



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2024 – 10:31 AM EST

PDB ID : 3X2Q
Title : X-ray structure of cyanide-bound bovine heart cytochrome c oxidase in the fully oxidized state at 2.0 angstrom resolution
Authors : Yano, N.; Muramoto, K.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2014-12-26
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

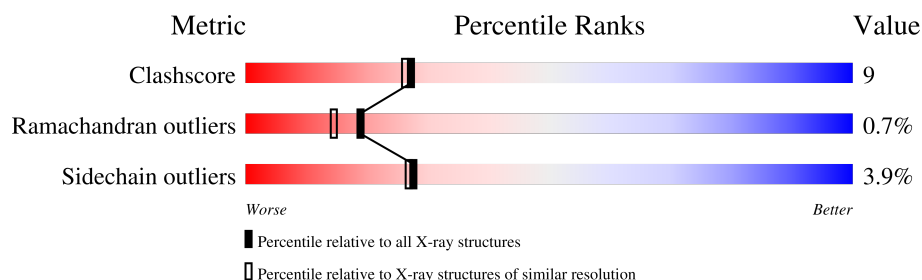
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)











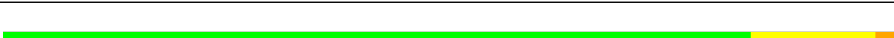


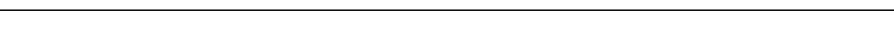
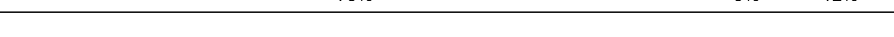
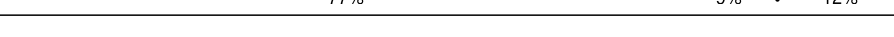



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	514	
1	N	514	
2	B	227	
2	O	227	
3	C	261	
3	P	261	
4	D	147	

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Mol	Chain	Length	Quality of chain
4	Q	147	 82% 12% . . .
5	E	109	 82% 13% . .
5	R	109	 86% 7% . .
6	F	98	 79% 18% . .
6	S	98	 76% 17% 7%
7	G	85	 71% 18% 11% .
7	T	85	 68% 19% 12% .
8	H	85	 76% 12% . . 7%
8	U	85	 74% 14% . . 7%
9	I	74	 85% 9% 5%
9	V	74	 84% 14% .
10	J	59	 90% 7% . .
10	W	59	 93% . . .
11	K	56	 79% 9% 12%
11	X	56	 77% 9% . 12%
12	L	47	 79% 17% . .
12	Y	47	 77% 19% . .
13	M	46	 74% 17% . 7%
13	Z	46	 78% 15% 7%

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
24	CDL	G	103	-	-	X	-
24	CDL	T	102	-	-	X	-
25	PEK	T	101	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32060 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	3	0
			4051	2708	626	681	36			
1	N	514	Total	C	N	O	S	0	3	0
			4051	2708	626	681	36			

- 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	3	0
			2134	1427	339	353	15			
3	P	259	Total	C	N	O	S	0	3	0
			2134	1427	339	353	15			

- 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	74	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	74	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	0	ACE	-	acetylation	UNP P04038
V	0	ACE	-	acetylation	UNP P04038

- 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			
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			

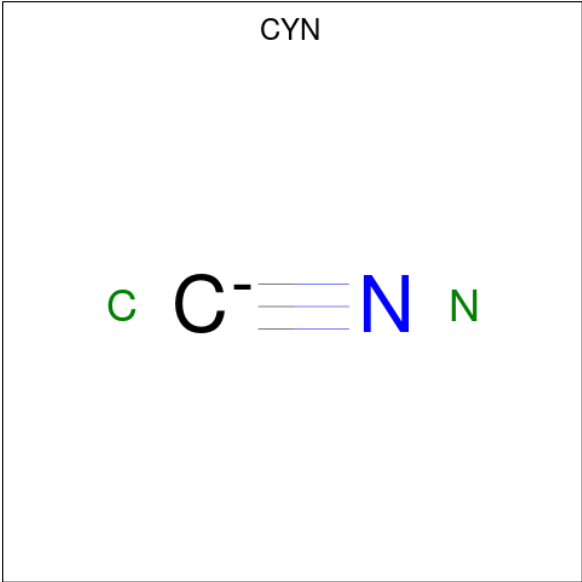
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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.

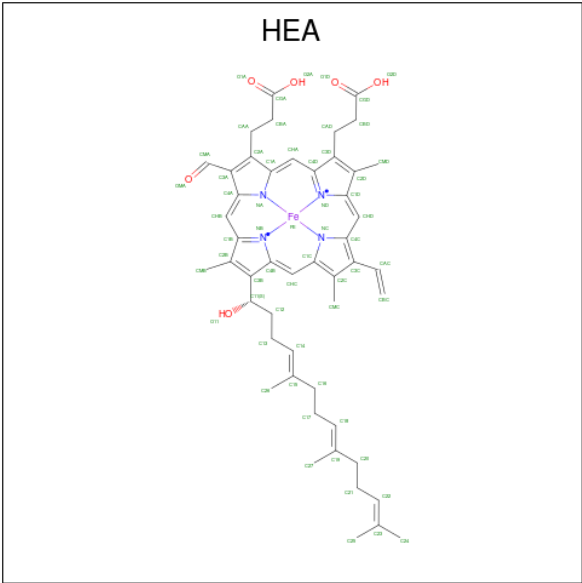
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is CYANIDE ION (three-letter code: CYN) (formula: CN).



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

- Molecule 15 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

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

- Molecule 16 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

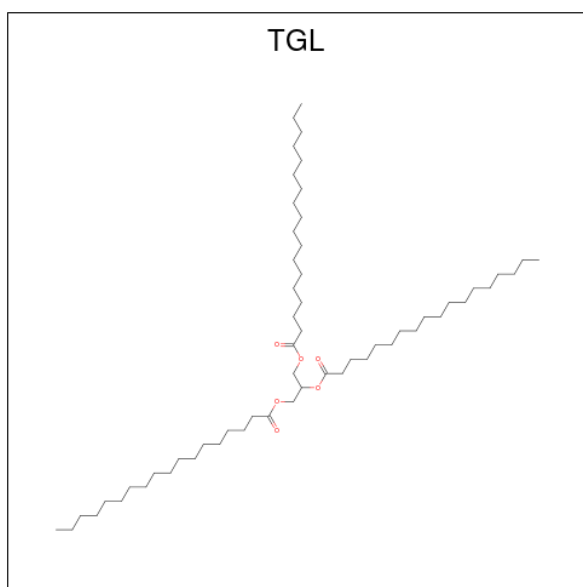
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (three-letter code: NA) (formula: Na).

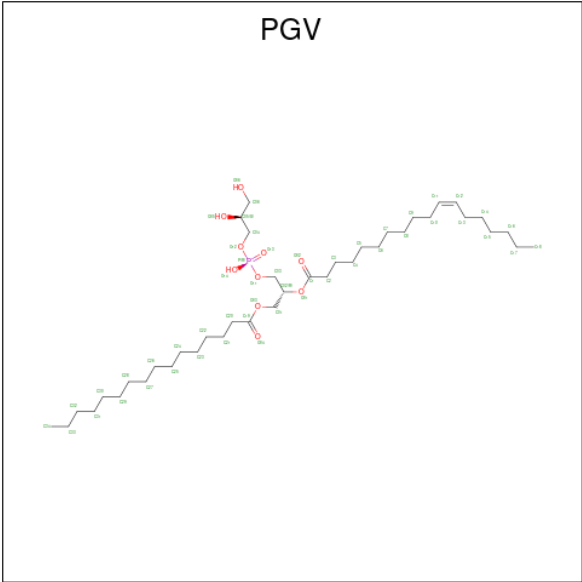
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Na	0	0
			1	1		
18	N	1	Total	Na	0	0
			1	1		

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



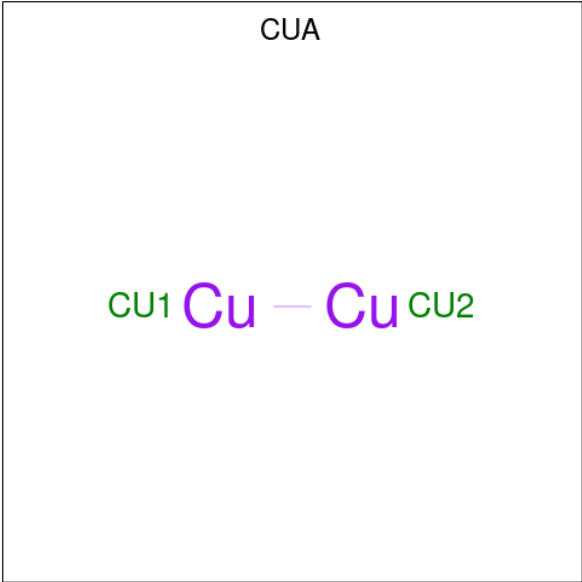
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

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



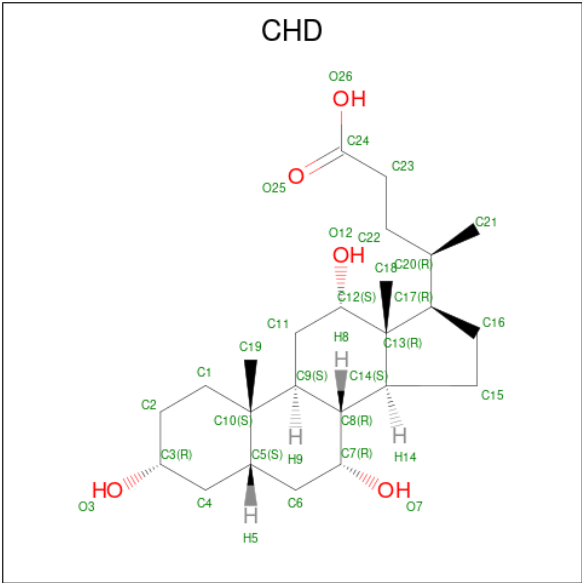
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: 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 (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



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		

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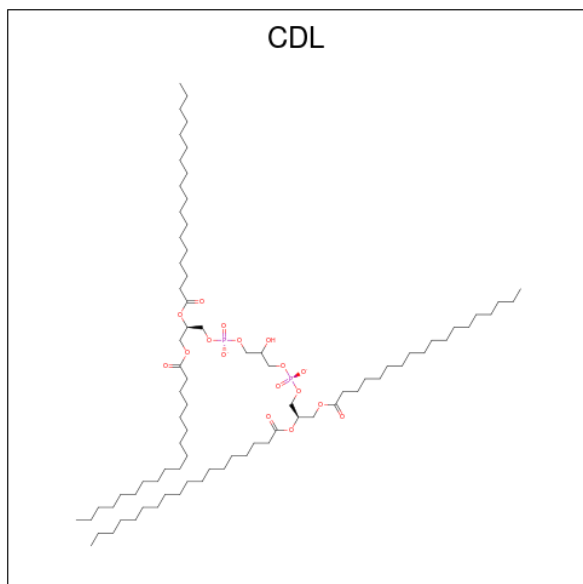
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	C	O	0	0
			29	24	5		
22	O	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		

- Molecule 23 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

- Molecule 24 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



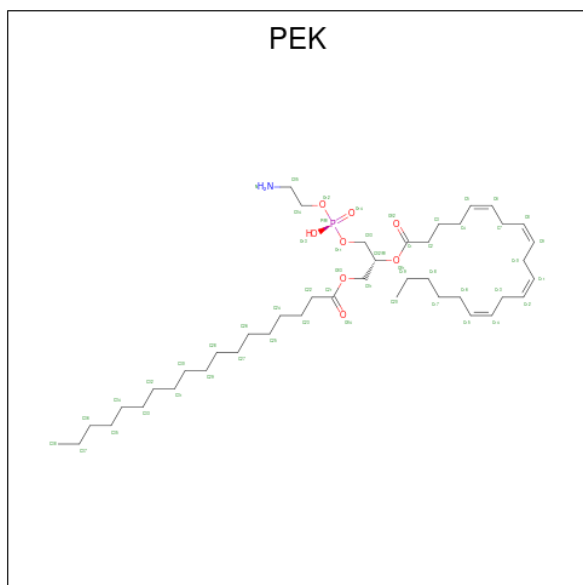
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	C	1	Total	C	O	P	0	0
			100	81	17	2		
24	G	1	Total	C	O	P	0	0
			100	81	17	2		
24	P	1	Total	C	O	P	0	0
			100	81	17	2		

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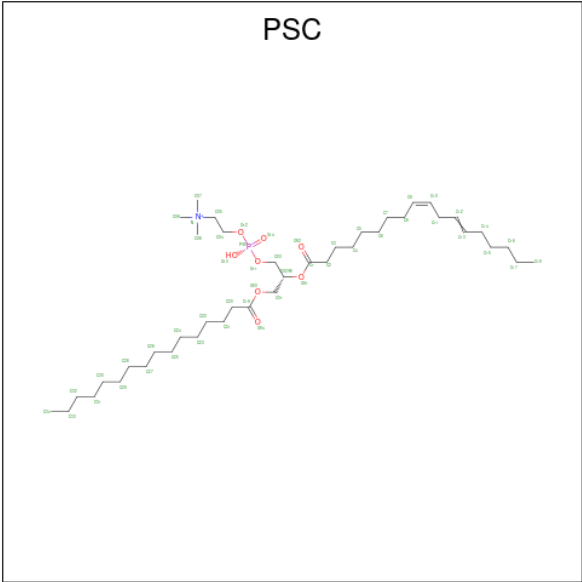
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	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 (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 (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).

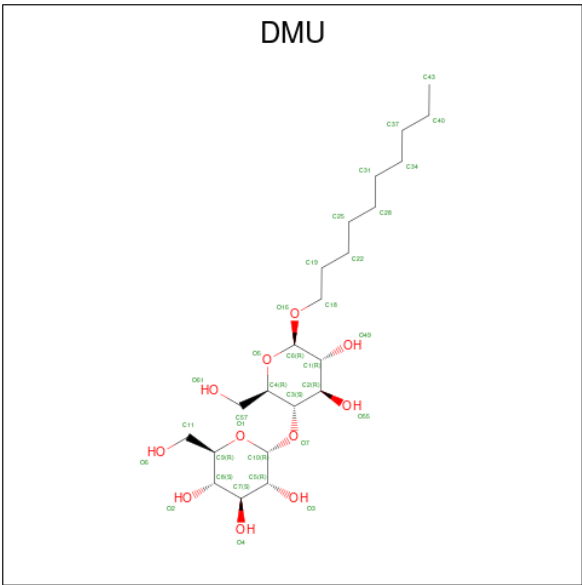


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 28 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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	P	1	Total	C	O	0	0
			33	22	11		
28	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	188	Total	O	0	0
			188	188		
29	B	121	Total	O	0	0
			121	121		
29	C	77	Total	O	0	0
			77	77		
29	D	78	Total	O	0	0
			78	78		
29	E	58	Total	O	0	0
			58	58		
29	F	58	Total	O	0	0
			58	58		
29	G	27	Total	O	0	0
			27	27		
29	H	34	Total	O	0	0
			34	34		

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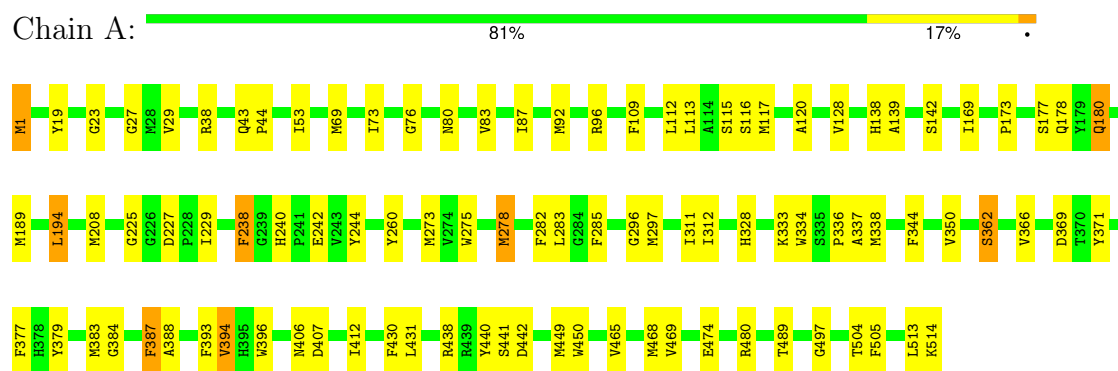
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	I	29	Total 29	O 29	0	0
29	J	15	Total 15	O 15	0	0
29	K	20	Total 20	O 20	0	0
29	L	16	Total 16	O 16	0	0
29	M	14	Total 14	O 14	0	0
29	N	156	Total 156	O 156	0	0
29	O	91	Total 91	O 91	0	0
29	P	76	Total 76	O 76	0	0
29	Q	46	Total 46	O 46	0	0
29	R	42	Total 42	O 42	0	0
29	S	38	Total 38	O 38	0	0
29	T	23	Total 23	O 23	0	0
29	U	28	Total 28	O 28	0	0
29	V	14	Total 14	O 14	0	0
29	W	4	Total 4	O 4	0	0
29	X	15	Total 15	O 15	0	0
29	Y	11	Total 11	O 11	0	0
29	Z	7	Total 7	O 7	0	0

3 Residue-property plots

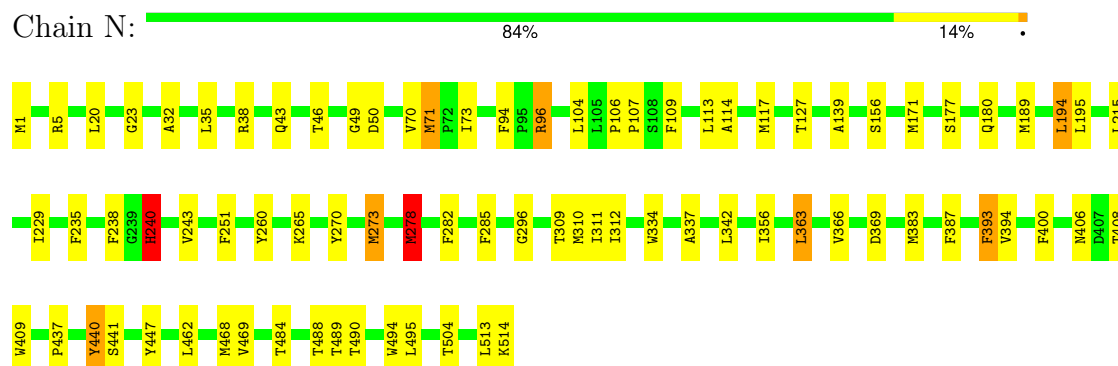
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Note EDS failed to run properly.

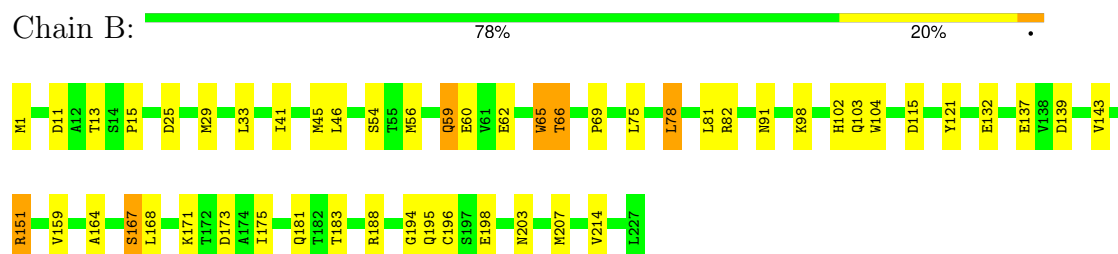
- Molecule 1: Cytochrome c oxidase subunit 1



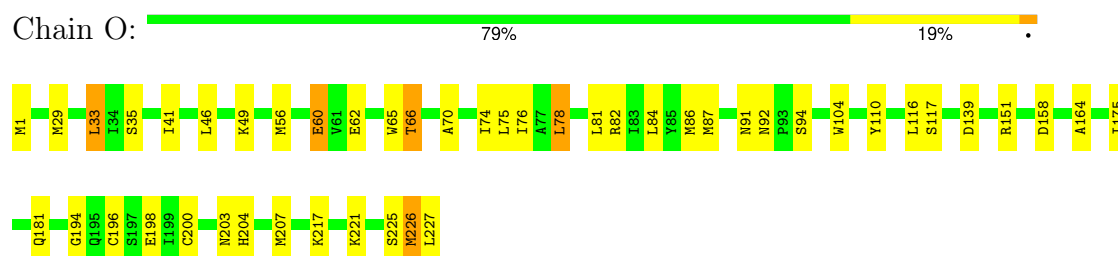
- Molecule 1: Cytochrome c oxidase subunit 1



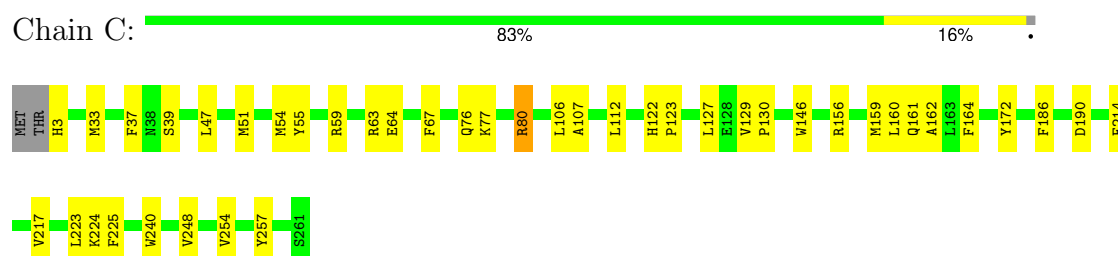
- Molecule 2: Cytochrome c oxidase subunit 2



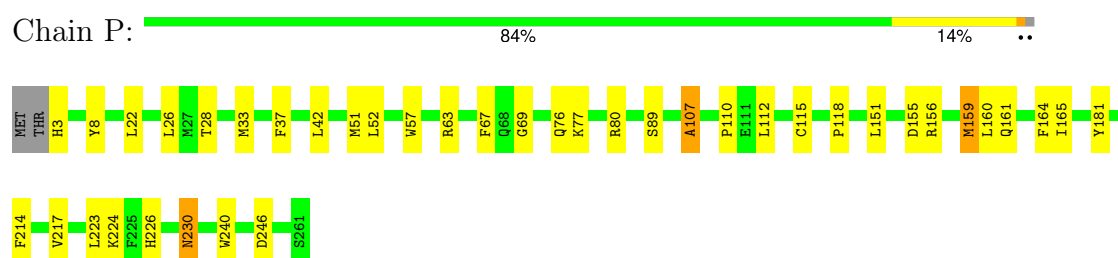
- Molecule 2: Cytochrome c oxidase subunit 2



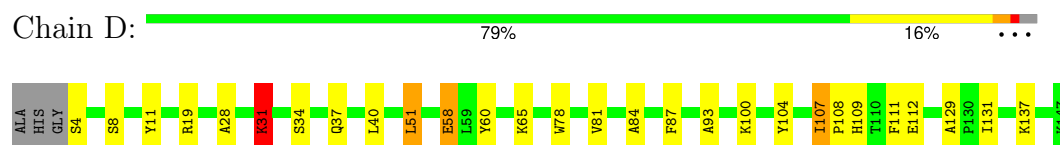
- Molecule 3: Cytochrome c oxidase subunit 3



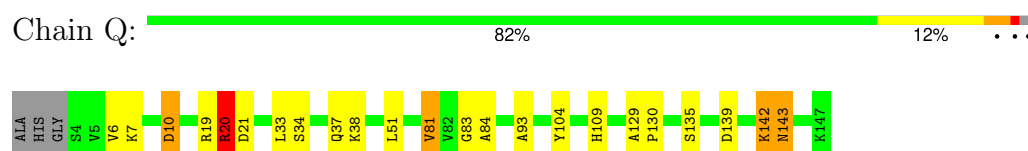
- Molecule 3: Cytochrome c oxidase subunit 3



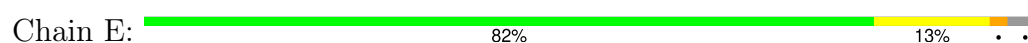
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

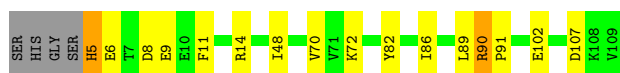


- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

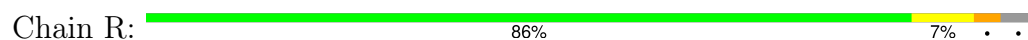


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial





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



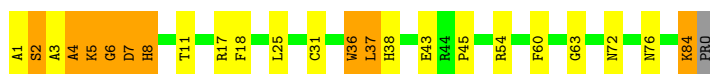
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



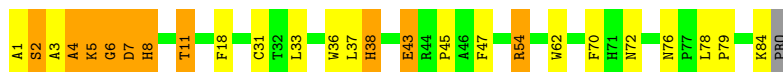
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



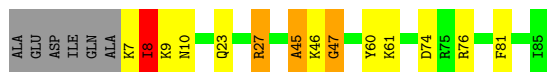
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



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

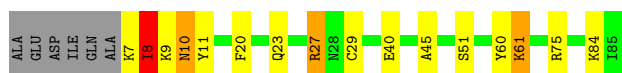


- Molecule 8: Cytochrome c oxidase subunit 6B1

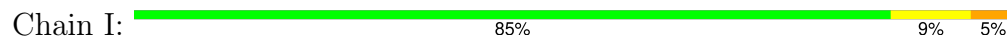


- Molecule 8: Cytochrome c oxidase subunit 6B1

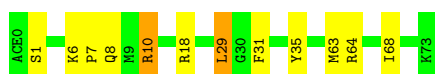
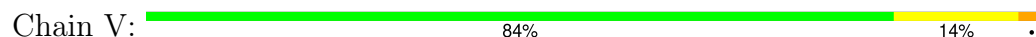




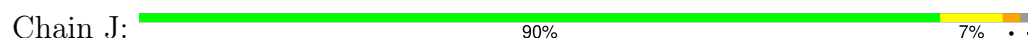
- Molecule 9: Cytochrome c oxidase subunit 6C



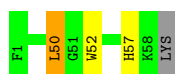
- Molecule 9: Cytochrome c oxidase subunit 6C



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



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



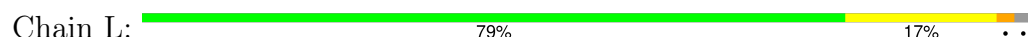
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

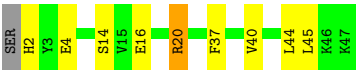


- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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

