



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 31, 2025 – 09:02 PM JST

PDB ID : 5X1B / pdb_00005x1b
Title : CO bound cytochrome c oxidase at 20 nsec after pump laser irradiation to release CO from O2 reduction center
Authors : Shimada, A.; Kubo, M.; Baba, S.; Yamashita, K.; Hirata, K.; Ueno, G.; Nomura, T.; Kimura, T.; Shinzawa-Itoh, K.; Baba, J.; Hatano, K.; Eto, Y.; Miyamoto, A.; Murakami, H.; Kumasaka, T.; Owada, S.; Tono, K.; Yabashi, M.; Yamaguchi, Y.; Yanagisawa, S.; Sakaguchi, M.; Ogura, T.; Komiya, R.; Yan, J.; Yamashita, E.; Yamamoto, M.; Ago, H.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2017-01-25
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
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)

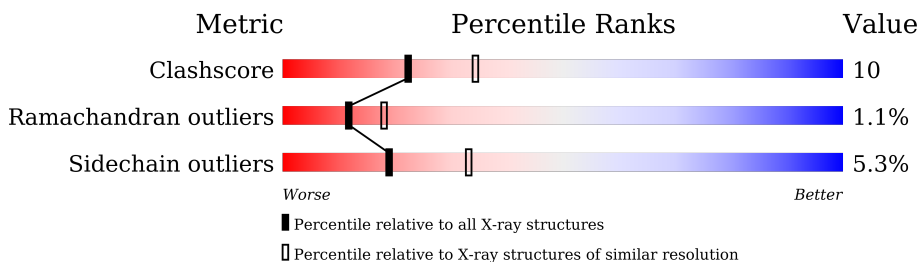
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)


















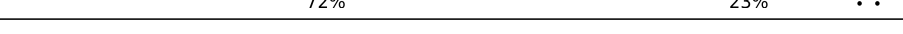


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

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	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	EDO	A	614	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 31717 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	1	0
			4030	2694	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	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	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			

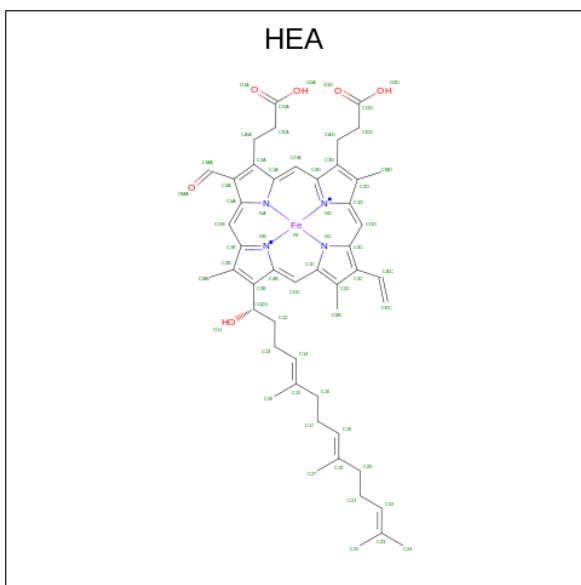
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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: $C_{49}H_{56}FeN_4O_6$).



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		

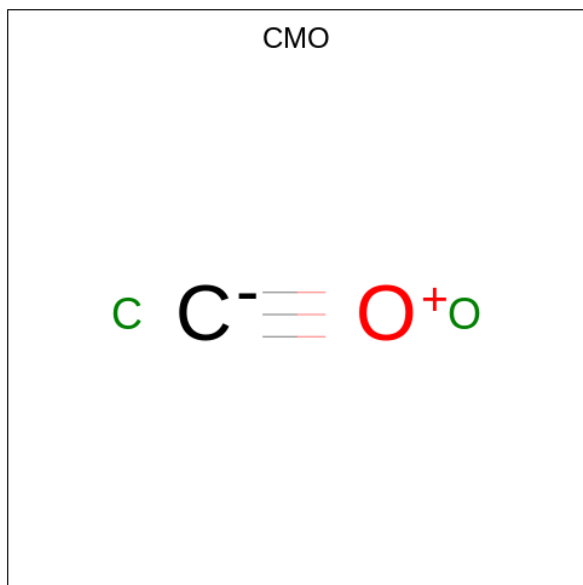
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

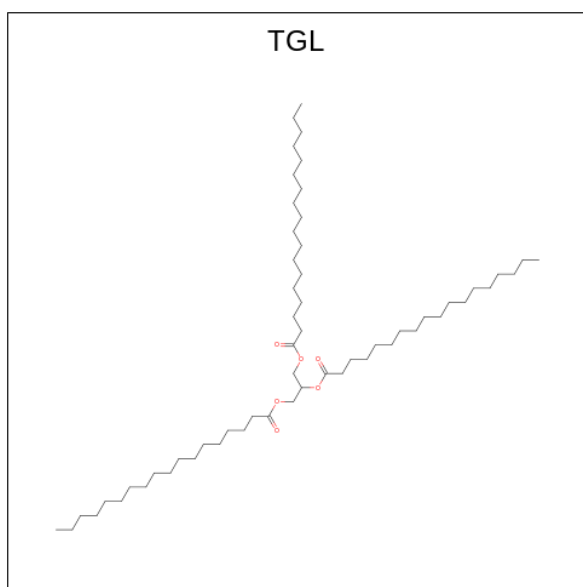
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



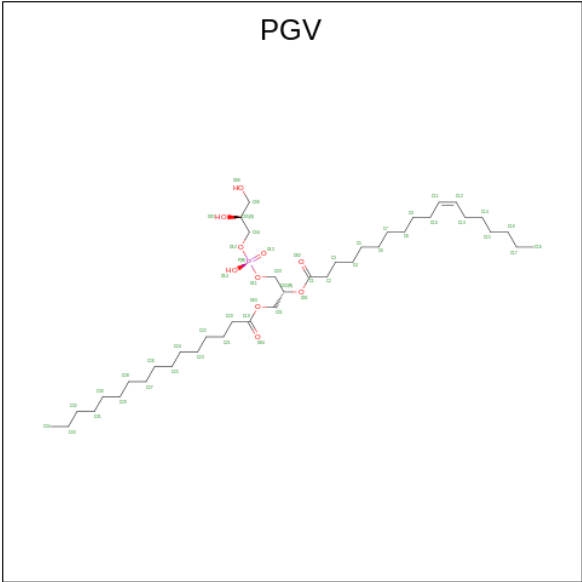
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			2	1	1		
18	N	1	Total	C	O	0	0
			2	1	1		

- Molecule 19 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



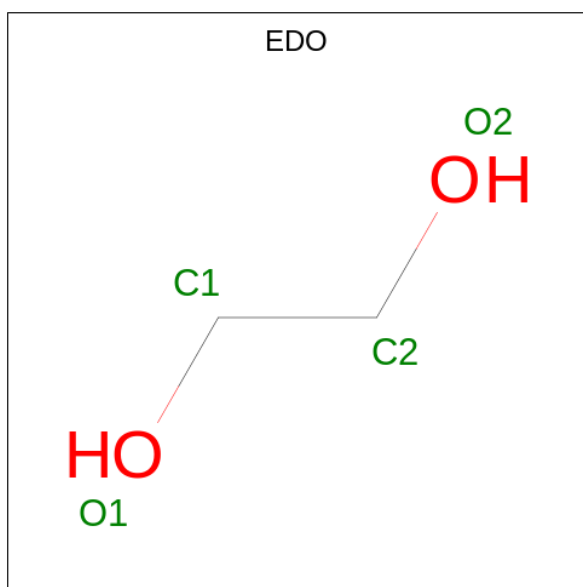
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: 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	G	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		

- Molecule 21 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



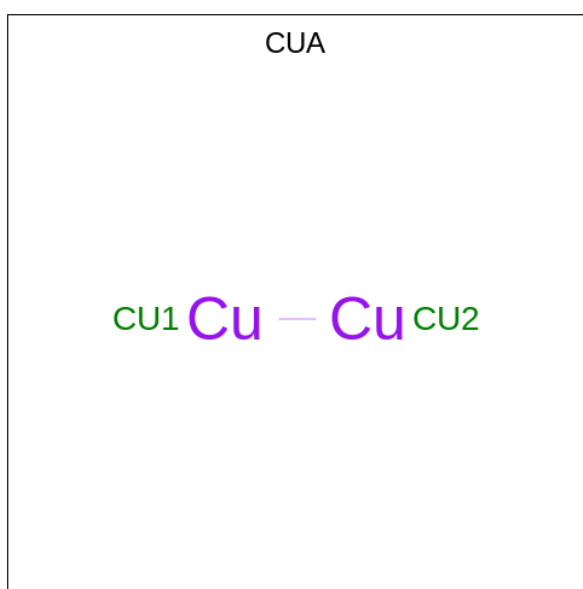
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21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

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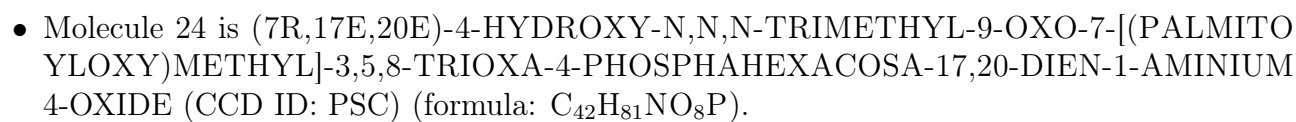
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	K	1	Total	C	O	0	0
			4	2	2		
21	L	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	T	1	Total	C	O	0	0
			4	2	2		

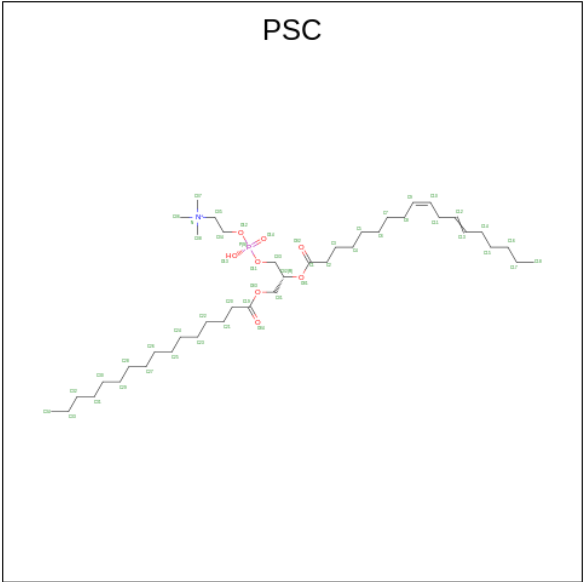
- Molecule 22 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



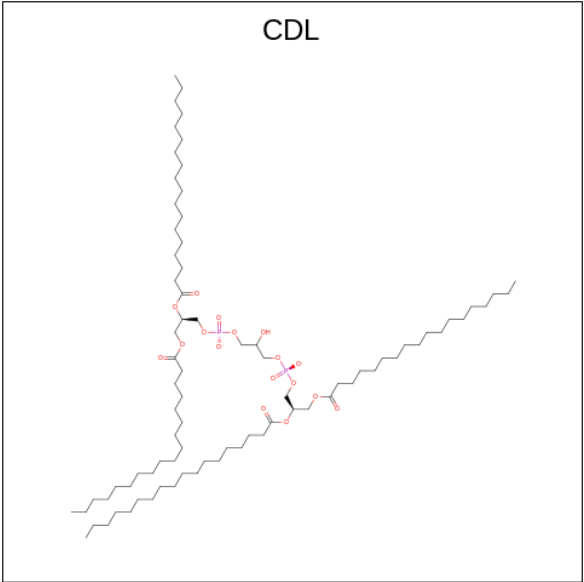


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
24	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

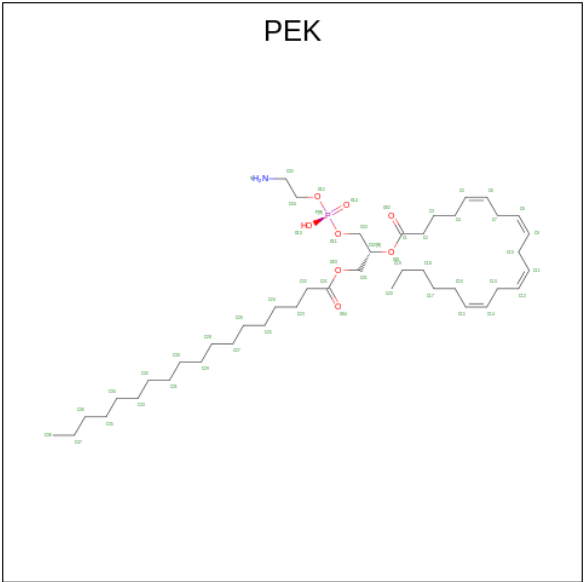
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	C	1	Total	X	0	0
			1	1		
25	P	1	Total	X	0	0
			1	1		

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



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

- 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: C₄₃H₇₈NO₈P).

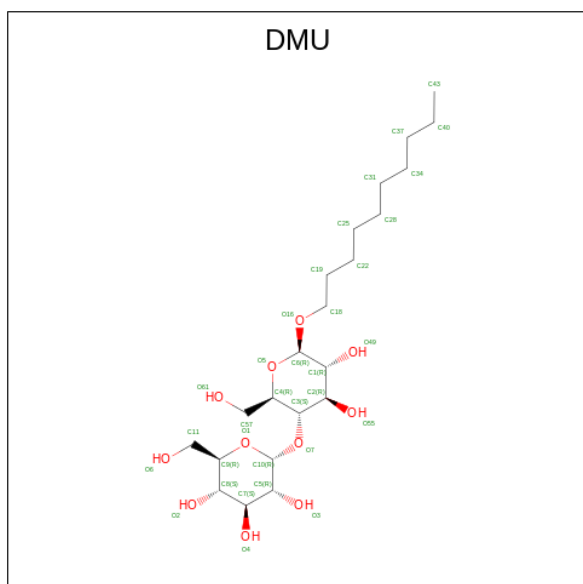


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 29 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



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

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	125	Total	O		0	0
			125	125			
30	B	77	Total	O		0	1
			78	78			
30	C	70	Total	O		0	0
			70	70			
30	D	41	Total	O		0	0
			41	41			
30	E	24	Total	O		0	0
			24	24			
30	F	36	Total	O		0	0
			36	36			
30	G	31	Total	O		0	0
			31	31			
30	H	33	Total	O		0	0
			33	33			
30	I	12	Total	O		0	0
			12	12			
30	J	19	Total	O		0	0
			19	19			
30	K	19	Total	O		0	0
			19	19			
30	L	14	Total	O		0	0
			14	14			
30	M	15	Total	O		0	0
			15	15			
30	N	117	Total	O		0	0
			117	117			
30	O	76	Total	O		0	1
			77	77			
30	P	54	Total	O		0	0
			54	54			
30	Q	29	Total	O		0	0
			29	29			
30	R	29	Total	O		0	0
			29	29			

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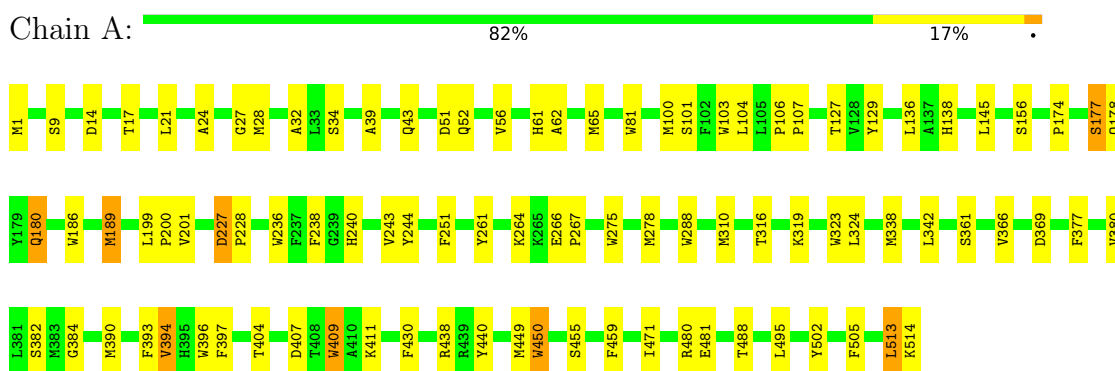
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	S	43	Total 43	O 43	0	0
30	T	20	Total 20	O 20	0	0
30	U	31	Total 31	O 31	0	0
30	V	19	Total 19	O 19	0	0
30	W	17	Total 17	O 17	0	0
30	X	9	Total 9	O 9	0	0
30	Y	6	Total 6	O 6	0	0
30	Z	4	Total 4	O 4	0	0

3 Residue-property plots

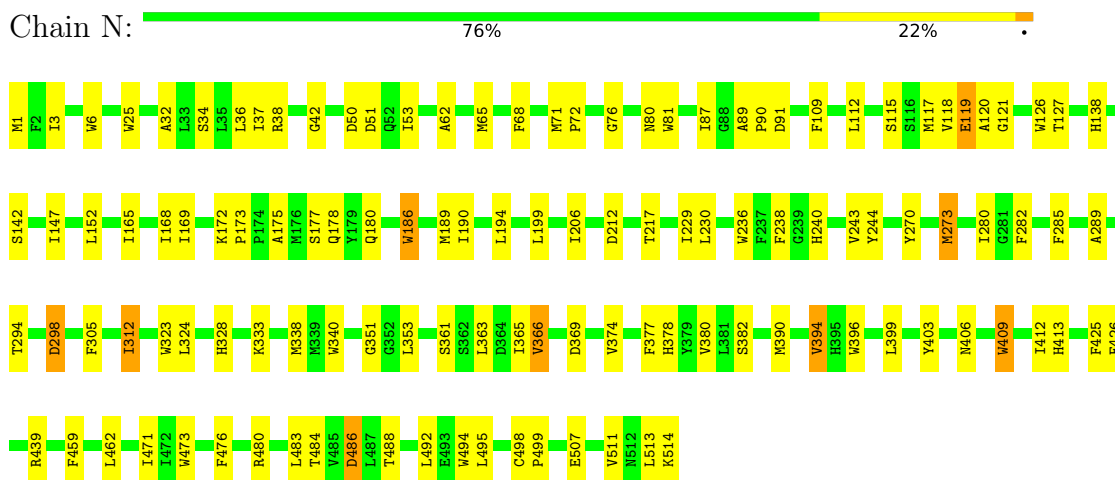
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

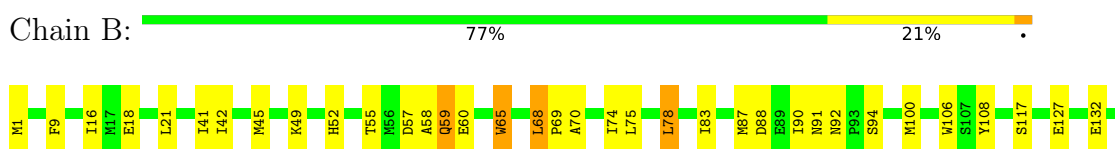
• Molecule 1: Cytochrome c oxidase subunit 1

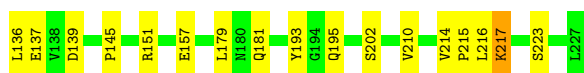


• Molecule 1: Cytochrome c oxidase subunit 1

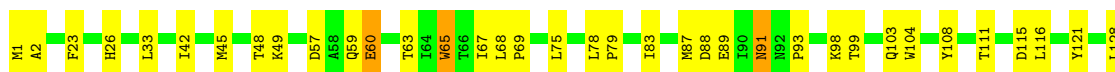


• Molecule 2: Cytochrome c oxidase subunit 2

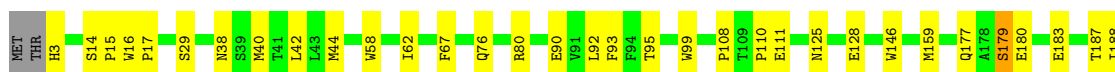
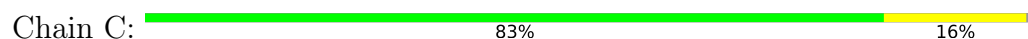




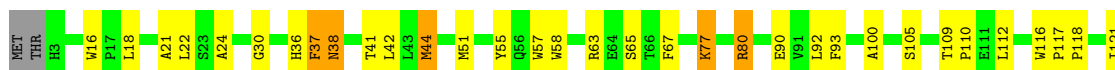
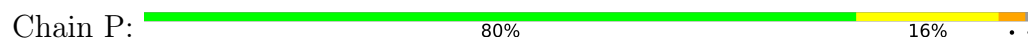
• Molecule 2: Cytochrome c oxidase subunit 2



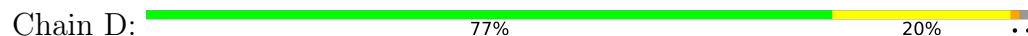
• Molecule 3: Cytochrome c oxidase subunit 3



• Molecule 3: Cytochrome c oxidase subunit 3




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

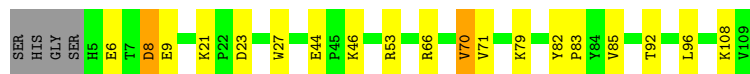


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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

Chain E:  79% 16% . .




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

Chain R:  69% 27% . .




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

Chain F:  76% 21% .



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

Chain S:  80% 15% . .



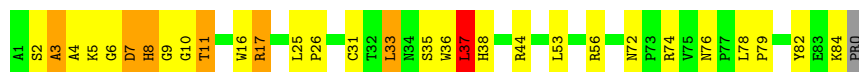
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:  61% 28% 8% . .



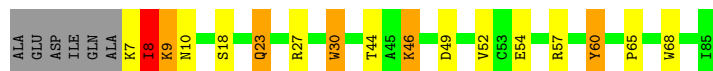
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:  64% 27% 7% . .



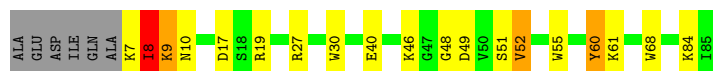
- Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:  73% 13% 6% . 7%




- Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:  71% 18% . . 7%



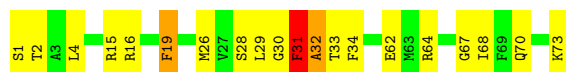
- Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:  84% 12% .




- Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:  73% 23% . .



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

Chain J:  81% 15% . .



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

Chain W:  69% 25% . .



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

Chain K:  70% 18% 12%



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

Chain X:  64% 18% 5% 12%



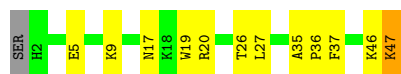
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:  72% 23% ..



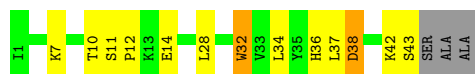
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:  72% 23% ..



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

Chain M:  65% 24% • 7%



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

Chain Z:  61% 24% 9% 7%



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	185.85Å 209.49Å 179.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40	Depositor
% Data completeness (in resolution range)	97.7 (15.00-2.40)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.182 , 0.230	Depositor
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.221	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.045 for l,-k,h	Xtriage
Total number of atoms	31717	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: UNX, TPO, CU, MG, FME, CUA, CDL, PEK, DMU, PGV, SAC, ZN, EDO, CMO, NA, CHD, TGL, HEA, PSC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.91	10/4164 (0.2%)	0.89	4/5689 (0.1%)
1	N	0.86	11/4156 (0.3%)	0.82	0/5678
2	B	0.81	2/1860 (0.1%)	0.90	1/2534 (0.0%)
2	O	0.73	2/1860 (0.1%)	0.83	0/2534
3	C	0.92	7/2197 (0.3%)	0.81	0/3005
3	P	0.89	4/2197 (0.2%)	0.80	0/3005
4	D	0.82	4/1229 (0.3%)	0.79	0/1658
4	Q	0.76	4/1229 (0.3%)	0.74	0/1658
5	E	0.67	1/871 (0.1%)	0.80	0/1182
5	R	0.65	0/871	0.74	0/1182
6	F	0.74	1/765 (0.1%)	0.86	2/1038 (0.2%)
6	S	0.72	0/765	0.82	1/1038 (0.1%)
7	G	0.86	1/690 (0.1%)	0.87	1/937 (0.1%)
7	T	0.80	1/690 (0.1%)	0.83	1/937 (0.1%)
8	H	0.85	2/682 (0.3%)	0.86	0/921
8	U	0.79	3/682 (0.4%)	0.79	0/921
9	I	0.69	0/605	0.83	0/802
9	V	0.60	0/605	0.80	1/802 (0.1%)
10	J	0.72	0/471	0.75	0/636
10	W	0.66	1/471 (0.2%)	0.77	0/636
11	K	0.81	1/398 (0.3%)	0.76	0/546
11	X	0.80	2/398 (0.5%)	0.75	0/546
12	L	0.80	0/393	0.76	0/526
12	Y	0.75	1/393 (0.3%)	0.75	0/526
13	M	0.81	1/345 (0.3%)	0.78	0/470
13	Z	0.68	0/345	0.75	0/470
All	All	0.82	59/29332 (0.2%)	0.82	11/39877 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
7	T	0	2
All	All	0	3

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	58	TRP	CD2-CE2	7.46	1.50	1.41
1	N	126	TRP	CD2-CE2	7.33	1.50	1.41
1	A	396	TRP	CD2-CE2	6.55	1.49	1.41
2	B	106	TRP	CD2-CE2	6.42	1.49	1.41
1	N	340	TRP	CD2-CE2	6.38	1.49	1.41

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASP	CB-CG-OD1	7.54	125.08	118.30
1	A	438	ARG	NE-CZ-NH1	-6.50	117.05	120.30
6	S	96	LEU	CA-CB-CG	6.36	129.92	115.30
7	G	37	LEU	CA-CB-CG	6.03	129.17	115.30
6	F	48	LEU	CB-CG-CD2	-6.00	100.81	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	11	TPO	Peptide
7	T	10	GLY	Peptide
7	T	11	TPO	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	4030	0	4009	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4027	0	4002	99	0
2	B	1824	0	1833	34	0
2	O	1824	0	1833	38	0
3	C	2110	0	2027	31	0
3	P	2110	0	2027	40	0
4	D	1195	0	1183	21	0
4	Q	1195	0	1183	31	0
5	E	852	0	845	8	0
5	R	852	0	845	21	0
6	F	748	0	728	13	0
6	S	748	0	728	18	0
7	G	675	0	643	29	0
7	T	675	0	643	23	0
8	H	662	0	623	13	0
8	U	662	0	623	9	0
9	I	601	0	613	8	0
9	V	601	0	613	23	0
10	J	460	0	459	8	0
10	W	460	0	459	11	0
11	K	384	0	366	6	0
11	X	384	0	366	12	0
12	L	380	0	380	12	0
12	Y	380	0	380	13	0
13	M	335	0	352	9	0
13	Z	335	0	352	15	0
14	A	120	0	108	12	0
14	N	120	0	108	13	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	2	0	0	1	0
18	N	2	0	0	0	0
19	A	63	0	110	3	0
19	D	63	0	110	1	0
19	L	63	0	110	4	0
19	N	189	0	330	11	0
20	A	102	0	152	3	0
20	C	102	0	152	0	0
20	G	51	0	76	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	N	102	0	152	8	0
20	P	51	0	76	3	0
21	A	20	0	30	9	0
21	B	8	0	12	1	0
21	C	12	0	18	0	0
21	F	4	0	6	0	0
21	G	4	0	6	0	0
21	K	12	0	18	0	0
21	L	4	0	6	0	0
21	N	4	0	6	1	0
21	T	4	0	6	1	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	29	0	39	1	0
23	C	58	0	78	3	0
23	J	29	0	39	1	0
23	O	29	0	39	1	0
23	P	58	0	78	2	0
23	W	29	0	38	1	0
24	B	52	0	80	12	0
24	R	52	0	80	6	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	200	0	312	15	0
26	P	100	0	156	7	0
26	T	100	0	156	13	0
27	C	53	0	77	3	0
27	G	106	0	154	10	0
27	P	53	0	77	4	0
27	T	106	0	154	4	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	M	33	0	42	1	0
29	Z	33	0	42	1	0
30	A	125	0	0	22	0
30	B	78	0	0	6	0
30	C	70	0	0	18	0
30	D	41	0	0	2	0
30	E	24	0	0	2	0
30	F	36	0	0	2	0
30	G	31	0	0	2	0
30	H	33	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	I	12	0	0	0	0
30	J	19	0	0	2	0
30	K	19	0	0	3	0
30	L	14	0	0	2	0
30	M	15	0	0	1	0
30	N	117	0	0	16	0
30	O	77	0	0	8	0
30	P	54	0	0	5	0
30	Q	29	0	0	7	0
30	R	29	0	0	3	0
30	S	43	0	0	4	0
30	T	20	0	0	6	0
30	U	31	0	0	3	0
30	V	19	0	0	4	0
30	W	17	0	0	1	0
30	X	9	0	0	4	0
30	Y	6	0	0	1	0
30	Z	4	0	0	0	0
All	All	31717	0	31348	645	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 10.

