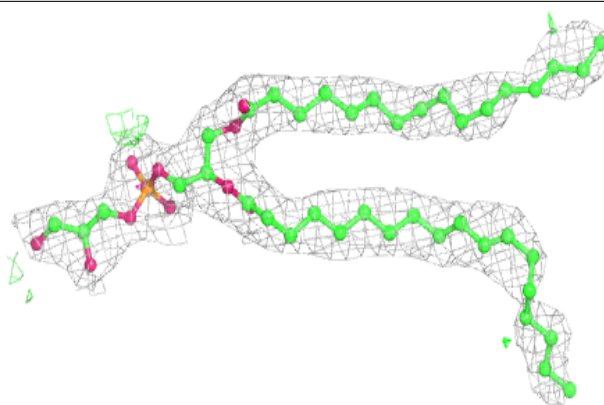
**Electron density around PEK C 302:**

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

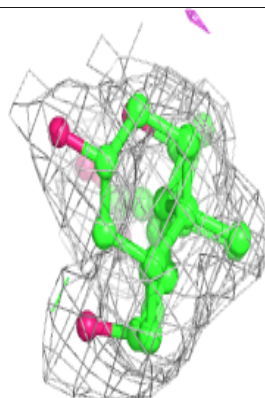
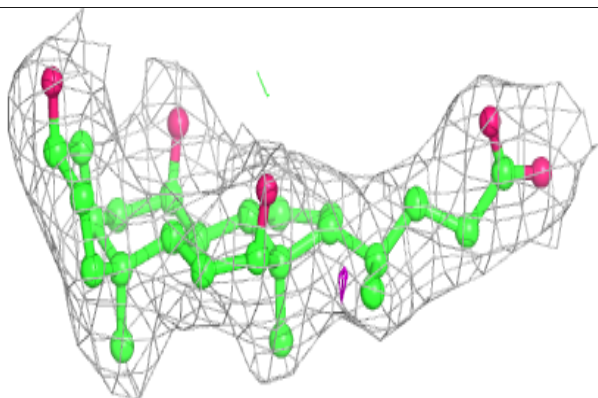
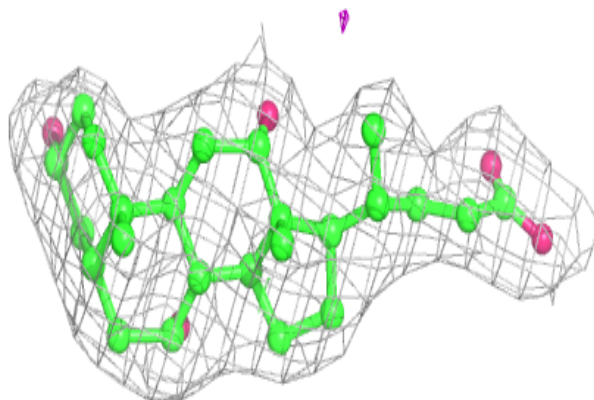


Electron density around PGV C 303:

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

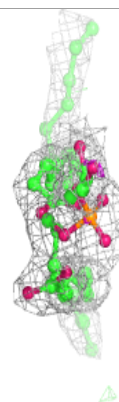
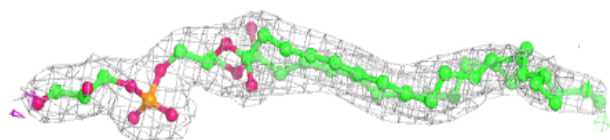
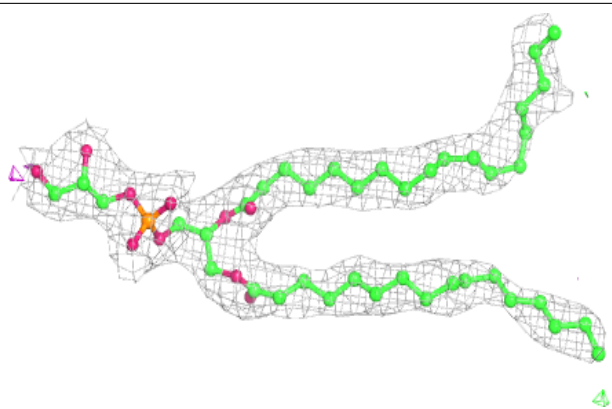
**Electron density around CHD P 306:**