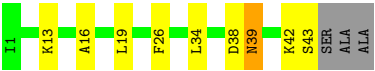




• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.68Å 206.68Å 178.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.9 (40.00-2.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.187 , 0.214	Depositor
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.465	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
Total number of atoms	32060	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, CYN, NA, FME, ZN, UNX, DMU, PEK, TGL, PGV, CHD, MG, CDL, PSC, TPO, CU, ACE, 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	1.51	29/4180 (0.7%)	1.15	18/5710 (0.3%)
1	N	1.34	15/4180 (0.4%)	0.99	10/5710 (0.2%)
2	B	1.45	11/1860 (0.6%)	1.16	13/2534 (0.5%)
2	O	1.14	3/1860 (0.2%)	1.01	3/2534 (0.1%)
3	C	1.35	5/2221 (0.2%)	0.96	1/3035 (0.0%)
3	P	1.31	6/2221 (0.3%)	0.93	2/3035 (0.1%)
4	D	1.48	10/1229 (0.8%)	1.14	6/1658 (0.4%)
4	Q	1.03	1/1229 (0.1%)	0.92	3/1658 (0.2%)
5	E	1.27	3/871 (0.3%)	1.11	3/1182 (0.3%)
5	R	1.15	3/871 (0.3%)	0.97	2/1182 (0.2%)
6	F	1.31	0/765	1.08	2/1038 (0.2%)
6	S	1.20	0/765	1.02	0/1038
7	G	1.33	3/690 (0.4%)	1.01	4/937 (0.4%)
7	T	1.31	4/690 (0.6%)	1.07	2/937 (0.2%)
8	H	1.26	1/682 (0.1%)	1.01	3/921 (0.3%)
8	U	1.04	0/682	0.91	1/921 (0.1%)
9	I	1.36	0/612	1.14	3/812 (0.4%)
9	V	1.09	0/612	1.07	3/812 (0.4%)
10	J	1.21	0/471	0.94	0/636
10	W	1.07	0/471	0.92	0/636
11	K	1.38	1/398 (0.3%)	1.11	2/546 (0.4%)
11	X	1.07	1/398 (0.3%)	0.85	0/546
12	L	1.38	3/393 (0.8%)	1.02	1/526 (0.2%)
12	Y	1.16	0/393	0.82	0/526
13	M	1.38	2/345 (0.6%)	1.04	0/470
13	Z	1.05	0/345	0.87	0/470
All	All	1.32	101/29434 (0.3%)	1.03	82/40010 (0.2%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
6	F	0	1
6	S	0	1
10	J	0	1
10	W	0	1
All	All	0	6

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	80	GLU	CG-CD	9.50	1.66	1.51
2	B	167	SER	CB-OG	-8.83	1.30	1.42
1	A	371	TYR	CD1-CE1	8.27	1.51	1.39
7	T	36	TRP	CB-CG	8.23	1.65	1.50
5	R	80	GLU	CB-CG	8.14	1.67	1.52

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	MET	CG-SD-CE	-19.27	69.37	100.20
4	D	19	ARG	NE-CZ-NH1	-13.36	113.62	120.30
1	A	96	ARG	NE-CZ-NH2	-11.58	114.51	120.30
4	Q	20	ARG	NE-CZ-NH2	-10.39	115.10	120.30
1	A	278	MET	CG-SD-CE	-9.12	85.61	100.20

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
6	F	93	PRO	Peptide
10	J	57	HIS	Peptide
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4051	0	4029	55	0
1	N	4051	0	4029	56	0
2	B	1824	0	1833	26	0
2	O	1824	0	1833	31	0
3	C	2134	0	2051	31	0
3	P	2134	0	2051	36	0
4	D	1195	0	1183	15	0
4	Q	1195	0	1183	20	0
5	E	852	0	845	11	0
5	R	852	0	845	8	0
6	F	748	0	728	16	0
6	S	748	0	728	29	0
7	G	675	0	643	27	0
7	T	675	0	643	45	0
8	H	662	0	623	7	0
8	U	662	0	623	12	0
9	I	601	0	613	12	0
9	V	601	0	613	10	0
10	J	460	0	459	4	0
10	W	460	0	459	2	0
11	K	384	0	366	2	0
11	X	384	0	366	4	0
12	L	380	0	380	10	0
12	Y	380	0	380	15	0
13	M	335	0	352	2	0
13	Z	335	0	352	2	0
14	A	2	0	0	0	0
14	N	2	0	0	0	0
15	A	120	0	108	9	0
15	N	120	0	108	8	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	1	0	0	1	0
18	N	1	0	0	0	0
19	A	63	0	110	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	63	0	110	12	0
19	L	63	0	110	14	0
19	N	126	0	220	22	0
19	Q	63	0	110	2	0
20	A	102	0	152	8	0
20	C	102	0	152	5	0
20	N	102	0	152	10	0
20	P	102	0	152	5	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	2	0
22	C	58	0	78	6	0
22	O	29	0	39	1	0
22	P	58	0	78	8	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	100	0	156	17	0
24	G	100	0	156	26	0
24	P	100	0	156	20	0
24	T	100	0	156	27	0
25	C	53	0	77	6	0
25	G	106	0	154	13	0
25	P	106	0	154	13	0
25	T	53	0	77	22	0
26	E	52	0	80	16	0
26	O	52	0	80	17	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	41	4	0
28	M	33	0	42	0	0
28	P	33	0	42	3	0
28	Z	33	0	42	0	0
29	A	188	0	0	10	0
29	B	121	0	0	3	0
29	C	77	0	0	1	0
29	D	78	0	0	4	0
29	E	58	0	0	2	0
29	F	58	0	0	4	0
29	G	27	0	0	3	0
29	H	34	0	0	0	0
29	I	29	0	0	4	0
29	J	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	K	20	0	0	1	0
29	L	16	0	0	2	0
29	M	14	0	0	0	0
29	N	156	0	0	3	0
29	O	91	0	0	3	0
29	P	76	0	0	9	0
29	Q	46	0	0	4	0
29	R	42	0	0	1	0
29	S	38	0	0	3	0
29	T	23	0	0	2	0
29	U	28	0	0	3	0
29	V	14	0	0	0	0
29	W	4	0	0	0	0
29	X	15	0	0	1	0
29	Y	11	0	0	0	0
29	Z	7	0	0	0	0
All	All	32060	0	31341	561	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 9.

The worst 5 of 561 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)
25:P:309:PEK:H383	24:T:102:CDL:C27	1.43	1.46
1:A:297:MET:SD	1:A:297:MET:CE	2.04	1.45
25:C:306:PEK:H383	24:G:103:CDL:C27	1.49	1.38
1:A:312[A]:ILE:HD12	29:A:740:HOH:O	1.21	1.31
6:S:43:LYS:H	6:S:43:LYS:CD	1.43	1.26

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	515/514 (100%)	502 (98%)	12 (2%)	1 (0%)	44	42
1	N	515/514 (100%)	501 (97%)	14 (3%)	0	100	100
2	B	225/227 (99%)	216 (96%)	9 (4%)	0	100	100
2	O	225/227 (99%)	218 (97%)	6 (3%)	1 (0%)	30	27
3	C	260/261 (100%)	256 (98%)	4 (2%)	0	100	100
3	P	260/261 (100%)	255 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	132 (93%)	10 (7%)	0	100	100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	5	2
6	S	96/98 (98%)	91 (95%)	2 (2%)	3 (3%)	3	1
7	G	81/85 (95%)	70 (86%)	6 (7%)	5 (6%)	1	0
7	T	81/85 (95%)	66 (82%)	10 (12%)	5 (6%)	1	0
8	H	77/85 (91%)	70 (91%)	3 (4%)	4 (5%)	1	0
8	U	77/85 (91%)	71 (92%)	2 (3%)	4 (5%)	1	0
9	I	72/74 (97%)	71 (99%)	1 (1%)	0	100	100
9	V	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
All	All	3518/3616 (97%)	3388 (96%)	105 (3%)	25 (1%)	19	14

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	4	ALA
7	G	7	ASP
8	H	8	ILE
8	H	45	ALA

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	429/426 (101%)	418 (97%)	11 (3%)	41	44
1	N	429/426 (101%)	421 (98%)	8 (2%)	52	57
2	B	210/210 (100%)	198 (94%)	12 (6%)	17	14
2	O	210/210 (100%)	200 (95%)	10 (5%)	21	19
3	C	227/226 (100%)	224 (99%)	3 (1%)	65	71
3	P	227/226 (100%)	223 (98%)	4 (2%)	54	59
4	D	128/129 (99%)	123 (96%)	5 (4%)	27	27
4	Q	128/129 (99%)	122 (95%)	6 (5%)	22	20
5	E	92/95 (97%)	91 (99%)	1 (1%)	70	76
5	R	92/95 (97%)	88 (96%)	4 (4%)	25	23
6	F	81/81 (100%)	77 (95%)	4 (5%)	21	18
6	S	81/81 (100%)	77 (95%)	4 (5%)	21	18
7	G	67/68 (98%)	61 (91%)	6 (9%)	8	5
7	T	67/68 (98%)	61 (91%)	6 (9%)	8	5
8	H	71/75 (95%)	67 (94%)	4 (6%)	17	15
8	U	71/75 (95%)	64 (90%)	7 (10%)	6	4
9	I	58/58 (100%)	54 (93%)	4 (7%)	13	9
9	V	58/58 (100%)	55 (95%)	3 (5%)	19	17
10	J	49/50 (98%)	48 (98%)	1 (2%)	50	55
10	W	49/50 (98%)	48 (98%)	1 (2%)	50	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	39/46 (85%)	38 (97%)	1 (3%)	41	44
11	X	39/46 (85%)	37 (95%)	2 (5%)	20	17
12	L	39/40 (98%)	39 (100%)	0	100	100
12	Y	39/40 (98%)	36 (92%)	3 (8%)	10	7
13	M	37/38 (97%)	32 (86%)	5 (14%)	3	2
13	Z	37/38 (97%)	33 (89%)	4 (11%)	5	3
All	All	3054/3084 (99%)	2935 (96%)	119 (4%)	27	27

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	38	ARG
11	X	7	PRO
2	O	91	ASN
10	W	50	LEU
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	195	GLN
6	S	54	ASN
3	P	50	ASN
4	Q	143	ASN
6	S	94	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	A	1	1	8,9,10	1.07	0	8,9,11	5.58	3 (37%)
2	FME	B	1	2	8,9,10	2.01	1 (12%)	8,9,11	7.80	4 (50%)
1	FME	N	1	1	8,9,10	1.44	1 (12%)	8,9,11	6.15	3 (37%)
7	TPO	G	11	7	8,10,11	1.77	2 (25%)	10,14,16	1.52	2 (20%)
7	TPO	T	11	7	8,10,11	2.14	2 (25%)	10,14,16	1.75	1 (10%)
2	FME	O	1	2	8,9,10	0.88	0	8,9,11	4.35	5 (62%)

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	A	1	1	-	3/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	4/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
7	TPO	T	11	7	-	4/9/11/13	-
2	FME	O	1	2	-	1/7/9/11	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CA-N	4.46	1.53	1.46
7	T	11	TPO	P-O1P	3.45	1.61	1.50
1	N	1	FME	CA-N	3.30	1.51	1.46
7	G	11	TPO	P-O1P	3.21	1.60	1.50
7	T	11	TPO	P-OG1	2.97	1.64	1.59

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-20.20	91.75	122.82
1	N	1	FME	CA-N-CN	-16.07	98.11	122.82
1	A	1	FME	CA-N-CN	-15.24	99.38	122.82
2	O	1	FME	CA-N-CN	-10.62	106.50	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	O1-CN-N	6.69	142.60	125.32

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	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
7	T	11	TPO	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 and 2 are unknown - leaving 44 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	$\# Z > 2$
14	CYN	N	601	16	1,1,1	0.23	0	-		
24	CDL	C	303	-	99,99,99	1.49	13 (13%)	105,111,111	1.44	12 (11%)
19	TGL	N	610	-	62,62,62	1.58	6 (9%)	65,65,65	1.68	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PSC	O	303	-	51,51,51	1.21	3 (5%)	57,59,59	1.34	5 (8%)
19	TGL	N	609	-	62,62,62	1.35	6 (9%)	65,65,65	1.47	10 (15%)
25	PEK	G	102	-	52,52,52	0.98	3 (5%)	55,57,57	1.54	8 (14%)
25	PEK	P	309	-	52,52,52	1.21	2 (3%)	55,57,57	1.20	4 (7%)
28	DMU	Z	101	-	34,34,34	0.65	0	45,45,45	1.89	10 (22%)
20	PGV	C	307	-	50,50,50	1.44	4 (8%)	53,56,56	1.45	8 (15%)
20	PGV	N	608	-	50,50,50	1.05	3 (6%)	53,56,56	1.30	4 (7%)
24	CDL	G	103	-	99,99,99	1.50	12 (12%)	105,111,111	1.42	17 (16%)
25	PEK	C	306	-	52,52,52	1.15	2 (3%)	55,57,57	1.20	5 (9%)
22	CHD	P	307	-	32,32,32	0.81	1 (3%)	51,51,51	2.97	22 (43%)
22	CHD	B	302	-	32,32,32	1.11	3 (9%)	51,51,51	1.71	11 (21%)
15	HEA	A	602	1	58,67,67	1.76	14 (24%)	63,103,103	2.74	27 (42%)
19	TGL	A	607	-	62,62,62	1.42	7 (11%)	65,65,65	2.29	16 (24%)
22	CHD	C	305	-	32,32,32	1.24	4 (12%)	51,51,51	1.74	12 (23%)
15	HEA	N	602	1	58,67,67	1.56	11 (18%)	63,103,103	2.80	30 (47%)
21	CUA	O	301	2	0,1,1	-	-	-		
28	DMU	M	101	-	34,34,34	0.60	0	45,45,45	1.94	12 (26%)
28	DMU	P	301	-	34,34,34	0.95	1 (2%)	45,45,45	2.39	12 (26%)
20	PGV	A	608	-	50,50,50	0.97	2 (4%)	53,56,56	1.46	5 (9%)
28	DMU	G	101	-	34,34,34	0.86	2 (5%)	45,45,45	2.45	13 (28%)
25	PEK	T	101	-	52,52,52	1.22	2 (3%)	55,57,57	1.27	6 (10%)
19	TGL	Q	201	-	62,62,62	1.37	6 (9%)	65,65,65	1.48	9 (13%)
19	TGL	L	101	-	62,62,62	1.58	7 (11%)	65,65,65	1.68	14 (21%)
22	CHD	C	304	-	32,32,32	0.77	1 (3%)	51,51,51	2.63	23 (45%)
15	HEA	N	603	1	58,67,67	1.66	12 (20%)	63,103,103	1.99	26 (41%)
20	PGV	A	609	-	50,50,50	1.24	2 (4%)	53,56,56	1.47	9 (16%)
21	CUA	B	301	2	0,1,1	-	-	-		
22	CHD	P	308	-	32,32,32	1.18	3 (9%)	51,51,51	1.85	17 (33%)
22	CHD	O	302	-	32,32,32	1.10	3 (9%)	51,51,51	1.69	10 (19%)
24	CDL	P	306	-	99,99,99	1.49	12 (12%)	105,111,111	1.40	11 (10%)
25	PEK	P	304	-	52,52,52	0.86	3 (5%)	55,57,57	1.67	9 (16%)
25	PEK	G	104	-	52,52,52	1.13	2 (3%)	55,57,57	1.18	6 (10%)
20	PGV	P	302	-	50,50,50	1.15	2 (4%)	53,56,56	1.25	3 (5%)
15	HEA	A	603	1	58,67,67	1.65	12 (20%)	63,103,103	2.31	24 (38%)
26	PSC	E	201	-	51,51,51	1.31	3 (5%)	57,59,59	1.25	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	C	302	-	50,50,50	0.93	3 (6%)	53,56,56	1.10	4 (7%)
20	PGV	N	607	-	50,50,50	1.03	2 (4%)	53,56,56	1.57	7 (13%)
20	PGV	P	305	-	50,50,50	0.90	2 (4%)	53,56,56	1.14	5 (9%)
24	CDL	T	102	-	99,99,99	1.45	12 (12%)	105,111,111	1.38	12 (11%)
19	TGL	D	201	-	62,62,62	1.49	7 (11%)	65,65,65	1.48	14 (21%)
14	CYN	A	601	16	1,1,1	0.22	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
19	TGL	N	610	-	-	36/65/65/65	-
26	PSC	O	303	-	-	35/55/55/55	-
19	TGL	N	609	-	-	33/65/65/65	-
25	PEK	G	102	-	-	23/56/56/56	-
25	PEK	P	309	-	-	22/56/56/56	-
28	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
20	PGV	C	307	-	-	30/55/55/55	-
20	PGV	N	608	-	-	13/55/55/55	-
24	CDL	G	103	-	-	56/110/110/110	-
25	PEK	C	306	-	-	31/56/56/56	-
22	CHD	P	307	-	-	8/9/74/74	0/4/4/4
22	CHD	B	302	-	-	2/9/74/74	0/4/4/4
15	HEA	A	602	1	-	5/32/76/76	-
19	TGL	A	607	-	-	36/65/65/65	-
22	CHD	C	305	-	-	1/9/74/74	0/4/4/4
15	HEA	N	602	1	-	7/32/76/76	-
28	DMU	M	101	-	-	7/19/59/59	0/2/2/2
28	DMU	P	301	-	-	7/19/59/59	0/2/2/2
20	PGV	A	608	-	-	10/55/55/55	-
28	DMU	G	101	-	-	12/19/59/59	0/2/2/2
25	PEK	T	101	-	-	36/56/56/56	-
19	TGL	Q	201	-	-	36/65/65/65	-
19	TGL	L	101	-	-	36/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	C	304	-	-	5/9/74/74	0/4/4/4
15	HEA	N	603	1	-	4/32/76/76	-
20	PGV	A	609	-	-	32/55/55/55	-
22	CHD	P	308	-	-	1/9/74/74	0/4/4/4
22	CHD	O	302	-	-	2/9/74/74	0/4/4/4
24	CDL	P	306	-	-	72/110/110/110	-
25	PEK	P	304	-	-	26/56/56/56	-
25	PEK	G	104	-	-	32/56/56/56	-
20	PGV	P	302	-	-	33/55/55/55	-
15	HEA	A	603	1	-	5/32/76/76	-
26	PSC	E	201	-	-	36/55/55/55	-
20	PGV	C	302	-	-	16/55/55/55	-
20	PGV	N	607	-	-	29/55/55/55	-
20	PGV	P	305	-	-	16/55/55/55	-
24	CDL	T	102	-	-	54/110/110/110	-
19	TGL	D	201	-	-	39/65/65/65	-
24	CDL	C	303	-	-	67/110/110/110	-

The worst 5 of 195 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	610	TGL	OG2-CB1	6.08	1.51	1.34
20	C	307	PGV	O01-C1	6.07	1.51	1.34
19	L	101	TGL	OG2-CB1	5.98	1.51	1.34
20	C	307	PGV	O03-C19	5.86	1.50	1.33
24	P	306	CDL	OA8-CA7	5.44	1.49	1.33

The worst 5 of 471 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	602	HEA	C17-C18-C19	-10.69	103.15	127.62
15	A	602	HEA	C20-C19-C18	-9.49	99.87	121.17
28	P	301	DMU	O16-C6-C1	9.42	122.58	108.27
19	A	607	TGL	CG2-OG2-CB1	9.15	139.70	117.80
28	G	101	DMU	O1-C9-C11	8.13	126.60	106.44

There are no chirality outliers.

5 of 957 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	602	HEA	C16-C17-C18-C19
19	A	607	TGL	CB2-CB1-OG2-CG2
19	D	201	TGL	CC2-CC1-OG3-CG3
20	A	609	PGV	C03-O11-P-O12
20	A	609	PGV	C03-O11-P-O13

There are no ring outliers.

37 monomers are involved in 286 short contacts:

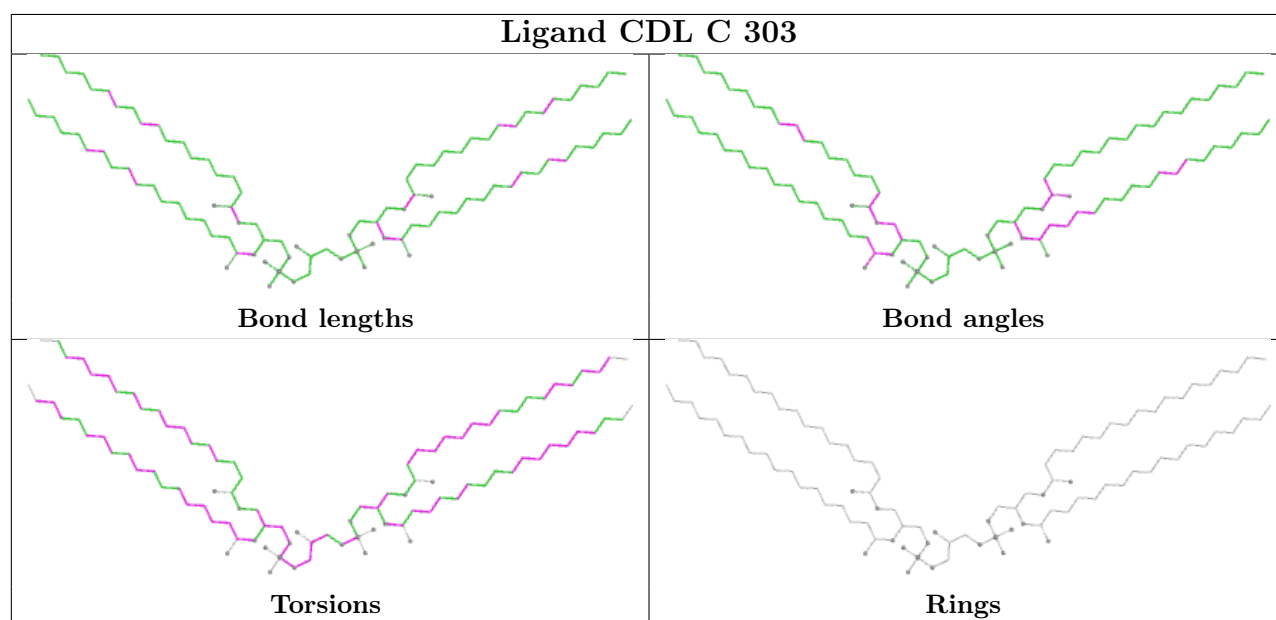
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	303	CDL	17	0
19	N	610	TGL	14	0
26	O	303	PSC	17	0
19	N	609	TGL	8	0
25	G	102	PEK	2	0
25	P	309	PEK	8	0
20	C	307	PGV	3	0
20	N	608	PGV	1	0
24	G	103	CDL	26	0
25	C	306	PEK	6	0
22	P	307	CHD	7	0
22	B	302	CHD	2	0
15	A	602	HEA	7	0
19	A	607	TGL	6	0
22	C	305	CHD	1	0
15	N	602	HEA	6	0
28	P	301	DMU	3	0
28	G	101	DMU	4	0
25	T	101	PEK	22	0
19	Q	201	TGL	2	0
19	L	101	TGL	14	0
22	C	304	CHD	5	0
15	N	603	HEA	2	0
20	A	609	PGV	8	0
22	P	308	CHD	1	0
22	O	302	CHD	1	0
24	P	306	CDL	20	0
25	P	304	PEK	5	0
25	G	104	PEK	11	0
20	P	302	PGV	2	0
15	A	603	HEA	2	0
26	E	201	PSC	16	0
20	C	302	PGV	2	0

