



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:26 PM UTC

PDB ID : 8GBT / pdb_00008gbt
Title : Time-resolve SFX structure of a photoproduct of carbon monoxide complex of bovine cytochrome c oxidase
Authors : Ishigami, I.; Yeh, S.-R.; Rousseau, D.L.
Deposited on : 2023-02-28
Resolution : 2.80 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

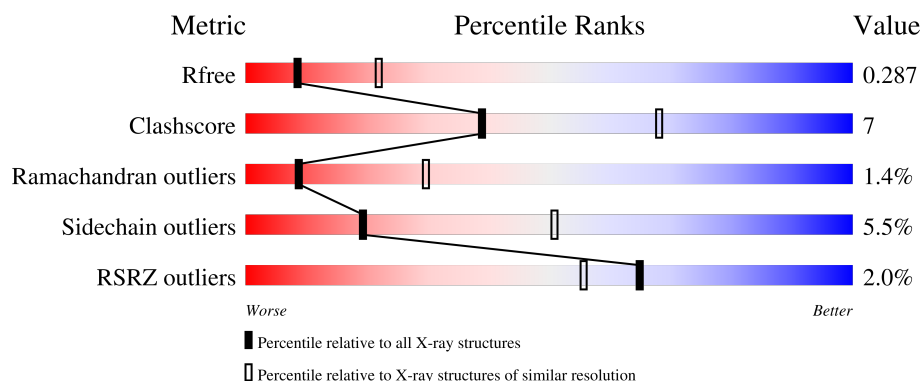
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



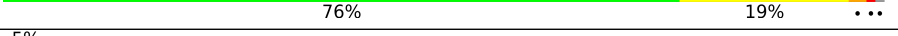
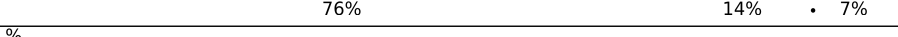
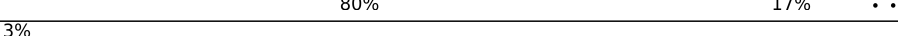
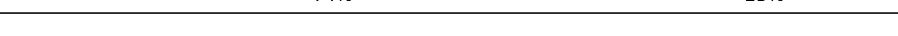
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	
1	N	514	
2	B	227	
2	O	227	
3	C	261	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	DMU	G	102	X	-	-	-
28	DMU	M	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	DMU	Q	201	X	-	-	-
28	DMU	T	102	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 30981 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	T	84	Total	C	N	O	P	S	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	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			
9	V	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			

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

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

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

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

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

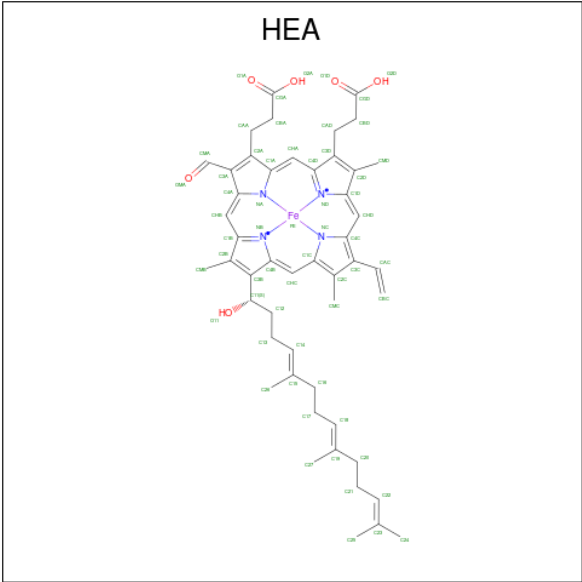
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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 HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

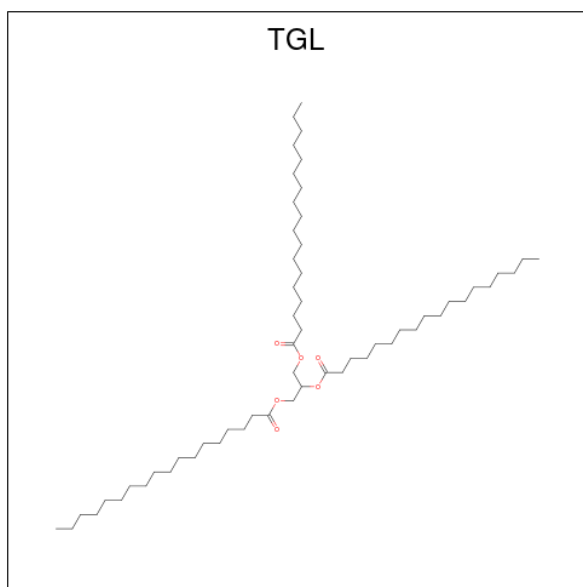
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

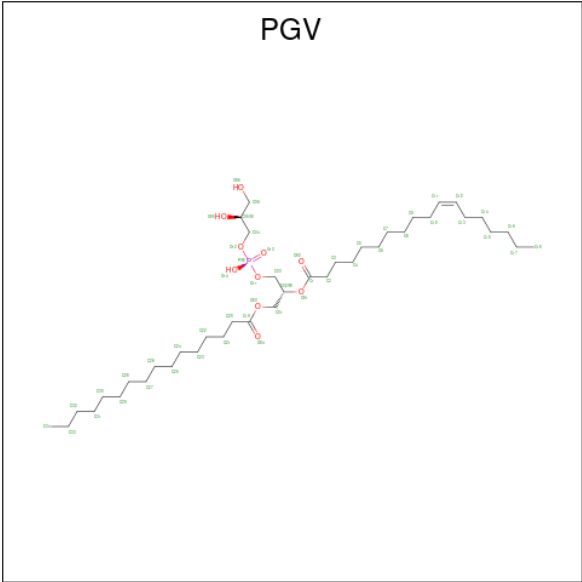
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



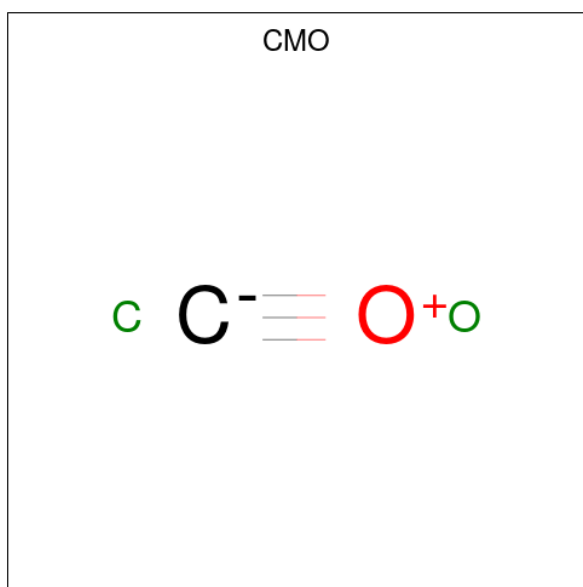
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	I	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 19 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P) (labeled as "Ligand of Interest" by depositor).



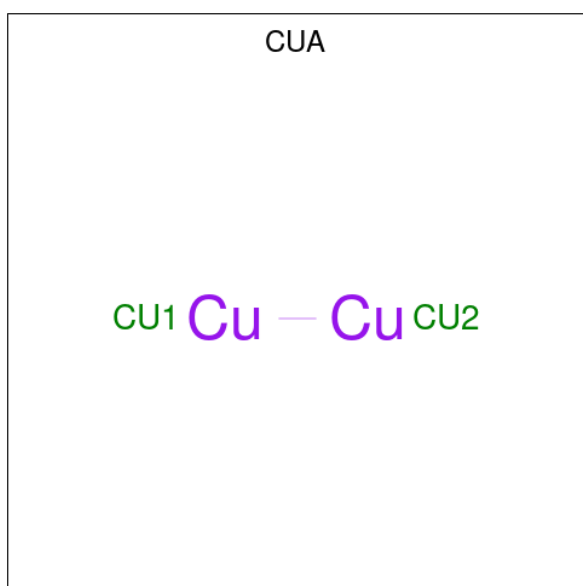
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	M	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	U	1	Total	C	O	P	0	0
			51	40	10	1		
19	Z	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 20 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



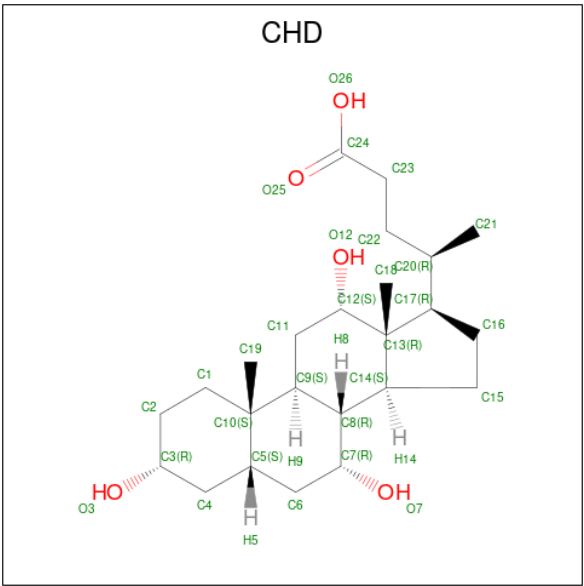
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			2	1	1		
20	N	1	Total	C	O	0	0
			2	1	1		

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



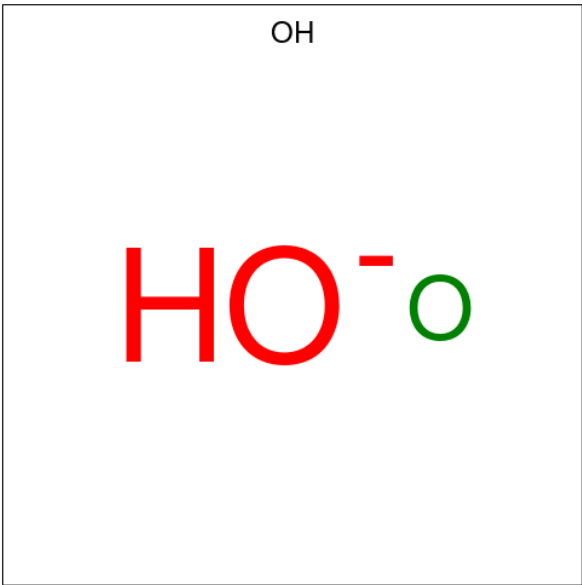
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	Cu	0	0
			2	2		
21	O	1	Total	Cu	0	0
			2	2		

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



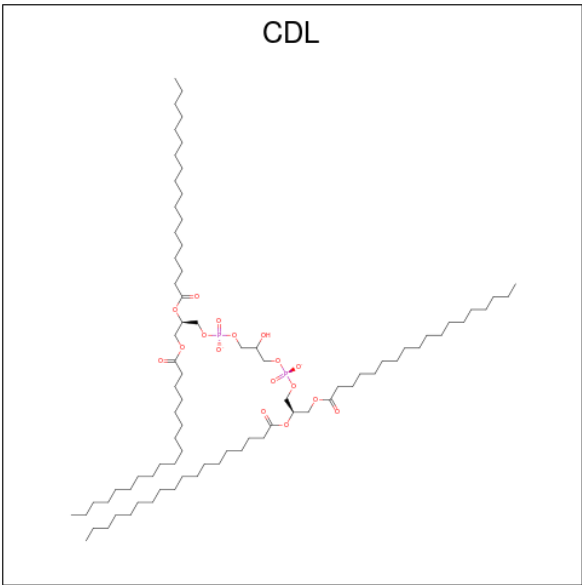
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	N	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0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

- Molecule 23 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	O		0	1
			1	1			
23	P	1	Total	O		0	1
			1	1			

- Molecule 24 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



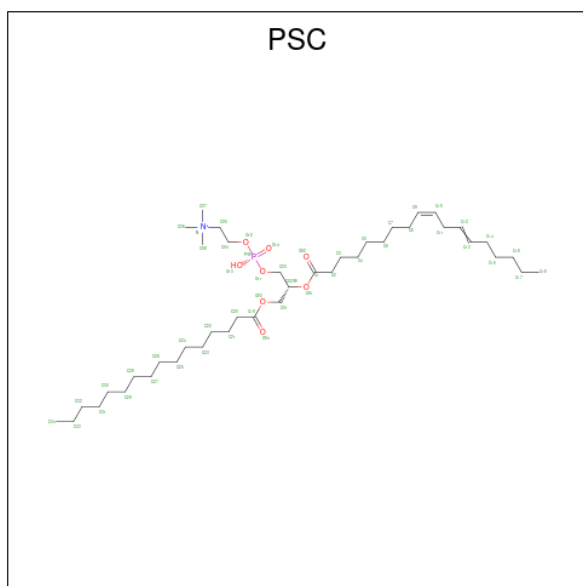
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	C	1	Total	C	O	P	0	0
			100	81	17	2		
24	G	1	Total	C	O	P	0	0
			100	81	17	2		

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

- Molecule 25 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: $C_{42}H_{81}NO_8P$) (labeled as "Ligand of Interest" by depositor).

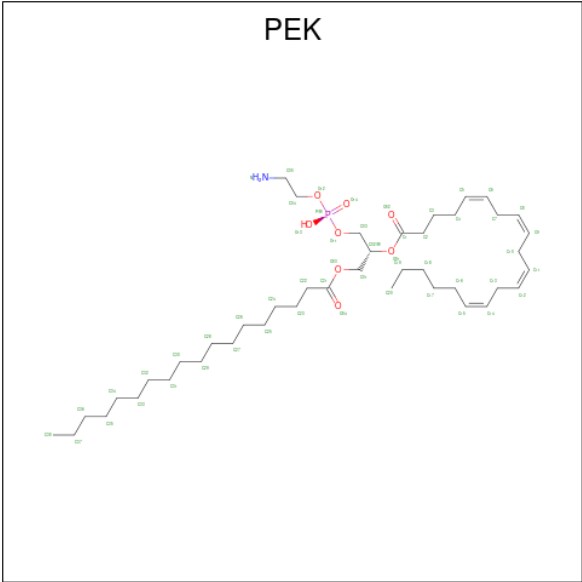


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	E	1	Total	C	N	O	P	0
			52	42	1	8	1	
25	R	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

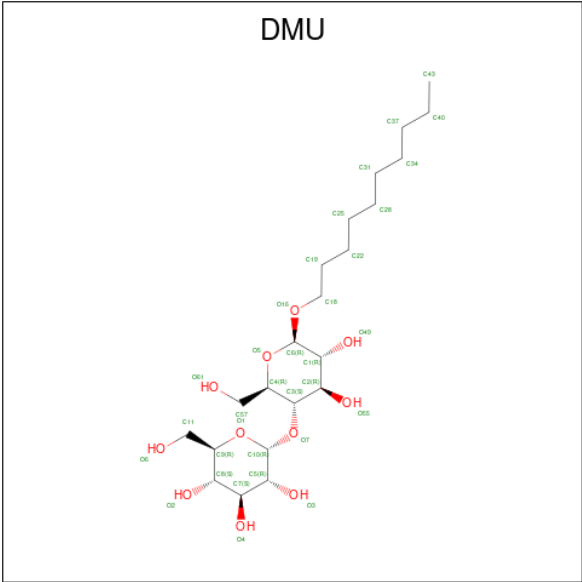
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	F	1	Total	Zn	0	0
			1	1		
26	S	1	Total	Zn	0	0
			1	1		

- Molecule 27 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: $C_{43}H_{78}NO_8P$).



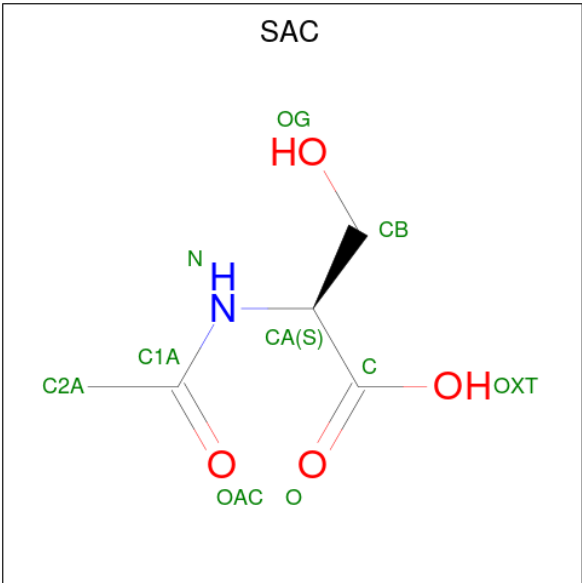
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 28 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁) (labeled as "Ligand of Interest" by depositor).



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

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



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

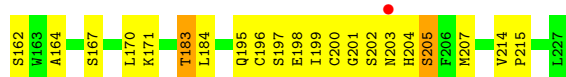
- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	43	Total	O	0	0
			43	43		
30	B	21	Total	O	0	0
			21	21		
30	C	23	Total	O	0	0
			23	23		
30	D	11	Total	O	0	0
			11	11		
30	E	10	Total	O	0	0
			10	10		
30	F	7	Total	O	0	0
			7	7		
30	G	11	Total	O	0	0
			11	11		
30	H	1	Total	O	0	0
			1	1		
30	I	2	Total	O	0	0
			2	2		
30	K	4	Total	O	0	0
			4	4		
30	L	4	Total	O	0	0
			4	4		
30	M	3	Total	O	0	0
			3	3		
30	N	31	Total	O	0	0
			31	31		
30	O	21	Total	O	0	0
			21	21		
30	P	12	Total	O	0	0
			12	12		
30	Q	7	Total	O	0	0
			7	7		
30	R	8	Total	O	0	0
			8	8		
30	S	5	Total	O	0	0
			5	5		

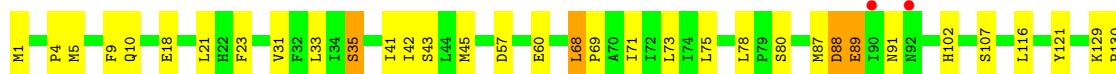
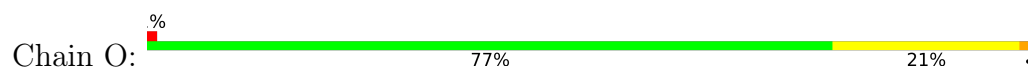
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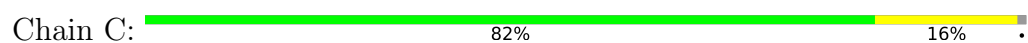
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	T	7	Total 7	O 7	0	0
30	U	1	Total 1	O 1	0	0
30	V	8	Total 8	O 8	0	0
30	W	1	Total 1	O 1	0	0
30	Y	2	Total 2	O 2	0	0
30	Z	2	Total 2	O 2	0	0



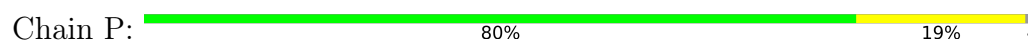
• Molecule 2: Cytochrome c oxidase subunit 2



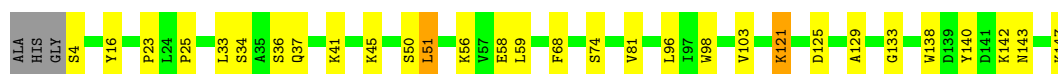
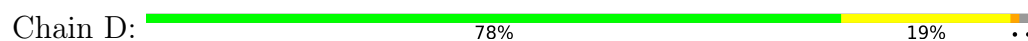
• Molecule 3: Cytochrome c oxidase subunit 3



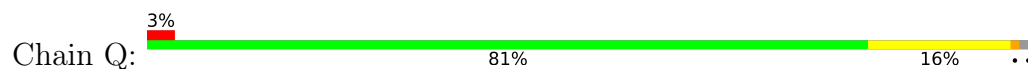
• Molecule 3: Cytochrome c oxidase subunit 3



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



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



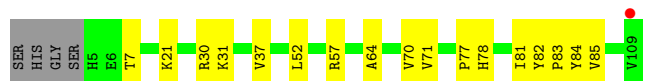
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:  81% 14% . .



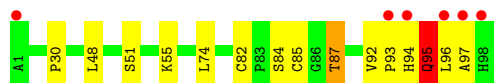
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:  81% 16% .



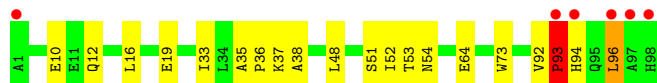
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:  6% 85% 13% ..



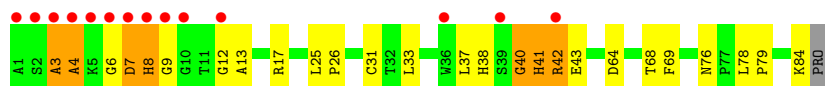
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:  6% 80% 18% ..



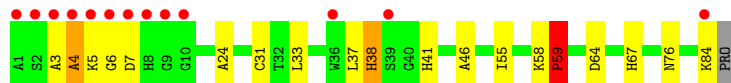
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:  16% 68% 22% 8% .



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

Chain T:  15% 76% 19% ...

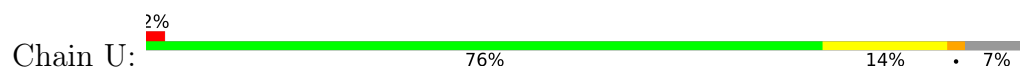


- Molecule 8: Cytochrome c oxidase subunit 6B1

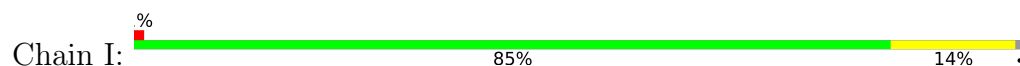
Chain H:  5% 79% 9% . . 7%



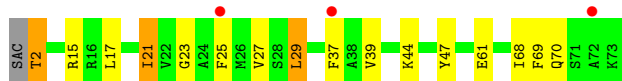
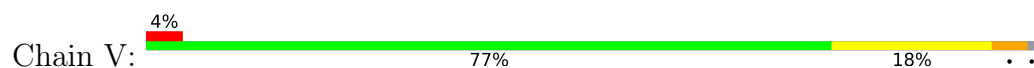
- Molecule 8: Cytochrome c oxidase subunit 6B1



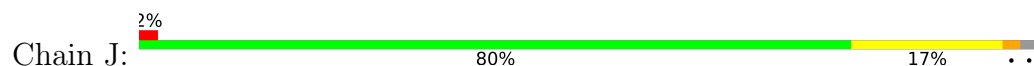
- Molecule 9: Cytochrome c oxidase subunit 6C



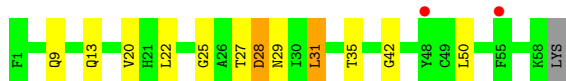
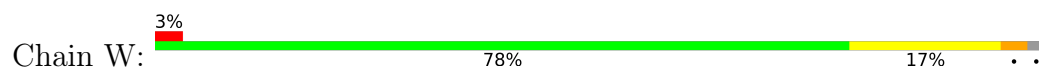
- Molecule 9: Cytochrome c oxidase subunit 6C



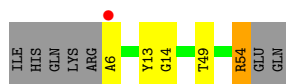
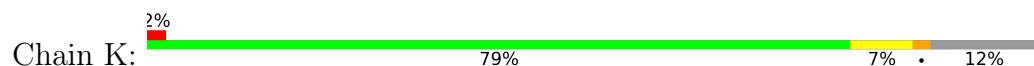
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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

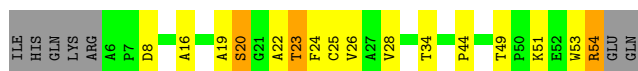


- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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

Chain X:  59% 23% 5% 12%



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

Chain L:  2% 87% 9% ..



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

Chain Y:  2% 74% 23% .



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

Chain M:  83% 11% 7%



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

Chain Z:  59% 33% . 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	178.30Å 189.00Å 209.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.00 – 2.80 32.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (32.00-2.80) 99.4 (32.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.223 , 0.269 (Not available) , 0.287	Depositor DCC
R_{free} test set	8688 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	30981	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.00	1/4156 (0.0%)	1.51	7/5678 (0.1%)
1	N	1.04	1/4156 (0.0%)	1.54	8/5678 (0.1%)
2	B	0.98	1/1860 (0.1%)	1.40	3/2534 (0.1%)
2	O	1.02	1/1860 (0.1%)	1.43	0/2534
3	C	0.96	0/2197	1.51	0/3005
3	P	0.98	0/2197	1.54	0/3005
4	D	0.99	0/1229	1.48	0/1658
4	Q	1.00	0/1229	1.47	0/1658
5	E	0.96	0/871	1.49	0/1182
5	R	0.99	0/871	1.53	0/1182
6	F	1.01	0/765	1.42	0/1038
6	S	1.04	0/765	1.42	0/1038
7	G	0.99	0/690	1.38	0/937
7	T	1.02	0/690	1.44	0/937
8	H	1.00	1/682 (0.1%)	1.45	0/921
8	U	0.99	0/682	1.50	0/921
9	I	0.99	0/605	1.58	0/802
9	V	0.98	0/605	1.58	2/802 (0.2%)
10	J	0.96	0/471	1.56	0/636
10	W	0.99	0/471	1.63	2/636 (0.3%)
11	K	1.01	0/398	1.35	0/546
11	X	1.03	0/398	1.48	0/546
12	L	0.98	0/393	1.47	1/526 (0.2%)
12	Y	1.01	0/393	1.47	0/526
13	M	0.96	0/345	1.50	0/470
13	Z	1.02	0/345	1.47	0/470
All	All	1.00	5/29324 (0.0%)	1.49	23/39866 (0.1%)

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
7	G	0	1
7	T	0	2
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	198	GLU	C-O	6.38	1.31	1.23
8	H	9	LYS	N-CA	6.29	1.50	1.46
2	B	198	GLU	C-O	5.91	1.31	1.23
1	A	240	HIS	CE1-NE2	5.48	1.38	1.32
1	N	240	HIS	CE1-NE2	5.27	1.37	1.32

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	HIS	CA-CB-CG	-7.50	106.30	113.80
1	N	240	HIS	CA-CB-CG	-6.88	106.92	113.80
2	B	158	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	45	GLY	CA-C-O	-6.08	118.07	122.45
1	A	377	PHE	CA-CB-CG	5.42	119.22	113.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
7	G	12	GLY	Peptide
6	S	93	PRO	Peptide
7	T	5	LYS	Peptide
7	T	6	GLY	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	47	0
1	N	4027	0	4001	90	0
2	B	1824	0	1833	25	0
2	O	1824	0	1833	27	0
3	C	2110	0	2027	28	0
3	P	2110	0	2027	32	0
4	D	1195	0	1183	15	0
4	Q	1195	0	1183	15	0
5	E	852	0	845	13	0
5	R	852	0	845	9	0
6	F	748	0	728	10	0
6	S	748	0	728	9	0
7	G	675	0	644	15	0
7	T	675	0	644	9	0
8	H	662	0	623	13	0
8	U	662	0	623	6	0
9	I	592	0	604	4	0
9	V	592	0	604	9	0
10	J	460	0	459	8	0
10	W	460	0	459	6	0
11	K	384	0	366	3	0
11	X	384	0	366	10	0
12	L	380	0	380	2	0
12	Y	380	0	380	5	0
13	M	335	0	352	2	0
13	Z	335	0	352	13	0
14	A	120	0	108	7	0
14	N	120	0	108	7	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	63	0	110	2	0
18	I	63	0	110	1	0
18	L	63	0	110	1	0
18	N	126	0	220	1	0
18	Y	63	0	110	0	0
19	A	51	0	76	0	0
19	C	102	0	152	2	0
19	M	51	0	76	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	51	0	76	1	0
19	P	51	0	76	2	0
19	U	51	0	76	2	0
19	Z	51	0	76	3	0
20	A	2	0	0	1	0
20	N	2	0	0	0	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	0	0
22	C	58	0	78	3	0
22	G	29	0	39	1	0
22	J	29	0	39	4	0
22	N	29	0	39	5	0
22	P	58	0	78	3	0
23	C	1	0	0	1	0
23	P	1	0	0	1	0
24	C	100	0	156	2	0
24	G	100	0	156	7	0
24	P	100	0	156	0	0
24	T	100	0	156	6	0
25	E	52	0	80	10	0
25	R	52	0	80	3	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	G	159	0	231	6	0
27	P	53	0	77	2	0
27	T	106	0	154	1	0
28	G	33	0	42	0	0
28	M	33	0	42	0	0
28	Q	33	0	42	2	0
28	T	33	0	41	0	0
29	I	9	0	8	2	0
29	V	9	0	8	0	0
30	A	43	0	0	1	0
30	B	21	0	0	2	0
30	C	23	0	0	8	0
30	D	11	0	0	0	0
30	E	10	0	0	0	0
30	F	7	0	0	0	0
30	G	11	0	0	2	0
30	H	1	0	0	0	0
30	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	K	4	0	0	2	0
30	L	4	0	0	0	0
30	M	3	0	0	0	0
30	N	31	0	0	3	0
30	O	21	0	0	7	0
30	P	12	0	0	0	0
30	Q	7	0	0	2	0
30	R	8	0	0	0	0
30	S	5	0	0	0	0
30	T	7	0	0	0	0
30	U	1	0	0	1	0
30	V	8	0	0	2	0
30	W	1	0	0	0	0
30	Y	2	0	0	0	0
30	Z	2	0	0	3	0
All	All	30981	0	31315	419	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 7.