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

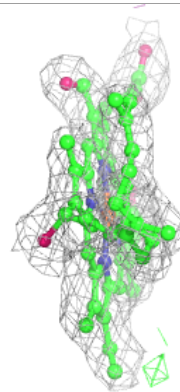
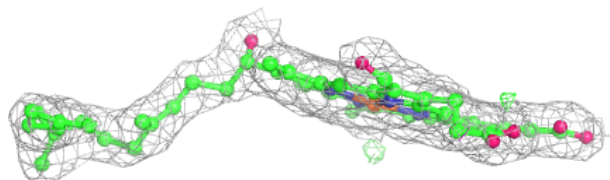
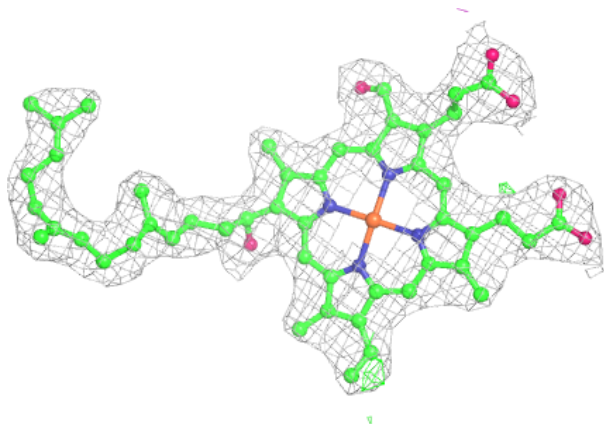


Electron density around PGV P 303:

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

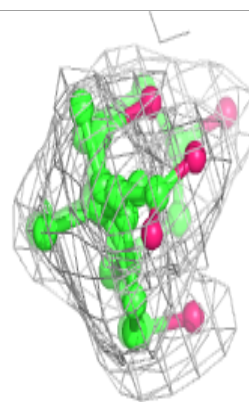
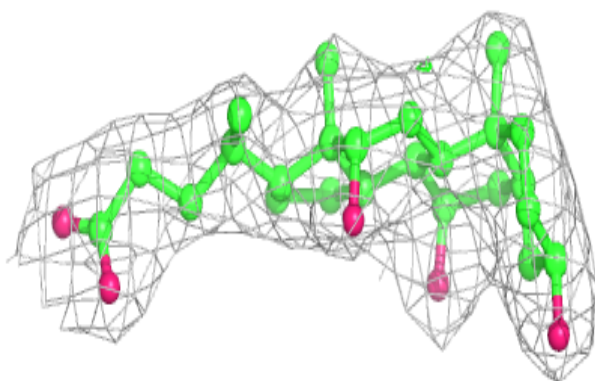
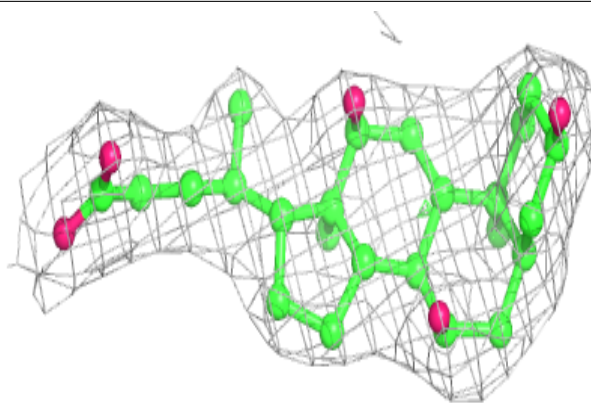
**Electron density around HEA N 602:**

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

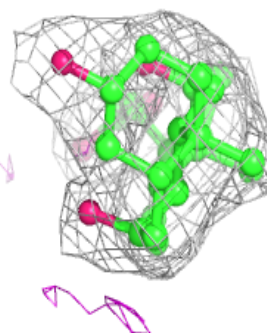
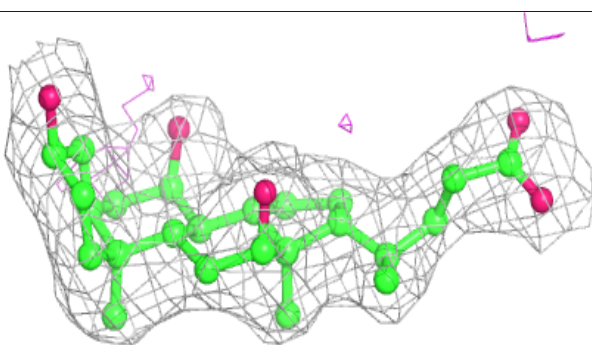
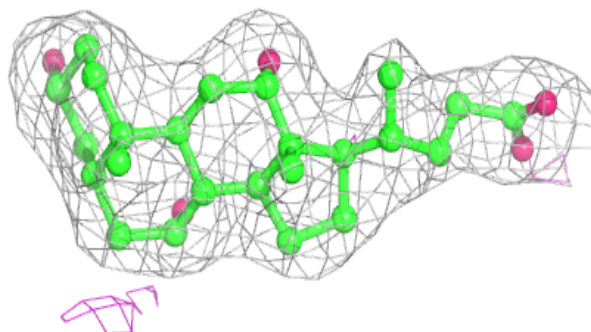


