



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 11:14 PM UTC

PDB ID : 2DYS / pdb_00002dys
Title : Bovine heart cytochrome C oxidase modified by DCCD
Authors : Shinzawa-Itoh, K.; Aoyama, H.; Muramoto, K.; Kurauchi, T.; Mizushima, T.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2006-09-16
Resolution : 2.20 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

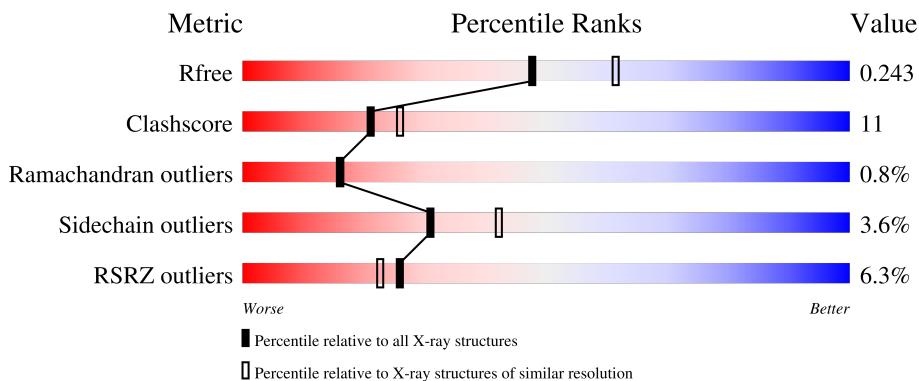
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

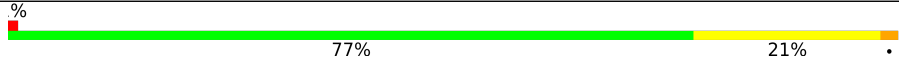
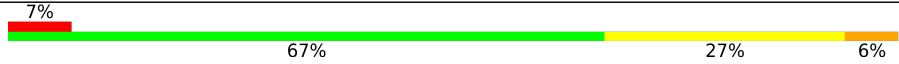
The reported resolution of this entry is 2.20 Å.

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






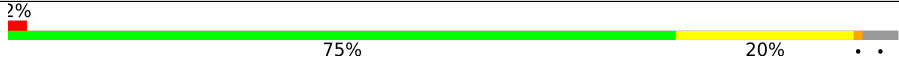
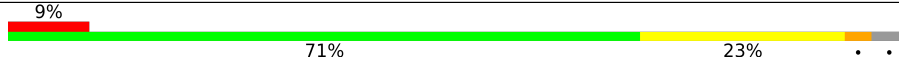
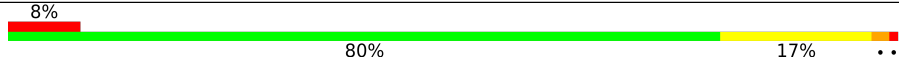
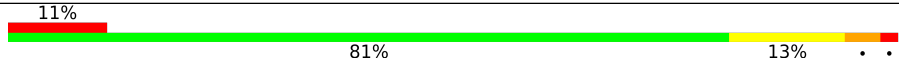
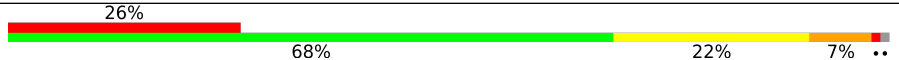
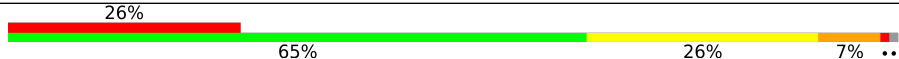
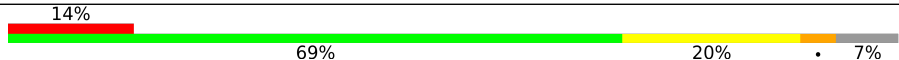



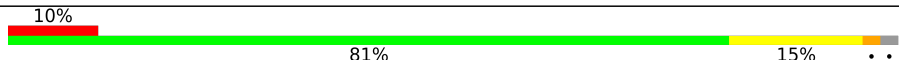
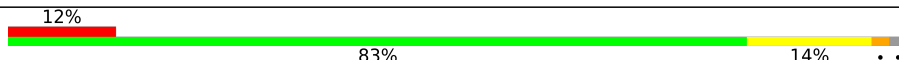
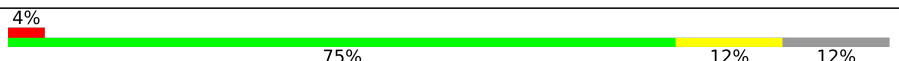
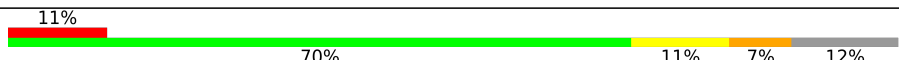
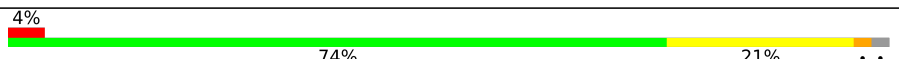
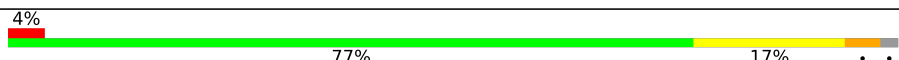
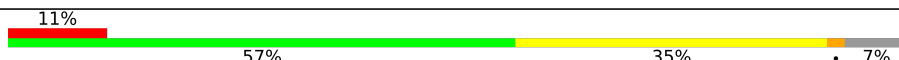
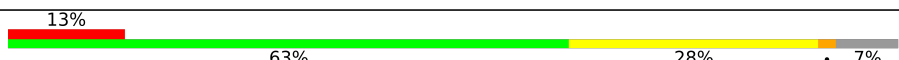
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	 79% 20% .
1	N	514	 77% 21% .
2	B	227	 71% 26% .
2	O	227	 67% 27% 6% .
3	C	261	 79% 20% .

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	TGL	L	101	-	-	X	-
21	PSC	B	303	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	PSC	O	304	-	-	X	-
22	CHD	C	310	X	-	-	-
22	CHD	J	101	X	-	-	-
22	CHD	P	310	X	-	-	-
22	CHD	W	101	X	-	-	-
23	DCW	C	301	-	-	X	-
24	DMU	C	302	X	-	-	-
24	DMU	M	101	X	-	-	-
24	DMU	P	302	X	-	-	-
24	DMU	Z	101	X	-	-	-
27	CDL	T	102	-	-	X	-

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 32170 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	4027	2691	623	678	35	0	0	0
1	N	514	4027	2691	623	678	35	0	0	0

- 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	1824	1185	281	340	18	0	0	0
2	O	227	1824	1185	281	340	18	0	0	0

- 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	2109	1412	336	349	12	0	0	0
3	P	259	2109	1412	336	349	12	0	0	0

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

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

- Molecule 5 is a protein called Cytochrome c oxidase polypeptide Va.

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

- Molecule 6 is a protein called Cytochrome c oxidase polypeptide Vb.

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

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide VIa-heart.

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

- Molecule 8 is a protein called Cytochrome c oxidase subunit VIb isoform 1.

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

- Molecule 9 is a protein called Cytochrome c oxidase polypeptide VIc.

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

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide VIIa-heart.

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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 COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

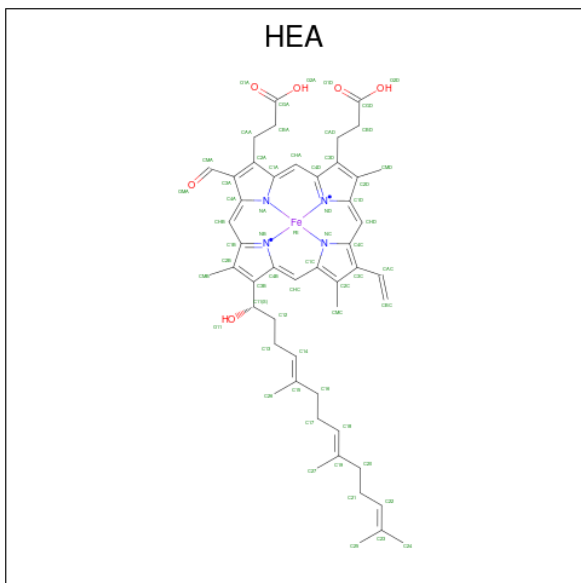
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

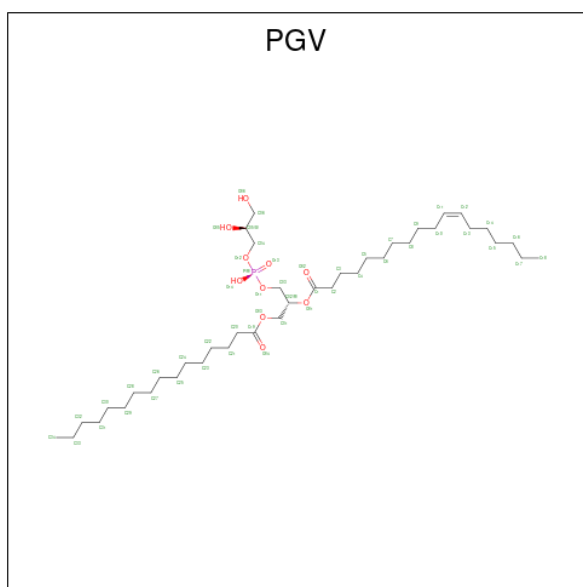
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

- Molecule 17 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



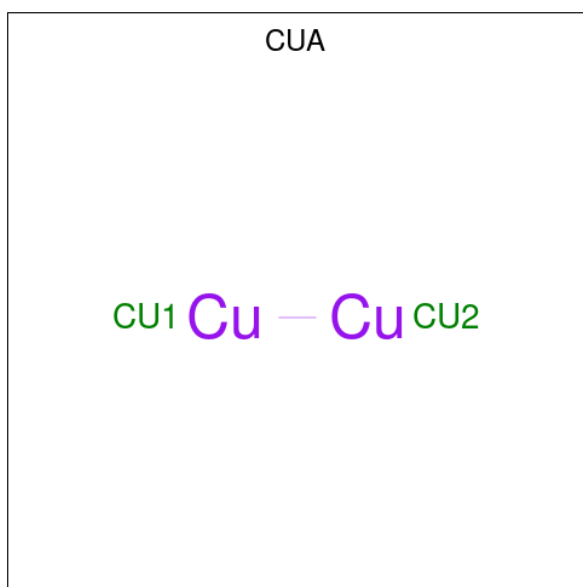
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0

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



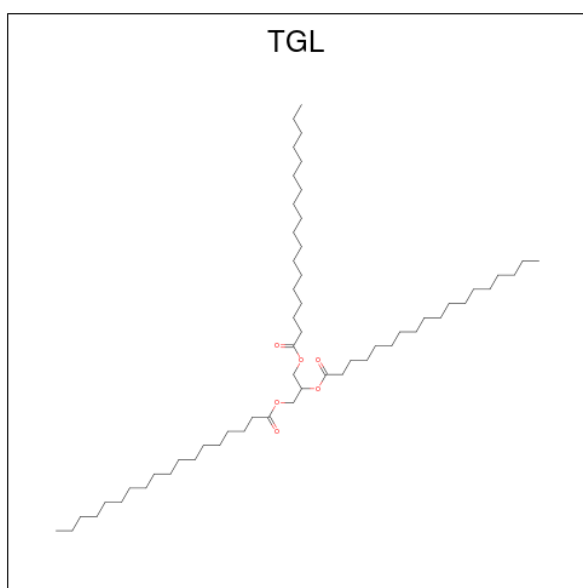
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			P
18	A	1	51	40	10	1	0	0
18	A	1	51	40	10	1	0	0
18	C	1	51	40	10	1	0	0
18	C	1	51	40	10	1	0	0
18	N	1	51	40	10	1	0	0
18	N	1	51	40	10	1	0	0
18	P	1	51	40	10	1	0	0
18	P	1	51	40	10	1	0	0

- Molecule 19 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 20 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



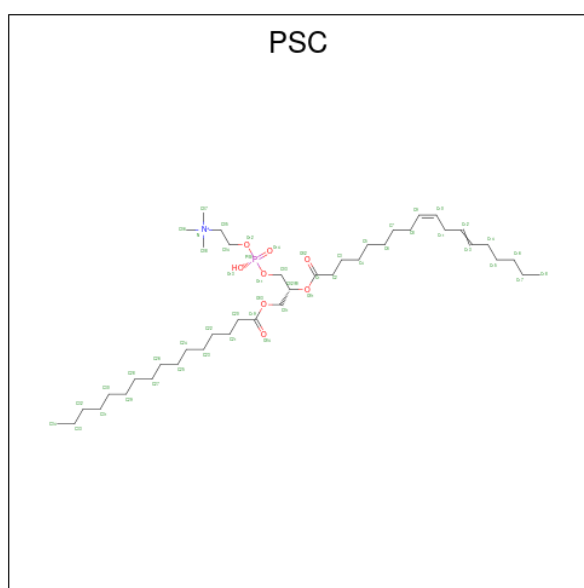
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	B	1	Total C O 63 57 6	0	0
20	D	1	Total C O 63 57 6	0	0

Continued on next page...

Continued from previous page...

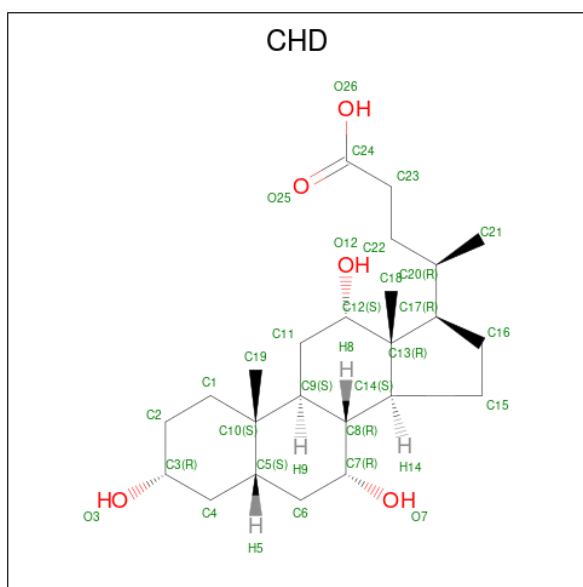
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	O	1	Total	C	O	0	0
			63	57	6		

- Molecule 21 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



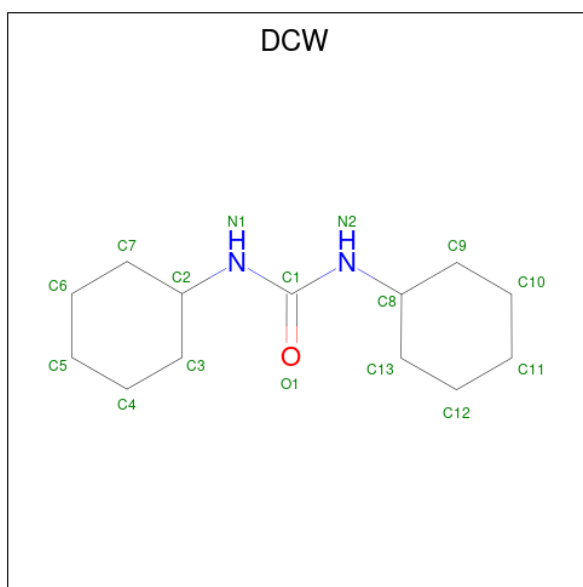
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
21	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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



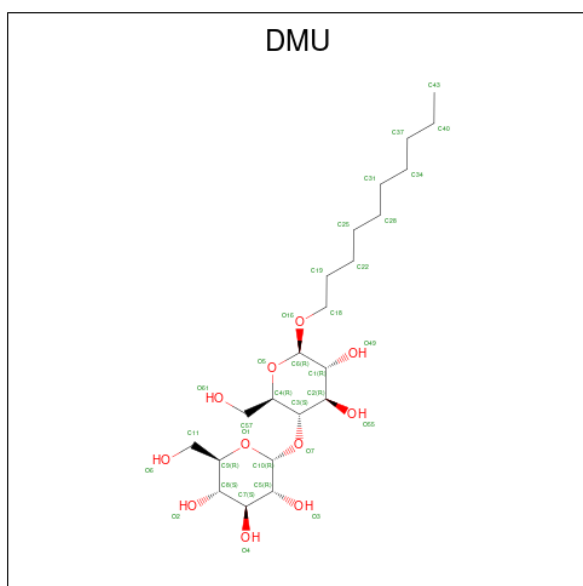
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

- Molecule 23 is DICYCLOHEXYLUREA (CCD ID: DCW) (formula: $C_{13}H_{24}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
23	C	1	16	13	2	1	0	0
23	P	1	16	13	2	1	0	0

- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

Continued on next page...

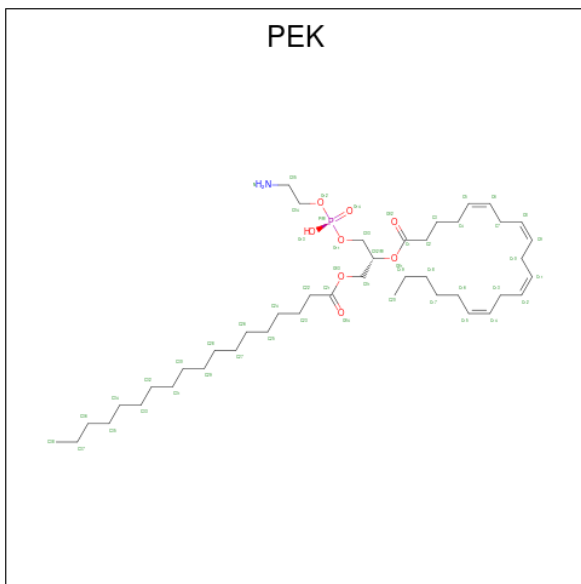
Continued from previous page...

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

- Molecule 25 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

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

- Molecule 26 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



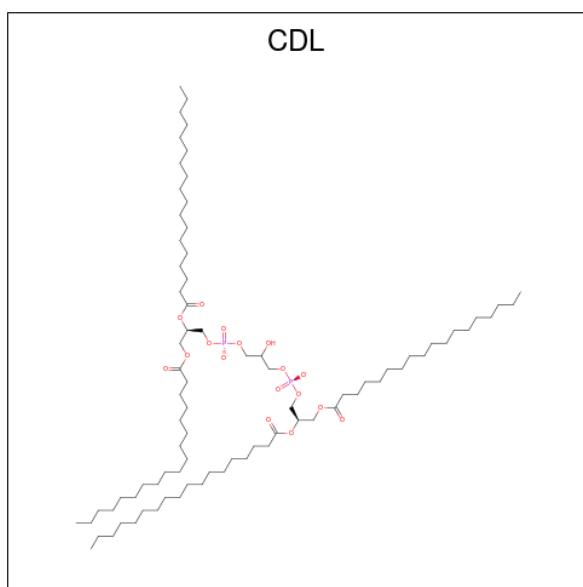
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

Continued on next page...

Continued from previous page...

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

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

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	199	Total O 199 199	0	0
29	B	119	Total O 119 119	0	0
29	C	82	Total O 82 82	0	0
29	D	79	Total O 79 79	0	0
29	E	58	Total O 58 58	0	0
29	F	64	Total O 64 64	0	0
29	G	35	Total O 35 35	0	0
29	H	39	Total O 39 39	0	0
29	I	29	Total O 29 29	0	0
29	J	14	Total O 14 14	0	0
29	K	21	Total O 21 21	0	0
29	L	17	Total O 17 17	0	0
29	M	14	Total O 14 14	0	0
29	N	176	Total O 176 176	0	0
29	O	103	Total O 103 103	0	0
29	P	74	Total O 74 74	0	0
29	Q	46	Total O 46 46	0	0
29	R	41	Total O 41 41	0	0
29	S	56	Total O 56 56	0	0
29	T	30	Total O 30 30	0	0
29	U	39	Total O 39 39	0	0

Continued on next page...

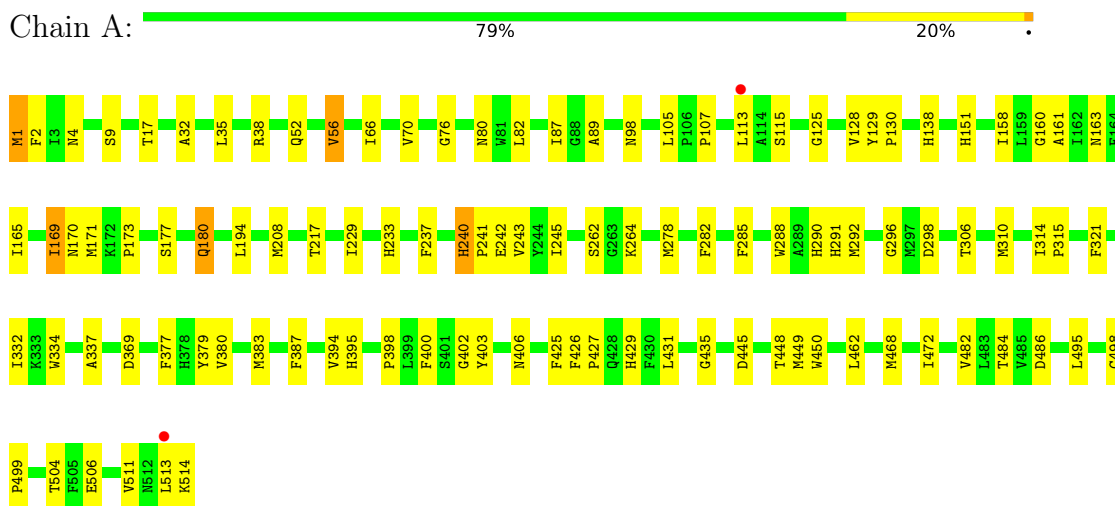
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	V	19	Total O 19 19	0	0
29	W	14	Total O 14 14	0	0
29	X	17	Total O 17 17	0	0
29	Y	13	Total O 13 13	0	0
29	Z	10	Total O 10 10	0	0

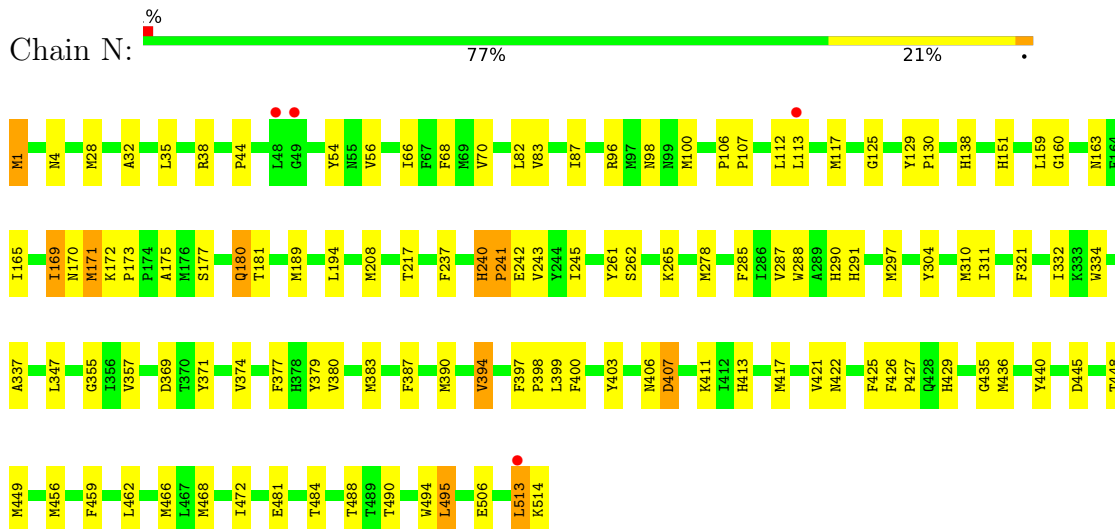
3 Residue-property plots

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

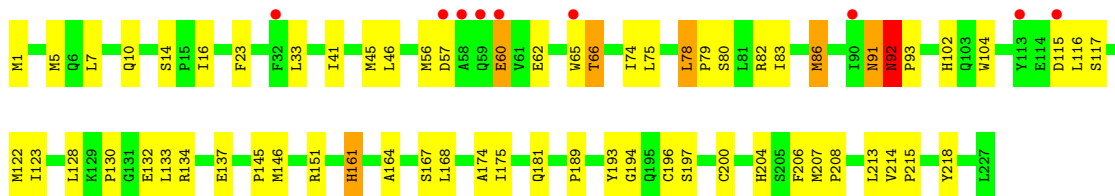


- Molecule 1: Cytochrome c oxidase subunit 1

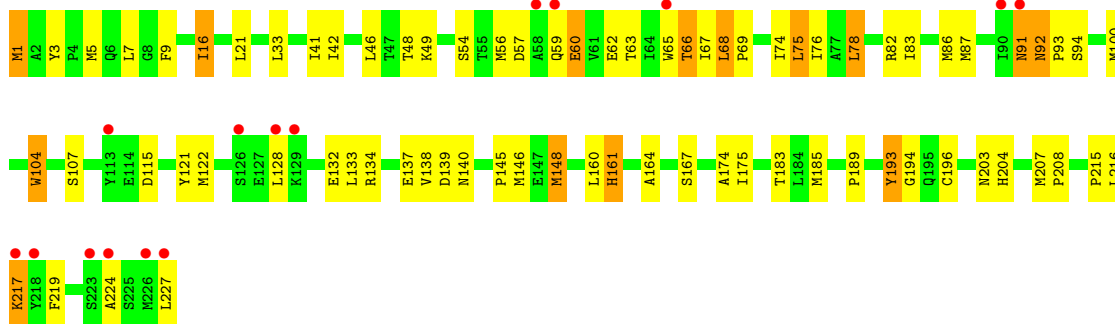


- Molecule 2: Cytochrome c oxidase subunit 2

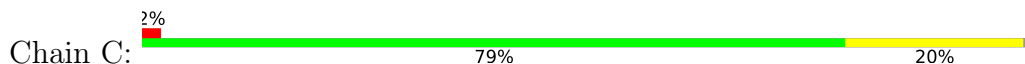




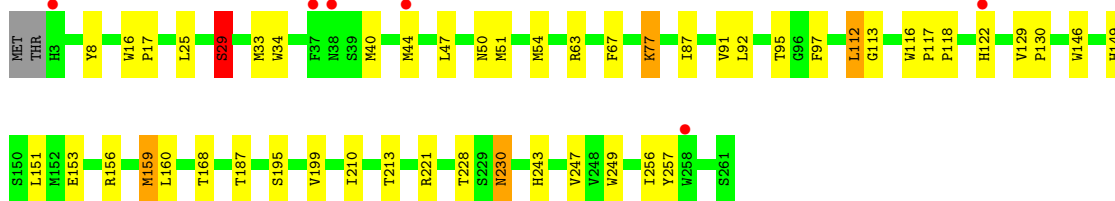
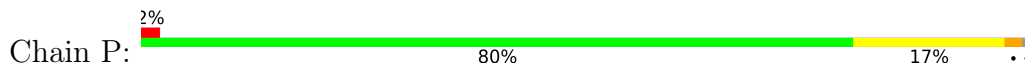
• Molecule 2: Cytochrome c oxidase subunit 2



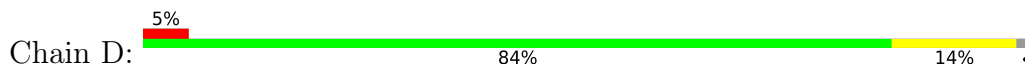
• Molecule 3: Cytochrome c oxidase subunit 3



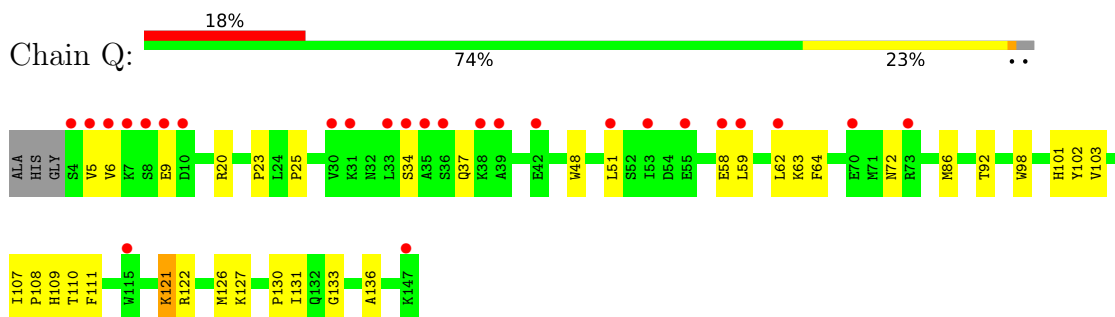
• Molecule 3: Cytochrome c oxidase subunit 3



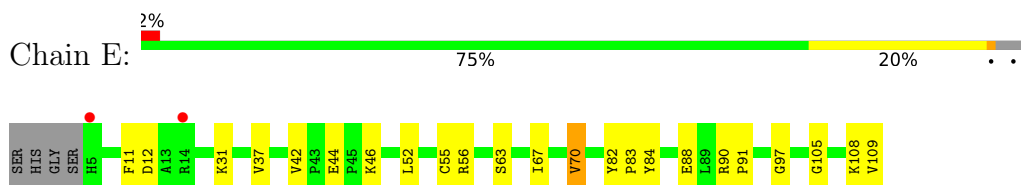
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



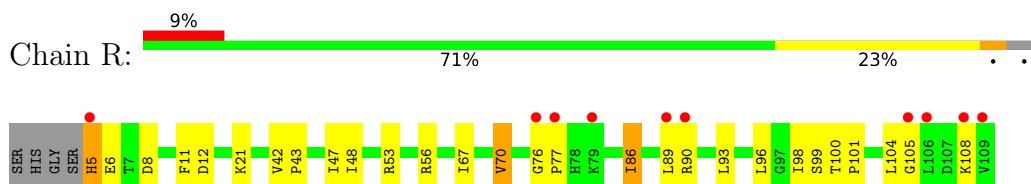
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



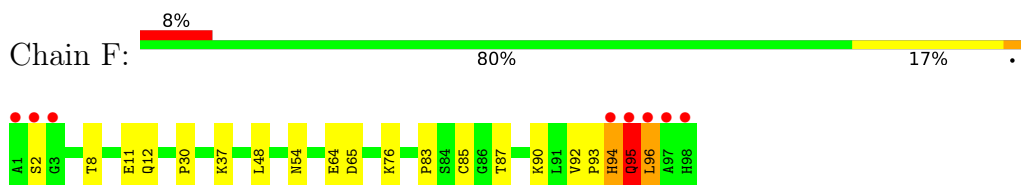
- Molecule 5: Cytochrome c oxidase polypeptide Va



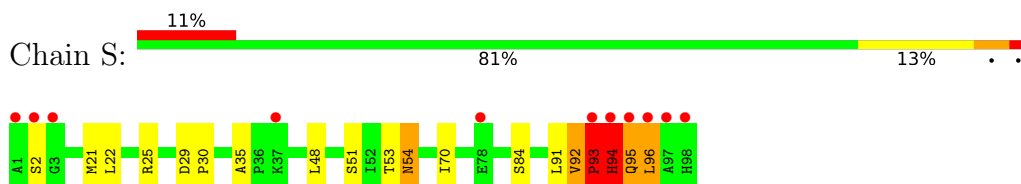
- Molecule 5: Cytochrome c oxidase polypeptide Va