The worst 5 of 419 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)
18:N:608:TGL:CC1	30:N:701:HOH:O	2.24	0.85
3:P:47:LEU:O	3:P:51:MET:HG2	1.79	0.81
30:C:412:HOH:O	10:J:46:SER:CB	2.34	0.75
7:G:76:ASN:HD21	27:G:101:PEK:HN2	1.35	0.75
3:P:232:HIS:NE2	23:P:301[H]:OH:O	2.23	0.72

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	379/514 (74%)	359 (95%)	20 (5%)	0	100	100
1	N	512/514 (100%)	471 (92%)	39 (8%)	2 (0%)	30	60
2	B	13/227 (6%)	11 (85%)	2 (15%)	0	100	100
2	O	225/227 (99%)	204 (91%)	20 (9%)	1 (0%)	30	60
3	C	257/261 (98%)	240 (93%)	14 (5%)	3 (1%)	10	34
3	P	257/261 (98%)	240 (93%)	16 (6%)	1 (0%)	30	60
4	D	142/147 (97%)	132 (93%)	9 (6%)	1 (1%)	18	47
4	Q	142/147 (97%)	120 (84%)	17 (12%)	5 (4%)	3	10
5	E	103/109 (94%)	97 (94%)	6 (6%)	0	100	100
5	R	103/109 (94%)	94 (91%)	9 (9%)	0	100	100
6	F	96/98 (98%)	84 (88%)	10 (10%)	2 (2%)	5	20
6	S	96/98 (98%)	80 (83%)	11 (12%)	5 (5%)	1	5
7	G	81/85 (95%)	60 (74%)	13 (16%)	8 (10%)	0	1
7	T	81/85 (95%)	60 (74%)	13 (16%)	8 (10%)	0	1
8	H	77/85 (91%)	62 (80%)	13 (17%)	2 (3%)	4	15
8	U	77/85 (91%)	61 (79%)	13 (17%)	3 (4%)	2	8
9	I	70/73 (96%)	61 (87%)	9 (13%)	0	100	100
9	V	70/73 (96%)	61 (87%)	8 (11%)	1 (1%)	9	30
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
11	K	47/56 (84%)	40 (85%)	7 (15%)	0	100	100
11	X	47/56 (84%)	38 (81%)	9 (19%)	0	100	100
12	L	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
12	Y	44/47 (94%)	39 (89%)	3 (7%)	2 (4%)	2	7
13	M	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
13	Z	41/46 (89%)	31 (76%)	9 (22%)	1 (2%)	4	17
All	All	3157/3614 (87%)	2829 (90%)	283 (9%)	45 (1%)	9	30

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	3	ALA
7	G	4	ALA

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Mol	Chain	Res	Type
7	G	7	ASP
8	H	8	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	414 (97%)	12 (3%)	38	73
1	N	426/426 (100%)	409 (96%)	17 (4%)	28	63
2	B	210/210 (100%)	194 (92%)	16 (8%)	12	36
2	O	210/210 (100%)	191 (91%)	19 (9%)	9	28
3	C	224/226 (99%)	218 (97%)	6 (3%)	39	74
3	P	224/226 (99%)	214 (96%)	10 (4%)	24	58
4	D	128/129 (99%)	117 (91%)	11 (9%)	10	31
4	Q	128/129 (99%)	123 (96%)	5 (4%)	28	64
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	69
5	R	92/95 (97%)	89 (97%)	3 (3%)	33	69
6	F	81/81 (100%)	78 (96%)	3 (4%)	30	65
6	S	81/81 (100%)	76 (94%)	5 (6%)	16	45
7	G	67/68 (98%)	62 (92%)	5 (8%)	12	37
7	T	67/68 (98%)	63 (94%)	4 (6%)	17	47
8	H	71/75 (95%)	67 (94%)	4 (6%)	19	50
8	U	71/75 (95%)	66 (93%)	5 (7%)	14	40
9	I	57/57 (100%)	52 (91%)	5 (9%)	9	29
9	V	57/57 (100%)	51 (90%)	6 (10%)	6	22
10	J	49/50 (98%)	44 (90%)	5 (10%)	7	23
10	W	49/50 (98%)	45 (92%)	4 (8%)	10	33
11	K	39/46 (85%)	37 (95%)	2 (5%)	21	54
11	X	39/46 (85%)	33 (85%)	6 (15%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	39/40 (98%)	37 (95%)	2 (5%)	21	54
12	Y	39/40 (98%)	34 (87%)	5 (13%)	4	15
13	M	37/38 (97%)	35 (95%)	2 (5%)	20	51
13	Z	37/38 (97%)	35 (95%)	2 (5%)	20	51
All	All	3040/3082 (99%)	2873 (94%)	167 (6%)	19	51

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	P	38	ASN
8	U	66	ILE
3	P	127	LEU
6	S	33	ILE
10	W	20	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
3	P	50	ASN
5	R	94	ASN
3	P	149	HIS
3	P	230	ASN
7	T	76	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	B	1	2	8,9,10	0.62	0	8,9,11	1.45	2 (25%)
2	FME	O	1	2	8,9,10	0.48	0	8,9,11	1.37	2 (25%)
7	TPO	T	11	7	8,10,11	0.85	0	10,14,16	0.79	0
7	TPO	G	11	7	8,10,11	0.77	0	10,14,16	0.81	0
1	FME	A	1	1	8,9,10	0.48	0	8,9,11	0.99	0
1	FME	N	1	1	8,9,10	0.52	0	8,9,11	0.84	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
2	FME	B	1	2	-	1/7/9/11	-
2	FME	O	1	2	-	1/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-
7	TPO	G	11	7	-	3/9/11/13	-
1	FME	A	1	1	-	4/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-3.22	117.87	122.82
2	O	1	FME	CA-N-CN	-2.95	118.29	122.82
2	O	1	FME	C-CA-N	2.21	113.77	109.50
2	B	1	FME	C-CA-N	2.03	113.42	109.50

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

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

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 58 ligands modelled in this entry, 8 are monoatomic and 2 are modelled with single atom - leaving 48 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	$\# Z > 2$
28	DMU	G	102	-	34,34,34	0.74	1 (2%)	45,45,45	1.06	5 (11%)
18	TGL	L	101	-	62,62,62	0.35	0	65,65,65	0.54	1 (1%)
14	HEA	N	601	1	67,67,67	2.39	25 (37%)	81,103,103	2.54	33 (40%)
18	TGL	I	101	-	62,62,62	0.35	0	65,65,65	0.51	1 (1%)
18	TGL	N	606	-	62,62,62	0.28	0	65,65,65	0.29	0
20	CMO	A	608	14	0,1,1	-	-	-	-	-
21	CUA	O	301	2	0,1,1	-	-	-	-	-
19	PGV	M	101	-	50,50,50	0.39	0	53,56,56	0.59	2 (3%)
27	PEK	P	303	-	52,52,52	0.29	0	55,57,57	0.40	0
24	CDL	T	104	-	99,99,99	0.32	0	105,111,111	0.46	1 (0%)
24	CDL	P	305	-	99,99,99	0.32	0	105,111,111	0.40	1 (0%)
22	CHD	P	302	-	32,32,32	0.56	0	51,51,51	0.77	1 (1%)
27	PEK	T	101	-	52,52,52	0.32	0	55,57,57	0.36	0
14	HEA	A	602	1,20	67,67,67	2.37	26 (38%)	81,103,103	2.57	33 (40%)
19	PGV	C	303	-	50,50,50	0.30	0	53,56,56	0.55	1 (1%)
27	PEK	T	103	-	52,52,52	0.36	0	55,57,57	0.50	0
22	CHD	N	609	-	32,32,32	0.64	0	51,51,51	1.23	8 (15%)
22	CHD	P	306	-	32,32,32	0.69	0	51,51,51	1.34	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PGV	A	607	-	50,50,50	0.33	0	53,56,56	0.50	0
18	TGL	N	608	-	62,62,62	0.32	0	65,65,65	0.50	1 (1%)
19	PGV	P	304	-	50,50,50	0.29	0	53,56,56	0.44	0
28	DMU	Q	201	-	34,34,34	0.73	1 (2%)	45,45,45	1.38	7 (15%)
19	PGV	C	304	-	50,50,50	0.36	0	53,56,56	0.64	1 (1%)
20	CMO	N	610	14	0,1,1	-	-	-	-	-
22	CHD	J	101	-	32,32,32	0.63	0	51,51,51	0.93	3 (5%)
14	HEA	N	602	1,20	67,67,67	2.32	29 (43%)	81,103,103	2.61	32 (39%)
22	CHD	B	302	-	32,32,32	0.60	0	51,51,51	0.81	1 (1%)
29	SAC	I	102	-	7,8,9	0.57	0	7,9,11	1.14	1 (14%)
18	TGL	Y	101	-	62,62,62	0.29	0	65,65,65	0.31	0
24	CDL	C	305	-	99,99,99	0.30	0	105,111,111	0.33	0
25	PSC	R	201	-	51,51,51	0.29	0	57,59,59	0.43	0
19	PGV	N	607	-	50,50,50	0.32	0	53,56,56	0.40	0
22	CHD	C	301	-	32,32,32	0.59	0	51,51,51	0.74	0
25	PSC	E	201	-	51,51,51	0.30	0	57,59,59	0.43	0
27	PEK	G	106	-	52,52,52	0.32	0	55,57,57	0.44	0
28	DMU	M	102	-	34,34,34	0.78	1 (2%)	45,45,45	1.63	11 (24%)
14	HEA	A	601	1	67,67,67	2.33	26 (38%)	81,103,103	2.50	26 (32%)
19	PGV	U	101	-	50,50,50	0.36	0	53,56,56	0.63	1 (1%)
21	CUA	B	301	2	0,1,1	-	-	-	-	-
22	CHD	G	105	-	32,32,32	0.64	0	51,51,51	1.00	2 (3%)
27	PEK	G	101	-	52,52,52	0.31	0	55,57,57	0.35	0
19	PGV	Z	101	-	50,50,50	0.35	0	53,56,56	0.48	0
29	SAC	V	101	-	7,8,9	0.56	0	7,9,11	1.03	1 (14%)
28	DMU	T	102	-	34,34,34	0.92	1 (2%)	45,45,45	1.88	7 (15%)
22	CHD	C	306	-	32,32,32	0.57	0	51,51,51	0.84	1 (1%)
24	CDL	G	104	-	99,99,99	0.33	0	105,111,111	0.49	1 (0%)
27	PEK	G	103	-	52,52,52	0.31	0	55,57,57	0.42	0
18	TGL	A	606	-	62,62,62	0.36	0	65,65,65	0.50	1 (1%)

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
28	DMU	G	102	-	2/2/10/10	9/19/59/59	0/2/2/2
18	TGL	L	101	-	-	35/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	N	601	1	-	5/36/76/76	-
18	TGL	I	101	-	-	29/65/65/65	-
18	TGL	N	606	-	-	30/65/65/65	-
19	PGV	M	101	-	-	30/55/55/55	-
27	PEK	P	303	-	-	19/56/56/56	-
24	CDL	T	104	-	-	57/110/110/110	-
24	CDL	P	305	-	-	54/110/110/110	-
22	CHD	P	302	-	-	3/9/74/74	0/4/4/4
27	PEK	T	101	-	-	27/56/56/56	-
14	HEA	A	602	1,20	-	5/36/76/76	-
19	PGV	C	303	-	-	16/55/55/55	-
27	PEK	T	103	-	-	29/56/56/56	-
22	CHD	N	609	-	-	4/9/74/74	0/4/4/4
22	CHD	P	306	-	-	3/9/74/74	0/4/4/4
19	PGV	A	607	-	-	17/55/55/55	-
18	TGL	N	608	-	-	26/65/65/65	-
19	PGV	P	304	-	-	21/55/55/55	-
28	DMU	Q	201	-	2/2/10/10	8/19/59/59	0/2/2/2
19	PGV	C	304	-	-	27/55/55/55	-
22	CHD	J	101	-	-	6/9/74/74	0/4/4/4
14	HEA	N	602	1,20	-	8/36/76/76	-
22	CHD	B	302	-	-	5/9/74/74	0/4/4/4
29	SAC	I	102	-	-	3/7/8/10	-
18	TGL	Y	101	-	-	31/65/65/65	-
24	CDL	C	305	-	-	60/110/110/110	-
25	PSC	R	201	-	-	21/55/55/55	-
19	PGV	N	607	-	-	24/55/55/55	-
22	CHD	C	301	-	-	2/9/74/74	0/4/4/4
25	PSC	E	201	-	-	26/55/55/55	-
27	PEK	G	106	-	-	31/56/56/56	-
28	DMU	M	102	-	2/2/10/10	9/19/59/59	0/2/2/2
14	HEA	A	601	1	-	7/36/76/76	-
19	PGV	U	101	-	-	32/55/55/55	-
22	CHD	G	105	-	-	4/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PEK	G	101	-	-	17/56/56/56	-
19	PGV	Z	101	-	-	25/55/55/55	-
29	SAC	V	101	-	-	1/7/8/10	-
28	DMU	T	102	-	3/3/10/10	8/19/59/59	0/2/2/2
22	CHD	C	306	-	-	3/9/74/74	0/4/4/4
24	CDL	G	104	-	-	54/110/110/110	-
27	PEK	G	103	-	-	26/56/56/56	-
18	TGL	A	606	-	-	35/65/65/65	-

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	C3B-C2B	5.97	1.48	1.34
14	N	601	HEA	C3B-C2B	5.77	1.47	1.34
14	A	602	HEA	CHB-C4A	5.54	1.49	1.38
14	N	602	HEA	FE-ND	5.31	2.11	1.94
14	N	601	HEA	CHB-C4A	5.26	1.48	1.38

The worst 5 of 190 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601	HEA	C3A-C2A-C1A	-7.85	99.62	107.05
14	A	601	HEA	C3A-C2A-C1A	-7.46	99.99	107.05
14	N	601	HEA	C3B-C4B-NB	7.11	118.01	109.84
14	N	602	HEA	C3A-C2A-C1A	-6.98	100.44	107.05
14	N	602	HEA	C2A-C1A-NA	6.93	117.00	110.32

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	G	102	DMU	C6
28	G	102	DMU	C5
28	M	102	DMU	C6
28	M	102	DMU	C5
28	Q	201	DMU	C6

5 of 892 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	I	101	TGL	CB2-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
18	L	101	TGL	CB2-CB1-OG2-CG2
19	A	607	PGV	C04-O12-P-O13
19	C	303	PGV	C04-C05-C06-O06
19	C	304	PGV	C04-O12-P-O11

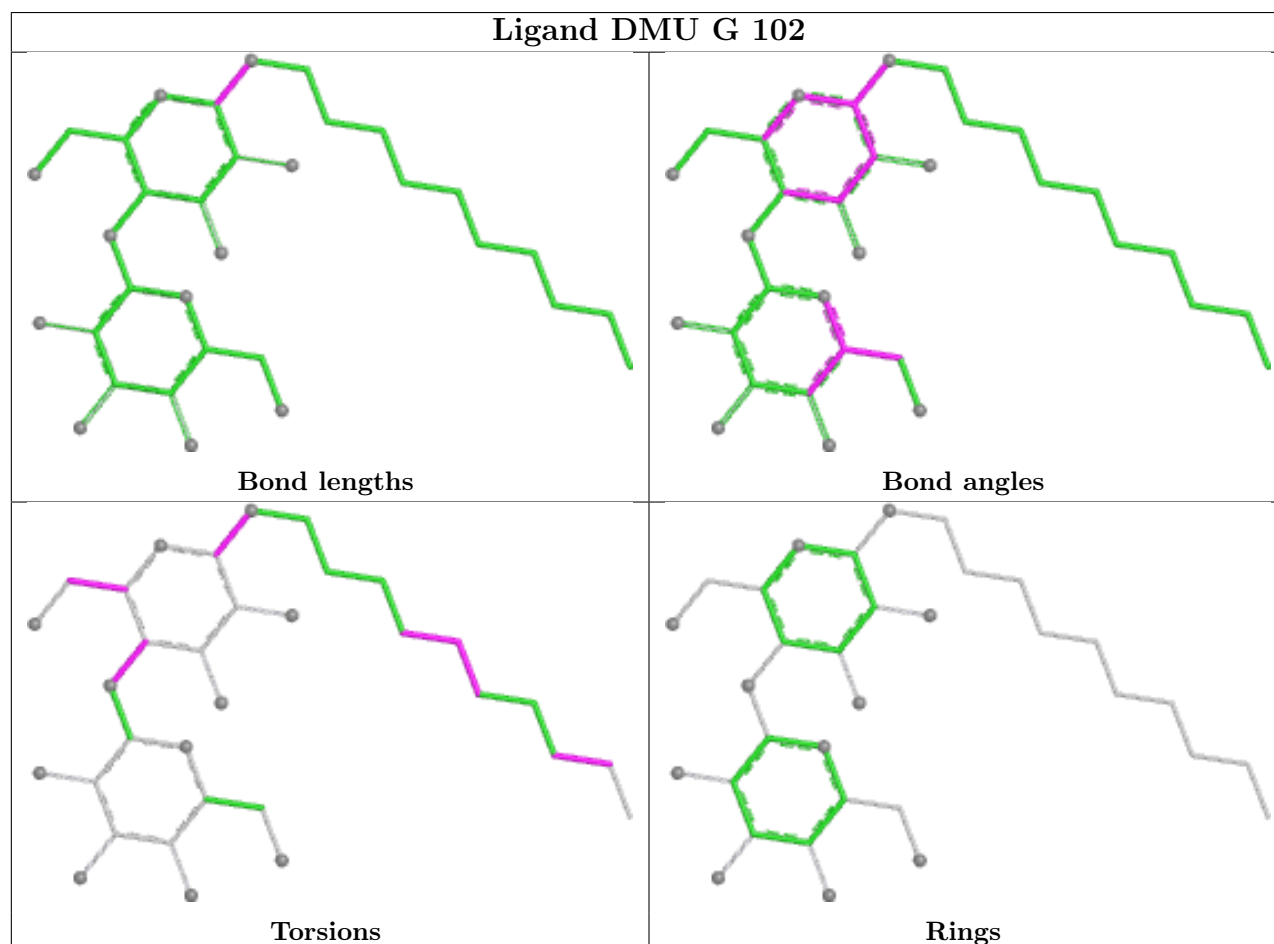
There are no ring outliers.

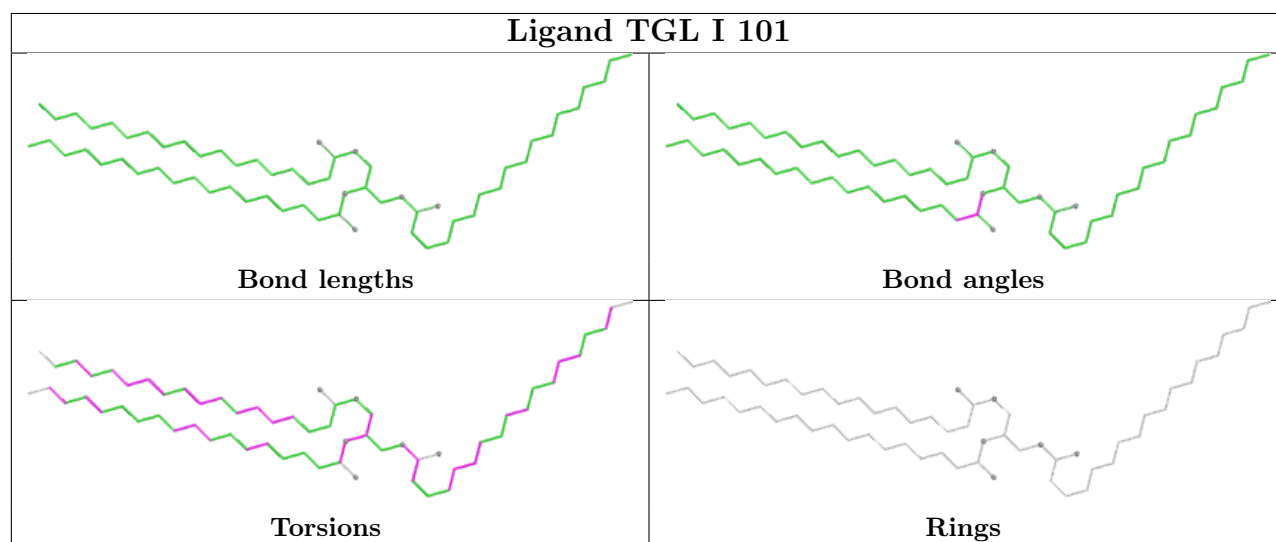
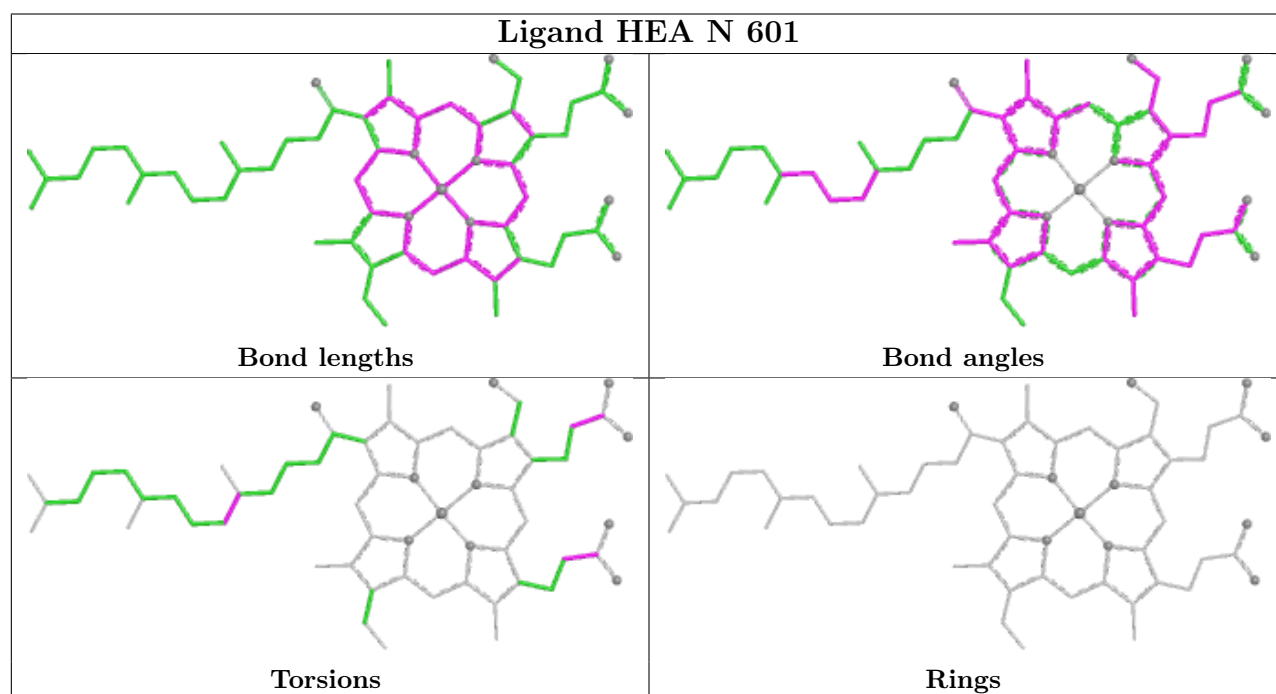
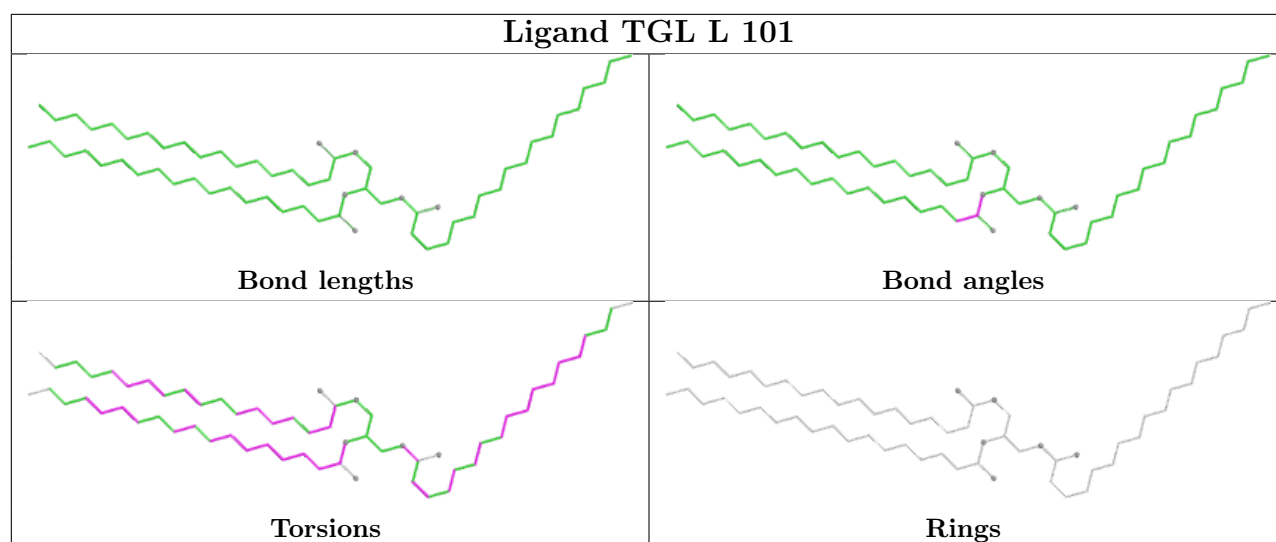
31 monomers are involved in 83 short contacts:

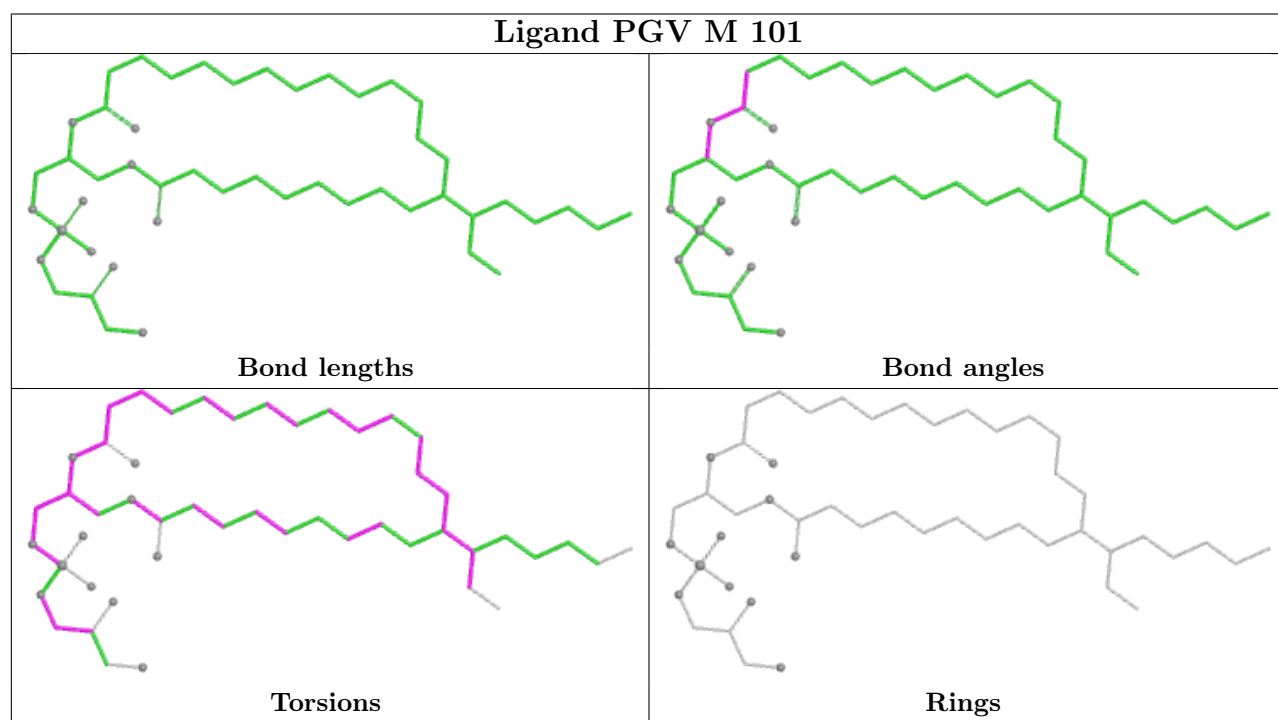
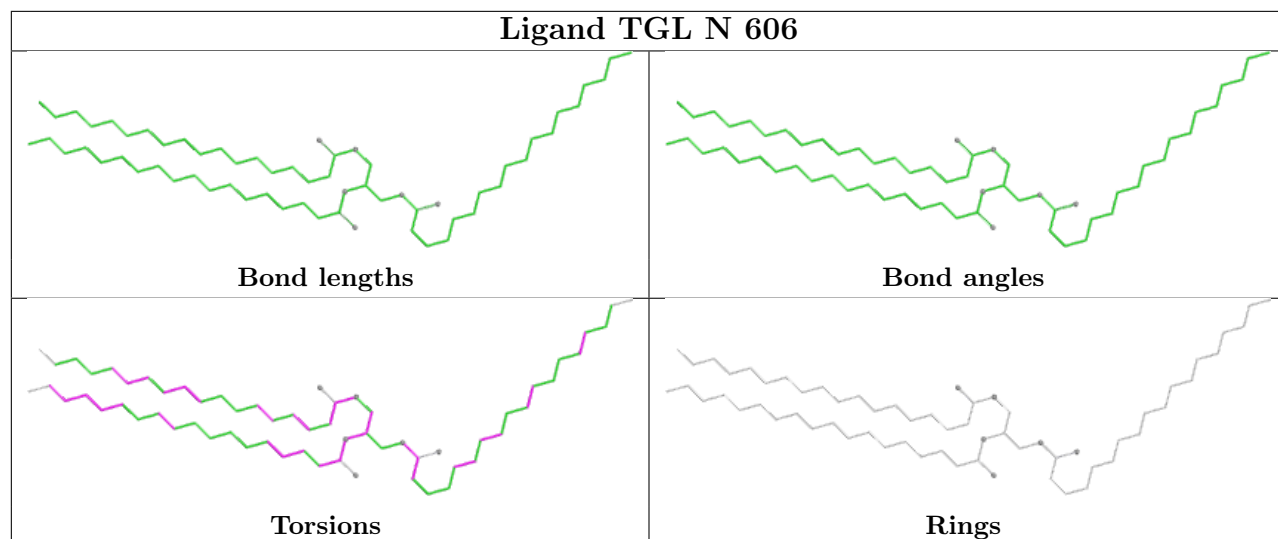
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	L	101	TGL	1	0
14	N	601	HEA	3	0
18	I	101	TGL	1	0
20	A	608	CMO	1	0
27	P	303	PEK	2	0
24	T	104	CDL	6	0
27	T	101	PEK	1	0
14	A	602	HEA	3	0
19	C	303	PGV	2	0
22	N	609	CHD	5	0
22	P	306	CHD	3	0
18	N	608	TGL	1	0
19	P	304	PGV	2	0
28	Q	201	DMU	2	0
22	J	101	CHD	4	0
14	N	602	HEA	4	0
29	I	102	SAC	2	0
24	C	305	CDL	2	0
25	R	201	PSC	3	0
19	N	607	PGV	1	0
22	C	301	CHD	2	0
25	E	201	PSC	10	0
14	A	601	HEA	4	0
19	U	101	PGV	2	0
22	G	105	CHD	1	0
27	G	101	PEK	3	0
19	Z	101	PGV	3	0
22	C	306	CHD	1	0
24	G	104	CDL	7	0
27	G	103	PEK	3	0
18	A	606	TGL	2	0