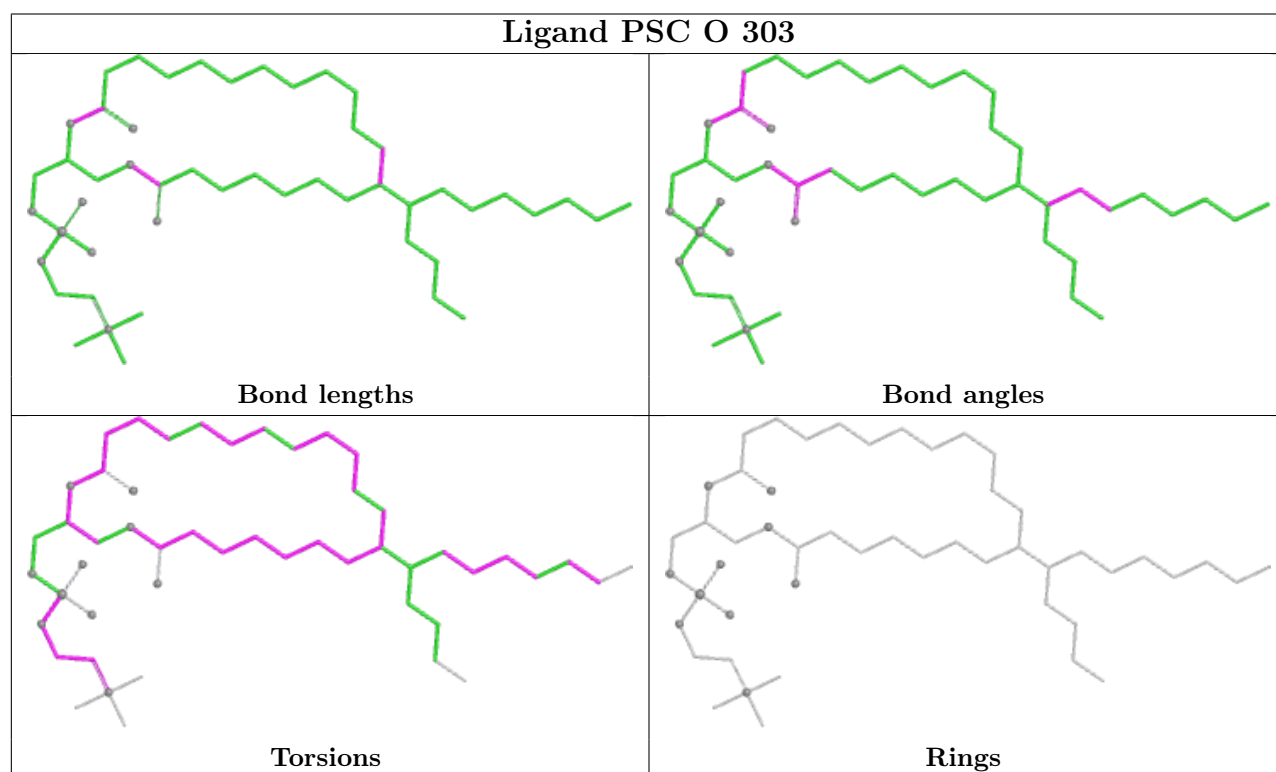
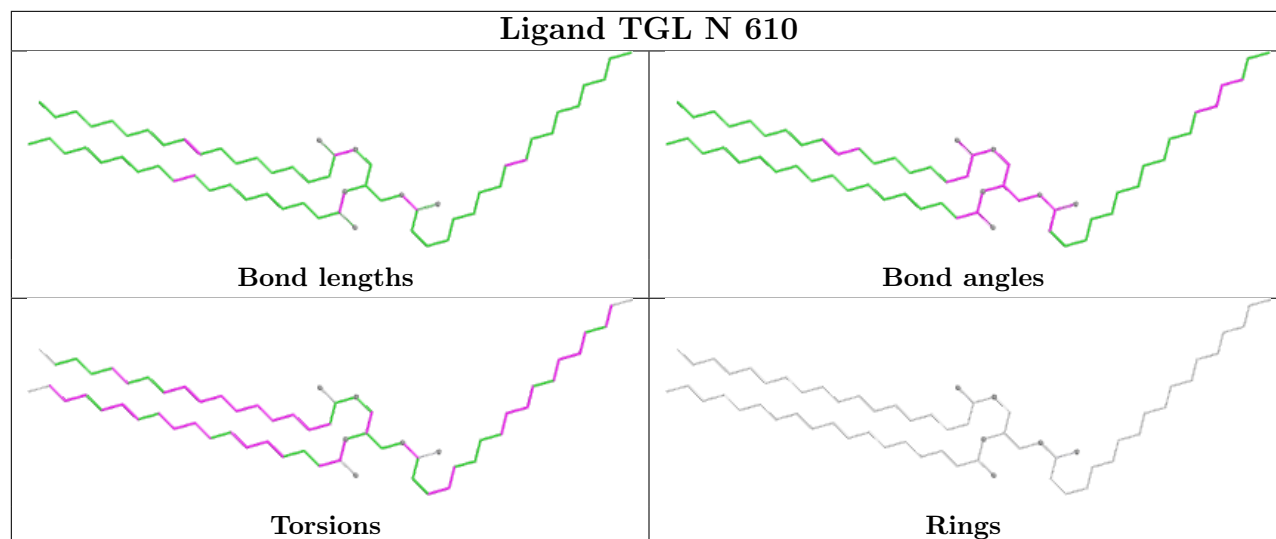
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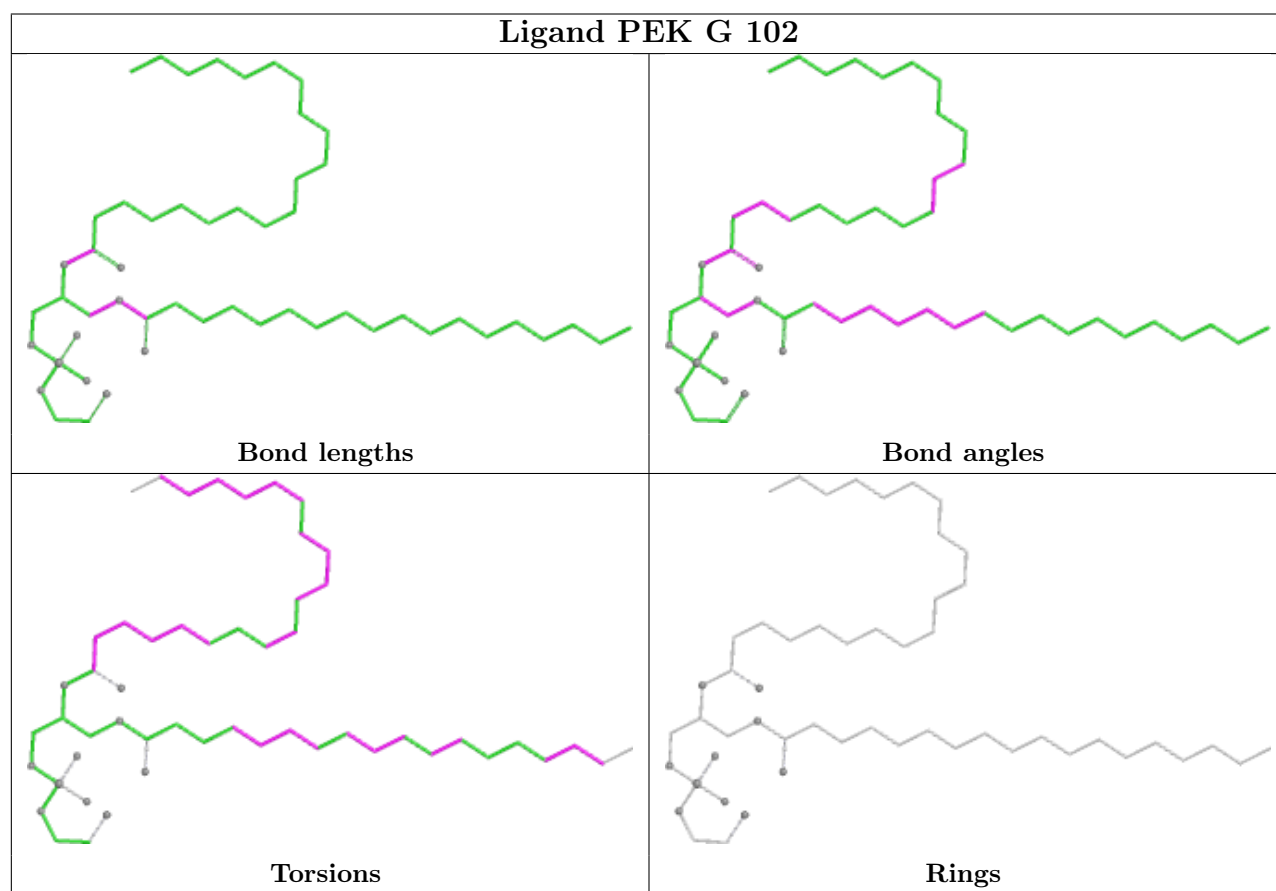
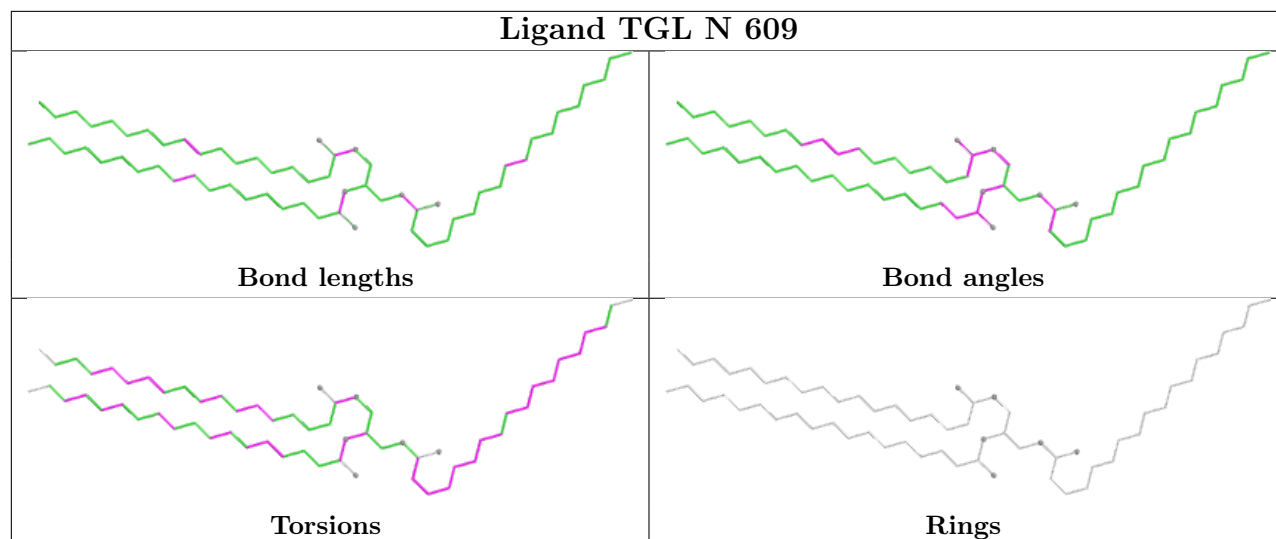
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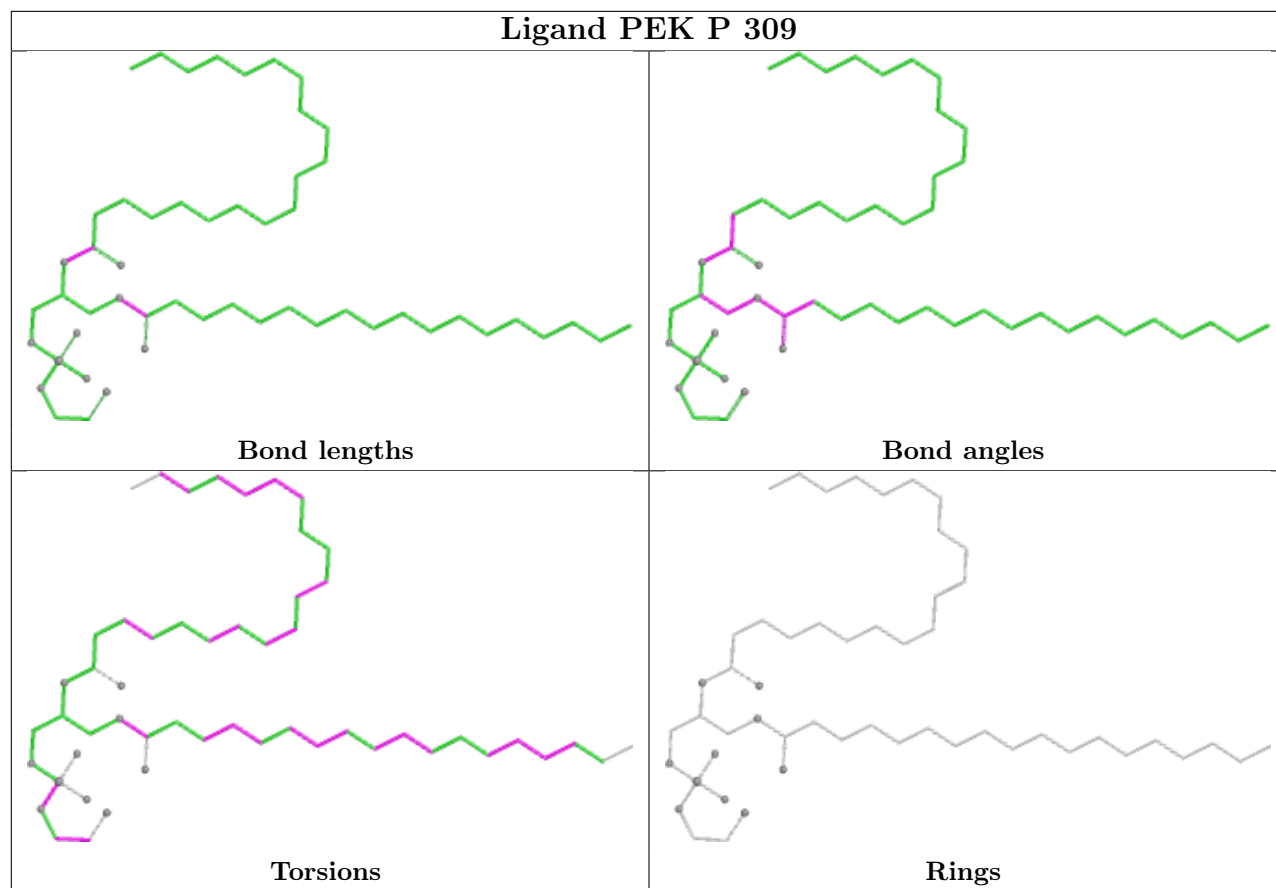
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	N	607	PGV	9	0
20	P	305	PGV	3	0
24	T	102	CDL	27	0
19	D	201	TGL	12	0

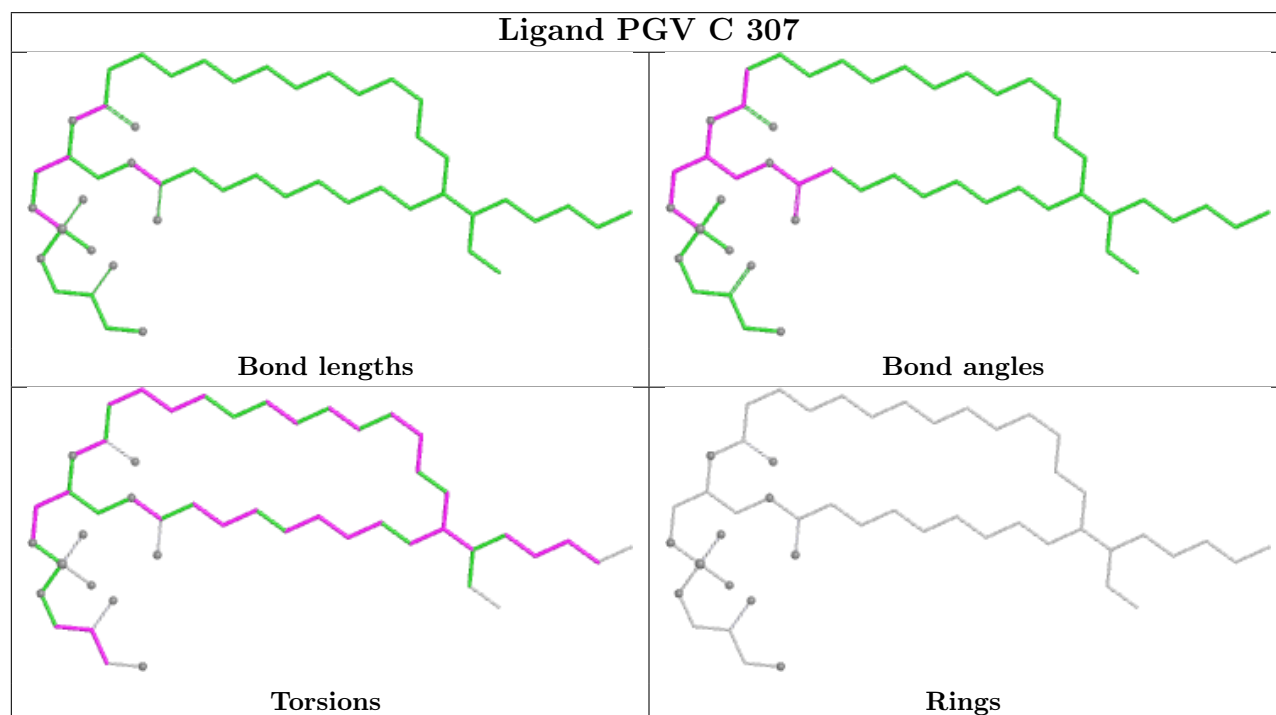
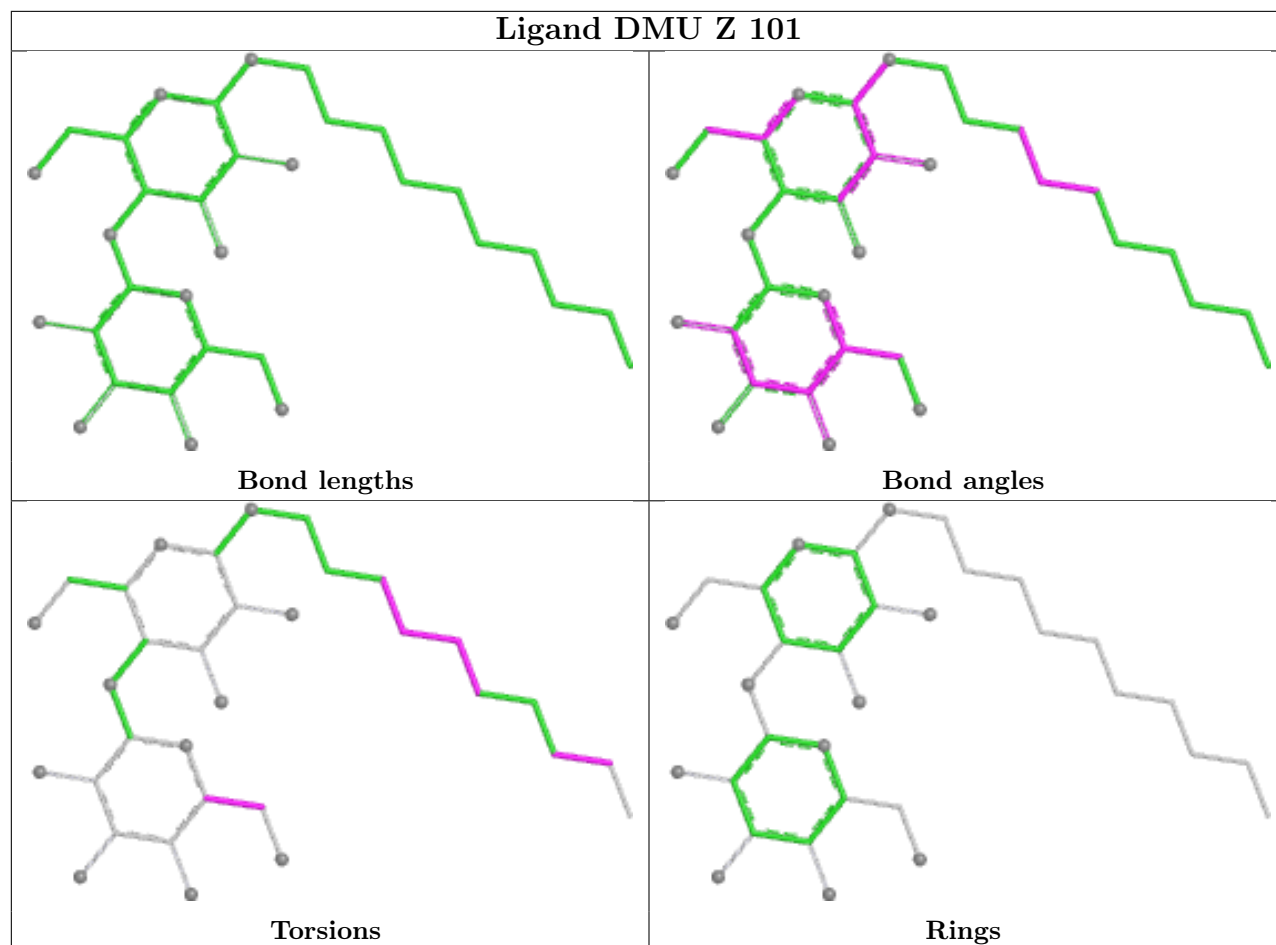
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

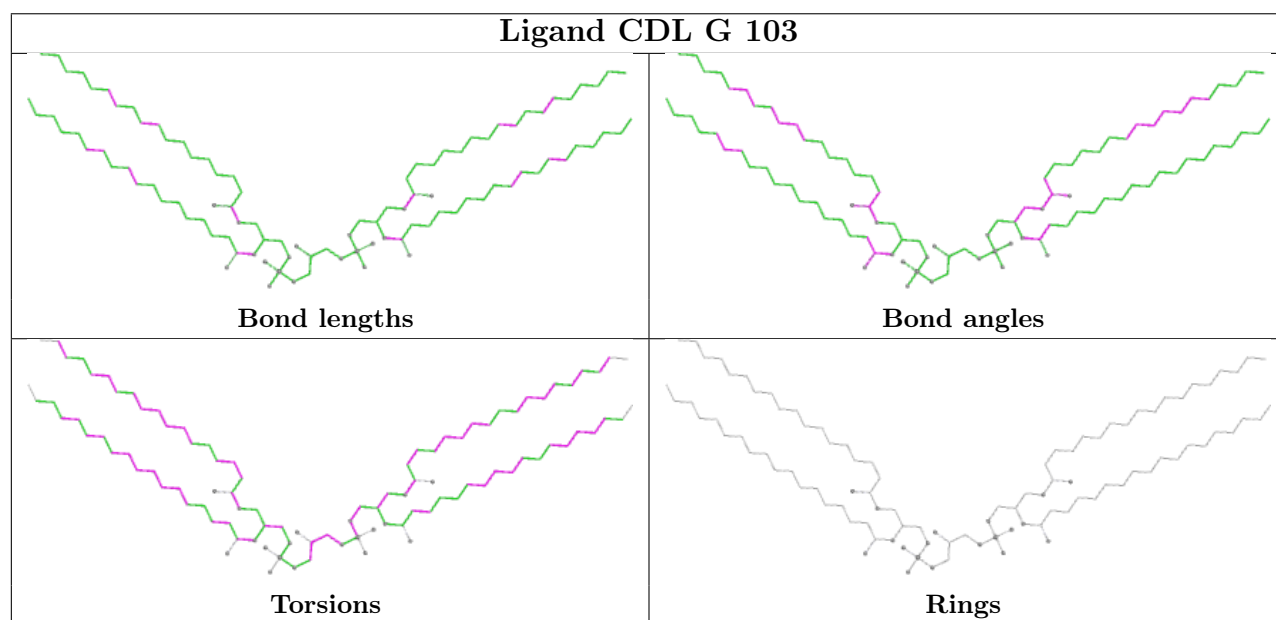
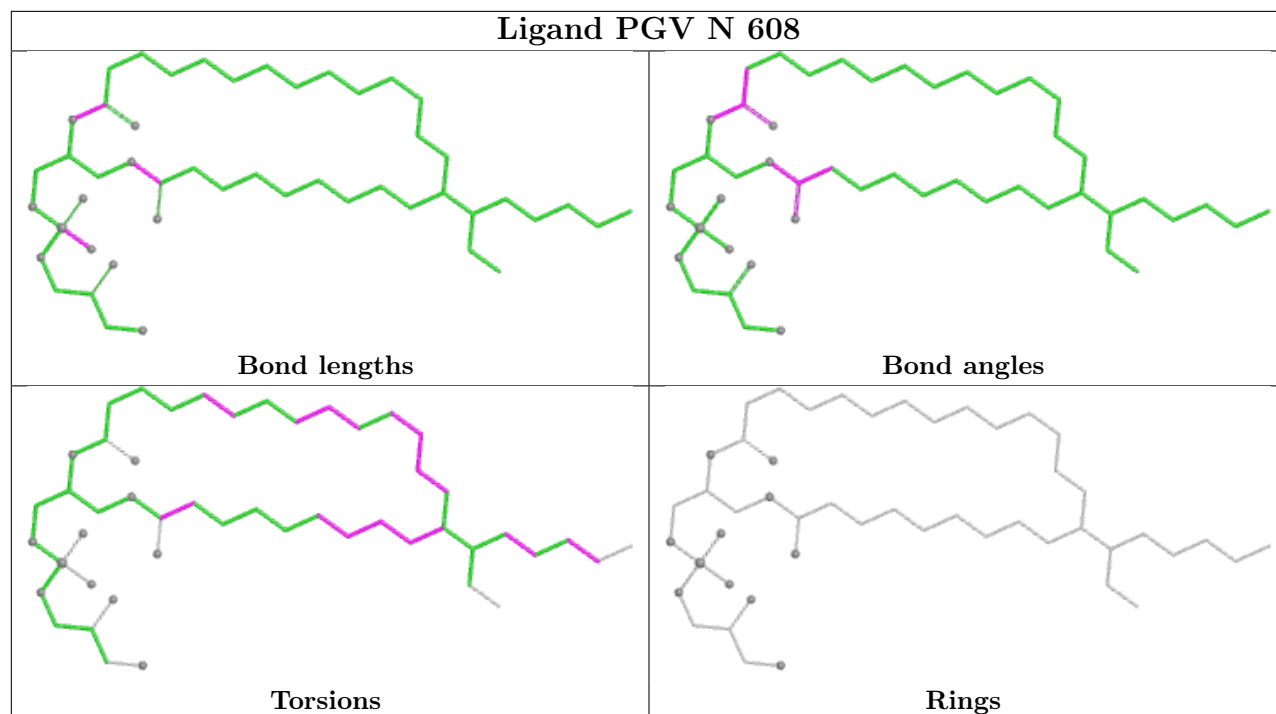




