



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:34 PM UTC

PDB ID : 8GCQ / pdb_00008gcq
Title : SFX structure of oxidized cytochrome c oxidase at 2.38 Angstrom resolution
Authors : Ishigami, I.; Yeh, S.-R.; Rousseau, D.L.
Deposited on : 2023-03-02
Resolution : 2.38 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

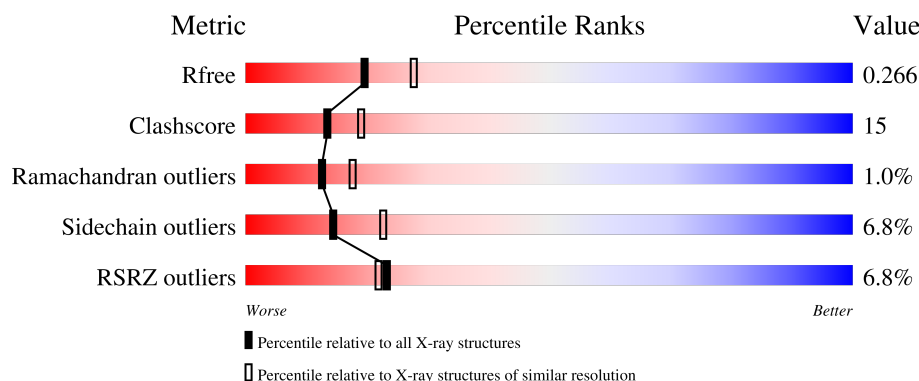
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	59% 36% 5%
1	N	514	4% 56% 41% .
2	B	227	3% 63% 33% ..
2	O	227	11% 67% 30% .
3	C	261	% 67% 30% ..

Continued on next page...

Continued from previous page...

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	47	
13	Z	47	

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
23	CHD	T	103	X	-	-	-
23	CHD	Y	101	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	DMU	C	309	X	-	-	-
26	DMU	C	310	X	-	-	-
26	DMU	G	101	X	-	-	-
26	DMU	M	101	X	-	-	-
26	DMU	P	302	X	-	-	-
26	DMU	Q	201	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 31457 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	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- 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	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	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	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0
7	T	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0

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

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

- Molecule 9 is a protein called Cytochrome c oxidase 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	0	0
			592	385	106	97	4			

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

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

Continued on next page...

Continued from previous page...

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	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

- Molecule 12 is a protein called Cytochrome c oxidase subunit 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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	SER	-	expression tag	UNP P10175
Z	0	SER	-	expression tag	UNP P10175

- Molecule 14 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

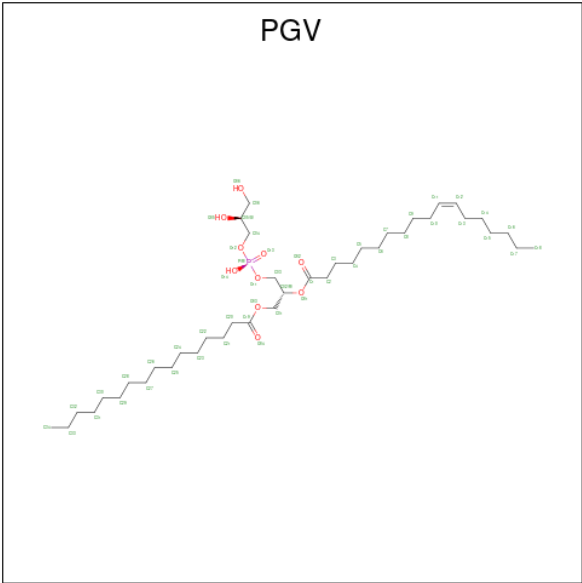
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 17 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P) (labeled as "Ligand of Interest" by depositor).



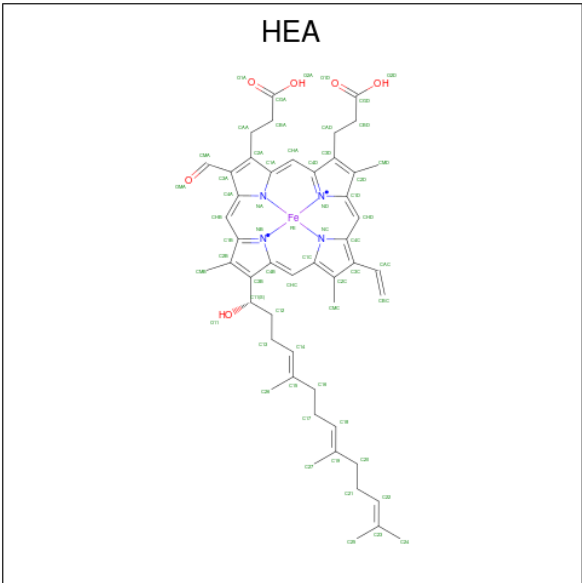
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	O	P	0	0
			51	40	10	1		
17	C	1	Total	C	O	P	0	0
			51	40	10	1		
17	C	1	Total	C	O	P	0	0
			51	40	10	1		
17	H	1	Total	C	O	P	0	0
			51	40	10	1		
17	N	1	Total	C	O	P	0	0
			51	40	10	1		

Continued on next page...

Continued from previous page...

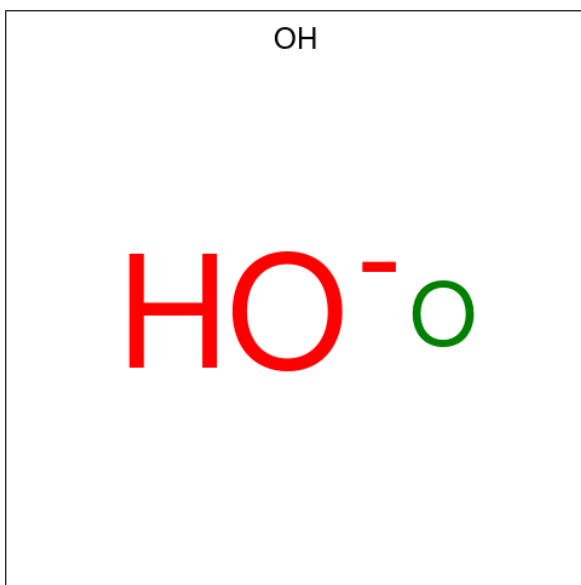
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	N	1	Total	C	O	P	0	0
			51	40	10	1		
17	P	1	Total	C	O	P	0	0
			51	40	10	1		
17	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 18 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



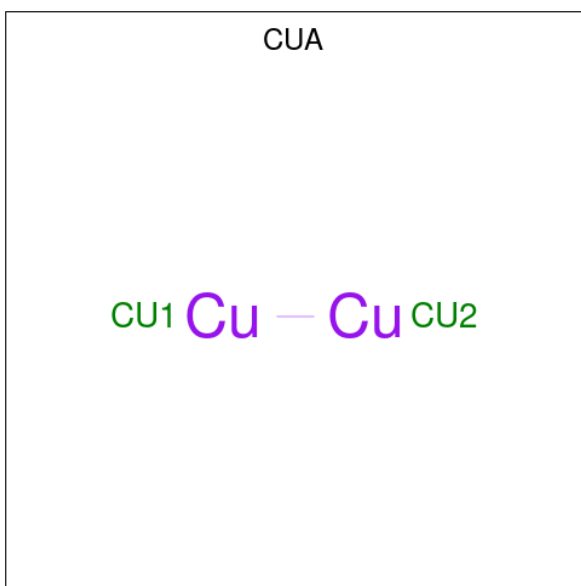
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 19 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



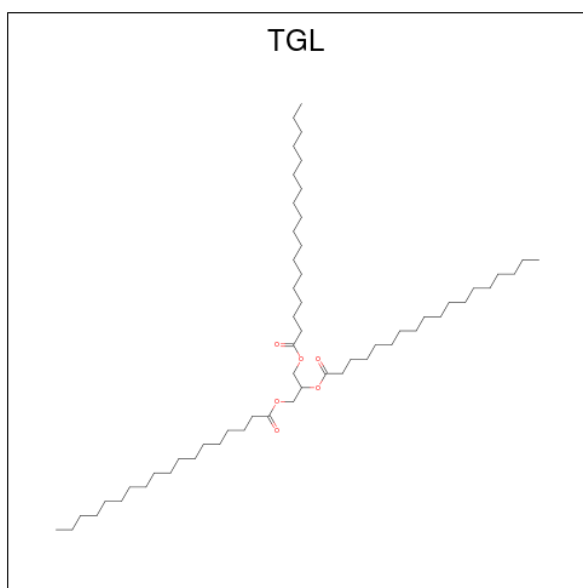
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total O 1 1	0	0
19	N	1	Total O 1 1	0	0

- Molecule 20 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



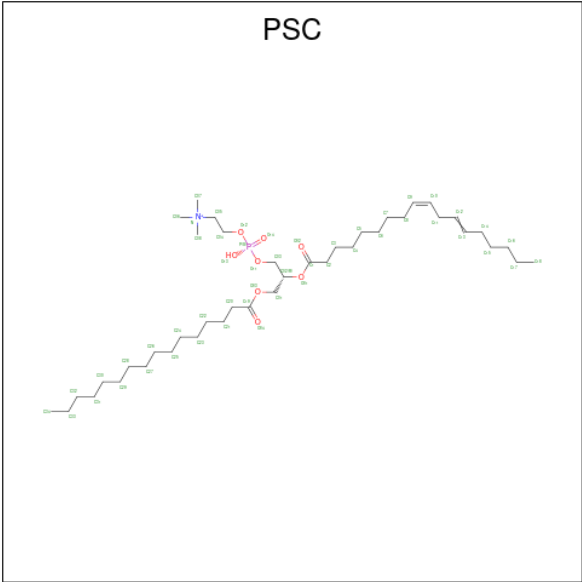
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	B	1	Total Cu 2 2	0	0
20	O	1	Total Cu 2 2	0	0

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



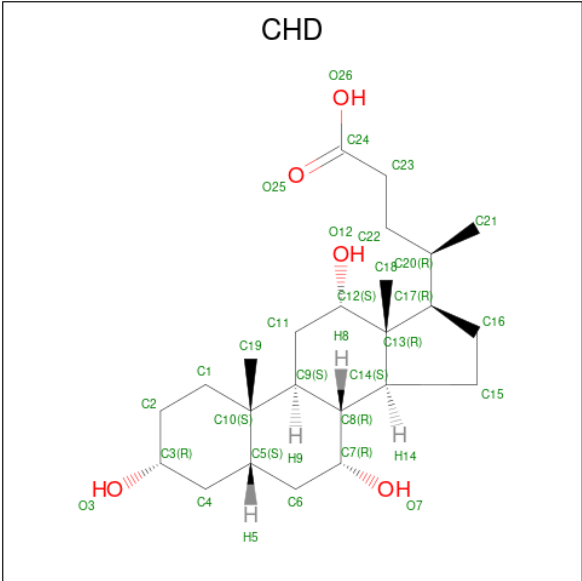
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	O	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: $C_{42}H_{81}NO_8P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$) (labeled as "Ligand of Interest" by depositor).



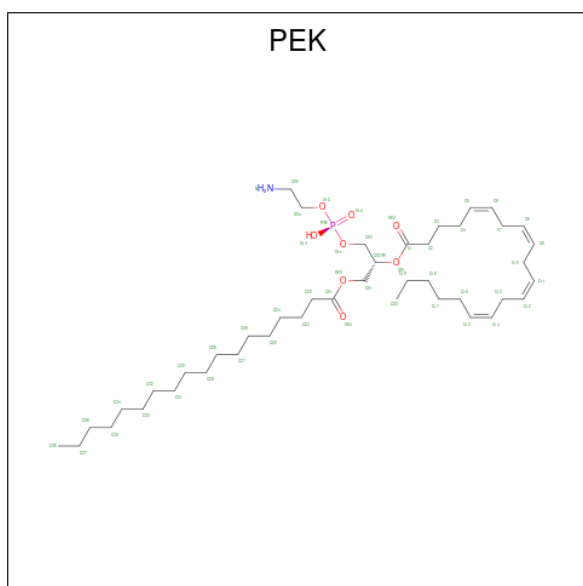
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			29	24	5		

Continued on next page...

Continued from previous page...

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

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



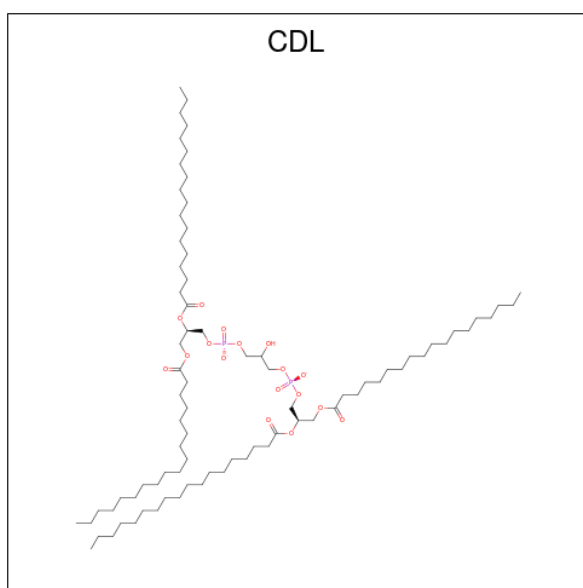
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

Continued on next page...

Continued from previous page...

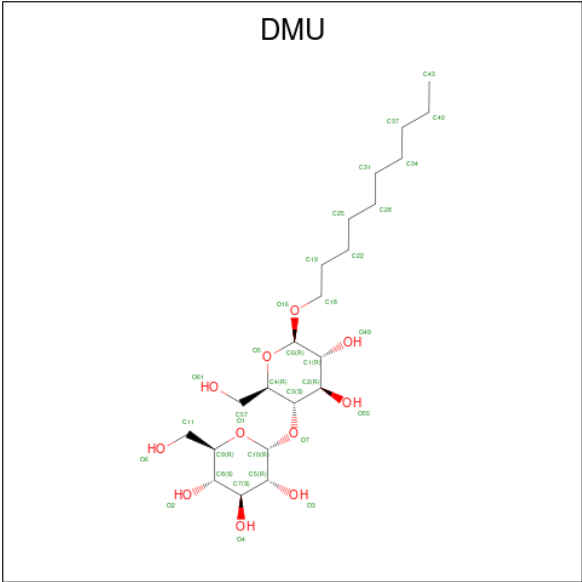
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 25 is CARDIOLIPIN (CCD ID: 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	C	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	P	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$) (labeled as "Ligand of Interest" by depositor).

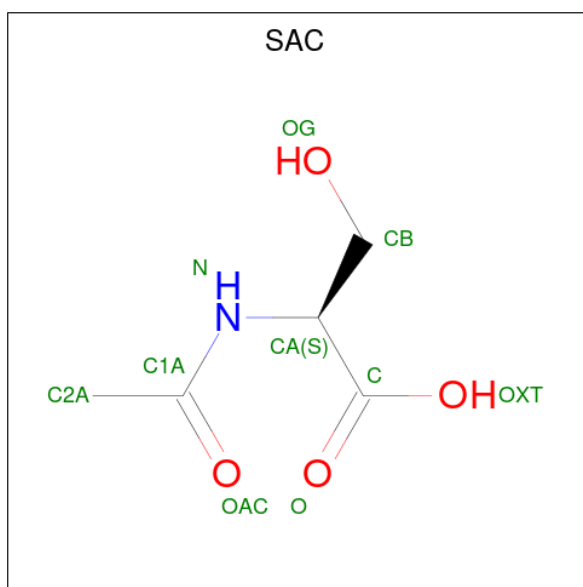


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	C	1	Total	C	O	0	0
			33	22	11		
26	C	1	Total	C	O	0	0
			33	22	11		
26	G	1	Total	C	O	0	0
			33	22	11		
26	M	1	Total	C	O	0	0
			33	22	11		
26	P	1	Total	C	O	0	0
			33	22	11		
26	Q	1	Total	C	O	0	0
			33	22	11		

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

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

- Molecule 28 is N-ACETYL-SERINE (CCD ID: SAC) (formula: C₅H₉NO₄) (labeled as "Lig- and of Interest" by depositor).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	104	Total	O	0	0
			104	104		
29	B	46	Total	O	0	0
			46	46		
29	C	44	Total	O	0	0
			44	44		
29	D	23	Total	O	0	0
			23	23		
29	E	23	Total	O	0	0
			23	23		
29	F	20	Total	O	0	0
			20	20		
29	G	13	Total	O	0	0
			13	13		
29	H	26	Total	O	0	0
			26	26		
29	I	8	Total	O	0	0
			8	8		
29	J	11	Total	O	0	0
			11	11		

Continued on next page...

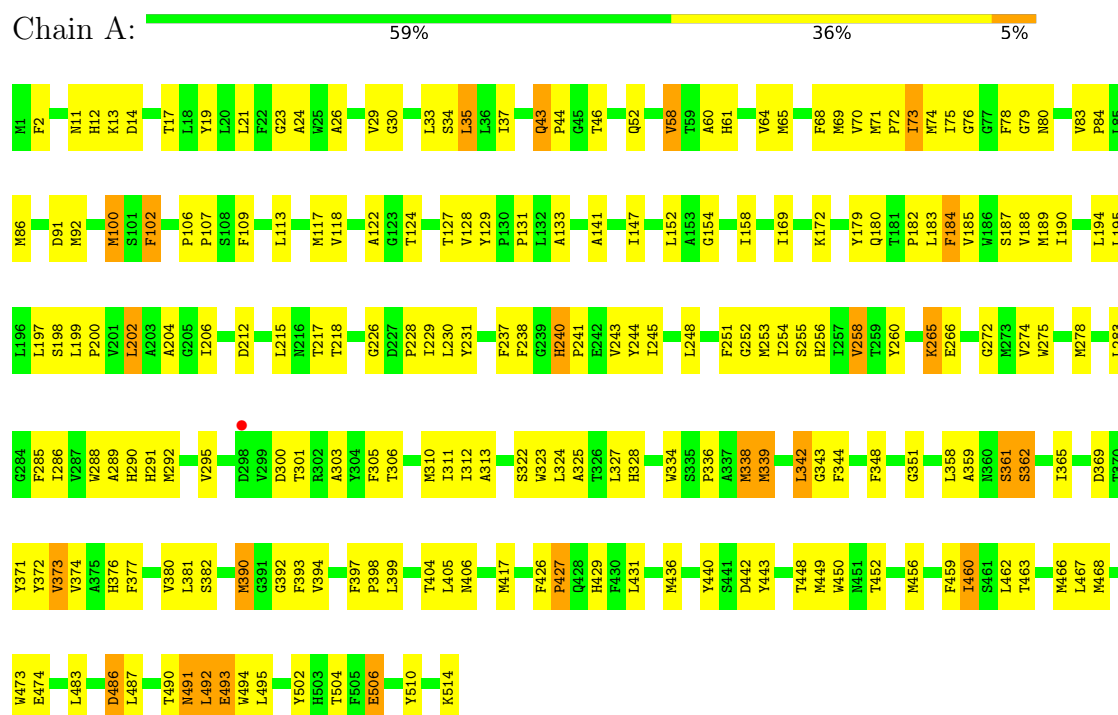
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	K	8	Total 8	O 8	0	0
29	L	13	Total 13	O 13	0	0
29	M	7	Total 7	O 7	0	0
29	N	74	Total 74	O 74	0	0
29	O	39	Total 39	O 39	0	0
29	P	40	Total 40	O 40	0	0
29	Q	28	Total 28	O 28	0	0
29	R	8	Total 8	O 8	0	0
29	S	19	Total 19	O 19	0	0
29	T	17	Total 17	O 17	0	0
29	U	7	Total 7	O 7	0	0
29	V	6	Total 6	O 6	0	0
29	W	5	Total 5	O 5	0	0
29	X	8	Total 8	O 8	0	0
29	Y	1	Total 1	O 1	0	0
29	Z	3	Total 3	O 3	0	0

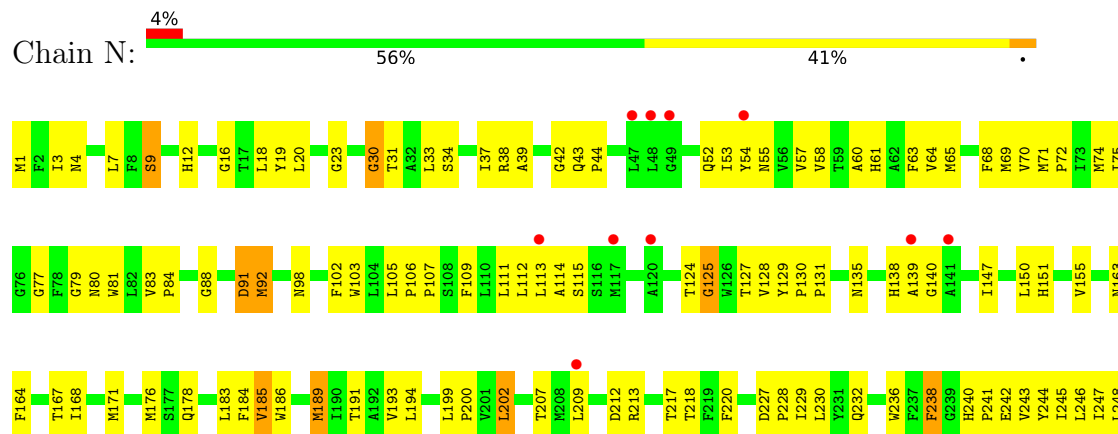
3 Residue-property plots [i](#)

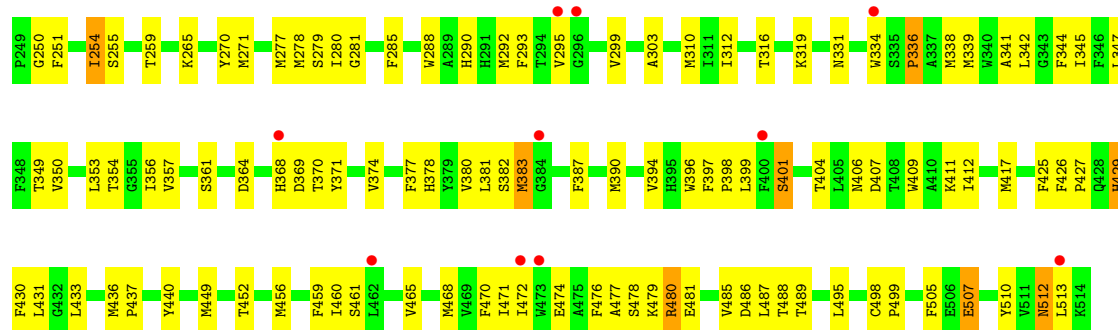
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Cytochrome c oxidase subunit 1

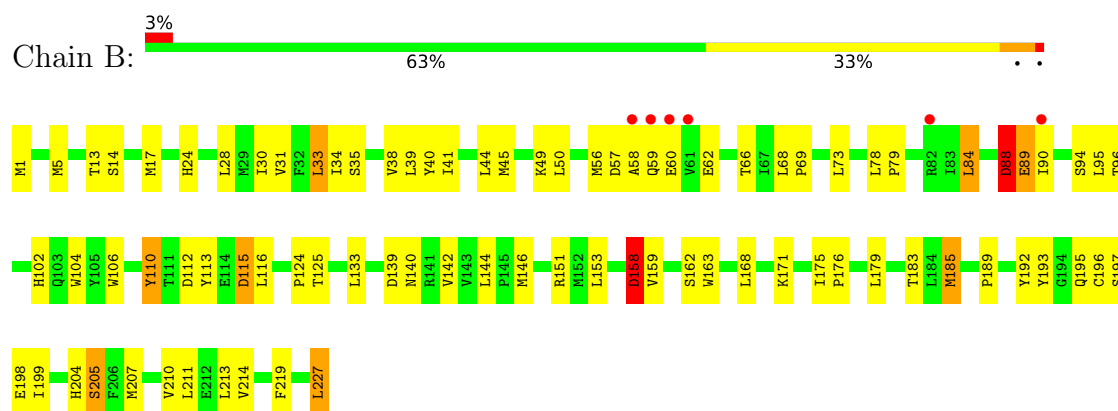


• Molecule 1: Cytochrome c oxidase subunit 1

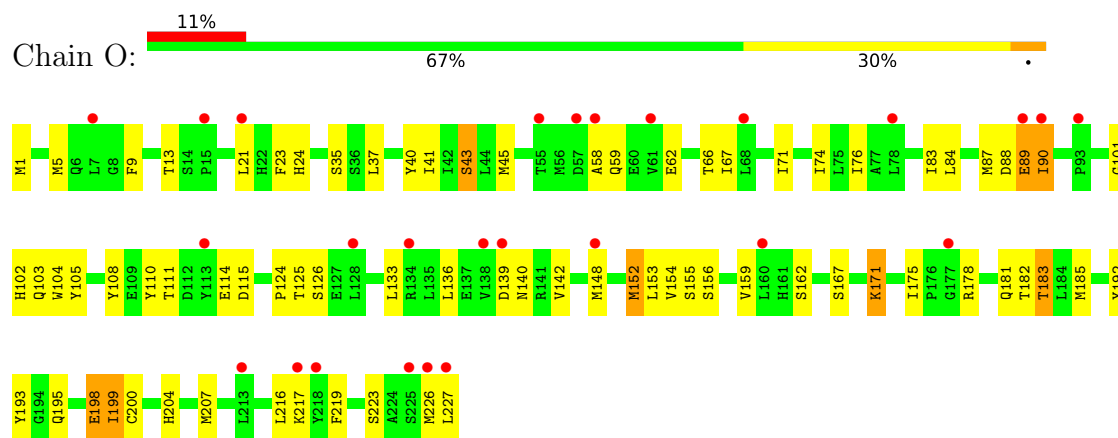




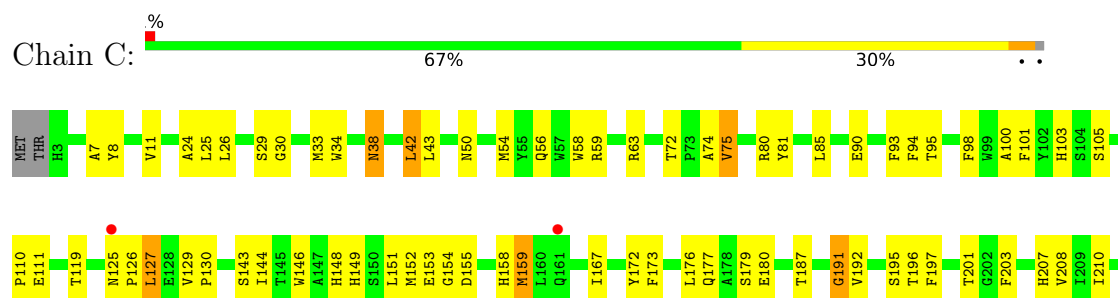
• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2

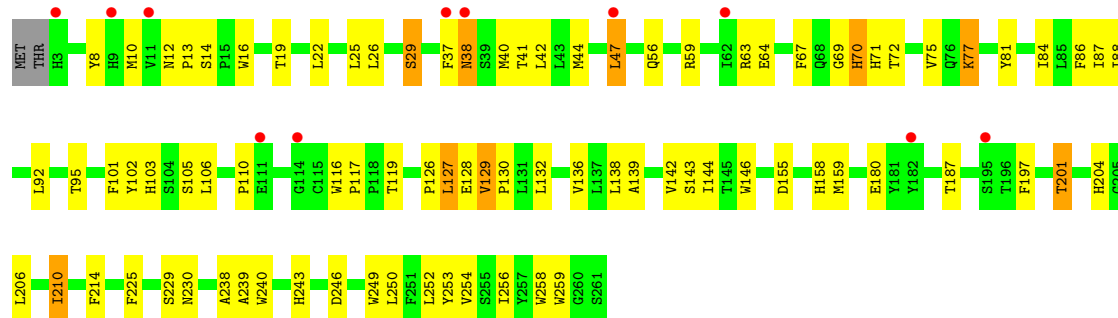


• Molecule 3: Cytochrome c oxidase subunit 3

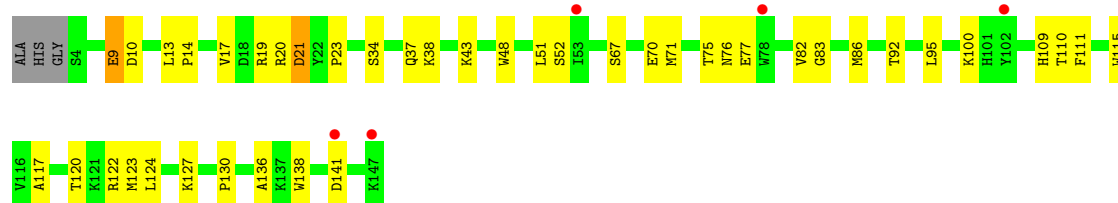




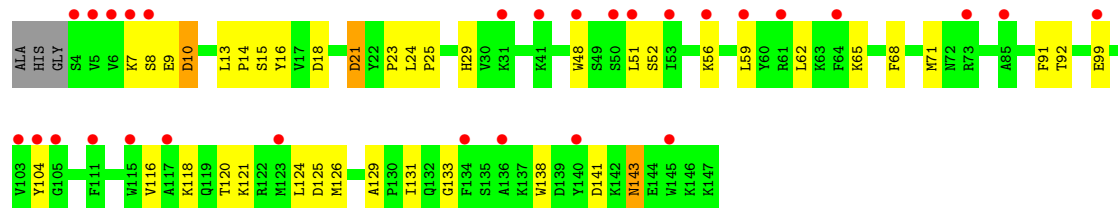
• Molecule 3: Cytochrome c oxidase subunit 3



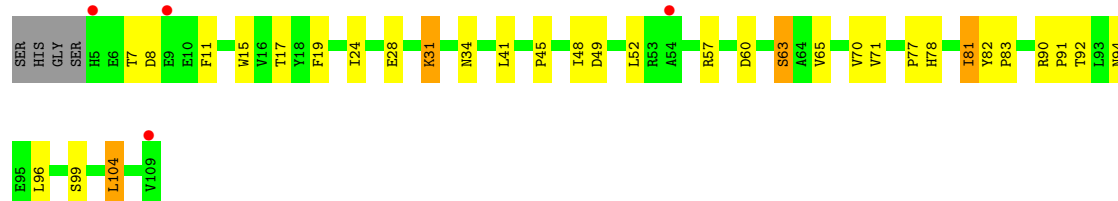
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



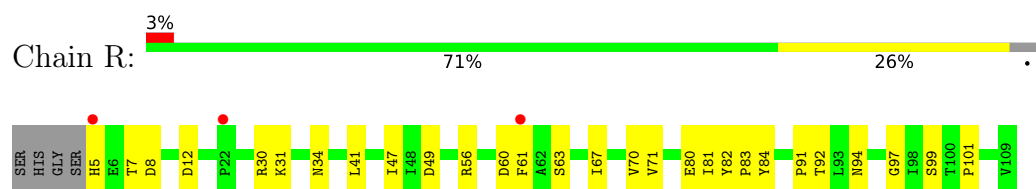
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



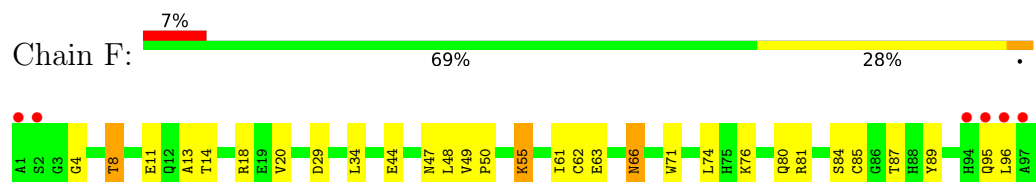
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



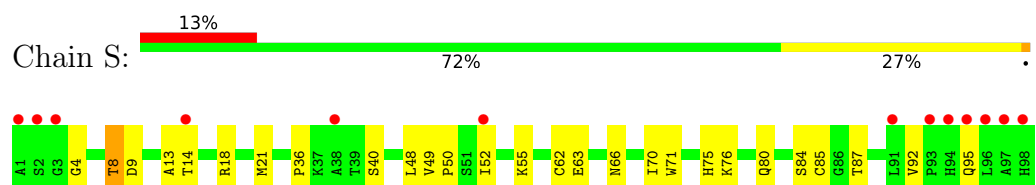
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



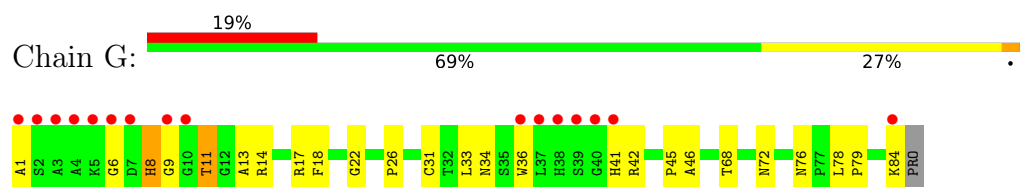
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



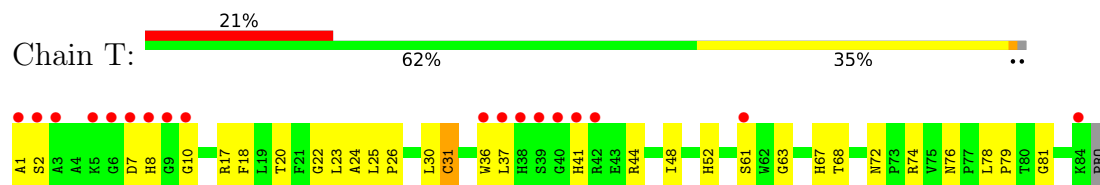
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



