



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2023 – 12:51 PM JST

PDB ID : 5ZCP
Title : azide-bound cytochrome c oxidase structure determined using the crystals exposed to 20 mM azide solution for 2 days
Authors : Shimada, A.; Hatano, K.; Tadehara, H.; Tsukihara, T.
Deposited on : 2018-02-19
Resolution : 1.65 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

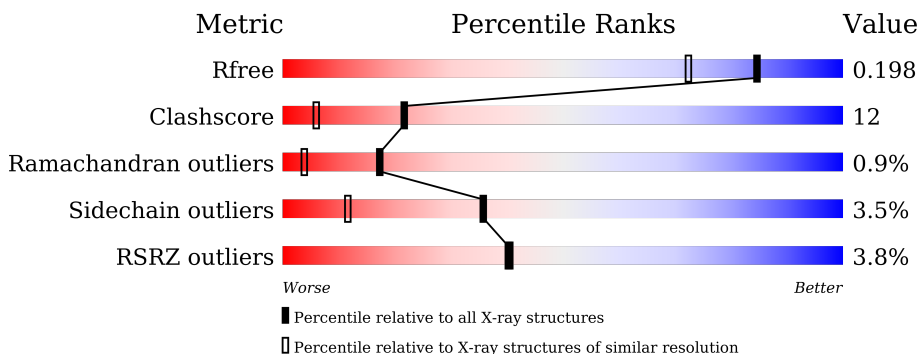
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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.



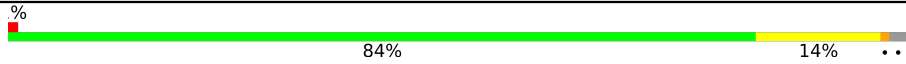
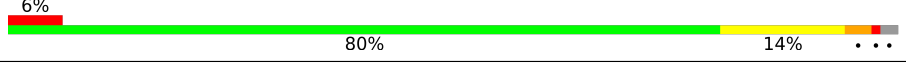



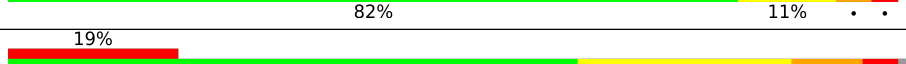
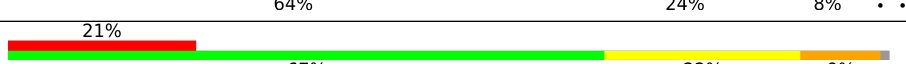
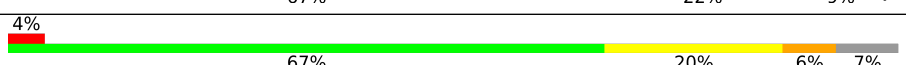
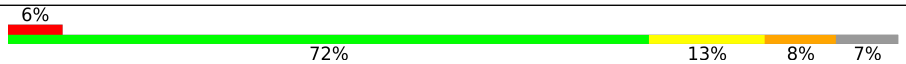
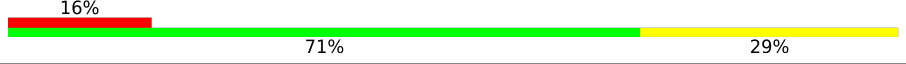
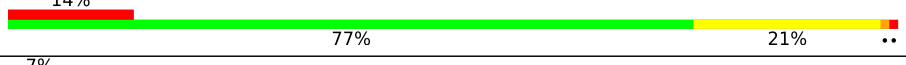
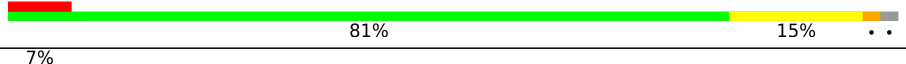
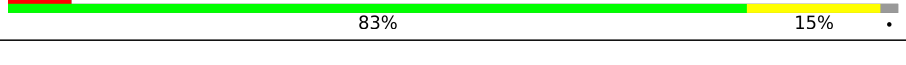

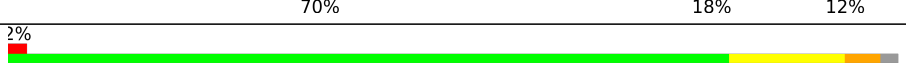



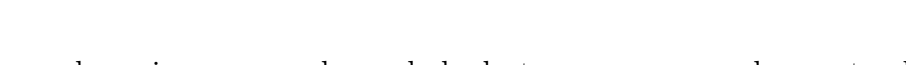
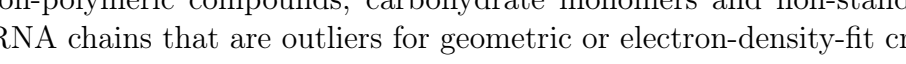
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	80% (green), 18% (yellow), 2% (orange), 2% (red)
1	N	514	79% (green), 19% (yellow), 2% (orange), 0% (red)
2	B	227	3% (red), 68% (green), 27% (yellow), 2% (orange)
2	O	227	3% (red), 78% (green), 18% (yellow), 3% (orange)
3	C	261	0% (red), 82% (green), 15% (yellow), 3% (orange)
3	P	261	0% (red), 82% (green), 16% (yellow), 2% (orange)

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	AZI	A	607[A]	-	-	X	-
18	AZI	A	607[B]	-	-	X	-
21	EDO	A	616	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	EDO	D	202	-	-	X	-
27	CDL	N	601	-	-	X	-
27	CDL	P	305	-	-	X	-
9	SAC	V	1	-	X	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33609 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
			Total	C	N	O	S			
1	A	514	Total	C	N	O	S	0	22	0
			4193	2793	649	709	42			
1	N	514	Total	C	N	O	S	0	20	0
			4179	2786	647	704	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	Total	C	N	O	S	0	9	0
			1899	1234	292	353	20			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	288	347	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			
3	P	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	144	Total	C	N	O	S	0	4	0
			1233	803	204	222	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1224	797	202	221	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	1	0
			863	550	148	163	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	4	0
			778	481	139	152	6			
6	S	98	Total	C	N	O	S	0	2	0
			763	473	136	148	6			

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

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

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

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

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

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

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

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

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

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

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

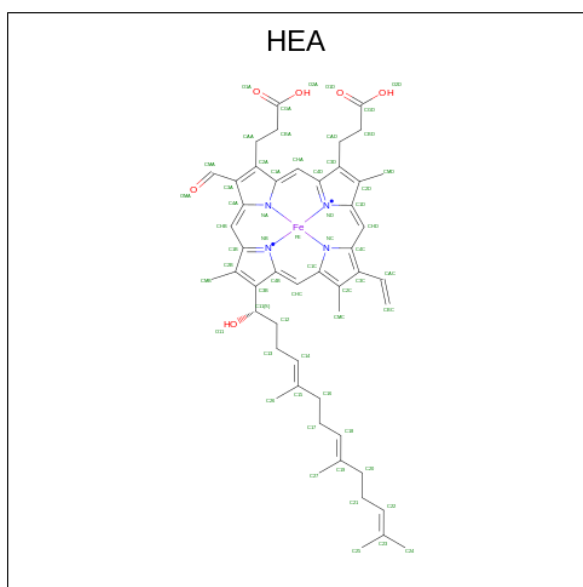
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- 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		

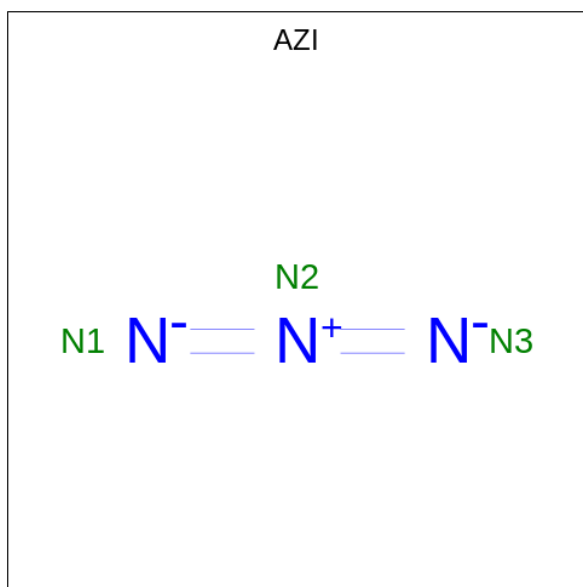
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

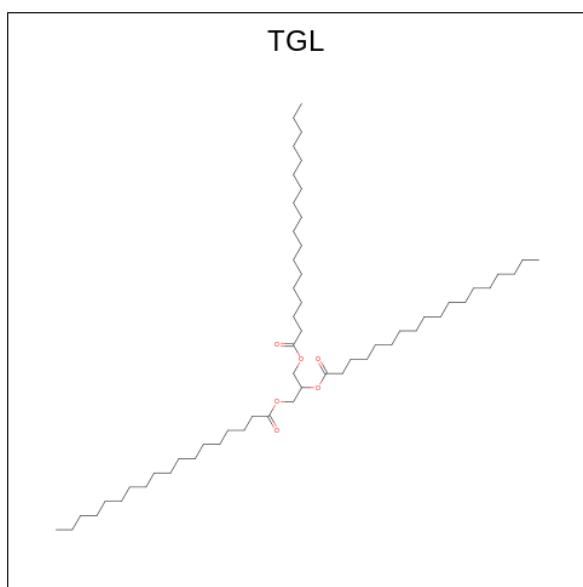
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is AZIDE ION (three-letter code: AZI) (formula: N₃).



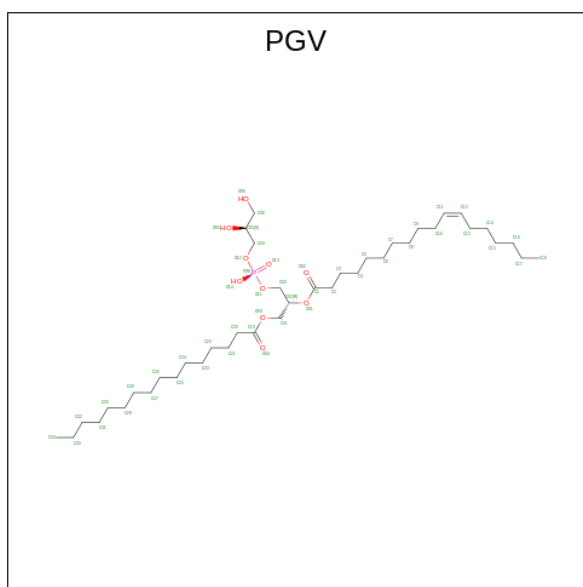
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total N 3 3	0	1
18	A	1	Total N 6 6	0	1
18	N	1	Total N 3 3	0	1
18	N	1	Total N 6 6	0	1

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



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

- Molecule 20 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



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

- Molecule 21 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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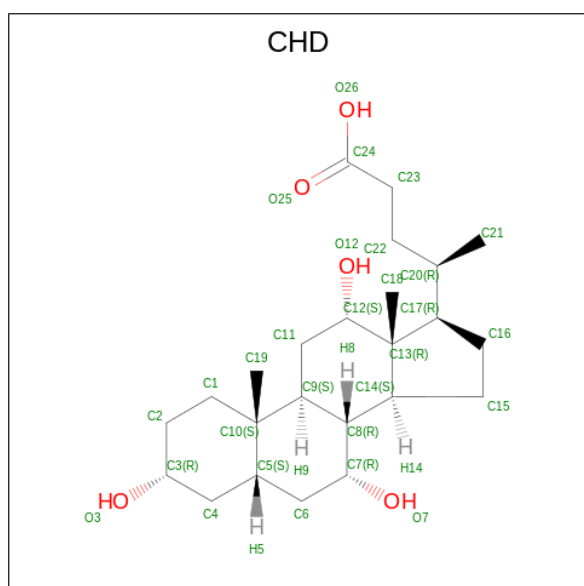
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4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

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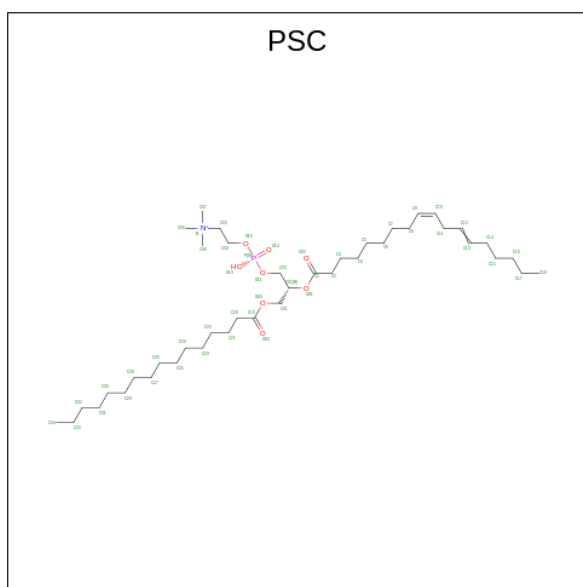
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	O	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	R	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	T	1	Total	C	O	0	0
			4	2	2		
21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

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



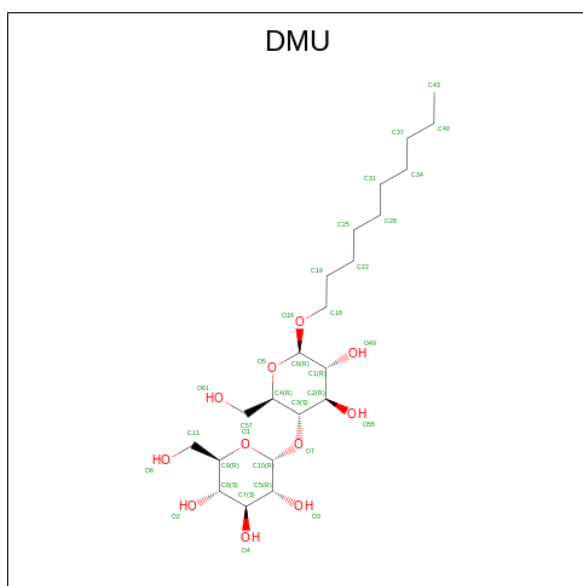
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		

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

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

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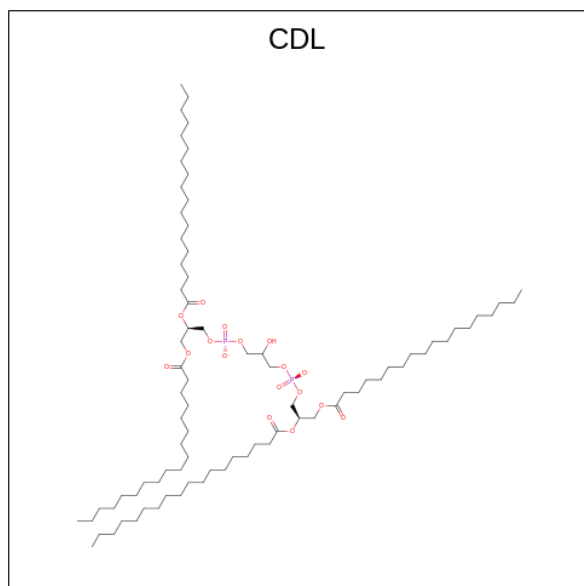
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total	C	O	0	0
			33	22	11		
25	C	1	Total	C	O	0	0
			33	22	11		
25	M	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22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

- Molecule 26 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

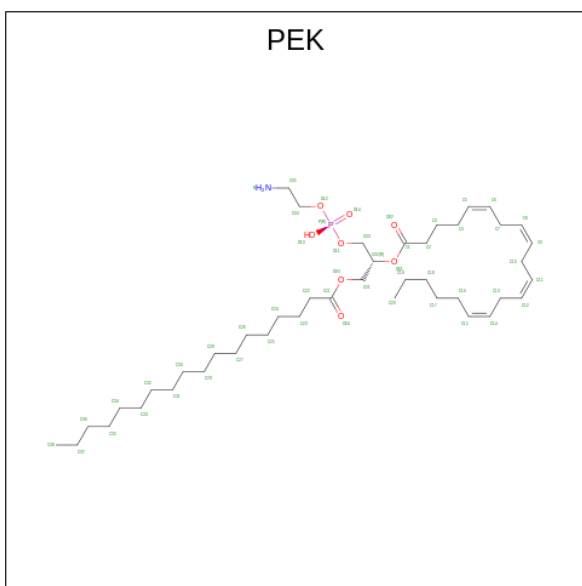
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	C	1	Total	X	0	0
			1	1		
26	P	1	Total	X	0	0
			1	1		

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



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

- Molecule 28 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
28	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	235	Total 235	O 235	0	0
30	B	161	Total 162	O 162	0	1
30	C	110	Total 110	O 110	0	0
30	D	118	Total 118	O 118	0	0
30	E	93	Total 93	O 93	0	0
30	F	94	Total 94	O 94	0	0
30	G	42	Total 42	O 42	0	0
30	H	42	Total 42	O 42	0	0
30	I	27	Total 27	O 27	0	0
30	J	23	Total 23	O 23	0	0
30	K	26	Total 26	O 26	0	0
30	L	38	Total 38	O 38	0	0
30	M	25	Total 25	O 25	0	0
30	N	203	Total 203	O 203	0	0
30	O	99	Total 100	O 100	0	1
30	P	95	Total 95	O 95	0	0
30	Q	29	Total 29	O 29	0	0
30	R	40	Total 40	O 40	0	0

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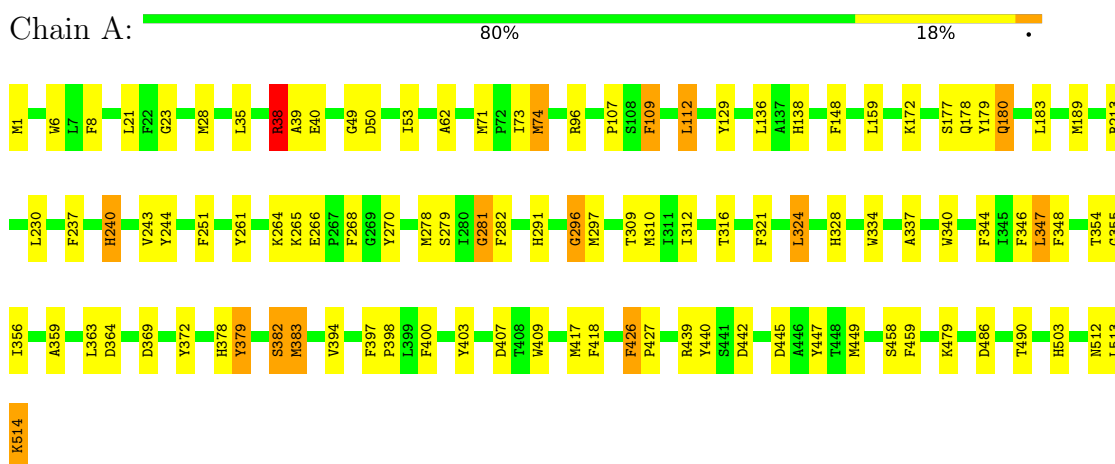
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	S	45	Total O 45 45	0	0
30	T	35	Total O 35 35	0	0
30	U	29	Total O 29 29	0	0
30	V	16	Total O 16 16	0	0
30	W	7	Total O 7 7	0	0
30	X	11	Total O 11 11	0	0
30	Y	12	Total O 12 12	0	0
30	Z	12	Total O 12 12	0	0

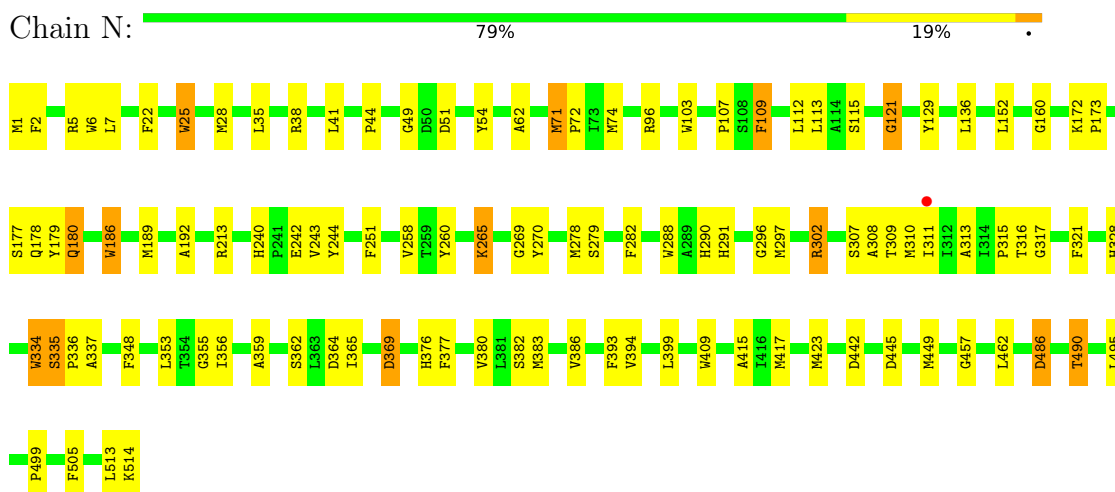
3 Residue-property plots [i](#)

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

- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 1: Cytochrome c oxidase subunit 1

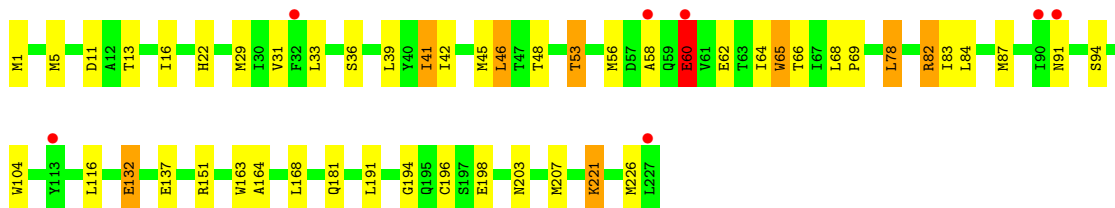
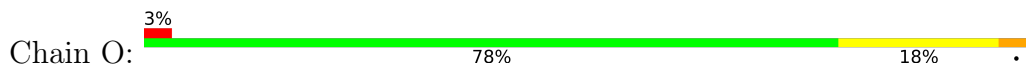


- Molecule 2: Cytochrome c oxidase subunit 2

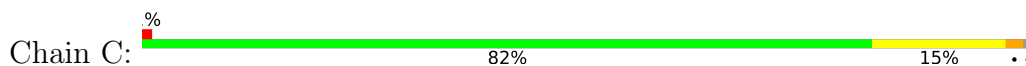




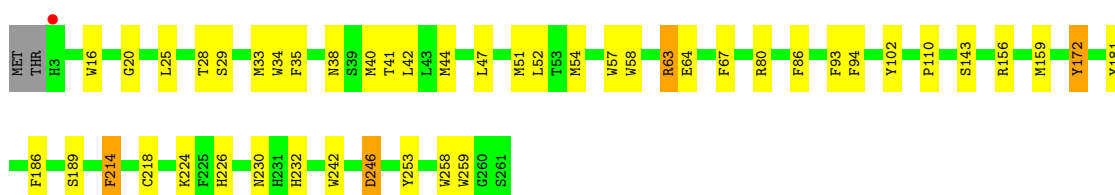
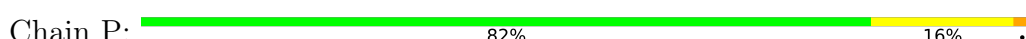
• Molecule 2: Cytochrome c oxidase subunit 2



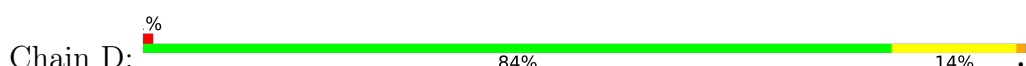
• Molecule 3: Cytochrome c oxidase subunit 3



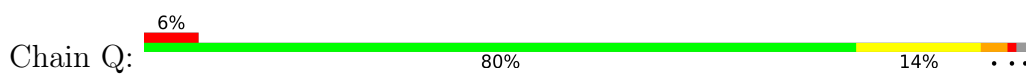
• Molecule 3: Cytochrome c oxidase subunit 3



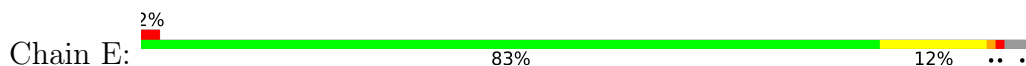
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



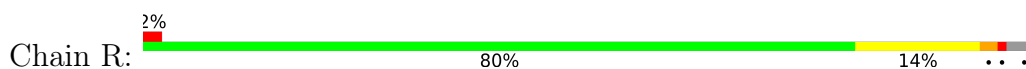
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



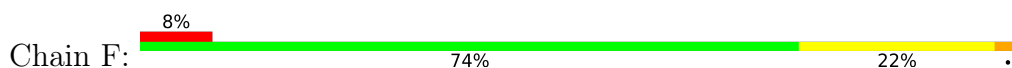
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



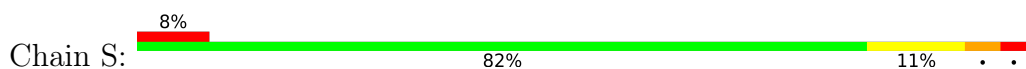
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



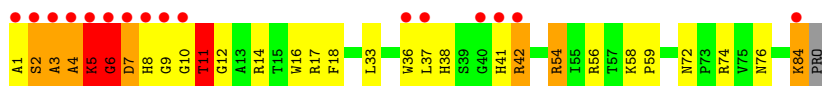
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



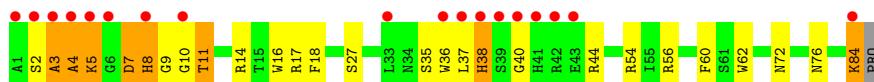
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



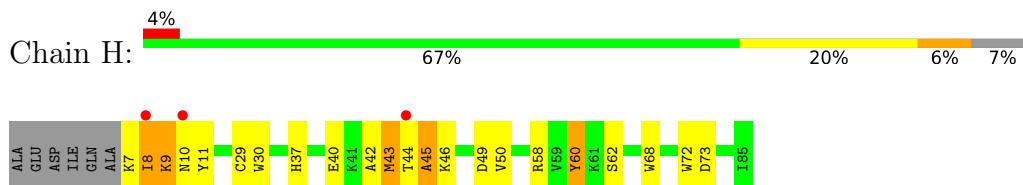
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



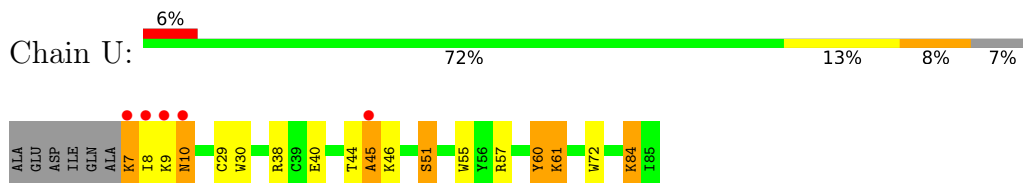
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



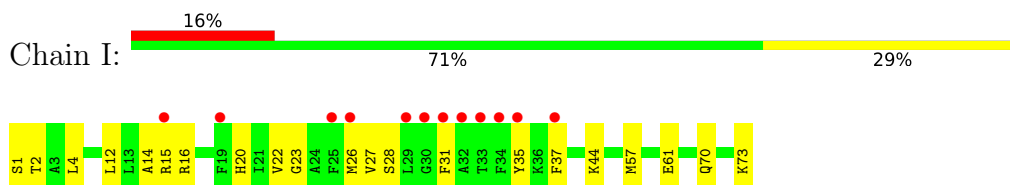
- Molecule 8: Cytochrome c oxidase subunit 6B1



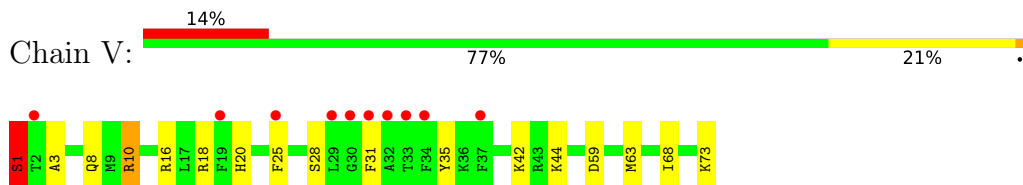
- Molecule 8: Cytochrome c oxidase subunit 6B1



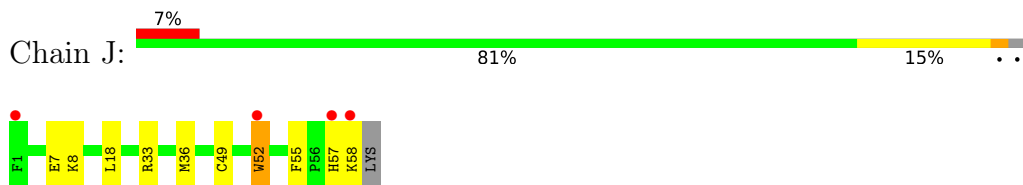
- Molecule 9: Cytochrome c oxidase subunit 6C



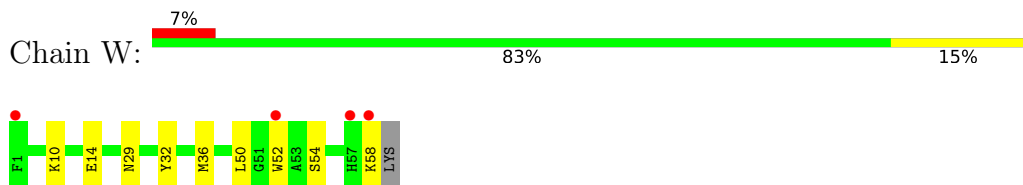
- Molecule 9: Cytochrome c oxidase subunit 6C



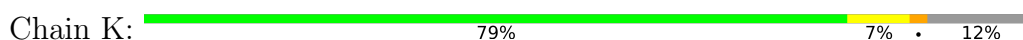
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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

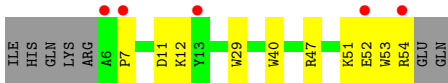


- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

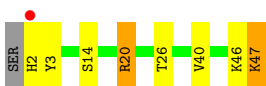
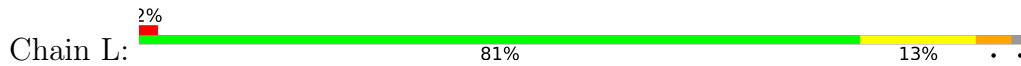




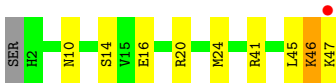
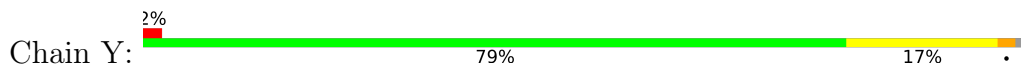
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



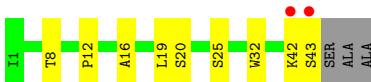
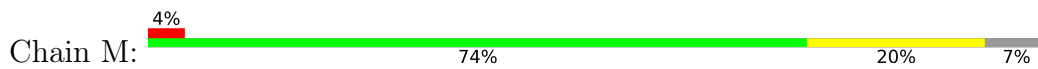
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



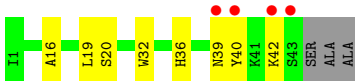
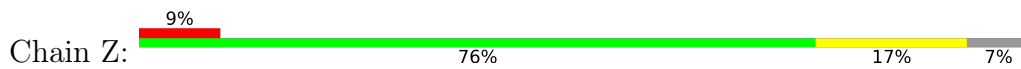
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.32Å 206.17Å 177.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.65 137.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-1.65) 99.6 (137.00-1.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 1.65Å)	Xtrriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.175 , 0.197 0.176 , 0.198	Depositor DCC
R_{free} test set	39973 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtrriage
Anisotropy	0.590	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.005 for l,-k,h	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33609	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: HEA, EDO, UNX, PGV, TGL, CHD, DMU, CUA, MG, CU, CDL, PSC, PEK, NA, AZI, ZN, TPO, SAC, 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	1.62	23/4322 (0.5%)	1.43	39/5897 (0.7%)
1	N	1.58	30/4308 (0.7%)	1.39	29/5878 (0.5%)
2	B	1.52	12/1937 (0.6%)	1.37	14/2637 (0.5%)
2	O	1.30	8/1908 (0.4%)	1.16	7/2597 (0.3%)
3	C	1.53	15/2272 (0.7%)	1.28	8/3102 (0.3%)
3	P	1.57	19/2272 (0.8%)	1.32	14/3102 (0.5%)
4	D	1.51	4/1268 (0.3%)	1.29	8/1709 (0.5%)
4	Q	1.17	4/1259 (0.3%)	1.23	4/1698 (0.2%)
5	E	1.50	6/871 (0.7%)	1.62	8/1182 (0.7%)
5	R	1.33	4/882 (0.5%)	1.25	5/1196 (0.4%)
6	F	1.37	2/795 (0.3%)	1.21	1/1079 (0.1%)
6	S	1.25	0/780	1.20	2/1058 (0.2%)
7	G	1.46	3/702 (0.4%)	1.21	6/953 (0.6%)
7	T	1.51	6/702 (0.9%)	1.19	3/953 (0.3%)
8	H	1.34	4/682 (0.6%)	1.03	1/921 (0.1%)
8	U	1.12	3/682 (0.4%)	0.95	1/921 (0.1%)
9	I	1.26	2/605 (0.3%)	1.19	2/802 (0.2%)
9	V	1.09	0/605	1.11	3/802 (0.4%)
10	J	1.34	1/471 (0.2%)	1.17	1/636 (0.2%)
10	W	1.31	1/480 (0.2%)	1.20	1/648 (0.2%)
11	K	1.36	2/398 (0.5%)	1.16	1/546 (0.2%)
11	X	1.19	3/405 (0.7%)	0.93	1/556 (0.2%)
12	L	1.45	0/393	1.30	2/526 (0.4%)
12	Y	1.34	0/401	1.09	0/536
13	M	1.48	3/345 (0.9%)	1.15	0/470
13	Z	1.28	2/345 (0.6%)	0.97	0/470
All	All	1.46	157/30090 (0.5%)	1.29	161/40875 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	N	0	2
6	F	0	1
6	S	0	2
7	G	0	1
9	V	0	1
All	All	0	11

The worst 5 of 157 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	89	SER	CB-OG	8.75	1.53	1.42
2	B	198	GLU	CD-OE2	-8.56	1.16	1.25
4	D	58	GLU	CD-OE1	8.47	1.34	1.25
1	N	409	TRP	CD2-CE2	8.41	1.51	1.41
2	B	108	TYR	CE1-CZ	8.16	1.49	1.38

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	90	ARG	NE-CZ-NH1	25.98	133.29	120.30
4	Q	20	ARG	NE-CZ-NH2	-19.33	110.63	120.30
5	E	90	ARG	NE-CZ-NH2	-19.32	110.64	120.30
1	N	71	MET	CG-SD-CE	-16.18	74.31	100.20
4	Q	20	ARG	NE-CZ-NH1	16.03	128.32	120.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
1	A	379	TYR	Mainchain
1	A	38	ARG	Sidechain
6	F	93	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4193	0	4162	97	0
1	N	4179	0	4154	95	0
2	B	1899	0	1898	63	0
2	O	1870	0	1868	45	0
3	C	2185	0	2097	46	0
3	P	2185	0	2097	34	0
4	D	1233	0	1223	37	0
4	Q	1224	0	1211	20	0
5	E	852	0	845	4	0
5	R	863	0	857	6	0
6	F	778	0	754	26	0
6	S	763	0	742	22	0
7	G	686	0	652	28	0
7	T	686	0	651	23	0
8	H	662	0	623	18	0
8	U	662	0	623	9	0
9	I	601	0	613	19	0
9	V	601	0	613	14	0
10	J	460	0	459	7	0
10	W	469	0	464	4	0
11	K	384	0	366	2	0
11	X	391	0	374	3	0
12	L	380	0	380	16	0
12	Y	388	0	388	13	0
13	M	335	0	352	8	0
13	Z	335	0	352	8	0
14	A	180	0	162	25	0
14	N	180	0	162	28	0
15	A	1	0	0	1	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	9	0	0	8	0
18	N	9	0	0	3	0
19	A	126	0	220	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	63	0	110	13	0
19	N	63	0	110	7	0
19	Q	63	0	110	12	0
19	Y	63	0	110	20	0
20	A	102	0	152	13	0
20	C	102	0	152	4	0
20	N	102	0	152	10	0
20	P	102	0	152	3	0
21	A	36	0	52	8	0
21	B	16	0	24	2	0
21	C	4	0	6	0	0
21	D	8	0	12	9	0
21	E	12	0	18	0	0
21	F	12	0	18	0	0
21	G	8	0	12	3	0
21	L	4	0	6	0	0
21	M	4	0	6	0	0
21	N	36	0	54	1	0
21	O	4	0	6	0	0
21	P	8	0	12	0	0
21	R	4	0	6	0	0
21	S	12	0	18	0	0
21	T	4	0	6	0	0
21	W	4	0	6	0	0
21	Y	4	0	6	0	0
22	B	29	0	39	0	0
22	C	58	0	78	6	0
22	G	29	0	39	1	0
22	J	29	0	38	1	0
22	P	58	0	78	6	0
22	W	29	0	38	1	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	52	0	80	15	0
24	N	52	0	80	16	0
25	C	99	0	126	15	0
25	M	33	0	42	0	0
25	P	99	0	126	15	0
25	Z	33	0	42	0	0
26	C	1	0	0	0	0
26	P	1	0	0	1	0
27	C	100	0	156	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	N	100	0	156	29	0
27	P	100	0	156	24	0
27	T	100	0	156	16	0
28	C	106	0	154	15	0
28	G	106	0	154	8	0
28	P	53	0	77	6	0
28	T	53	0	77	3	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	A	235	0	0	32	0
30	B	162	0	0	25	2
30	C	110	0	0	3	0
30	D	118	0	0	13	1
30	E	93	0	0	1	0
30	F	94	0	0	5	0
30	G	42	0	0	5	0
30	H	42	0	0	1	0
30	I	27	0	0	5	1
30	J	23	0	0	2	0
30	K	26	0	0	1	0
30	L	38	0	0	4	1
30	M	25	0	0	7	1
30	N	203	0	0	14	0
30	O	100	0	0	1	0
30	P	95	0	0	3	0
30	Q	29	0	0	5	0
30	R	40	0	0	1	0
30	S	45	0	0	3	0
30	T	35	0	0	3	0
30	U	29	0	0	0	0
30	V	16	0	0	3	0
30	W	7	0	0	0	0
30	X	11	0	0	0	0
30	Y	12	0	0	0	0
30	Z	12	0	0	0	0
All	All	33609	0	32570	772	3

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 12.