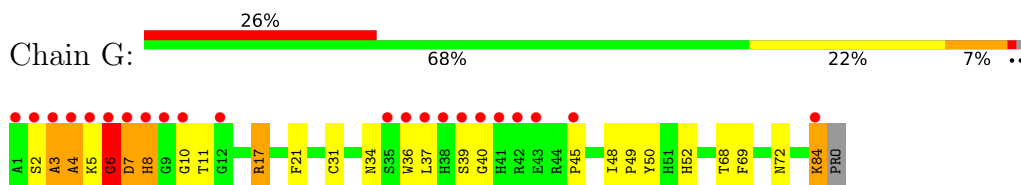
- Molecule 6: Cytochrome c oxidase polypeptide Vb



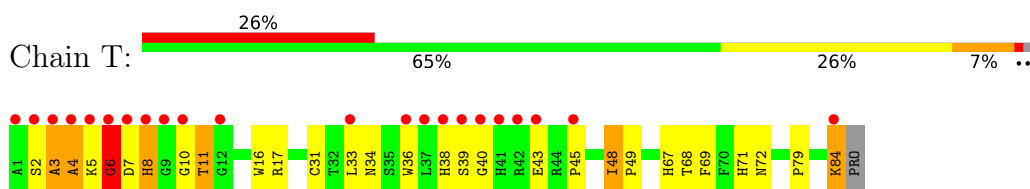
- Molecule 6: Cytochrome c oxidase polypeptide Vb



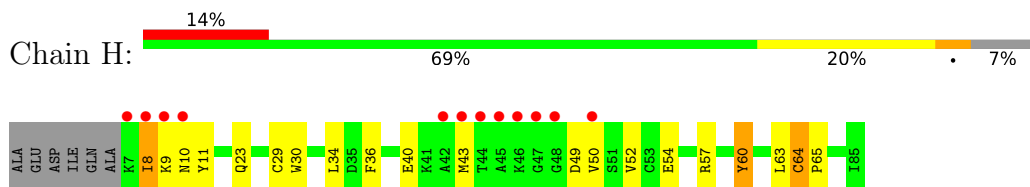
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



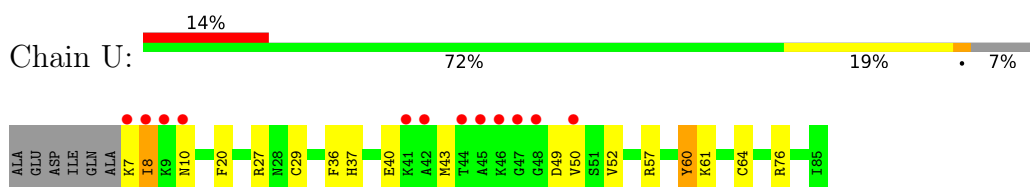
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



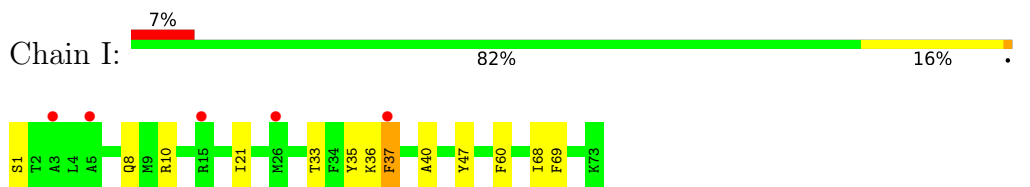
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



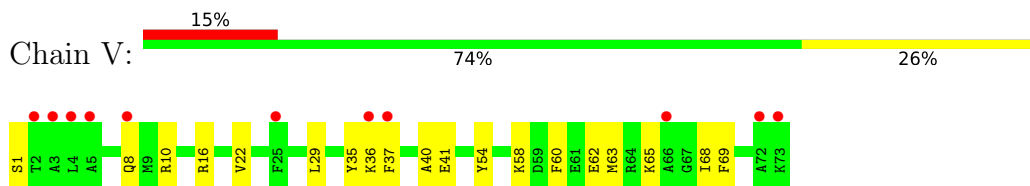
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



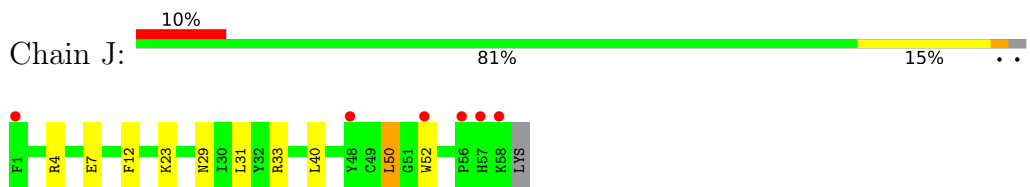
- Molecule 9: Cytochrome c oxidase polypeptide VIc



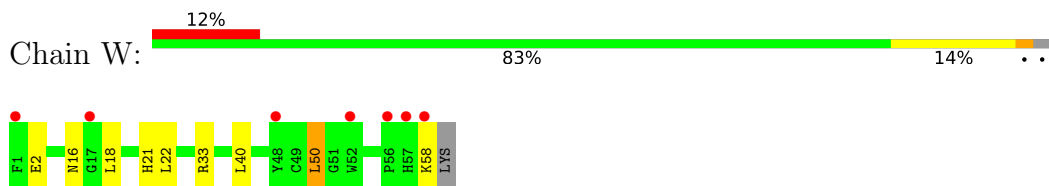
- Molecule 9: Cytochrome c oxidase polypeptide VIc



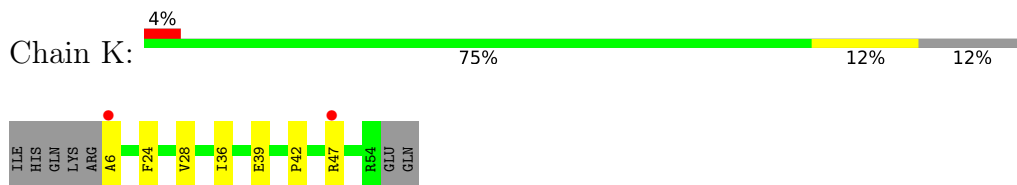
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



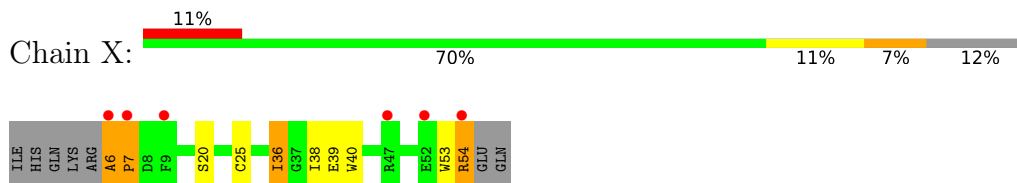
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



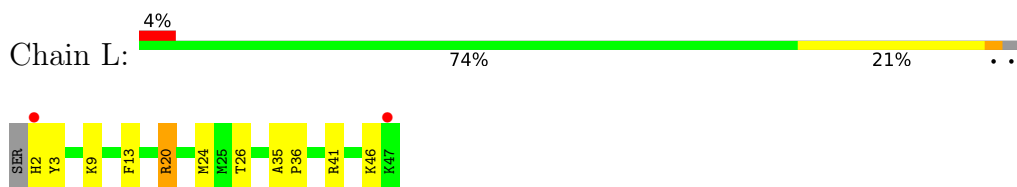
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



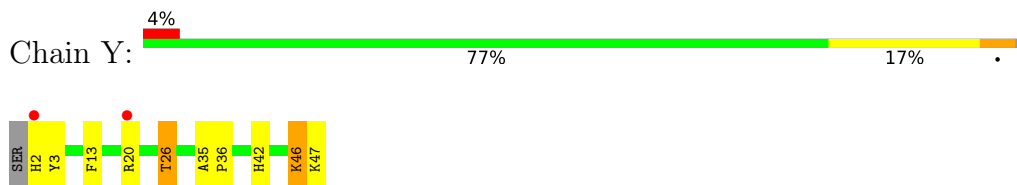
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



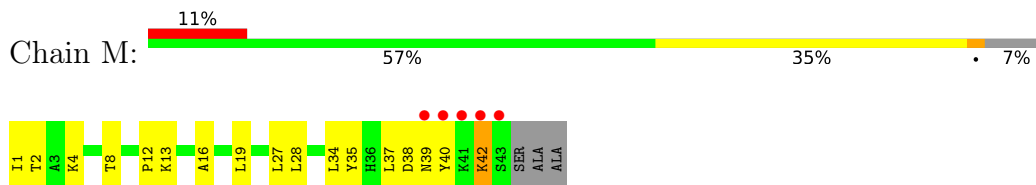
- Molecule 12: Cytochrome c oxidase polypeptide VIIc



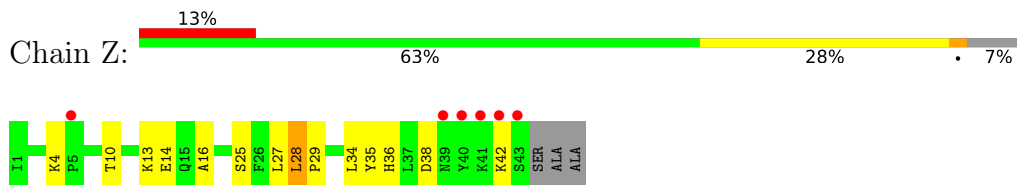
- Molecule 12: Cytochrome c oxidase polypeptide VIIc



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.13Å 207.23Å 178.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 40.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.20) 99.2 (40.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.20Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.242 0.207 , 0.243	Depositor DCC
R_{free} test set	16860 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.006 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32170	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: DMU, MG, PSC, SAC, CDL, UNX, PGV, ZN, CUA, NA, HEA, DCW, CU, PEK, TPO, TGL, CHD, 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	0.75	2/4156 (0.0%)	1.13	28/5678 (0.5%)
1	N	0.68	1/4156 (0.0%)	1.10	27/5678 (0.5%)
2	B	0.69	0/1860	1.07	7/2534 (0.3%)
2	O	0.66	0/1860	1.10	6/2534 (0.2%)
3	C	0.68	0/2196	1.01	7/3003 (0.2%)
3	P	0.64	0/2196	1.01	10/3003 (0.3%)
4	D	0.65	0/1229	1.01	1/1658 (0.1%)
4	Q	0.68	2/1229 (0.2%)	1.00	2/1658 (0.1%)
5	E	0.68	0/871	0.95	1/1182 (0.1%)
5	R	0.62	0/871	1.12	5/1182 (0.4%)
6	F	0.69	0/765	1.18	7/1038 (0.7%)
6	S	0.70	0/765	1.20	9/1038 (0.9%)
7	G	0.75	0/690	1.11	5/937 (0.5%)
7	T	0.74	0/690	1.12	7/937 (0.7%)
8	H	0.63	0/682	1.08	6/921 (0.7%)
8	U	0.58	0/682	1.07	3/921 (0.3%)
9	I	0.63	0/605	0.98	1/802 (0.1%)
9	V	0.58	0/605	0.92	1/802 (0.1%)
10	J	0.61	0/471	1.01	0/636
10	W	0.55	0/471	1.10	0/636
11	K	0.70	0/398	1.16	3/546 (0.5%)
11	X	0.57	0/398	1.06	4/546 (0.7%)
12	L	0.63	0/393	0.99	2/526 (0.4%)
12	Y	0.58	0/393	1.06	2/526 (0.4%)
13	M	0.68	0/345	1.05	4/470 (0.9%)
13	Z	0.61	0/345	1.05	2/470 (0.4%)
All	All	0.68	5/29322 (0.0%)	1.07	150/39862 (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	1
1	N	0	2
9	I	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	83	VAL	CA-CB	7.35	1.57	1.54
4	Q	5	VAL	CA-CB	6.13	1.60	1.53
1	A	511	VAL	CA-CB	5.31	1.61	1.54
4	Q	6	VAL	CA-CB	5.28	1.61	1.54
1	A	130	PRO	CA-C	5.08	1.56	1.52

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	42	VAL	N-CA-C	-10.17	96.38	107.77
1	A	125	GLY	N-CA-C	-8.40	102.32	112.48
6	S	94	HIS	N-CA-C	8.30	128.49	110.80
1	A	56	VAL	N-CA-C	-8.25	102.39	110.72
1	N	125	GLY	N-CA-C	-8.13	102.64	112.48

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
9	I	47	TYR	Sidechain
1	N	240	HIS	Sidechain
1	N	304	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	71	0
1	N	4027	0	4001	81	0
2	B	1824	0	1833	46	0
2	O	1824	0	1833	59	0
3	C	2109	0	2027	45	0
3	P	2109	0	2027	44	0
4	D	1195	0	1183	19	0
4	Q	1195	0	1183	25	0
5	E	852	0	845	15	0
5	R	852	0	845	16	0
6	F	748	0	728	9	0
6	S	748	0	728	13	0
7	G	675	0	644	24	0
7	T	675	0	644	29	0
8	H	662	0	623	12	0
8	U	662	0	623	17	0
9	I	601	0	613	7	0
9	V	601	0	613	13	0
10	J	460	0	459	8	0
10	W	460	0	459	8	0
11	K	384	0	366	4	0
11	X	384	0	366	11	0
12	L	380	0	380	14	0
12	Y	380	0	380	9	0
13	M	335	0	352	10	0
13	Z	335	0	352	8	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	3	0
17	N	120	0	108	5	0
18	A	102	0	152	16	0
18	C	102	0	152	10	0
18	N	102	0	152	13	0
18	P	102	0	152	9	0
19	B	2	0	0	0	0
19	O	2	0	0	0	0
20	B	63	0	110	6	0
20	D	63	0	110	6	0
20	L	63	0	110	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	N	126	0	220	19	0
20	O	63	0	110	7	0
21	B	52	0	80	23	0
21	O	52	0	80	21	0
22	B	29	0	39	1	0
22	C	58	0	77	1	0
22	J	29	0	39	2	0
22	O	29	0	39	0	0
22	P	58	0	78	2	0
22	W	29	0	39	4	0
23	C	16	0	23	9	0
23	P	16	0	23	8	0
24	C	33	0	37	5	0
24	M	33	0	37	1	0
24	P	33	0	37	5	0
24	Z	33	0	37	1	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	106	0	154	18	0
26	G	53	0	77	11	0
26	P	106	0	154	17	0
26	T	53	0	77	8	0
27	C	100	0	156	15	0
27	G	100	0	156	15	0
27	P	100	0	156	14	0
27	T	100	0	156	21	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	199	0	0	6	0
29	B	119	0	0	2	0
29	C	82	0	0	2	0
29	D	79	0	0	2	0
29	E	58	0	0	3	0
29	F	64	0	0	2	0
29	G	35	0	0	1	0
29	H	39	0	0	1	0
29	I	29	0	0	4	0
29	J	14	0	0	1	0
29	K	21	0	0	0	0
29	L	17	0	0	2	0
29	M	14	0	0	1	0
29	N	176	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	O	103	0	0	5	0
29	P	74	0	0	3	0
29	Q	46	0	0	2	0
29	R	41	0	0	1	0
29	S	56	0	0	3	0
29	T	30	0	0	3	0
29	U	39	0	0	0	0
29	V	19	0	0	0	0
29	W	14	0	0	2	0
29	X	17	0	0	0	0
29	Y	13	0	0	1	0
29	Z	10	0	0	1	0
All	All	32170	0	31343	685	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 685 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)
10:W:33:ARG:HG2	22:W:101:CHD:H152	1.31	1.10
21:B:303:PSC:H343	21:B:303:PSC:H142	1.31	1.07
21:O:304:PSC:H142	21:O:304:PSC:H343	1.28	1.06
7:G:84:LYS:H	7:G:84:LYS:HD2	1.22	1.05
12:L:20:ARG:HH12	20:L:101:TGL:HC61	1.15	1.05

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	493 (96%)	19 (4%)	0	100	100
1	N	512/514 (100%)	493 (96%)	19 (4%)	0	100	100
2	B	225/227 (99%)	209 (93%)	14 (6%)	2 (1%)	14	14
2	O	225/227 (99%)	206 (92%)	18 (8%)	1 (0%)	30	34
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	140 (99%)	2 (1%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
6	F	96/98 (98%)	87 (91%)	6 (6%)	3 (3%)	3	1
6	S	96/98 (98%)	87 (91%)	5 (5%)	4 (4%)	2	1
7	G	81/85 (95%)	64 (79%)	9 (11%)	8 (10%)	0	0
7	T	81/85 (95%)	65 (80%)	8 (10%)	8 (10%)	0	0
8	H	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	9	8
8	U	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	9	8
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3329 (95%)	147 (4%)	28 (1%)	16	16

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	39	SER
6	S	94	HIS

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	426/426 (100%)	418 (98%)	8 (2%)	50 66
1	N	426/426 (100%)	416 (98%)	10 (2%)	44 59
2	B	210/210 (100%)	199 (95%)	11 (5%)	21 26
2	O	210/210 (100%)	195 (93%)	15 (7%)	13 16
3	C	224/226 (99%)	218 (97%)	6 (3%)	39 53
3	P	224/226 (99%)	219 (98%)	5 (2%)	45 61
4	D	128/129 (99%)	126 (98%)	2 (2%)	55 71
4	Q	128/129 (99%)	125 (98%)	3 (2%)	44 59
5	E	92/95 (97%)	89 (97%)	3 (3%)	33 45
5	R	92/95 (97%)	87 (95%)	5 (5%)	20 25
6	F	81/81 (100%)	78 (96%)	3 (4%)	30 41
6	S	81/81 (100%)	78 (96%)	3 (4%)	30 41
7	G	67/68 (98%)	64 (96%)	3 (4%)	24 33
7	T	67/68 (98%)	64 (96%)	3 (4%)	24 33
8	H	71/75 (95%)	68 (96%)	3 (4%)	26 36
8	U	71/75 (95%)	69 (97%)	2 (3%)	38 52
9	I	57/57 (100%)	54 (95%)	3 (5%)	20 26
9	V	57/57 (100%)	54 (95%)	3 (5%)	20 26
10	J	49/50 (98%)	47 (96%)	2 (4%)	27 37
10	W	49/50 (98%)	48 (98%)	1 (2%)	48 64
11	K	39/46 (85%)	39 (100%)	0	100 100
11	X	39/46 (85%)	37 (95%)	2 (5%)	21 27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	39/40 (98%)	37 (95%)	2 (5%)	21	27
12	Y	39/40 (98%)	38 (97%)	1 (3%)	40	55
13	M	37/38 (97%)	30 (81%)	7 (19%)	1	1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	6
All	All	3040/3082 (99%)	2930 (96%)	110 (4%)	31	42

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	241	PRO
2	O	78	LEU
13	Z	42	LYS
9	V	8	GLN
1	N	369	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	178	GLN
2	O	52	HIS
7	T	66	ASN
1	N	180	GLN
1	N	491	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SAC	I	1	9	7,8,9	2.48	2 (28%)	7,9,11	1.62	2 (28%)
9	SAC	V	1	9	7,8,9	2.85	2 (28%)	7,9,11	1.94	3 (42%)
1	FME	N	1	1	8,9,10	0.84	0	8,9,11	1.14	1 (12%)
1	FME	A	1	1	8,9,10	0.75	0	8,9,11	1.36	1 (12%)
7	TPO	T	11	7	8,10,11	1.38	2 (25%)	10,14,16	1.14	1 (10%)
2	FME	O	1	2	8,9,10	0.65	0	8,9,11	1.66	2 (25%)
2	FME	B	1	2	8,9,10	0.83	0	8,9,11	1.59	2 (25%)
7	TPO	G	11	7	8,10,11	1.78	1 (12%)	10,14,16	1.09	0

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.25	1.35	1.23
9	I	1	SAC	OAC-C1A	5.18	1.34	1.23
9	V	1	SAC	CA-N	5.01	1.53	1.46
7	G	11	TPO	CB-CA	3.81	1.61	1.53
9	I	1	SAC	CA-N	3.75	1.52	1.46

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	C-CA-N	3.70	116.64	109.50
2	B	1	FME	C-CA-N	3.09	115.47	109.50
1	A	1	FME	CA-N-CN	-2.97	118.25	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	C2A-C1A-N	2.94	121.00	116.12
2	B	1	FME	CA-N-CN	-2.76	118.58	122.82

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	N	1	FME	2	0
1	A	1	FME	4	0
7	T	11	TPO	1	0
2	O	1	FME	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 46 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
26	PEK	C	306	-	52,52,52	1.70	9 (17%)	55,57,57	1.12	5 (9%)
20	TGL	N	607	-	62,62,62	0.91	2 (3%)	65,65,65	1.39	9 (13%)
20	TGL	D	201	-	62,62,62	1.01	4 (6%)	65,65,65	1.44	11 (16%)
22	CHD	J	101	-	32,32,32	1.05	2 (6%)	51,51,51	3.66	25 (49%)
24	DMU	P	302	-	34,34,34	2.65	13 (38%)	45,45,45	4.22	18 (40%)
24	DMU	Z	101	-	34,34,34	3.08	10 (29%)	45,45,45	4.12	19 (42%)
18	PGV	C	308	-	50,50,50	1.47	6 (12%)	53,56,56	0.88	2 (3%)
26	PEK	G	102	-	52,52,52	1.92	12 (23%)	55,57,57	1.30	5 (9%)
27	CDL	G	101	-	99,99,99	1.21	10 (10%)	105,111,111	0.99	9 (8%)
22	CHD	O	302	-	32,32,32	0.77	0	51,51,51	1.89	14 (27%)
18	PGV	A	606	-	50,50,50	1.18	3 (6%)	53,56,56	1.06	5 (9%)
20	TGL	B	302	-	62,62,62	0.81	2 (3%)	65,65,65	1.62	13 (20%)
22	CHD	C	304	-	32,32,32	0.97	2 (6%)	51,51,51	1.98	13 (25%)
24	DMU	C	302	-	34,34,34	2.77	14 (41%)	45,45,45	4.13	18 (40%)
26	PEK	P	306	-	52,52,52	1.67	10 (19%)	55,57,57	1.13	5 (9%)
20	TGL	L	101	-	62,62,62	1.33	6 (9%)	65,65,65	1.82	12 (18%)
27	CDL	P	309	-	99,99,99	0.96	7 (7%)	105,111,111	1.02	6 (5%)
23	DCW	P	301	3	17,17,17	1.64	4 (23%)	21,21,21	0.89	1 (4%)
22	CHD	P	304	-	32,32,32	0.80	1 (3%)	51,51,51	1.89	14 (27%)
20	TGL	N	606	-	62,62,62	1.45	6 (9%)	65,65,65	1.78	14 (21%)
23	DCW	C	301	3	17,17,17	1.37	2 (11%)	21,21,21	1.03	2 (9%)
17	HEA	N	605	1	67,67,67	1.27	6 (8%)	81,103,103	1.46	13 (16%)
18	PGV	C	307	-	50,50,50	0.99	3 (6%)	53,56,56	1.00	5 (9%)
27	CDL	C	309	-	99,99,99	0.92	5 (5%)	105,111,111	1.01	7 (6%)
19	CUA	O	301	2	0,1,1	-	-	-	-	-
22	CHD	P	310	-	32,32,32	0.96	1 (3%)	51,51,51	3.56	26 (50%)
22	CHD	W	101	-	32,32,32	1.18	2 (6%)	51,51,51	3.70	26 (50%)
18	PGV	A	607	-	50,50,50	1.01	3 (6%)	53,56,56	1.08	3 (5%)
27	CDL	T	102	-	99,99,99	1.19	11 (11%)	105,111,111	1.02	9 (8%)
19	CUA	B	301	2	0,1,1	-	-	-	-	-
21	PSC	B	303	-	51,51,51	1.34	5 (9%)	57,59,59	1.04	1 (1%)
26	PEK	C	305	-	52,52,52	1.44	5 (9%)	55,57,57	1.04	2 (3%)
18	PGV	N	608	-	50,50,50	1.22	4 (8%)	53,56,56	1.04	4 (7%)
17	HEA	N	604	1	67,67,67	1.21	5 (7%)	81,103,103	1.38	10 (12%)
18	PGV	N	609	-	50,50,50	1.13	4 (8%)	53,56,56	1.13	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	HEA	A	605	1	67,67,67	1.45	12 (17%)	81,103,103	1.42	10 (12%)
18	PGV	P	308	-	50,50,50	1.46	7 (14%)	53,56,56	0.91	3 (5%)
18	PGV	P	307	-	50,50,50	0.95	2 (4%)	53,56,56	0.88	2 (3%)
24	DMU	M	101	-	34,34,34	3.19	8 (23%)	45,45,45	4.21	19 (42%)
17	HEA	A	604	1	67,67,67	1.24	5 (7%)	81,103,103	1.25	9 (11%)
21	PSC	O	304	-	51,51,51	1.31	4 (7%)	57,59,59	1.06	3 (5%)
26	PEK	P	305	-	52,52,52	1.52	7 (13%)	55,57,57	1.11	5 (9%)
22	CHD	B	304	-	32,32,32	0.93	1 (3%)	51,51,51	1.89	11 (21%)
22	CHD	C	310	-	32,32,32	1.05	2 (6%)	51,51,51	3.50	27 (52%)
20	TGL	O	303	-	62,62,62	0.89	2 (3%)	65,65,65	1.56	10 (15%)
26	PEK	T	101	-	52,52,52	2.07	13 (25%)	55,57,57	1.31	5 (9%)

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
26	PEK	C	306	-	-	16/56/56/56	-
22	CHD	J	101	-	5/5/12/12	8/9/74/74	0/4/4/4
20	TGL	D	201	-	-	15/65/65/65	-
20	TGL	N	607	-	-	16/65/65/65	-
24	DMU	P	302	-	6/6/10/10	10/19/59/59	0/2/2/2
24	DMU	Z	101	-	5/5/10/10	9/19/59/59	0/2/2/2
18	PGV	C	308	-	-	34/55/55/55	-
26	PEK	G	102	-	-	29/56/56/56	-
27	CDL	G	101	-	-	61/110/110/110	-
22	CHD	O	302	-	-	3/9/74/74	0/4/4/4
18	PGV	A	606	-	-	33/55/55/55	-
20	TGL	B	302	-	-	13/65/65/65	-
22	CHD	C	304	-	-	2/9/74/74	0/4/4/4
24	DMU	C	302	-	6/6/10/10	9/19/59/59	0/2/2/2
26	PEK	P	306	-	-	17/56/56/56	-
20	TGL	L	101	-	-	15/65/65/65	-
27	CDL	P	309	-	-	69/110/110/110	-
23	DCW	P	301	3	-	2/8/24/24	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	P	304	-	-	2/9/74/74	0/4/4/4
20	TGL	N	606	-	-	17/65/65/65	-
23	DCW	C	301	3	-	3/8/24/24	0/2/2/2
17	HEA	N	605	1	-	7/36/76/76	-
18	PGV	C	307	-	-	15/55/55/55	-
27	CDL	C	309	-	-	70/110/110/110	-
22	CHD	P	310	-	5/5/12/12	8/9/74/74	0/4/4/4
22	CHD	W	101	-	5/5/12/12	8/9/74/74	0/4/4/4
18	PGV	A	607	-	-	12/55/55/55	-
27	CDL	T	102	-	-	61/110/110/110	-
21	PSC	B	303	-	-	39/55/55/55	-
26	PEK	C	305	-	-	25/56/56/56	-
18	PGV	N	608	-	-	32/55/55/55	-
17	HEA	N	604	1	-	7/36/76/76	-
18	PGV	N	609	-	-	12/55/55/55	-
17	HEA	A	605	1	-	6/36/76/76	-
18	PGV	P	308	-	-	34/55/55/55	-
18	PGV	P	307	-	-	14/55/55/55	-
24	DMU	M	101	-	5/5/10/10	10/19/59/59	0/2/2/2
17	HEA	A	604	1	-	10/36/76/76	-
21	PSC	O	304	-	-	38/55/55/55	-
26	PEK	P	305	-	-	25/56/56/56	-
22	CHD	B	304	-	-	2/9/74/74	0/4/4/4
22	CHD	C	310	-	5/5/12/12	8/9/74/74	0/4/4/4
20	TGL	O	303	-	-	13/65/65/65	-
26	PEK	T	101	-	-	29/56/56/56	-

The worst 5 of 242 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	101	DMU	O7-C3	-7.59	1.24	1.43
24	M	101	DMU	O16-C6	-7.32	1.28	1.40
24	Z	101	DMU	O7-C3	-7.11	1.25	1.43
24	M	101	DMU	O1-C9	-6.73	1.27	1.44
24	Z	101	DMU	O16-C18	-6.70	1.24	1.43

The worst 5 of 435 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	302	DMU	O16-C6-C1	11.55	125.81	108.27
24	C	302	DMU	O16-C6-C1	11.24	125.34	108.27
22	P	310	CHD	C17-C13-C14	10.84	110.98	100.11
22	J	101	CHD	C17-C13-C14	10.60	110.75	100.11
22	W	101	CHD	C17-C13-C14	10.53	110.68	100.11

5 of 42 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	310	CHD	C9
22	C	310	CHD	C8
22	C	310	CHD	C12
22	C	310	CHD	C14
22	C	310	CHD	C3

5 of 868 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C04-O12-P-O11
18	A	606	PGV	C04-O12-P-O13
18	A	606	PGV	C04-O12-P-O14
18	A	606	PGV	C02-C03-O11-P
18	A	606	PGV	C05-C04-O12-P

There are no ring outliers.