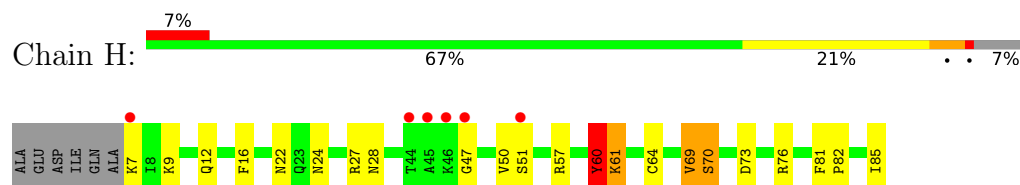
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



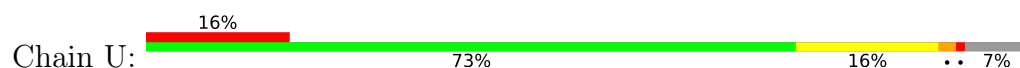
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

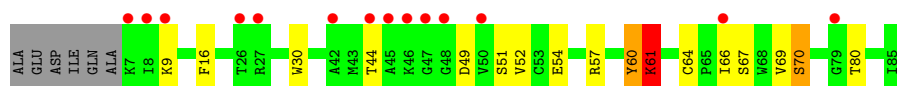


- Molecule 8: Cytochrome c oxidase subunit 6B1

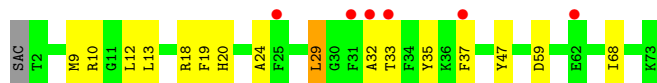
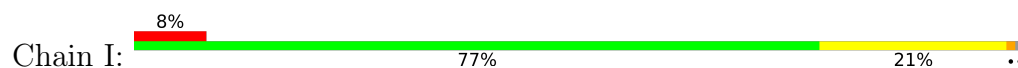


- Molecule 8: Cytochrome c oxidase subunit 6B1

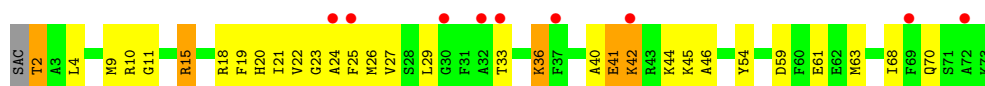




- Molecule 9: Cytochrome c oxidase subunit 6C



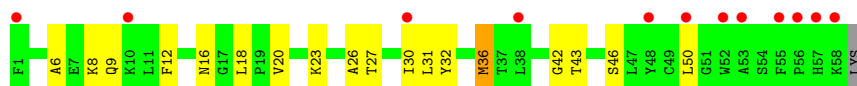
- Molecule 9: Cytochrome c oxidase subunit 6C



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



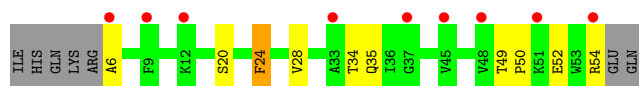
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



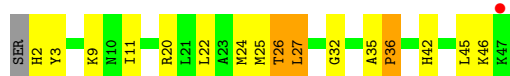
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



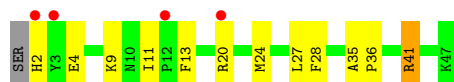
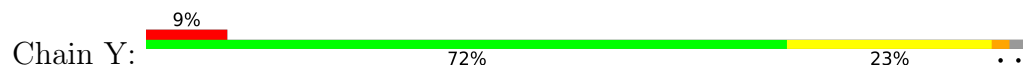
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



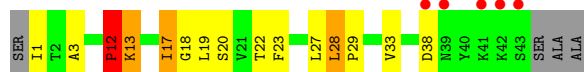
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	178.60Å 189.50Å 211.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 2.38 33.00 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.00-2.38) 99.7 (33.00-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.232 , 0.266 0.234 , 0.266	Depositor DCC
R_{free} test set	14182 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	31457	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.15	5/4156 (0.1%)	1.65	34/5678 (0.6%)
1	N	1.09	0/4156	1.60	30/5678 (0.5%)
2	B	1.14	2/1860 (0.1%)	1.50	3/2534 (0.1%)
2	O	1.07	1/1860 (0.1%)	1.48	1/2534 (0.0%)
3	C	1.05	1/2197 (0.0%)	1.61	15/3005 (0.5%)
3	P	1.06	0/2197	1.60	13/3005 (0.4%)
4	D	1.09	0/1229	1.49	1/1658 (0.1%)
4	Q	1.07	0/1229	1.46	0/1658
5	E	1.03	0/871	1.56	3/1182 (0.3%)
5	R	1.01	0/871	1.56	4/1182 (0.3%)
6	F	1.09	0/765	1.47	1/1038 (0.1%)
6	S	1.11	1/765 (0.1%)	1.48	1/1038 (0.1%)
7	G	1.02	0/690	1.36	0/937
7	T	1.04	0/690	1.40	1/937 (0.1%)
8	H	1.09	1/682 (0.1%)	1.50	5/921 (0.5%)
8	U	0.99	0/682	1.46	2/921 (0.2%)
9	I	1.00	0/605	1.57	0/802
9	V	1.02	0/605	1.62	2/802 (0.2%)
10	J	1.07	0/471	1.70	6/636 (0.9%)
10	W	1.08	0/471	1.60	0/636
11	K	1.13	0/398	1.51	0/546
11	X	1.08	0/398	1.51	2/546 (0.4%)
12	L	1.09	0/393	1.53	2/526 (0.4%)
12	Y	1.03	0/393	1.48	2/526 (0.4%)
13	M	1.15	2/345 (0.6%)	1.61	2/470 (0.4%)
13	Z	1.02	0/345	1.47	2/470 (0.4%)
All	All	1.08	13/29324 (0.0%)	1.56	132/39866 (0.3%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	12	PRO	C-O	-6.30	1.15	1.24
2	O	198	GLU	C-O	6.03	1.31	1.23
13	M	28	LEU	N-CA	5.97	1.50	1.46
3	C	43	LEU	C-O	5.81	1.30	1.24
1	A	265	LYS	C-O	-5.53	1.17	1.24

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	VAL	N-CA-C	-7.33	103.19	110.30
1	A	240	HIS	CA-CB-CG	-7.29	106.51	113.80
1	A	184	PHE	N-CA-C	-7.26	103.37	111.28
1	A	58	VAL	O-C-N	7.15	128.92	121.91
1	N	336	PRO	CA-C-N	7.14	130.17	120.38

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	4027	0	4002	208	0
1	N	4027	0	4002	189	0
2	B	1824	0	1833	75	0
2	O	1824	0	1833	58	0
3	C	2110	0	2027	57	0
3	P	2110	0	2027	69	0
4	D	1195	0	1183	33	0
4	Q	1195	0	1183	37	0
5	E	852	0	845	24	0
5	R	852	0	845	21	0
6	F	748	0	728	17	0
6	S	748	0	728	16	0
7	G	675	0	643	21	0
7	T	675	0	643	27	0
8	H	662	0	623	16	0
8	U	662	0	623	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	592	0	604	14	0
9	V	592	0	604	20	0
10	J	460	0	459	12	0
10	W	460	0	459	13	0
11	K	384	0	366	14	0
11	X	384	0	366	7	0
12	L	380	0	380	13	0
12	Y	380	0	380	9	0
13	M	335	0	352	9	0
13	Z	335	0	352	7	0
14	A	1	0	0	0	0
14	N	1	0	0	0	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	51	0	76	3	0
17	C	102	0	152	3	0
17	H	51	0	76	1	0
17	N	102	0	152	2	0
17	P	102	0	152	2	0
18	A	120	0	108	15	0
18	N	120	0	108	11	0
19	A	1	0	0	0	0
19	N	1	0	0	0	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	63	0	110	2	0
21	D	63	0	110	2	0
21	L	63	0	110	8	0
21	N	126	0	220	7	0
21	O	63	0	110	0	0
22	B	52	0	80	1	0
22	V	52	0	80	2	0
23	C	58	0	78	3	0
23	J	29	0	39	1	0
23	O	29	0	39	0	0
23	P	58	0	78	2	0
23	T	58	0	78	3	0
23	W	29	0	39	0	0
23	Y	29	0	39	2	0
24	C	159	0	231	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	P	106	0	154	3	0
24	T	53	0	77	1	0
25	C	200	0	312	3	0
25	P	200	0	312	9	0
26	C	66	0	84	6	0
26	G	33	0	42	0	0
26	M	33	0	42	1	0
26	P	33	0	42	0	0
26	Q	33	0	42	0	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	I	9	0	8	0	0
28	V	9	0	8	1	0
29	A	104	0	0	68	0
29	B	46	0	0	16	0
29	C	44	0	0	9	0
29	D	23	0	0	10	0
29	E	23	0	0	4	0
29	F	20	0	0	2	0
29	G	13	0	0	5	0
29	H	26	0	0	10	0
29	I	8	0	0	4	0
29	J	11	0	0	8	0
29	K	8	0	0	5	0
29	L	13	0	0	6	0
29	M	7	0	0	2	0
29	N	74	0	0	47	0
29	O	39	0	0	13	0
29	P	40	0	0	22	0
29	Q	28	0	0	12	0
29	R	8	0	0	0	0
29	S	19	0	0	2	0
29	T	17	0	0	4	0
29	U	7	0	0	0	0
29	V	6	0	0	0	0
29	W	5	0	0	1	0
29	X	8	0	0	5	0
29	Y	1	0	0	0	0
29	Z	3	0	0	0	0
All	All	31457	0	31478	914	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 15.

The worst 5 of 914 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:HIS:NE2	1:A:244:TYR:CE2	1.81	1.47
1:A:240:HIS:NE2	1:A:244:TYR:HE2	0.90	1.37
1:N:240:HIS:NE2	1:N:244:TYR:HE2	1.27	1.30
1:A:394:VAL:HA	29:A:722:HOH:O	1.31	1.28
1:N:240:HIS:NE2	1:N:244:TYR:CE2	2.04	1.26

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	512/514 (100%)	455 (89%)	52 (10%)	5 (1%)	12	17
1	N	512/514 (100%)	451 (88%)	60 (12%)	1 (0%)	43	56
2	B	225/227 (99%)	199 (88%)	22 (10%)	4 (2%)	6	8
2	O	225/227 (99%)	194 (86%)	27 (12%)	4 (2%)	6	8
3	C	257/261 (98%)	240 (93%)	15 (6%)	2 (1%)	16	23
3	P	257/261 (98%)	226 (88%)	30 (12%)	1 (0%)	30	40
4	D	142/147 (97%)	124 (87%)	17 (12%)	1 (1%)	18	26
4	Q	142/147 (97%)	130 (92%)	10 (7%)	2 (1%)	9	11
5	E	103/109 (94%)	93 (90%)	9 (9%)	1 (1%)	12	17
5	R	103/109 (94%)	99 (96%)	4 (4%)	0	100	100
6	F	96/98 (98%)	86 (90%)	9 (9%)	1 (1%)	12	17
6	S	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
7	G	81/85 (95%)	68 (84%)	12 (15%)	1 (1%)	10	14
7	T	81/85 (95%)	66 (82%)	13 (16%)	2 (2%)	4	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	4	4
8	U	77/85 (91%)	65 (84%)	10 (13%)	2 (3%)	4	4
9	I	70/73 (96%)	64 (91%)	5 (7%)	1 (1%)	9	11
9	V	70/73 (96%)	62 (89%)	7 (10%)	1 (1%)	9	11
10	J	56/59 (95%)	50 (89%)	5 (9%)	1 (2%)	6	8
10	W	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
11	K	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
11	X	47/56 (84%)	43 (92%)	4 (8%)	0	100	100
12	L	44/47 (94%)	39 (89%)	4 (9%)	1 (2%)	5	5
12	Y	44/47 (94%)	41 (93%)	2 (4%)	1 (2%)	5	5
13	M	41/47 (87%)	35 (85%)	4 (10%)	2 (5%)	1	1
13	Z	41/47 (87%)	37 (90%)	4 (10%)	0	100	100
All	All	3502/3616 (97%)	3123 (89%)	343 (10%)	36 (1%)	12	17

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	59	GLN
2	B	89	GLU
7	G	41	HIS
10	J	26	ALA
12	L	46	LYS

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	426/426 (100%)	406 (95%)	20 (5%)	23	37
1	N	426/426 (100%)	404 (95%)	22 (5%)	21	33
2	B	210/210 (100%)	197 (94%)	13 (6%)	16	26
2	O	210/210 (100%)	193 (92%)	17 (8%)	11	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	224/226 (99%)	210 (94%)	14 (6%)	16	26
3	P	224/226 (99%)	212 (95%)	12 (5%)	20	32
4	D	128/129 (99%)	119 (93%)	9 (7%)	14	21
4	Q	128/129 (99%)	119 (93%)	9 (7%)	14	21
5	E	92/95 (97%)	85 (92%)	7 (8%)	12	19
5	R	92/95 (97%)	88 (96%)	4 (4%)	26	41
6	F	81/81 (100%)	73 (90%)	8 (10%)	7	10
6	S	81/81 (100%)	75 (93%)	6 (7%)	13	19
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	13
7	T	67/68 (98%)	63 (94%)	4 (6%)	17	28
8	H	71/75 (95%)	68 (96%)	3 (4%)	26	42
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	15
9	I	57/57 (100%)	52 (91%)	5 (9%)	9	14
9	V	57/57 (100%)	47 (82%)	10 (18%)	2	2
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	43
10	W	49/50 (98%)	44 (90%)	5 (10%)	7	9
11	K	39/46 (85%)	34 (87%)	5 (13%)	4	5
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	34
12	L	39/40 (98%)	34 (87%)	5 (13%)	4	5
12	Y	39/40 (98%)	37 (95%)	2 (5%)	21	34
13	M	37/39 (95%)	33 (89%)	4 (11%)	6	8
13	Z	37/39 (95%)	30 (81%)	7 (19%)	1	2
All	All	3040/3084 (99%)	2833 (93%)	207 (7%)	14	23

5 of 207 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	383	MET
3	P	70	HIS
12	Y	27	LEU
1	N	471	ILE
2	O	152	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	26	HIS
5	R	78	HIS
8	U	31	GLN
2	O	91	ASN
3	P	68	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	N	1	1	8,9,10	0.50	0	8,9,11	0.91	1 (12%)
2	FME	O	1	2	8,9,10	0.68	0	8,9,11	0.99	0
1	FME	A	1	1	8,9,10	0.64	0	8,9,11	0.96	0
7	TPO	G	11	7	8,10,11	0.94	1 (12%)	10,14,16	0.98	1 (10%)
2	FME	B	1	2	8,9,10	0.39	0	8,9,11	1.02	0
7	TPO	T	11	7	8,10,11	0.84	0	10,14,16	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	N	1	1	-	3/7/9/11	-
2	FME	O	1	2	-	2/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
7	TPO	G	11	7	-	7/9/11/13	-
2	FME	B	1	2	-	1/7/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TPO	T	11	7	-	5/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	2.18	1.63	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	11	TPO	O-C-CA	-2.03	119.54	124.77
1	N	1	FME	O-C-CA	-2.01	119.59	124.77

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	FME	4	0
7	G	11	TPO	2	0
2	B	1	FME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 8 are monoatomic and 2 are modelled with single atom - leaving 50 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
22	PSC	V	101	-	51,51,51	0.31	0	57,59,59	0.45	0
18	HEA	A	606	1	67,67,67	2.37	25 (37%)	81,103,103	2.67	34 (41%)
17	PGV	A	604	-	50,50,50	0.32	0	53,56,56	0.51	0
25	CDL	P	309	-	99,99,99	0.31	0	105,111,111	0.38	0
23	CHD	T	101	-	32,32,32	0.65	0	51,51,51	1.43	11 (21%)
26	DMU	G	101	-	34,34,34	0.84	1 (2%)	45,45,45	1.10	3 (6%)
17	PGV	P	306	-	50,50,50	0.32	0	53,56,56	0.39	0
17	PGV	N	610	-	50,50,50	0.32	0	53,56,56	0.39	0
28	SAC	I	101	-	7,8,9	0.57	0	7,9,11	1.11	1 (14%)
26	DMU	M	101	-	34,34,34	0.67	0	45,45,45	1.55	8 (17%)
25	CDL	C	308	-	99,99,99	0.32	0	105,111,111	0.39	0
24	PEK	C	311	-	52,52,52	0.38	0	55,57,57	0.45	0
24	PEK	P	304	-	52,52,52	0.29	0	55,57,57	0.51	0
18	HEA	N	607	1	67,67,67	2.46	23 (34%)	81,103,103	2.76	32 (39%)
22	PSC	B	303	-	51,51,51	0.29	0	57,59,59	0.38	0
21	TGL	L	101	-	62,62,62	0.27	0	65,65,65	0.34	0
23	CHD	P	303	-	32,32,32	0.66	1 (3%)	51,51,51	1.13	3 (5%)
23	CHD	C	302	-	32,32,32	0.67	0	51,51,51	0.94	1 (1%)
17	PGV	H	101	-	50,50,50	0.31	0	53,56,56	0.42	0
25	CDL	C	306	-	99,99,99	0.30	0	105,111,111	0.38	0
21	TGL	O	301	-	62,62,62	0.27	0	65,65,65	0.36	0
23	CHD	J	101	-	32,32,32	0.63	0	51,51,51	1.06	3 (5%)
23	CHD	P	308	-	32,32,32	0.58	0	51,51,51	0.90	0
24	PEK	P	301	-	52,52,52	0.31	0	55,57,57	0.36	0
21	TGL	N	609	-	62,62,62	0.27	0	65,65,65	0.24	0
24	PEK	C	303	-	52,52,52	0.29	0	55,57,57	0.66	1 (1%)
23	CHD	O	303	-	32,32,32	0.56	0	51,51,51	1.04	3 (5%)
17	PGV	N	605	-	50,50,50	0.31	0	53,56,56	0.74	2 (3%)
23	CHD	C	307	-	32,32,32	0.64	0	51,51,51	1.07	2 (3%)
21	TGL	N	604	-	62,62,62	0.22	0	65,65,65	0.34	0
18	HEA	A	605	19,1	67,67,67	2.46	23 (34%)	81,103,103	2.81	30 (37%)
23	CHD	W	101	-	32,32,32	0.60	0	51,51,51	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DMU	C	310	-	34,34,34	0.83	1 (2%)	45,45,45	1.28	5 (11%)
24	PEK	T	102	-	52,52,52	0.33	0	55,57,57	0.72	1 (1%)
20	CUA	O	302	2	0,1,1	-	-	-	-	-
18	HEA	N	606	19,1	67,67,67	2.51	25 (37%)	81,103,103	2.57	28 (34%)
28	SAC	V	102	-	7,8,9	0.55	0	7,9,11	1.50	1 (14%)
25	CDL	P	307	-	99,99,99	0.31	0	105,111,111	0.47	1 (0%)
26	DMU	P	302	-	34,34,34	0.64	1 (2%)	45,45,45	1.29	7 (15%)
26	DMU	C	309	-	34,34,34	0.92	1 (2%)	45,45,45	1.39	7 (15%)
21	TGL	D	201	-	62,62,62	0.23	0	65,65,65	0.28	0
26	DMU	Q	201	-	34,34,34	0.65	1 (2%)	45,45,45	1.15	5 (11%)
20	CUA	B	301	2	0,1,1	-	-	-	-	-
23	CHD	Y	101	-	32,32,32	0.63	0	51,51,51	0.95	1 (1%)
21	TGL	B	302	-	62,62,62	0.35	0	65,65,65	0.40	0
24	PEK	C	304	-	52,52,52	0.29	0	55,57,57	0.38	0
23	CHD	T	103	-	32,32,32	0.63	0	51,51,51	0.92	2 (3%)
17	PGV	C	301	-	50,50,50	0.35	0	53,56,56	0.68	2 (3%)
17	PGV	P	305	-	50,50,50	0.33	0	53,56,56	0.53	0
17	PGV	C	305	-	50,50,50	0.37	0	53,56,56	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSC	V	101	-	-	30/55/55/55	-
18	HEA	A	606	1	-	7/36/76/76	-
17	PGV	A	604	-	-	31/55/55/55	-
25	CDL	P	309	-	-	49/110/110/110	-
23	CHD	T	101	-	-	7/9/74/74	0/4/4/4
26	DMU	G	101	-	2/2/10/10	13/19/59/59	0/2/2/2
17	PGV	P	306	-	-	33/55/55/55	-
17	PGV	N	610	-	-	34/55/55/55	-
28	SAC	I	101	-	-	2/7/8/10	-
26	DMU	M	101	-	2/2/10/10	7/19/59/59	0/2/2/2
25	CDL	C	308	-	-	56/110/110/110	-
24	PEK	C	311	-	-	24/56/56/56	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PEK	P	304	-	-	20/56/56/56	-
18	HEA	N	607	1	-	5/36/76/76	-
22	PSC	B	303	-	-	28/55/55/55	-
21	TGL	L	101	-	-	34/65/65/65	-
23	CHD	P	303	-	-	7/9/74/74	0/4/4/4
23	CHD	C	302	-	-	3/9/74/74	0/4/4/4
17	PGV	H	101	-	-	30/55/55/55	-
25	CDL	C	306	-	-	56/110/110/110	-
21	TGL	O	301	-	-	34/65/65/65	-
23	CHD	J	101	-	-	3/9/74/74	0/4/4/4
23	CHD	P	308	-	-	3/9/74/74	0/4/4/4
24	PEK	P	301	-	-	32/56/56/56	-
21	TGL	N	609	-	-	34/65/65/65	-
24	PEK	C	303	-	-	17/56/56/56	-
23	CHD	O	303	-	-	2/9/74/74	0/4/4/4
17	PGV	N	605	-	-	21/55/55/55	-
23	CHD	C	307	-	-	6/9/74/74	0/4/4/4
21	TGL	N	604	-	-	38/65/65/65	-
18	HEA	A	605	19,1	-	9/36/76/76	-
23	CHD	W	101	-	-	1/9/74/74	0/4/4/4
26	DMU	C	310	-	2/2/10/10	9/19/59/59	0/2/2/2
24	PEK	T	102	-	-	33/56/56/56	-
18	HEA	N	606	19,1	-	9/36/76/76	-
28	SAC	V	102	-	-	2/7/8/10	-
25	CDL	P	307	-	-	61/110/110/110	-
26	DMU	P	302	-	2/2/10/10	9/19/59/59	0/2/2/2
26	DMU	C	309	-	2/2/10/10	9/19/59/59	0/2/2/2
21	TGL	D	201	-	-	39/65/65/65	-
26	DMU	Q	201	-	2/2/10/10	9/19/59/59	0/2/2/2
23	CHD	Y	101	-	1/1/12/12	5/9/74/74	0/4/4/4
21	TGL	B	302	-	-	34/65/65/65	-
24	PEK	C	304	-	-	25/56/56/56	-
23	CHD	T	103	-	1/1/12/12	3/9/74/74	0/4/4/4
17	PGV	C	301	-	-	16/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PGV	P	305	-	-	24/55/55/55	-
17	PGV	C	305	-	-	17/55/55/55	-

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	607	HEA	C3B-C2B	6.35	1.49	1.34
18	A	606	HEA	CHB-C4A	5.69	1.49	1.38
18	N	607	HEA	FE-ND	5.49	2.11	1.94
18	N	607	HEA	C3D-C2D	5.41	1.48	1.36
18	N	606	HEA	C4B-NB	-5.38	1.30	1.40

The worst 5 of 194 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	607	HEA	C3A-C2A-C1A	-8.87	98.66	107.05
18	N	607	HEA	C3C-C4C-NC	7.83	116.39	109.80
18	A	605	HEA	C3A-C2A-C1A	-7.70	99.76	107.05
18	A	605	HEA	C1D-C2D-C3D	-7.57	99.02	106.98
18	N	607	HEA	C2D-C1D-ND	7.54	118.50	109.84

5 of 14 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	T	103	CHD	C9
23	Y	101	CHD	C3
26	C	309	DMU	C6
26	C	309	DMU	C5
26	C	310	DMU	C6

5 of 980 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	604	PGV	C03-O11-P-O12
17	A	604	PGV	C04-O12-P-O11
17	A	604	PGV	C04-O12-P-O13
17	A	604	PGV	C04-O12-P-O14
17	A	604	PGV	C04-C05-C06-O06

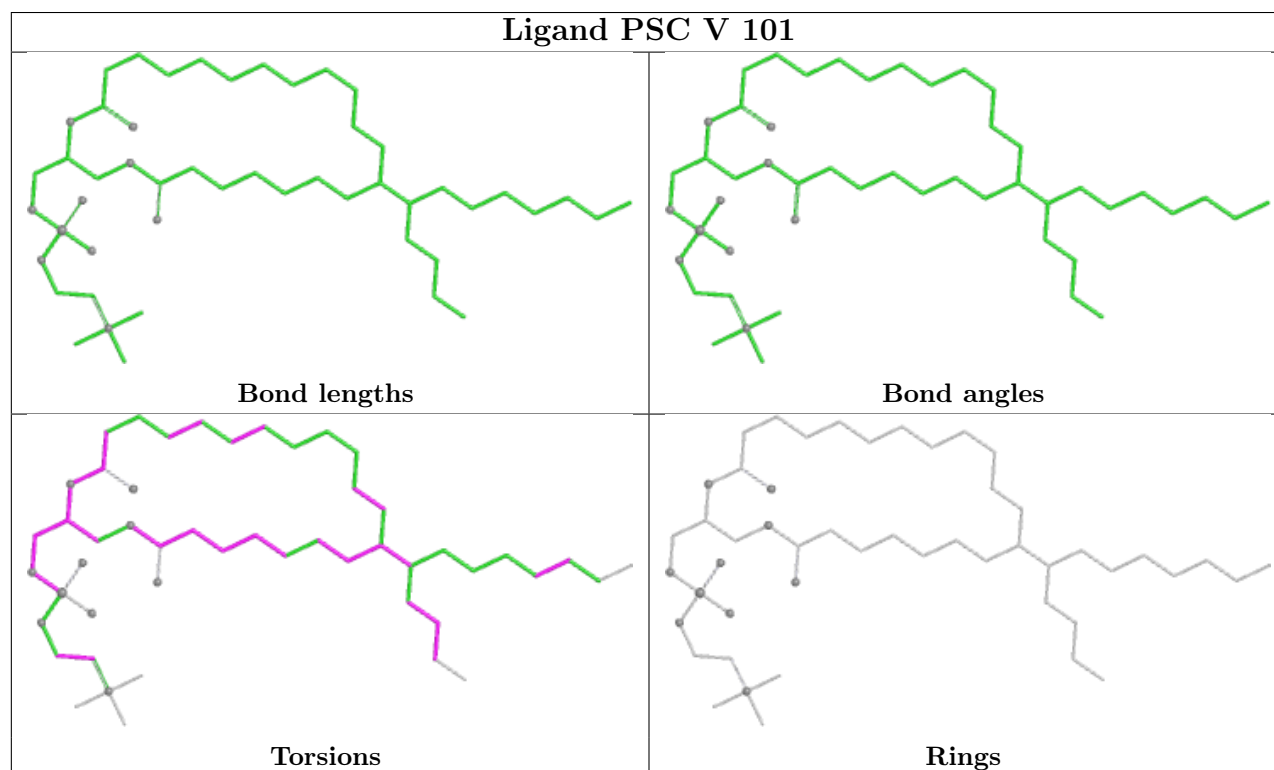
There are no ring outliers.

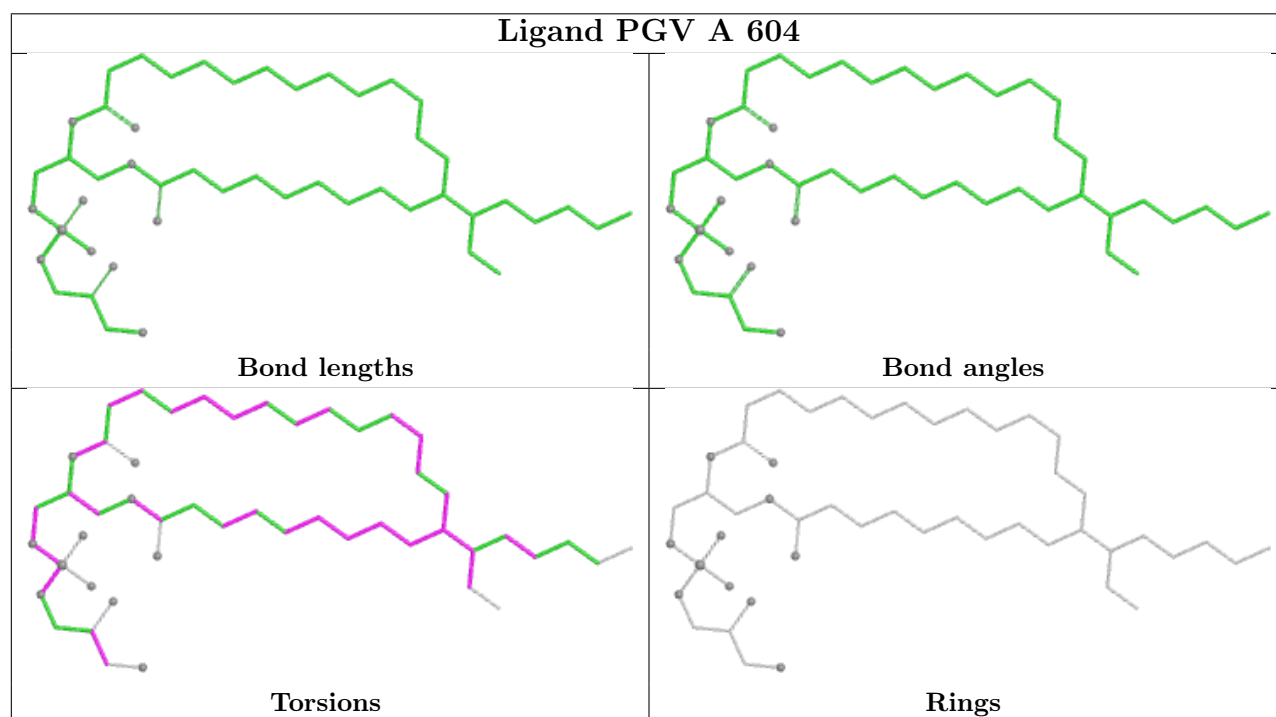
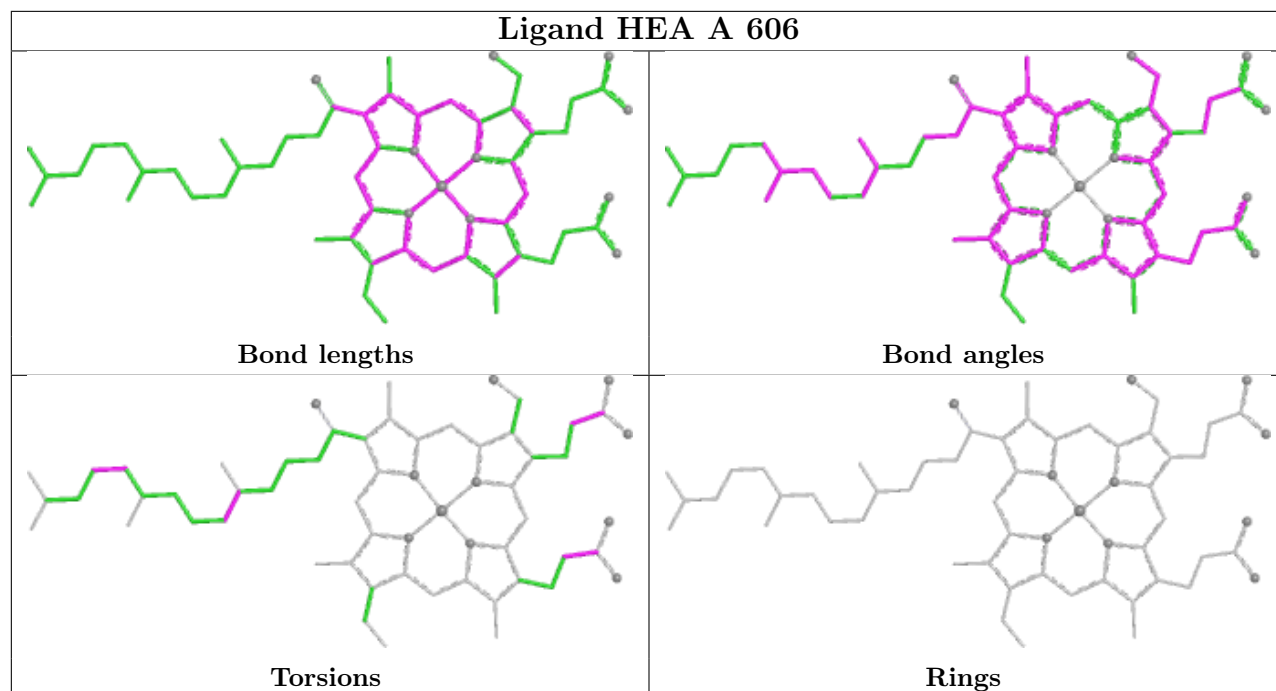
40 monomers are involved in 98 short contacts:

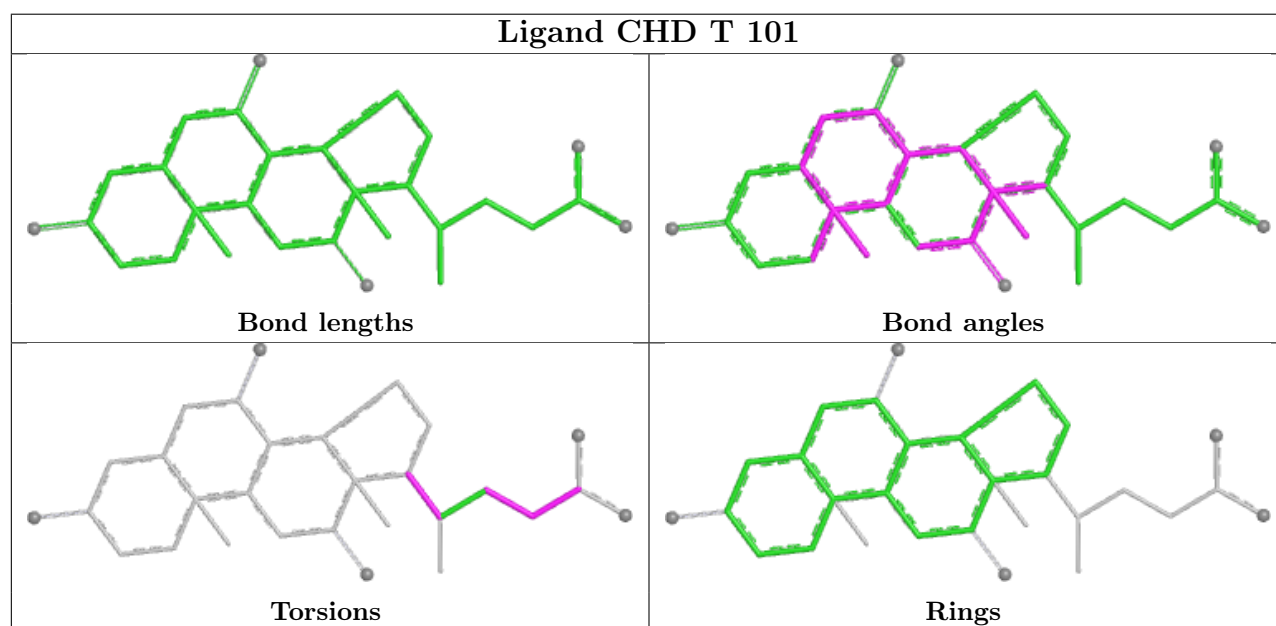
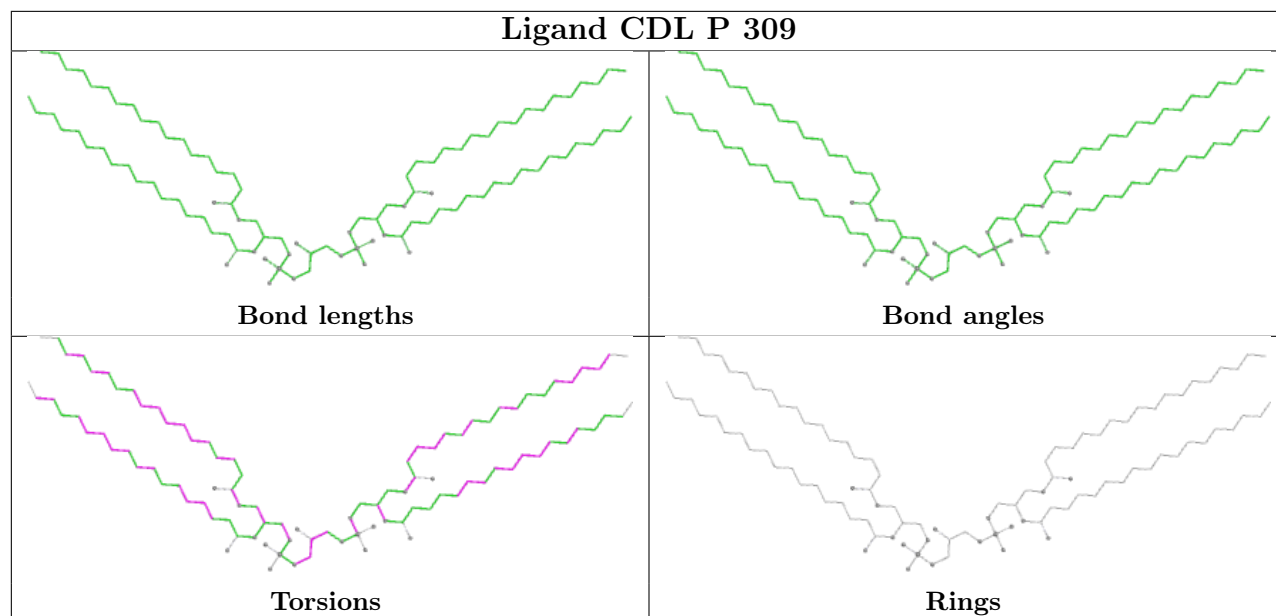
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	V	101	PSC	2	0
18	A	606	HEA	9	0
17	A	604	PGV	3	0
25	P	309	CDL	8	0
23	T	101	CHD	1	0
17	P	306	PGV	1	0
17	N	610	PGV	1	0
26	M	101	DMU	1	0
25	C	308	CDL	2	0
24	C	311	PEK	2	0
24	P	304	PEK	2	0
18	N	607	HEA	9	0
22	B	303	PSC	1	0
21	L	101	TGL	8	0
23	P	303	CHD	1	0
23	C	302	CHD	2	0
17	H	101	PGV	1	0
25	C	306	CDL	1	0
23	J	101	CHD	1	0
23	P	308	CHD	1	0
24	P	301	PEK	1	0
21	N	609	TGL	1	0
24	C	303	PEK	5	0
17	N	605	PGV	1	0
23	C	307	CHD	1	0
21	N	604	TGL	6	0
18	A	605	HEA	6	0
26	C	310	DMU	1	0
24	T	102	PEK	1	0
18	N	606	HEA	2	0
28	V	102	SAC	1	0
25	P	307	CDL	1	0
26	C	309	DMU	5	0
21	D	201	TGL	2	0
23	Y	101	CHD	2	0
21	B	302	TGL	2	0
23	T	103	CHD	2	0
17	C	301	PGV	1	0
17	P	305	PGV	1	0
17	C	305	PGV	2	0

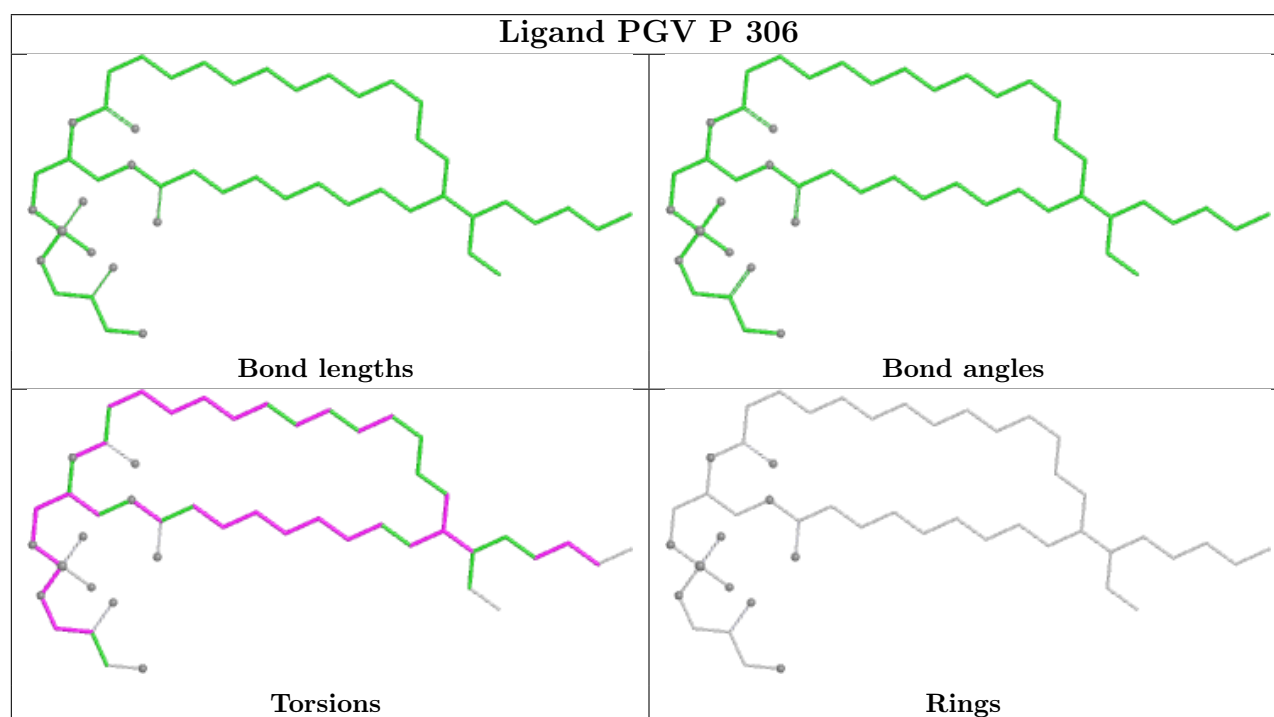
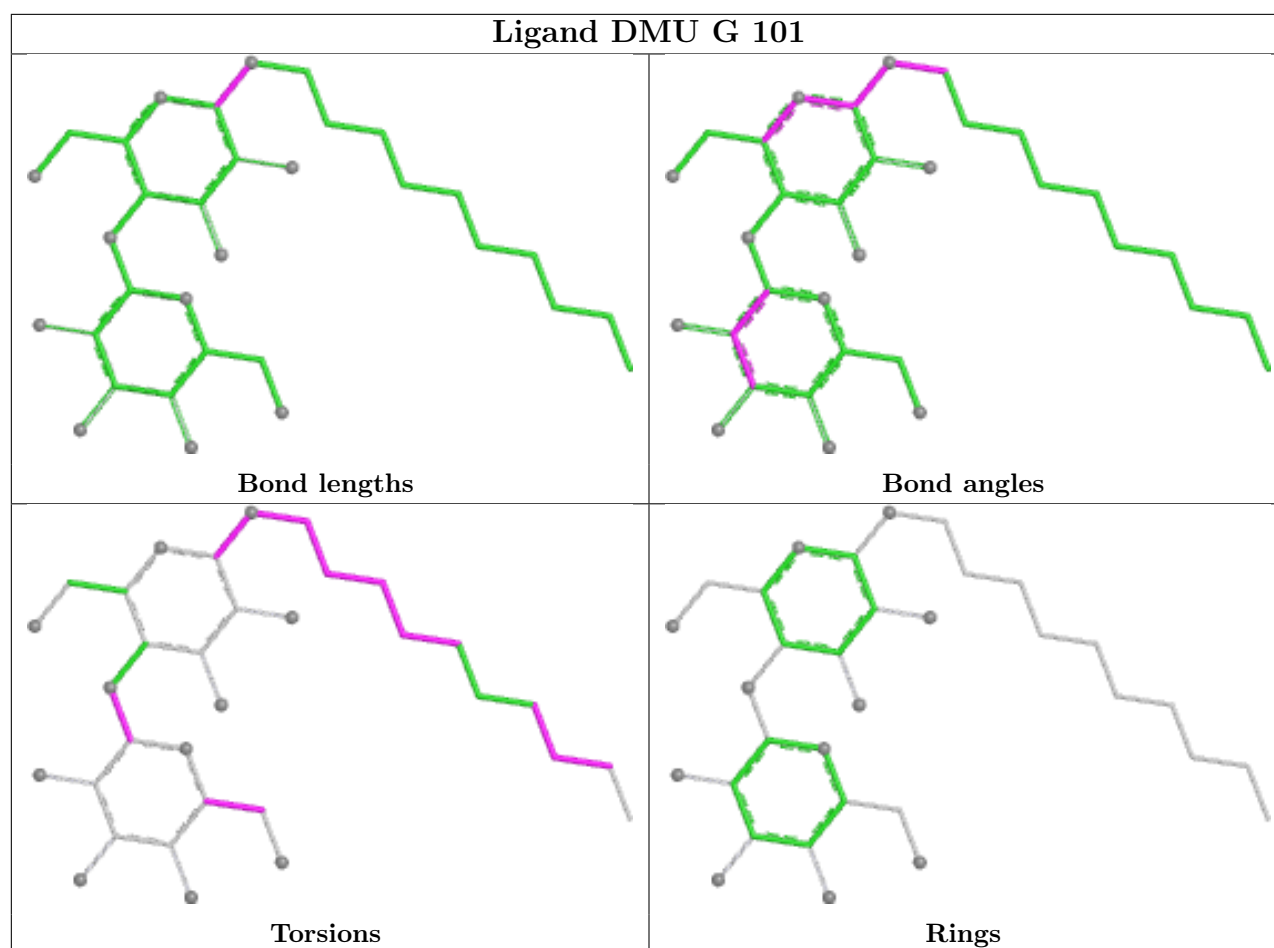
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

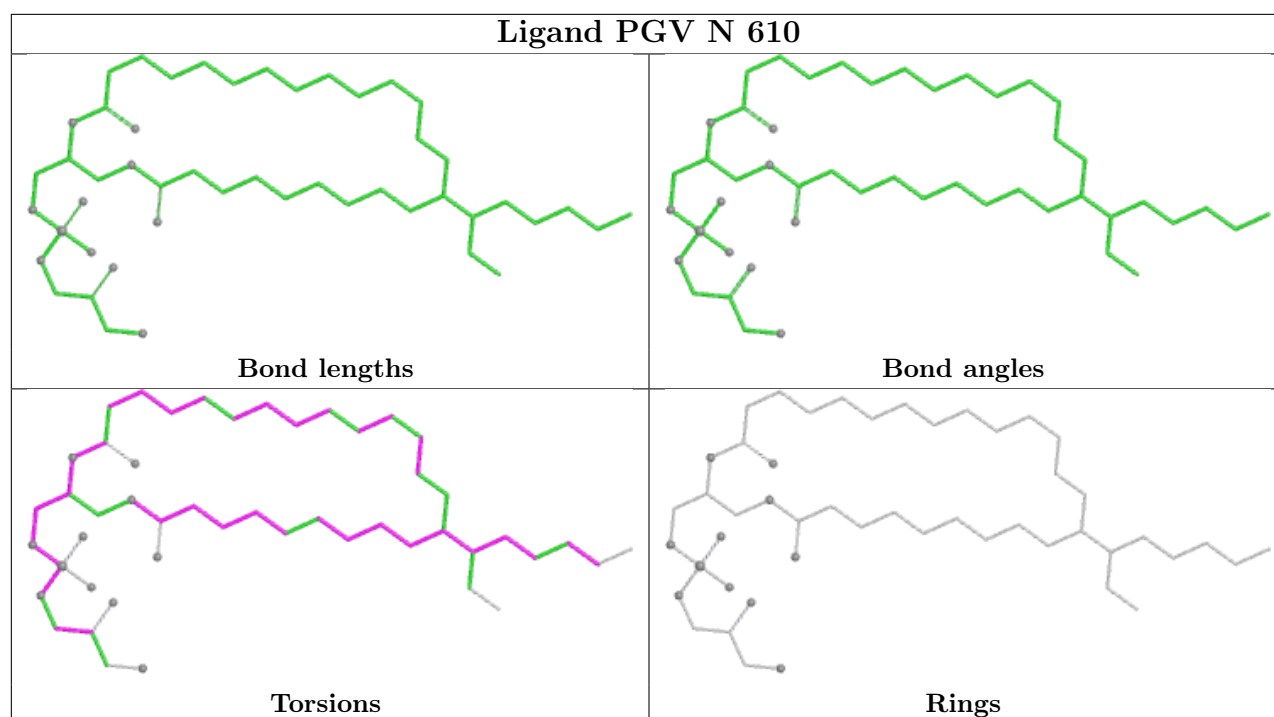
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

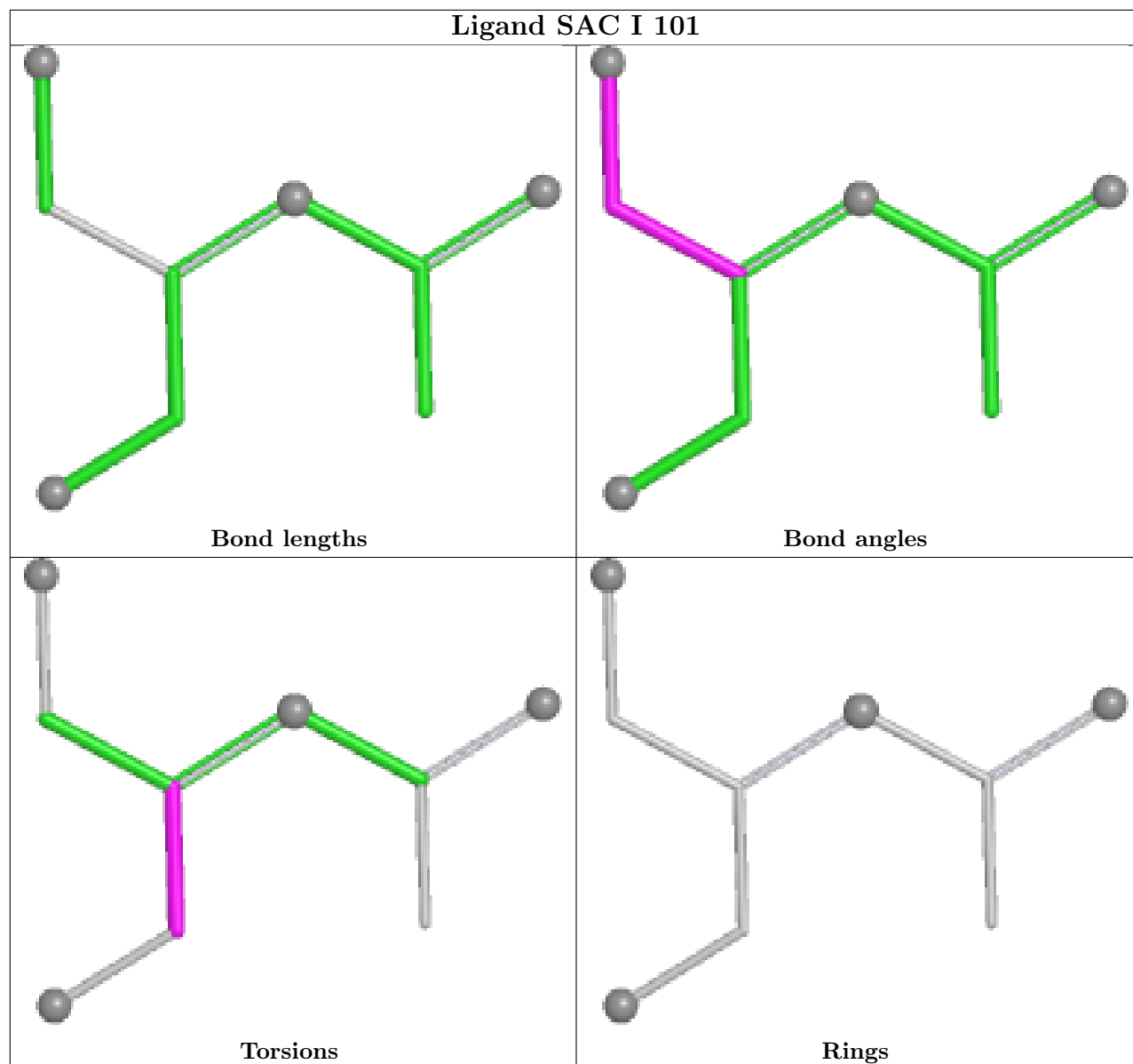


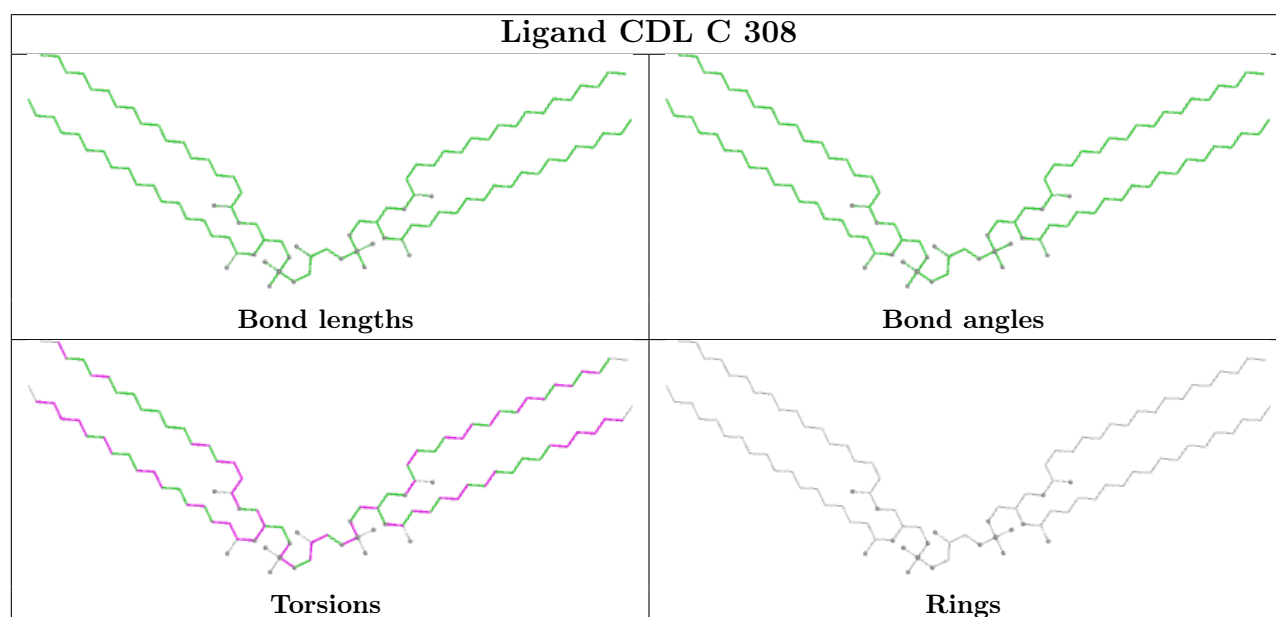
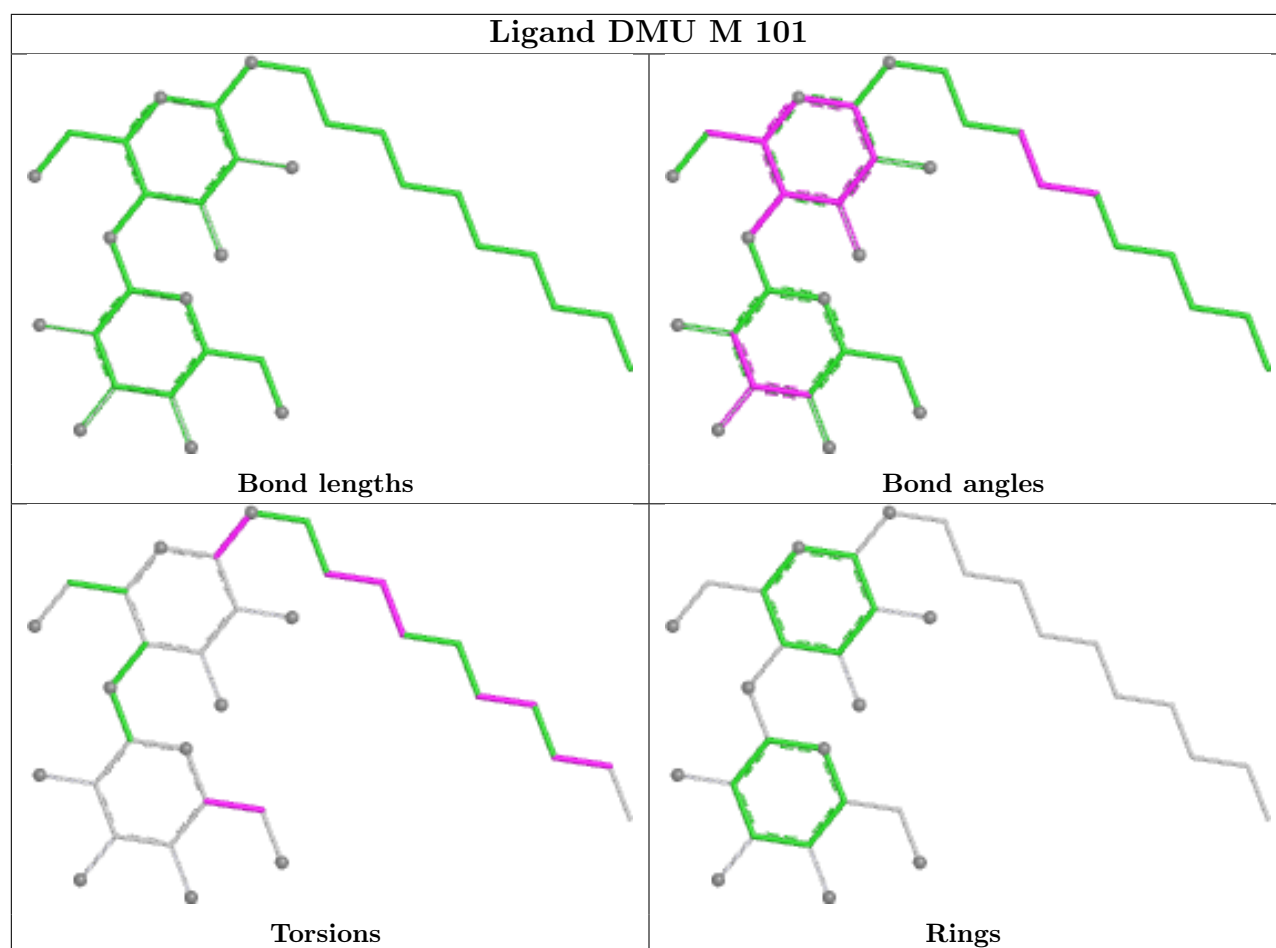