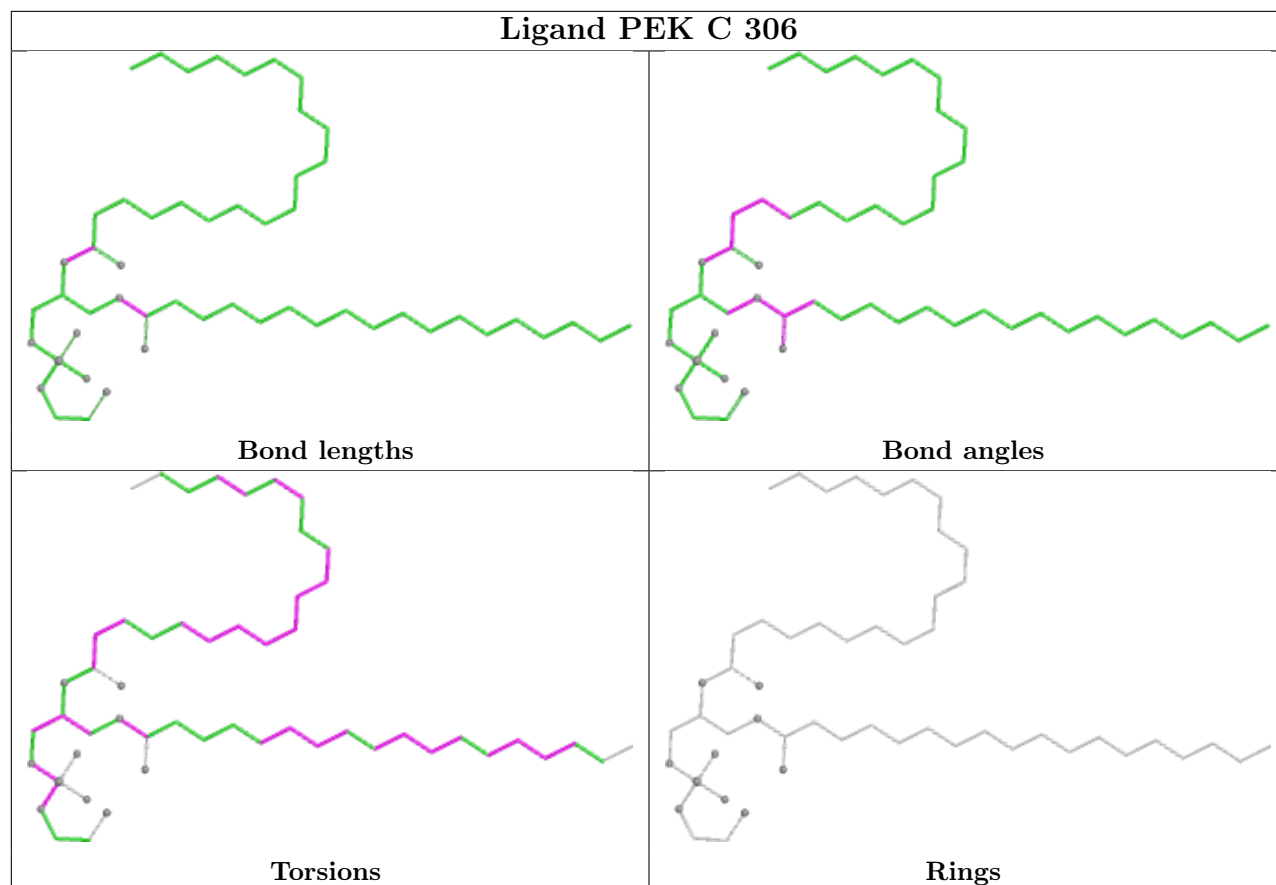




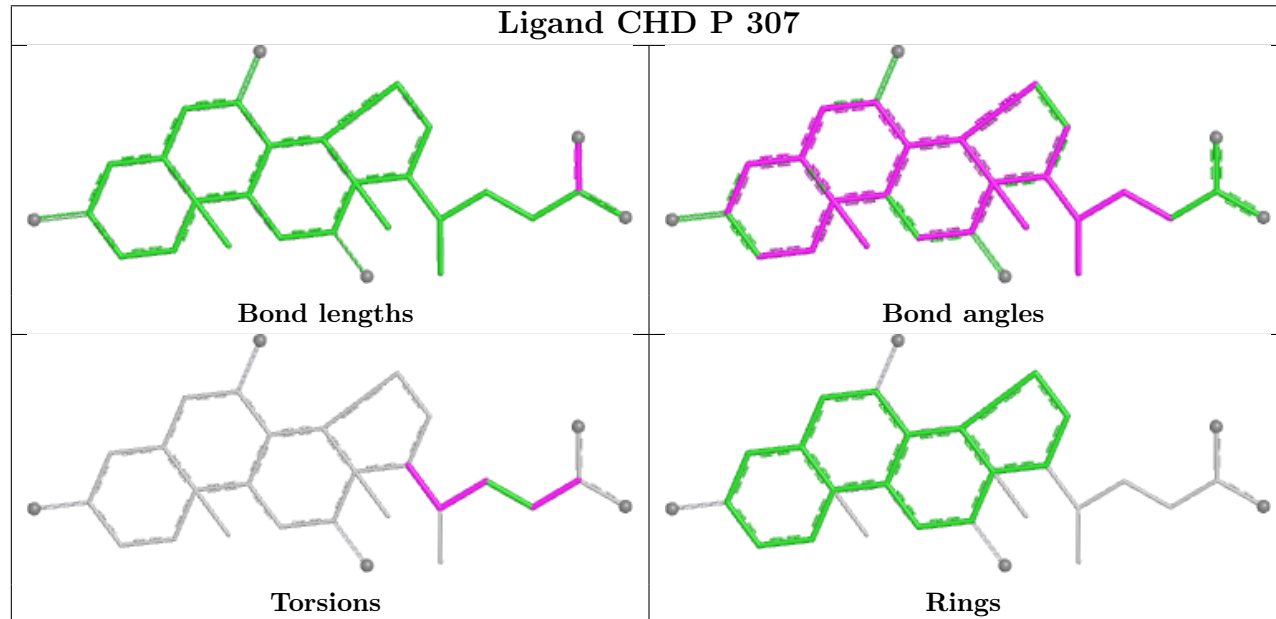


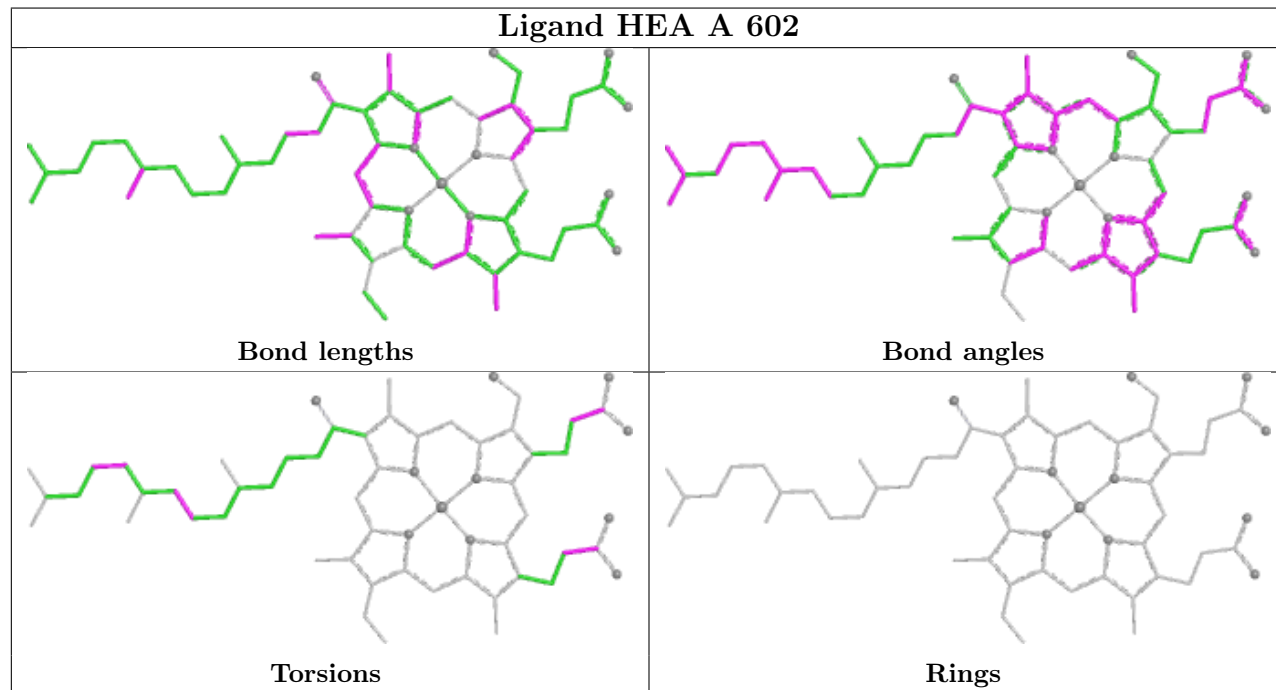
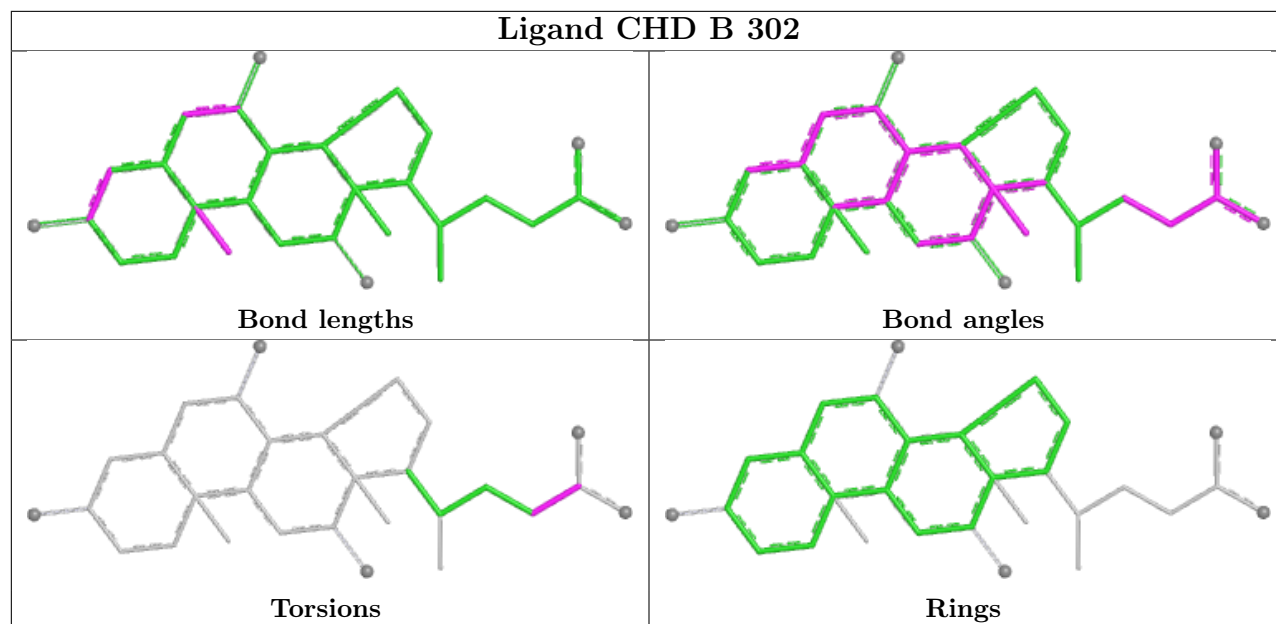


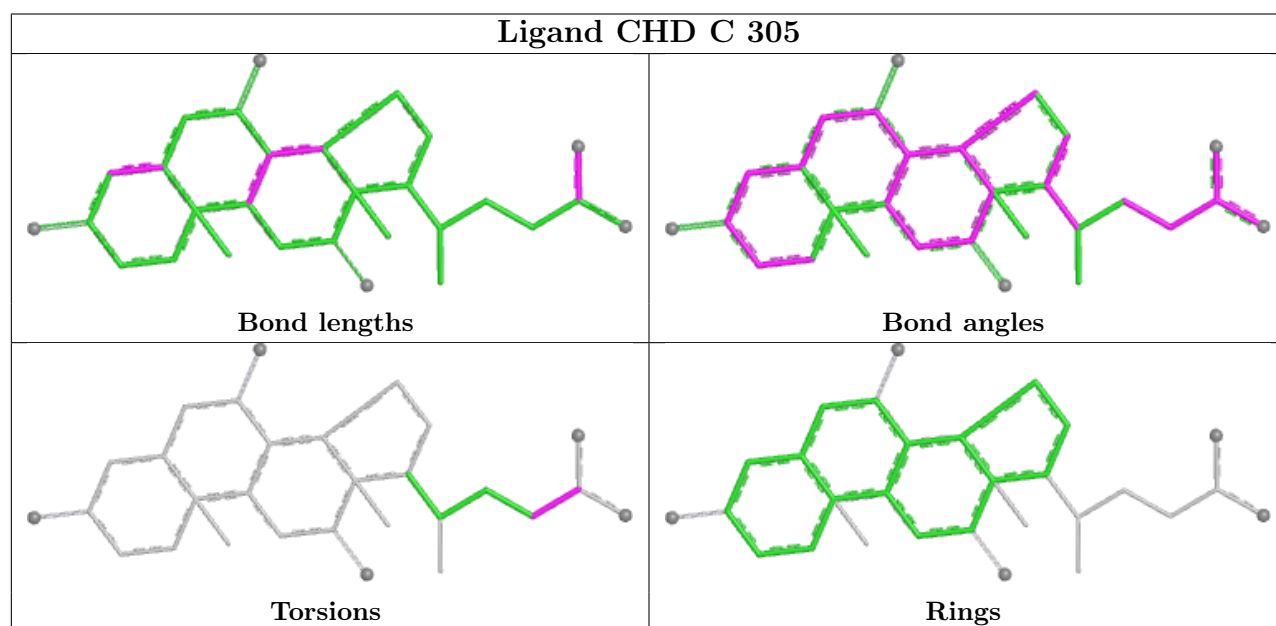
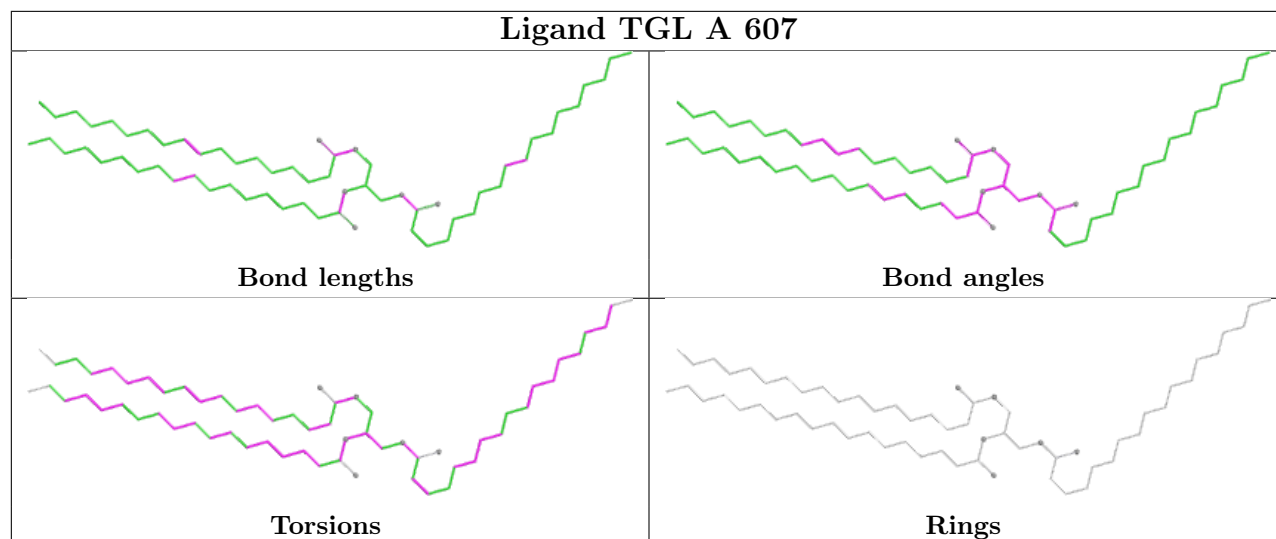
Ligand PEK C 306

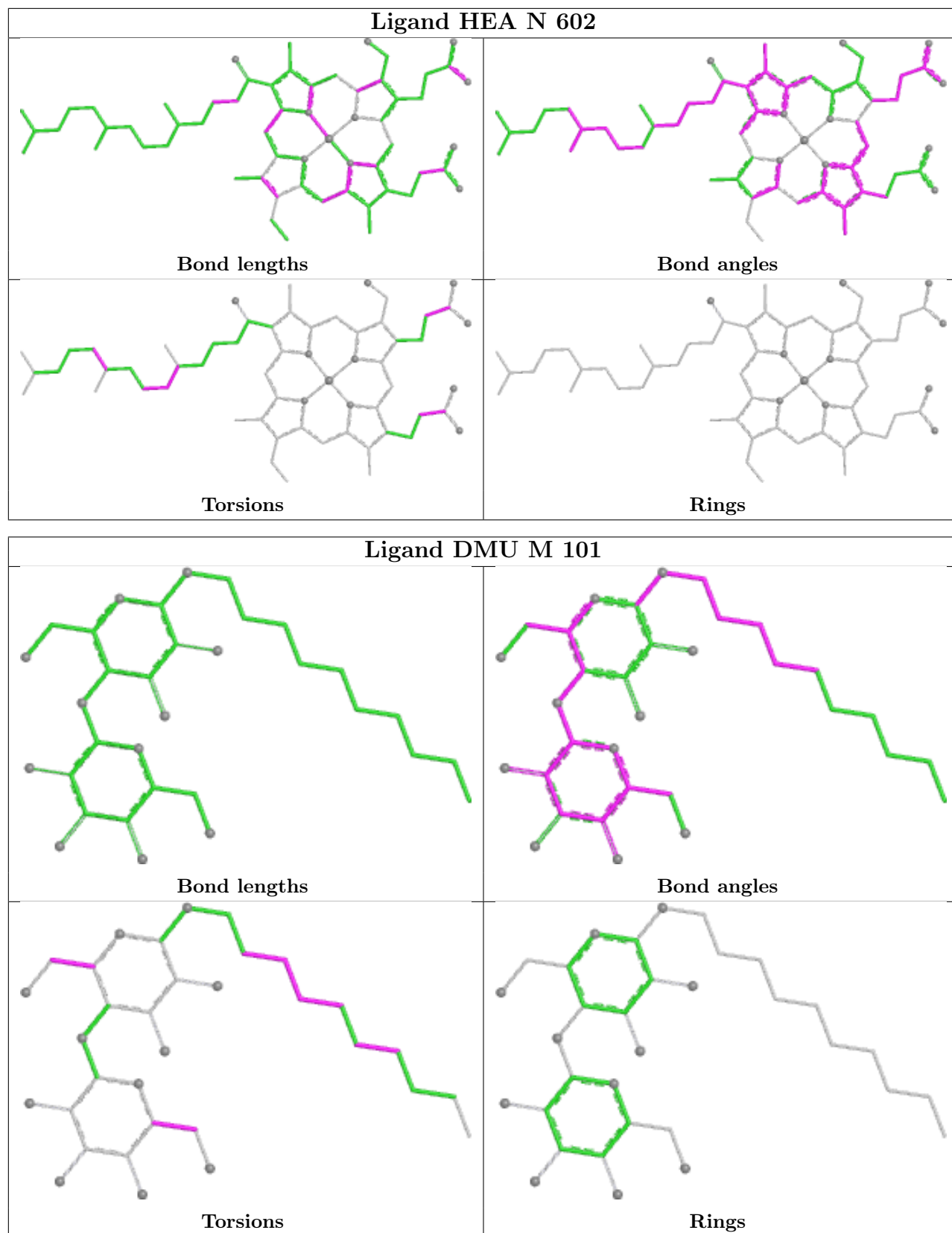


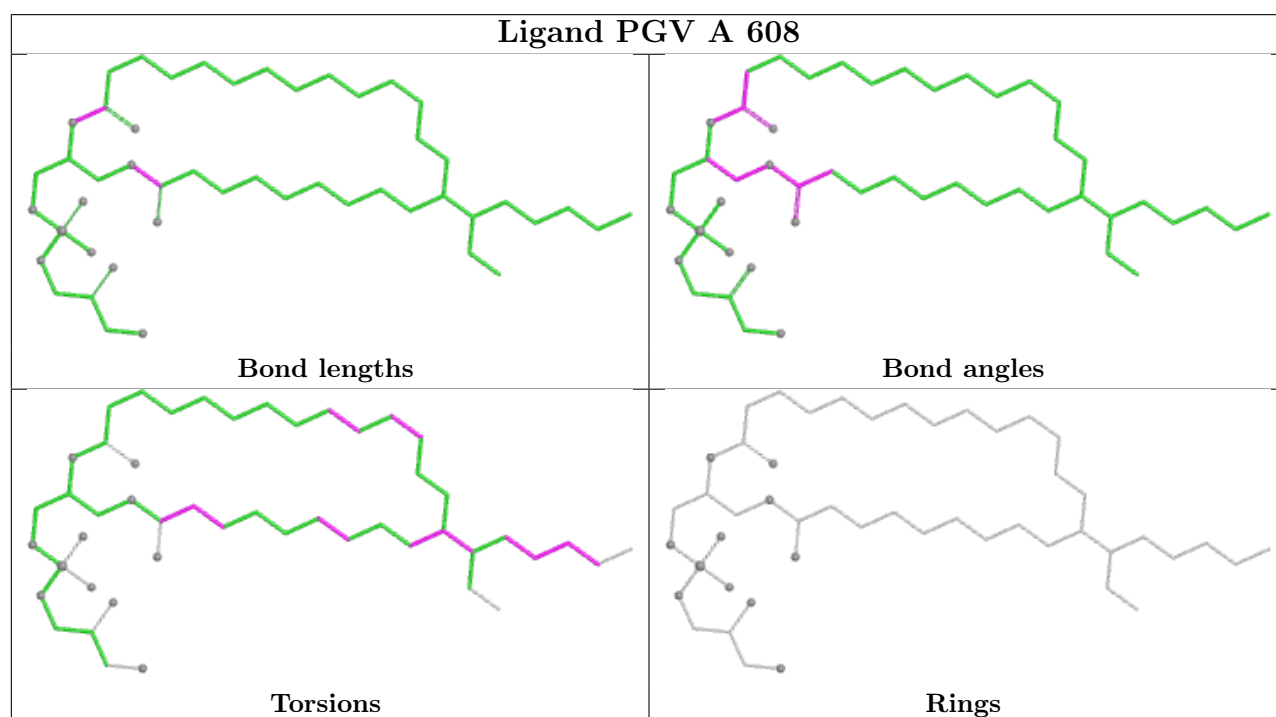
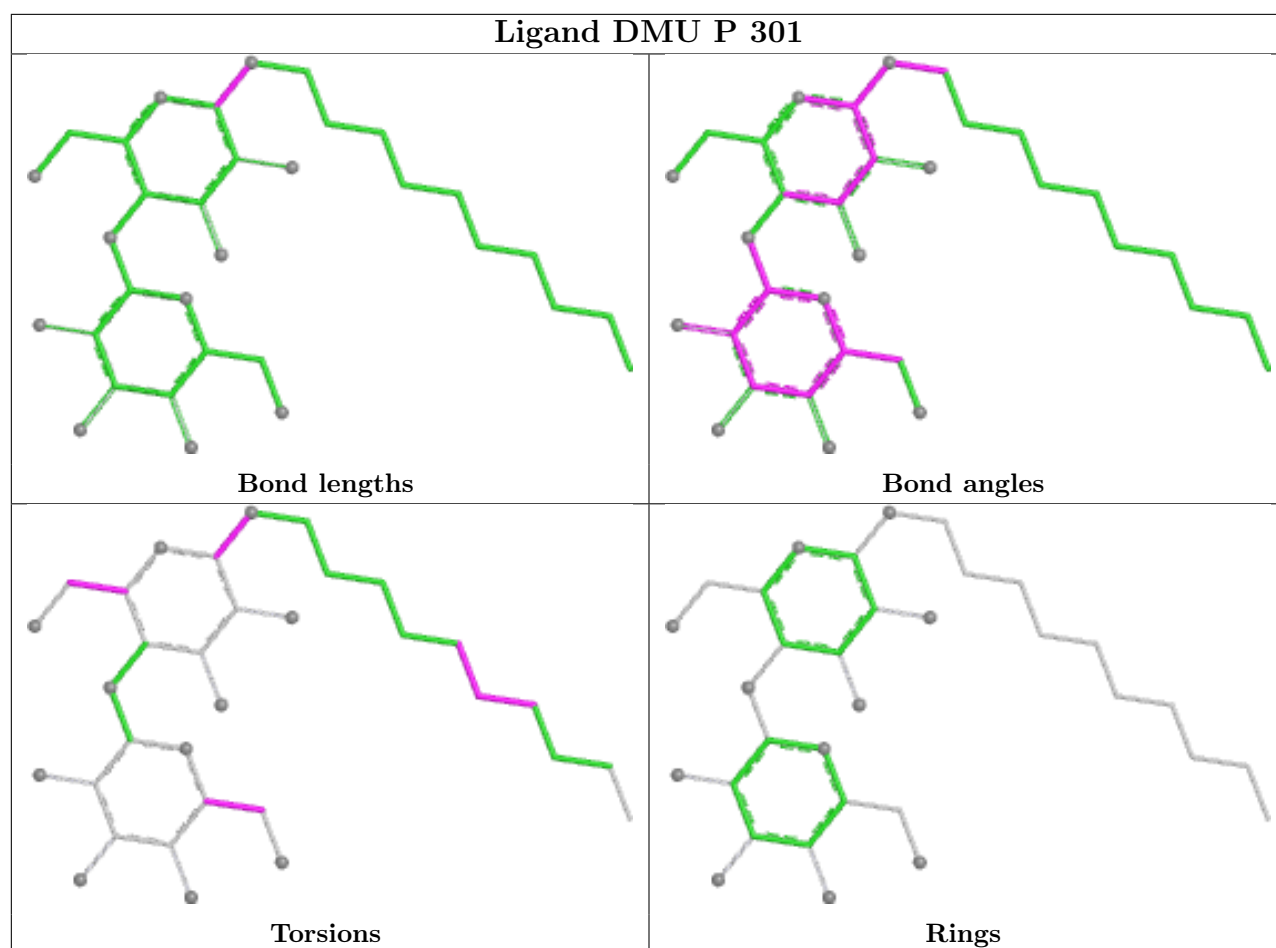
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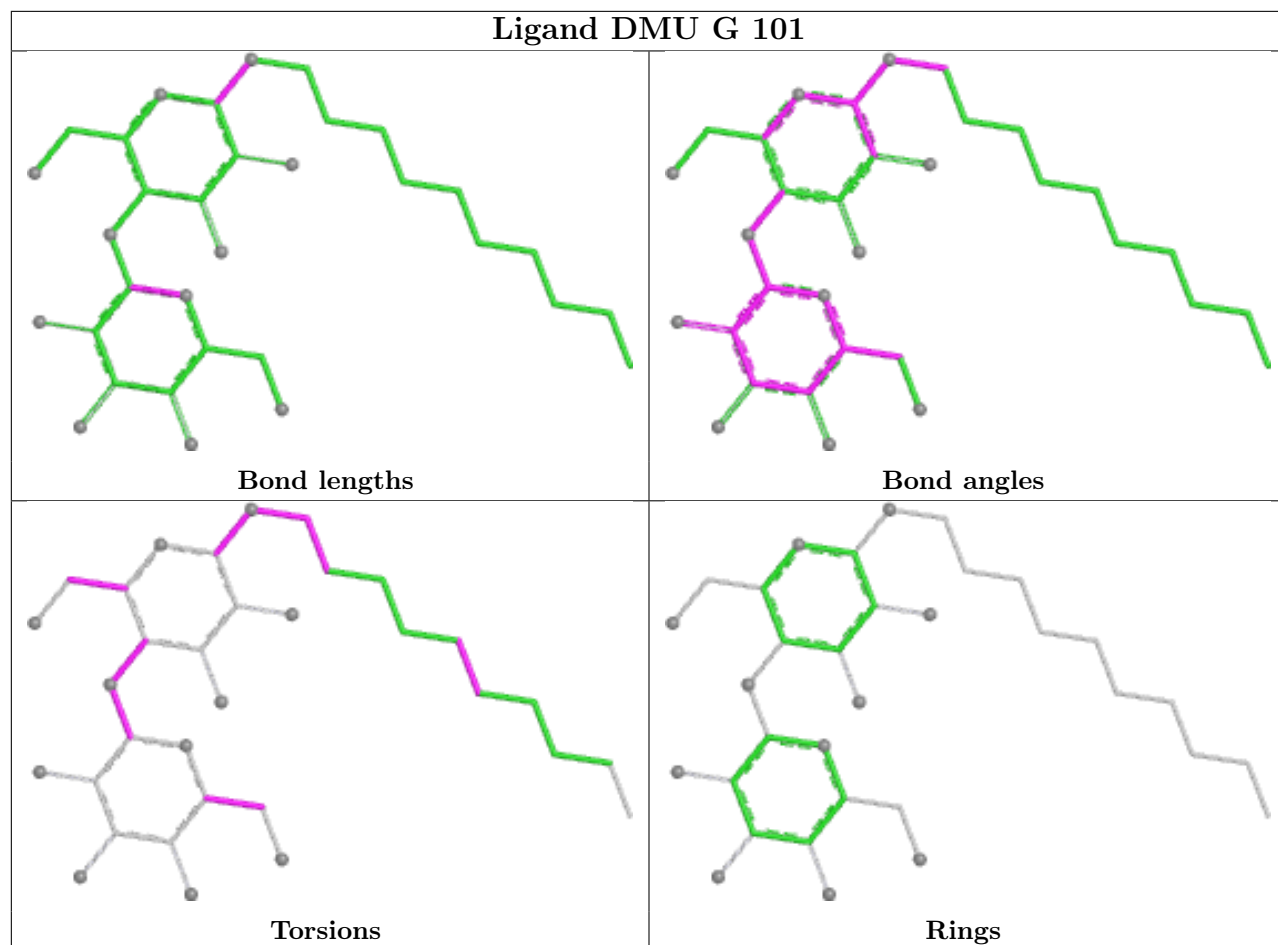