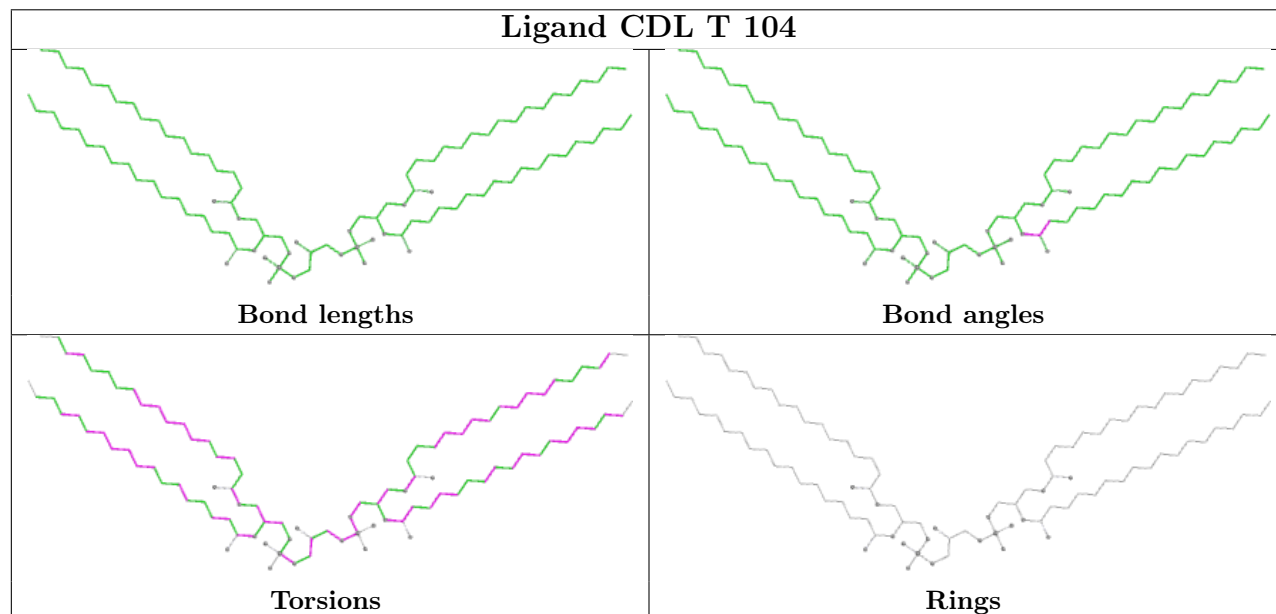
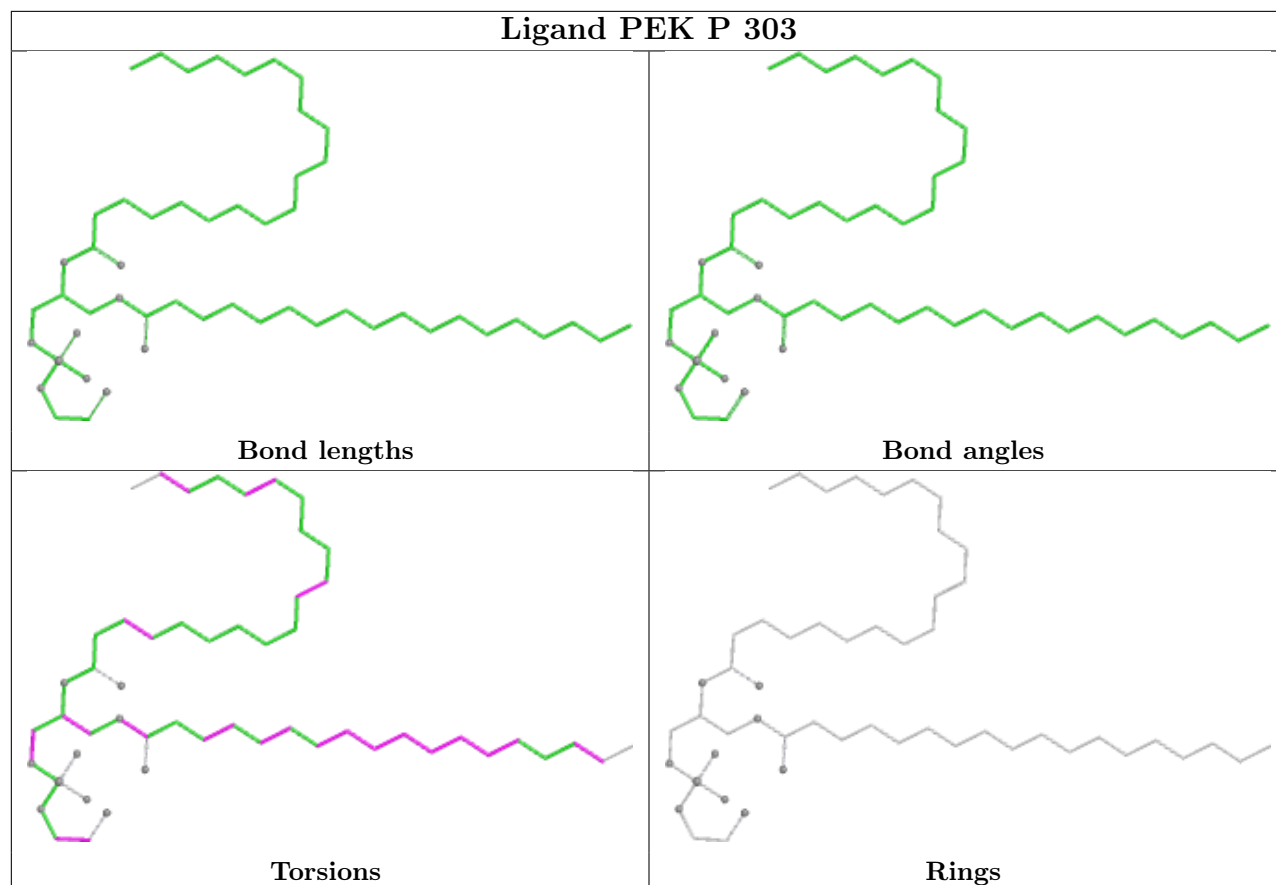
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

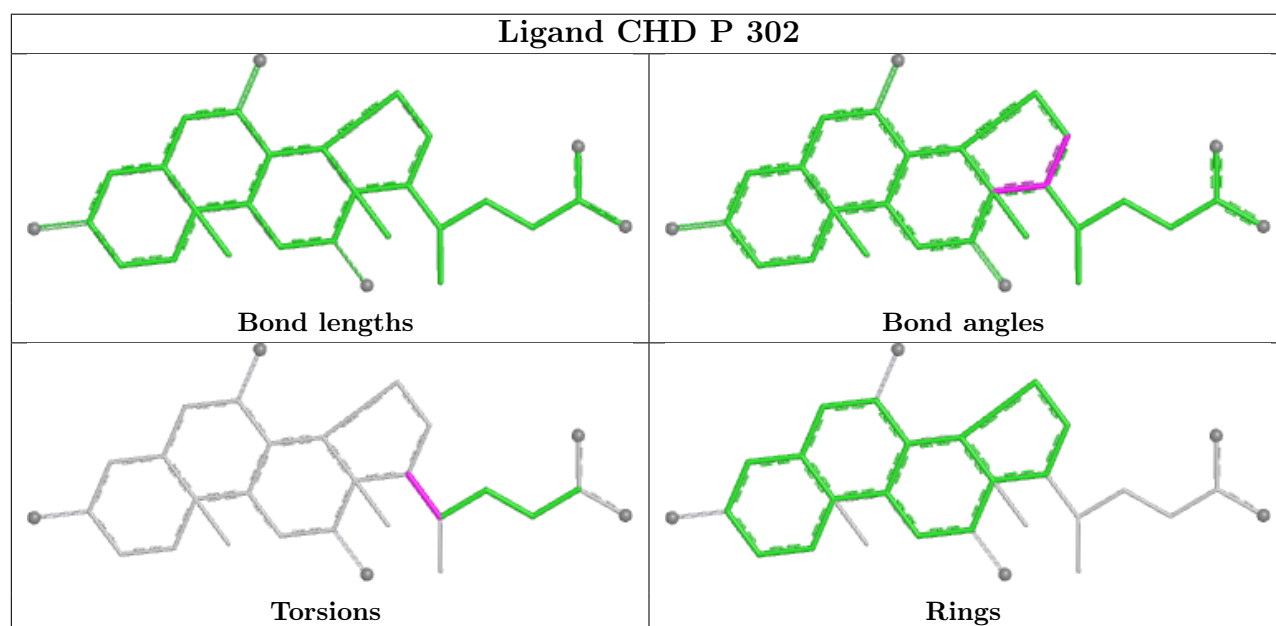
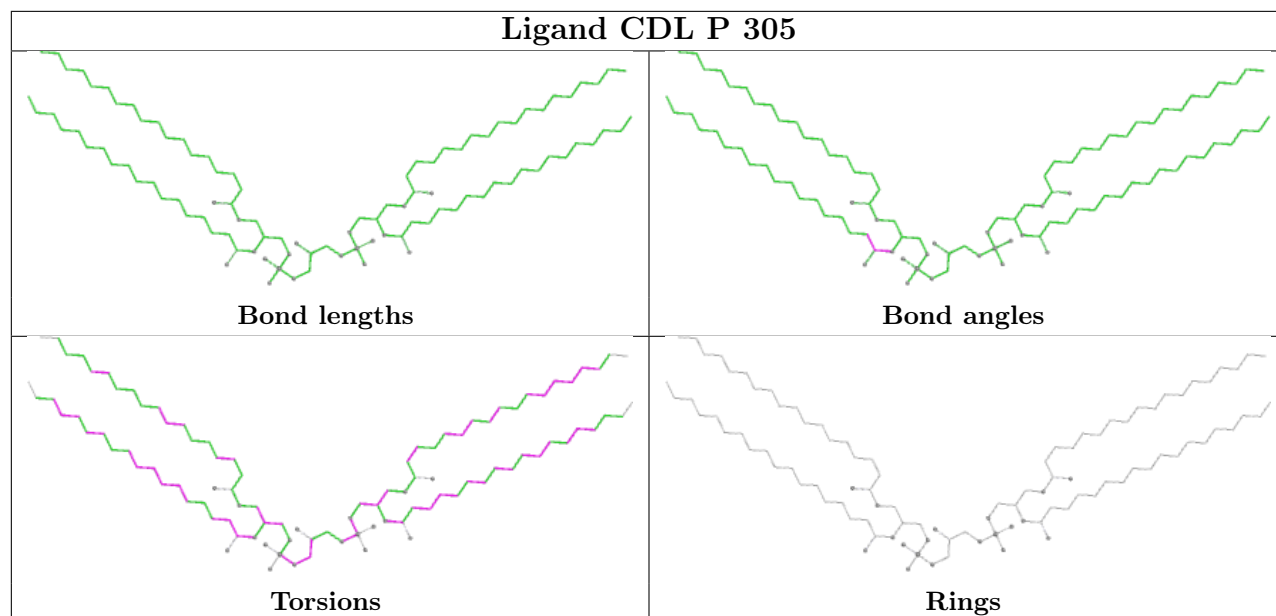
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

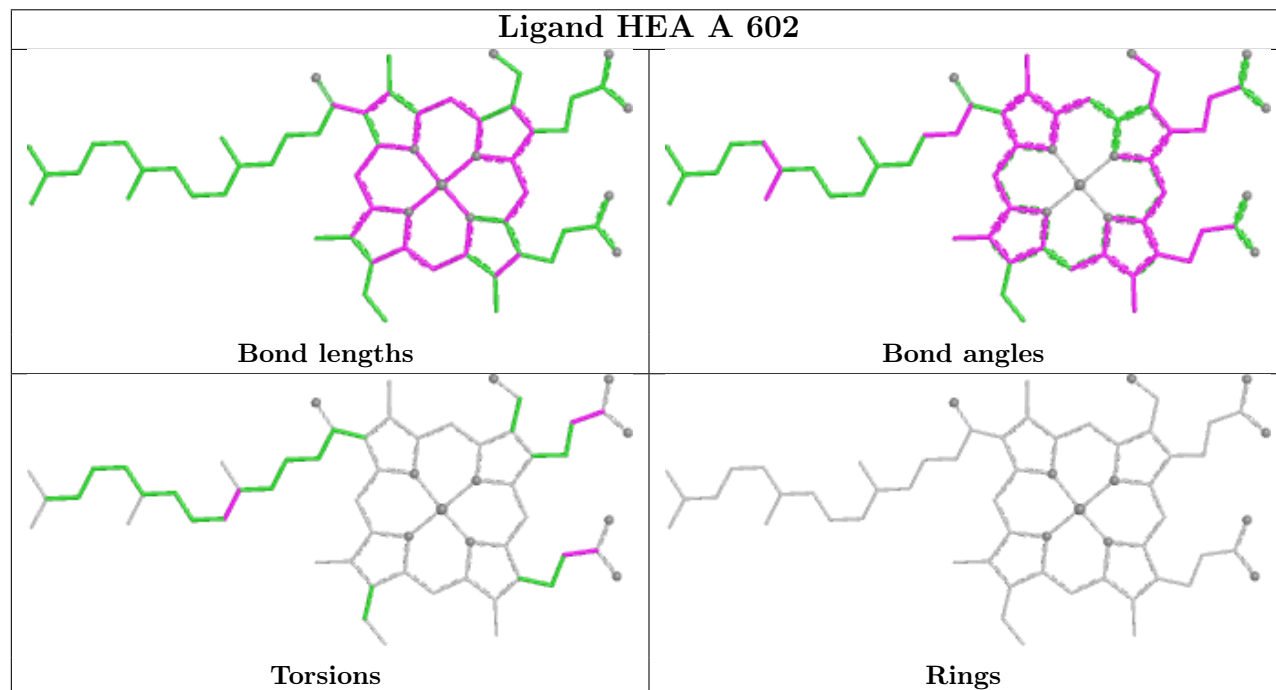
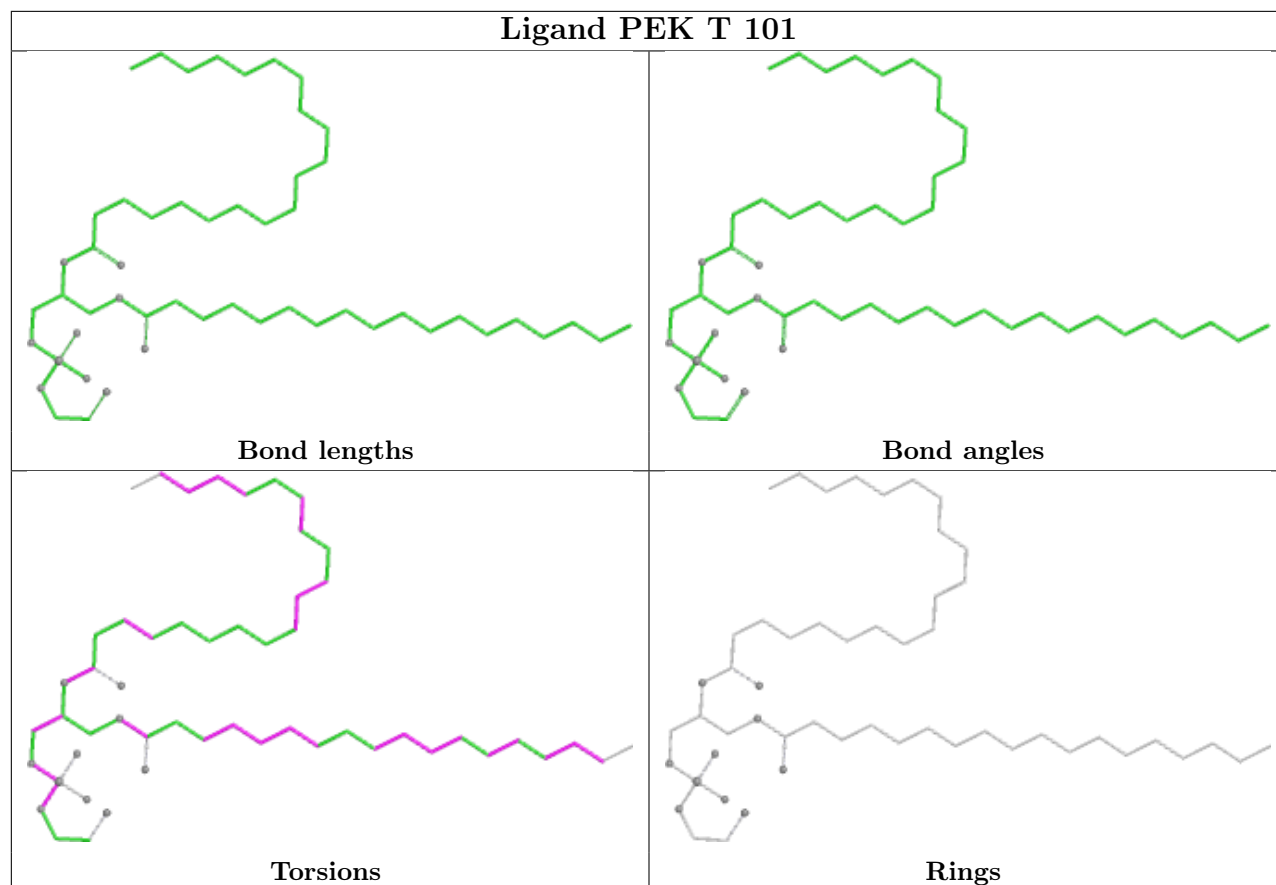


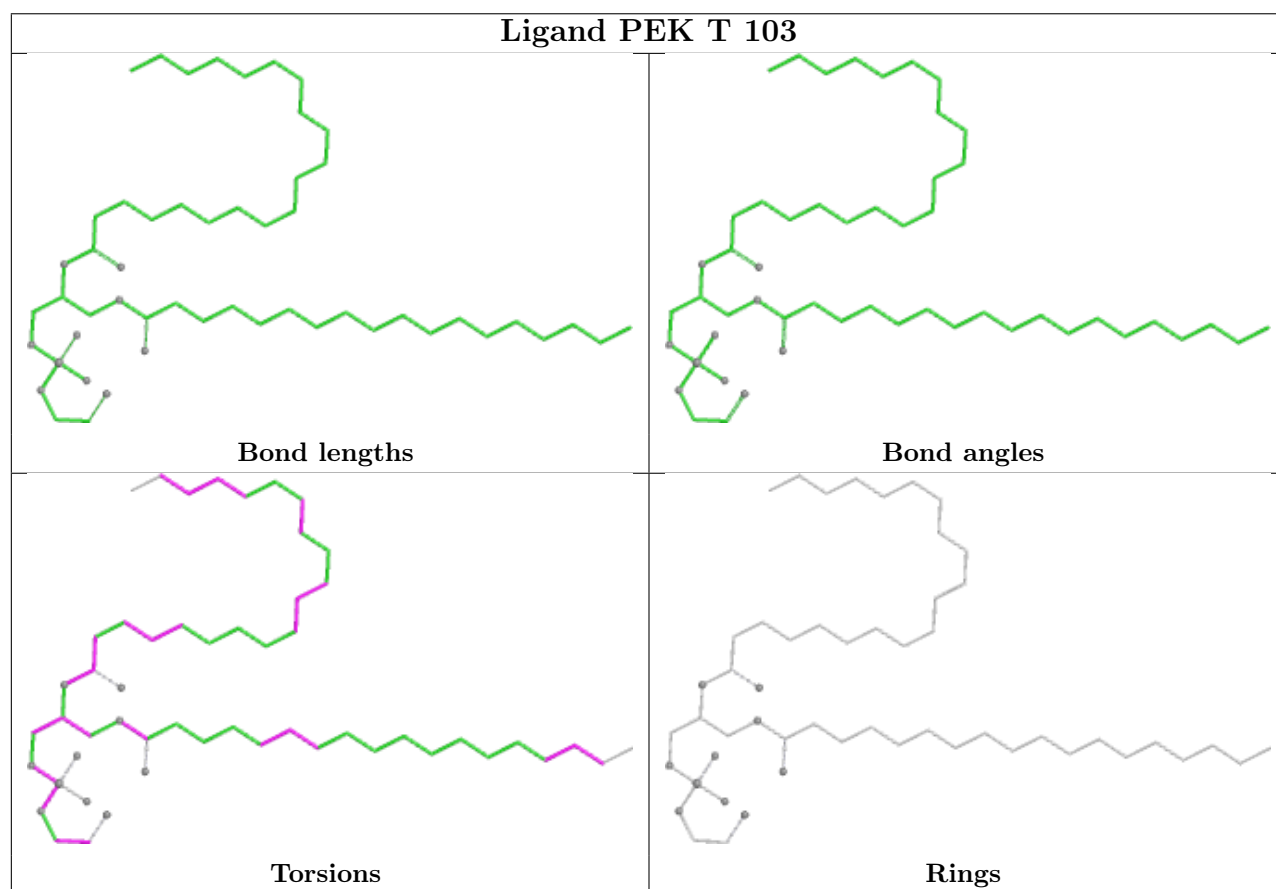
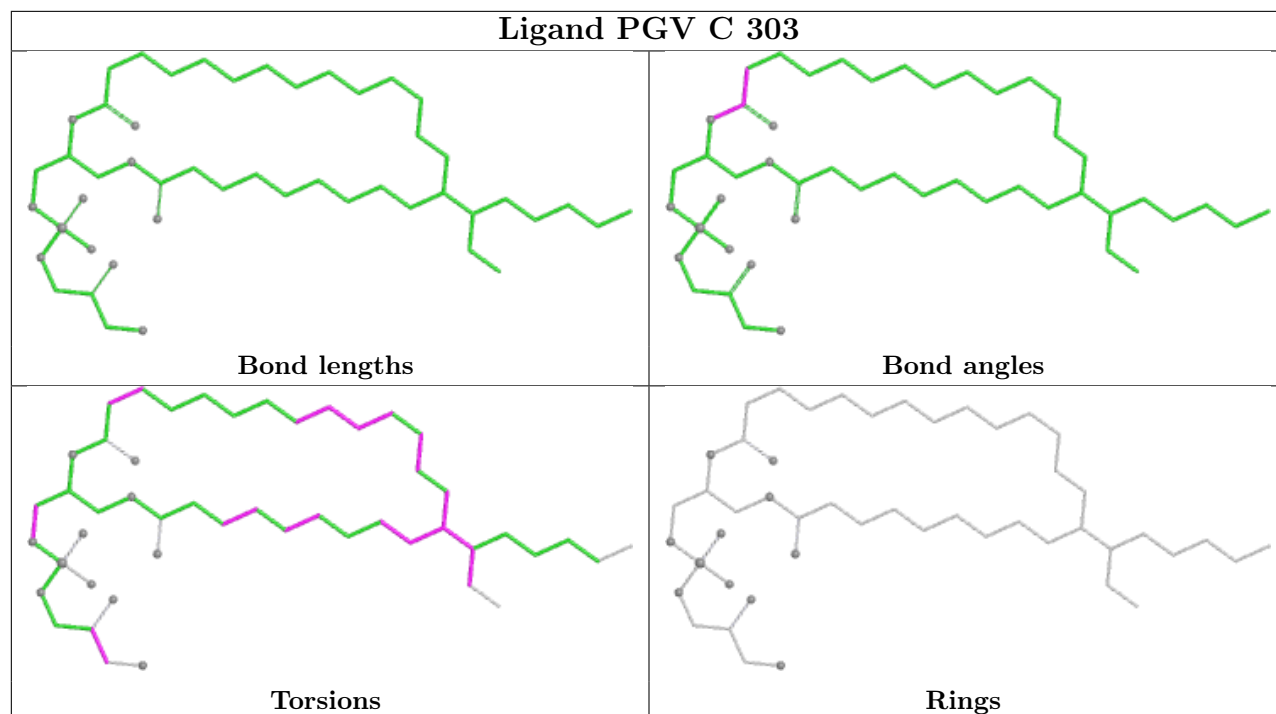


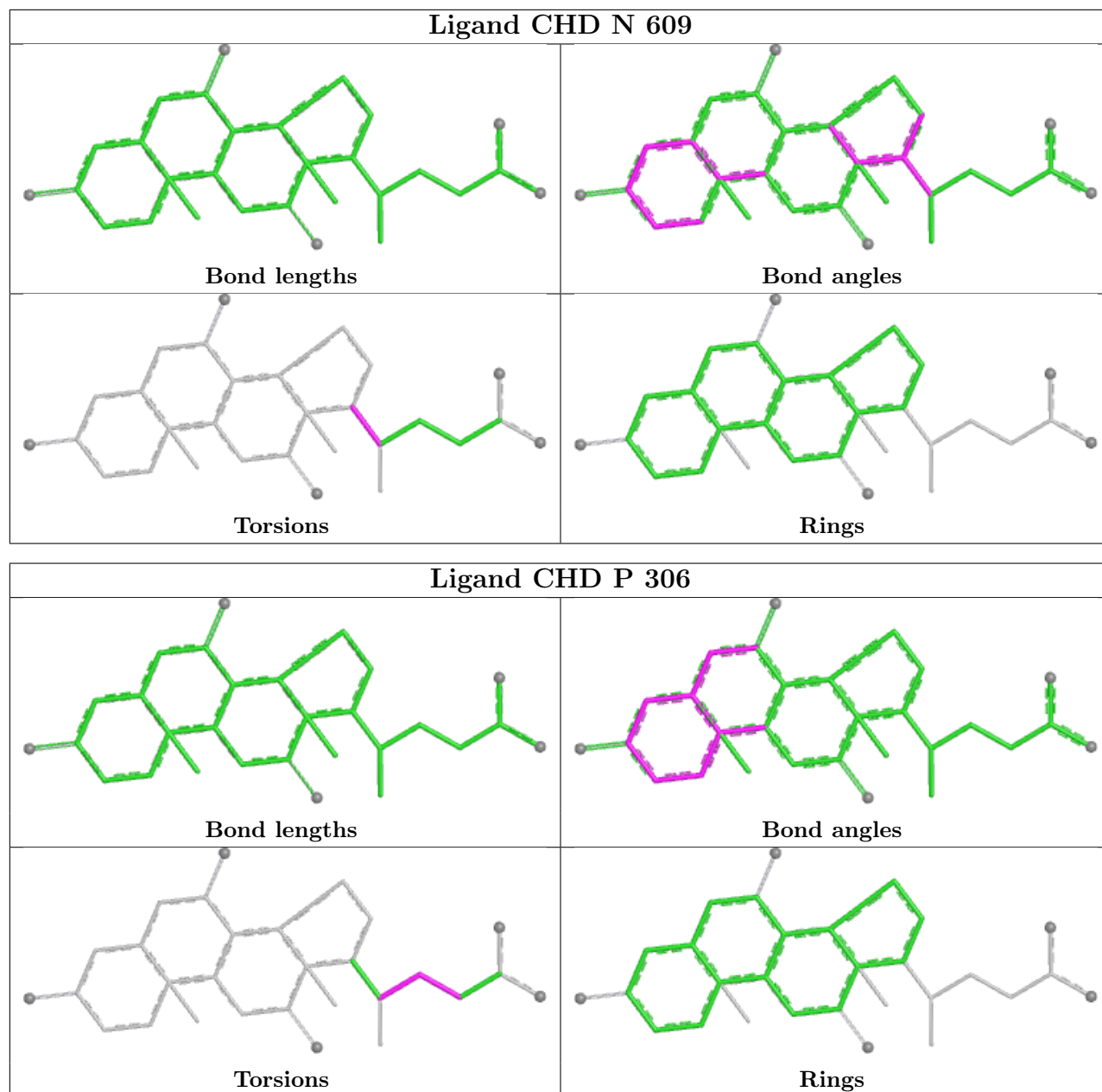


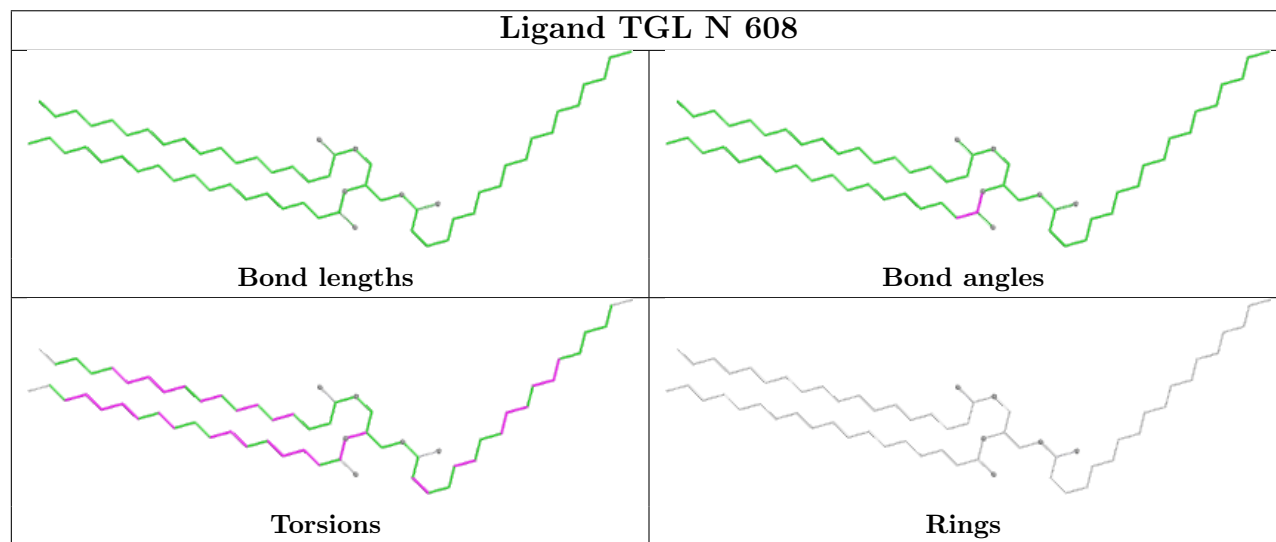
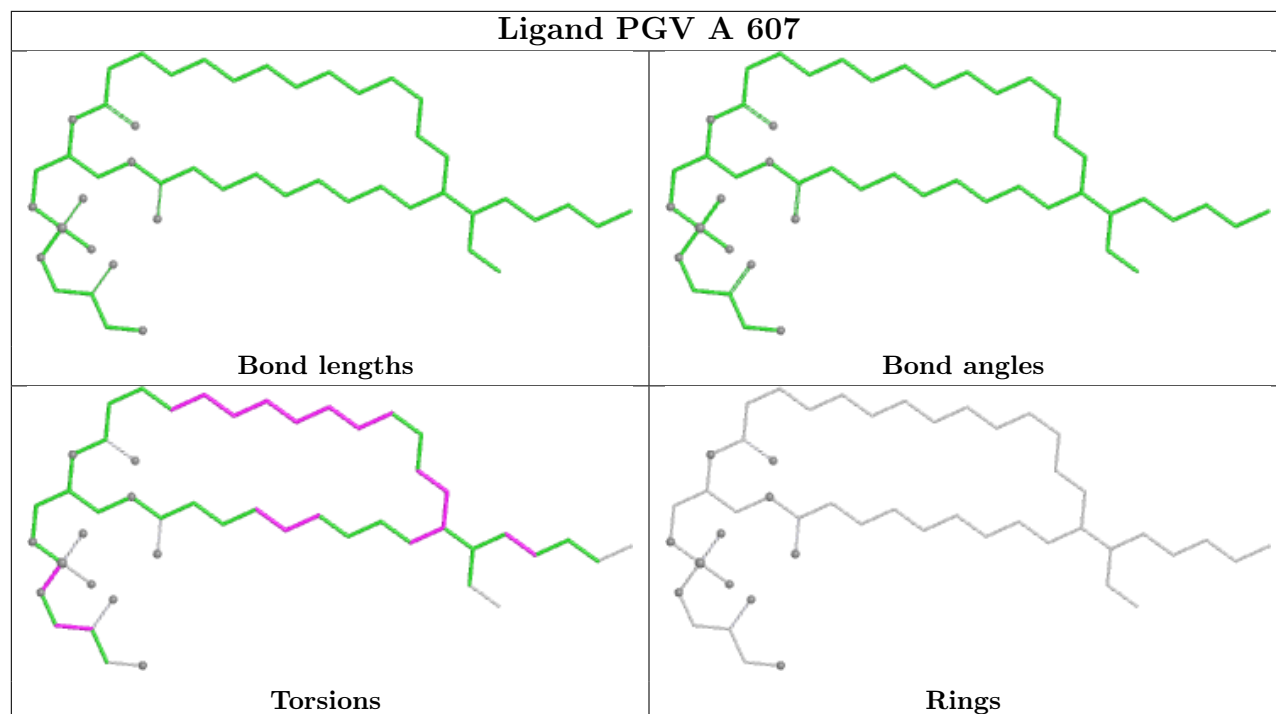