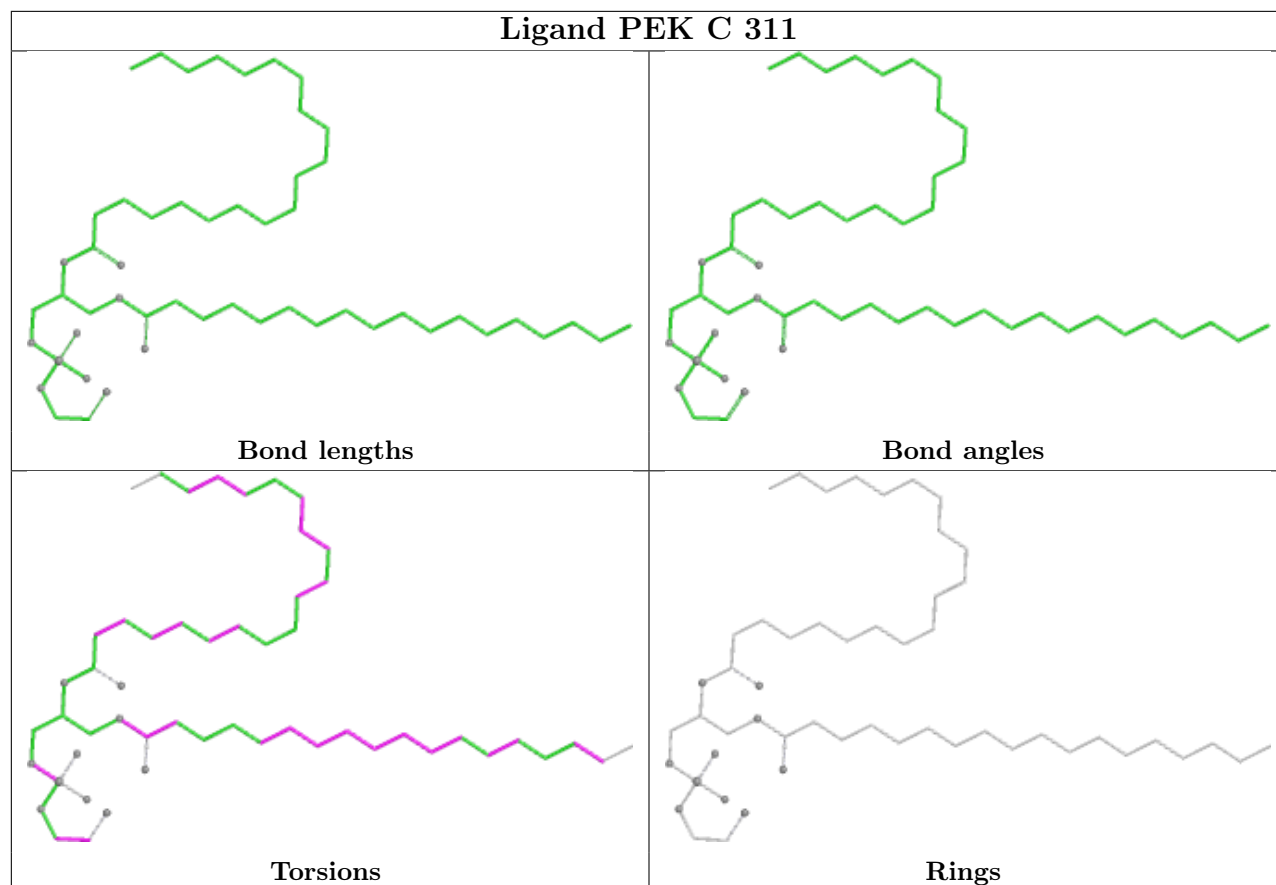




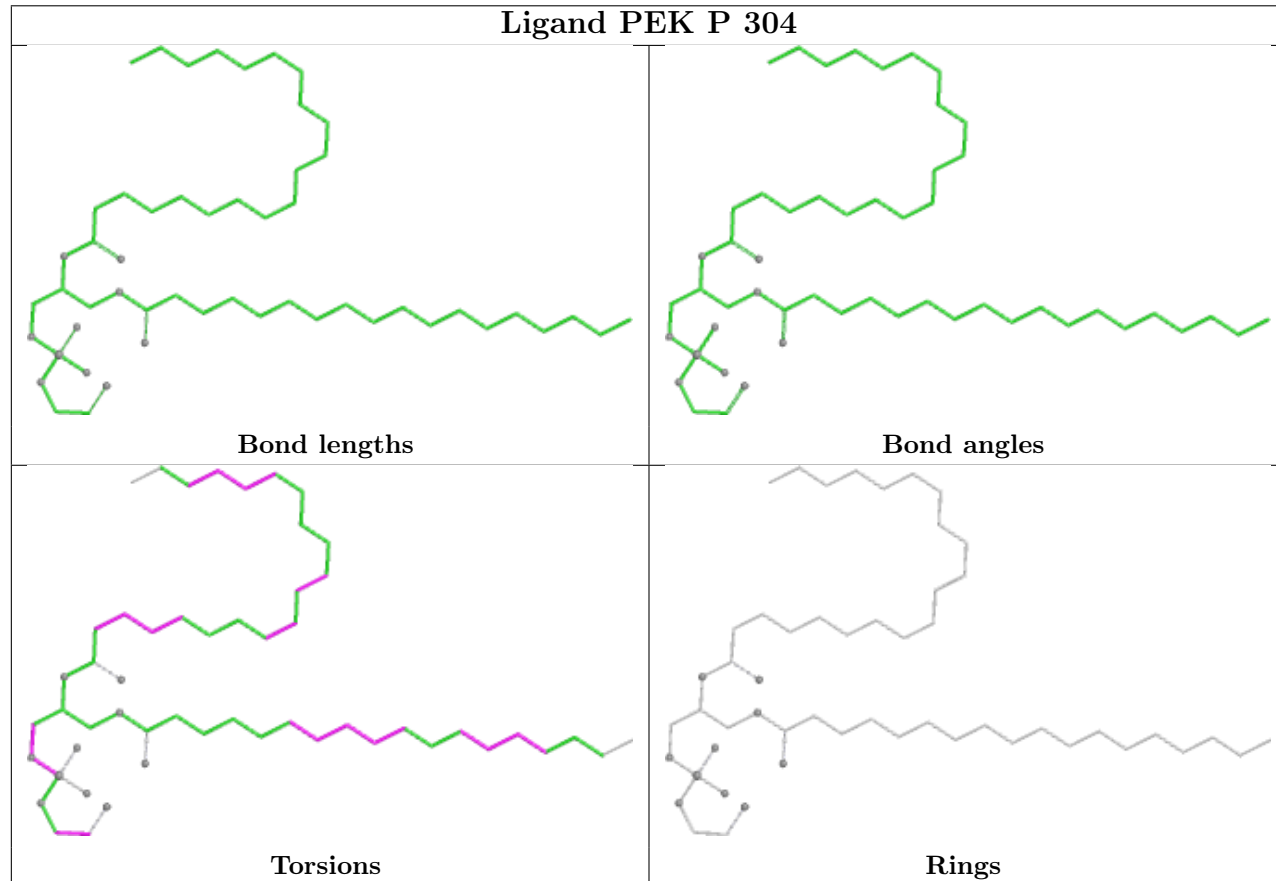


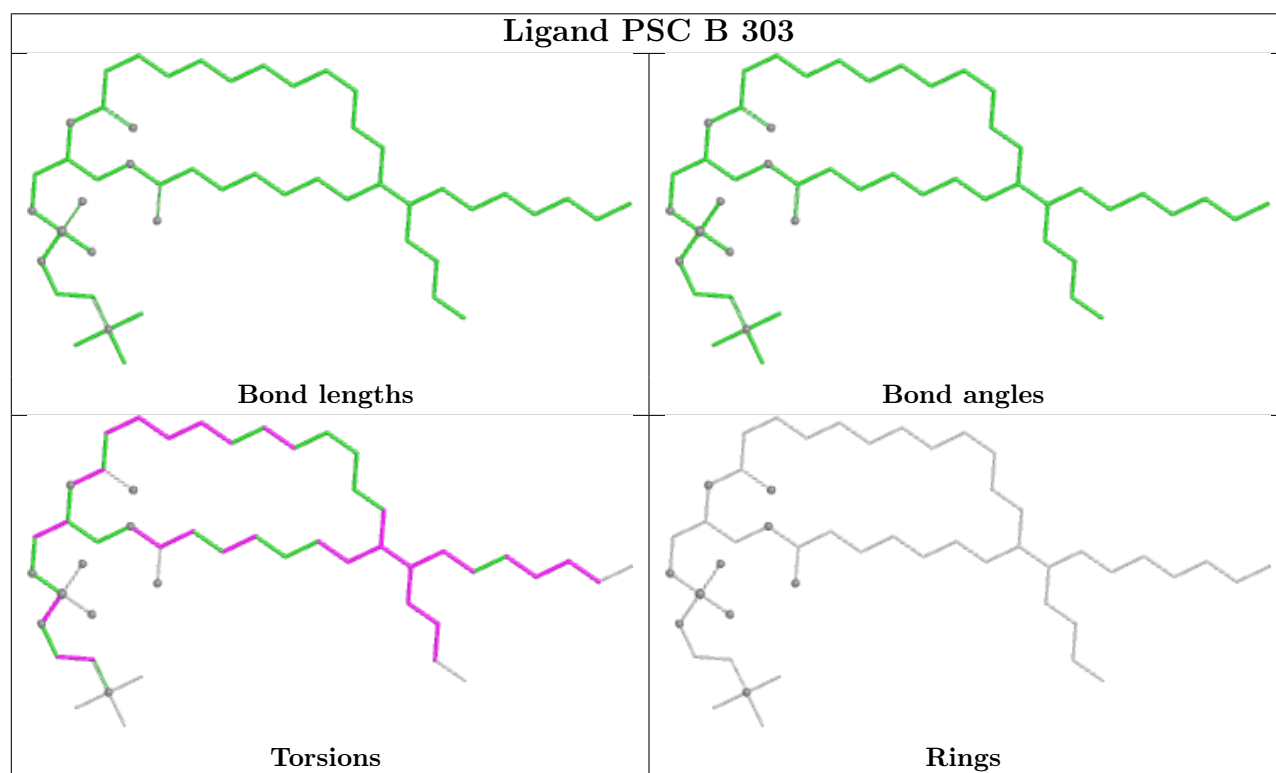
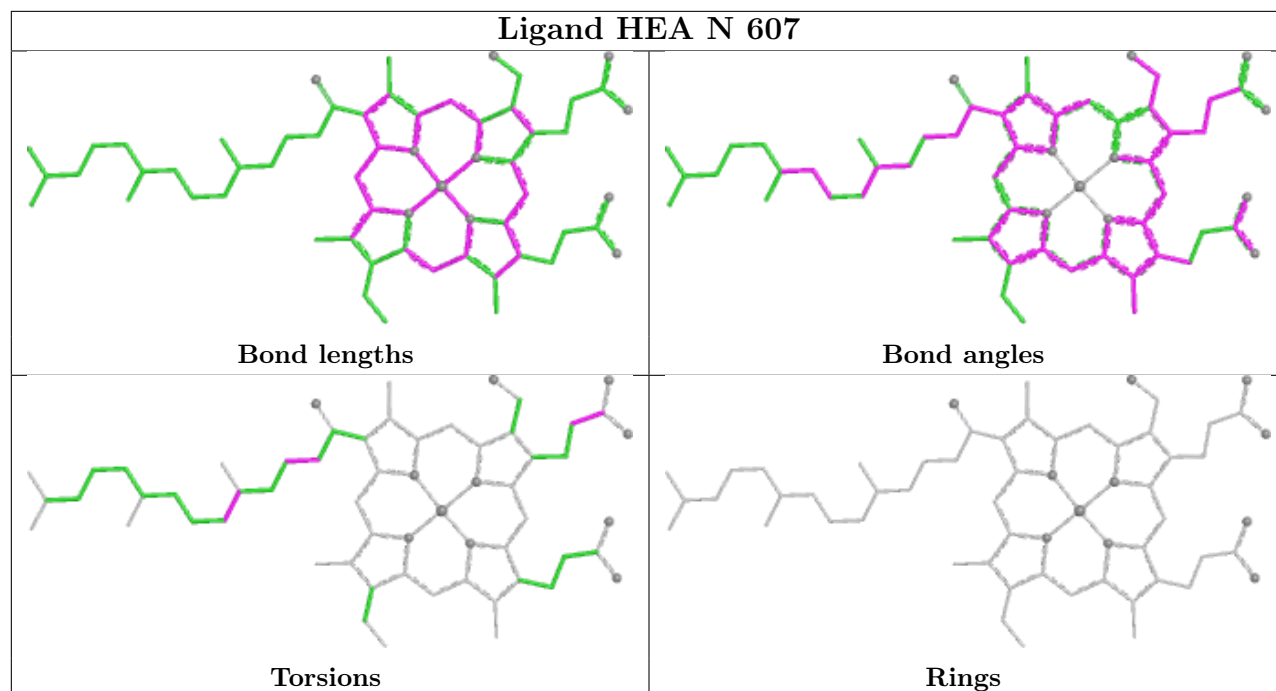


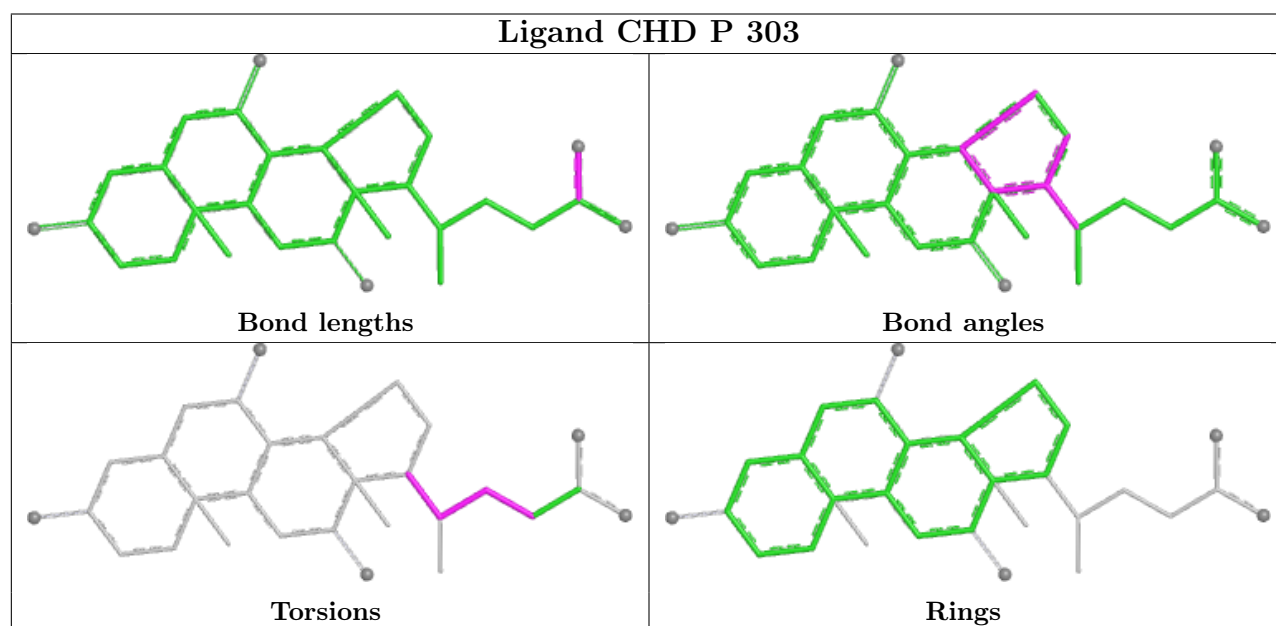
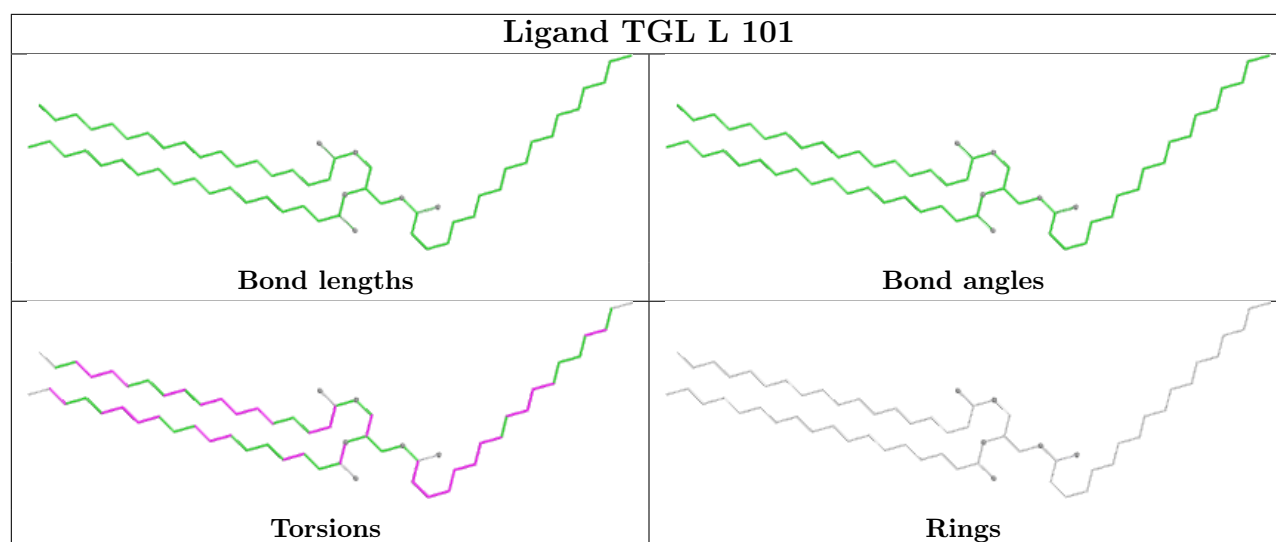
Ligand PEK C 311

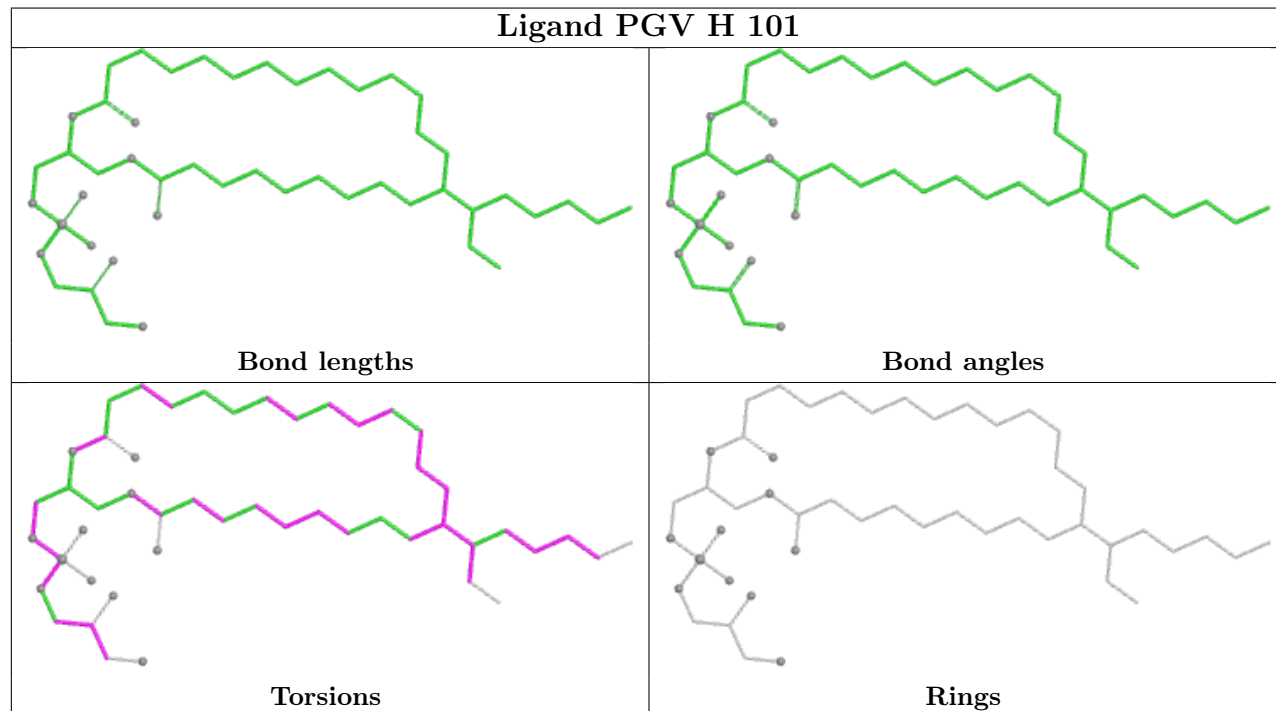
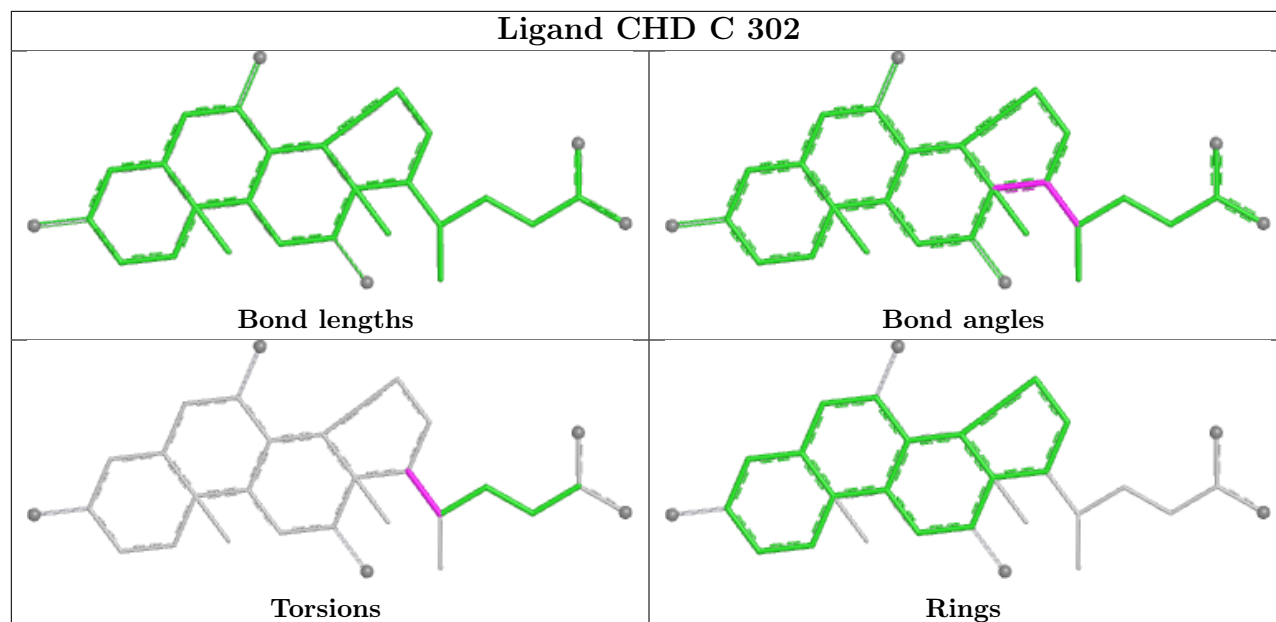


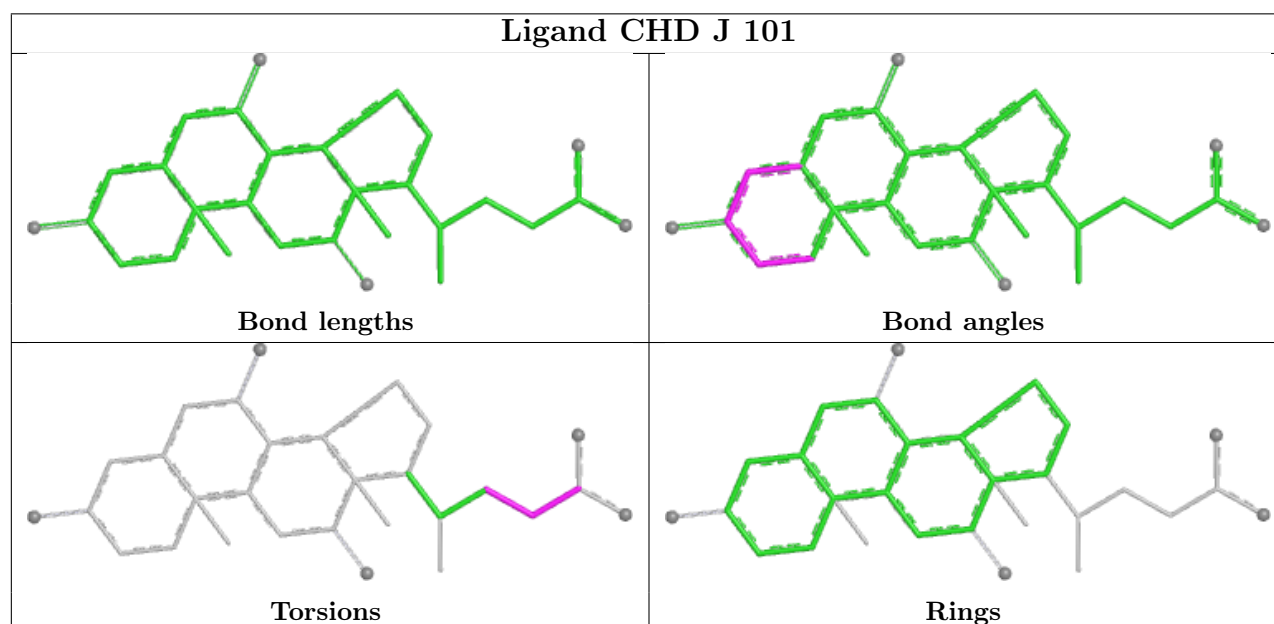
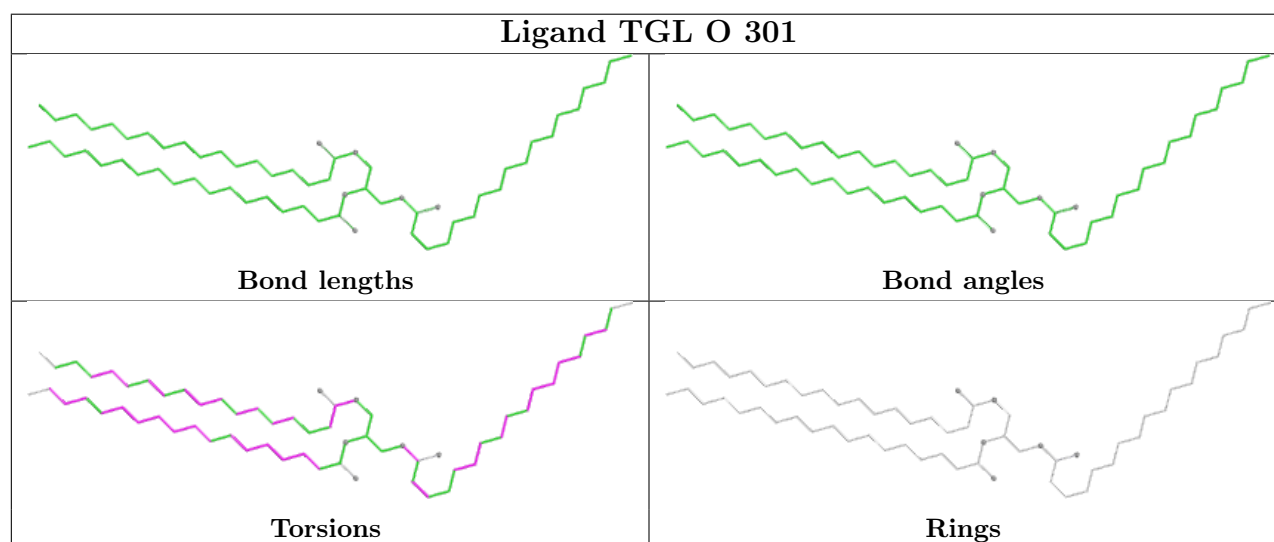
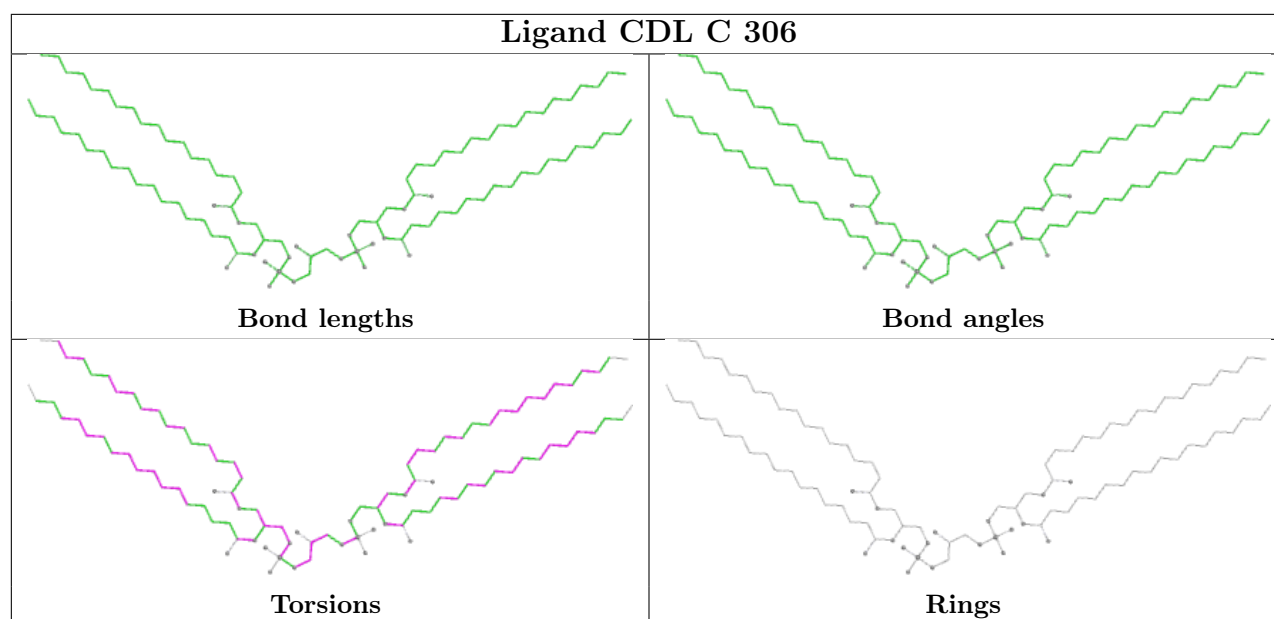
Ligand PEK P 304

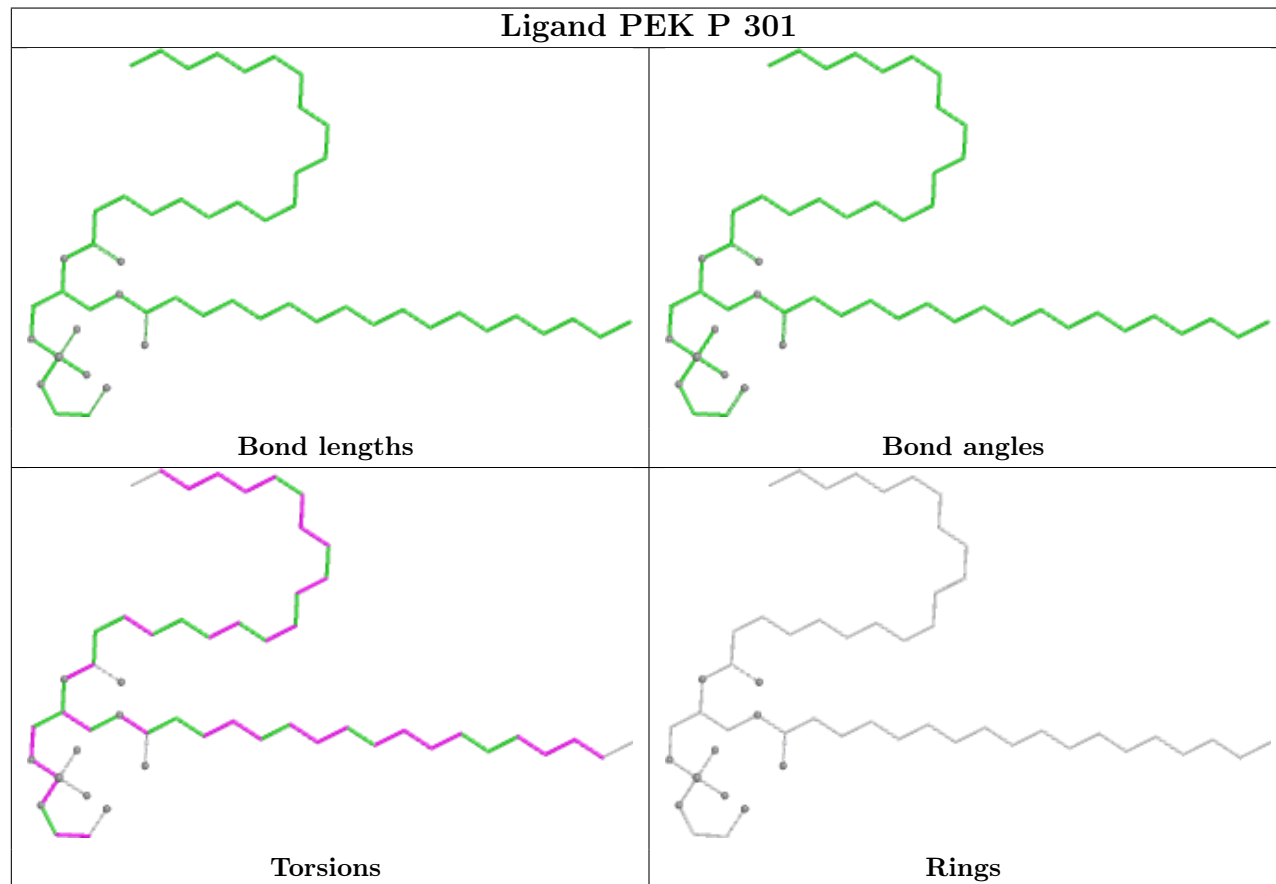
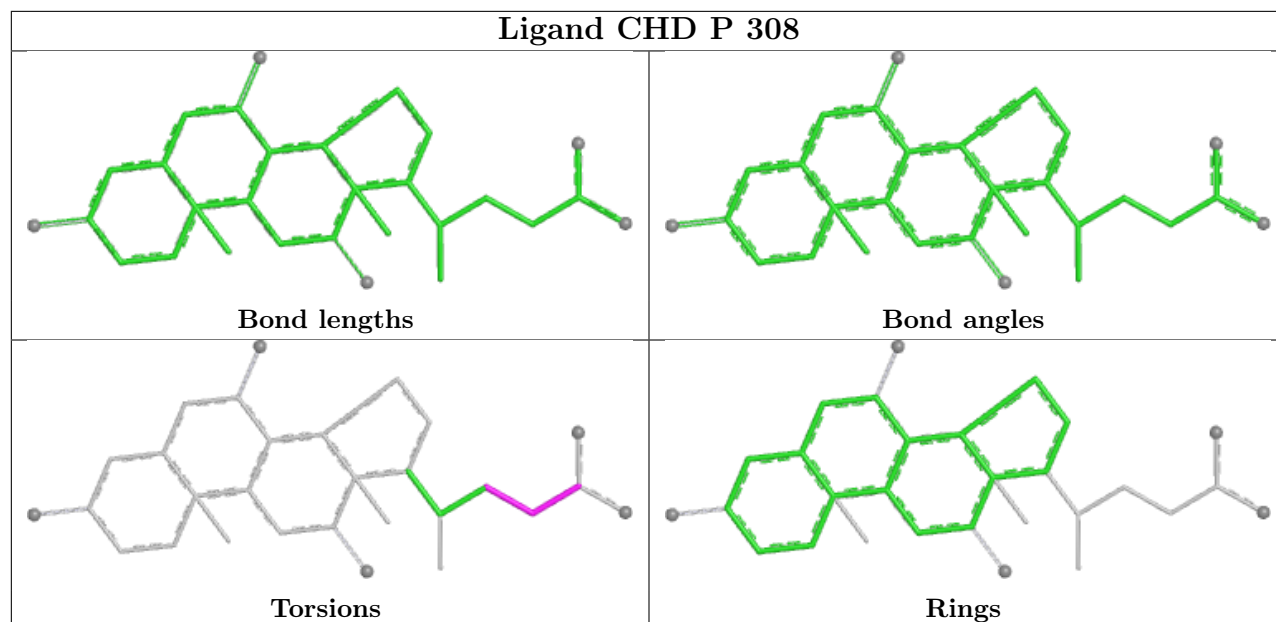


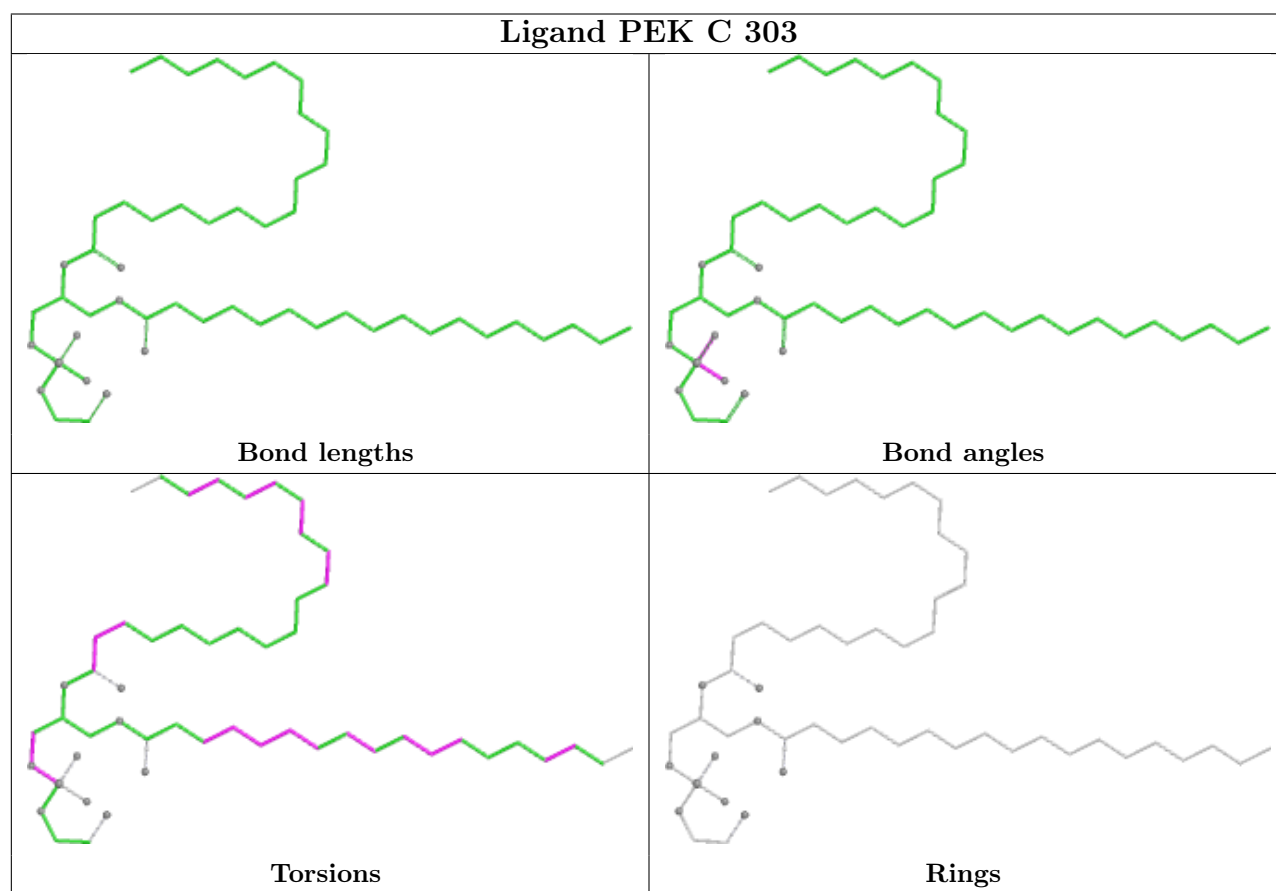
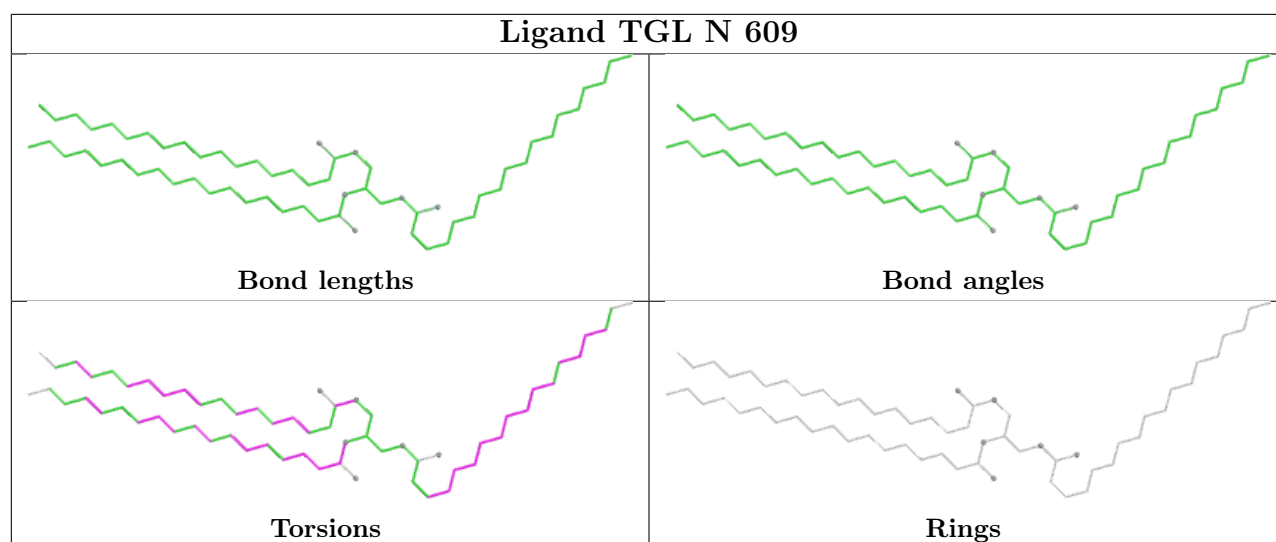


