



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 04:13 am BST

PDB ID : 5Z85
Title : The structure of azide-bound cytochrome c oxidase determined using the another batch crystals exposed to 20 mM azide solution for 2 days
Authors : Shimada, A.; Hatano, K.; Tadehara, H.; Tsukihara, T.
Deposited on : 2018-01-31
Resolution : 1.85 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 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) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

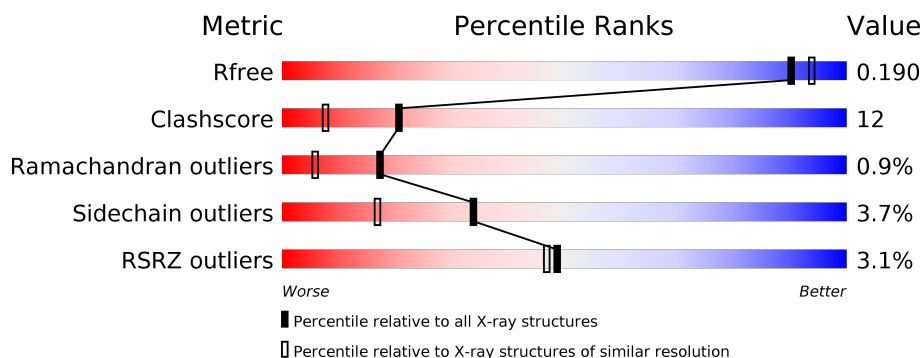
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div></div> <div>82%16%•</div> </div>
1	N	514	<div> <div></div> <div>82%16%•</div> </div>
2	B	227	<div> <div>%</div> <div>73%24%•</div> </div>
2	O	227	<div> <div>%</div> <div>76%22%•</div> </div>
3	C	261	<div> <div></div> <div>82%17%••</div> </div>
3	P	261	<div> <div>%</div> <div>80%19%••</div> </div>

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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
14	HEA	A	601	X	-	-	-
14	HEA	A	602[A]	X	-	-	-
14	HEA	A	602[B]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	601	X	-	-	-
14	HEA	N	602[A]	X	-	-	-
14	HEA	N	602[B]	X	-	-	-
18	AZI	A	607	-	-	X	-
18	AZI	N	607	-	-	X	-
21	EDO	A	612	-	-	X	-
21	EDO	A	614	-	X	X	-
21	EDO	A	618	-	-	X	-
21	EDO	C	318	-	-	-	X
21	EDO	D	202	-	-	X	-
21	EDO	D	203	-	-	X	-
21	EDO	D	204	-	-	-	X
21	EDO	N	618	-	-	X	-
21	EDO	N	621	-	-	X	-
21	EDO	Q	204	-	-	X	-
27	CDL	C	305	-	-	X	-
27	CDL	G	102	-	-	X	-
27	CDL	P	306	-	-	X	-
27	CDL	T	103	-	-	X	-
7	TPO	T	11	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33411 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	18	0
			4165	2777	645	703	40			
1	N	514	Total	C	N	O	S	0	18	0
			4160	2774	642	702	42			

- 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	4	0
			1859	1211	285	344	19			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	288	347	20			

- 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	7	0
			2171	1449	347	360	15			
3	P	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			

- 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	1	0
			1204	783	198	219	4			
4	Q	144	Total	C	N	O	S	0	2	0
			1213	791	198	220	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	3	0
			771	477	138	150	6			
6	S	98	Total	C	N	O	S	0	2	0
			763	473	136	148	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 686	C 440	N 130	O 114	P 1	S 1	0	1	0
7	T	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0

- 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	1	0
			391	255	66	68	2			

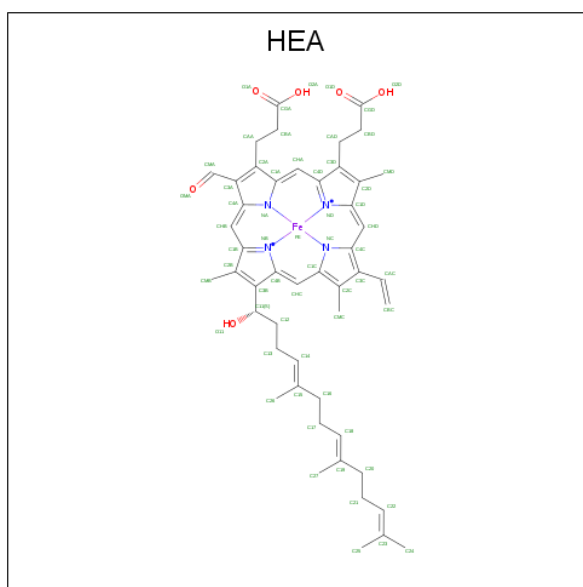
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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	1	0
			388	259	65	61	3			

- 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 (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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 120	C 98	Fe 2	N 8	O 12	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 120	C 98	Fe 2	N 8	O 12	0	1

- Molecule 15 is COPPER (II) ION (three-letter code: 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		

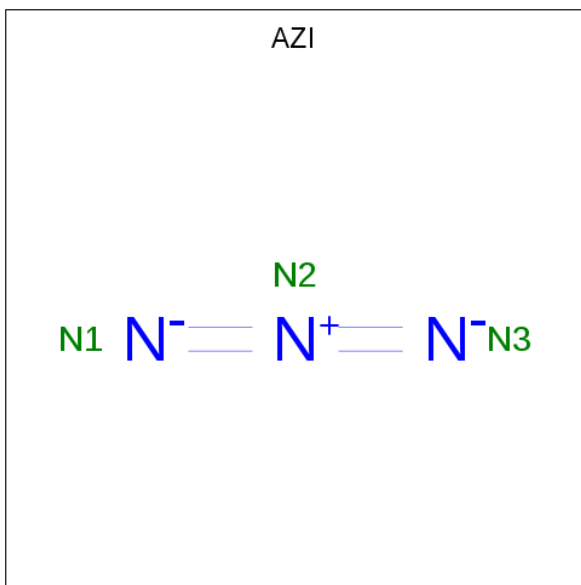
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: NA) (formula: Na).