41 monomers are involved in 283 short contacts:

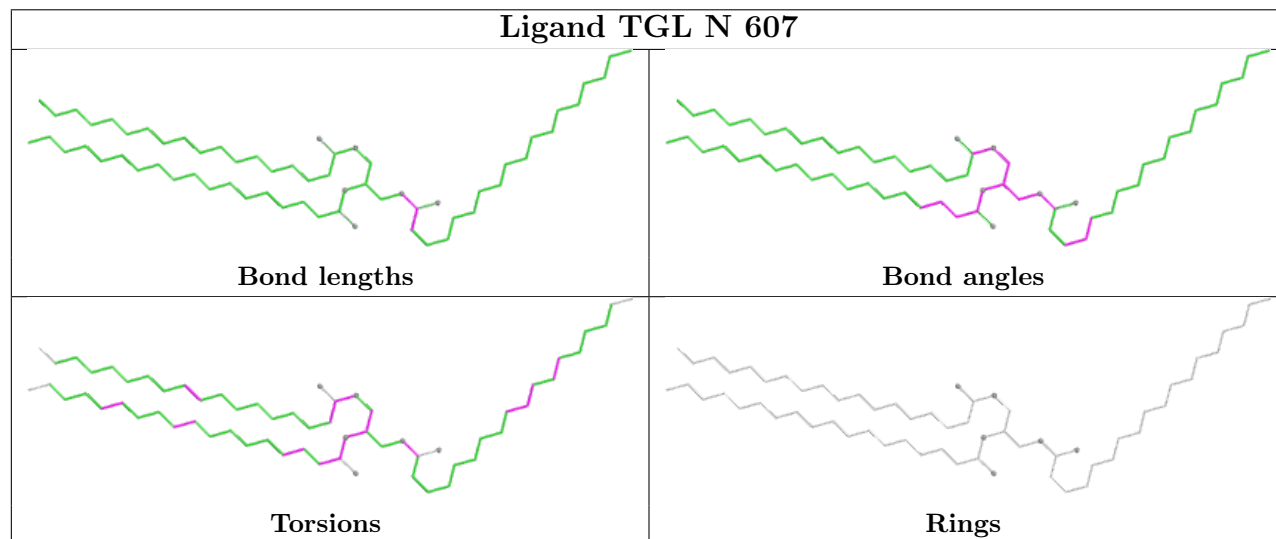
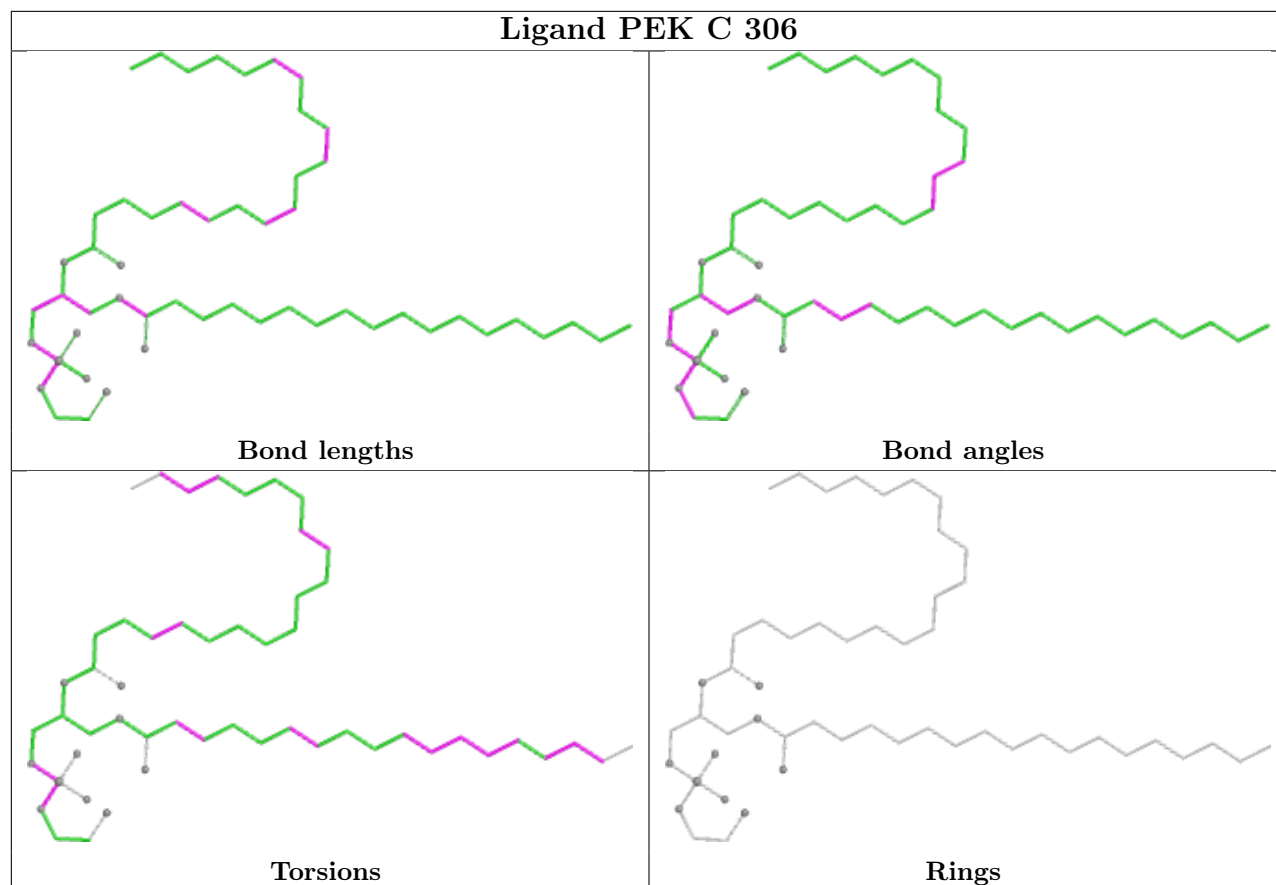
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	306	PEK	7	0
20	N	607	TGL	5	0
20	D	201	TGL	6	0
22	J	101	CHD	2	0
24	P	302	DMU	5	0
24	Z	101	DMU	1	0
18	C	308	PGV	1	0
26	G	102	PEK	11	0
27	G	101	CDL	15	0
18	A	606	PGV	8	0
20	B	302	TGL	6	0
24	C	302	DMU	5	0
26	P	306	PEK	6	0

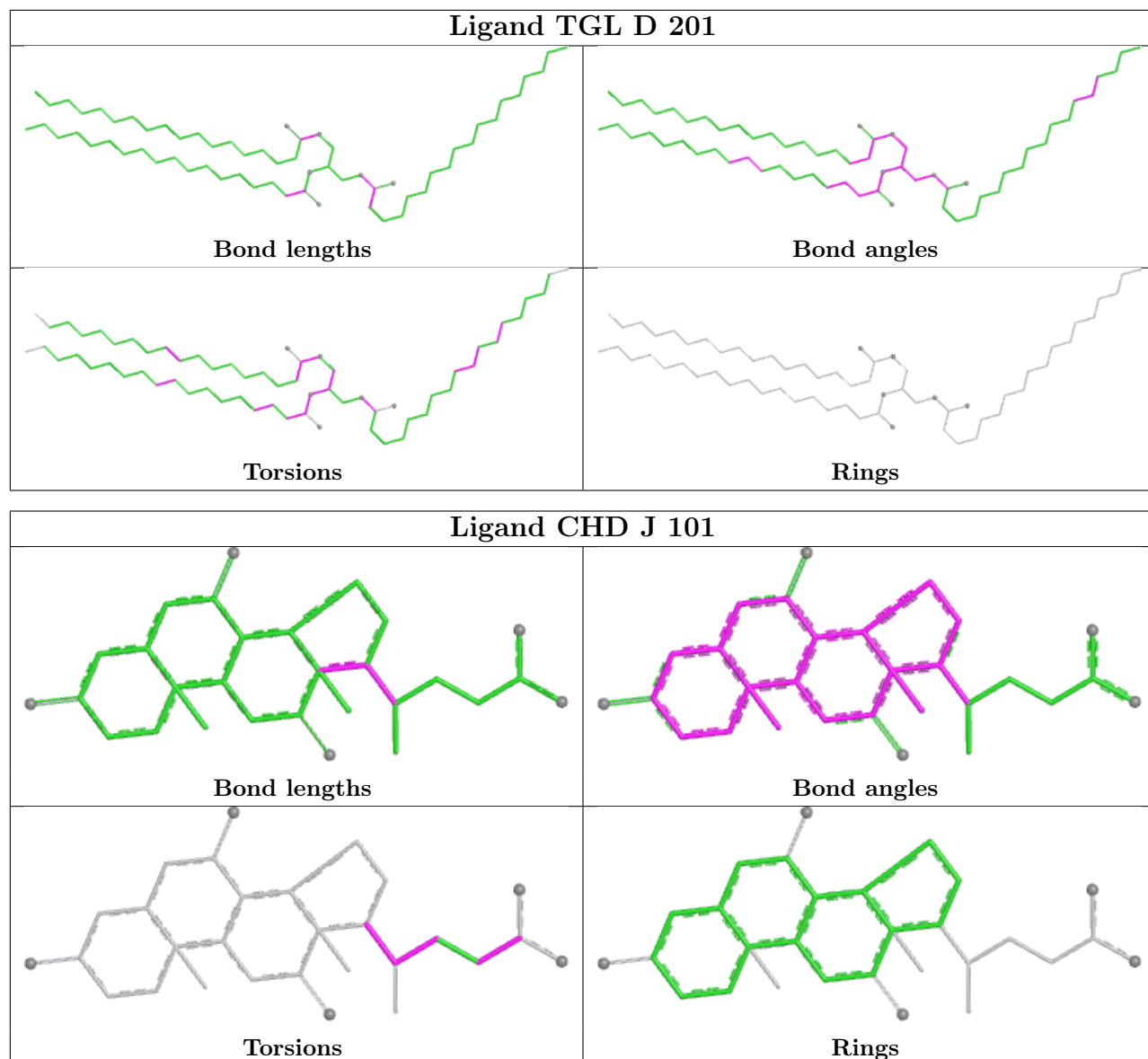
Continued on next page...

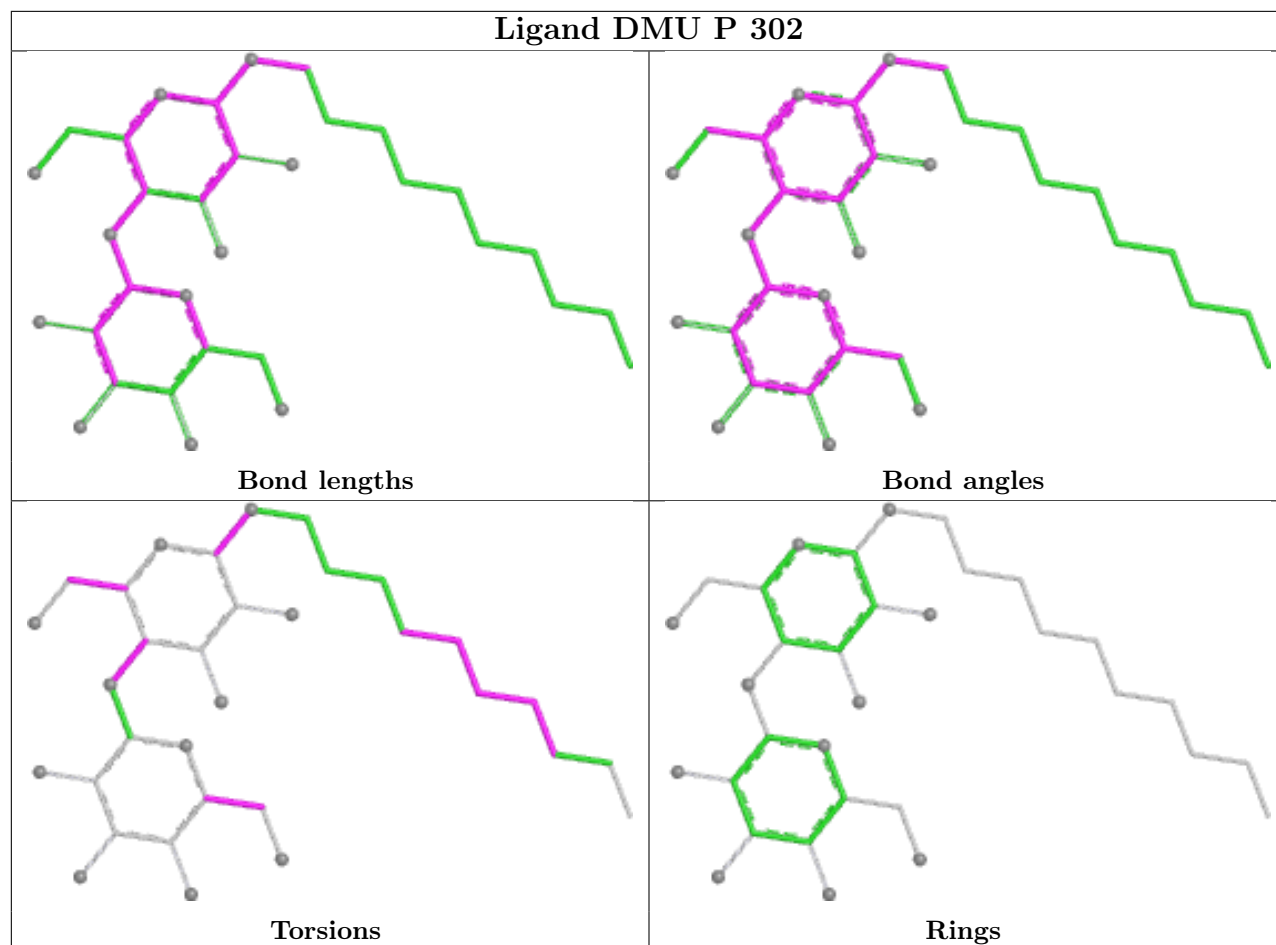
Continued from previous page...

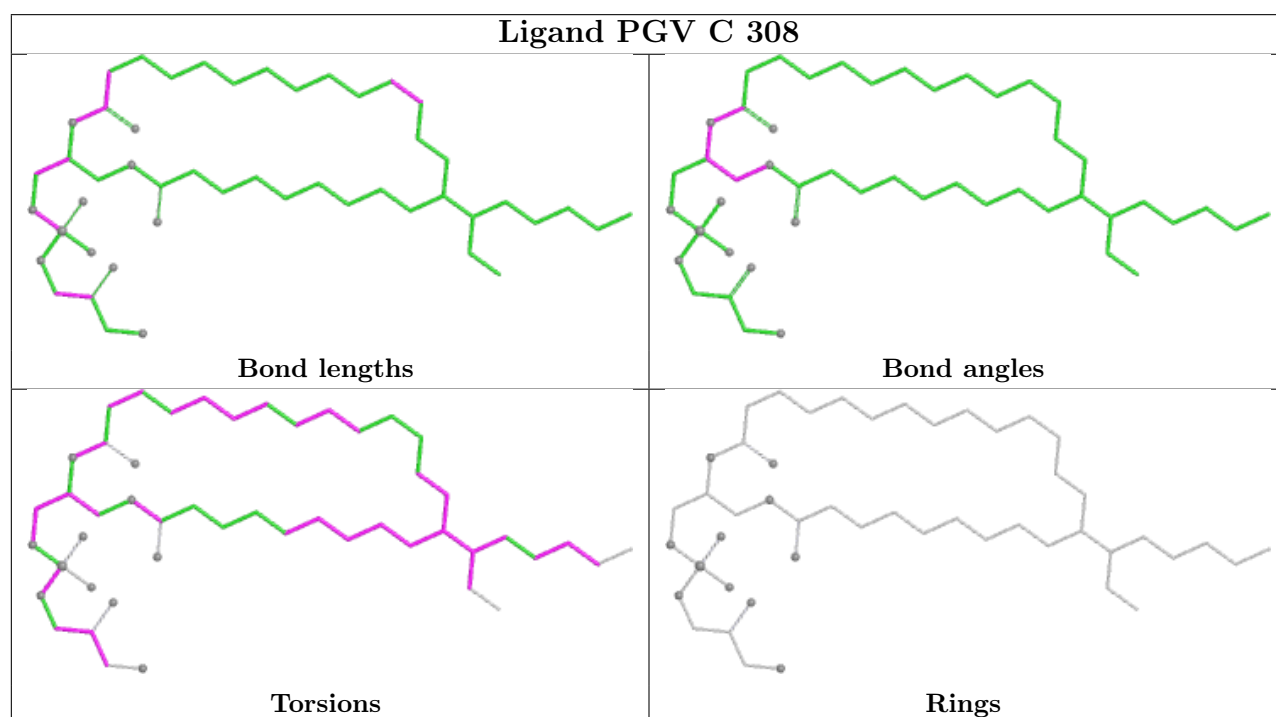
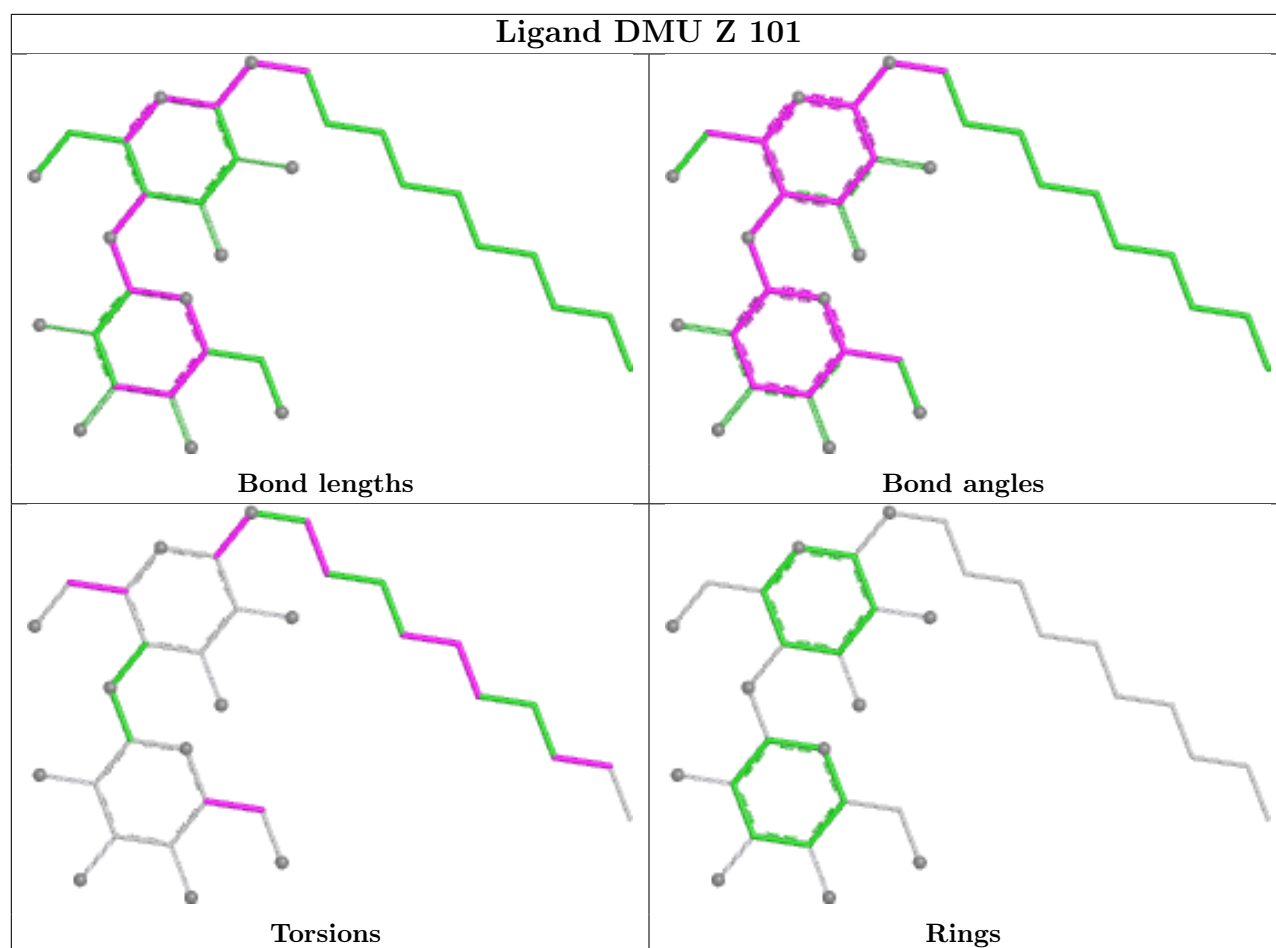
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	L	101	TGL	23	0
27	P	309	CDL	14	0
23	P	301	DCW	8	0
20	N	606	TGL	14	0
23	C	301	DCW	9	0
17	N	605	HEA	2	0
18	C	307	PGV	9	0
27	C	309	CDL	15	0
22	P	310	CHD	2	0
22	W	101	CHD	4	0
18	A	607	PGV	8	0
27	T	102	CDL	21	0
21	B	303	PSC	23	0
26	C	305	PEK	11	0
18	N	608	PGV	7	0
17	N	604	HEA	3	0
18	N	609	PGV	6	0
17	A	605	HEA	2	0
18	P	308	PGV	1	0
18	P	307	PGV	8	0
24	M	101	DMU	1	0
17	A	604	HEA	1	0
21	O	304	PSC	21	0
26	P	305	PEK	11	0
22	B	304	CHD	1	0
22	C	310	CHD	1	0
20	O	303	TGL	7	0
26	T	101	PEK	8	0

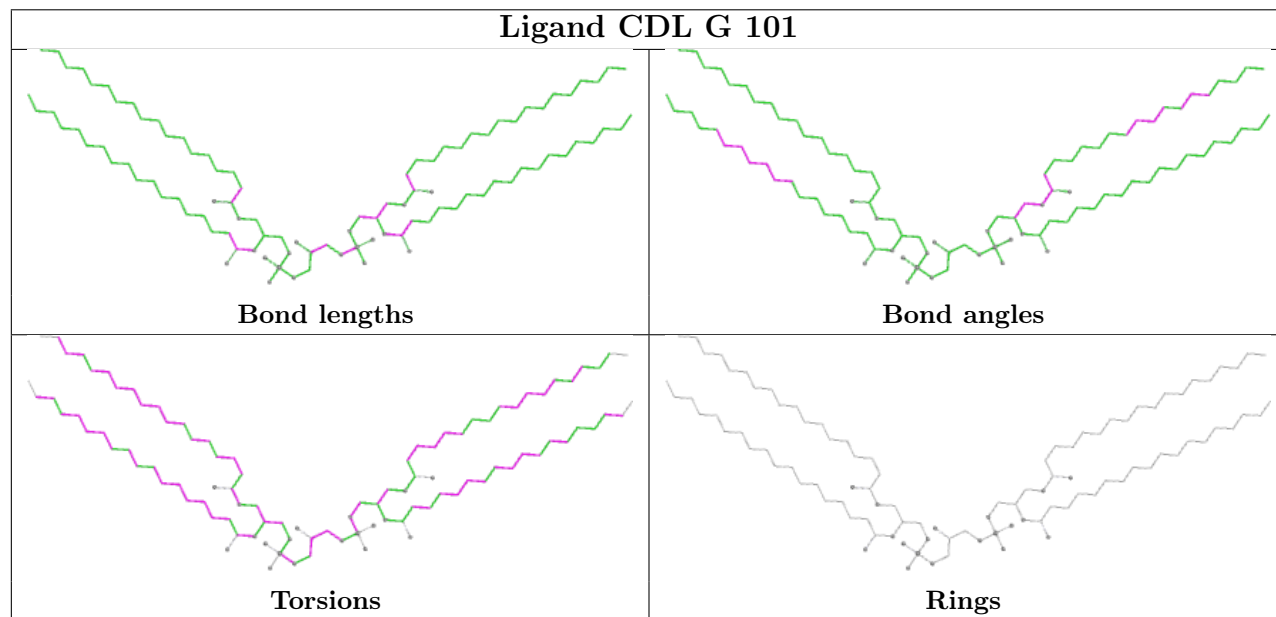
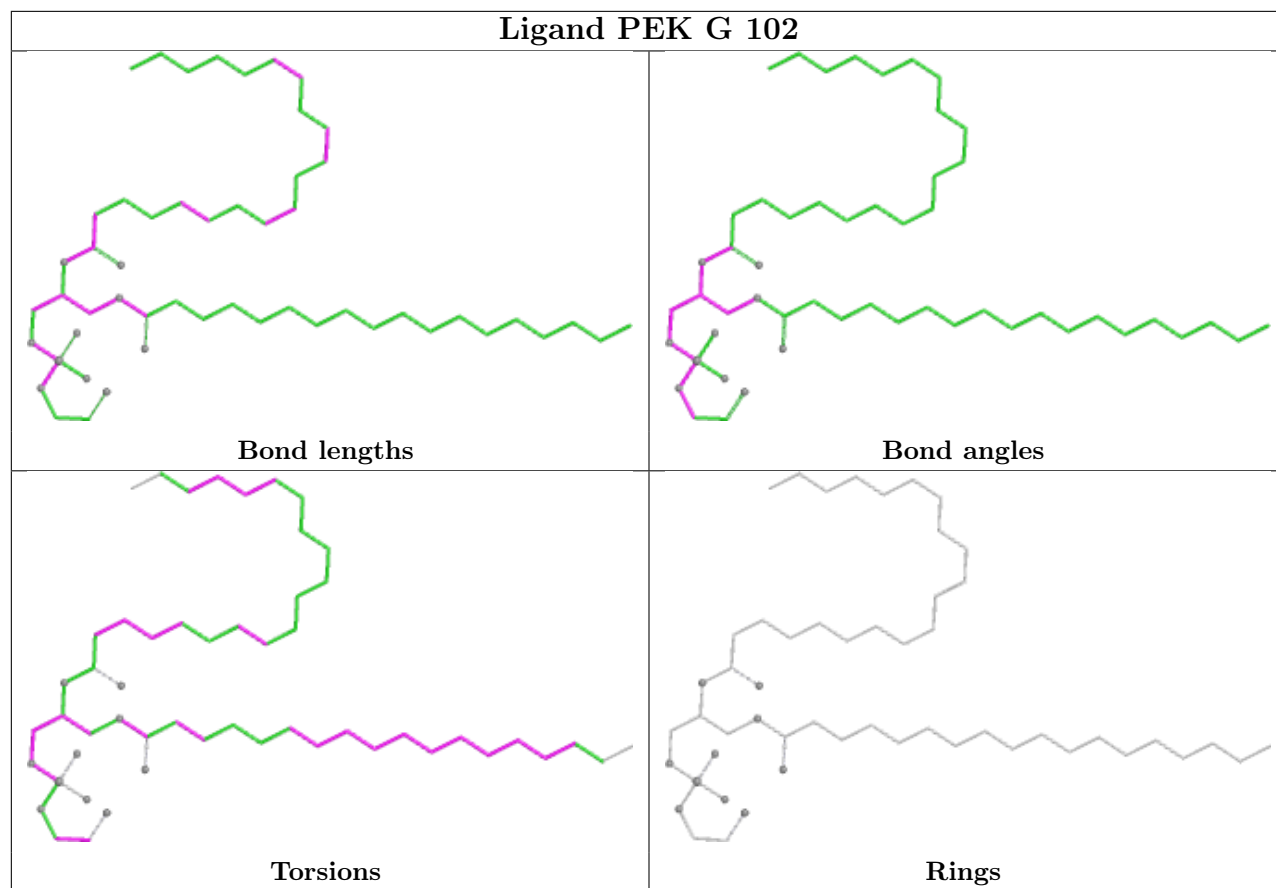
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

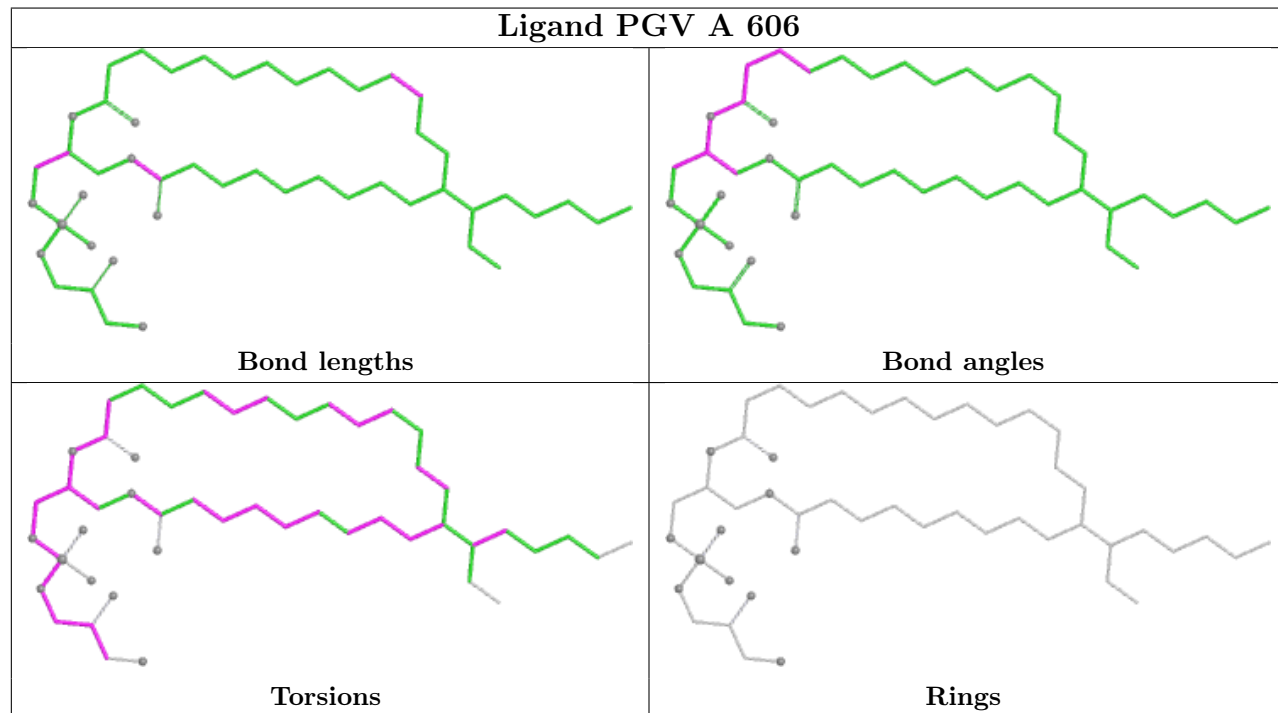
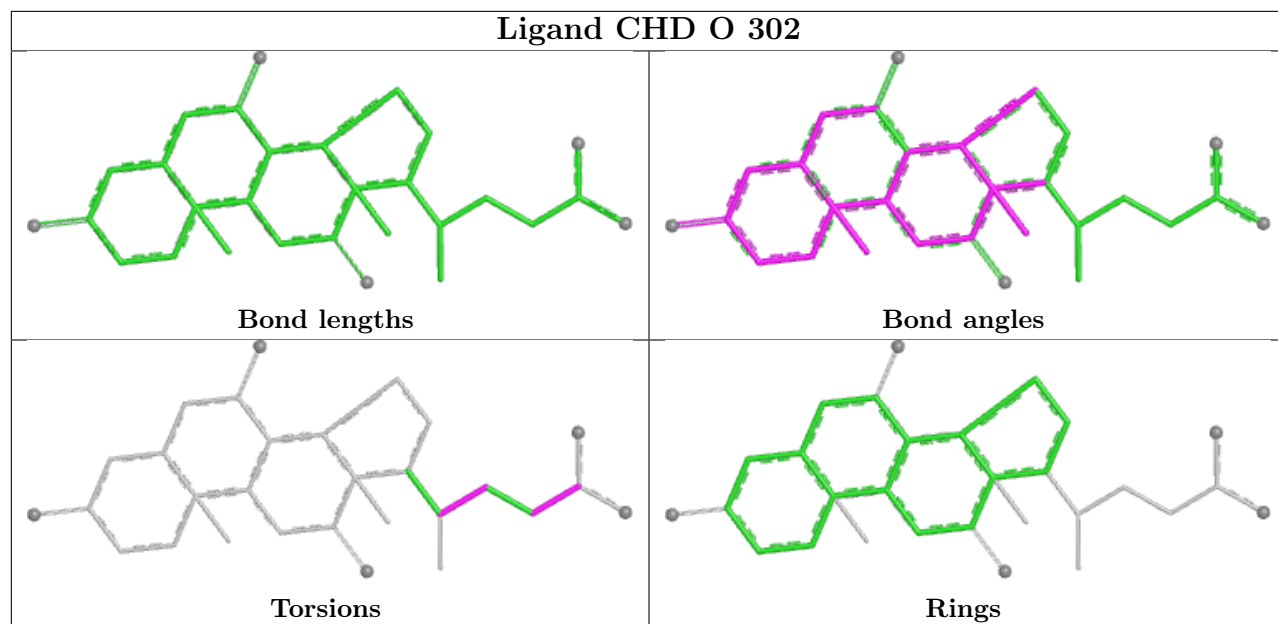