The worst 5 of 772 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:MET:CG	1:A:74:MET:CB	1.75	1.61
6:S:43:LYS:H	6:S:43:LYS:CD	1.08	1.49
20:N:609:PGV:H011	20:N:609:PGV:C2	1.38	1.33
24:B:303:PSC:O02	9:I:14:ALA:HB2	1.16	1.31
30:A:709:HOH:O	19:D:201:TGL:HG11	1.23	1.29

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:491:HOH:O	30:D:341:HOH:O[2_584]	1.22	0.98
30:I:126:HOH:O	30:M:216:HOH:O[2_584]	1.92	0.28
30:B:541:HOH:O	30:L:228:HOH:O[2_584]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	534/514 (104%)	516 (97%)	18 (3%)	0	100	100
1	N	532/514 (104%)	515 (97%)	17 (3%)	0	100	100
2	B	234/227 (103%)	227 (97%)	5 (2%)	2 (1%)	17	4
2	O	230/227 (101%)	223 (97%)	7 (3%)	0	100	100
3	C	266/261 (102%)	262 (98%)	4 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	146/147 (99%)	142 (97%)	4 (3%)	0	100	100
4	Q	145/147 (99%)	138 (95%)	4 (3%)	3 (2%)	7	0
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	104/109 (95%)	103 (99%)	0	1 (1%)	15	3
6	F	100/98 (102%)	96 (96%)	1 (1%)	3 (3%)	4	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S	98/98 (100%)	91 (93%)	3 (3%)	4 (4%)	3	0
7	G	82/85 (96%)	68 (83%)	9 (11%)	5 (6%)	1	0
7	T	82/85 (96%)	70 (85%)	8 (10%)	4 (5%)	2	0
8	H	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	3	0
8	U	77/85 (91%)	68 (88%)	5 (6%)	4 (5%)	2	0
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
12	Y	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	6	0
13	M	41/46 (89%)	38 (93%)	2 (5%)	1 (2%)	6	0
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3597/3614 (100%)	3457 (96%)	109 (3%)	31 (1%)	17	4

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	2	SER
7	G	3	ALA
7	G	4	ALA
7	G	5	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/426 (105%)	438 (98%)	9 (2%)	55	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	445/426 (104%)	439 (99%)	6 (1%)	69	50
2	B	219/210 (104%)	209 (95%)	10 (5%)	27	6
2	O	215/210 (102%)	208 (97%)	7 (3%)	38	12
3	C	233/226 (103%)	229 (98%)	4 (2%)	60	39
3	P	233/226 (103%)	229 (98%)	4 (2%)	60	39
4	D	132/129 (102%)	130 (98%)	2 (2%)	65	44
4	Q	131/129 (102%)	125 (95%)	6 (5%)	27	6
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	12
5	R	93/95 (98%)	88 (95%)	5 (5%)	22	4
6	F	85/81 (105%)	81 (95%)	4 (5%)	26	6
6	S	83/81 (102%)	73 (88%)	10 (12%)	5	0
7	G	68/68 (100%)	61 (90%)	7 (10%)	7	1
7	T	68/68 (100%)	60 (88%)	8 (12%)	5	1
8	H	71/75 (95%)	67 (94%)	4 (6%)	21	4
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	1
9	I	57/57 (100%)	55 (96%)	2 (4%)	36	11
9	V	57/57 (100%)	54 (95%)	3 (5%)	22	4
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	32
10	W	50/50 (100%)	48 (96%)	2 (4%)	31	9
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	40/46 (87%)	37 (92%)	3 (8%)	13	2
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	21
12	Y	40/40 (100%)	39 (98%)	1 (2%)	47	22
13	M	37/38 (97%)	37 (100%)	0	100	100
13	Z	37/38 (97%)	37 (100%)	0	100	100
All	All	3131/3082 (102%)	3023 (97%)	108 (3%)	36	12

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	91	ASN
5	R	45	PRO
9	V	8	GLN

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Mol	Chain	Res	Type
2	O	221	LYS
4	Q	20	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
4	Q	37	GLN
6	S	94	HIS
4	Q	101	HIS
6	S	54	ASN
6	S	98	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	N	1	1	8,9,10	1.26	1 (12%)	7,9,11	1.30	1 (14%)
9	SAC	V	1	9	7,8,9	1.66	1 (14%)	8,9,11	1.35	2 (25%)
7	TPO	G	11	7	8,10,11	2.03	3 (37%)	10,14,16	0.88	0
7	TPO	T	11	7	8,10,11	1.74	2 (25%)	10,14,16	1.28	1 (10%)
2	FME	O	1	2	8,9,10	1.26	1 (12%)	7,9,11	2.00	2 (28%)
9	SAC	I	1	9	7,8,9	1.50	1 (14%)	8,9,11	1.89	2 (25%)
1	FME	A	1	1	8,9,10	0.96	1 (12%)	7,9,11	1.84	3 (42%)
2	FME	B	1	2	8,9,10	2.06	4 (50%)	7,9,11	1.90	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	N	1	1	-	3/7/9/11	-
9	SAC	V	1	9	-	7/7/8/10	-
7	TPO	G	11	7	-	4/9/11/13	-
7	TPO	T	11	7	-	5/9/11/13	-
2	FME	O	1	2	-	0/7/9/11	-
9	SAC	I	1	9	-	4/7/8/10	-
1	FME	A	1	1	-	2/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.24	1.52	1.46
2	B	1	FME	CB-CA	3.59	1.59	1.53
9	I	1	SAC	CA-N	3.50	1.51	1.46
7	G	11	TPO	P-O1P	3.29	1.61	1.50
7	T	11	TPO	P-O1P	3.09	1.60	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	1	SAC	OG-CB-CA	-3.53	101.96	110.97
9	I	1	SAC	C-CA-N	3.46	115.97	109.73
2	O	1	FME	CA-N-CN	3.36	127.98	122.82
1	A	1	FME	CE-SD-CG	3.23	111.50	100.40
2	B	1	FME	C-CA-N	-3.20	103.96	109.73

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	O-C-CA-CB
7	G	11	TPO	CA-CB-OG1-P
9	I	1	SAC	C-CA-CB-OG

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 111 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 101 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	CHD	P	301	-	32,32,32	1.60	8 (25%)	51,51,51	2.05	16 (31%)
21	EDO	F	103	-	3,3,3	1.11	0	2,2,2	0.11	0
21	EDO	N	619	-	3,3,3	1.21	0	2,2,2	0.19	0
21	EDO	N	621	-	3,3,3	0.79	0	2,2,2	1.29	0
20	PGV	N	609	-	50,50,50	1.20	2 (4%)	53,56,56	1.23	6 (11%)
19	TGL	Y	101	-	62,62,62	1.49	5 (8%)	65,65,65	1.81	10 (15%)
28	PEK	P	308	-	52,52,52	1.24	2 (3%)	55,57,57	1.37	5 (9%)
22	CHD	C	301	-	32,32,32	1.77	6 (18%)	51,51,51	2.31	19 (37%)
21	EDO	S	102	-	3,3,3	1.07	0	2,2,2	0.43	0
18	AZI	N	607[B]	14	0,2,2	-	-	0,1,1	-	-
20	PGV	N	610	-	50,50,50	1.15	6 (12%)	53,56,56	1.48	9 (16%)
22	CHD	C	306	-	32,32,32	1.30	5 (15%)	51,51,51	3.30	19 (37%)
21	EDO	W	102	-	3,3,3	0.49	0	2,2,2	0.65	0
21	EDO	N	616	-	3,3,3	1.04	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CHD	W	101	-	32,32,32	1.27	4 (12%)	51,51,51	2.62	27 (52%)
21	EDO	E	201	-	3,3,3	0.70	0	2,2,2	0.77	0
28	PEK	G	101	-	52,52,52	1.08	6 (11%)	55,57,57	1.45	8 (14%)
21	EDO	G	104	-	3,3,3	0.99	0	2,2,2	0.62	0
24	PSC	B	303	-	51,51,51	1.28	4 (7%)	57,59,59	1.38	4 (7%)
21	EDO	A	616	-	3,3,3	3.00	1 (33%)	2,2,2	5.57	1 (50%)
21	EDO	B	306	-	3,3,3	0.58	0	2,2,2	0.30	0
21	EDO	D	203	-	3,3,3	0.56	0	2,2,2	0.35	0
18	AZI	A	606[B]	14	0,2,2	-	-	0,1,1	-	-
25	DMU	Z	101	-	34,34,34	0.80	1 (2%)	45,45,45	1.21	3 (6%)
20	PGV	P	302	-	50,50,50	1.16	2 (4%)	53,56,56	1.32	4 (7%)
21	EDO	L	101	-	3,3,3	0.74	0	2,2,2	0.84	0
21	EDO	A	612	-	3,3,3	0.40	0	2,2,2	1.48	0
14	HEA	A	602[A]	18,1	57,67,67	1.61	12 (21%)	61,103,103	2.18	20 (32%)
21	EDO	N	620	-	3,3,3	0.57	0	2,2,2	0.05	0
27	CDL	P	305	-	99,99,99	1.53	18 (18%)	105,111,111	1.63	18 (17%)
28	PEK	G	103	-	52,52,52	1.11	2 (3%)	55,57,57	1.19	4 (7%)
21	EDO	F	104	-	3,3,3	0.68	0	2,2,2	0.34	0
25	DMU	C	302	-	34,34,34	0.75	1 (2%)	45,45,45	1.47	7 (15%)
18	AZI	N	608[A]	15,14	0,2,2	-	-	0,1,1	-	-
22	CHD	B	301	-	32,32,32	1.79	10 (31%)	51,51,51	2.26	22 (43%)
20	PGV	P	304	-	50,50,50	1.07	4 (8%)	53,56,56	1.35	6 (11%)
27	CDL	T	102	-	99,99,99	1.45	13 (13%)	105,111,111	1.36	17 (16%)
21	EDO	S	104	-	3,3,3	0.63	0	2,2,2	1.66	1 (50%)
21	EDO	S	103	-	3,3,3	1.30	0	2,2,2	0.49	0
21	EDO	F	102	-	3,3,3	0.94	0	2,2,2	0.20	0
14	HEA	N	603[B]	18,1	57,67,67	1.36	6 (10%)	61,103,103	2.27	23 (37%)
21	EDO	G	105	-	3,3,3	0.59	0	2,2,2	0.30	0
21	EDO	N	615	-	3,3,3	0.69	0	2,2,2	1.27	0
28	PEK	T	101	-	52,52,52	1.37	6 (11%)	55,57,57	2.47	8 (14%)
21	EDO	B	304	-	3,3,3	0.16	0	2,2,2	1.40	0
22	CHD	G	102	-	32,32,32	1.98	10 (31%)	51,51,51	1.98	14 (27%)
14	HEA	A	601	1	57,67,67	1.67	11 (19%)	61,103,103	2.69	25 (40%)
14	HEA	A	602[B]	18,1	57,67,67	1.57	9 (15%)	61,103,103	2.35	21 (34%)
25	DMU	C	311	-	34,34,34	1.04	1 (2%)	45,45,45	2.33	13 (28%)
21	EDO	E	203	-	3,3,3	0.77	0	2,2,2	0.53	0
27	CDL	C	305	-	99,99,99	1.50	17 (17%)	105,111,111	1.53	15 (14%)
22	CHD	P	306	-	32,32,32	1.49	6 (18%)	51,51,51	3.47	22 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	TGL	D	201	-	62,62,62	2.00	5 (8%)	65,65,65	2.58	11 (16%)
18	AZI	N	608[B]	15	0,2,2	-	-	0,1,1	-	-
22	CHD	J	101	-	32,32,32	0.91	0	51,51,51	2.27	20 (39%)
21	EDO	A	618	-	3,3,3	0.41	0	2,2,2	1.03	0
21	EDO	B	305	-	3,3,3	1.59	0	2,2,2	0.24	0
21	EDO	P	311	-	3,3,3	0.87	0	2,2,2	0.50	0
20	PGV	C	304	-	50,50,50	0.98	3 (6%)	53,56,56	1.12	4 (7%)
25	DMU	M	101	-	34,34,34	0.90	1 (2%)	45,45,45	1.44	6 (13%)
19	TGL	A	608	-	62,62,62	1.31	6 (9%)	65,65,65	2.24	10 (15%)
25	DMU	P	307	-	34,34,34	0.94	1 (2%)	45,45,45	1.46	8 (17%)
21	EDO	N	617	-	3,3,3	0.65	0	2,2,2	0.84	0
21	EDO	C	312	-	3,3,3	0.64	0	2,2,2	0.60	0
21	EDO	A	613	-	3,3,3	0.58	0	2,2,2	1.32	0
20	PGV	A	609	-	50,50,50	1.19	5 (10%)	53,56,56	1.30	6 (11%)
20	PGV	A	610	-	50,50,50	1.41	5 (10%)	53,56,56	1.88	7 (13%)
21	EDO	E	202	-	3,3,3	0.93	0	2,2,2	0.66	0
21	EDO	P	312	-	3,3,3	0.77	0	2,2,2	1.65	1 (50%)
23	CUA	B	302	30,2	0,1,1	-	-	-	-	-
21	EDO	N	613	-	3,3,3	1.61	1 (33%)	2,2,2	0.51	0
18	AZI	A	607[A]	15,14	0,2,2	-	-	0,1,1	-	-
21	EDO	A	614	-	3,3,3	1.58	1 (33%)	2,2,2	0.78	0
21	EDO	Y	102	-	3,3,3	0.53	0	2,2,2	0.61	0
21	EDO	D	202	-	3,3,3	1.05	0	2,2,2	0.36	0
24	PSC	N	612	-	51,51,51	1.29	3 (5%)	57,59,59	1.19	4 (7%)
21	EDO	T	103	-	3,3,3	1.00	0	2,2,2	0.82	0
21	EDO	A	620	-	3,3,3	0.45	0	2,2,2	0.84	0
21	EDO	N	614	-	3,3,3	0.47	0	2,2,2	1.07	0
21	EDO	R	201	-	3,3,3	0.87	0	2,2,2	0.63	0
28	PEK	C	307	-	52,52,52	1.50	4 (7%)	55,57,57	1.50	9 (16%)
21	EDO	B	307	-	3,3,3	0.67	0	2,2,2	0.04	0
19	TGL	A	611	-	62,62,62	1.28	3 (4%)	65,65,65	1.83	13 (20%)
25	DMU	C	310	-	34,34,34	0.91	1 (2%)	45,45,45	2.51	13 (28%)
21	EDO	A	617	-	3,3,3	1.38	0	2,2,2	0.41	0
21	EDO	A	619	-	3,3,3	0.26	0	2,2,2	0.78	0
18	AZI	A	607[B]	15	0,2,2	-	-	0,1,1	-	-
21	EDO	O	302	-	3,3,3	0.65	0	2,2,2	0.58	0
19	TGL	Q	201	-	62,62,62	1.51	4 (6%)	65,65,65	1.47	7 (10%)
25	DMU	P	309	-	34,34,34	0.81	1 (2%)	45,45,45	2.15	12 (26%)
20	PGV	C	308	-	50,50,50	1.26	2 (4%)	53,56,56	1.44	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	DMU	P	310	-	34,34,34	1.11	2 (5%)	45,45,45	1.79	10 (22%)
19	TGL	N	611	-	62,62,62	1.12	4 (6%)	65,65,65	1.69	10 (15%)
21	EDO	N	618	-	3,3,3	0.64	0	2,2,2	0.66	0
21	EDO	A	615	-	3,3,3	0.62	0	2,2,2	1.83	1 (50%)
14	HEA	N	602	1	57,67,67	1.74	17 (29%)	61,103,103	2.07	19 (31%)
14	HEA	N	603[A]	18,1	57,67,67	1.65	13 (22%)	61,103,103	2.16	26 (42%)
28	PEK	C	309	-	52,52,52	1.19	2 (3%)	55,57,57	1.37	5 (9%)
23	CUA	O	301	2	0,1,1	-	-	-	-	-
27	CDL	N	601	-	99,99,99	1.53	15 (15%)	105,111,111	1.51	16 (15%)
21	EDO	M	102	-	3,3,3	0.24	0	2,2,2	1.04	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	P	301	-	-	3/9/74/74	0/4/4/4
21	EDO	F	103	-	-	0/1/1/1	-
21	EDO	N	619	-	-	0/1/1/1	-
21	EDO	N	621	-	-	1/1/1/1	-
20	PGV	N	609	-	-	35/55/55/55	-
19	TGL	Y	101	-	-	34/65/65/65	-
28	PEK	P	308	-	-	25/56/56/56	-
22	CHD	C	301	-	-	2/9/74/74	0/4/4/4
21	EDO	S	102	-	-	0/1/1/1	-
20	PGV	N	610	-	-	11/55/55/55	-
22	CHD	C	306	-	-	5/9/74/74	0/4/4/4
21	EDO	W	102	-	-	0/1/1/1	-
21	EDO	N	616	-	-	0/1/1/1	-
22	CHD	W	101	-	-	8/9/74/74	0/4/4/4
21	EDO	E	201	-	-	0/1/1/1	-
28	PEK	G	101	-	-	19/56/56/56	-
21	EDO	G	104	-	-	0/1/1/1	-
24	PSC	B	303	-	-	33/55/55/55	-
21	EDO	A	616	-	-	1/1/1/1	-
21	EDO	B	306	-	-	0/1/1/1	-
21	EDO	D	203	-	-	0/1/1/1	-
25	DMU	Z	101	-	-	7/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	P	302	-	-	24/55/55/55	-
21	EDO	L	101	-	-	1/1/1/1	-
21	EDO	A	612	-	-	1/1/1/1	-
14	HEA	A	602[A]	18,1	-	6/32/76/76	-
21	EDO	N	620	-	-	0/1/1/1	-
27	CDL	P	305	-	-	54/110/110/110	-
28	PEK	G	103	-	-	31/56/56/56	-
21	EDO	F	104	-	-	0/1/1/1	-
25	DMU	C	302	-	-	9/19/59/59	0/2/2/2
22	CHD	B	301	-	-	2/9/74/74	0/4/4/4
20	PGV	P	304	-	-	13/55/55/55	-
27	CDL	T	102	-	-	51/110/110/110	-
21	EDO	S	104	-	-	0/1/1/1	-
21	EDO	S	103	-	-	0/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
14	HEA	N	603[B]	18,1	-	5/32/76/76	-
21	EDO	G	105	-	-	0/1/1/1	-
21	EDO	N	615	-	-	0/1/1/1	-
28	PEK	T	101	-	-	23/56/56/56	-
21	EDO	B	304	-	-	1/1/1/1	-
22	CHD	G	102	-	-	2/9/74/74	0/4/4/4
14	HEA	A	601	1	-	7/32/76/76	-
14	HEA	A	602[B]	18,1	-	4/32/76/76	-
25	DMU	C	311	-	-	8/19/59/59	0/2/2/2
21	EDO	E	203	-	-	0/1/1/1	-
27	CDL	C	305	-	-	53/110/110/110	-
22	CHD	P	306	-	-	5/9/74/74	0/4/4/4
19	TGL	D	201	-	-	36/65/65/65	-
22	CHD	J	101	-	-	5/9/74/74	0/4/4/4
21	EDO	A	618	-	-	1/1/1/1	-
21	EDO	B	305	-	-	1/1/1/1	-
21	EDO	P	311	-	-	0/1/1/1	-
20	PGV	C	304	-	-	17/55/55/55	-
25	DMU	M	101	-	-	4/19/59/59	0/2/2/2
19	TGL	A	608	-	-	34/65/65/65	-
25	DMU	P	307	-	-	5/19/59/59	0/2/2/2
21	EDO	N	617	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	C	312	-	-	0/1/1/1	-
21	EDO	A	613	-	-	1/1/1/1	-
20	PGV	A	609	-	-	8/55/55/55	-
20	PGV	A	610	-	-	28/55/55/55	-
21	EDO	E	202	-	-	1/1/1/1	-
21	EDO	P	312	-	-	0/1/1/1	-
21	EDO	N	613	-	-	0/1/1/1	-
21	EDO	A	614	-	-	0/1/1/1	-
21	EDO	Y	102	-	-	1/1/1/1	-
21	EDO	D	202	-	-	1/1/1/1	-
24	PSC	N	612	-	-	28/55/55/55	-
21	EDO	T	103	-	-	0/1/1/1	-
21	EDO	A	620	-	-	0/1/1/1	-
21	EDO	N	614	-	-	0/1/1/1	-
21	EDO	R	201	-	-	0/1/1/1	-
28	PEK	C	307	-	-	31/56/56/56	-
21	EDO	B	307	-	-	0/1/1/1	-
19	TGL	A	611	-	-	39/65/65/65	-
25	DMU	C	310	-	-	7/19/59/59	0/2/2/2
21	EDO	A	617	-	-	0/1/1/1	-
21	EDO	A	619	-	-	1/1/1/1	-
21	EDO	O	302	-	-	0/1/1/1	-
19	TGL	Q	201	-	-	30/65/65/65	-
25	DMU	P	309	-	-	7/19/59/59	0/2/2/2
20	PGV	C	308	-	-	23/55/55/55	-
25	DMU	P	310	-	-	10/19/59/59	0/2/2/2
19	TGL	N	611	-	-	39/65/65/65	-
21	EDO	N	618	-	-	1/1/1/1	-
21	EDO	A	615	-	-	1/1/1/1	-
14	HEA	N	602	1	-	6/32/76/76	-
14	HEA	N	603[A]	18,1	-	4/32/76/76	-
28	PEK	C	309	-	-	26/56/56/56	-
27	CDL	N	601	-	-	59/110/110/110	-
21	EDO	M	102	-	-	0/1/1/1	-

The worst 5 of 277 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	201	TGL	OB1-CB1	10.00	1.52	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	201	TGL	OG2-CB1	7.60	1.55	1.34
19	Y	101	TGL	OG2-CB1	6.73	1.53	1.34
19	Q	201	TGL	OG2-CB1	6.52	1.52	1.34
28	C	307	PEK	O01-C1	6.35	1.52	1.34

The worst 5 of 592 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	306	CHD	C23-C22-C20	-17.95	81.74	114.52
22	P	306	CHD	C23-C22-C20	-17.82	81.97	114.52
28	T	101	PEK	C2-C3-C4	15.35	140.59	113.23
19	D	201	TGL	OG2-CB1-CB2	-12.32	84.94	111.50
25	C	311	DMU	O16-C6-C1	11.07	125.59	108.30

There are no chirality outliers.

5 of 939 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602[B]	HEA	C4D-C3D-CAD-CBD
19	A	611	TGL	CB2-CB1-OG2-CG2
19	A	611	TGL	OB1-CB1-OG2-CG2
19	D	201	TGL	CG2-CG1-OG1-CA1
19	Y	101	TGL	CA2-CA1-OG1-CG1

There are no ring outliers.

58 monomers are involved in 363 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	P	301	CHD	1	0
21	N	621	EDO	1	0
20	N	609	PGV	9	0
19	Y	101	TGL	20	0
28	P	308	PEK	6	0
22	C	301	CHD	1	0
18	N	607[B]	AZI	1	0
20	N	610	PGV	1	0
22	C	306	CHD	5	0
22	W	101	CHD	1	0
28	G	101	PEK	7	0
24	B	303	PSC	15	0
21	A	616	EDO	2	0

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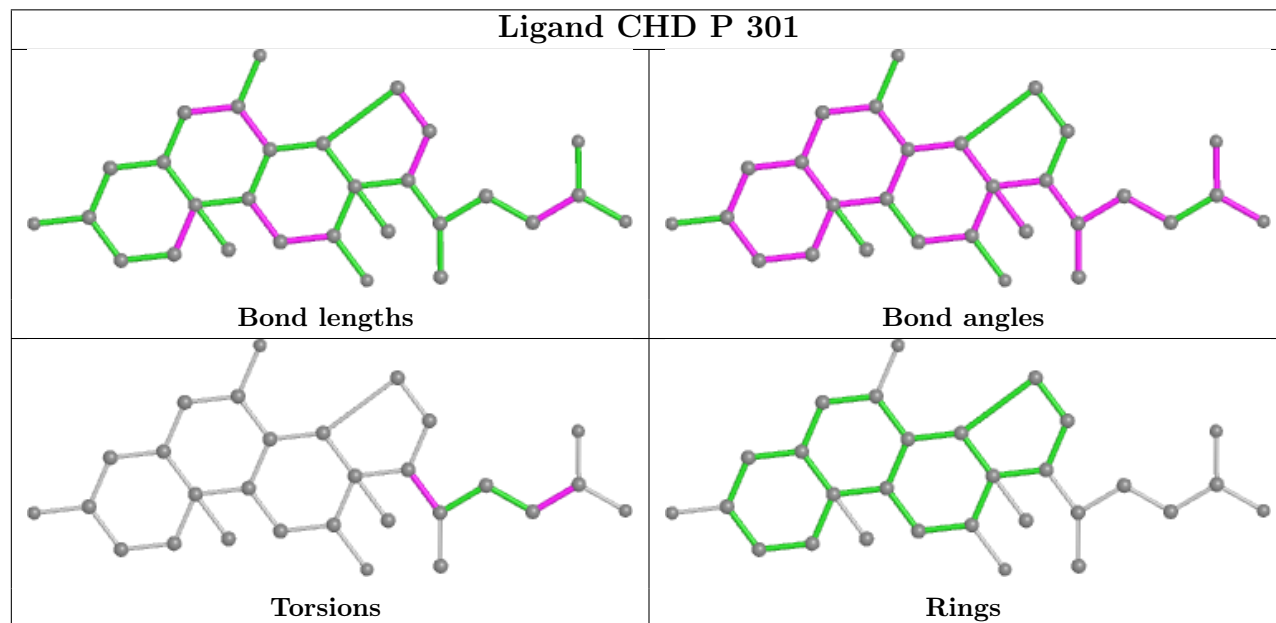
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	606[B]	AZI	1	0
20	P	302	PGV	1	0
14	A	602[A]	HEA	5	0
27	P	305	CDL	24	0
28	G	103	PEK	1	0
25	C	302	DMU	12	0
18	N	608[A]	AZI	1	0
20	P	304	PGV	2	0
27	T	102	CDL	16	0
14	N	603[B]	HEA	12	0
21	G	105	EDO	3	0
28	T	101	PEK	3	0
21	B	304	EDO	2	0
22	G	102	CHD	1	0
14	A	601	HEA	8	0
14	A	602[B]	HEA	12	0
27	C	305	CDL	17	0
22	P	306	CHD	5	0
19	D	201	TGL	13	0
18	N	608[B]	AZI	1	0
22	J	101	CHD	1	0
21	A	618	EDO	2	0
20	C	304	PGV	3	0
19	A	608	TGL	5	0
25	P	307	DMU	11	0
20	A	609	PGV	4	0
20	A	610	PGV	9	0
18	A	607[A]	AZI	2	0
21	D	202	EDO	9	0
24	N	612	PSC	16	0
21	A	620	EDO	1	0
28	C	307	PEK	11	0
19	A	611	TGL	6	0
25	C	310	DMU	3	0
21	A	619	EDO	3	0
18	A	607[B]	AZI	5	0
19	Q	201	TGL	12	0
25	P	309	DMU	3	0
20	C	308	PGV	1	0
25	P	310	DMU	2	0
19	N	611	TGL	7	0
14	N	602	HEA	11	0

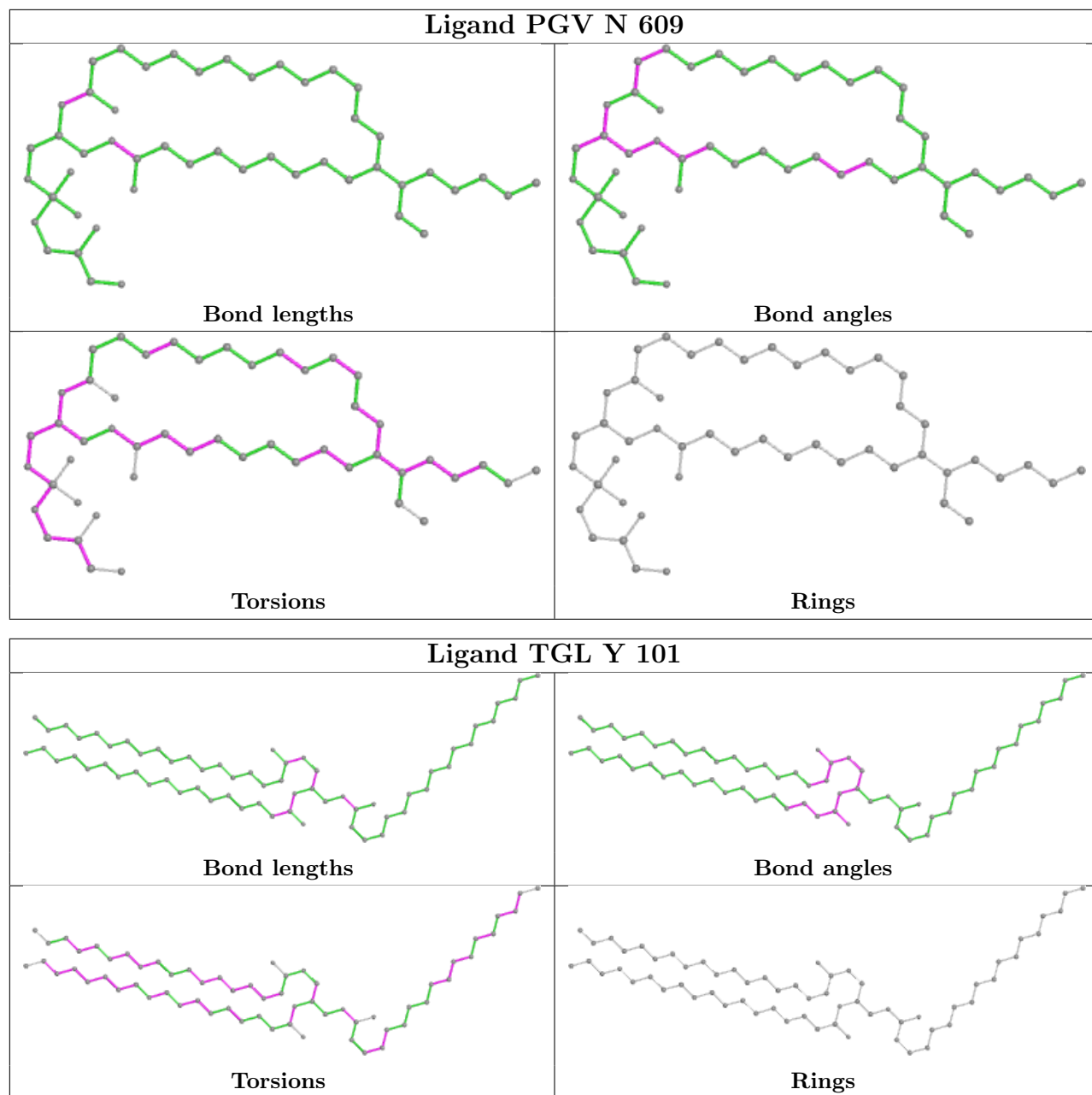
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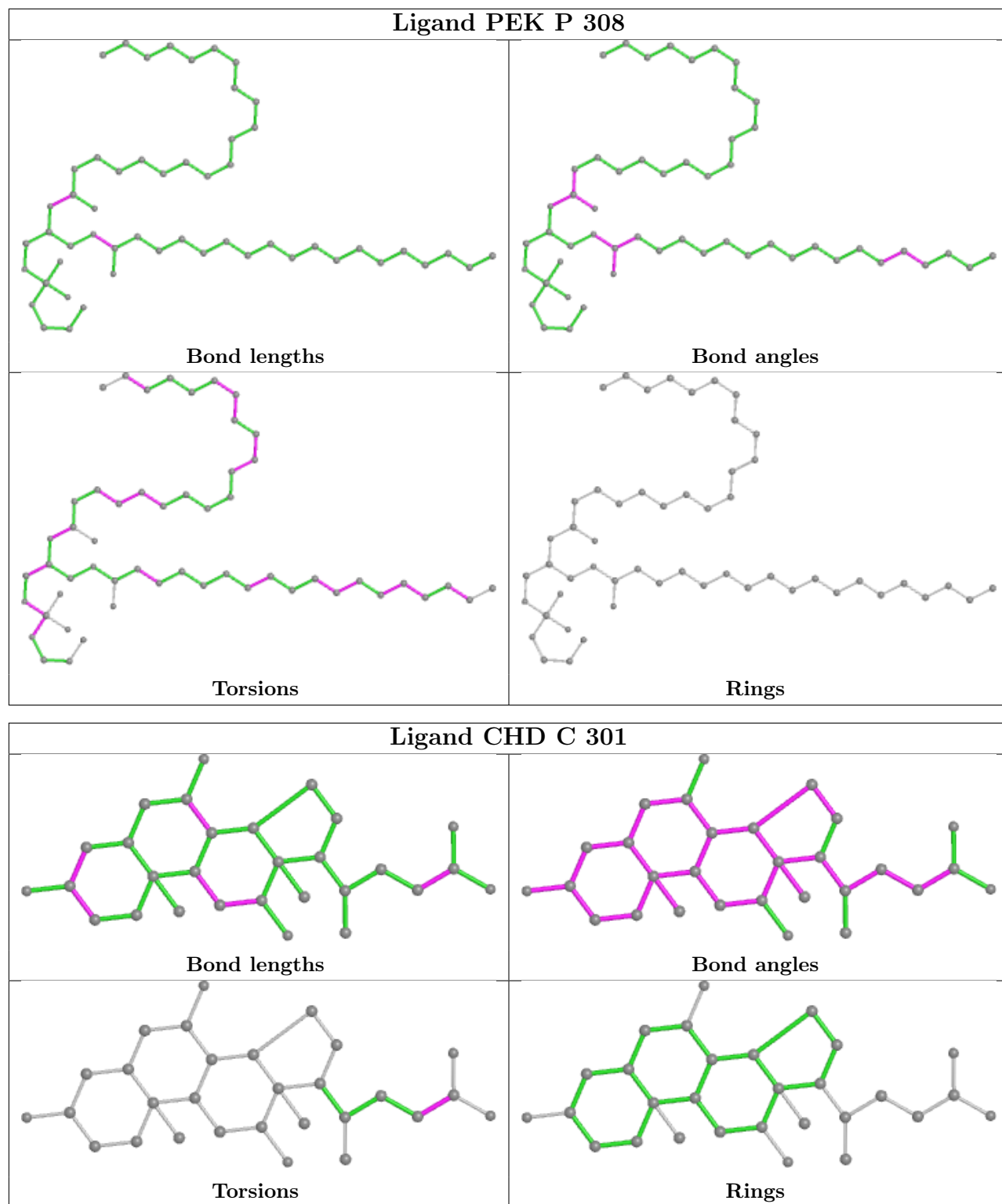
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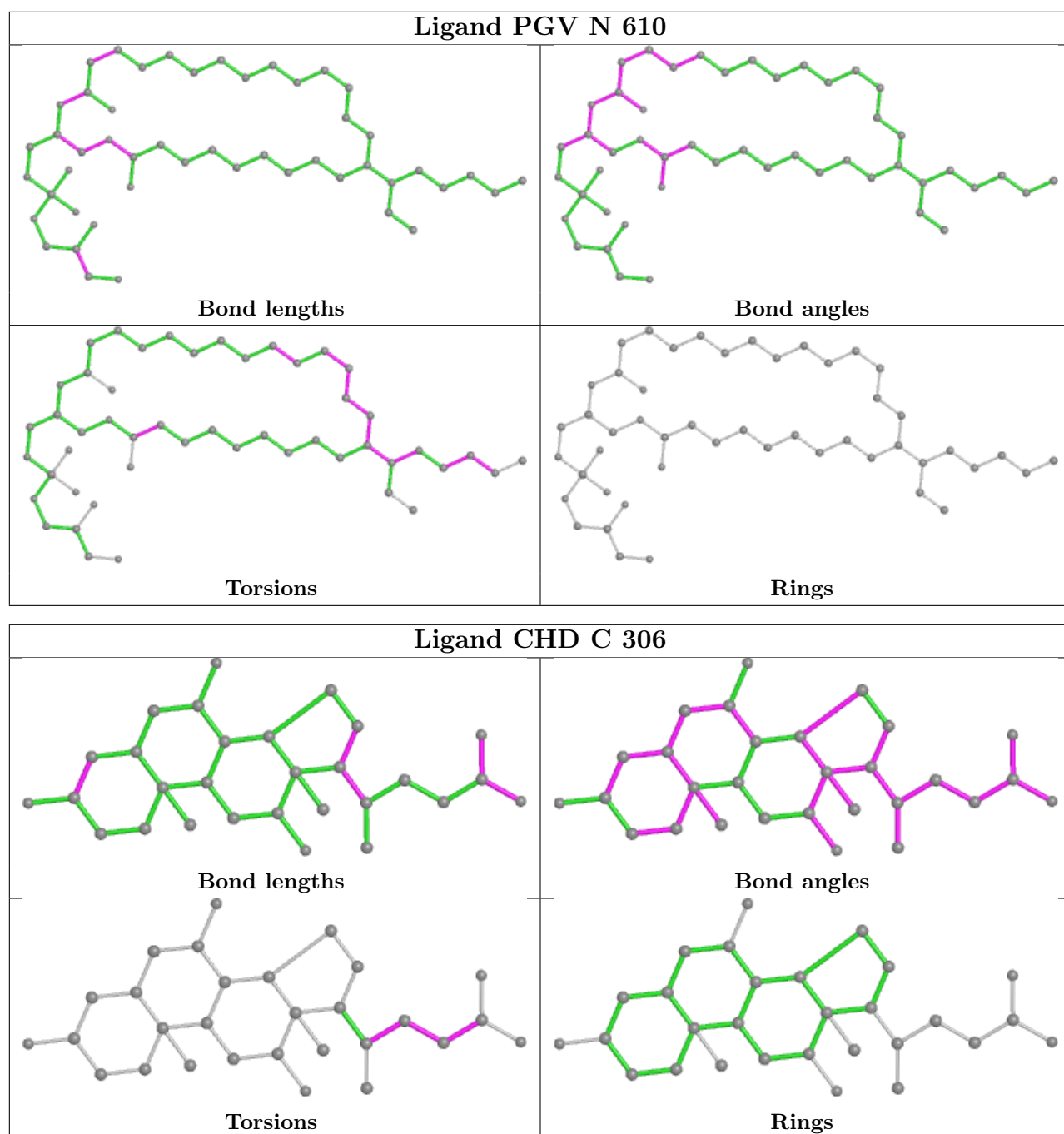
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	603[A]	HEA	5	0
28	C	309	PEK	4	0
27	N	601	CDL	29	0