The worst 5 of 645 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:240:HIS:NE2	1:N:244:TYR:CE2	1.73	1.45
1:A:240:HIS:NE2	1:A:244:TYR:HE2	1.01	1.42
1:A:240:HIS:NE2	1:A:244:TYR:CE2	1.78	1.30
1:A:240:HIS:CD2	1:A:244:TYR:HE2	1.49	1.29
1:N:240:HIS:NE2	1:N:244:TYR:HE2	0.80	1.28

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	513/514 (100%)	494 (96%)	19 (4%)	0	100	100
1	N	512/514 (100%)	488 (95%)	23 (4%)	1 (0%)	44	59
2	B	225/227 (99%)	213 (95%)	11 (5%)	1 (0%)	30	44
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	14	22
3	C	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
3	P	257/261 (98%)	248 (96%)	6 (2%)	3 (1%)	11	16
4	D	142/147 (97%)	133 (94%)	9 (6%)	0	100	100
4	Q	142/147 (97%)	130 (92%)	9 (6%)	3 (2%)	5	7
5	E	103/109 (94%)	98 (95%)	4 (4%)	1 (1%)	13	20
5	R	103/109 (94%)	99 (96%)	3 (3%)	1 (1%)	13	20
6	F	96/98 (98%)	87 (91%)	7 (7%)	2 (2%)	5	7
6	S	96/98 (98%)	90 (94%)	5 (5%)	1 (1%)	13	20
7	G	81/85 (95%)	69 (85%)	8 (10%)	4 (5%)	2	1
7	T	81/85 (95%)	68 (84%)	5 (6%)	8 (10%)	0	0
8	H	77/85 (91%)	67 (87%)	9 (12%)	1 (1%)	10	15
8	U	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	1	1
9	I	71/73 (97%)	66 (93%)	5 (7%)	0	100	100
9	V	71/73 (97%)	64 (90%)	6 (8%)	1 (1%)	9	13
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	7	9
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	41 (87%)	5 (11%)	1 (2%)	5	7
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
13	M	41/46 (89%)	40 (98%)	0	1 (2%)	5	5
13	Z	41/46 (89%)	38 (93%)	2 (5%)	1 (2%)	5	5
All	All	3505/3614 (97%)	3301 (94%)	167 (5%)	37 (1%)	12	18

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	97	ALA
7	G	3	ALA
7	G	4	ALA
7	G	8	HIS
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	427/426 (100%)	411 (96%)	16 (4%)	29	48
1	N	426/426 (100%)	408 (96%)	18 (4%)	25	43
2	B	210/210 (100%)	198 (94%)	12 (6%)	17	29
2	O	210/210 (100%)	198 (94%)	12 (6%)	17	29
3	C	224/226 (99%)	220 (98%)	4 (2%)	54	73
3	P	224/226 (99%)	216 (96%)	8 (4%)	30	49
4	D	128/129 (99%)	125 (98%)	3 (2%)	45	66
4	Q	128/129 (99%)	121 (94%)	7 (6%)	18	31
5	E	92/95 (97%)	86 (94%)	6 (6%)	14	24
5	R	92/95 (97%)	87 (95%)	5 (5%)	18	32
6	F	81/81 (100%)	77 (95%)	4 (5%)	21	36
6	S	81/81 (100%)	74 (91%)	7 (9%)	8	14
7	G	67/68 (98%)	61 (91%)	6 (9%)	8	12
7	T	67/68 (98%)	63 (94%)	4 (6%)	16	27
8	H	71/75 (95%)	63 (89%)	8 (11%)	4	7
8	U	71/75 (95%)	65 (92%)	6 (8%)	8	14
9	I	57/57 (100%)	52 (91%)	5 (9%)	8	13
9	V	57/57 (100%)	51 (90%)	6 (10%)	5	8
10	J	49/50 (98%)	46 (94%)	3 (6%)	15	27
10	W	49/50 (98%)	43 (88%)	6 (12%)	4	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	39/46 (85%)	37 (95%)	2 (5%)	20	35
11	X	39/46 (85%)	37 (95%)	2 (5%)	20	35
12	L	39/40 (98%)	37 (95%)	2 (5%)	20	35
12	Y	39/40 (98%)	37 (95%)	2 (5%)	20	35
13	M	37/38 (97%)	35 (95%)	2 (5%)	18	32
13	Z	37/38 (97%)	32 (86%)	5 (14%)	3	4
All	All	3041/3082 (99%)	2880 (95%)	161 (5%)	19	33

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	Q	31	LYS
9	V	31	PHE
5	R	36	LEU
7	T	17	ARG
10	W	29	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	181	GLN
7	T	8	HIS
3	P	68	GLN
4	Q	109	HIS
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 ⓘ

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SAC	I	1	9	7,8,9	1.30	1 (14%)	8,9,11	0.99	0
7	TPO	T	11	7	8,10,11	1.73	2 (25%)	10,14,16	1.02	1 (10%)
1	FME	A	1	1	8,9,10	0.44	0	7,9,11	1.97	4 (57%)
1	FME	N	1	1	8,9,10	0.45	0	7,9,11	1.59	2 (28%)
7	TPO	G	11	7	8,10,11	1.45	1 (12%)	10,14,16	0.92	1 (10%)
2	FME	O	1	2	8,9,10	0.85	0	7,9,11	1.63	1 (14%)
2	FME	B	1	2	8,9,10	0.97	0	7,9,11	1.45	3 (42%)
9	SAC	V	1	9	7,8,9	1.70	1 (14%)	8,9,11	1.82	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SAC	I	1	9	-	4/7/8/10	-
7	TPO	T	11	7	-	2/9/11/13	-
1	FME	A	1	1	-	3/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-
7	TPO	G	11	7	-	2/9/11/13	-
2	FME	O	1	2	-	0/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
9	SAC	V	1	9	-	4/7/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	CA-N	4.27	1.52	1.46
9	I	1	SAC	CA-N	3.22	1.50	1.46
7	T	11	TPO	P-O1P	2.85	1.59	1.50
7	G	11	TPO	P-O1P	2.83	1.59	1.50
7	T	11	TPO	P-OG1	2.33	1.63	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	C-CA-N	3.75	116.49	109.73
2	O	1	FME	CA-N-CN	3.70	128.51	122.82
1	N	1	FME	C-CA-N	2.76	114.71	109.73
1	A	1	FME	C-CA-N	2.75	114.69	109.73
1	A	1	FME	CE-SD-CG	2.60	109.33	100.40

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
7	G	11	TPO	N-CA-CB-OG1
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 62 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	$\# Z > 2$
21	EDO	G	104	-	3,3,3	0.40	0	2,2,2	0.56	0
21	EDO	L	102	-	3,3,3	0.46	0	2,2,2	0.40	0
23	CHD	W	101	-	32,32,32	0.91	1 (3%)	51,51,51	2.11	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	P	303	-	50,50,50	0.93	2 (4%)	53,56,56	1.08	5 (9%)
20	PGV	N	607	-	50,50,50	1.09	2 (4%)	53,56,56	1.07	4 (7%)
14	HEA	N	602	1	57,67,67	1.70	11 (19%)	61,103,103	1.48	10 (16%)
19	TGL	D	201	-	62,62,62	1.13	3 (4%)	65,65,65	0.99	5 (7%)
21	EDO	C	310	-	3,3,3	0.53	0	2,2,2	0.33	0
21	EDO	K	102	-	3,3,3	0.50	0	2,2,2	0.26	0
23	CHD	C	305	-	32,32,32	0.99	1 (3%)	51,51,51	1.25	7 (13%)
29	DMU	M	101	-	34,34,34	0.53	0	45,45,45	1.14	4 (8%)
19	TGL	A	607	-	62,62,62	1.23	4 (6%)	65,65,65	1.38	10 (15%)
23	CHD	P	305	-	32,32,32	0.59	0	51,51,51	1.81	13 (25%)
21	EDO	B	305	-	3,3,3	0.39	0	2,2,2	0.49	0
23	CHD	B	302	-	32,32,32	0.81	0	51,51,51	1.26	4 (7%)
21	EDO	C	311	-	3,3,3	0.53	0	2,2,2	0.30	0
29	DMU	Z	101	-	34,34,34	0.53	0	45,45,45	1.13	4 (8%)
18	CMO	N	606	-	0,1,1	-	-	-	-	-
27	PEK	C	306	-	52,52,52	1.03	2 (3%)	55,57,57	0.90	3 (5%)
23	CHD	C	304	-	32,32,32	0.62	0	51,51,51	1.97	16 (31%)
14	HEA	N	601	1	57,67,67	1.61	9 (15%)	61,103,103	1.42	9 (14%)
22	CUA	B	301	2	0,1,1	-	-	-	-	-
21	EDO	A	610	-	3,3,3	0.52	0	2,2,2	0.57	0
23	CHD	P	306	-	32,32,32	0.74	1 (3%)	51,51,51	1.53	12 (23%)
23	CHD	J	101	-	32,32,32	0.66	0	51,51,51	1.54	10 (19%)
21	EDO	A	611	-	3,3,3	0.37	0	2,2,2	0.61	0
20	PGV	C	308	-	50,50,50	1.21	2 (4%)	53,56,56	1.01	3 (5%)
19	TGL	N	609	-	62,62,62	1.12	3 (4%)	65,65,65	1.29	8 (12%)
26	CDL	C	303	-	99,99,99	1.39	12 (12%)	105,111,111	1.22	7 (6%)
26	CDL	C	307	-	99,99,99	1.43	13 (13%)	105,111,111	1.23	8 (7%)
20	PGV	N	608	-	50,50,50	0.90	3 (6%)	53,56,56	1.17	4 (7%)
27	PEK	T	101	-	52,52,52	1.16	2 (3%)	55,57,57	1.06	4 (7%)
14	HEA	A	601	1	57,67,67	1.56	8 (14%)	61,103,103	2.23	24 (39%)
22	CUA	O	301	2	0,1,1	-	-	-	-	-
19	TGL	N	611	-	62,62,62	1.18	3 (4%)	65,65,65	1.24	7 (10%)
27	PEK	T	102	-	52,52,52	1.19	2 (3%)	55,57,57	1.13	4 (7%)
24	PSC	B	303	-	51,51,51	1.28	3 (5%)	57,59,59	1.07	5 (8%)
14	HEA	A	602	1	57,67,67	1.66	12 (21%)	61,103,103	1.67	12 (19%)
21	EDO	A	612	-	3,3,3	0.52	0	2,2,2	0.10	0
27	PEK	G	101	-	52,52,52	0.94	2 (3%)	55,57,57	1.23	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	B	304	-	3,3,3	0.40	0	2,2,2	0.60	0
26	CDL	P	304	-	99,99,99	1.39	12 (12%)	105,111,111	1.16	7 (6%)
20	PGV	C	302	-	50,50,50	0.92	2 (4%)	53,56,56	0.93	4 (7%)
19	TGL	L	101	-	62,62,62	1.19	3 (4%)	65,65,65	1.25	5 (7%)
18	CMO	A	606	15	0,1,1	-	-	-	-	-
21	EDO	N	612	-	3,3,3	0.56	0	2,2,2	0.16	0
26	CDL	T	103	-	99,99,99	1.37	12 (12%)	105,111,111	1.31	11 (10%)
21	EDO	T	104	-	3,3,3	0.45	0	2,2,2	0.26	0
27	PEK	P	302	-	52,52,52	0.87	2 (3%)	55,57,57	1.35	5 (9%)
20	PGV	A	609	-	50,50,50	1.10	2 (4%)	53,56,56	1.08	5 (9%)
21	EDO	A	613	-	3,3,3	0.54	0	2,2,2	0.24	0
21	EDO	K	103	-	3,3,3	0.56	0	2,2,2	0.11	0
21	EDO	F	102	-	3,3,3	0.57	0	2,2,2	0.06	0
24	PSC	R	201	-	51,51,51	1.22	3 (5%)	57,59,59	0.99	4 (7%)
20	PGV	A	608	-	50,50,50	0.79	2 (4%)	53,56,56	1.44	5 (9%)
21	EDO	C	309	-	3,3,3	0.38	0	2,2,2	0.68	0
27	PEK	G	102	-	52,52,52	1.21	2 (3%)	55,57,57	1.06	5 (9%)
19	TGL	N	610	-	62,62,62	1.13	3 (4%)	65,65,65	1.13	6 (9%)
20	PGV	G	103	-	50,50,50	1.07	2 (4%)	53,56,56	0.95	2 (3%)
23	CHD	O	302	-	32,32,32	1.04	2 (6%)	51,51,51	1.46	8 (15%)
21	EDO	A	614	-	3,3,3	0.59	0	2,2,2	0.11	0
21	EDO	K	101	-	3,3,3	0.47	0	2,2,2	0.33	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
21	EDO	G	104	-	-	0/1/1/1	-
21	EDO	L	102	-	-	1/1/1/1	-
23	CHD	W	101	-	-	6/9/74/74	0/4/4/4
20	PGV	N	607	-	-	33/55/55/55	-
14	HEA	N	602	1	-	6/32/76/76	-
19	TGL	D	201	-	-	38/65/65/65	-
21	EDO	C	310	-	-	1/1/1/1	-
21	EDO	K	102	-	-	1/1/1/1	-
23	CHD	C	305	-	-	2/9/74/74	0/4/4/4
29	DMU	M	101	-	-	5/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	A	607	-	-	36/65/65/65	-
23	CHD	P	305	-	-	9/9/74/74	0/4/4/4
21	EDO	B	305	-	-	0/1/1/1	-
23	CHD	B	302	-	-	2/9/74/74	0/4/4/4
21	EDO	C	311	-	-	0/1/1/1	-
29	DMU	Z	101	-	-	9/19/59/59	0/2/2/2
27	PEK	C	306	-	-	30/56/56/56	-
23	CHD	C	304	-	-	5/9/74/74	0/4/4/4
14	HEA	N	601	1	-	5/32/76/76	-
21	EDO	A	610	-	-	1/1/1/1	-
23	CHD	P	306	-	-	3/9/74/74	0/4/4/4
23	CHD	J	101	-	-	9/9/74/74	0/4/4/4
21	EDO	A	611	-	-	1/1/1/1	-
20	PGV	C	308	-	-	32/55/55/55	-
19	TGL	N	609	-	-	37/65/65/65	-
26	CDL	C	303	-	-	65/110/110/110	-
26	CDL	C	307	-	-	64/110/110/110	-
20	PGV	N	608	-	-	22/55/55/55	-
27	PEK	T	101	-	-	22/56/56/56	-
14	HEA	A	601	1	-	8/32/76/76	-
19	TGL	N	611	-	-	34/65/65/65	-
27	PEK	T	102	-	-	29/56/56/56	-
24	PSC	B	303	-	-	30/55/55/55	-
14	HEA	A	602	1	-	3/32/76/76	-
21	EDO	A	612	-	-	1/1/1/1	-
27	PEK	G	101	-	-	21/56/56/56	-
21	EDO	B	304	-	-	1/1/1/1	-
26	CDL	P	304	-	-	66/110/110/110	-
20	PGV	C	302	-	-	15/55/55/55	-
19	TGL	L	101	-	-	35/65/65/65	-
21	EDO	N	612	-	-	0/1/1/1	-
26	CDL	T	103	-	-	63/110/110/110	-
21	EDO	T	104	-	-	1/1/1/1	-
27	PEK	P	302	-	-	17/56/56/56	-
20	PGV	A	609	-	-	31/55/55/55	-
21	EDO	A	613	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	K	103	-	-	0/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
24	PSC	R	201	-	-	29/55/55/55	-
20	PGV	A	608	-	-	11/55/55/55	-
21	EDO	C	309	-	-	1/1/1/1	-
20	PGV	G	103	-	-	33/55/55/55	-
27	PEK	G	102	-	-	35/56/56/56	-
19	TGL	N	610	-	-	42/65/65/65	-
20	PGV	P	303	-	-	21/55/55/55	-
23	CHD	O	302	-	-	4/9/74/74	0/4/4/4
21	EDO	A	614	-	-	0/1/1/1	-
21	EDO	K	101	-	-	1/1/1/1	-

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	101	TGL	OG2-CB1	5.59	1.50	1.34
19	A	607	TGL	OG1-CA1	5.58	1.49	1.33
27	T	102	PEK	O01-C1	5.50	1.49	1.34
19	A	607	TGL	OG2-CB1	5.44	1.49	1.34
20	C	308	PGV	O01-C1	5.43	1.49	1.34

The worst 5 of 290 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	C3D-C4D-ND	6.48	116.63	110.36
23	W	101	CHD	C13-C17-C20	5.97	126.63	119.50
19	N	611	TGL	OG2-CB1-CB2	5.80	124.01	111.50
19	N	609	TGL	OG2-CB1-CB2	5.64	123.66	111.50
26	T	103	CDL	OB6-CB5-C51	5.53	123.42	111.50

There are no chirality outliers.

5 of 978 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601	HEA	C1A-C2A-CAA-CBA
14	A	601	HEA	C3A-C2A-CAA-CBA
19	D	201	TGL	CC2-CC1-OG3-CG3
19	D	201	TGL	OC1-CC1-OG3-CG3
19	L	101	TGL	CB2-CB1-OG2-CG2

There are no ring outliers.

46 monomers are involved in 154 short contacts:

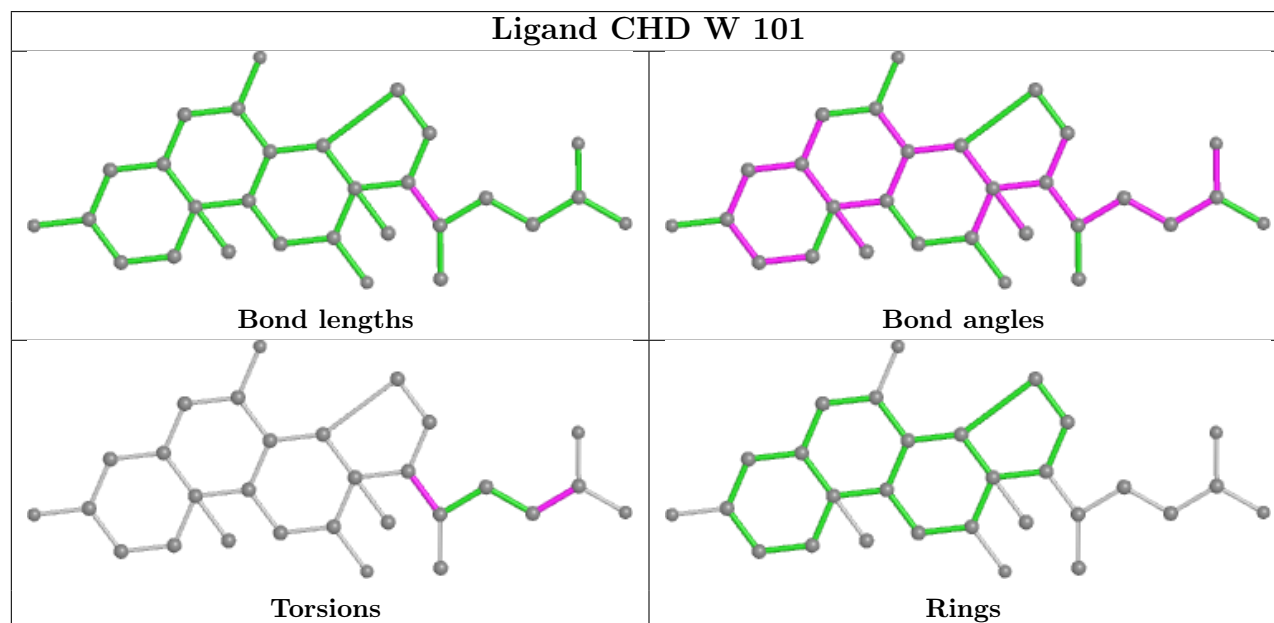
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	W	101	CHD	1	0
20	P	303	PGV	3	0
20	N	607	PGV	6	0
14	N	602	HEA	3	0
19	D	201	TGL	1	0
23	C	305	CHD	1	0
29	M	101	DMU	1	0
19	A	607	TGL	3	0
23	P	305	CHD	1	0
21	B	305	EDO	1	0
23	B	302	CHD	1	0
29	Z	101	DMU	1	0
27	C	306	PEK	3	0
23	C	304	CHD	2	0
14	N	601	HEA	10	0
21	A	610	EDO	1	0
23	P	306	CHD	1	0
23	J	101	CHD	1	0
19	N	609	TGL	5	0
26	C	303	CDL	2	0
26	C	307	CDL	13	0
20	N	608	PGV	2	0
27	T	101	PEK	3	0
14	A	601	HEA	6	0
19	N	611	TGL	4	0
27	T	102	PEK	1	0
24	B	303	PSC	12	0
14	A	602	HEA	6	0
21	A	612	EDO	2	0
27	G	101	PEK	4	0
26	P	304	CDL	7	0
19	L	101	TGL	4	0
18	A	606	CMO	1	0
21	N	612	EDO	1	0
26	T	103	CDL	13	0
21	T	104	EDO	1	0
27	P	302	PEK	4	0
20	A	609	PGV	2	0
21	A	613	EDO	2	0
24	R	201	PSC	6	0

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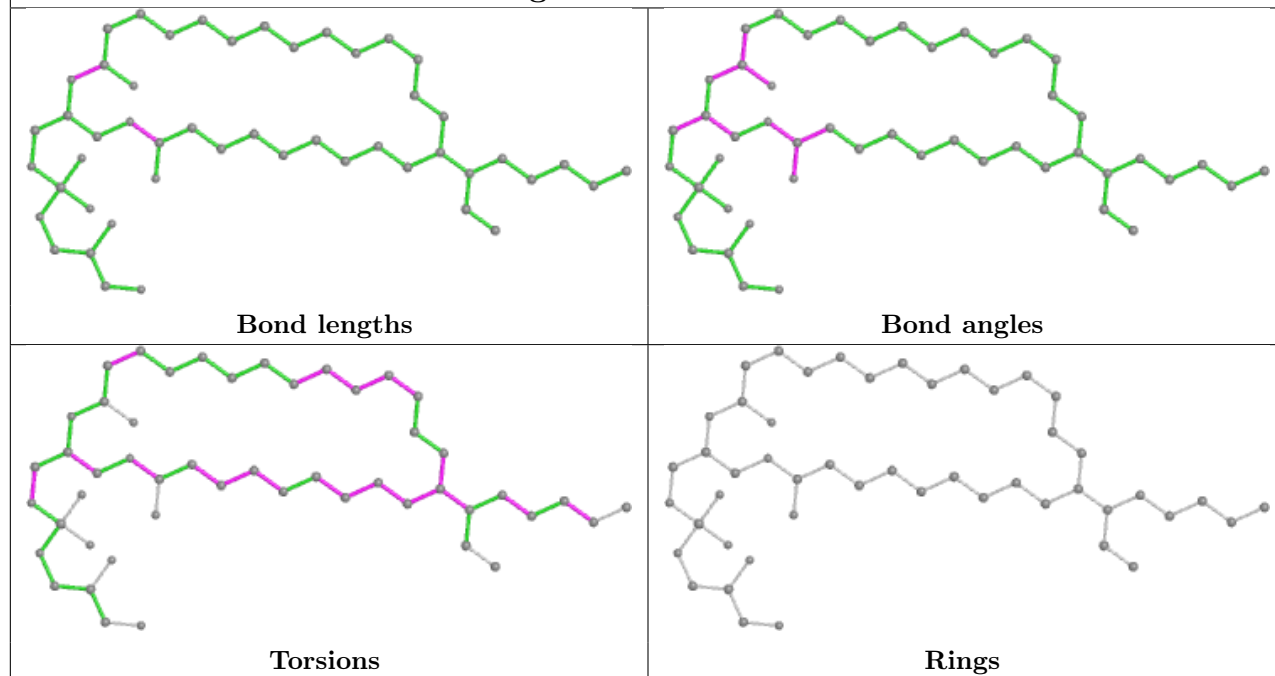
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	608	PGV	1	0
27	G	102	PEK	6	0
19	N	610	TGL	2	0
20	G	103	PGV	2	0
23	O	302	CHD	1	0
21	A	614	EDO	4	0