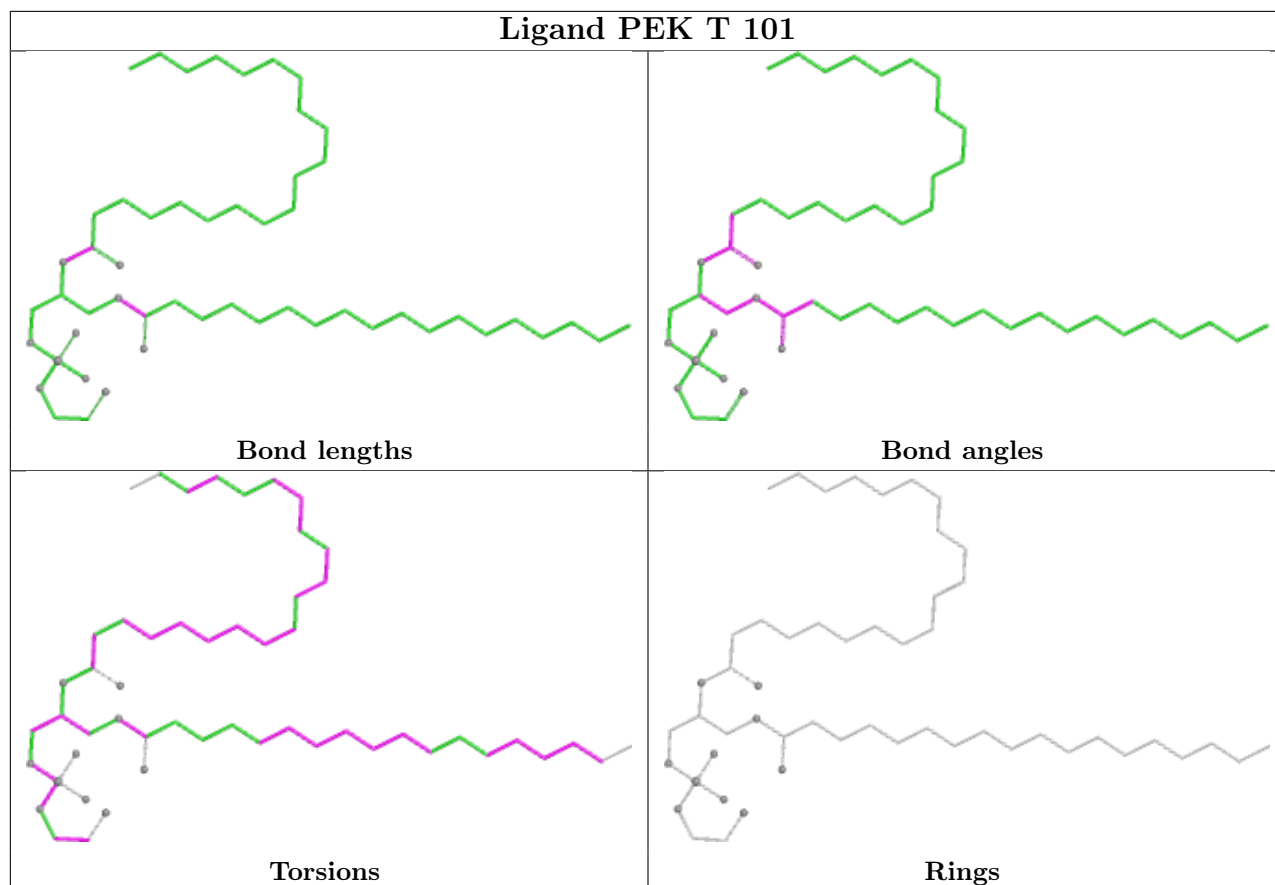




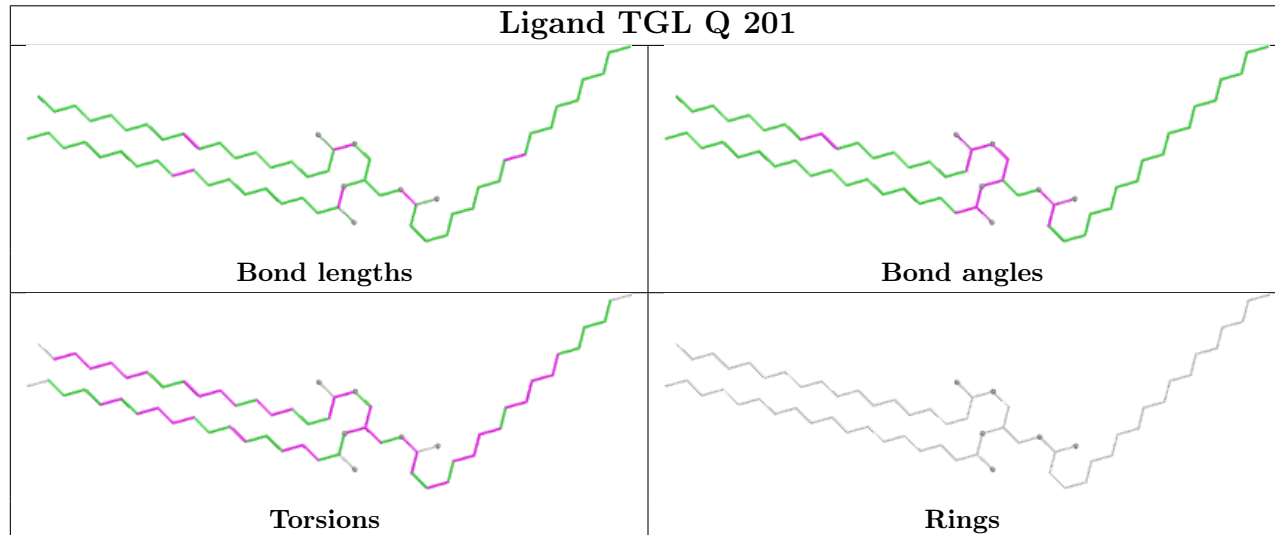


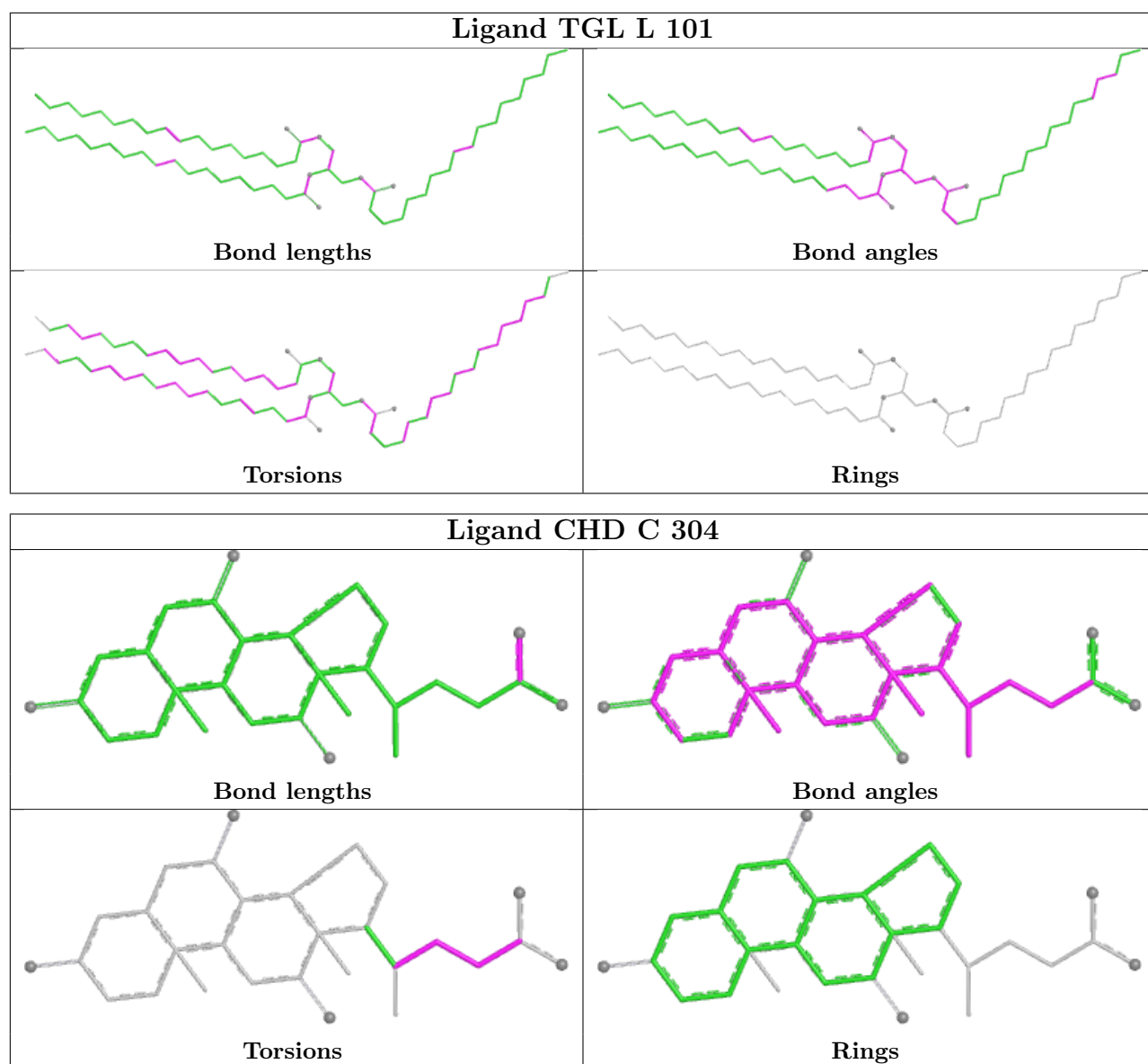


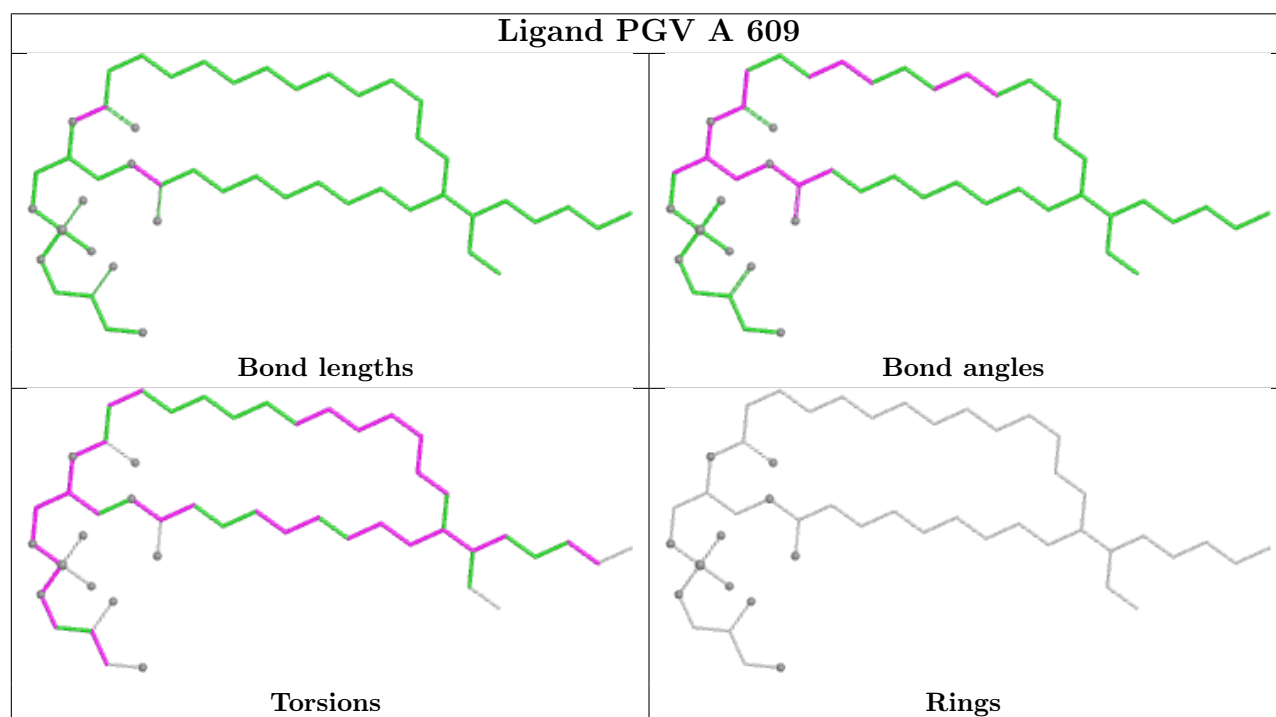
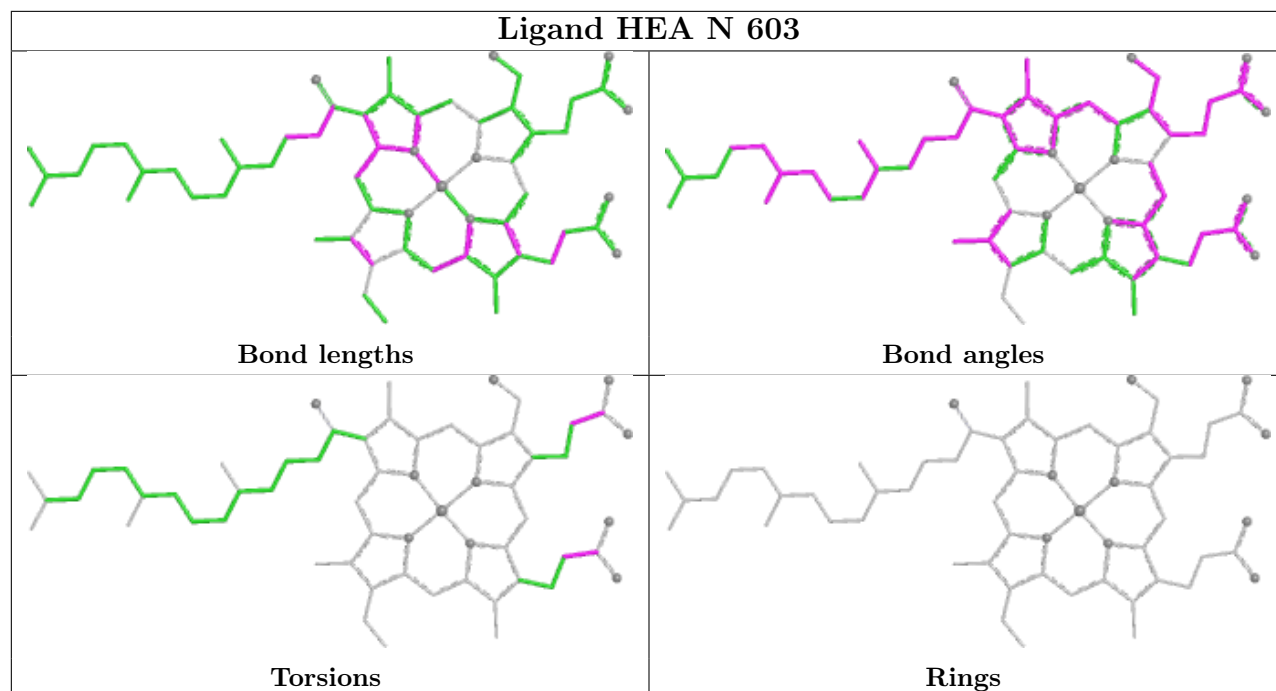
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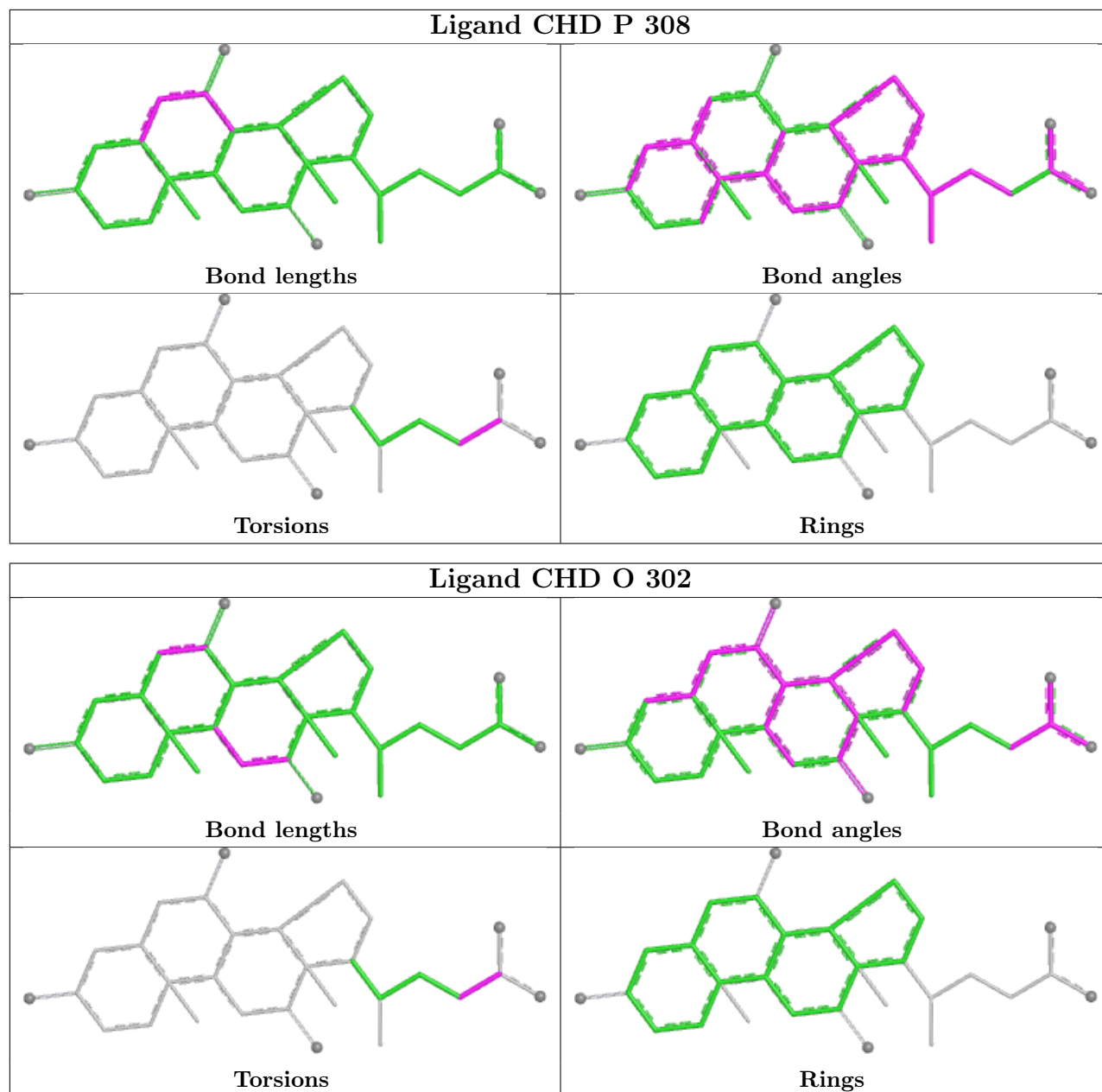


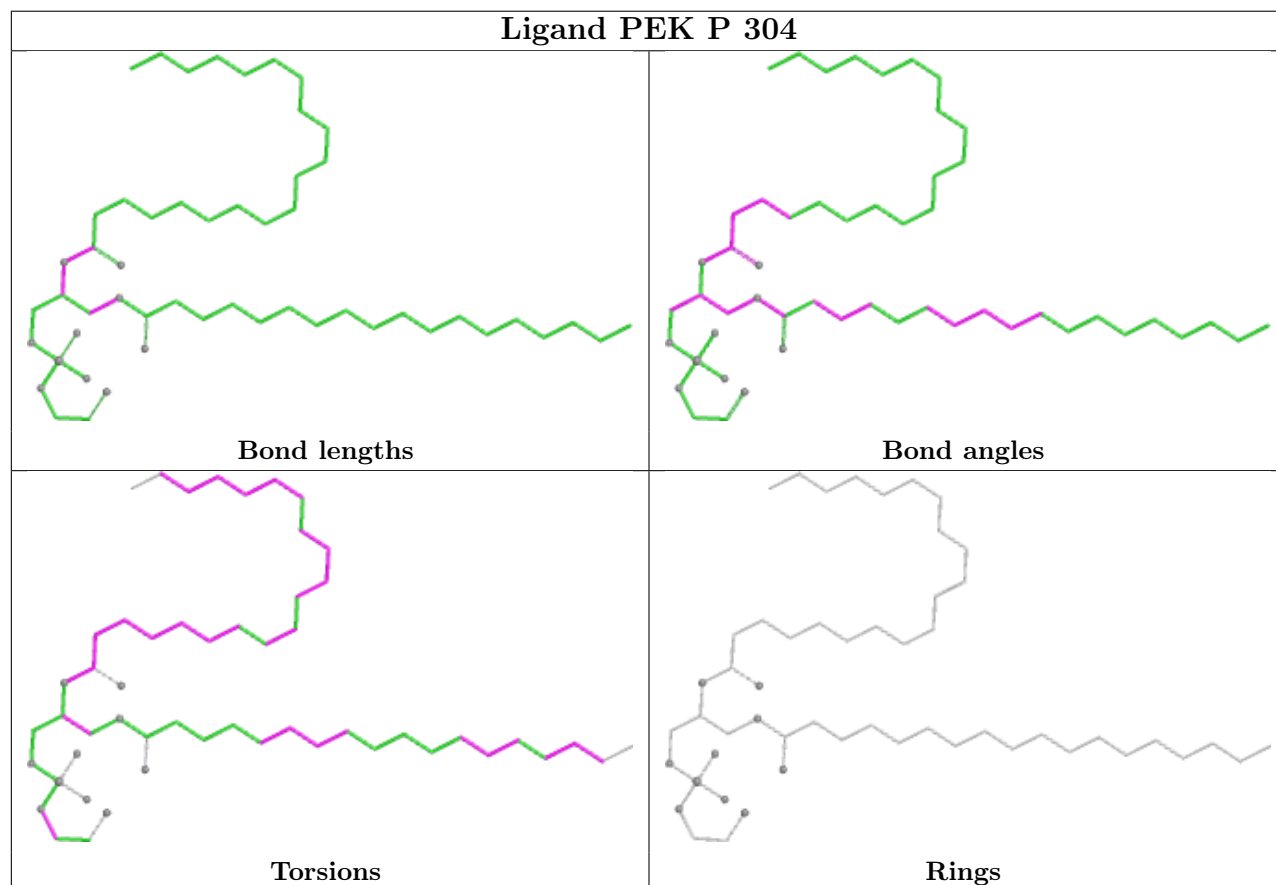
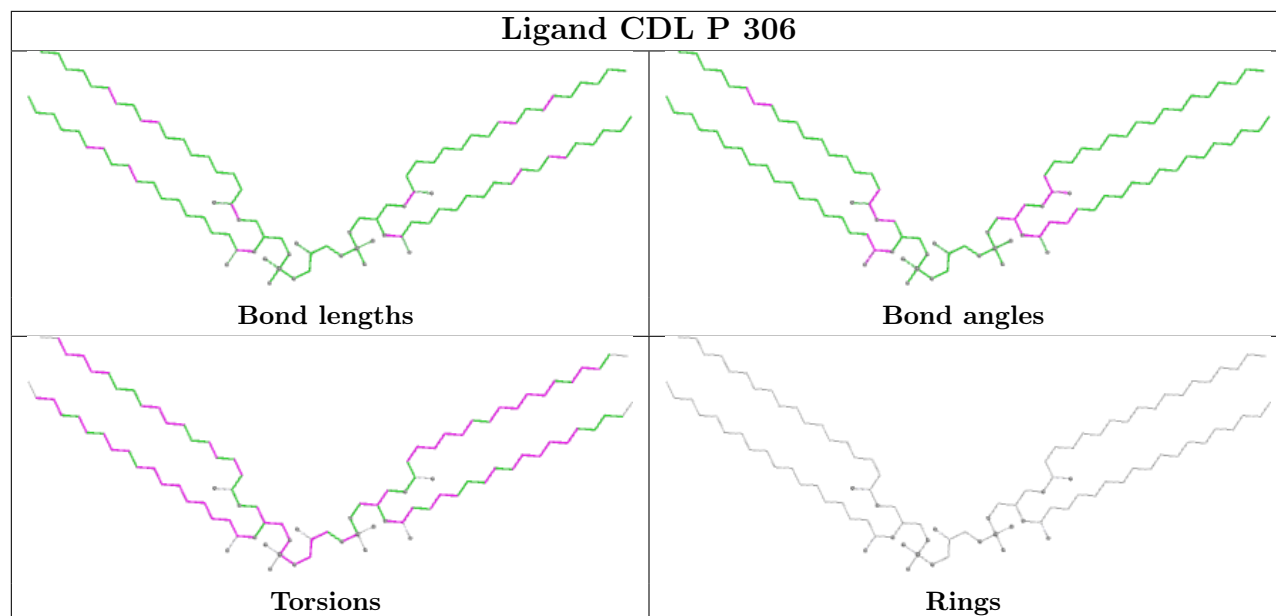
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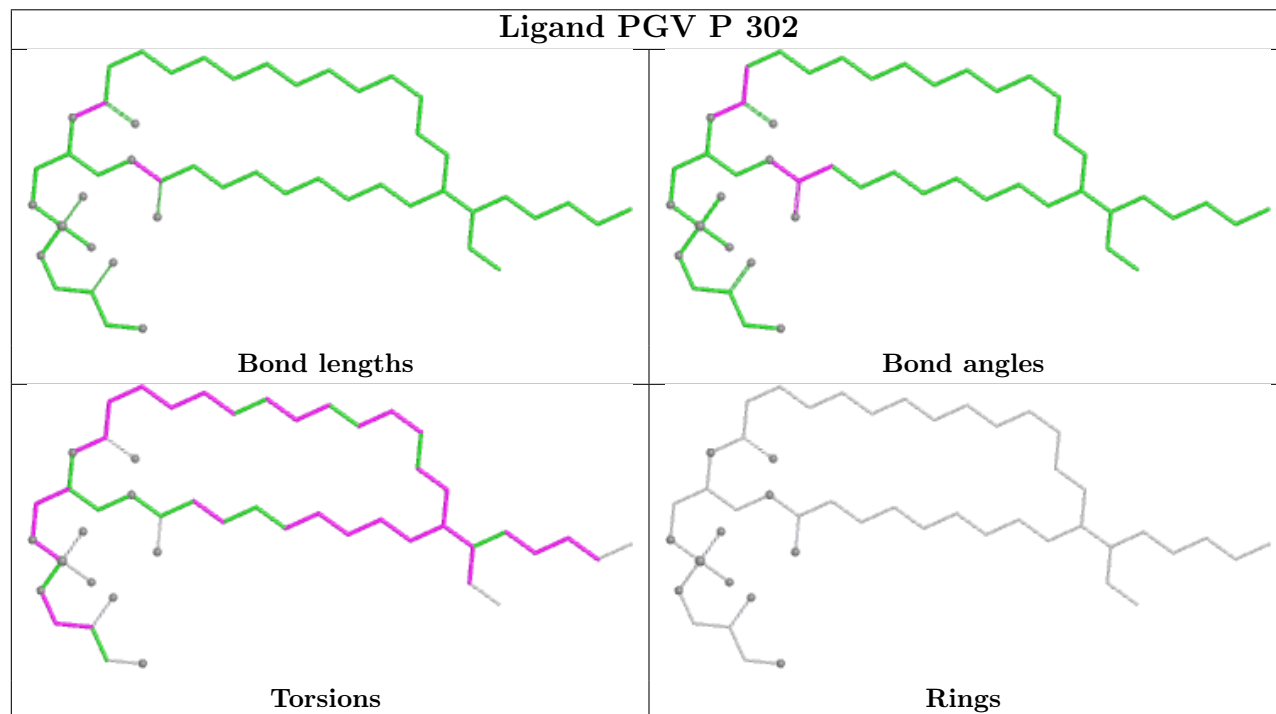
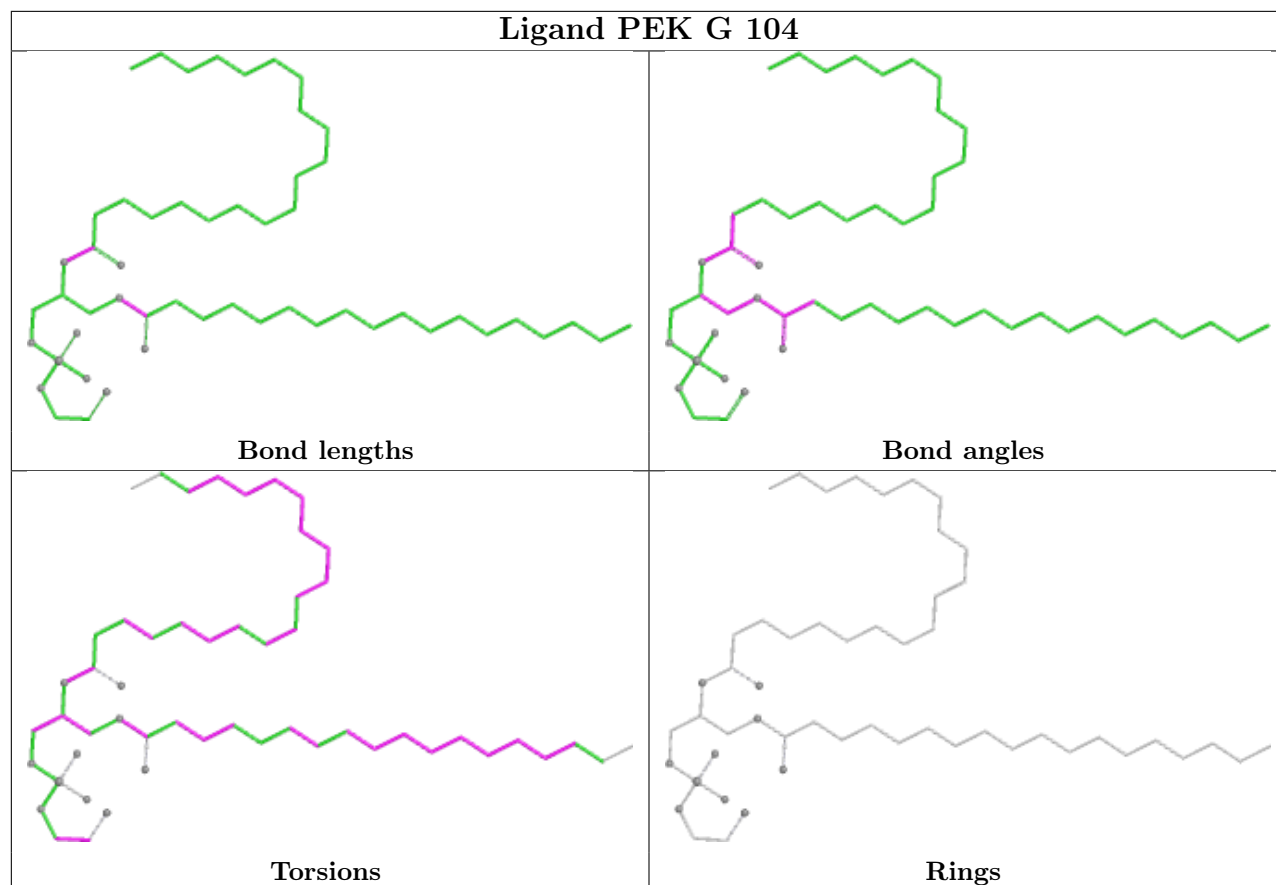