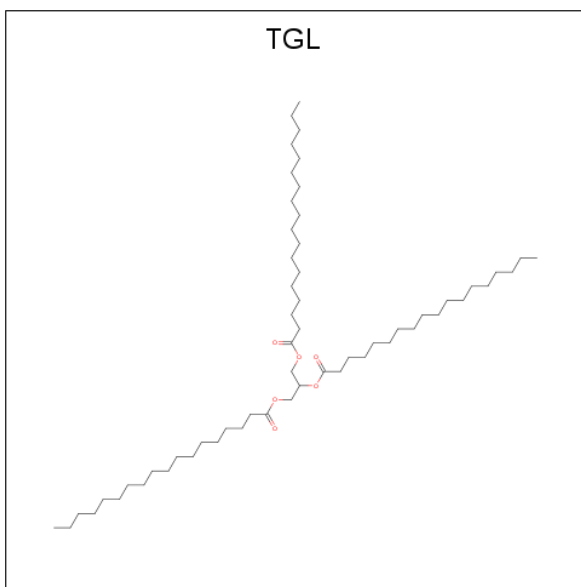
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is AZIDE ION (three-letter code: AZI) (formula: N₃).



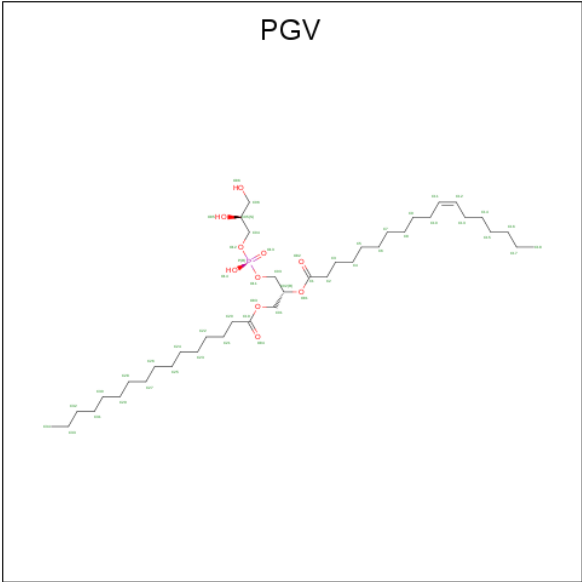
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total N 3 3	0	0
18	A	1	Total N 3 3	0	0
18	N	1	Total N 3 3	0	0
18	N	1	Total N 3 3	0	0

- 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	Q	1	Total	C	O	0	0
			63	57	6		
19	Y	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	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	M	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 1,2-ETHANEDIOL (three-letter code: 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	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	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	C	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	D	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0

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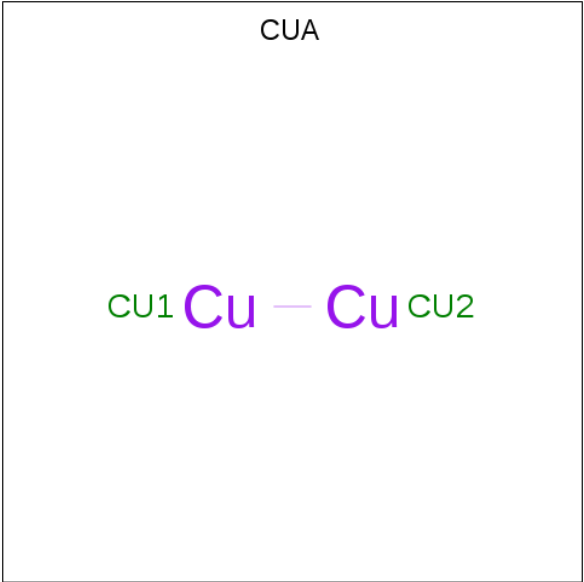
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	G	1	Total 4	C 2	O 2	0	0
21	H	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	Q	1	Total 4	C 2	O 2	0	0

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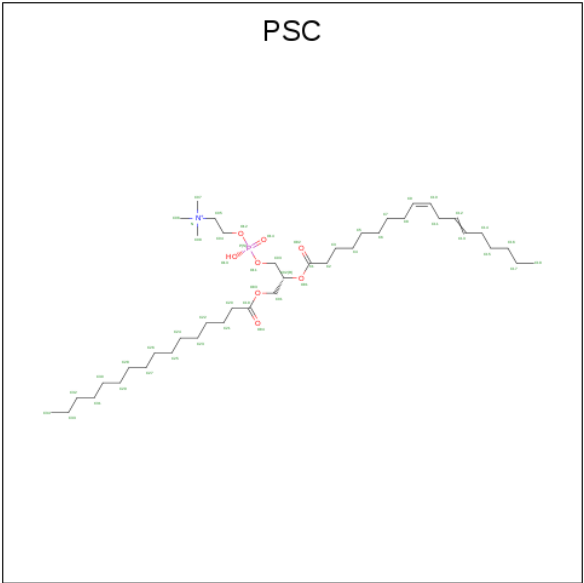
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	Q	1	Total 4	C 2	O 2	0	0
21	Q	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	T	1	Total 4	C 2	O 2	0	0
21	U	1	Total 4	C 2	O 2	0	0
21	V	1	Total 4	C 2	O 2	0	0

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: 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 (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