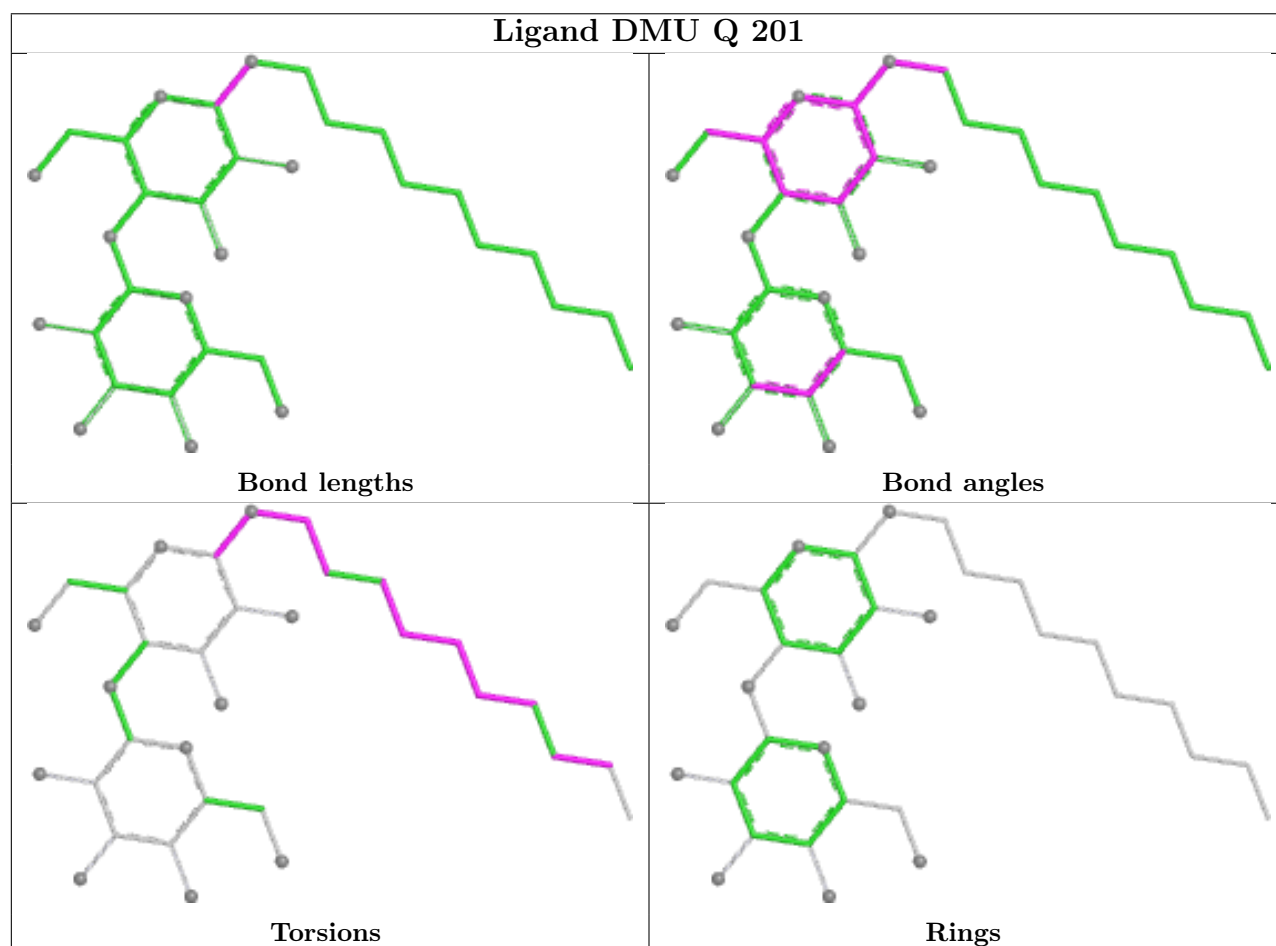
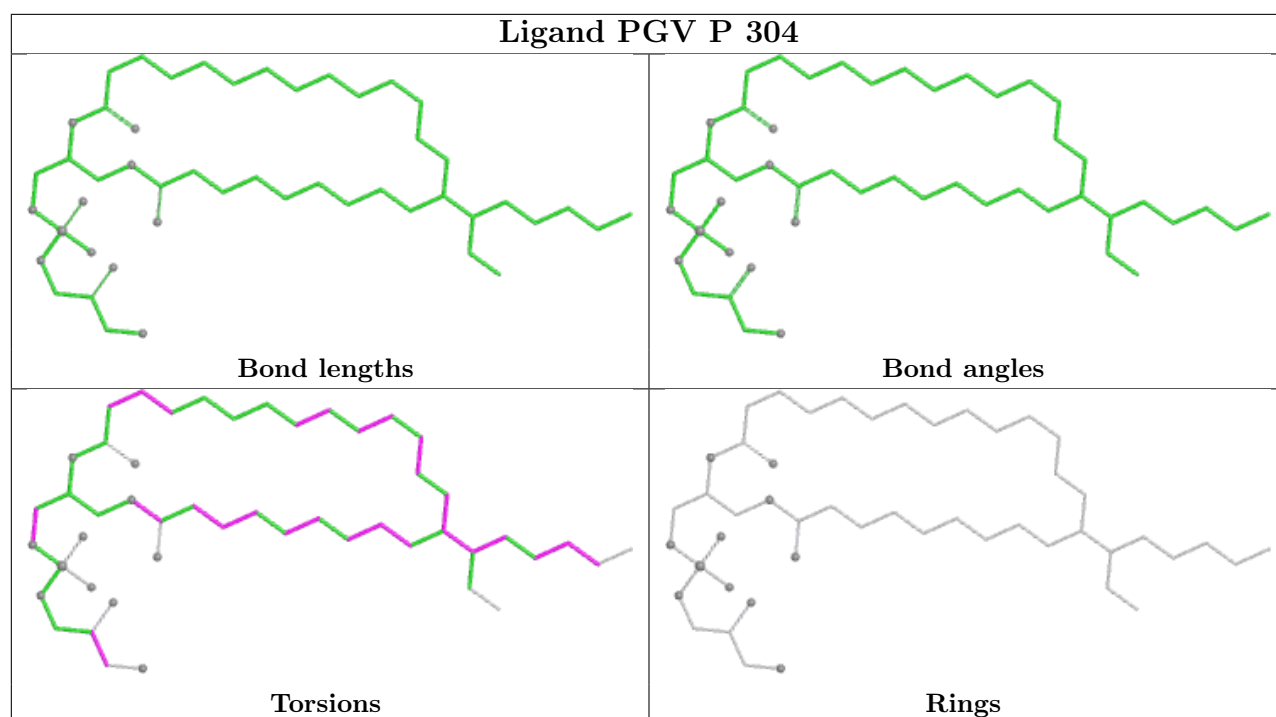


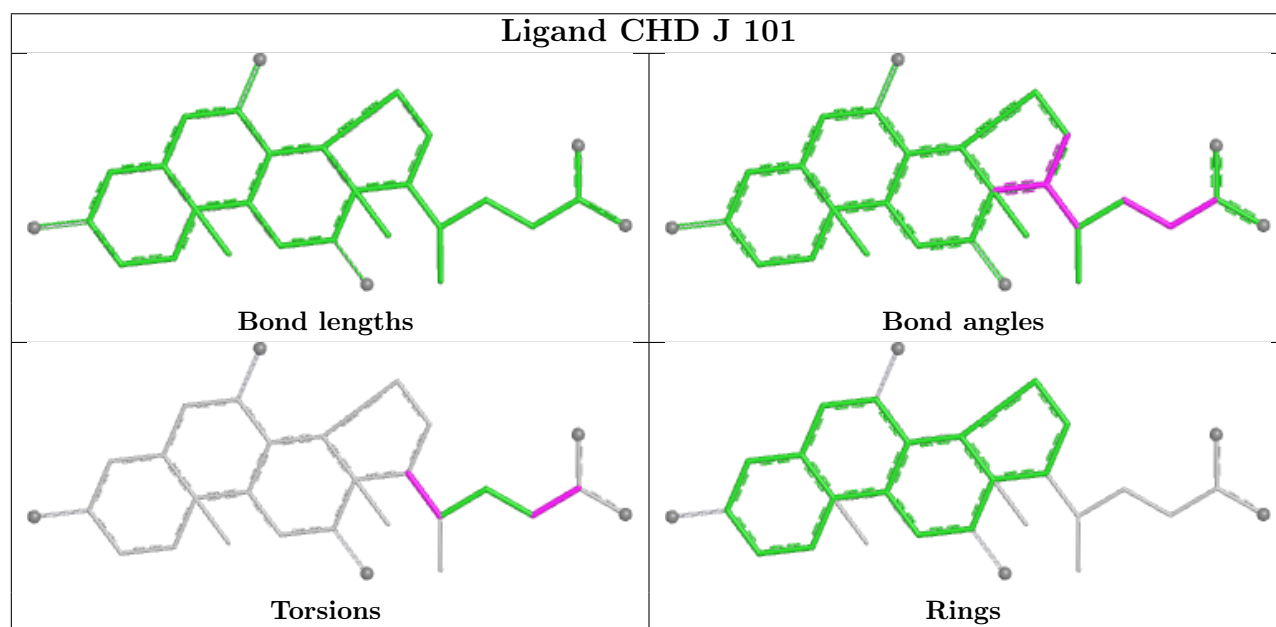
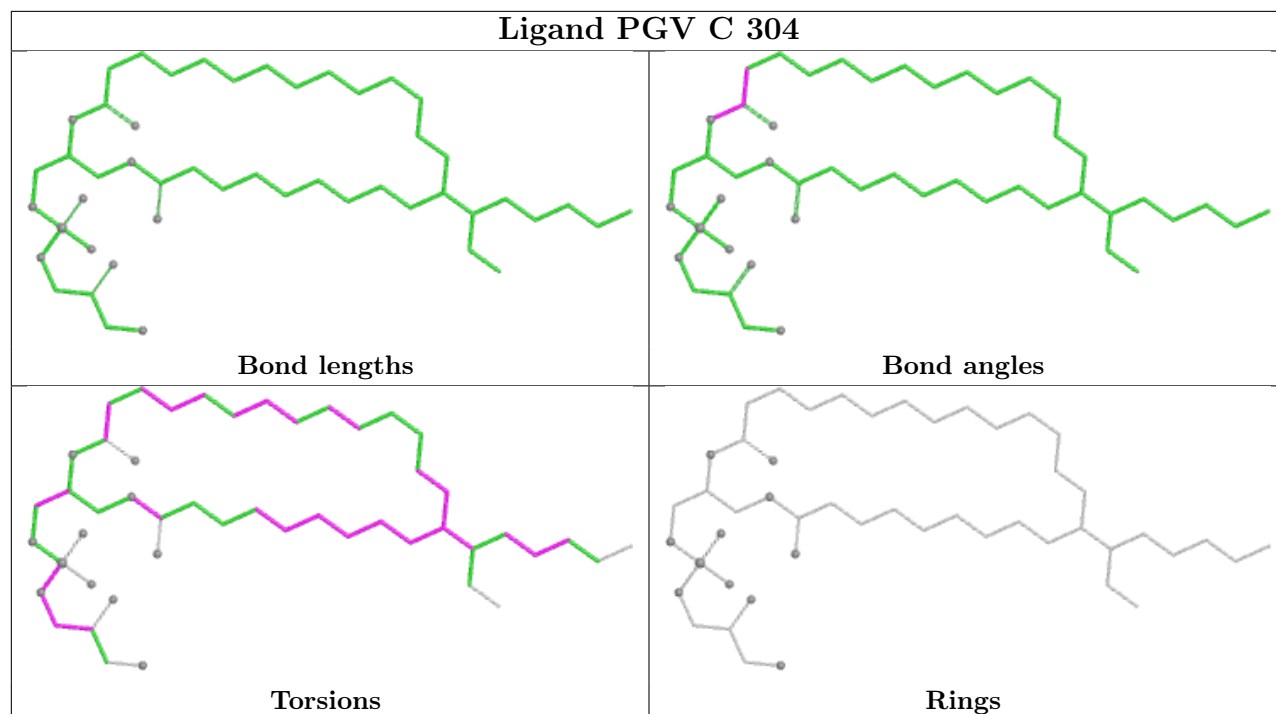


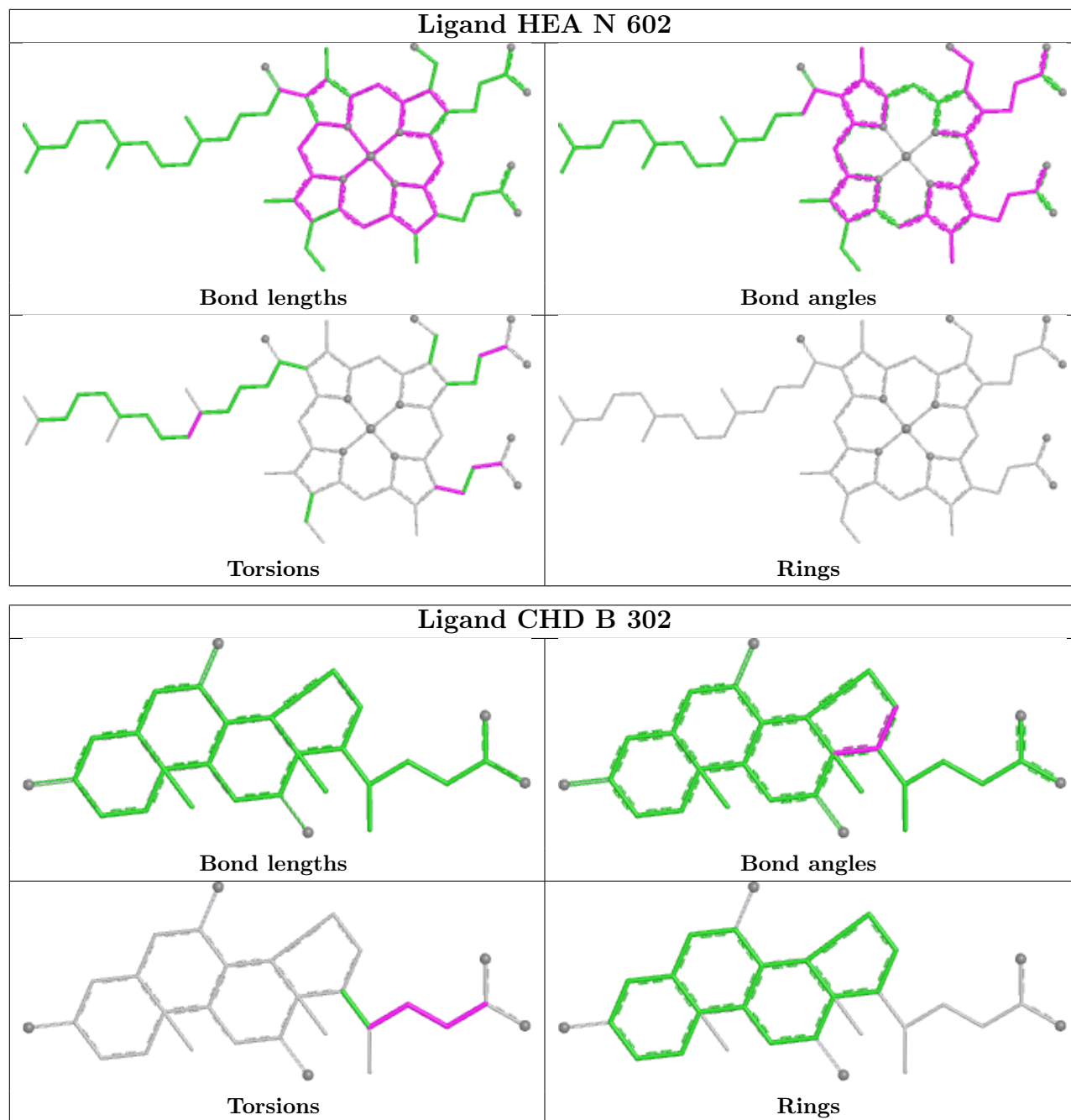


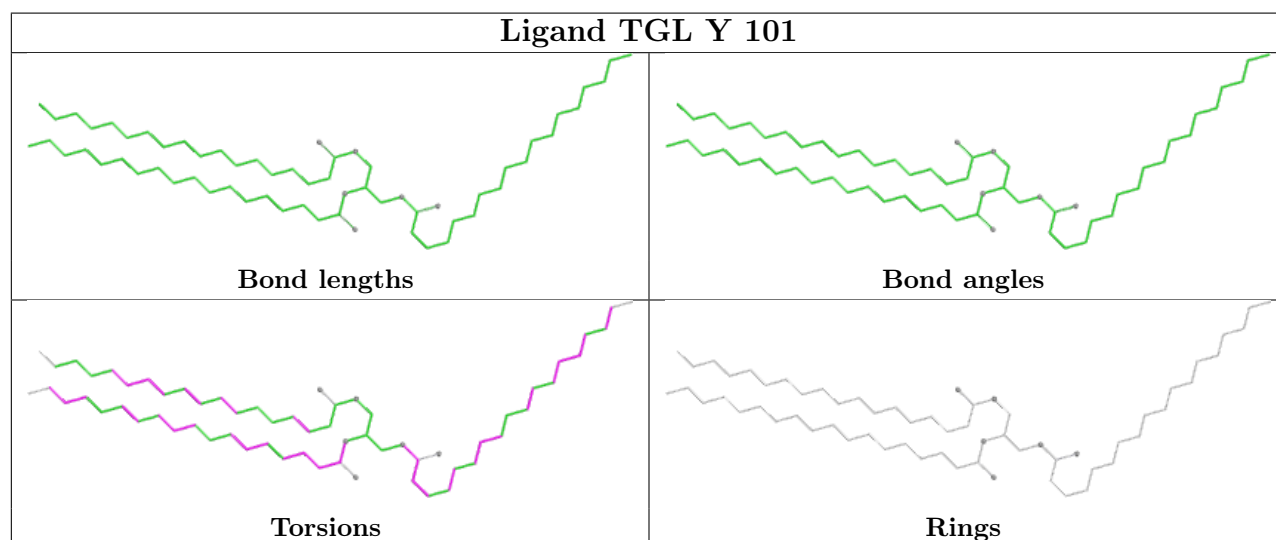
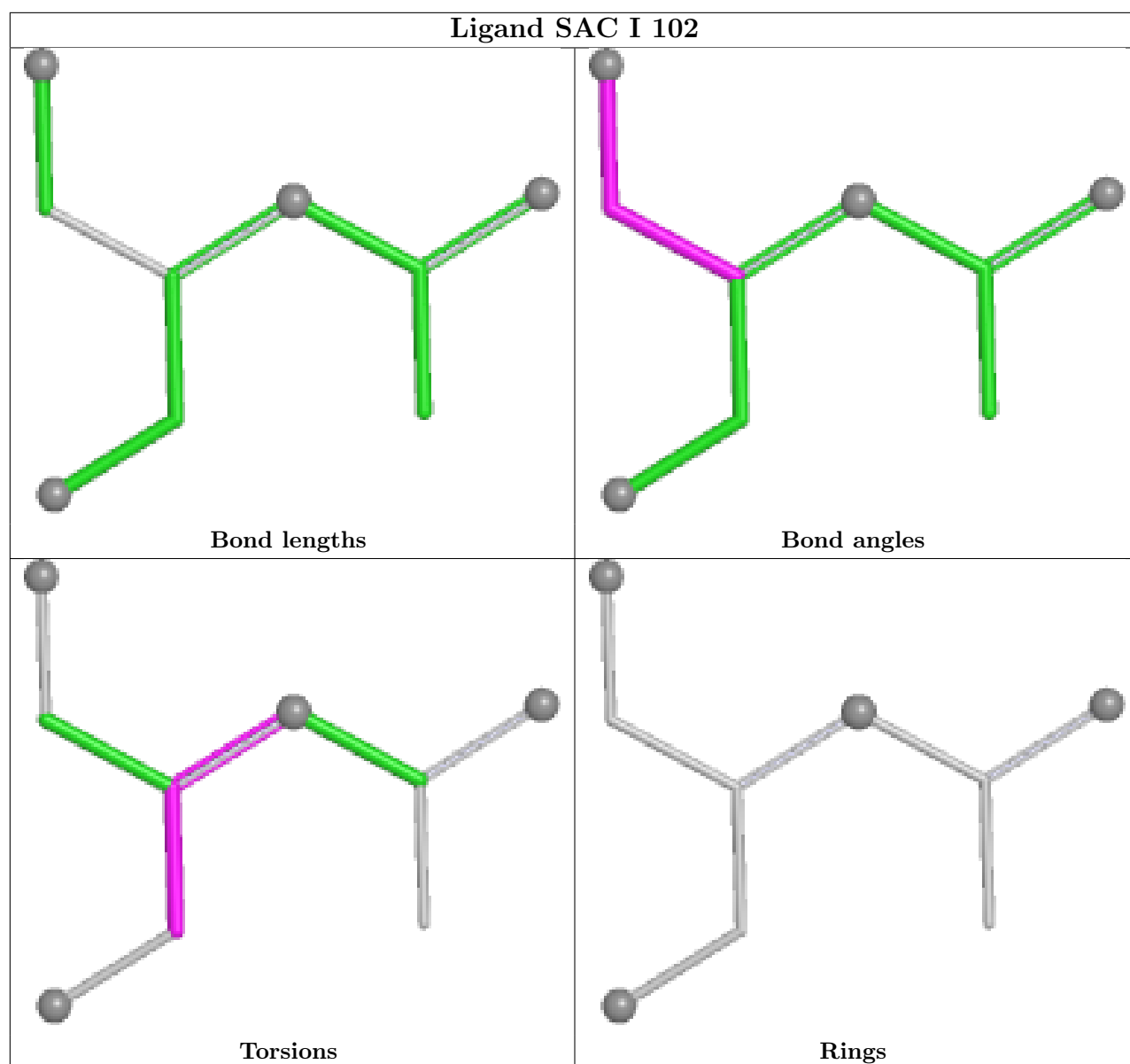


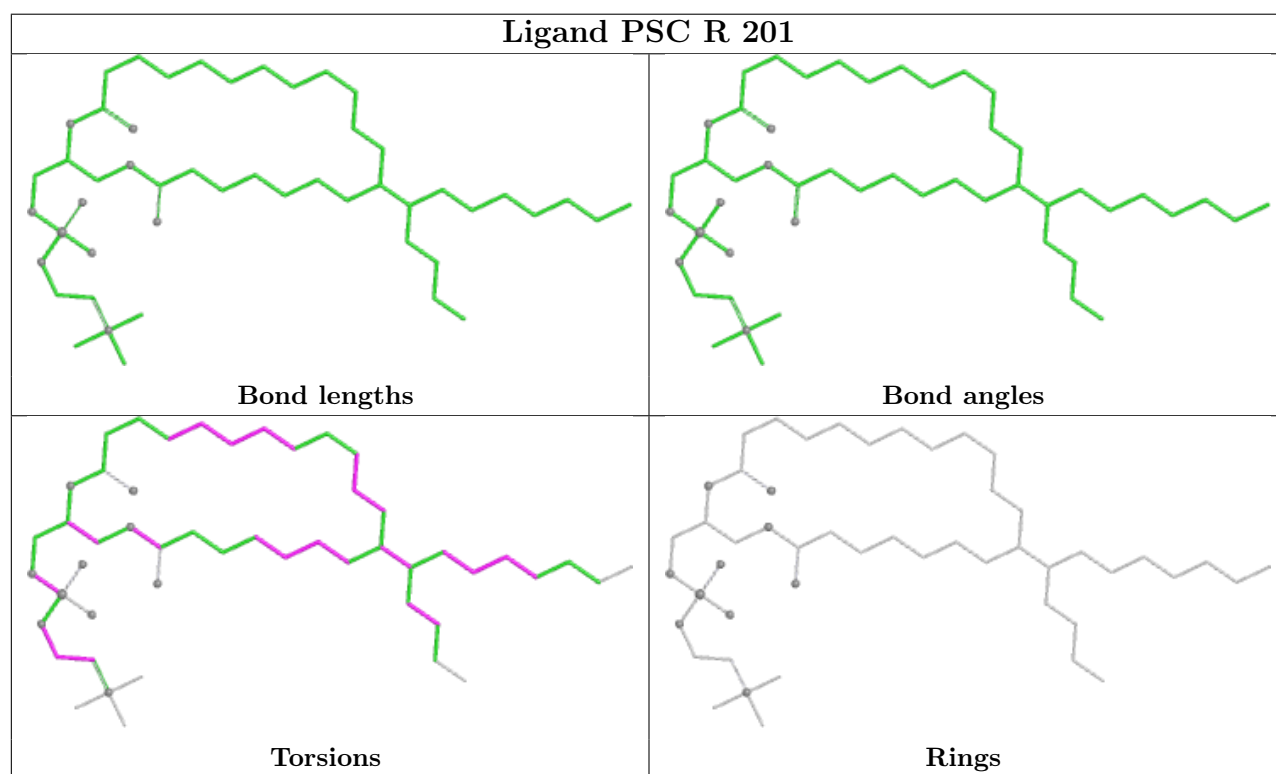
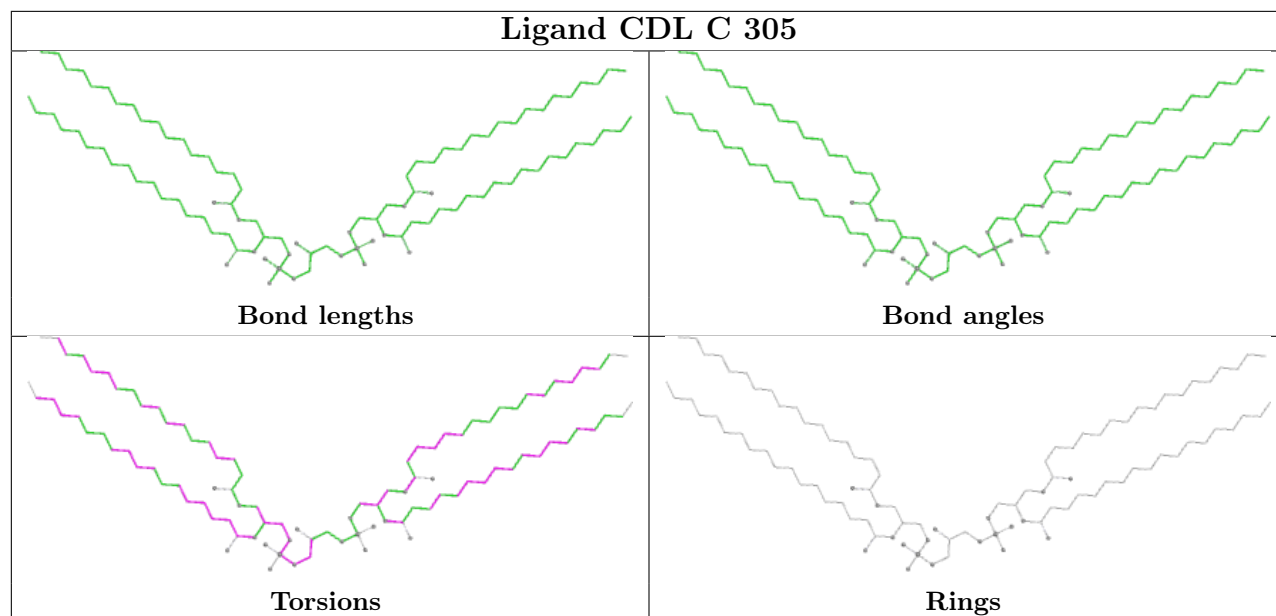