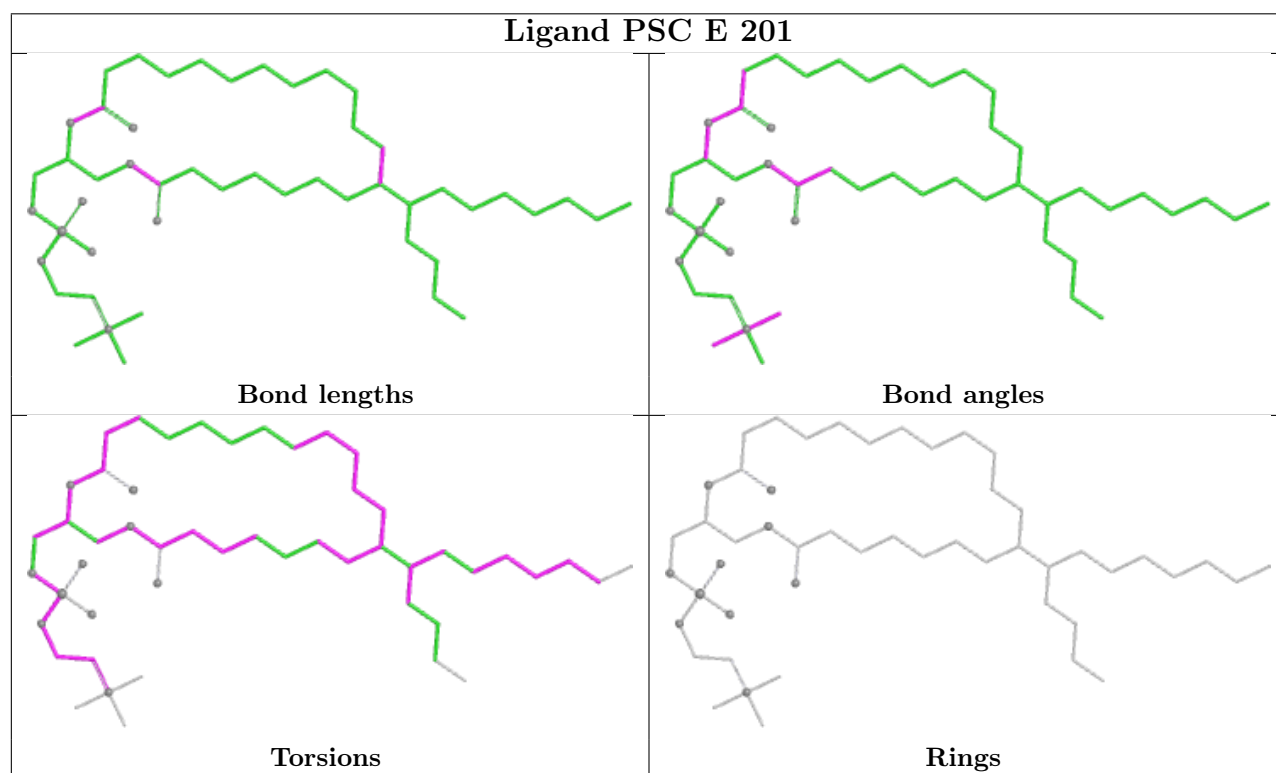
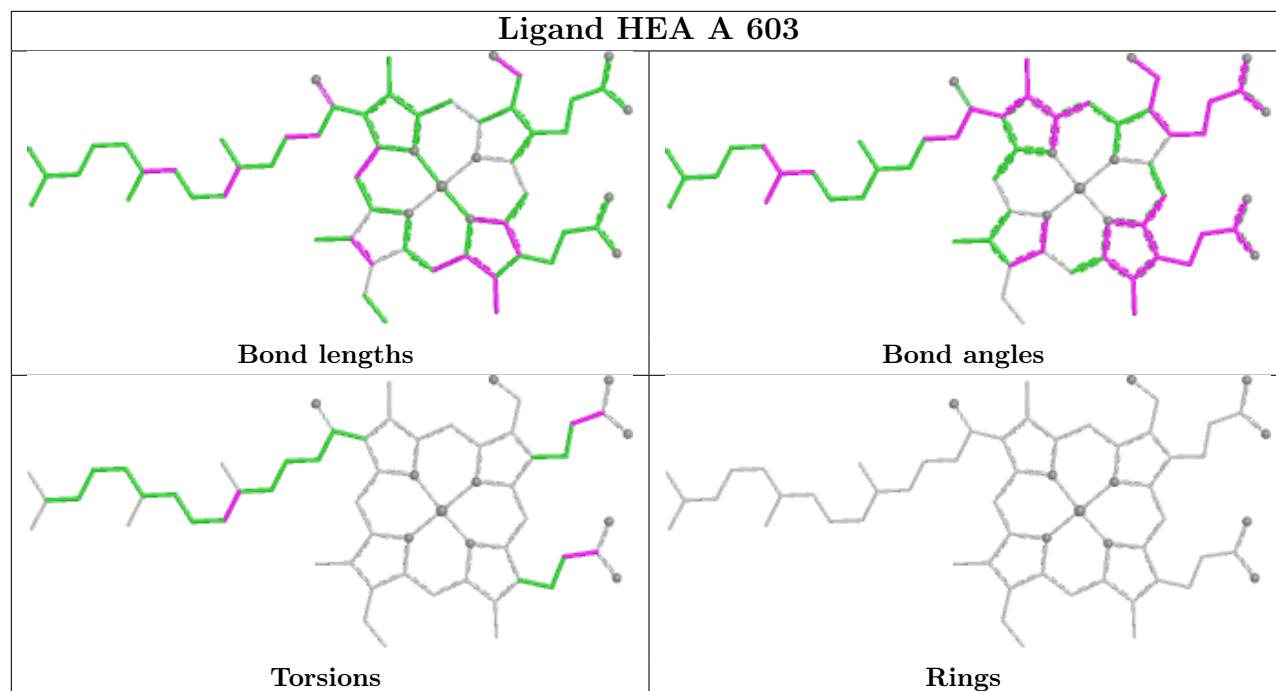


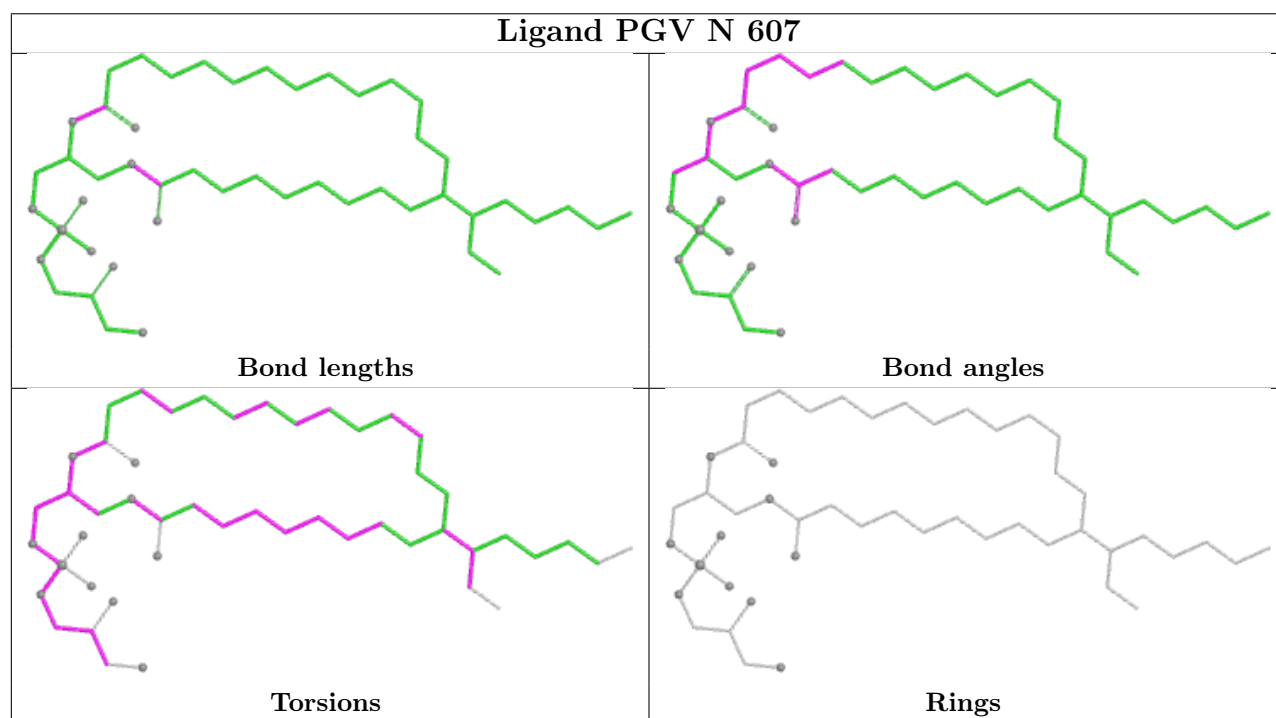
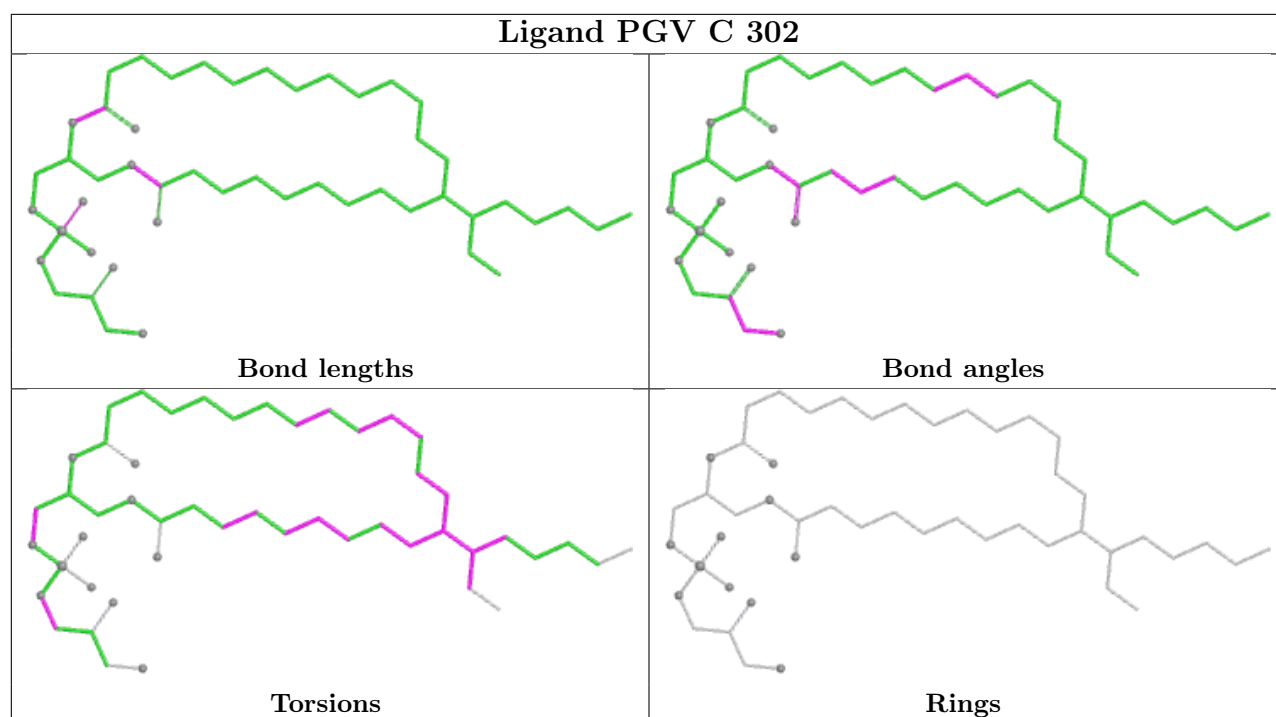


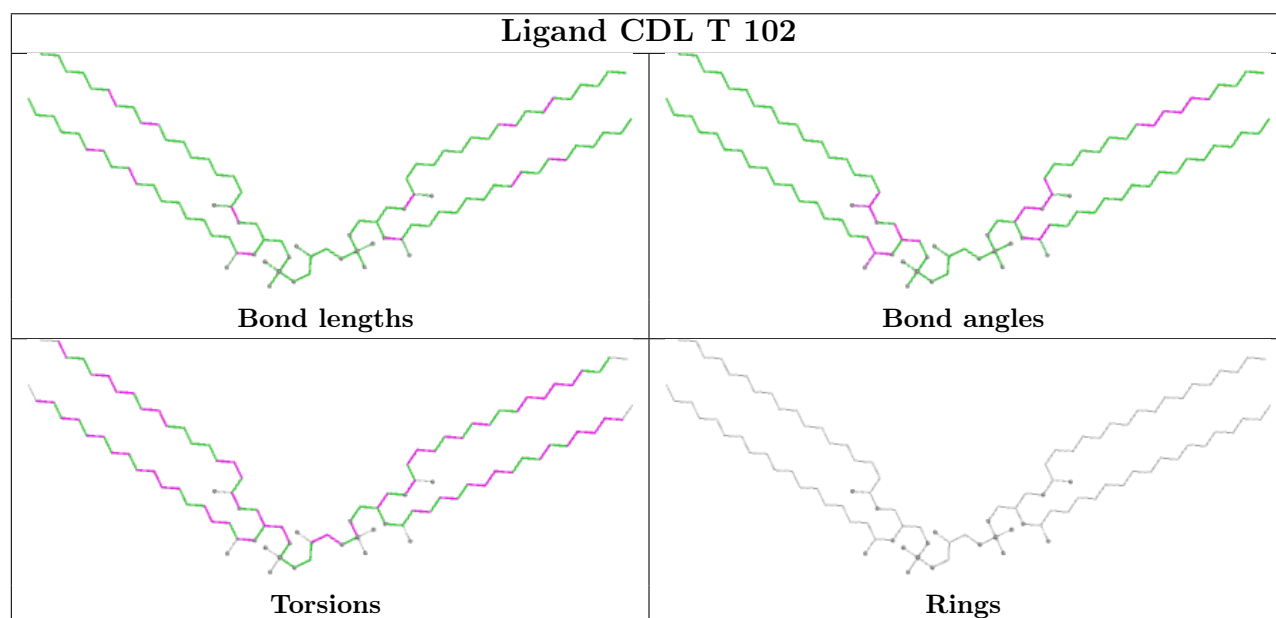
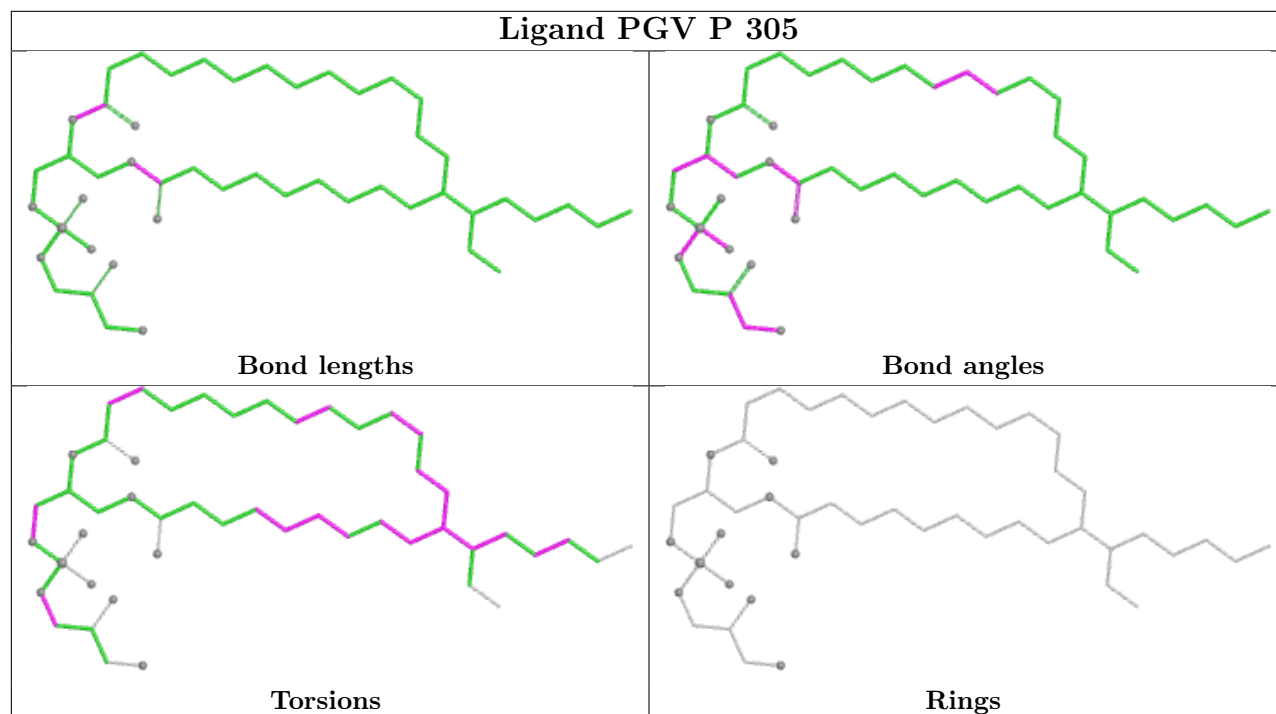


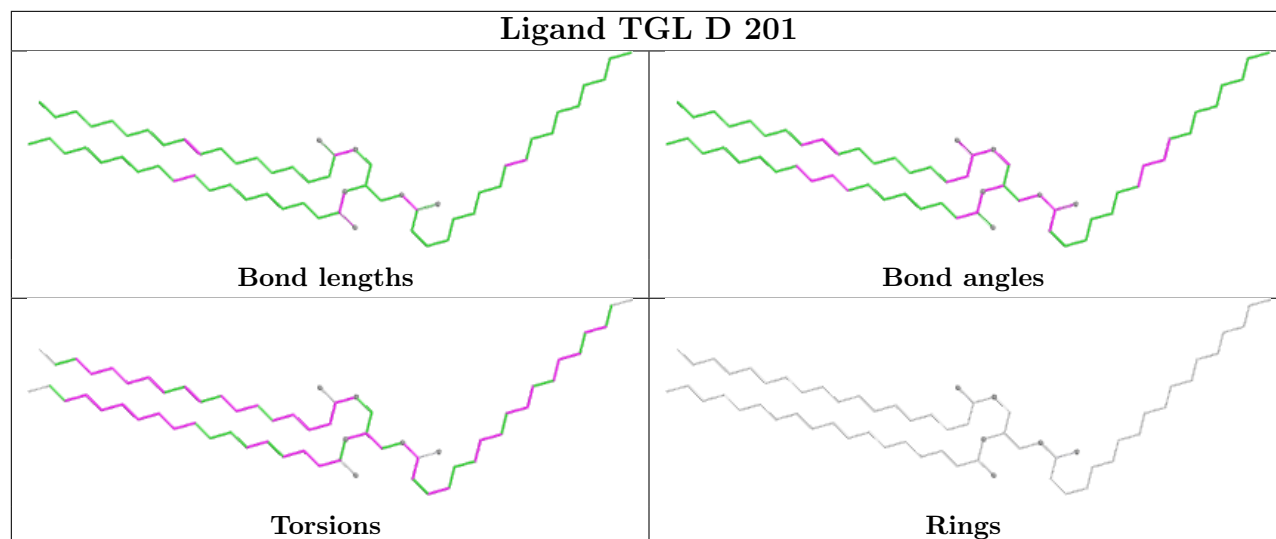












5.7 Other polymers [i](#)

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](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

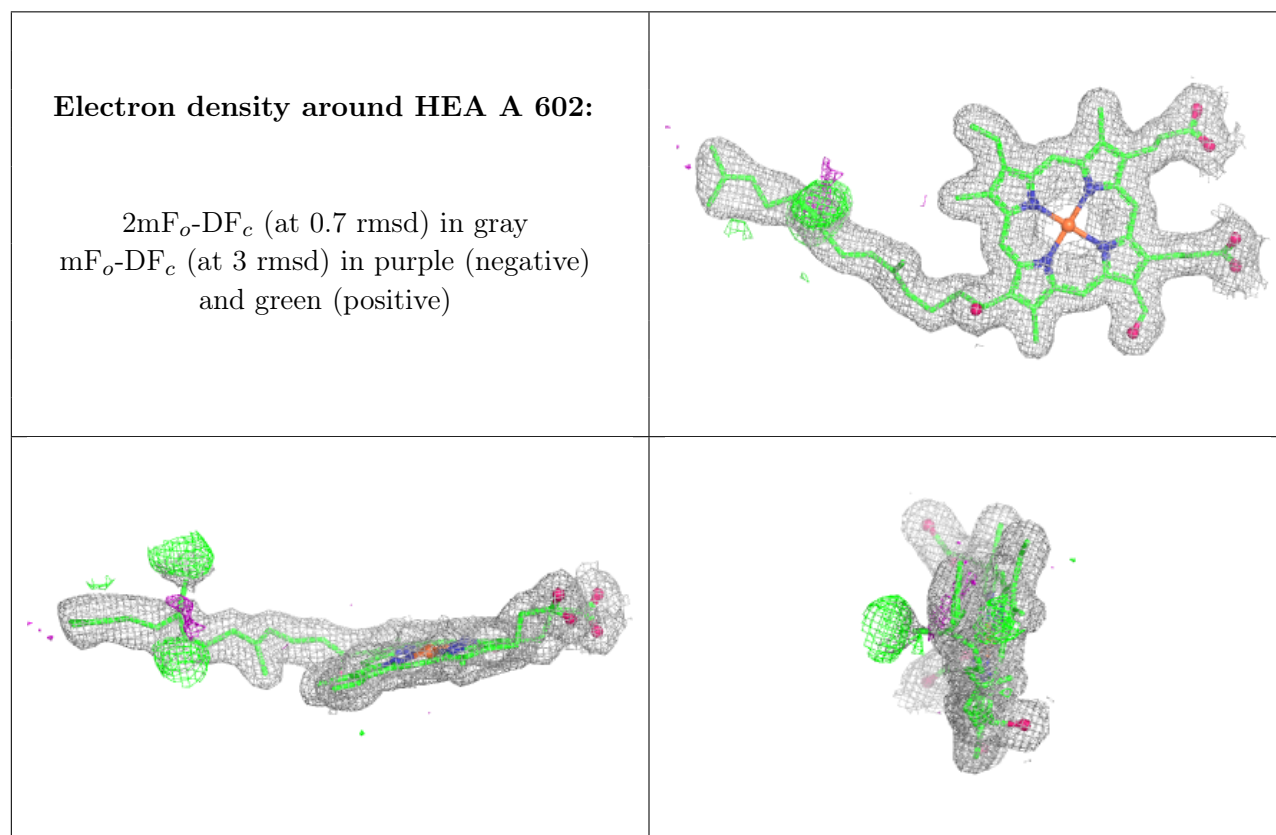
6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

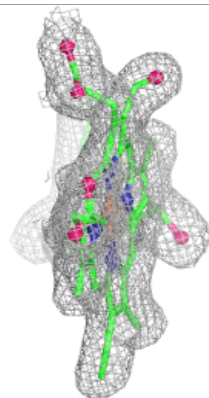
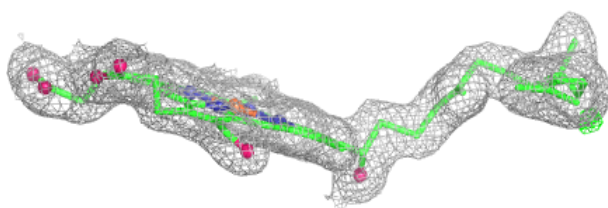
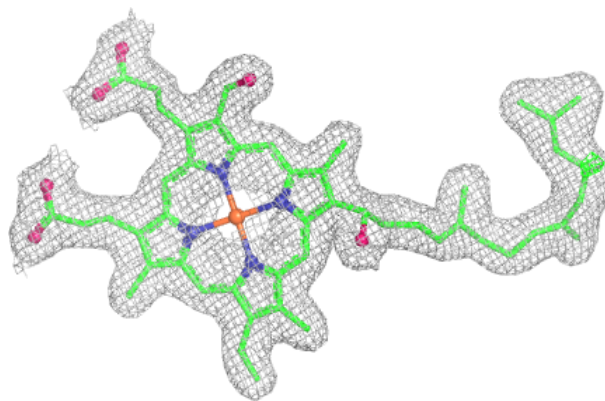
EDS failed to run properly - this section is therefore empty.

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.

