



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 03:45 AM UTC

PDB ID : 6NMP / pdb_00006nmp
Title : SFX structure of oxidized cytochrome c oxidase at room temperature
Authors : Rousseau, D.L.; Yeh, S.-R.; Ishigami, I.
Deposited on : 2019-01-11
Resolution : 2.90 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)
Xtrriage (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

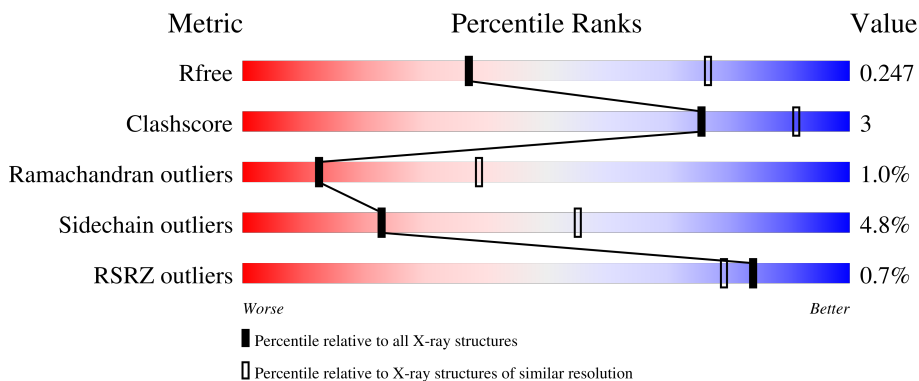
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	 90% 9% .
1	N	514	 87% 12% .
2	B	227	 86% 13% .
2	O	227	 88% 10% .
3	C	261	 93% 6% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	P	261	90% 9% .
4	D	147	90% 7% ..
4	Q	147	2% 88% 10% .
5	E	109	86% 10% .
5	R	109	89% 7% .
6	F	98	3% 90% 8% ..
6	S	98	3% 89% 9% .
7	G	85	5% 76% 16% 6% .
7	T	85	7% 78% 16% . . .
8	H	85	1% 80% 9% . . 7%
8	U	85	1% 82% 9% . 7%
9	I	73	1% 92% 8%
9	V	73	1% 84% 16%
10	J	59	92% 7% .
10	W	59	75% 22% . .
11	K	56	79% 9% 12%
11	X	56	77% 9% . 12%
12	L	47	89% 9% .
12	Y	47	83% 13% . .
13	M	46	80% 13% 7%
13	Z	46	74% 20% 7%

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 31210 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	2110	1412	336	350	12	0	0	0
3	P	259	2110	1412	336	350	12	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	144	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 subunit 5A, mitochondrial.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total	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 6B1.

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

- 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		

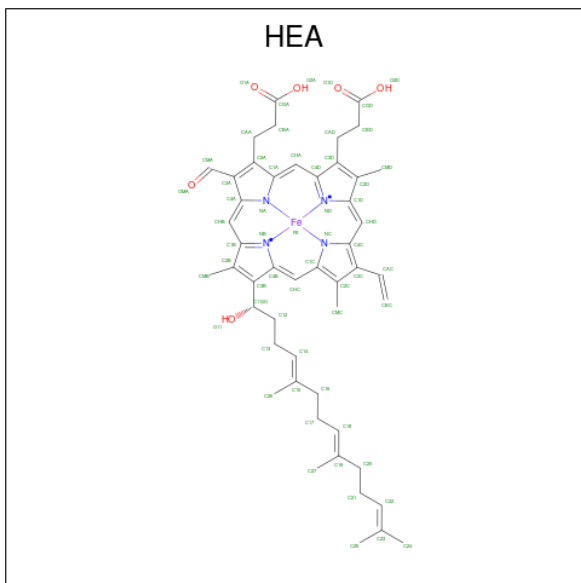
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

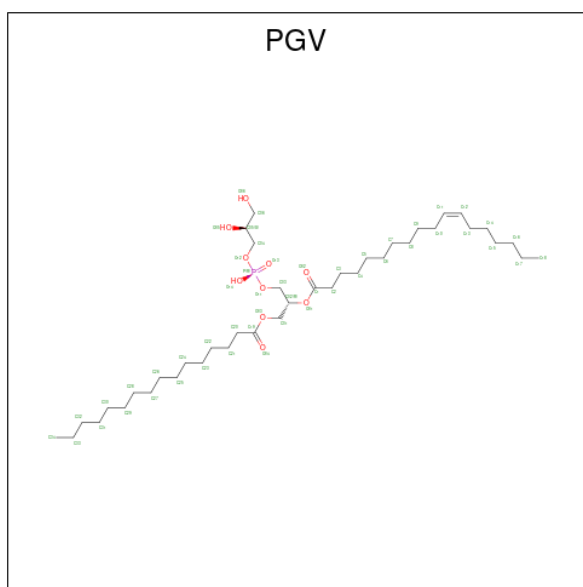
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

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



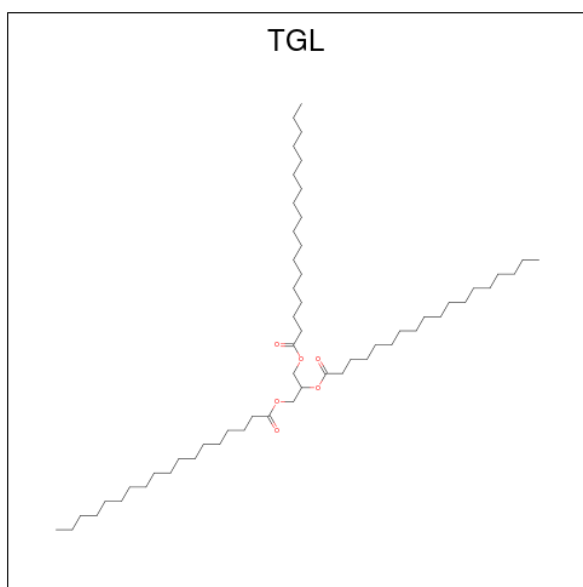
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0

- 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).



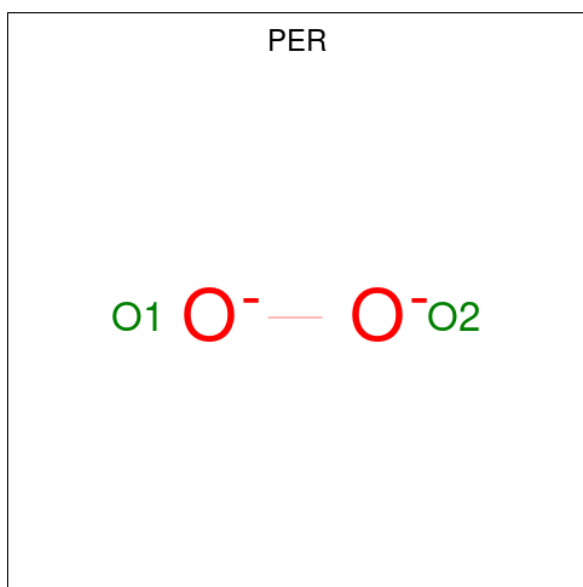
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
18	A	1	51	40	10	1	0	0
18	A	1	51	40	10	1	0	0
18	C	1	51	40	10	1	0	0
18	C	1	51	40	10	1	0	0
18	N	1	51	40	10	1	0	0
18	P	1	51	40	10	1	0	0
18	P	1	51	40	10	1	0	0
18	P	1	51	40	10	1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



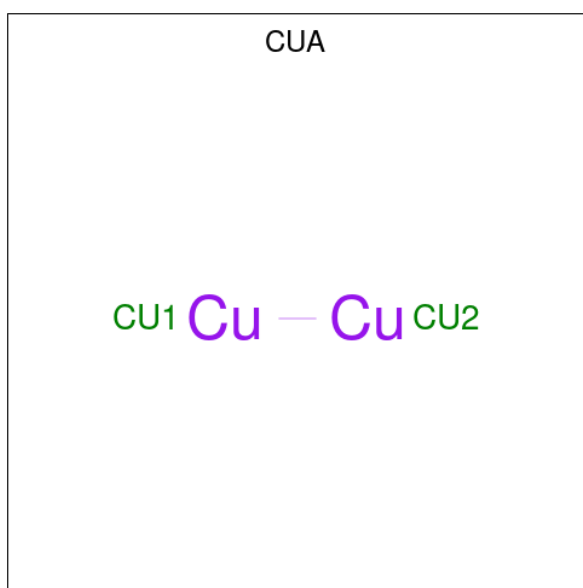
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	63	57	6	0	0
19	I	1	63	57	6	0	0
19	L	1	63	57	6	0	0
19	O	1	63	57	6	0	0
19	V	1	63	57	6	0	0
19	Y	1	63	57	6	0	0

- Molecule 20 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



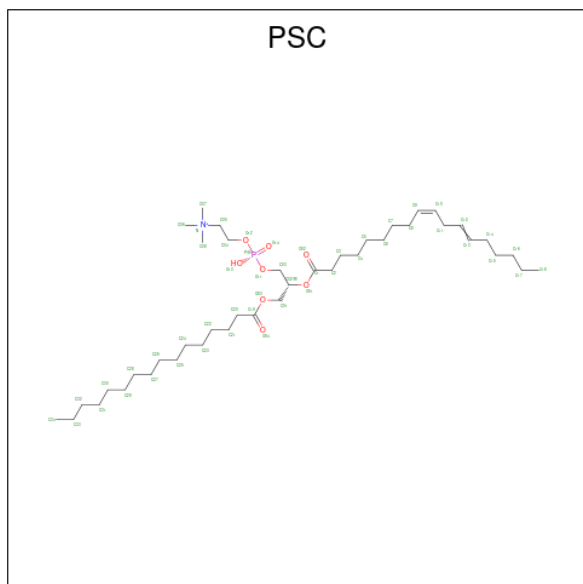
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total O 2 2	0	0
20	N	1	Total O 2 2	0	0

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



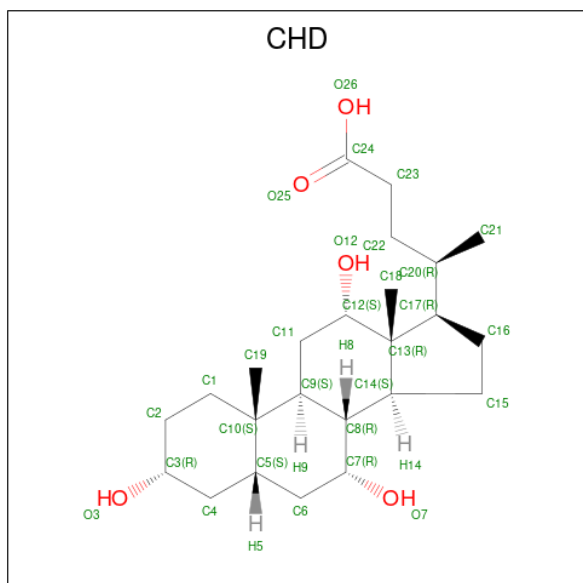
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total Cu 2 2	0	0
21	O	1	Total Cu 2 2	0	0

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



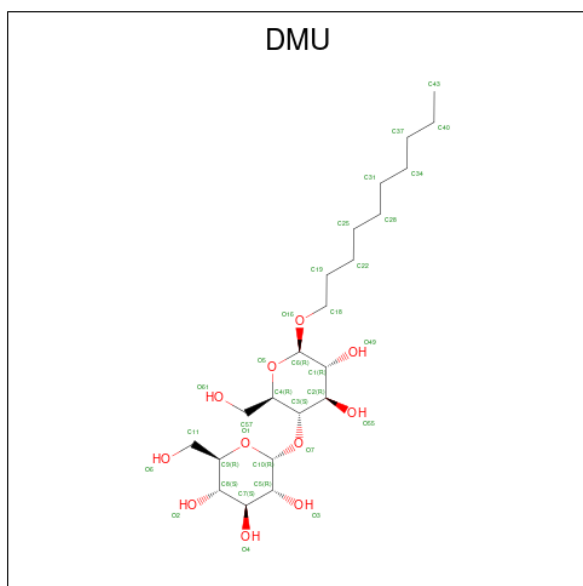
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
22	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



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

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



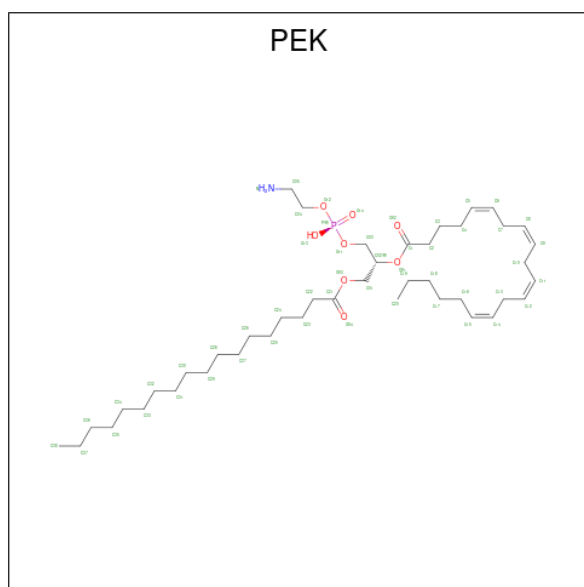
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	Q	1	Total	C	O	0	0
			33	22	11		

Continued on next page...

Continued from previous page...

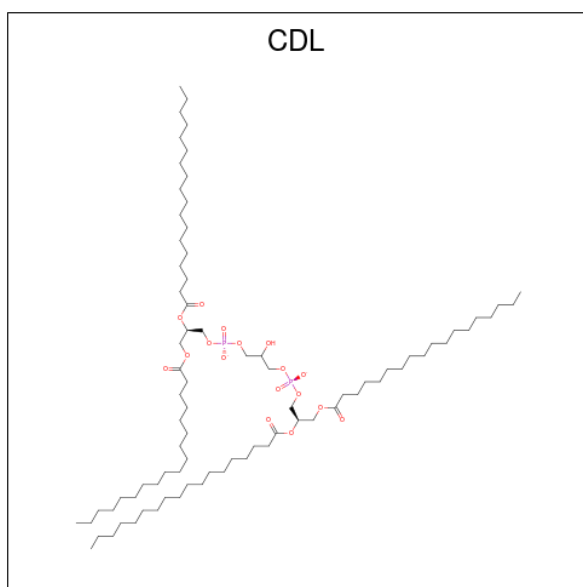
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	T	1	Total	C	O	0	0
			33	22	11		

- Molecule 25 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
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

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

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
28	A	79	79	79	0	0
28	B	55	55	55	0	0
28	C	28	28	28	0	0

Continued on next page...

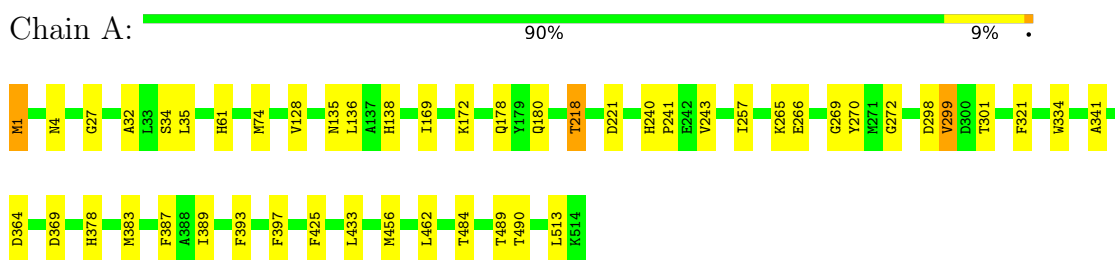
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	D	9	Total O 9 9	0	0
28	E	16	Total O 16 16	0	0
28	F	17	Total O 17 17	0	0
28	G	18	Total O 18 18	0	0
28	H	13	Total O 13 13	0	0
28	I	10	Total O 10 10	0	0
28	J	7	Total O 7 7	0	0
28	L	10	Total O 10 10	0	0
28	M	9	Total O 9 9	0	0
28	N	59	Total O 59 59	0	0
28	O	29	Total O 29 29	0	0
28	P	30	Total O 30 30	0	0
28	Q	19	Total O 19 19	0	0
28	R	14	Total O 14 14	0	0
28	S	7	Total O 7 7	0	0
28	T	14	Total O 14 14	0	0
28	U	11	Total O 11 11	0	0
28	V	12	Total O 12 12	0	0
28	W	4	Total O 4 4	0	0
28	Y	4	Total O 4 4	0	0
28	Z	2	Total O 2 2	0	0

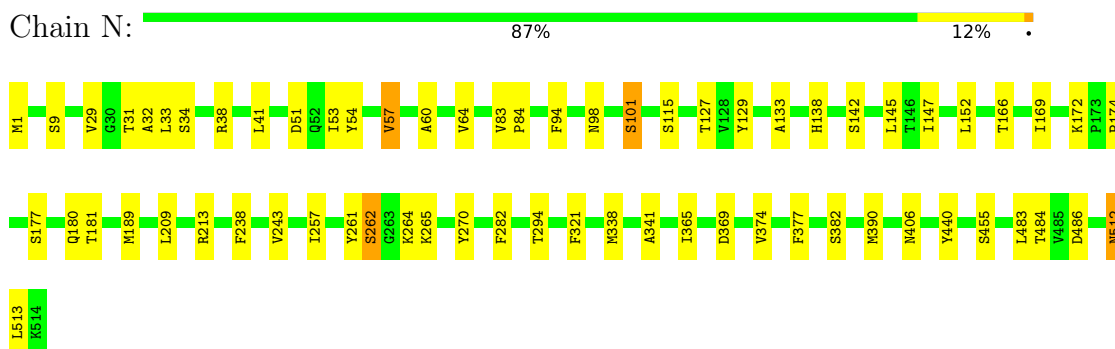
3 Residue-property plots [i](#)

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

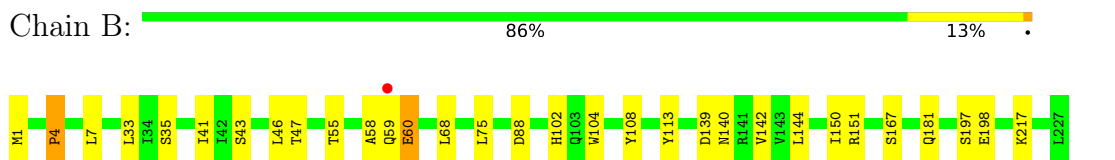
- Molecule 1: Cytochrome c oxidase subunit 1



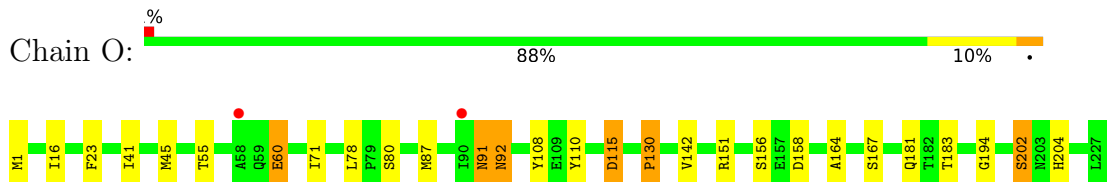
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2




- Molecule 3: Cytochrome c oxidase subunit 3

Chain C:  93% 6%




- Molecule 3: Cytochrome c oxidase subunit 3

Chain P:  90% 9%




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

Chain D:  90% 7%




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

Chain Q:  88% 10% 2%




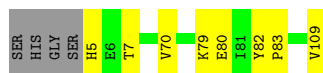
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:  86% 10%




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

Chain R:  89% 7%

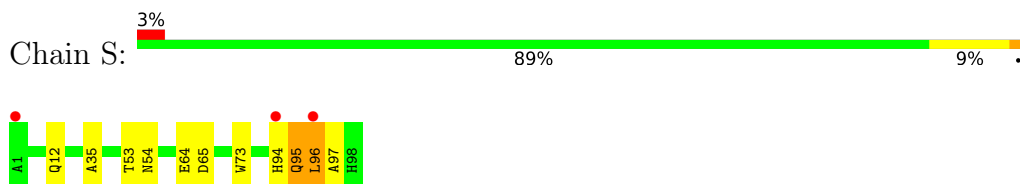


- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

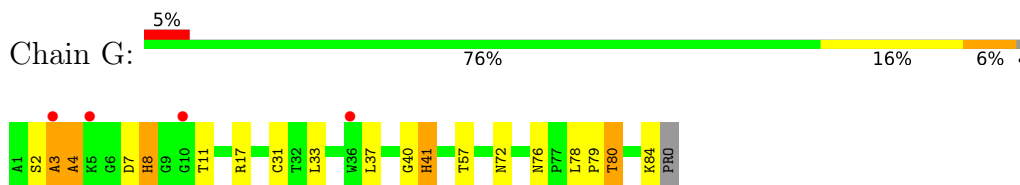
Chain F:  90% 8% 3%



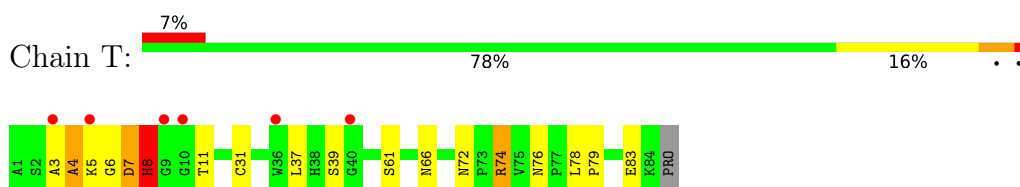
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



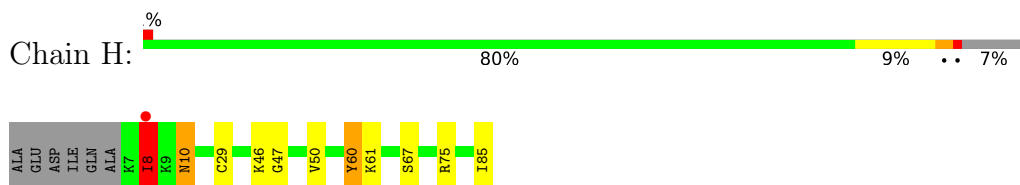
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



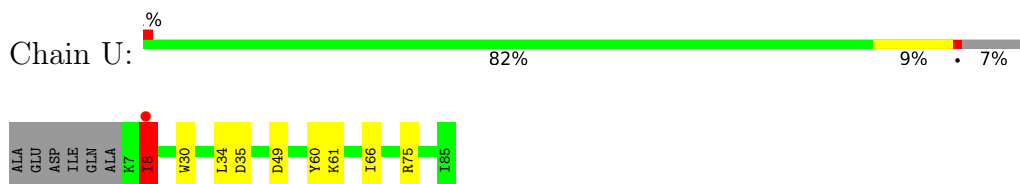
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



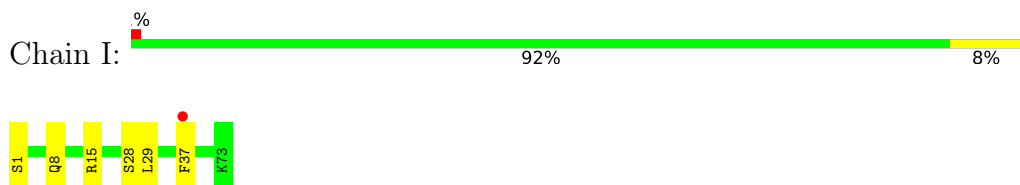
- Molecule 8: Cytochrome c oxidase subunit 6B1



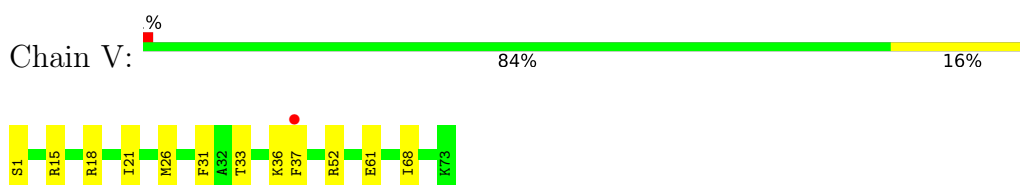
- Molecule 8: Cytochrome c oxidase subunit 6B1




- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 9: Cytochrome c oxidase subunit 6C



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

Chain J:  92% 7%




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

Chain W:  75% 22%




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

Chain K:  79% 9% 12%




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

Chain X:  77% 9% 12%




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

Chain L:  89% 9%




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

Chain Y:  83% 13%



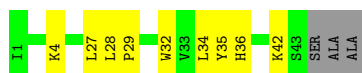
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:  80% 13% 7%



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

Chain Z:  74% 20% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	178.70Å 189.80Å 211.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.00-2.90) 99.2 (15.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.192 , 0.244 0.201 , 0.247	Depositor DCC
R_{free} test set	7805 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtrriage
Anisotropy	0.122	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 91.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31210	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: PGV, PEK, SAC, CU, PER, PSC, TPO, DMU, MG, ZN, FME, NA, HEA, CHD, TGL, CUA, CDL

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	0/4156	0.99	1/5678 (0.0%)
1	N	0.72	0/4156	1.00	1/5678 (0.0%)
2	B	0.74	1/1860 (0.1%)	0.97	0/2534
2	O	0.74	1/1860 (0.1%)	0.93	0/2534
3	C	0.71	0/2197	0.97	0/3005
3	P	0.69	0/2197	0.95	0/3005
4	D	0.66	0/1229	0.91	0/1658
4	Q	0.74	0/1229	0.99	1/1658 (0.1%)
5	E	0.69	0/871	0.93	0/1182
5	R	0.68	0/871	0.94	0/1182
6	F	0.78	0/765	0.99	0/1038
6	S	0.69	0/765	0.90	0/1038
7	G	0.81	0/690	0.92	0/937
7	T	0.80	0/690	0.96	0/937
8	H	0.76	0/682	0.97	0/921
8	U	0.74	0/682	0.98	0/921
9	I	0.74	0/605	0.98	0/802
9	V	0.73	0/605	1.03	0/802
10	J	0.68	0/471	1.04	0/636
10	W	0.71	0/471	1.06	0/636
11	K	0.77	0/398	0.99	0/546
11	X	0.70	0/398	0.93	0/546
12	L	0.72	0/393	0.91	0/526
12	Y	0.72	0/393	1.01	0/526
13	M	0.72	0/345	1.00	0/470
13	Z	0.67	0/345	1.02	0/470
All	All	0.73	2/29324 (0.0%)	0.97	3/39866 (0.0%)

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
6	F	0	1
6	S	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	6.18	1.31	1.23
2	O	158	ASP	CA-C	5.36	1.54	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	GLU	N-CA-C	6.60	114.07	108.13
4	Q	133	GLY	N-CA-C	5.24	119.47	112.77
1	N	169	ILE	CB-CA-C	-5.05	105.43	112.04

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
6	S	94	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	24	0
1	N	4027	0	4001	39	0
2	B	1824	0	1833	14	0
2	O	1824	0	1833	13	0
3	C	2110	0	2027	10	0
3	P	2110	0	2027	12	0
4	D	1195	0	1183	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	1195	0	1183	9	0
5	E	852	0	845	6	0
5	R	852	0	845	1	0
6	F	748	0	728	2	0
6	S	748	0	728	4	0
7	G	675	0	643	11	0
7	T	675	0	643	11	0
8	H	662	0	623	3	0
8	U	662	0	623	4	0
9	I	601	0	613	1	0
9	V	601	0	613	0	0
10	J	460	0	459	1	0
10	W	460	0	459	5	0
11	K	384	0	366	2	0
11	X	384	0	366	3	0
12	L	380	0	380	2	0
12	Y	380	0	380	4	0
13	M	335	0	352	1	0
13	Z	335	0	352	5	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	4	0
17	N	120	0	108	3	0
18	A	102	0	152	1	0
18	C	102	0	152	0	0
18	N	51	0	76	2	0
18	P	153	0	228	1	0
19	A	63	0	110	1	0
19	I	63	0	110	3	0
19	L	63	0	110	1	0
19	O	63	0	110	0	0
19	V	63	0	110	0	0
19	Y	63	0	110	2	0
20	A	2	0	0	1	0
20	N	2	0	0	1	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	O	52	0	80	4	0
23	B	29	0	39	0	0
23	C	58	0	78	1	0
23	J	29	0	39	0	0
23	O	29	0	39	1	0
23	P	58	0	78	0	0
23	W	29	0	39	2	0
24	C	33	0	42	0	0
24	M	33	0	42	0	0
24	Q	33	0	42	2	0
24	T	33	0	42	0	0
25	C	106	0	154	1	0
25	G	106	0	154	1	0
25	P	53	0	77	3	0
25	T	53	0	77	1	0
26	C	100	0	156	4	0
26	G	100	0	156	1	0
26	P	100	0	156	2	0
26	T	100	0	156	2	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	79	0	0	0	0
28	B	55	0	0	2	0
28	C	28	0	0	0	0
28	D	9	0	0	0	0
28	E	16	0	0	0	0
28	F	17	0	0	1	0
28	G	18	0	0	0	0
28	H	13	0	0	1	0
28	I	10	0	0	0	0
28	J	7	0	0	0	0
28	L	10	0	0	0	0
28	M	9	0	0	0	0
28	N	59	0	0	4	0
28	O	29	0	0	1	0
28	P	30	0	0	0	0
28	Q	19	0	0	3	0
28	R	14	0	0	0	0
28	S	7	0	0	0	0
28	T	14	0	0	0	0
28	U	11	0	0	0	0
28	V	12	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	W	4	0	0	1	0
28	Y	4	0	0	0	0
28	Z	2	0	0	0	0
All	All	31210	0	31316	185	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 3.