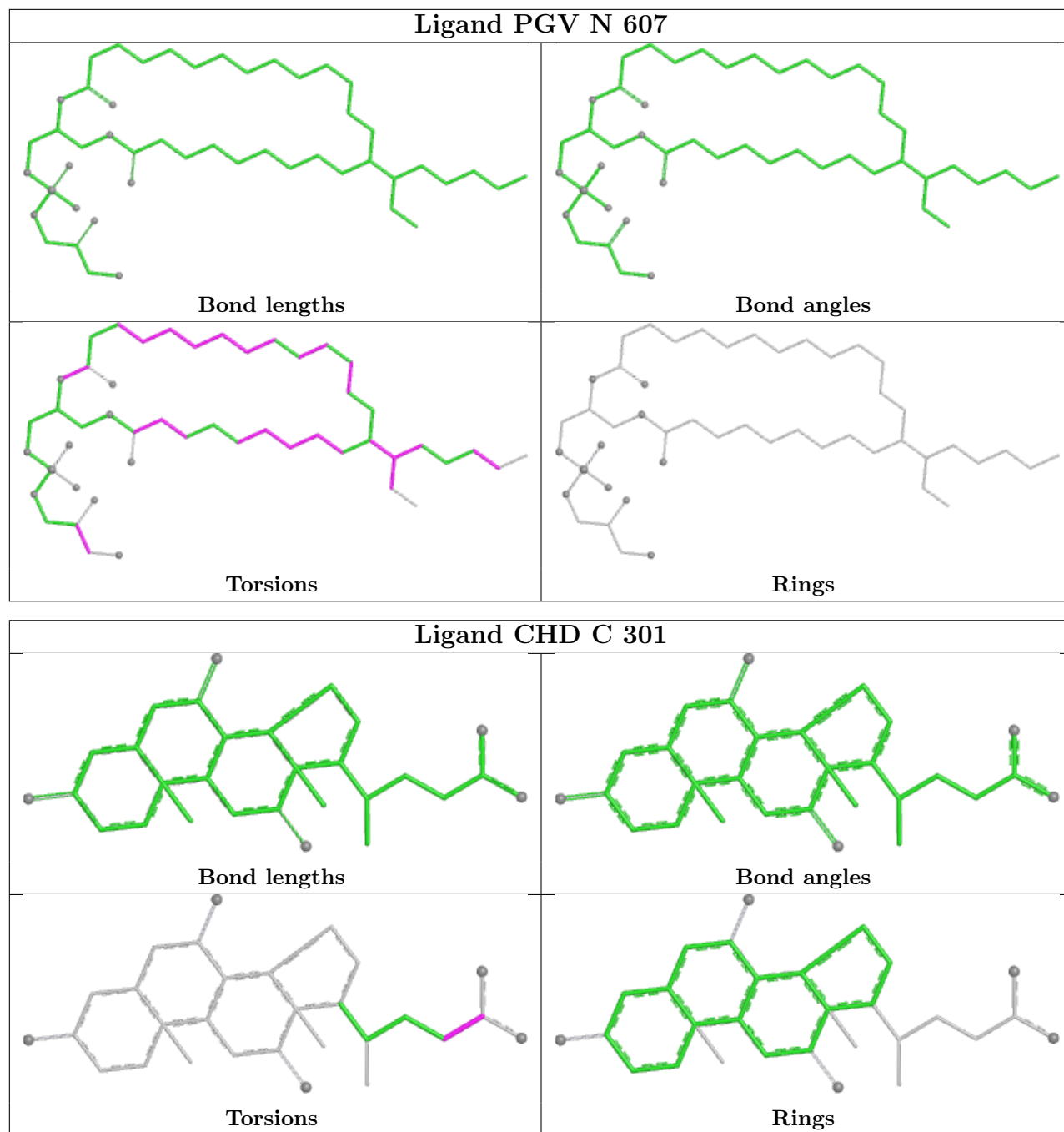




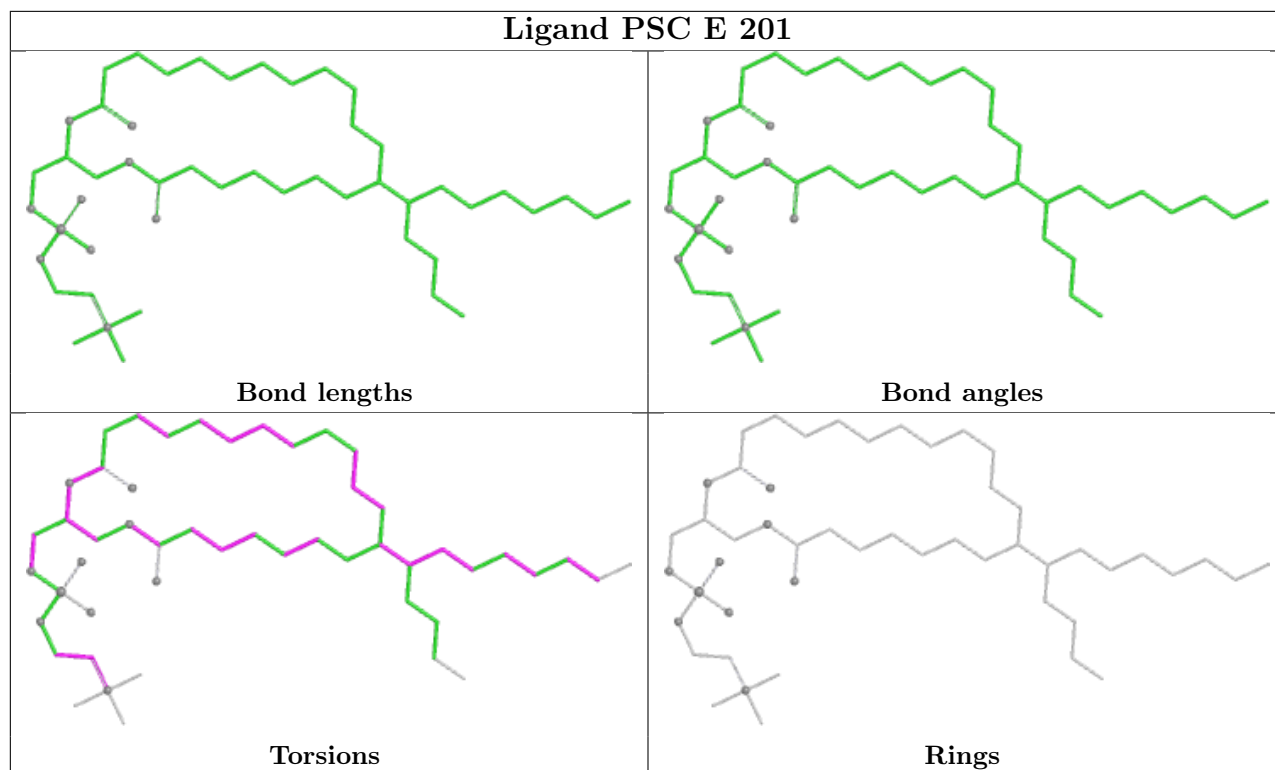




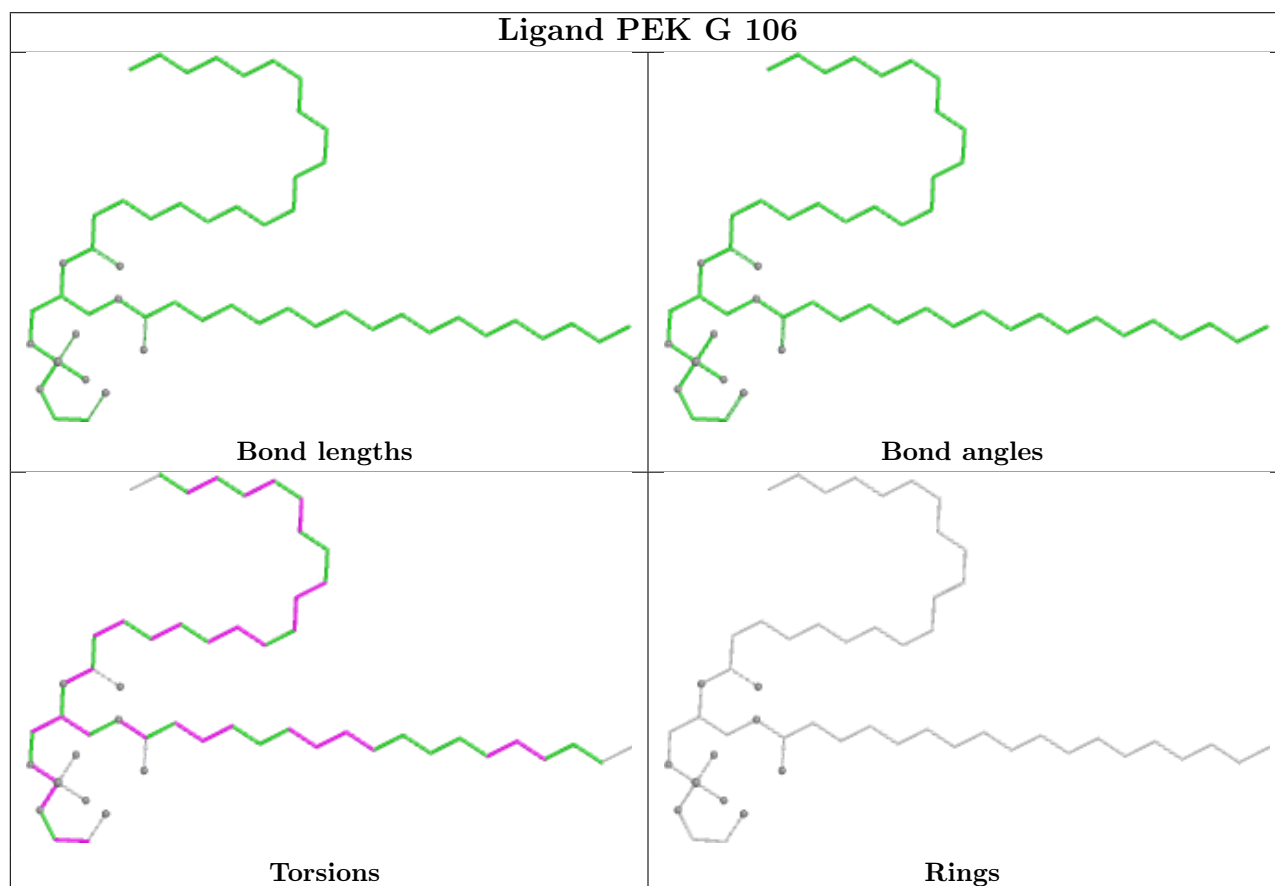


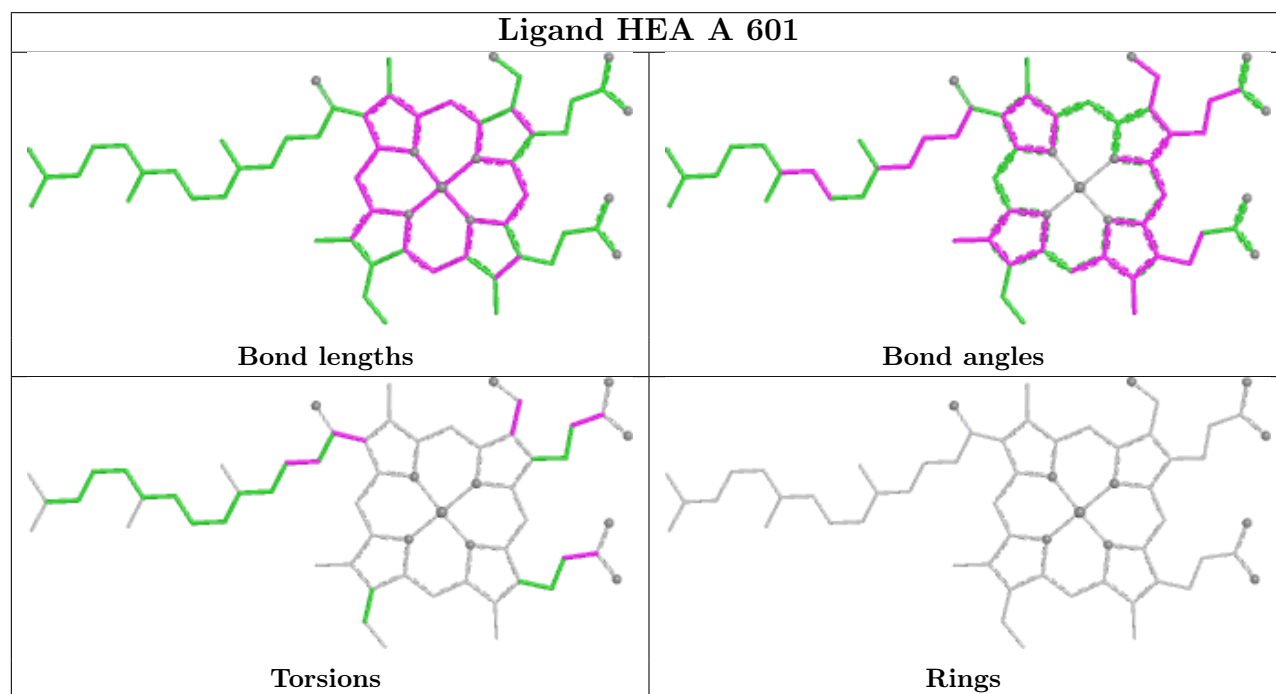
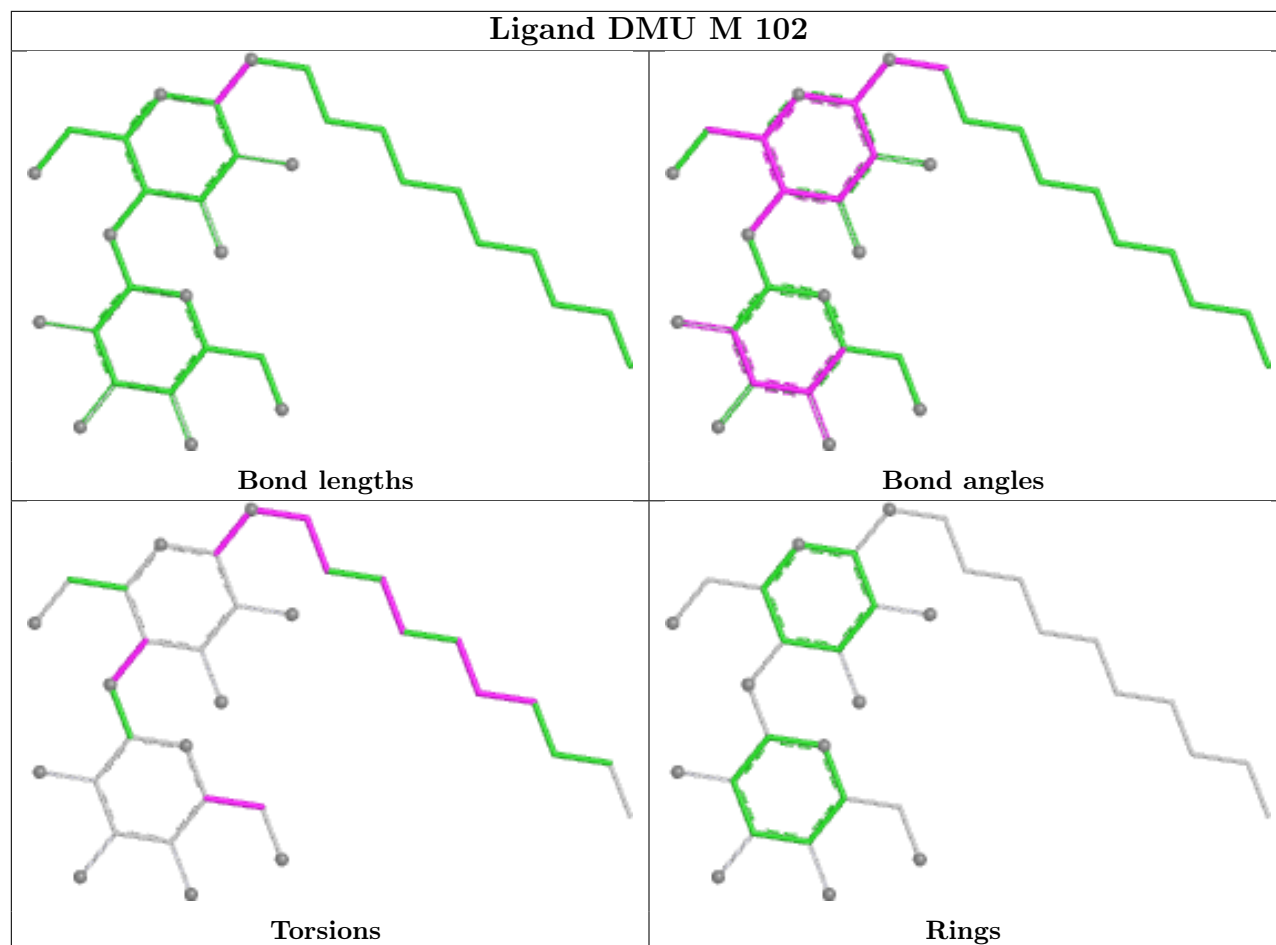


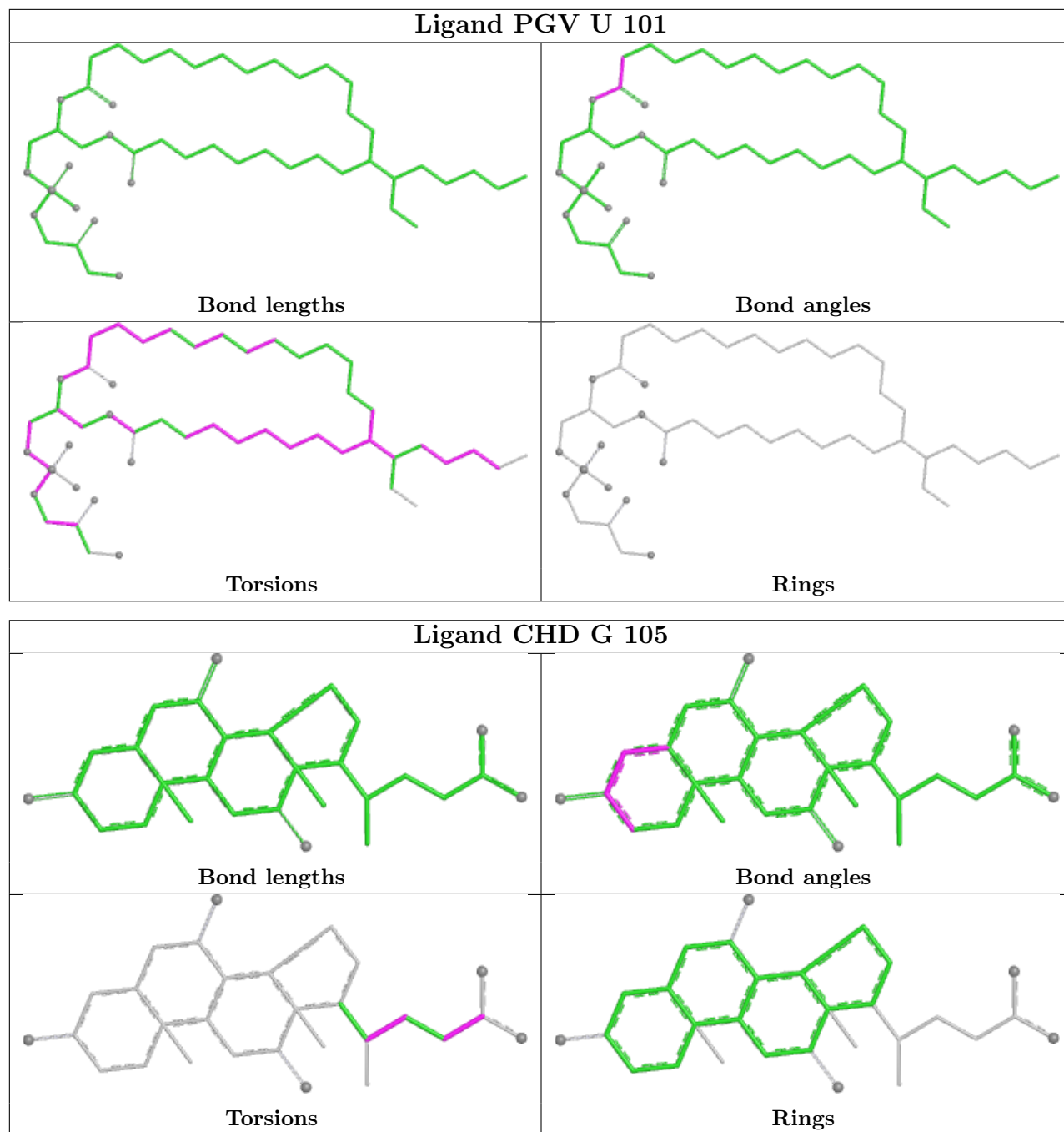
Ligand PSC E 201

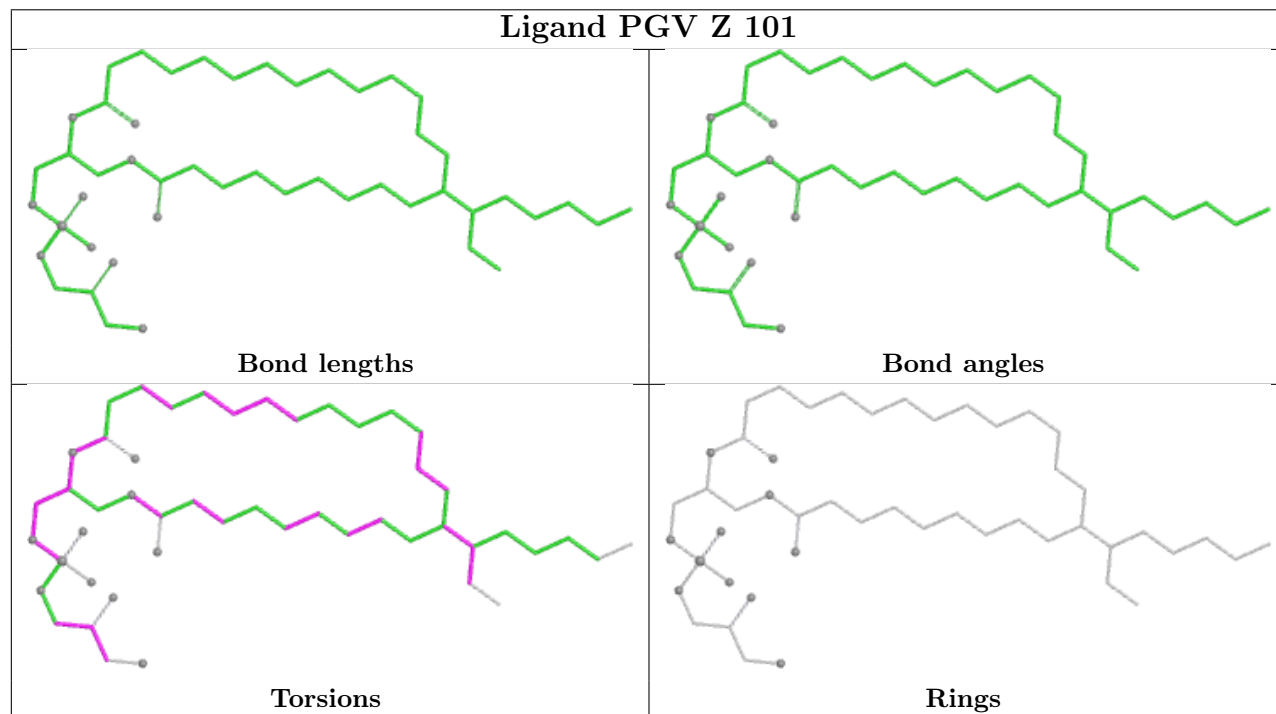
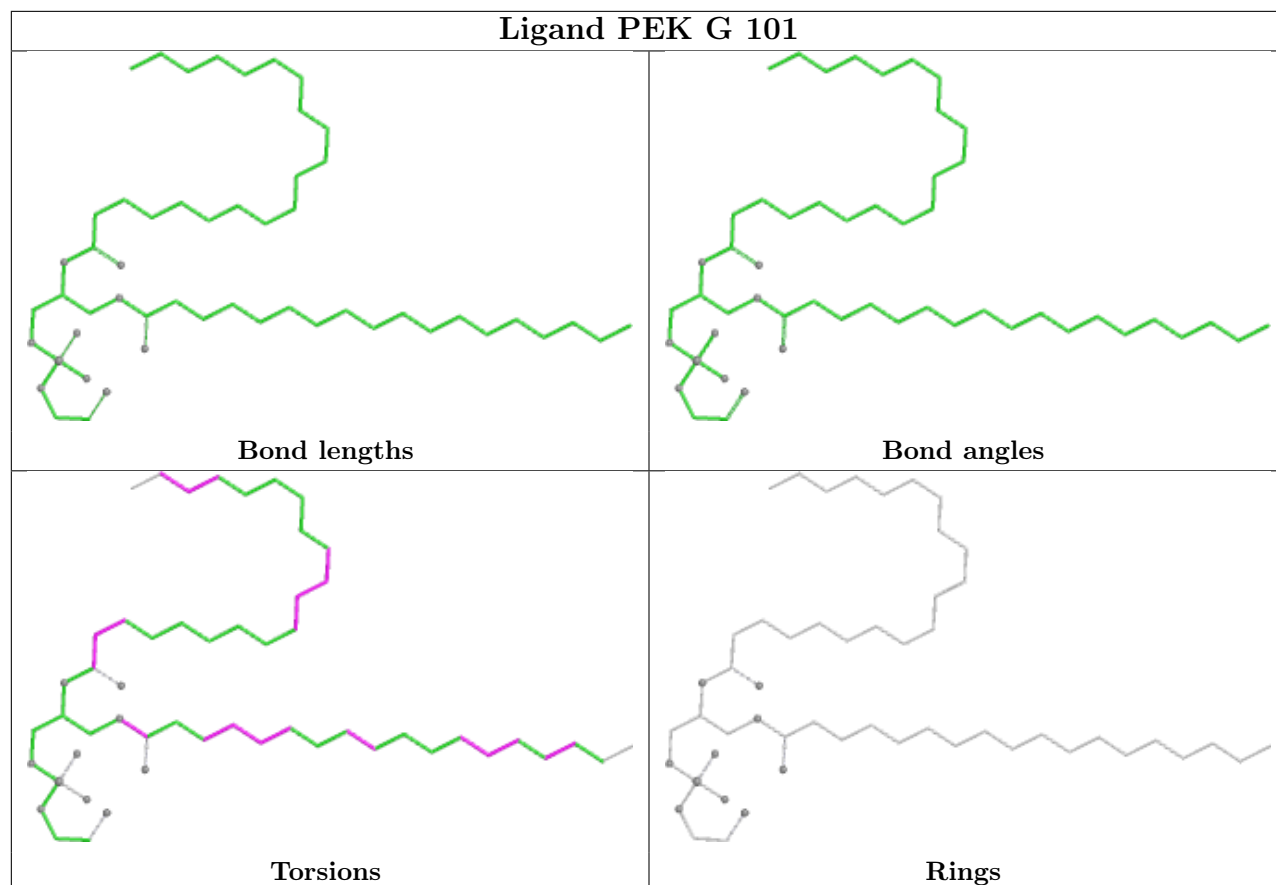