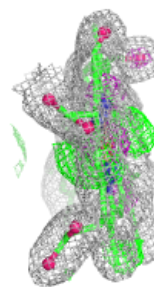
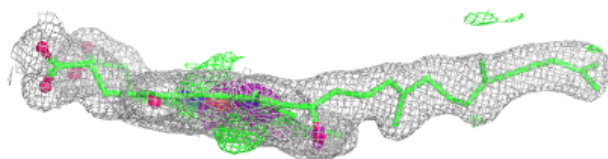
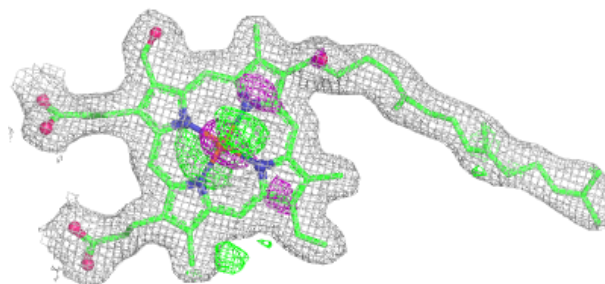


Electron density around HEA A 603:

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

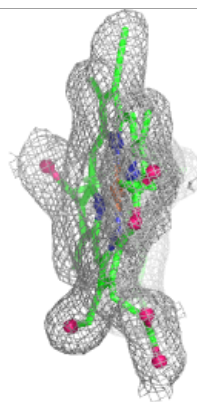
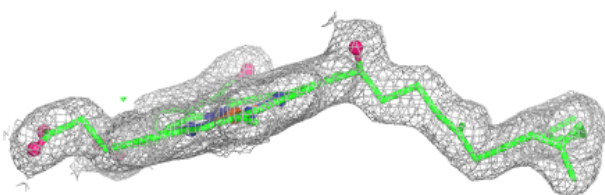
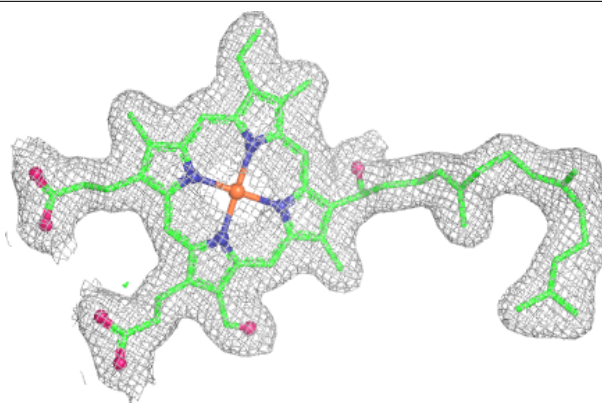
**Electron density around HEA N 602:**

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

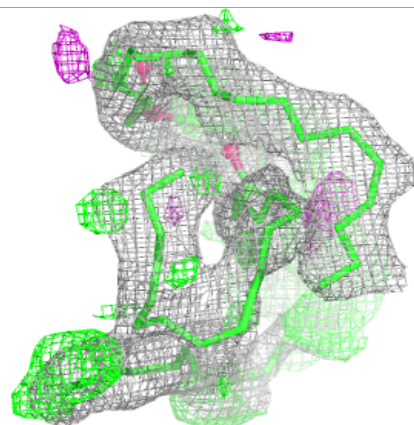
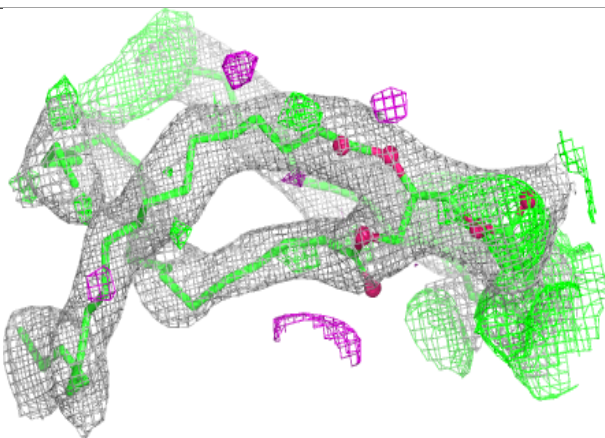
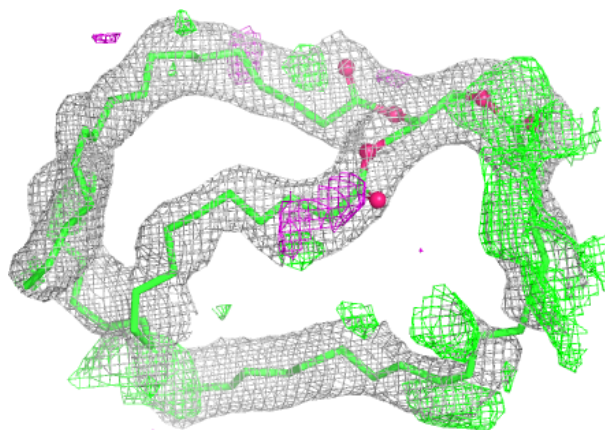


Electron density around HEA N 603:

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

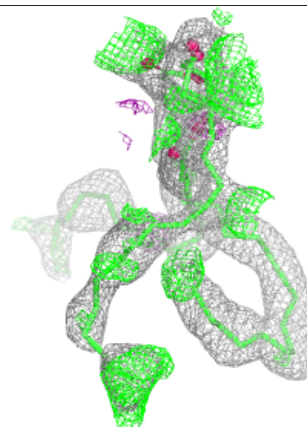
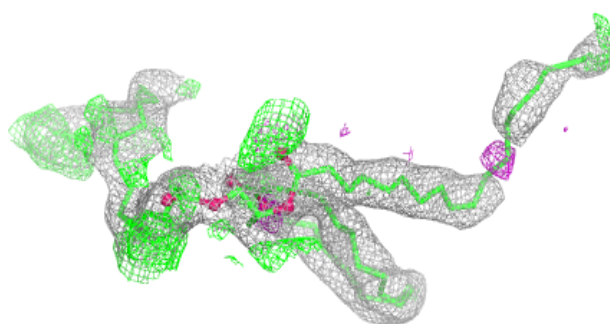
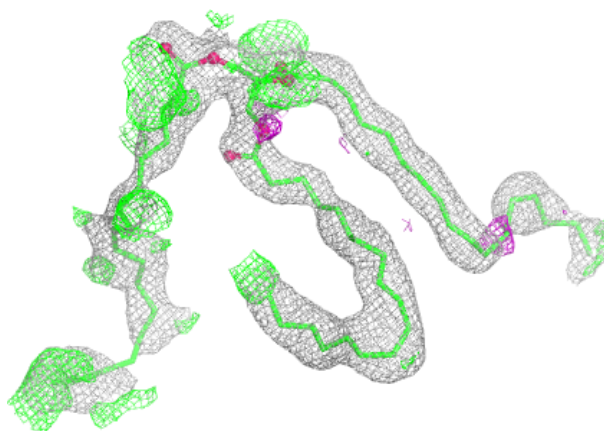
**Electron density around TGL A 607:**

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



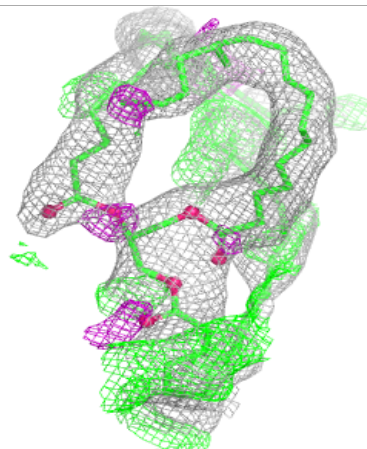
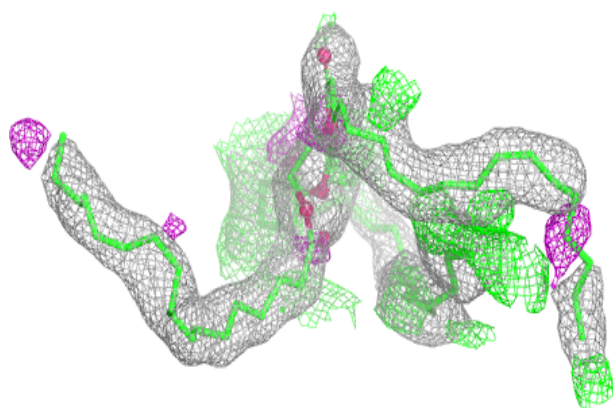
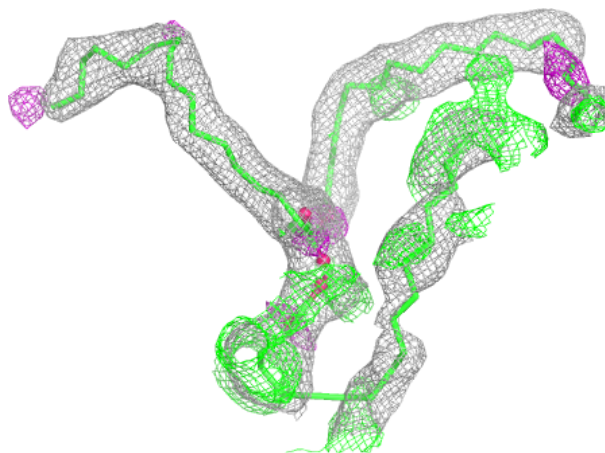
Electron density around TGL D 201:

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



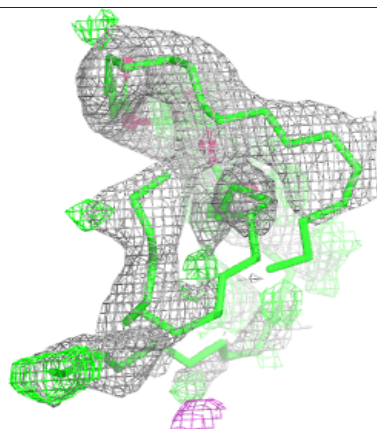
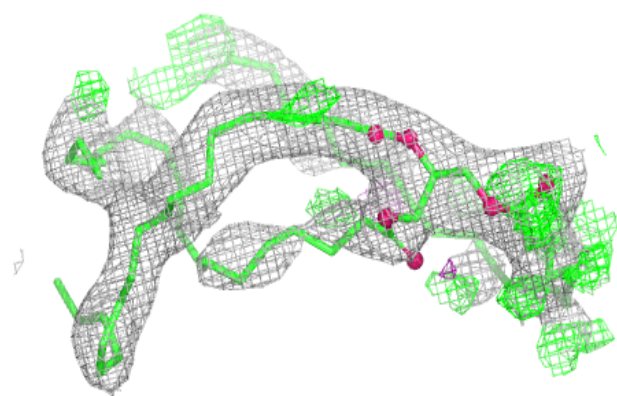
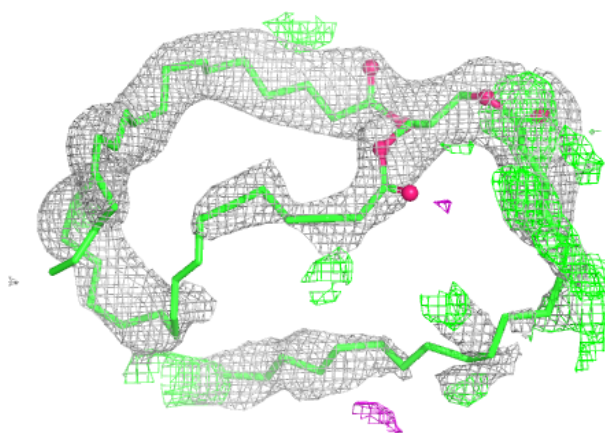
Electron density around TGL L 101:

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



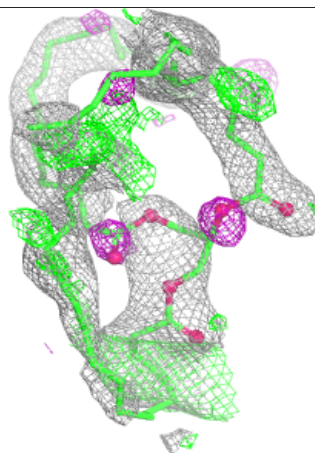
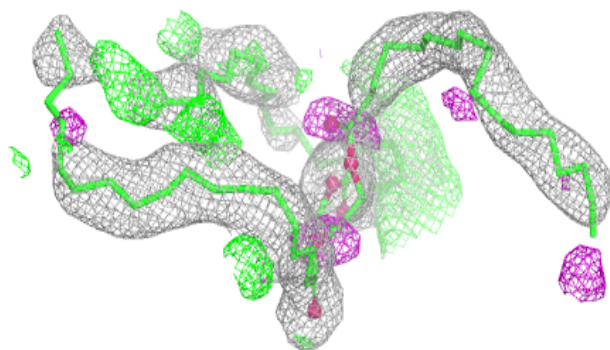
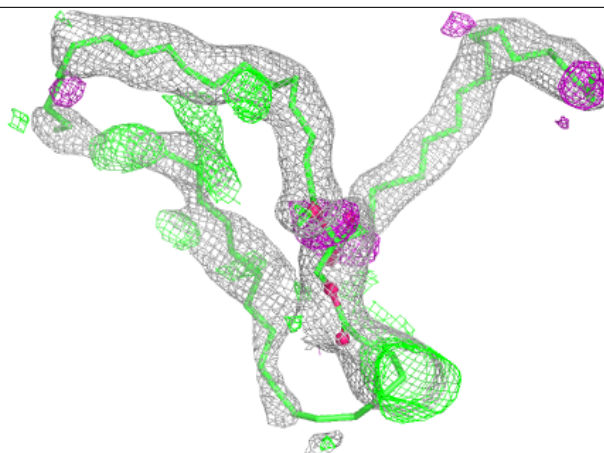
Electron density around TGL N 609:

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

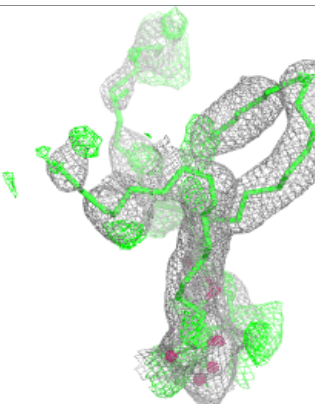
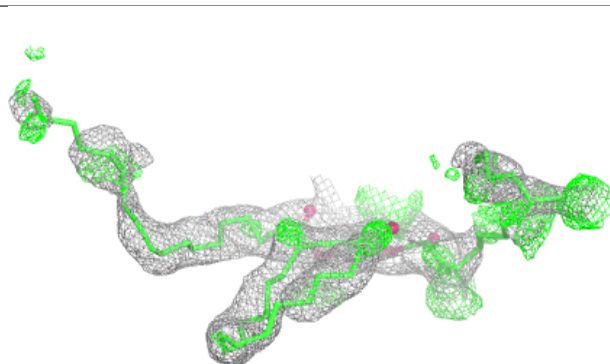
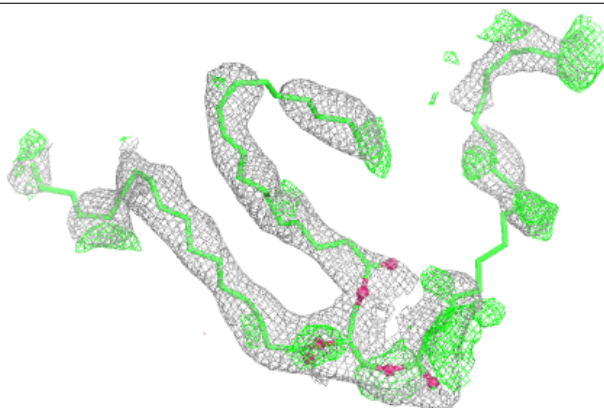


Electron density around TGL N 610:

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

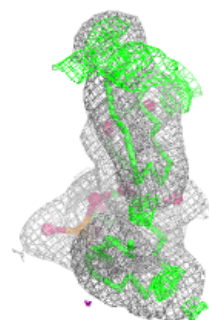
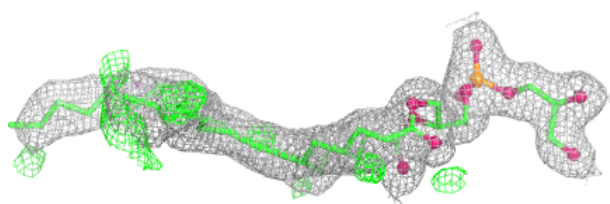
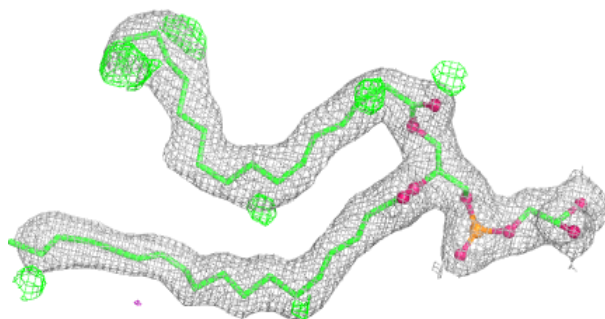
**Electron density around TGL Q 201:**

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

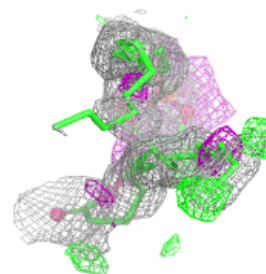
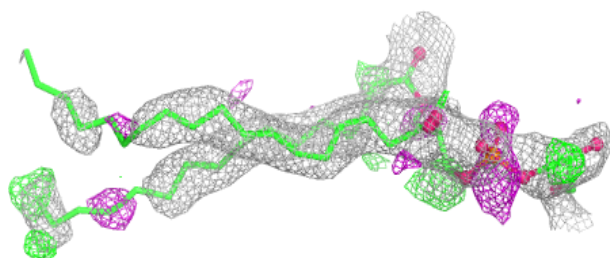
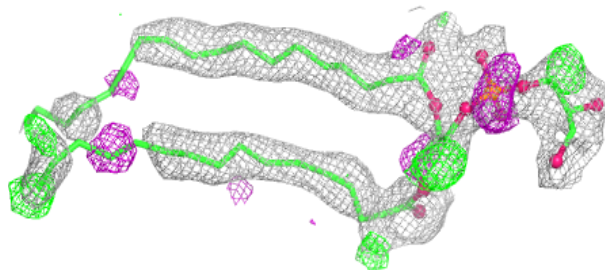


Electron density around PGV A 608:

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

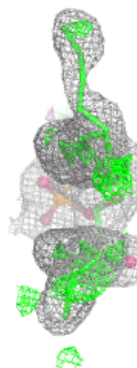
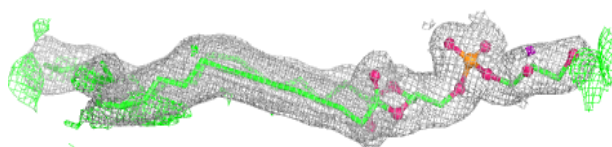
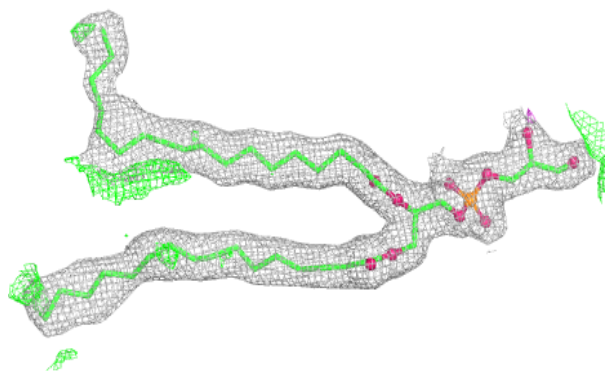
**Electron density around PGV A 609:**

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

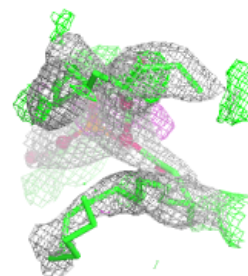
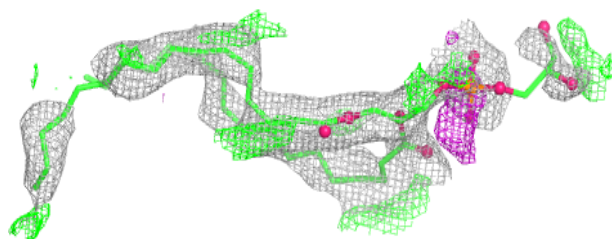
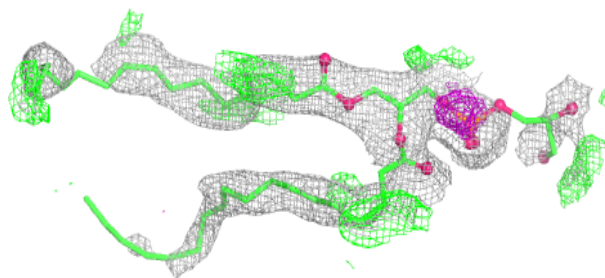


Electron density around PGV C 302:

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

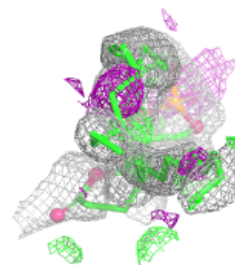
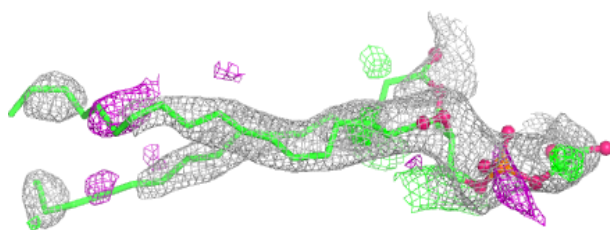
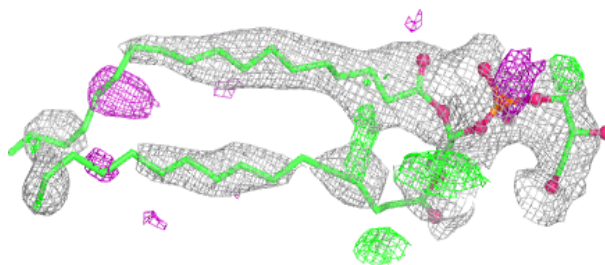
**Electron density around PGV C 307:**

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

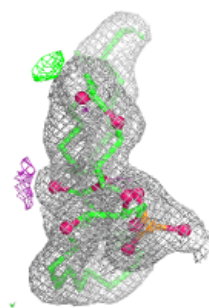
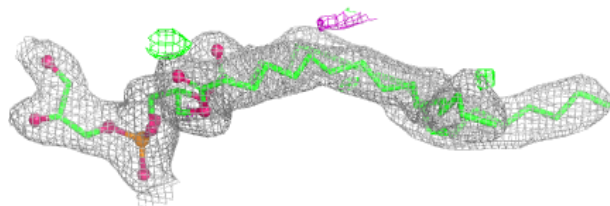
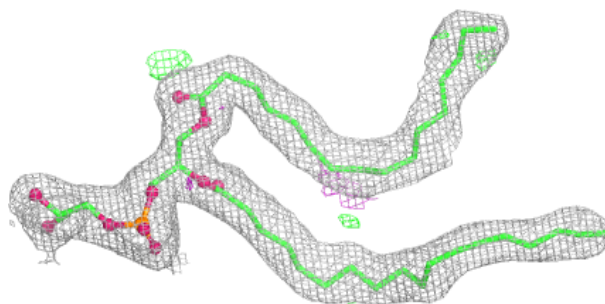


Electron density around PGV N 607:

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

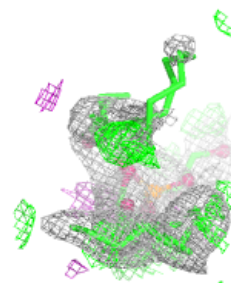
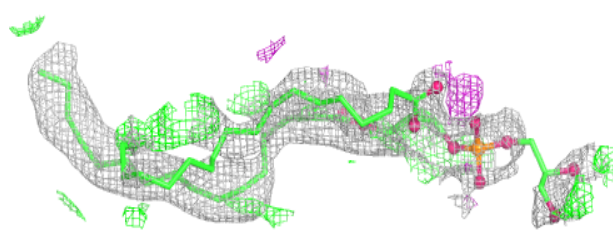
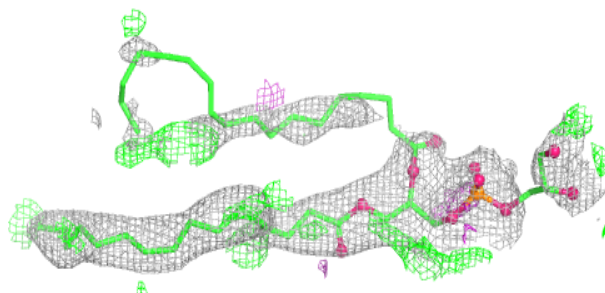
**Electron density around PGV N 608:**

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

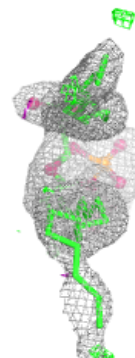
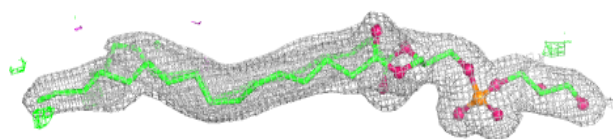
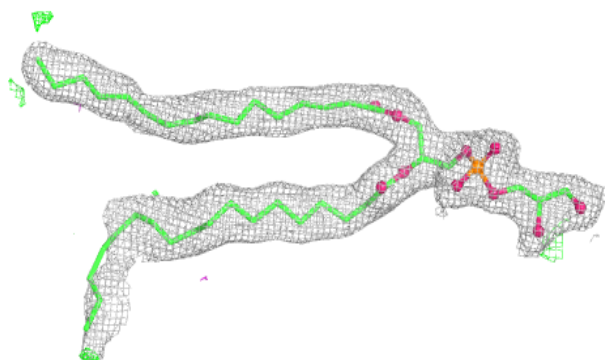


Electron density around PGV P 302:

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

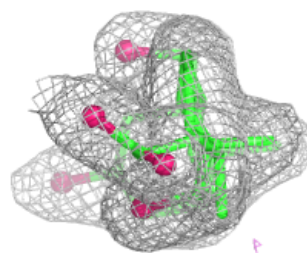
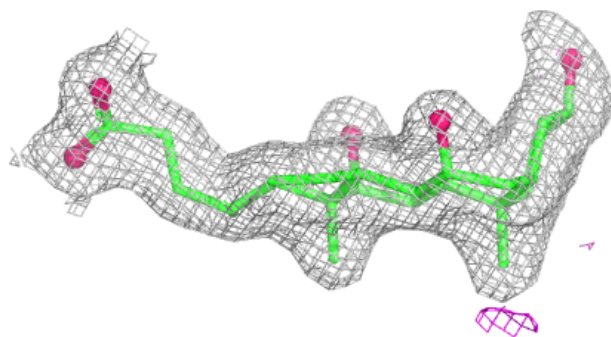
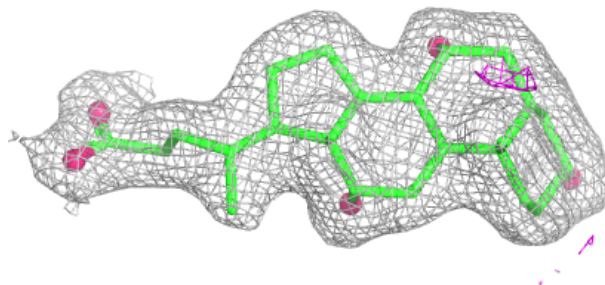
**Electron density around PGV P 305:**

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

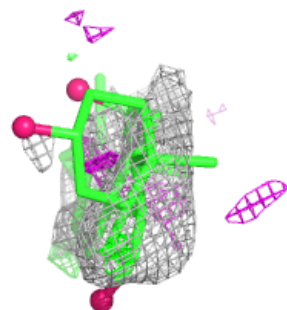
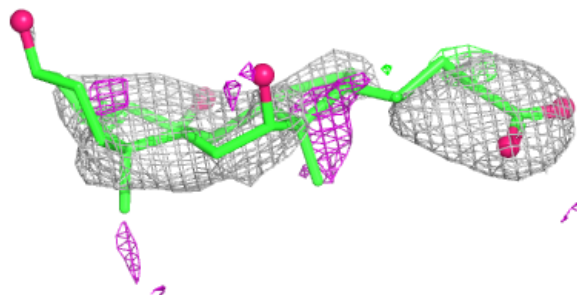
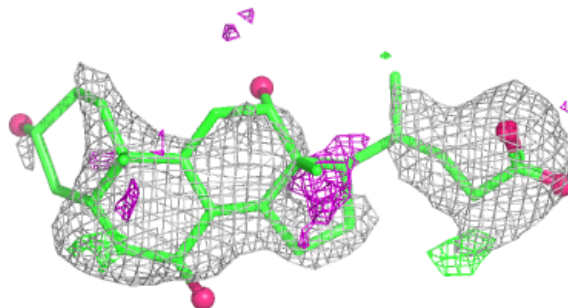


Electron density around CHD B 302:

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

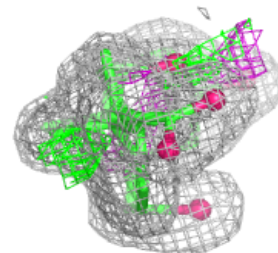
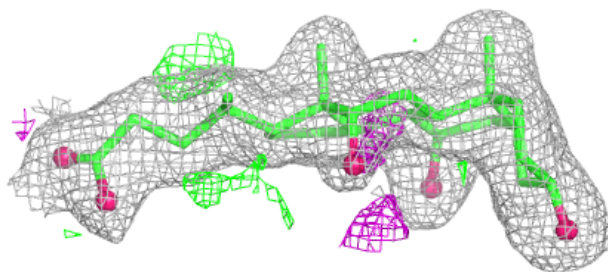
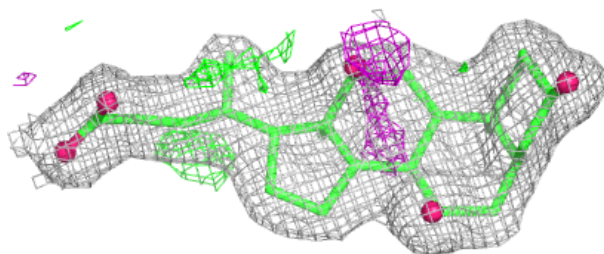
**Electron density around CHD C 304:**