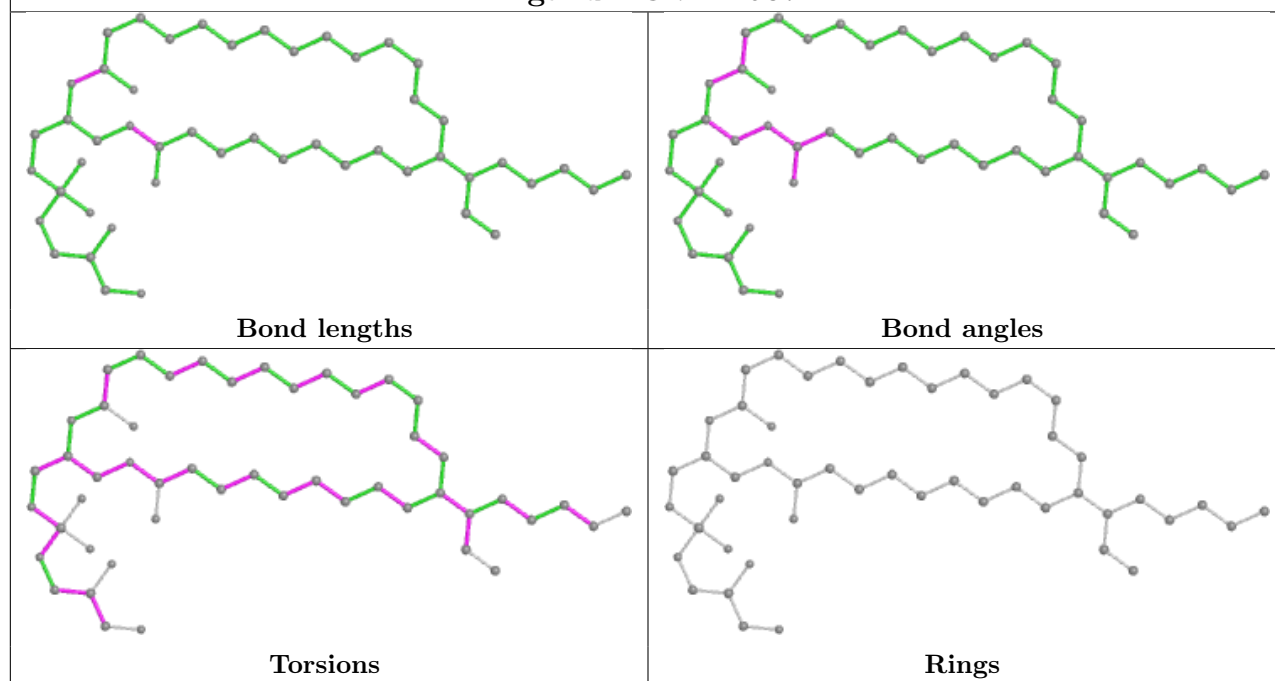
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

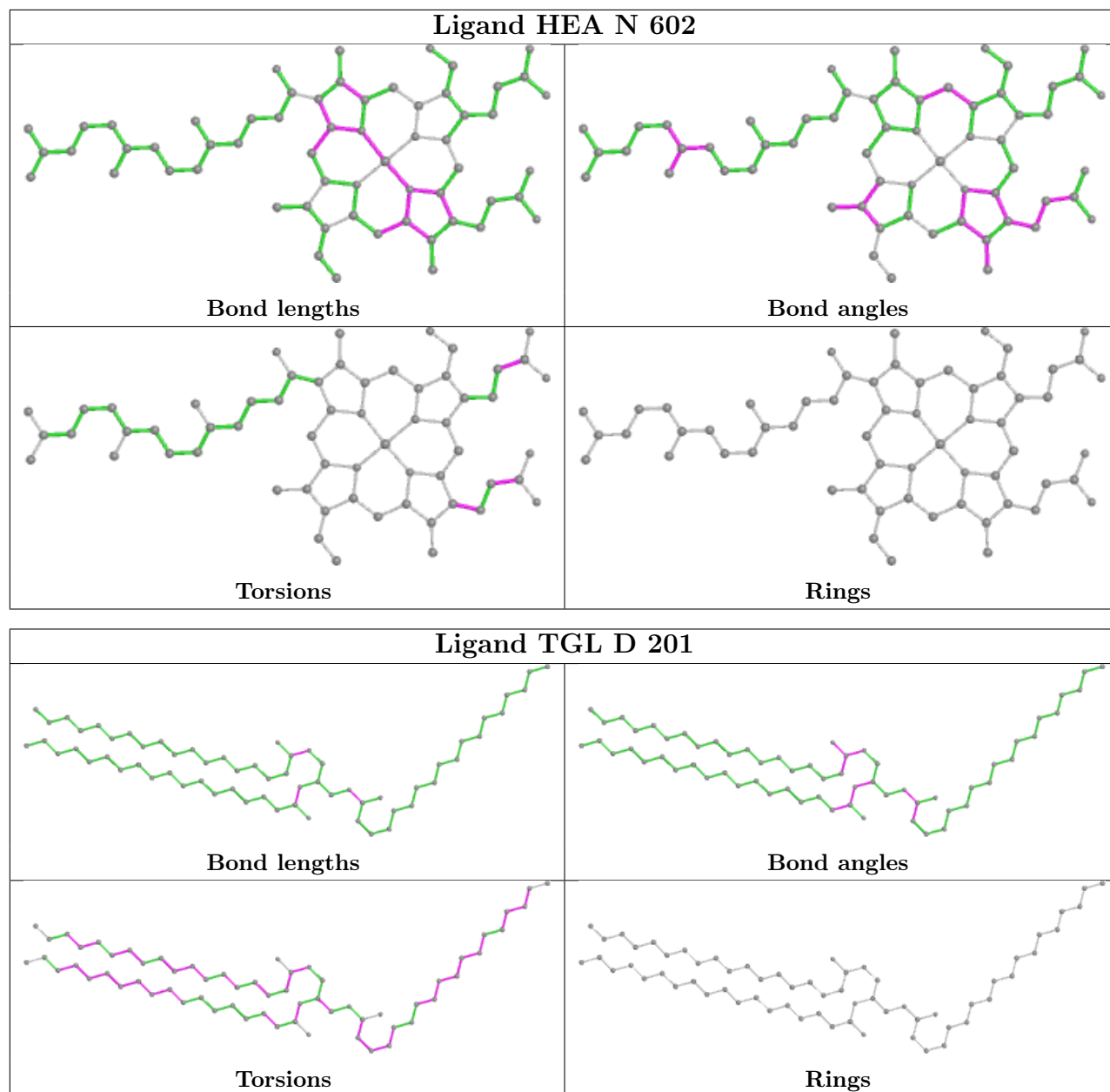


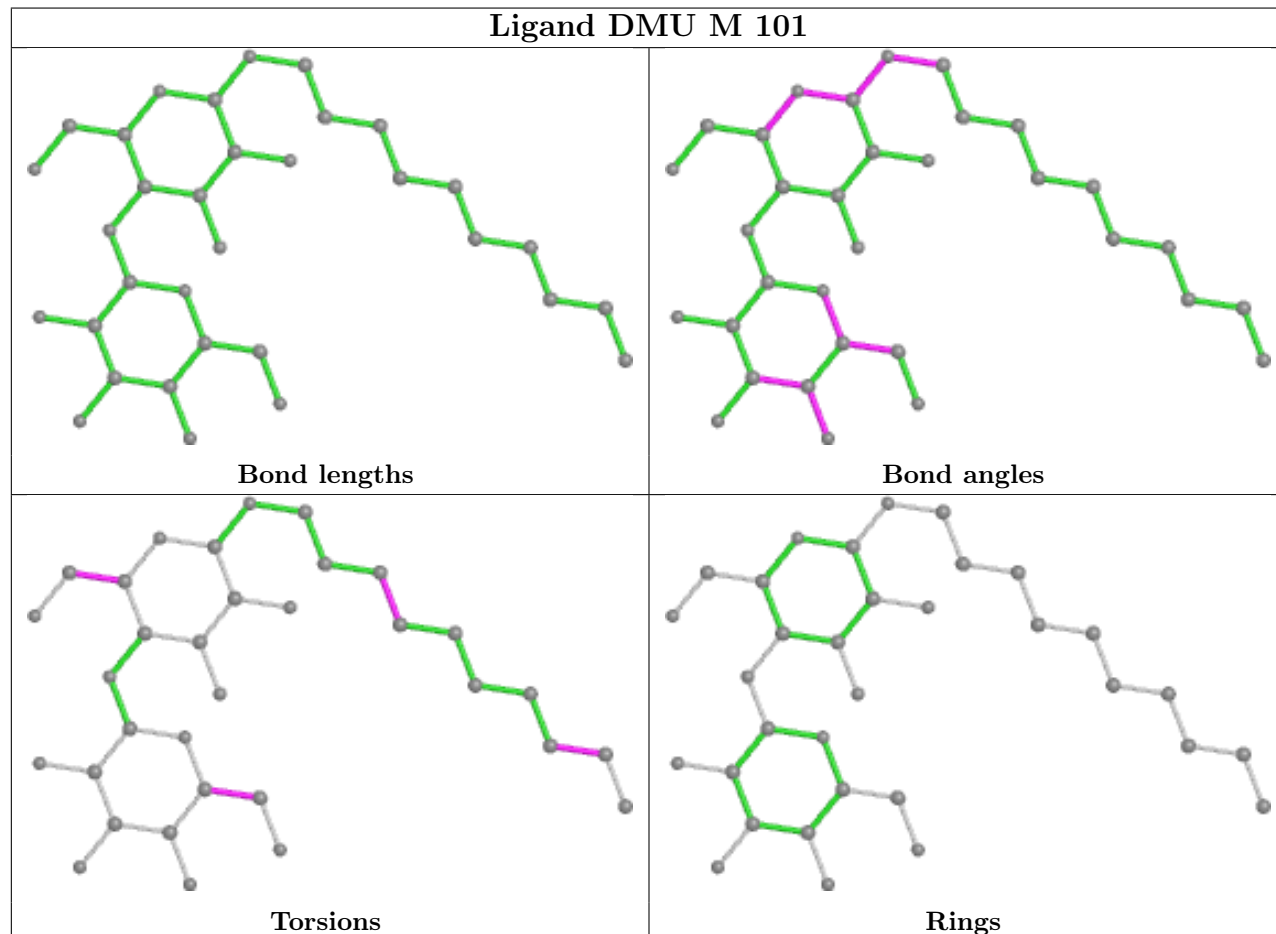
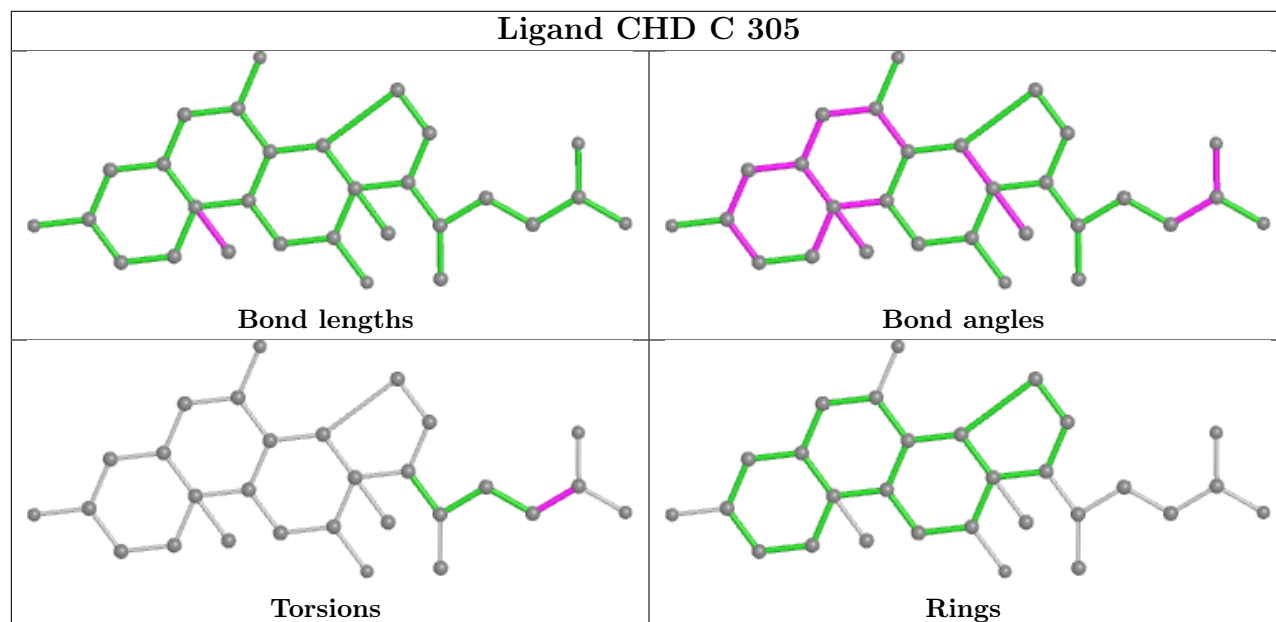
Ligand PGV P 303