The worst 5 of 185 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)
20:N:607:PER:O1	20:N:607:PER:O2	1.61	1.19
20:A:609:PER:O1	20:A:609:PER:O2	1.61	1.18
7:T:31:CYS:SG	26:T:103:CDL:H532	2.20	0.81
8:H:10:ASN:HA	28:H:107:HOH:O	1.82	0.79
7:G:76:ASN:HD21	25:G:101:PEK:HN2	1.33	0.77

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%)	492 (96%)	19 (4%)	1 (0%)	43 72
1	N	512/514 (100%)	481 (94%)	30 (6%)	1 (0%)	43 72
2	B	225/227 (99%)	209 (93%)	14 (6%)	2 (1%)	14 41
2	O	225/227 (99%)	202 (90%)	19 (8%)	4 (2%)	6 25
3	C	257/261 (98%)	248 (96%)	8 (3%)	1 (0%)	30 59
3	P	257/261 (98%)	245 (95%)	11 (4%)	1 (0%)	30 59
4	D	142/147 (97%)	131 (92%)	11 (8%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	142/147 (97%)	130 (92%)	12 (8%)	0	100	100
5	E	103/109 (94%)	95 (92%)	8 (8%)	0	100	100
5	R	103/109 (94%)	99 (96%)	4 (4%)	0	100	100
6	F	96/98 (98%)	83 (86%)	10 (10%)	3 (3%)	3	14
6	S	96/98 (98%)	82 (85%)	12 (12%)	2 (2%)	5	21
7	G	81/85 (95%)	64 (79%)	11 (14%)	6 (7%)	1	2
7	T	81/85 (95%)	62 (76%)	12 (15%)	7 (9%)	0	1
8	H	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	2	10
8	U	77/85 (91%)	67 (87%)	9 (12%)	1 (1%)	9	32
9	I	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	9	30
9	V	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	9	30
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	6	25
11	K	47/56 (84%)	41 (87%)	5 (11%)	1 (2%)	5	21
11	X	47/56 (84%)	40 (85%)	7 (15%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	39 (89%)	5 (11%)	0	100	100
13	M	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3504/3614 (97%)	3236 (92%)	232 (7%)	36 (1%)	12	39

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	VAL
2	B	59	GLN
6	F	94	HIS
7	G	4	ALA
9	I	37	PHE

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%)	415 (97%)	11 (3%)	40	73
1	N	426/426 (100%)	407 (96%)	19 (4%)	24	58
2	B	210/210 (100%)	199 (95%)	11 (5%)	21	52
2	O	210/210 (100%)	199 (95%)	11 (5%)	21	52
3	C	224/226 (99%)	222 (99%)	2 (1%)	70	90
3	P	224/226 (99%)	218 (97%)	6 (3%)	39	73
4	D	128/129 (99%)	122 (95%)	6 (5%)	23	56
4	Q	128/129 (99%)	124 (97%)	4 (3%)	35	69
5	E	92/95 (97%)	91 (99%)	1 (1%)	65	88
5	R	92/95 (97%)	86 (94%)	6 (6%)	15	44
6	F	81/81 (100%)	75 (93%)	6 (7%)	13	38
6	S	81/81 (100%)	77 (95%)	4 (5%)	22	54
7	G	67/68 (98%)	63 (94%)	4 (6%)	17	47
7	T	67/68 (98%)	63 (94%)	4 (6%)	17	47
8	H	71/75 (95%)	62 (87%)	9 (13%)	4	14
8	U	71/75 (95%)	66 (93%)	5 (7%)	14	40
9	I	57/57 (100%)	54 (95%)	3 (5%)	20	52
9	V	57/57 (100%)	47 (82%)	10 (18%)	2	6
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	61
10	W	49/50 (98%)	44 (90%)	5 (10%)	7	23
11	K	39/46 (85%)	37 (95%)	2 (5%)	21	53
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	53
12	L	39/40 (98%)	37 (95%)	2 (5%)	21	53
12	Y	39/40 (98%)	34 (87%)	5 (13%)	4	14
13	M	37/38 (97%)	32 (86%)	5 (14%)	4	12
13	Z	37/38 (97%)	35 (95%)	2 (5%)	20	51
All	All	3040/3082 (99%)	2893 (95%)	147 (5%)	23	55

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	T	39	SER
12	Y	26	THR
8	U	49	ASP
9	V	52	ARG
8	H	75	ARG

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

Mol	Chain	Res	Type
2	O	140	ASN
4	Q	76	ASN
10	W	21	HIS
2	O	181	GLN
3	P	68	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	N	1	1	8,9,10	0.50	0	8,9,11	1.53	1 (12%)
2	FME	O	1	2	8,9,10	0.53	0	8,9,11	2.27	3 (37%)
7	TPO	T	11	7	8,10,11	1.14	1 (12%)	10,14,16	0.81	0
9	SAC	I	1	9	7,8,9	1.96	1 (14%)	7,9,11	1.63	2 (28%)
1	FME	A	1	1	8,9,10	0.59	0	8,9,11	1.63	2 (25%)
7	TPO	G	11	7	8,10,11	1.27	1 (12%)	10,14,16	0.91	1 (10%)
9	SAC	V	1	9	7,8,9	1.57	1 (14%)	7,9,11	1.49	2 (28%)
2	FME	B	1	2	8,9,10	0.67	0	8,9,11	2.30	3 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	N	1	1	-	6/7/9/11	-
2	FME	O	1	2	-	1/7/9/11	-
7	TPO	T	11	7	-	3/9/11/13	-
9	SAC	I	1	9	-	4/7/8/10	-
1	FME	A	1	1	-	4/7/9/11	-
7	TPO	G	11	7	-	2/9/11/13	-
9	SAC	V	1	9	-	5/7/8/10	-
2	FME	B	1	2	-	1/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	CA-N	4.90	1.53	1.46
9	V	1	SAC	CA-N	3.94	1.52	1.46
7	G	11	TPO	P-OG1	2.39	1.63	1.59
7	T	11	TPO	P-OG1	2.26	1.63	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-5.03	115.08	122.82
2	O	1	FME	CA-N-CN	-4.89	115.30	122.82
1	A	1	FME	CA-N-CN	-3.28	117.78	122.82
2	O	1	FME	C-CA-N	2.99	115.28	109.50
2	B	1	FME	C-CA-N	2.94	115.18	109.50

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-OG1
9	I	1	SAC	CB-CA-N-C1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 8 are monoatomic - 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$
18	PGV	A	606	-	50,50,50	1.06	2 (4%)	53,56,56	1.11	5 (9%)
19	TGL	I	101	-	62,62,62	1.03	3 (4%)	65,65,65	1.34	8 (12%)
26	CDL	G	102	-	99,99,99	1.00	4 (4%)	105,111,111	0.91	6 (5%)
19	TGL	A	608	-	62,62,62	1.16	3 (4%)	65,65,65	0.89	4 (6%)
18	PGV	N	606	-	50,50,50	1.04	2 (4%)	53,56,56	1.07	3 (5%)
23	CHD	W	101	-	32,32,32	0.68	0	51,51,51	1.71	8 (15%)
17	HEA	A	604	1	67,67,67	2.39	27 (40%)	81,103,103	2.43	27 (33%)
22	PSC	B	302	-	51,51,51	1.09	3 (5%)	57,59,59	1.40	8 (14%)
25	PEK	G	101	-	52,52,52	0.90	2 (3%)	55,57,57	0.71	1 (1%)
20	PER	N	607	14,17	1,1,1	1.33	0	-		
26	CDL	P	306	-	99,99,99	1.02	4 (4%)	105,111,111	1.14	6 (5%)
18	PGV	C	301	-	50,50,50	0.93	3 (6%)	53,56,56	0.73	0
18	PGV	P	301	-	50,50,50	0.93	2 (4%)	53,56,56	1.02	3 (5%)
18	PGV	P	305	-	50,50,50	1.18	2 (4%)	53,56,56	1.16	3 (5%)
20	PER	A	609	14,17	1,1,1	1.32	0	-		
18	PGV	A	607	-	50,50,50	1.12	2 (4%)	53,56,56	1.10	3 (5%)
17	HEA	A	605	20,1	67,67,67	2.46	28 (41%)	81,103,103	2.65	28 (34%)
18	PGV	C	305	-	50,50,50	1.01	2 (4%)	53,56,56	0.90	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHD	C	307	-	32,32,32	0.67	0	51,51,51	1.49	6 (11%)
17	HEA	N	605	20,1	67,67,67	2.43	28 (41%)	81,103,103	2.48	29 (35%)
23	CHD	B	303	-	32,32,32	0.66	0	51,51,51	1.25	5 (9%)
19	TGL	O	304	-	62,62,62	1.04	3 (4%)	65,65,65	0.92	4 (6%)
24	DMU	Q	201	-	34,34,34	0.84	0	45,45,45	1.29	4 (8%)
23	CHD	C	303	-	32,32,32	0.57	0	51,51,51	1.03	2 (3%)
25	PEK	T	102	-	52,52,52	1.01	2 (3%)	55,57,57	0.86	2 (3%)
19	TGL	V	101	-	62,62,62	1.03	3 (4%)	65,65,65	0.97	6 (9%)
21	CUA	B	301	2	0,1,1	-	-	-	-	-
25	PEK	G	103	-	52,52,52	1.03	2 (3%)	55,57,57	0.96	4 (7%)
22	PSC	O	303	-	51,51,51	1.05	2 (3%)	57,59,59	1.49	8 (14%)
25	PEK	C	304	-	52,52,52	1.00	2 (3%)	55,57,57	0.89	3 (5%)
21	CUA	O	301	2	0,1,1	-	-	-	-	-
26	CDL	T	103	-	99,99,99	1.05	4 (4%)	105,111,111	0.93	6 (5%)
19	TGL	L	101	-	62,62,62	1.06	3 (4%)	65,65,65	0.78	3 (4%)
25	PEK	C	308	-	52,52,52	1.06	2 (3%)	55,57,57	1.03	3 (5%)
24	DMU	C	302	-	34,34,34	1.56	7 (20%)	45,45,45	1.86	9 (20%)
24	DMU	T	101	-	34,34,34	1.48	5 (14%)	45,45,45	1.54	9 (20%)
25	PEK	P	303	-	52,52,52	0.90	2 (3%)	55,57,57	0.74	2 (3%)
19	TGL	Y	101	-	62,62,62	1.08	3 (4%)	65,65,65	0.77	2 (3%)
23	CHD	O	302	-	32,32,32	0.64	0	51,51,51	1.42	8 (15%)
26	CDL	C	306	-	99,99,99	0.99	4 (4%)	105,111,111	1.11	8 (7%)
18	PGV	P	304	-	50,50,50	1.01	2 (4%)	53,56,56	0.92	4 (7%)
17	HEA	N	604	1	67,67,67	2.40	27 (40%)	81,103,103	2.42	26 (32%)
23	CHD	J	101	-	32,32,32	0.88	2 (6%)	51,51,51	2.23	17 (33%)
24	DMU	M	101	-	34,34,34	1.40	2 (5%)	45,45,45	1.24	4 (8%)
23	CHD	P	302	-	32,32,32	0.68	0	51,51,51	1.04	3 (5%)
23	CHD	P	307	-	32,32,32	0.58	0	51,51,51	1.46	6 (11%)

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
18	PGV	A	606	-	-	32/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	I	101	-	-	38/65/65/65	-
26	CDL	G	102	-	-	42/110/110/110	-
19	TGL	A	608	-	-	33/65/65/65	-
18	PGV	N	606	-	-	33/55/55/55	-
23	CHD	W	101	-	-	7/9/74/74	0/4/4/4
17	HEA	A	604	1	-	9/36/76/76	-
22	PSC	B	302	-	-	25/55/55/55	-
25	PEK	G	101	-	-	21/56/56/56	-
26	CDL	P	306	-	-	69/110/110/110	-
18	PGV	C	301	-	-	18/55/55/55	-
18	PGV	P	301	-	-	16/55/55/55	-
18	PGV	P	305	-	-	29/55/55/55	-
18	PGV	A	607	-	-	25/55/55/55	-
23	CHD	C	307	-	-	4/9/74/74	0/4/4/4
17	HEA	A	605	20,1	-	7/36/76/76	-
18	PGV	C	305	-	-	25/55/55/55	-
17	HEA	N	605	20,1	-	8/36/76/76	-
23	CHD	B	303	-	-	6/9/74/74	0/4/4/4
19	TGL	O	304	-	-	41/65/65/65	-
24	DMU	Q	201	-	-	10/19/59/59	0/2/2/2
23	CHD	C	303	-	-	2/9/74/74	0/4/4/4
25	PEK	T	102	-	-	22/56/56/56	-
19	TGL	V	101	-	-	34/65/65/65	-
25	PEK	G	103	-	-	19/56/56/56	-
22	PSC	O	303	-	-	30/55/55/55	-
25	PEK	C	304	-	-	24/56/56/56	-
26	CDL	T	103	-	-	58/110/110/110	-
19	TGL	L	101	-	-	31/65/65/65	-
25	PEK	C	308	-	-	20/56/56/56	-
24	DMU	C	302	-	-	10/19/59/59	0/2/2/2
24	DMU	T	101	-	-	8/19/59/59	0/2/2/2
25	PEK	P	303	-	-	20/56/56/56	-
19	TGL	Y	101	-	-	28/65/65/65	-
23	CHD	O	302	-	-	4/9/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CDL	C	306	-	-	61/110/110/110	-
18	PGV	P	304	-	-	14/55/55/55	-
17	HEA	N	604	1	-	10/36/76/76	-
23	CHD	J	101	-	-	5/9/74/74	0/4/4/4
24	DMU	M	101	-	-	9/19/59/59	0/2/2/2
23	CHD	P	302	-	-	2/9/74/74	0/4/4/4
23	CHD	P	307	-	-	5/9/74/74	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	101	DMU	O16-C6	6.88	1.51	1.40
17	N	605	HEA	FE-ND	5.72	2.12	1.94
17	A	605	HEA	FE-ND	5.48	2.11	1.94
17	N	604	HEA	C3B-C2B	5.45	1.47	1.34
17	A	605	HEA	C3B-C2B	5.40	1.47	1.34

The worst 5 of 298 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	604	HEA	C3A-C2A-C1A	-8.76	98.76	107.05
17	N	605	HEA	C3A-C2A-C1A	-7.59	99.86	107.05
17	A	605	HEA	C3C-C4C-NC	7.53	116.14	109.80
17	N	604	HEA	C2A-C1A-NA	7.48	117.54	110.32
17	A	605	HEA	C3A-C2A-C1A	-7.48	99.97	107.05

There are no chirality outliers.

5 of 914 torsion outliers are listed below:

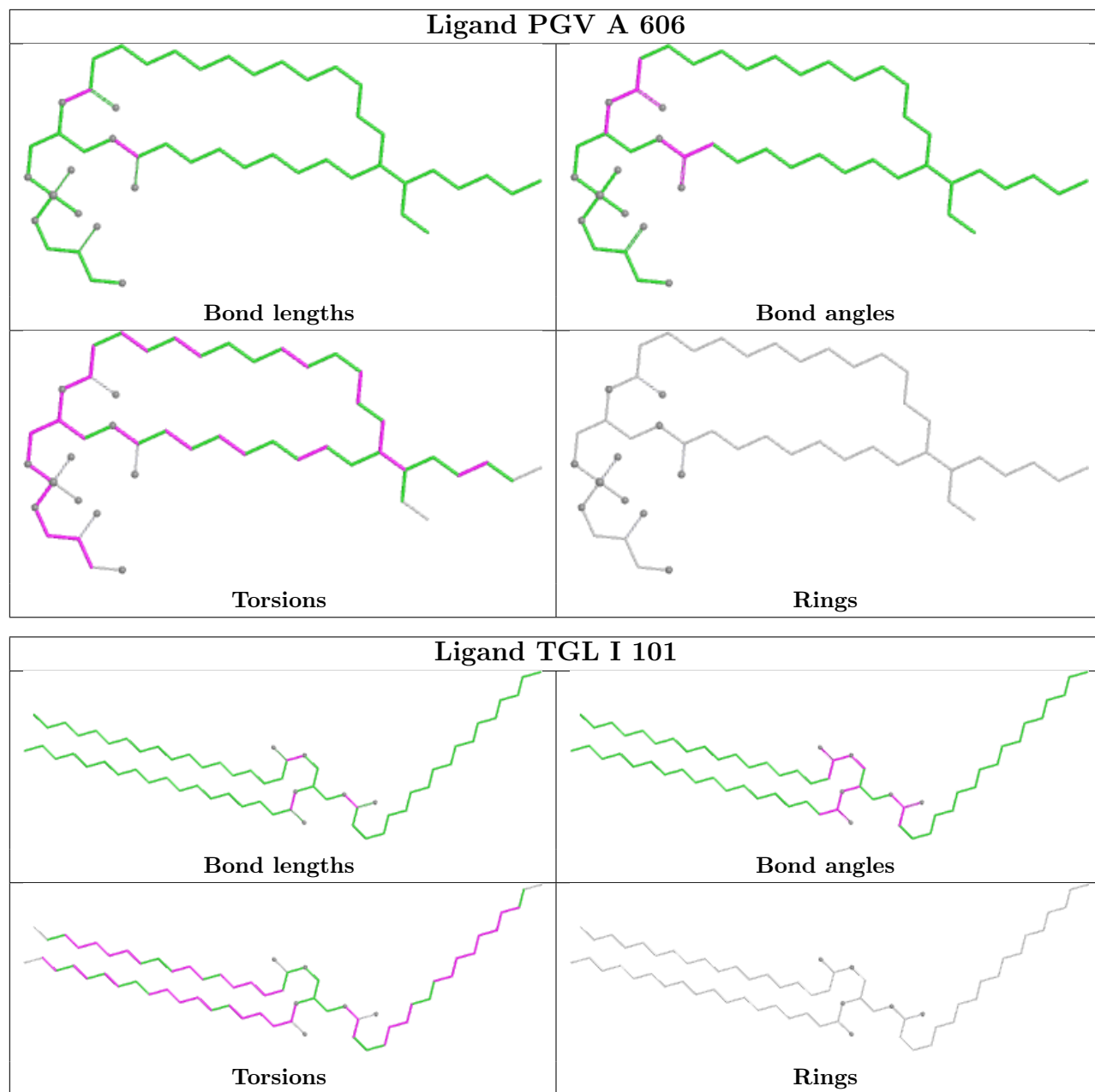
Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C03-O11-P-O12
18	A	606	PGV	C03-O11-P-O14
18	A	606	PGV	C04-O12-P-O11
18	A	606	PGV	C04-O12-P-O13
18	A	606	PGV	C04-O12-P-O14

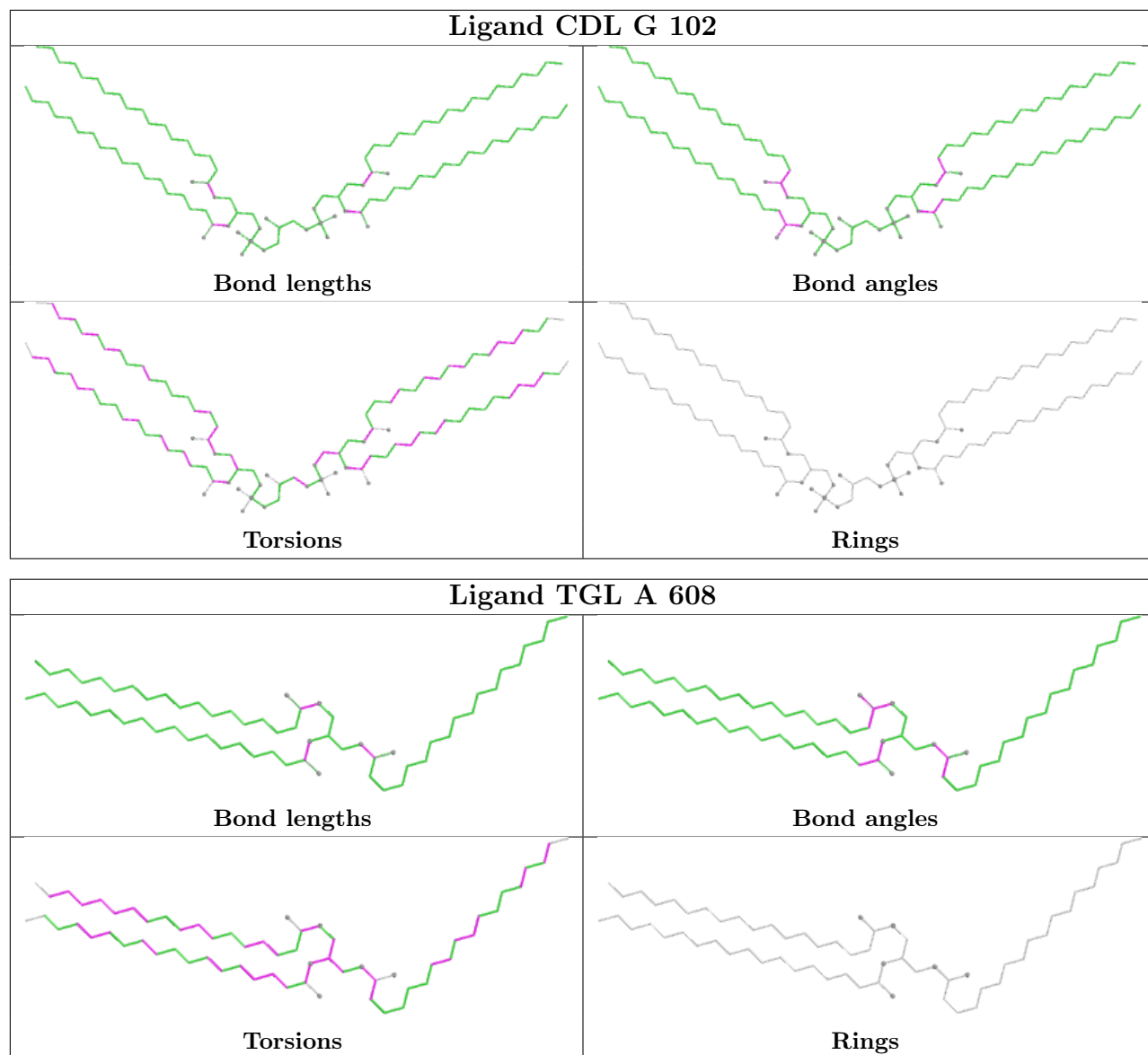
There are no ring outliers.

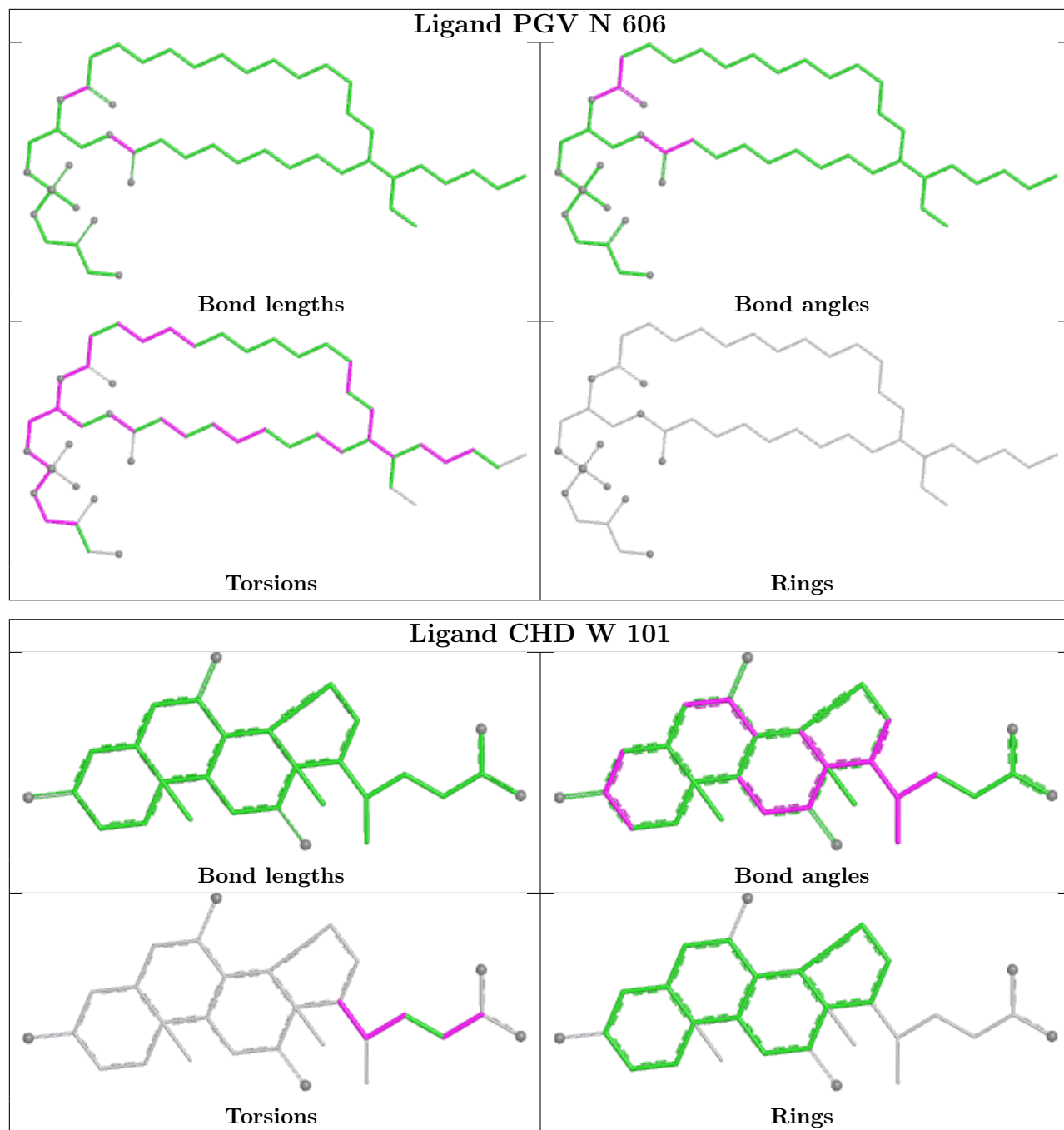
27 monomers are involved in 46 short contacts:

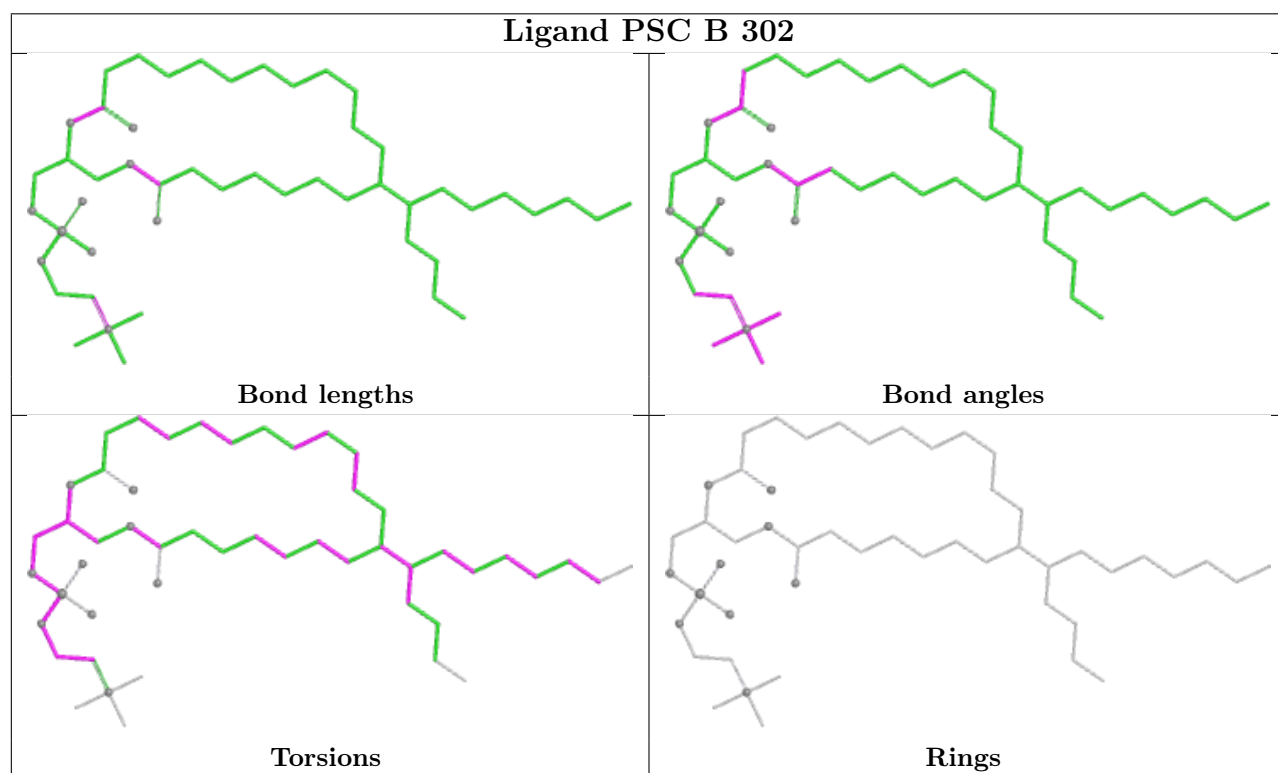
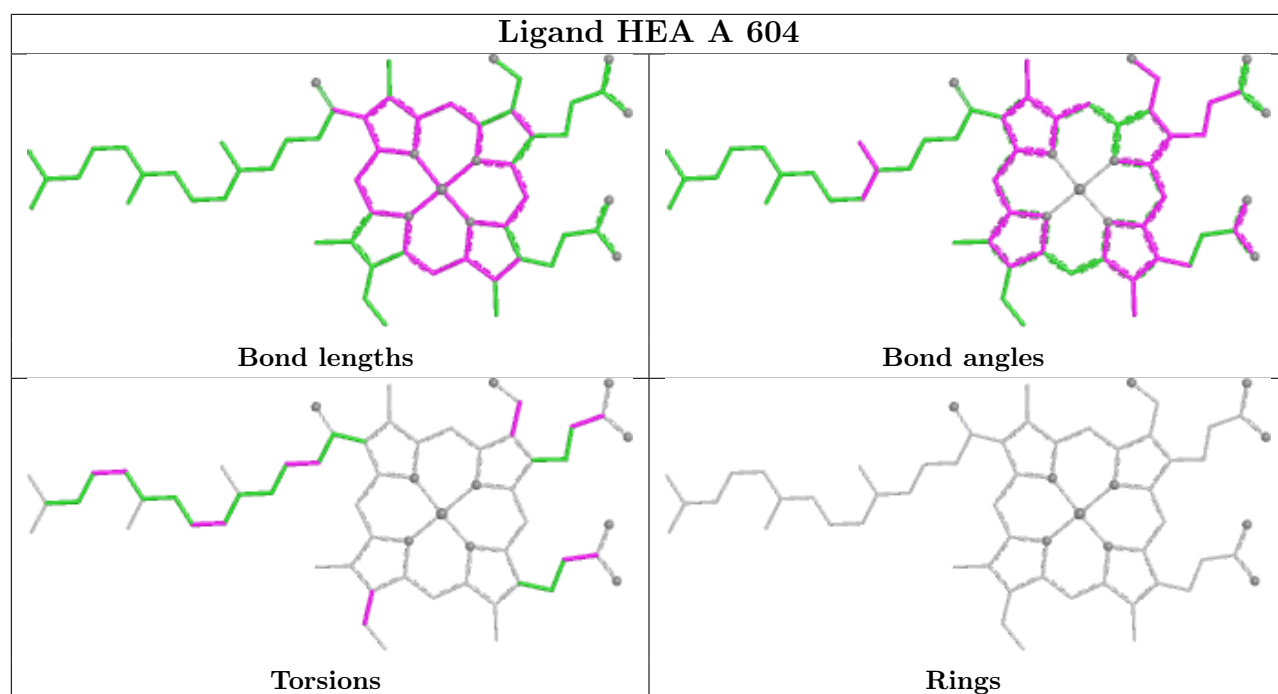
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	606	PGV	1	0
19	I	101	TGL	3	0
26	G	102	CDL	1	0
19	A	608	TGL	1	0
18	N	606	PGV	2	0
23	W	101	CHD	2	0
17	A	604	HEA	3	0
22	B	302	PSC	3	0
25	G	101	PEK	1	0
20	N	607	PER	1	0
26	P	306	CDL	2	0
20	A	609	PER	1	0
17	A	605	HEA	1	0
17	N	605	HEA	1	0
24	Q	201	DMU	2	0
23	C	303	CHD	1	0
25	T	102	PEK	1	0
22	O	303	PSC	4	0
26	T	103	CDL	2	0
19	L	101	TGL	1	0
25	C	308	PEK	1	0
25	P	303	PEK	3	0
19	Y	101	TGL	2	0
23	O	302	CHD	1	0
26	C	306	CDL	4	0
18	P	304	PGV	1	0
17	N	604	HEA	2	0