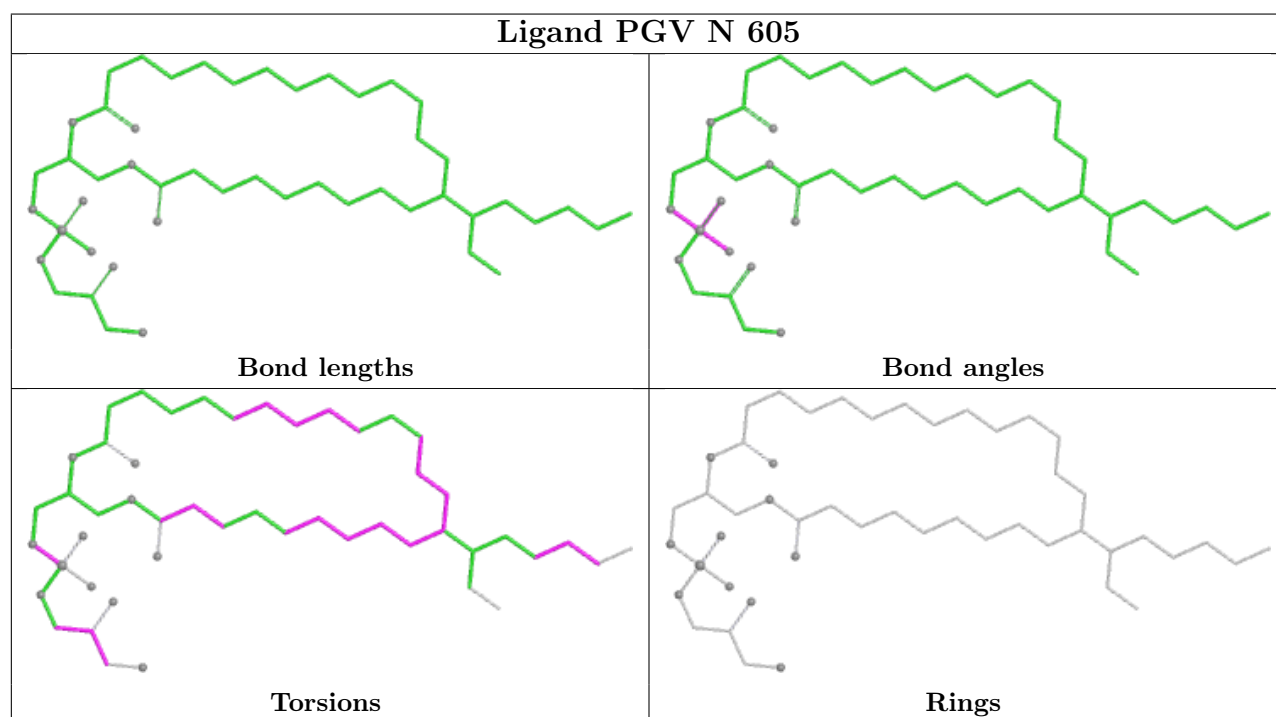
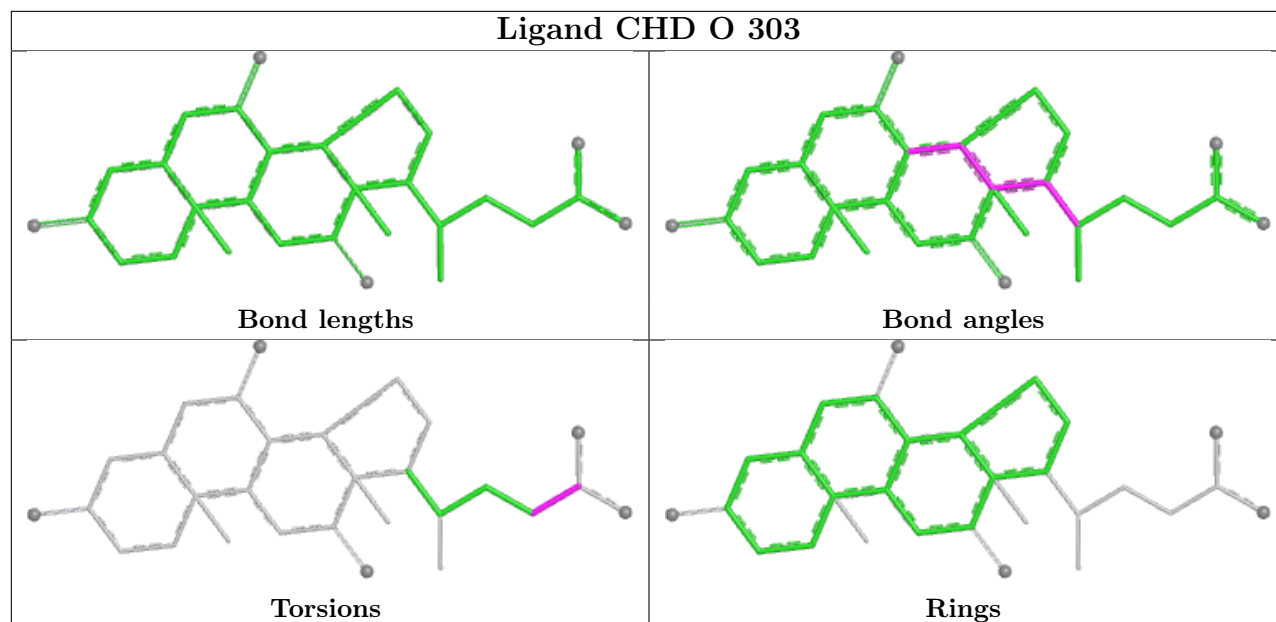


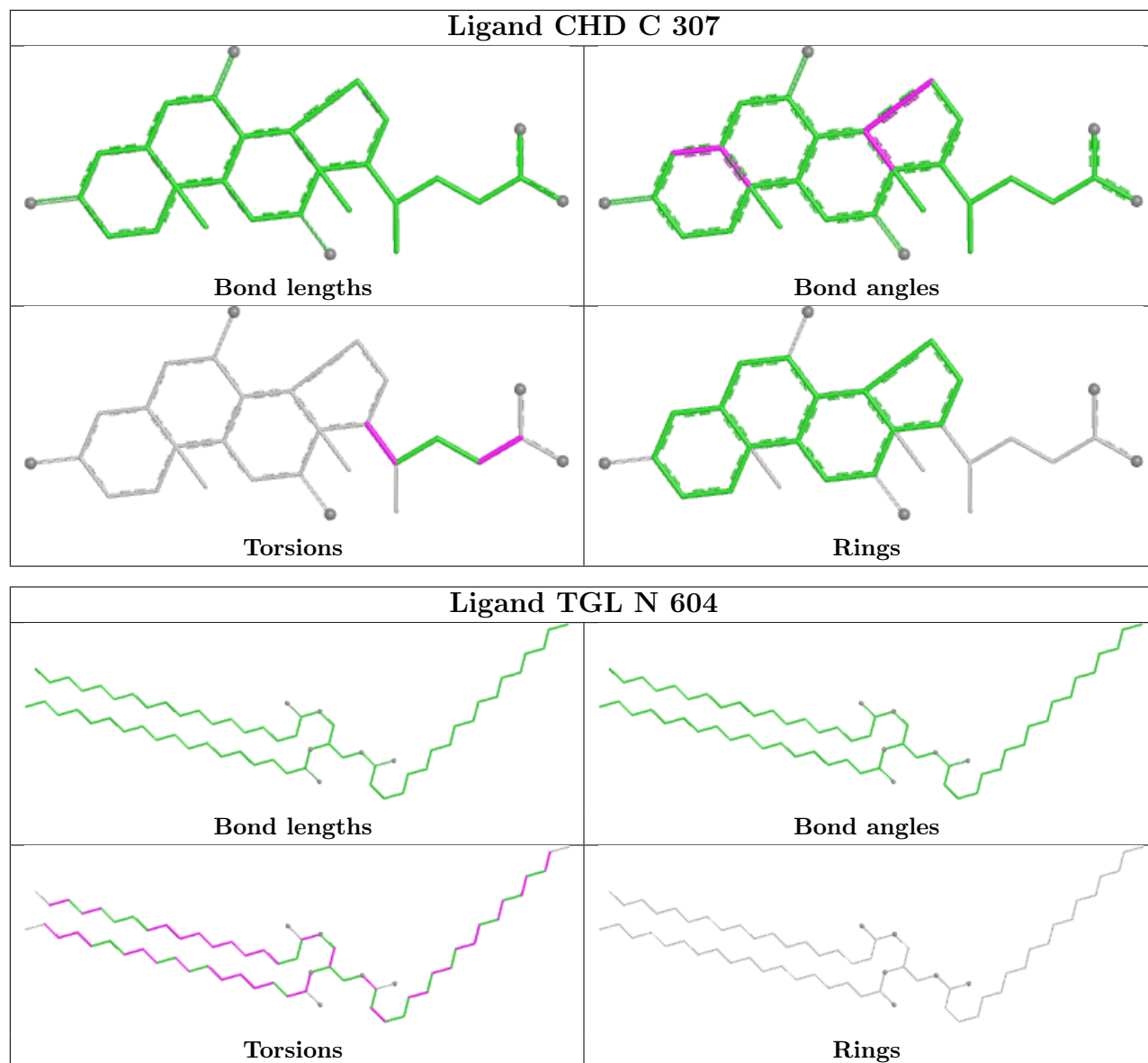


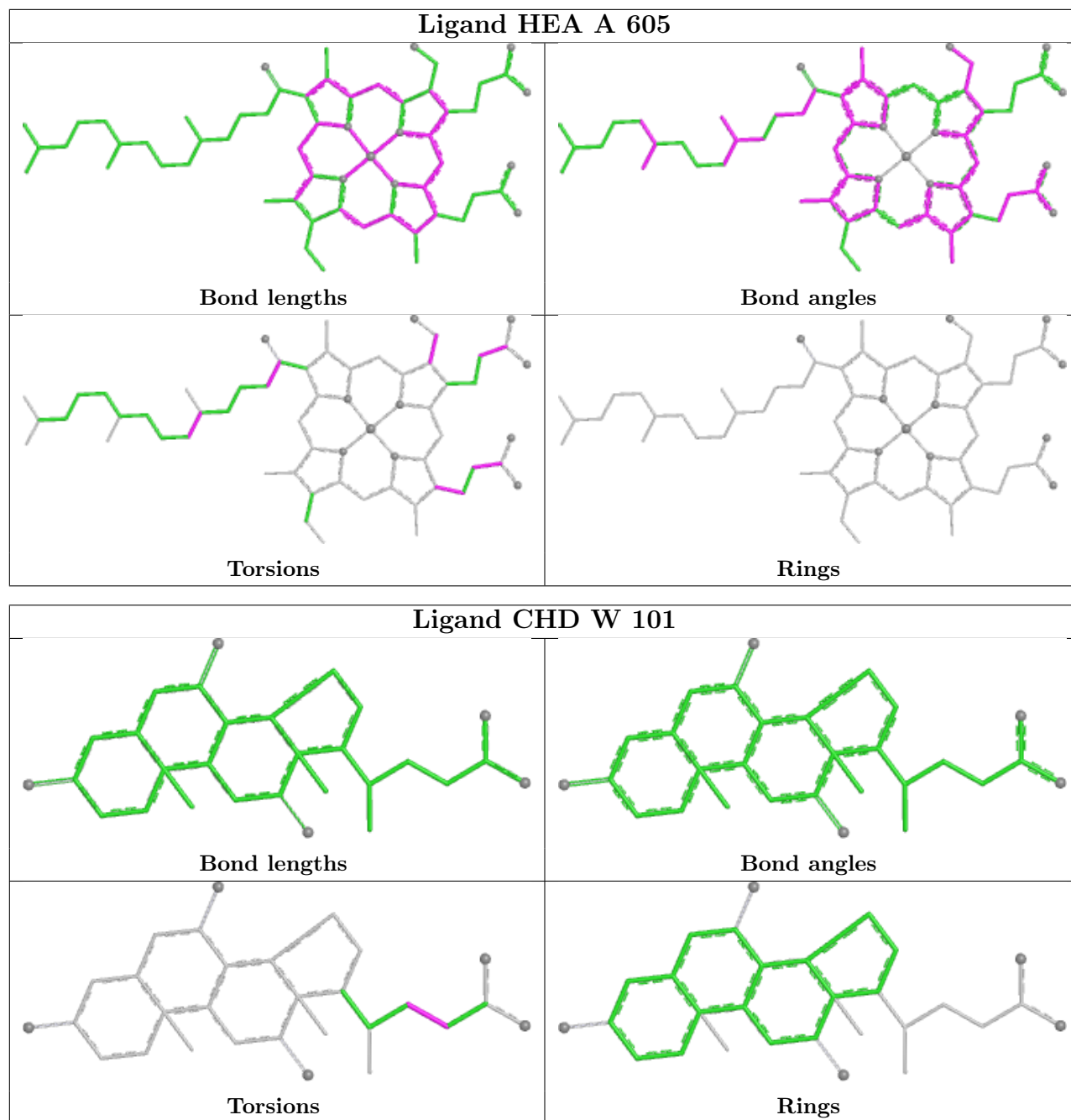


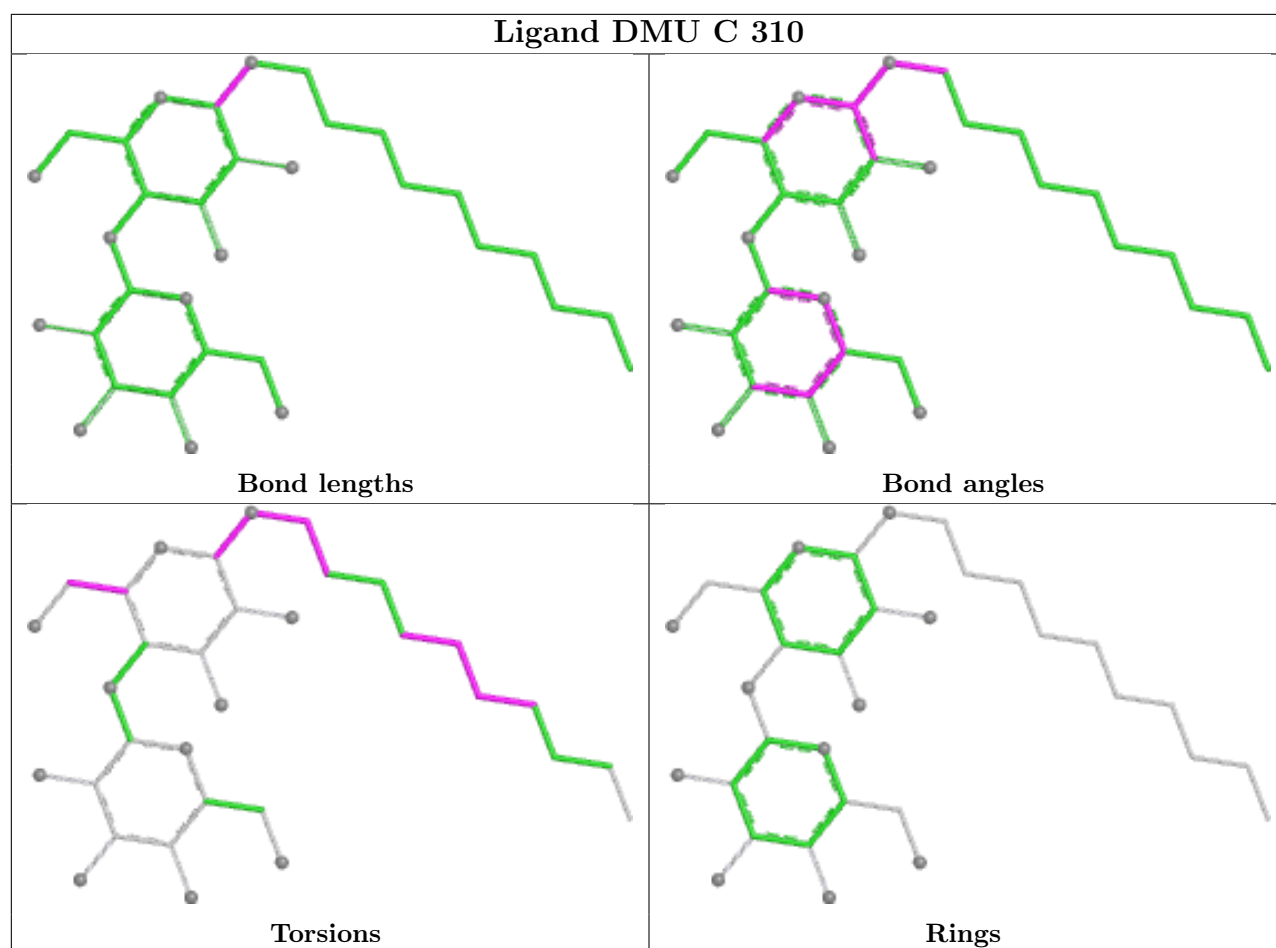


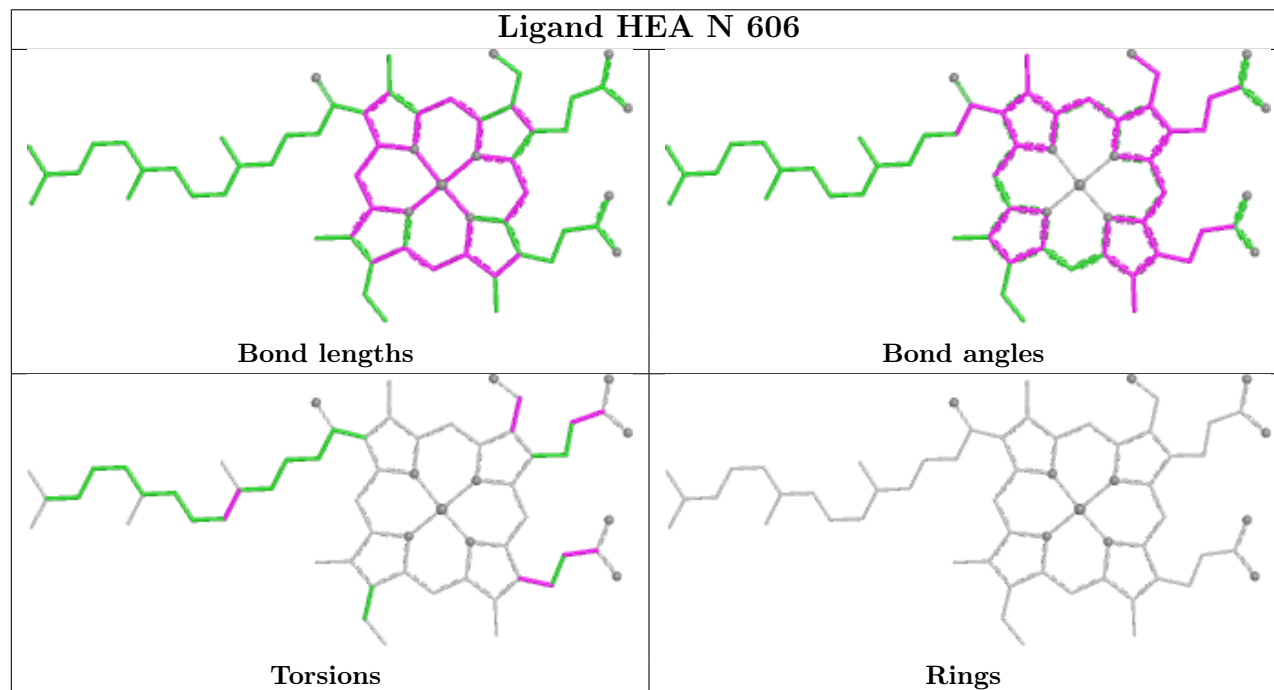
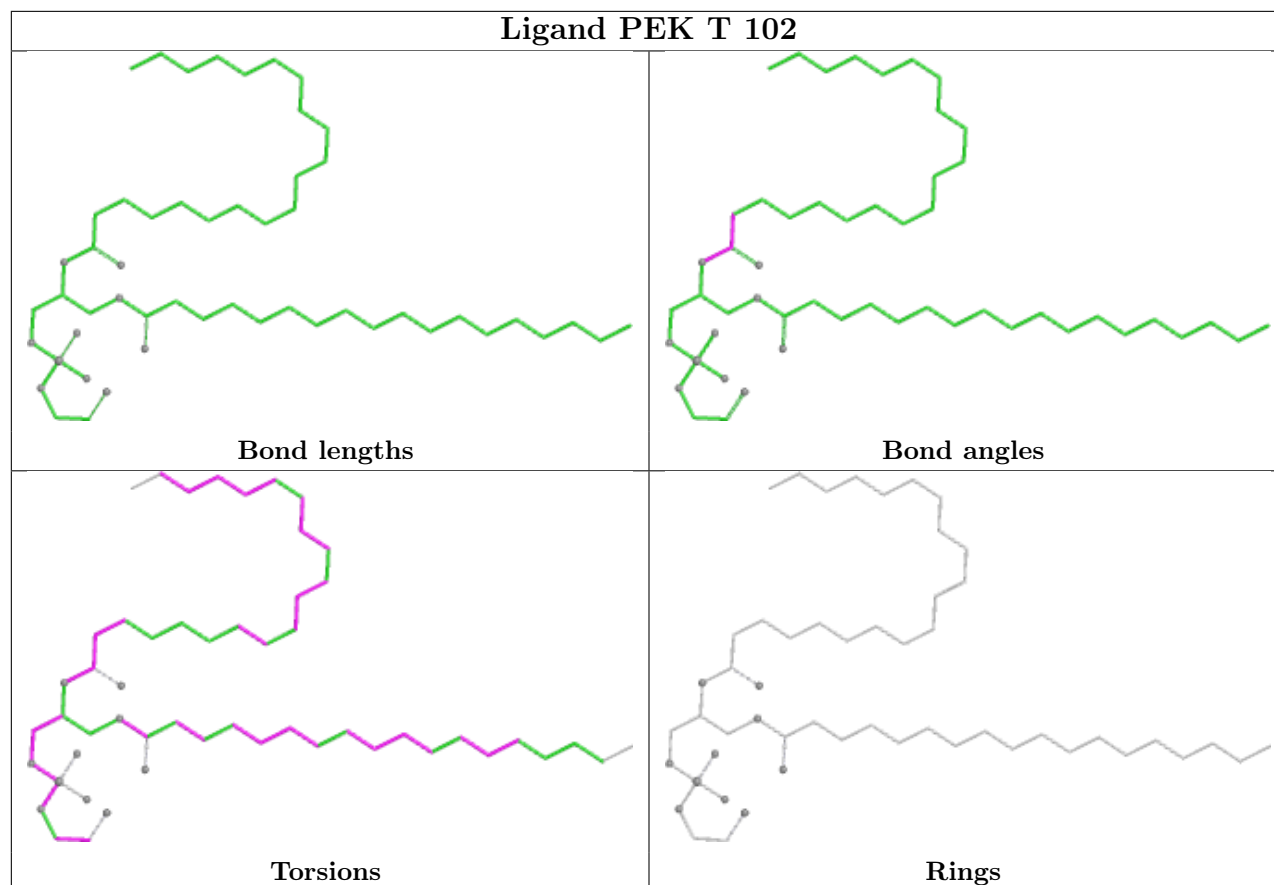


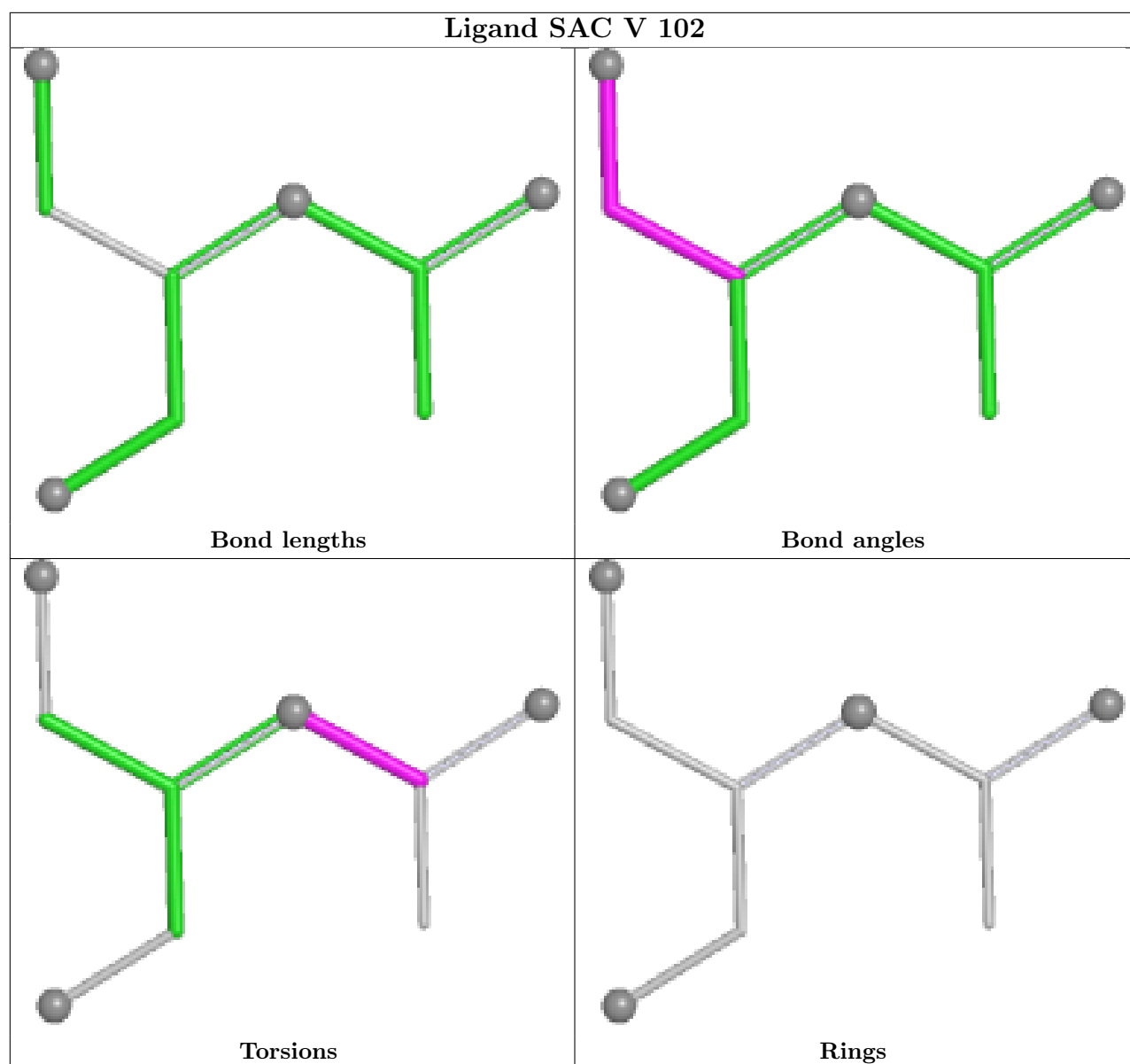


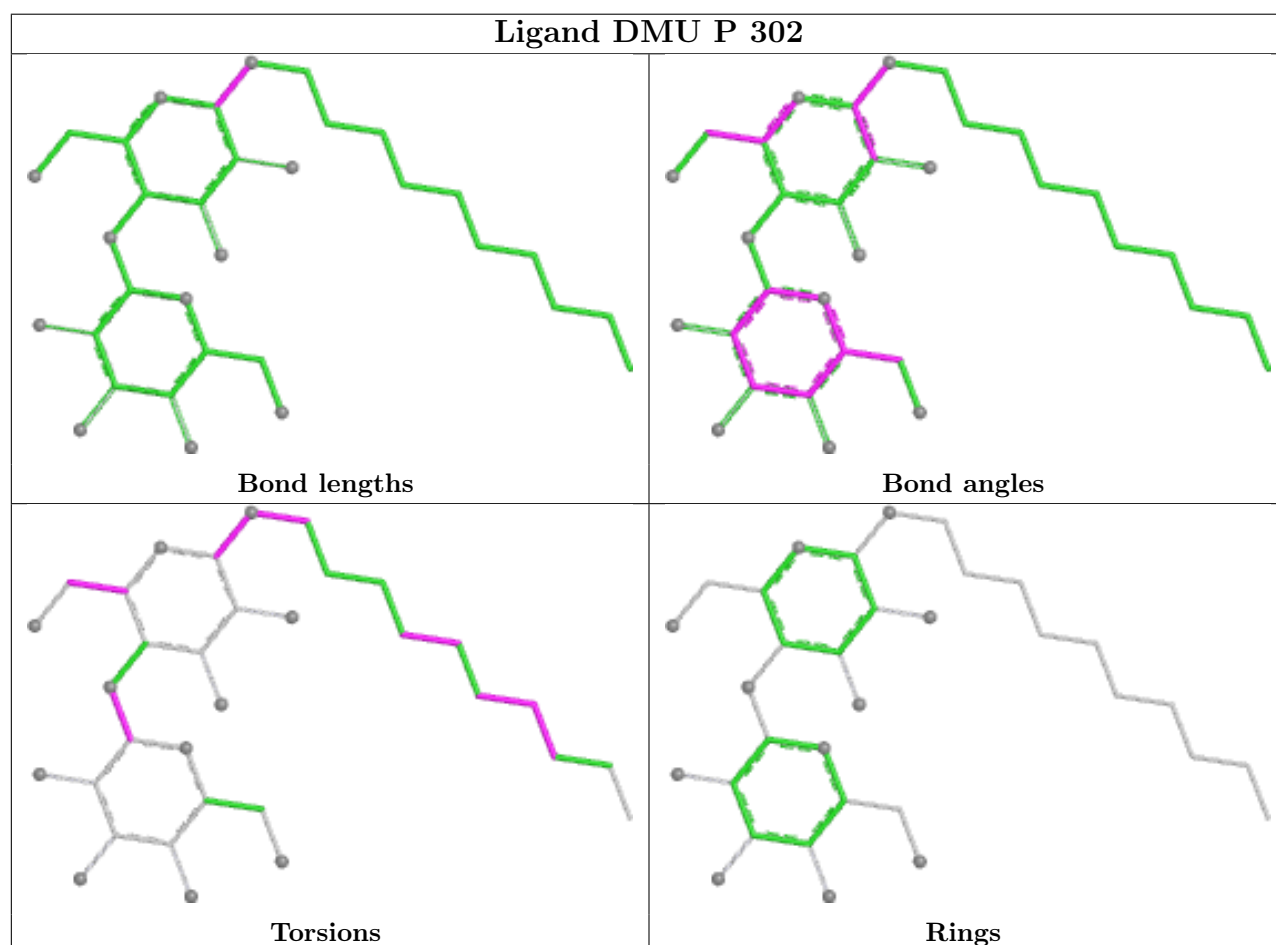
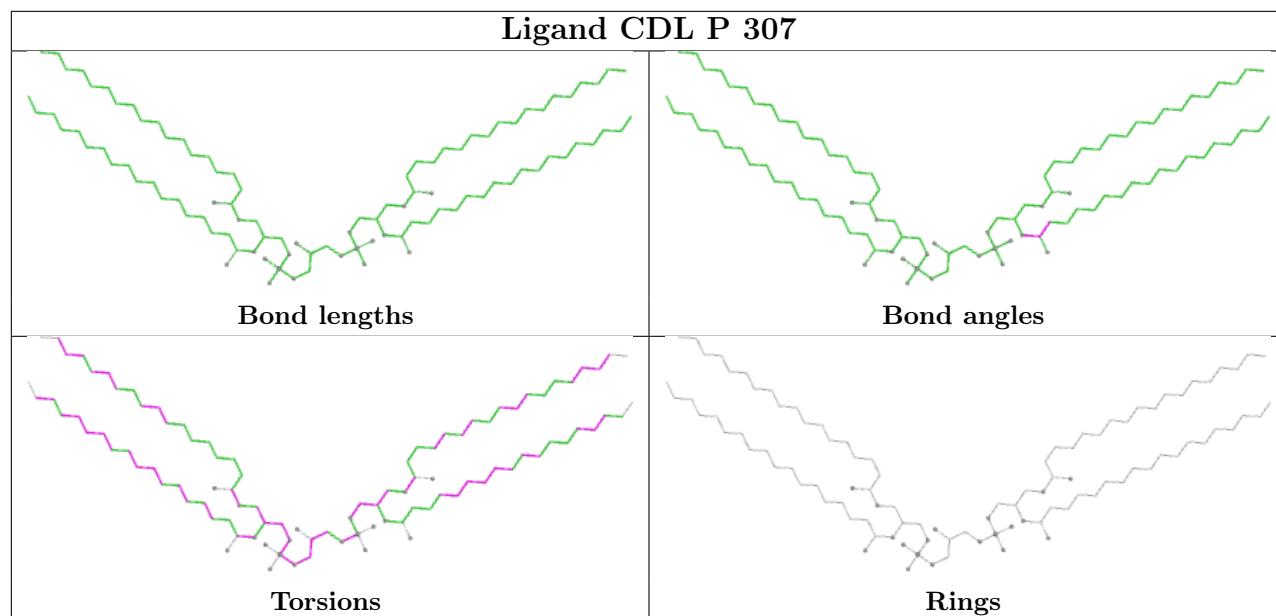