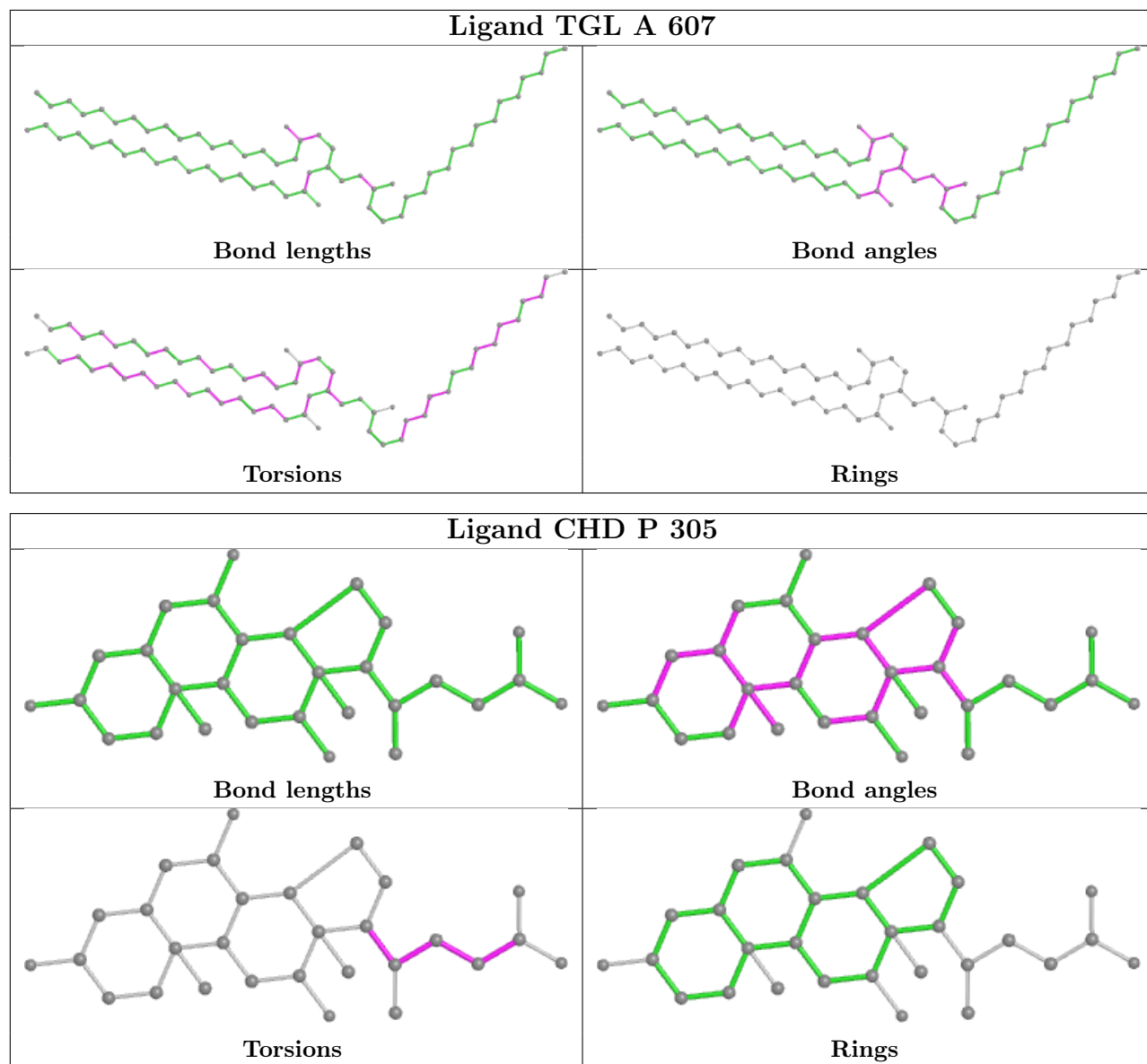


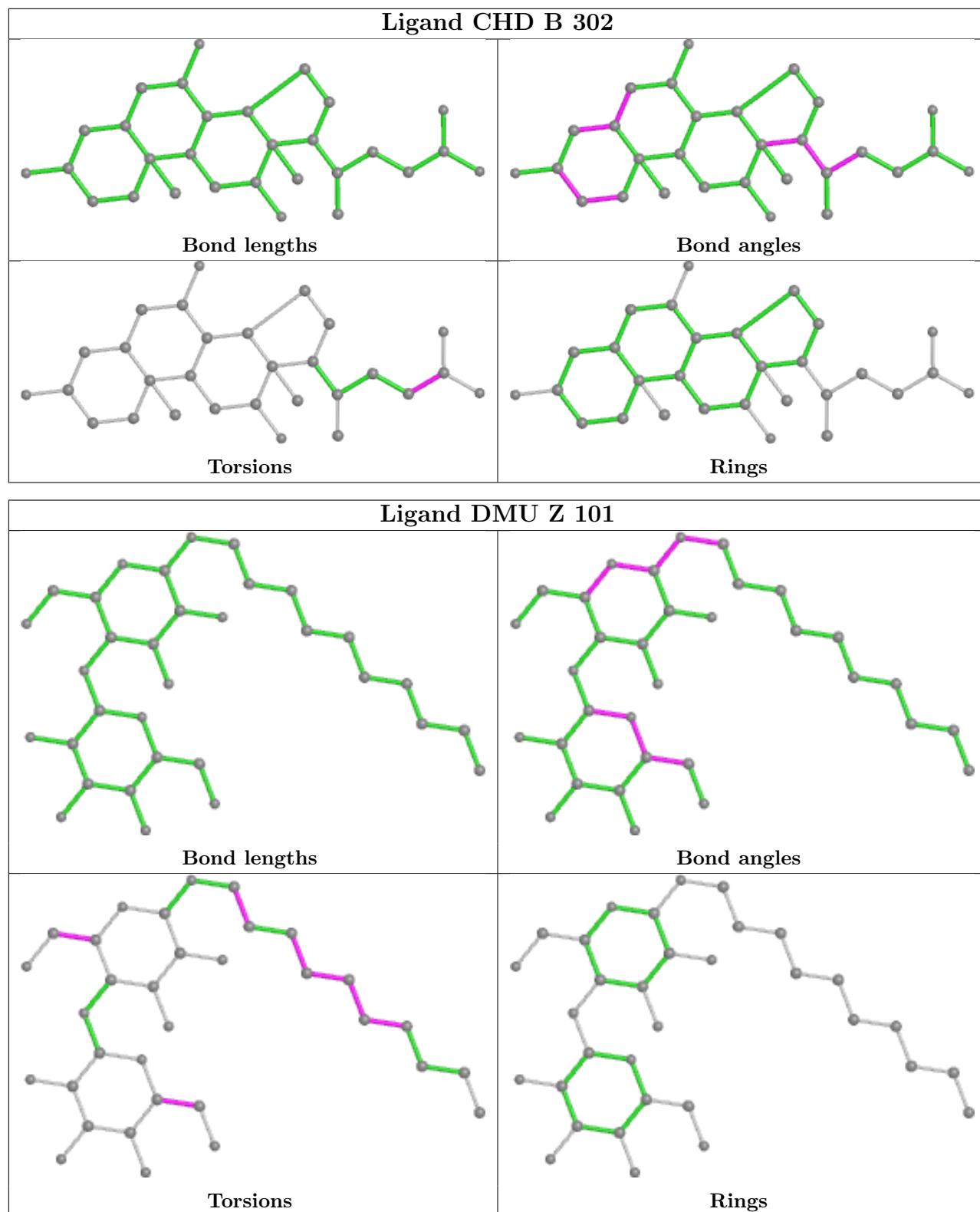
Ligand PGV N 607



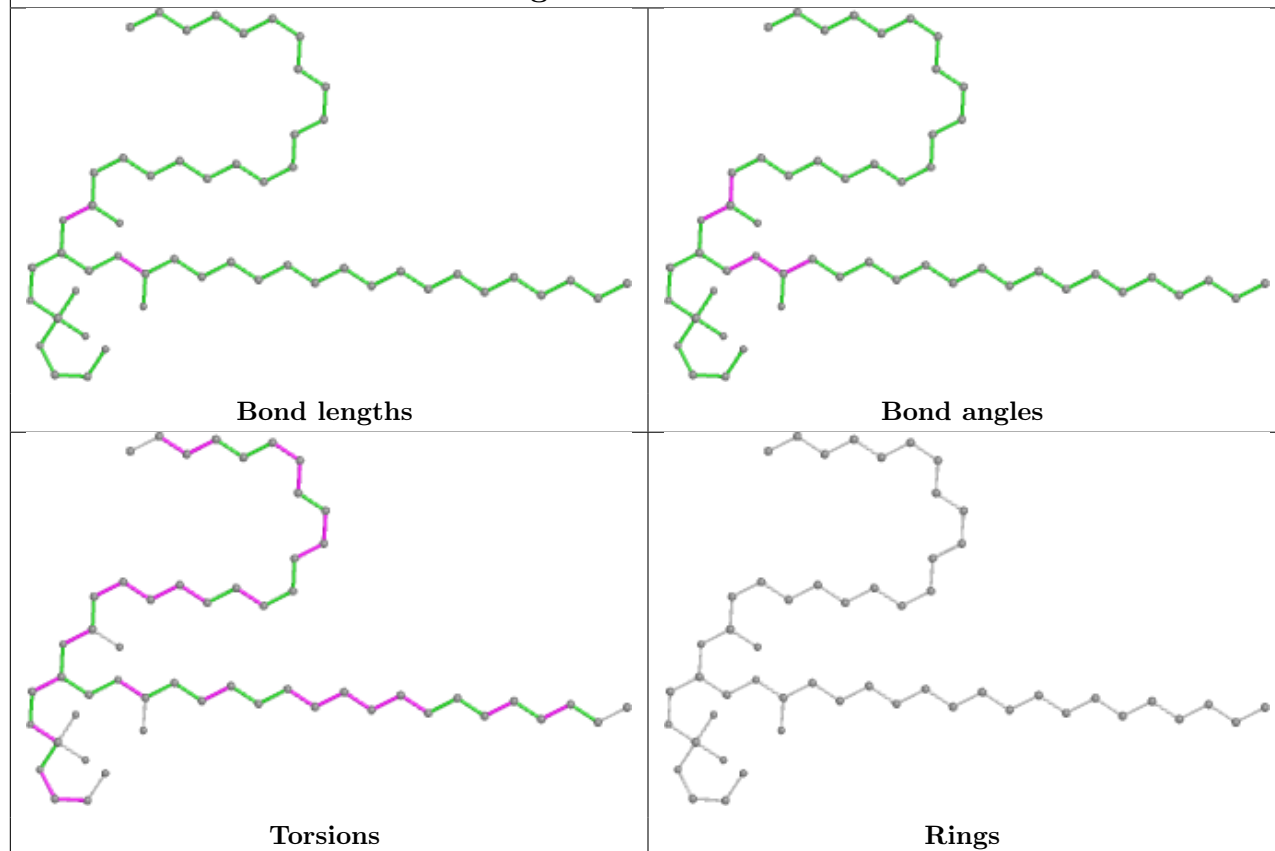




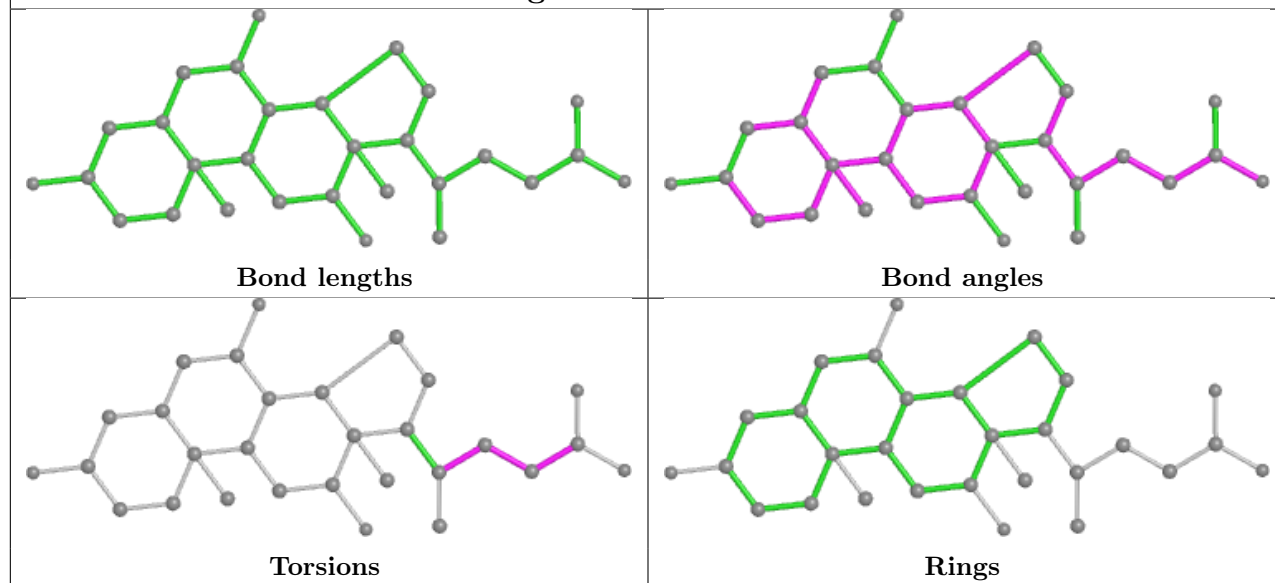


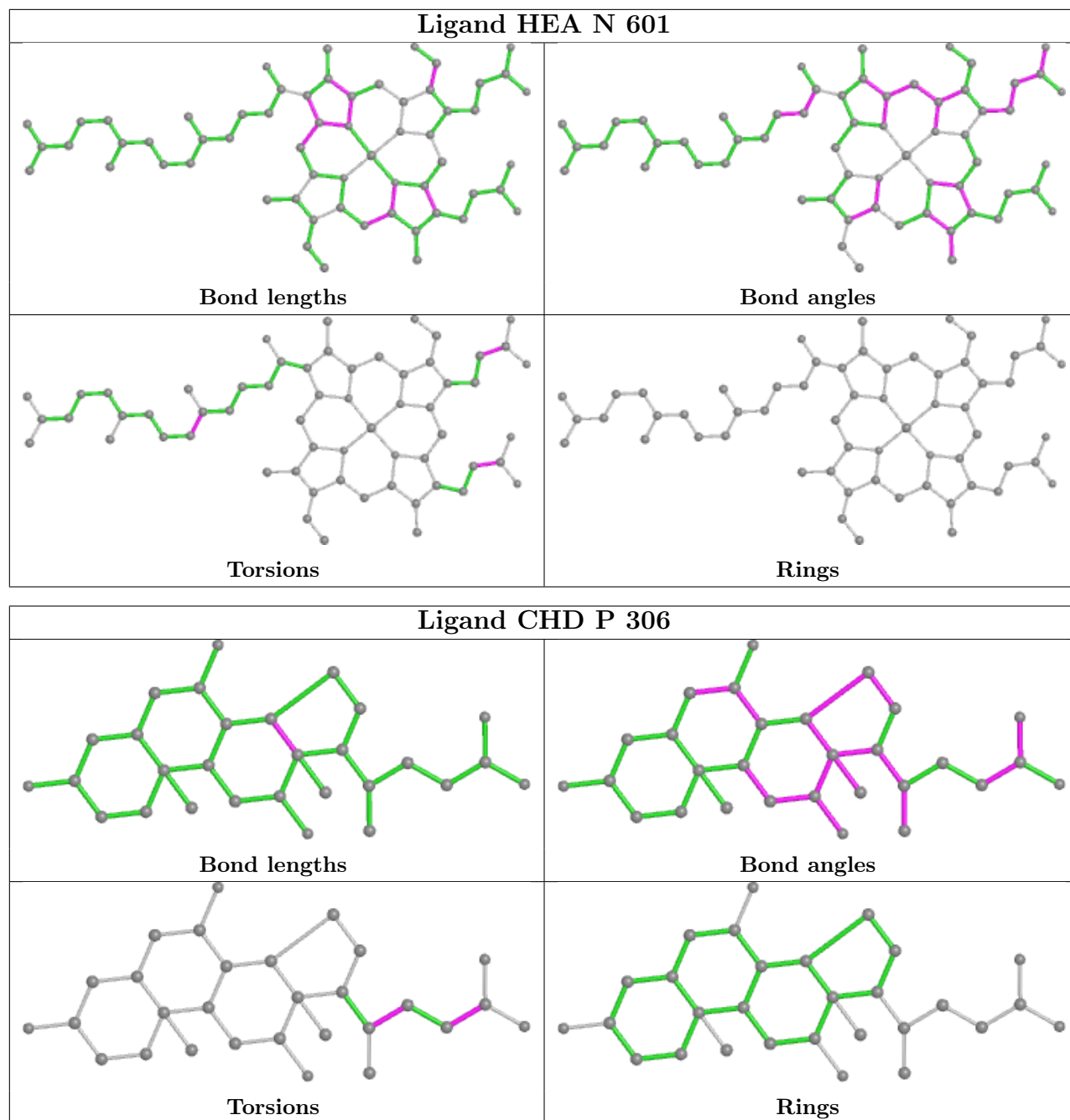


Ligand PEK C 306

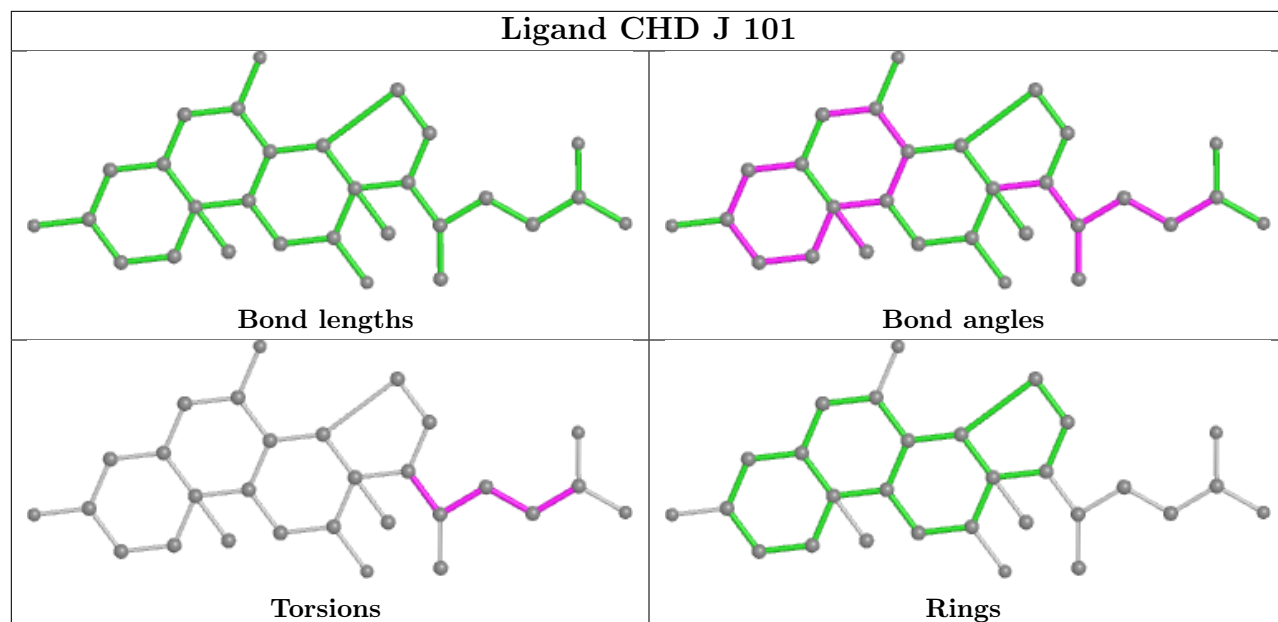


Ligand CHD C 304

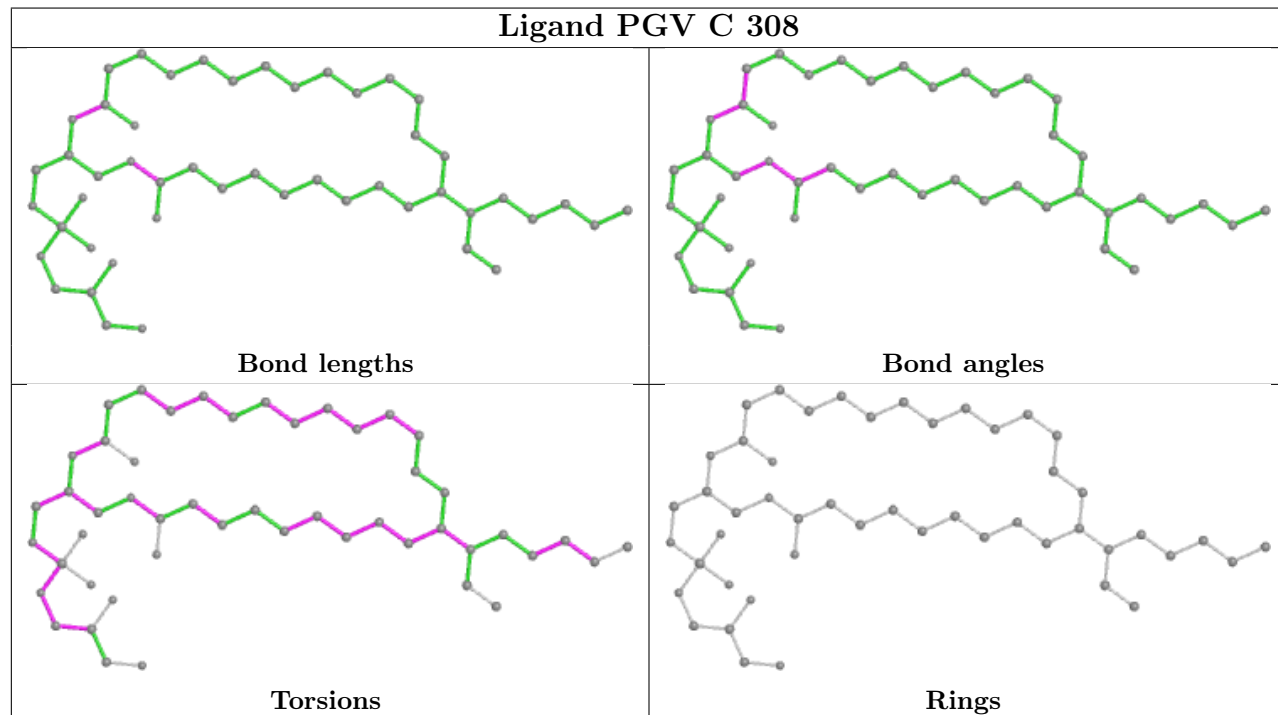


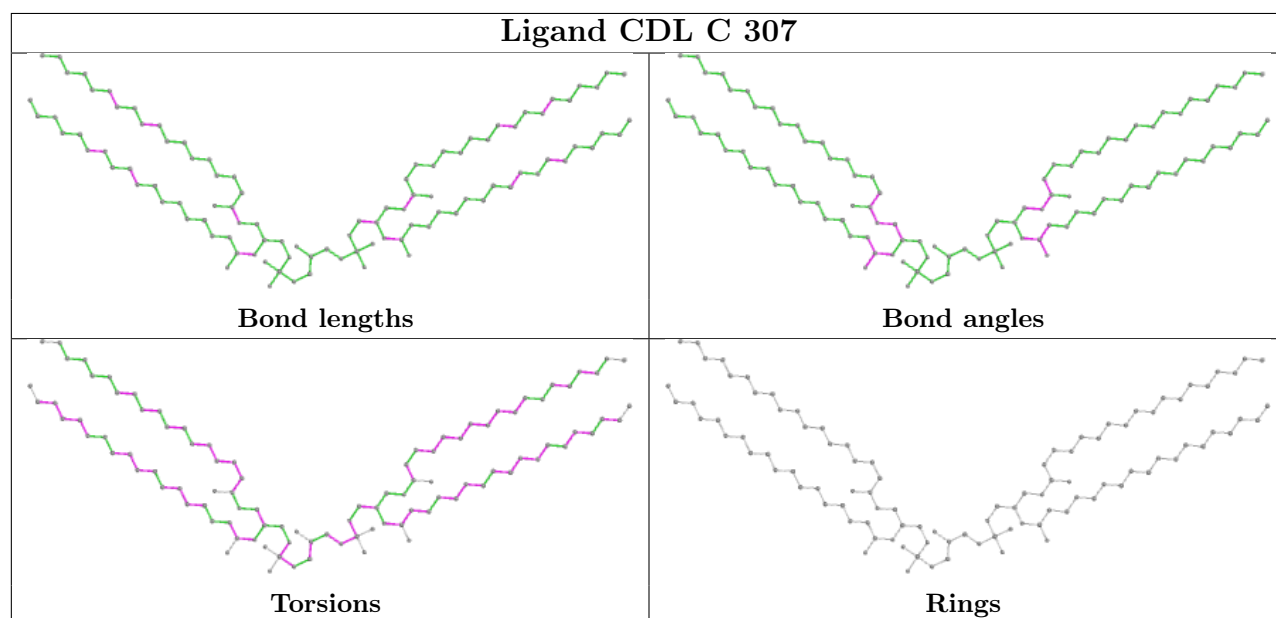
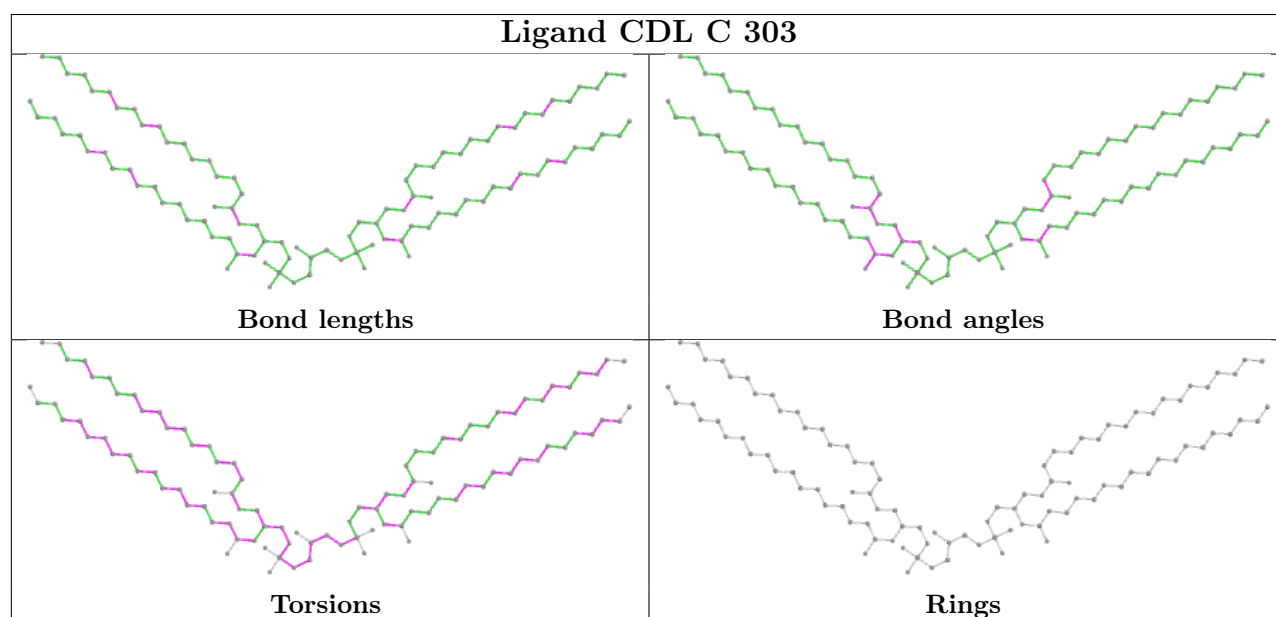
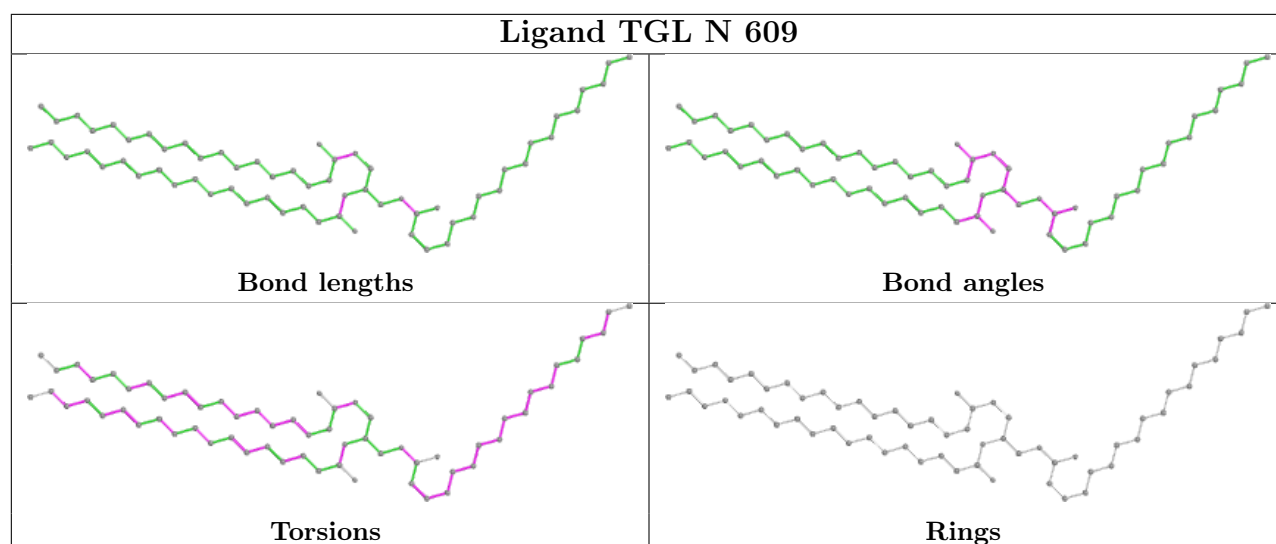


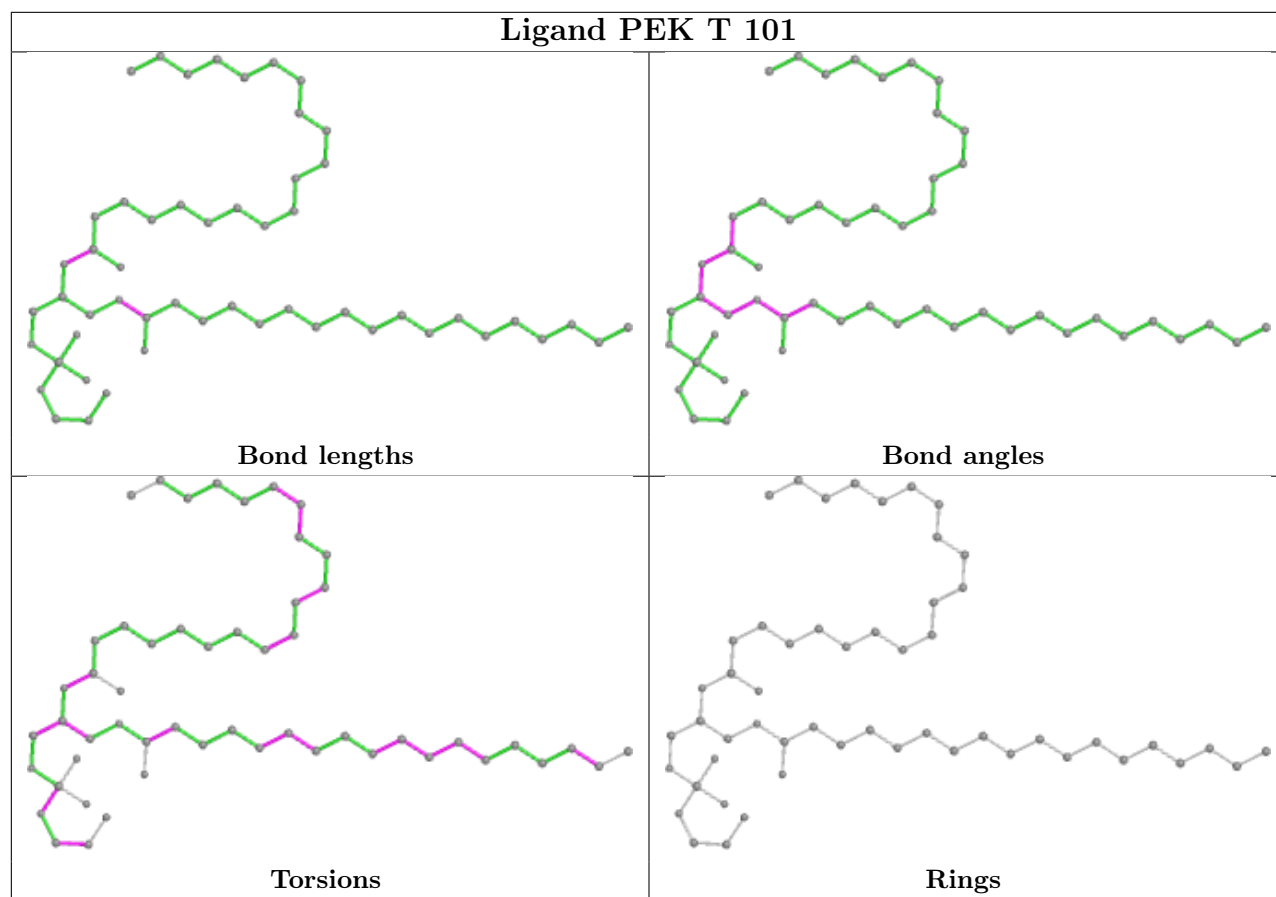
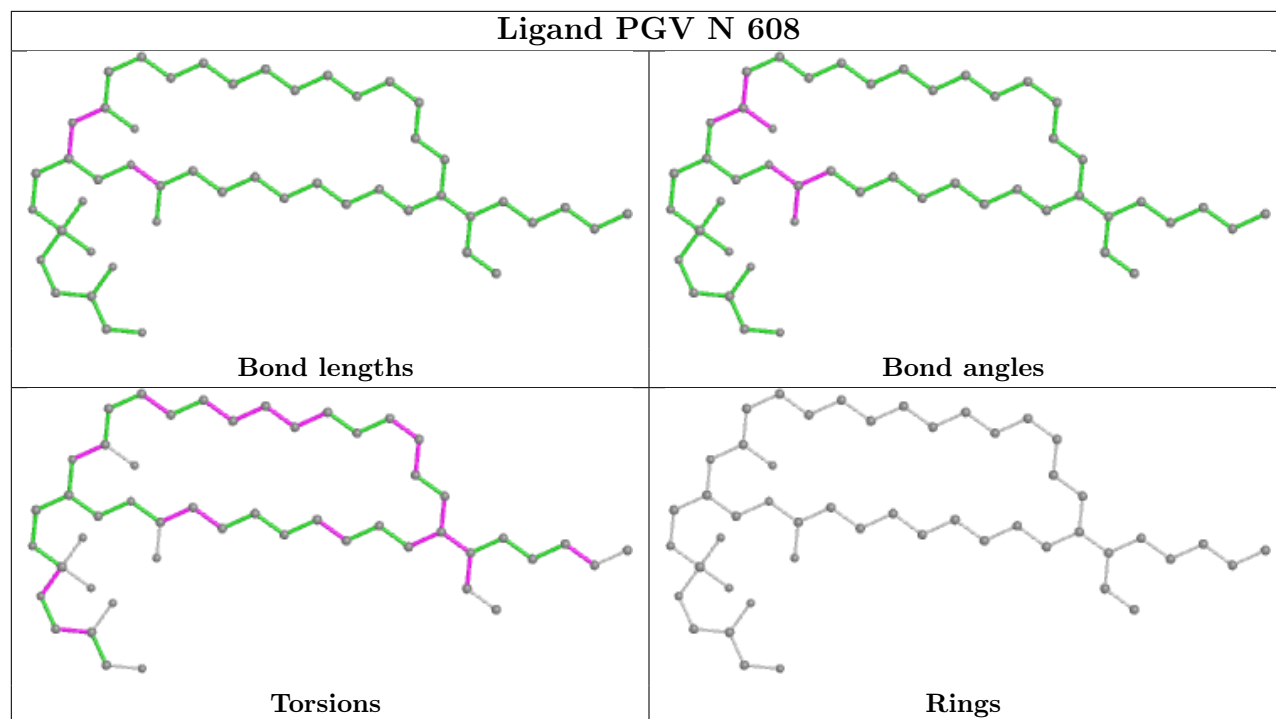
Ligand CHD J 101