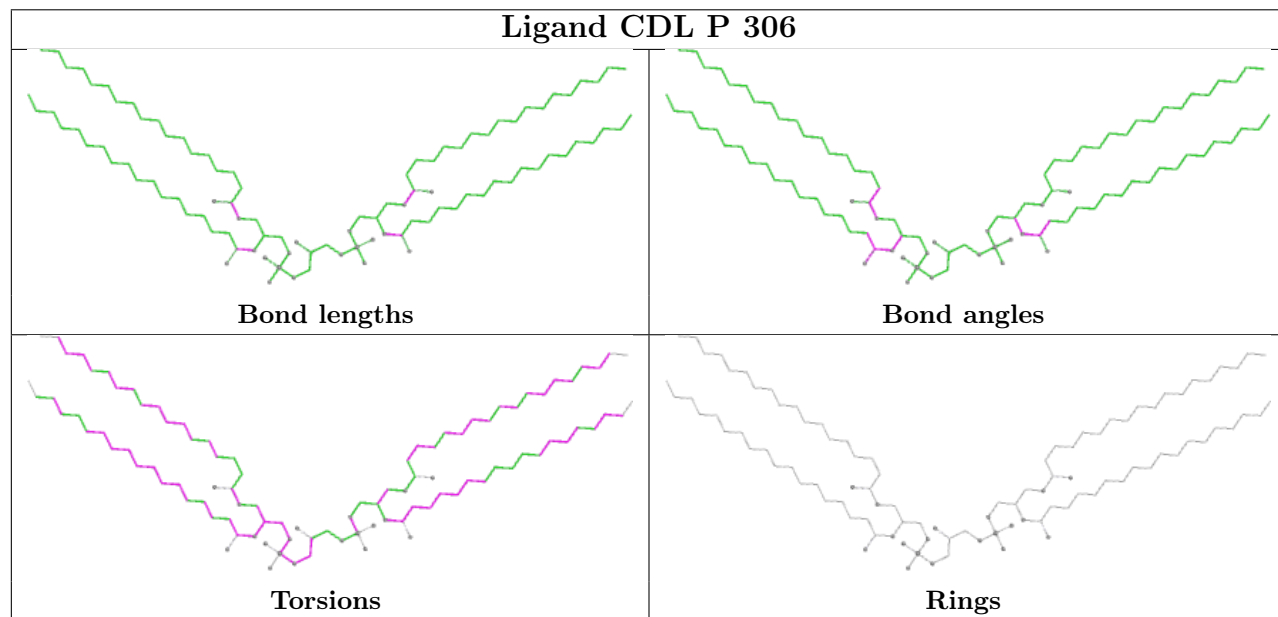
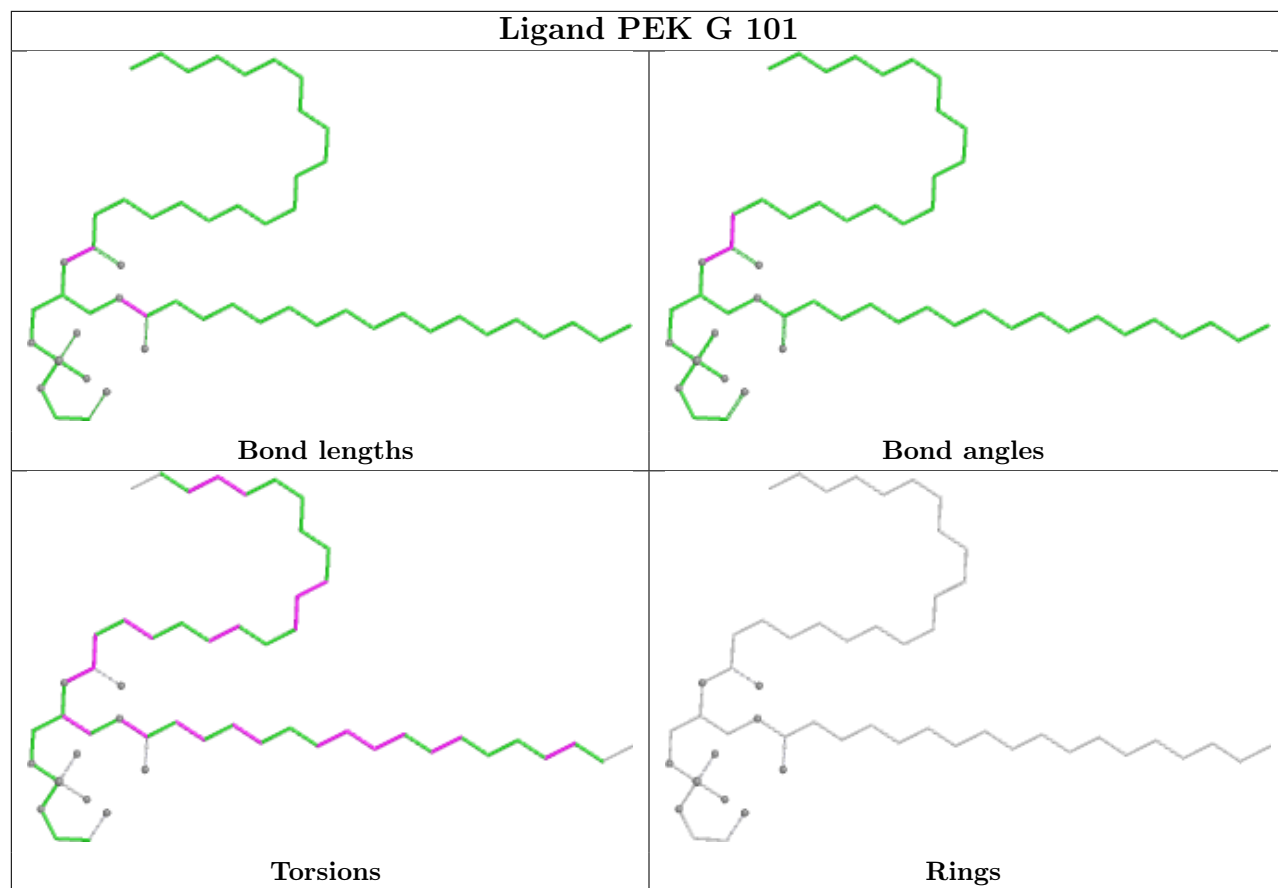
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

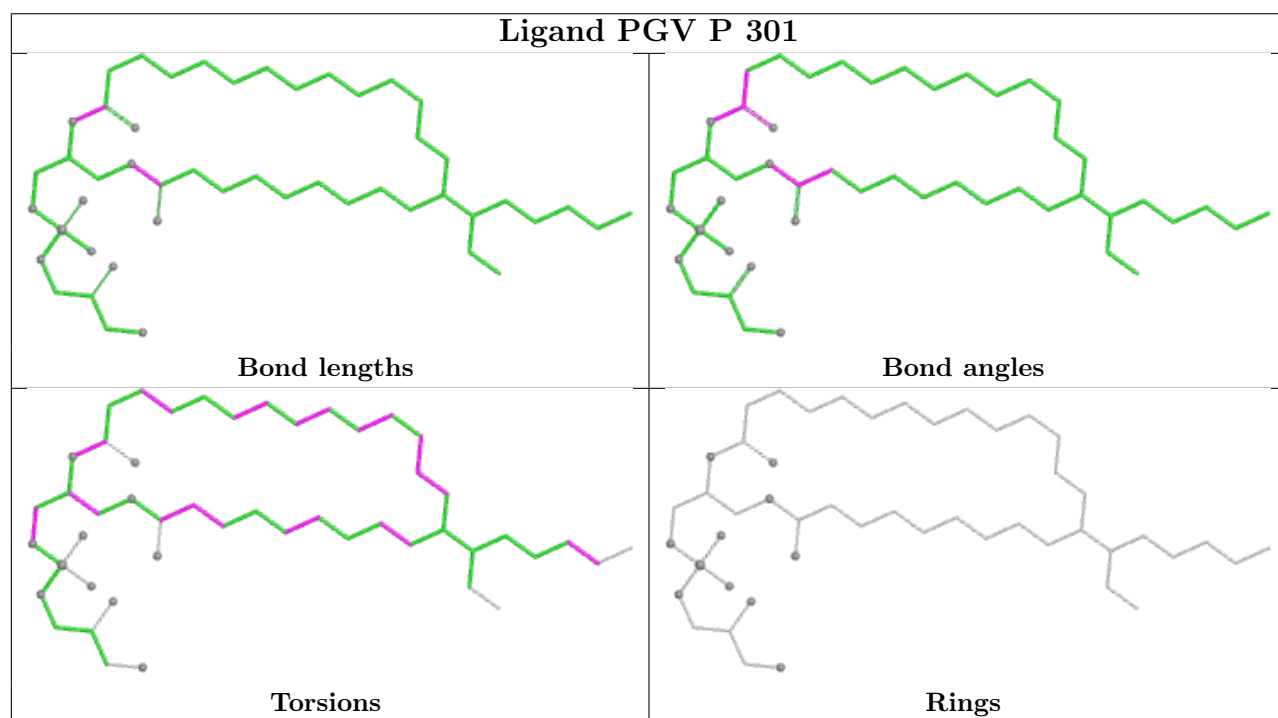
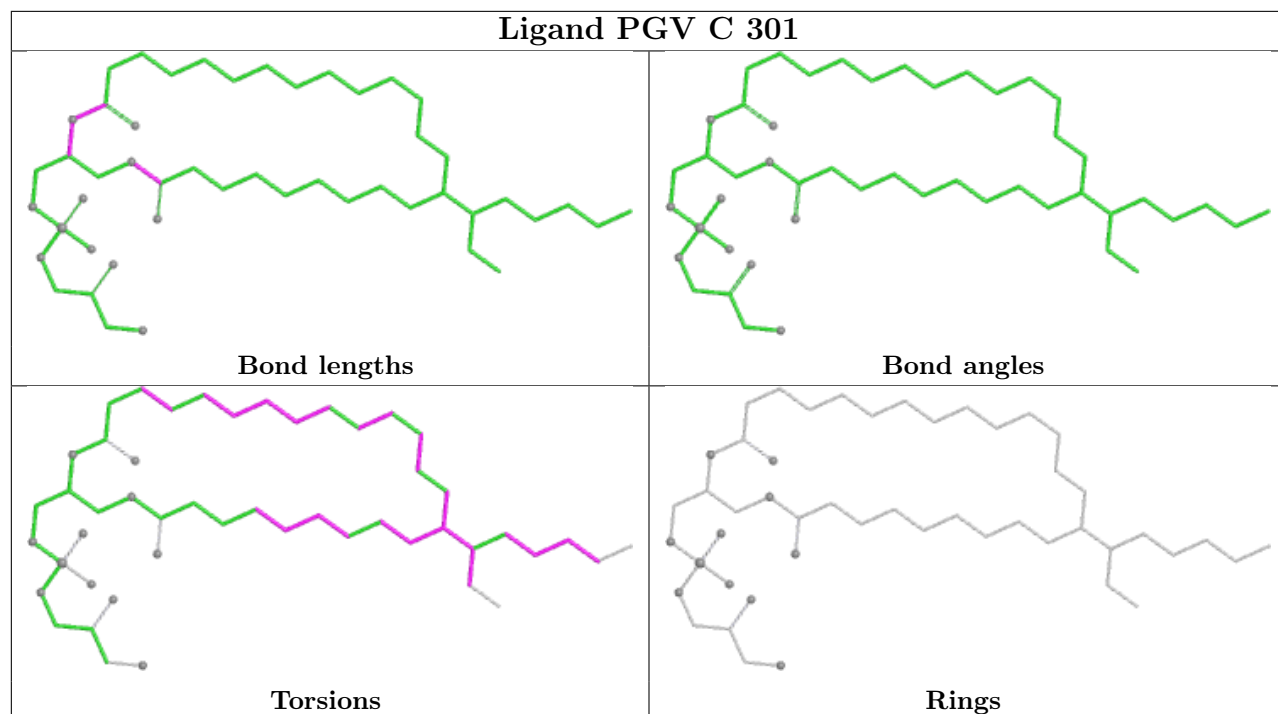


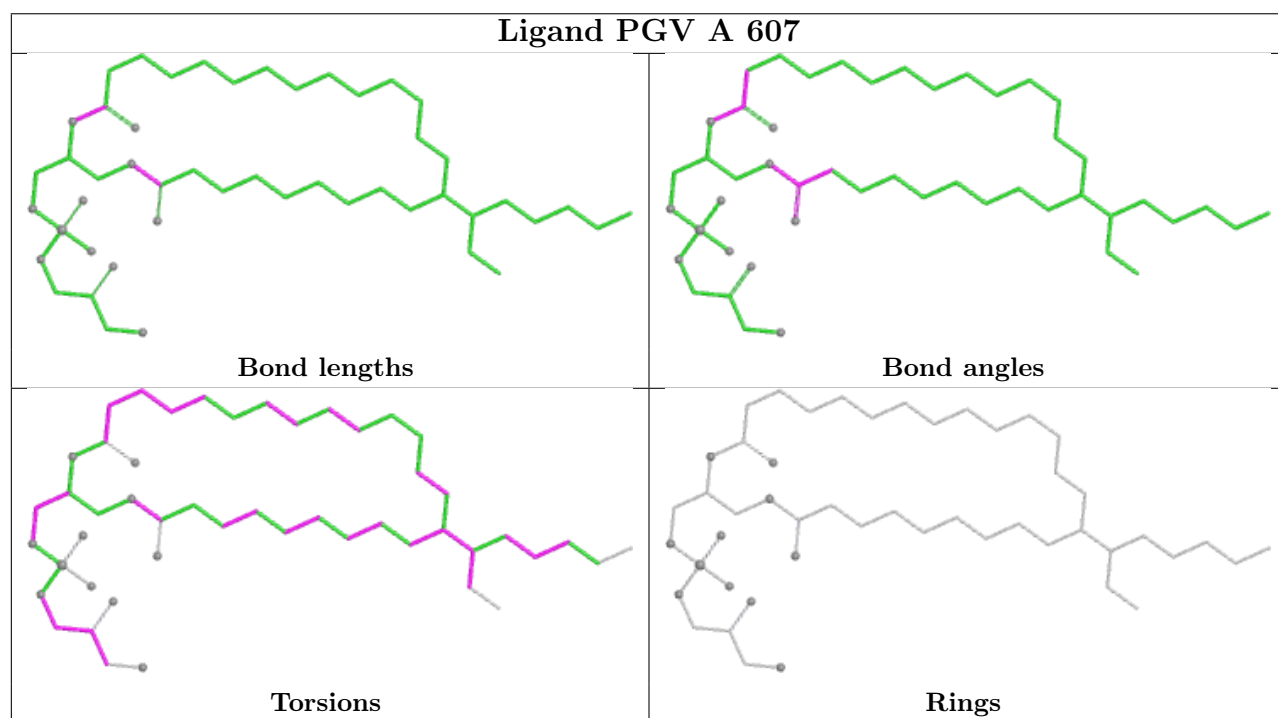
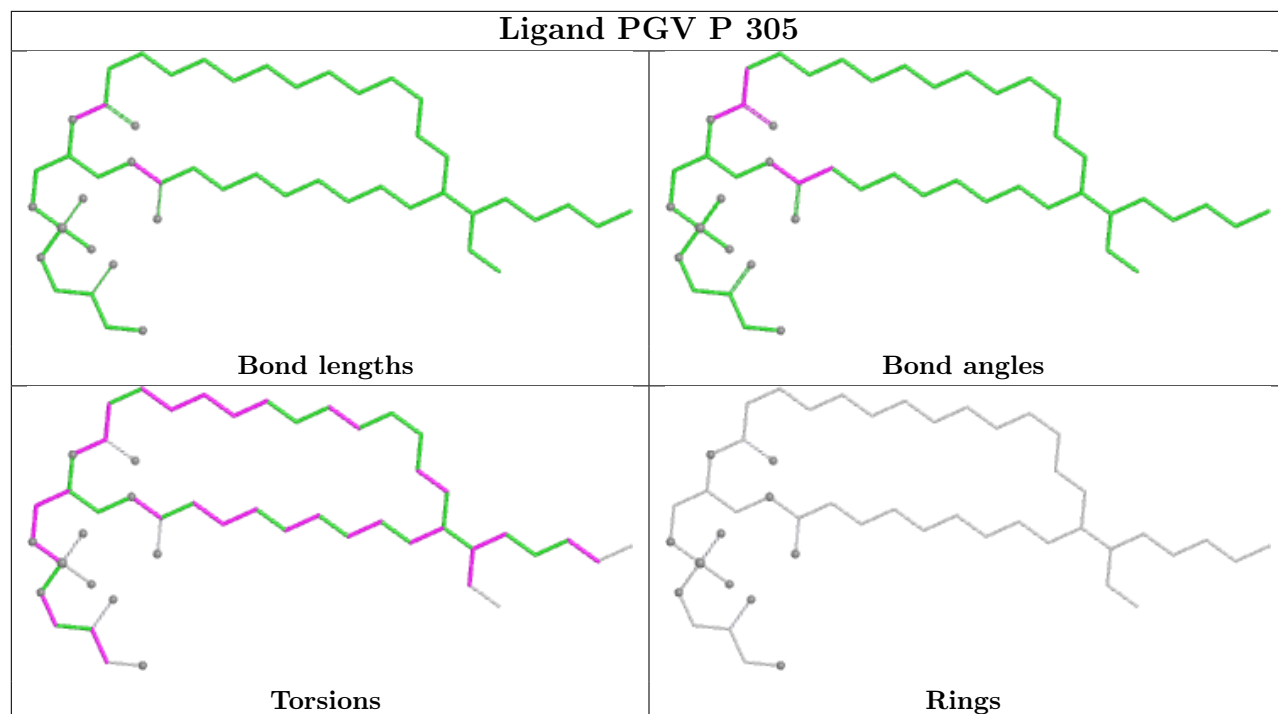


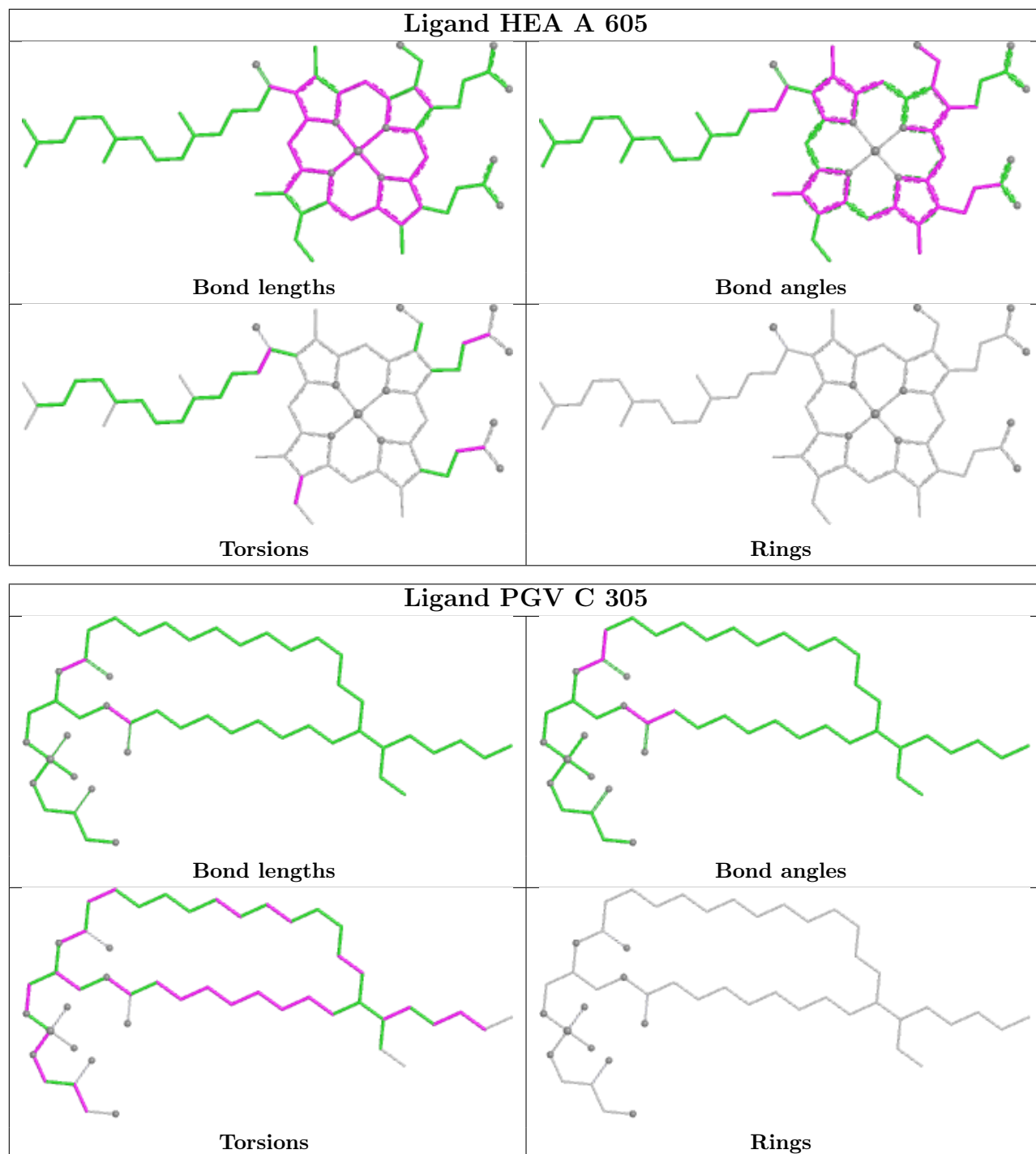


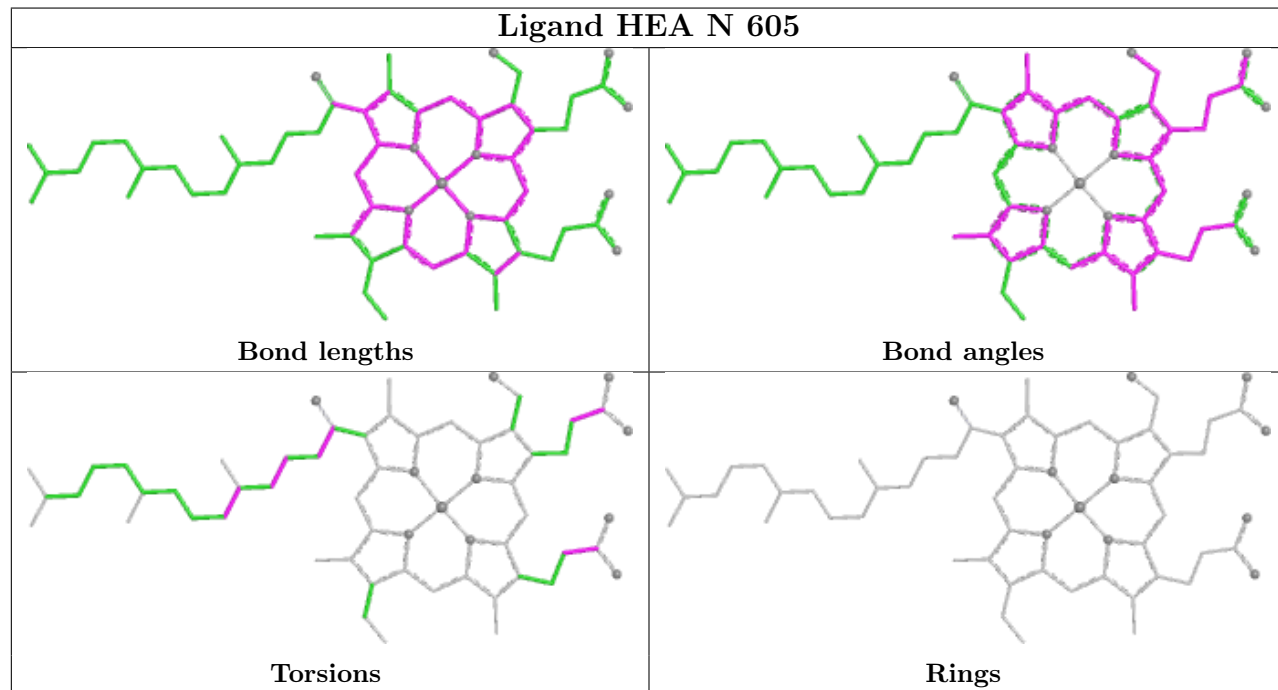
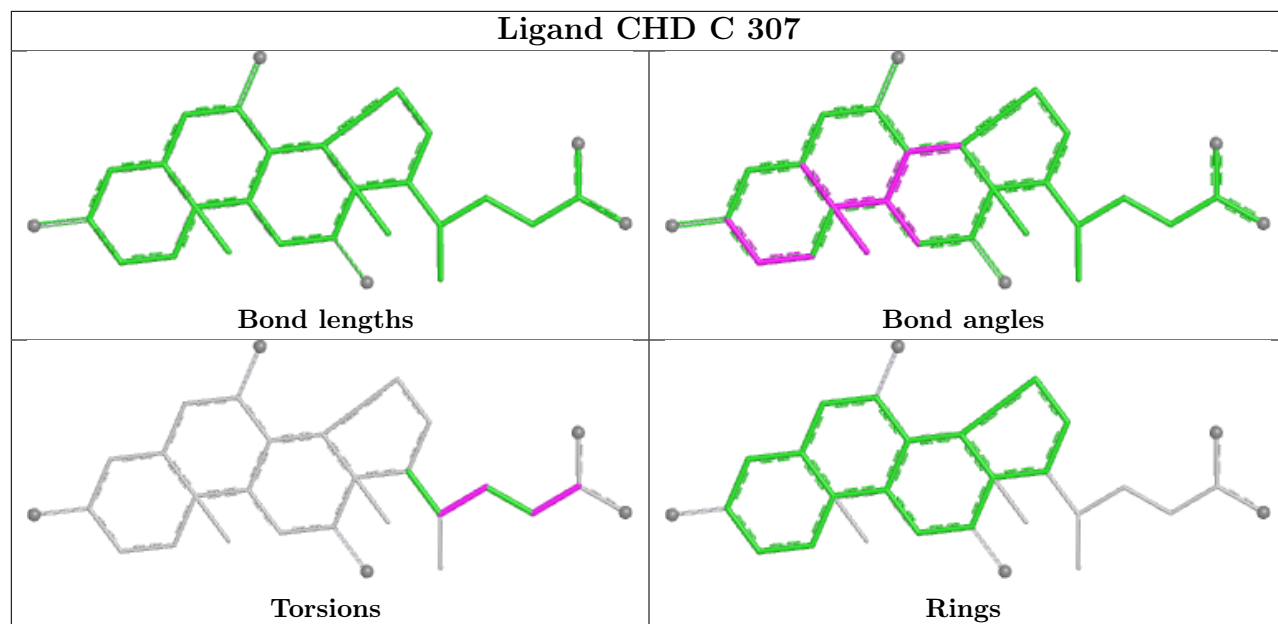