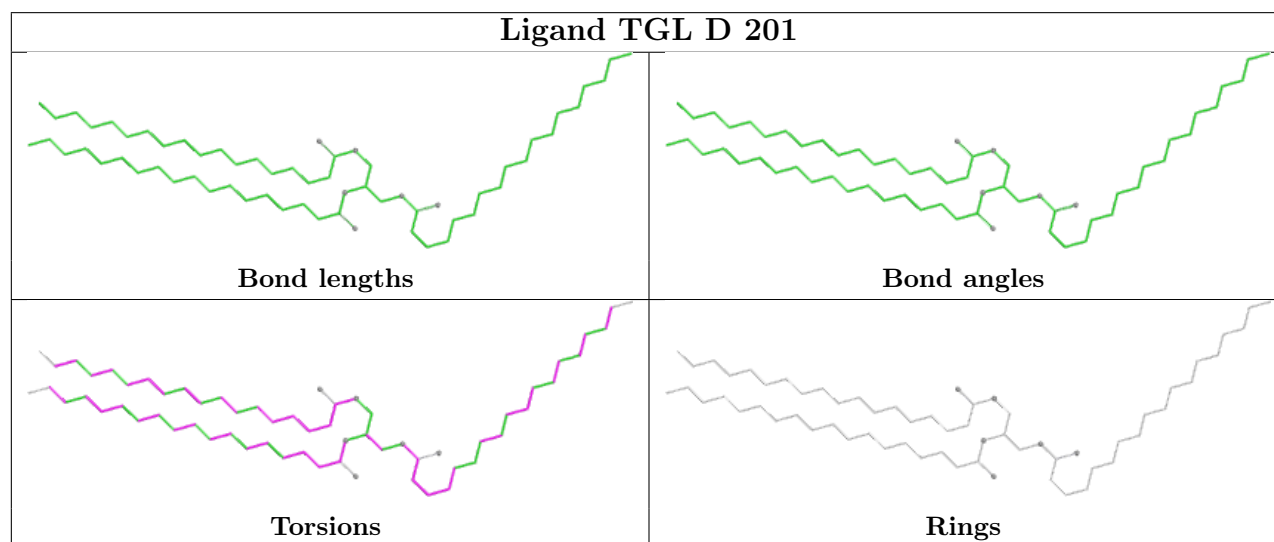
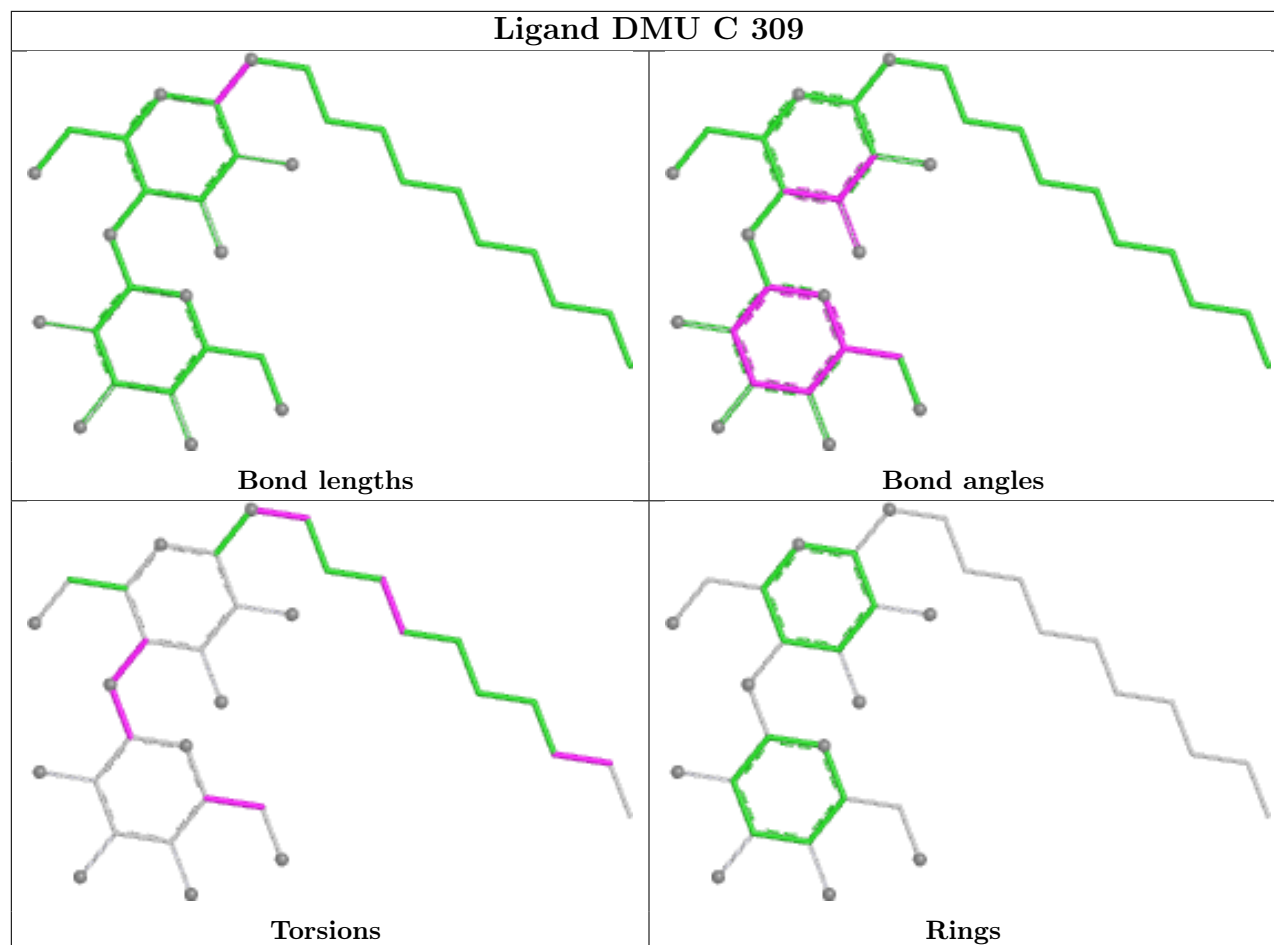


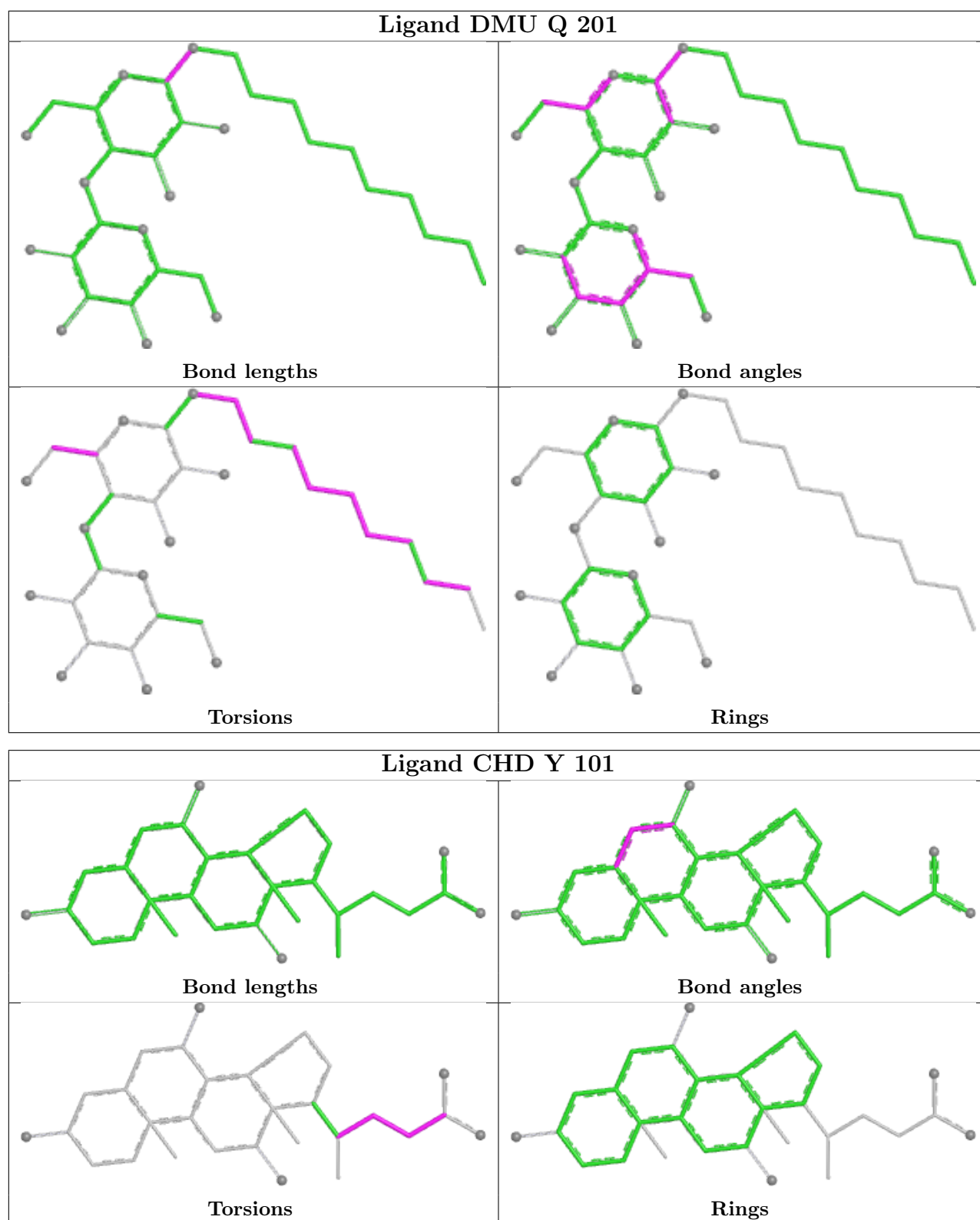


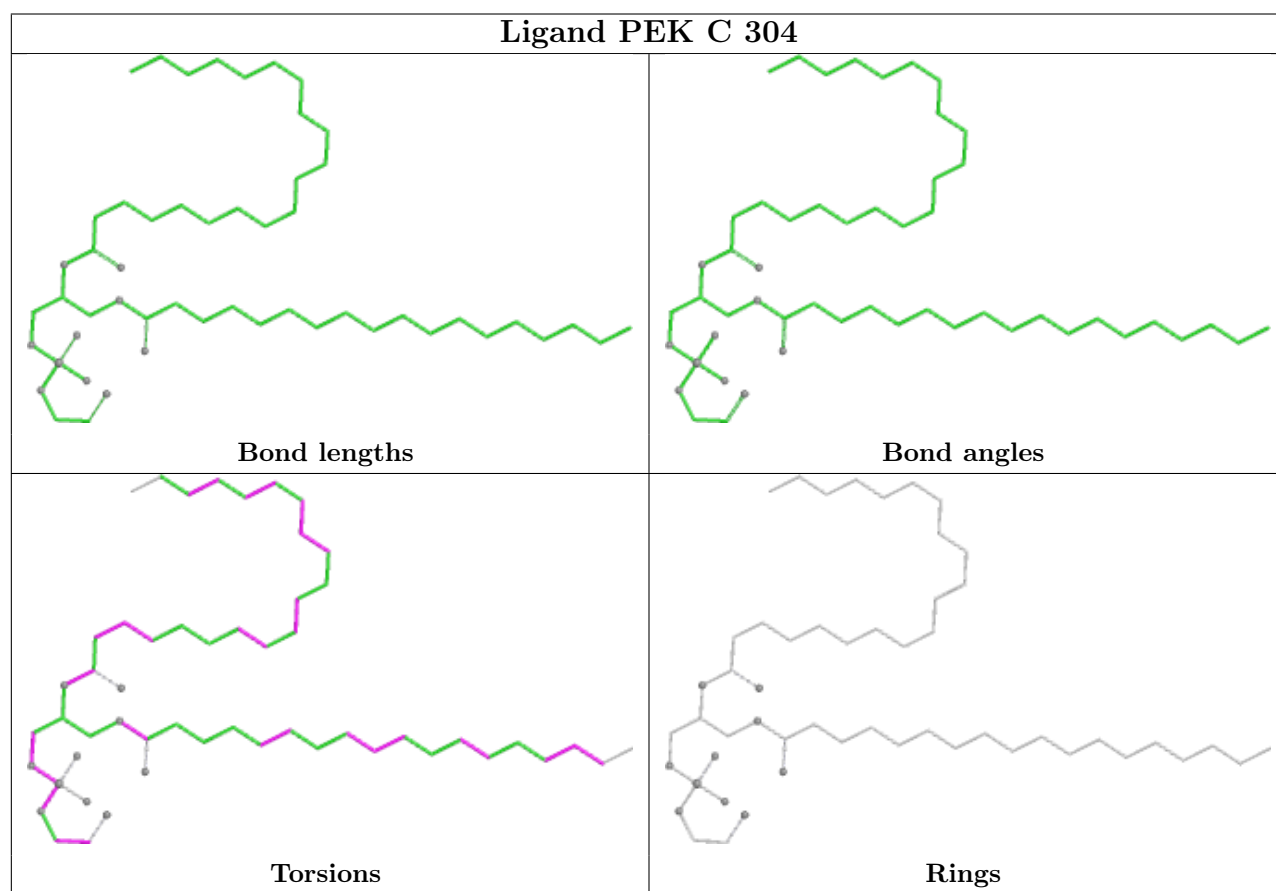
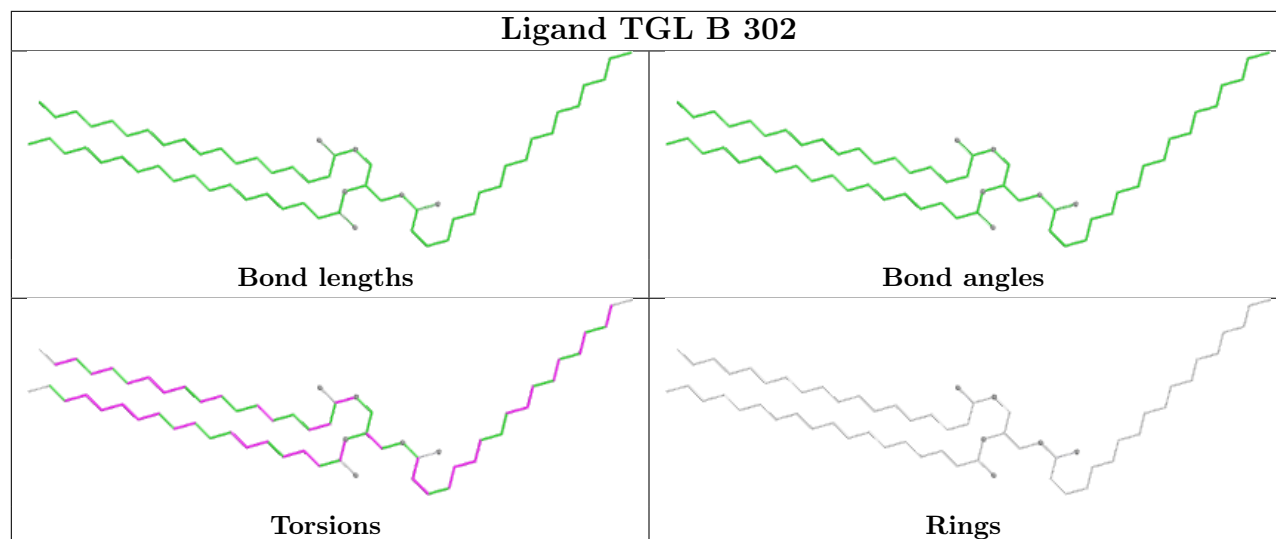


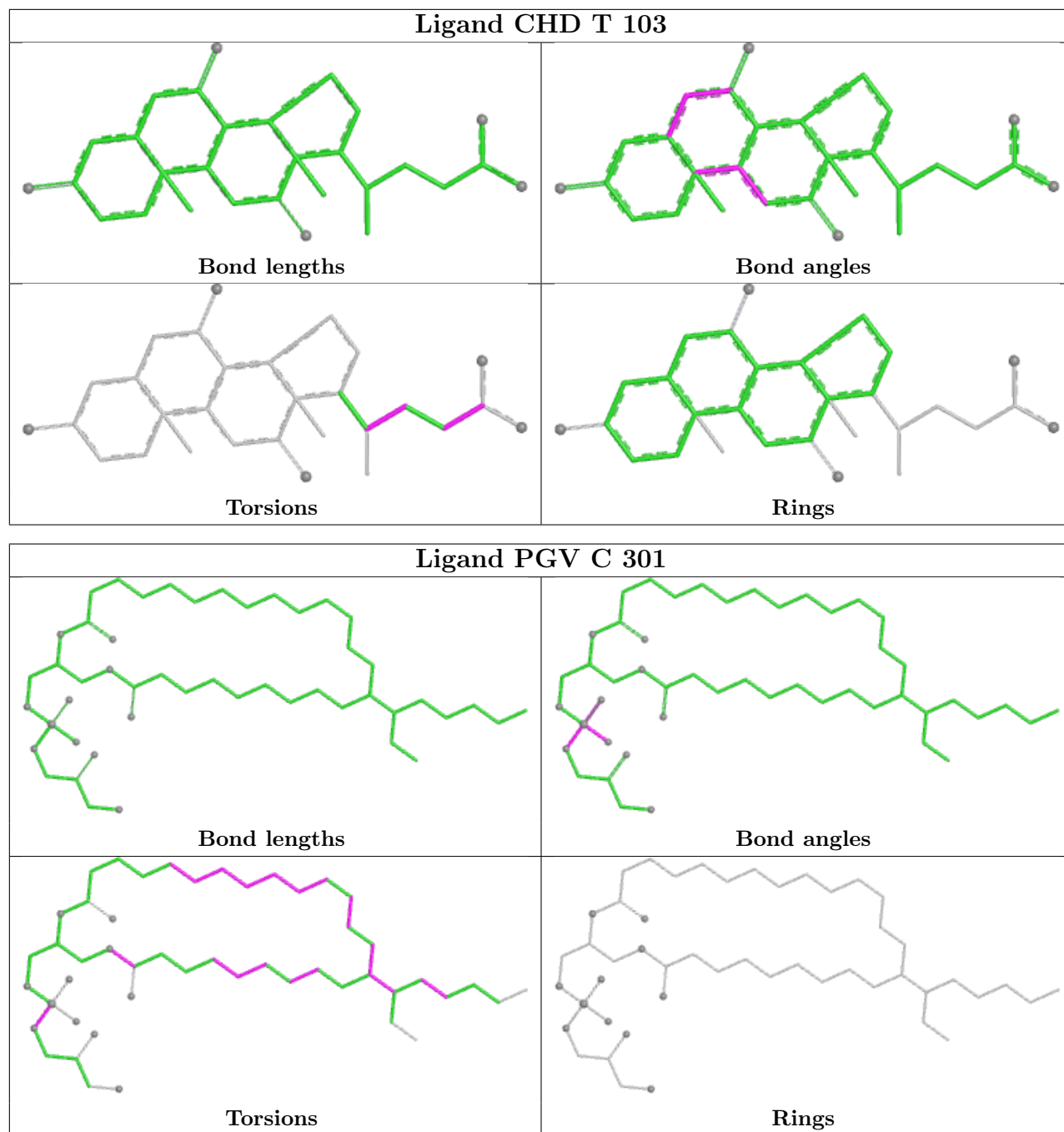


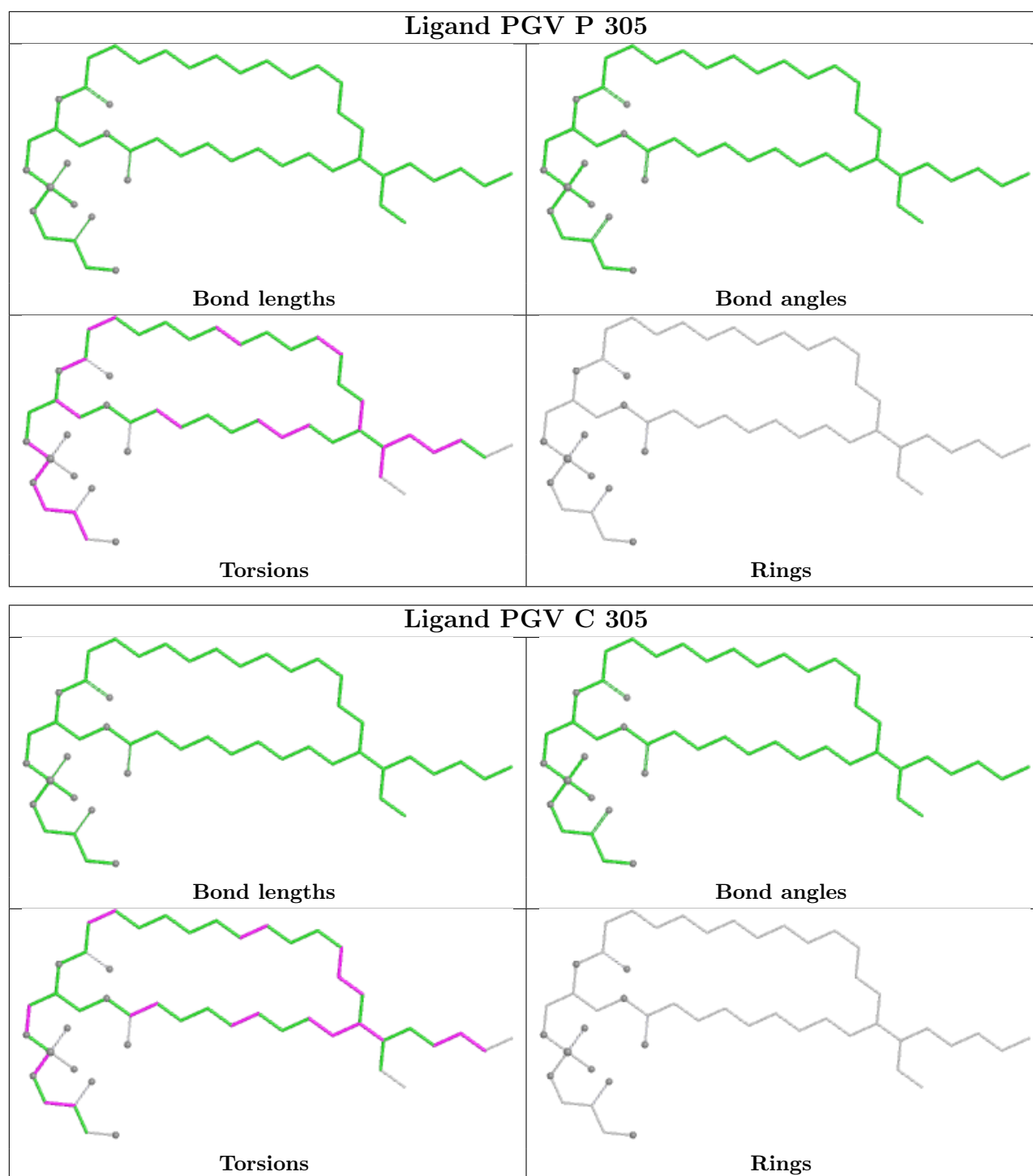












5.7 Other polymers [i](#)

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%)	-0.25	1 (0%) 91 90	5, 15, 24, 48	0
1	N	513/514 (99%)	0.33	20 (3%) 43 43	12, 27, 44, 62	0
2	B	226/227 (99%)	0.05	6 (2%) 56 56	8, 20, 45, 91	0
2	O	226/227 (99%)	0.90	26 (11%) 9 8	19, 39, 65, 116	0
3	C	259/261 (99%)	-0.00	2 (0%) 82 82	10, 20, 33, 50	0
3	P	259/261 (99%)	0.40	11 (4%) 40 40	13, 28, 49, 78	0
4	D	144/147 (97%)	0.11	5 (3%) 47 47	12, 27, 47, 59	0
4	Q	144/147 (97%)	1.35	29 (20%) 3 2	24, 52, 76, 185	0
5	E	105/109 (96%)	0.03	4 (3%) 44 44	15, 26, 53, 83	0
5	R	105/109 (96%)	0.52	3 (2%) 53 53	23, 40, 58, 85	0
6	F	98/98 (100%)	0.46	7 (7%) 22 20	13, 27, 78, 119	0
6	S	98/98 (100%)	1.08	13 (13%) 7 6	21, 37, 103, 151	0
7	G	83/85 (97%)	1.14	16 (19%) 3 3	15, 33, 100, 116	0
7	T	83/85 (97%)	1.40	18 (21%) 2 2	14, 43, 92, 121	0
8	H	79/85 (92%)	0.47	6 (7%) 20 18	14, 28, 73, 83	0
8	U	79/85 (92%)	1.17	14 (17%) 4 3	29, 45, 87, 128	0
9	I	72/73 (98%)	0.56	6 (8%) 17 16	18, 36, 63, 76	0
9	V	72/73 (98%)	1.10	9 (12%) 8 7	30, 51, 72, 76	0
10	J	58/59 (98%)	0.34	3 (5%) 33 32	13, 31, 64, 92	0
10	W	58/59 (98%)	1.21	12 (20%) 2 2	32, 47, 89, 127	0
11	K	49/56 (87%)	0.19	1 (2%) 65 63	15, 28, 43, 47	0
11	X	49/56 (87%)	1.23	9 (18%) 3 3	34, 46, 69, 83	0
12	L	46/47 (97%)	0.02	1 (2%) 62 61	12, 20, 35, 77	0
12	Y	46/47 (97%)	1.02	4 (8%) 16 15	25, 41, 64, 76	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/47 (91%)	0.28	5 (11%) 9 8	14, 21, 74, 85	0
13	Z	43/47 (91%)	1.14	9 (20%) 2 2	29, 43, 73, 82	0
All	All	3550/3616 (98%)	0.42	240 (6%) 23 22	5, 28, 65, 185	0

The worst 5 of 240 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	14.0
4	Q	5	VAL	11.9
6	S	1	ALA	11.2
6	S	97	ALA	10.1
4	Q	7	LYS	8.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	G	11	11/12	0.61	0.27	81,114,143,143	0
7	TPO	T	11	11/12	0.74	0.27	85,108,132,134	0
1	FME	N	1	10/11	0.80	0.24	55,66,83,83	0
1	FME	A	1	10/11	0.90	0.13	31,37,45,48	0
2	FME	O	1	10/11	0.94	0.13	18,42,55,61	0
2	FME	B	1	10/11	0.96	0.08	23,25,26,26	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	SAC	I	101	9/10	0.64	0.23	82,90,98,99	0
26	DMU	P	302	33/33	0.67	0.20	45,87,96,102	0
23	CHD	Y	101	29/29	0.69	0.35	63,140,155,157	0
24	PEK	T	102	53/53	0.71	0.29	47,76,131,143	0
26	DMU	G	101	33/33	0.71	0.21	41,106,120,123	0
26	DMU	C	310	33/33	0.72	0.21	47,78,102,105	0
24	PEK	C	311	53/53	0.72	0.24	39,70,95,114	0
22	PSC	V	101	52/52	0.73	0.32	56,102,190,205	0
23	CHD	T	103	29/29	0.74	0.28	58,120,126,132	0
17	PGV	N	610	51/51	0.74	0.27	38,85,153,163	0
24	PEK	P	301	53/53	0.75	0.24	44,86,182,202	0
21	TGL	N	609	63/63	0.76	0.29	46,78,101,118	0
22	PSC	B	303	52/52	0.76	0.30	48,102,189,190	0
25	CDL	P	307	100/100	0.76	0.26	36,78,106,118	0
25	CDL	P	309	100/100	0.76	0.31	53,91,123,125	0
17	PGV	P	306	51/51	0.77	0.19	45,64,98,114	0
25	CDL	C	308	100/100	0.77	0.27	28,85,117,123	0
25	CDL	C	306	100/100	0.78	0.24	35,69,129,133	0
24	PEK	C	304	53/53	0.79	0.26	33,89,176,203	0
21	TGL	N	604	63/63	0.79	0.25	37,73,98,109	0
17	PGV	A	604	51/51	0.79	0.24	30,60,146,150	0
26	DMU	Q	201	33/33	0.79	0.16	35,57,71,74	0
17	PGV	H	101	51/51	0.79	0.22	57,69,86,88	0
26	DMU	C	309	33/33	0.80	0.17	23,71,87,95	0
28	SAC	V	102	9/10	0.80	0.14	60,74,78,79	0
23	CHD	W	101	29/29	0.81	0.19	58,83,95,96	0
21	TGL	D	201	63/63	0.84	0.22	36,60,93,97	0
21	TGL	L	101	63/63	0.85	0.19	13,53,77,82	0
23	CHD	C	307	29/29	0.85	0.14	32,50,56,60	0
23	CHD	J	101	29/29	0.85	0.13	53,61,64,69	0
21	TGL	B	302	63/63	0.86	0.22	21,56,94,98	0
21	TGL	O	301	63/63	0.88	0.19	33,61,87,93	0
23	CHD	P	308	29/29	0.88	0.14	52,72,76,80	0
23	CHD	O	303	29/29	0.90	0.10	24,27,30,33	0
23	CHD	P	303	29/29	0.91	0.09	16,24,28,30	0
16	NA	N	603	1/1	0.91	0.08	30,30,30,30	0
17	PGV	N	605	51/51	0.93	0.16	21,34,68,73	0
17	PGV	P	305	51/51	0.94	0.13	18,31,64,74	0
26	DMU	M	101	33/33	0.94	0.07	10,23,34,36	0
17	PGV	C	301	51/51	0.94	0.10	12,25,37,40	0
24	PEK	P	304	53/53	0.94	0.14	23,49,81,83	0
24	PEK	C	303	53/53	0.94	0.15	20,44,104,113	0
23	CHD	C	302	29/29	0.94	0.08	14,17,18,20	0

Continued on next page...

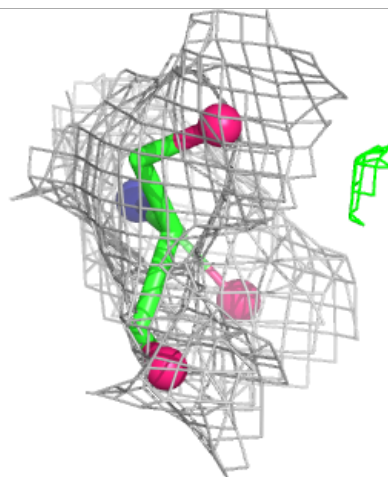
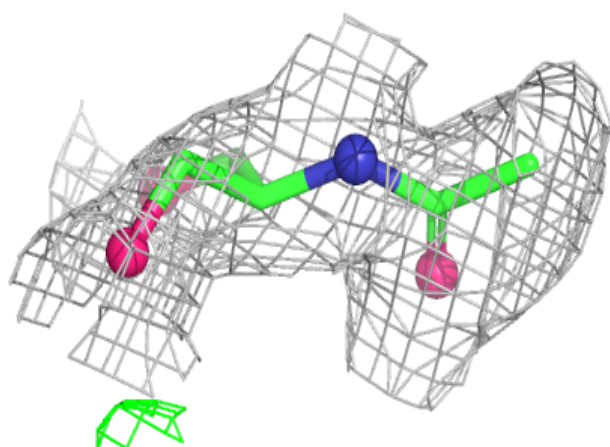
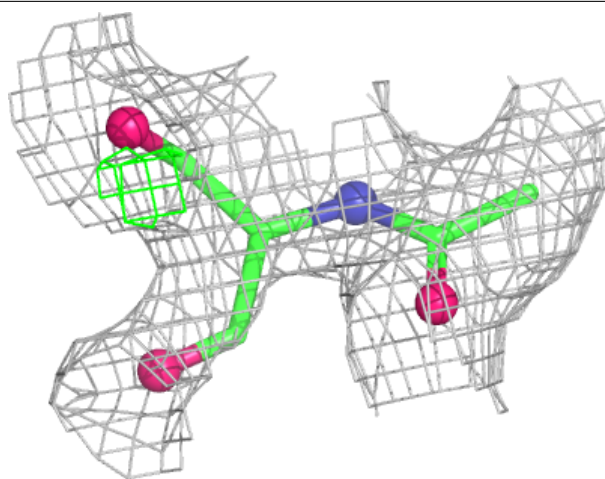
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CHD	T	101	29/29	0.95	0.08	11,13,15,17	0
17	PGV	C	305	51/51	0.95	0.12	14,26,74,81	0
18	HEA	N	607	60/60	0.96	0.11	24,29,53,58	0
18	HEA	N	606	60/60	0.97	0.08	16,20,33,37	0
16	NA	A	603	1/1	0.98	0.05	18,18,18,18	0
18	HEA	A	605	60/60	0.98	0.07	5,11,22,24	0
18	HEA	A	606	60/60	0.98	0.07	9,12,15,16	0
15	MG	A	602	1/1	0.98	0.03	15,15,15,15	0
15	MG	N	602	1/1	0.98	0.14	26,26,26,26	0
20	CUA	B	301	2/2	0.98	0.04	19,19,19,19	0
19	OH	N	608	1/1	0.99	0.04	14,14,14,14	0
20	CUA	O	302	2/2	0.99	0.02	29,29,29,34	0
14	CU	A	601	1/1	1.00	0.02	12,12,12,12	0
27	ZN	F	101	1/1	1.00	0.03	23,23,23,23	0
27	ZN	S	101	1/1	1.00	0.03	30,30,30,30	0
14	CU	N	601	1/1	1.00	0.02	29,29,29,29	0
19	OH	A	607	1/1	1.00	0.04	9,9,9,9	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.