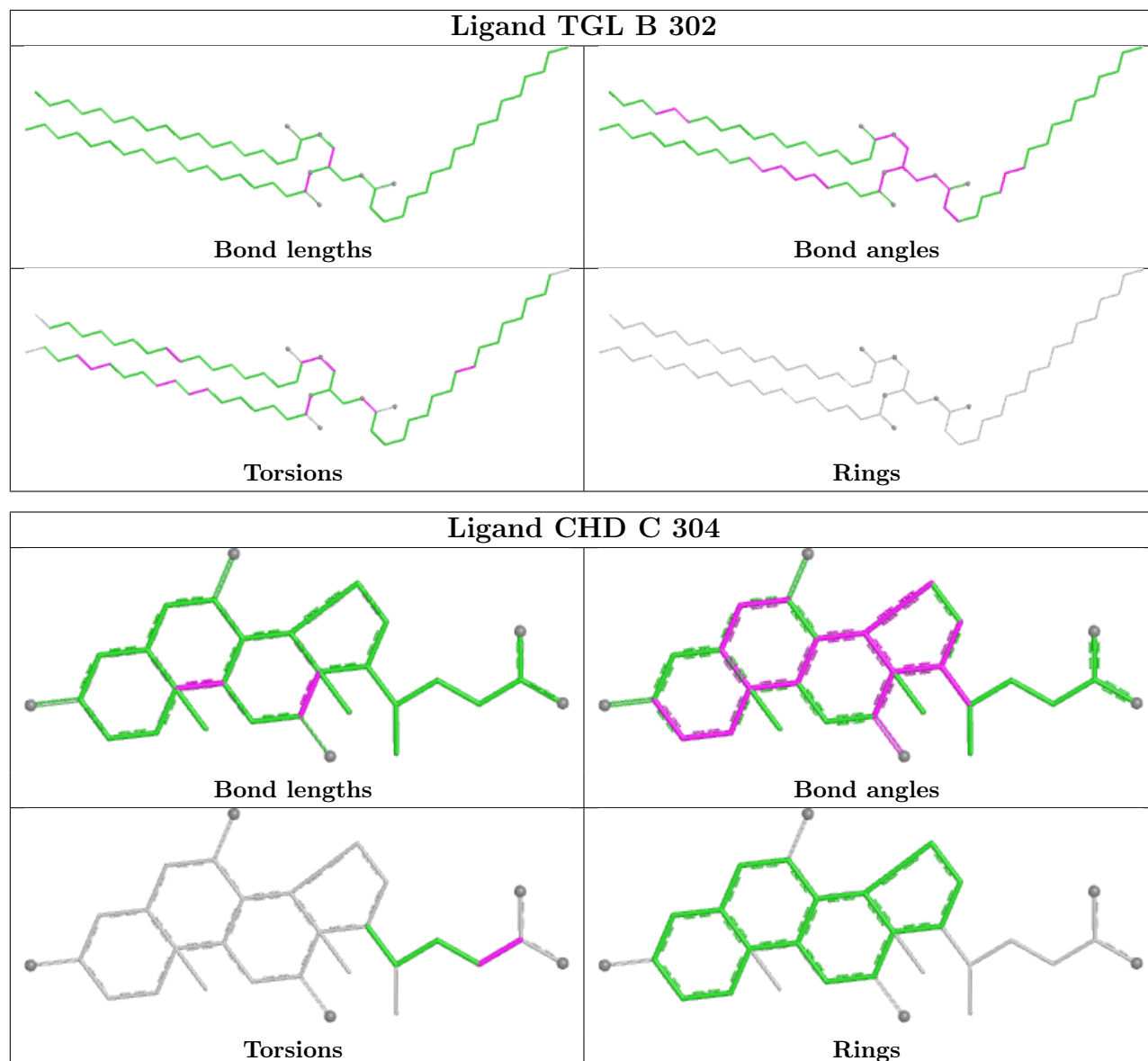


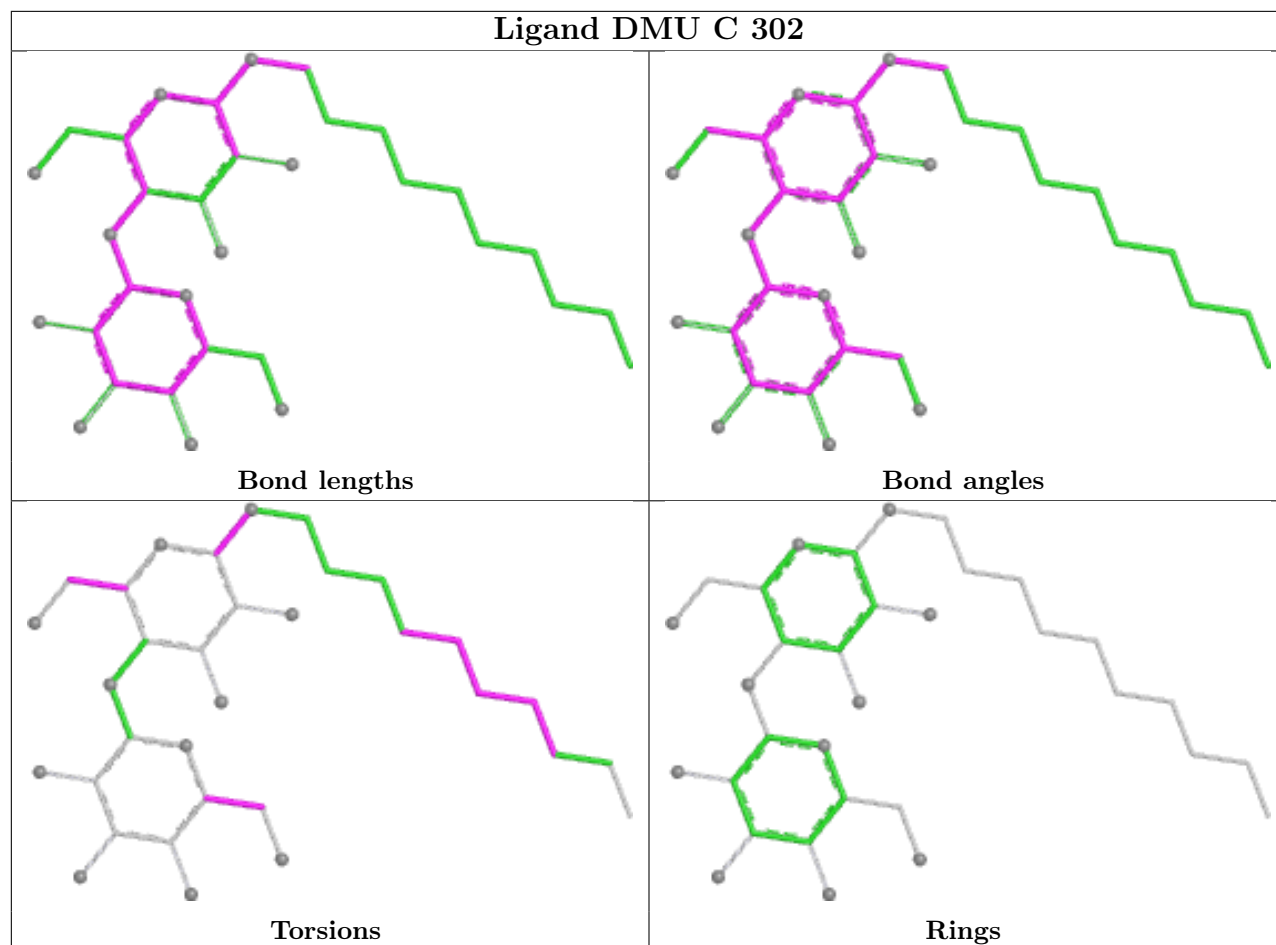


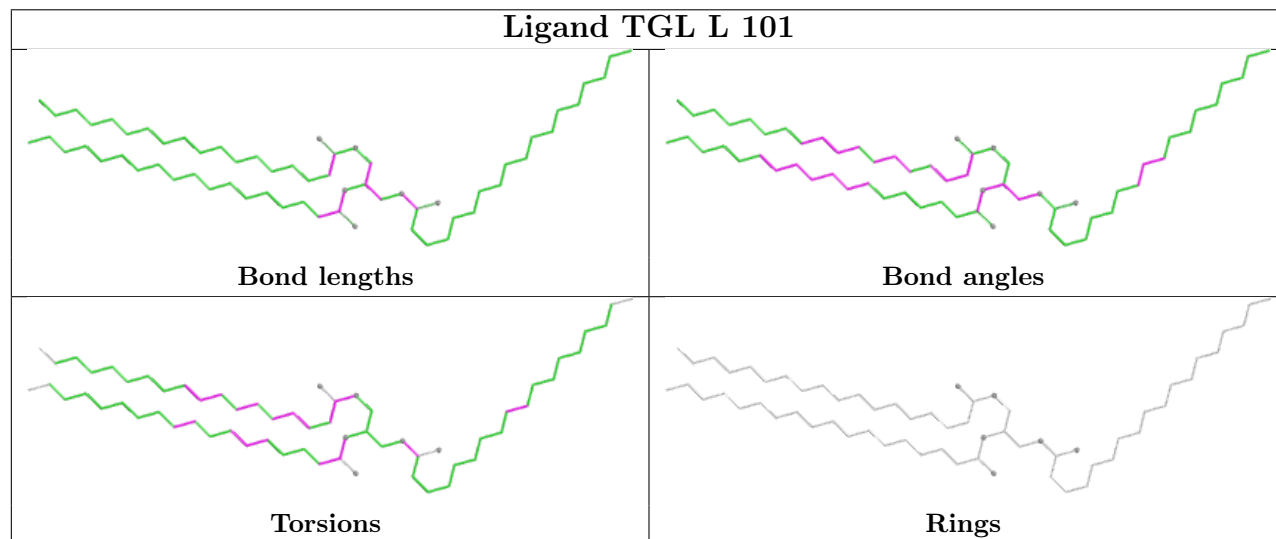
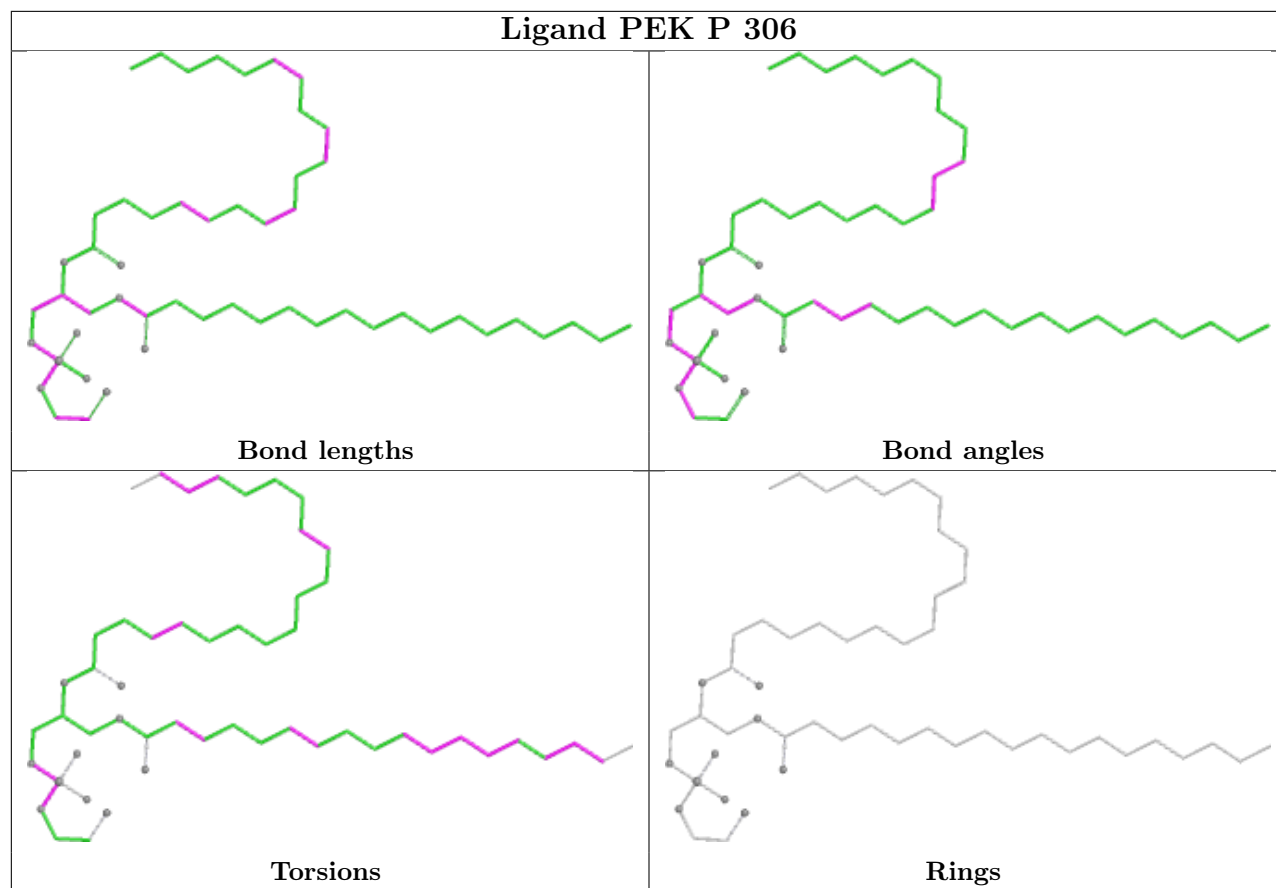


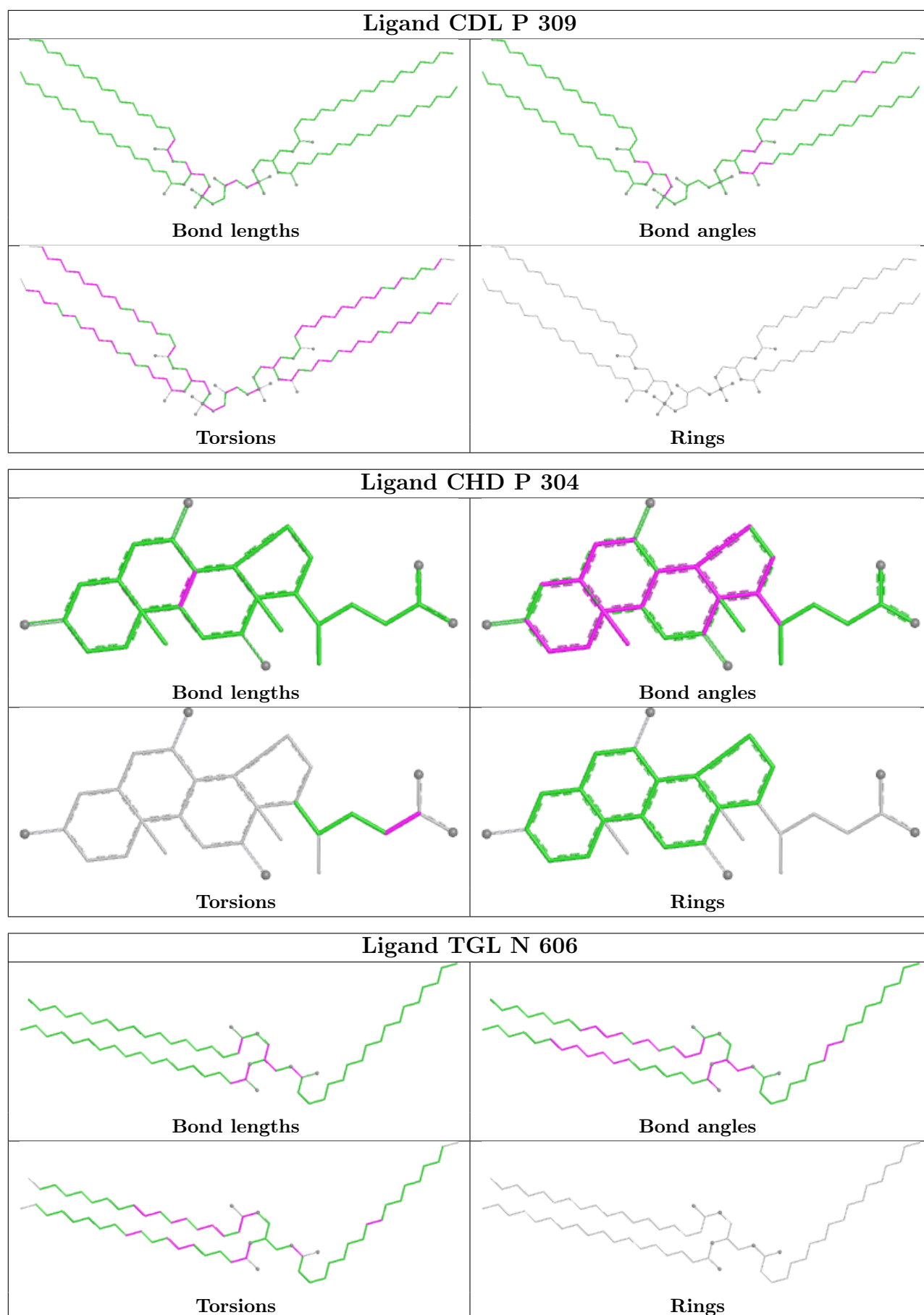


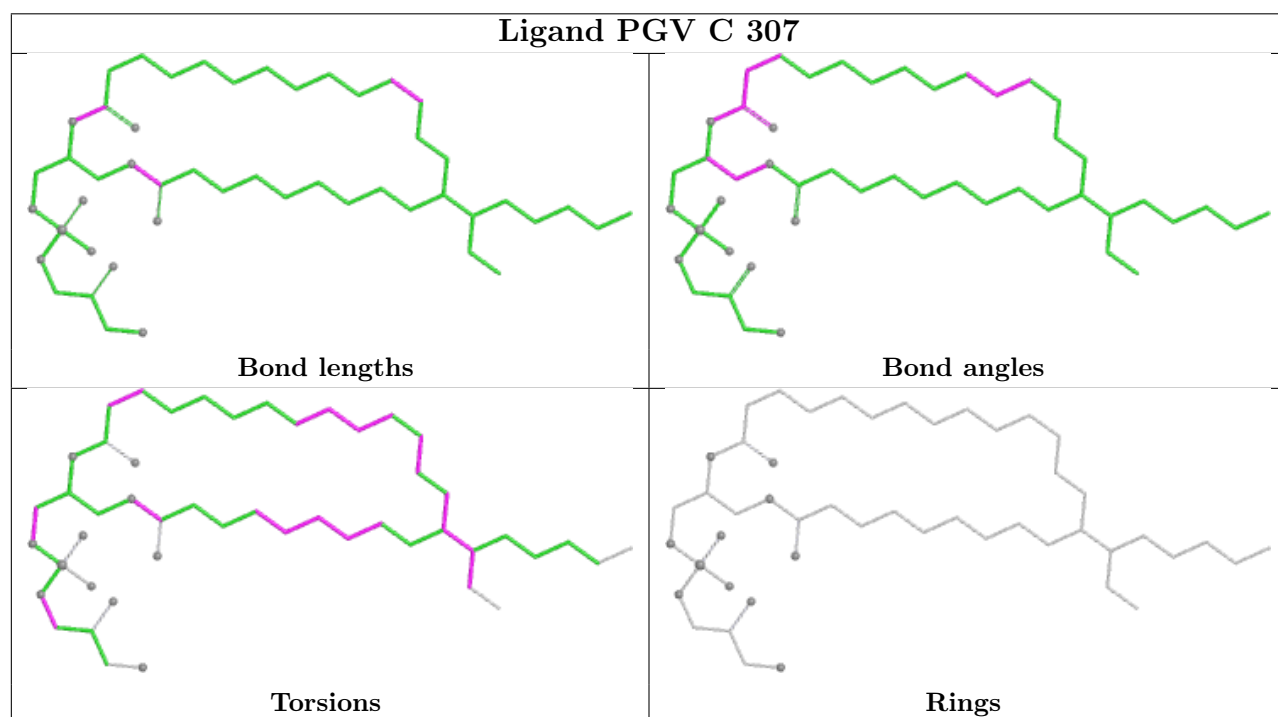
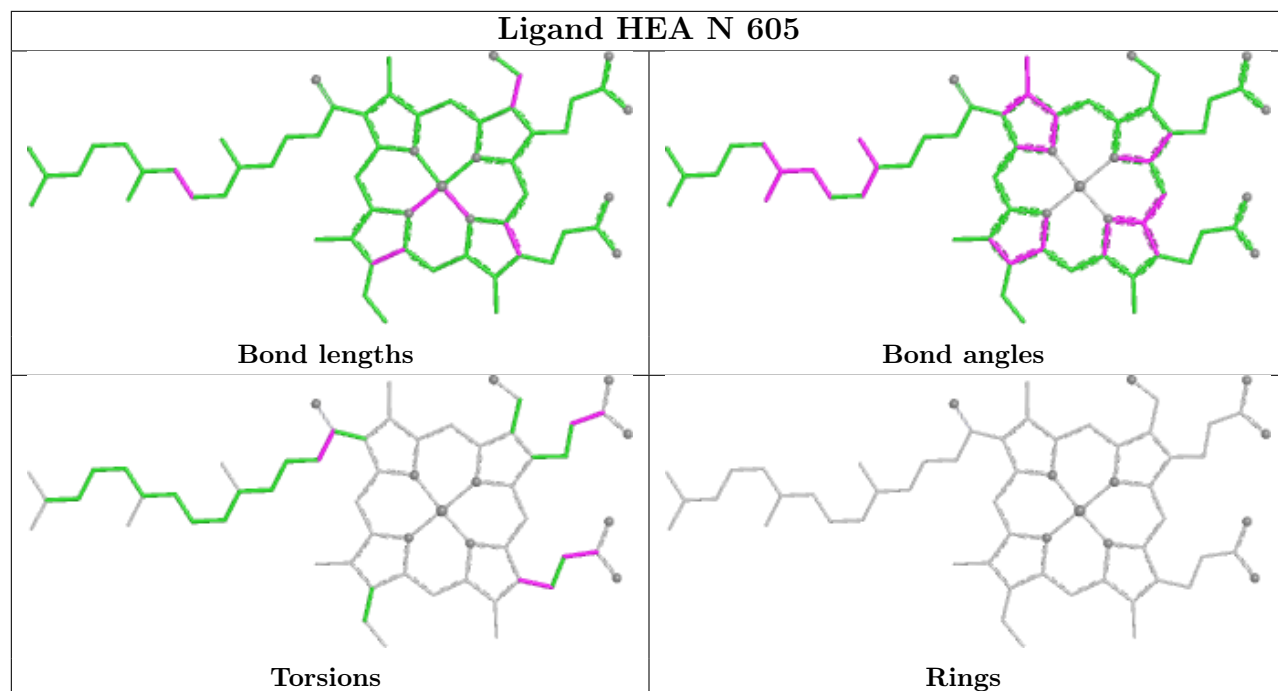


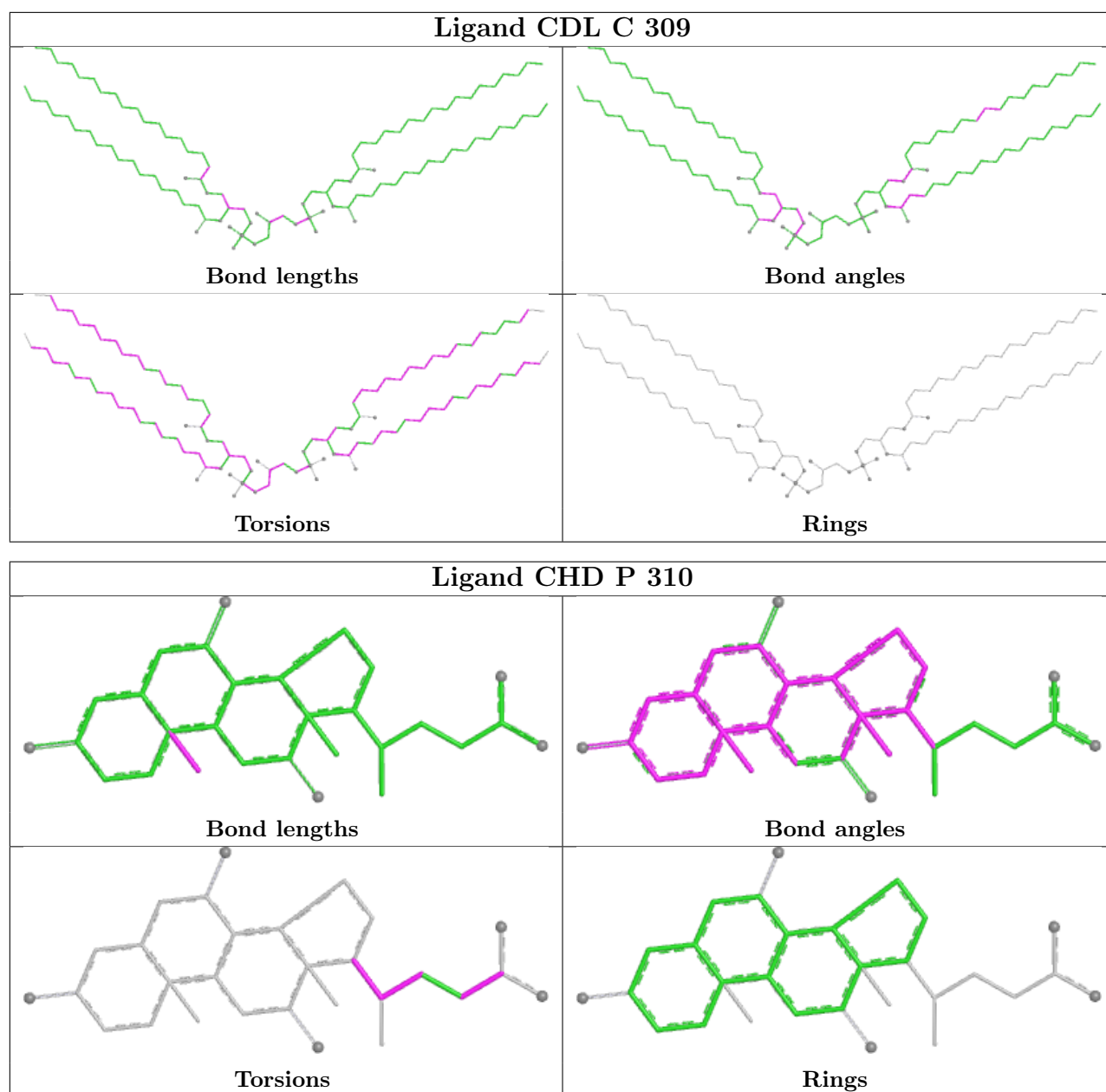


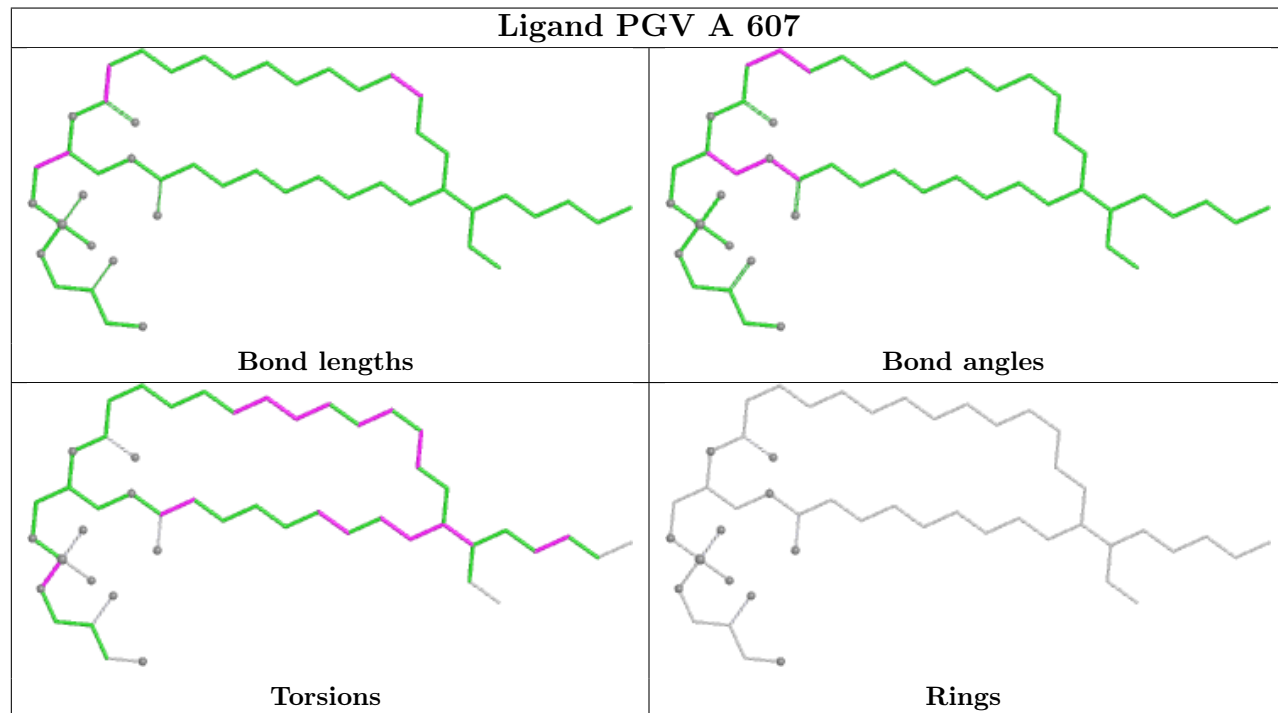
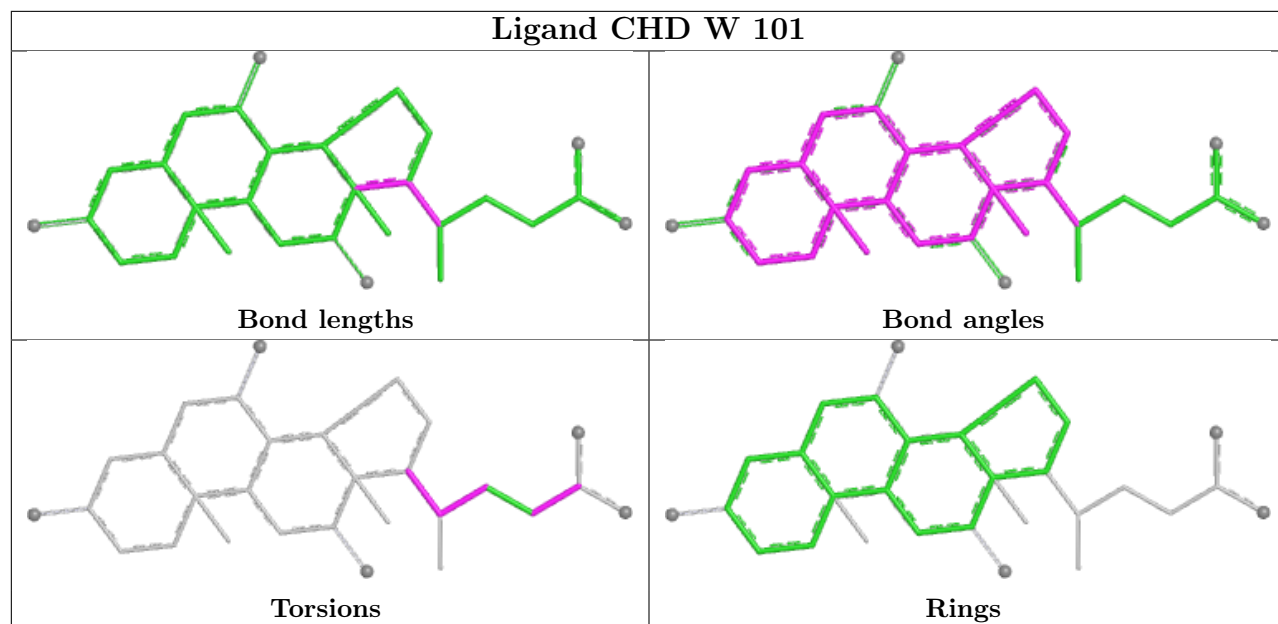