Electron density around CHD C 306:

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

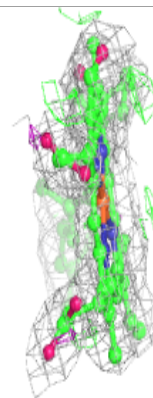
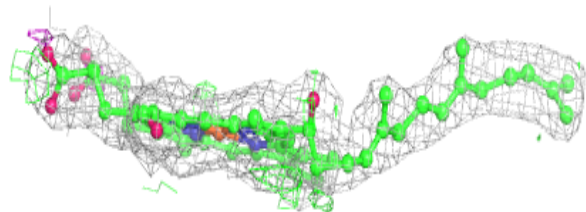
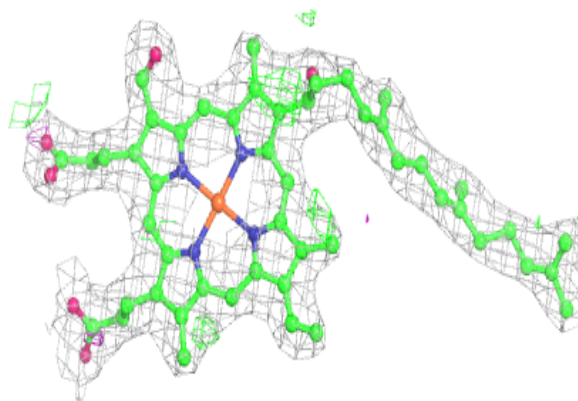
**Electron density around CHD G 103:**

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

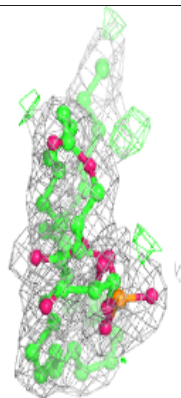
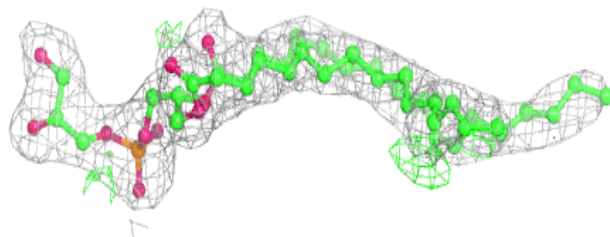
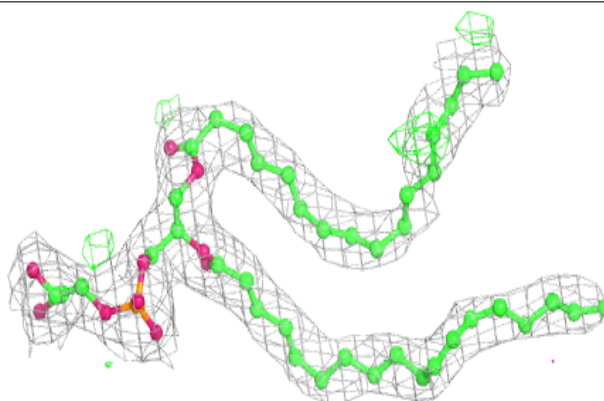


Electron density around HEA A 601:

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

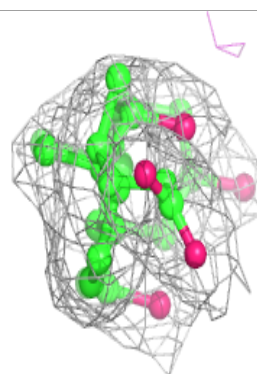
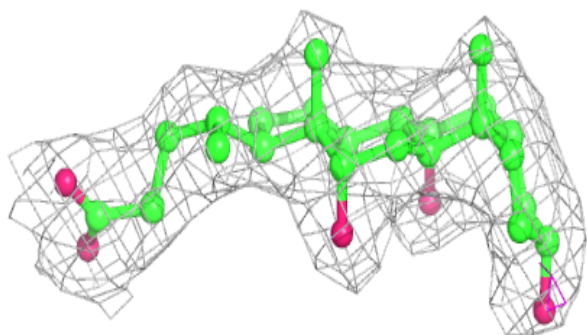
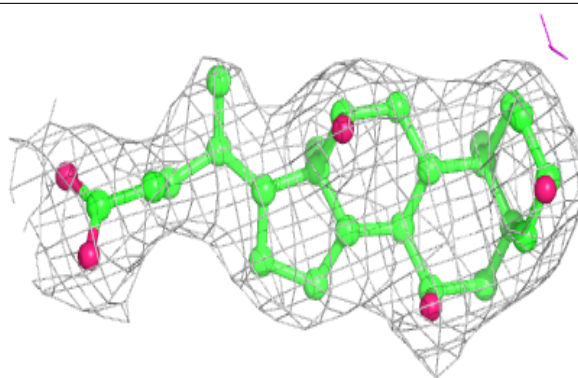
**Electron density around PGV P 301:**