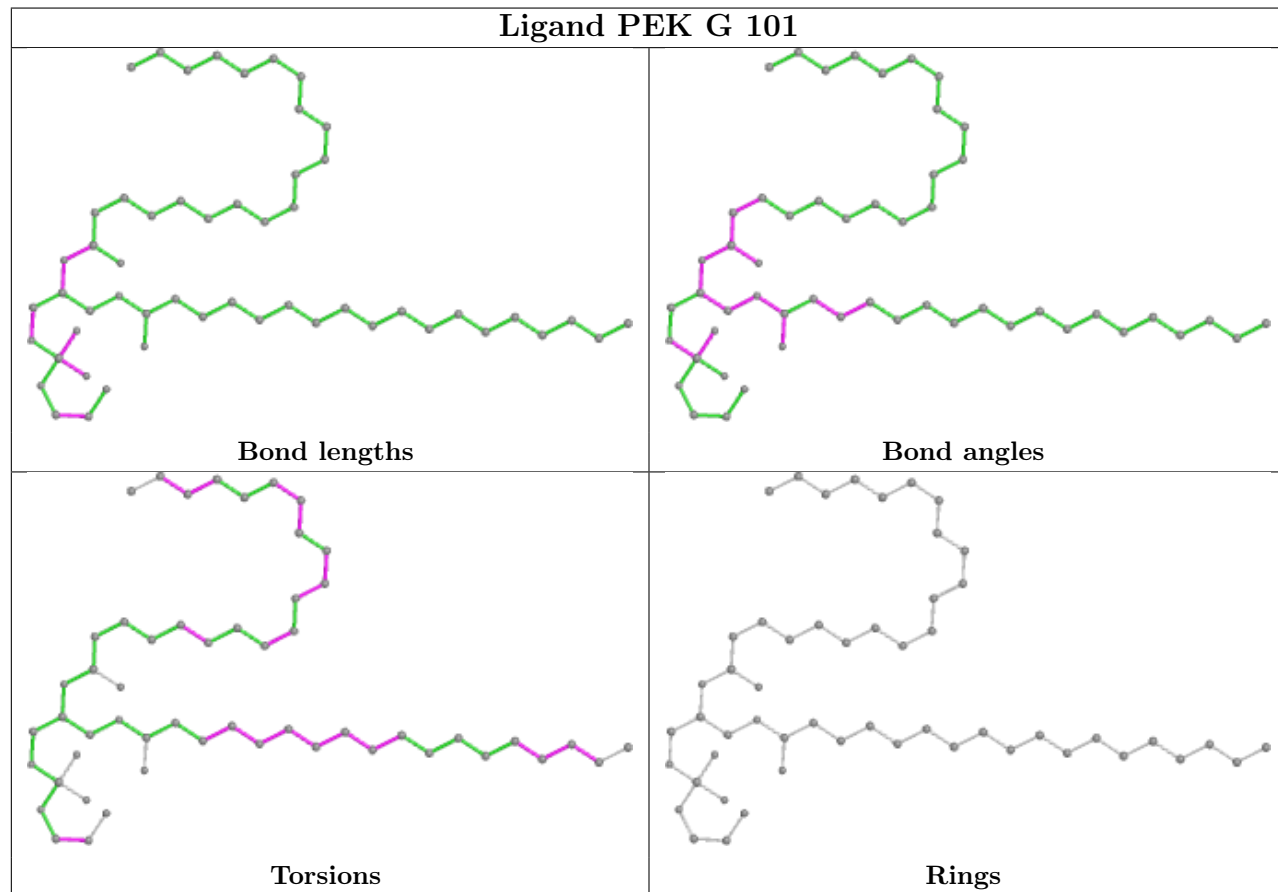
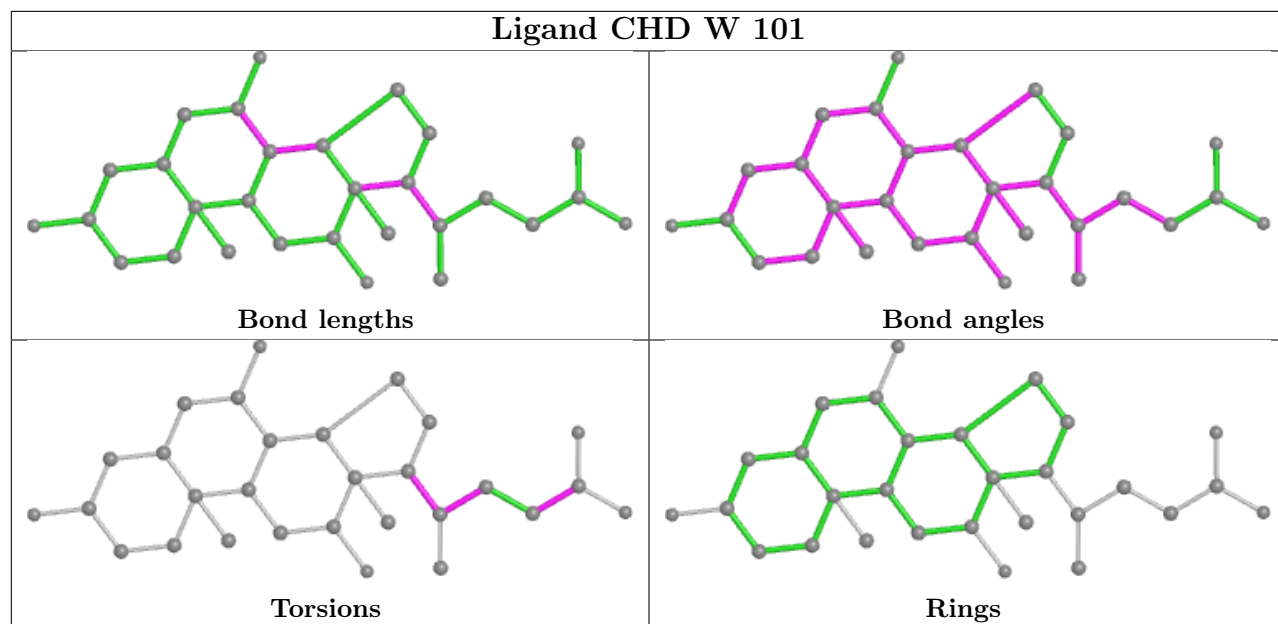
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

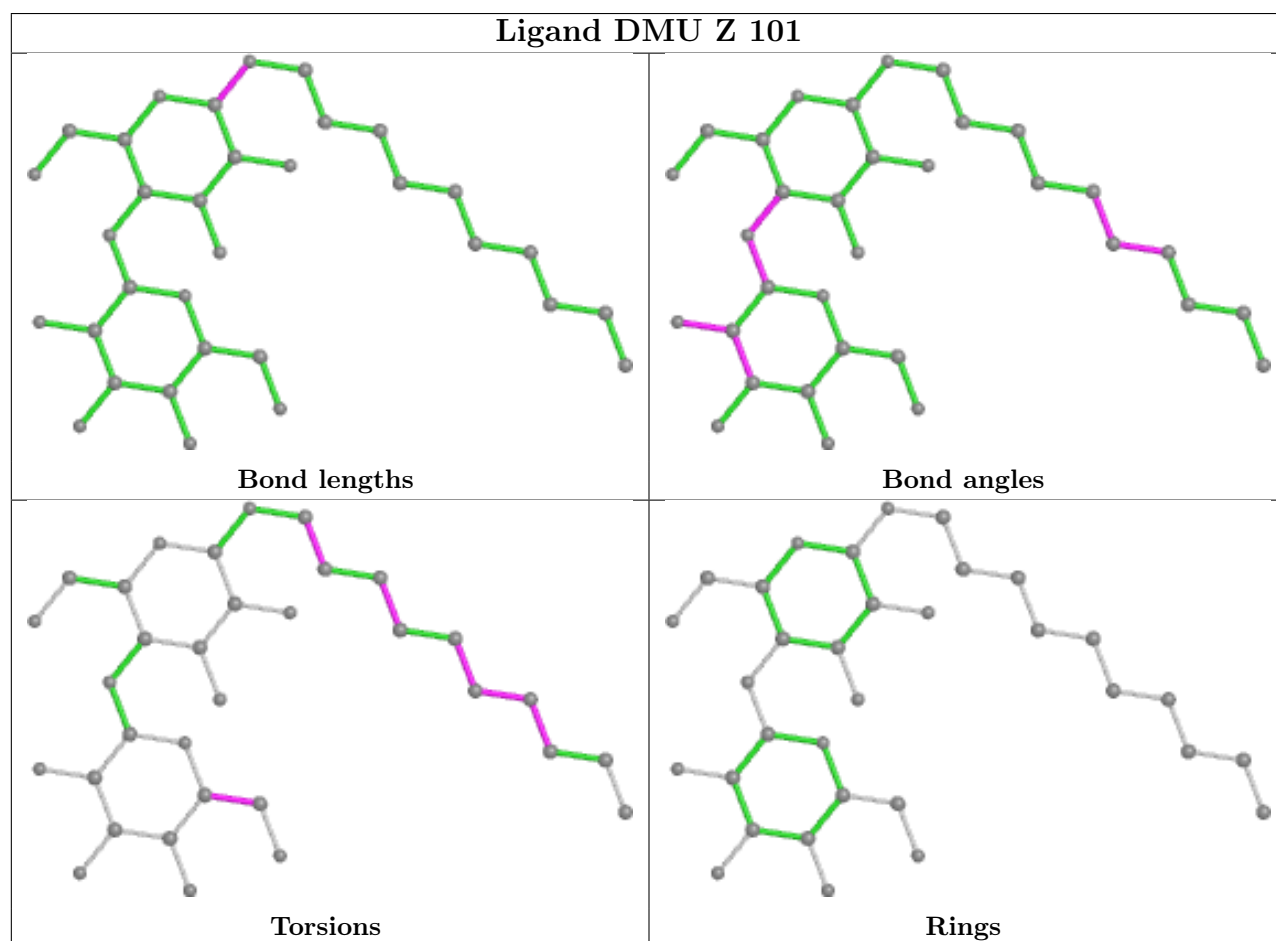
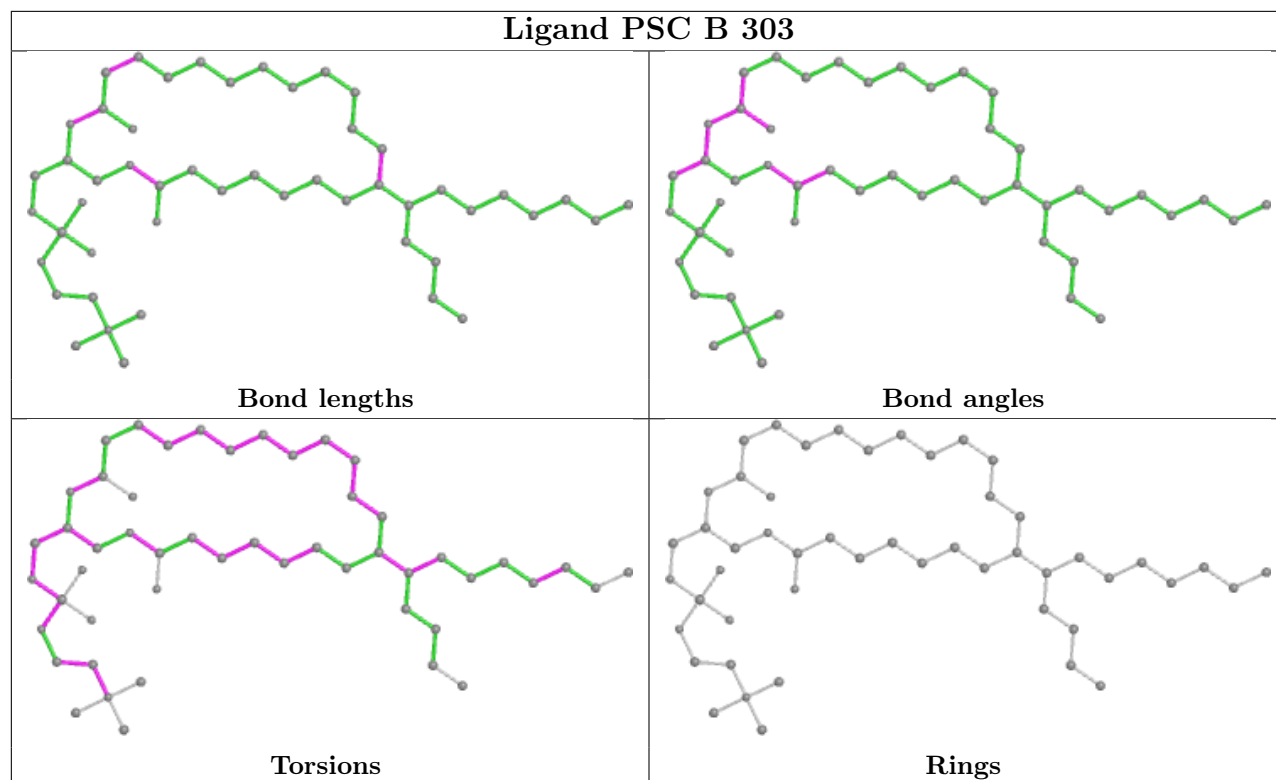


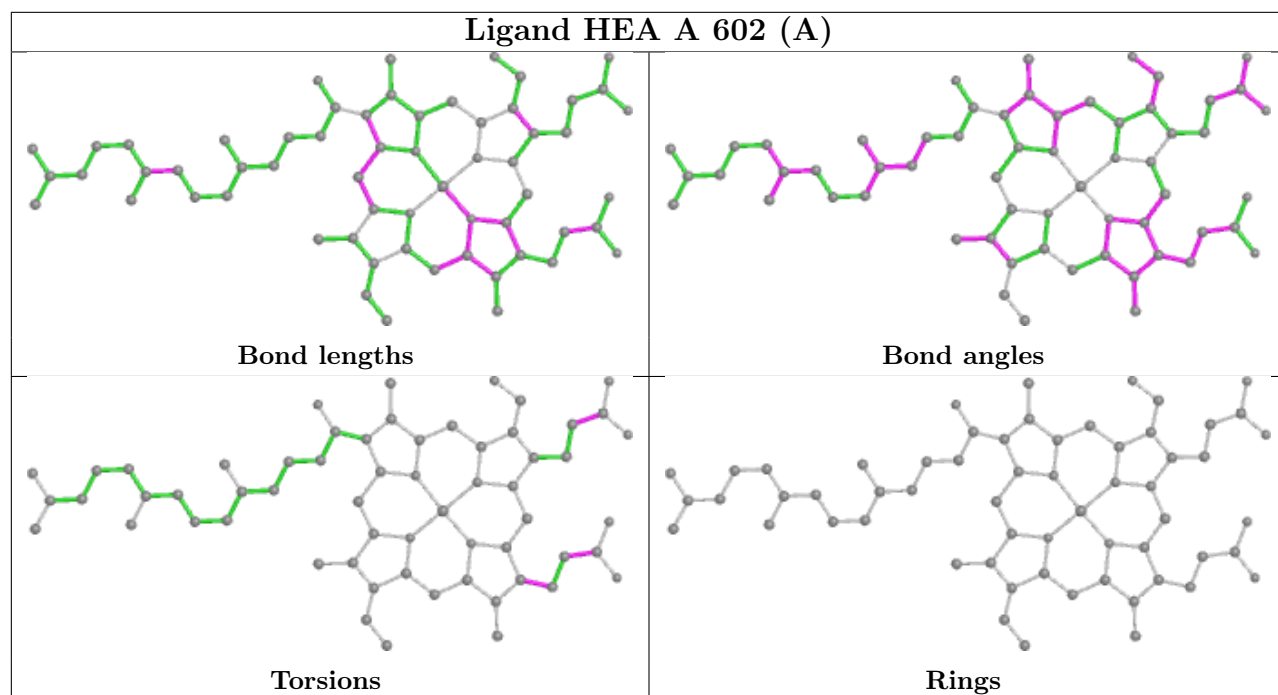
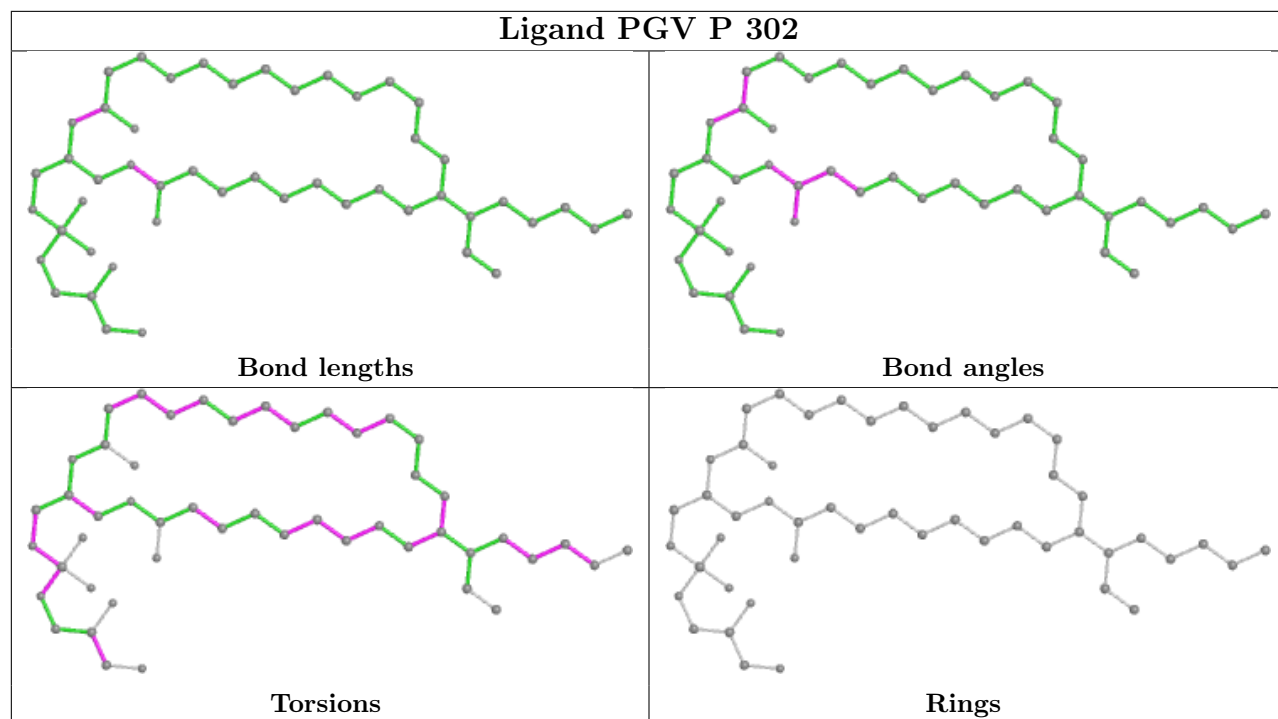


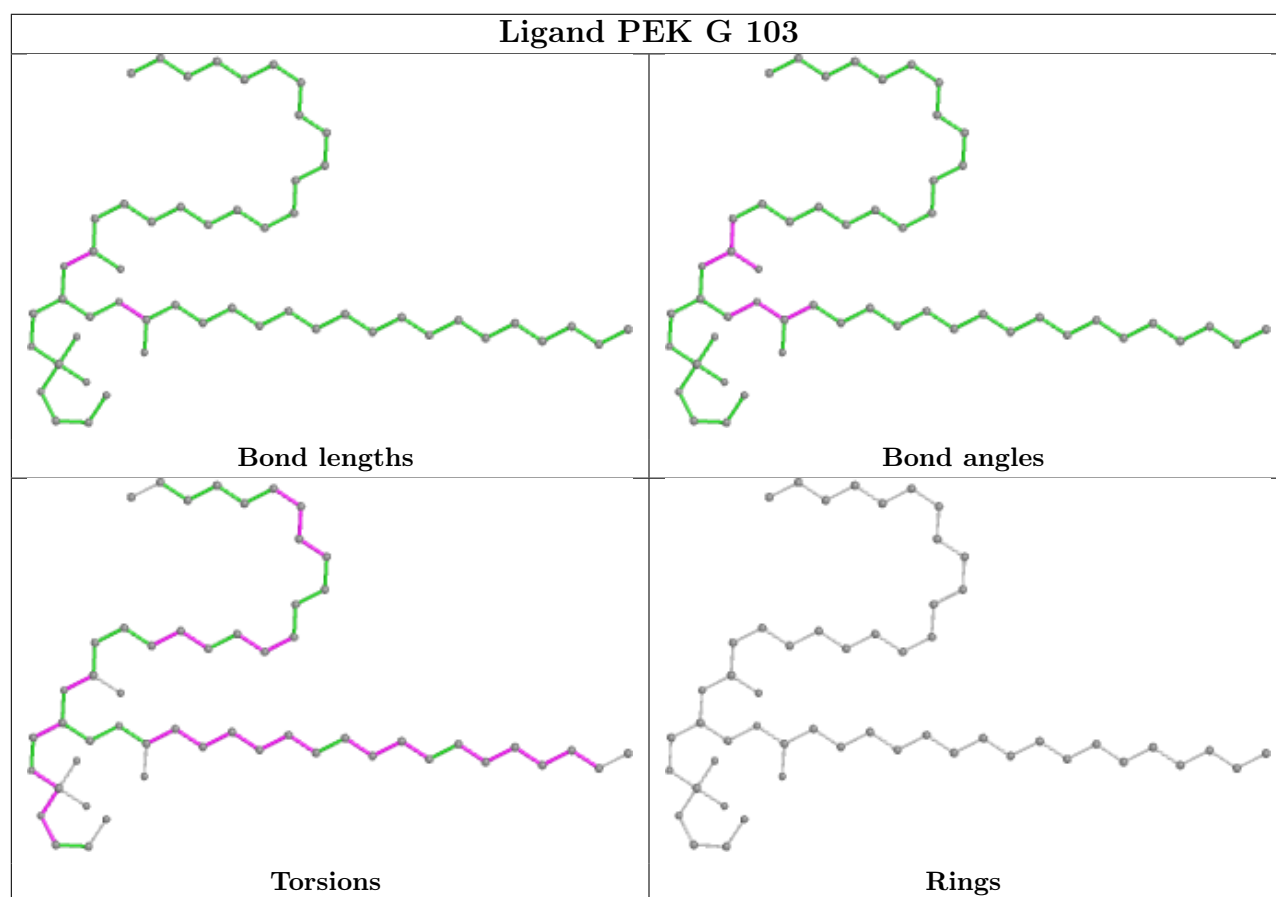
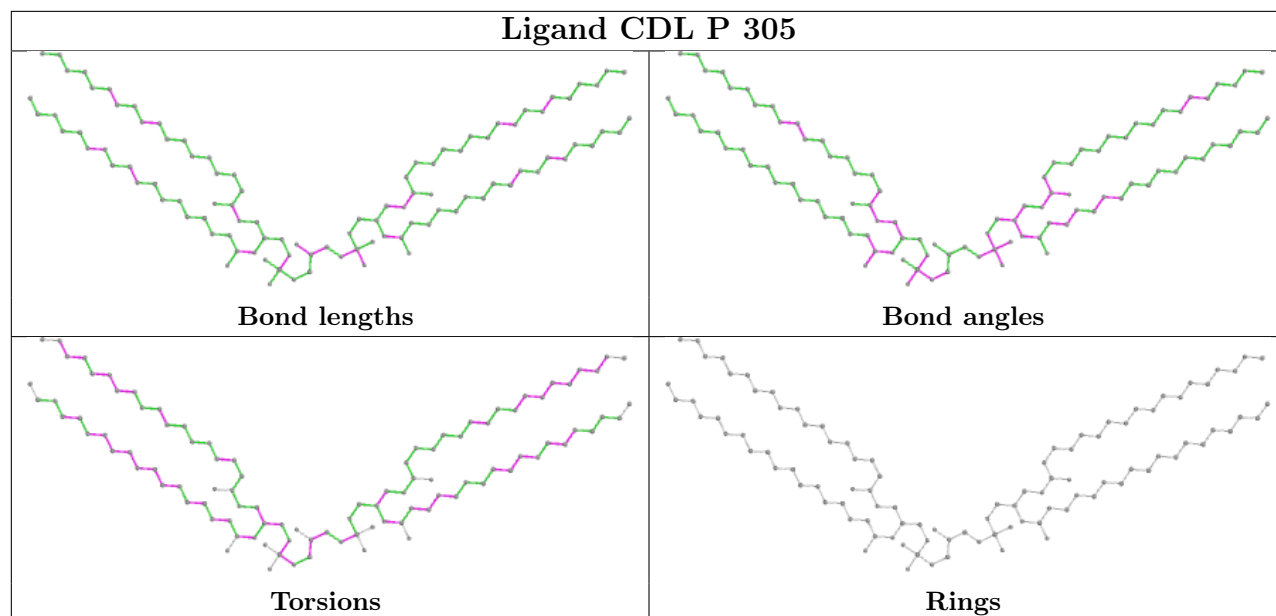