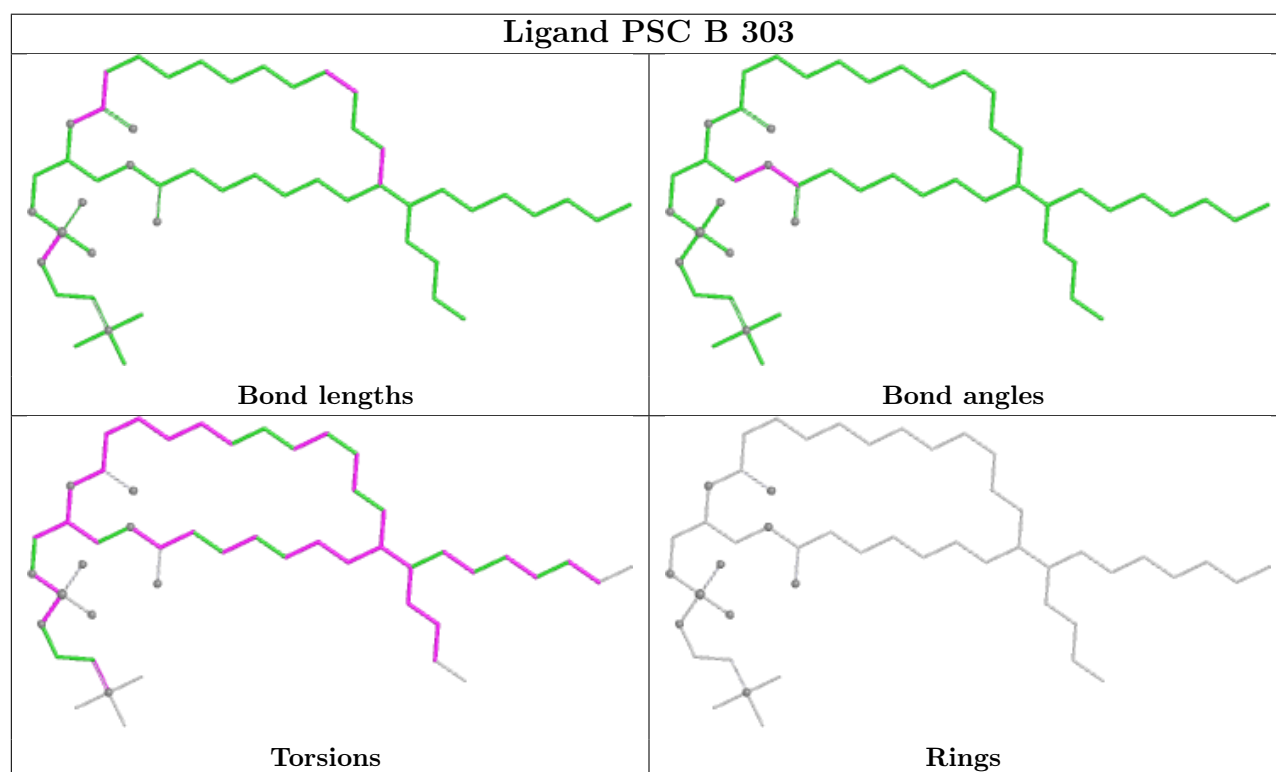
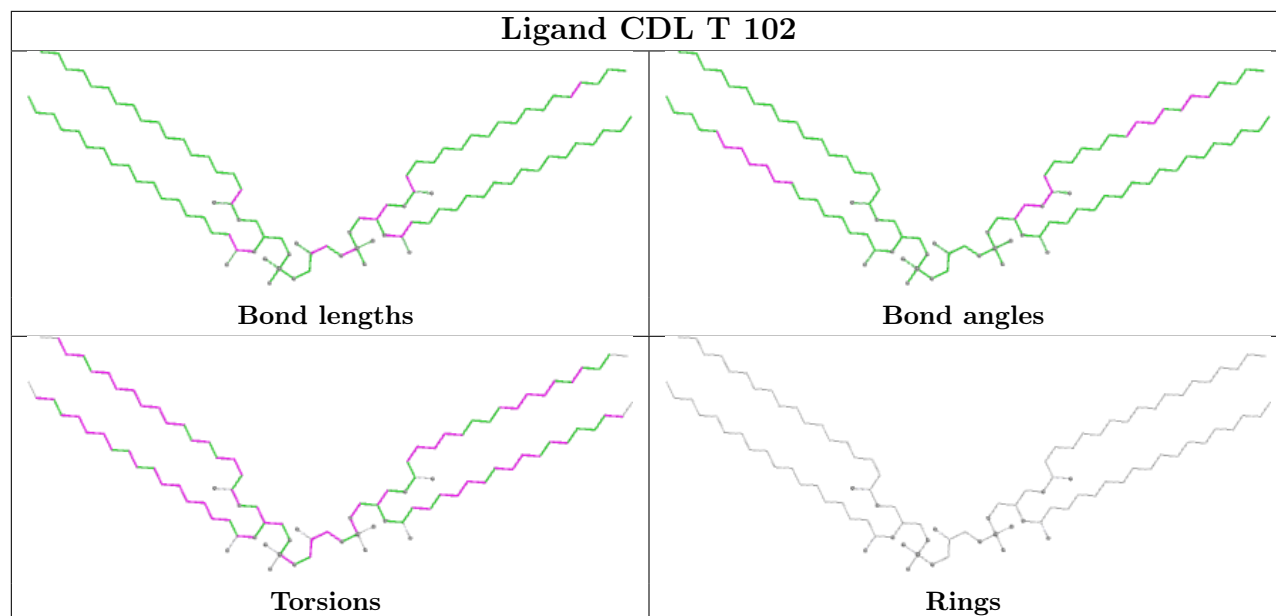


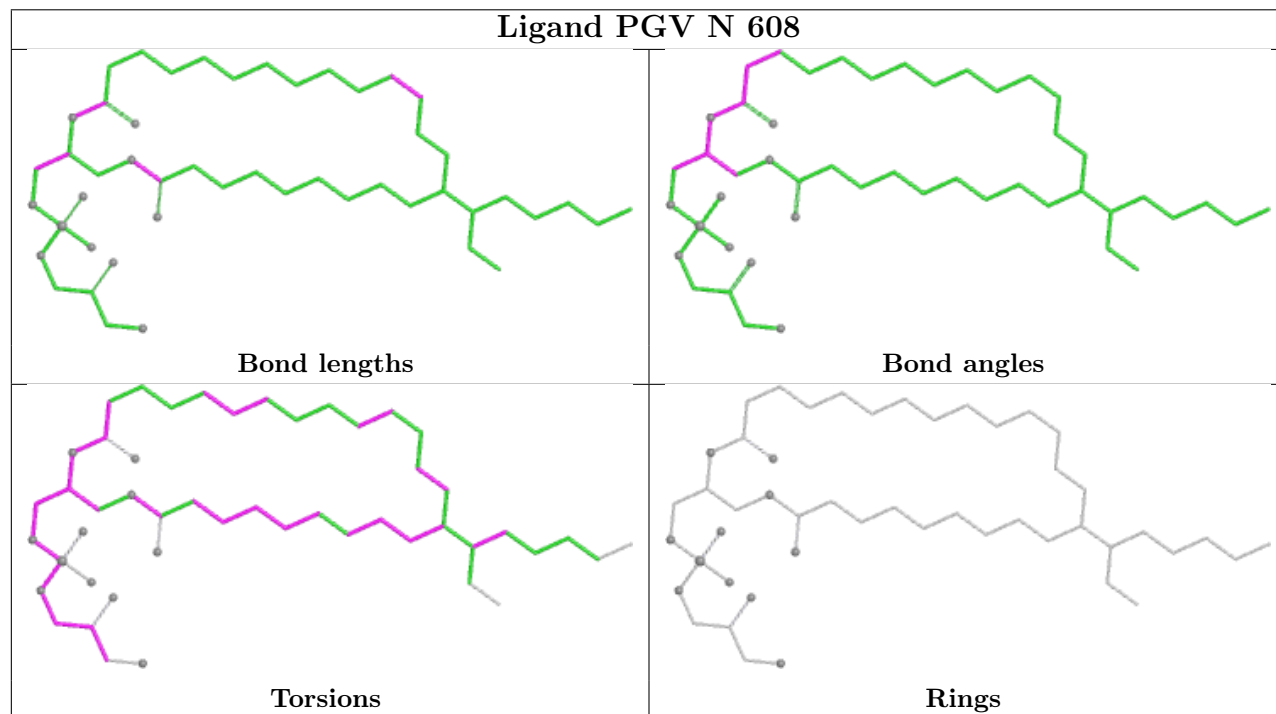
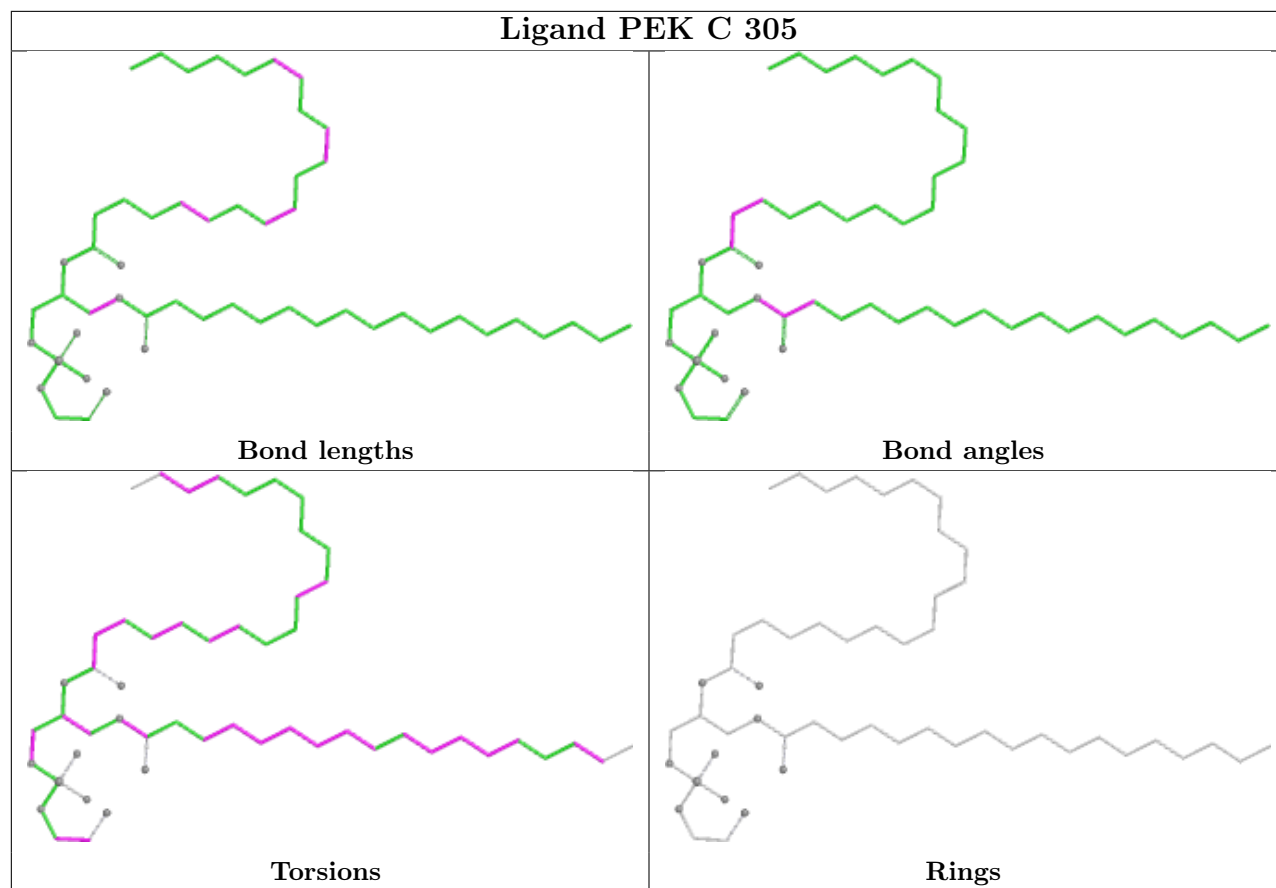


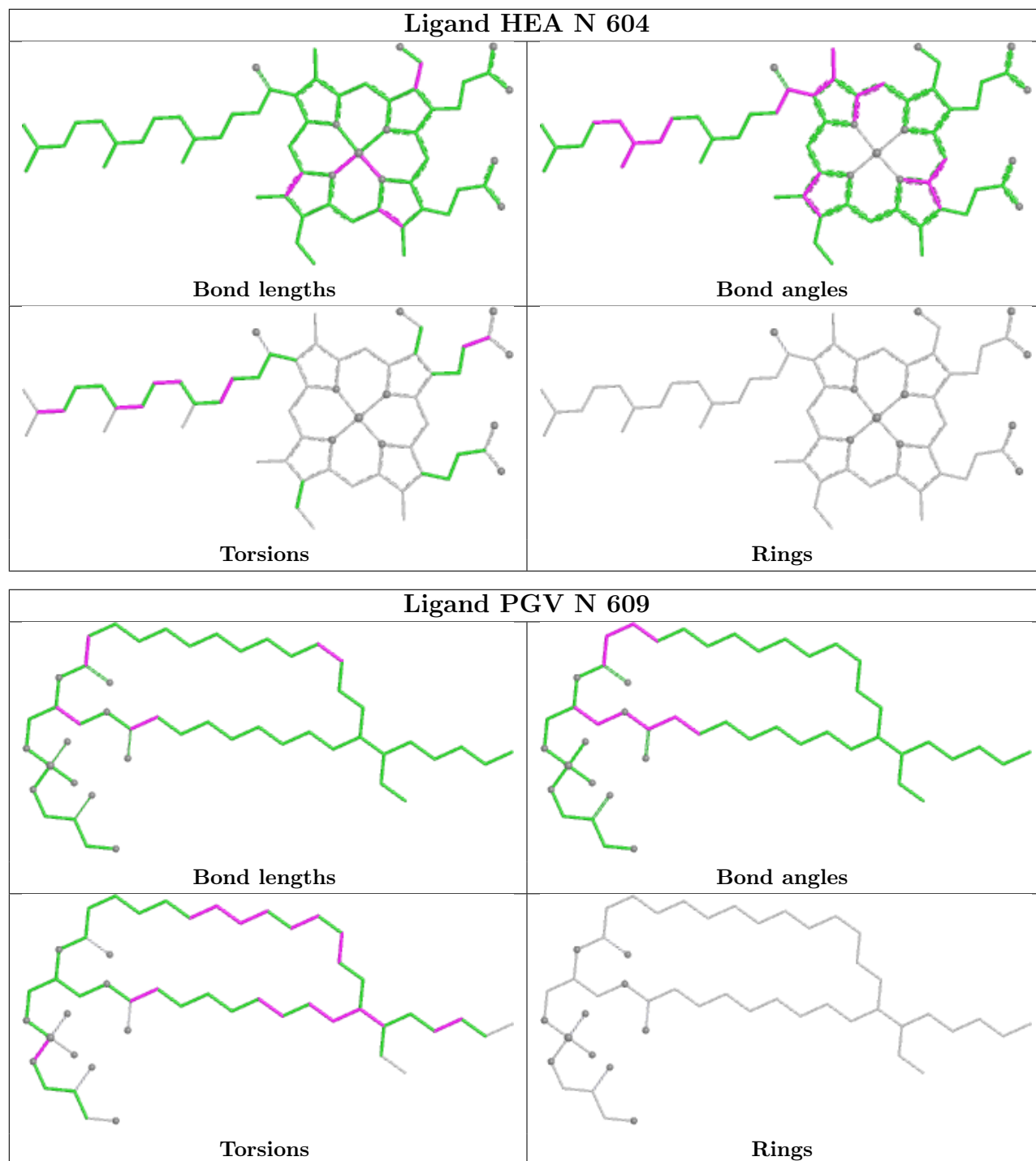


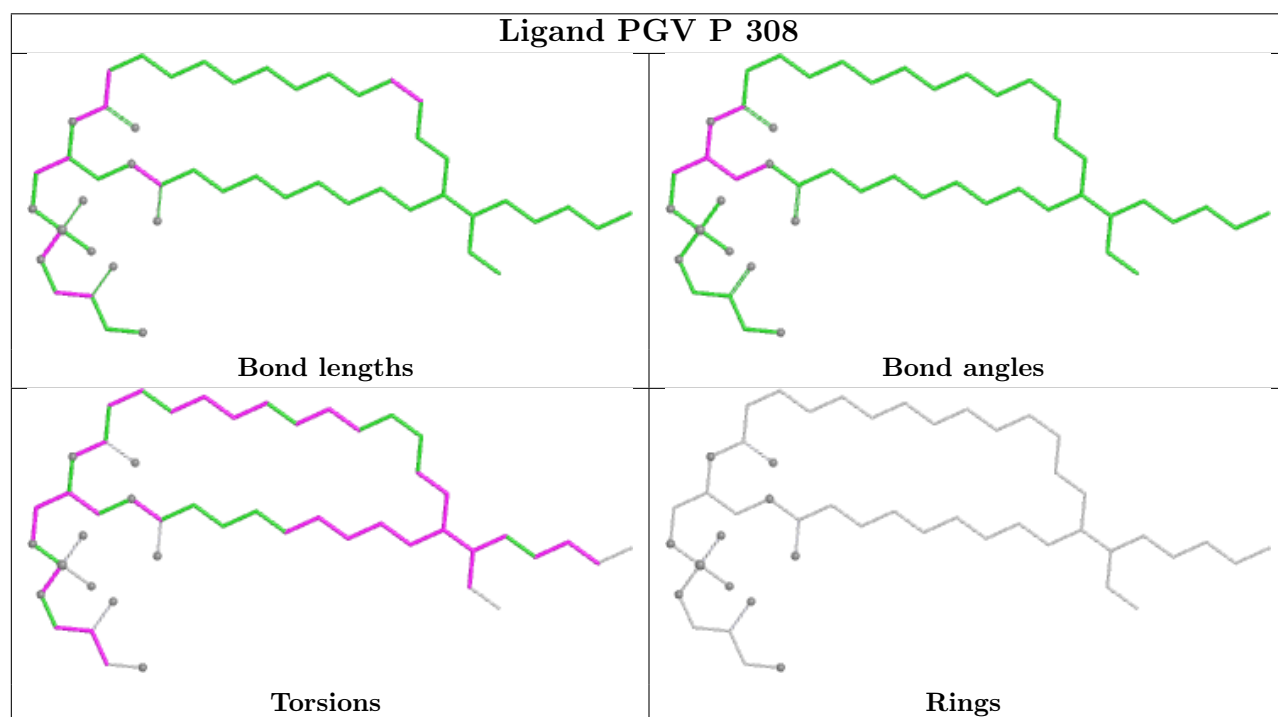
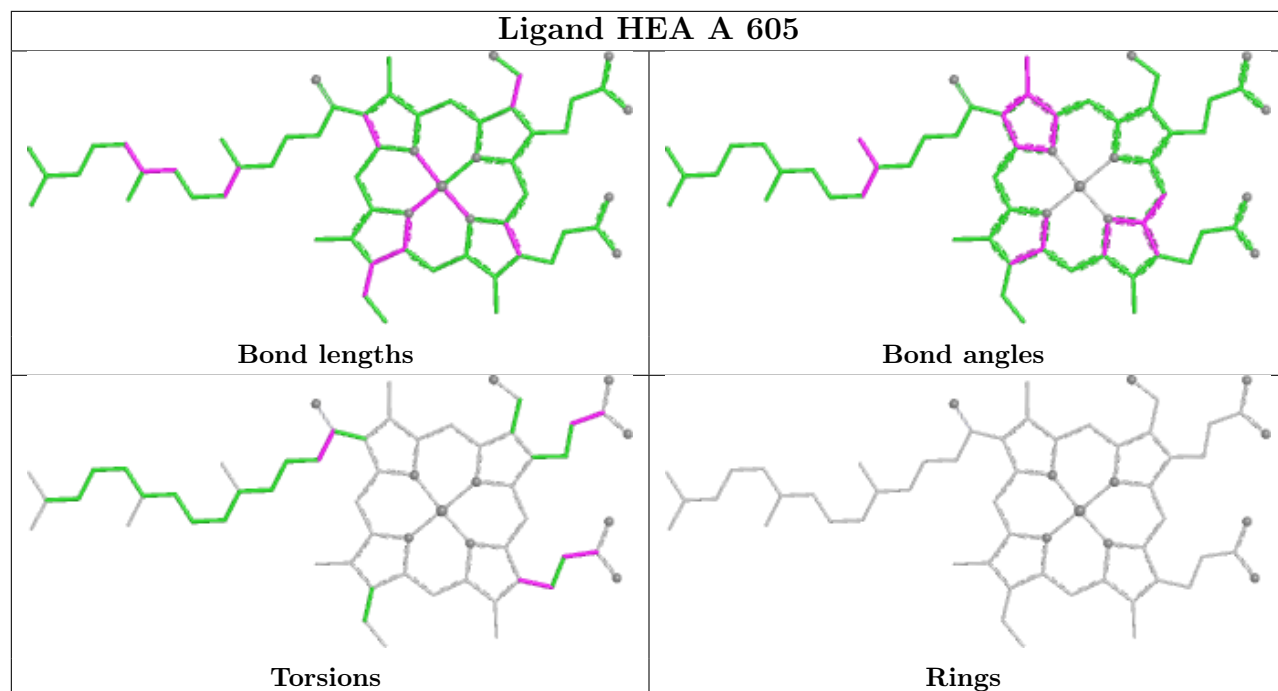


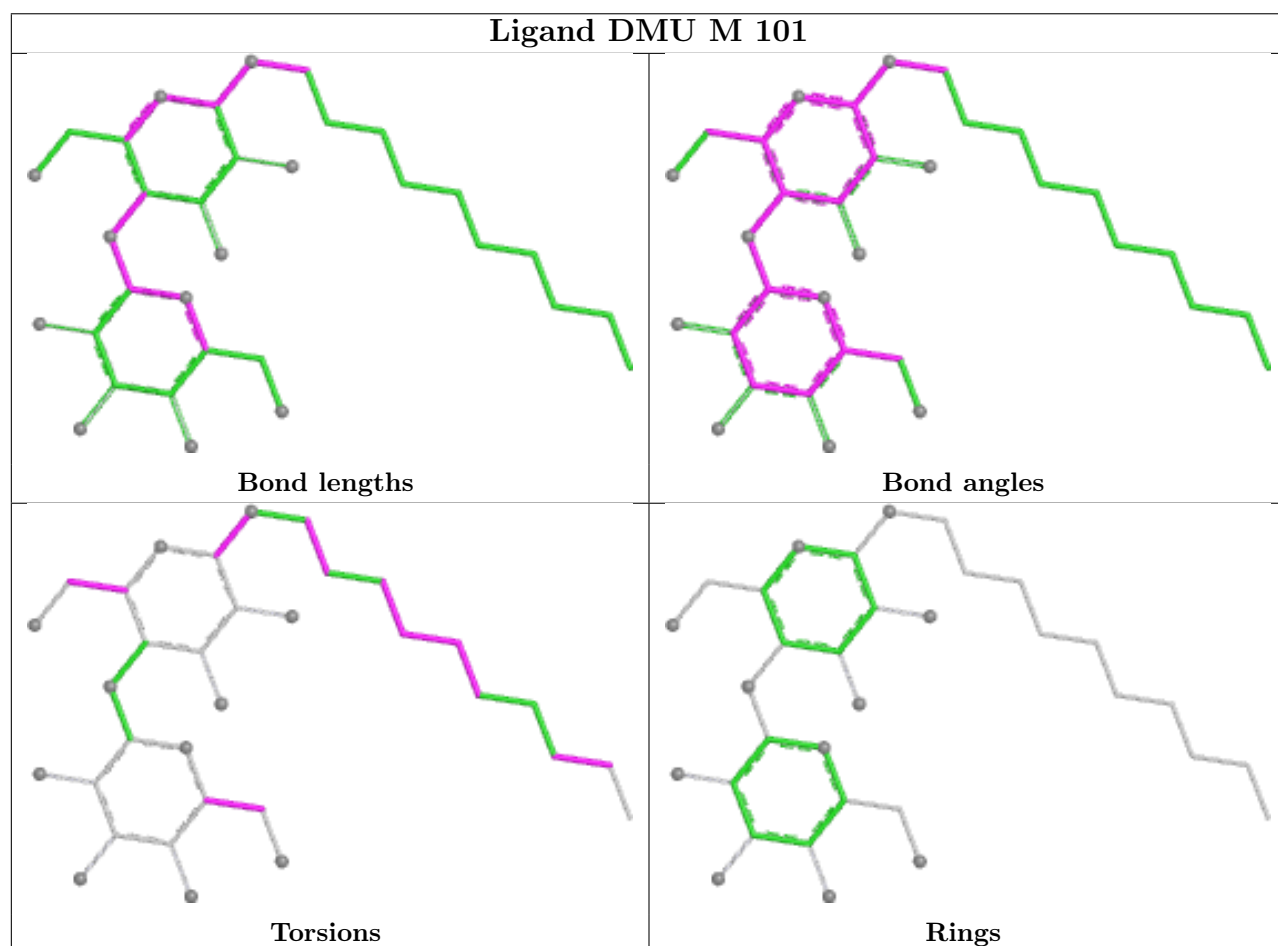
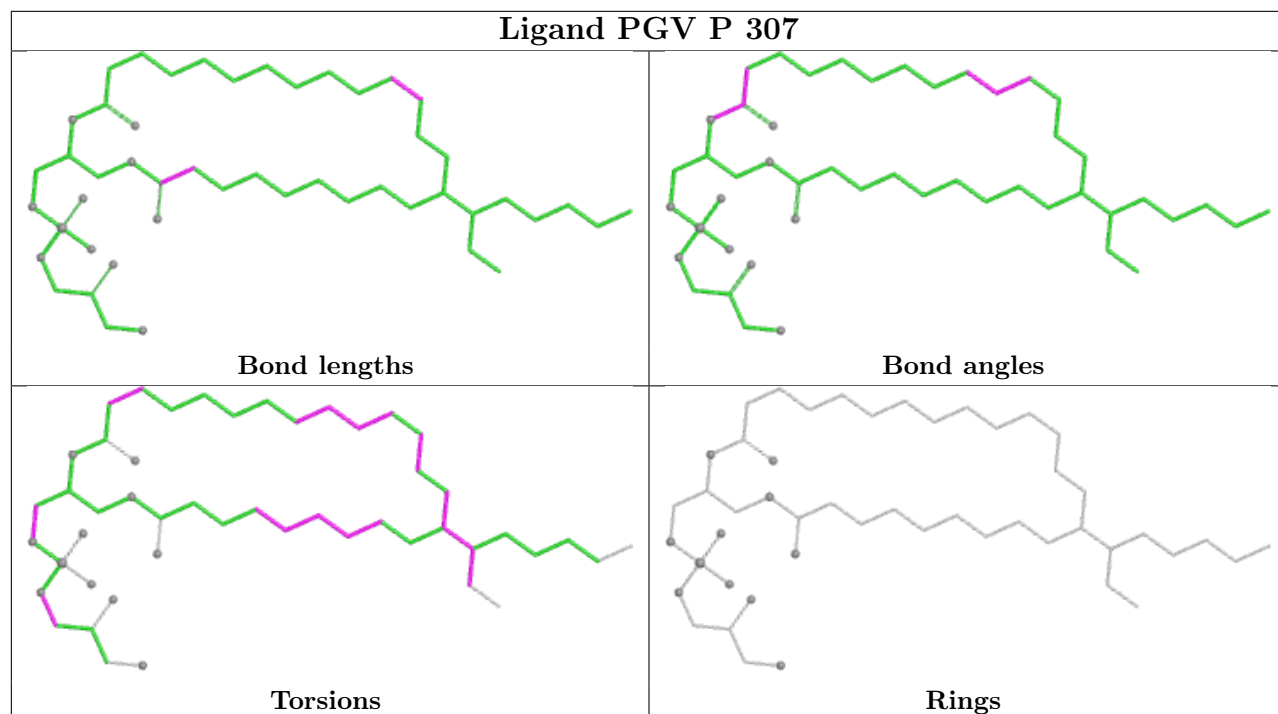


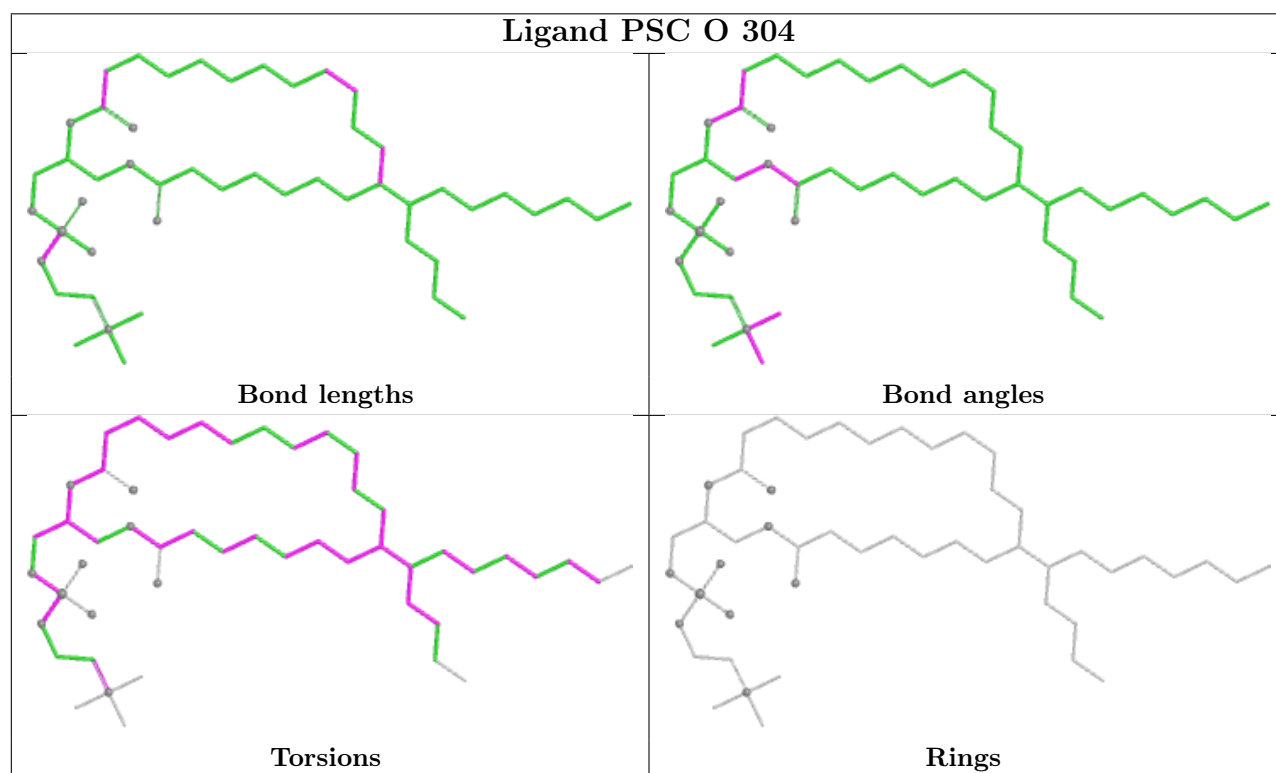
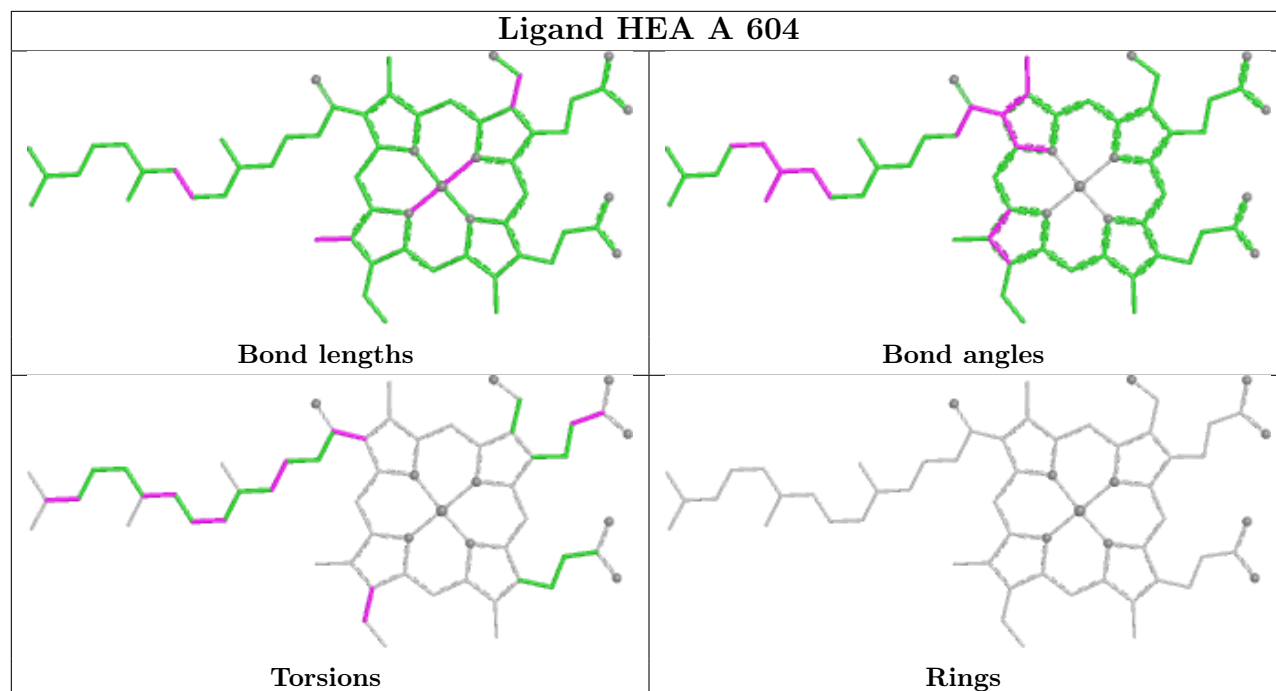