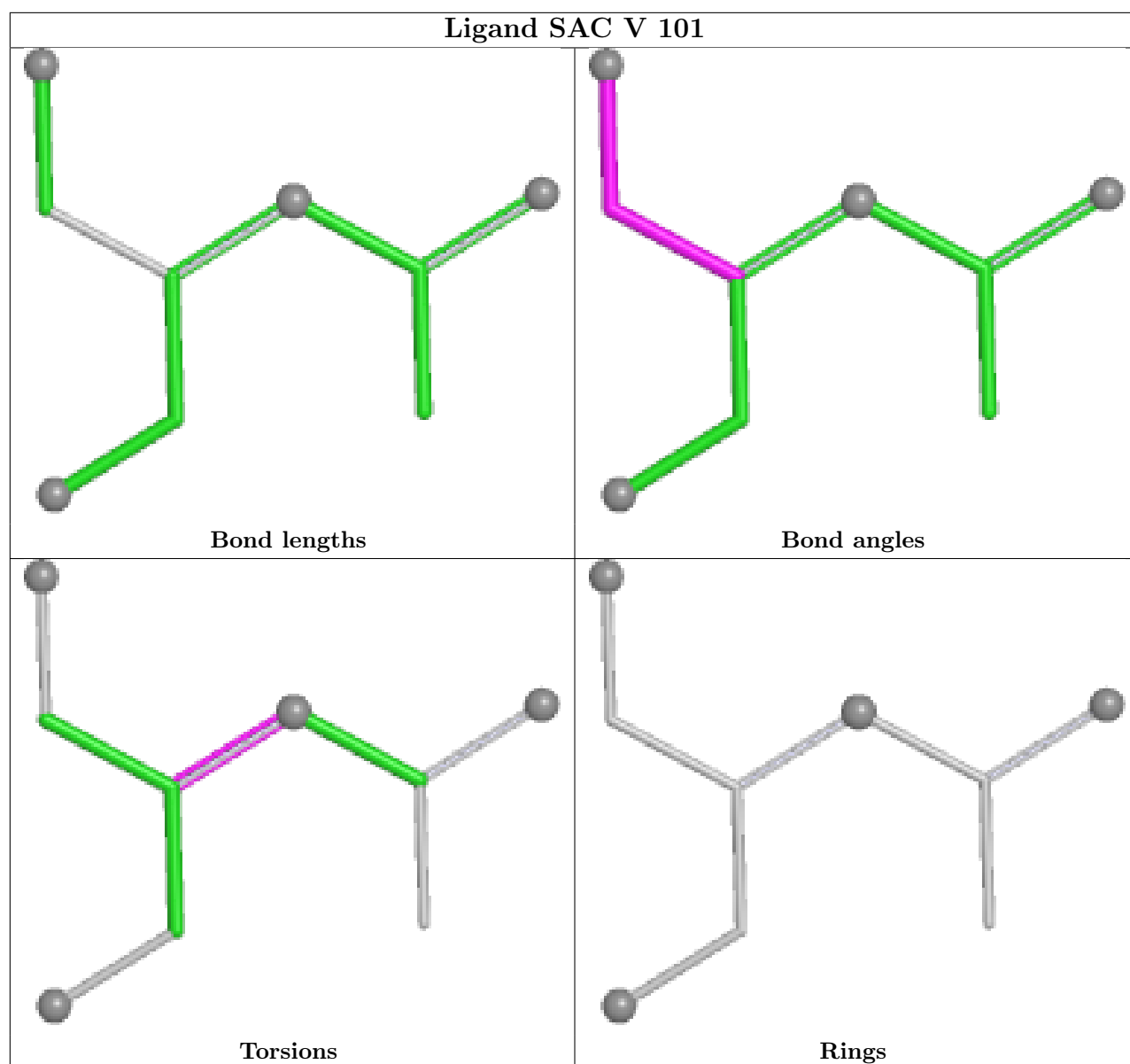
Ligand PEK G 106

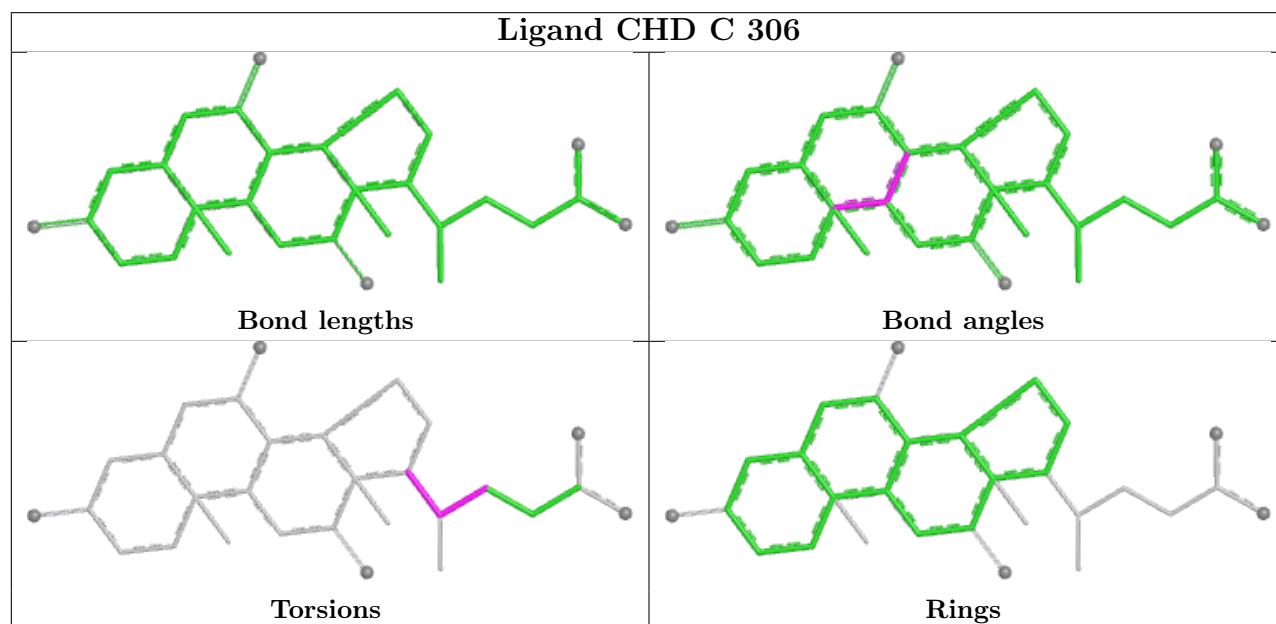
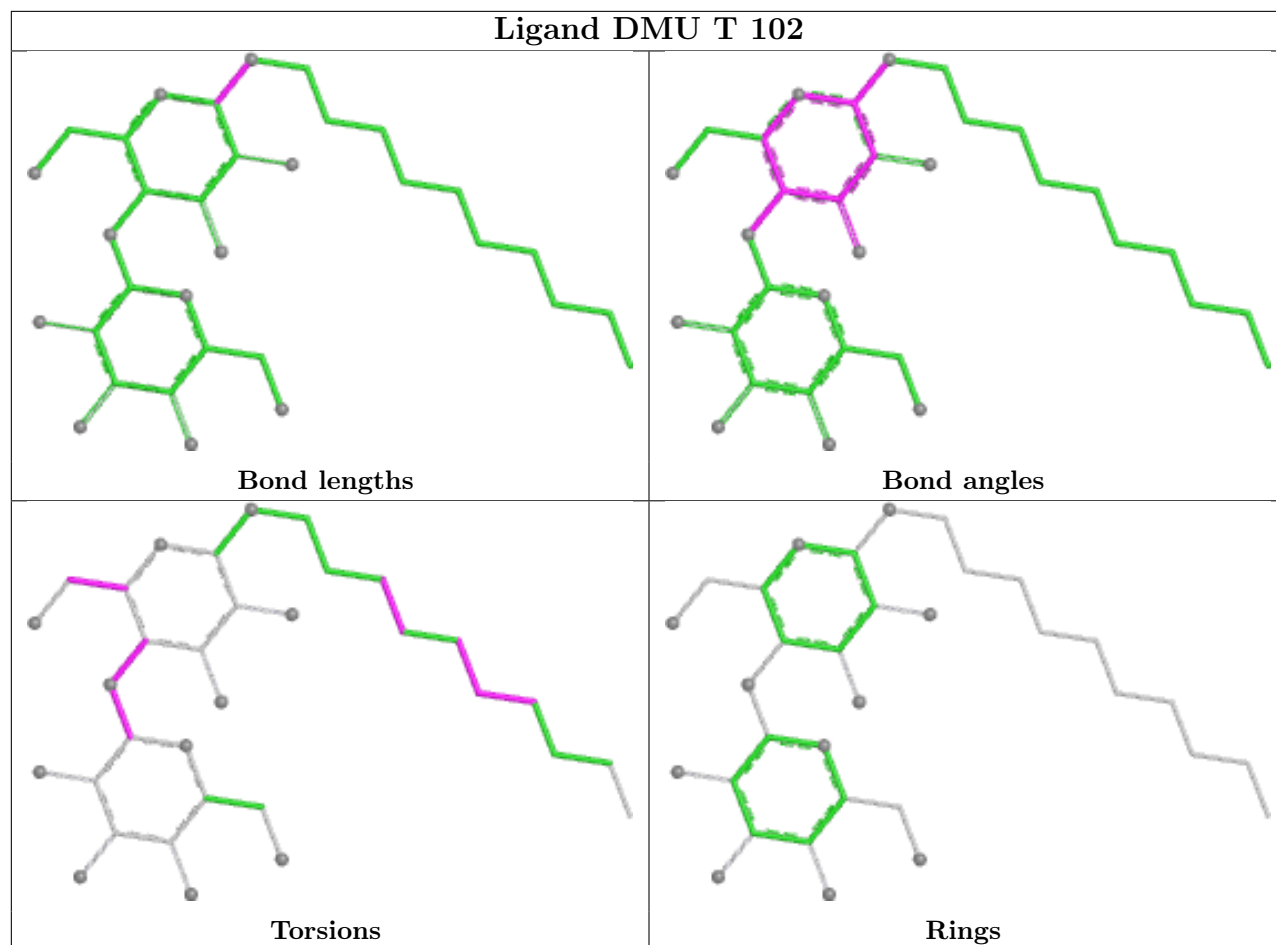


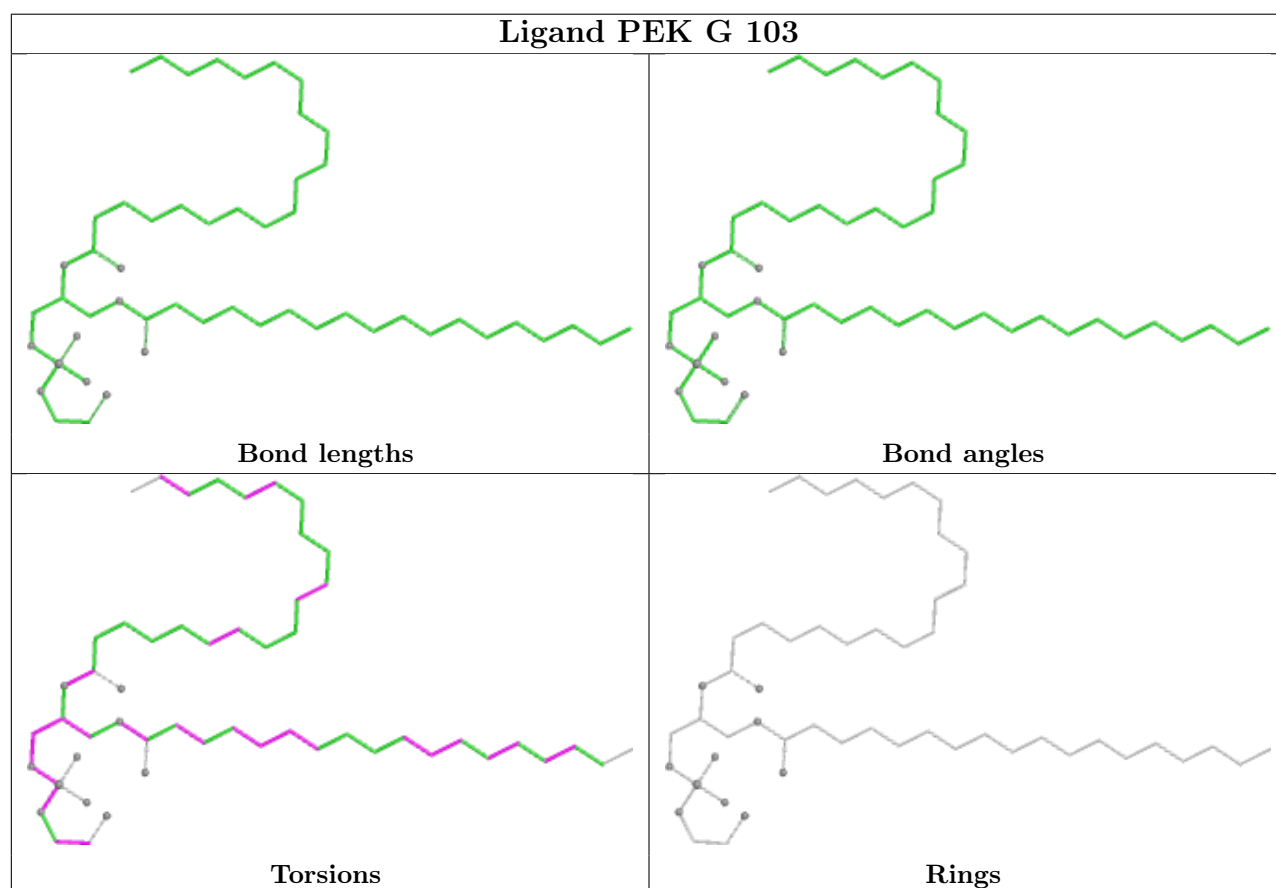
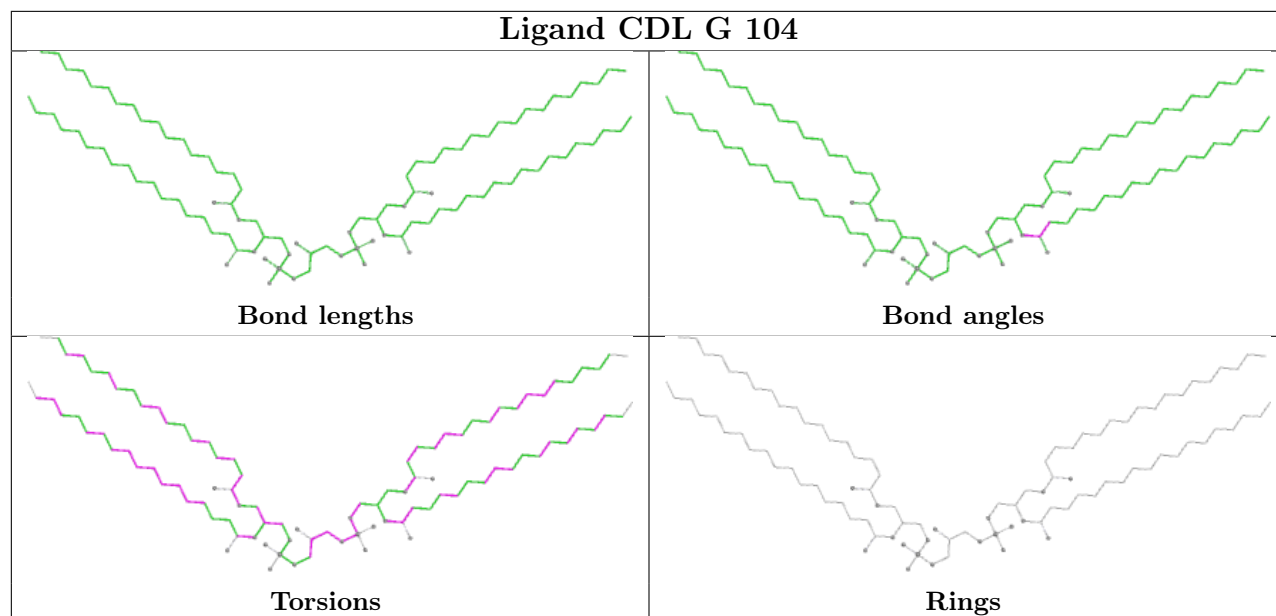


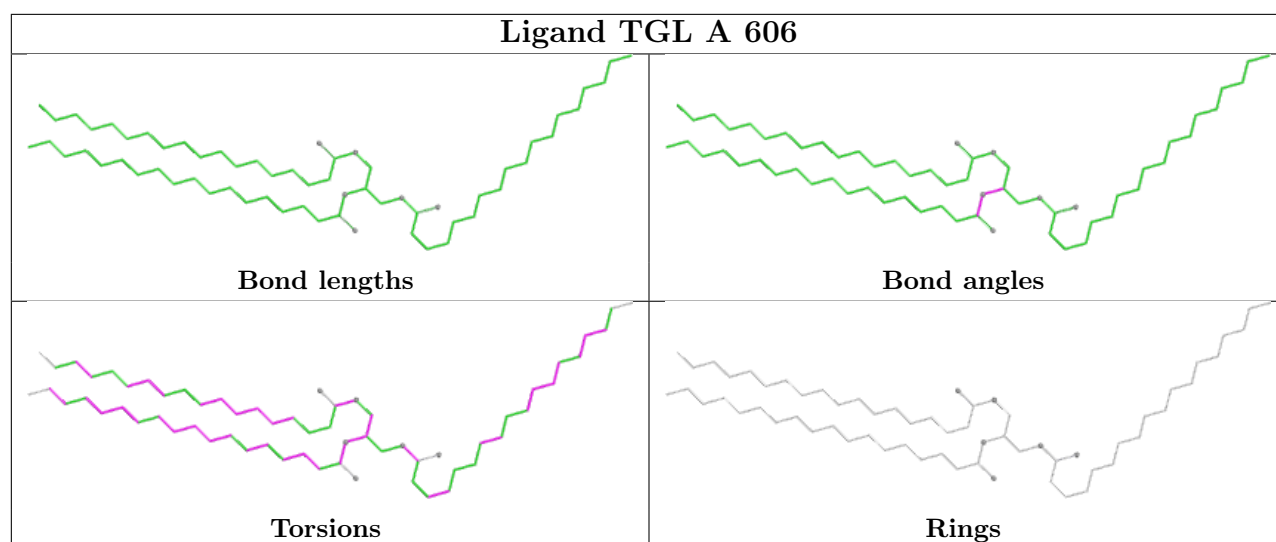












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.60	0 100 100	27, 39, 52, 90	0
1	N	513/514 (99%)	-0.29	1 (0%) 91 88	37, 52, 69, 92	0
2	B	226/227 (99%)	-0.35	4 (1%) 67 58	32, 47, 75, 138	0
2	O	226/227 (99%)	-0.04	3 (1%) 75 66	42, 63, 94, 133	0
3	C	259/261 (99%)	-0.49	0 100 100	33, 45, 62, 101	0
3	P	259/261 (99%)	-0.29	1 (0%) 88 84	37, 54, 78, 112	0
4	D	144/147 (97%)	-0.48	0 100 100	40, 50, 76, 98	0
4	Q	144/147 (97%)	0.16	5 (3%) 47 38	54, 75, 108, 166	0
5	E	105/109 (96%)	-0.50	0 100 100	36, 50, 82, 135	0
5	R	105/109 (96%)	-0.18	1 (0%) 79 72	47, 68, 89, 118	0
6	F	98/98 (100%)	-0.09	6 (6%) 27 20	38, 55, 121, 165	0
6	S	98/98 (100%)	0.07	6 (6%) 27 20	46, 64, 138, 178	0
7	G	83/85 (97%)	0.36	14 (16%) 4 3	39, 55, 142, 158	0
7	T	83/85 (97%)	0.39	13 (15%) 5 4	44, 67, 146, 162	0
8	H	79/85 (92%)	0.01	4 (5%) 33 25	42, 58, 119, 149	0
8	U	79/85 (92%)	0.20	2 (2%) 58 48	49, 72, 132, 149	0
9	I	72/73 (98%)	-0.20	1 (1%) 73 64	45, 58, 90, 101	0
9	V	72/73 (98%)	0.13	3 (4%) 40 32	51, 76, 104, 122	0
10	J	58/59 (98%)	-0.22	1 (1%) 69 60	44, 58, 94, 122	0
10	W	58/59 (98%)	0.24	2 (3%) 48 39	55, 73, 111, 142	0
11	K	49/56 (87%)	-0.41	1 (2%) 65 56	45, 56, 74, 101	0
11	X	49/56 (87%)	-0.01	0 100 100	54, 78, 97, 110	0
12	L	46/47 (97%)	-0.48	1 (2%) 62 52	36, 47, 73, 108	0
12	Y	46/47 (97%)	0.17	1 (2%) 62 52	51, 69, 105, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.38	0 100 100	34, 49, 87, 132	0
13	Z	43/46 (93%)	0.06	0 100 100	58, 71, 108, 147	0
All	All	3550/3614 (98%)	-0.24	70 (1%) 65 56	27, 54, 96, 178	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	10	GLY	6.1
6	S	97	ALA	5.8
7	G	5	LYS	5.8
7	G	2	SER	5.3
7	T	3	ALA	5.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	G	11	11/12	0.68	0.17	130,155,173,179	0
7	TPO	T	11	11/12	0.70	0.16	128,139,156,165	0
1	FME	N	1	10/11	0.79	0.19	85,93,132,138	0
1	FME	A	1	10/11	0.91	0.12	62,73,99,106	0
2	FME	O	1	10/11	0.96	0.10	50,65,73,73	0
2	FME	B	1	10/11	0.96	0.11	49,51,53,61	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($\text{\AA}^2$)	Q<0.9
29	SAC	V	101	9/10	0.52	0.14	106,135,145,154	0
28	DMU	T	102	33/33	0.68	0.21	94,128,165,185	0
16	MG	A	604	1/1	0.69	0.13	47,47,47,47	0
29	SAC	I	102	9/10	0.73	0.16	117,130,135,138	0
28	DMU	G	102	33/33	0.73	0.19	73,155,175,175	0
19	PGV	C	304	51/51	0.78	0.23	75,99,134,148	0
27	PEK	G	106	53/53	0.78	0.24	65,140,205,219	0
18	TGL	N	606	63/63	0.79	0.27	79,107,126,129	0
27	PEK	T	103	53/53	0.79	0.24	73,135,200,205	0
19	PGV	U	101	51/51	0.82	0.23	74,112,145,159	0
19	PGV	Z	101	51/51	0.82	0.23	65,104,165,168	0
22	CHD	J	101	29/29	0.82	0.16	75,108,123,130	0
22	CHD	N	609	29/29	0.83	0.22	108,129,146,153	0
18	TGL	A	606	63/63	0.84	0.22	66,95,108,110	0
19	PGV	M	101	51/51	0.84	0.21	64,99,161,175	0
18	TGL	Y	101	63/63	0.85	0.28	70,110,161,176	0
18	TGL	L	101	63/63	0.85	0.26	57,97,131,136	0
18	TGL	I	101	63/63	0.85	0.24	39,95,134,150	0
25	PSC	E	201	52/52	0.85	0.21	64,109,198,208	0
18	TGL	N	608	63/63	0.85	0.24	47,95,138,152	0
24	CDL	C	305	100/100	0.86	0.20	70,120,150,154	0
25	PSC	R	201	52/52	0.86	0.23	78,119,219,243	0
24	CDL	P	305	100/100	0.86	0.21	68,117,159,183	0
24	CDL	T	104	100/100	0.86	0.25	72,118,184,209	0
24	CDL	G	104	100/100	0.87	0.24	90,126,183,224	0
22	CHD	C	306	29/29	0.88	0.14	75,86,97,110	0
27	PEK	G	103	53/53	0.88	0.20	85,102,150,159	0
27	PEK	T	101	53/53	0.89	0.17	61,101,157,172	0
28	DMU	Q	201	33/33	0.90	0.11	70,96,112,116	0
22	CHD	P	306	29/29	0.92	0.12	80,89,94,99	0
22	CHD	P	302	29/29	0.93	0.09	42,47,50,51	0
28	DMU	M	102	33/33	0.93	0.09	45,60,78,79	0
27	PEK	P	303	53/53	0.94	0.16	60,78,128,137	0
22	CHD	C	301	29/29	0.94	0.08	35,38,41,41	0
17	NA	N	605	1/1	0.94	0.09	63,63,63,63	0
27	PEK	G	101	53/53	0.96	0.14	43,69,117,125	0
19	PGV	P	304	51/51	0.96	0.13	42,57,136,153	0
22	CHD	G	105	29/29	0.96	0.09	42,45,51,54	0
23	OH	C	302[H]	1/1	0.96	0.06	24,24,24,24	0
19	PGV	C	303	51/51	0.97	0.11	35,50,110,115	0
14	HEA	N	601	60/60	0.97	0.10	39,48,61,72	0
19	PGV	A	607	51/51	0.97	0.10	34,54,72,86	0
22	CHD	B	302	29/29	0.97	0.07	36,45,51,62	0

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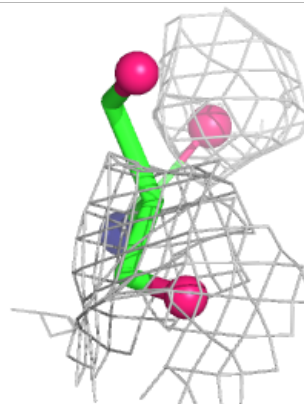
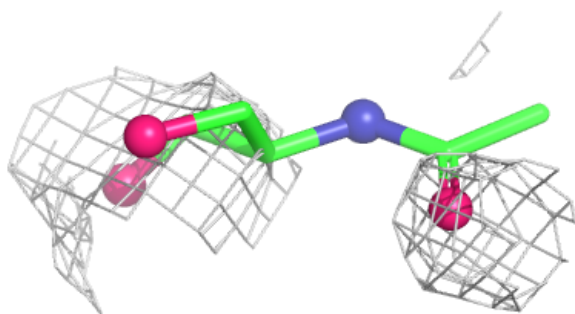
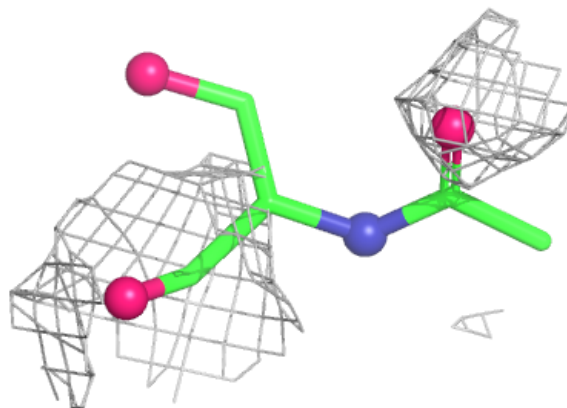
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	PGV	N	607	51/51	0.97	0.10	45,63,74,85	0
17	NA	A	605	1/1	0.98	0.06	38,38,38,38	0
14	HEA	A	601	60/60	0.98	0.07	27,36,56,59	0
14	HEA	N	602	60/60	0.98	0.07	34,39,55,56	0
14	HEA	A	602	60/60	0.98	0.06	24,34,48,55	0
16	MG	N	604	1/1	0.98	0.07	39,39,39,39	0
23	OH	P	301[H]	1/1	0.98	0.04	24,24,24,24	0
20	CMO	A	608	2/2	0.99	0.08	33,33,33,36	0
20	CMO	N	610	2/2	0.99	0.10	56,56,56,56	0
21	CUA	B	301	2/2	0.99	0.03	41,41,41,46	0
21	CUA	O	301	2/2	0.99	0.03	62,62,62,63	0
15	CU	N	603	1/1	0.99	0.04	55,55,55,55	0
26	ZN	S	101	1/1	0.99	0.03	67,67,67,67	0
26	ZN	F	101	1/1	1.00	0.02	67,67,67,67	0
15	CU	A	603	1/1	1.00	0.03	44,44,44,44	0

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

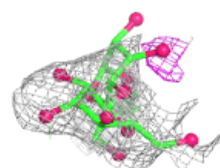
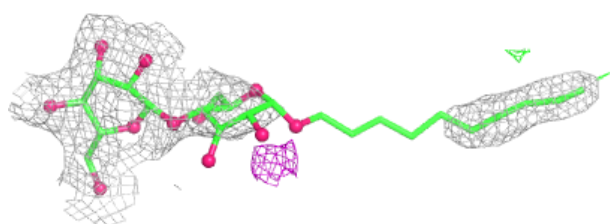
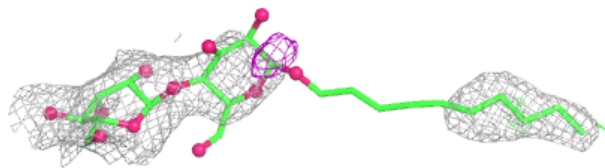
Electron density around SAC V 101:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



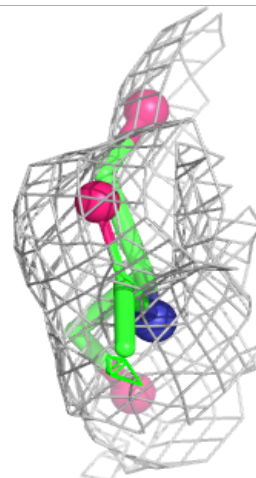
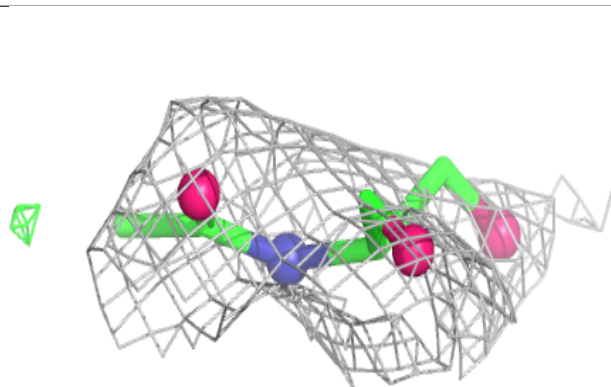
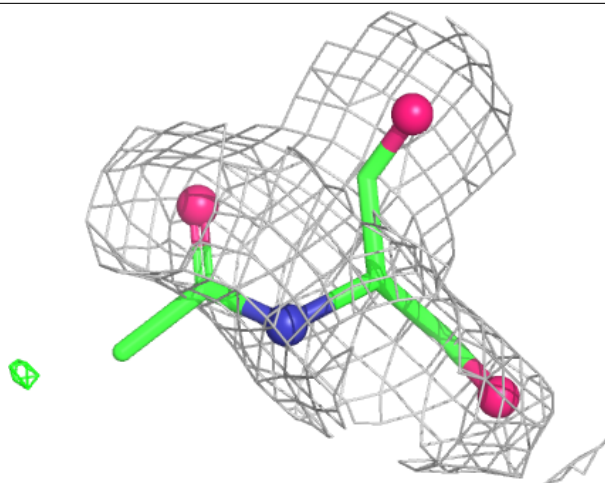
Electron density around DMU T 102:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