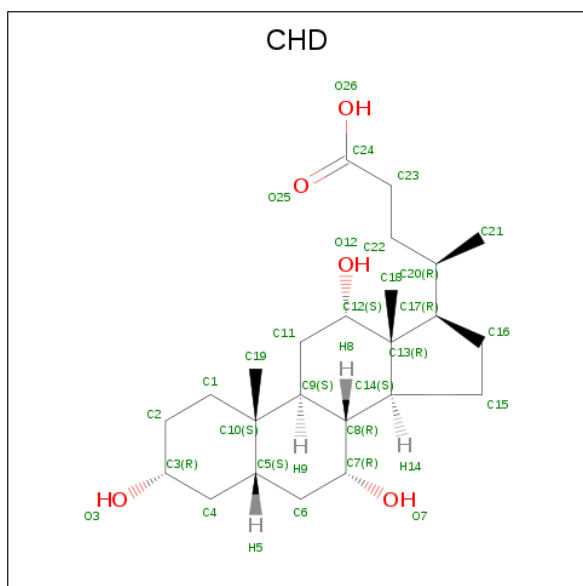
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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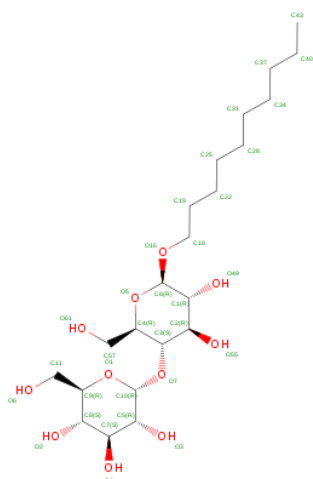
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 24 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



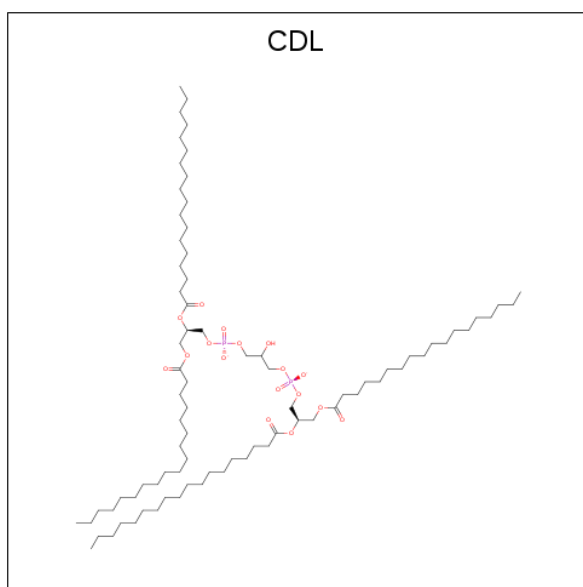
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			29	24	5		
24	C	1	Total	C	O	0	0
			29	24	5		
24	G	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	T	1	Total	C	O	0	0
			29	24	5		

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



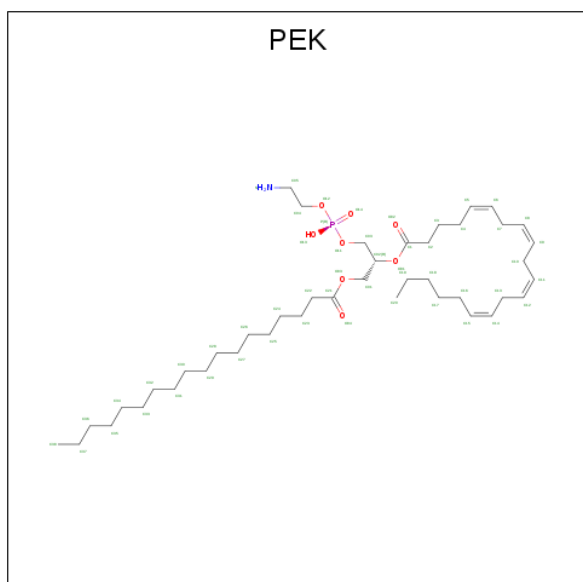
- Molecule 26 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



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

- Molecule 28 is (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
28	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	219	Total	O	0	0
			219	219		
30	B	131	Total	O	0	1
			132	132		
30	C	96	Total	O	0	0
			96	96		
30	D	93	Total	O	0	0
			93	93		
30	E	85	Total	O	0	0
			85	85		
30	F	78	Total	O	0	0
			78	78		
30	G	37	Total	O	0	0
			37	37		
30	H	30	Total	O	0	0
			30	30		
30	I	20	Total	O	0	0
			20	20		
30	J	22	Total	O	0	0
			22	22		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	17	Total 17	O 17	0	0
30	L	21	Total 21	O 21	0	0
30	M	22	Total 22	O 22	0	0
30	N	217	Total 217	O 217	0	0
30	O	114	Total 115	O 115	0	1
30	P	95	Total 95	O 95	0	0
30	Q	57	Total 57	O 57	0	0
30	R	56	Total 56	O 56	0	0
30	S	65	Total 65	O 65	0	0
30	T	33	Total 33	O 33	0	0
30	U	38	Total 38	O 38	0	0
30	V	16	Total 16	O 16	0	0
30	W	13	Total 13	O 13	0	0
30	X	15	Total 15	O 15	0	0
30	Y	14	Total 14	O 14	0	0
30	Z	12	Total 12	O 12	0	0