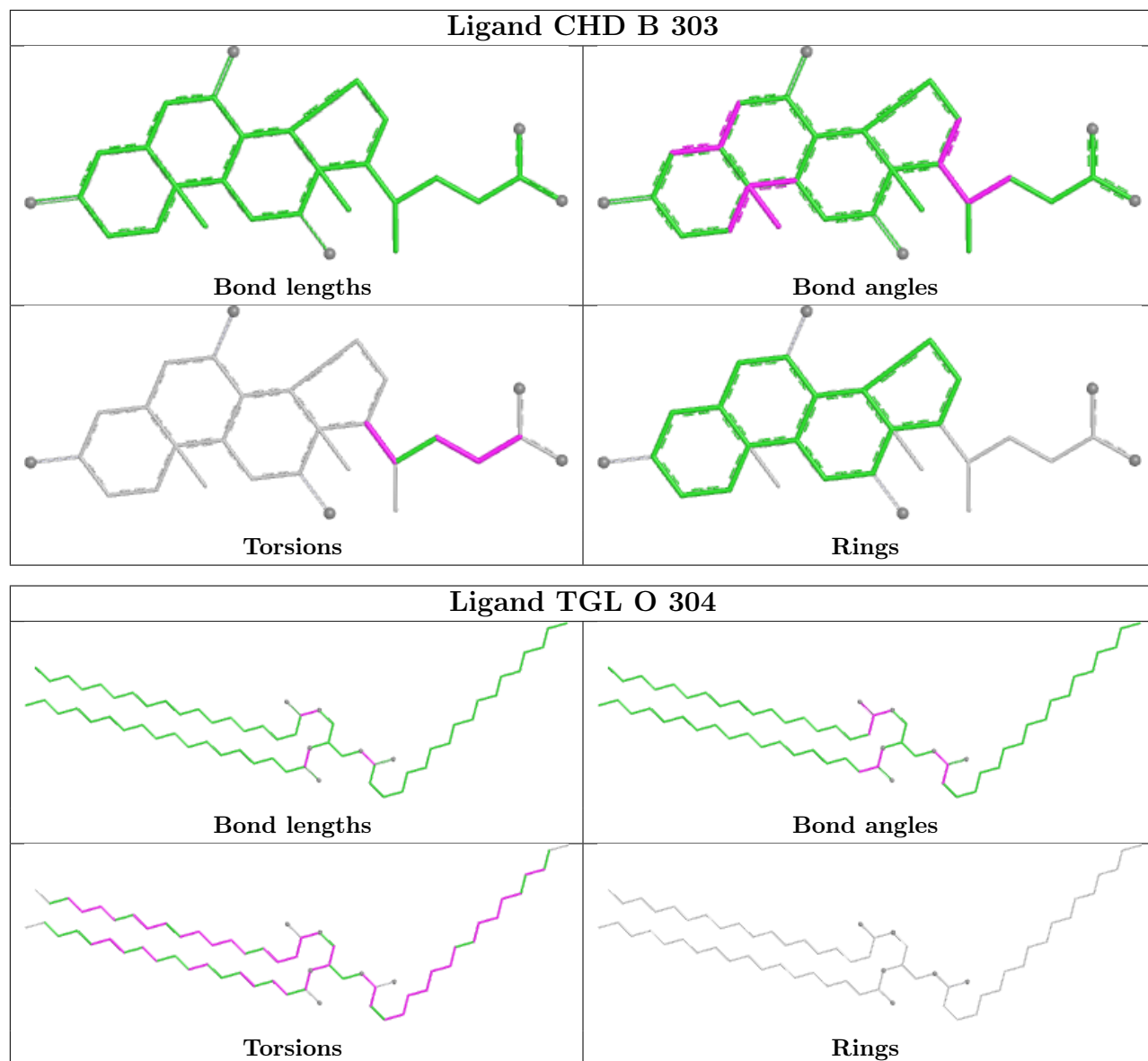


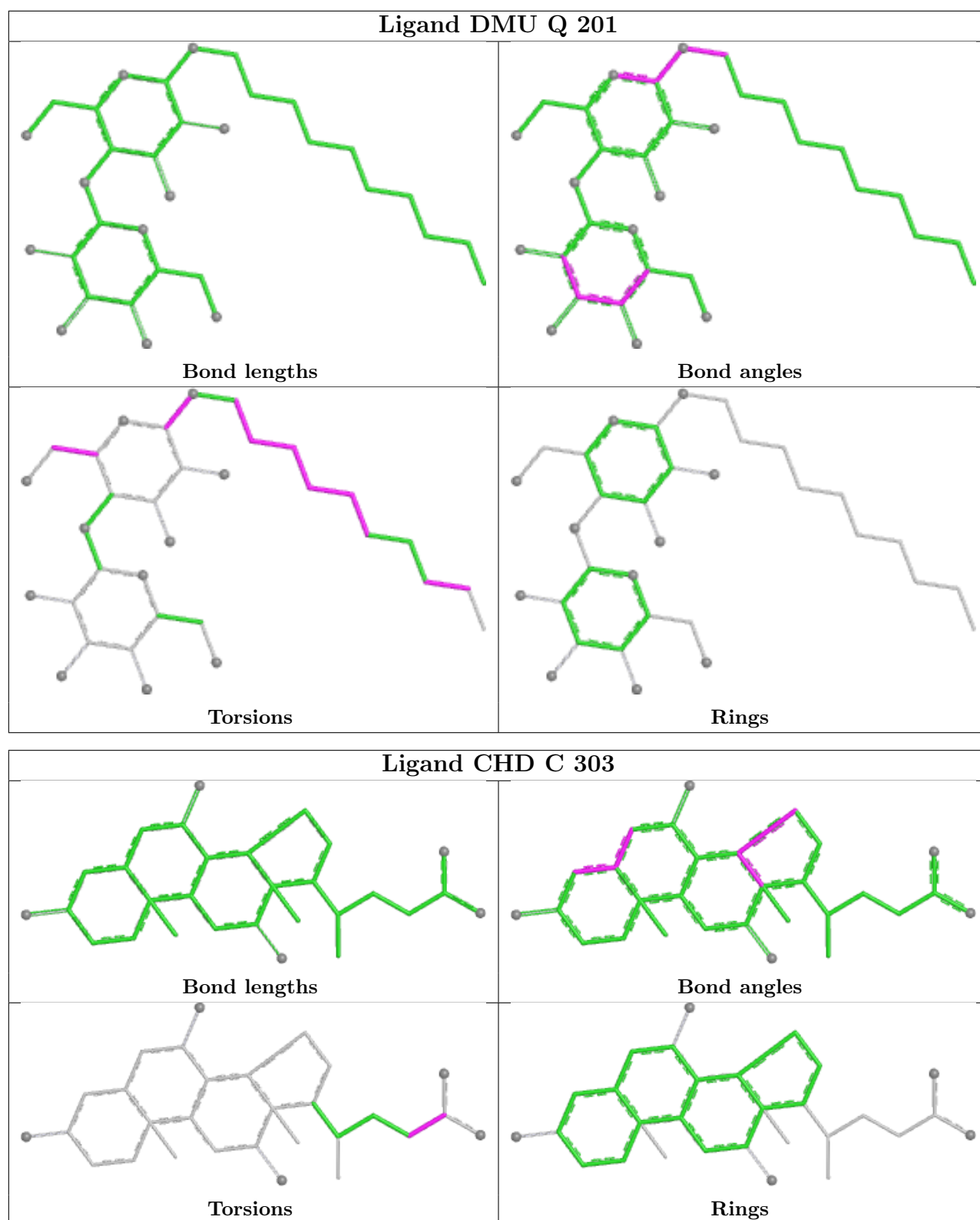


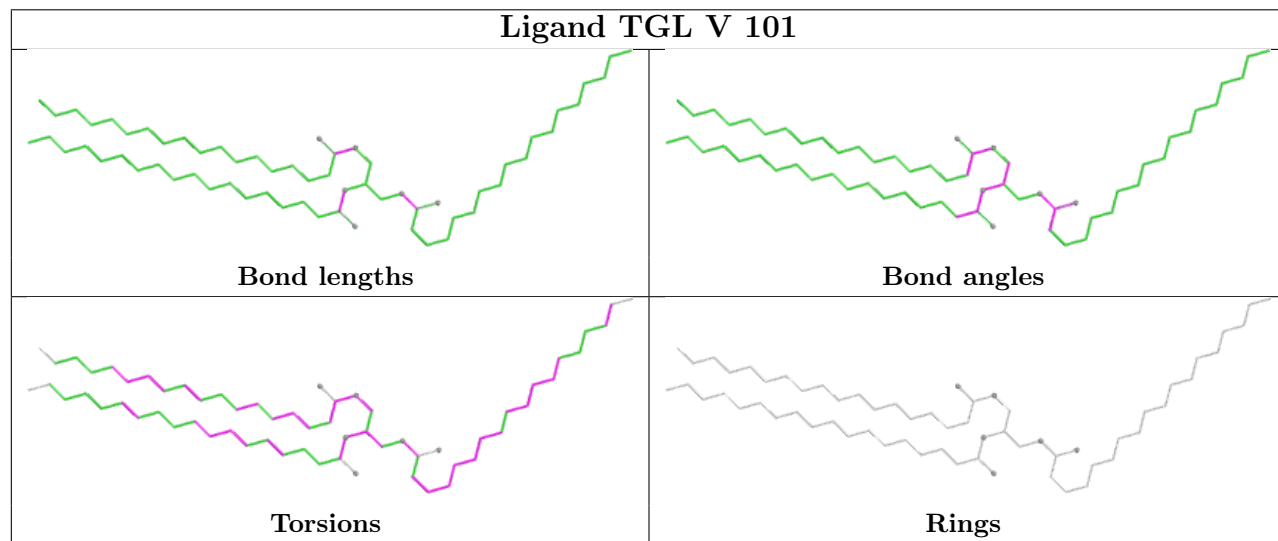
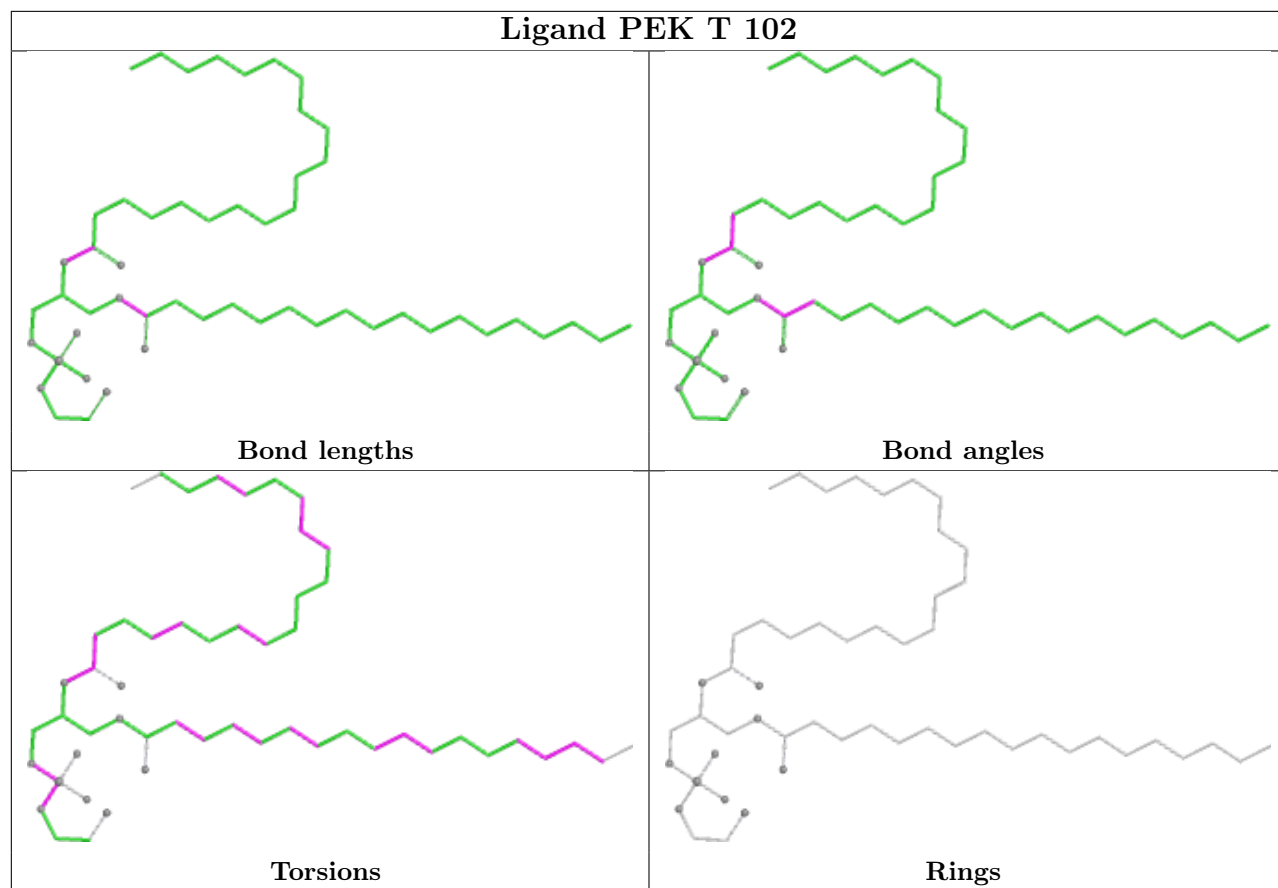


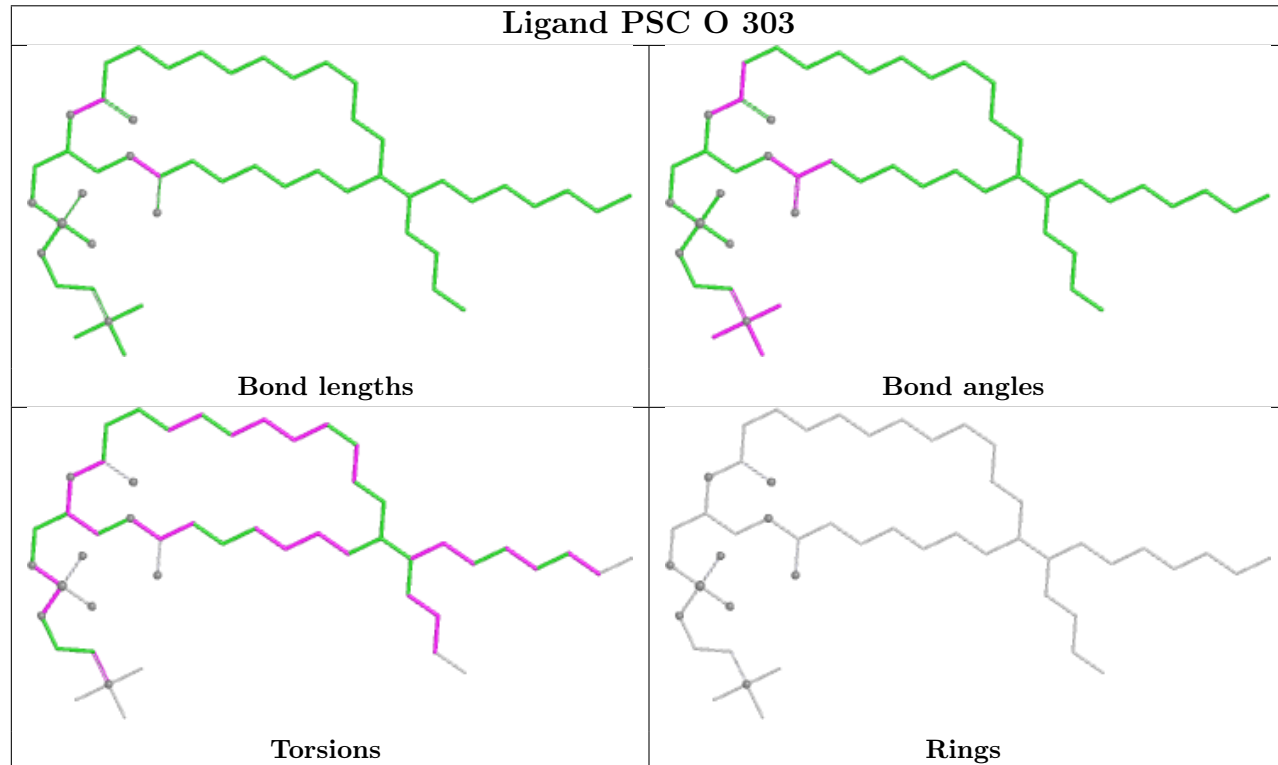
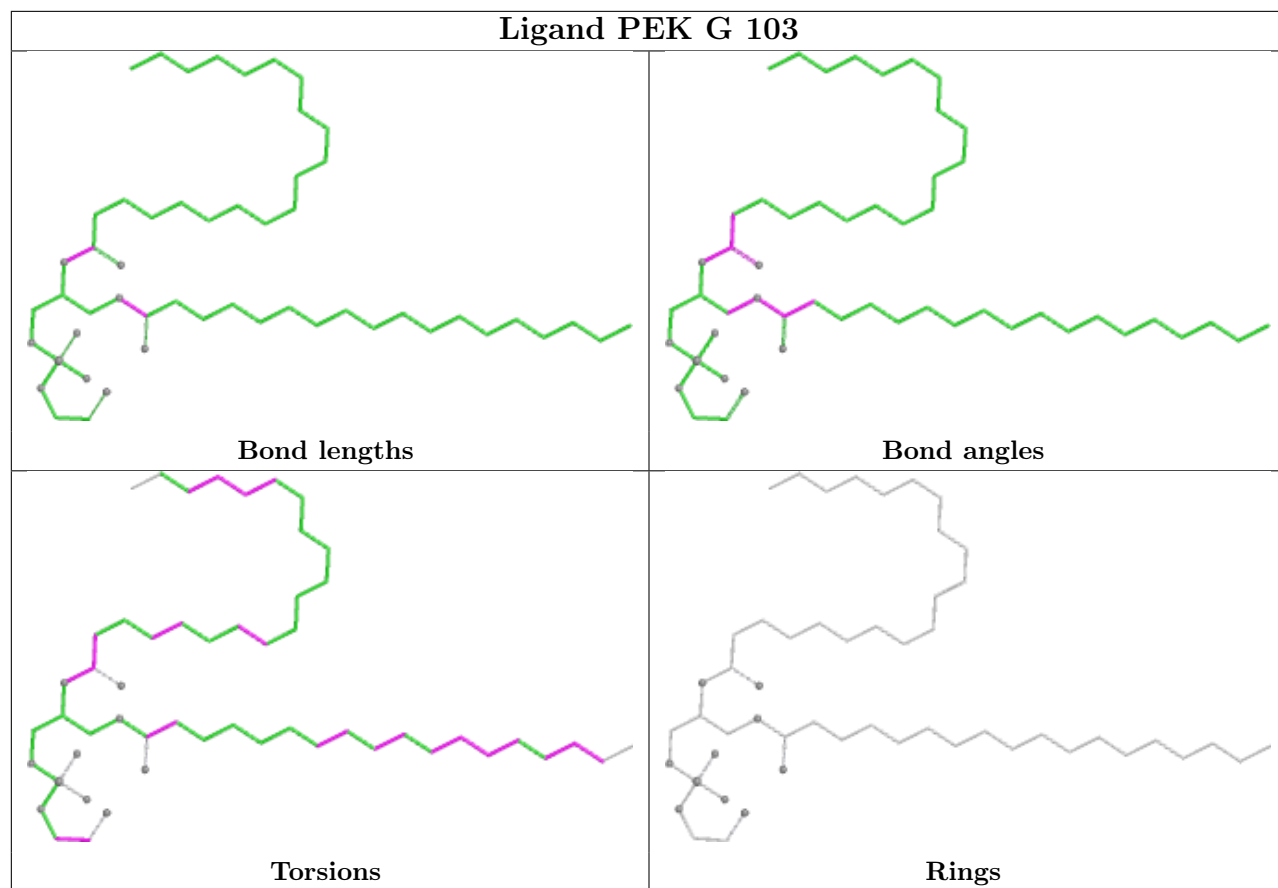


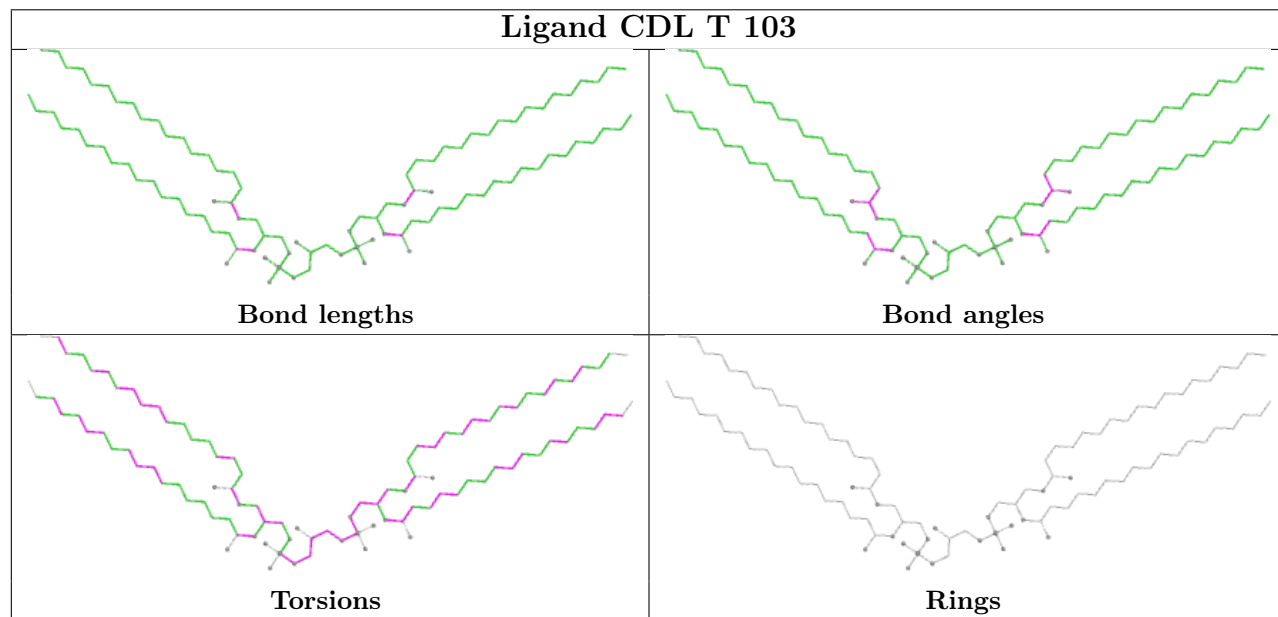
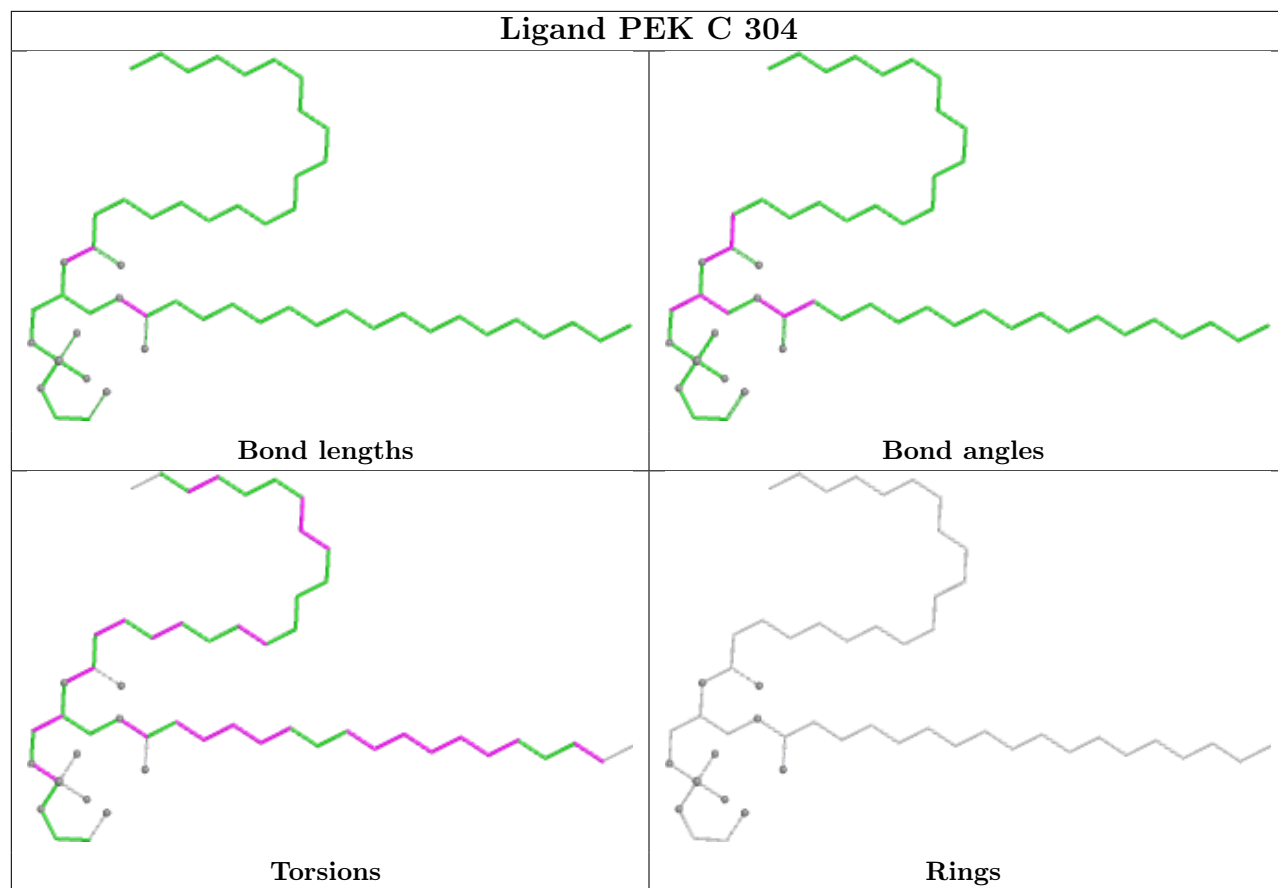