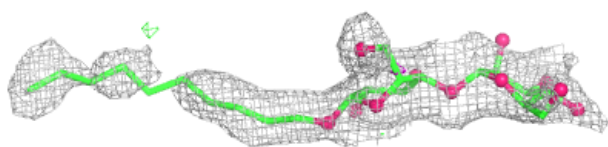
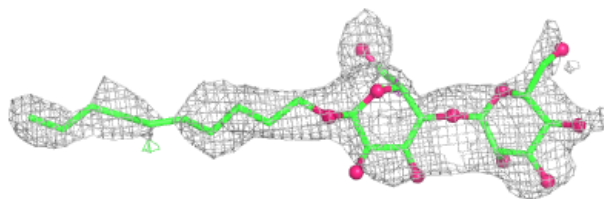
Electron density around SAC I 101:

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

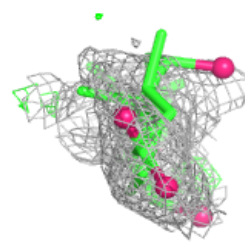
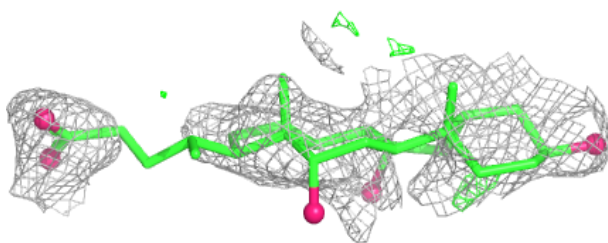
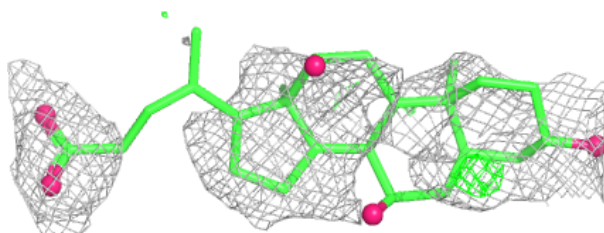


Electron density around DMU P 302:

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

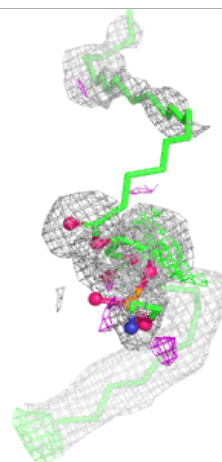
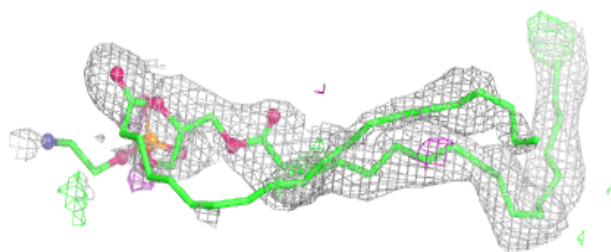
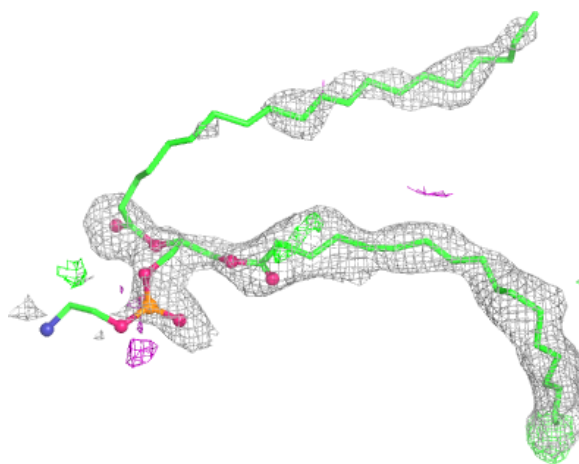
**Electron density around CHD Y 101:**

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



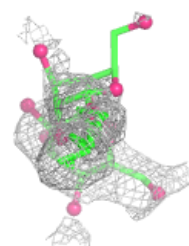
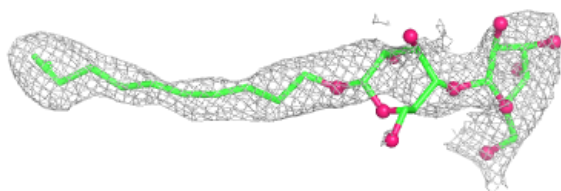
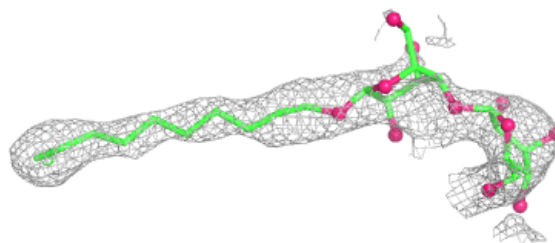
Electron density around PEK T 102:

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

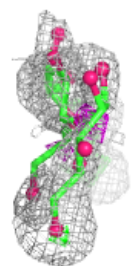
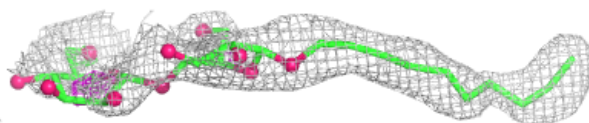
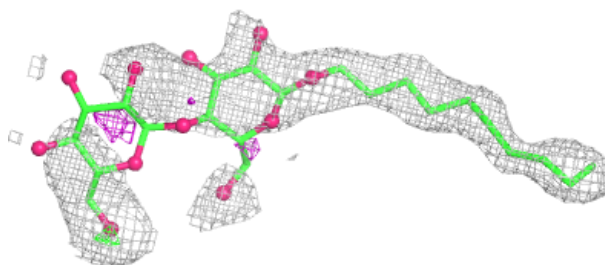


Electron density around DMU G 101:

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

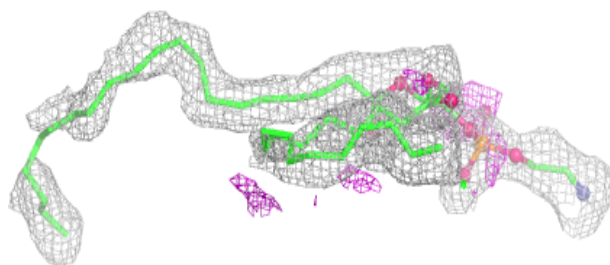
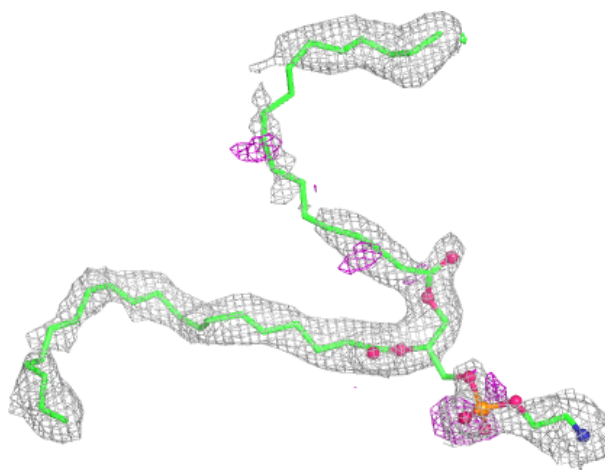
**Electron density around DMU C 310:**

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



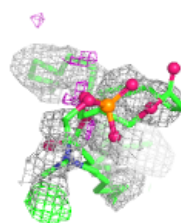
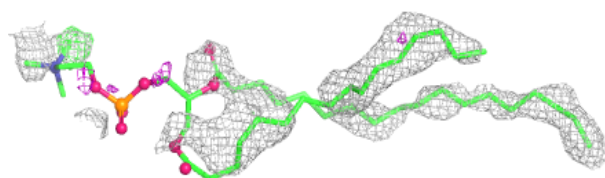
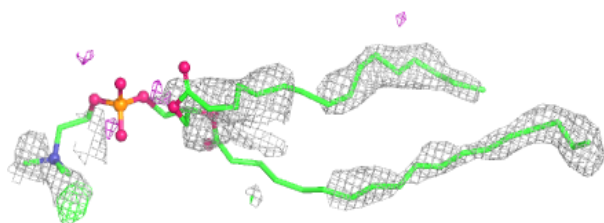
Electron density around PEK C 311:

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

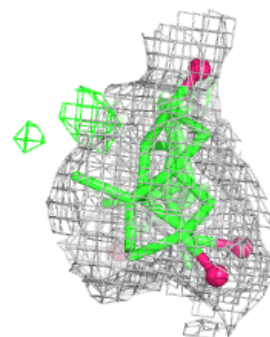
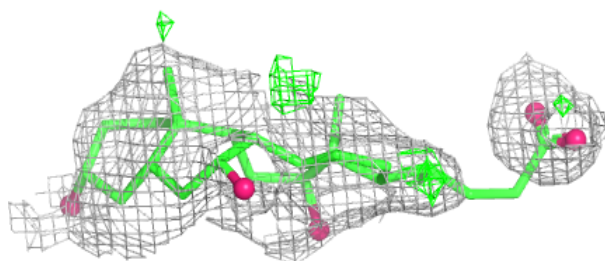


Electron density around PSC V 101:

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

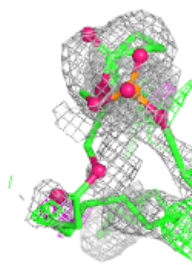
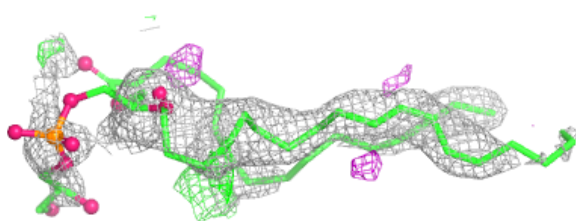
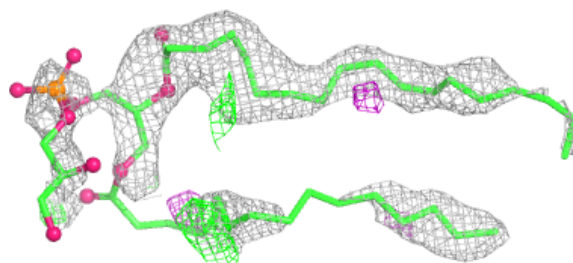
**Electron density around CHD T 103:**

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

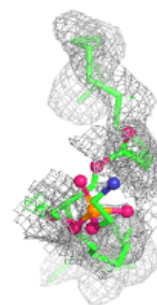
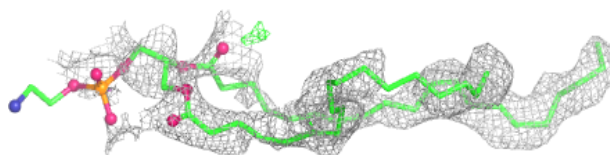
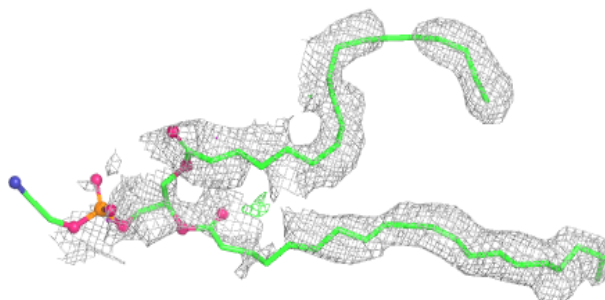


Electron density around PGV N 610:

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

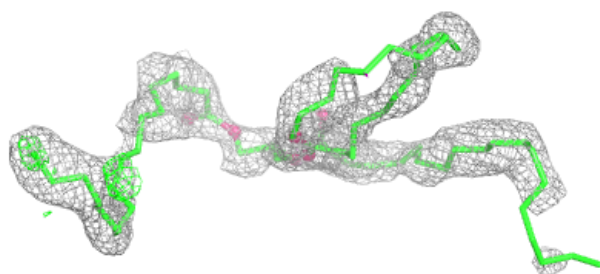
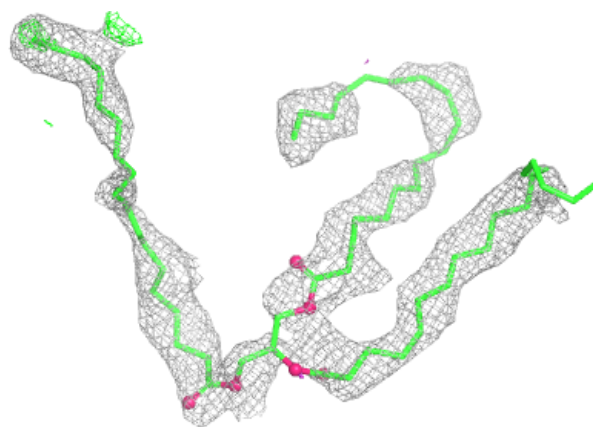
**Electron density around PEK P 301:**

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

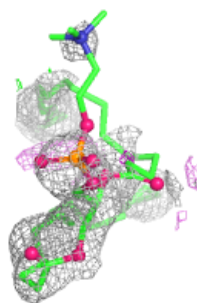
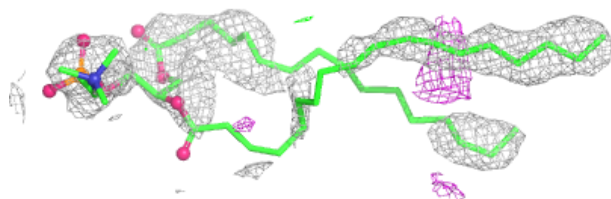
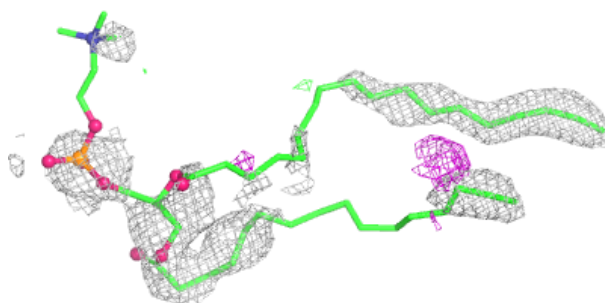


Electron density around TGL N 609:

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

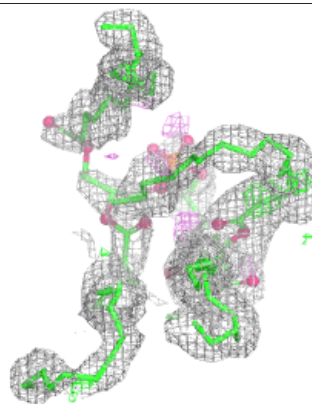
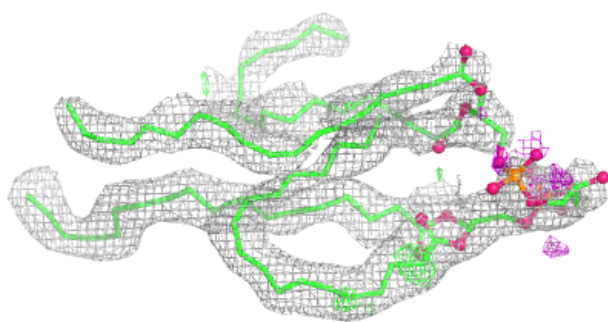
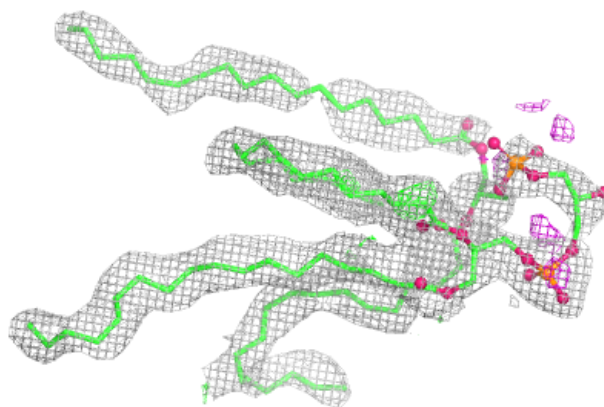
**Electron density around PSC B 303:**

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



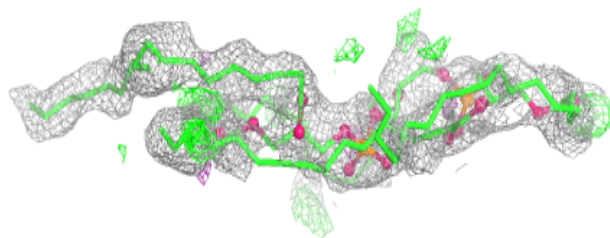
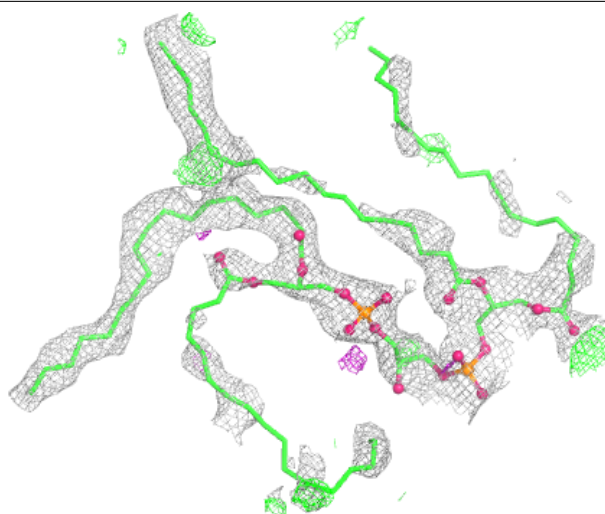
Electron density around CDL P 307:

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



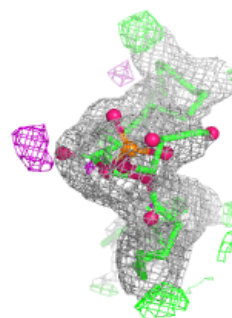
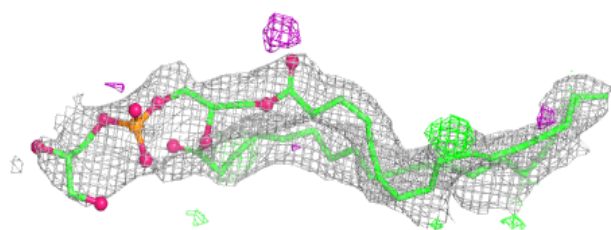
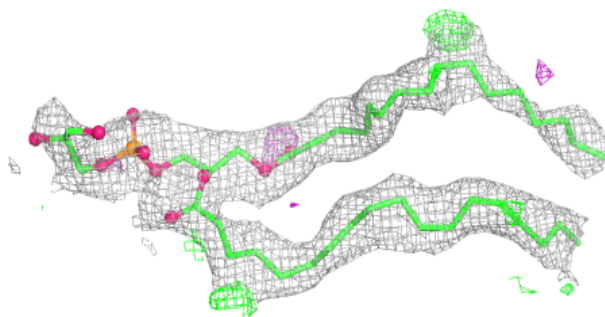
Electron density around CDL P 309:

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

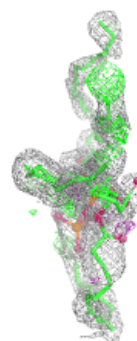
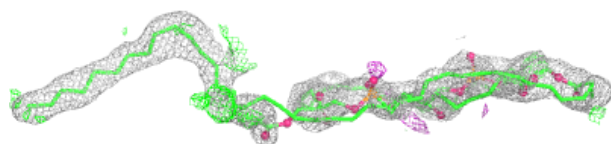
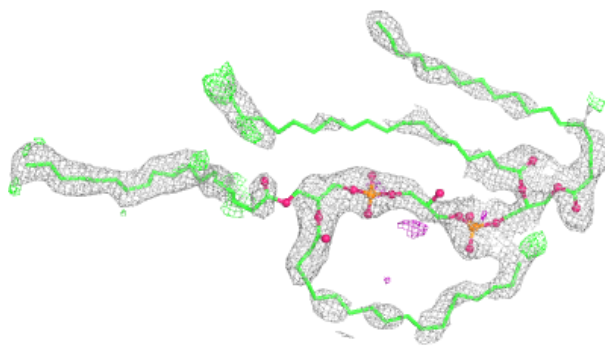


Electron density around PGV P 306:

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

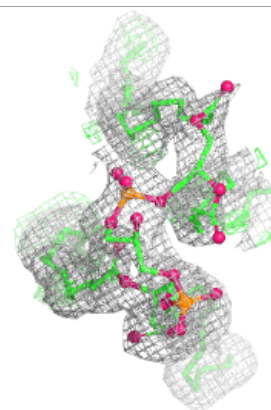
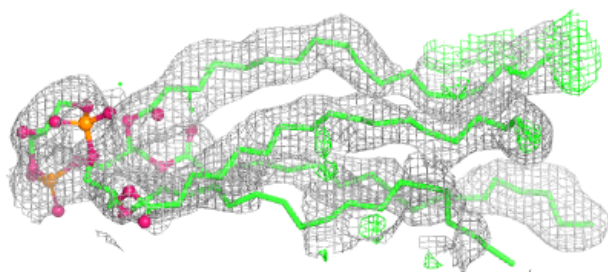
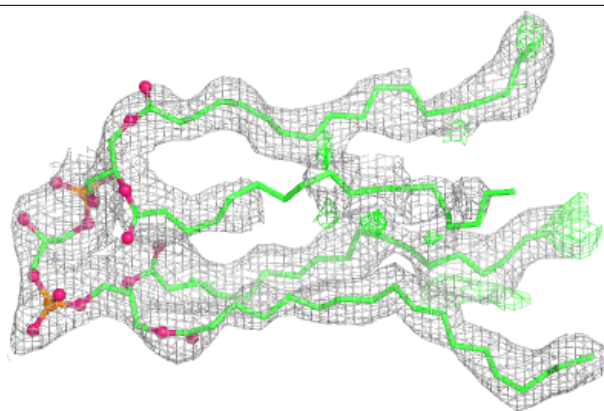
**Electron density around CDL C 308:**

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

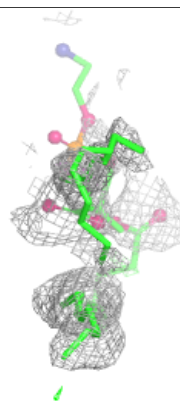
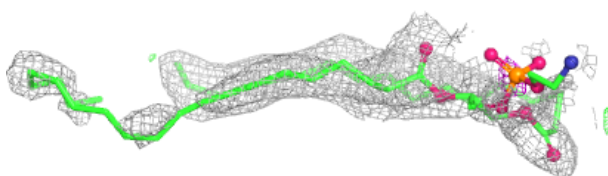
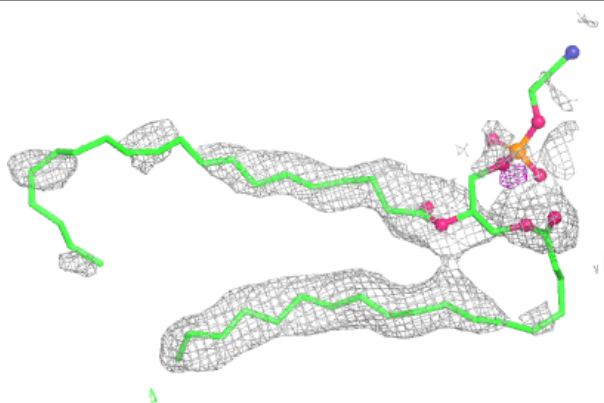


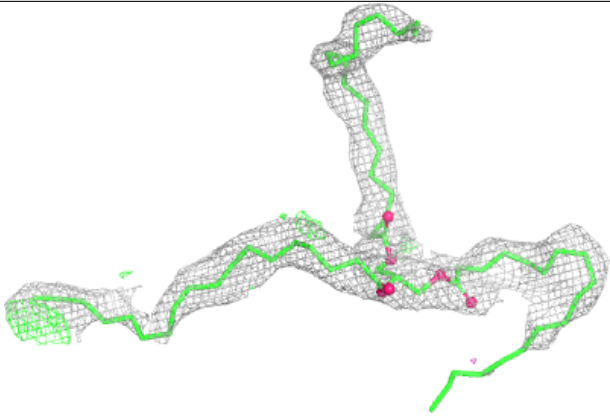
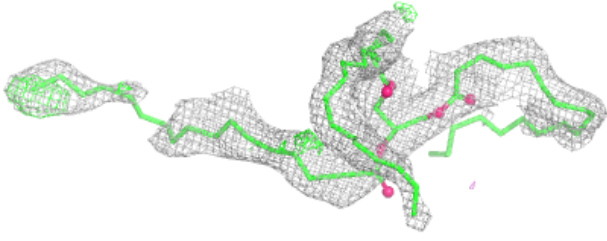
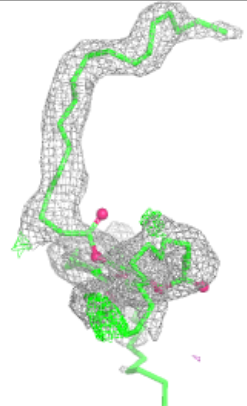
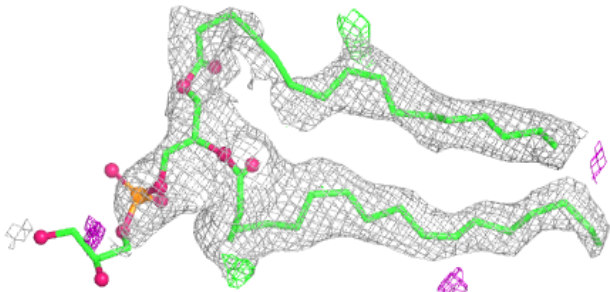
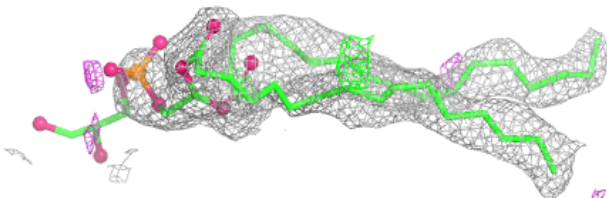
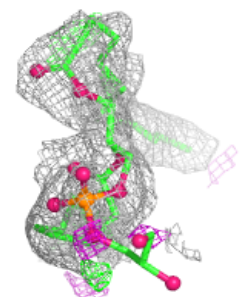
Electron density around CDL C 306:

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

**Electron density around PEK C 304:**

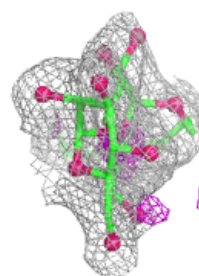
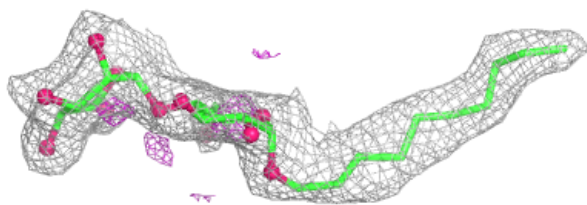
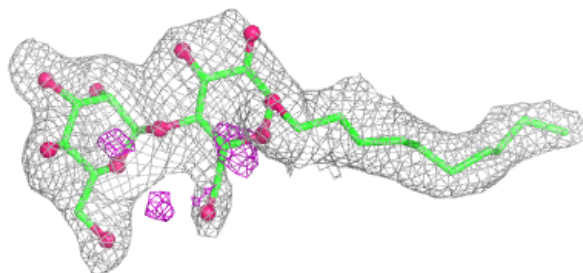
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



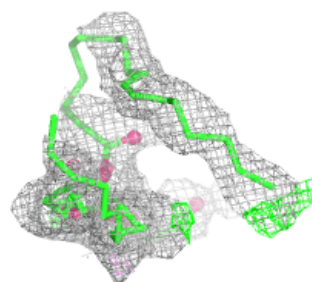
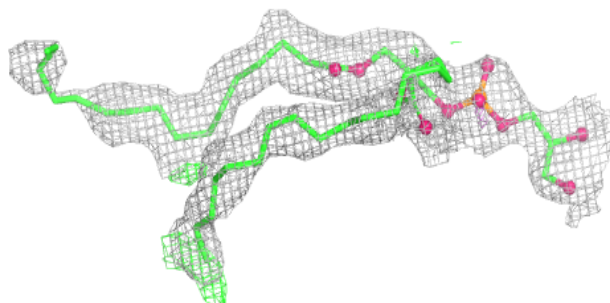
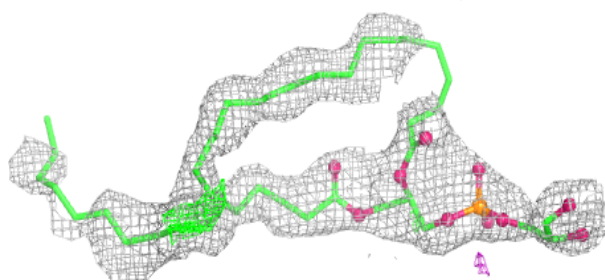
Electron density around TGL N 604: $2mF_o-DF_c$ (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	 A 3D visualization of the electron density map for TGL N 604. The map is shown as a gray mesh. The protein backbone is represented by a green line, and the side chains are shown as red spheres. The density map is shown in two views: a top-down view and a side view.
 A 3D visualization of the electron density map for TGL N 604. The map is shown as a gray mesh. The protein backbone is represented by a green line, and the side chains are shown as red spheres. The density map is shown in two views: a top-down view and a side view.	 A 3D visualization of the electron density map for TGL N 604. The map is shown as a gray mesh. The protein backbone is represented by a green line, and the side chains are shown as red spheres. The density map is shown in two views: a top-down view and a side view.
Electron density around PGV A 604: $2mF_o-DF_c$ (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	 A 3D visualization of the electron density map for PGV A 604. The map is shown as a gray mesh. The protein backbone is represented by a green line, and the side chains are shown as red spheres. The density map is shown in two views: a top-down view and a side view.
 A 3D visualization of the electron density map for PGV A 604. The map is shown as a gray mesh. The protein backbone is represented by a green line, and the side chains are shown as red spheres. The density map is shown in two views: a top-down view and a side view.	 A 3D visualization of the electron density map for PGV A 604. The map is shown as a gray mesh. The protein backbone is represented by a green line, and the side chains are shown as red spheres. The density map is shown in two views: a top-down view and a side view.