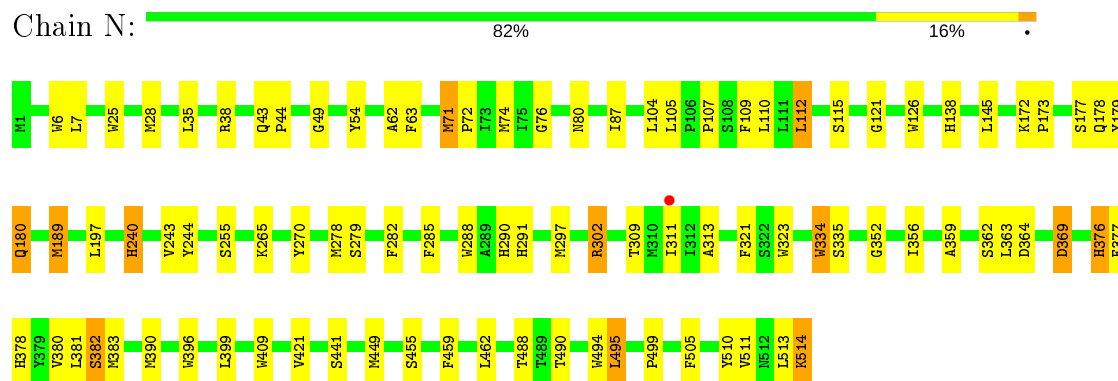
3 Residue-property plots

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

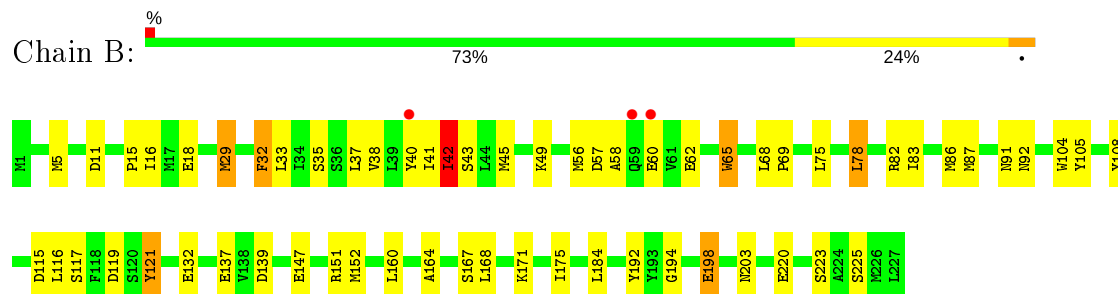
• Molecule 1: Cytochrome c oxidase subunit 1



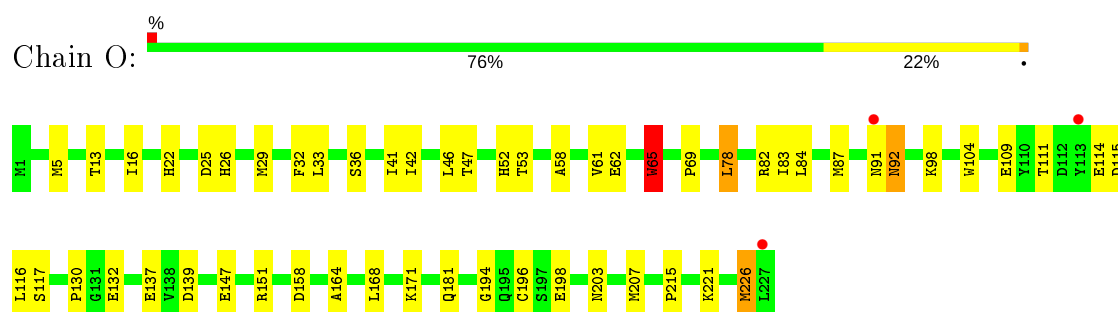
• Molecule 1: Cytochrome c oxidase subunit 1



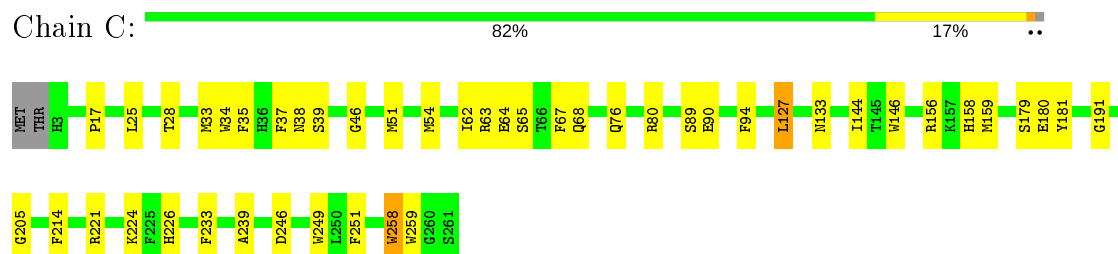
• Molecule 2: Cytochrome c oxidase subunit 2



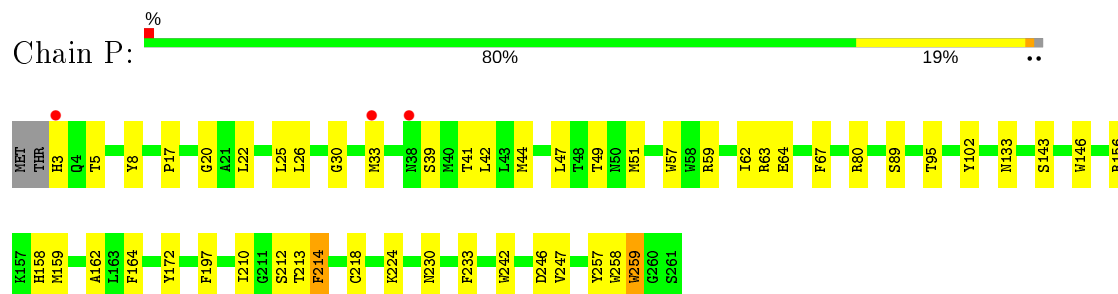
• Molecule 2: Cytochrome c oxidase subunit 2