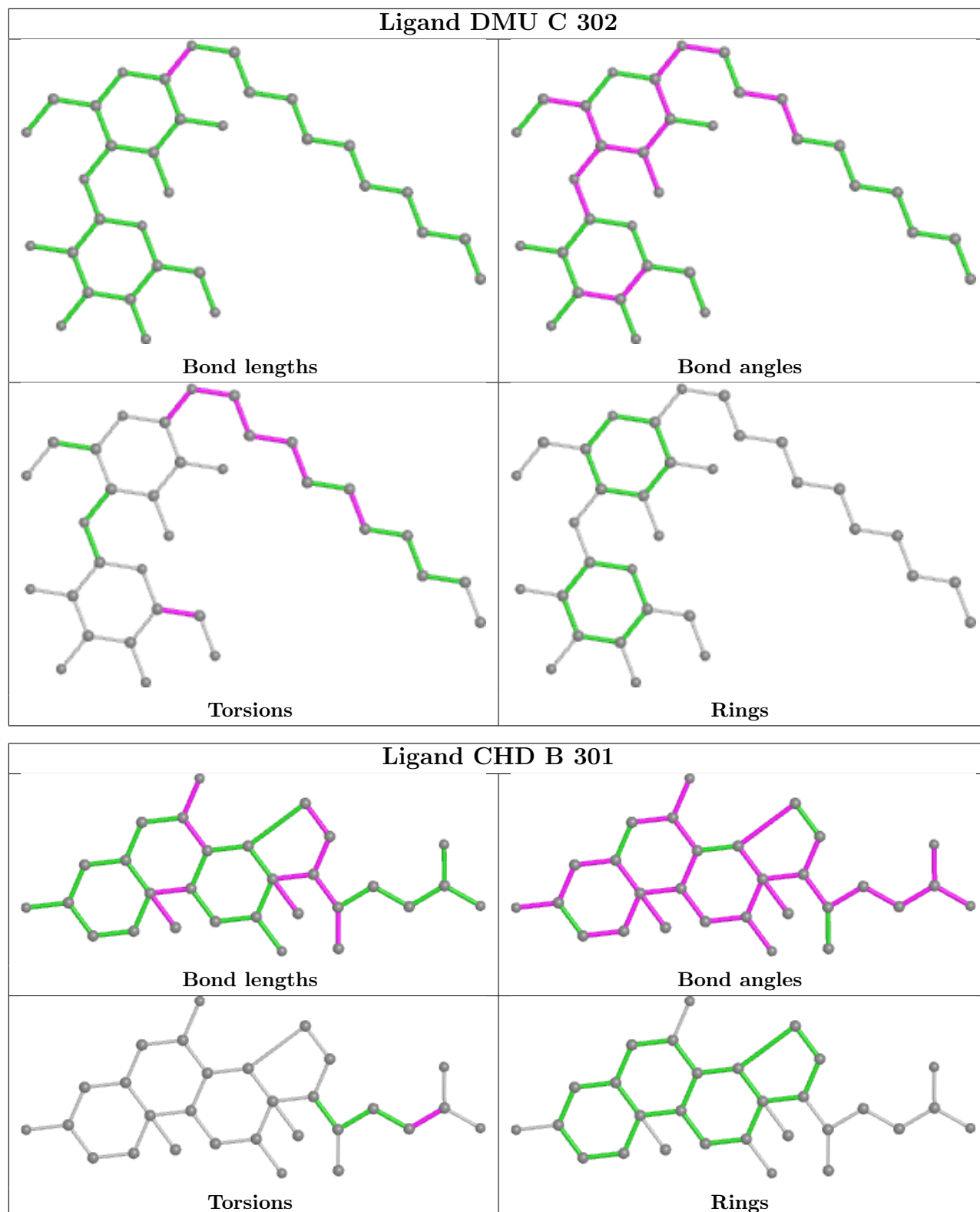


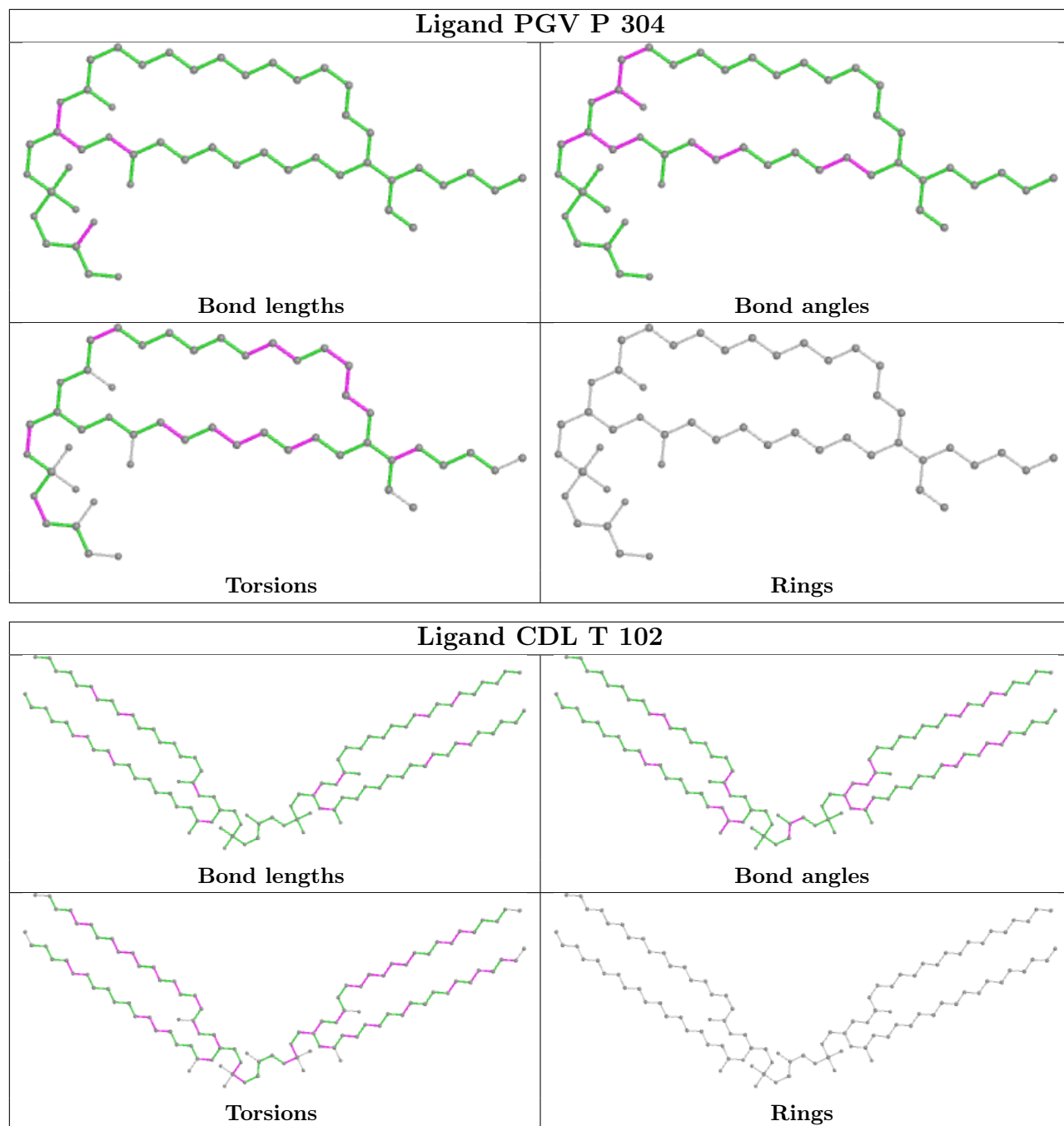


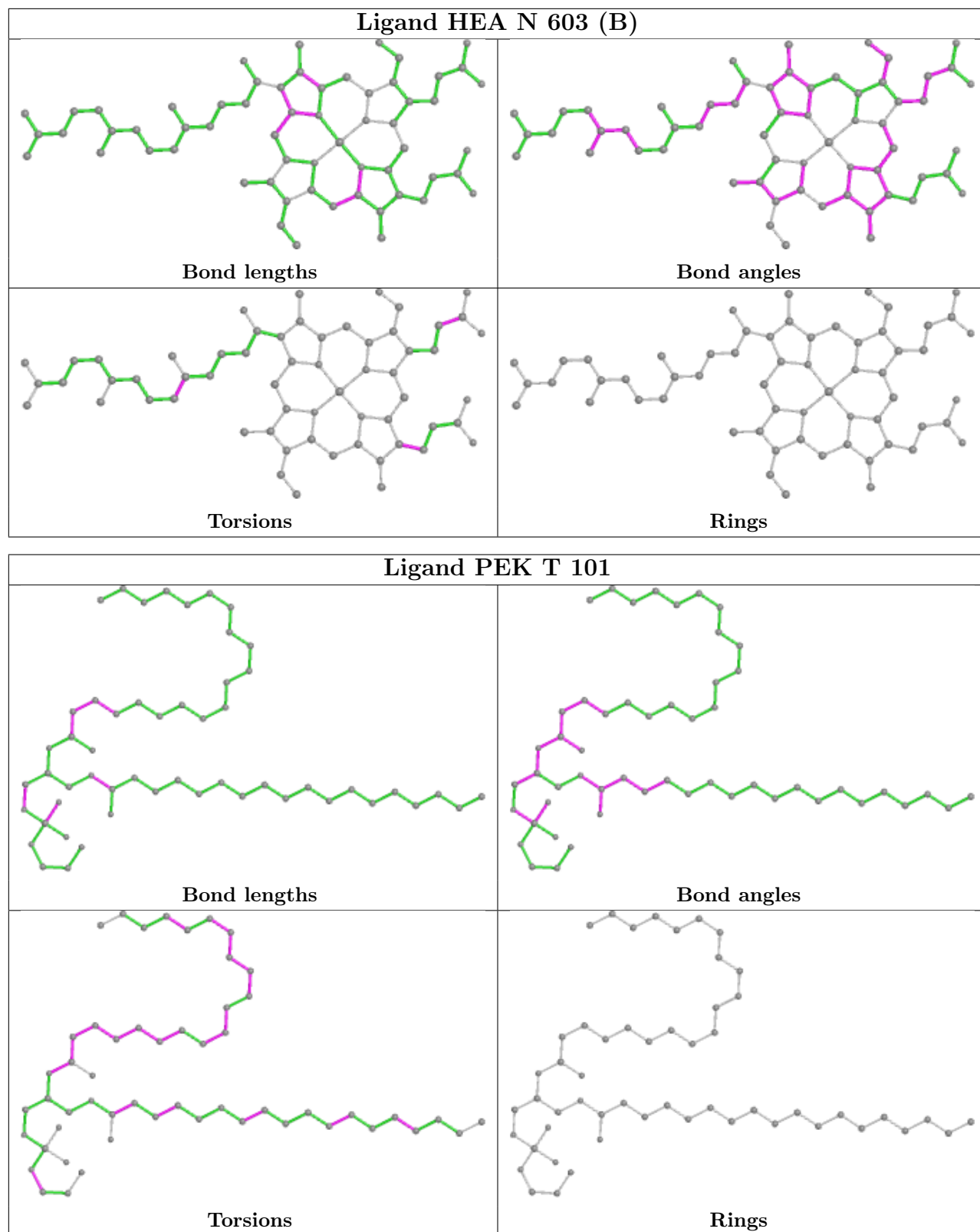


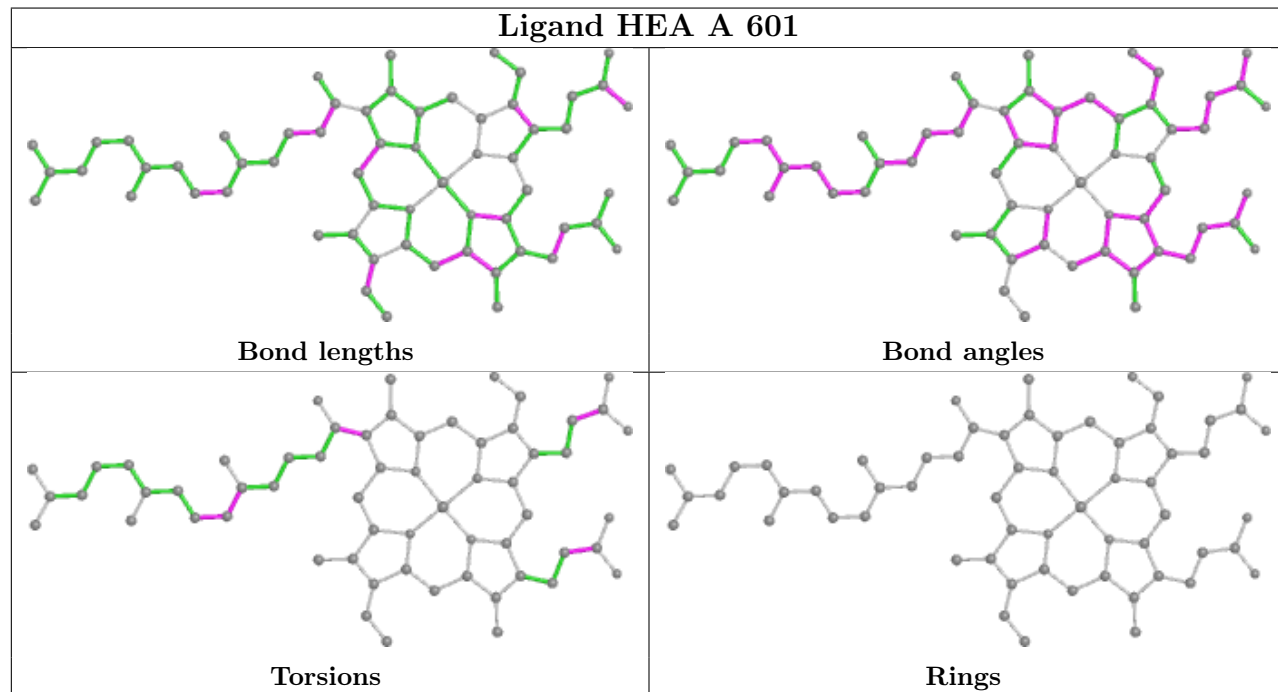
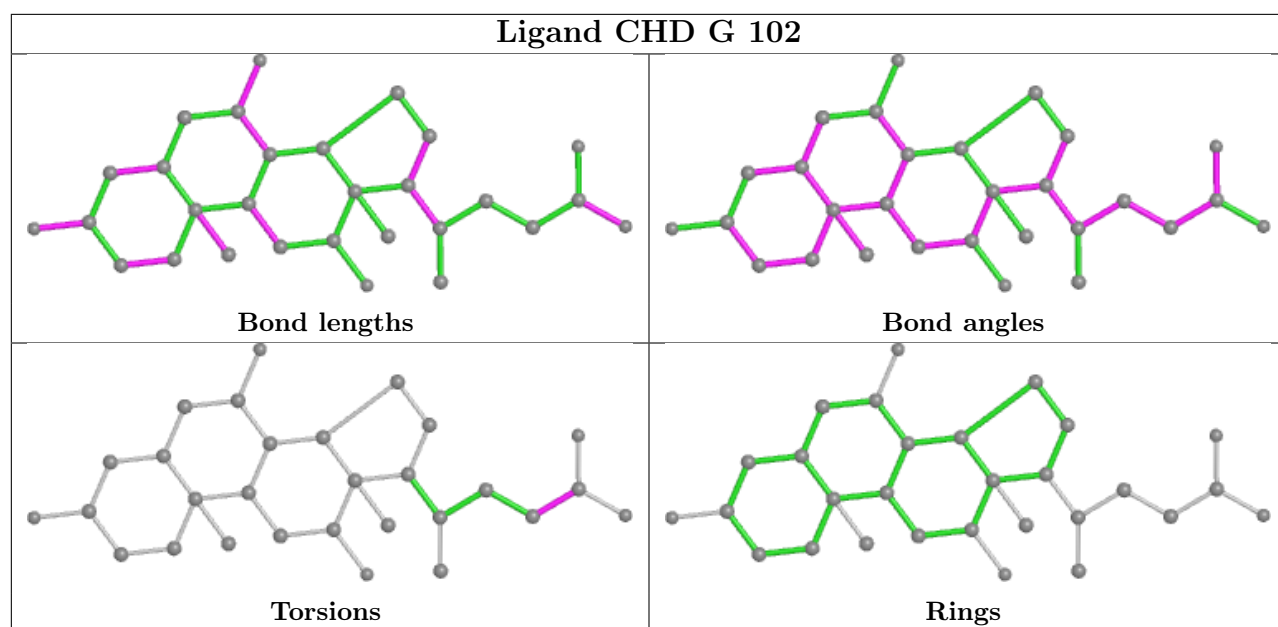


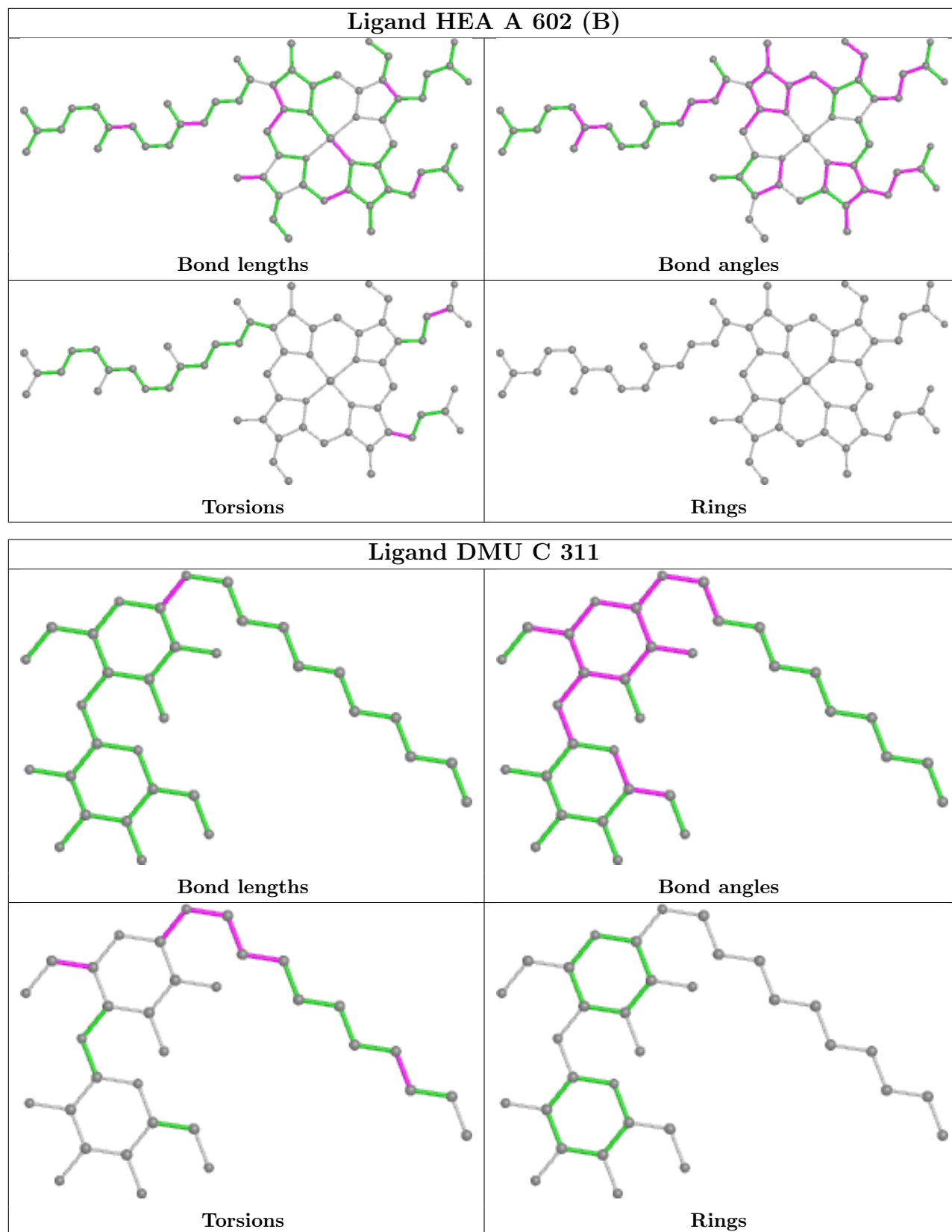


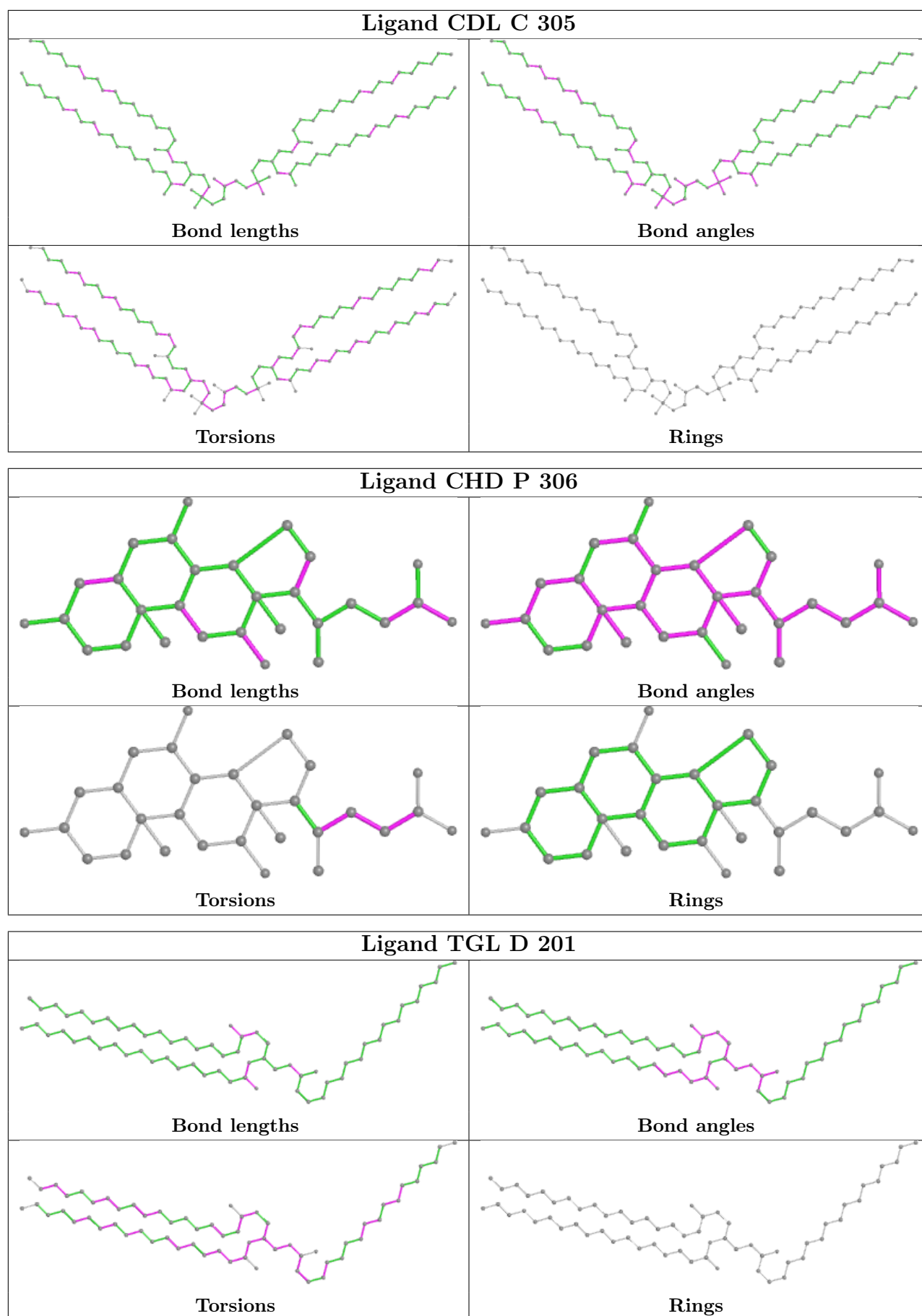


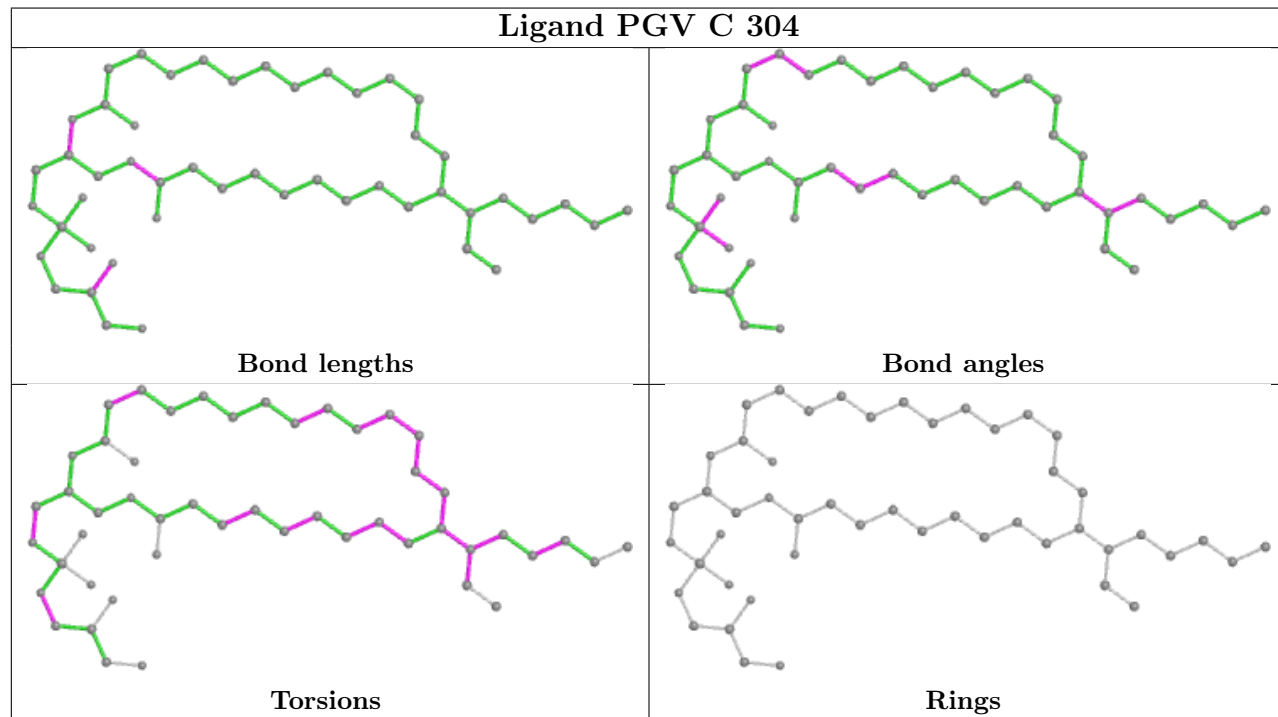
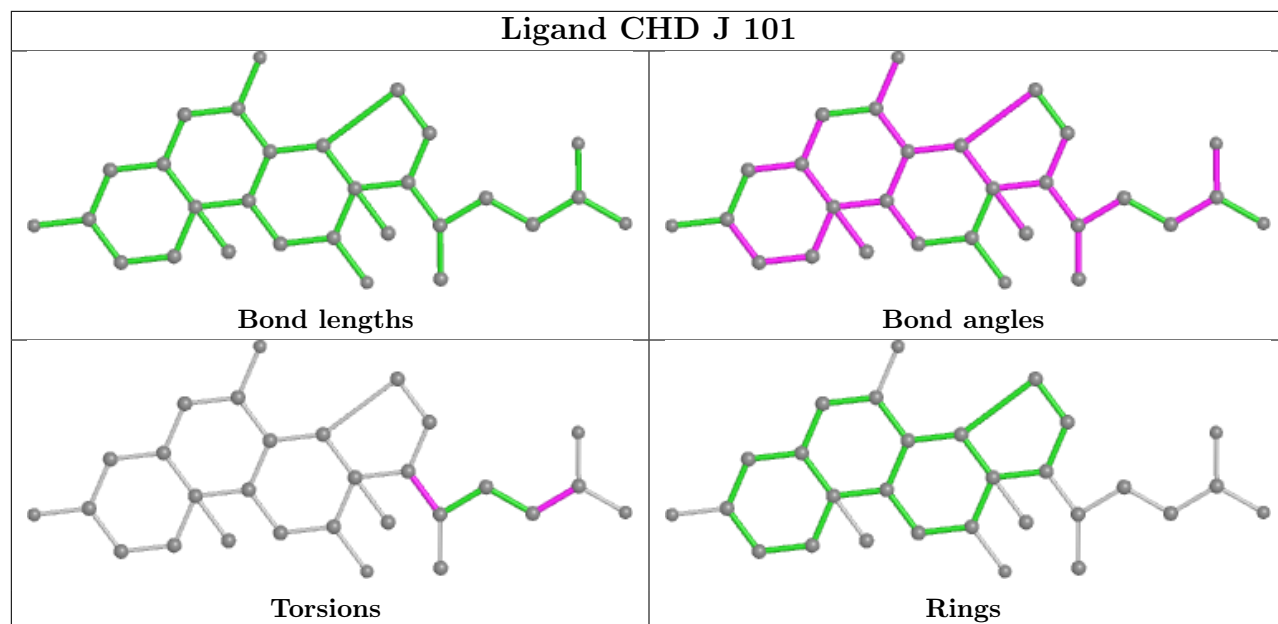


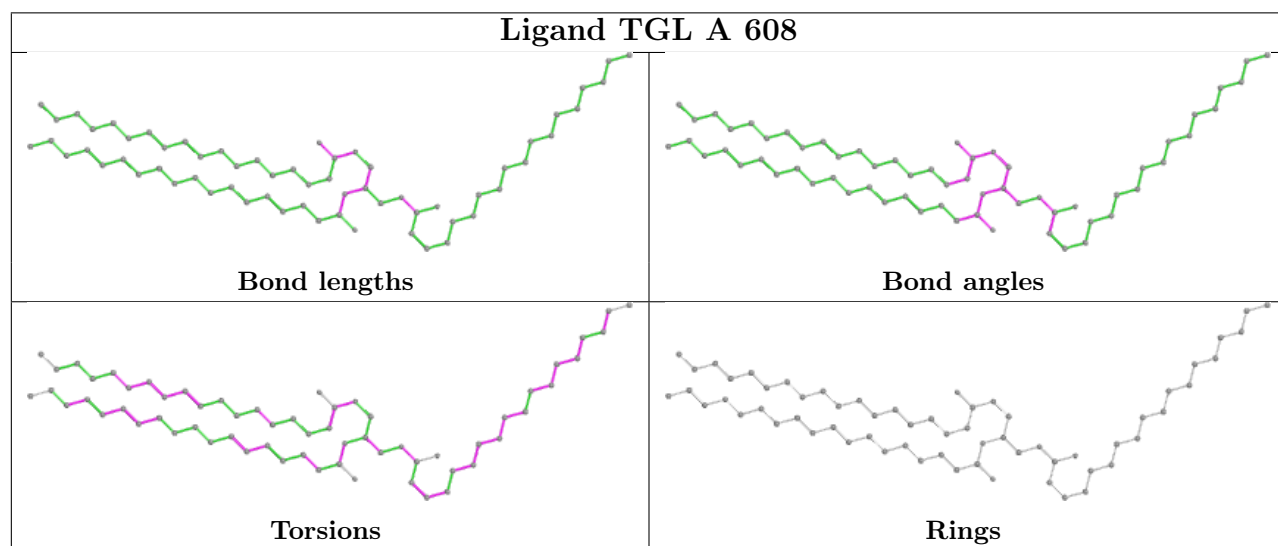
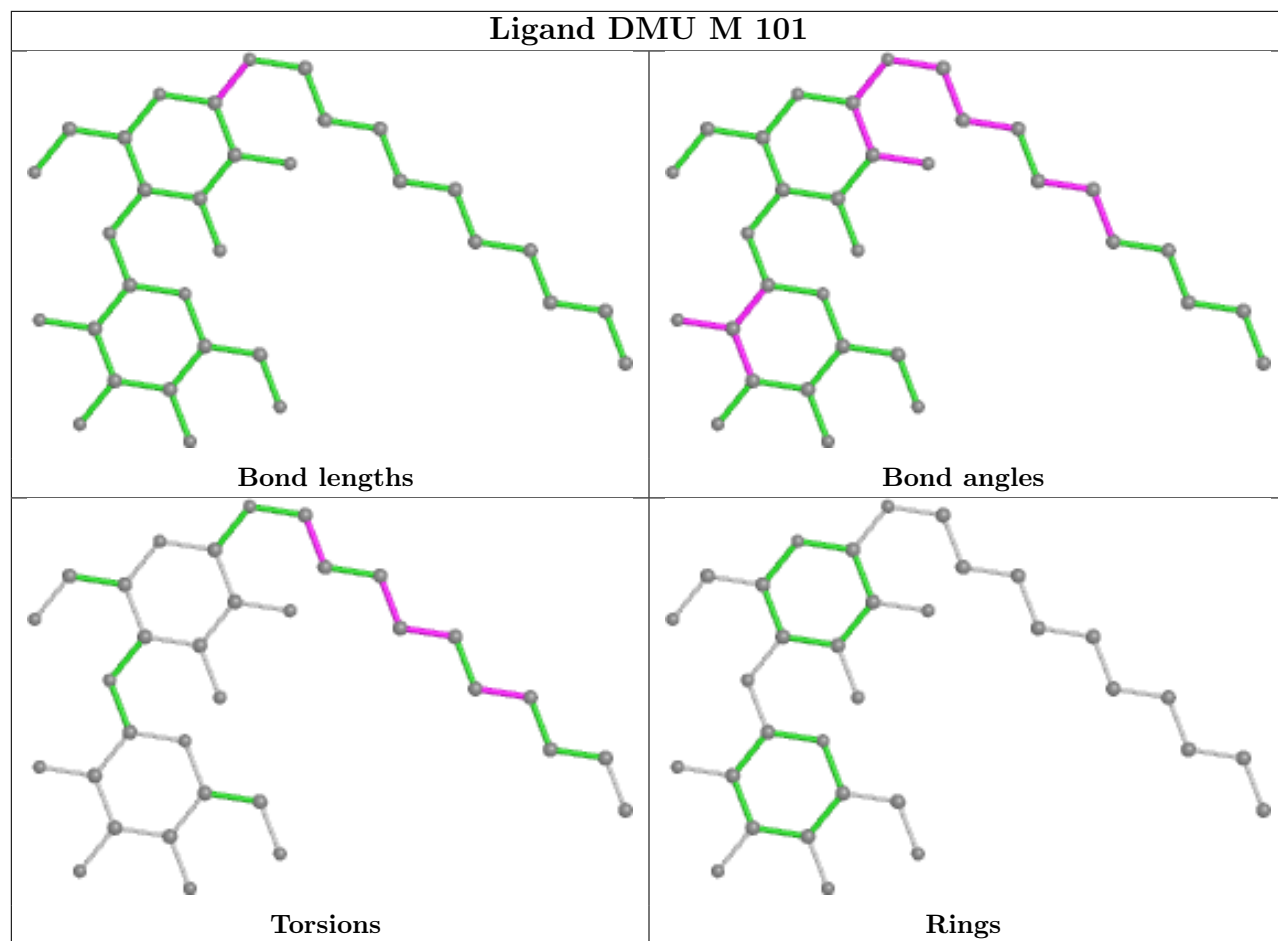


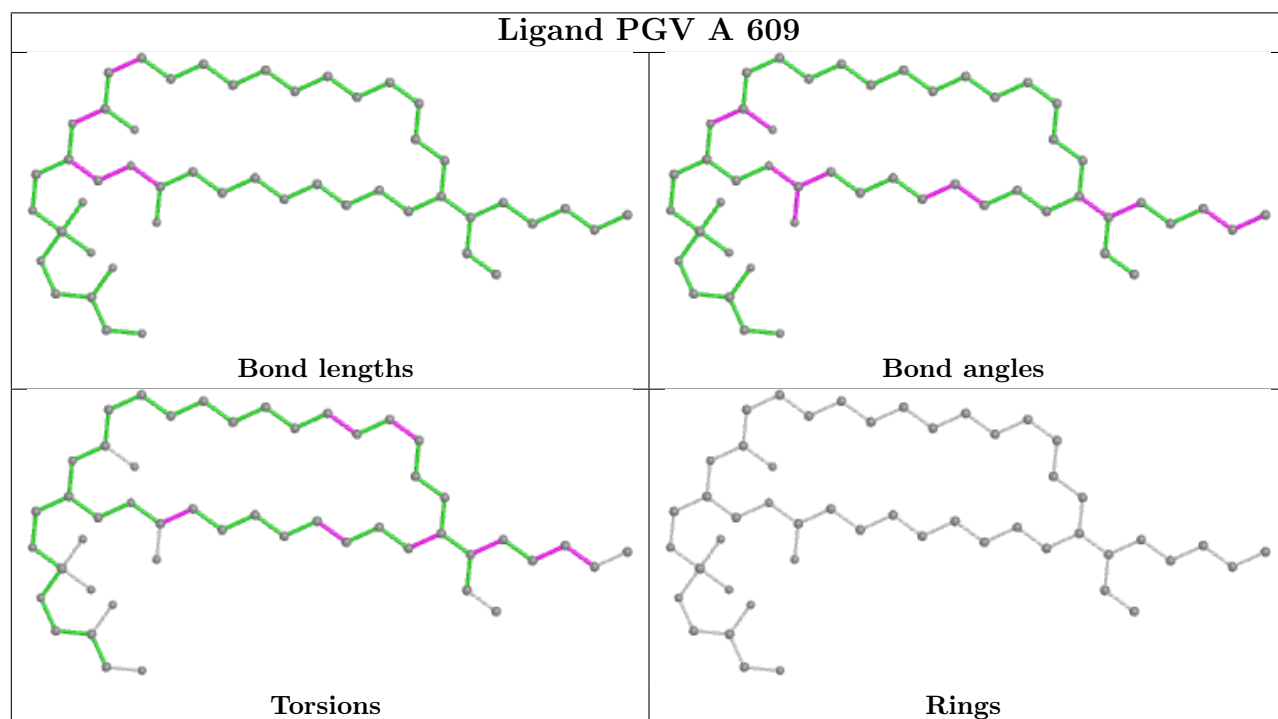
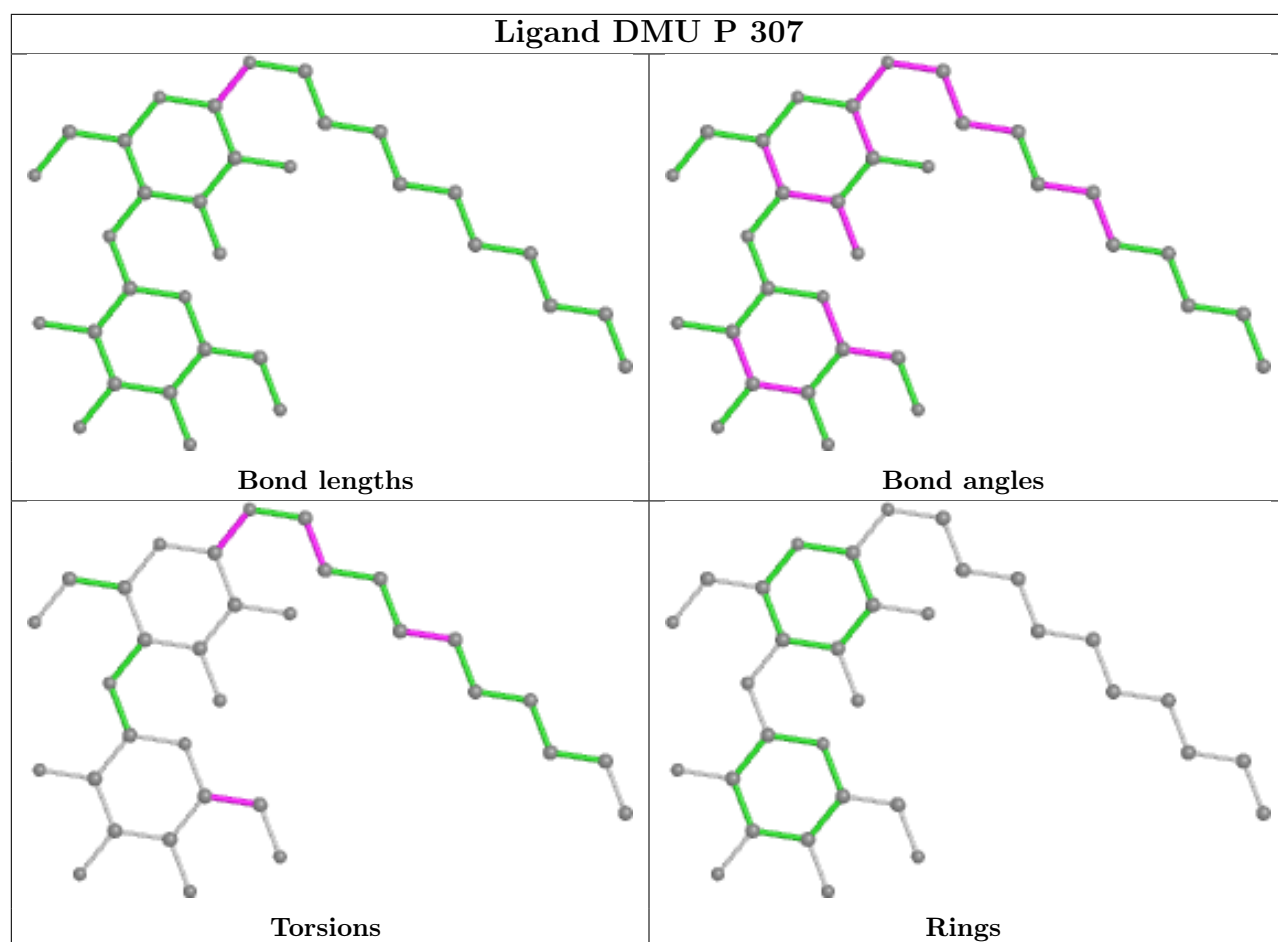