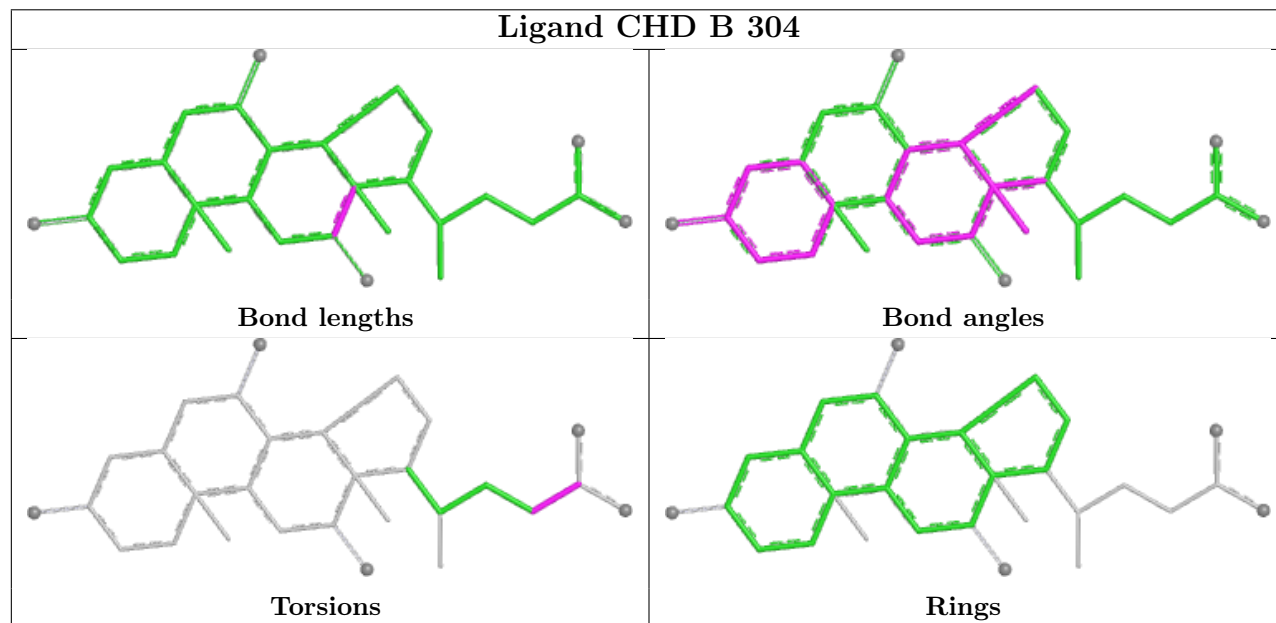
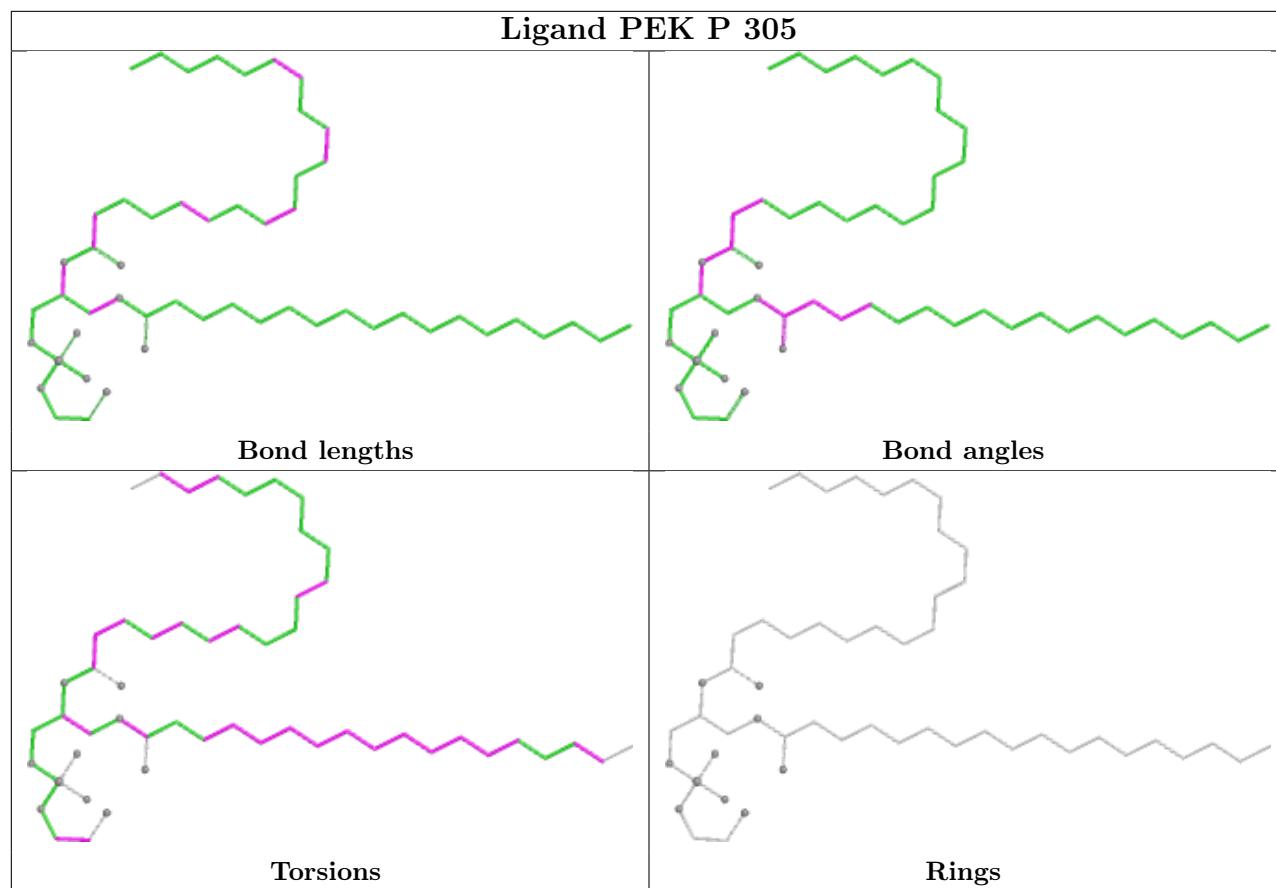


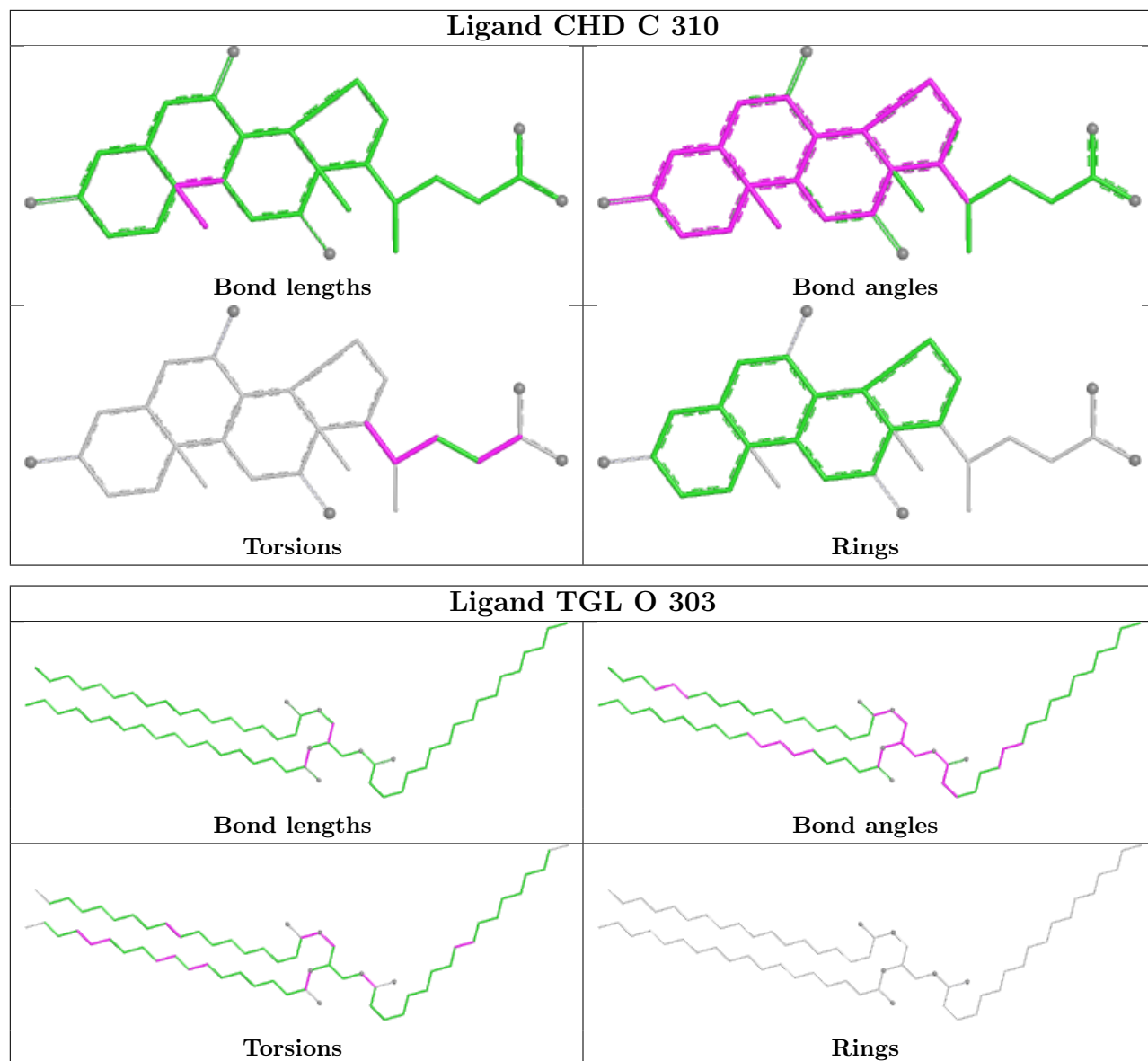


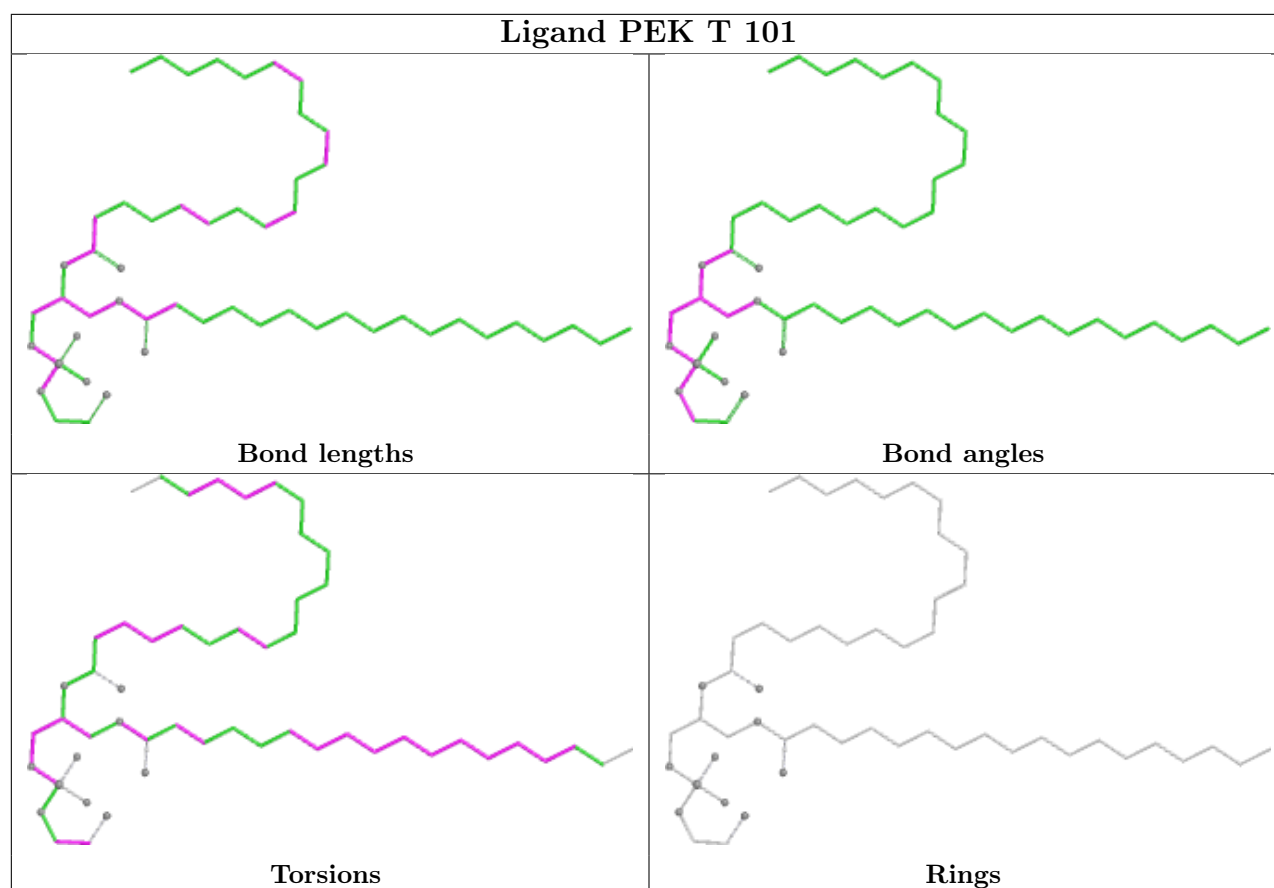












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	-0.68	2 (0%) 88 87	16, 25, 36, 67	0
1	N	513/514 (99%)	-0.33	4 (0%) 82 80	20, 32, 45, 70	0
2	B	226/227 (99%)	-0.17	9 (3%) 42 39	16, 31, 65, 95	0
2	O	226/227 (99%)	0.34	15 (6%) 24 21	27, 41, 71, 96	0
3	C	259/261 (99%)	-0.38	5 (1%) 66 63	20, 30, 50, 83	0
3	P	259/261 (99%)	-0.21	6 (2%) 61 58	23, 33, 56, 89	0
4	D	144/147 (97%)	0.10	7 (4%) 35 31	24, 36, 63, 90	0
4	Q	144/147 (97%)	1.30	26 (18%) 3 2	35, 53, 78, 108	0
5	E	105/109 (96%)	0.09	2 (1%) 66 63	26, 36, 68, 109	0
5	R	105/109 (96%)	0.71	10 (9%) 14 11	32, 45, 70, 111	0
6	F	98/98 (100%)	0.38	8 (8%) 17 15	22, 37, 100, 118	0
6	S	98/98 (100%)	0.91	11 (11%) 10 8	26, 43, 103, 115	0
7	G	83/85 (97%)	1.04	22 (26%) 1 1	23, 39, 103, 112	0
7	T	83/85 (97%)	1.19	22 (26%) 1 1	26, 45, 103, 113	0
8	H	79/85 (92%)	0.50	12 (15%) 5 4	25, 41, 99, 105	0
8	U	79/85 (92%)	0.85	12 (15%) 5 4	32, 48, 99, 109	0
9	I	72/73 (98%)	0.43	5 (6%) 23 20	27, 45, 74, 83	0
9	V	72/73 (98%)	1.05	11 (15%) 5 4	34, 56, 80, 97	0
10	J	58/59 (98%)	0.31	6 (10%) 12 9	27, 41, 79, 106	0
10	W	58/59 (98%)	0.85	7 (12%) 8 6	34, 49, 87, 110	0
11	K	49/56 (87%)	0.24	2 (4%) 41 38	29, 41, 57, 74	0
11	X	49/56 (87%)	0.95	6 (12%) 8 6	44, 56, 74, 88	0
12	L	46/47 (97%)	-0.20	2 (4%) 40 36	21, 32, 55, 92	0
12	Y	46/47 (97%)	0.41	2 (4%) 40 36	34, 43, 69, 98	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.02	5 (11%) 9 7	23, 32, 97, 108	0
13	Z	43/46 (93%)	0.66	6 (13%) 6 4	39, 47, 101, 112	0
All	All	3550/3614 (98%)	0.10	225 (6%) 26 23	16, 35, 74, 118	0

The worst 5 of 225 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	1	ALA	12.1
6	S	1	ALA	12.1
6	S	97	ALA	11.4
4	Q	5	VAL	11.3
4	Q	6	VAL	11.3

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
9	SAC	V	1	9/10	0.34	0.25	101,107,109,110	0
7	TPO	T	11	11/12	0.49	0.25	87,93,112,113	0
7	TPO	G	11	11/12	0.59	0.26	89,96,117,119	0
9	SAC	I	1	9/10	0.70	0.20	89,93,96,97	0
1	FME	A	1	10/11	0.79	0.18	50,60,76,86	0
1	FME	N	1	10/11	0.85	0.20	57,61,85,85	0
2	FME	O	1	10/11	0.93	0.13	40,42,47,54	0
2	FME	B	1	10/11	0.95	0.10	25,33,44,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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

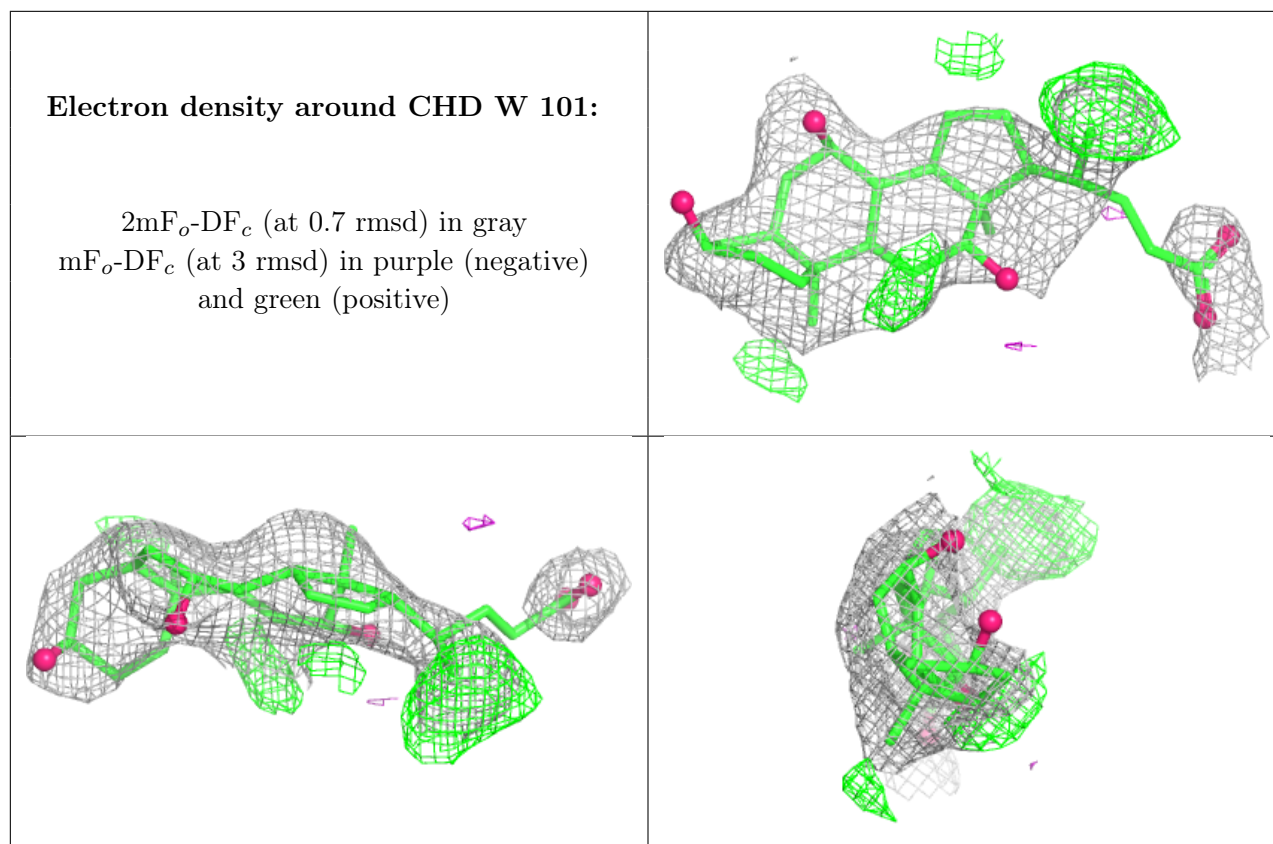
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	CHD	W	101	29/29	0.64	0.25	89,100,103,108	0
26	PEK	T	101	53/53	0.66	0.31	50,90,115,120	0
24	DMU	P	302	33/33	0.68	0.27	91,116,120,120	0
18	PGV	P	308	51/51	0.69	0.30	66,90,112,116	0
26	PEK	G	102	53/53	0.70	0.29	50,89,115,120	0
21	PSC	B	303	52/52	0.71	0.24	47,90,120,120	0
21	PSC	O	304	52/52	0.71	0.27	48,88,120,120	0
27	CDL	G	101	100/100	0.72	0.30	55,88,111,120	0
22	CHD	J	101	29/29	0.73	0.24	91,99,104,107	0
20	TGL	N	607	63/63	0.73	0.27	48,69,85,92	0
20	TGL	D	201	63/63	0.74	0.28	45,70,82,87	0
20	TGL	N	606	63/63	0.75	0.28	39,68,86,88	0
20	TGL	B	302	63/63	0.75	0.26	41,67,89,94	0
18	PGV	N	608	51/51	0.75	0.25	38,80,114,119	0
24	DMU	C	302	33/33	0.75	0.25	88,116,120,120	0
26	PEK	C	306	53/53	0.76	0.29	46,91,115,120	0
18	PGV	C	308	51/51	0.76	0.28	61,87,113,116	0
20	TGL	O	303	63/63	0.76	0.25	46,70,91,96	0
25	UNX	P	303	1/1	0.76	0.35	50,50,50,50	0
27	CDL	T	102	100/100	0.76	0.27	47,86,112,120	0
18	PGV	A	606	51/51	0.78	0.26	32,75,113,120	0
26	PEK	P	306	53/53	0.79	0.29	40,89,110,114	0
27	CDL	C	309	100/100	0.79	0.26	43,92,103,109	0
27	CDL	P	309	100/100	0.80	0.28	37,90,108,118	0
20	TGL	L	101	63/63	0.81	0.27	36,67,81,84	0
16	NA	A	603	1/1	0.81	0.18	44,44,44,44	0
24	DMU	Z	101	33/33	0.81	0.16	50,72,86,92	0
16	NA	N	603	1/1	0.83	0.18	50,50,50,50	0
22	CHD	P	310	29/29	0.84	0.20	78,91,94,99	0
25	UNX	C	303	1/1	0.86	0.43	45,45,45,45	0
22	CHD	C	310	29/29	0.86	0.20	75,92,97,101	0
24	DMU	M	101	33/33	0.89	0.14	45,63,80,87	0
23	DCW	C	301	16/16	0.93	0.12	46,50,53,54	0
23	DCW	P	301	16/16	0.93	0.13	52,59,70,70	0
26	PEK	P	305	53/53	0.93	0.15	24,46,73,77	0
26	PEK	C	305	53/53	0.94	0.14	17,43,71,73	0
18	PGV	N	609	51/51	0.95	0.13	25,43,64,77	0
22	CHD	P	304	29/29	0.95	0.07	25,32,40,46	0
22	CHD	C	304	29/29	0.96	0.06	25,31,37,39	0
15	MG	N	602	1/1	0.96	0.06	35,35,35,35	0
18	PGV	A	607	51/51	0.96	0.12	22,41,66,76	0
22	CHD	O	302	29/29	0.96	0.06	17,29,37,40	0

Continued on next page...

Continued from previous page...

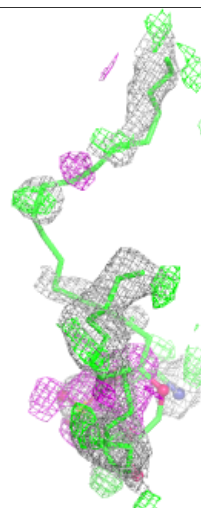
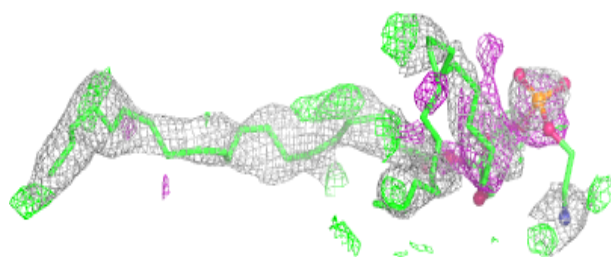
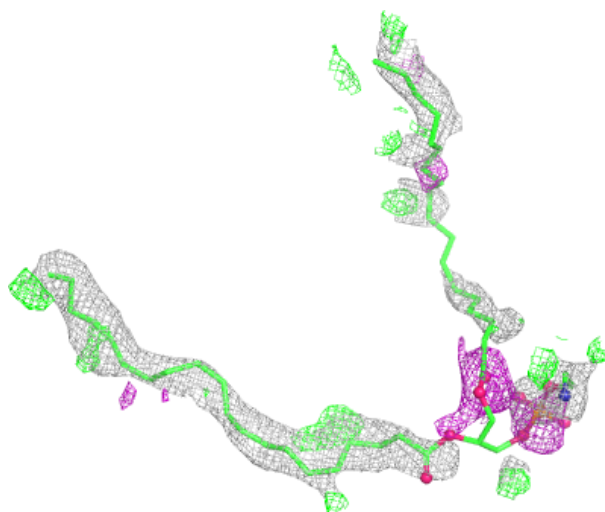
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CHD	B	304	29/29	0.96	0.06	20,27,34,38	0
18	PGV	P	307	51/51	0.97	0.11	23,36,68,73	0
18	PGV	C	307	51/51	0.97	0.10	22,33,65,72	0
15	MG	A	602	1/1	0.97	0.05	23,23,23,23	0
17	HEA	N	604	60/60	0.98	0.07	20,32,50,55	0
19	CUA	O	301	2/2	0.98	0.04	36,36,36,36	0
17	HEA	N	605	60/60	0.98	0.06	16,27,34,36	0
17	HEA	A	604	60/60	0.98	0.06	16,25,49,54	0
19	CUA	B	301	2/2	0.99	0.04	24,24,24,27	0
14	CU	A	601	1/1	0.99	0.02	23,23,23,23	0
17	HEA	A	605	60/60	0.99	0.05	10,24,31,33	0
14	CU	N	601	1/1	0.99	0.02	28,28,28,28	0
28	ZN	F	101	1/1	1.00	0.01	32,32,32,32	0
28	ZN	S	101	1/1	1.00	0.02	34,34,34,34	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.