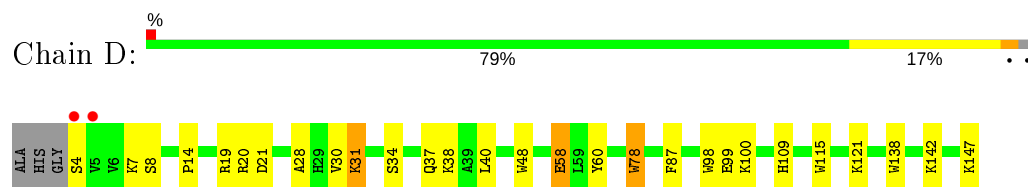
- Molecule 3: Cytochrome c oxidase subunit 3



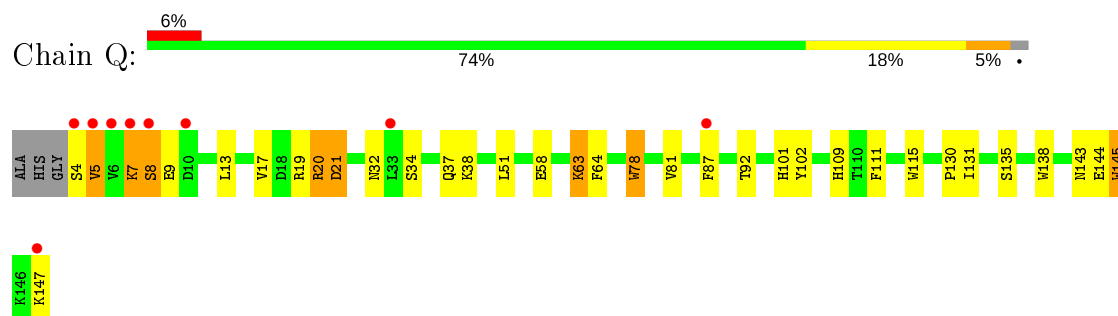
- Molecule 3: Cytochrome c oxidase subunit 3



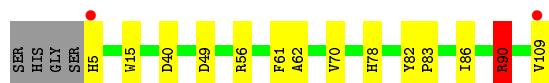
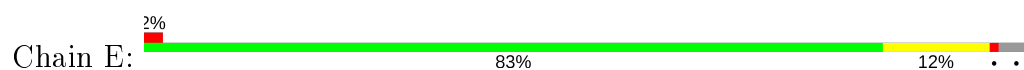
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



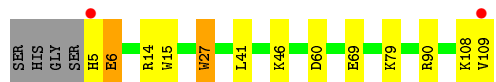
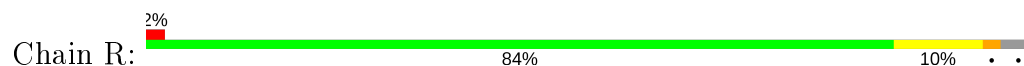
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



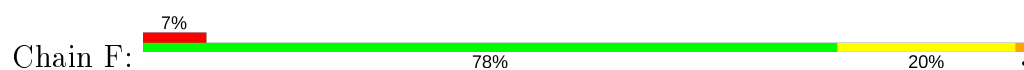
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



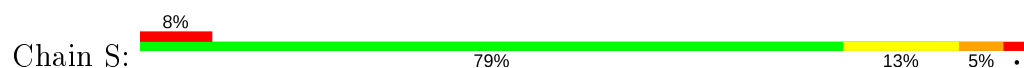
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



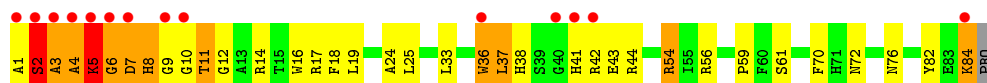
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



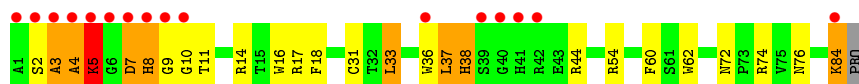
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



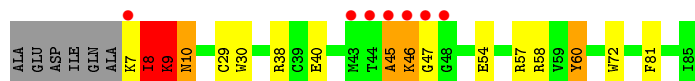
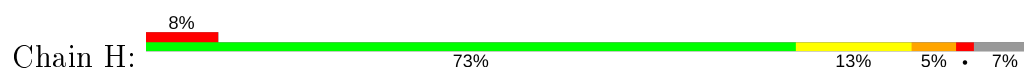
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



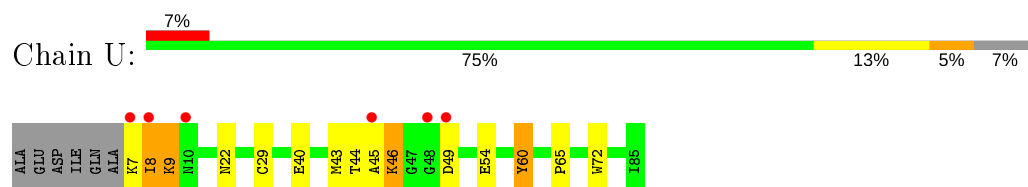
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



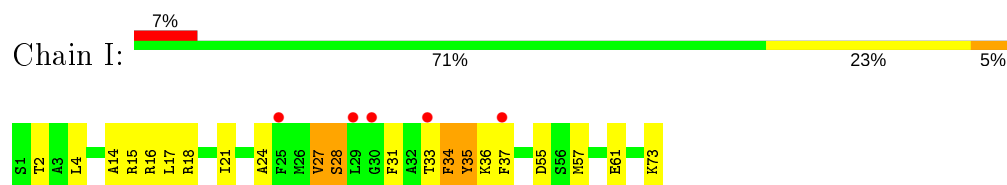
- Molecule 8: Cytochrome c oxidase subunit 6B1