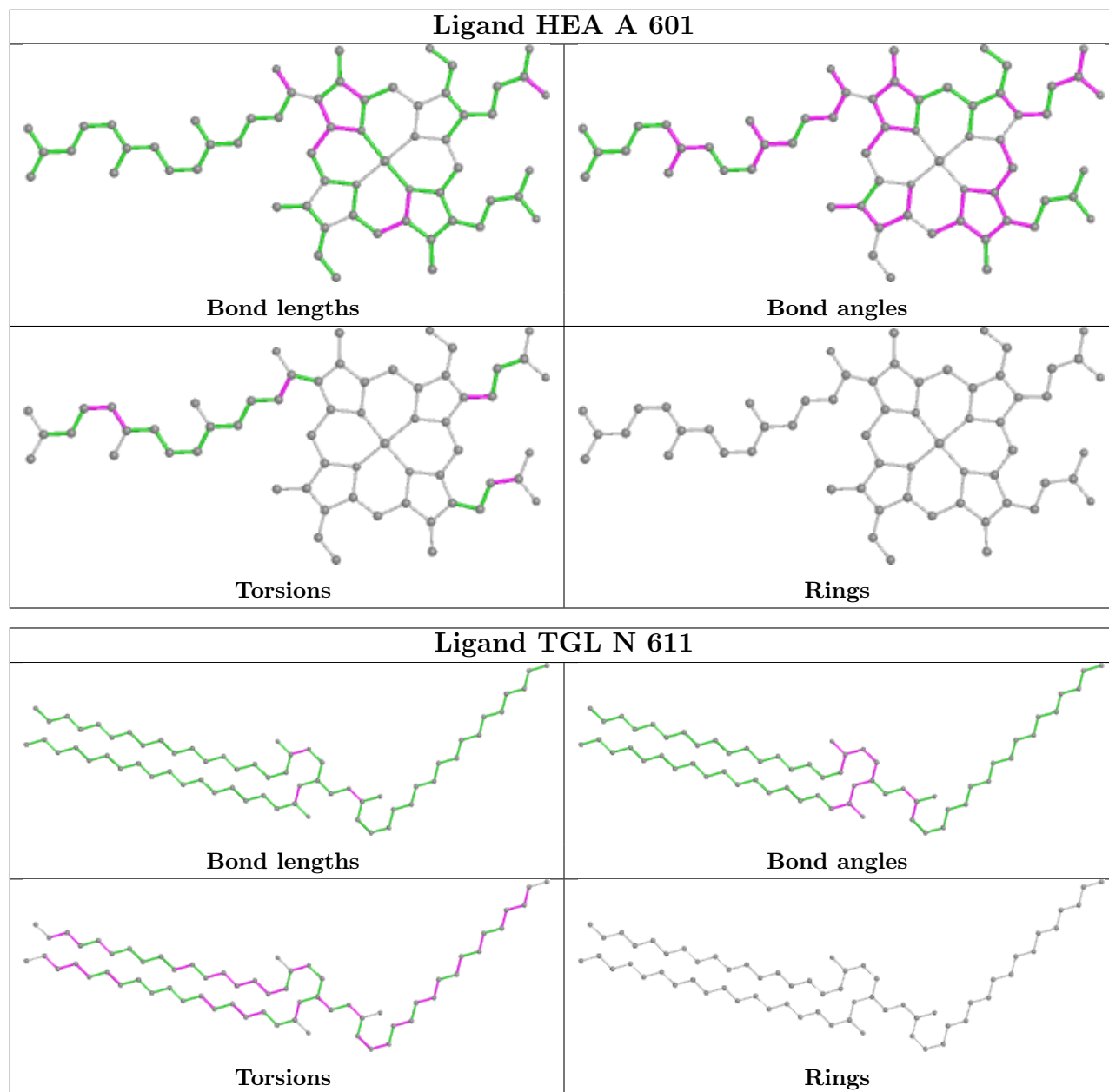


Ligand PGV C 308

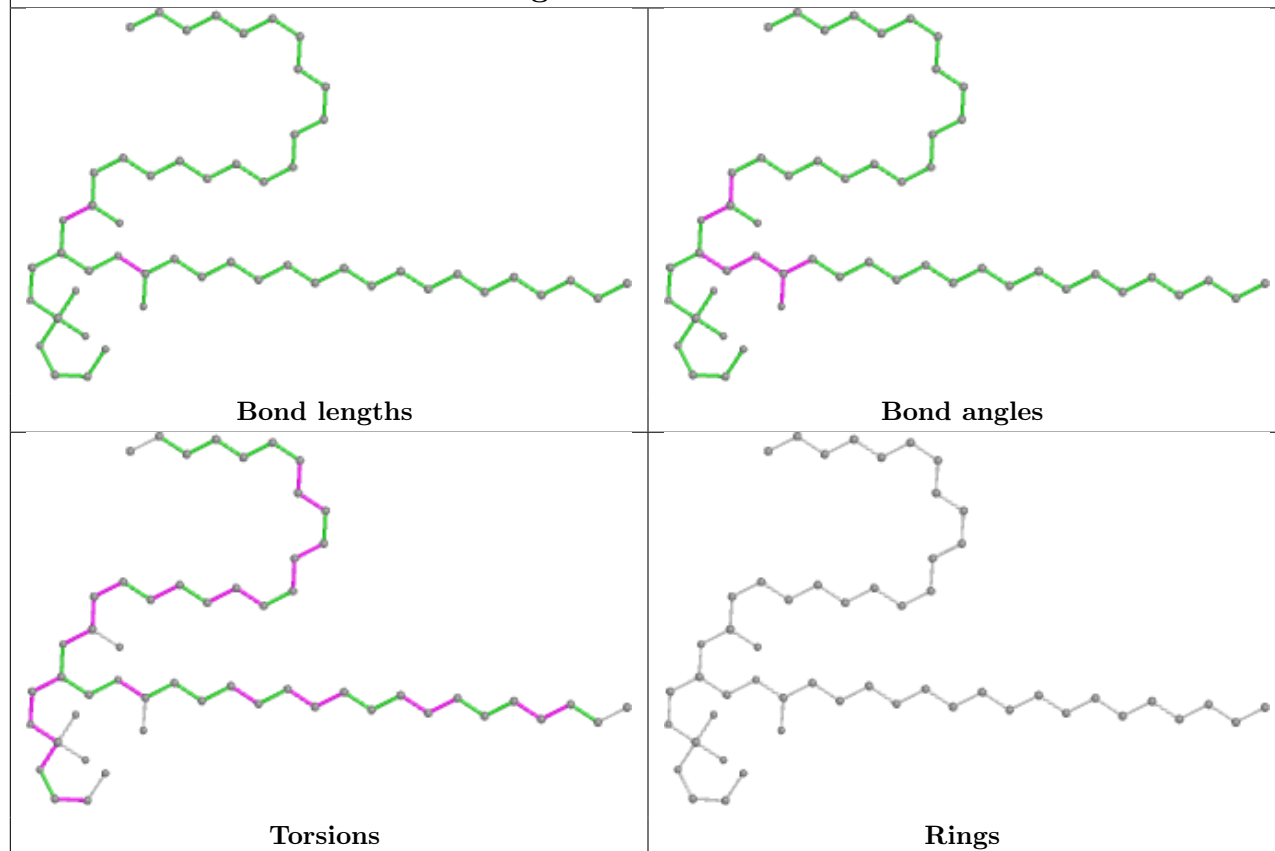




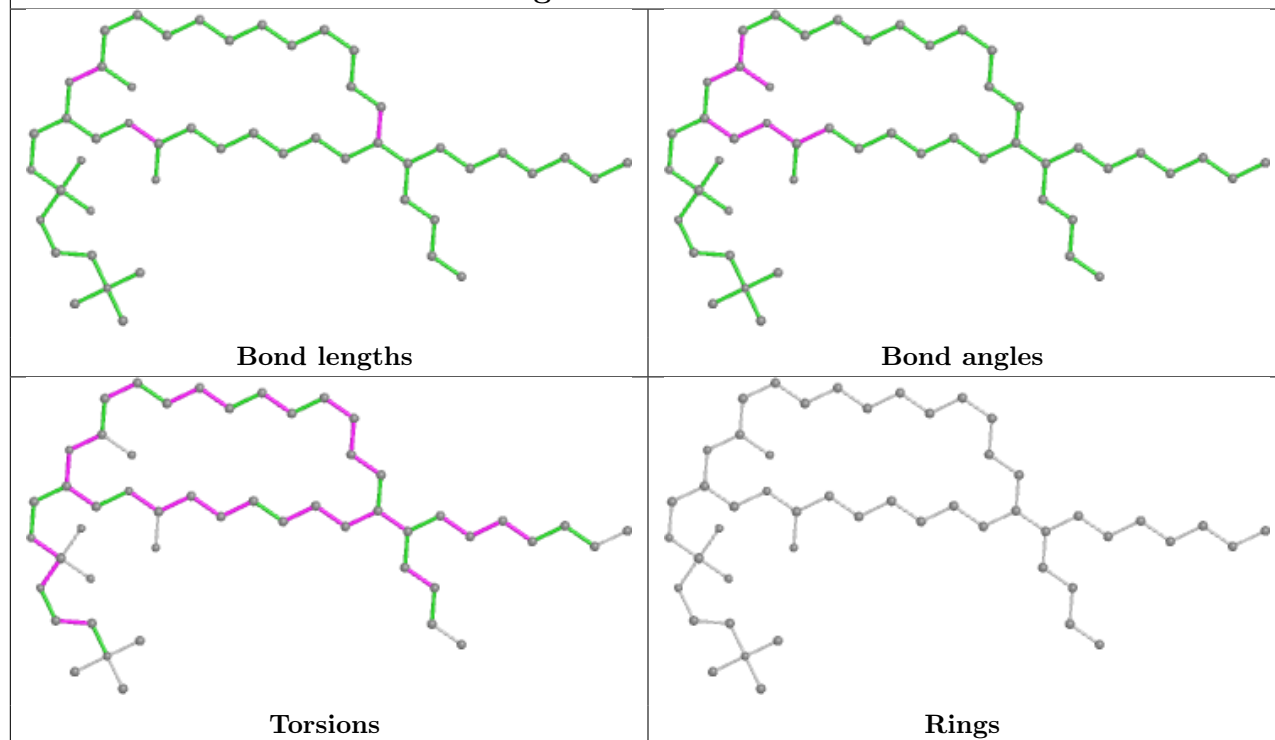


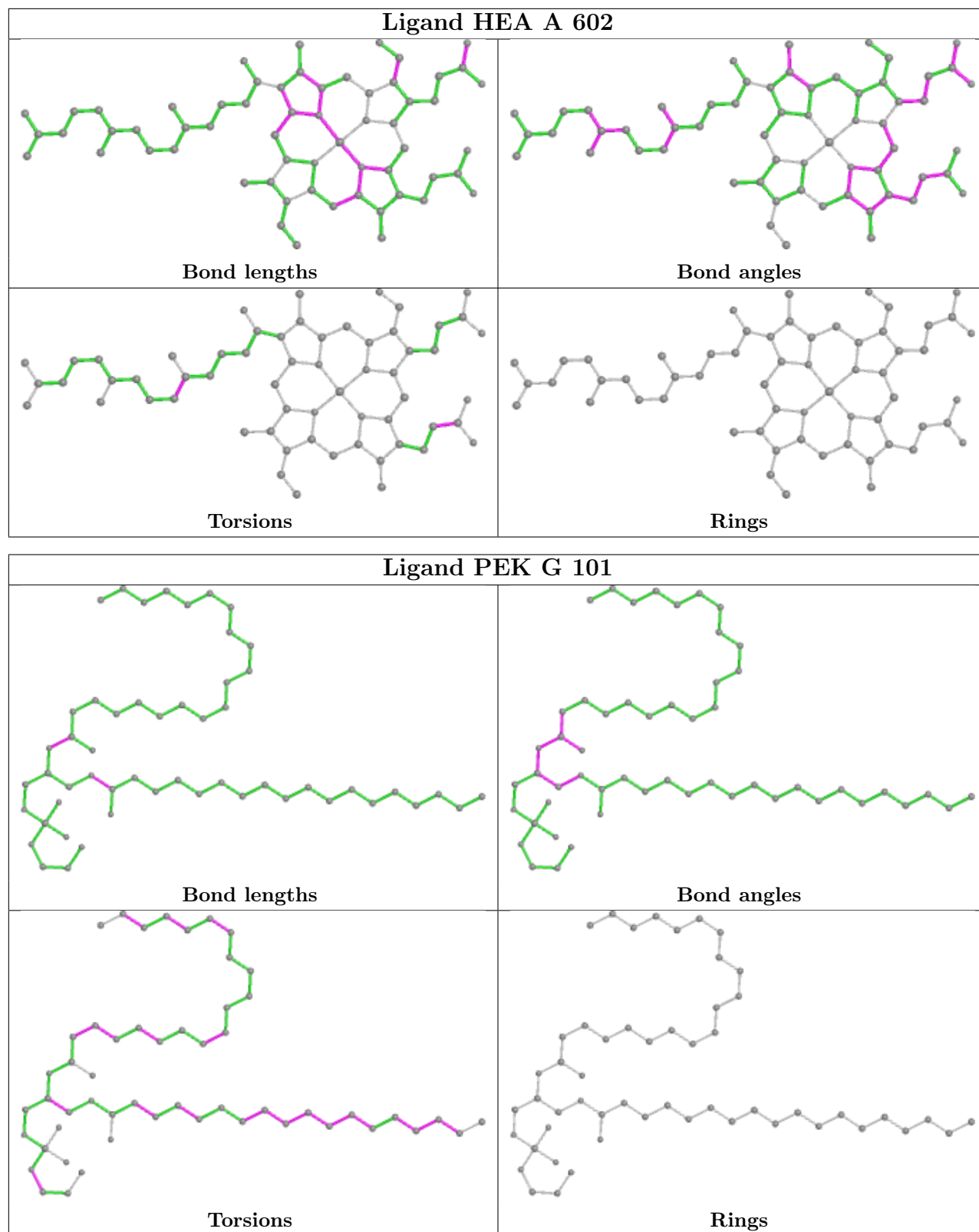


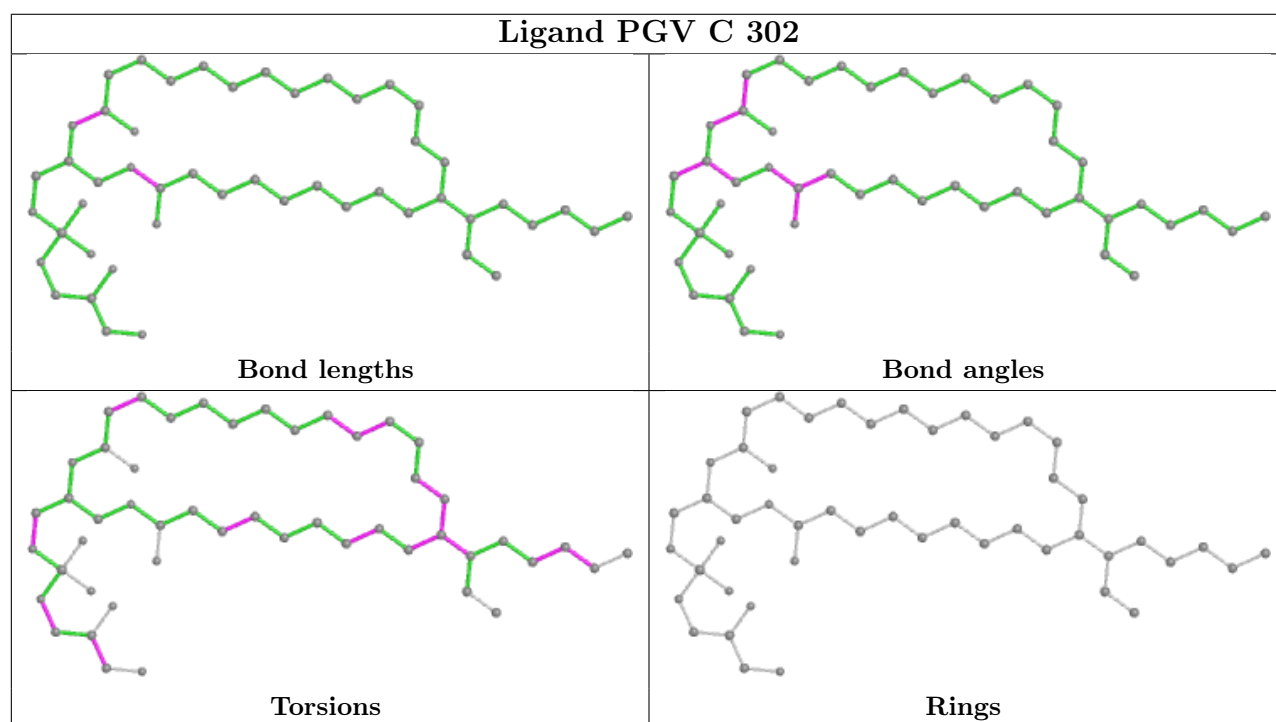
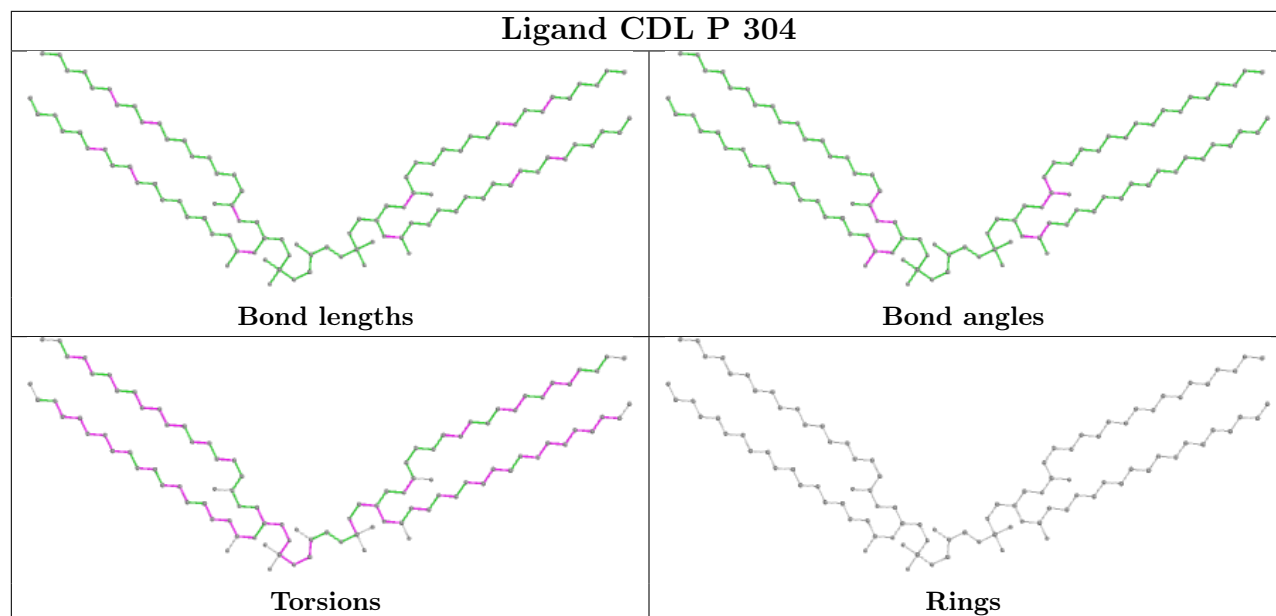
Ligand PEK T 102

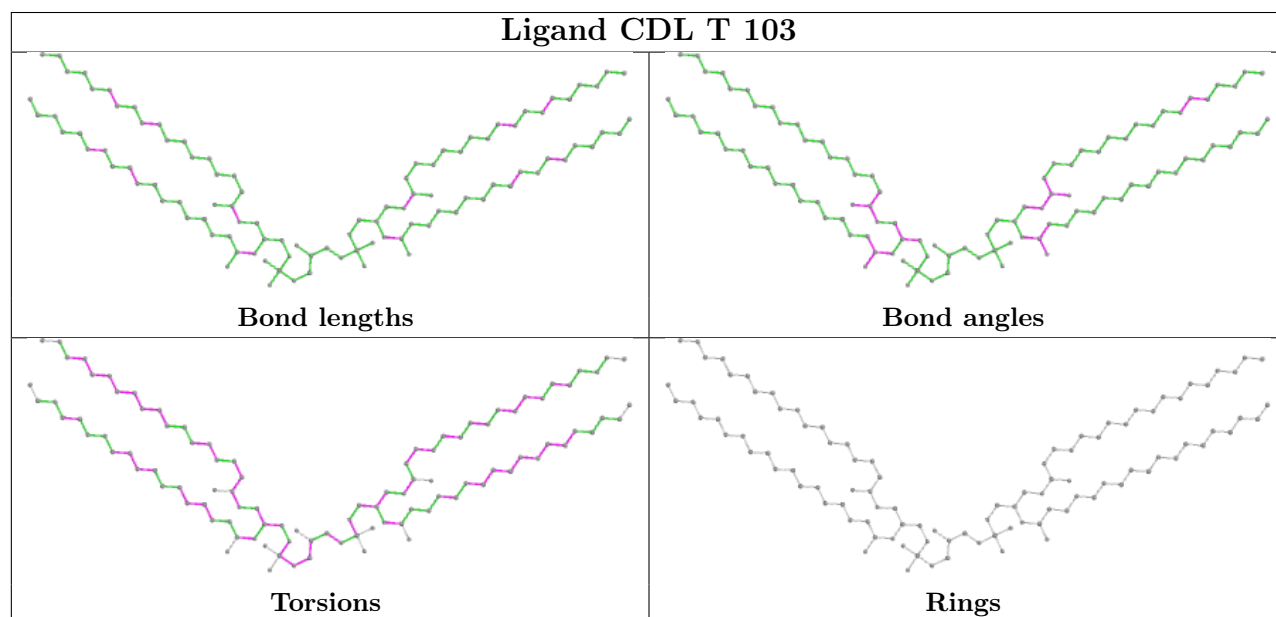
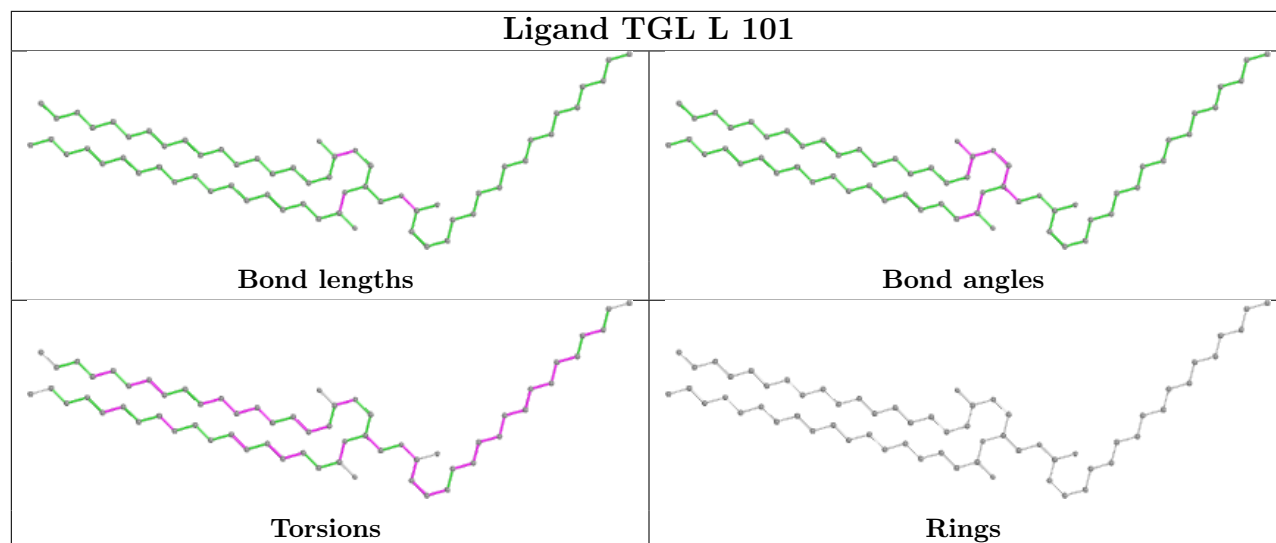