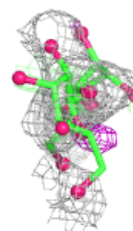
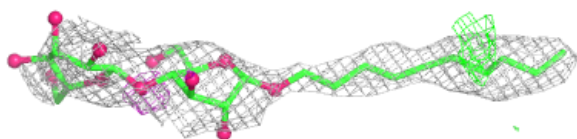
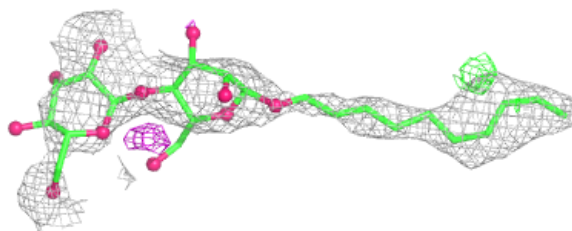
Electron density around SAC I 102:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

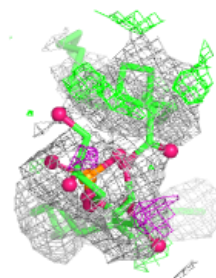
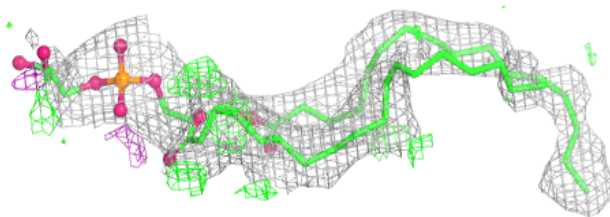
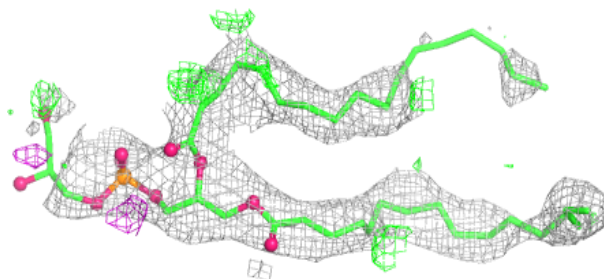


Electron density around DMU G 102:

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and green (positive)

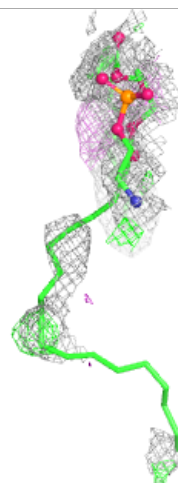
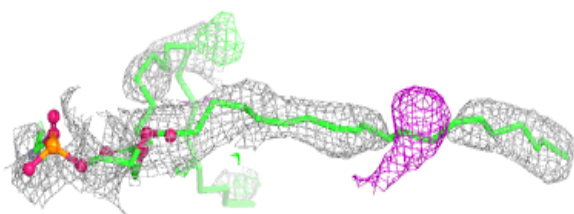
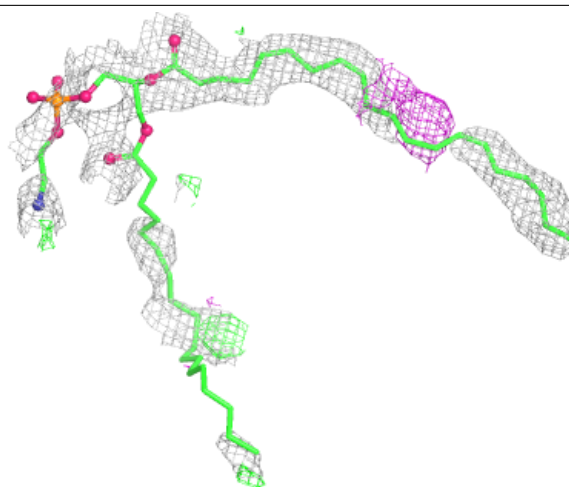
**Electron density around PGV C 304:**

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and green (positive)



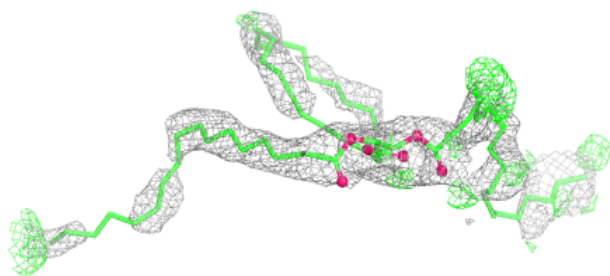
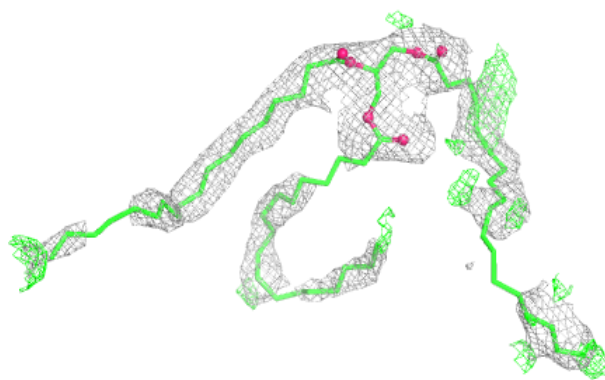
Electron density around PEK G 106:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



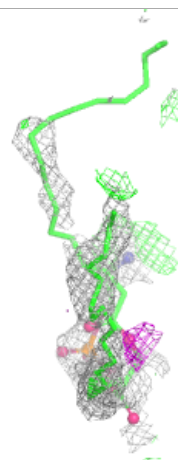
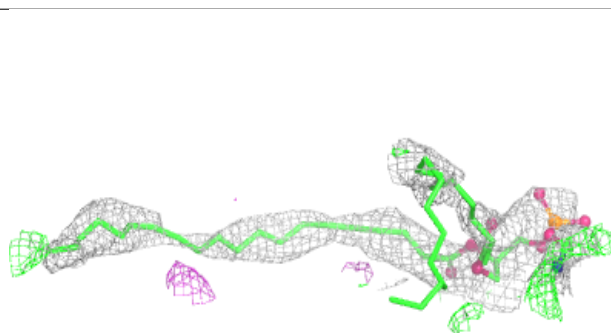
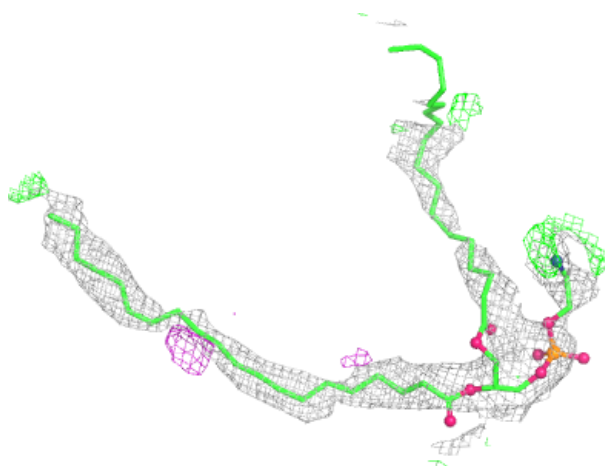
Electron density around TGL N 606:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



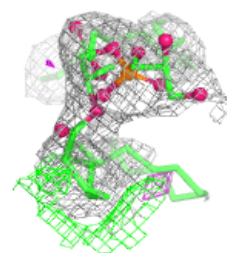
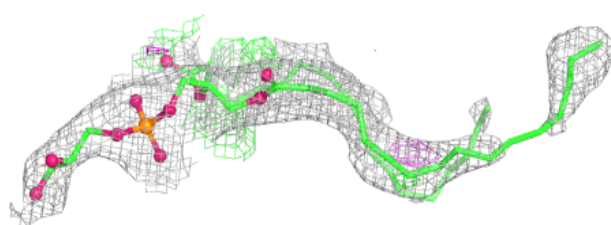
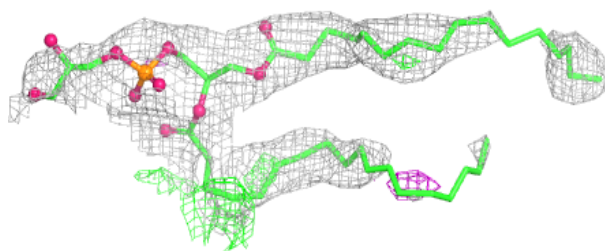
Electron density around PEK T 103:

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and green (positive)

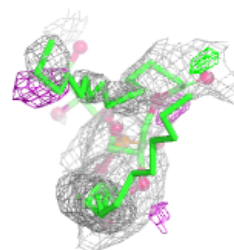
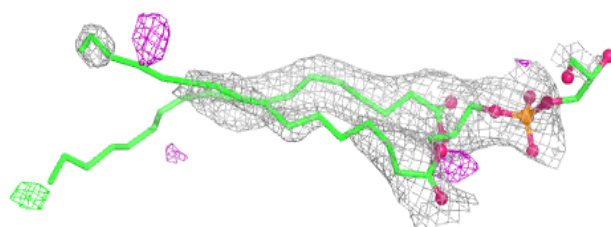
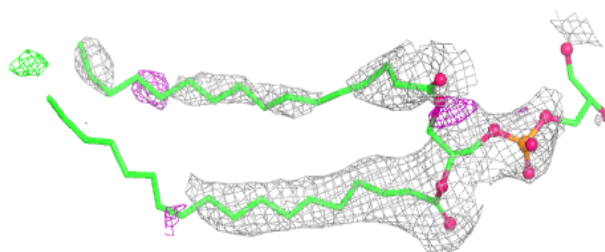


Electron density around PGV U 101:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

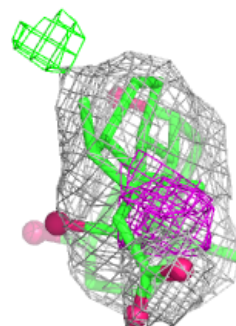
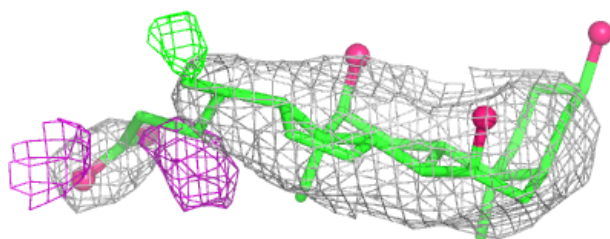
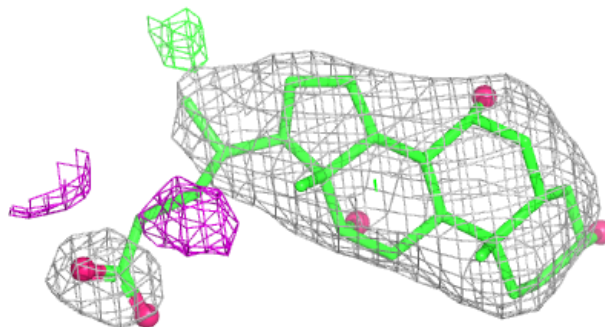
**Electron density around PGV Z 101:**

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

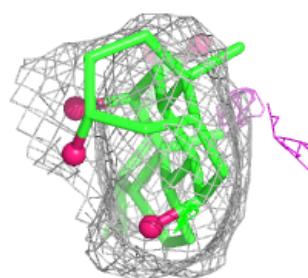
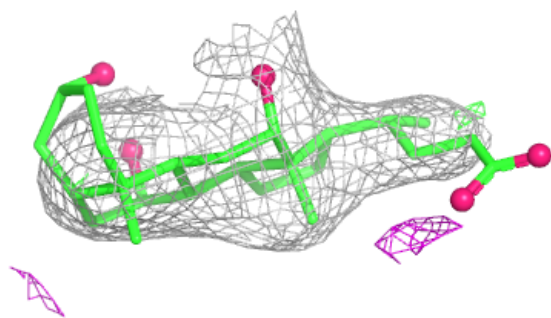
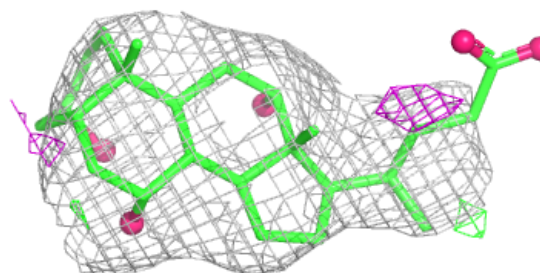


Electron density around CHD J 101:

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

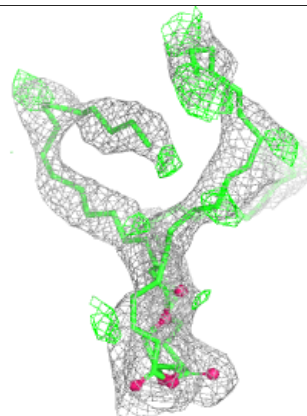
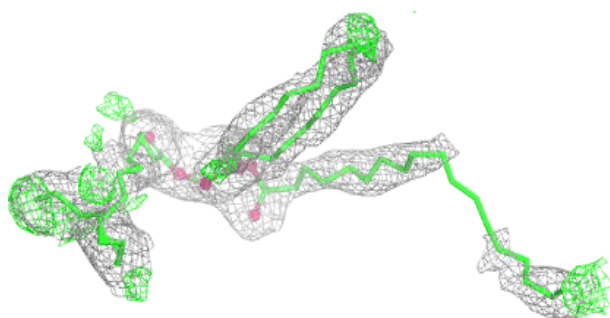
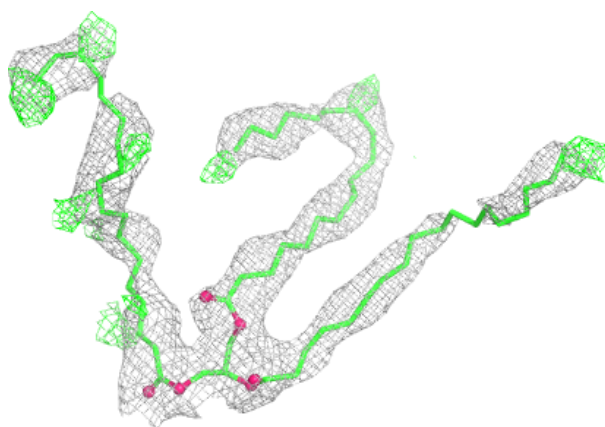
**Electron density around CHD N 609:**

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

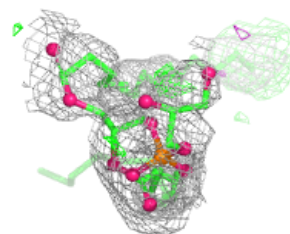
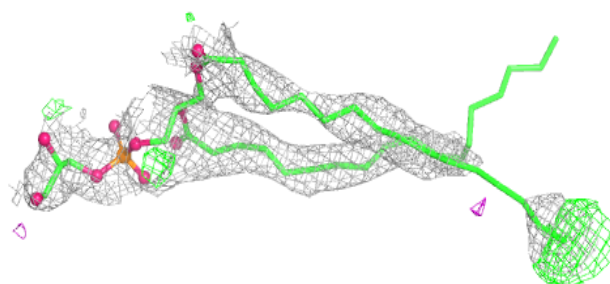
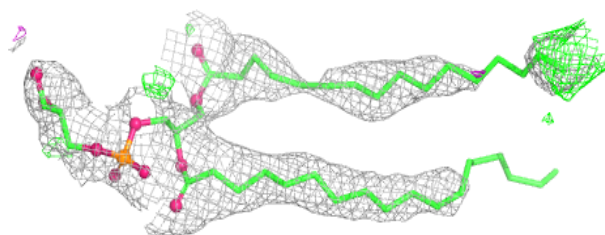


Electron density around TGL A 606:

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

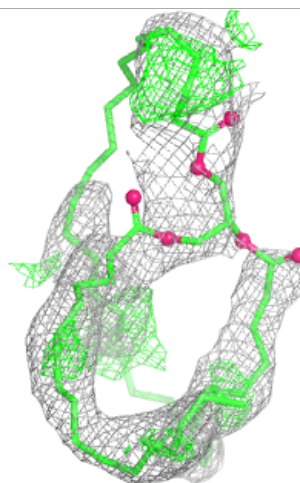
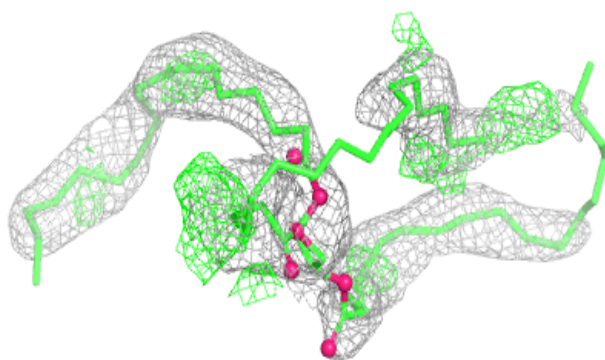
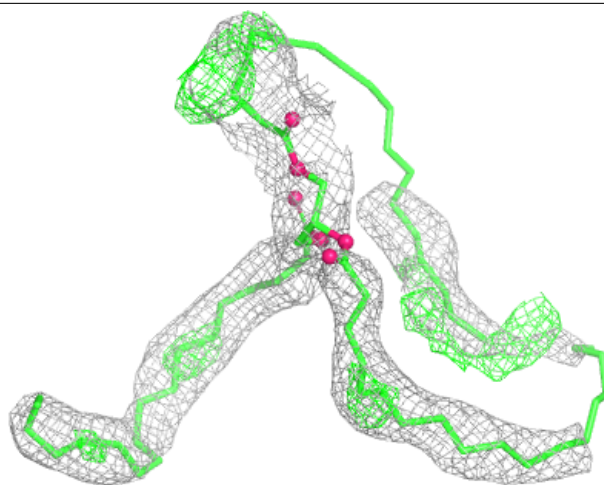
**Electron density around PGV M 101:**

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



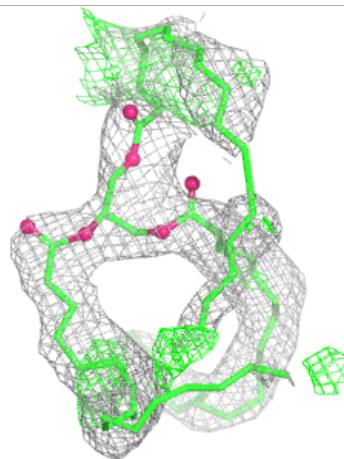
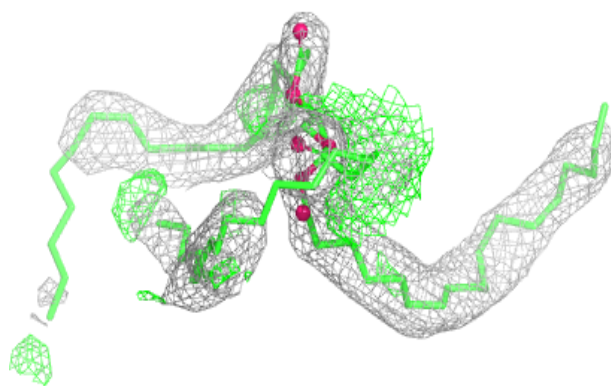
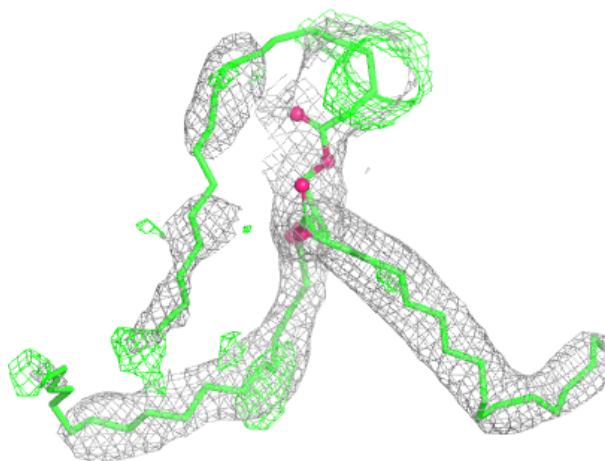
Electron density around TGL Y 101:

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



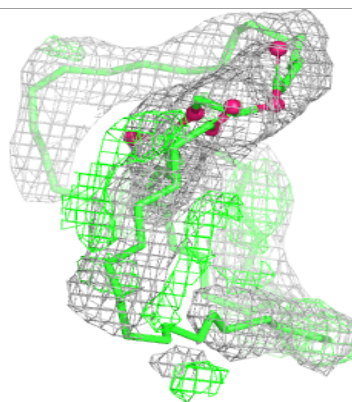
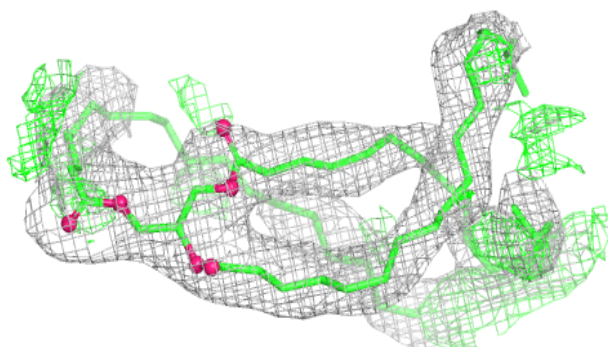
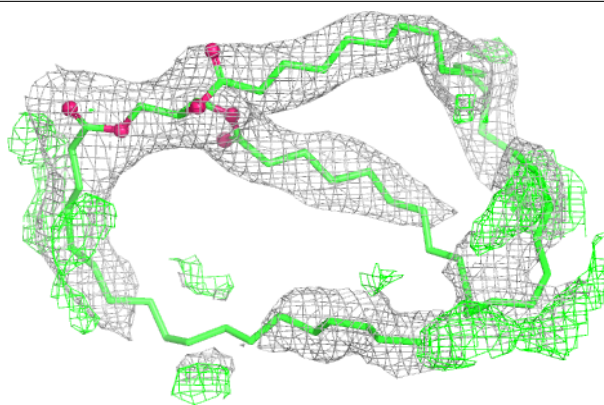
Electron density around TGL L 101:

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

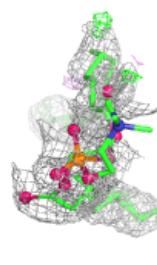
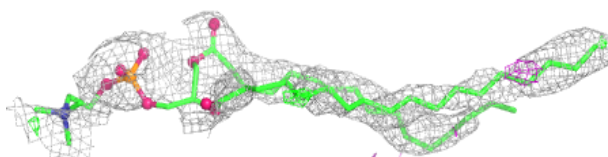
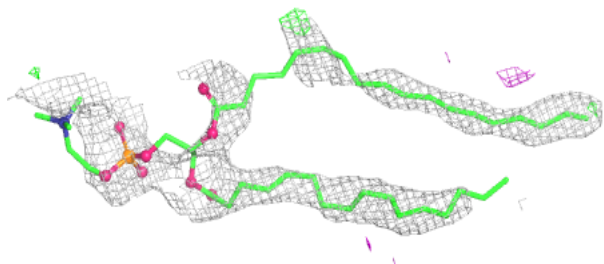


Electron density around TGL I 101:

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

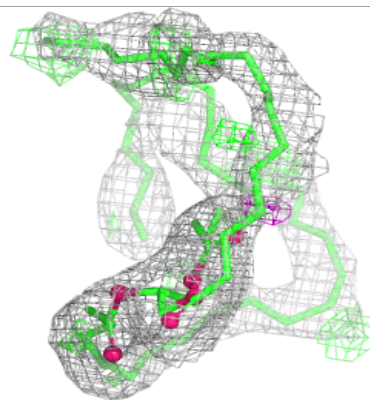
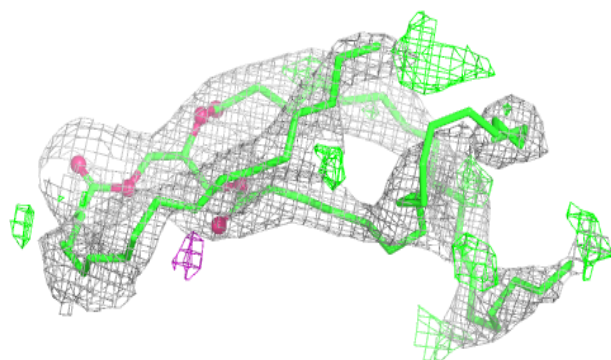
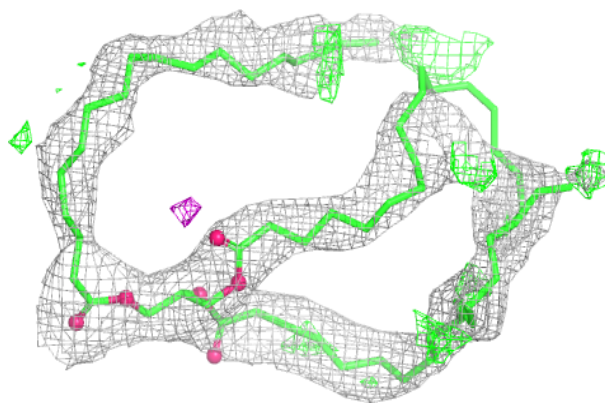
**Electron density around PSC E 201:**

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

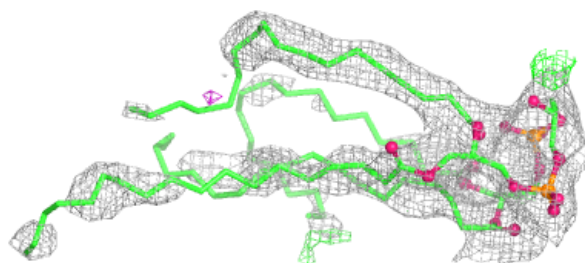
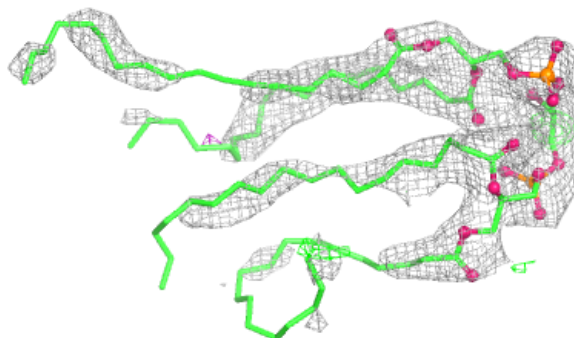


Electron density around TGL N 608:

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

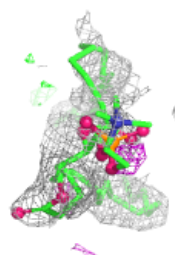
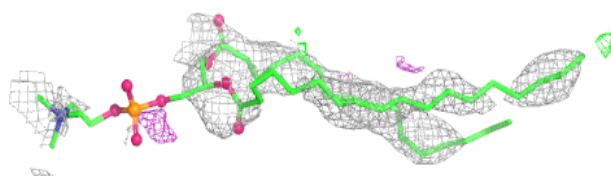
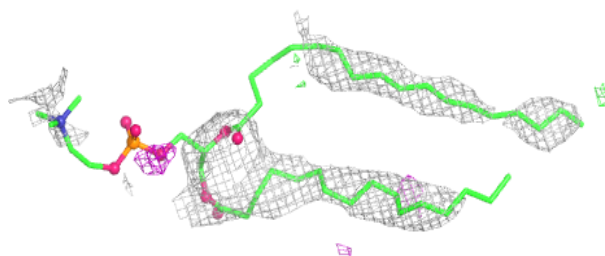
**Electron density around CDL C 305:**

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

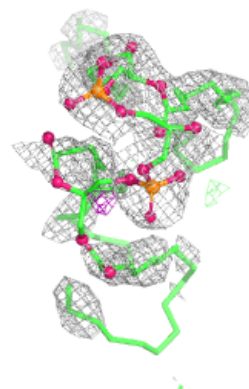
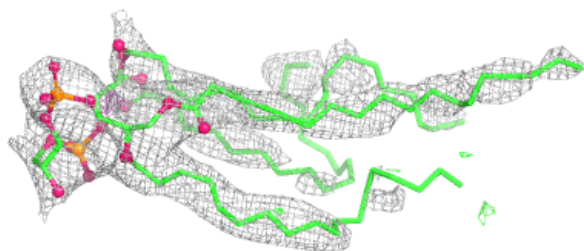
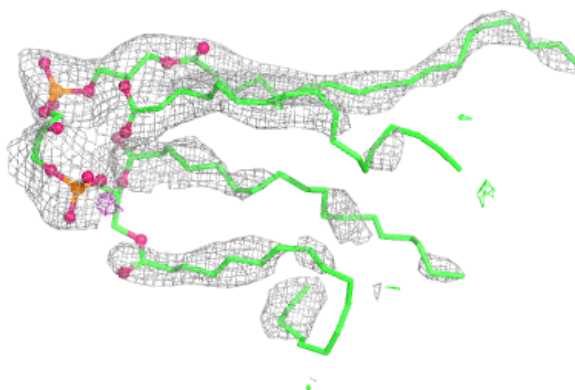


Electron density around PSC R 201:

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

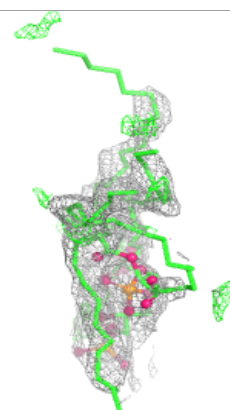
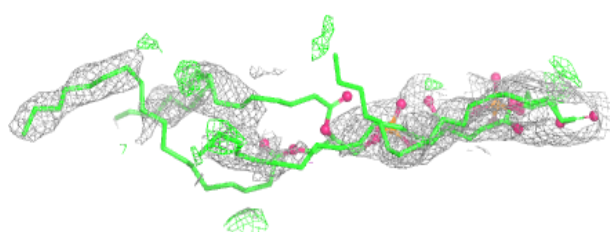
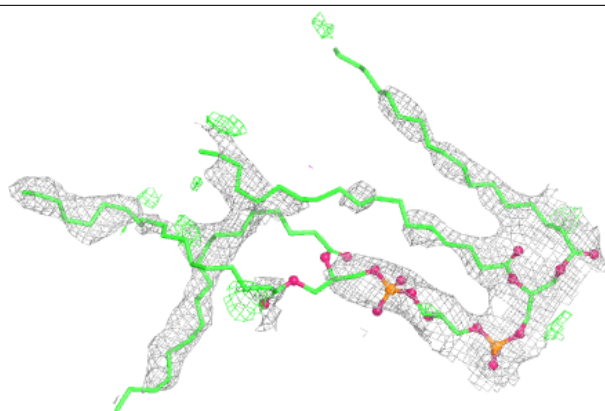
**Electron density around CDL P 305:**