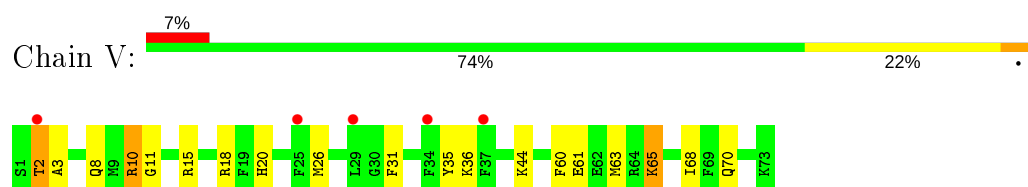
- Molecule 8: Cytochrome c oxidase subunit 6B1



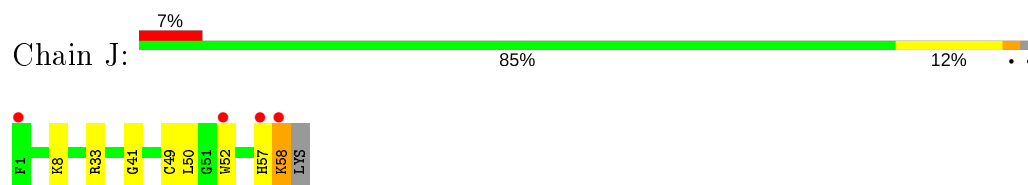
- Molecule 9: Cytochrome c oxidase subunit 6C



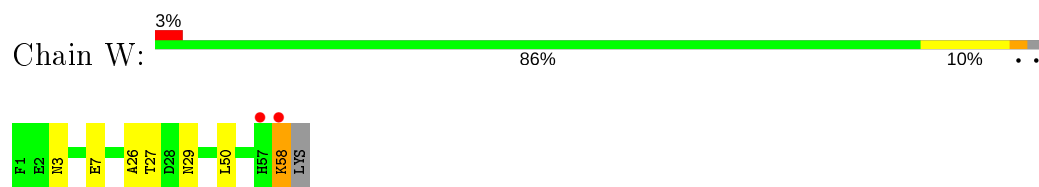
- Molecule 9: Cytochrome c oxidase subunit 6C



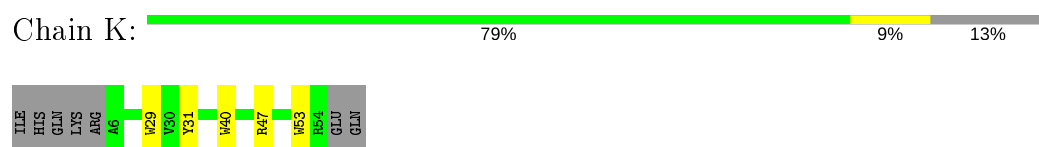
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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



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

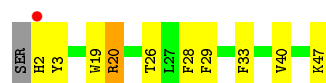
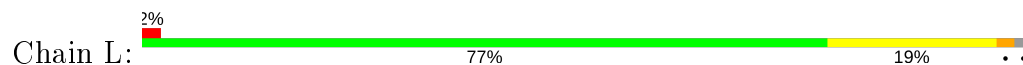


- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

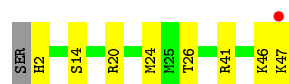
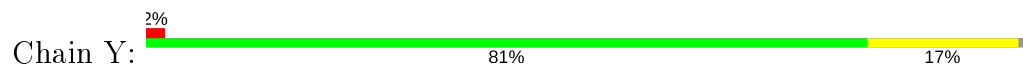




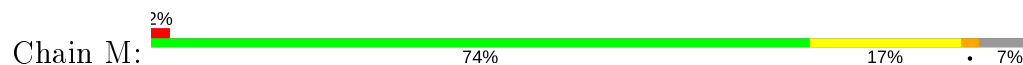
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



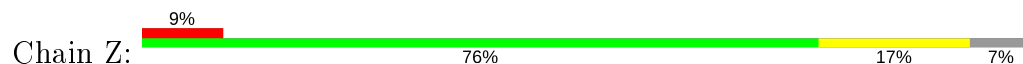
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.13Å 205.89Å 177.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 136.83 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.00-1.85) 99.4 (136.83-1.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.13 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, R_{free}	0.163 , 0.189 0.165 , 0.190	Depositor DCC
R_{free} test set	28242 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33411	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: AZI, ZN, CHD, HEA, SAC, TPO, PSC, PEK, MG, TGL, EDO, PGV, CDL, UNX, CUA, NA, FME, CU, DMU