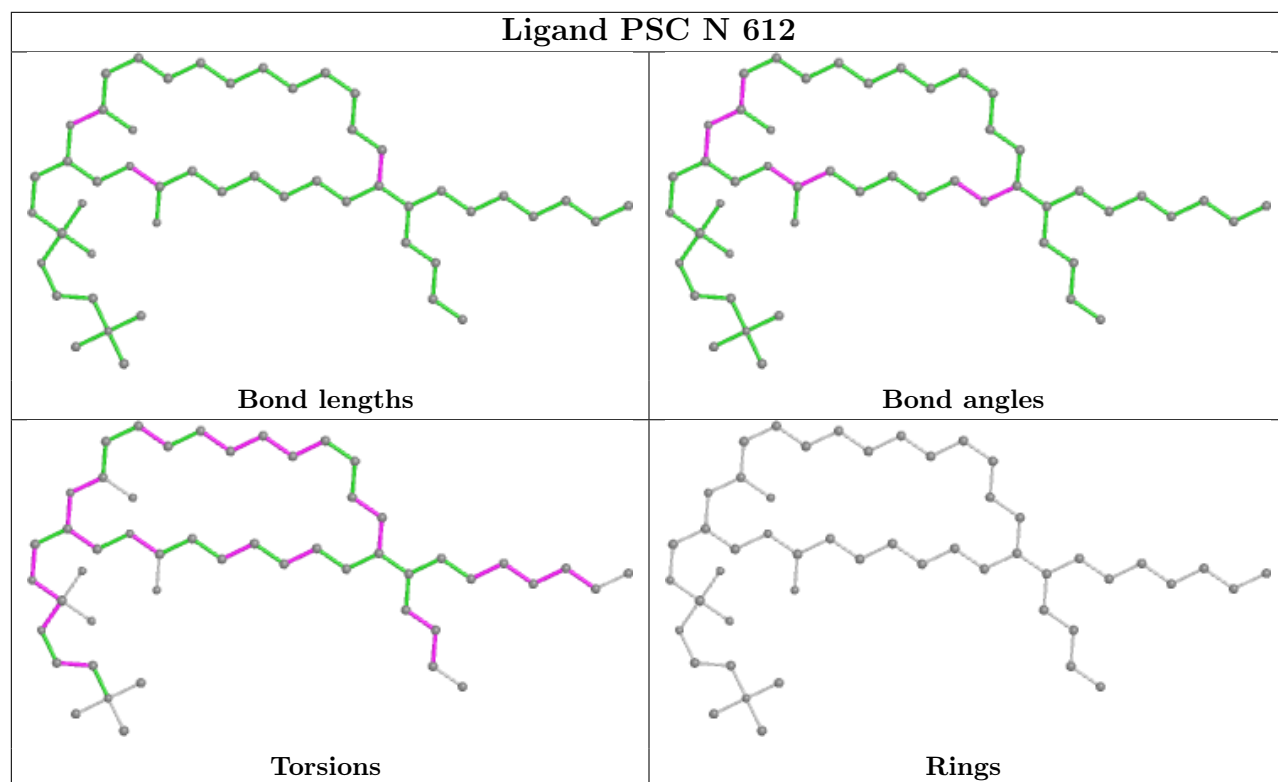
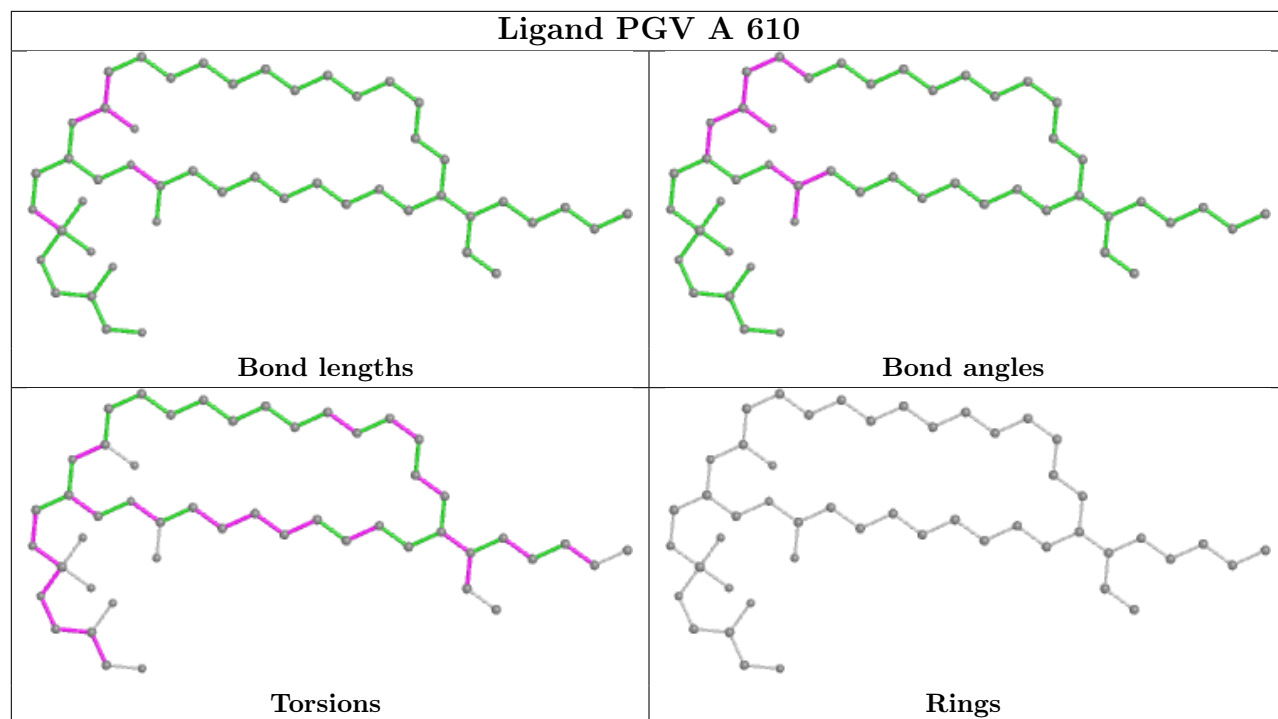


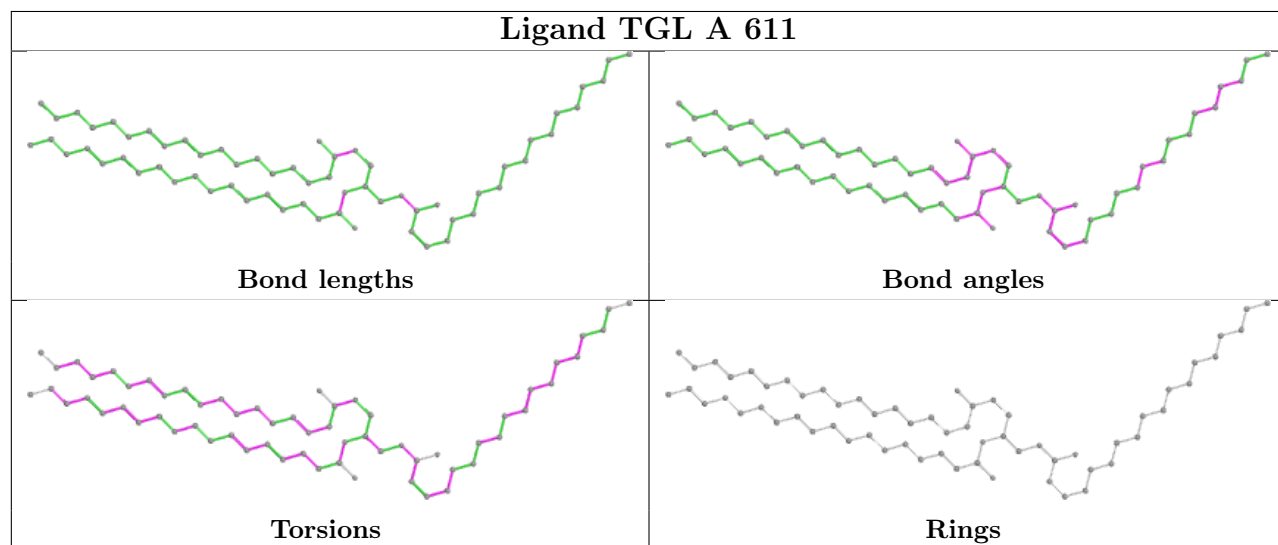
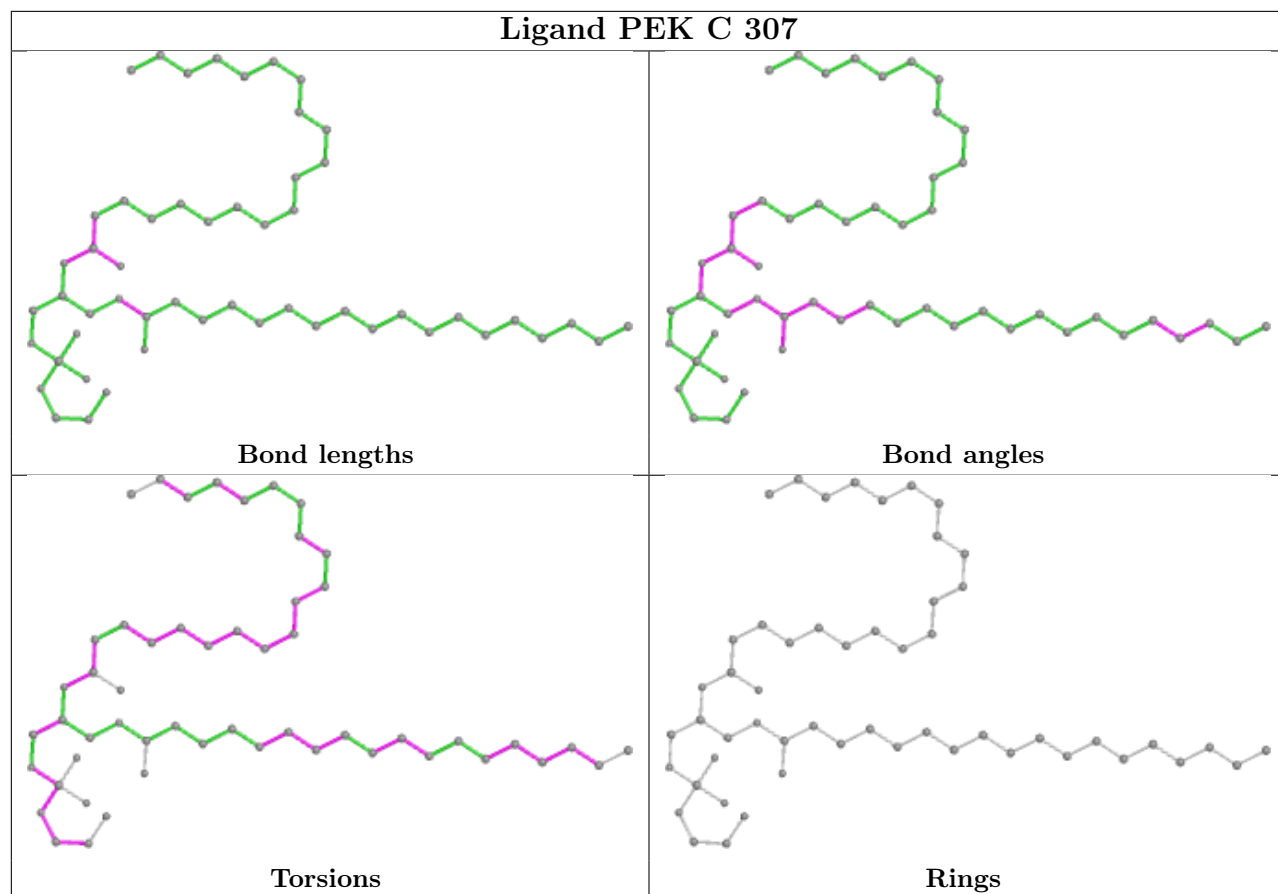


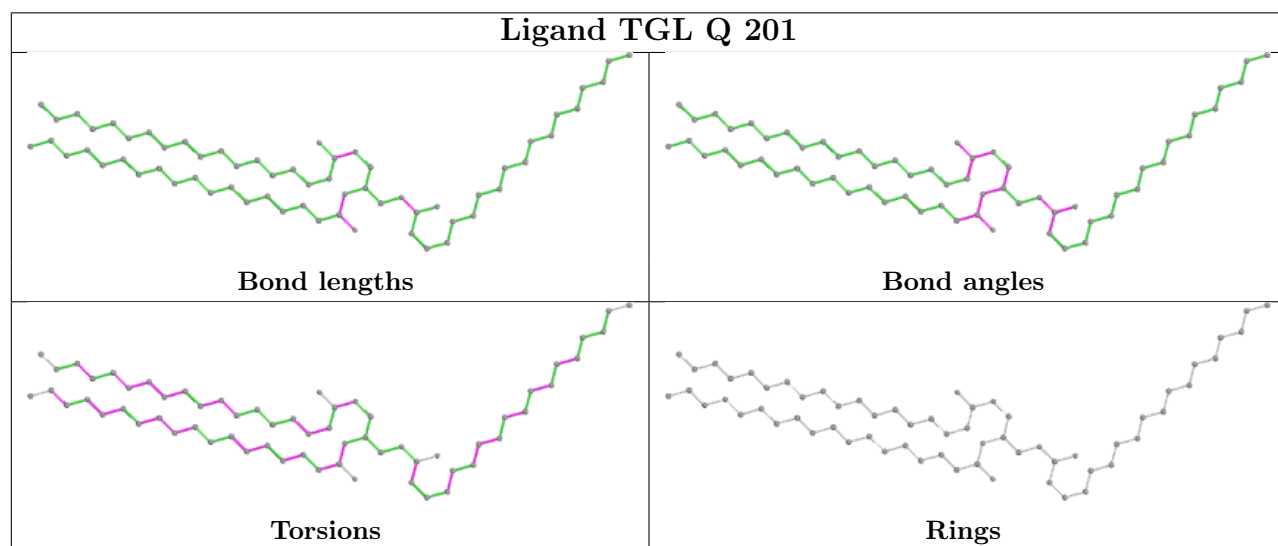
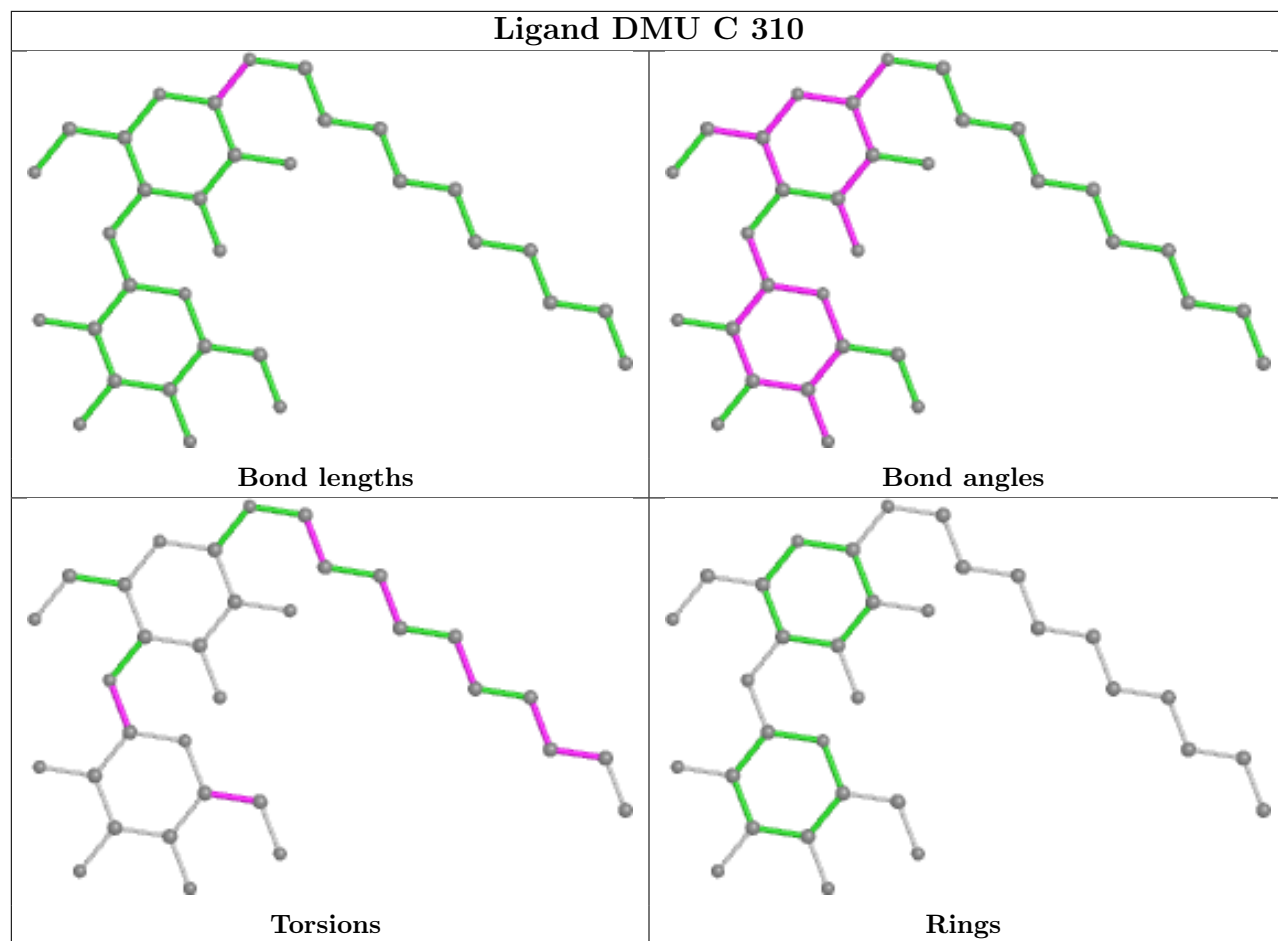


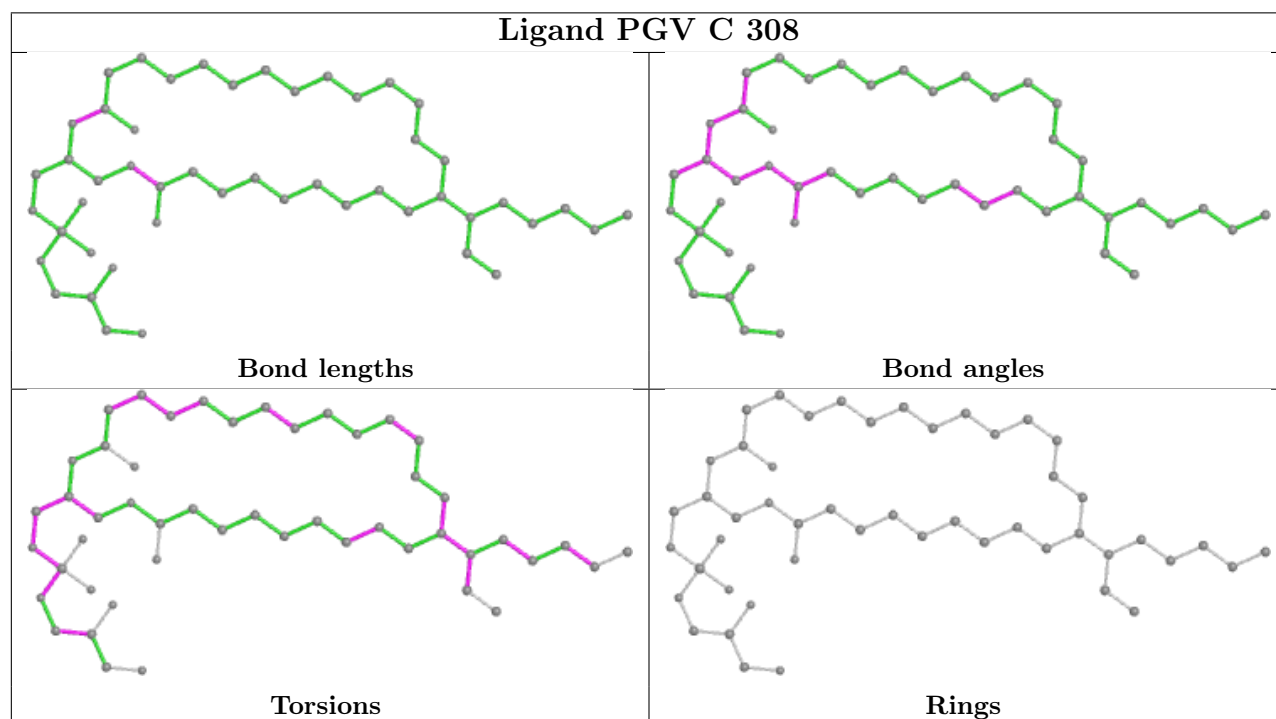
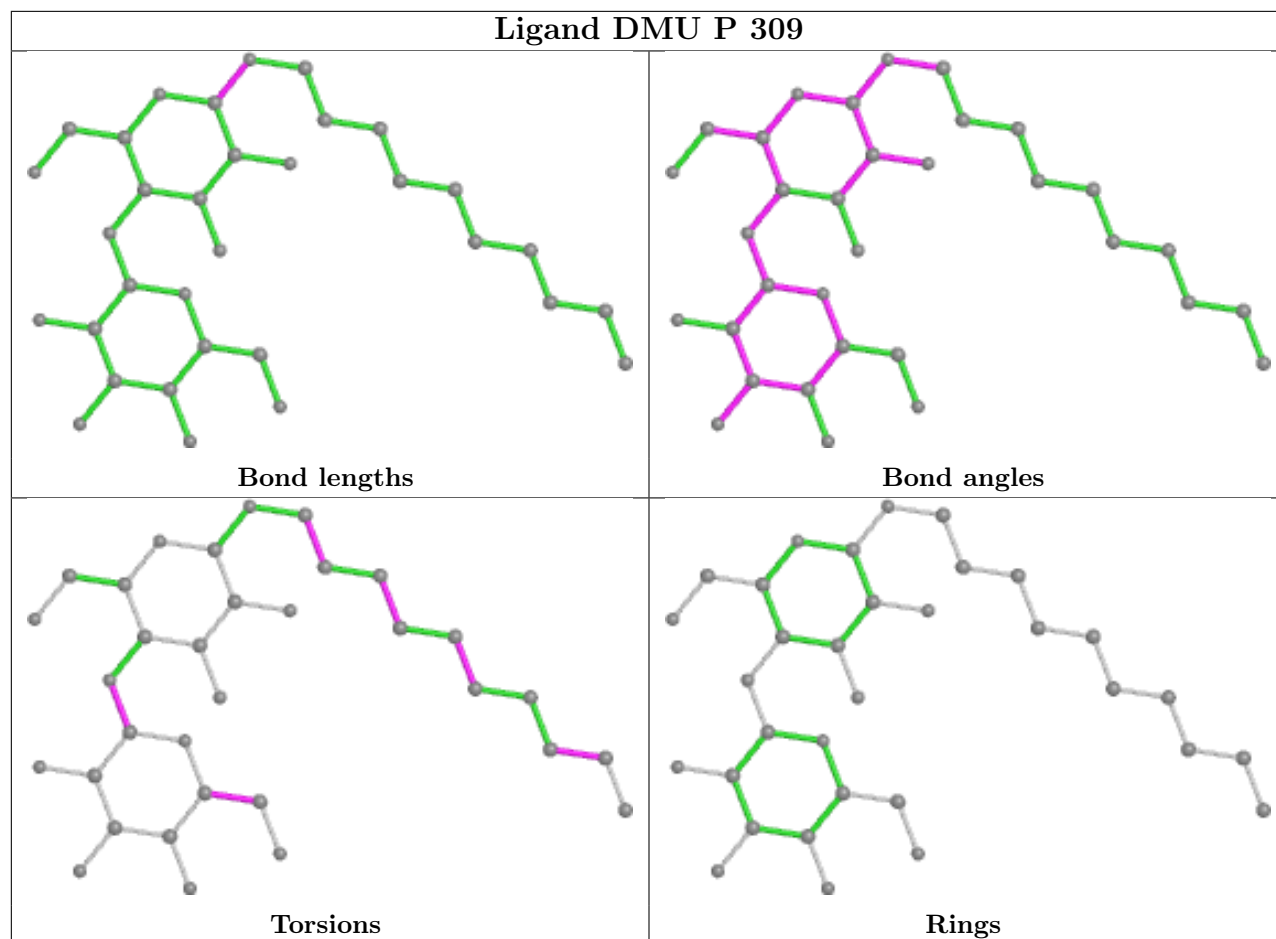


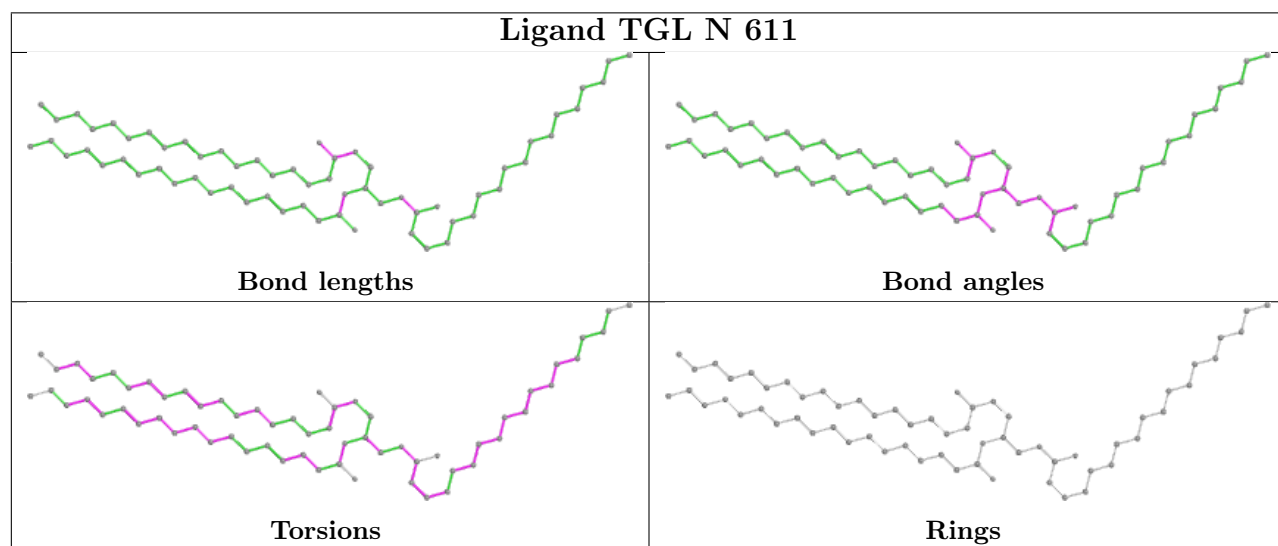
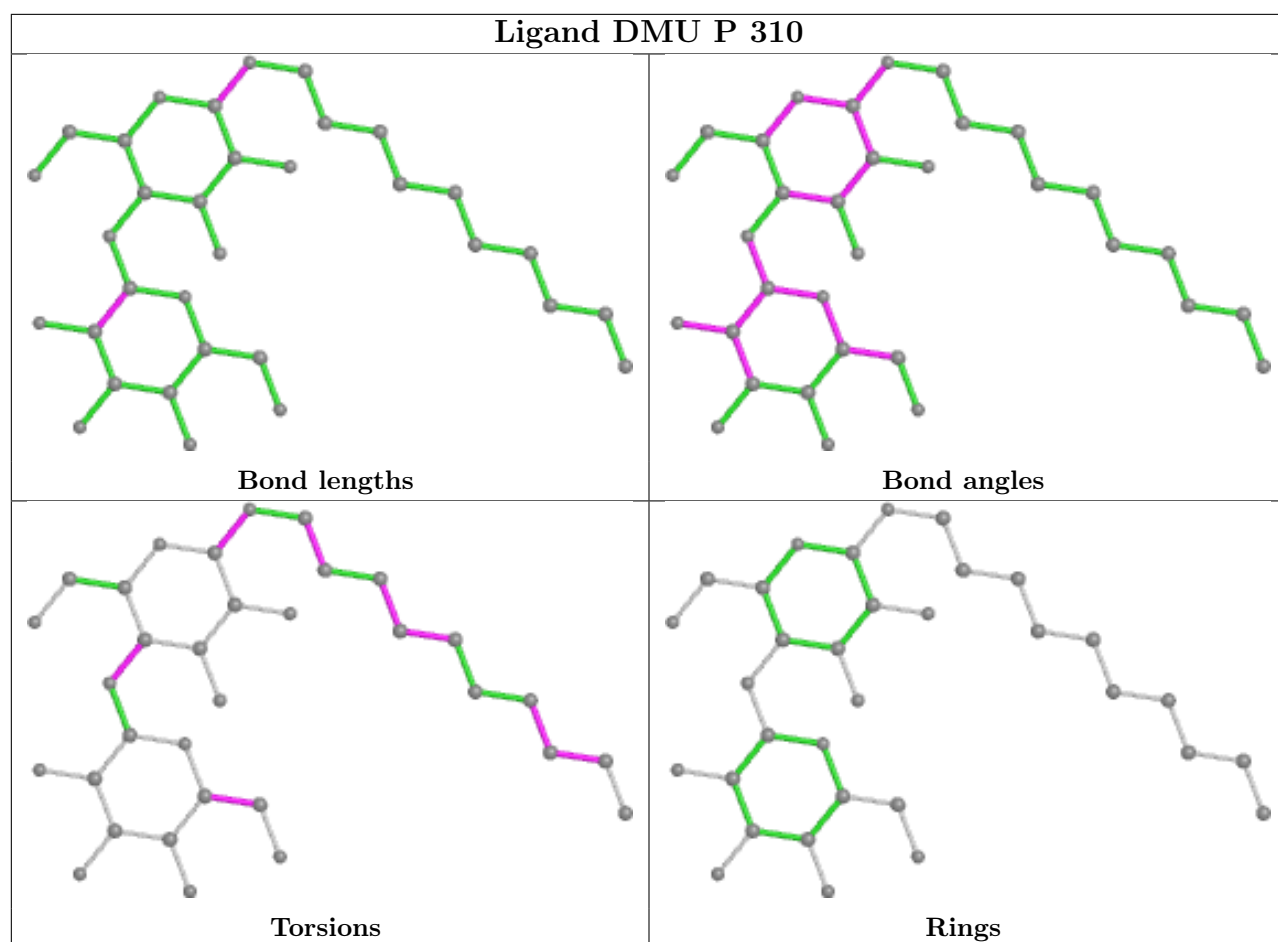


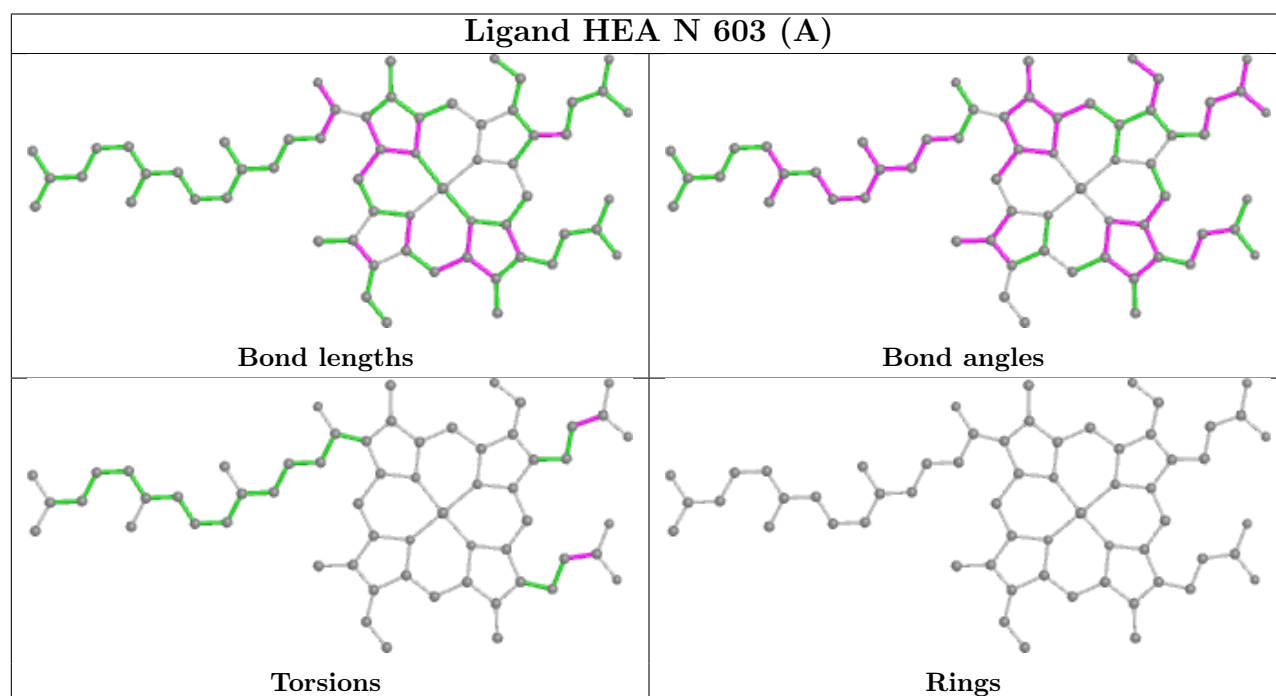
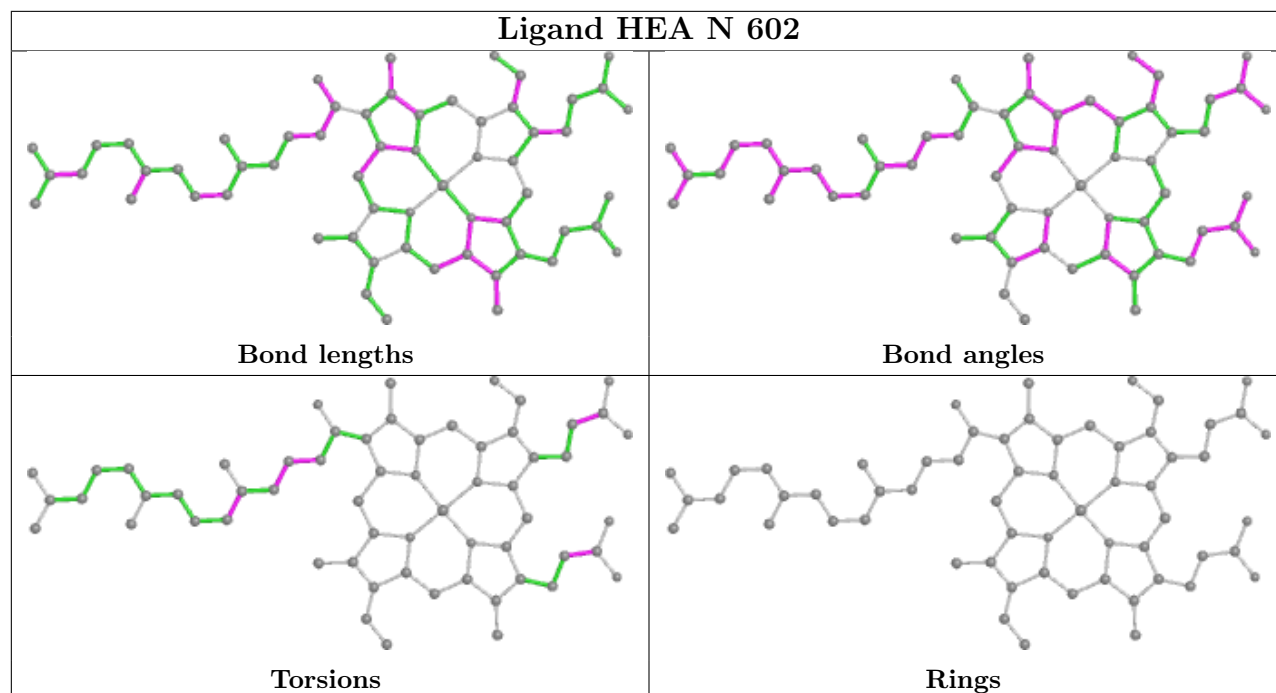