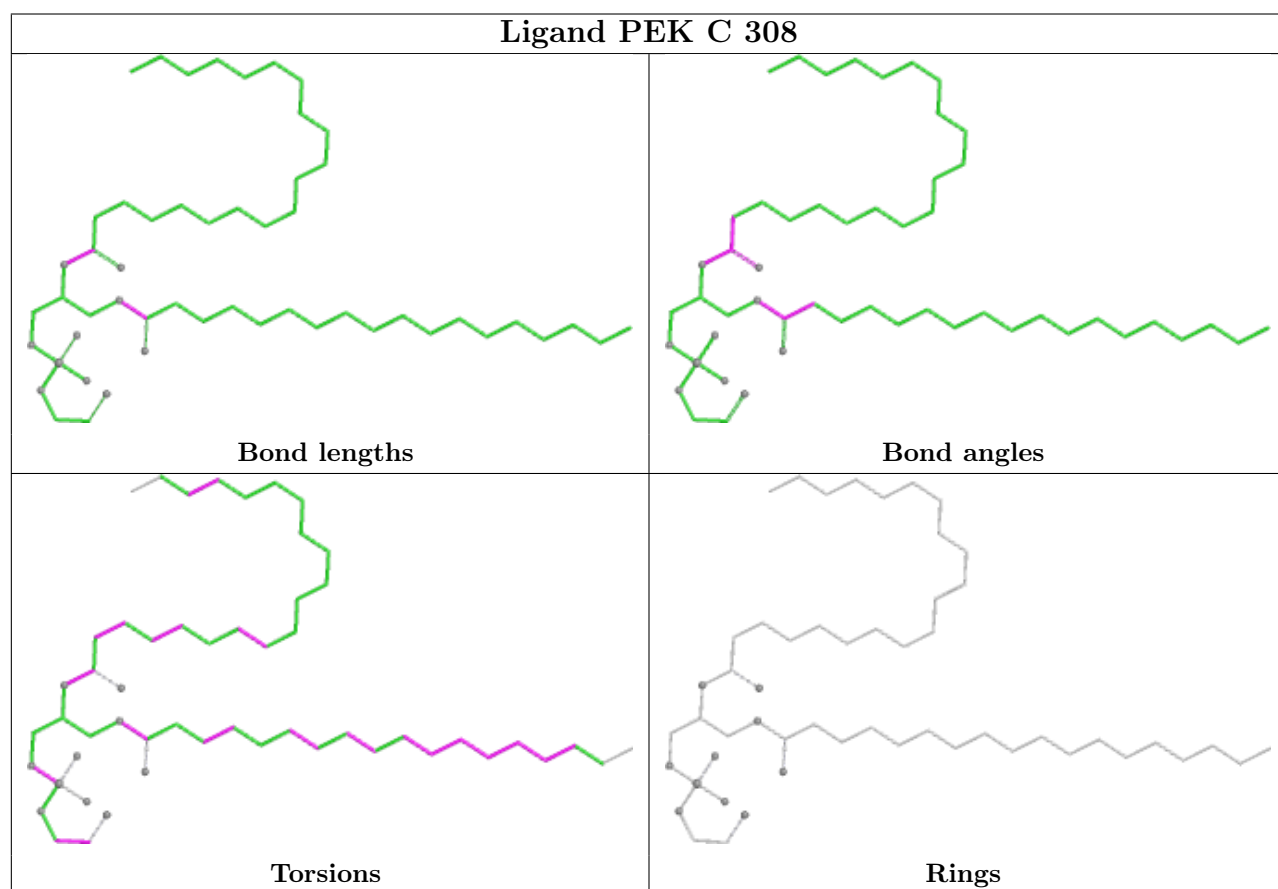
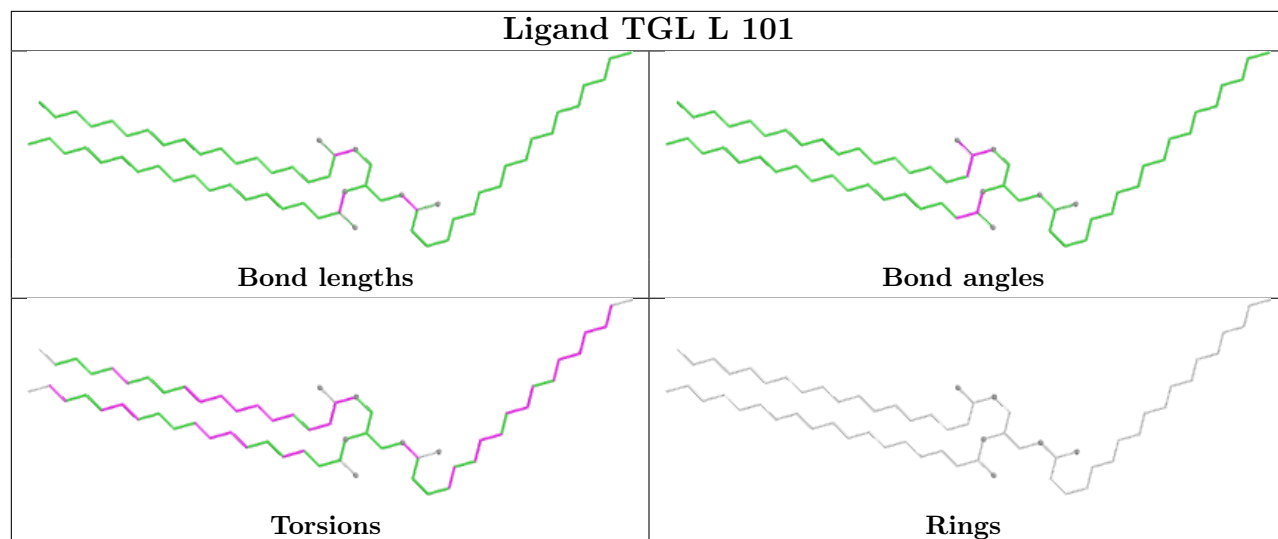


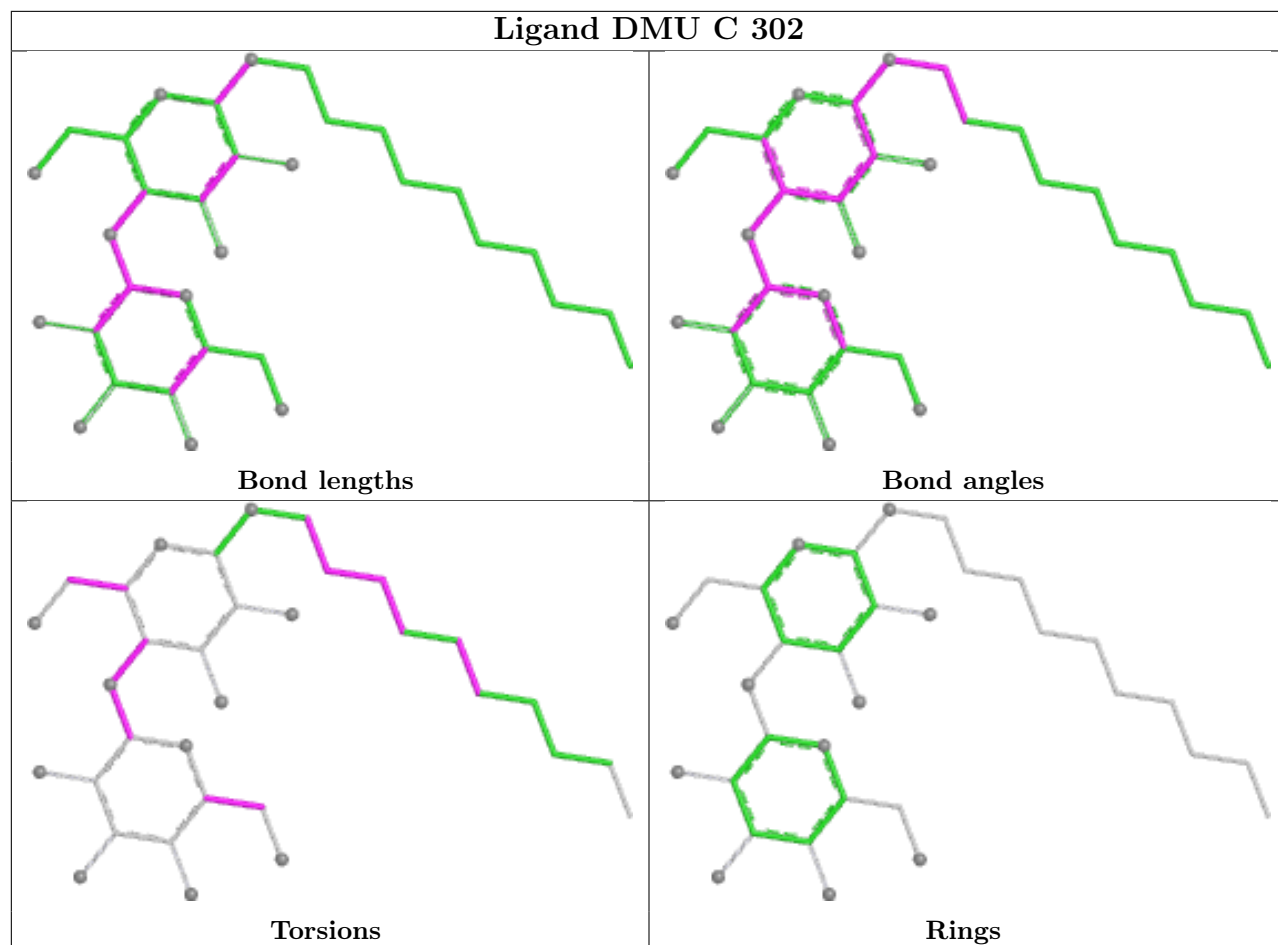


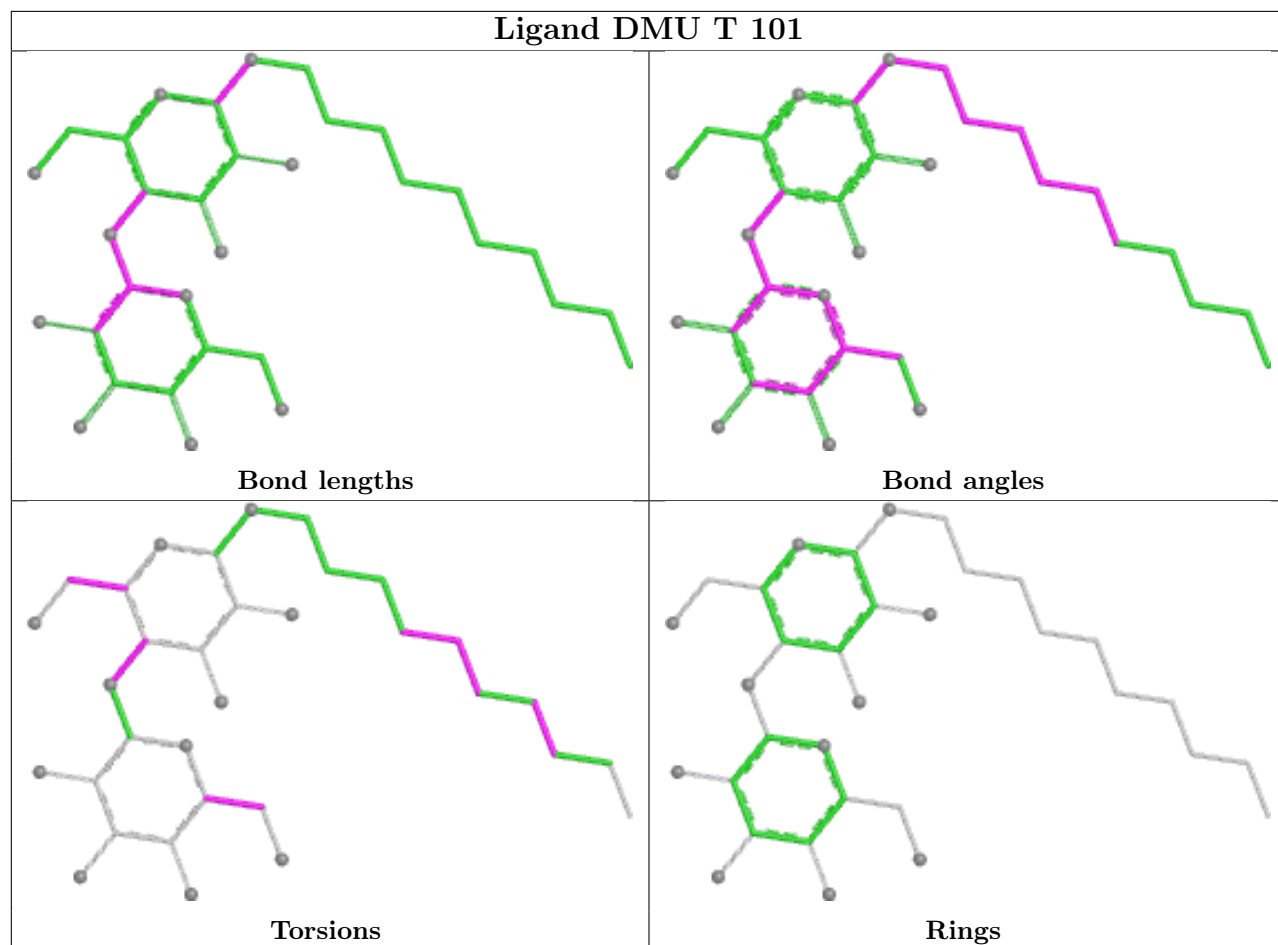


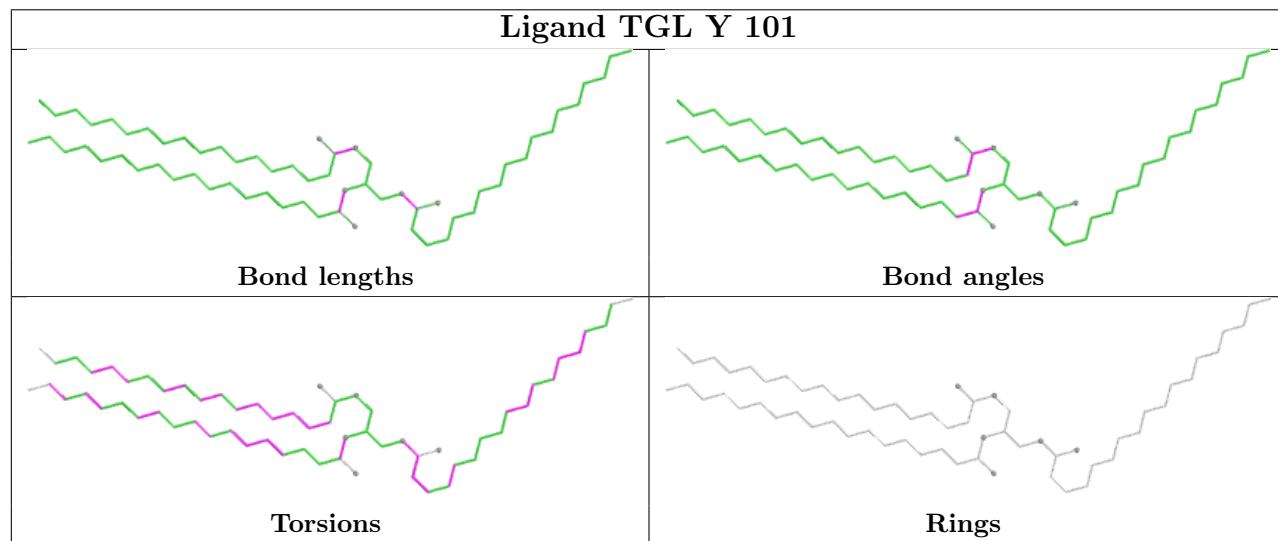
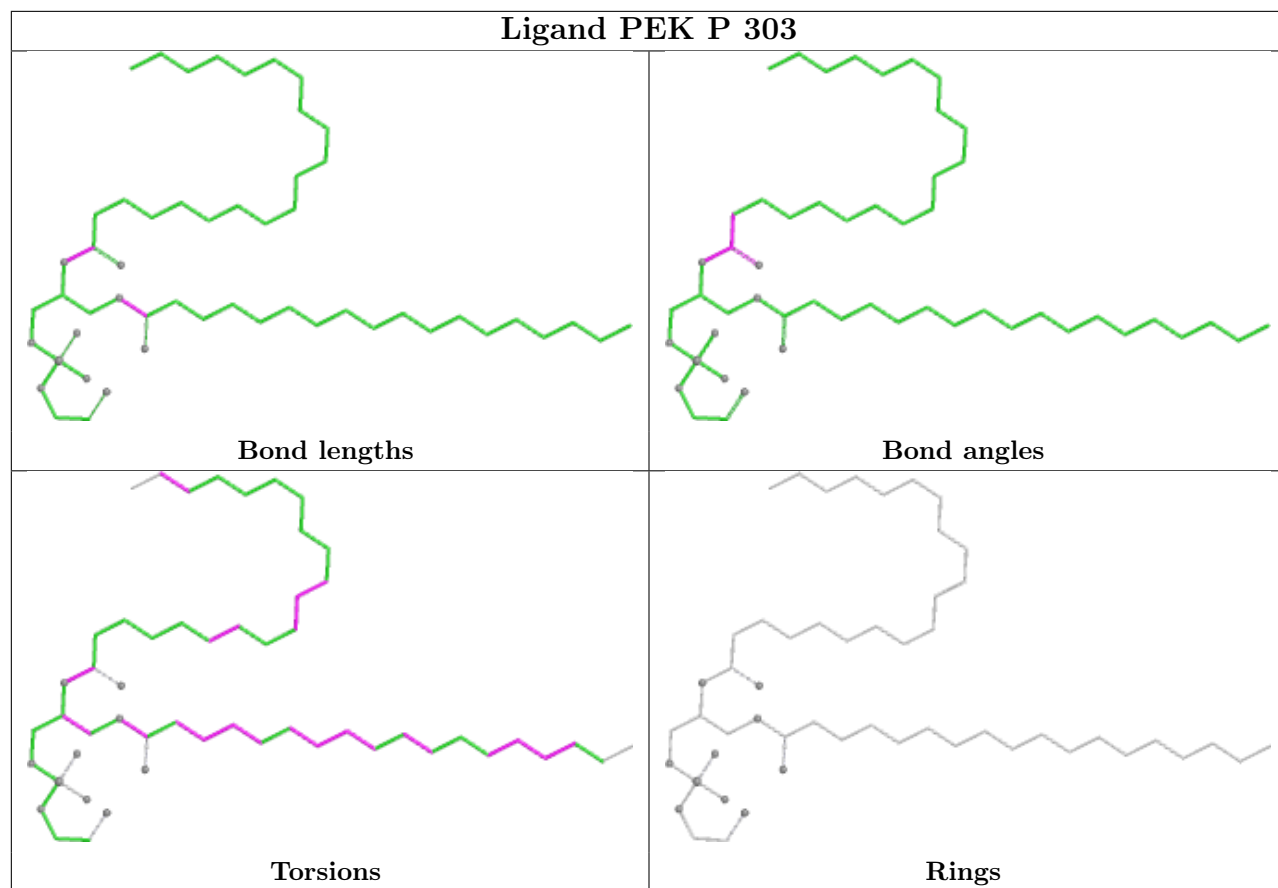


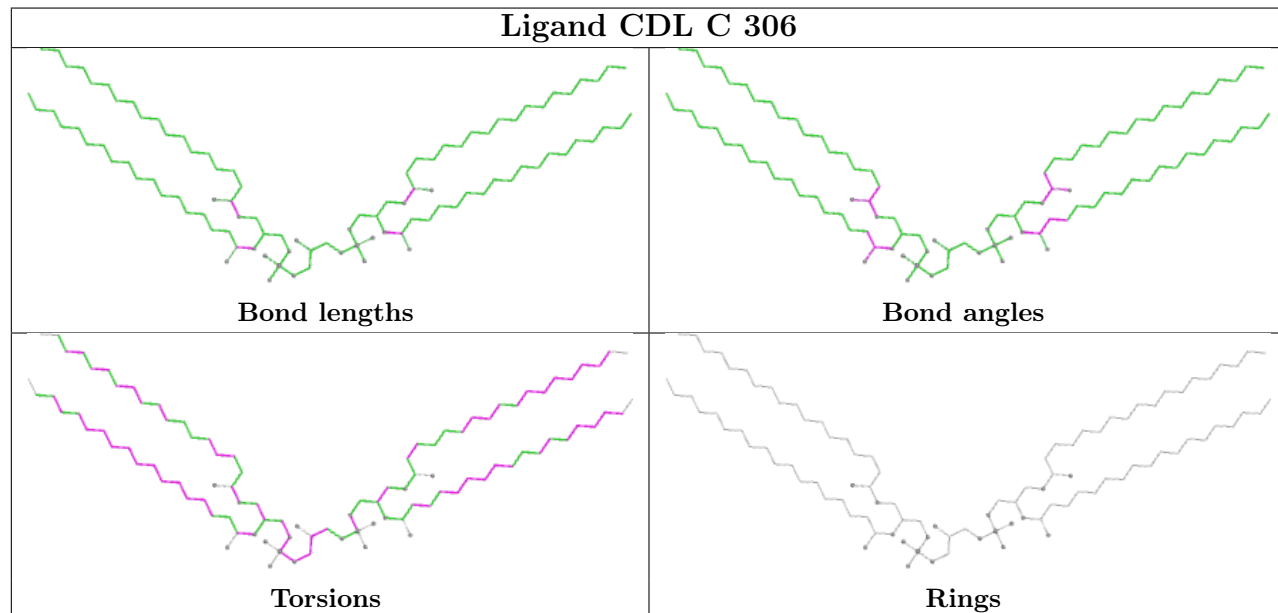
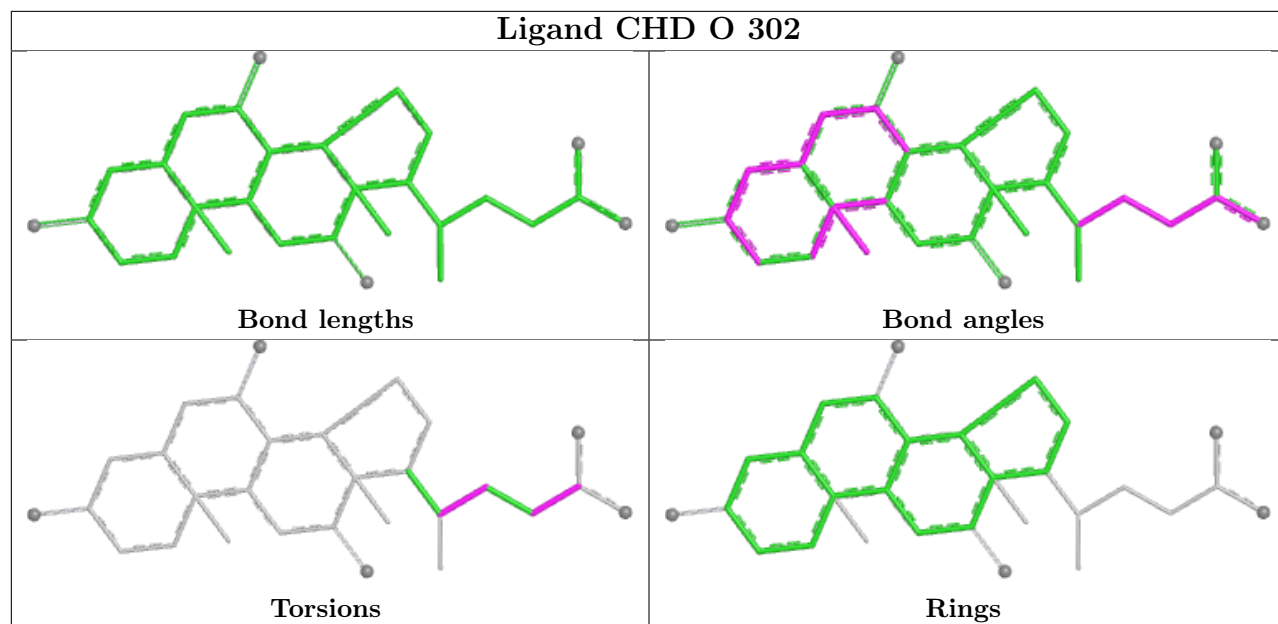


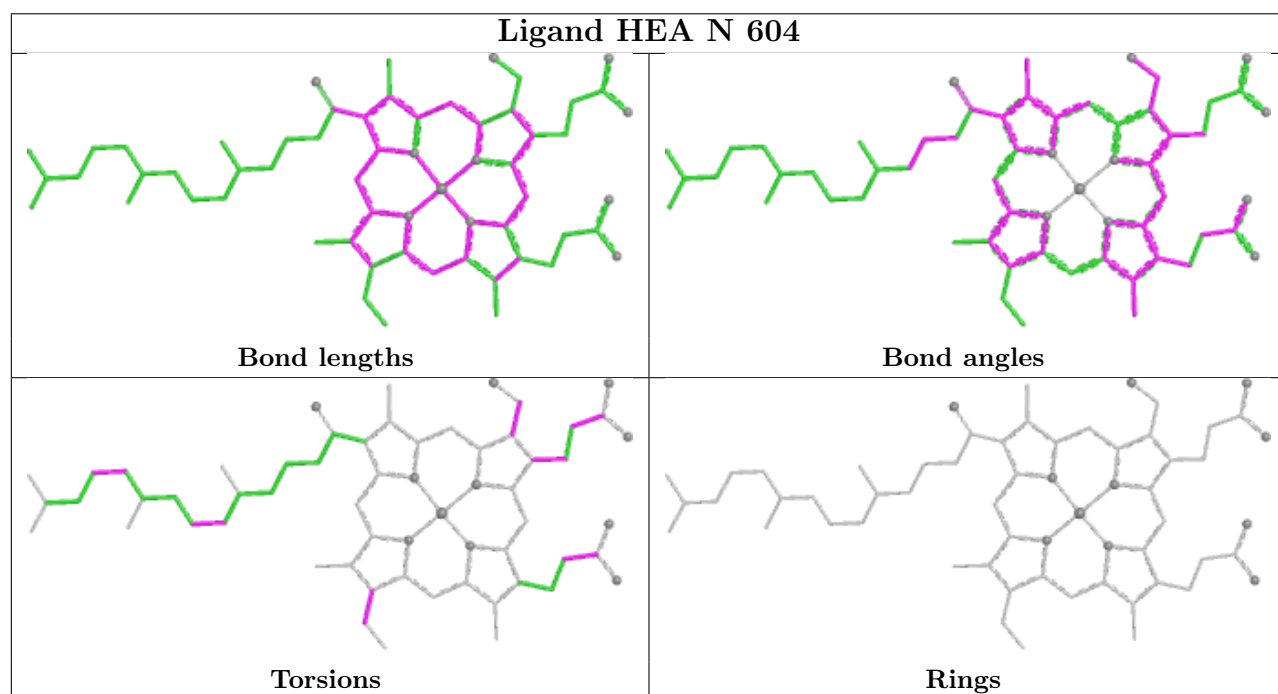
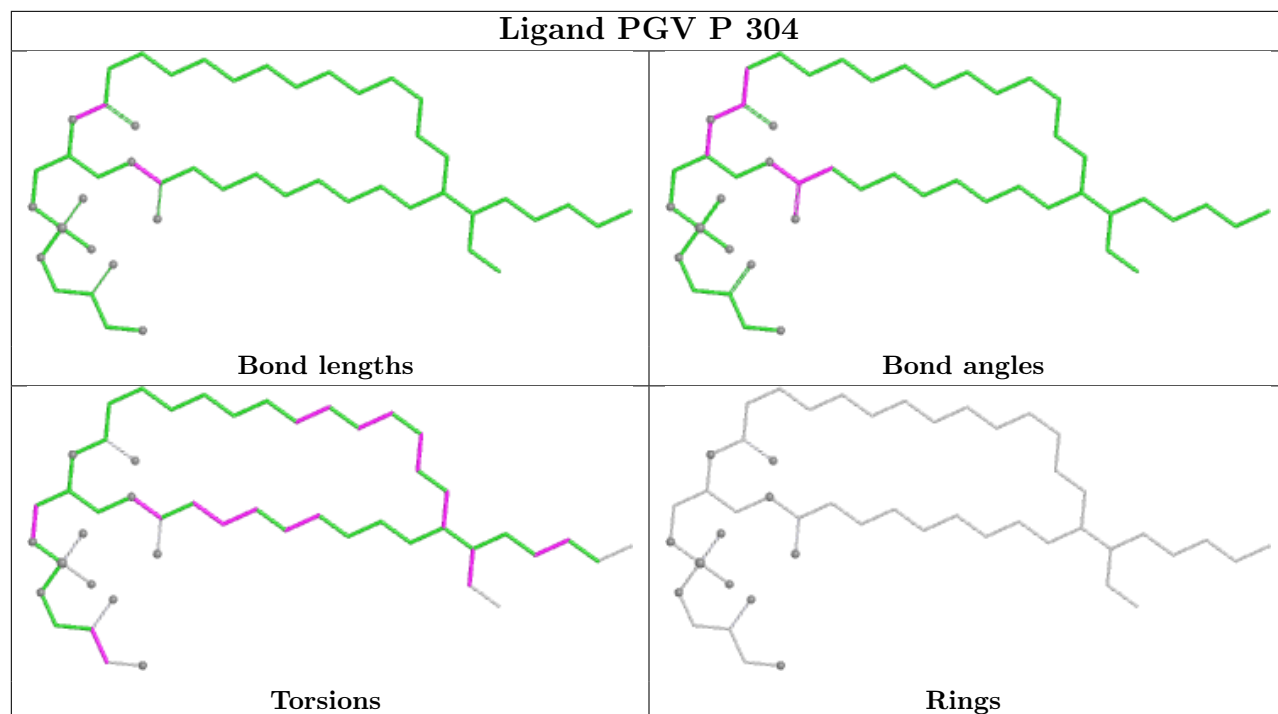