Ligand PSC B 303

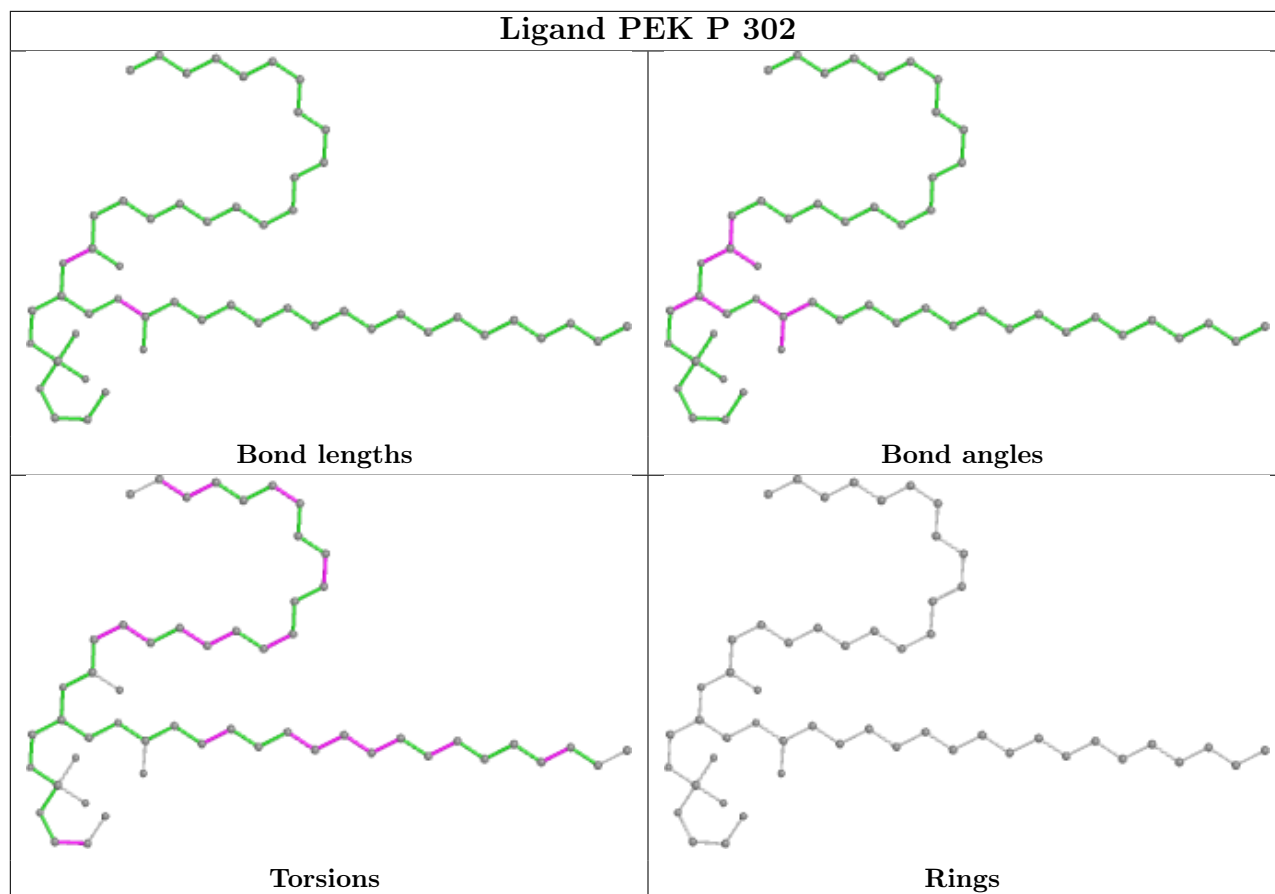




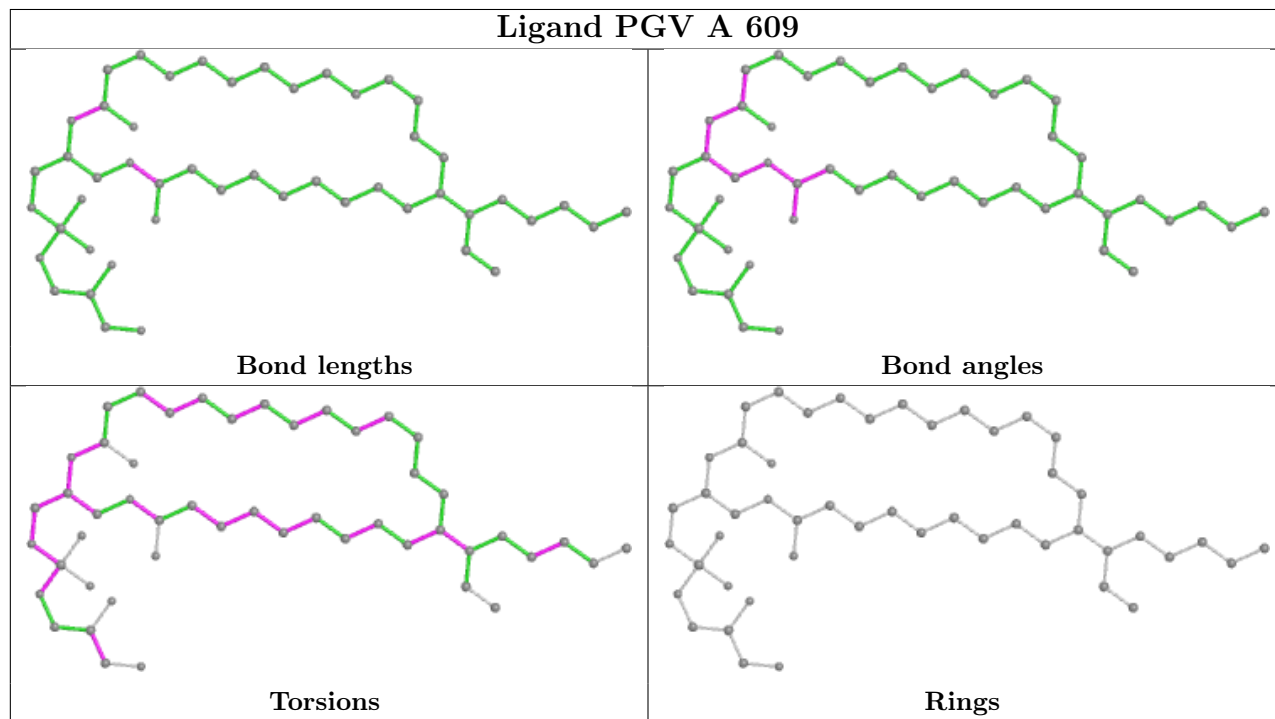




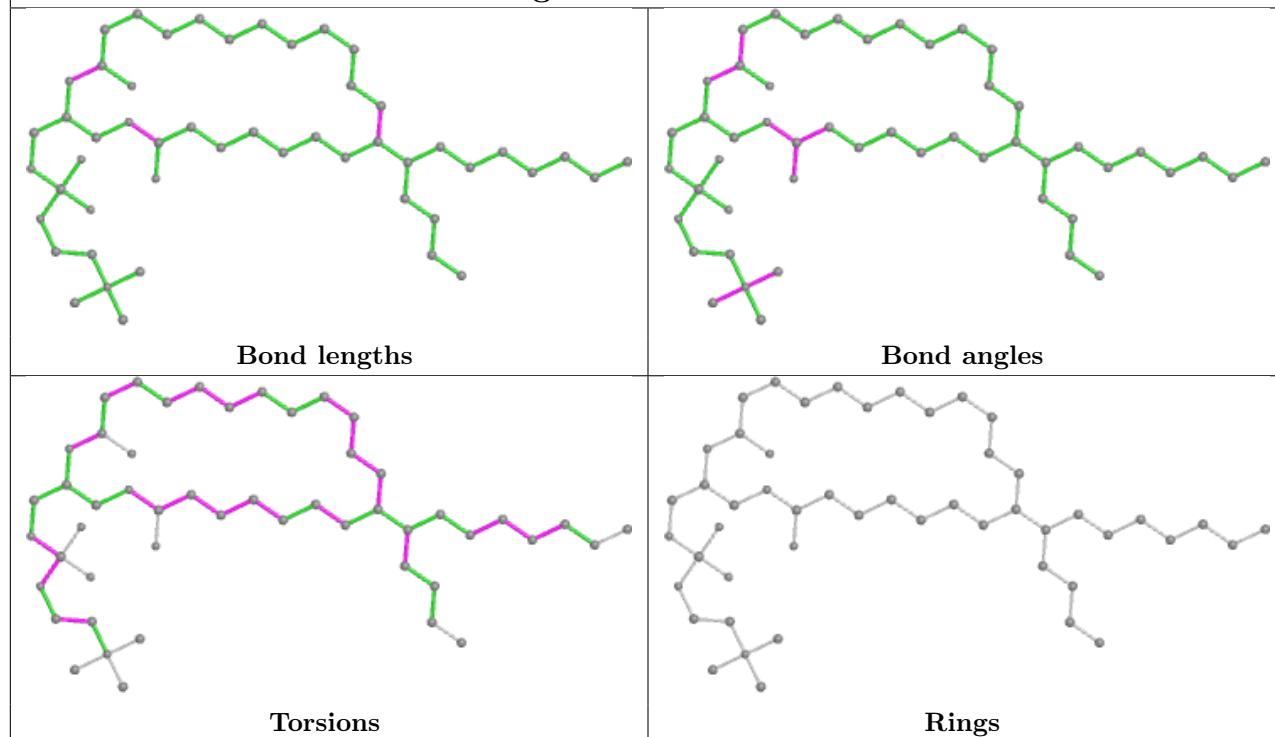
Ligand PEK P 302



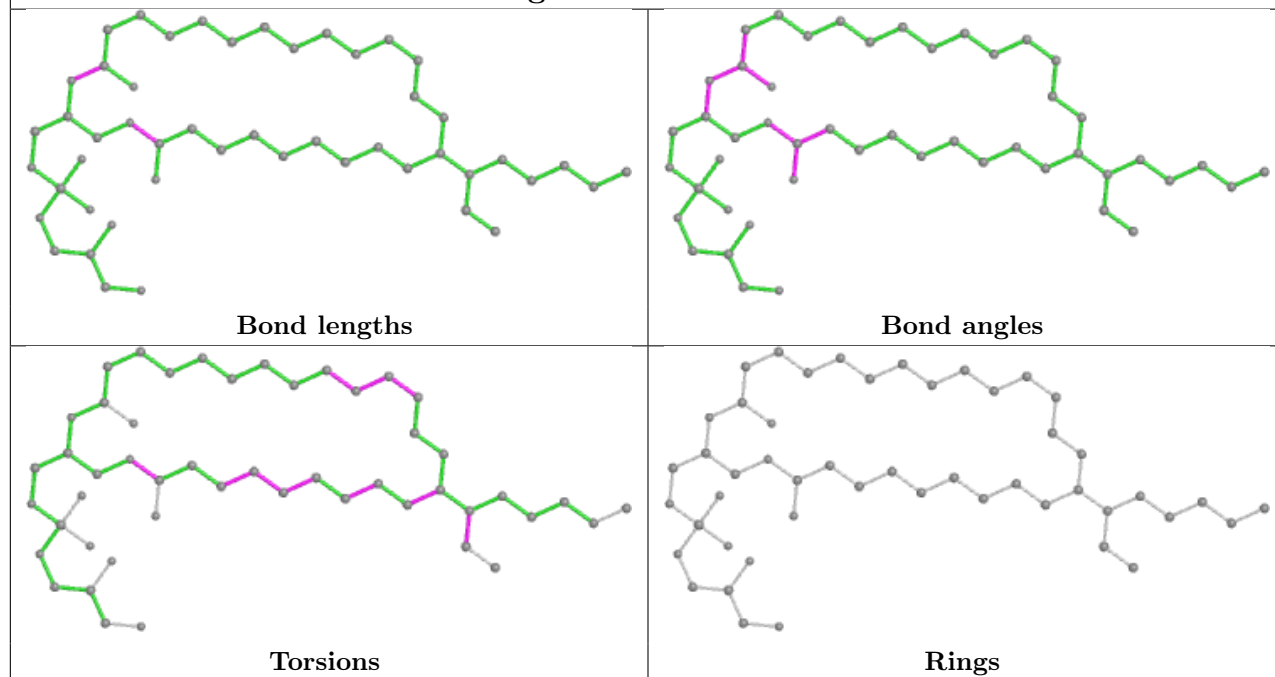
Ligand PGV A 609

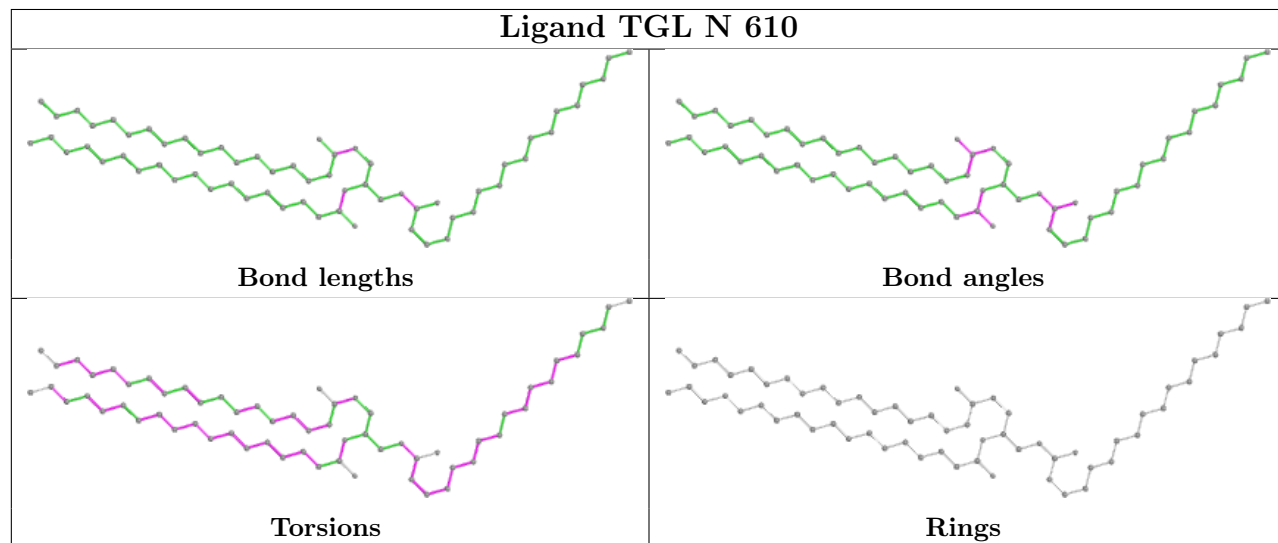
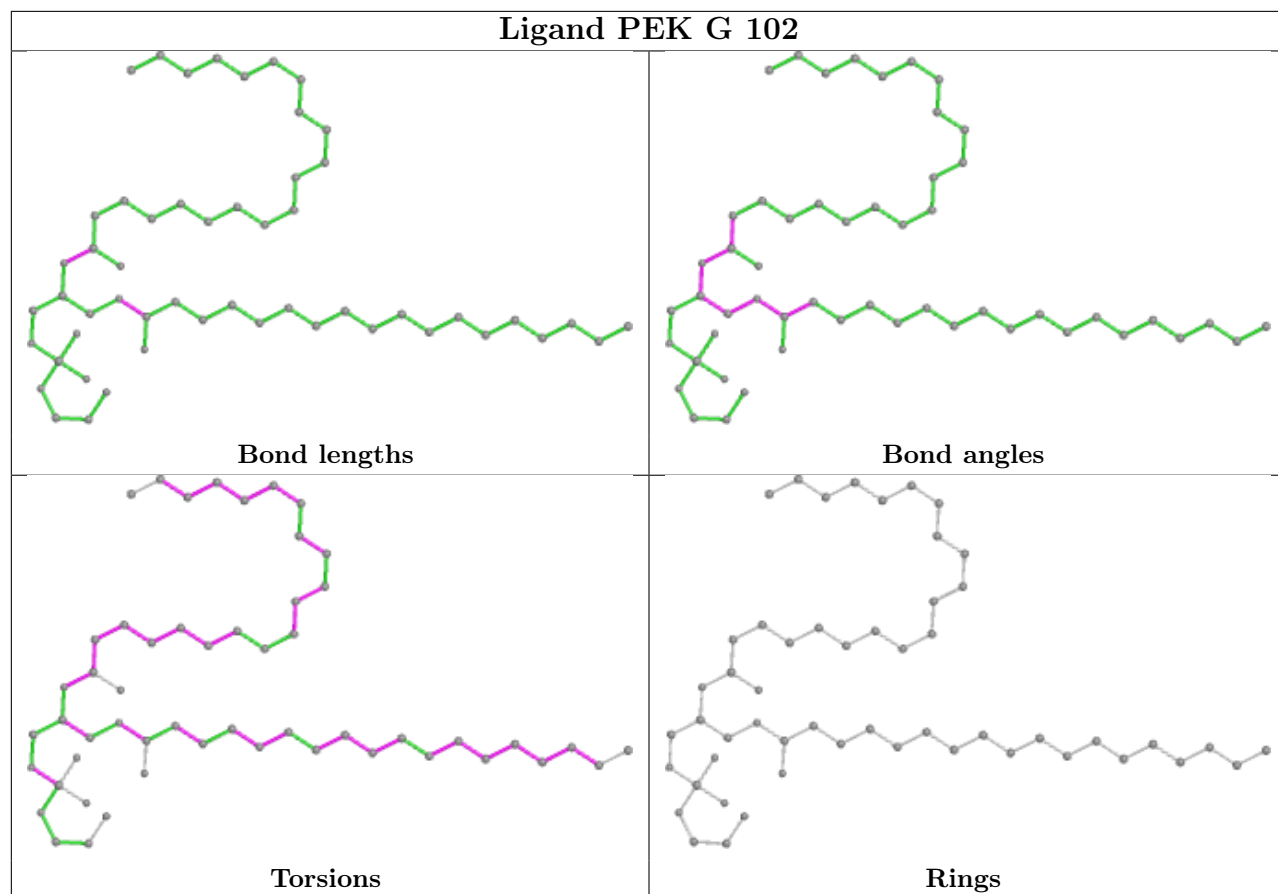


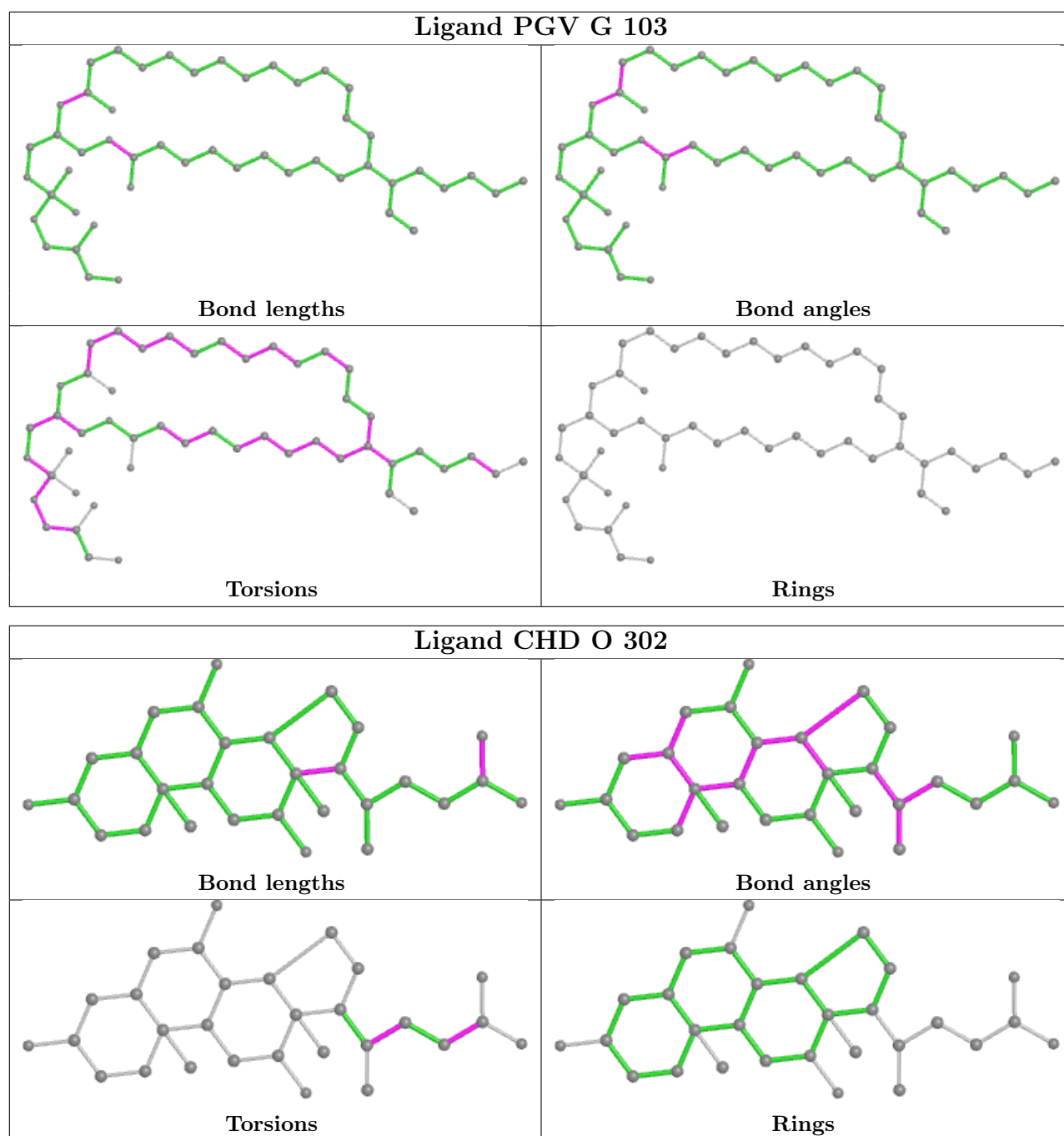
Ligand PSC R 201



Ligand PGV A 608







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 ⓘ

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

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

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

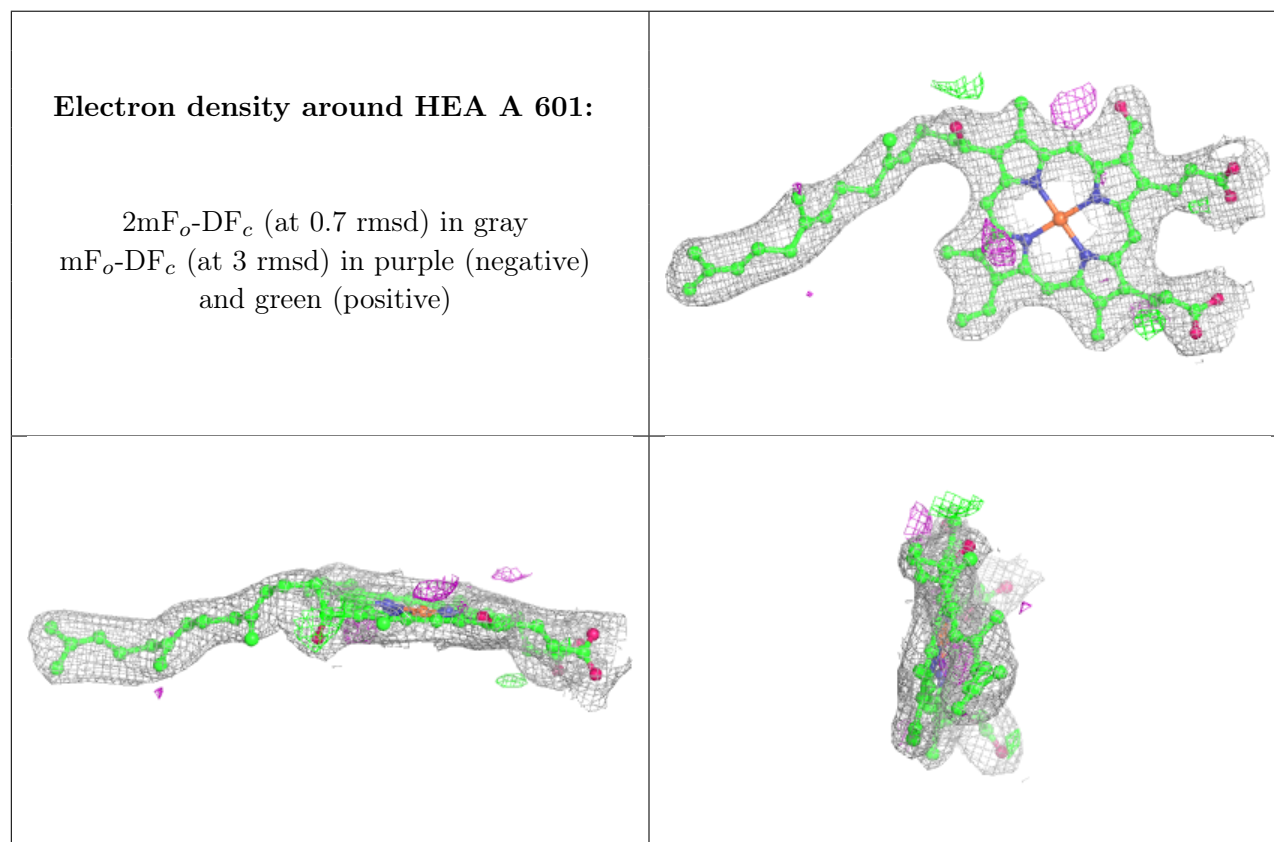
6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

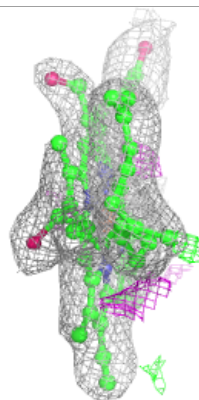
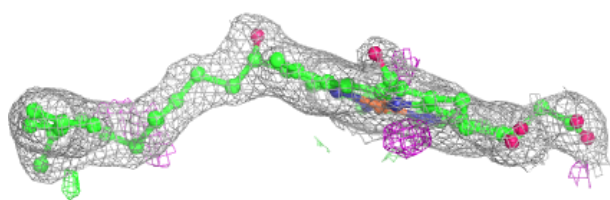
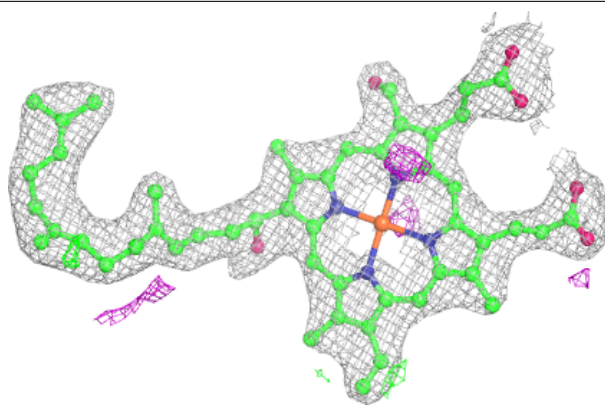
EDS failed to run properly - this section is therefore empty.

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.

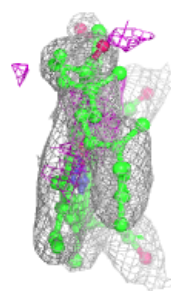
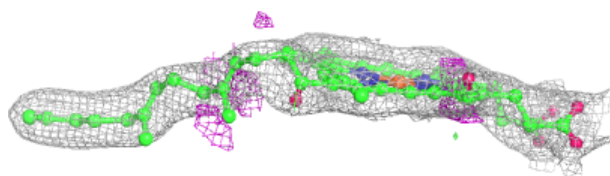
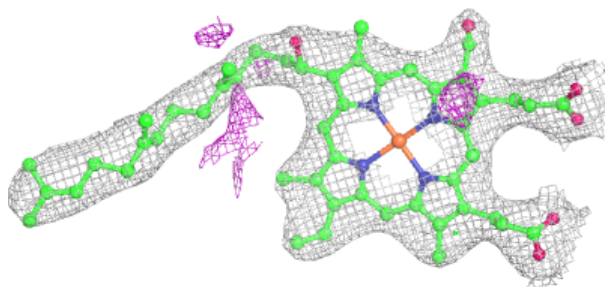


Electron density around HEA A 602:

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

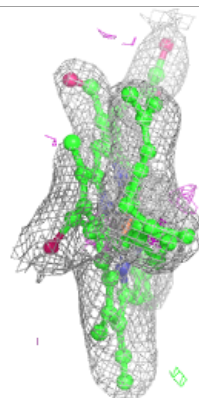
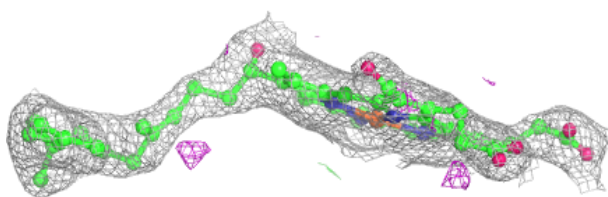
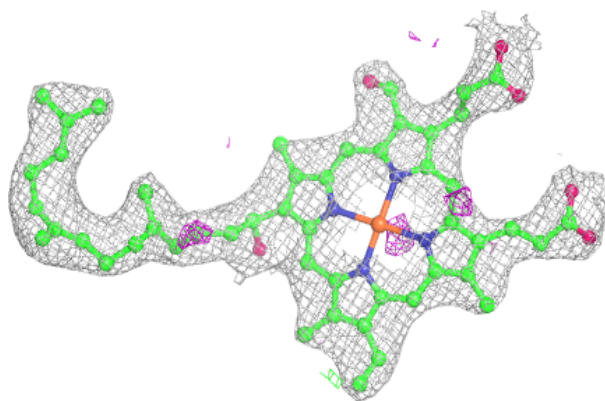
**Electron density around HEA N 601:**

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

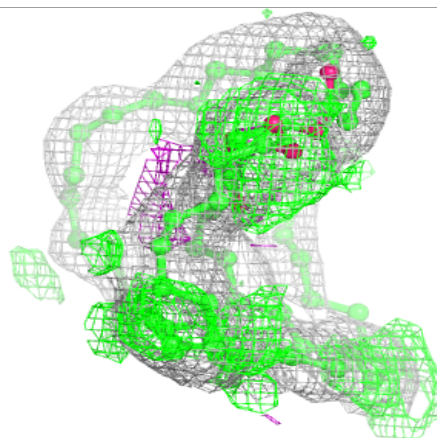
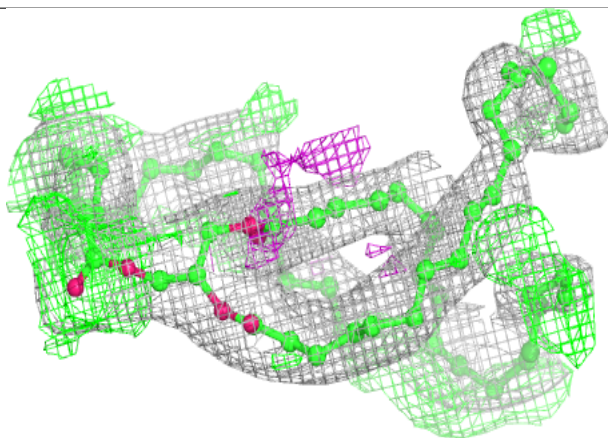
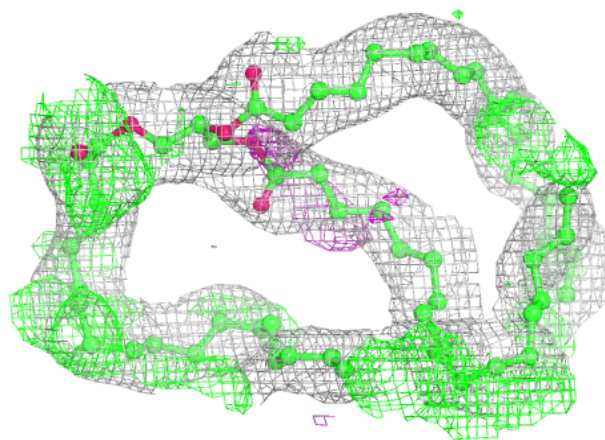