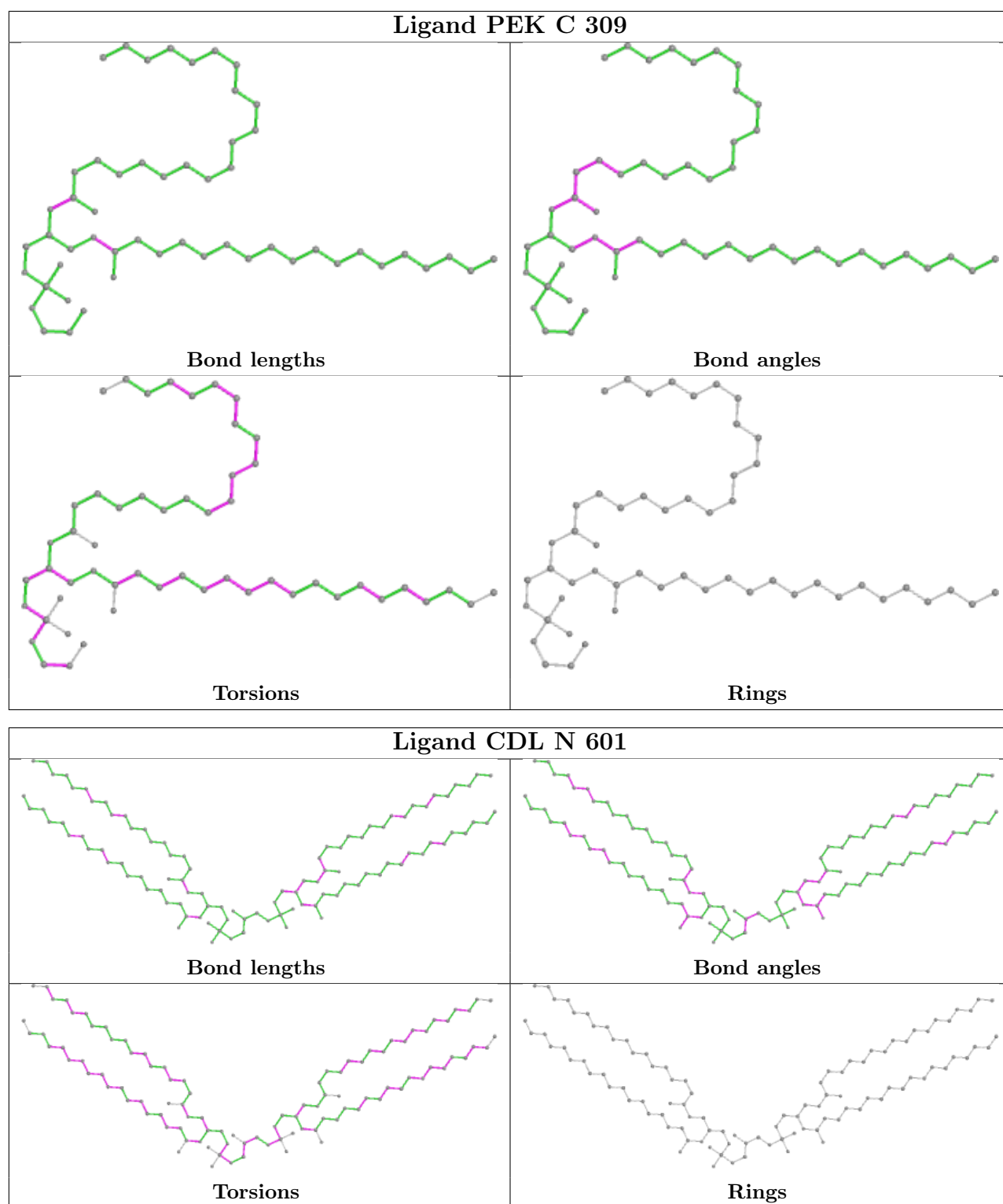












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.05	0 100 100	22, 27, 35, 70	0
1	N	513/514 (99%)	-0.16	1 (0%) 95 95	24, 31, 40, 74	0
2	B	226/227 (99%)	-0.01	7 (3%) 49 49	25, 35, 54, 68	0
2	O	226/227 (99%)	0.01	7 (3%) 49 49	30, 41, 65, 88	0
3	C	259/261 (99%)	-0.11	2 (0%) 86 88	24, 30, 40, 75	0
3	P	259/261 (99%)	-0.16	1 (0%) 92 93	25, 31, 42, 80	0
4	D	144/147 (97%)	-0.23	2 (1%) 75 79	28, 35, 57, 79	0
4	Q	144/147 (97%)	0.51	9 (6%) 20 19	35, 48, 74, 136	0
5	E	105/109 (96%)	-0.25	2 (1%) 66 69	27, 34, 57, 118	0
5	R	105/109 (96%)	-0.24	2 (1%) 66 69	33, 40, 58, 121	0
6	F	98/98 (100%)	0.52	8 (8%) 11 11	27, 37, 90, 148	0
6	S	98/98 (100%)	0.61	8 (8%) 11 11	27, 37, 99, 143	0
7	G	83/85 (97%)	1.01	16 (19%) 1 1	29, 39, 108, 141	0
7	T	83/85 (97%)	0.84	18 (21%) 0 0	28, 39, 101, 131	0
8	H	79/85 (92%)	0.14	3 (3%) 40 40	33, 44, 91, 101	0
8	U	79/85 (92%)	0.14	5 (6%) 20 19	37, 47, 103, 123	0
9	I	72/73 (98%)	0.62	12 (16%) 1 1	33, 44, 83, 90	0
9	V	72/73 (98%)	0.68	10 (13%) 2 2	32, 54, 80, 104	0
10	J	58/59 (98%)	0.41	4 (6%) 16 15	30, 39, 63, 121	0
10	W	58/59 (98%)	0.25	4 (6%) 16 15	33, 43, 69, 127	0
11	K	49/56 (87%)	-0.19	0 100 100	34, 41, 54, 61	0
11	X	49/56 (87%)	0.50	5 (10%) 6 5	43, 50, 70, 81	0
12	L	46/47 (97%)	0.06	1 (2%) 62 63	28, 33, 52, 91	0
12	Y	46/47 (97%)	0.06	1 (2%) 62 63	34, 40, 65, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.17	2 (4%) 31 30	30, 33, 68, 118	0
13	Z	43/46 (93%)	0.22	4 (9%) 8 7	39, 44, 78, 108	0
All	All	3550/3614 (98%)	0.08	134 (3%) 40 40	22, 35, 66, 148	0

The worst 5 of 134 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	23.5
6	F	97	ALA	17.7
4	Q	5	VAL	17.0
6	F	2	SER	16.2
10	J	58	LYS	15.3

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	0.39	0.37	90,110,131,132	0
7	TPO	T	11	11/12	0.64	0.36	94,107,122,130	0
9	SAC	V	1	9/10	0.68	0.41	102,119,126,133	0
9	SAC	I	1	9/10	0.89	0.26	60,74,81,81	0
1	FME	A	1	10/11	0.95	0.10	38,45,74,86	0
1	FME	N	1	10/11	0.96	0.13	42,51,69,79	0
2	FME	B	1	10/11	0.97	0.12	29,32,42,66	0
2	FME	O	1	10/11	0.97	0.10	38,39,48,53	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
22	CHD	W	101	29/29	0.64	0.35	61,91,115,121	0
25	DMU	C	302	33/33	0.67	0.34	30,73,105,109	0
28	PEK	C	307	53/53	0.67	0.21	38,77,135,141	0
27	CDL	T	102	100/100	0.69	0.26	49,89,137,155	0
21	EDO	D	203	4/4	0.69	0.20	63,67,71,74	0
27	CDL	N	601	100/100	0.70	0.29	54,90,129,155	0
19	TGL	Q	201	63/63	0.72	0.18	52,75,93,100	0
24	PSC	B	303	52/52	0.72	0.29	36,84,154,154	0
28	PEK	G	103	53/53	0.72	0.23	48,86,146,153	0
28	PEK	C	309	53/53	0.73	0.33	48,90,151,153	0
28	PEK	P	308	53/53	0.73	0.25	41,72,131,139	0
27	CDL	P	305	100/100	0.74	0.27	36,82,118,137	0
25	DMU	P	310	33/33	0.74	0.23	62,79,108,112	0
24	PSC	N	612	52/52	0.74	0.26	42,83,154,156	0
20	PGV	C	308	51/51	0.76	0.22	44,74,136,146	0
25	DMU	P	307	33/33	0.76	0.31	38,67,118,121	0
22	CHD	J	101	29/29	0.79	0.24	51,75,90,93	0
27	CDL	C	305	100/100	0.79	0.23	35,75,109,115	0
19	TGL	Y	101	63/63	0.79	0.23	45,74,111,138	0
20	PGV	P	302	51/51	0.80	0.26	51,81,132,151	0
21	EDO	A	613	4/4	0.81	0.20	49,53,56,57	0
20	PGV	N	609	51/51	0.82	0.24	43,77,115,131	0
25	DMU	C	310	33/33	0.82	0.25	52,73,102,105	0
21	EDO	G	105	4/4	0.83	0.26	53,56,64,79	0
19	TGL	A	611	63/63	0.83	0.18	34,60,92,110	0
25	DMU	P	309	33/33	0.83	0.19	45,72,92,97	0
21	EDO	N	621	4/4	0.84	0.26	41,51,53,61	0
21	EDO	L	101	4/4	0.84	0.24	55,62,78,81	0
25	DMU	C	311	33/33	0.85	0.18	46,77,99,109	0
20	PGV	A	610	51/51	0.85	0.21	34,75,106,125	0
21	EDO	A	618	4/4	0.85	0.32	51,51,53,63	0
19	TGL	D	201	63/63	0.85	0.18	32,62,89,92	0
21	EDO	N	616	4/4	0.86	0.16	52,54,55,56	0
21	EDO	A	615	4/4	0.86	0.13	53,63,65,70	0
19	TGL	N	611	63/63	0.87	0.17	51,77,97,104	0
22	CHD	C	306	29/29	0.88	0.17	43,49,54,66	0
21	EDO	A	617	4/4	0.88	0.15	40,42,43,44	0
22	CHD	P	306	29/29	0.88	0.18	43,49,52,68	0
25	DMU	Z	101	33/33	0.88	0.13	45,54,70,76	0
21	EDO	D	202	4/4	0.89	0.42	33,38,47,66	0
21	EDO	M	102	4/4	0.89	0.14	60,63,63,69	0
21	EDO	W	102	4/4	0.89	0.33	50,55,66,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
21	EDO	B	305	4/4	0.90	0.19	35,45,48,51	0
21	EDO	N	620	4/4	0.90	0.16	47,49,54,58	0
19	TGL	A	608	63/63	0.90	0.15	40,75,93,101	0
26	UNX	C	303	1/1	0.90	0.14	35,35,35,35	0
21	EDO	A	619	4/4	0.90	0.32	44,60,74,82	0
21	EDO	Y	102	4/4	0.90	0.26	61,65,66,67	0
21	EDO	N	617	4/4	0.91	0.17	52,55,58,61	0
25	DMU	M	101	33/33	0.92	0.08	38,44,58,67	0
21	EDO	A	614	4/4	0.92	0.10	30,31,32,37	0
21	EDO	B	306	4/4	0.93	0.19	50,51,55,57	0
21	EDO	F	104	4/4	0.94	0.11	36,36,38,42	0
21	EDO	A	620	4/4	0.94	0.15	52,56,57,64	0
21	EDO	B	304	4/4	0.94	0.25	46,59,60,85	0
21	EDO	E	203	4/4	0.94	0.08	42,42,50,55	0
21	EDO	P	312	4/4	0.94	0.12	33,36,43,49	0
21	EDO	N	613	4/4	0.95	0.10	33,34,37,41	0
21	EDO	R	201	4/4	0.95	0.08	44,45,45,45	0
21	EDO	S	103	4/4	0.95	0.07	39,42,45,47	0
21	EDO	S	104	4/4	0.95	0.17	40,52,60,65	0
21	EDO	B	307	4/4	0.95	0.11	29,30,35,37	0
21	EDO	E	202	4/4	0.95	0.08	38,40,44,47	0
21	EDO	N	619	4/4	0.95	0.13	40,43,46,49	0
21	EDO	A	616	4/4	0.95	0.12	22,27,28,42	0
22	CHD	P	301	29/29	0.95	0.07	28,32,36,39	0
21	EDO	F	103	4/4	0.95	0.09	37,41,42,52	0
28	PEK	T	101	53/53	0.95	0.13	29,49,85,92	0
21	EDO	O	302	4/4	0.96	0.10	38,39,40,42	0
21	EDO	T	103	4/4	0.96	0.09	36,37,42,44	0
18	AZI	N	607[B]	3/3	0.96	0.10	23,23,27,28	3
21	EDO	N	614	4/4	0.96	0.12	29,33,36,36	0
22	CHD	C	301	29/29	0.96	0.08	27,30,34,36	0
21	EDO	N	618	4/4	0.96	0.13	37,40,43,45	0
20	PGV	C	304	51/51	0.97	0.12	27,34,86,96	0
21	EDO	N	615	4/4	0.97	0.10	41,53,57,60	0
20	PGV	N	610	51/51	0.97	0.11	27,35,68,72	0
18	AZI	A	606[B]	3/3	0.97	0.11	22,22,23,24	3
22	CHD	B	301	29/29	0.97	0.09	25,30,33,41	0
28	PEK	G	101	53/53	0.97	0.12	29,46,79,95	0
21	EDO	A	612	4/4	0.97	0.12	37,41,41,53	0
21	EDO	C	312	4/4	0.97	0.40	41,43,72,85	0
22	CHD	G	102	29/29	0.97	0.09	28,30,36,39	0
18	AZI	N	608[A]	3/3	0.98	0.16	29,29,38,40	3

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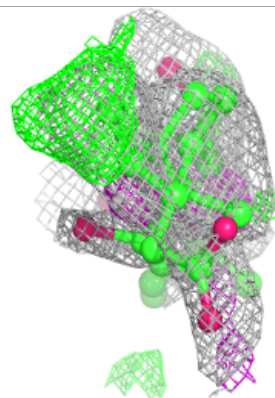
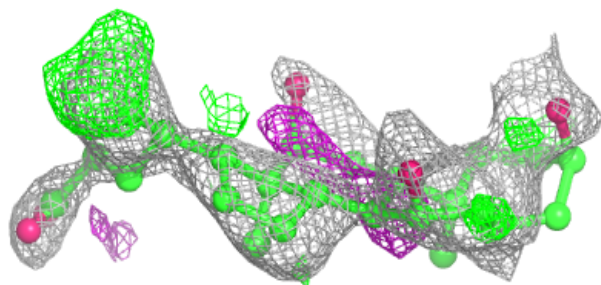
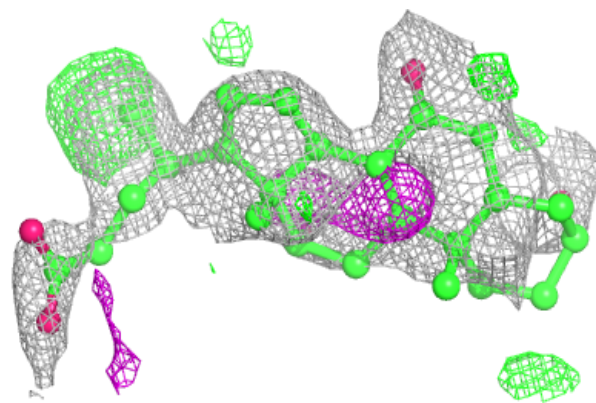
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
18	AZI	N	608[B]	3/3	0.98	0.16	24,24,26,26	3
14	HEA	A	602[B]	60/60	0.98	0.11	21,25,34,37	60
20	PGV	P	304	51/51	0.98	0.11	26,36,79,89	0
14	HEA	N	602	60/60	0.98	0.10	26,30,49,52	0
14	HEA	N	603[A]	60/60	0.98	0.11	21,25,28,30	60
26	UNX	P	303	1/1	0.98	0.06	32,32,32,32	0
14	HEA	N	603[B]	60/60	0.98	0.11	24,29,42,46	60
21	EDO	E	201	4/4	0.98	0.10	40,41,43,44	0
16	MG	N	605	1/1	0.98	0.06	31,31,31,31	0
17	NA	A	605	1/1	0.98	0.06	30,30,30,30	0
20	PGV	A	609	51/51	0.98	0.11	25,33,67,71	0
21	EDO	P	311	4/4	0.98	0.10	39,42,43,46	0
17	NA	N	606	1/1	0.98	0.05	35,35,35,35	0
21	EDO	G	104	4/4	0.98	0.10	34,37,38,41	0
14	HEA	A	601	60/60	0.98	0.10	21,24,48,50	0
14	HEA	A	602[A]	60/60	0.98	0.11	18,22,26,28	60
21	EDO	F	102	4/4	0.99	0.11	27,27,28,30	0
16	MG	A	604	1/1	0.99	0.09	26,26,26,26	0
18	AZI	A	607[A]	3/3	0.99	0.12	20,20,24,27	3
18	AZI	A	607[B]	3/3	0.99	0.12	23,23,24,29	3
21	EDO	S	102	4/4	0.99	0.07	29,29,30,30	0
29	ZN	F	101	1/1	0.99	0.12	31,31,31,31	0
29	ZN	S	101	1/1	0.99	0.13	33,33,33,33	0
15	CU	N	604	1/1	1.00	0.16	30,30,30,30	0
15	CU	A	603	1/1	1.00	0.15	26,26,26,26	0
23	CUA	B	302	2/2	1.00	0.15	27,27,27,28	0
23	CUA	O	301	2/2	1.00	0.12	32,32,32,32	0

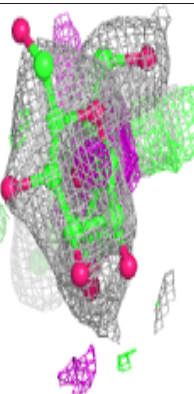
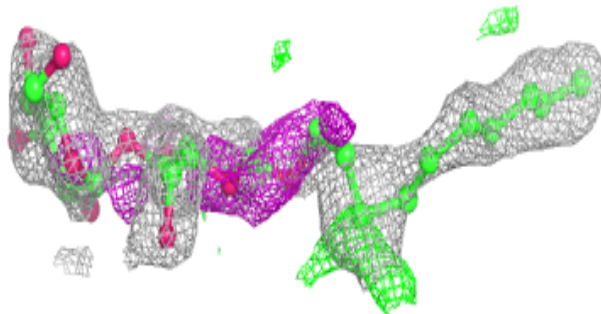
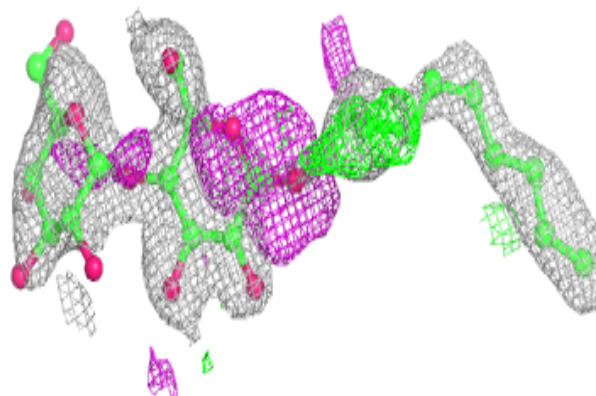
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

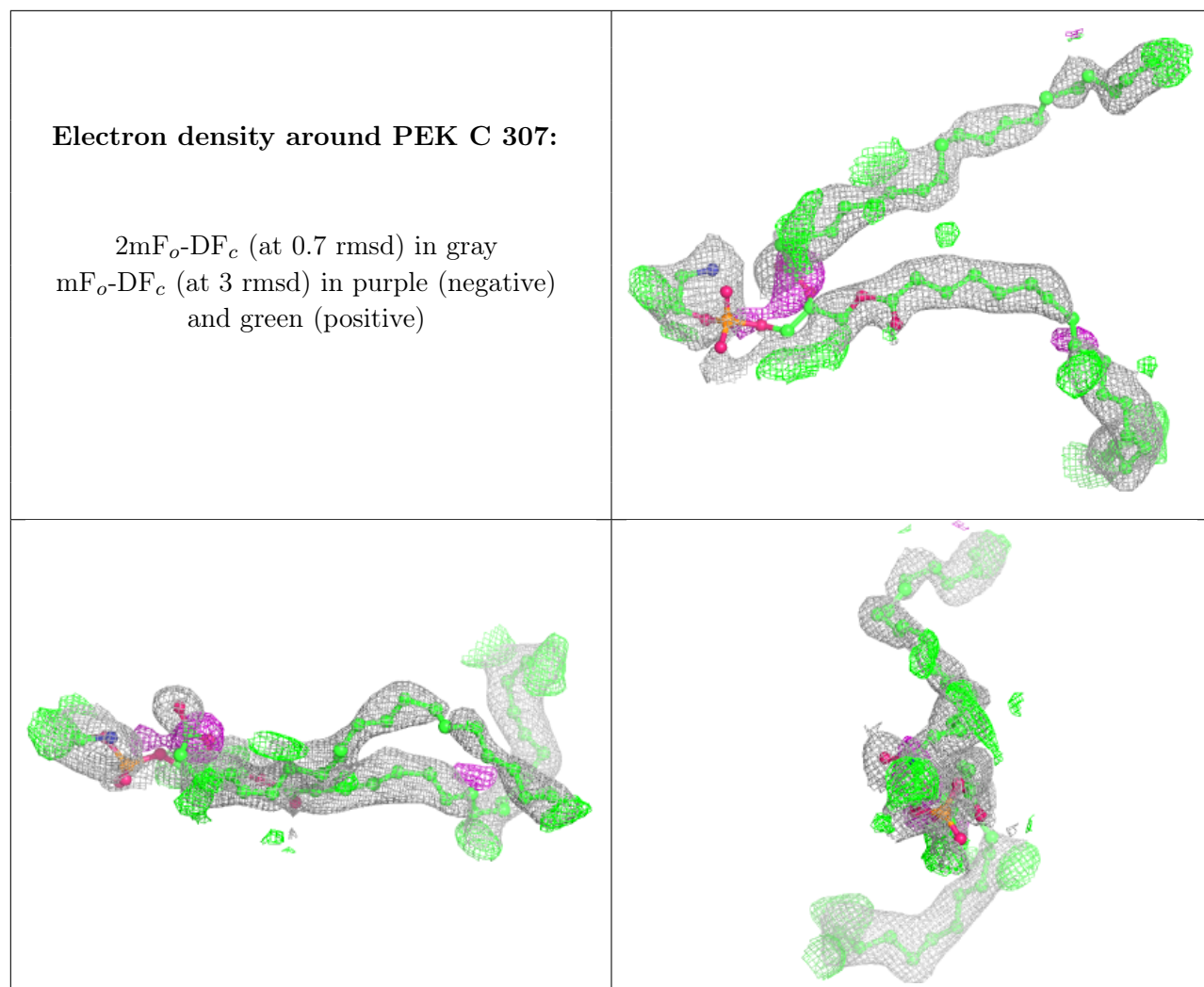
Electron density around CHD W 101:

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

**Electron density around DMU C 302:**

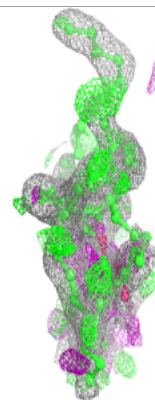
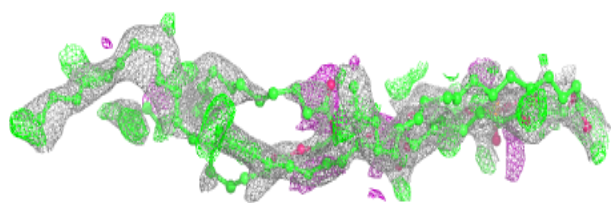
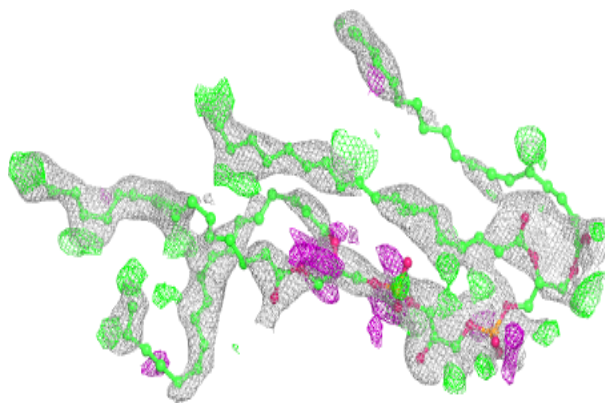
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



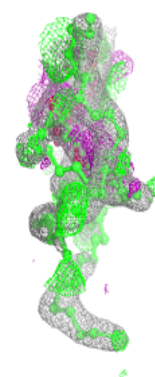
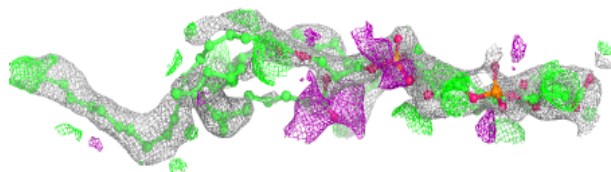
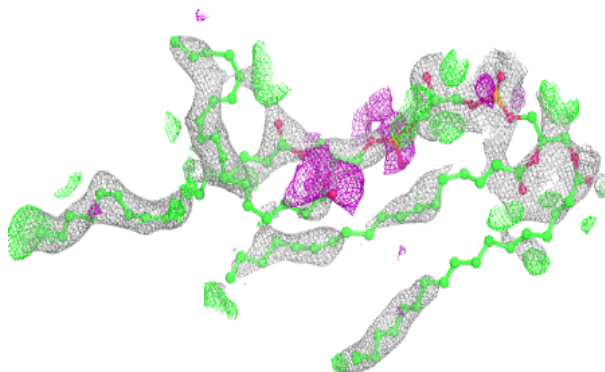


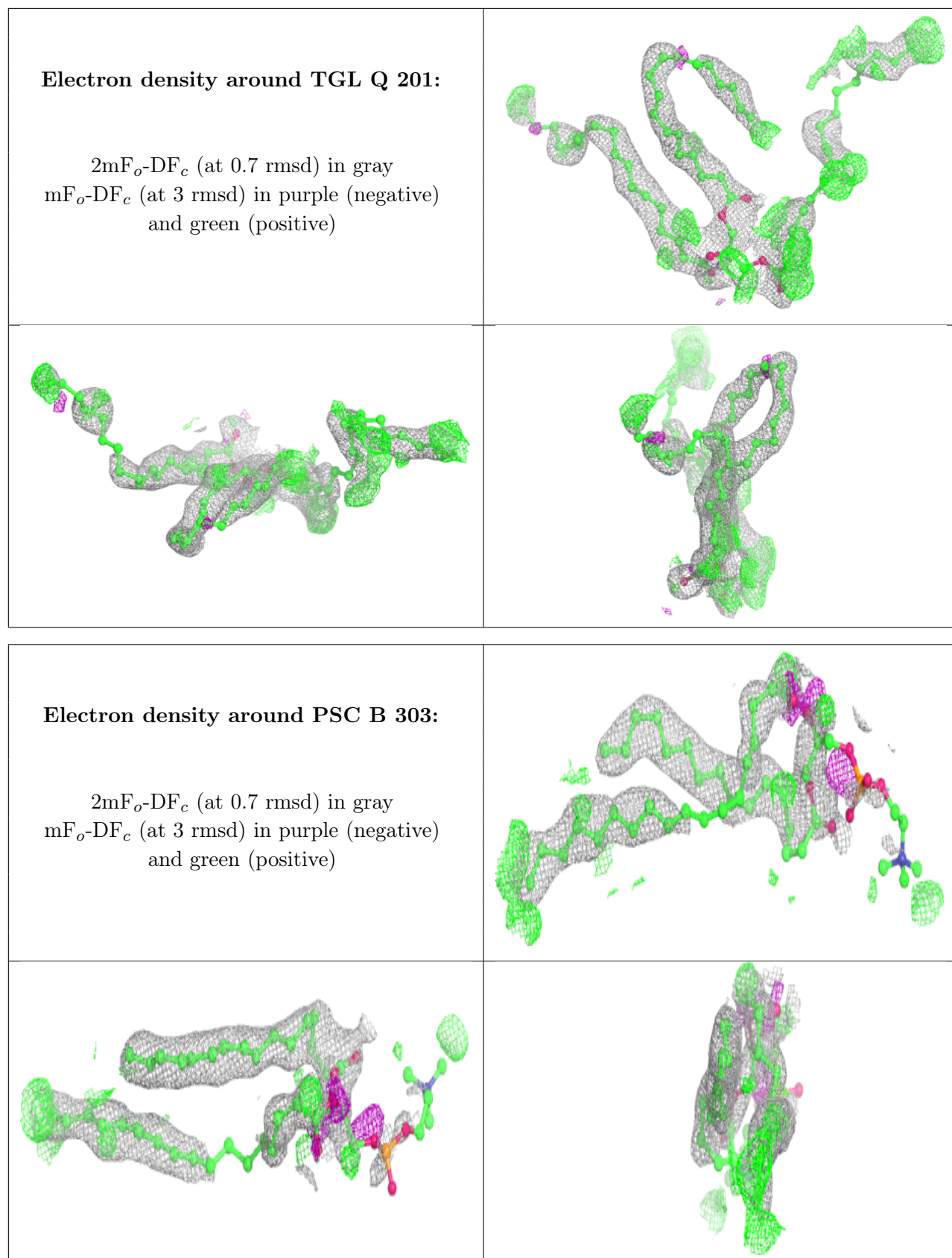
Electron density around CDL T 102:

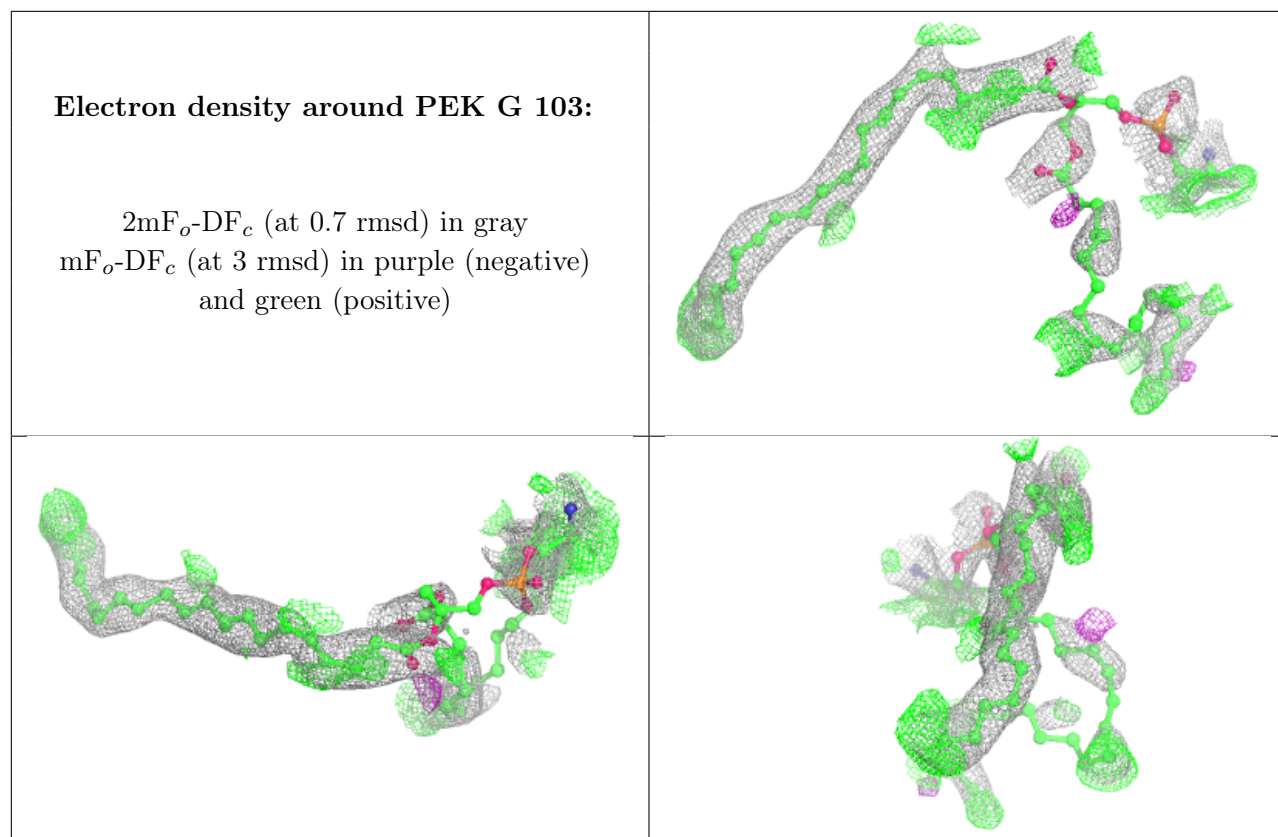
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CDL N 601:**

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

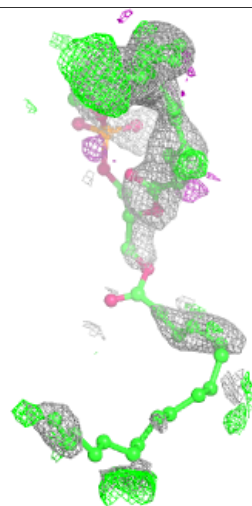
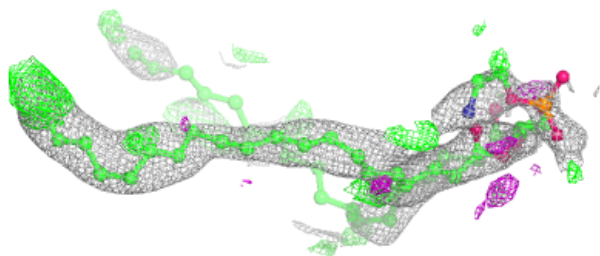
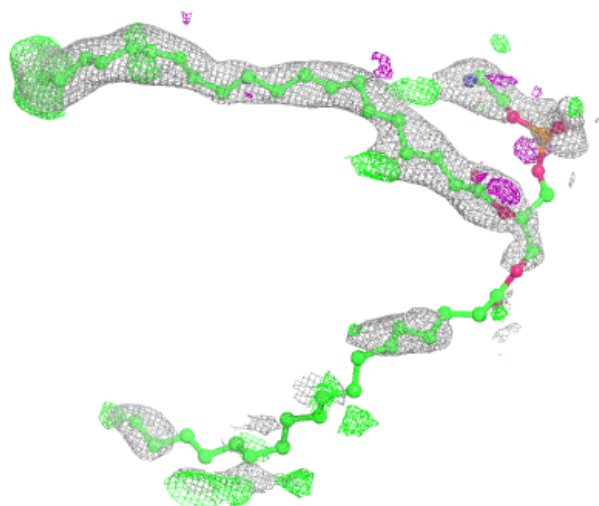


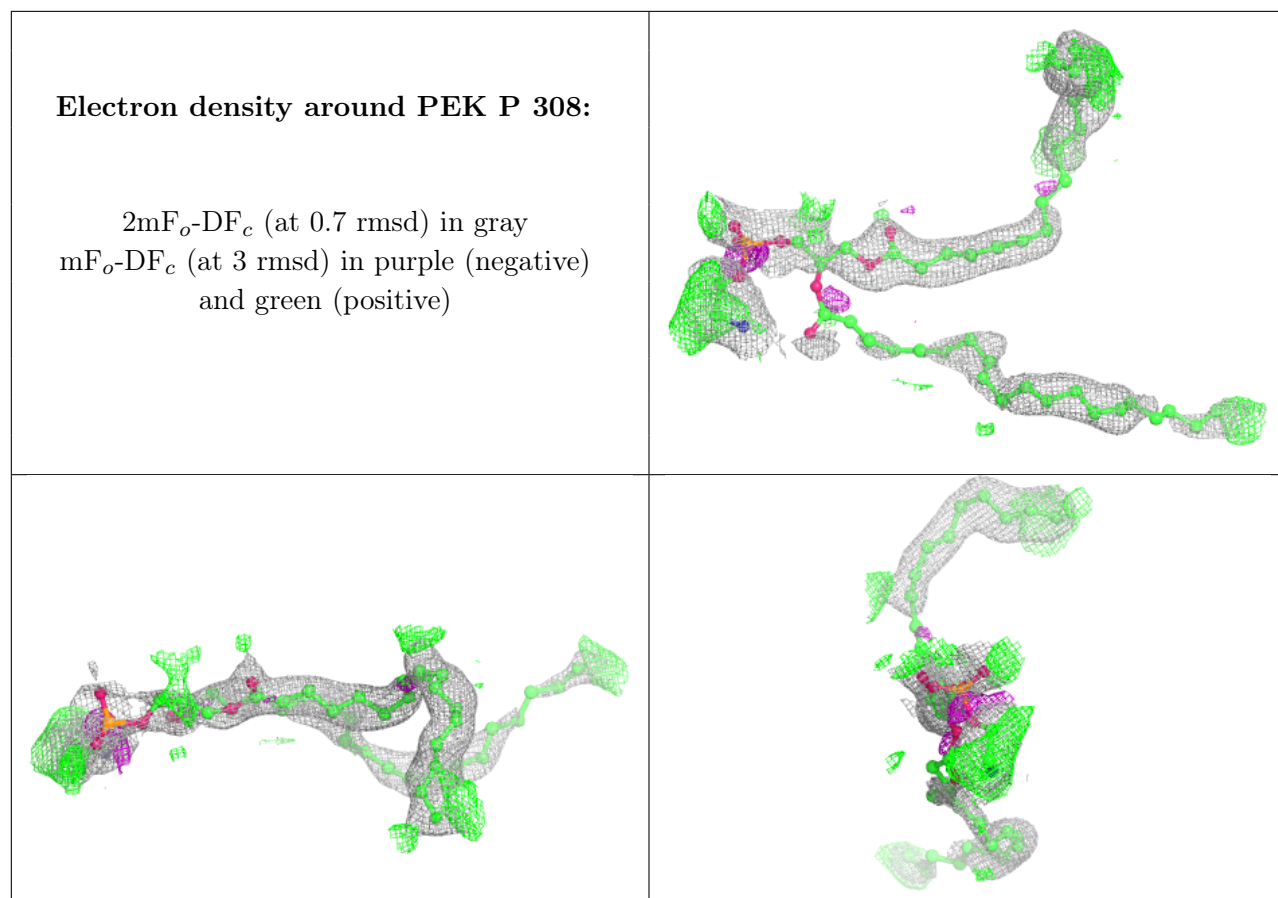




Electron density around PEK C 309:

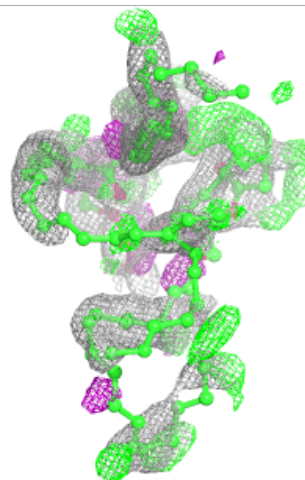
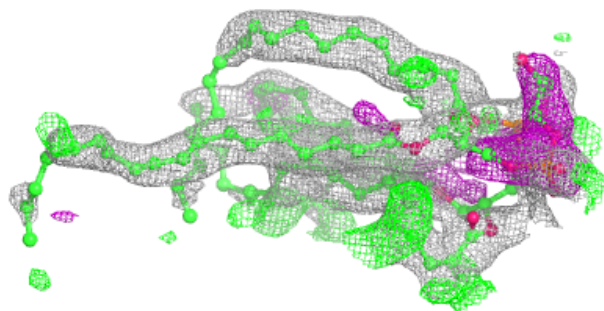
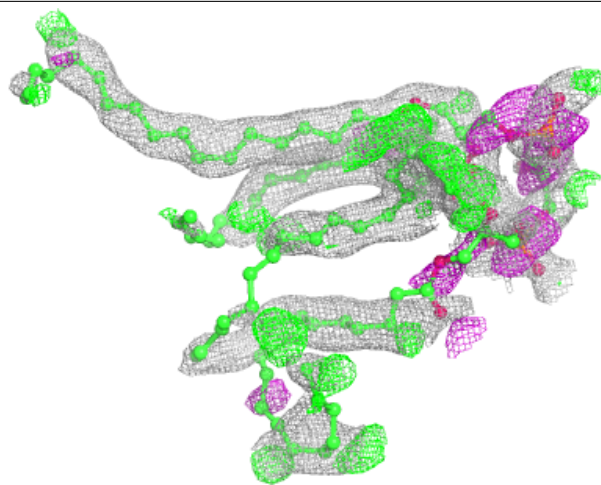
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





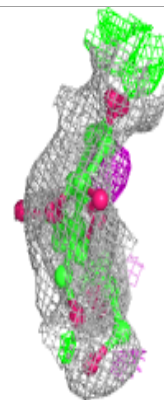
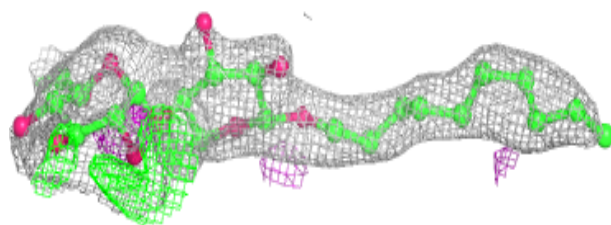
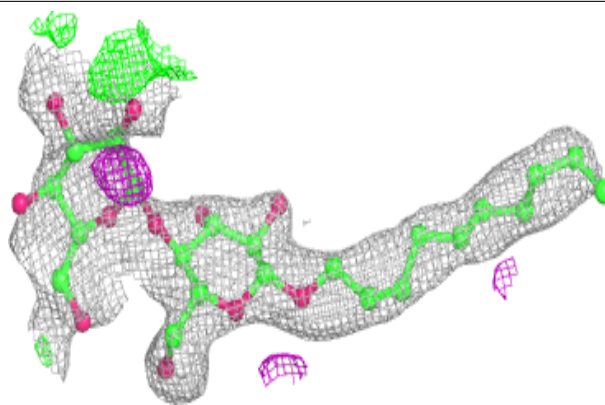
Electron density around CDL P 305:

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

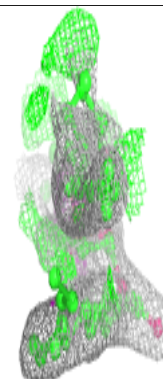
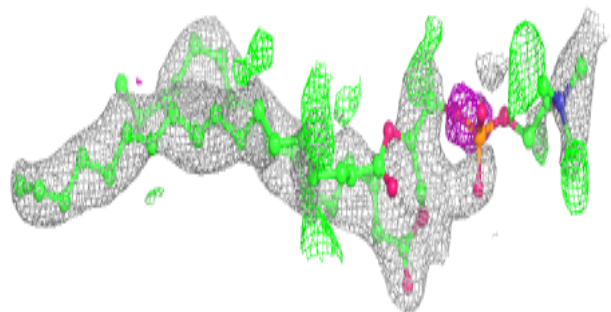
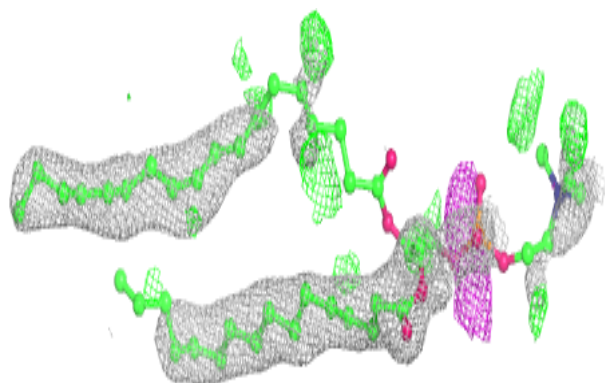


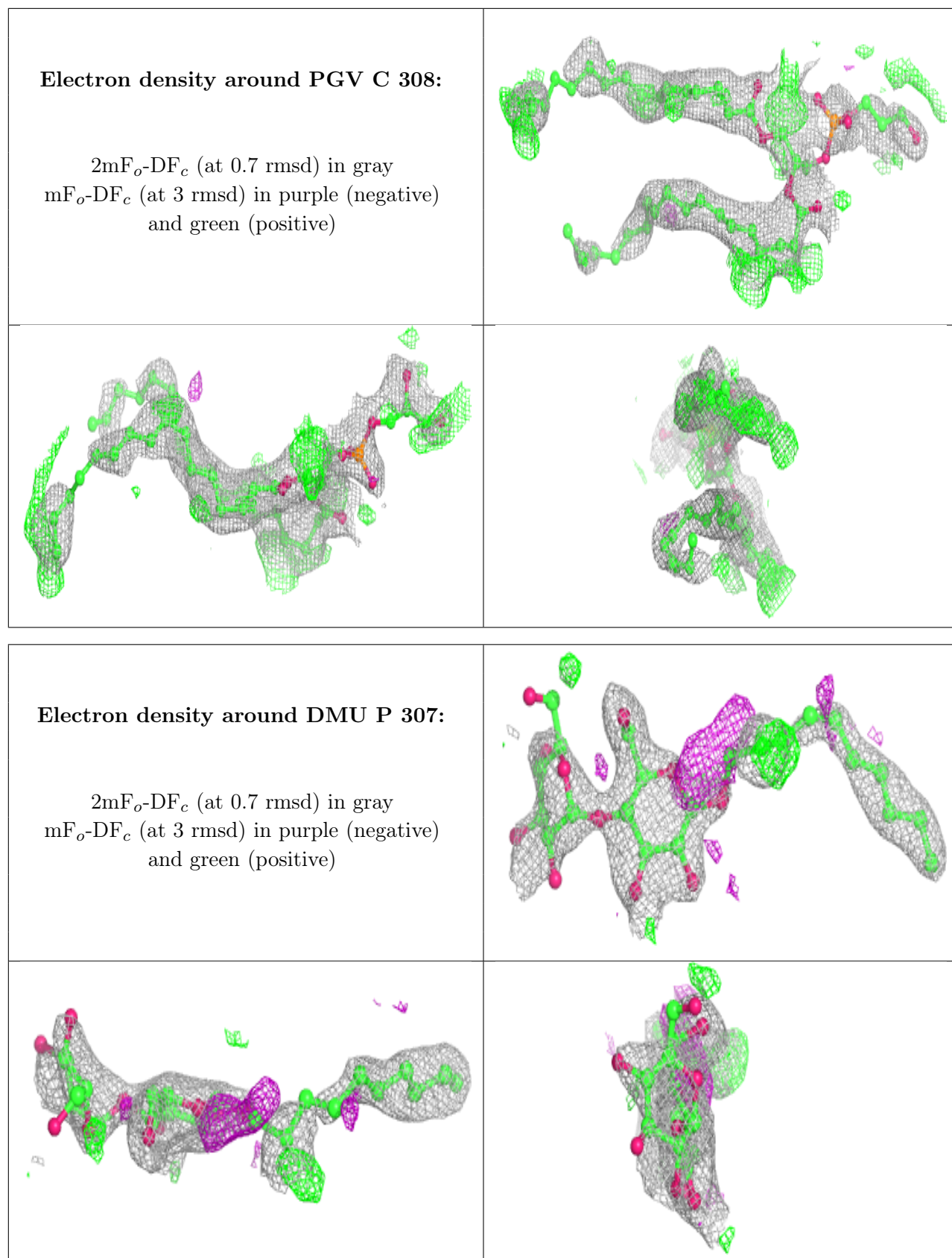
Electron density around DMU P 310:

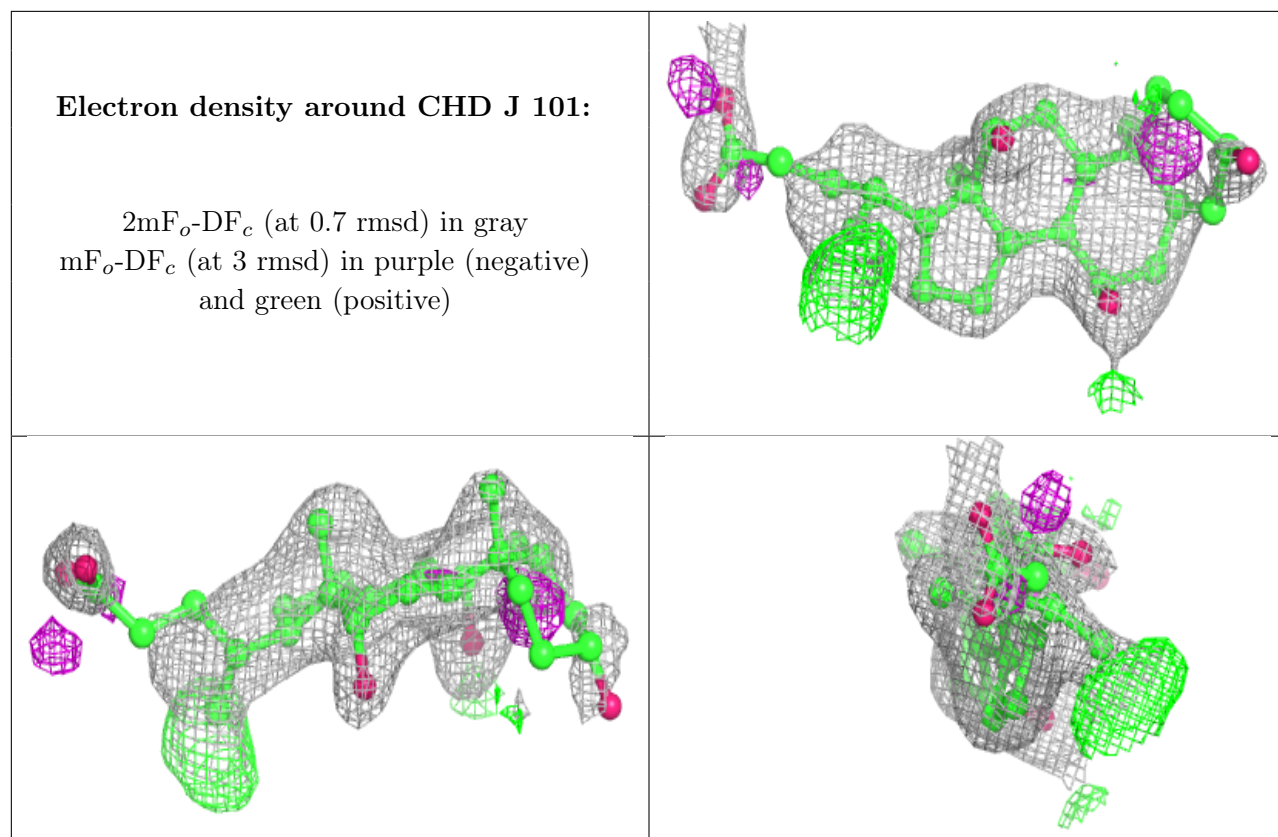
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PSC N 612:**

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

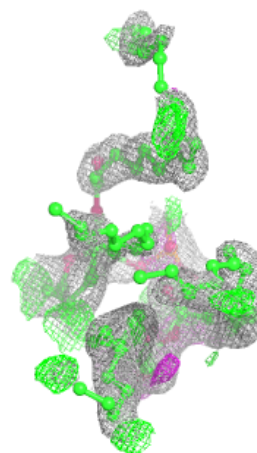
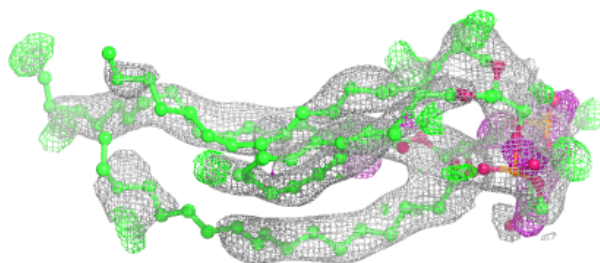
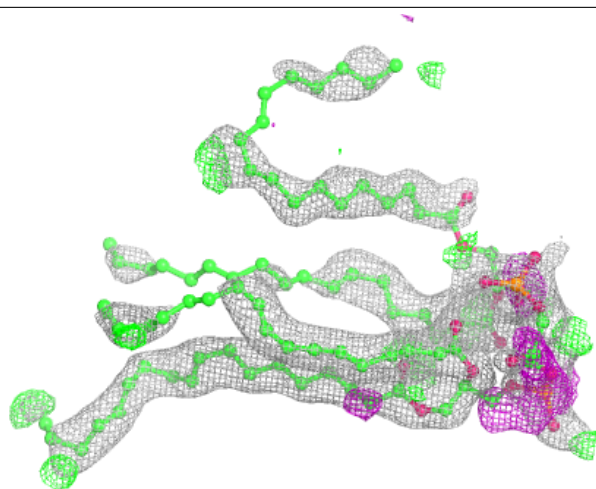






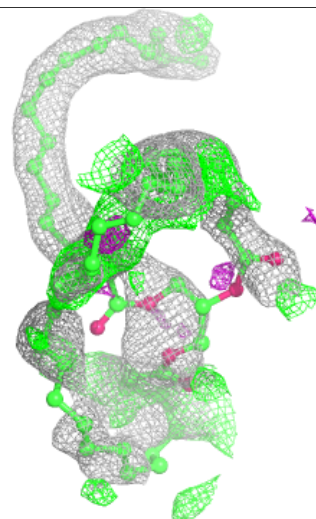
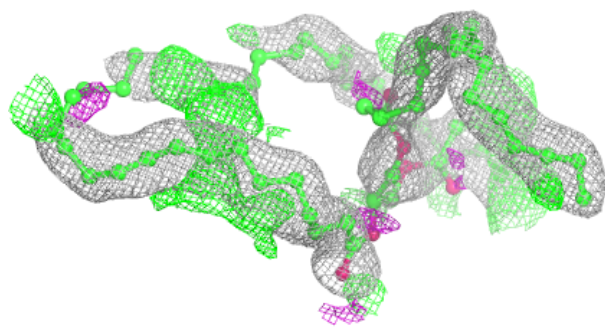
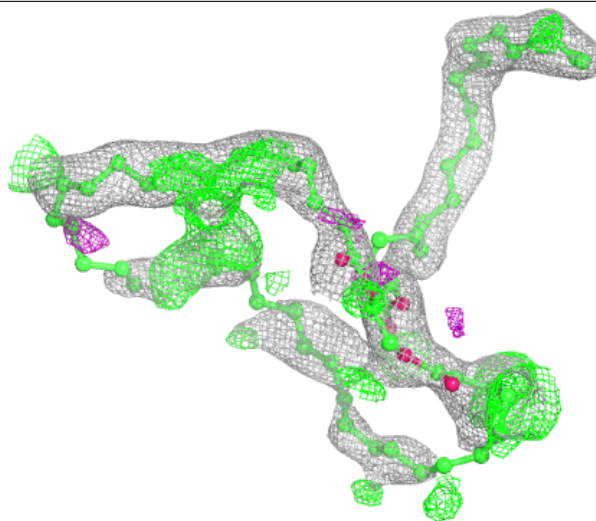
Electron density around CDL C 305:

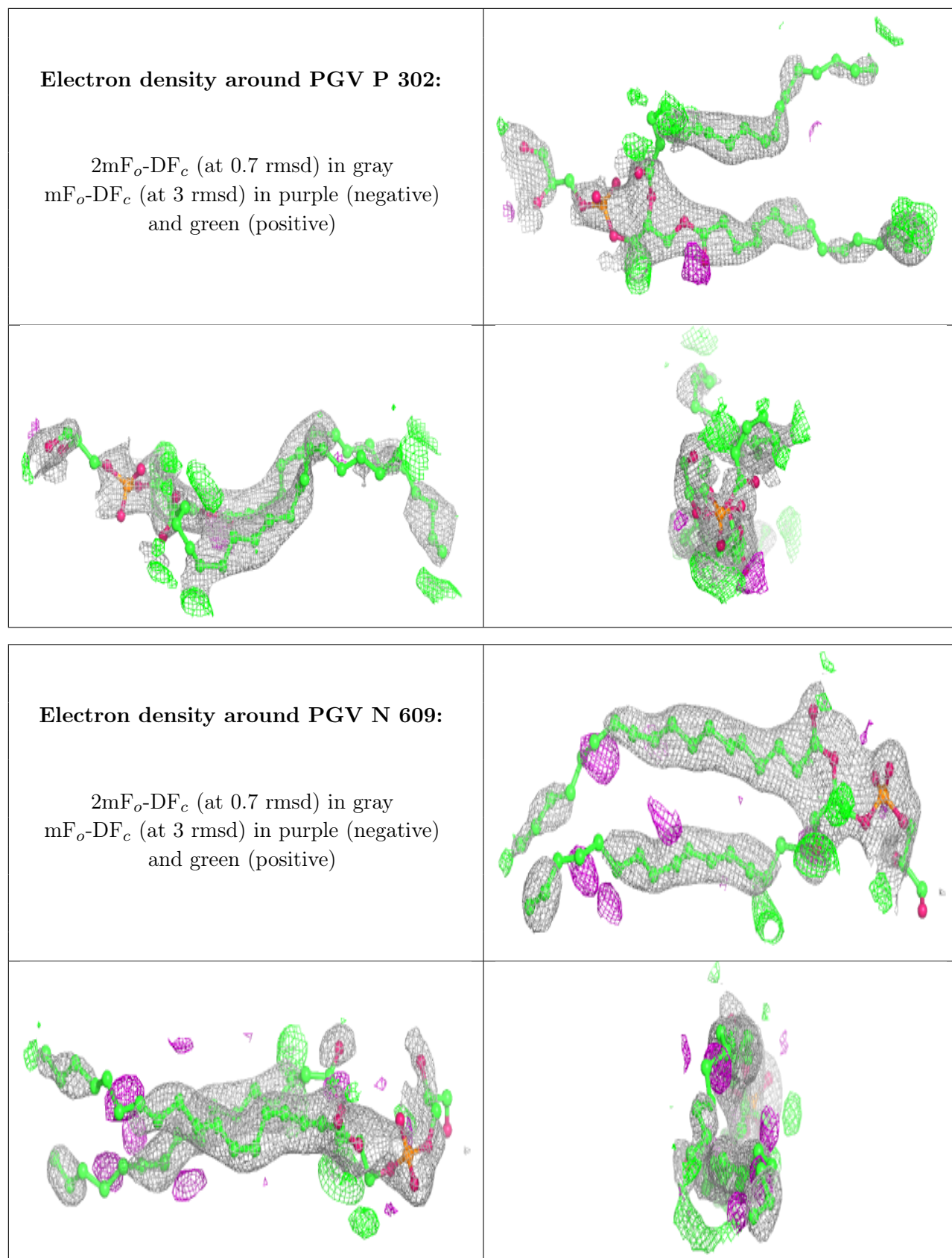
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

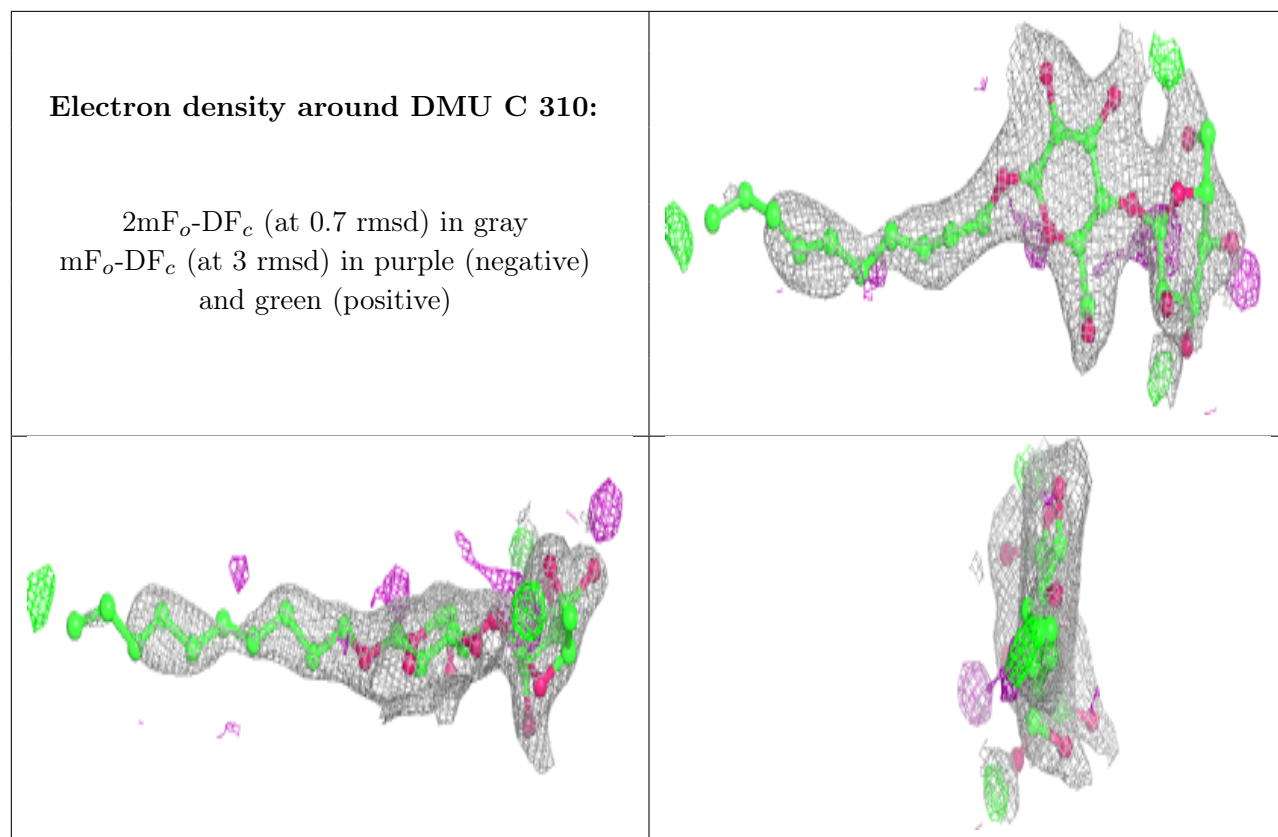


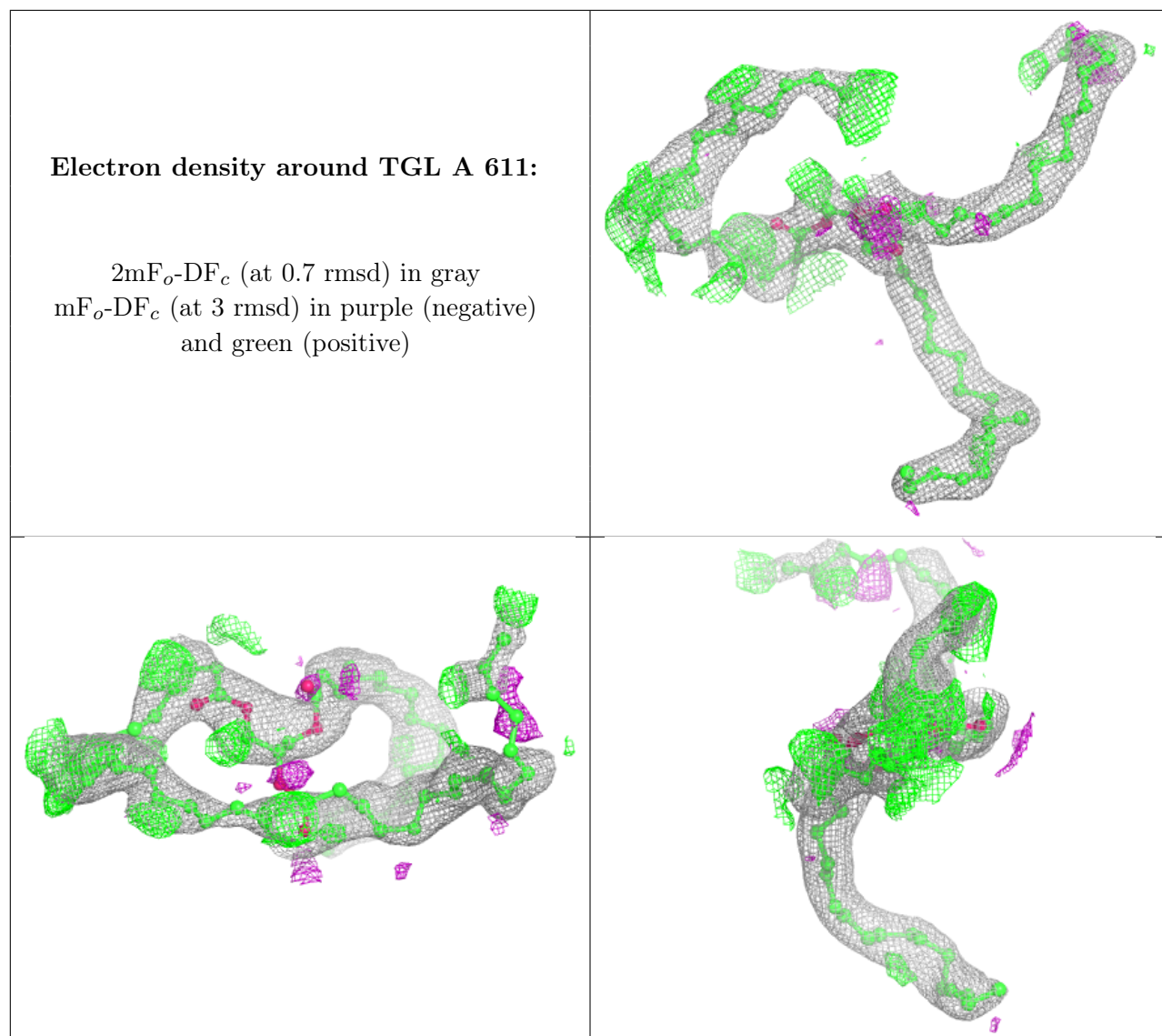
Electron density around TGL Y 101:

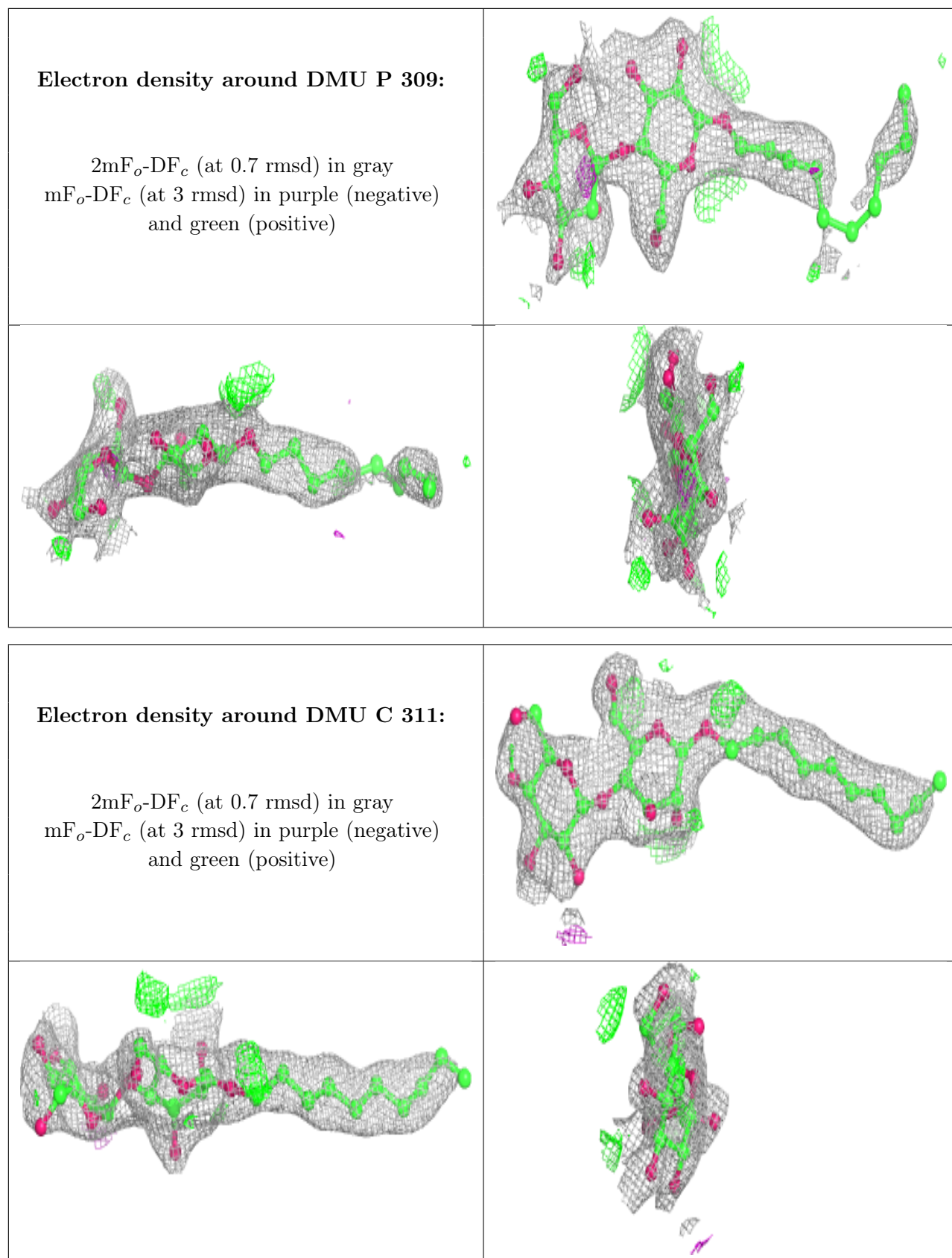
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





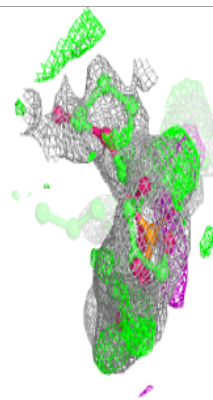
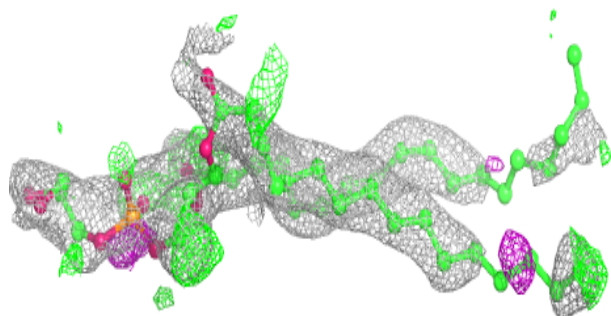
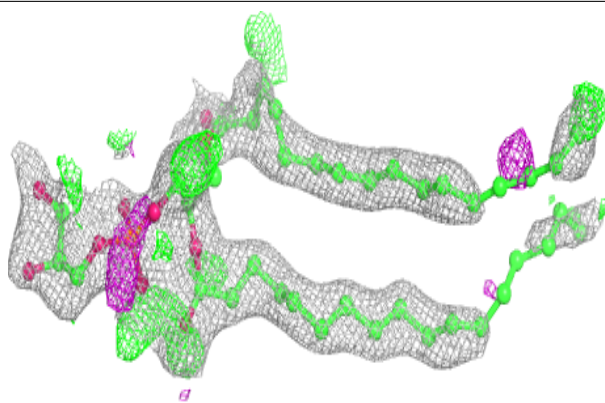




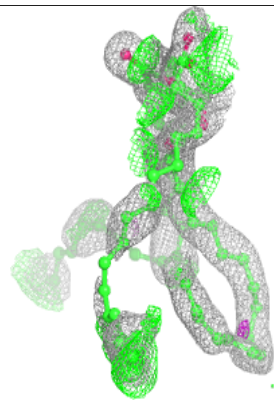
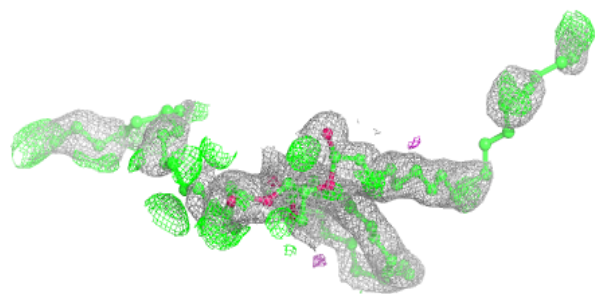
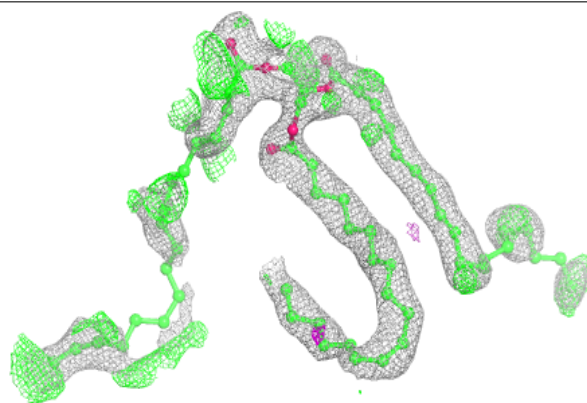


Electron density around PGV A 610:

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

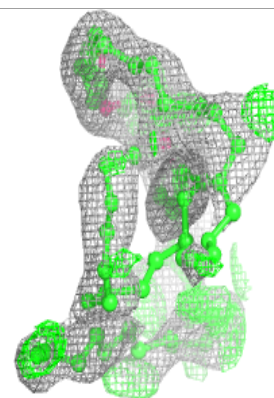
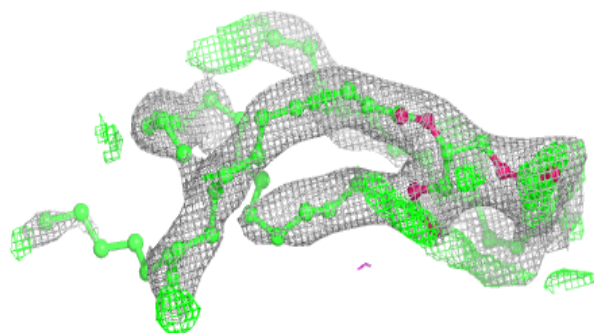
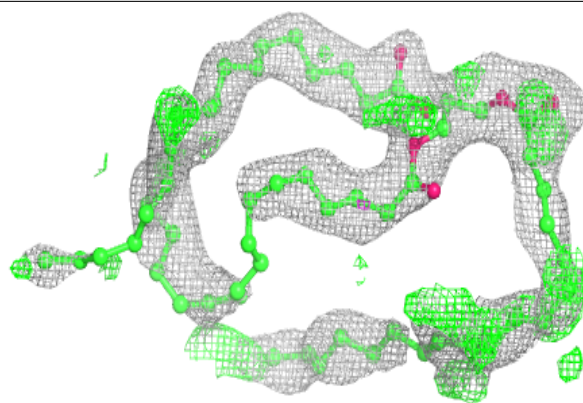
**Electron density around TGL D 201:**