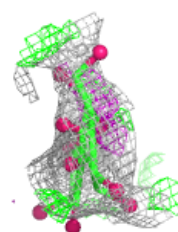
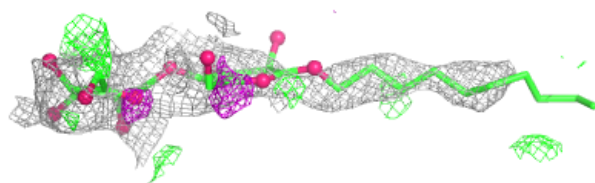
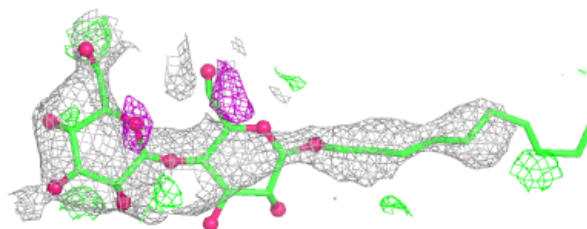
Electron density around PEK T 101:

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

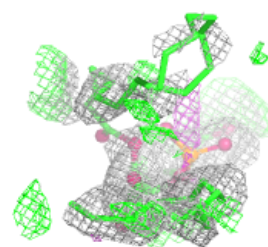
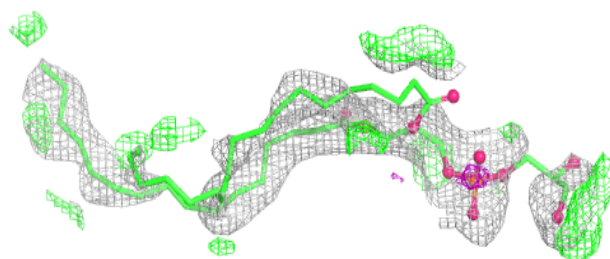
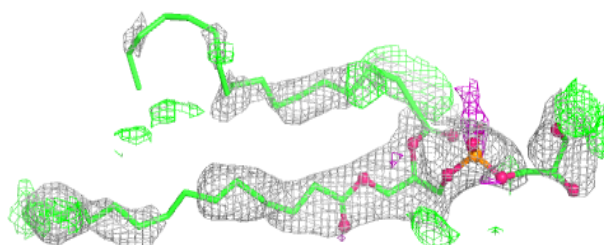


Electron density around DMU P 302:

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

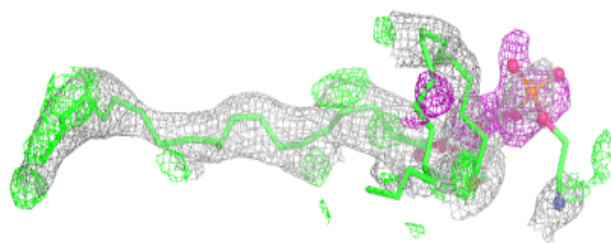
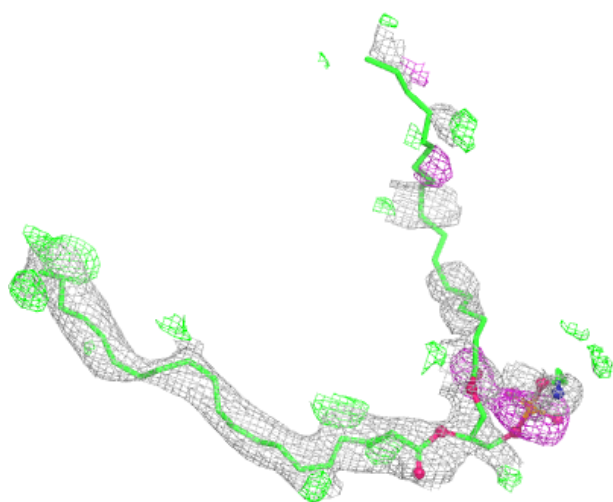
**Electron density around PGV P 308:**

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



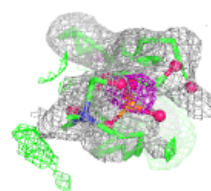
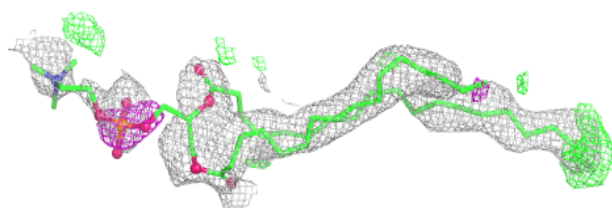
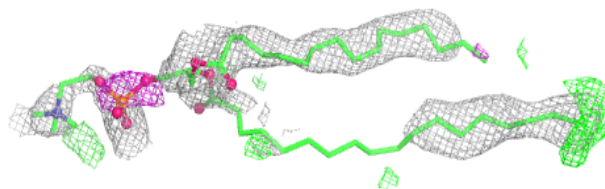
Electron density around PEK G 102:

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

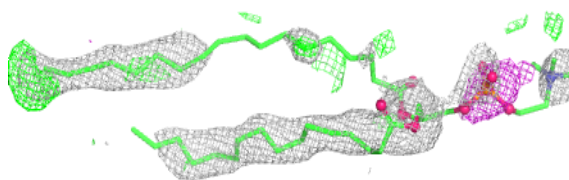


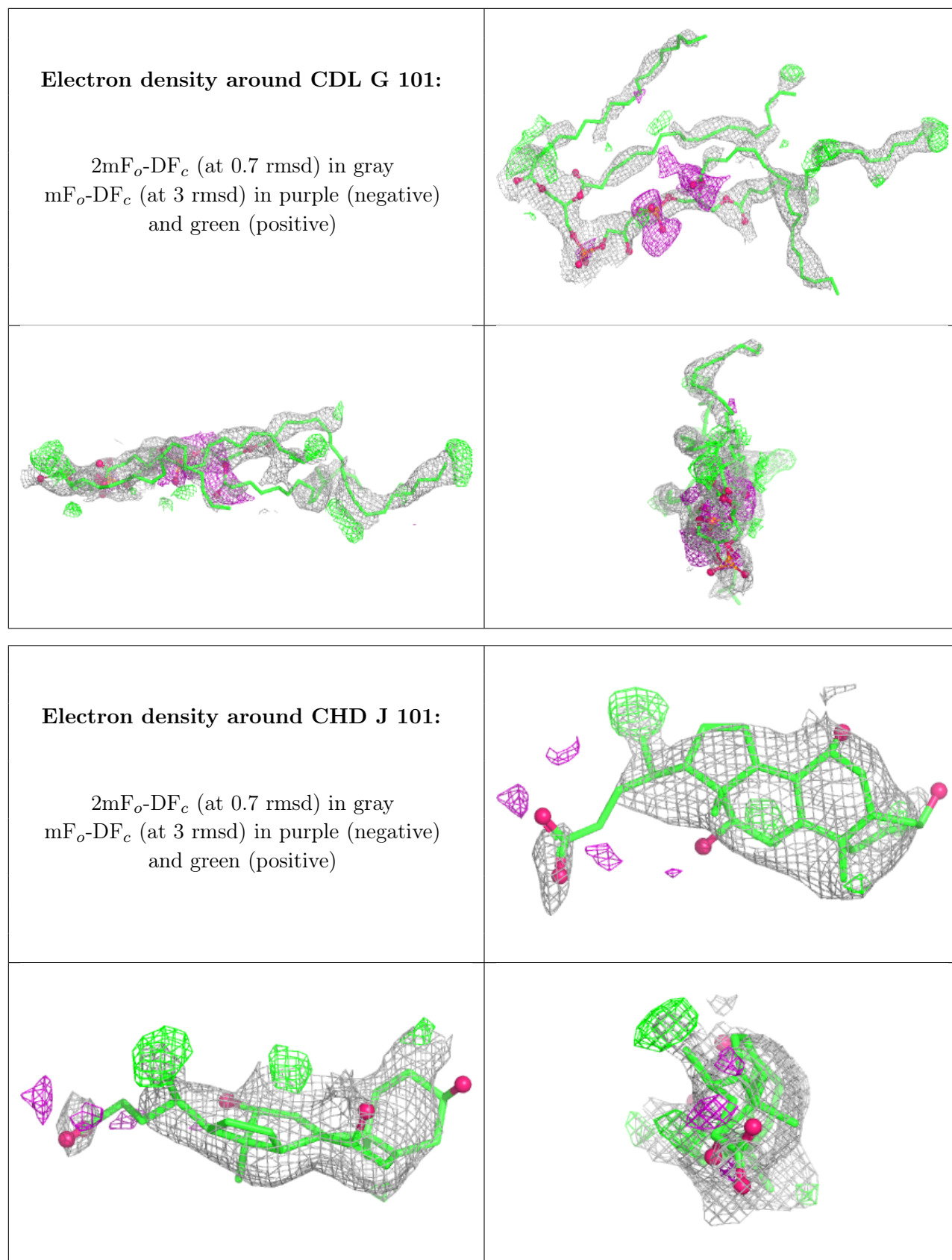
Electron density around PSC B 303:

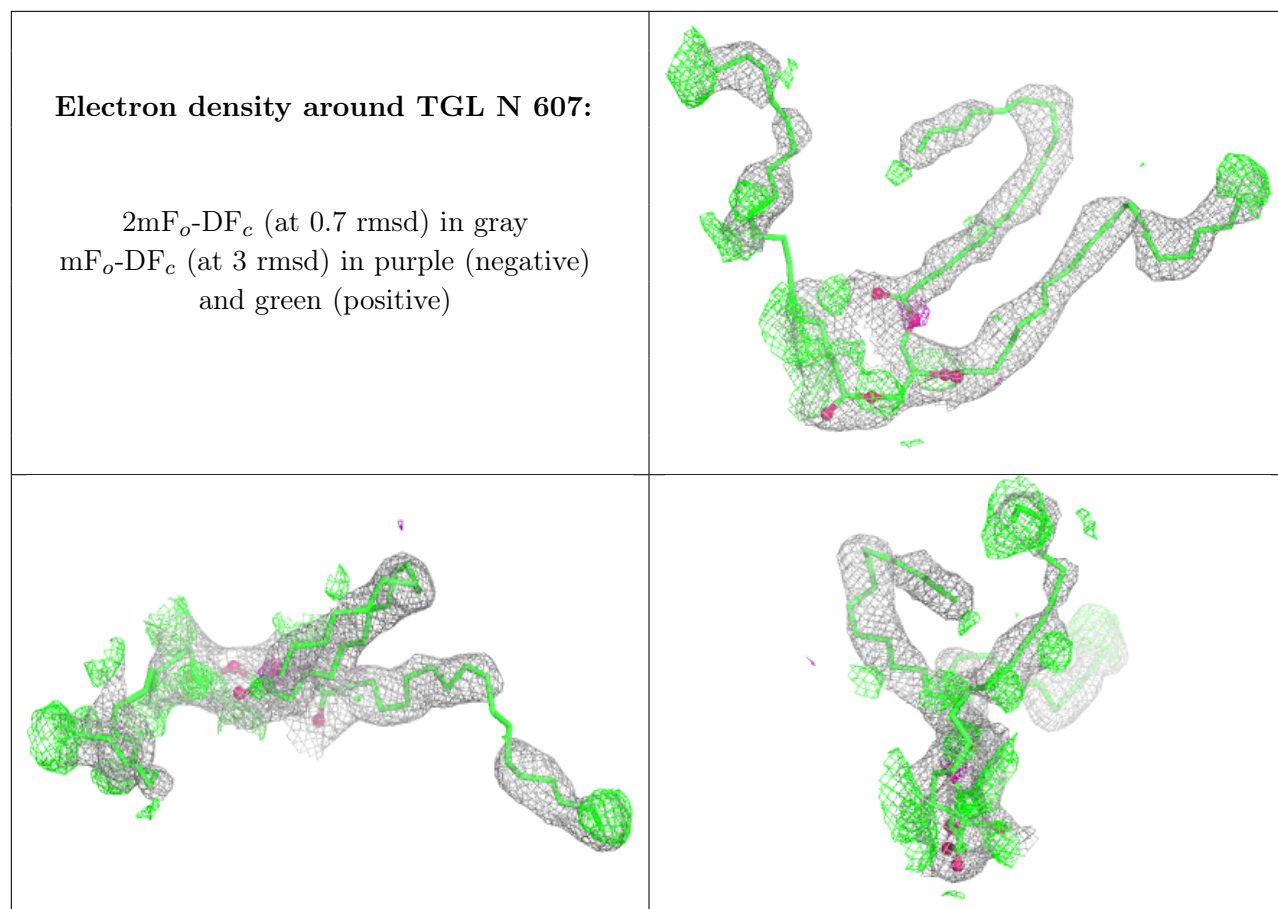
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

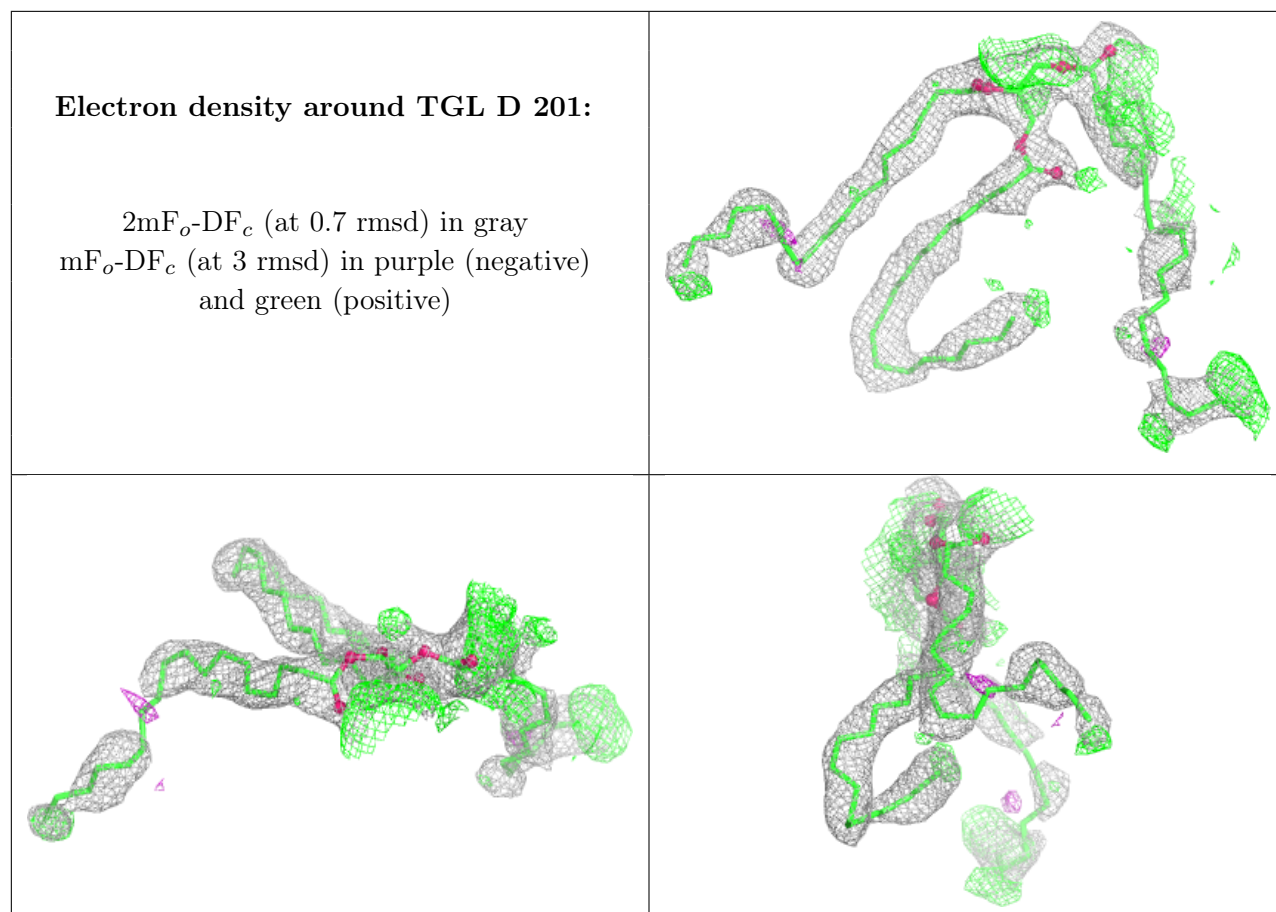
**Electron density around PSC O 304:**

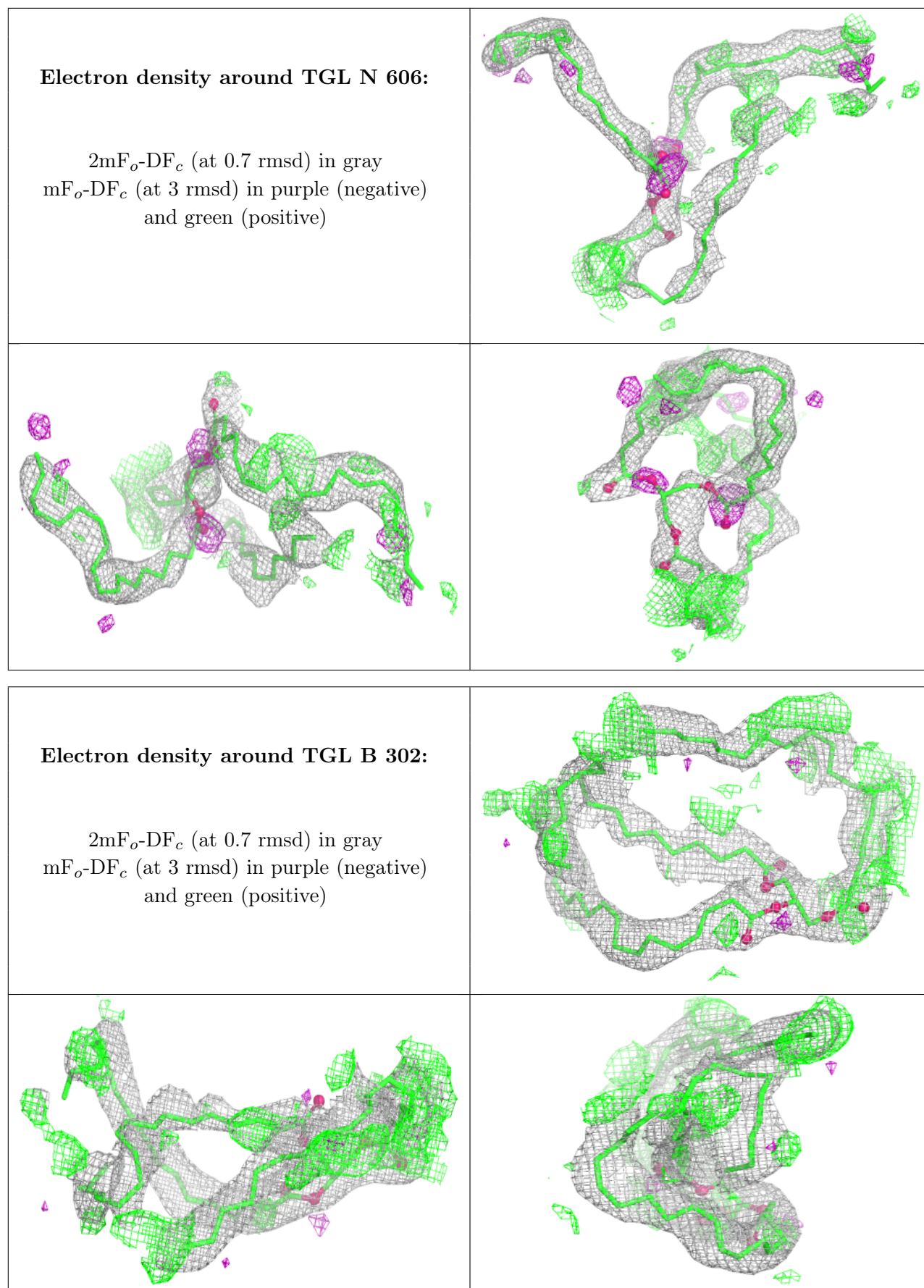
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





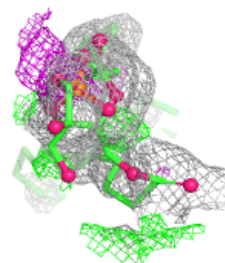
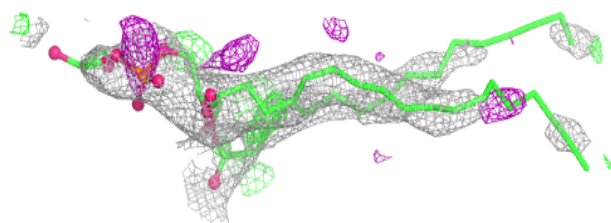
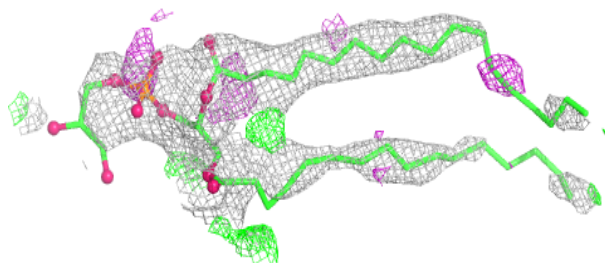




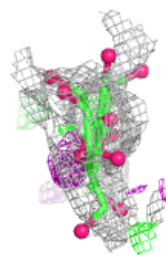
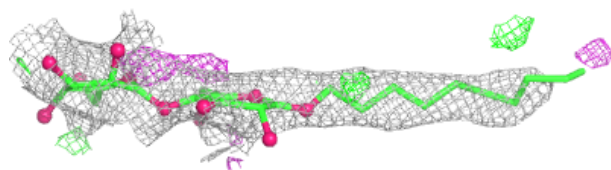
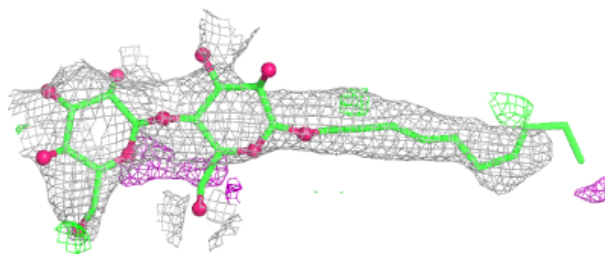


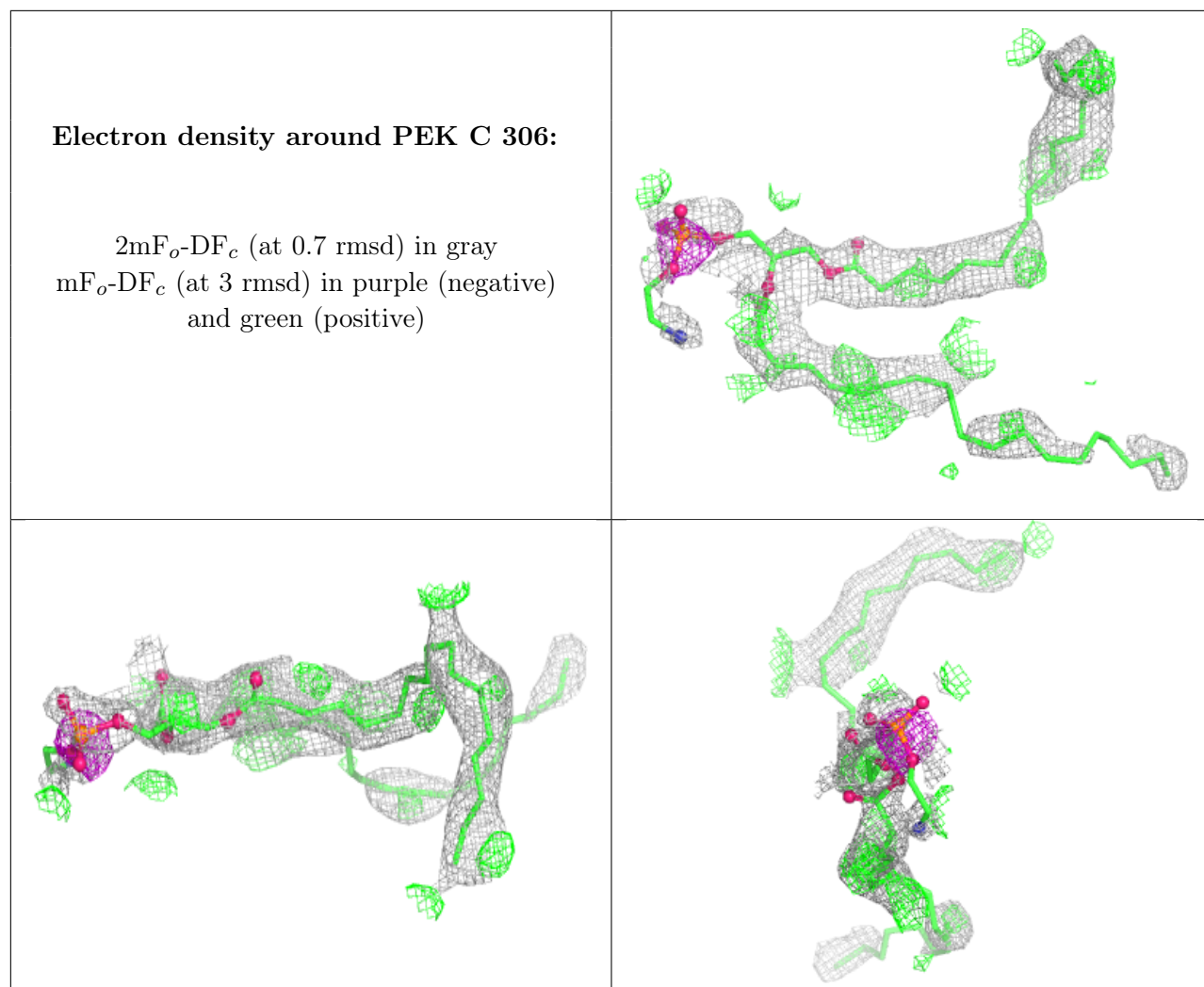
Electron density around PGV N 608:

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

**Electron density around DMU C 302:**

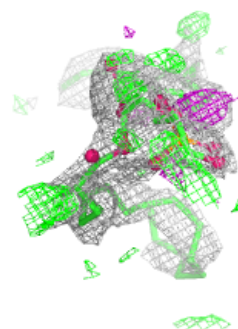
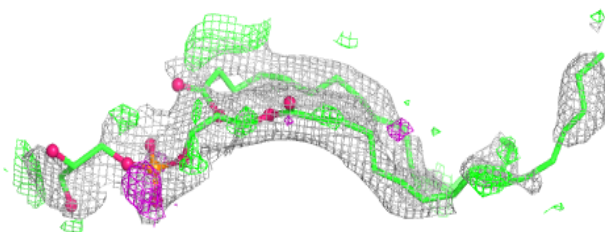
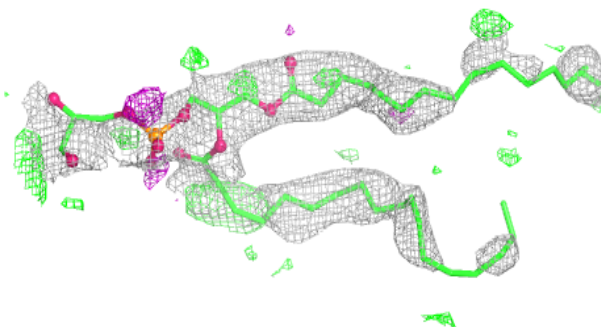
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



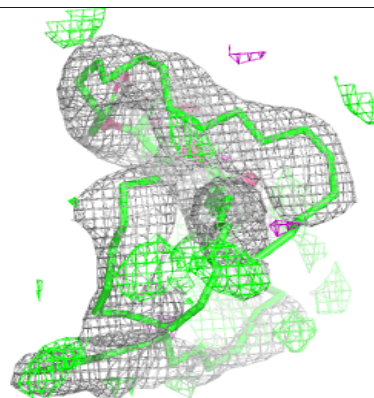
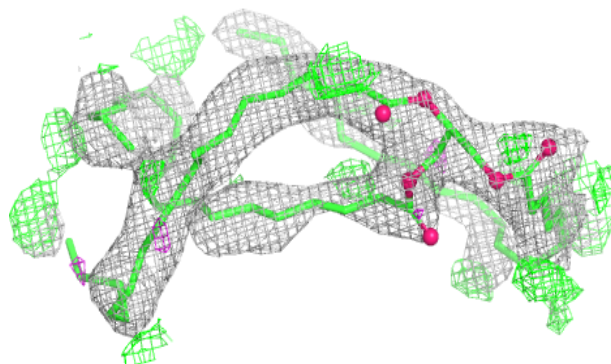
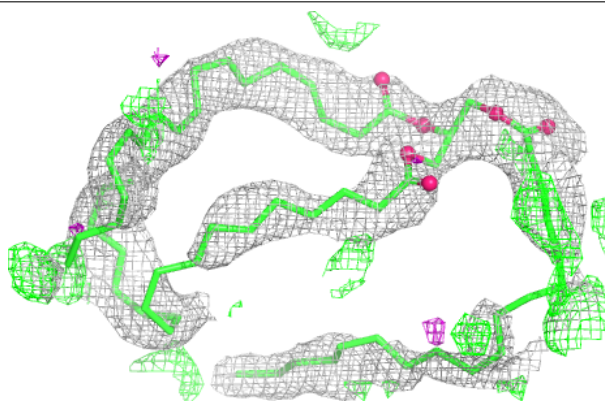


Electron density around PGV C 308:

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

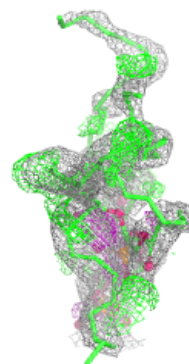
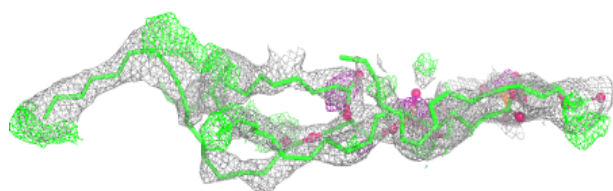
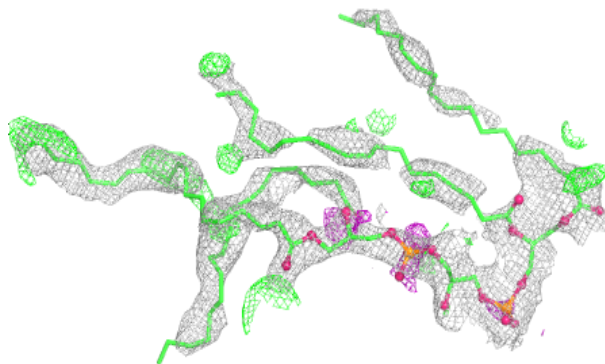
**Electron density around TGL O 303:**

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

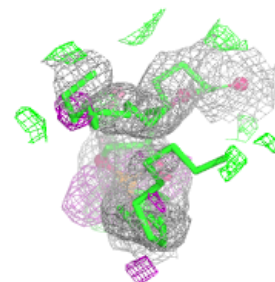
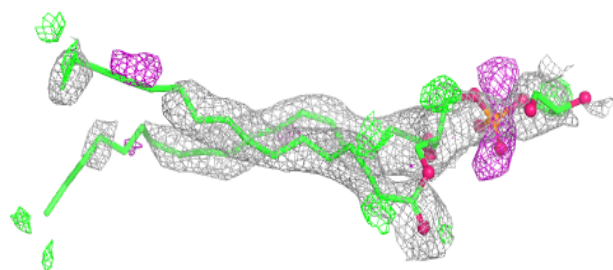
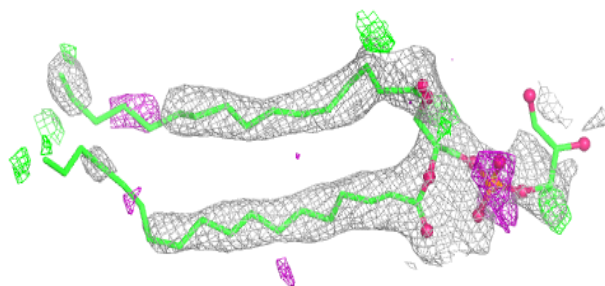


Electron density around CDL T 102:

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

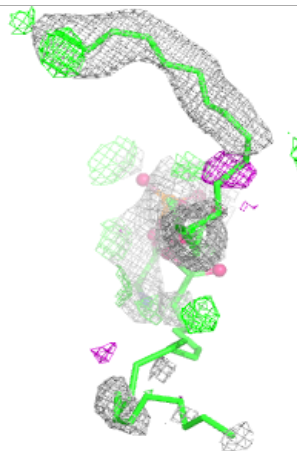
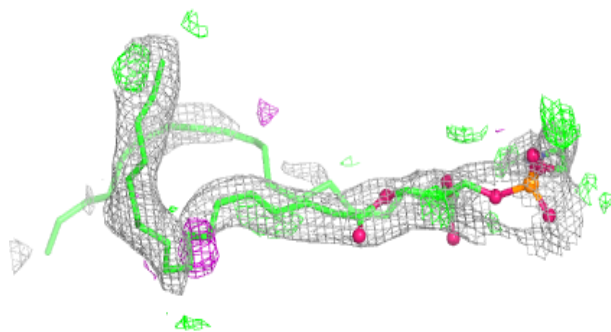
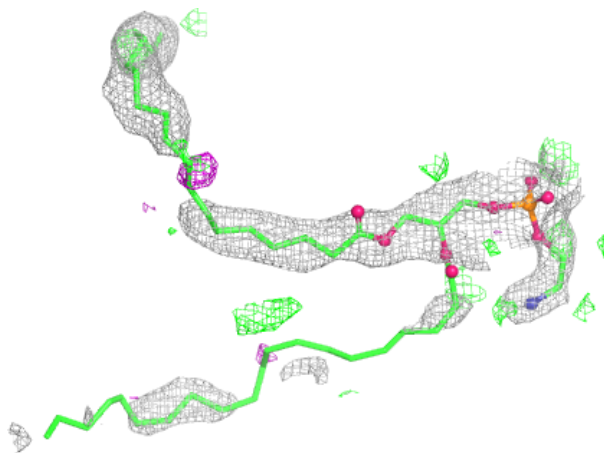
**Electron density around PGV A 606:**