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

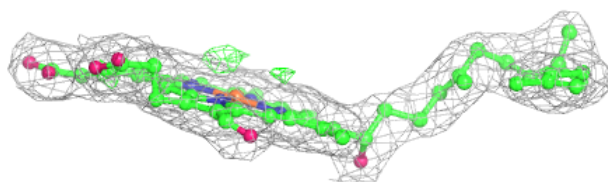
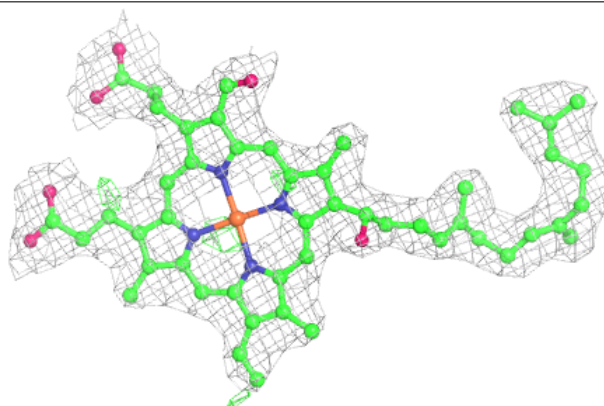


Electron density around CHD T 101:

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

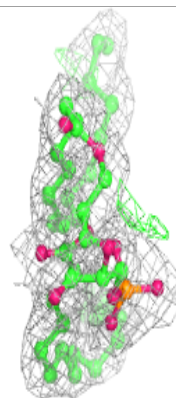
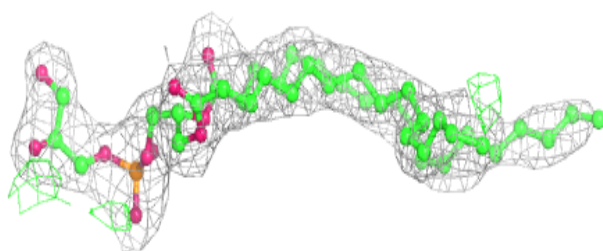
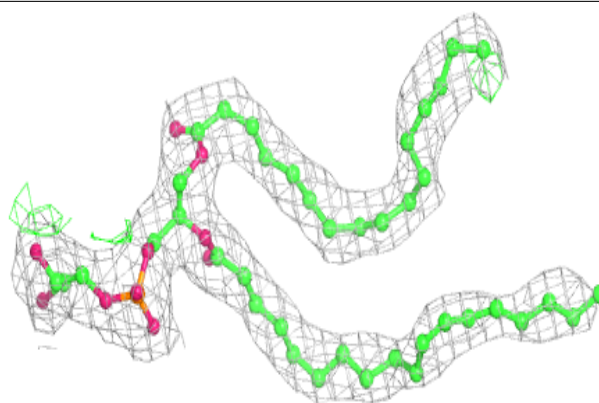
**Electron density around HEA A 602:**

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

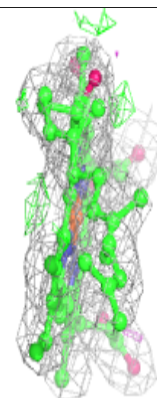
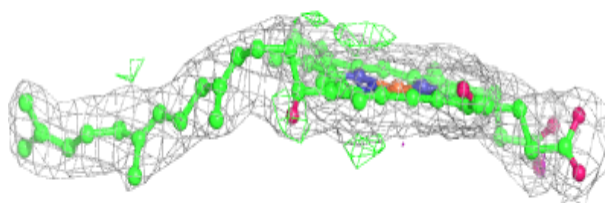
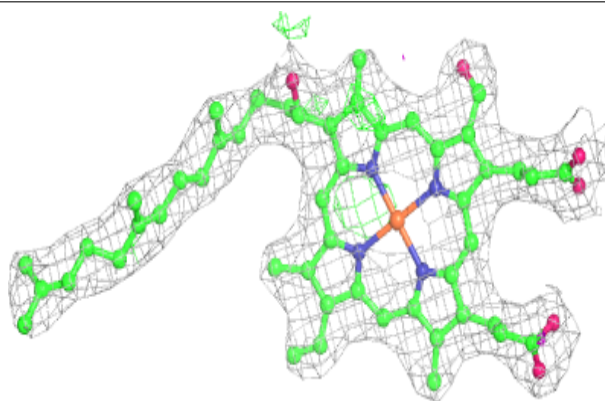


Electron density around PGV A 606:

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

**Electron density around 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.