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	1.63	25/4294 (0.6%)	1.33	26/5861 (0.4%)
1	N	1.55	25/4289 (0.6%)	1.22	14/5853 (0.2%)
2	B	1.49	9/1896 (0.5%)	1.28	16/2582 (0.6%)
2	O	1.25	5/1908 (0.3%)	1.16	5/2597 (0.2%)
3	C	1.57	15/2258 (0.7%)	1.13	2/3084 (0.1%)
3	P	1.56	15/2272 (0.7%)	1.14	5/3102 (0.2%)
4	D	1.52	8/1238 (0.6%)	1.23	6/1669 (0.4%)
4	Q	1.13	3/1248 (0.2%)	1.13	5/1684 (0.3%)
5	E	1.51	6/871 (0.7%)	1.46	6/1182 (0.5%)
5	R	1.26	3/871 (0.3%)	1.08	2/1182 (0.2%)
6	F	1.36	3/788 (0.4%)	1.16	2/1069 (0.2%)
6	S	1.29	0/780	1.18	4/1058 (0.4%)
7	G	1.51	5/702 (0.7%)	1.20	7/953 (0.7%)
7	T	1.47	4/690 (0.6%)	1.16	5/937 (0.5%)
8	H	1.34	5/682 (0.7%)	0.99	0/921
8	U	1.14	1/682 (0.1%)	0.93	0/921
9	I	1.27	2/605 (0.3%)	1.22	4/802 (0.5%)
9	V	1.06	0/605	1.11	2/802 (0.2%)
10	J	1.26	1/471 (0.2%)	1.10	1/636 (0.2%)
10	W	1.21	1/471 (0.2%)	1.03	0/636
11	K	1.40	4/398 (1.0%)	1.12	1/546 (0.2%)
11	X	1.09	2/405 (0.5%)	0.86	0/556
12	L	1.46	3/393 (0.8%)	1.25	2/526 (0.4%)
12	Y	1.22	0/401	1.03	0/536
13	M	1.39	2/345 (0.6%)	1.06	0/470
13	Z	1.20	0/345	0.95	0/470
All	All	1.45	147/29908 (0.5%)	1.19	115/40635 (0.3%)

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	2
1	N	0	1
4	Q	0	1
5	R	0	1
6	F	0	1
6	S	0	1
7	G	0	1
8	H	0	2
8	U	0	1
9	V	0	1
12	Y	0	1
All	All	0	13

The worst 5 of 147 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	89	SER	CB-OG	11.28	1.56	1.42
2	O	65	TRP	NE1-CE2	-10.74	1.23	1.37
2	B	198	GLU	CD-OE2	-10.28	1.14	1.25
2	B	65	TRP	CD2-CE2	9.24	1.52	1.41
2	O	65	TRP	CD2-CE2	9.08	1.52	1.41

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	90	ARG	NE-CZ-NH1	22.36	131.48	120.30
5	E	90	ARG	NE-CZ-NH2	-16.92	111.84	120.30
1	A	278	MET	CG-SD-CE	-16.40	73.96	100.20
4	Q	20	ARG	NE-CZ-NH2	-16.14	112.23	120.30
1	A	71	MET	CG-SD-CE	-15.80	74.93	100.20

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
6	F	93	PRO	Peptide
7	G	11	TPO	Peptide
8	H	8	ILE	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	4165	0	4137	80	0
1	N	4160	0	4132	89	0
2	B	1859	0	1869	44	0
2	O	1870	0	1868	41	0
3	C	2171	0	2085	43	0
3	P	2185	0	2097	52	0
4	D	1204	0	1195	23	0
4	Q	1213	0	1199	34	0
5	E	852	0	845	4	0
5	R	852	0	845	4	0
6	F	771	0	747	26	0
6	S	763	0	742	17	0
7	G	686	0	652	51	0
7	T	675	0	643	37	0
8	H	662	0	623	12	0
8	U	662	0	623	11	0
9	I	601	0	613	18	0
9	V	601	0	613	17	0
10	J	460	0	459	6	0
10	W	460	0	459	7	0
11	K	384	0	366	0	0
11	X	391	0	374	11	0
12	L	380	0	380	11	0
12	Y	388	0	388	11	0
13	M	335	0	352	5	0
13	Z	335	0	352	8	0
14	A	180	0	162	25	0
14	N	180	0	162	26	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	6	0	0	6	0
18	N	6	0	0	6	0
19	A	63	0	110	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	D	63	0	110	13	0
19	L	63	0	110	17	0
19	N	63	0	110	4	0
19	Q	63	0	110	12	0
19	Y	63	0	110	16	0
20	A	51	0	76	4	0
20	C	102	0	152	4	0
20	M	51	0	76	3	0
20	N	102	0	152	14	0
20	P	102	0	152	12	0
21	A	44	0	66	21	0
21	B	4	0	6	0	0
21	C	36	0	54	3	0
21	D	20	0	30	12	0
21	E	20	0	30	0	0
21	F	12	0	18	1	0
21	G	8	0	12	1	0
21	H	4	0	6	3	0
21	N	44	0	66	15	0
21	O	12	0	18	0	0
21	P	16	0	24	1	0
21	Q	12	0	18	6	0
21	R	20	0	30	3	0
21	S	12	0	18	3	0
21	T	4	0	6	0	0
21	U	4	0	6	0	0
21	V	4	0	6	0	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	52	0	80	13	0
23	O	52	0	80	16	0
24	C	58	0	78	5	0
24	G	29	0	39	1	0
24	P	58	0	77	6	0
24	T	29	0	39	0	0
25	C	99	0	126	18	0
25	M	33	0	42	0	0
25	P	99	0	126	14	0
25	Z	33	0	42	0	0
26	C	1	0	0	0	0
26	P	1	0	0	0	0
27	C	100	0	156	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	G	100	0	156	24	0
27	P	100	0	156	22	0
27	T	100	0	156	25	0
28	C	53	0	77	12	0
28	G	106	0	154	23	0
28	P	106	0	154	5	0
28	T	53	0	77	10	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	A	219	0	0	13	0
30	B	132	0	0	15	1
30	C	96	0	0	5	0
30	D	93	0	0	8	1
30	E	85	0	0	1	0
30	F	78	0	0	3	0
30	G	37	0	0	4	0
30	H	30	0	0	0	0
30	I	20	0	0	2	0
30	J	22	0	0	0	0
30	K	17	0	0	0	0
30	L	21	0	0	0	0
30	M	22	0	0	3	0
30	N	217	0	0	14	0
30	O	115	0	0	4	0
30	P	95	0	0	3	0
30	Q	57	0	0	10	0
30	R	56	0	0	4	0
30	S	65	0	0	1	0
30	T	33	0	0	0	0
30	U	38	0	0	3	0
30	V	16	0	0	3	0
30	W	13	0	0	1	0
30	X	15	0	0	2	0
30	Y	14	0	0	0	0
30	Z	12	0	0	2	0
All	All	33411	0	32479	789	1

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 12.