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

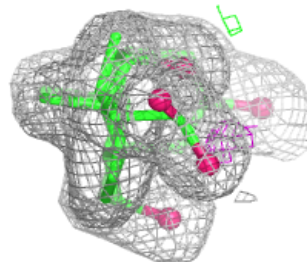
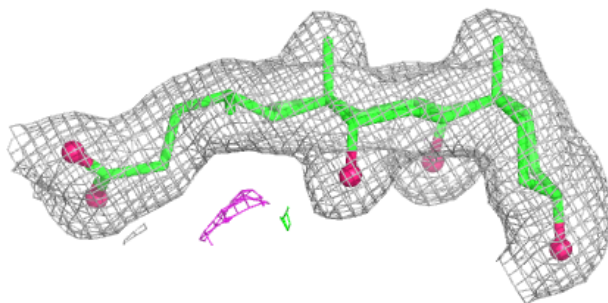
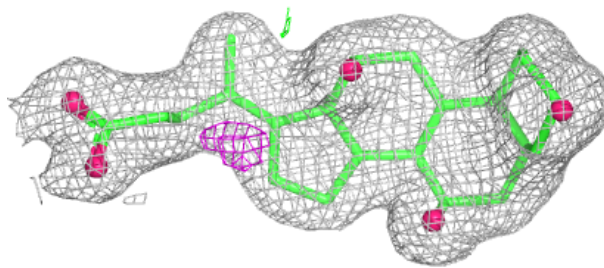


Electron density around CHD C 305:

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

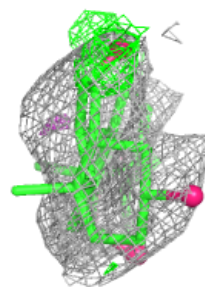
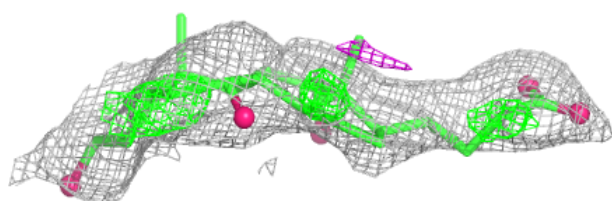
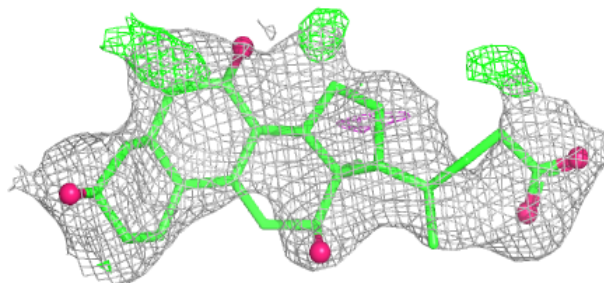
**Electron density around CHD O 302:**

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

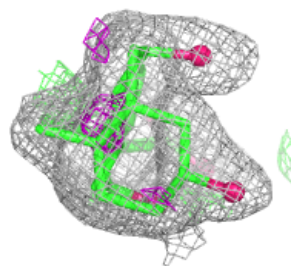
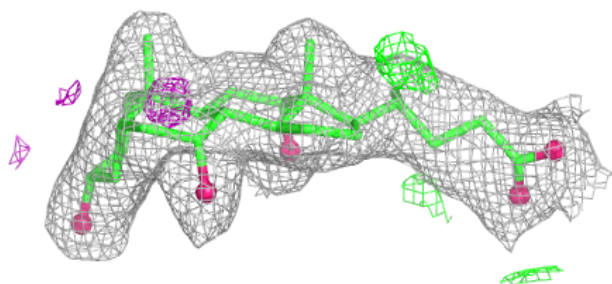
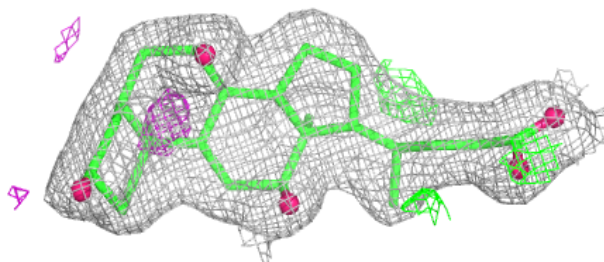


Electron density around CHD P 307:

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

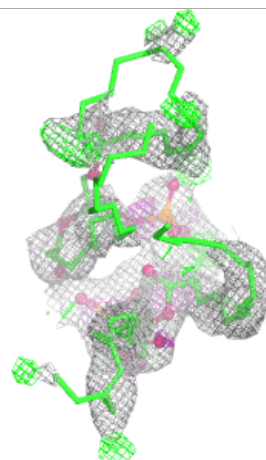
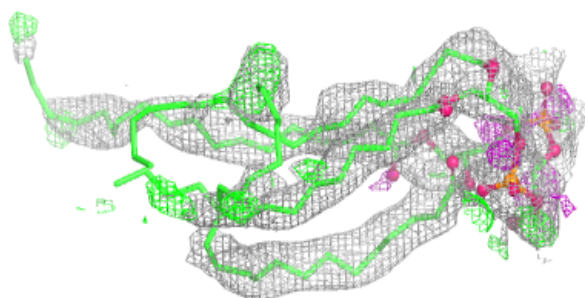
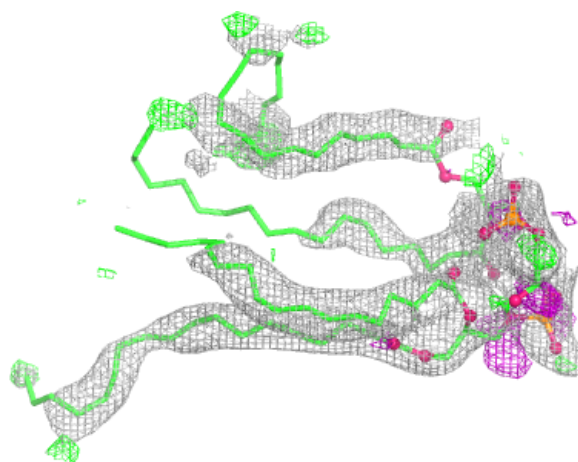
**Electron density around CHD P 308:**

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



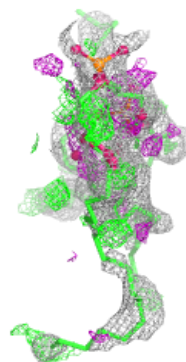
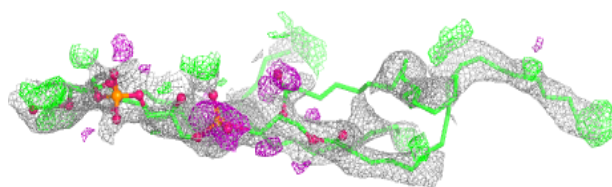
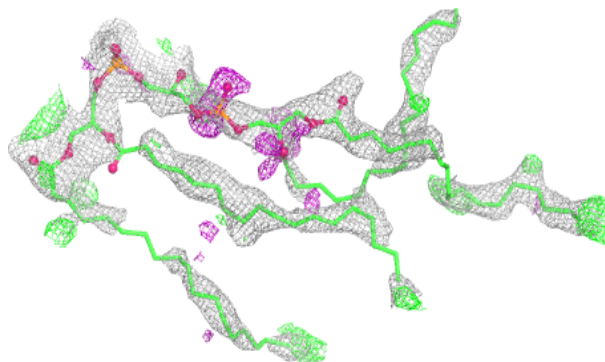
Electron density around CDL C 303:

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



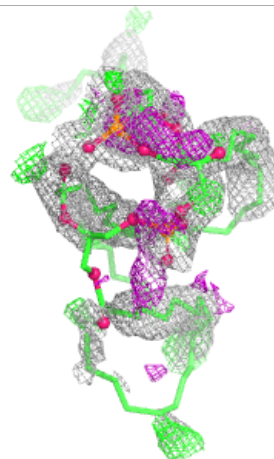
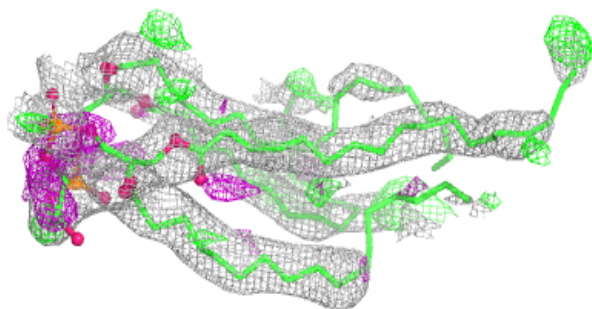
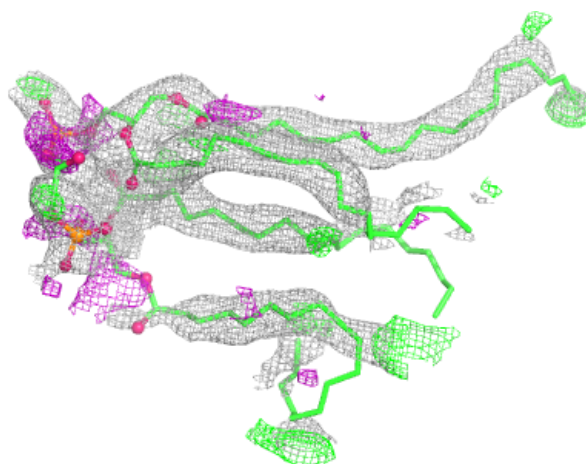
Electron density around CDL G 103:

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



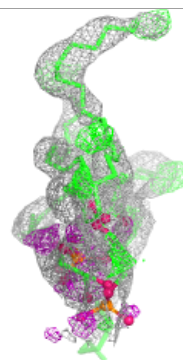
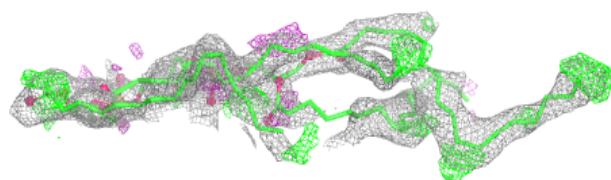
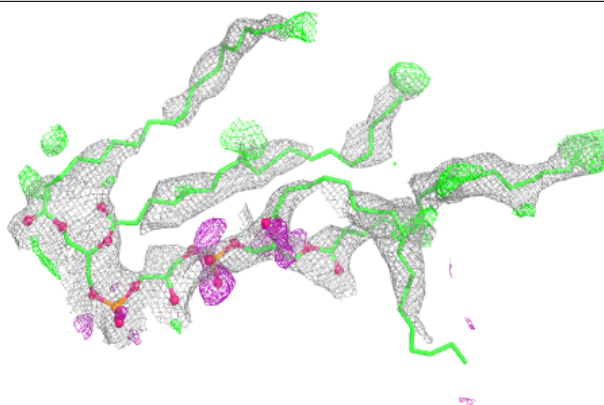
Electron density around CDL P 306:

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



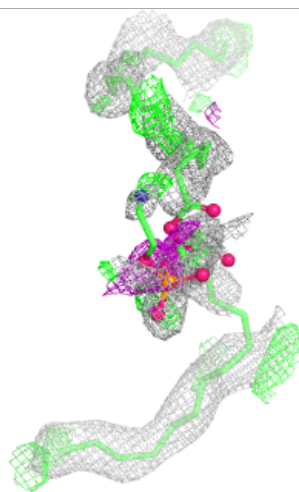
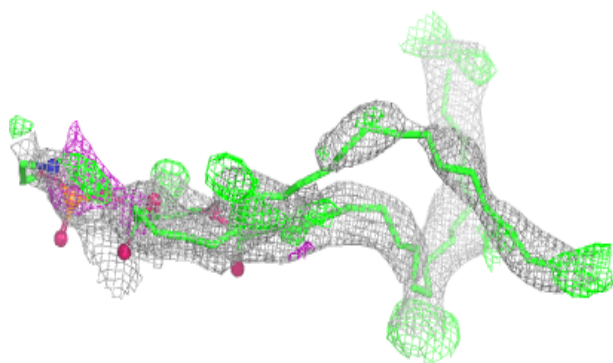
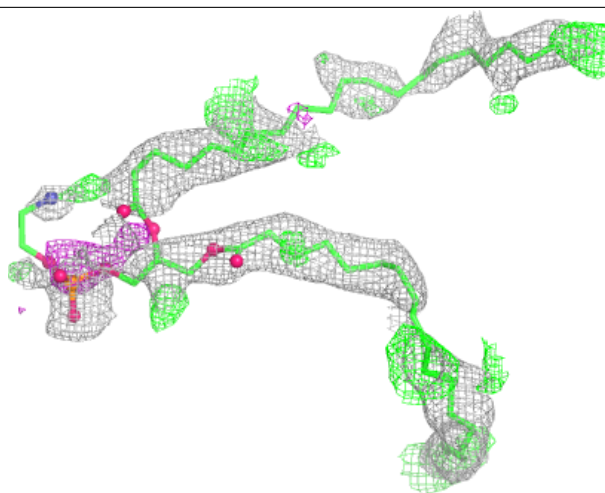
Electron density around CDL T 102:

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



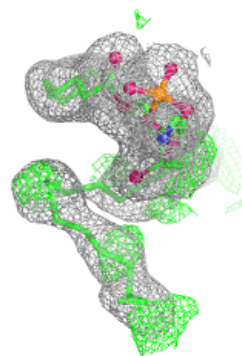
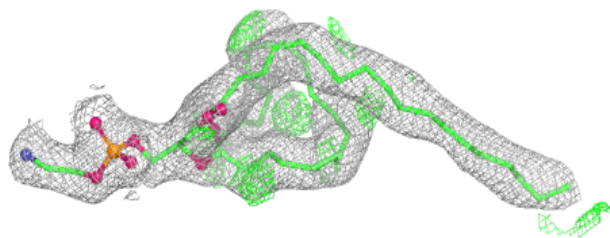
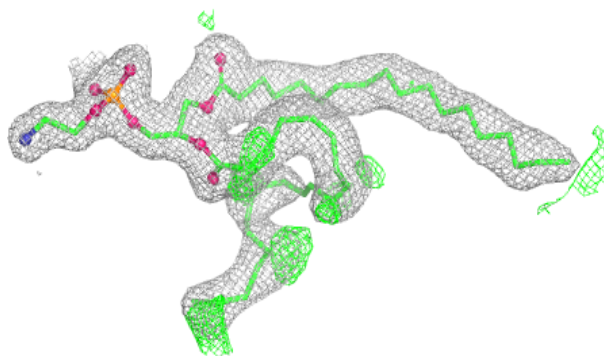
Electron density around PEK C 306:

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



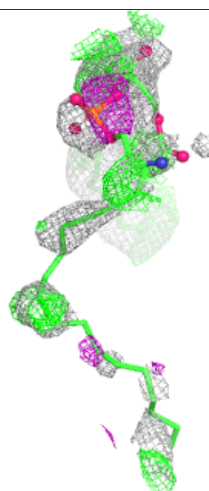
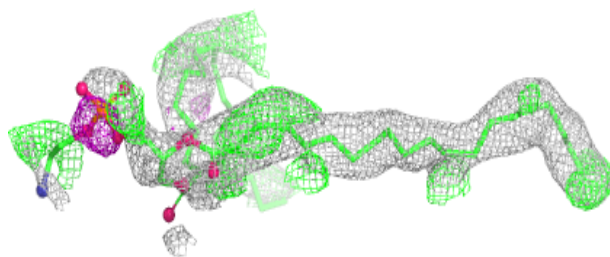
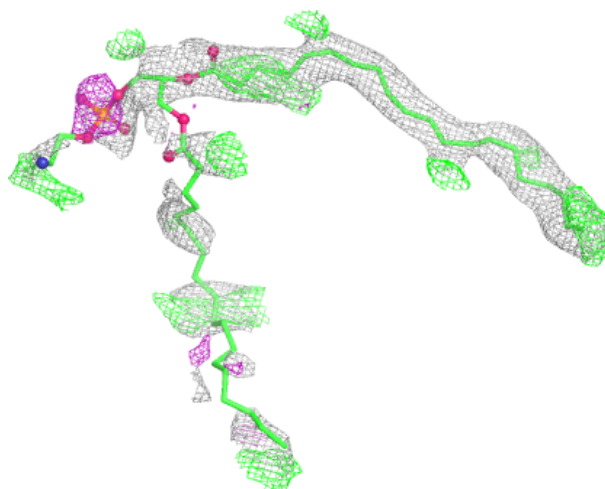
Electron density around PEK G 102:

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



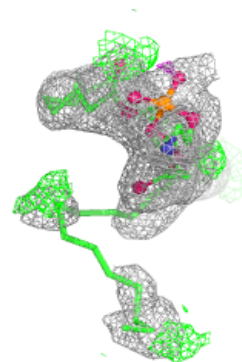
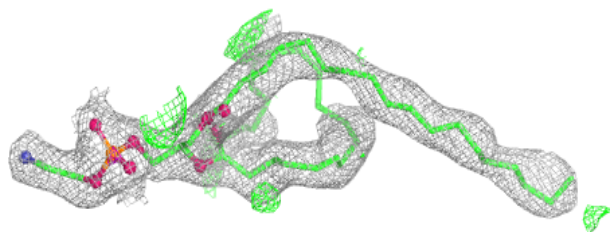
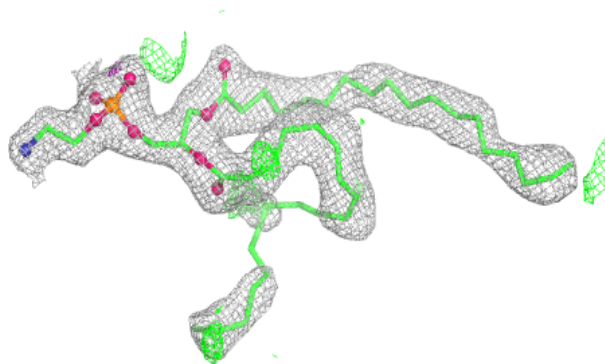
Electron density around PEK G 104:

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



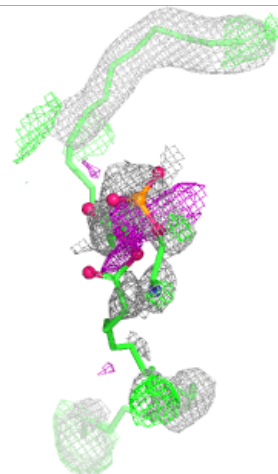
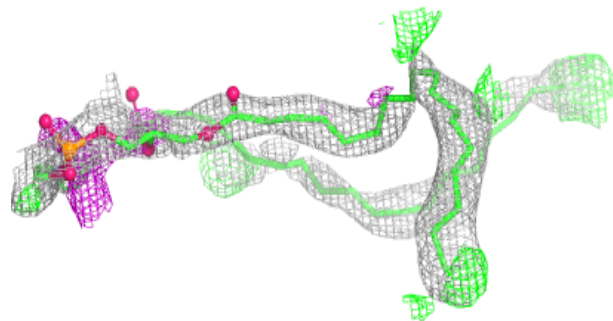
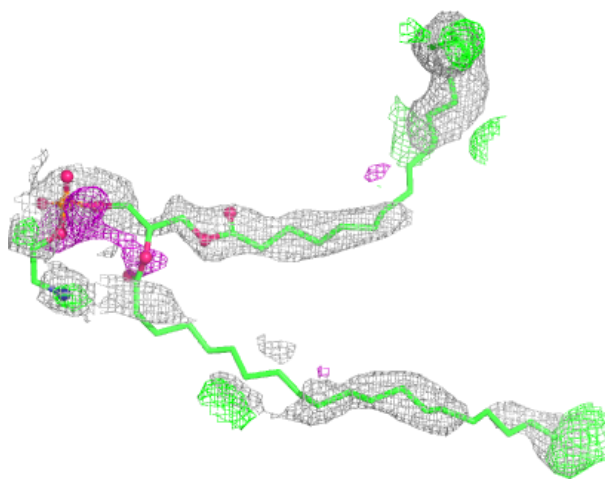
Electron density around PEK P 304:

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



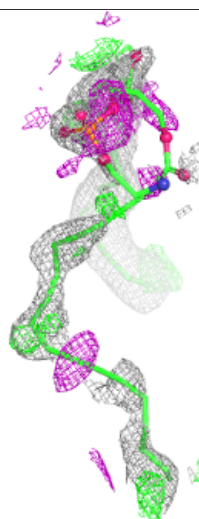
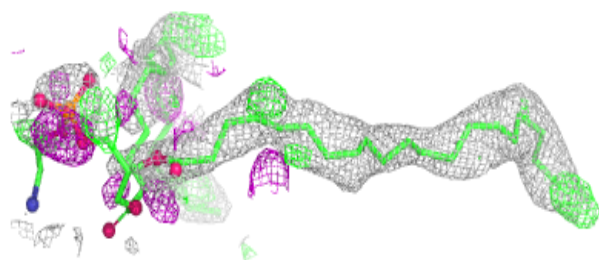
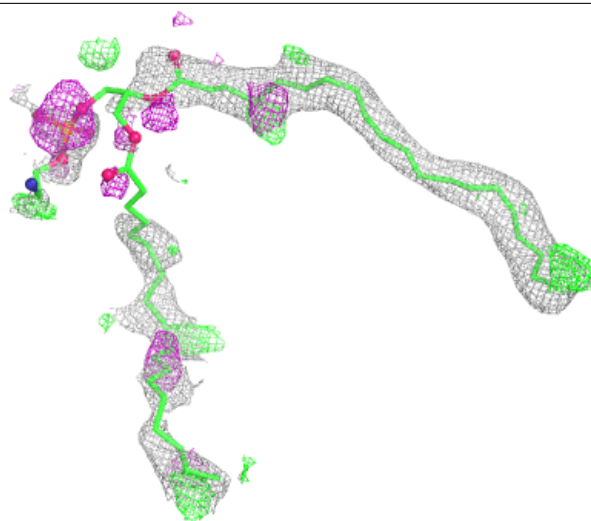
Electron density around PEK P 309:

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



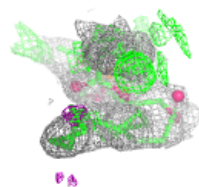
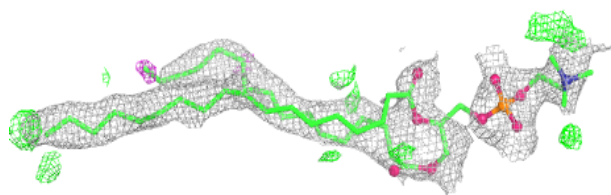
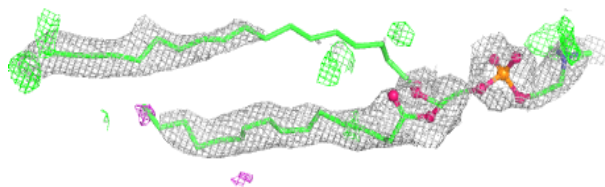
Electron density around PEK T 101:

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

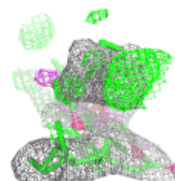
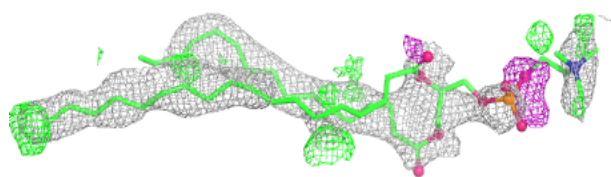
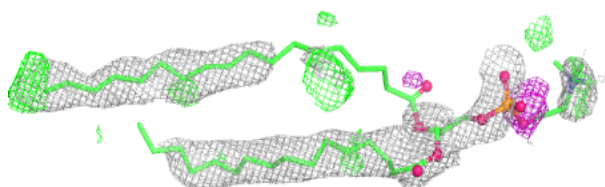


Electron density around PSC E 201:

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

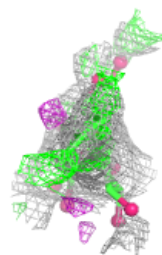
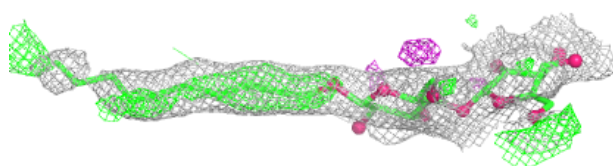
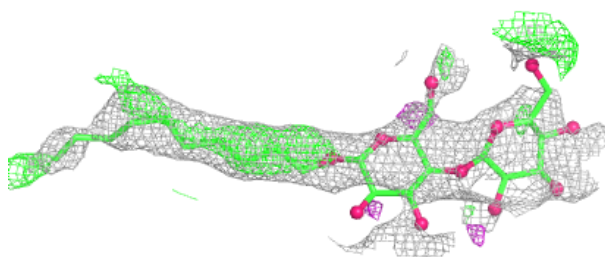
**Electron density around PSC O 303:**

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

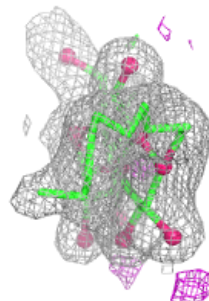
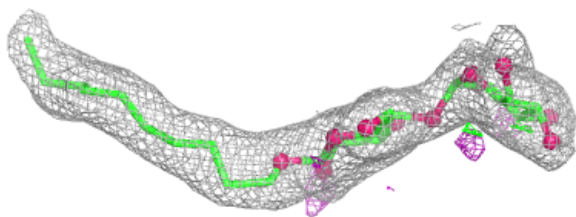
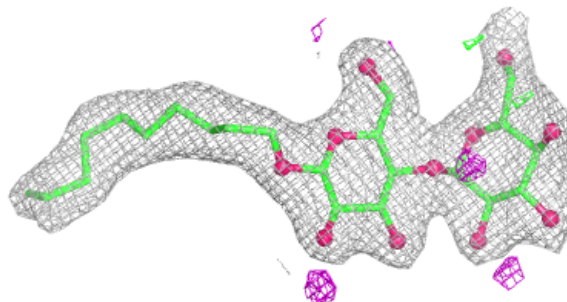


Electron density around DMU G 101:

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

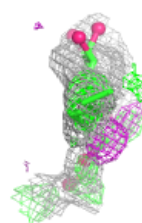
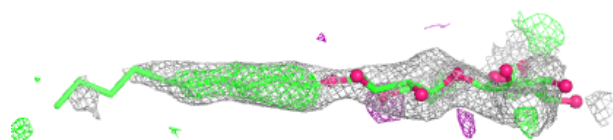
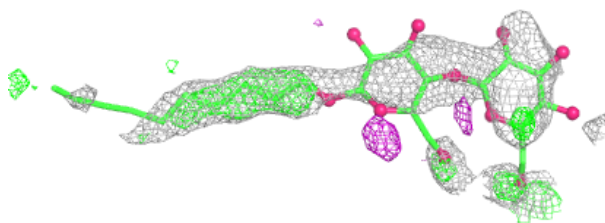
**Electron density around DMU M 101:**

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

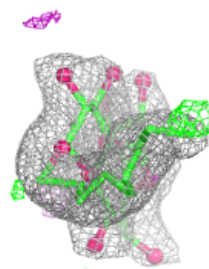
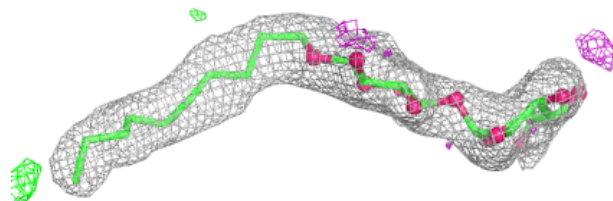
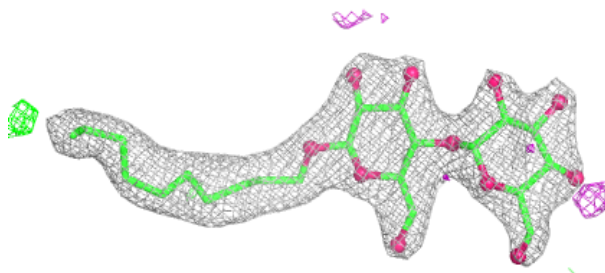


Electron density around DMU P 301:

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

**Electron density around DMU Z 101:**

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



6.5 Other polymers

EDS failed to run properly - this section is therefore empty.