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



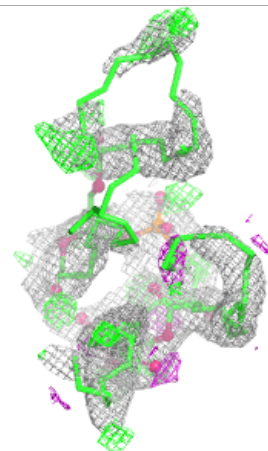
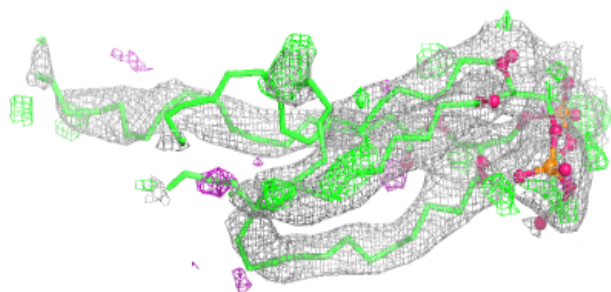
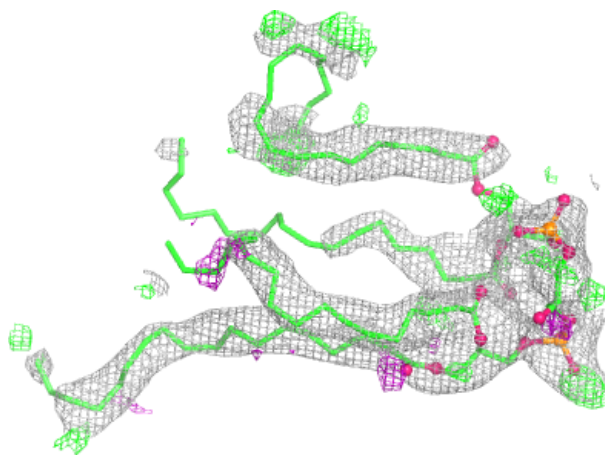
Electron density around PEK P 306:

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



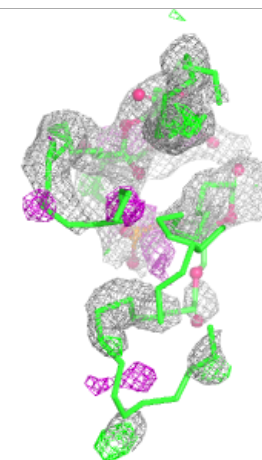
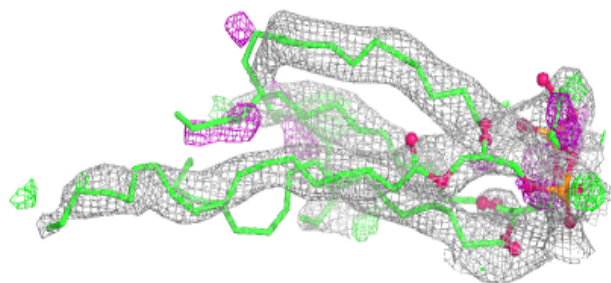
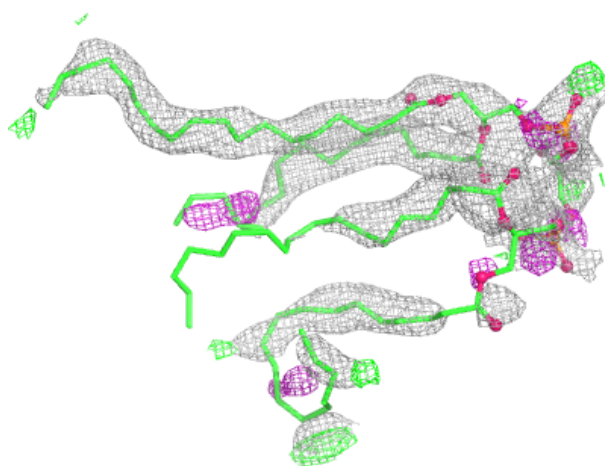
Electron density around CDL C 309:

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



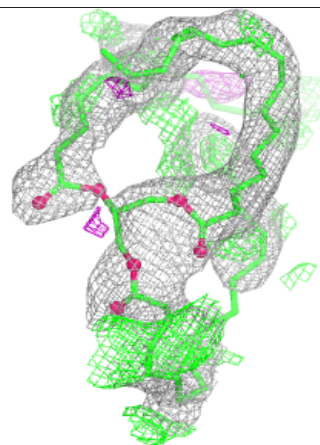
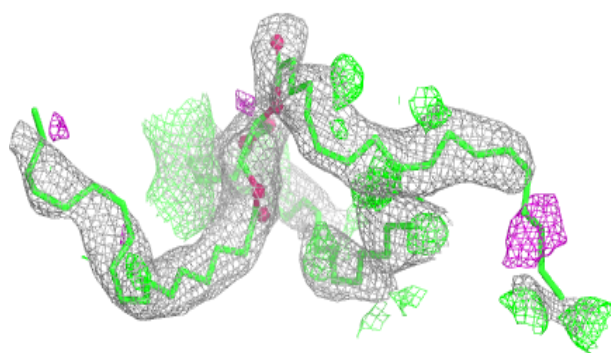
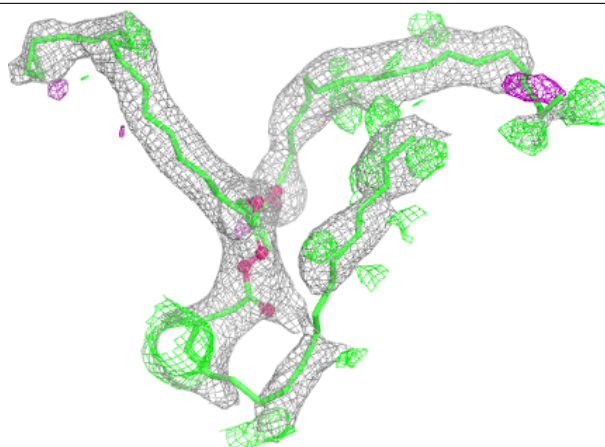
Electron density around CDL P 309:

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



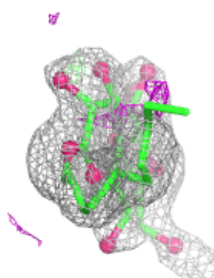
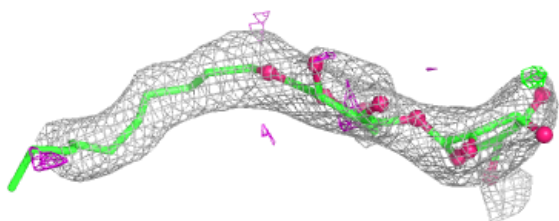
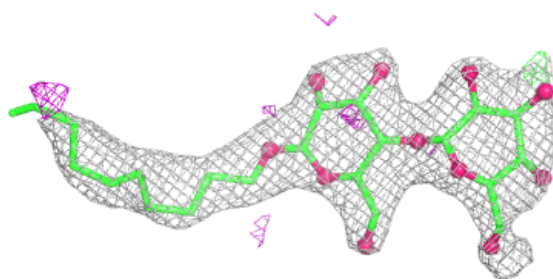
Electron density around TGL L 101:

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

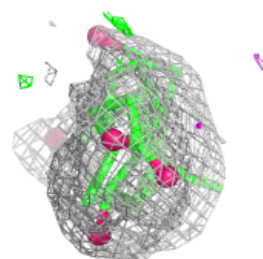
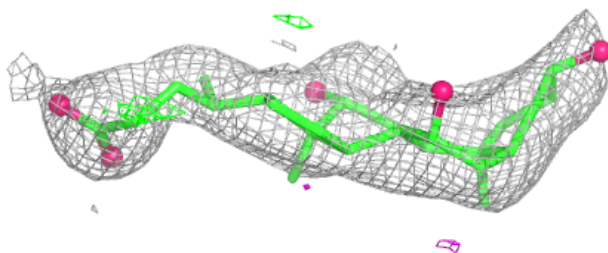
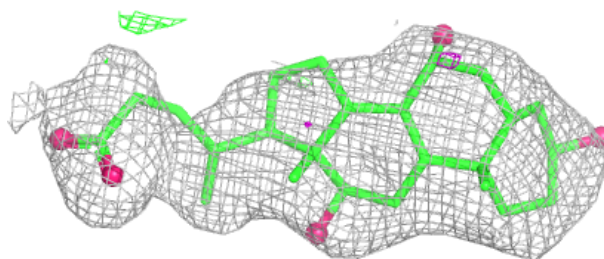


Electron density around DMU Z 101:

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

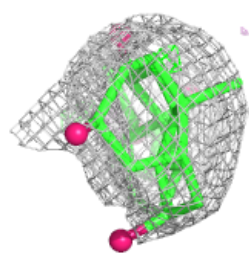
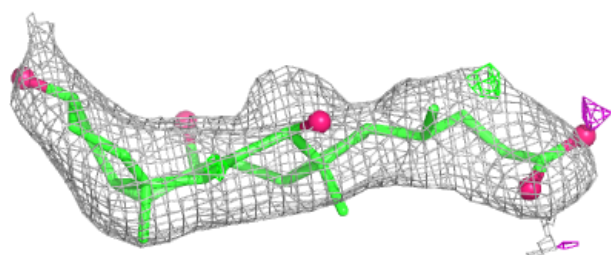
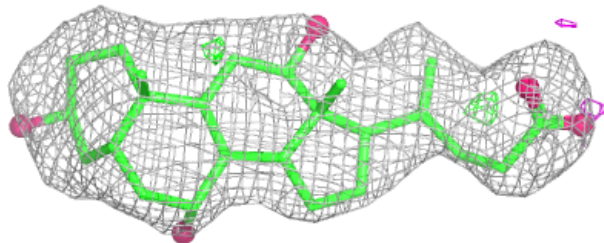
**Electron density around CHD P 310:**

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

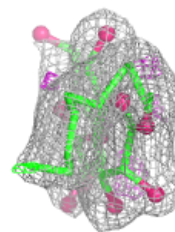
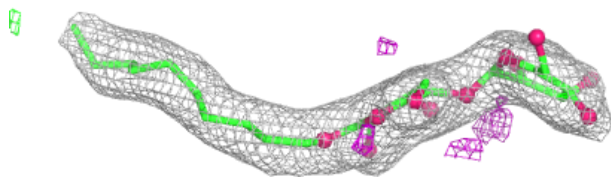
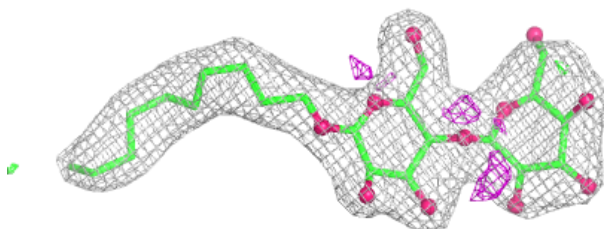


Electron density around CHD C 310:

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

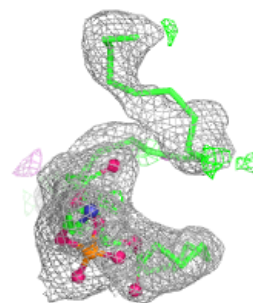
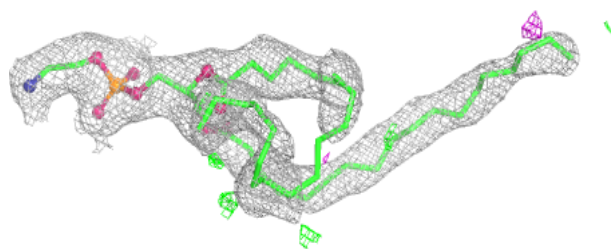
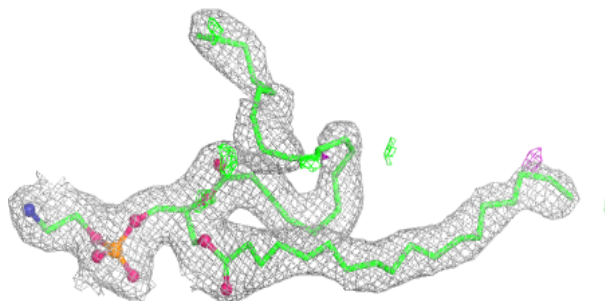
**Electron density around DMU M 101:**

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

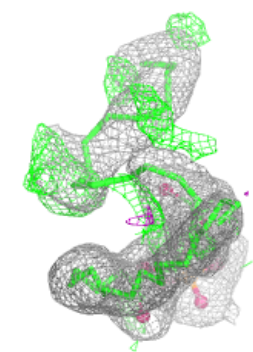
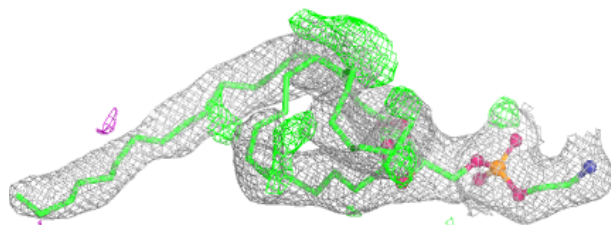
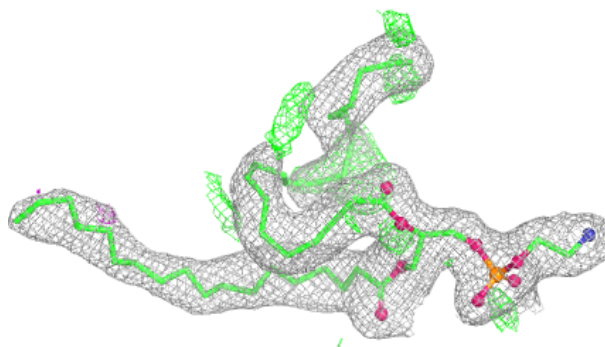


Electron density around PEK P 305:

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

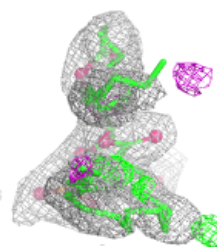
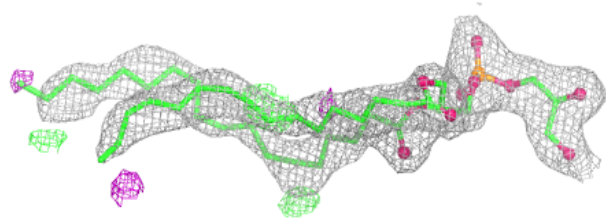
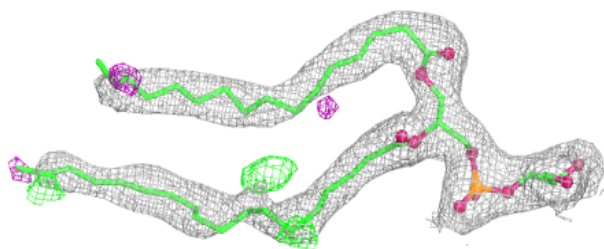
**Electron density around PEK C 305:**

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

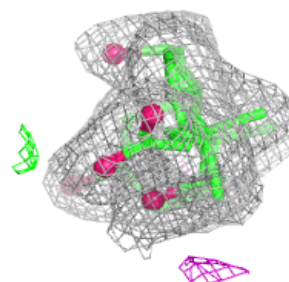
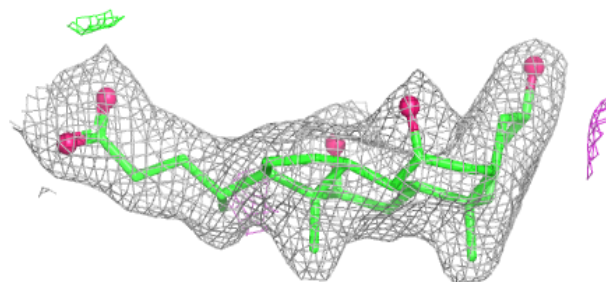
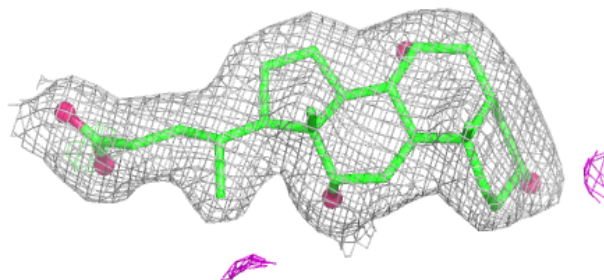


Electron density around PGV N 609:

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

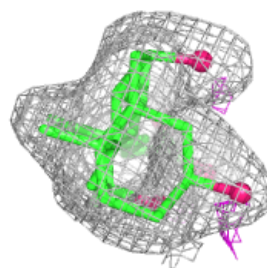
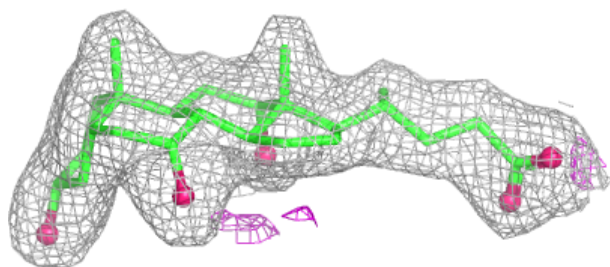
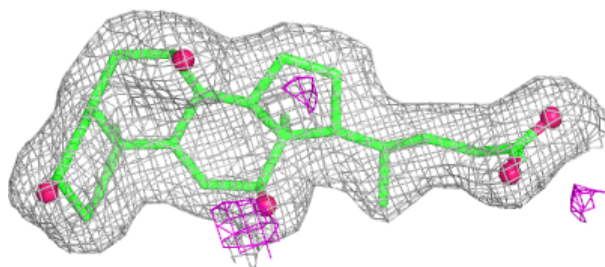
**Electron density around CHD P 304:**

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

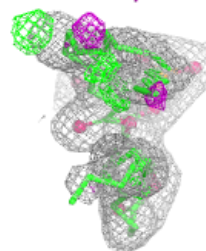
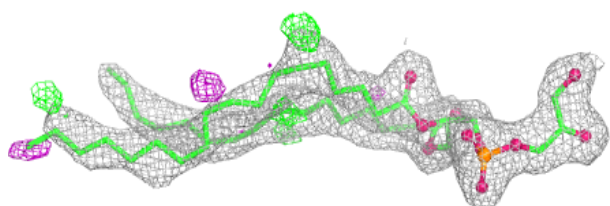
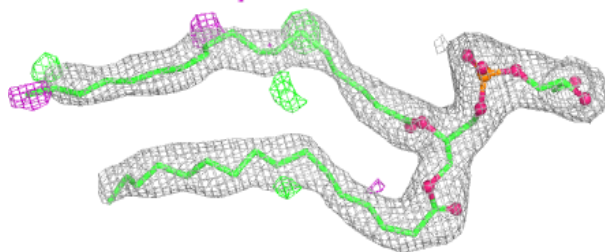


Electron density around CHD C 304:

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

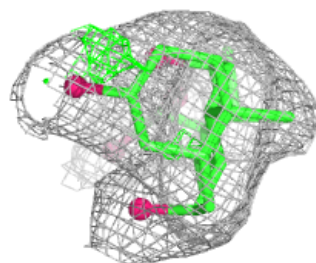
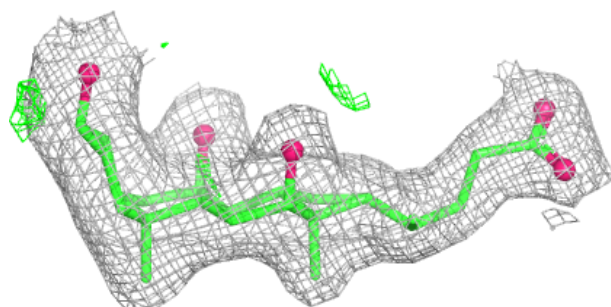
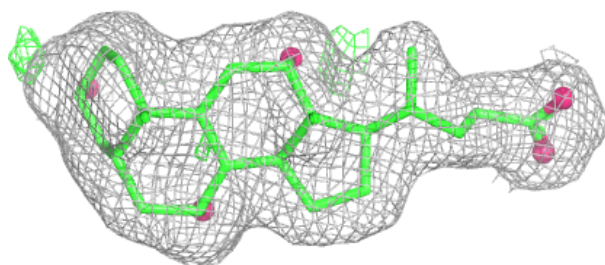
**Electron density around PGV A 607:**

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

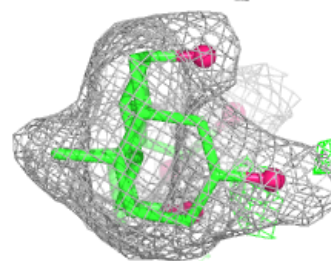
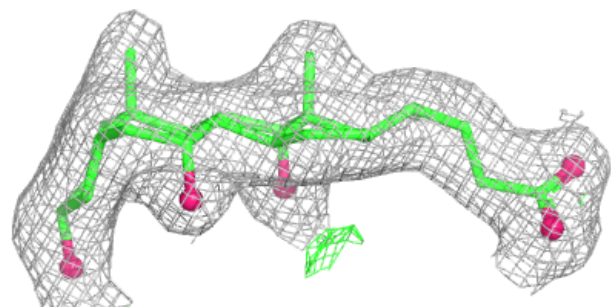
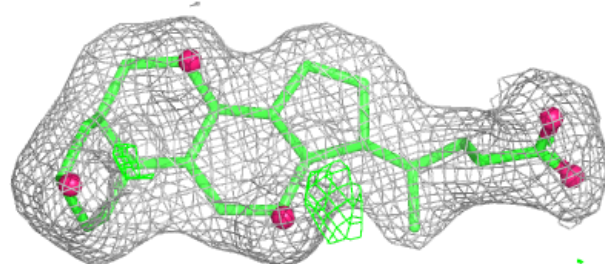


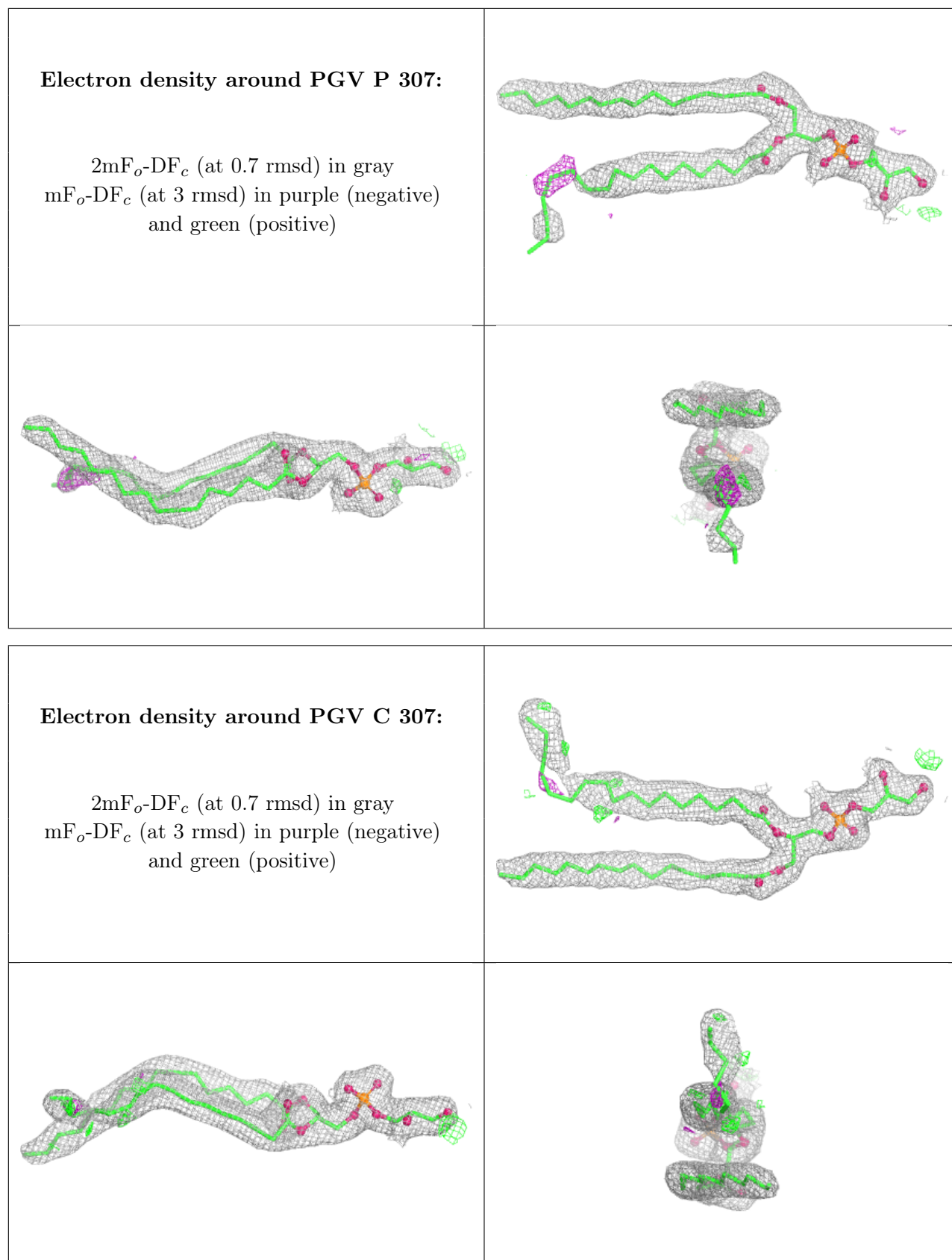
Electron density around CHD O 302:

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

**Electron density around CHD B 304:**

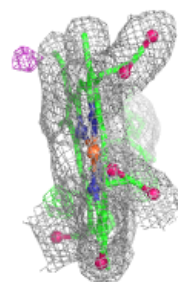
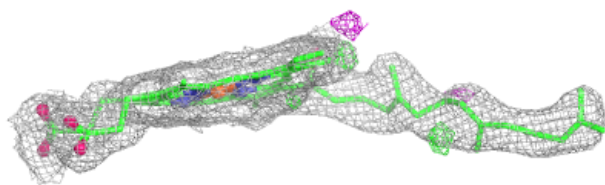
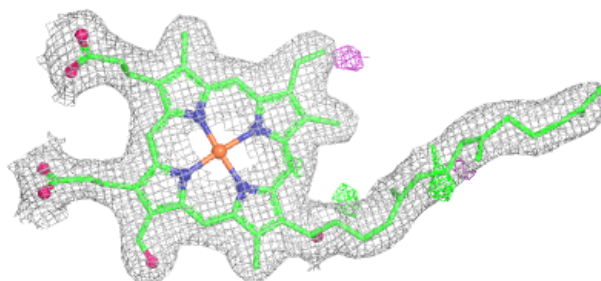
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



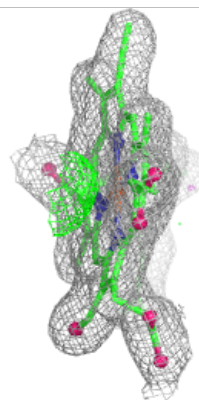
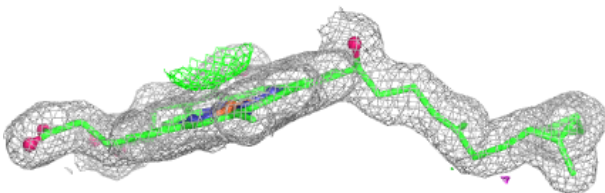
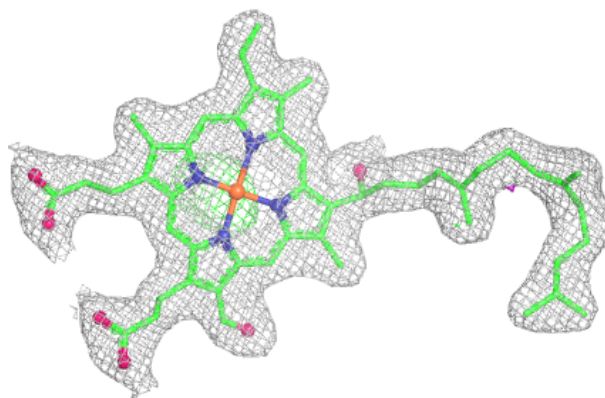


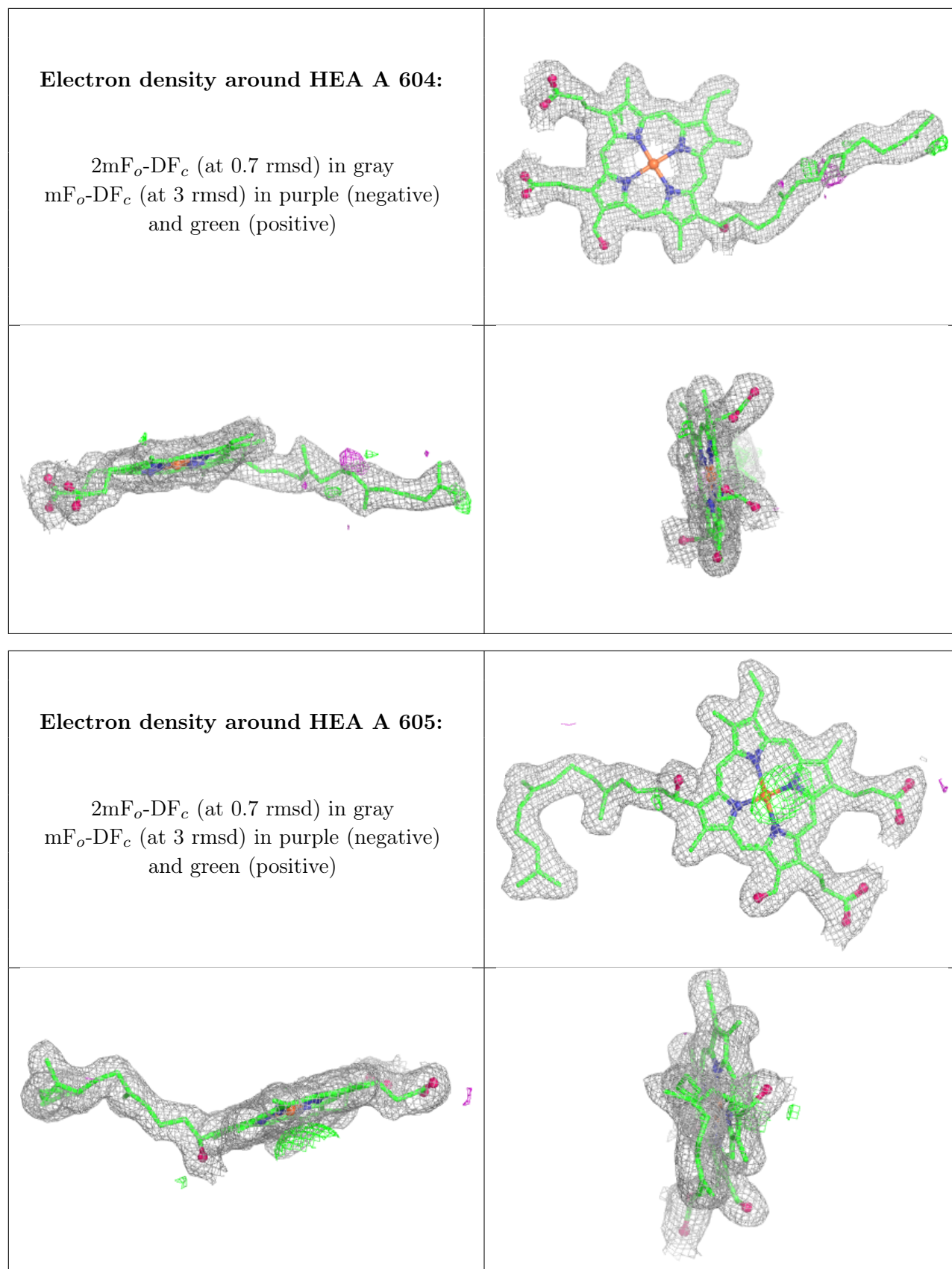
Electron density around HEA N 604:

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

**Electron density around HEA N 605:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.