Electron density around HEA N 602:

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

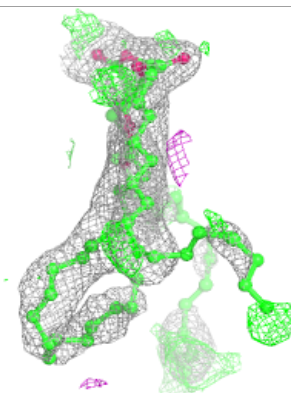
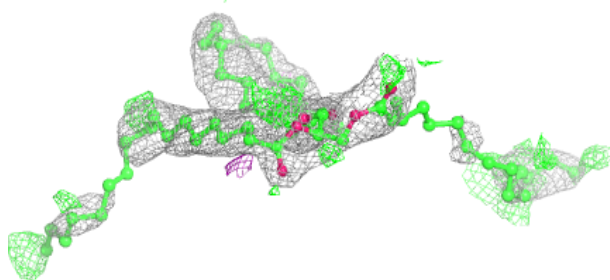
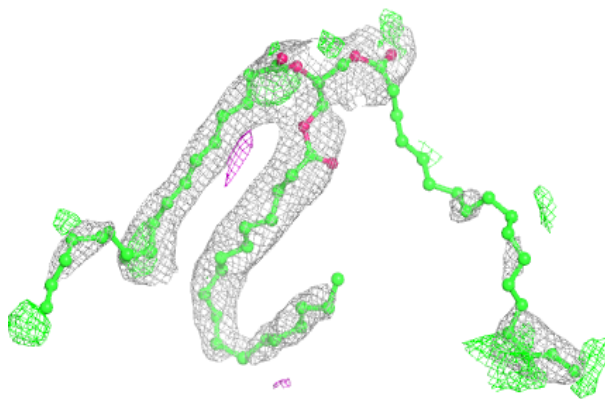
**Electron density around TGL A 607:**

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



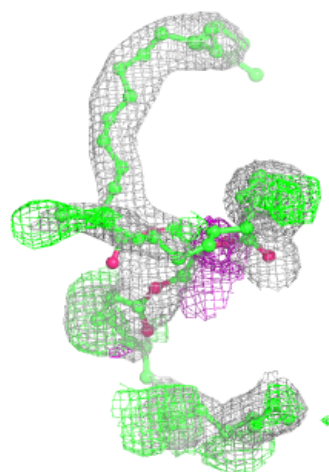
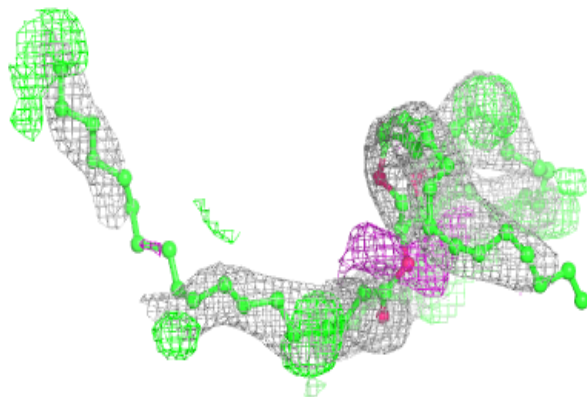
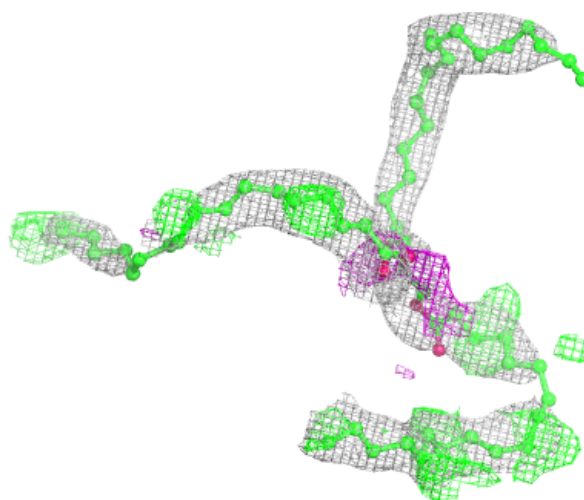
Electron density around TGL D 201:

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



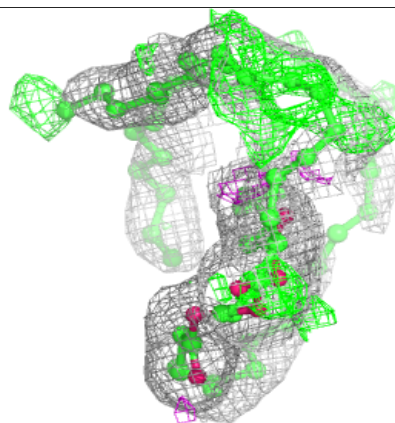
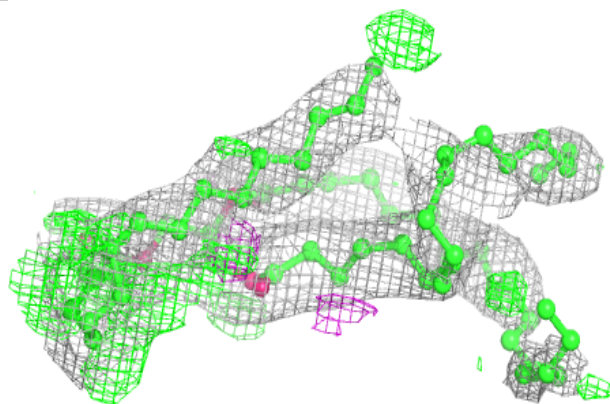
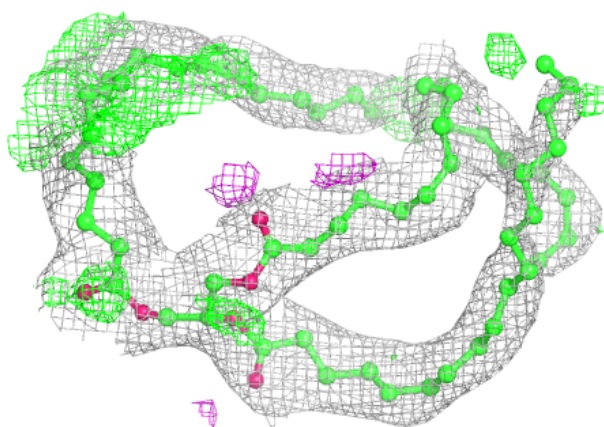
Electron density around TGL L 101:

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



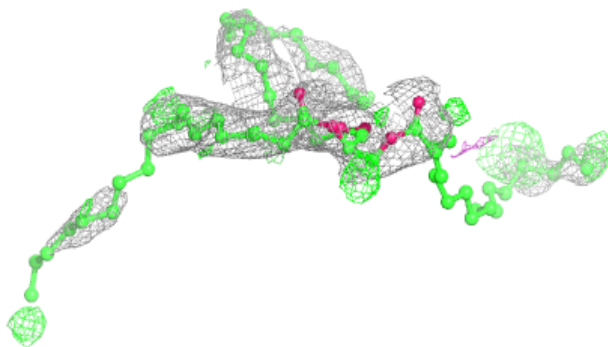
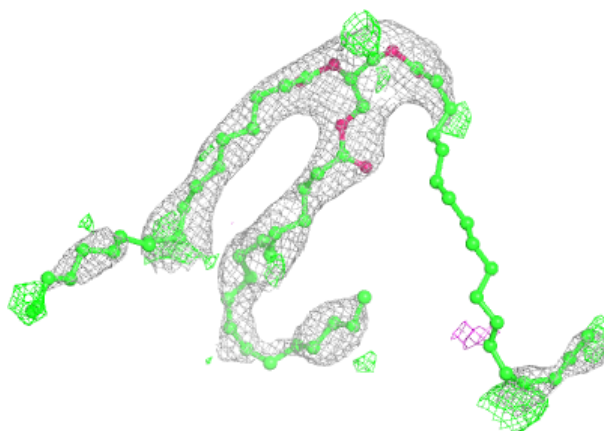
Electron density around TGL N 609:

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



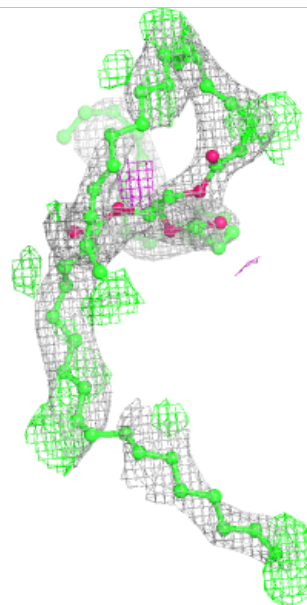
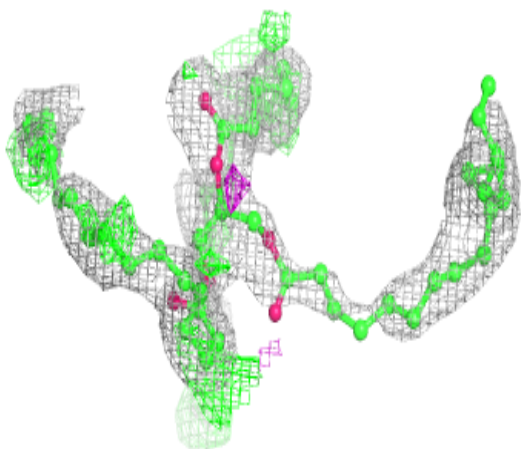
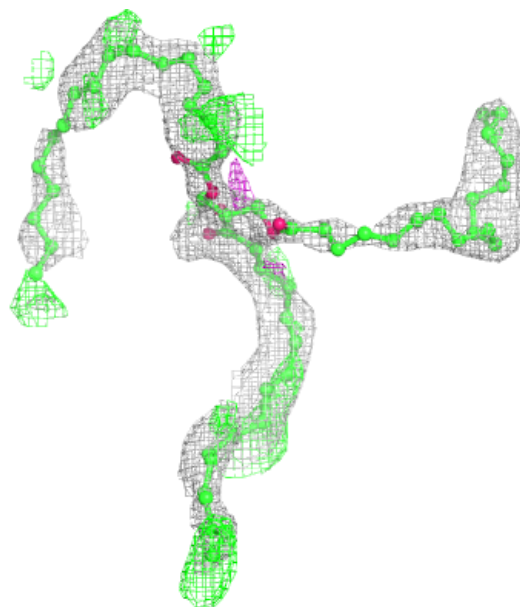
Electron density around TGL N 610:

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



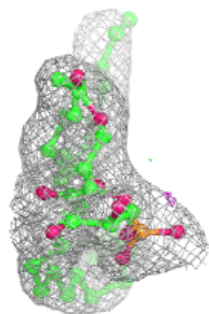
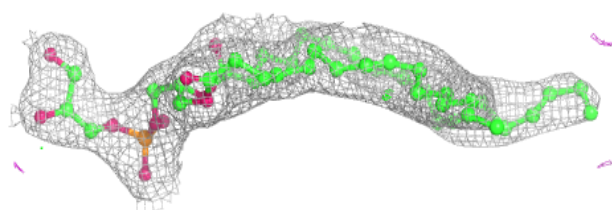
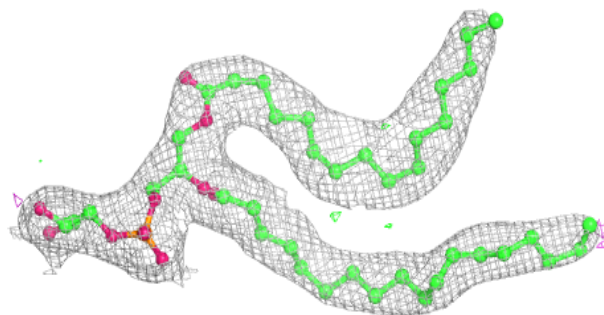
Electron density around TGL N 611:

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

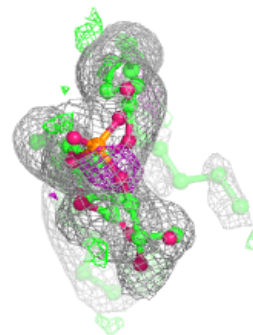
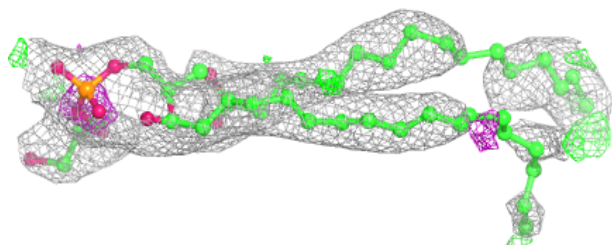
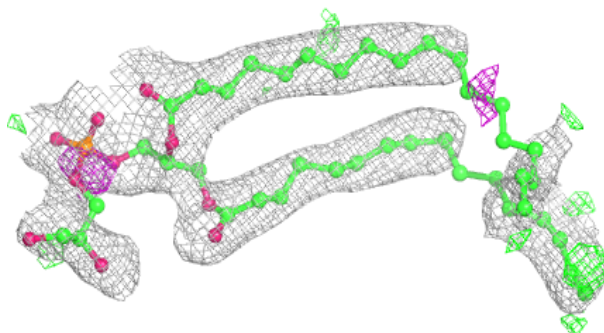


Electron density around PGV A 608:

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

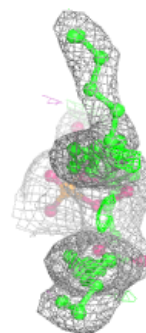
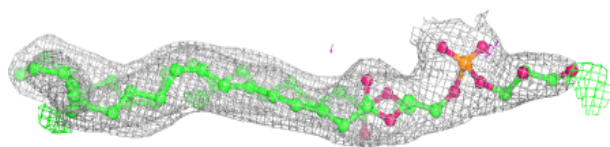
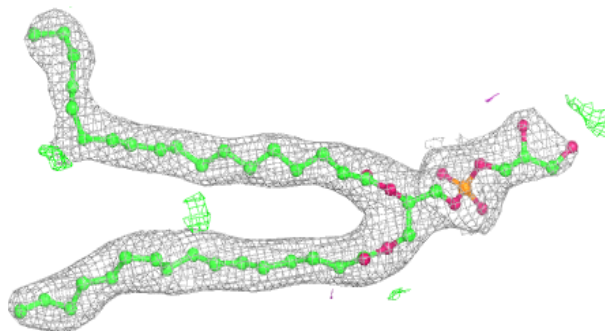
**Electron density around PGV A 609:**

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

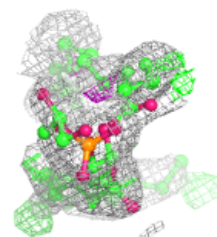
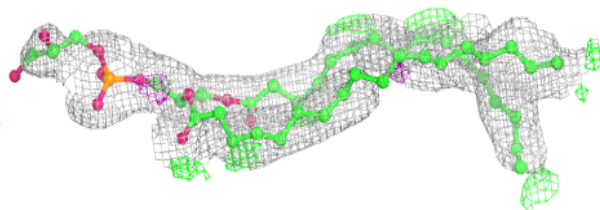
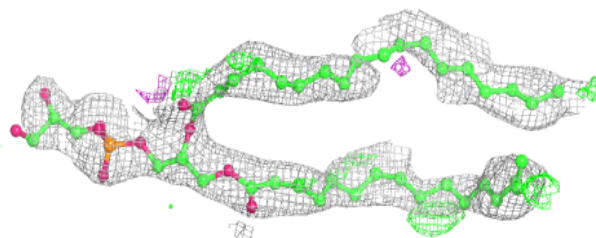


Electron density around PGV C 302:

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

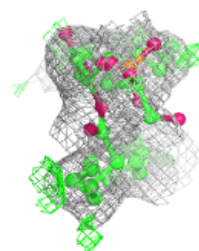
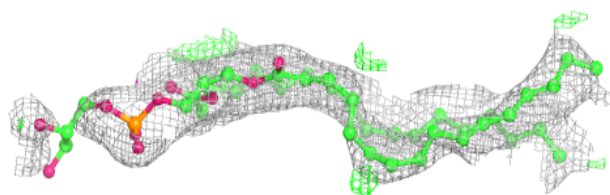
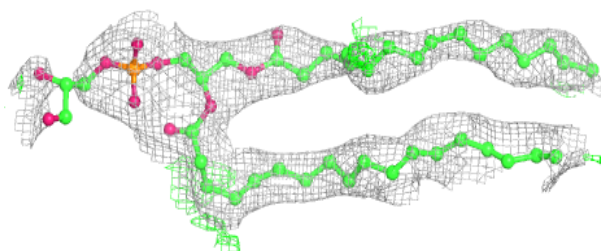
**Electron density around PGV C 308:**

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

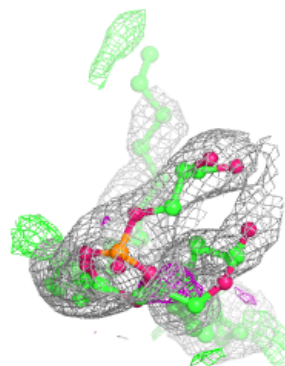
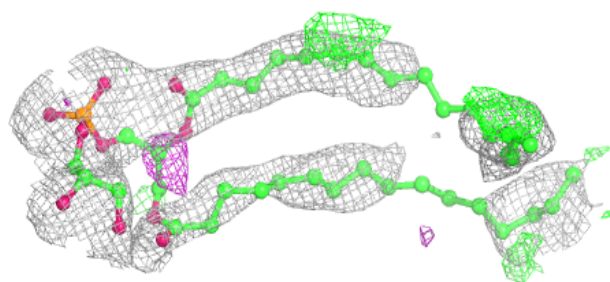
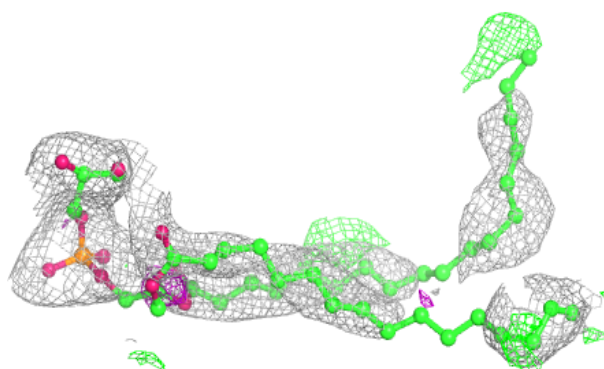


Electron density around PGV G 103:

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

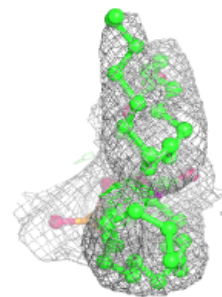
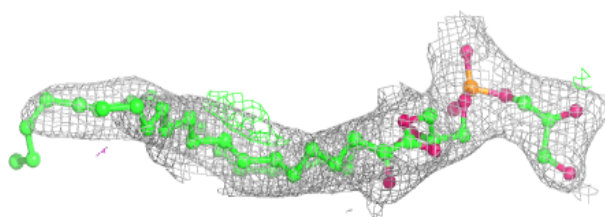
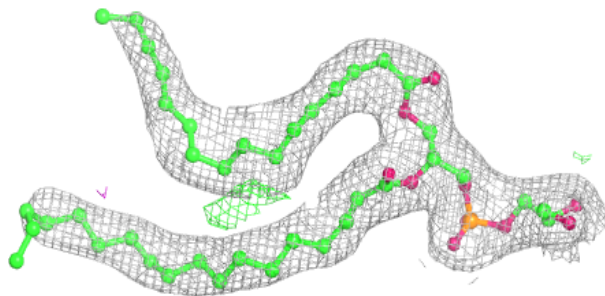
**Electron density around PGV N 607:**

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

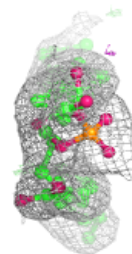
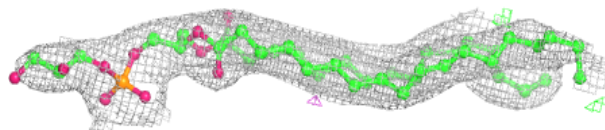
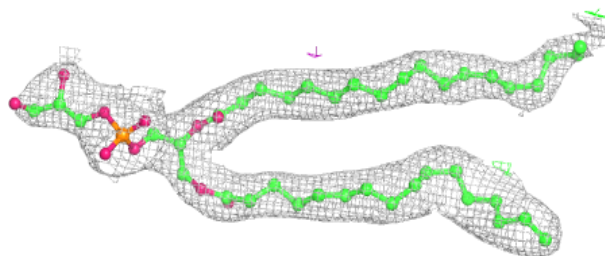


Electron density around PGV N 608:

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

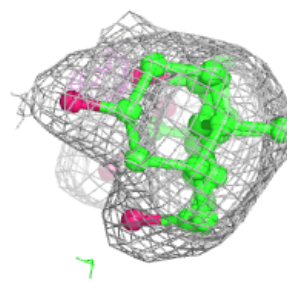
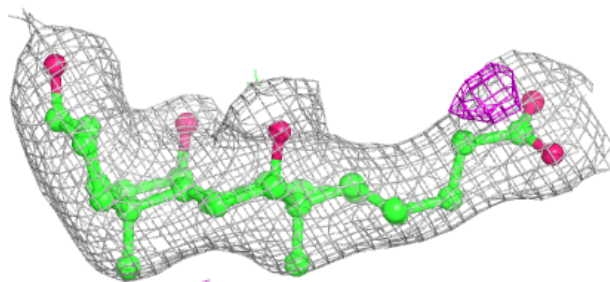
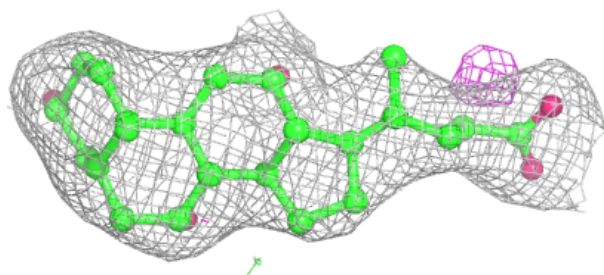
**Electron density around PGV P 303:**

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

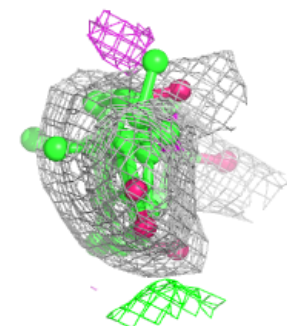
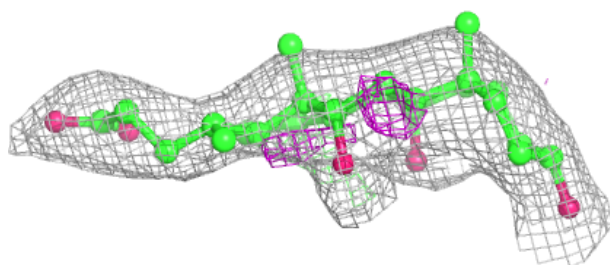
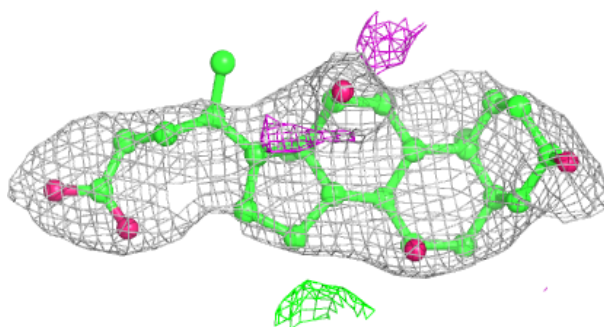


Electron density around CHD B 302:

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

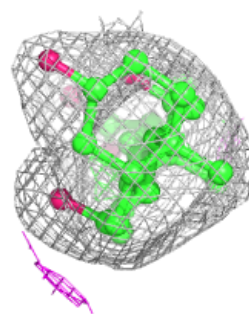
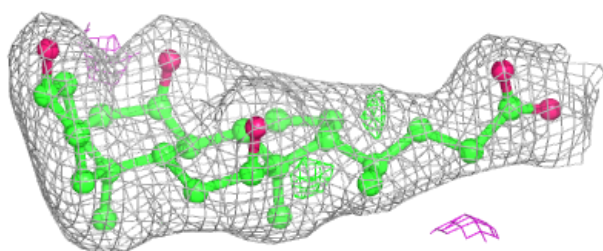
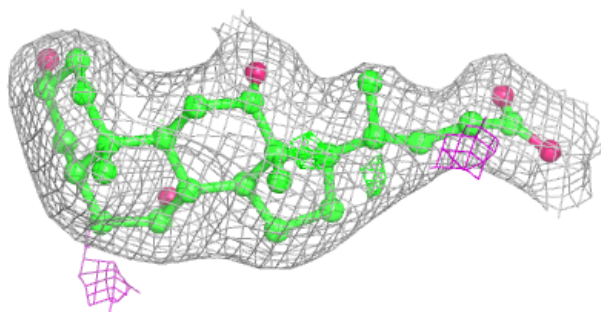
**Electron density around CHD C 304:**

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

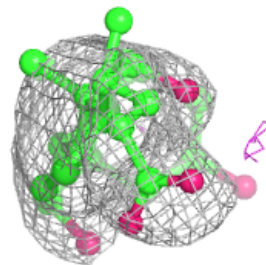
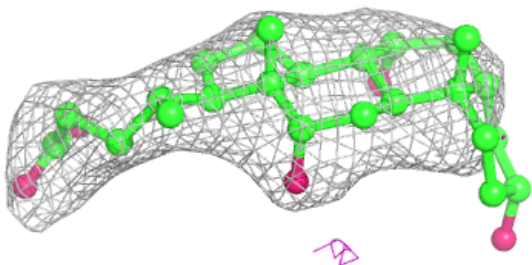
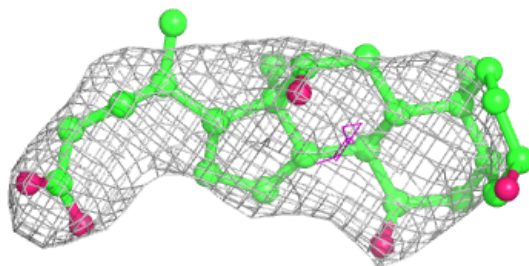