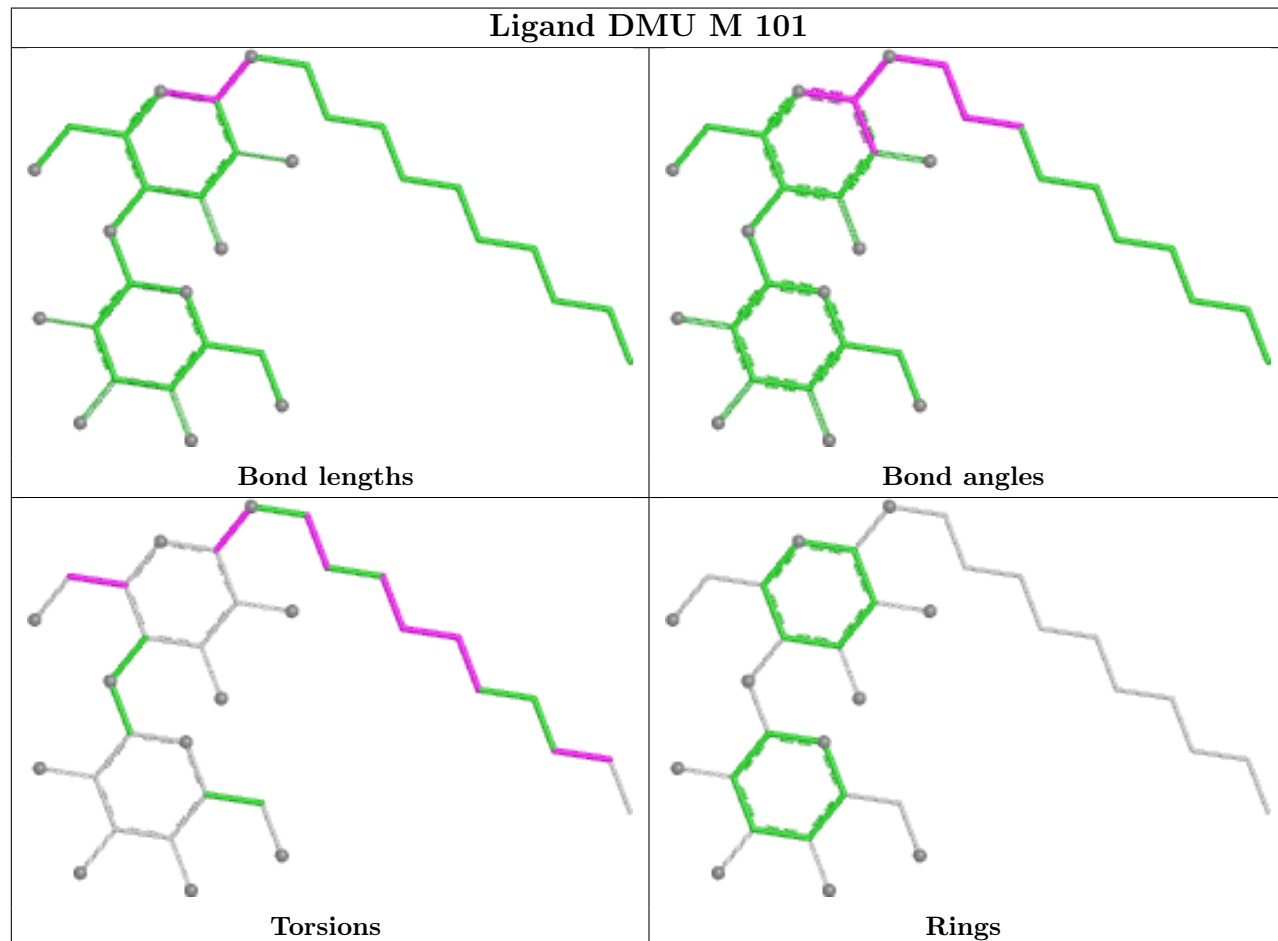
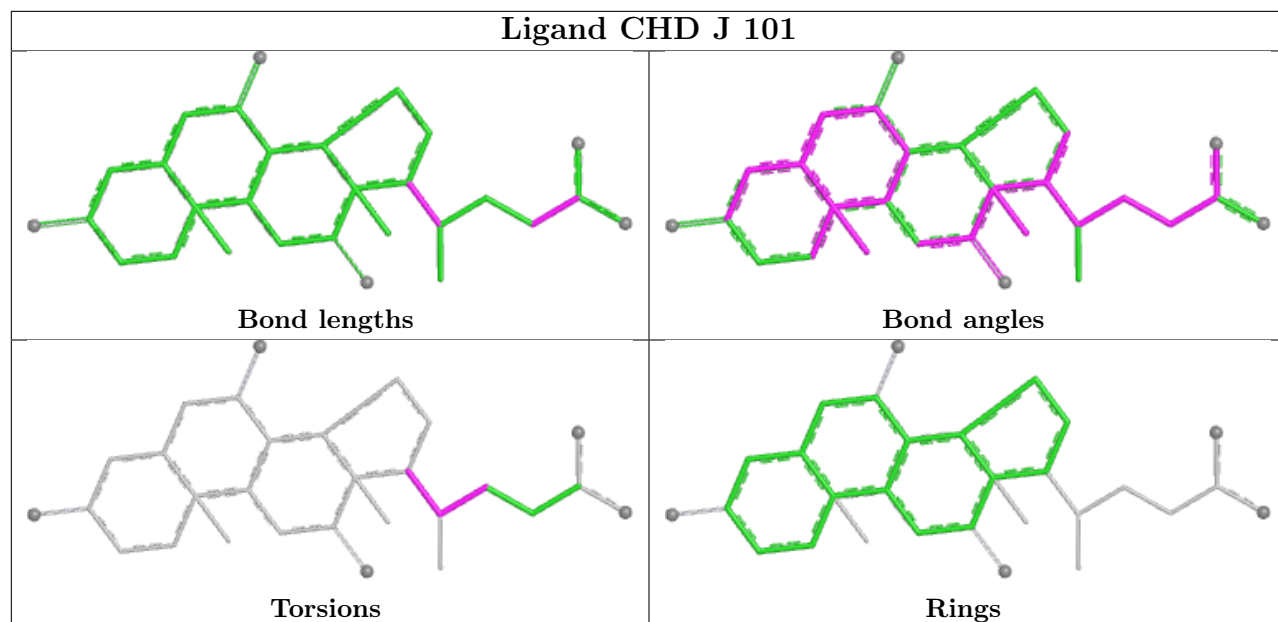


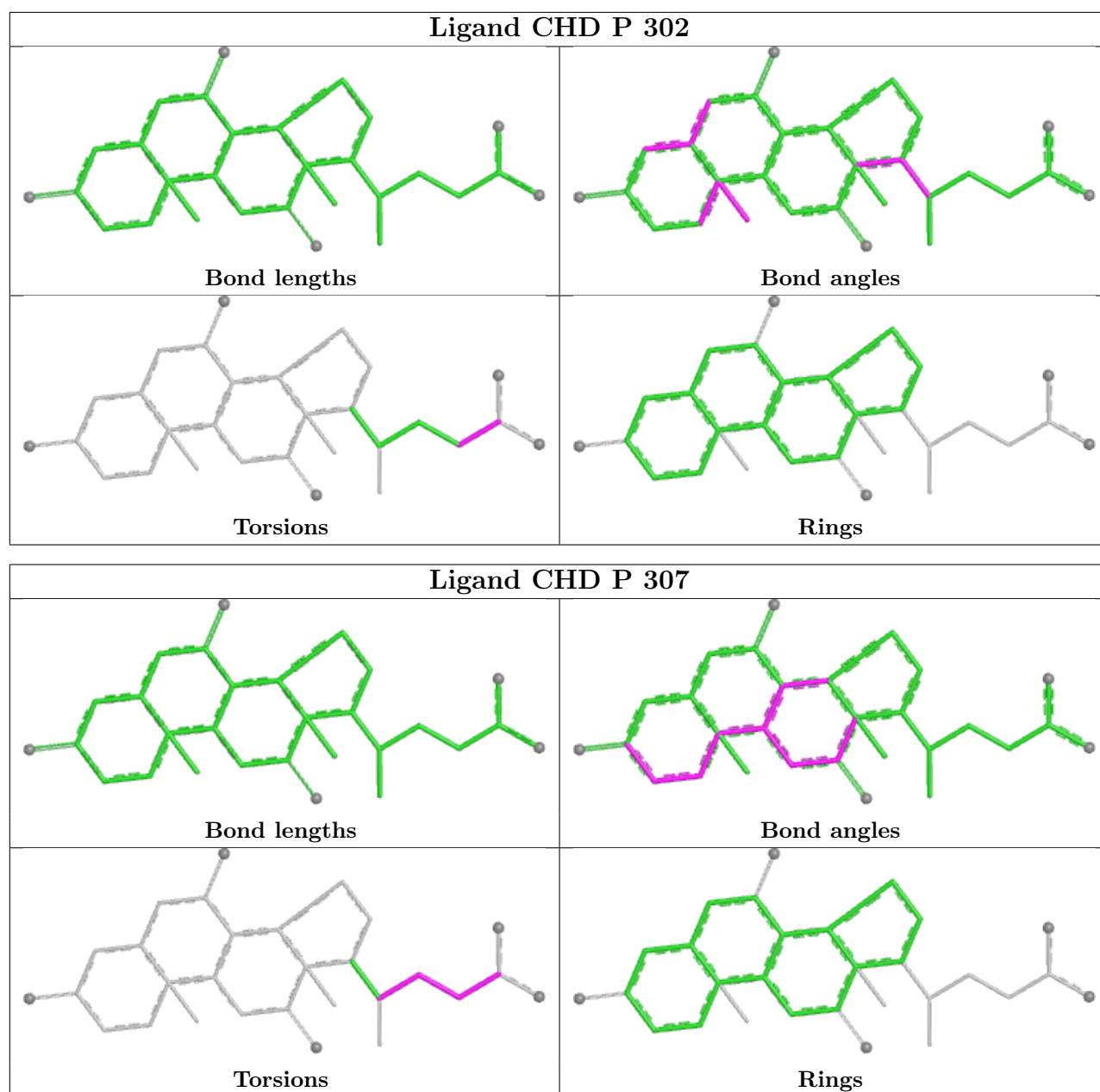












5.7 Other polymers [\(i\)](#)

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%)	-1.00	0 100 100	31, 41, 54, 91	0
1	N	513/514 (99%)	-0.72	0 100 100	36, 55, 75, 108	0
2	B	226/227 (99%)	-0.81	1 (0%) 88 85	33, 50, 83, 128	0
2	O	226/227 (99%)	-0.52	2 (0%) 81 75	49, 68, 104, 155	0
3	C	259/261 (99%)	-0.90	0 100 100	34, 46, 65, 98	0
3	P	259/261 (99%)	-0.71	0 100 100	42, 57, 80, 124	0
4	D	144/147 (97%)	-0.83	0 100 100	39, 53, 80, 110	0
4	Q	144/147 (97%)	-0.27	3 (2%) 63 54	56, 83, 120, 202	0
5	E	105/109 (96%)	-0.87	0 100 100	39, 53, 84, 140	0
5	R	105/109 (96%)	-0.65	0 100 100	52, 69, 90, 134	0
6	F	98/98 (100%)	-0.51	3 (3%) 51 42	38, 56, 130, 154	0
6	S	98/98 (100%)	-0.37	3 (3%) 51 42	47, 68, 152, 176	0
7	G	83/85 (97%)	-0.27	4 (4%) 35 28	40, 59, 144, 161	0
7	T	83/85 (97%)	-0.18	6 (7%) 21 17	43, 72, 144, 163	0
8	H	79/85 (92%)	-0.60	1 (1%) 75 67	43, 60, 119, 135	0
8	U	79/85 (92%)	-0.33	1 (1%) 75 67	54, 75, 129, 157	0
9	I	72/73 (98%)	-0.49	1 (1%) 73 65	46, 63, 93, 114	0
9	V	72/73 (98%)	-0.15	1 (1%) 73 65	49, 79, 112, 127	0
10	J	58/59 (98%)	-0.58	0 100 100	44, 60, 104, 138	0
10	W	58/59 (98%)	-0.18	0 100 100	61, 79, 130, 151	0
11	K	49/56 (87%)	-0.68	0 100 100	47, 60, 81, 96	0
11	X	49/56 (87%)	-0.26	0 100 100	59, 80, 104, 123	0
12	L	46/47 (97%)	-0.73	0 100 100	40, 49, 75, 124	0
12	Y	46/47 (97%)	-0.25	0 100 100	58, 76, 102, 137	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%)	-0.80	0 100 100	40, 48, 95, 139	0
13	Z	43/46 (93%)	-0.17	0 100 100	62, 74, 131, 153	0
All	All	3550/3614 (98%)	-0.66	26 (0%) 84 79	31, 56, 101, 202	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	1	ALA	7.3
4	Q	6	VAL	5.3
9	V	37	PHE	3.6
7	G	3	ALA	3.5
6	S	96	LEU	3.5

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	0.51	0.17	144,155,160,162	0
9	SAC	I	1	9/10	0.61	0.14	122,141,150,151	0
7	TPO	T	11	11/12	0.72	0.16	139,153,169,174	0
7	TPO	G	11	11/12	0.76	0.19	112,136,147,154	0
1	FME	N	1	10/11	0.82	0.14	86,103,121,132	0
1	FME	A	1	10/11	0.87	0.15	80,84,135,138	0
2	FME	O	1	10/11	0.94	0.09	60,73,78,88	0
2	FME	B	1	10/11	0.97	0.07	46,49,54,64	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.

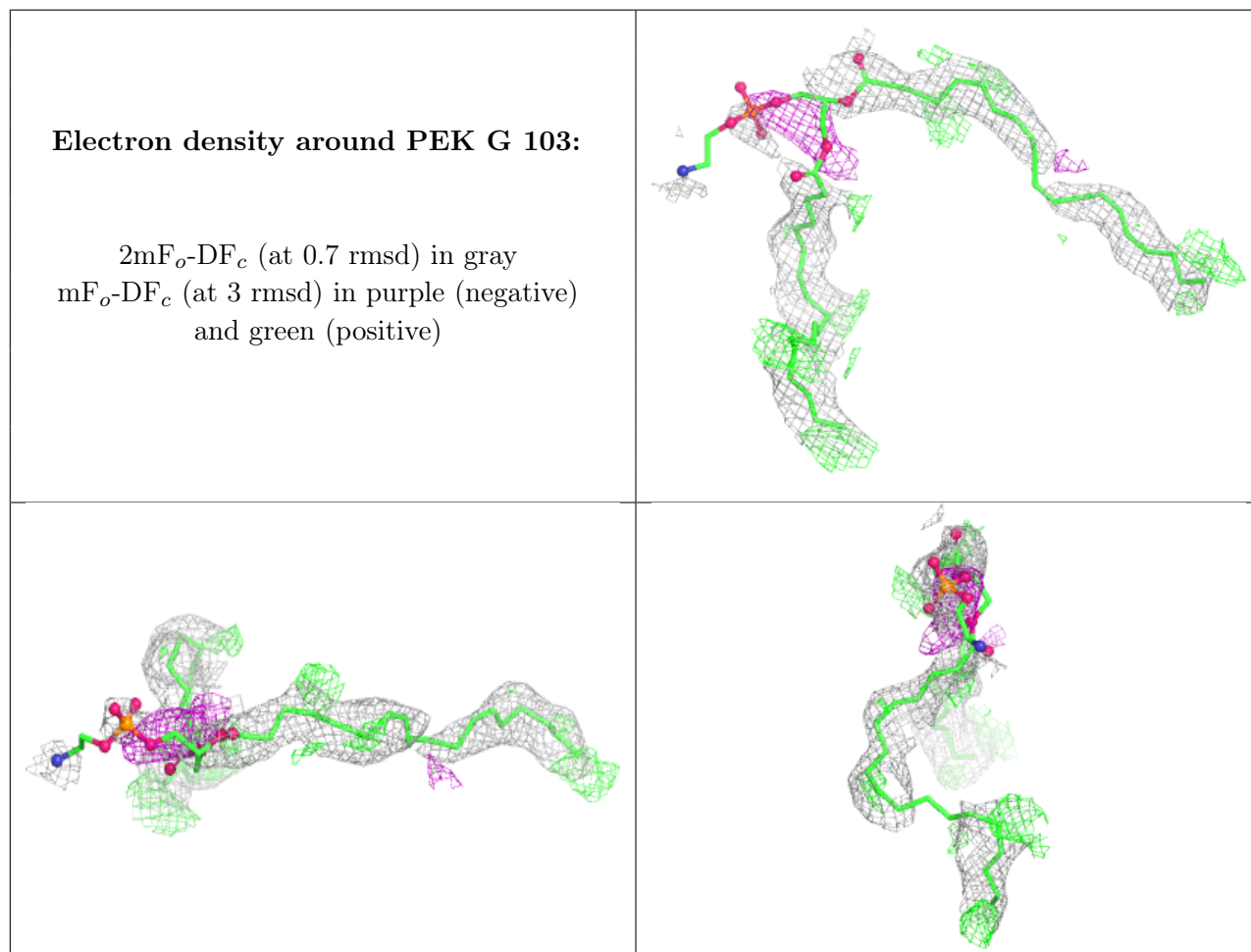
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	PEK	G	103	53/53	0.66	0.21	79,133,192,210	0
24	DMU	T	101	33/33	0.67	0.14	116,164,194,199	0
18	PGV	P	305	51/51	0.76	0.14	77,111,129,133	0
19	TGL	Y	101	63/63	0.79	0.16	76,102,153,164	0
18	PGV	N	606	51/51	0.79	0.14	59,100,150,166	0
25	PEK	C	308	53/53	0.79	0.18	71,111,178,196	0
19	TGL	O	304	63/63	0.79	0.15	89,112,126,138	0
23	CHD	W	101	29/29	0.80	0.14	105,123,144,151	0
25	PEK	C	304	53/53	0.80	0.14	75,104,180,197	0
23	CHD	J	101	29/29	0.82	0.14	82,94,112,120	0
18	PGV	A	607	51/51	0.82	0.13	76,107,130,136	0
25	PEK	T	102	53/53	0.82	0.13	73,108,155,162	0
19	TGL	A	608	63/63	0.83	0.13	57,92,112,120	0
26	CDL	C	306	100/100	0.83	0.14	60,109,150,157	0
26	CDL	G	102	100/100	0.83	0.15	78,128,168,200	0
26	CDL	P	306	100/100	0.83	0.13	66,112,142,143	0
26	CDL	T	103	100/100	0.83	0.15	76,113,183,211	0
18	PGV	A	606	51/51	0.84	0.14	57,108,156,190	0
19	TGL	I	101	63/63	0.85	0.13	44,91,123,136	0
19	TGL	L	101	63/63	0.85	0.16	58,93,123,133	0
24	DMU	C	302	33/33	0.85	0.13	112,136,174,194	0
22	PSC	O	303	52/52	0.85	0.15	79,119,224,231	0
22	PSC	B	302	52/52	0.86	0.15	69,119,211,230	0
19	TGL	V	101	63/63	0.86	0.12	50,93,138,147	0
24	DMU	Q	201	33/33	0.88	0.11	86,103,119,123	0
16	NA	N	603	1/1	0.89	0.14	64,64,64,64	0
23	CHD	C	307	29/29	0.91	0.10	77,85,92,93	0
23	CHD	P	307	29/29	0.93	0.09	85,103,118,128	0
24	DMU	M	101	33/33	0.93	0.08	50,57,74,75	0
25	PEK	P	303	53/53	0.94	0.09	56,83,135,148	0
23	CHD	P	302	29/29	0.95	0.07	45,49,60,63	0
18	PGV	P	304	51/51	0.96	0.09	45,54,149,162	0
25	PEK	G	101	53/53	0.96	0.08	37,67,111,123	0
18	PGV	P	301	51/51	0.96	0.08	37,65,89,93	0
23	CHD	C	303	29/29	0.97	0.05	36,41,44,48	0
15	MG	A	602	1/1	0.97	0.04	38,38,38,38	0
17	HEA	N	604	60/60	0.97	0.07	45,52,71,75	0
23	CHD	O	302	29/29	0.97	0.05	41,46,52,54	0
18	PGV	C	301	51/51	0.97	0.07	35,61,86,95	0
18	PGV	C	305	51/51	0.97	0.07	37,51,97,105	0
23	CHD	B	303	29/29	0.97	0.06	41,44,57,69	0
16	NA	A	603	1/1	0.98	0.04	39,39,39,39	0

Continued on next page...

Continued from previous page...

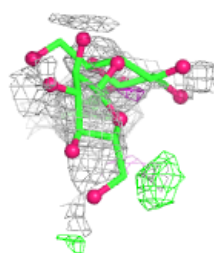
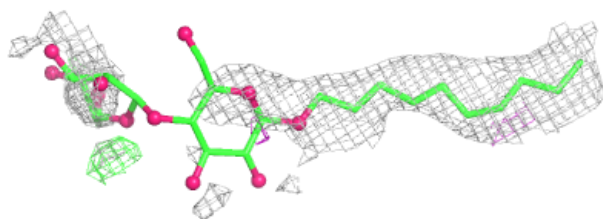
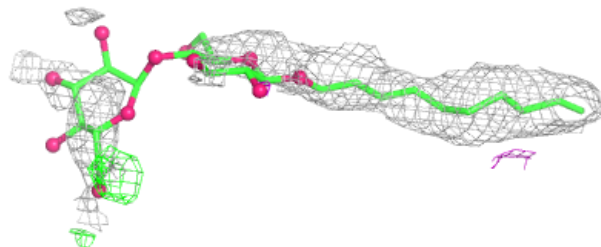
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	MG	N	602	1/1	0.98	0.06	46,46,46,46	0
17	HEA	A	604	60/60	0.98	0.06	33,39,78,81	0
17	HEA	A	605	60/60	0.99	0.05	28,34,47,55	0
17	HEA	N	605	60/60	0.99	0.05	39,43,47,52	0
20	PER	A	609	2/2	0.99	0.04	38,38,38,38	0
20	PER	N	607	2/2	0.99	0.06	50,50,50,53	0
21	CUA	B	301	2/2	0.99	0.03	42,42,42,43	0
21	CUA	O	301	2/2	0.99	0.03	62,62,62,62	0
14	CU	A	601	1/1	1.00	0.03	44,44,44,44	0
14	CU	N	601	1/1	1.00	0.04	58,58,58,58	0
27	ZN	F	101	1/1	1.00	0.01	54,54,54,54	0
27	ZN	S	101	1/1	1.00	0.01	65,65,65,65	0

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

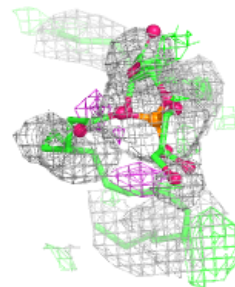
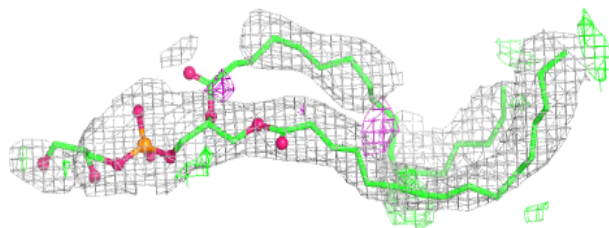
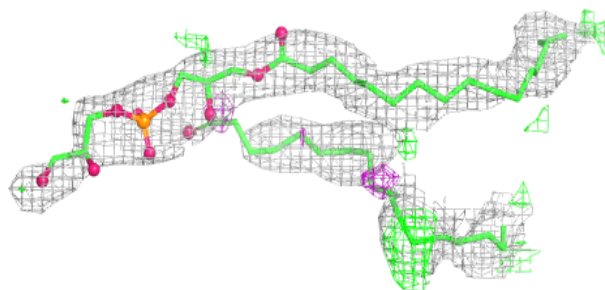


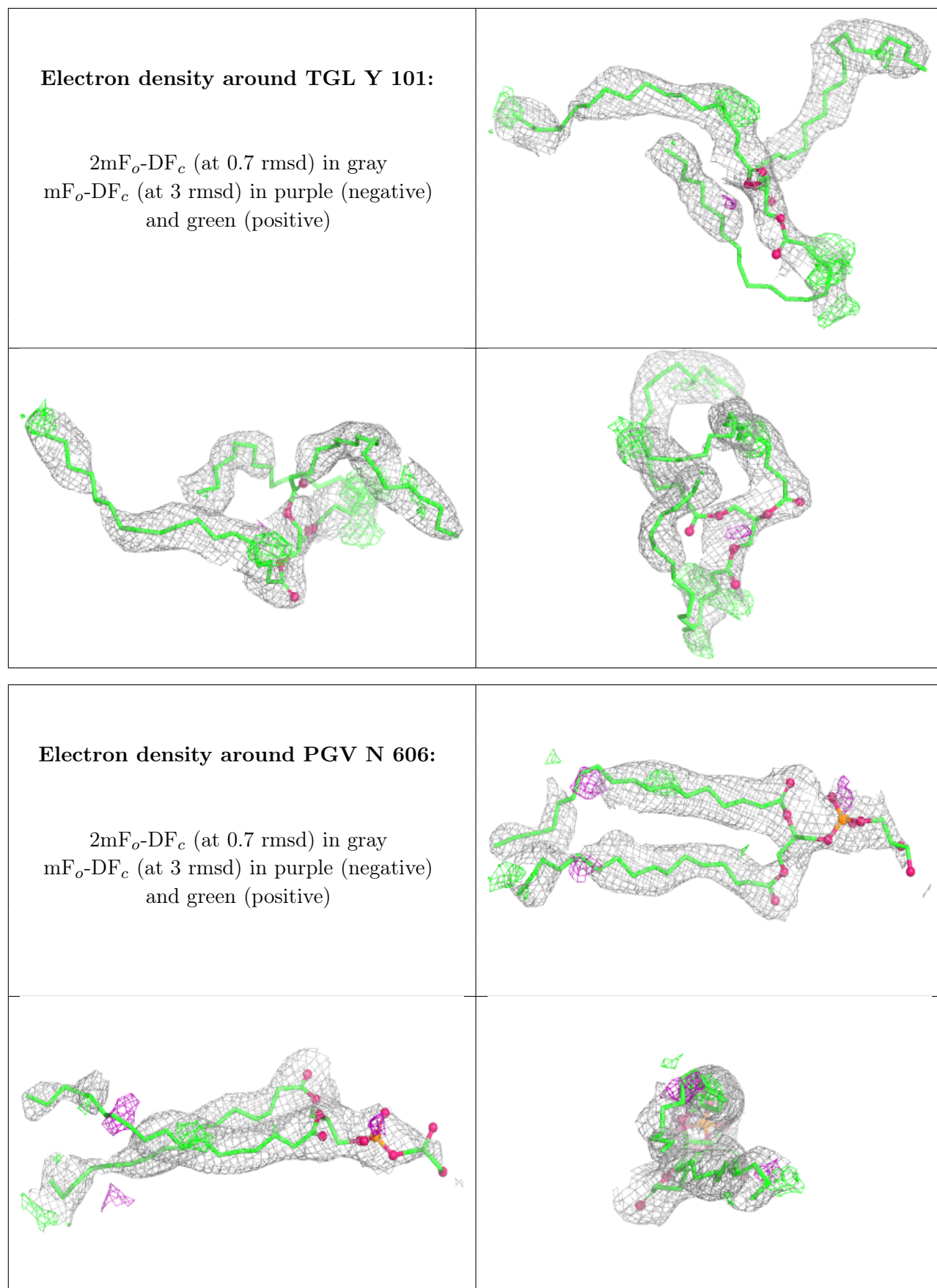
Electron density around DMU T 101:

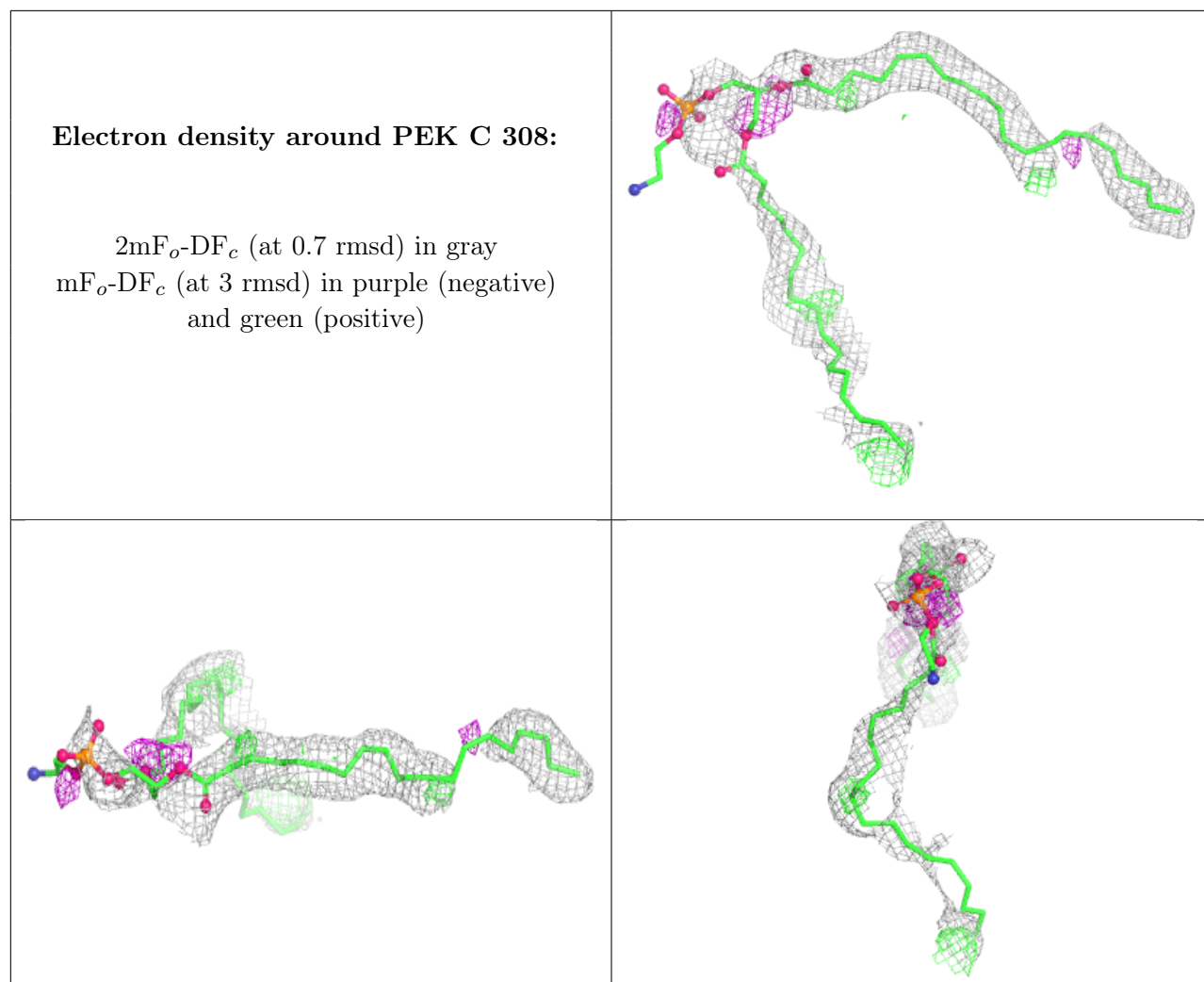
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