Electron density around DMU 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)

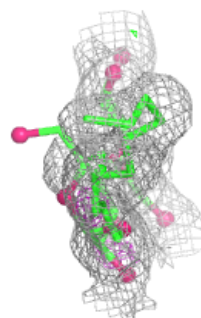
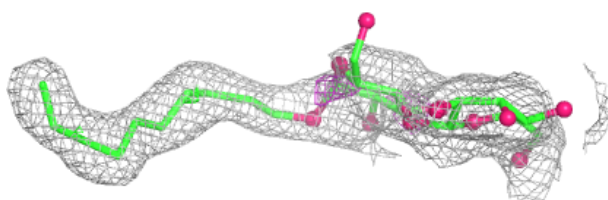
**Electron density around PGV H 101:**

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

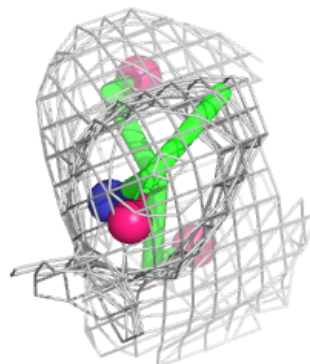
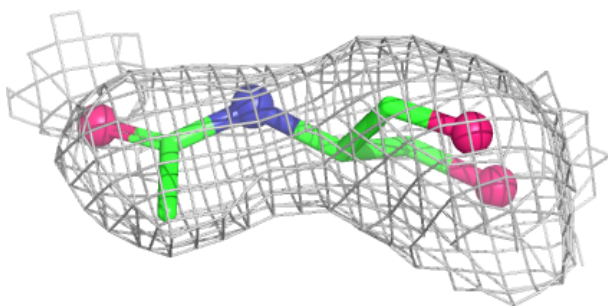
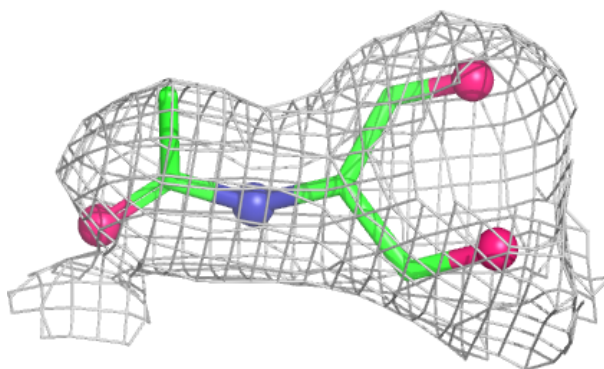


Electron density around DMU C 309:

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

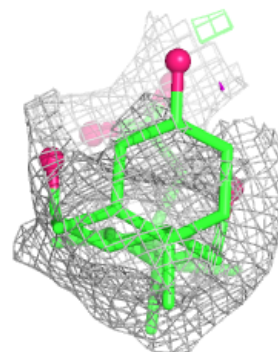
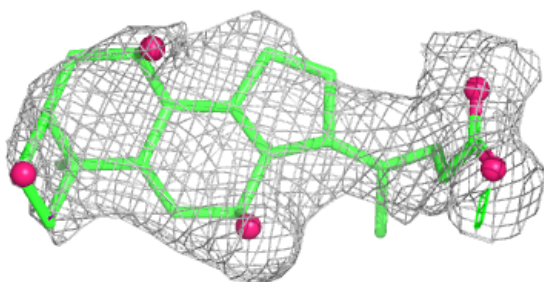
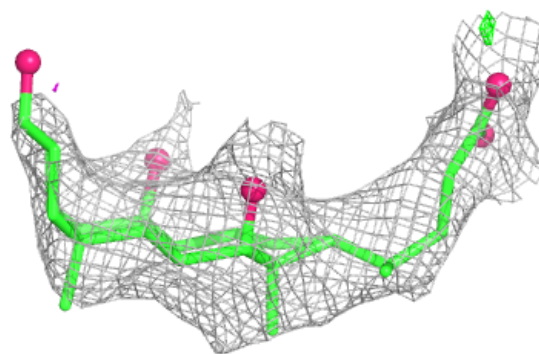
**Electron density around SAC V 102:**

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



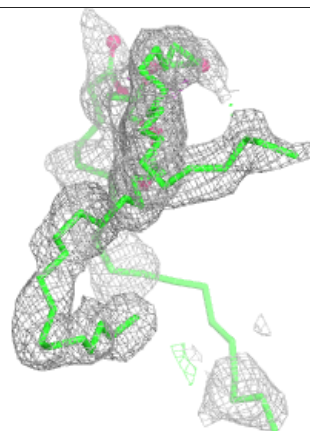
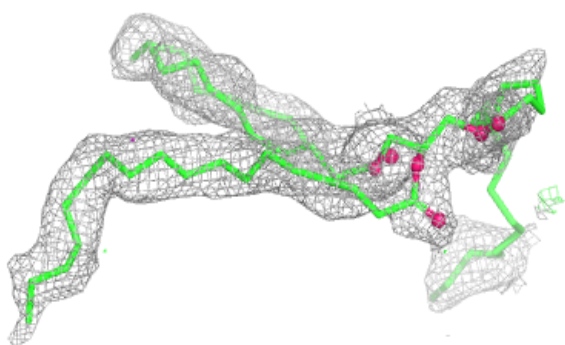
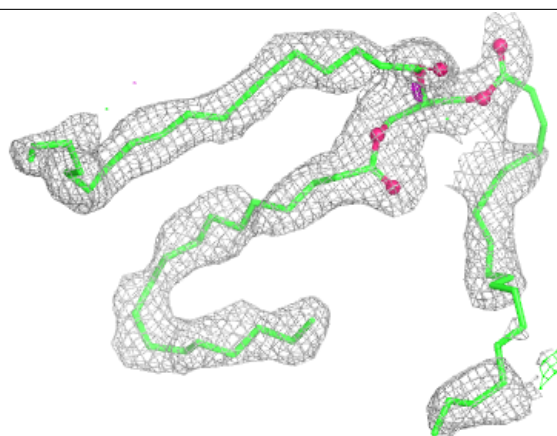
Electron density around CHD W 101:

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



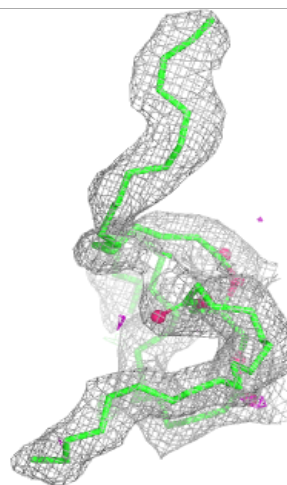
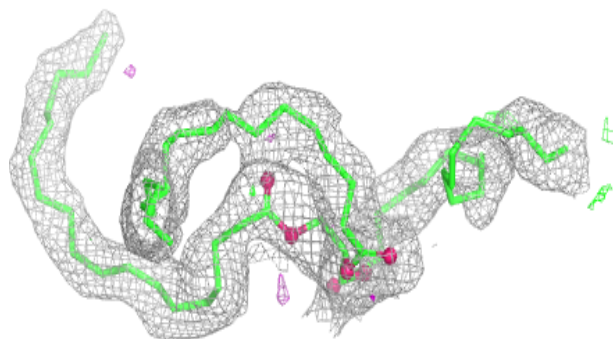
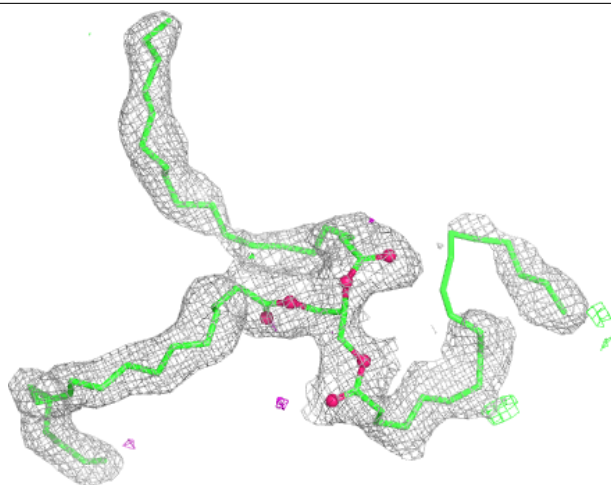
Electron density around TGL D 201:

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



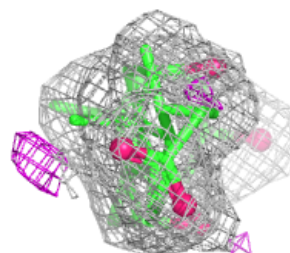
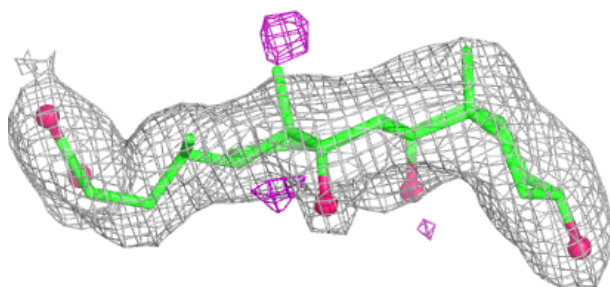
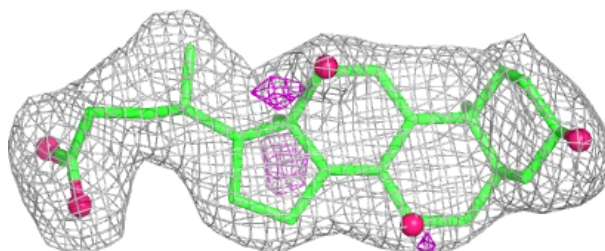
Electron density around TGL L 101:

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

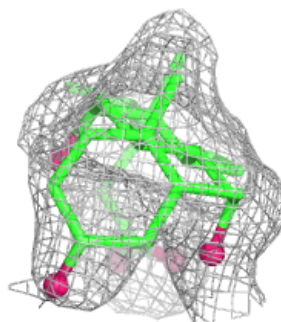
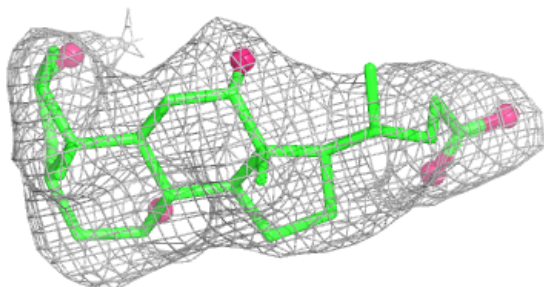
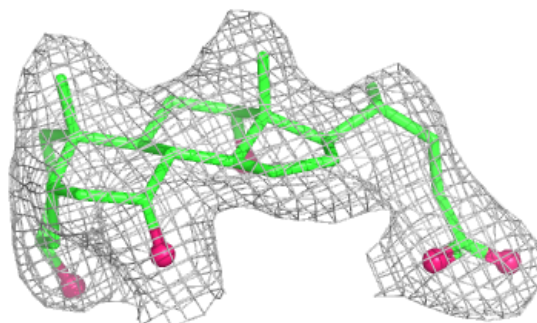


Electron density around CHD C 307:

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

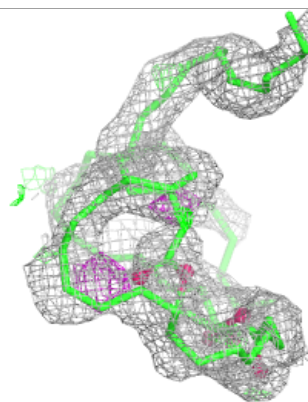
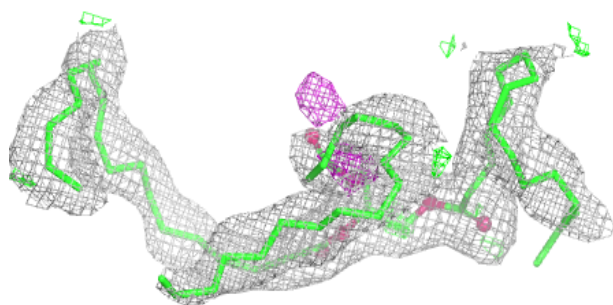
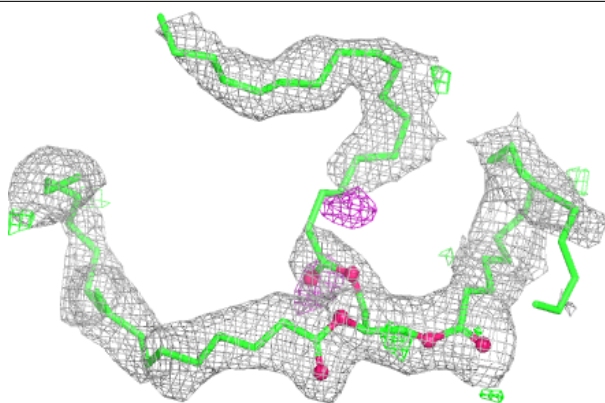
**Electron density around CHD J 101:**

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

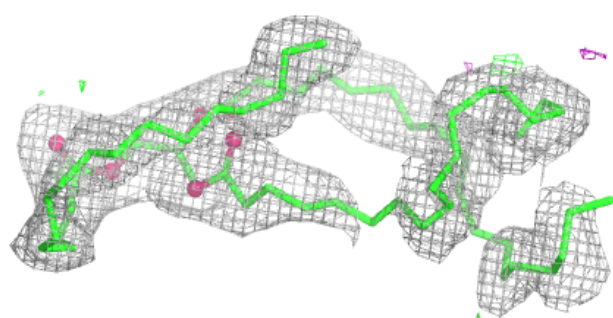
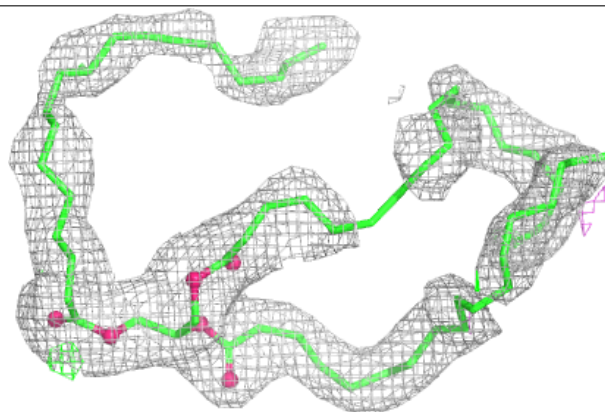


Electron density around TGL B 302:

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

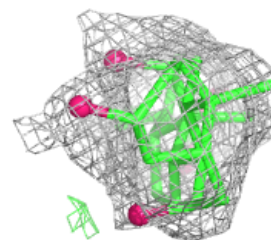
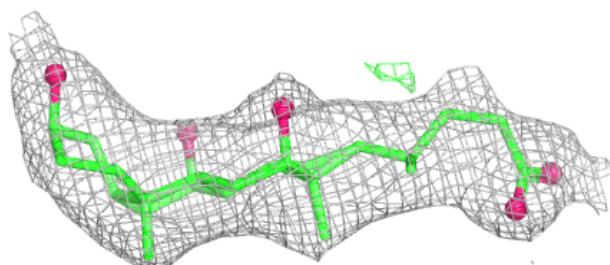
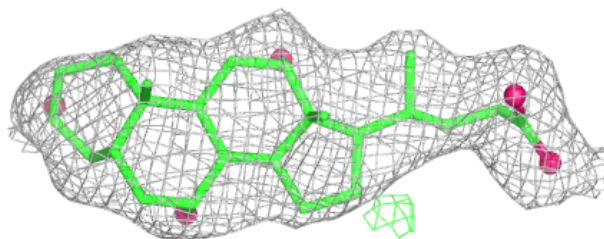
**Electron density around TGL O 301:**

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

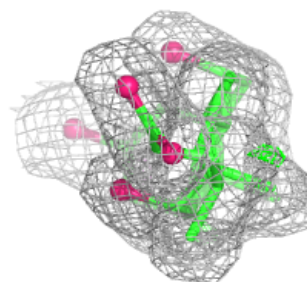
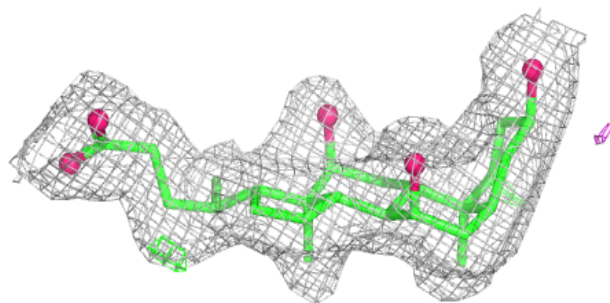
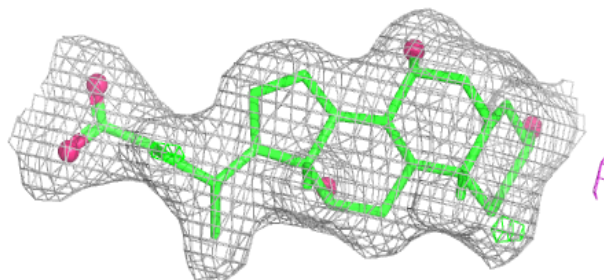


Electron density around CHD P 308:

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

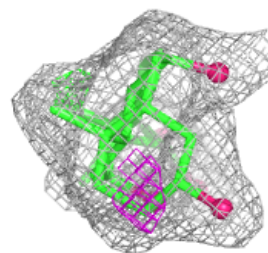
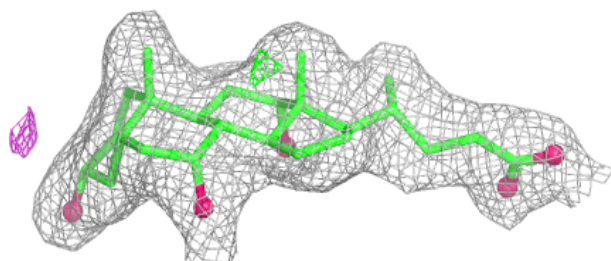
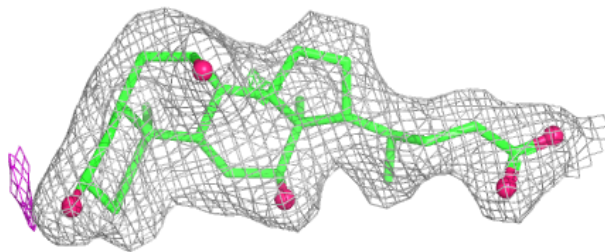
**Electron density around CHD O 303:**

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

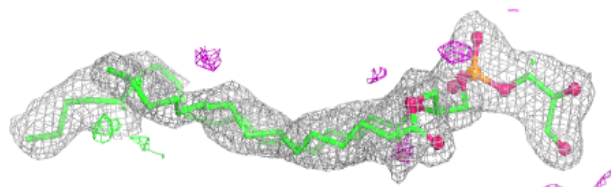
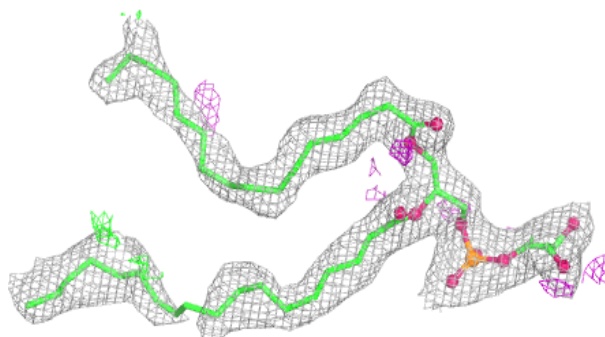


Electron density around CHD P 303:

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

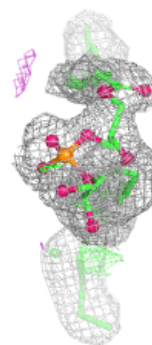
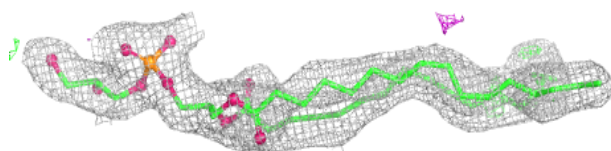
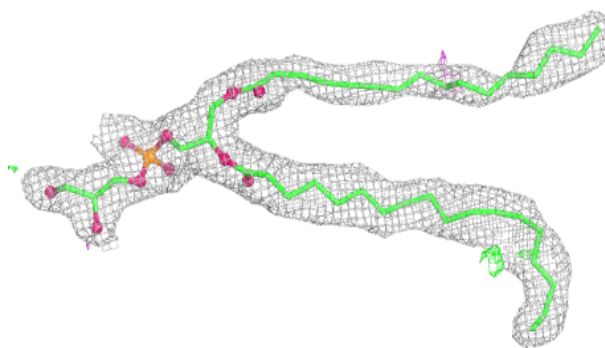
**Electron density around PGV N 605:**

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

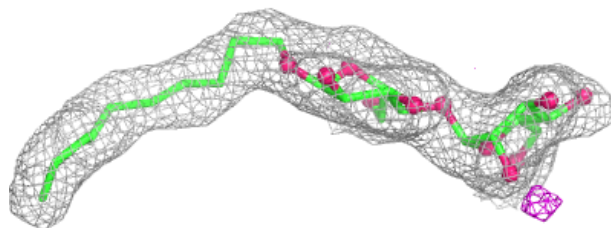
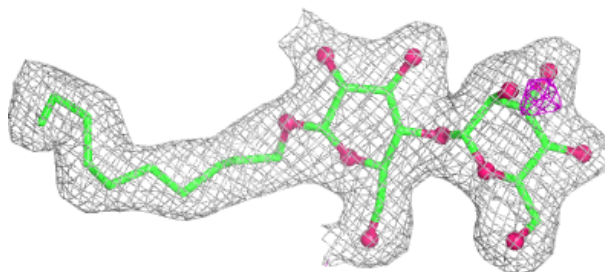


Electron density around PGV P 305:

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

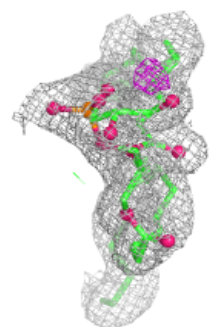
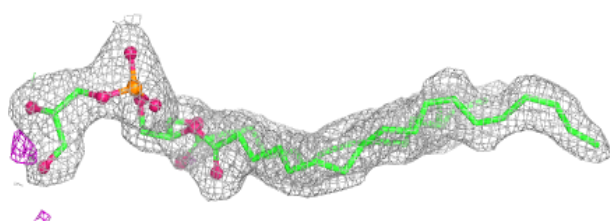
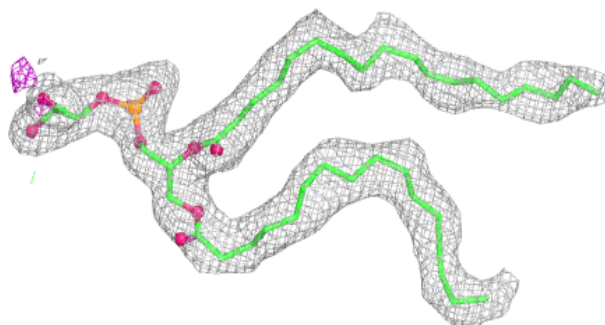
**Electron density around DMU M 101:**

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

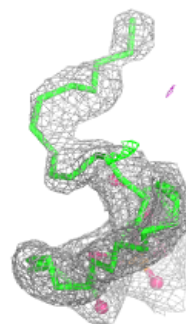
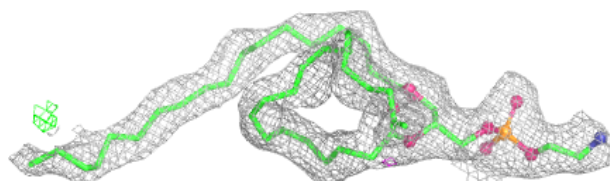
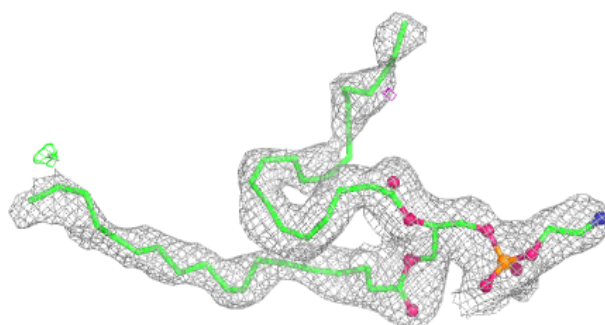


Electron density around PGV C 301:

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

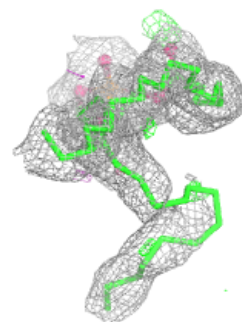
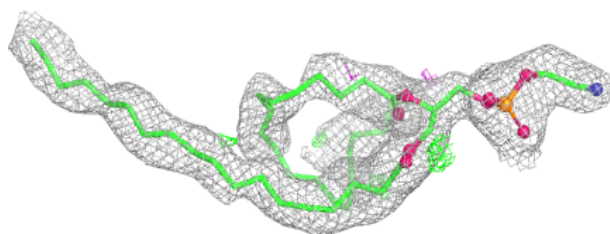
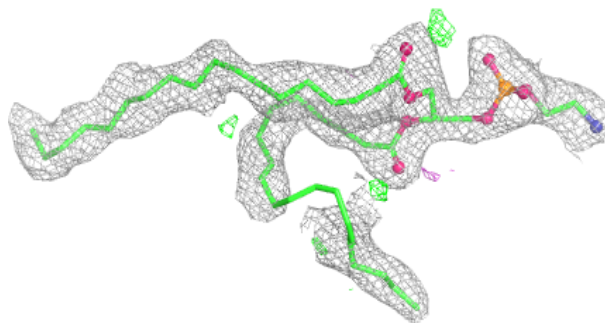
**Electron density around PEK P 304:**

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

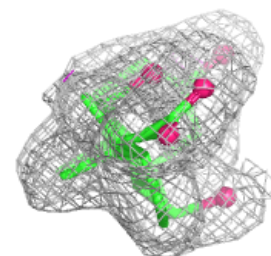
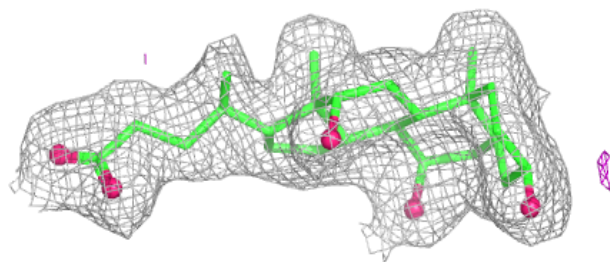
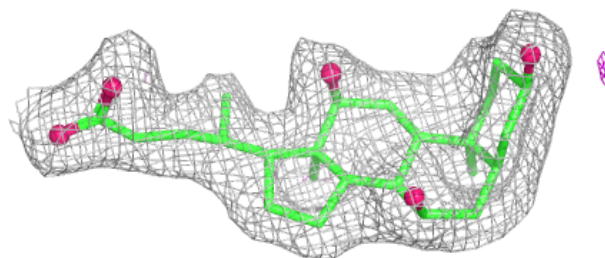


Electron density around PEK C 303:

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

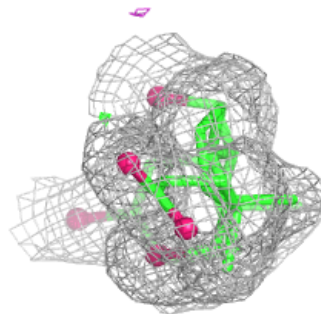
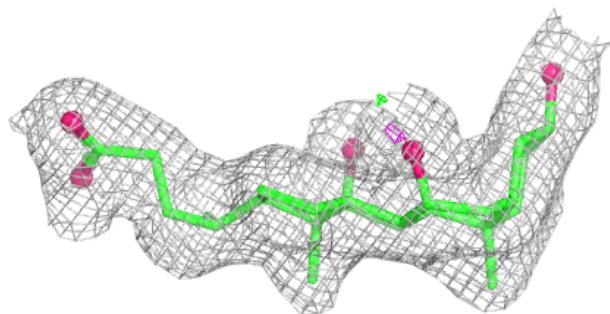
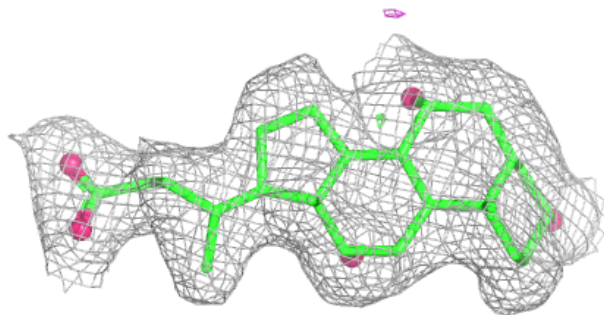
**Electron density around CHD C 302:**

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

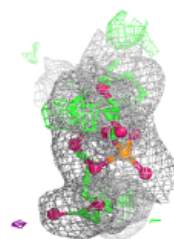
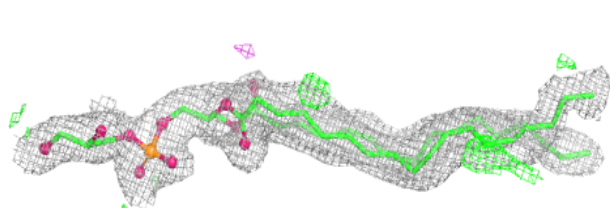
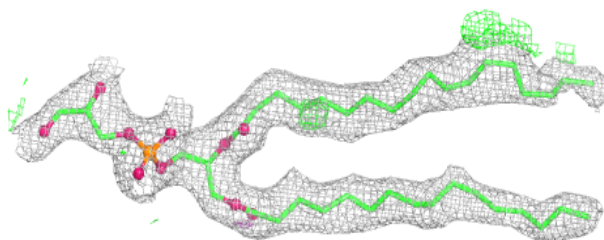


Electron density around CHD T 101:

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

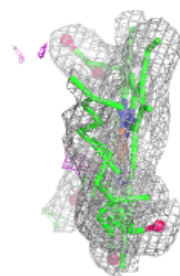
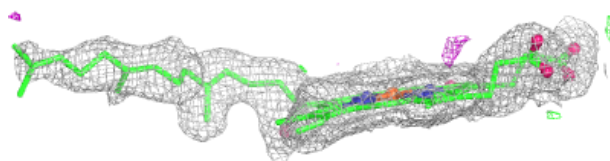
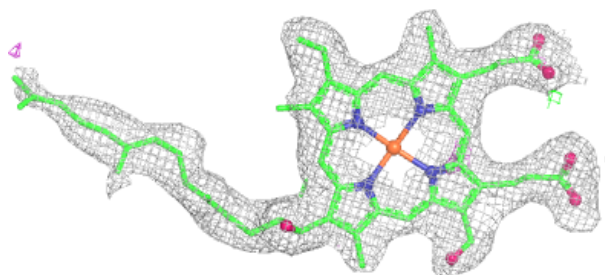
**Electron density around PGV C 305:**

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

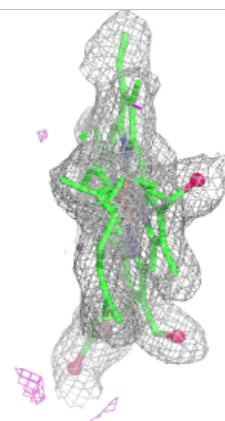
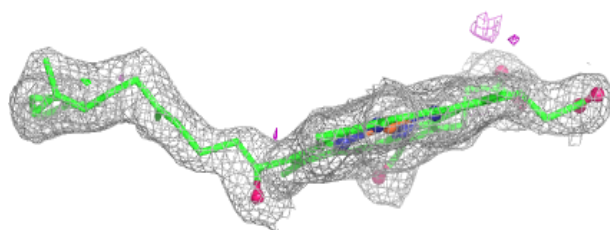
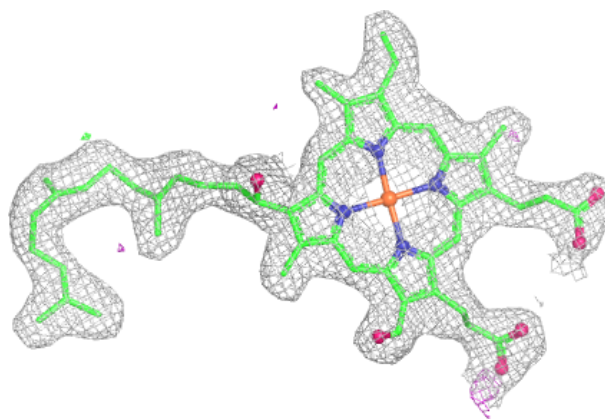


Electron density around HEA N 607:

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

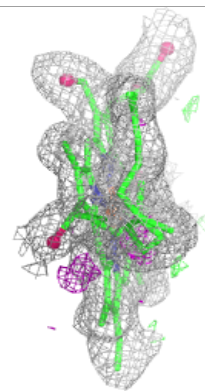
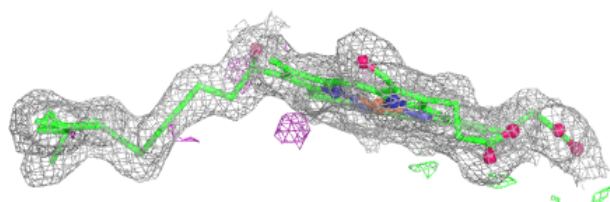
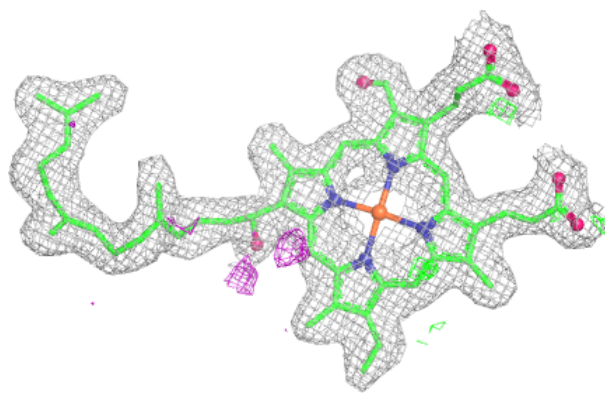
**Electron density around HEA N 606:**

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

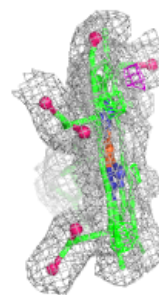
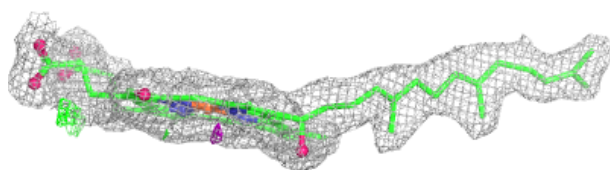
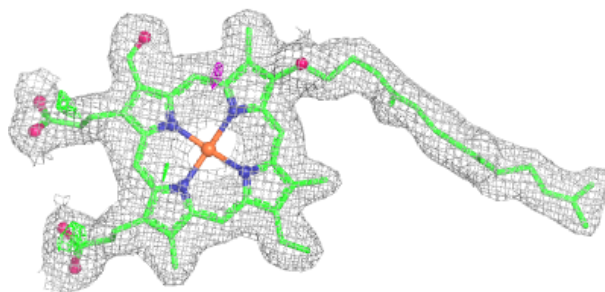


Electron density around HEA A 605:

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

**Electron density around HEA A 606:**

$2mF_o-DF_c$ (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.