Electron density around CHD C 305:

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

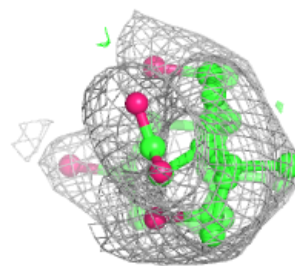
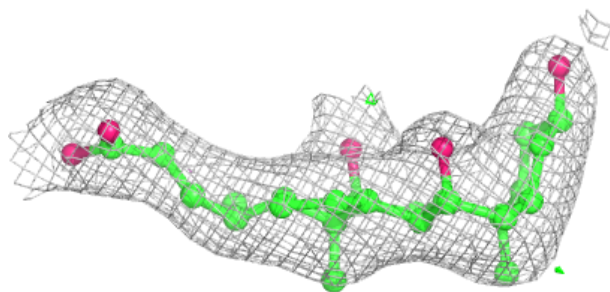
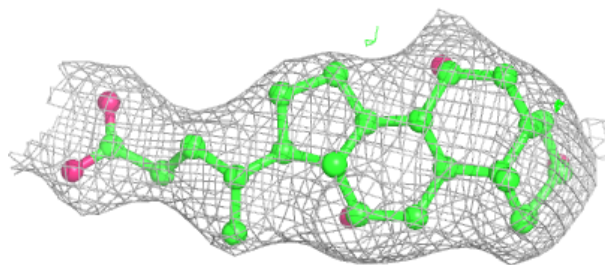
**Electron density around CHD J 101:**

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

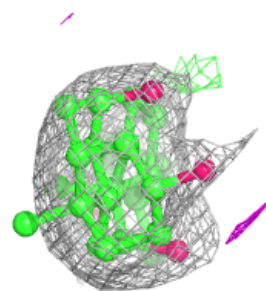
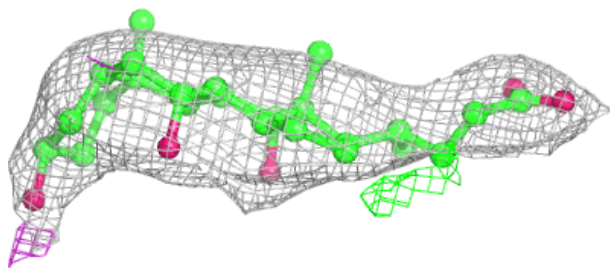
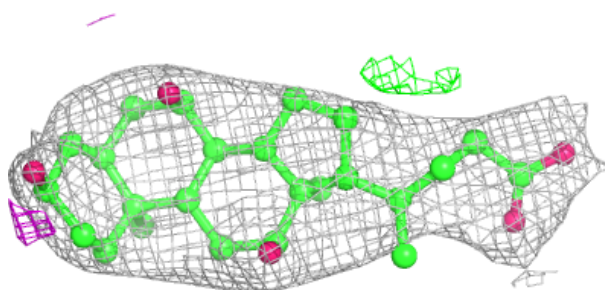


Electron density around CHD O 302:

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

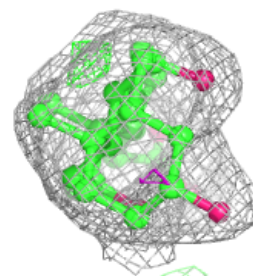
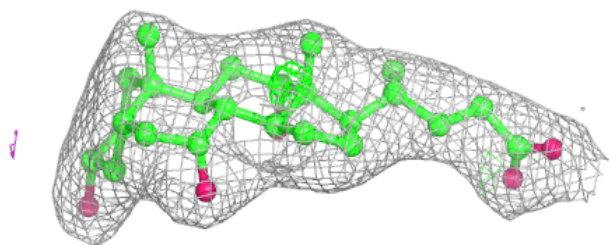
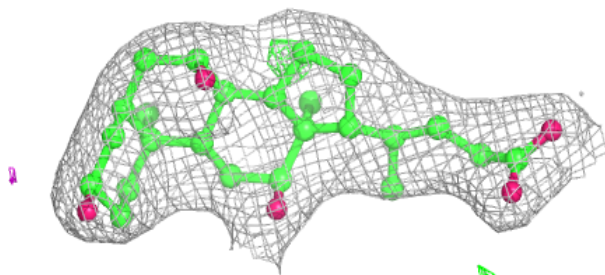
**Electron density around CHD P 305:**

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

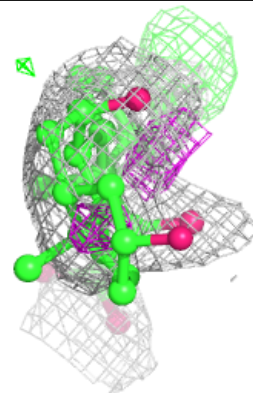
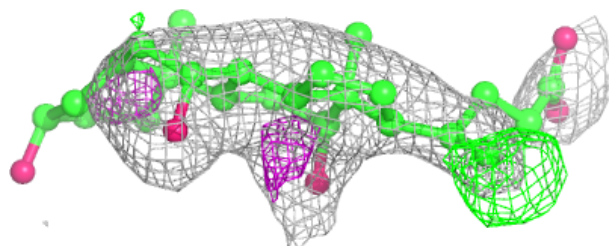
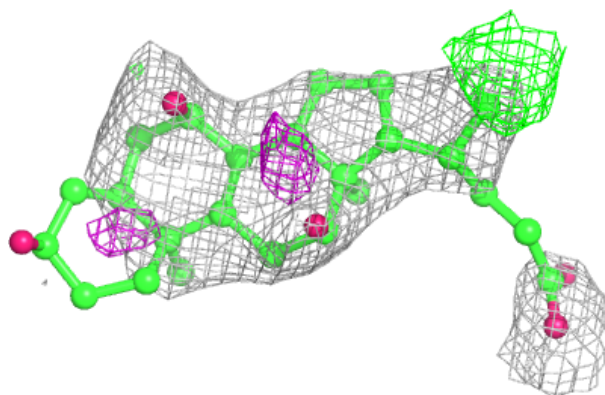


Electron density around CHD P 306:

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

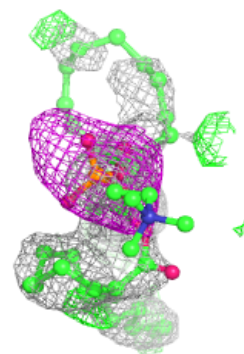
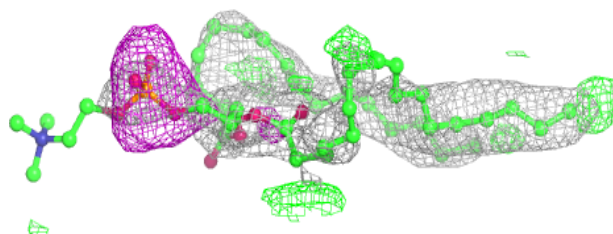
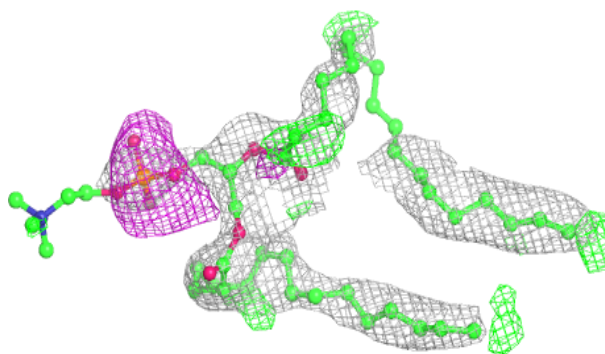
**Electron density around CHD W 101:**

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

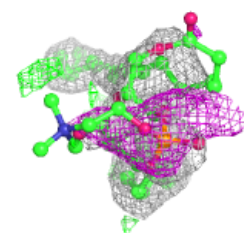
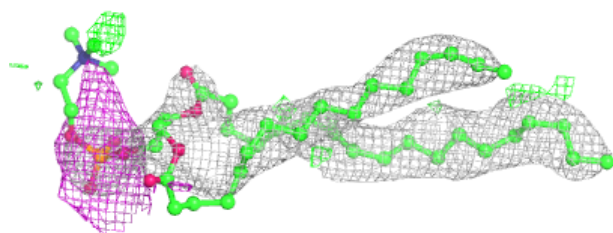
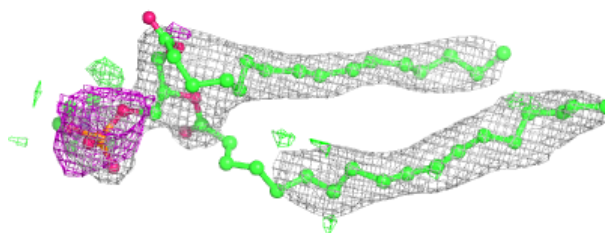


Electron density around PSC B 303:

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

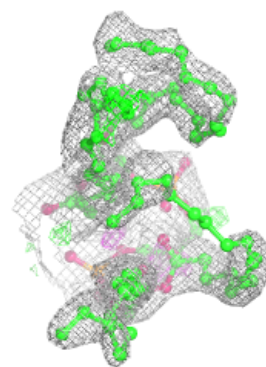
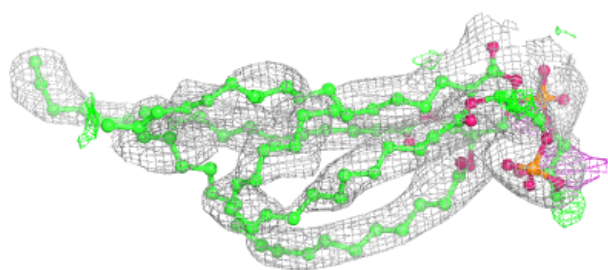
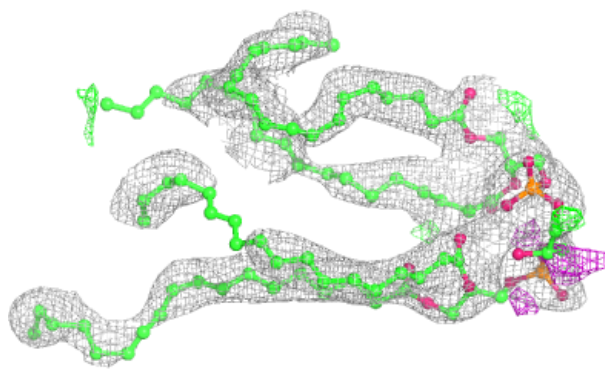
**Electron density around PSC R 201:**

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

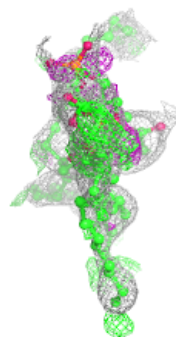
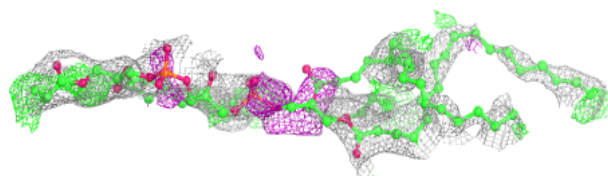
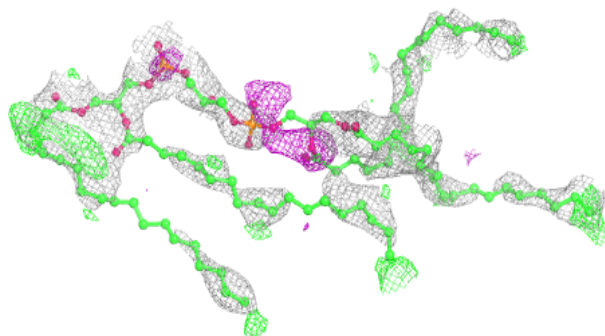


Electron density around CDL C 303:

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

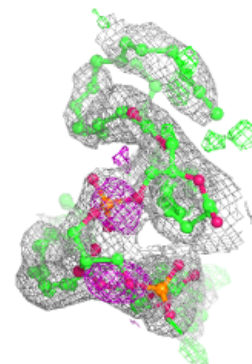
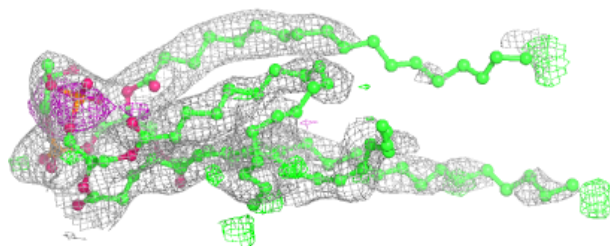
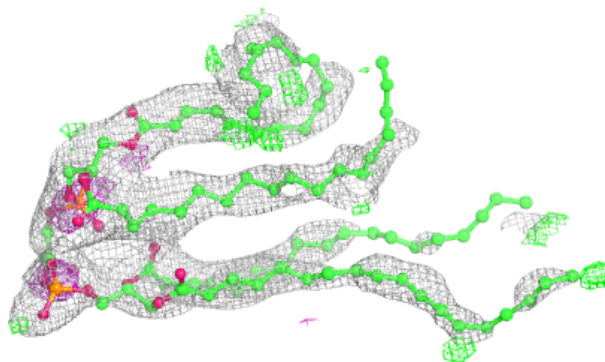
**Electron density around CDL C 307:**

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

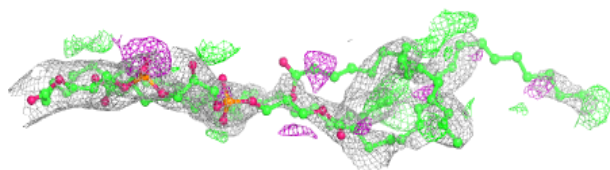
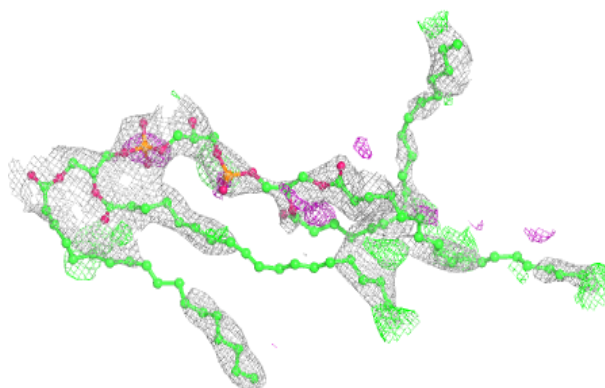


Electron density around CDL P 304:

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

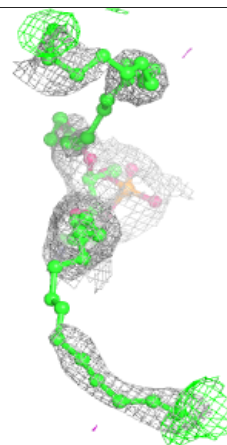
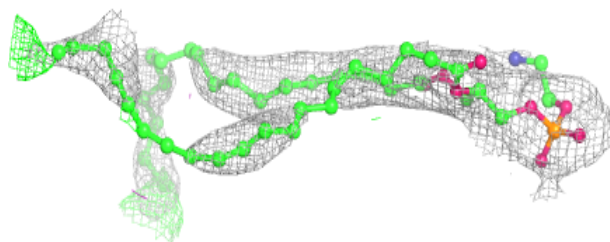
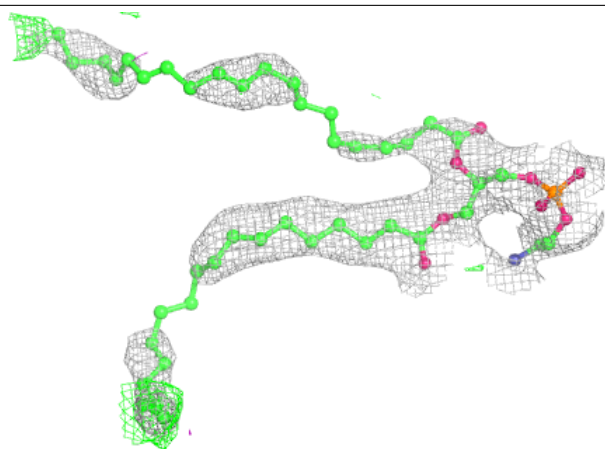
**Electron density around CDL T 103:**

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

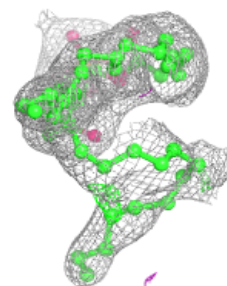
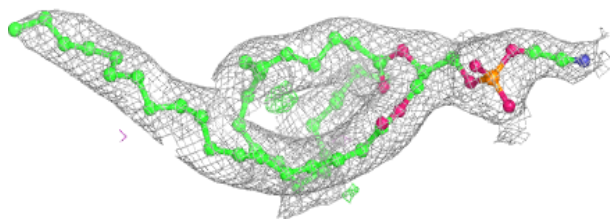
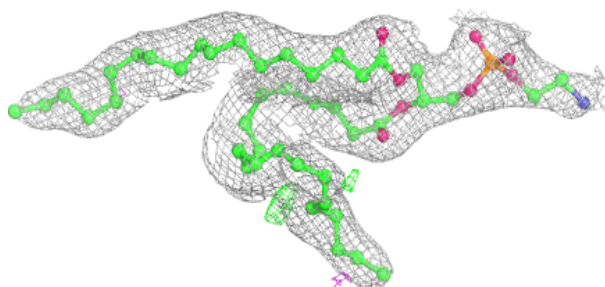


Electron density around PEK C 306:

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

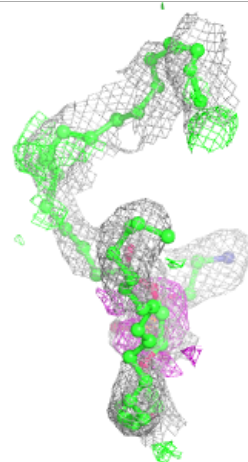
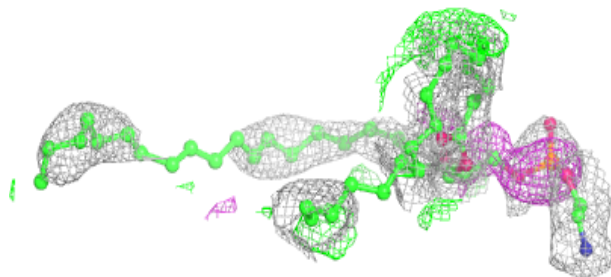
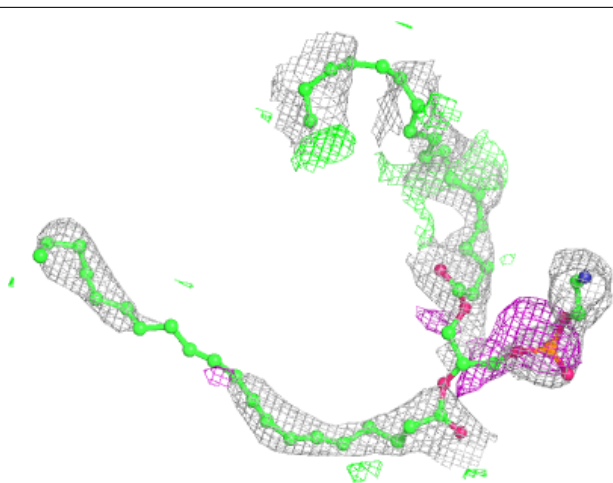
**Electron density around PEK G 101:**

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



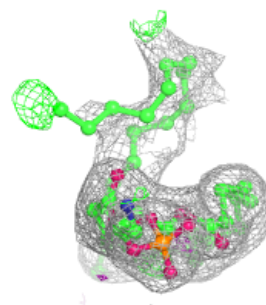
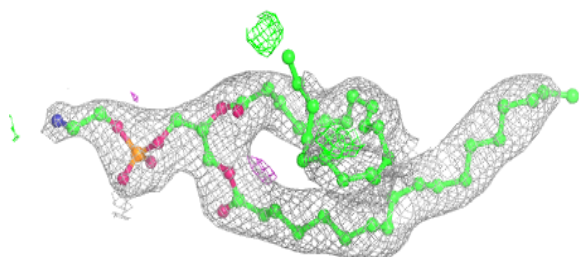
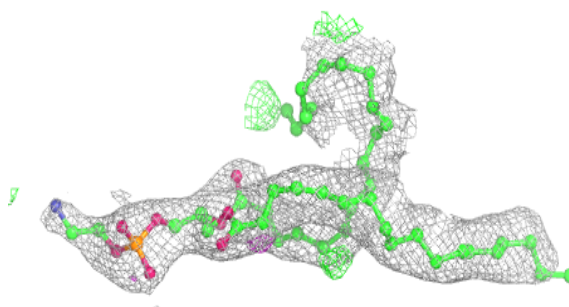
Electron density around PEK G 102:

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

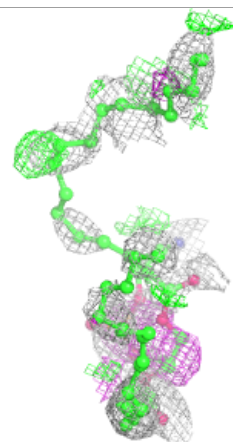
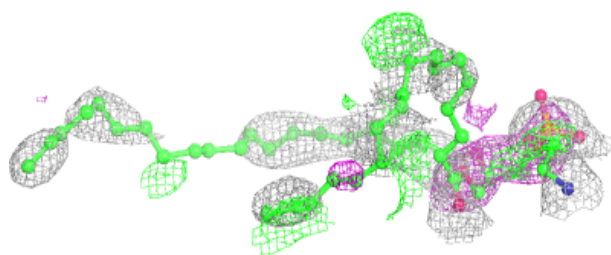
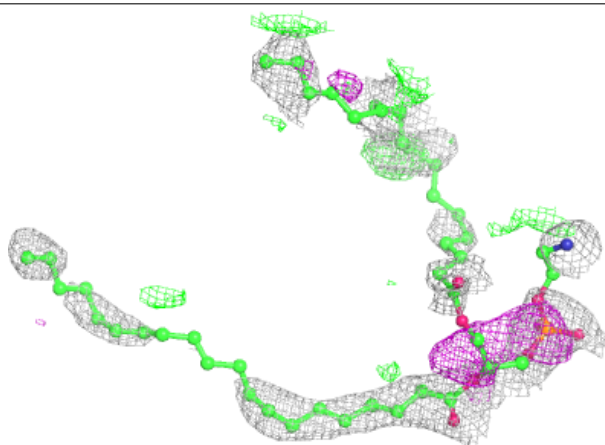


Electron density around PEK P 302:

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

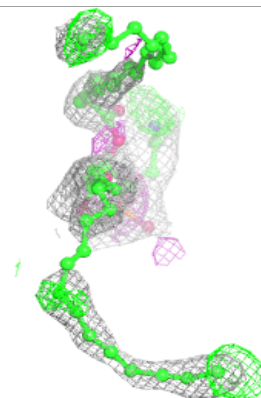
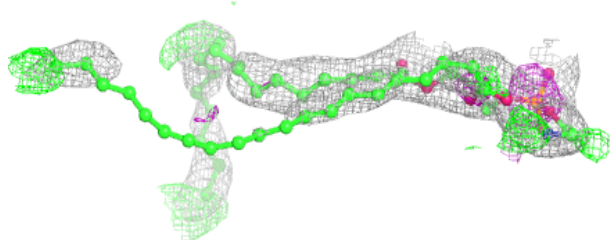
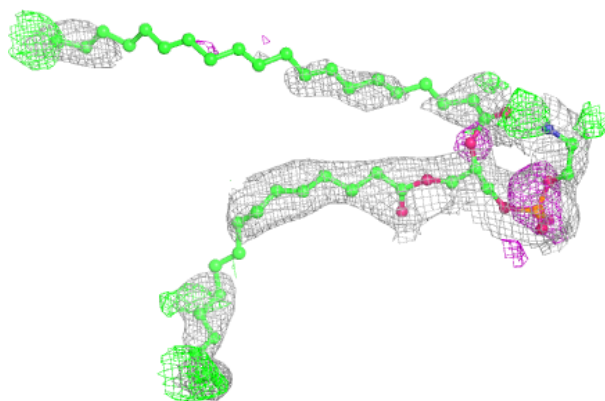
**Electron density around PEK T 101:**

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

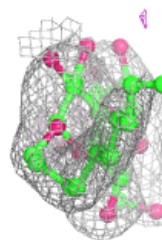
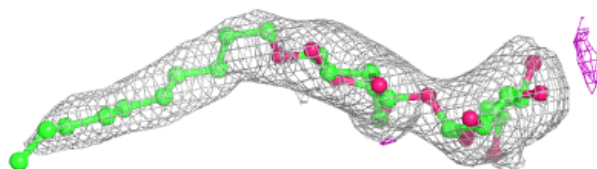
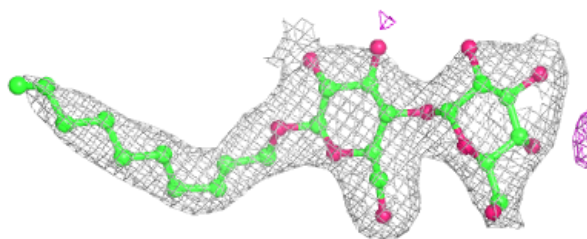


Electron density around PEK T 102:

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

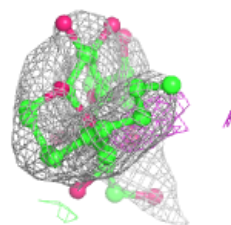
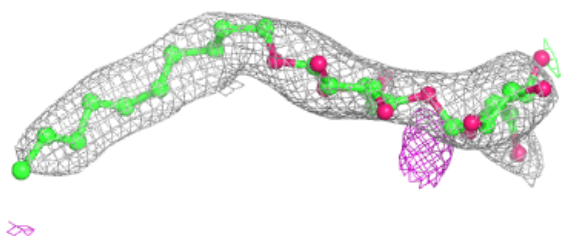
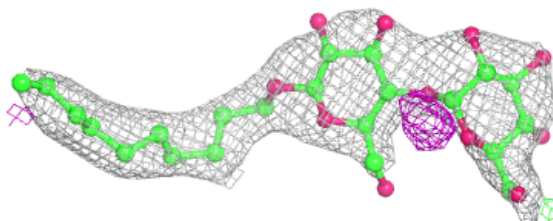
**Electron density around DMU M 101:**

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



Electron density around DMU 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.