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

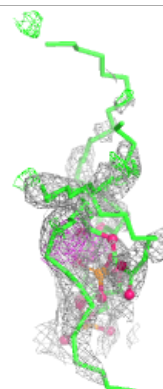
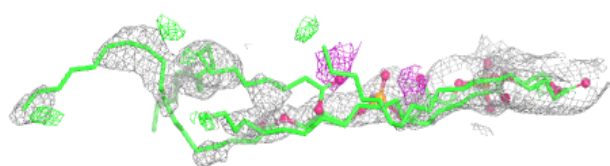
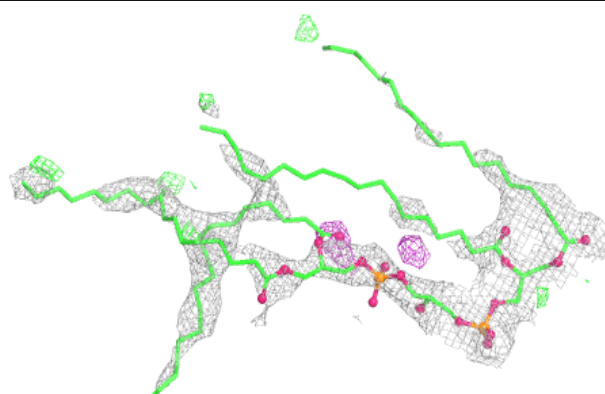


Electron density around CDL T 104:

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

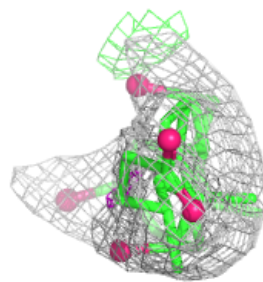
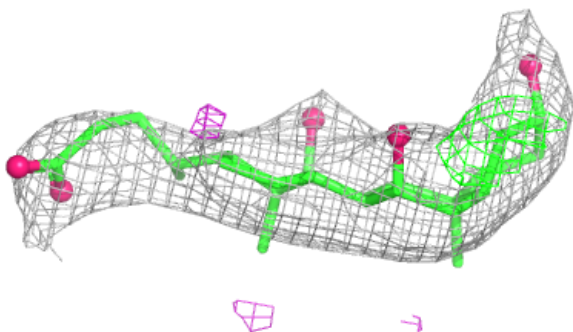
**Electron density around CDL G 104:**

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



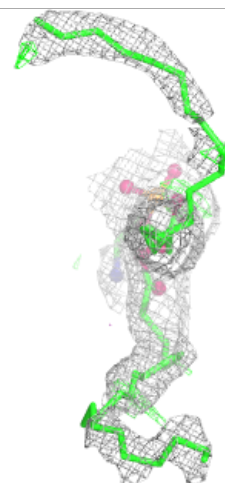
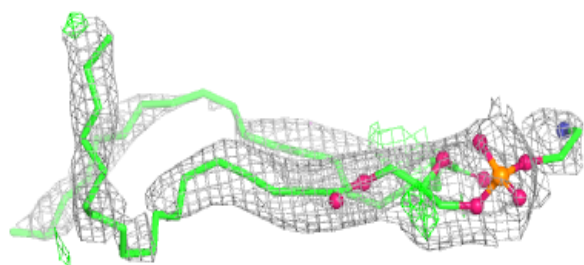
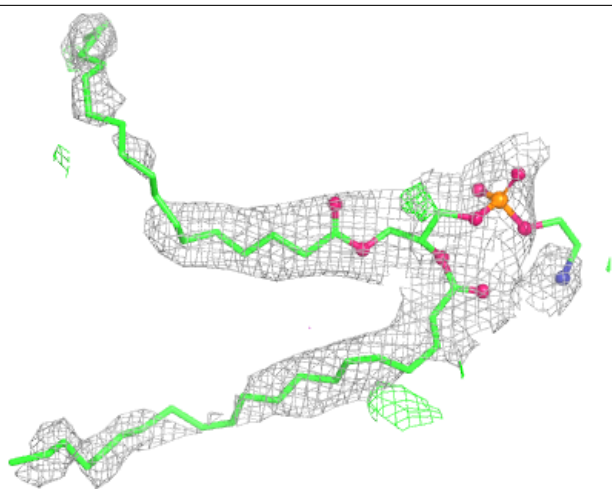
Electron density around CHD C 306:

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



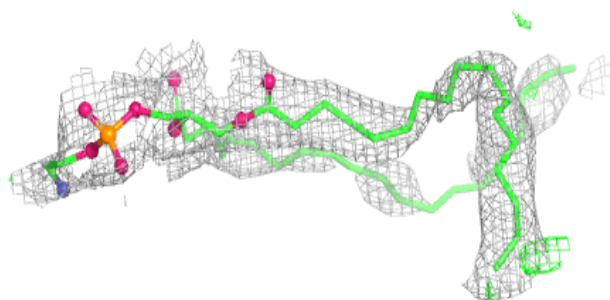
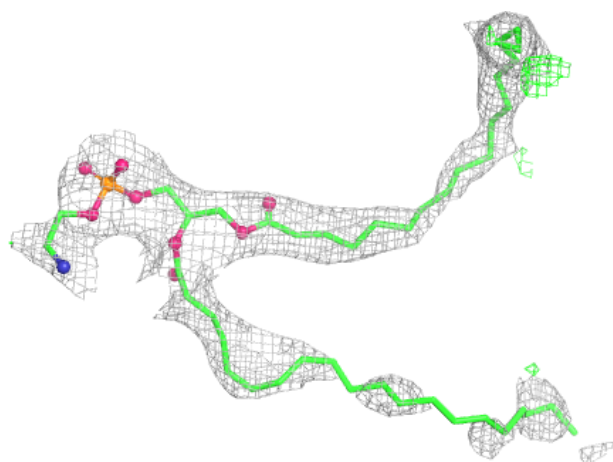
Electron density around PEK G 103:

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



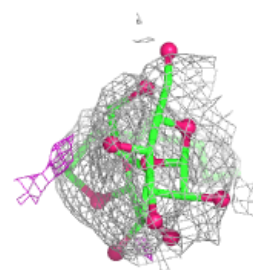
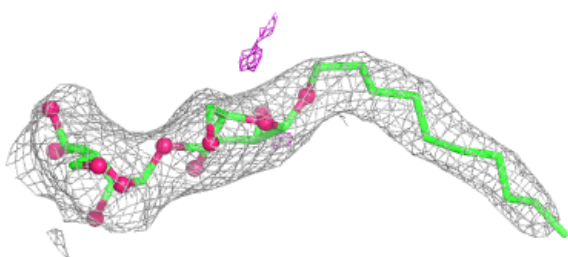
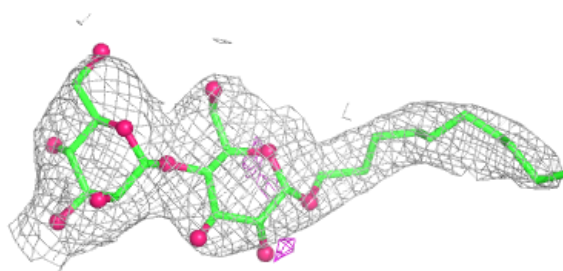
Electron density around PEK T 101:

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

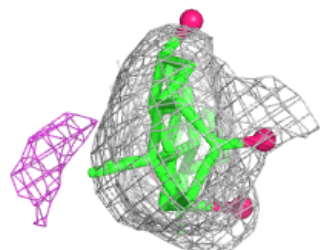
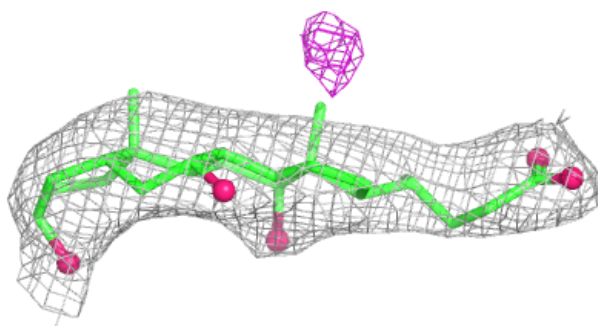
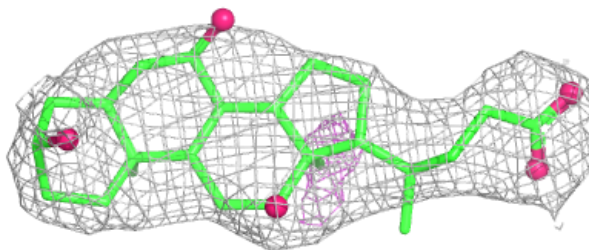


Electron density around DMU Q 201:

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

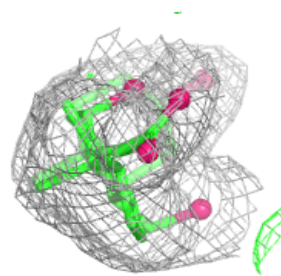
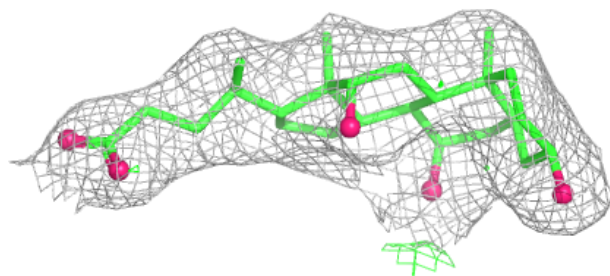
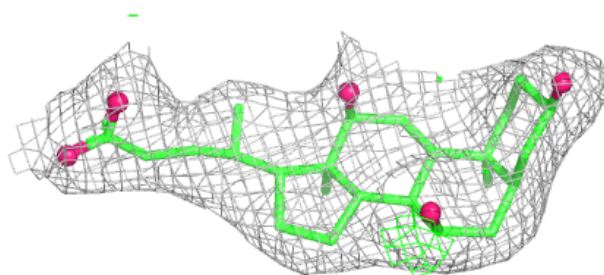
**Electron density around CHD P 306:**

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

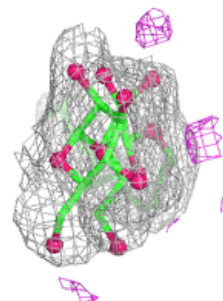
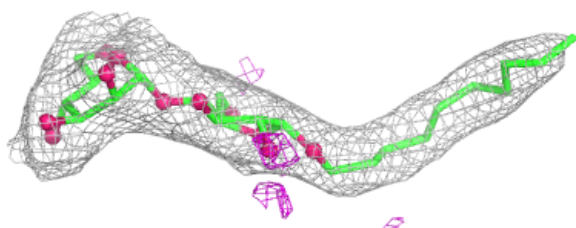
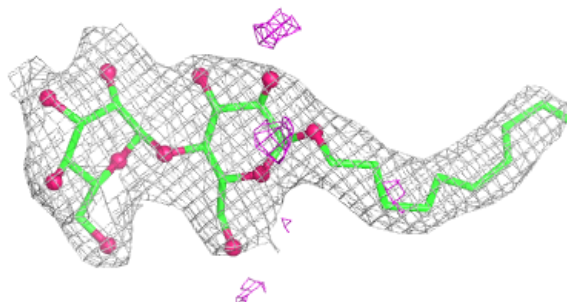


Electron density around CHD P 302:

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

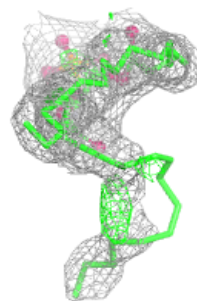
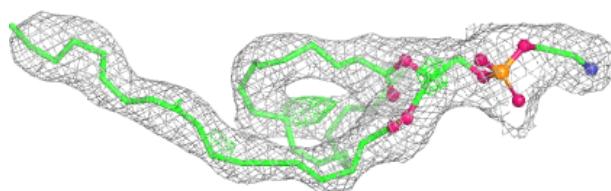
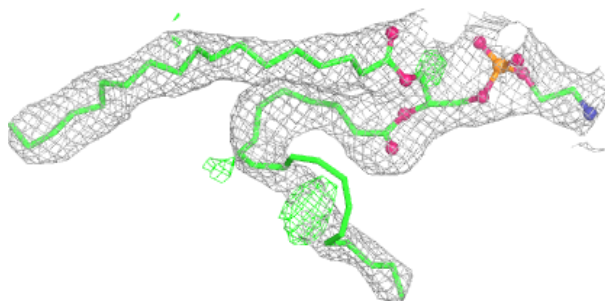
**Electron density around DMU M 102:**

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

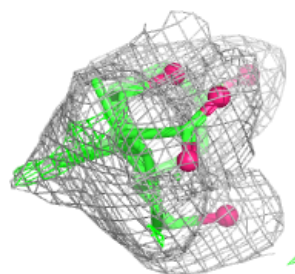
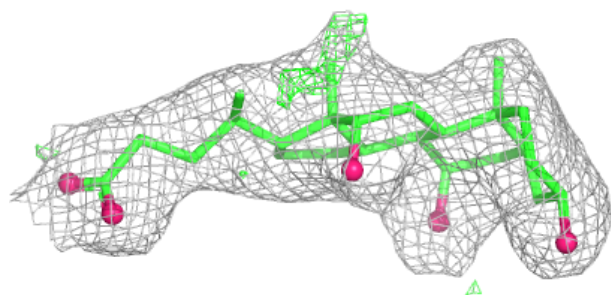
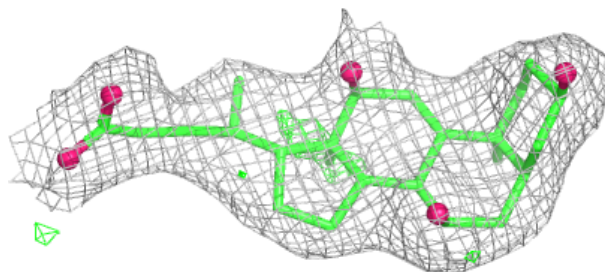


Electron density around PEK P 303:

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

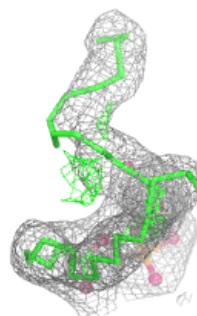
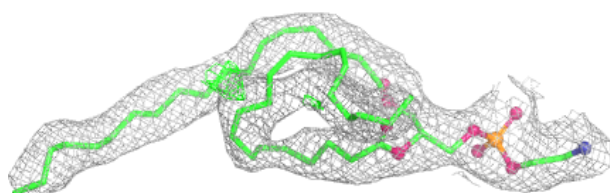
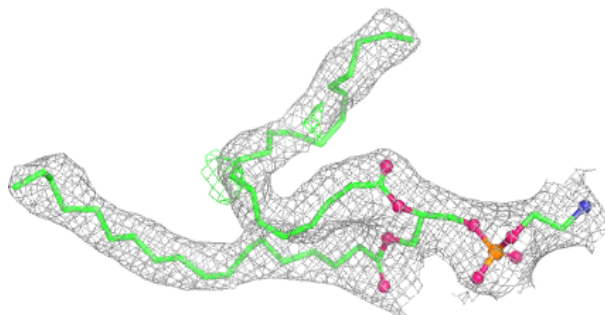
**Electron density around CHD C 301:**

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

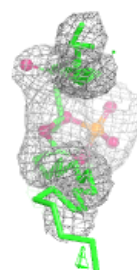
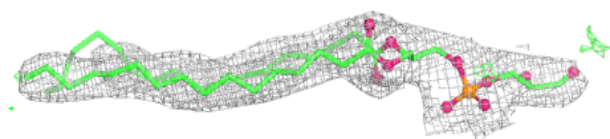
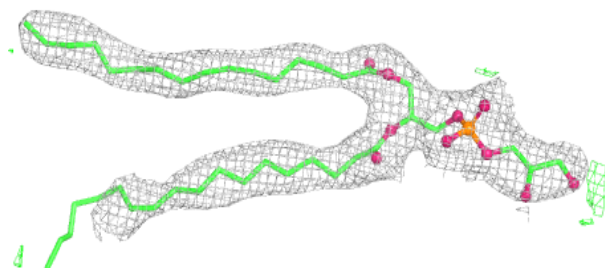


Electron density around PEK G 101:

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

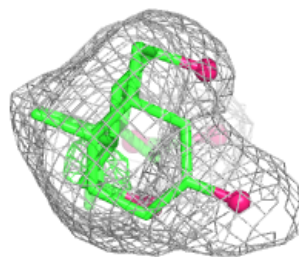
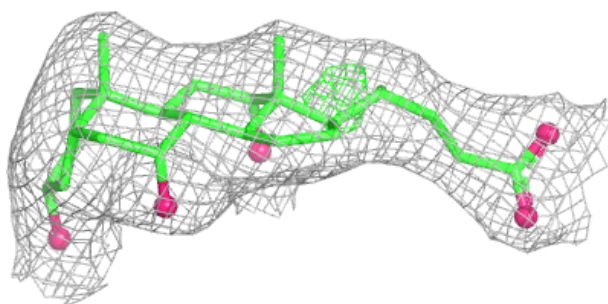
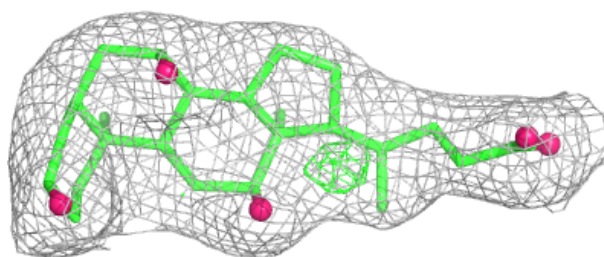
**Electron density around PGV P 304:**

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

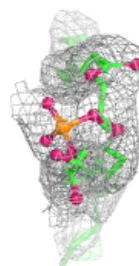
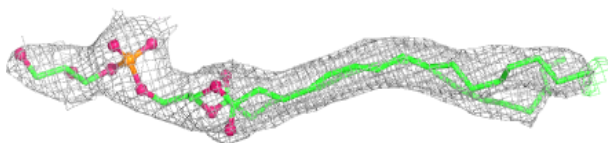
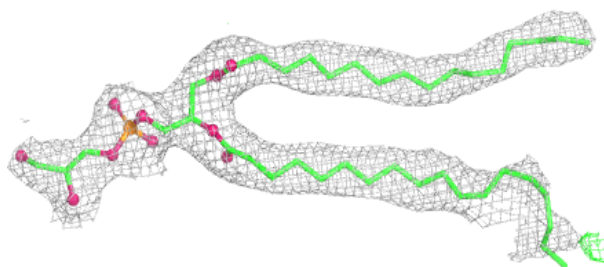


Electron density around CHD G 105:

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

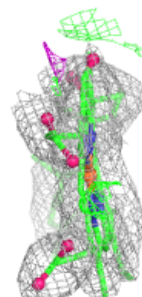
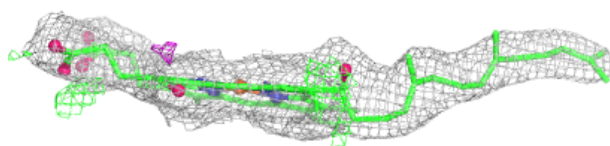
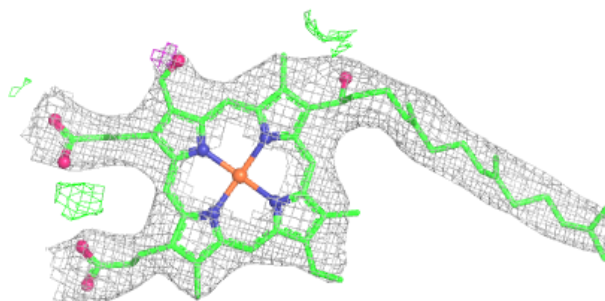
**Electron density around PGV C 303:**

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

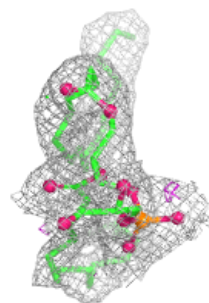
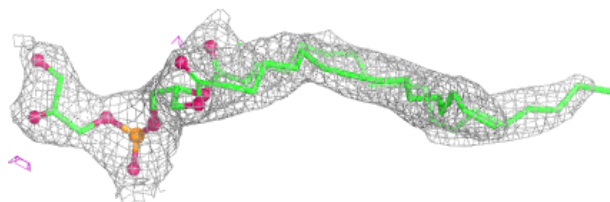
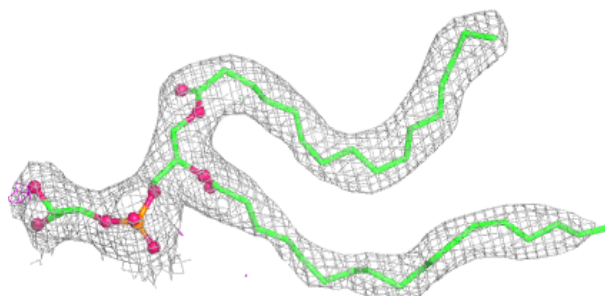


Electron density around HEA N 601:

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

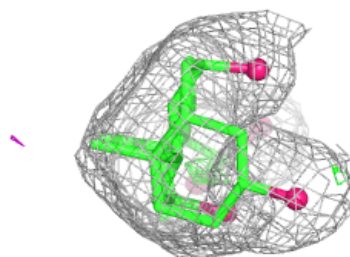
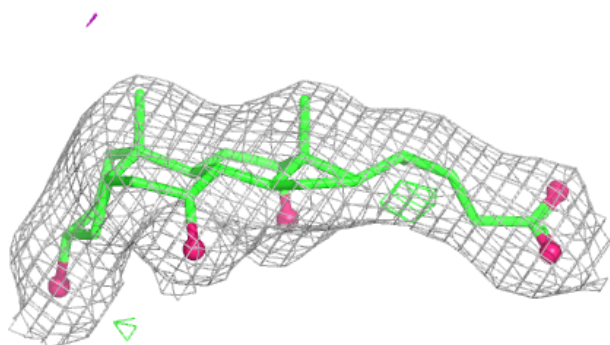
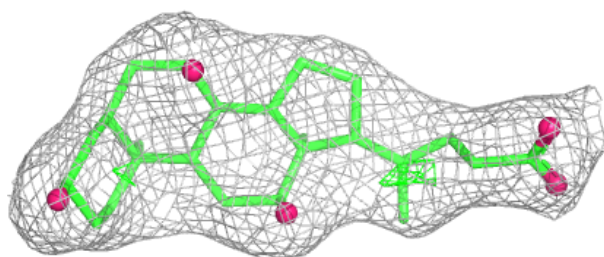
**Electron density around PGV A 607:**

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

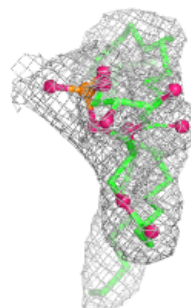
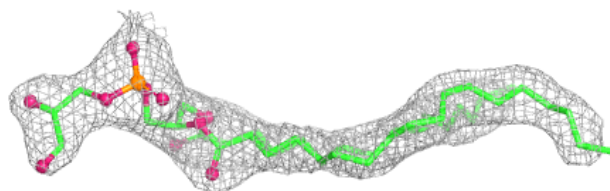
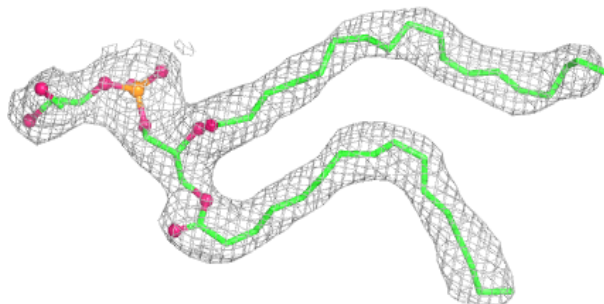


Electron density around CHD B 302:

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

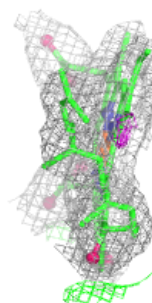
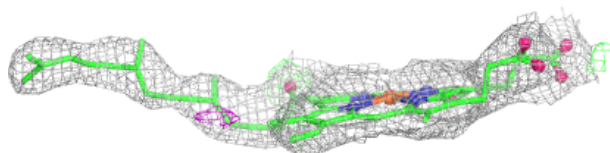
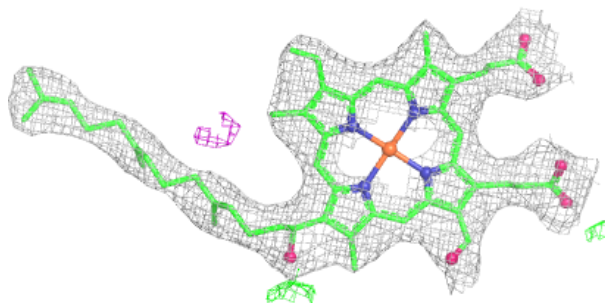
**Electron density around PGV N 607:**

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

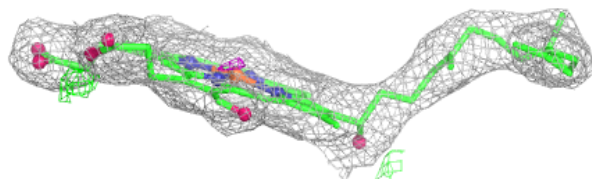
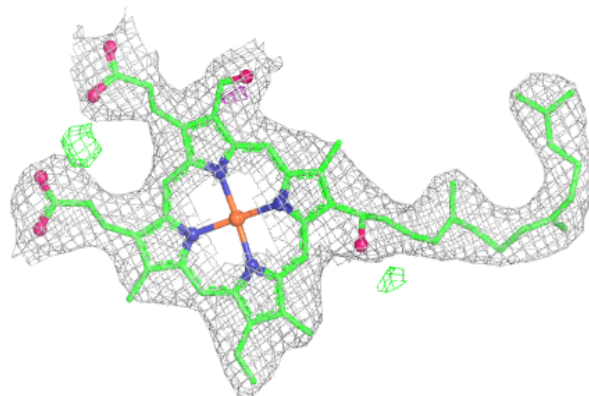


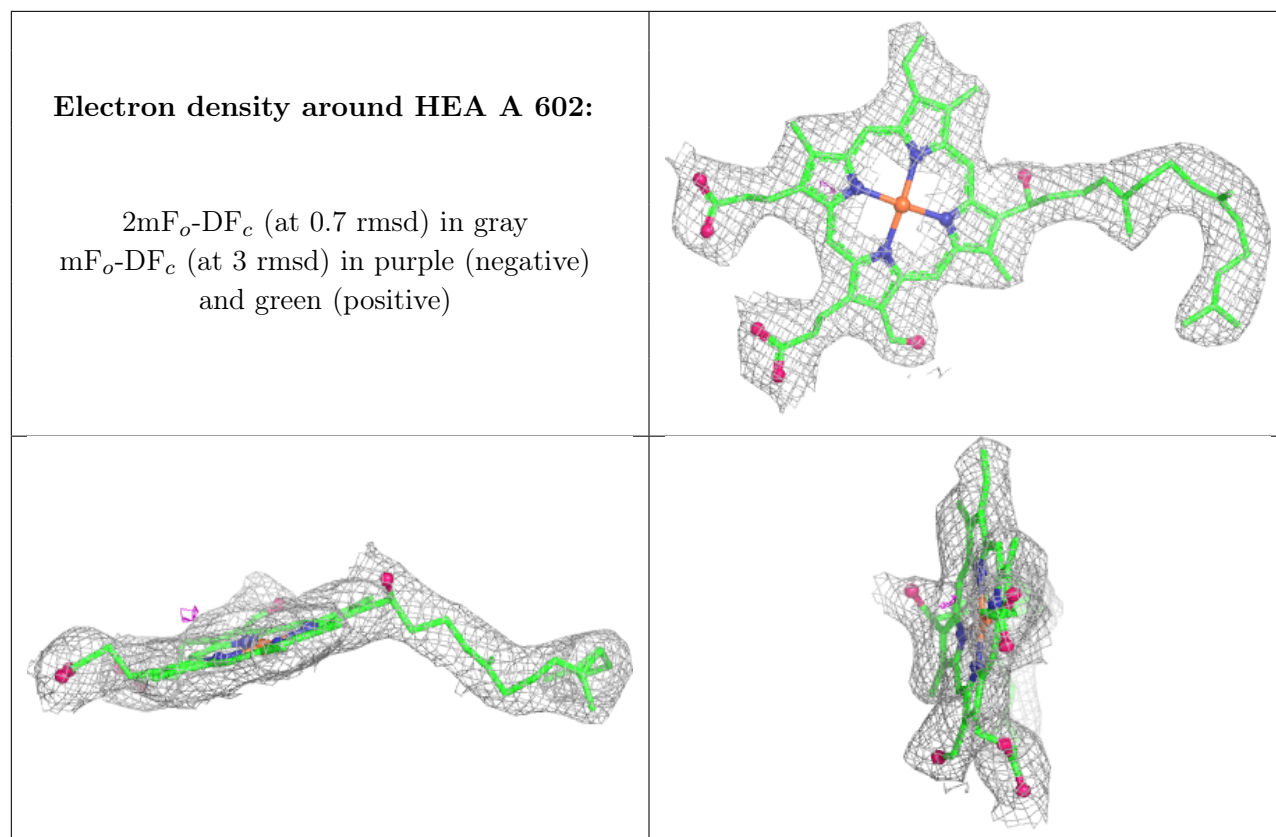
Electron density around HEA A 601:

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

**Electron density around HEA N 602:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.