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

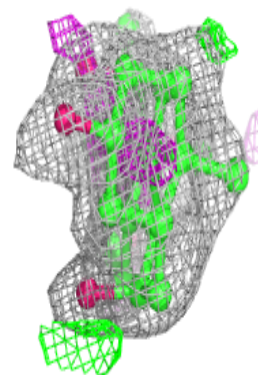
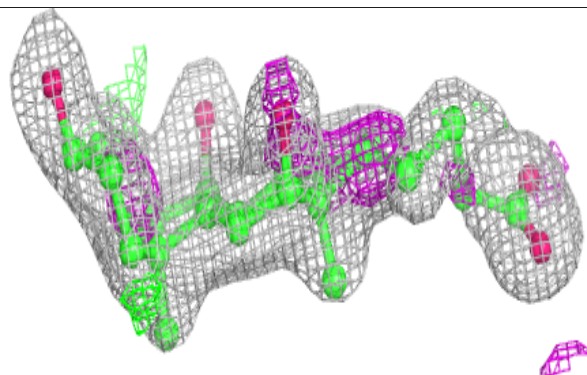
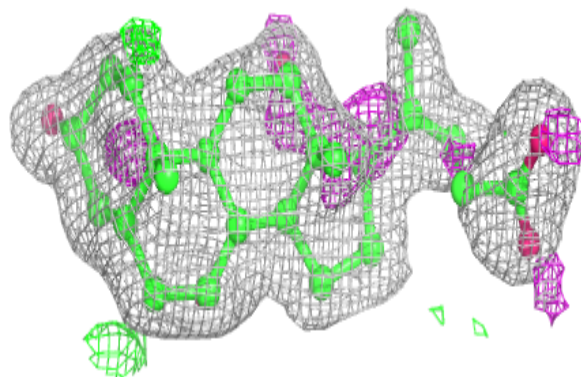


Electron density around TGL N 611:

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

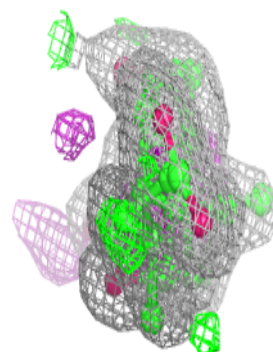
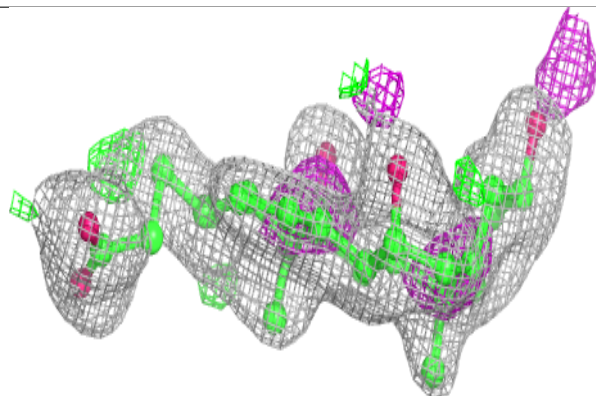
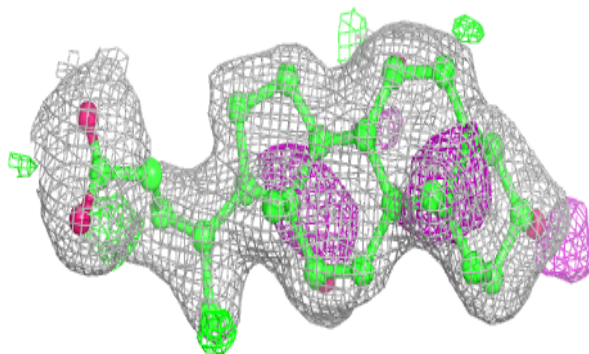
**Electron density around CHD C 306:**

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

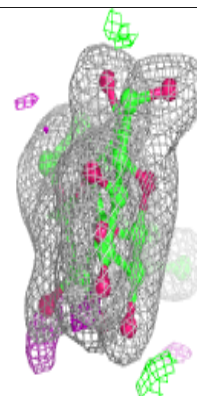
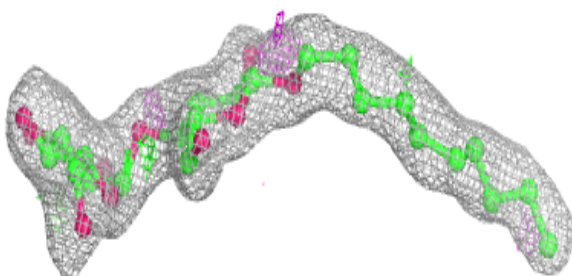
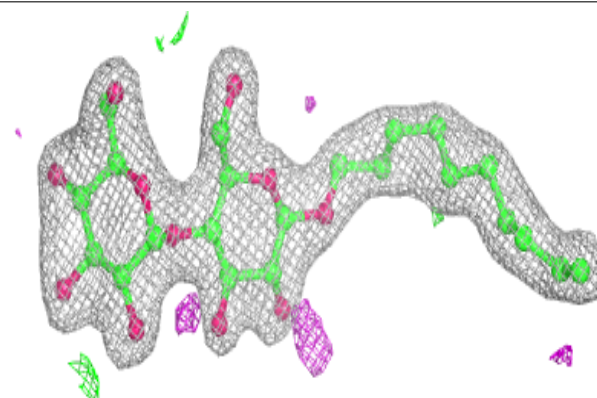


Electron density around CHD P 306:

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

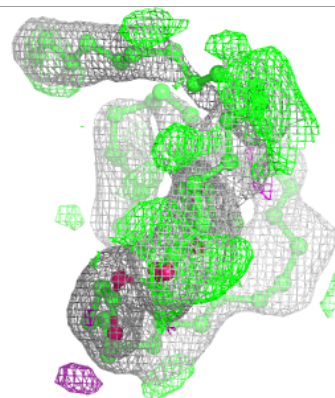
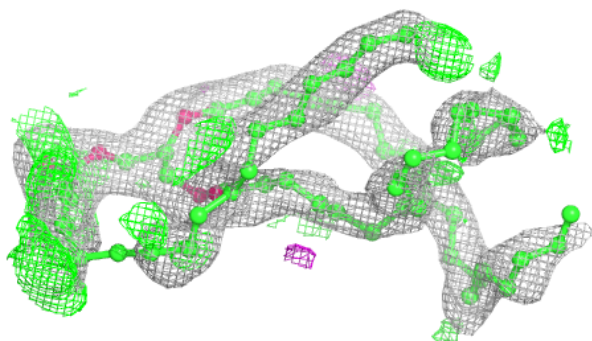
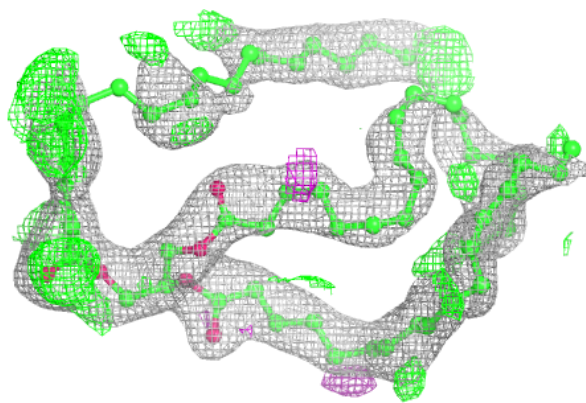
**Electron density around DMU Z 101:**

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

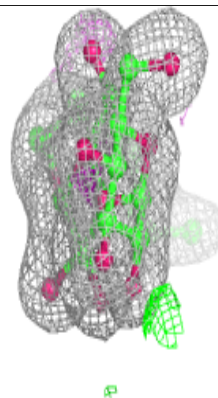
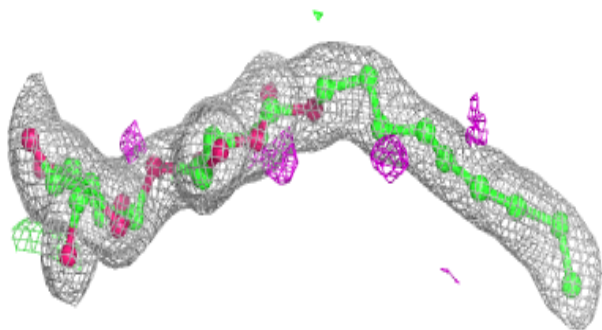
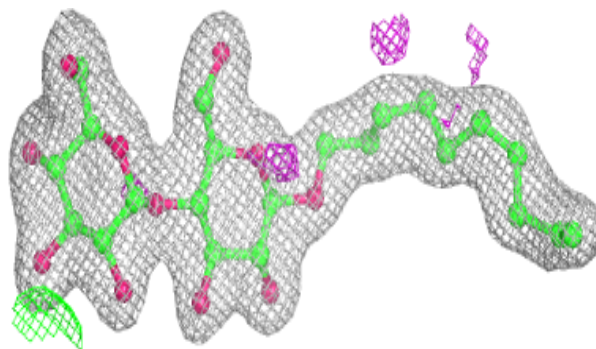


Electron density around TGL A 608:

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

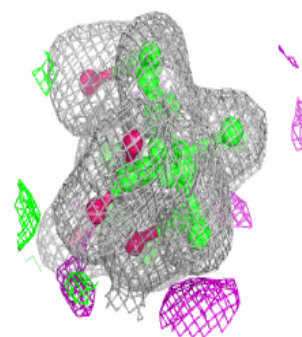
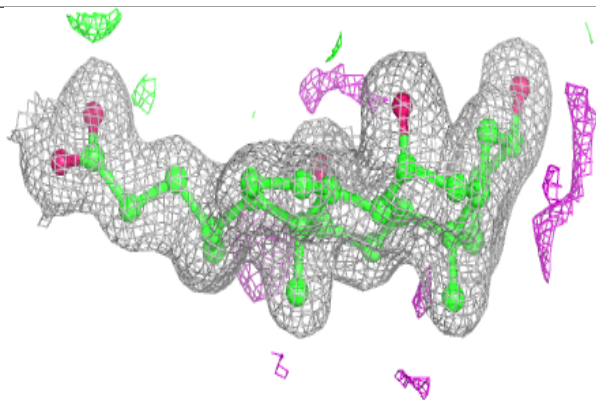
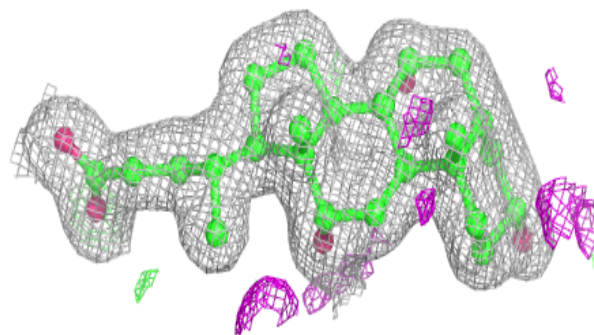
**Electron density around DMU M 101:**

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

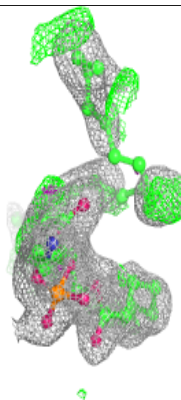
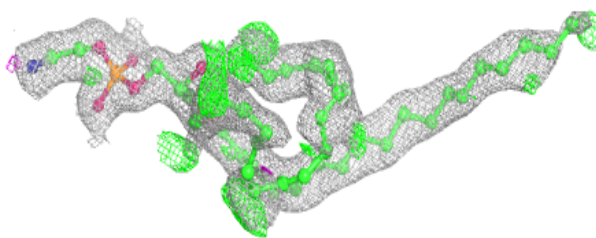
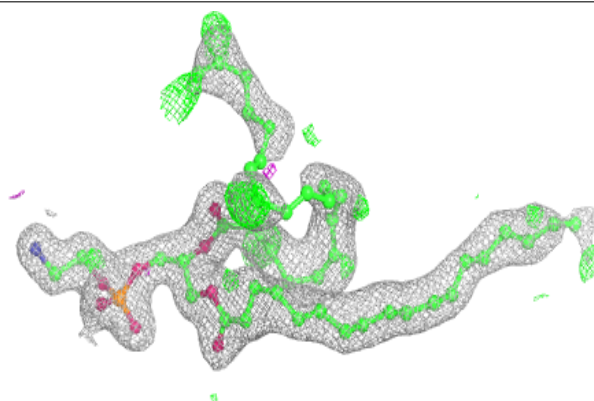


Electron density around CHD P 301:

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

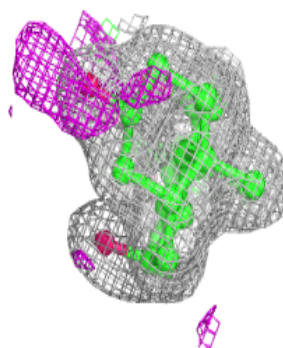
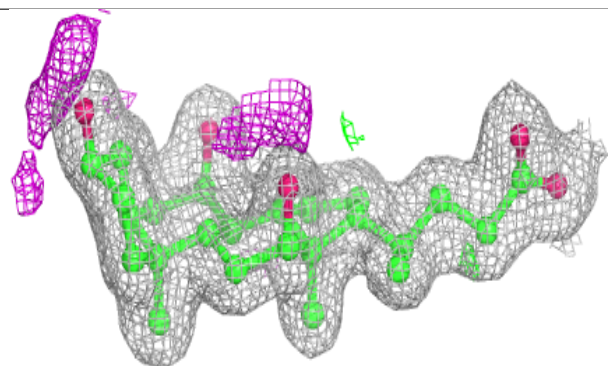
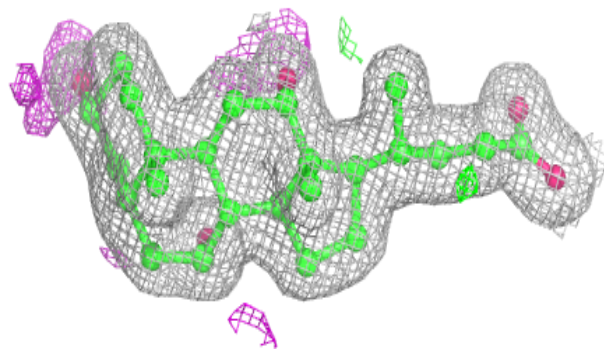
**Electron density around PEK T 101:**

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

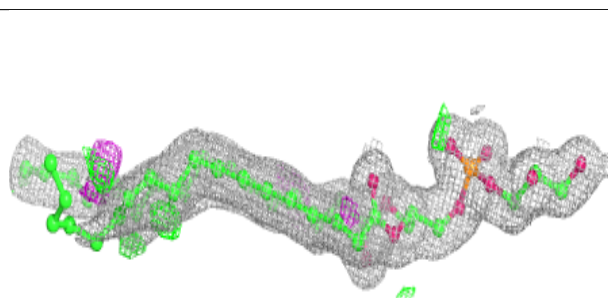
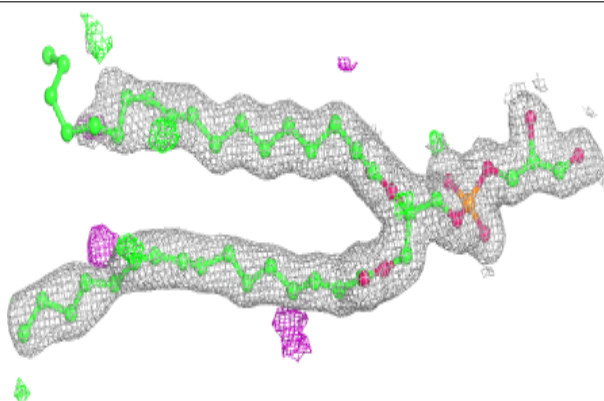


Electron density around CHD C 301:

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

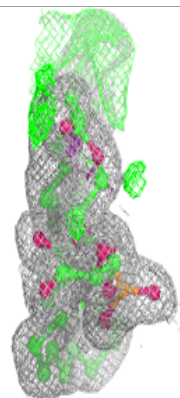
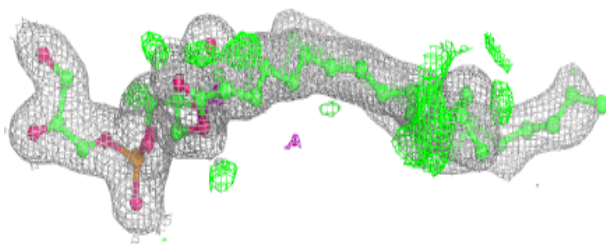
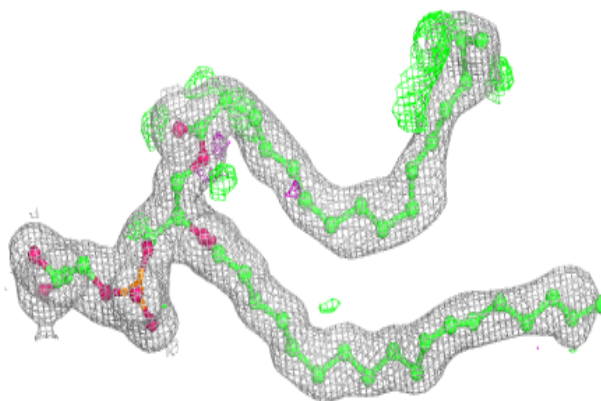
**Electron density around PGV C 304:**

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

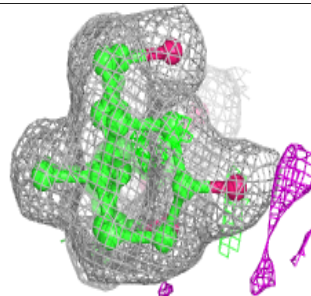
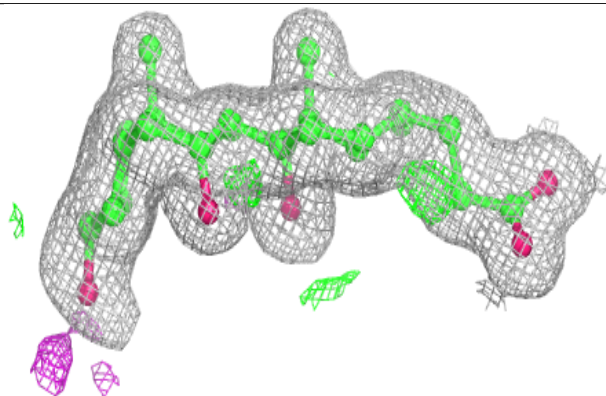
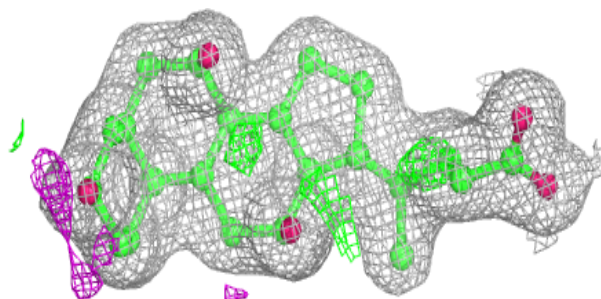


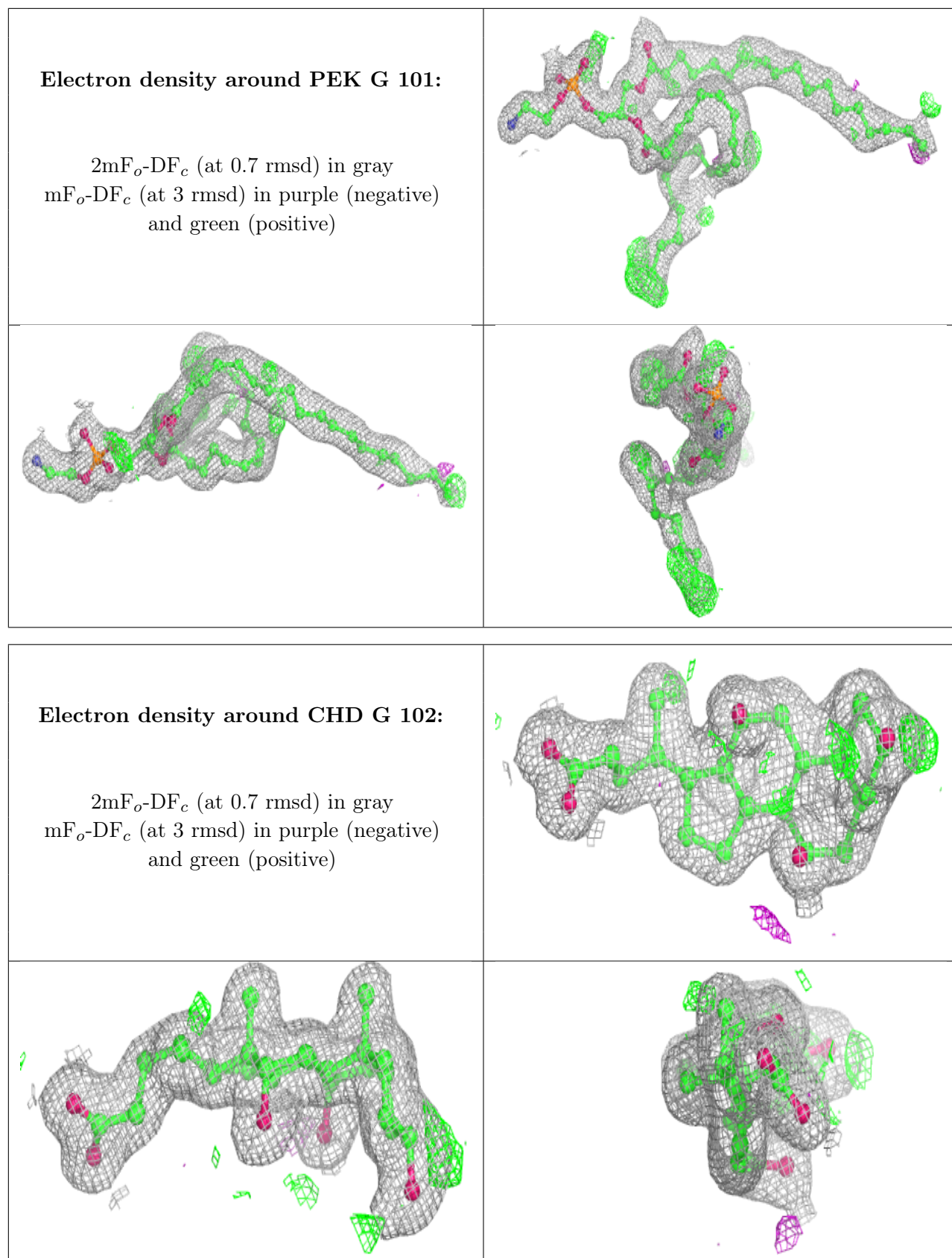
Electron density around PGV N 610:

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

**Electron density around CHD B 301:**

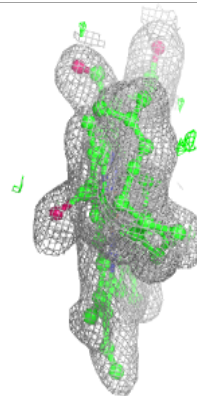
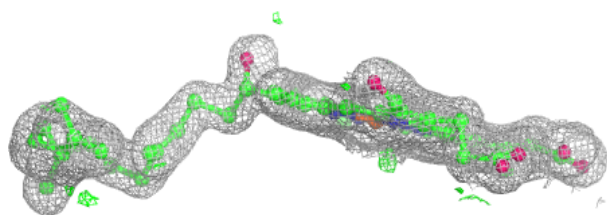
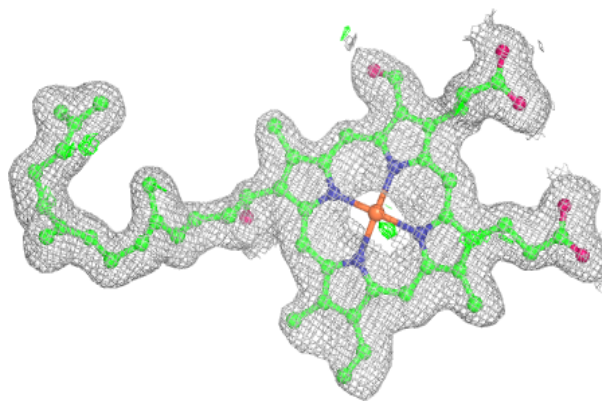
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



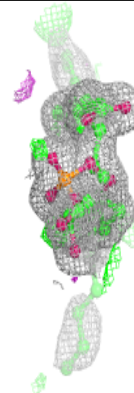
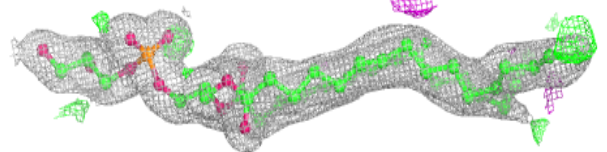
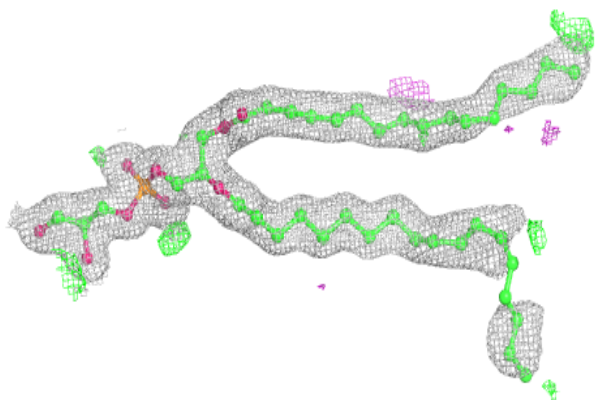


Electron density around HEA A 602 (B):

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

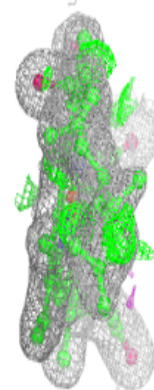
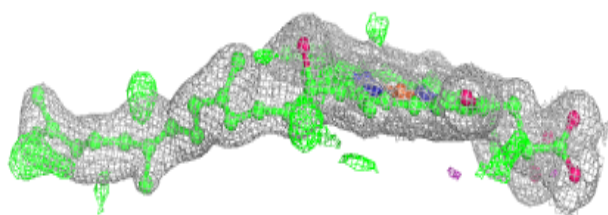
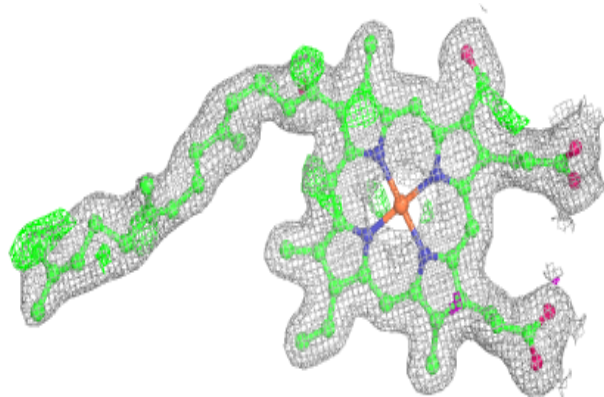
**Electron density around PGV P 304:**

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

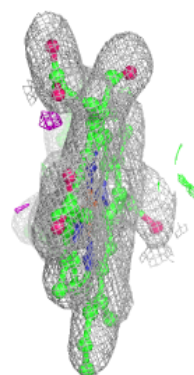
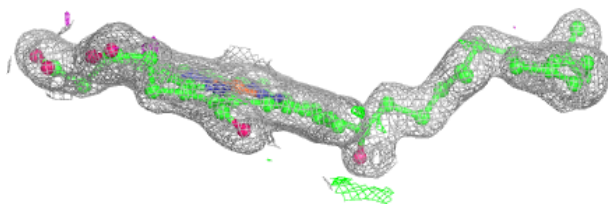
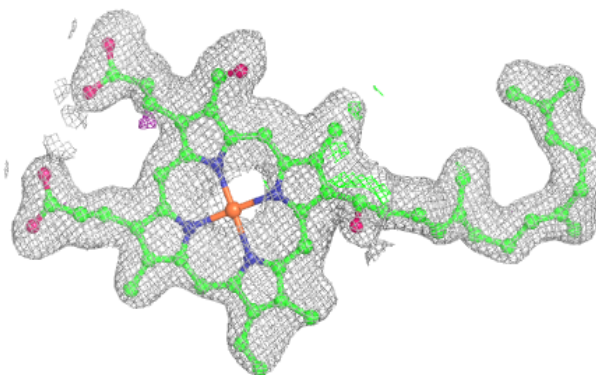


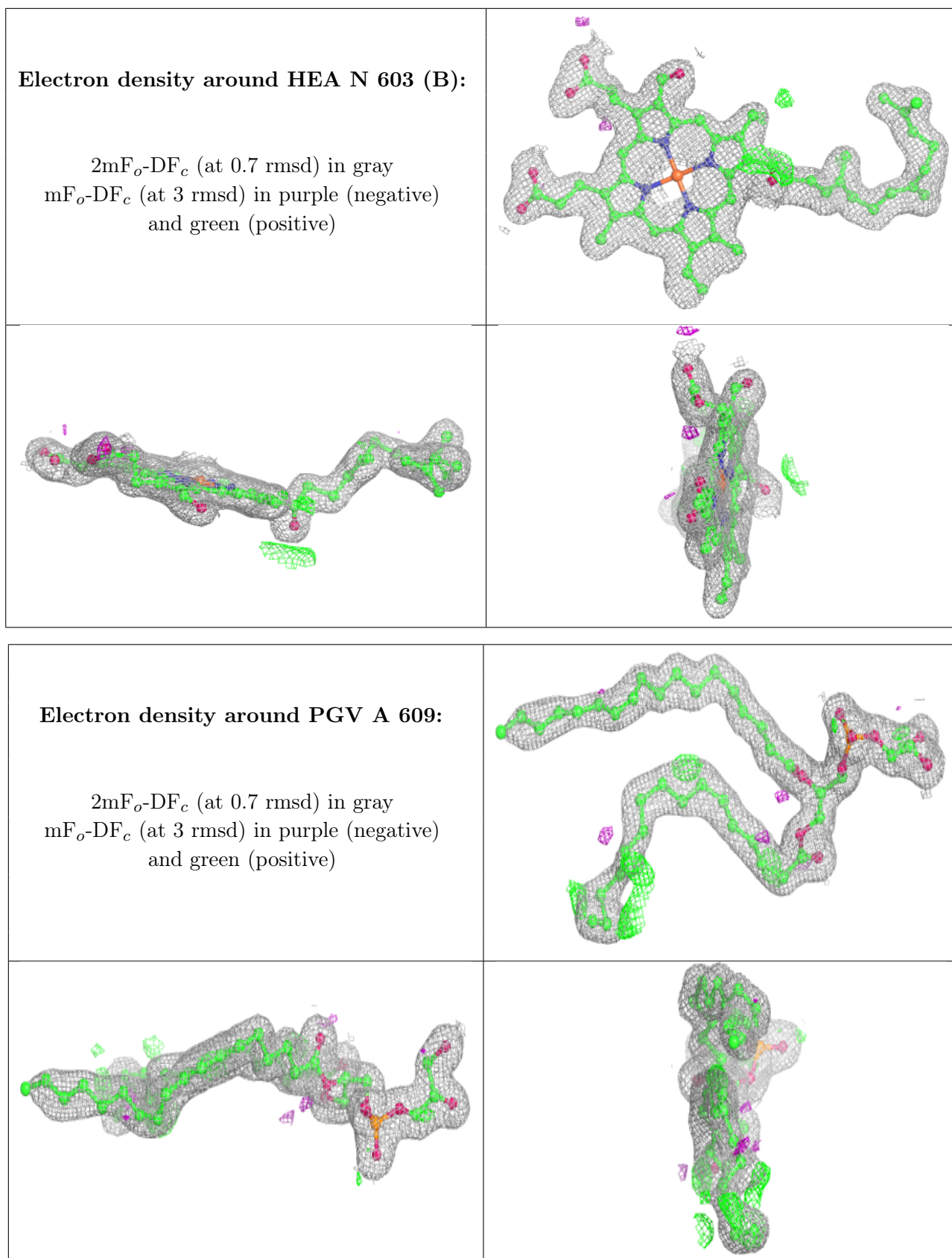
Electron density around HEA N 602:

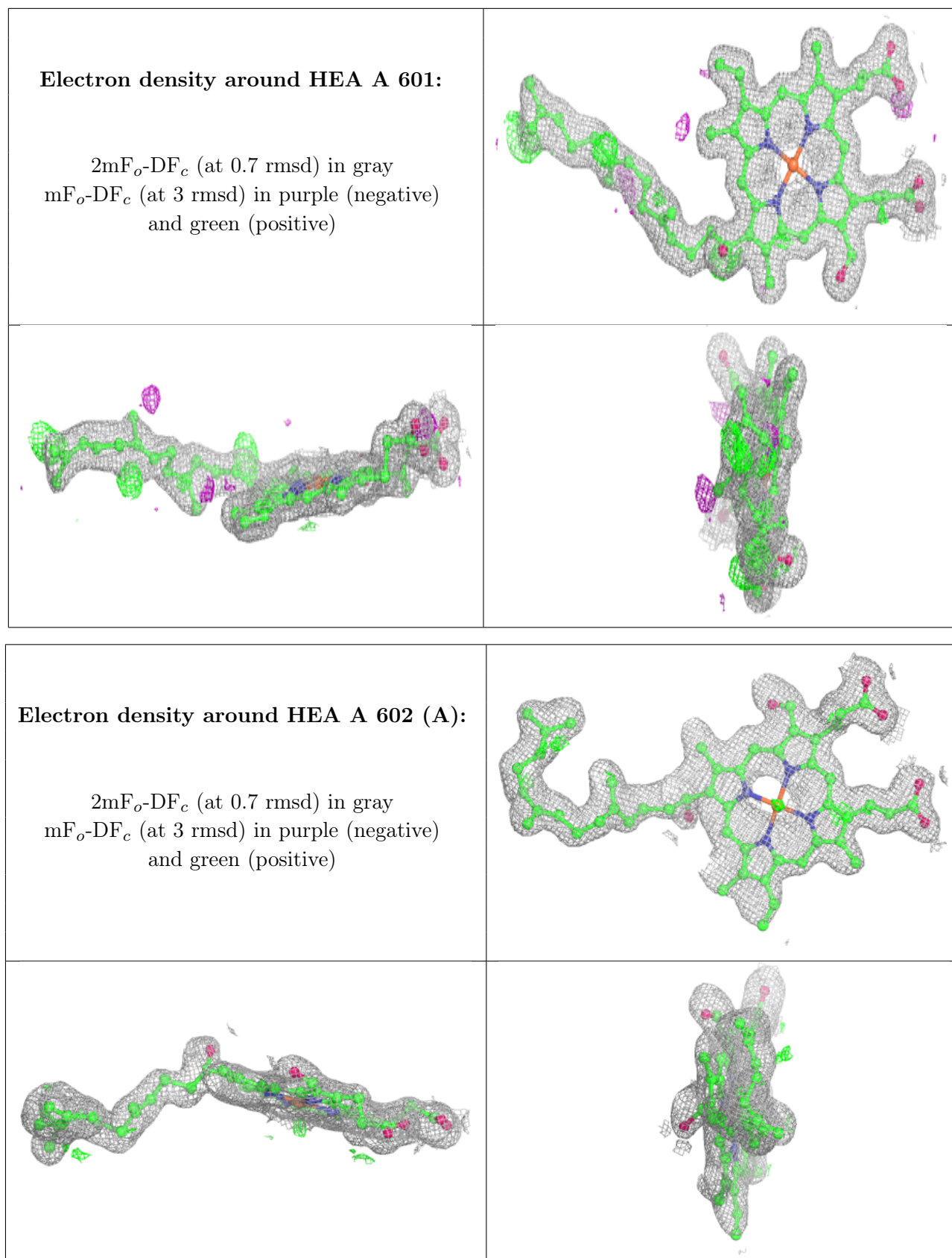
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around HEA N 603 (A):**

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







6.5 Other polymers [i](#)

There are no such residues in this entry.