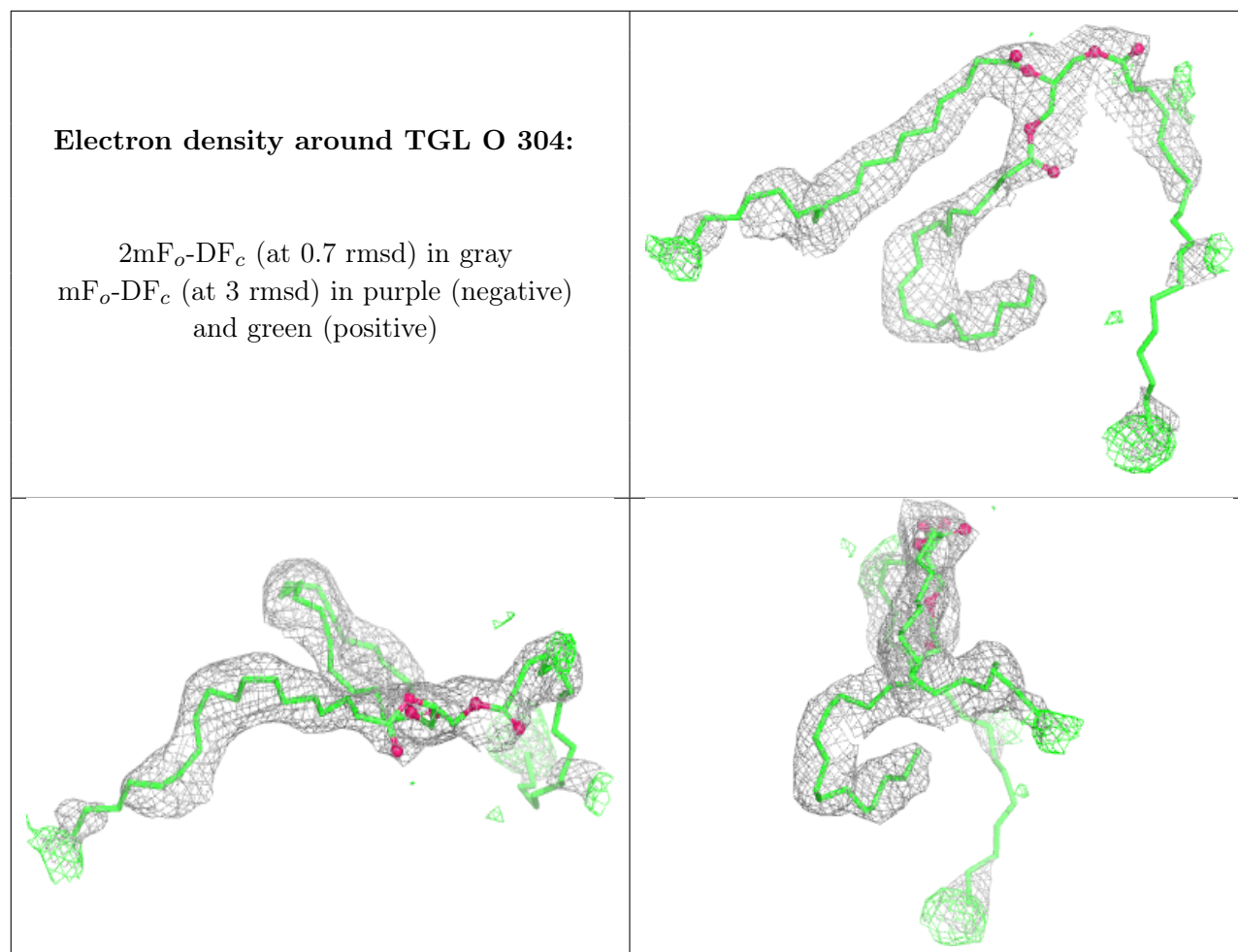
**Electron density around PGV P 305:**

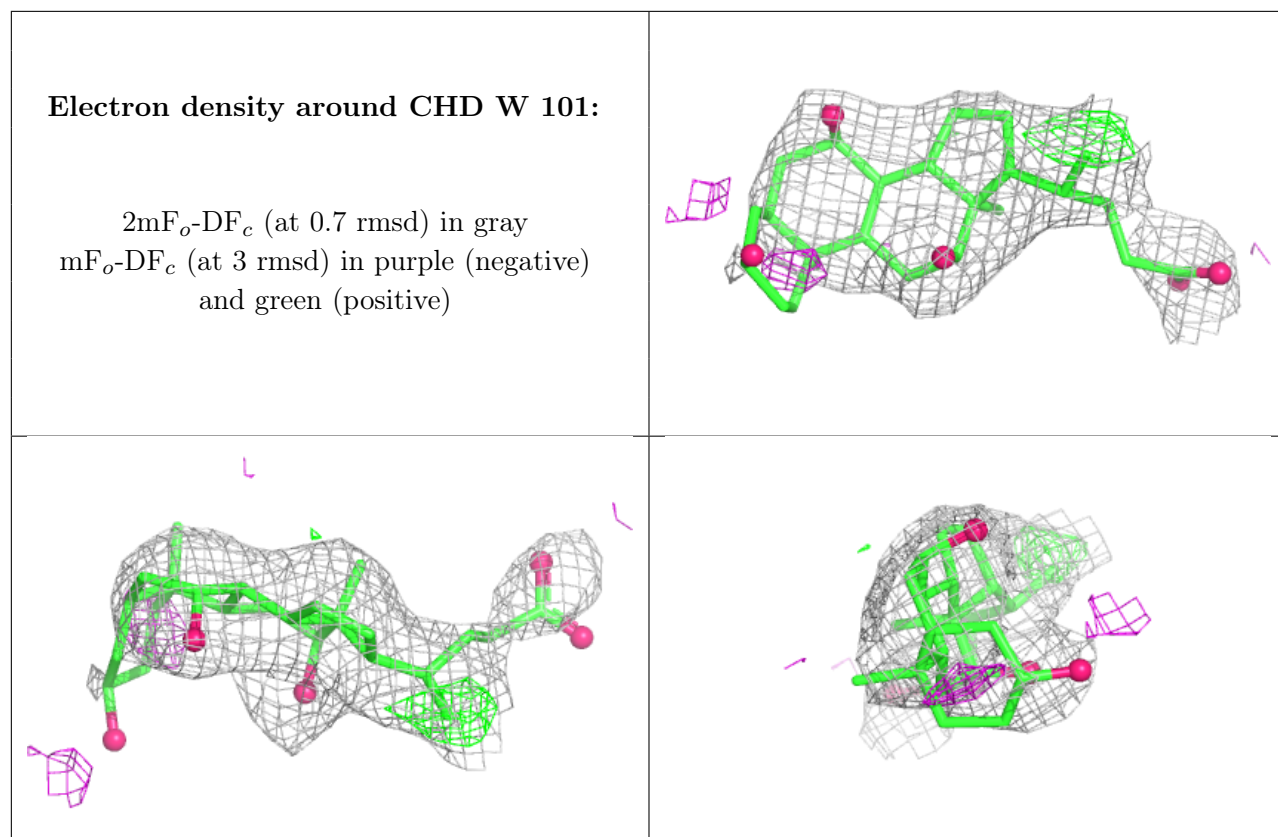
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





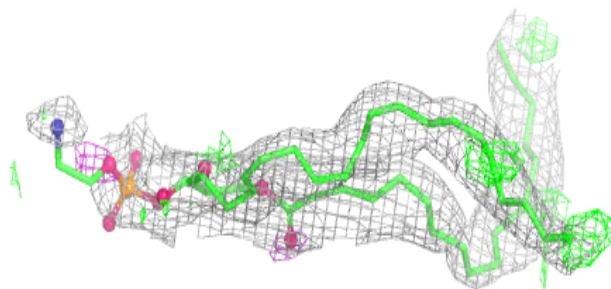
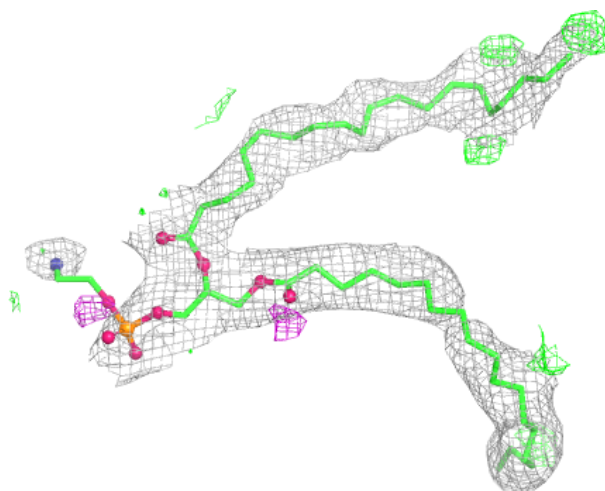






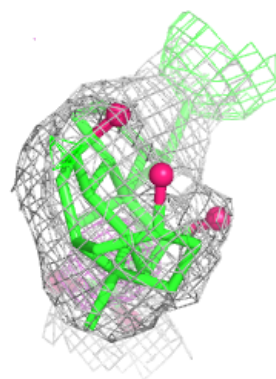
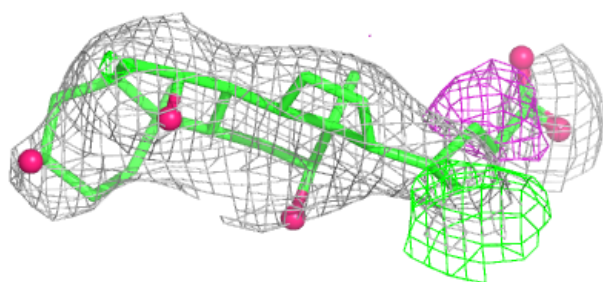
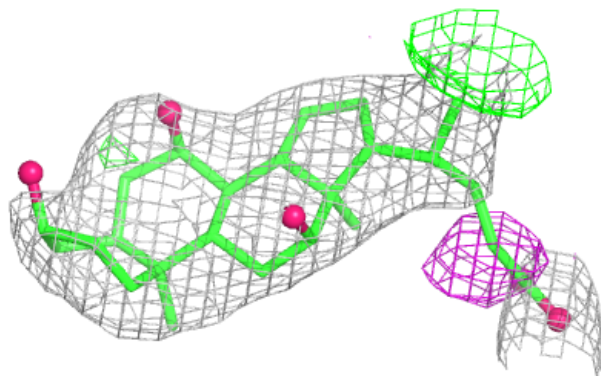
Electron density around PEK C 304:

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

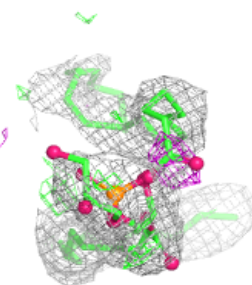
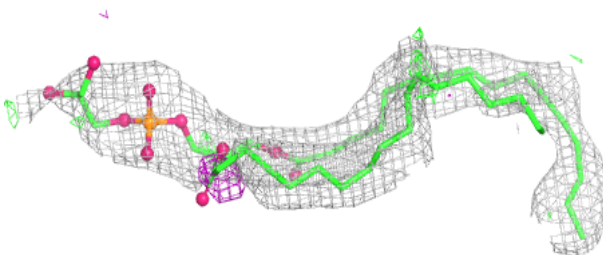
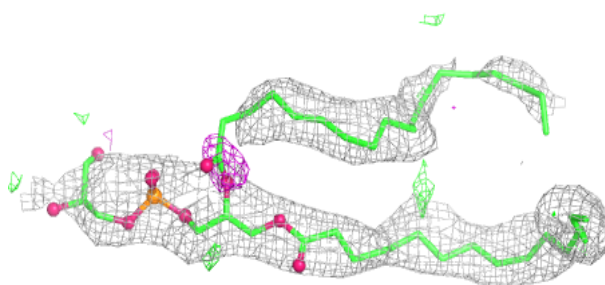


Electron density around CHD J 101:

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

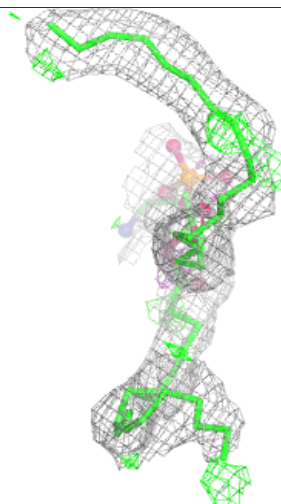
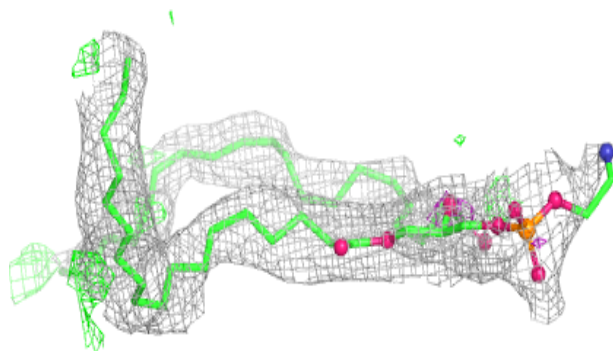
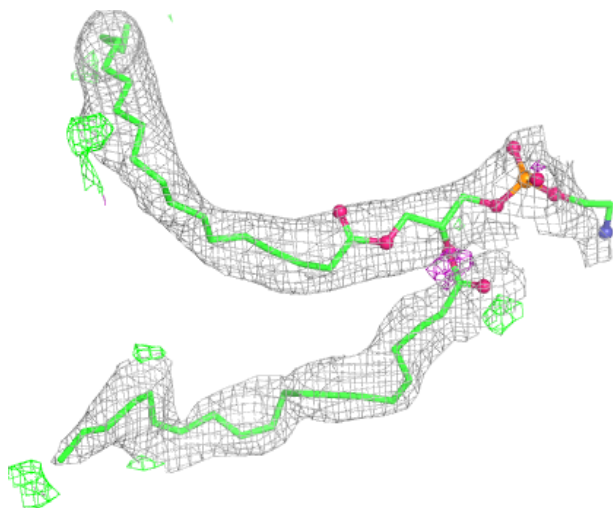
**Electron density around PGV A 607:**

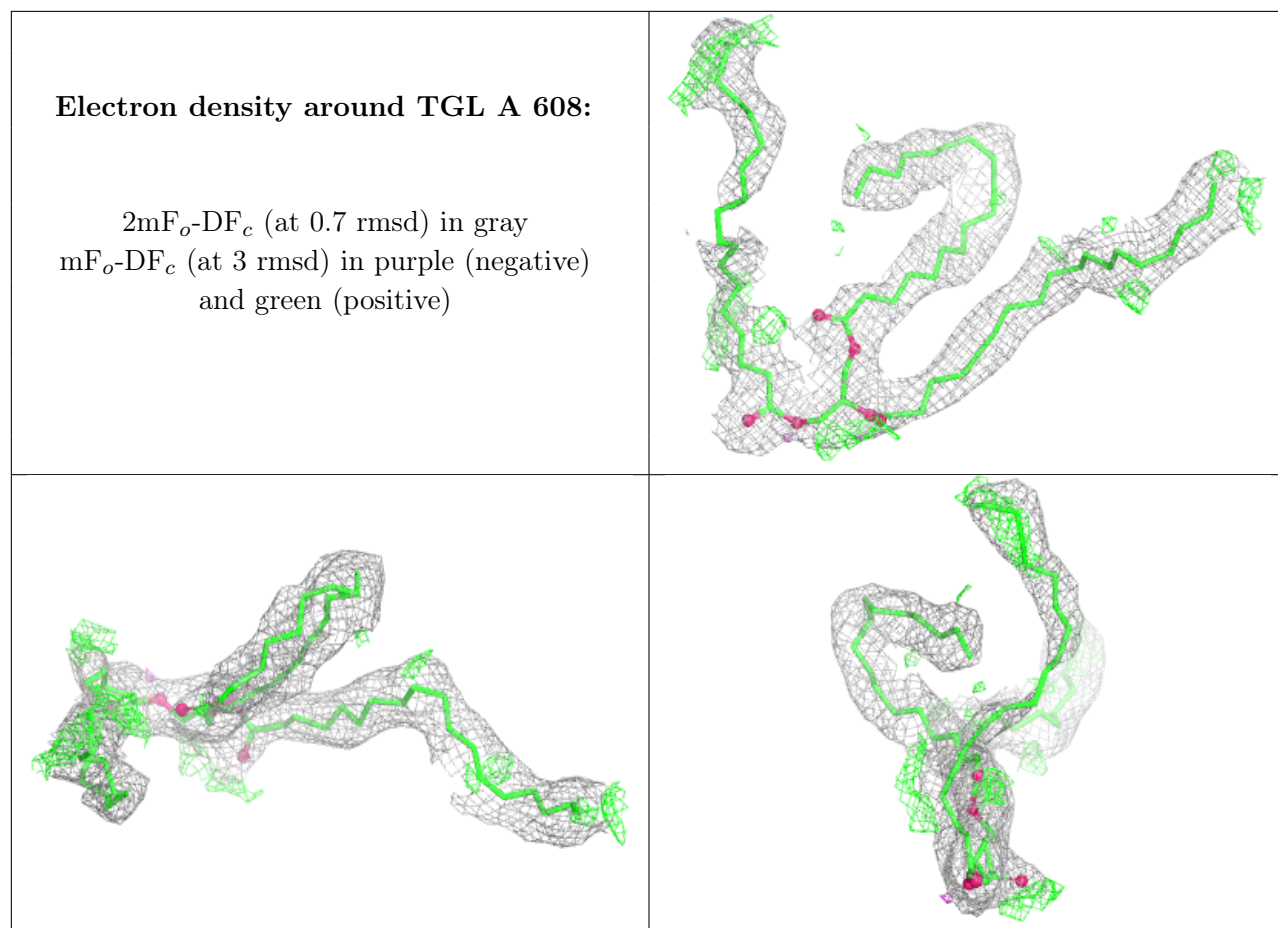
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEK T 102:

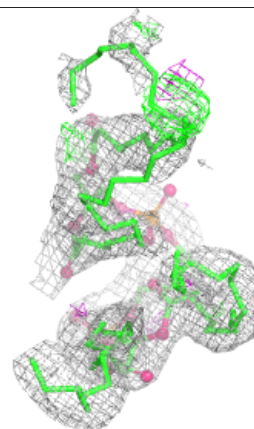
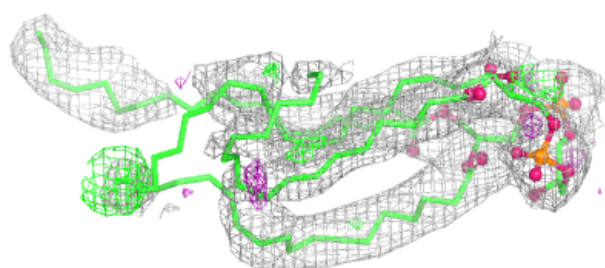
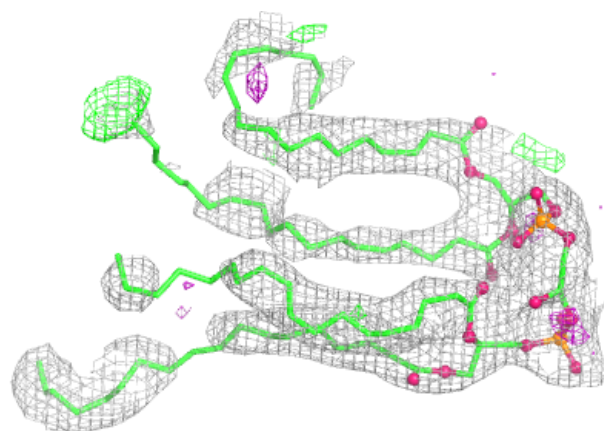
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



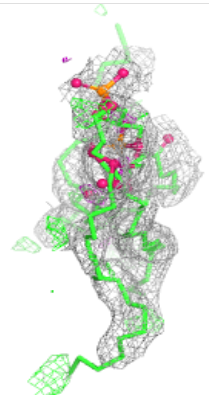
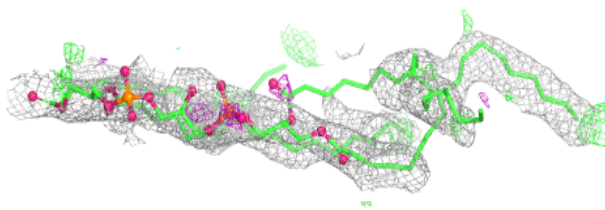
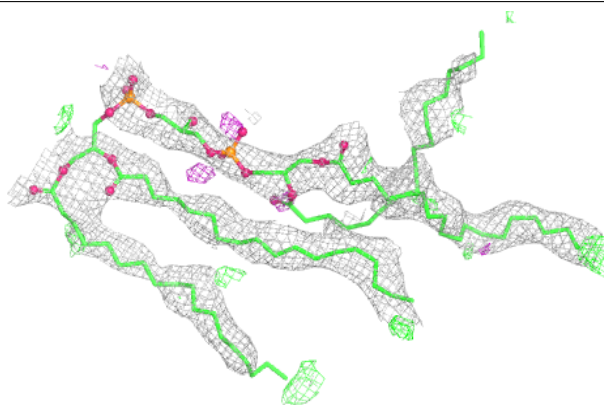


Electron density around CDL C 306:

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

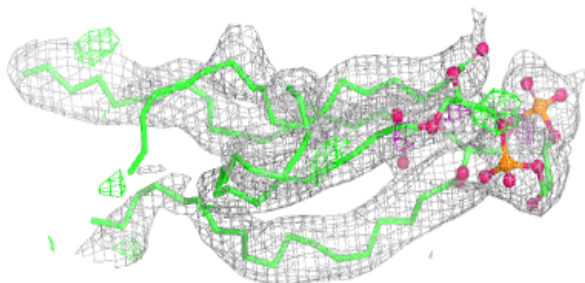
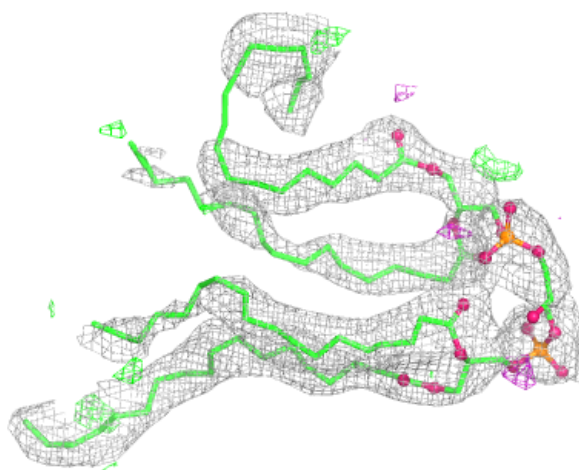
**Electron density around CDL G 102:**

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



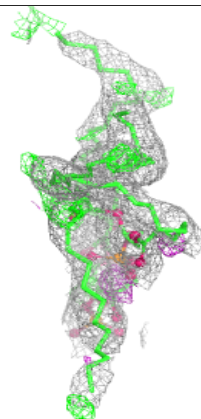
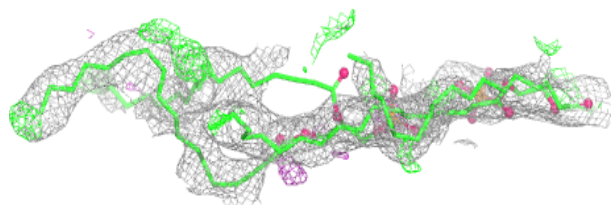
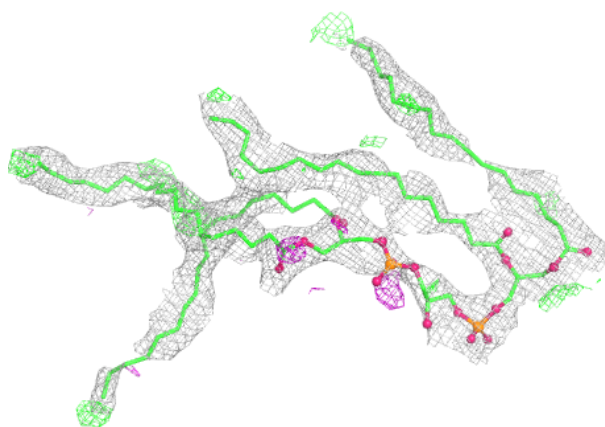
Electron density around CDL P 306:

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

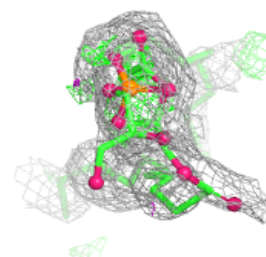
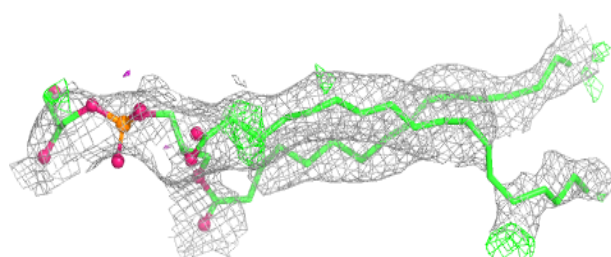
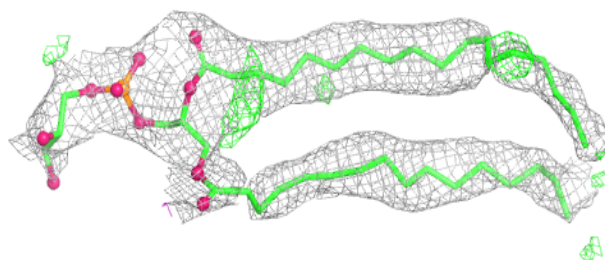


Electron density around CDL T 103:

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

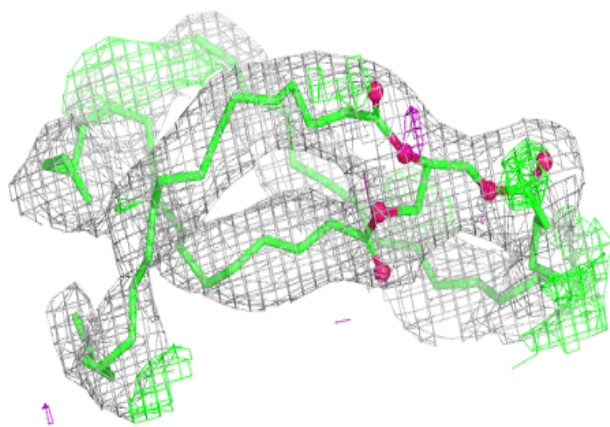
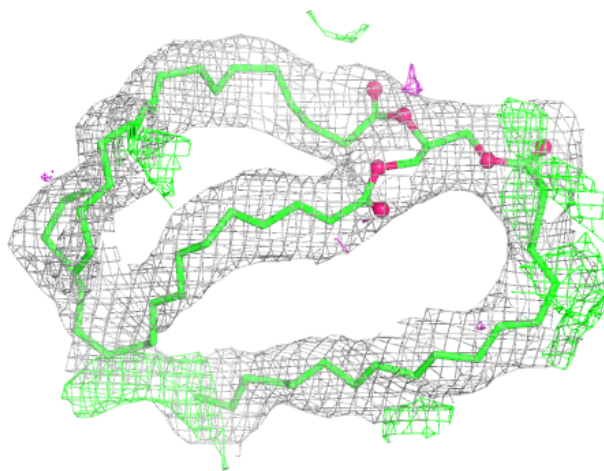
**Electron density around PGV A 606:**

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



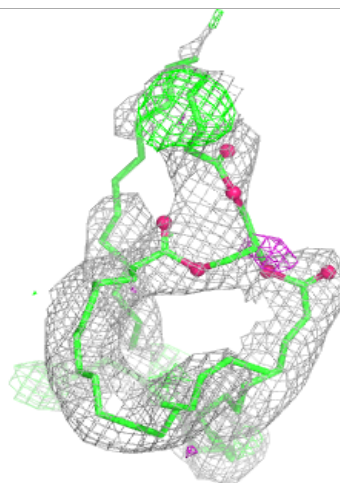
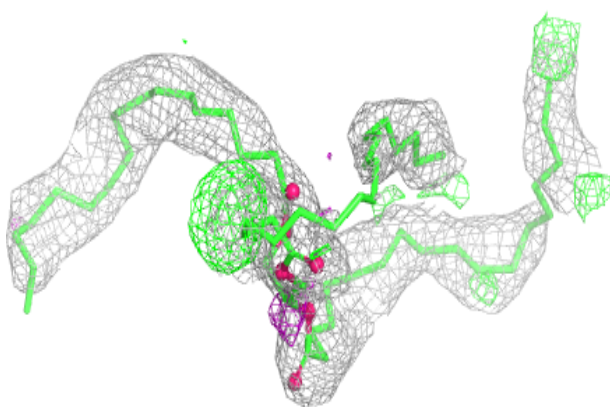
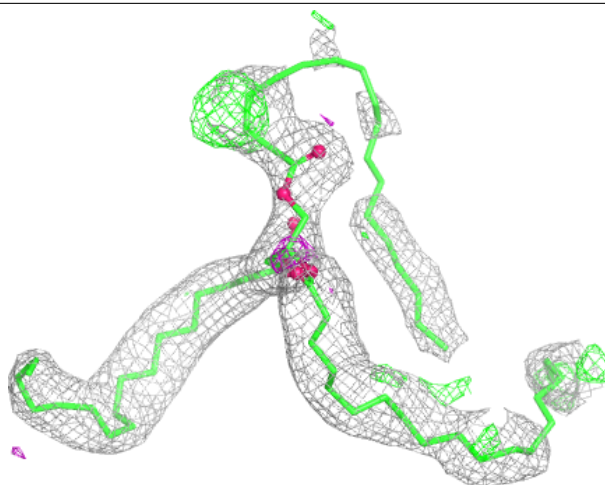
Electron density around TGL I 101:

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



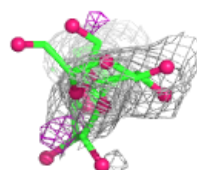
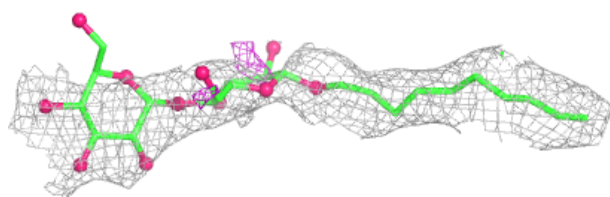
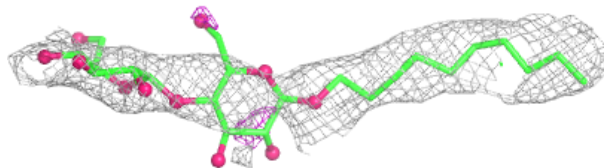
Electron density around TGL L 101:

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

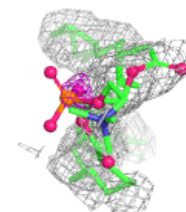
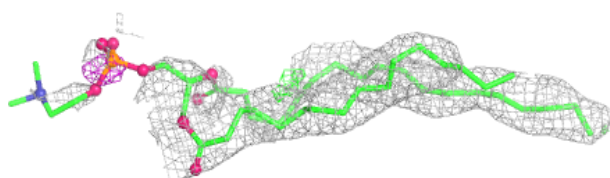
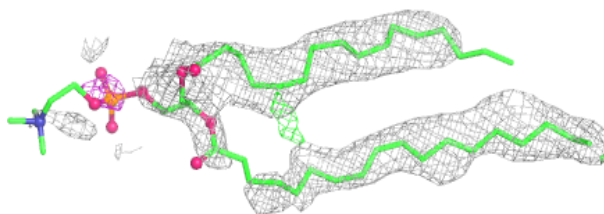


Electron density around DMU C 302:

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

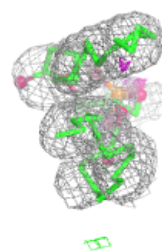
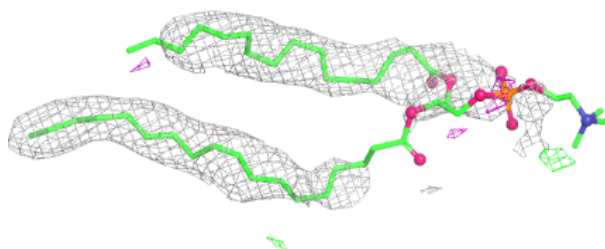
**Electron density around PSC O 303:**

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

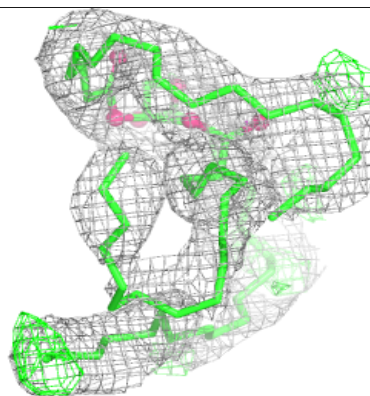
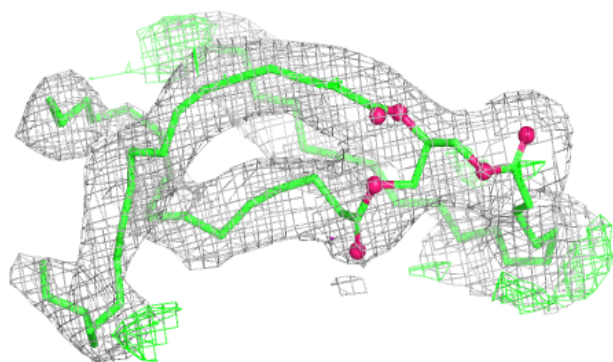
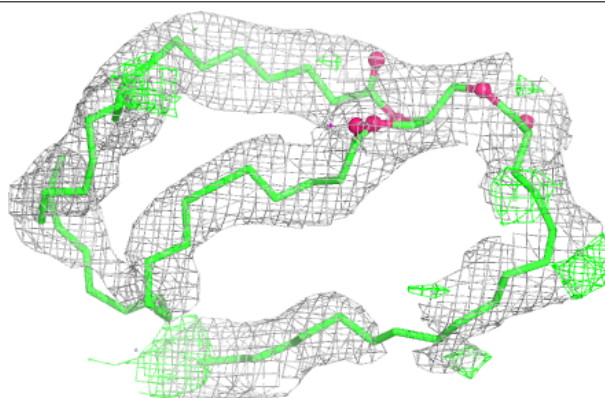


Electron density around PSC B 302:

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

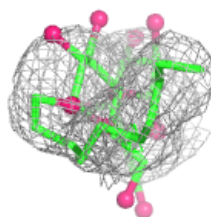
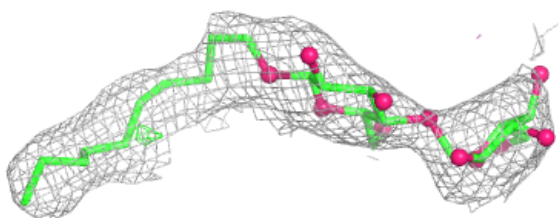
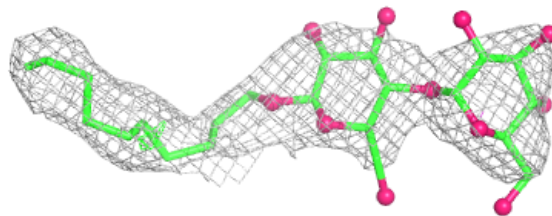
**Electron density around TGL V 101:**

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

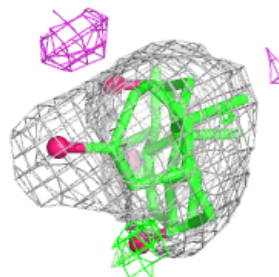
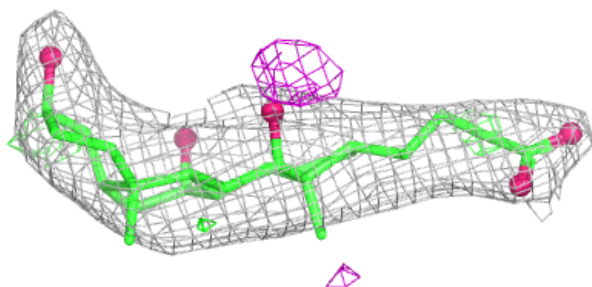
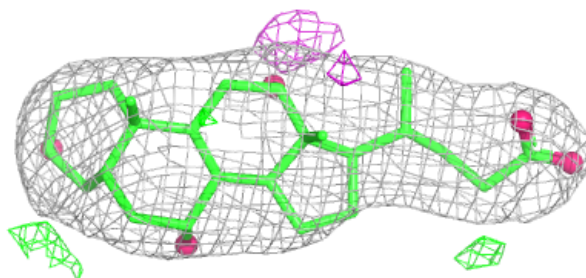


Electron density around DMU Q 201:

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

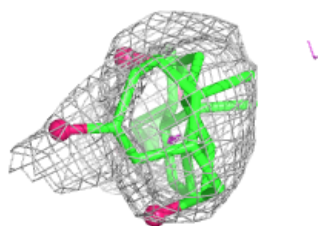
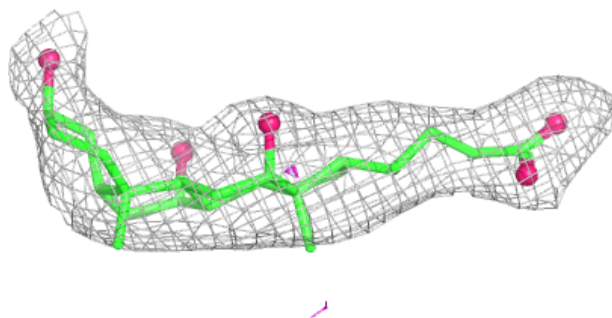
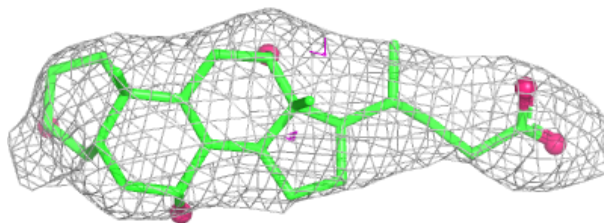
**Electron density around CHD C 307:**

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

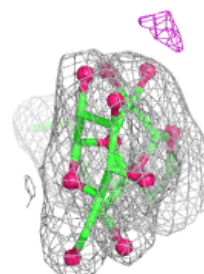
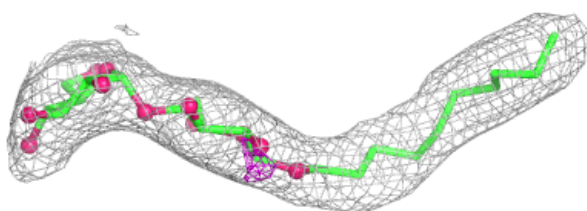
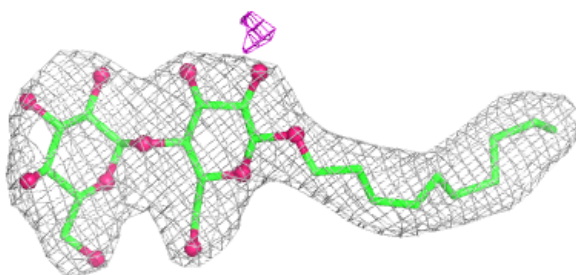


Electron density around CHD P 307:

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

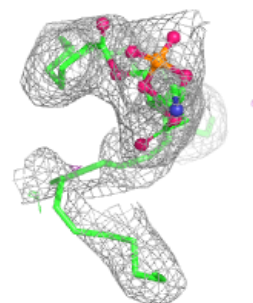
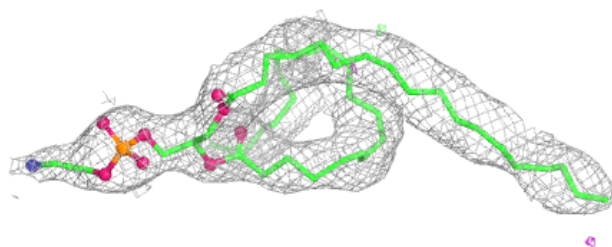
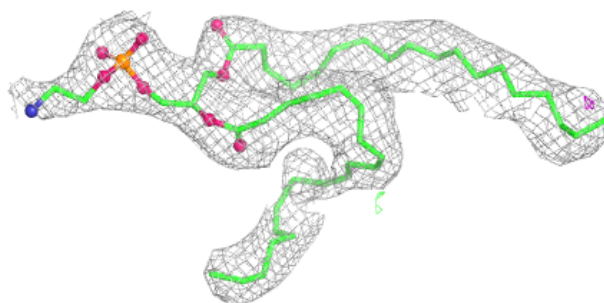
**Electron density around DMU M 101:**

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

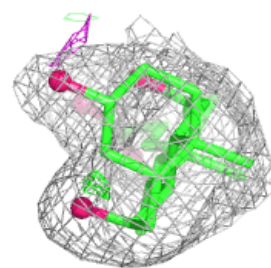
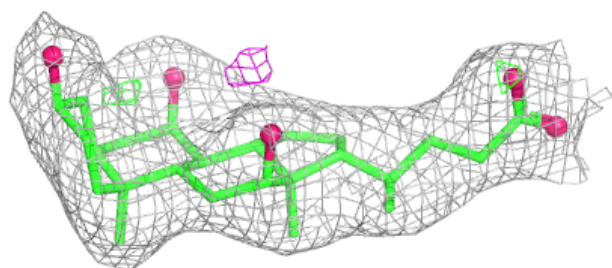
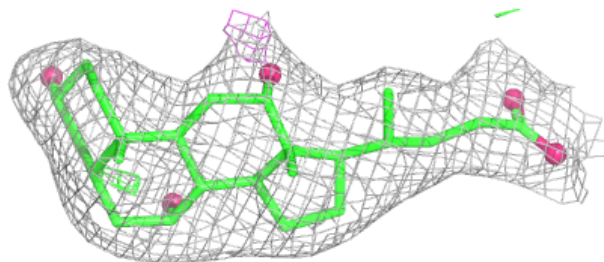


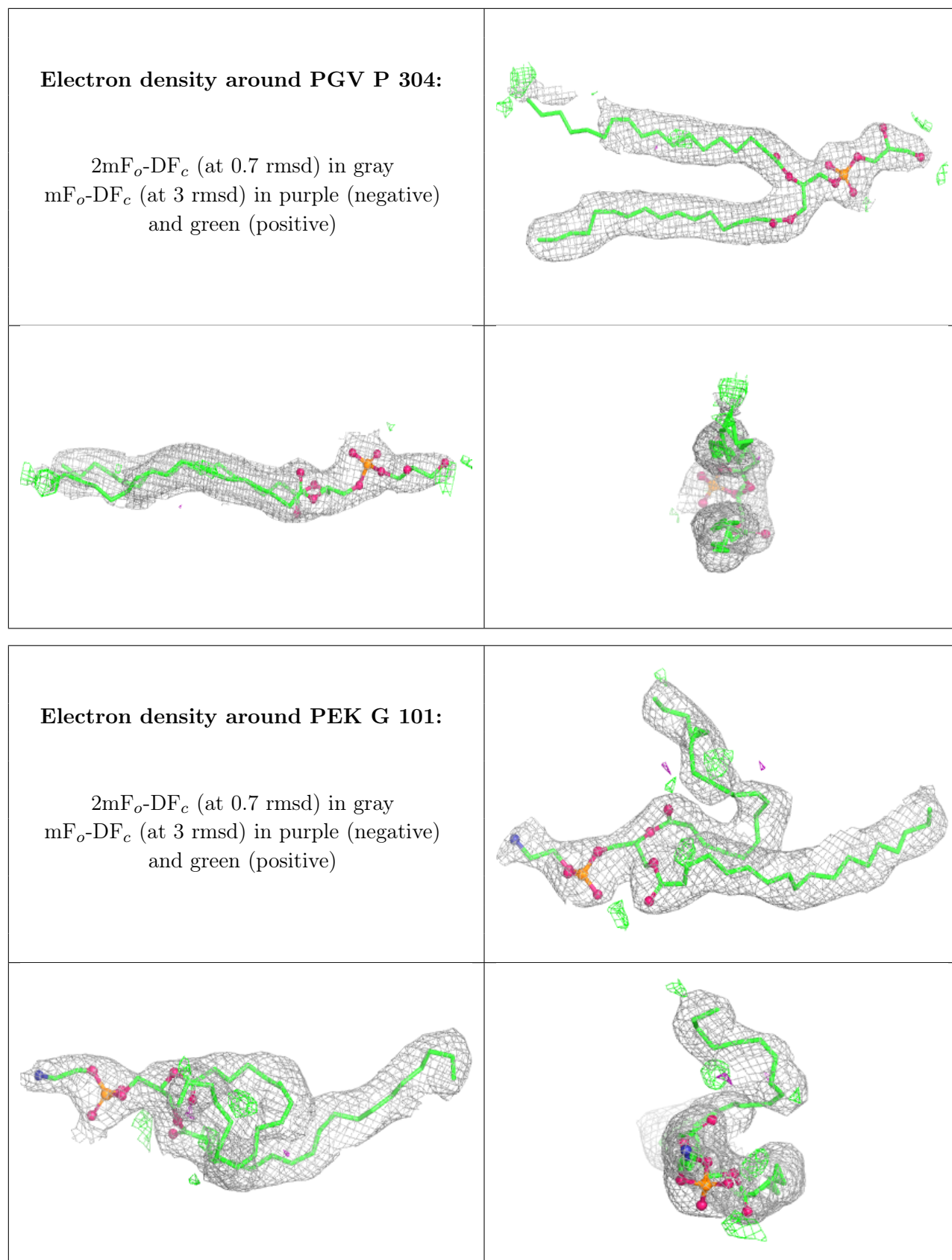
Electron density around PEK P 303:

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

**Electron density around CHD P 302:**

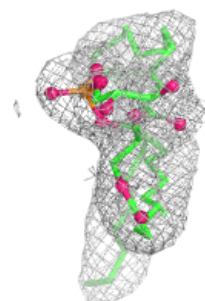
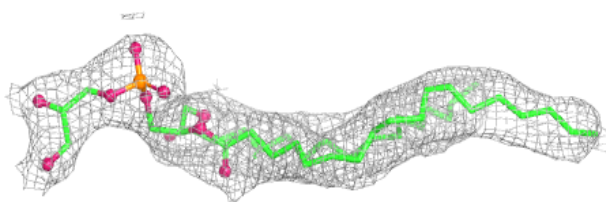
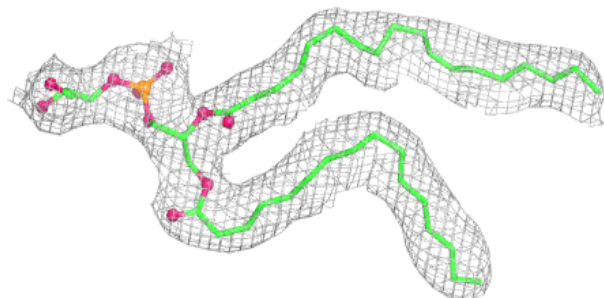
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



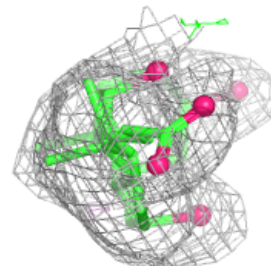
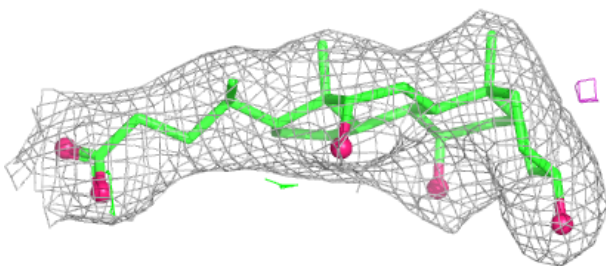
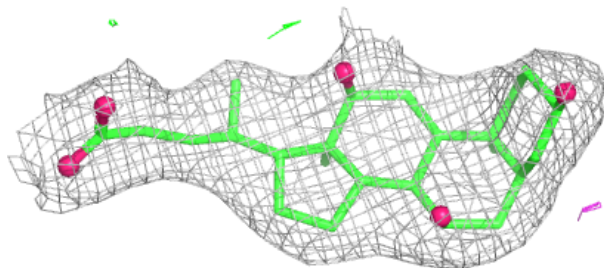


Electron density around PGV P 301:

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

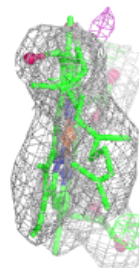
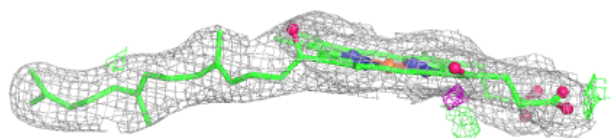
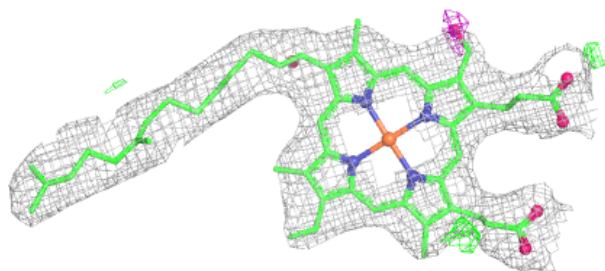
**Electron density around CHD C 303:**

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

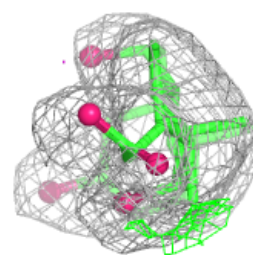
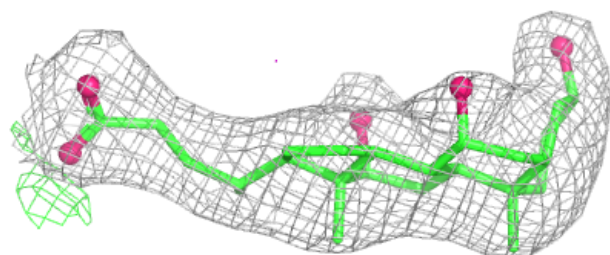
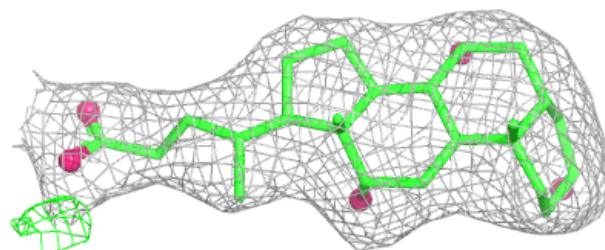


Electron density around HEA N 604:

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

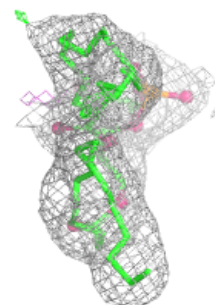
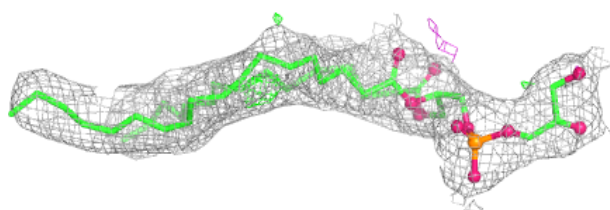
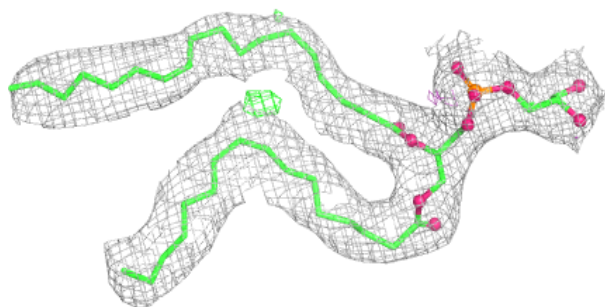
**Electron density around CHD O 302:**

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

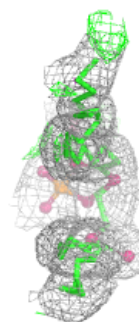
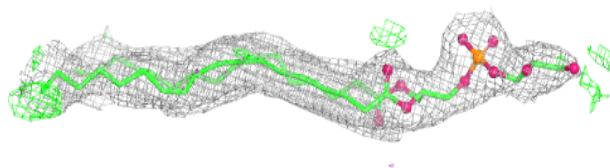
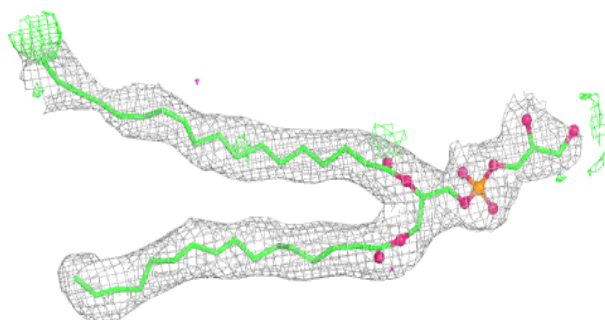


Electron density around PGV C 301:

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

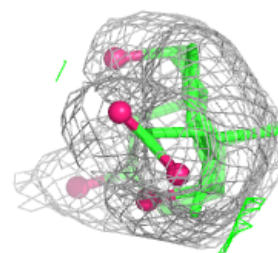
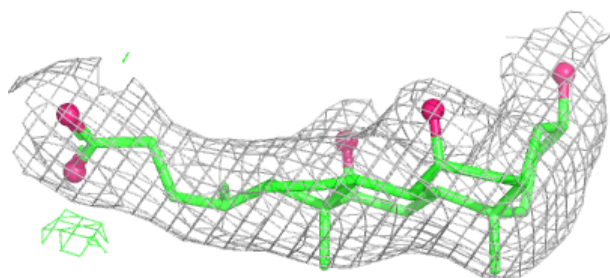
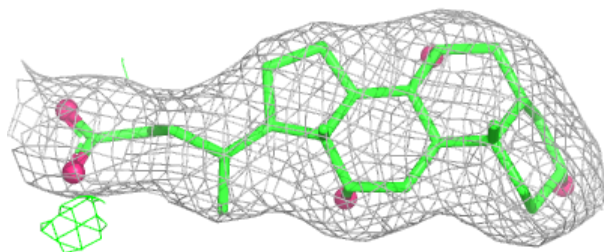
**Electron density around PGV C 305:**

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

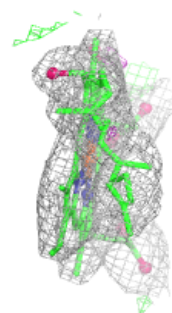
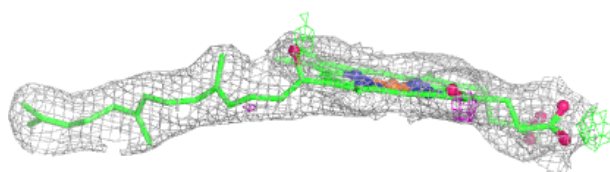
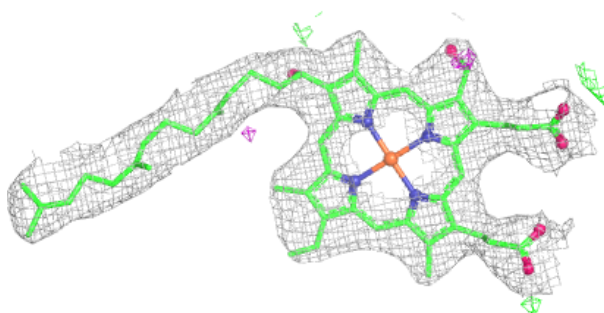


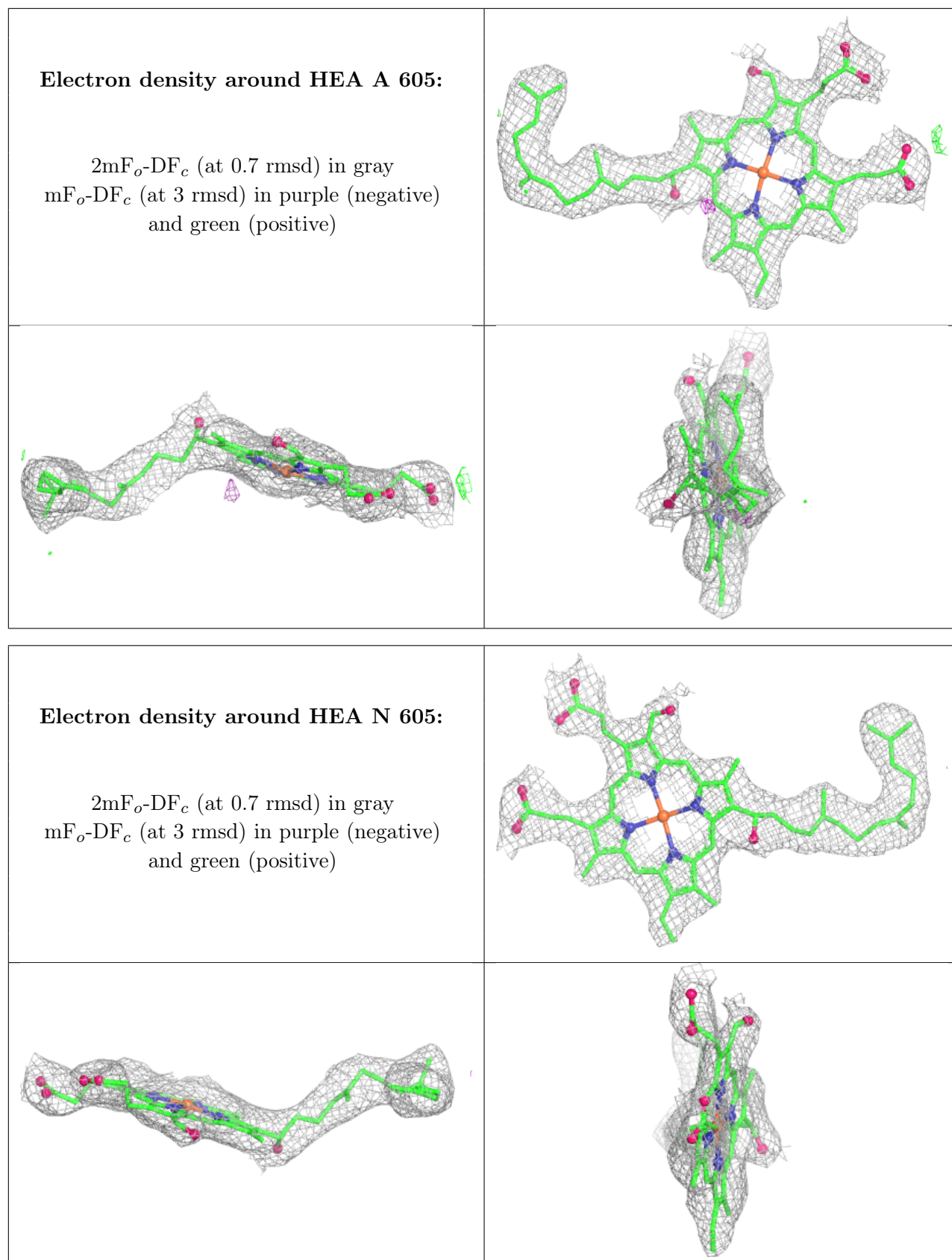
Electron density around CHD B 303:

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

**Electron density around HEA A 604:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.