The worst 5 of 789 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)
21:A:614:EDO:C1	21:A:614:EDO:C2	1.83	1.54
20:N:608:PGV:H011	20:N:608:PGV:C2	1.28	1.46
19:L:101:TGL:CC2	19:L:101:TGL:HC62	1.34	1.38
21:A:614:EDO:O1	21:A:614:EDO:C2	1.74	1.29
1:N:297[B]:MET:HB2	30:N:782:HOH:O	1.36	1.25

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:468:HOH:O	30:D:353:HOH:O[2_584]	1.99	0.21

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	530/514 (103%)	514 (97%)	16 (3%)	0	100	100
1	N	530/514 (103%)	516 (97%)	14 (3%)	0	100	100
2	B	229/227 (101%)	223 (97%)	6 (3%)	0	100	100
2	O	230/227 (101%)	224 (97%)	5 (2%)	1 (0%)	34	19
3	C	264/261 (101%)	260 (98%)	4 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	143/147 (97%)	139 (97%)	4 (3%)	0	100	100
4	Q	144/147 (98%)	138 (96%)	4 (3%)	2 (1%)	11	3
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	0	1 (1%)	15	5
6	F	99/98 (101%)	93 (94%)	2 (2%)	4 (4%)	3	0
6	S	98/98 (100%)	89 (91%)	4 (4%)	5 (5%)	2	0
7	G	82/85 (96%)	69 (84%)	6 (7%)	7 (8%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	T	81/85 (95%)	70 (86%)	7 (9%)	4 (5%)	2	0
8	H	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	3	0
8	U	77/85 (91%)	68 (88%)	6 (8%)	3 (4%)	3	0
9	I	71/73 (97%)	68 (96%)	1 (1%)	2 (3%)	5	0
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6	1
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3576/3614 (99%)	3444 (96%)	99 (3%)	33 (1%)	17	6

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
6	F	94	HIS
6	F	95	GLN
7	G	2	SER
7	G	4	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	443/426 (104%)	436 (98%)	7 (2%)	62	49
1	N	443/426 (104%)	434 (98%)	9 (2%)	55	40
2	B	214/210 (102%)	201 (94%)	13 (6%)	18	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	215/210 (102%)	207 (96%)	8 (4%)	34	17
3	C	231/226 (102%)	227 (98%)	4 (2%)	60	47
3	P	233/226 (103%)	228 (98%)	5 (2%)	53	38
4	D	129/129 (100%)	125 (97%)	4 (3%)	40	23
4	Q	130/129 (101%)	124 (95%)	6 (5%)	27	11
5	E	92/95 (97%)	88 (96%)	4 (4%)	29	12
5	R	92/95 (97%)	89 (97%)	3 (3%)	38	21
6	F	84/81 (104%)	80 (95%)	4 (5%)	25	10
6	S	83/81 (102%)	74 (89%)	9 (11%)	6	1
7	G	68/68 (100%)	59 (87%)	9 (13%)	4	0
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	1
8	H	71/75 (95%)	66 (93%)	5 (7%)	15	3
8	U	71/75 (95%)	67 (94%)	4 (6%)	21	7
9	I	57/57 (100%)	55 (96%)	2 (4%)	36	18
9	V	57/57 (100%)	53 (93%)	4 (7%)	15	3
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	40
10	W	49/50 (98%)	46 (94%)	3 (6%)	18	5
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	40/46 (87%)	40 (100%)	0	100	100
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	30
12	Y	40/40 (100%)	38 (95%)	2 (5%)	24	9
13	M	37/38 (97%)	35 (95%)	2 (5%)	22	8
13	Z	37/38 (97%)	35 (95%)	2 (5%)	22	8
All	All	3110/3082 (101%)	2993 (96%)	117 (4%)	34	16

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	58	LYS
2	O	33	LEU
9	V	65	LYS
13	M	38	ASP
1	N	180	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	180	GLN
3	P	50	ASN
10	W	29	ASN
2	O	10	GLN
2	O	181	GLN

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	$\# Z > 2$
1	FME	A	1	1	8,9,10	1.24	0	7,9,11	2.13	4 (57%)
9	SAC	I	1	9	7,8,9	1.37	1 (14%)	8,9,11	1.71	1 (12%)
9	SAC	V	1	9	7,8,9	1.71	1 (14%)	8,9,11	1.29	1 (12%)
7	TPO	G	11	7	8,10,11	2.12	2 (25%)	10,14,16	1.61	2 (20%)
2	FME	O	1	2	8,9,10	1.48	1 (12%)	7,9,11	1.73	2 (28%)
2	FME	B	1	2	8,9,10	1.85	2 (25%)	7,9,11	1.97	2 (28%)
1	FME	N	1	1	8,9,10	1.19	1 (12%)	7,9,11	1.36	0
7	TPO	T	11	7	8,10,11	1.70	1 (12%)	10,14,16	0.99	1 (10%)

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	-
9	SAC	I	1	9	-	4/7/8/10	-
9	SAC	V	1	9	-	5/7/8/10	-
7	TPO	G	11	7	-	6/9/11/13	-
2	FME	O	1	2	-	0/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-
7	TPO	T	11	7	-	3/9/11/13	-

The worst 5 of 9 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
7	T	11	TPO	P-O1P	3.51	1.61	1.50
7	G	11	TPO	P-OG1	3.20	1.65	1.59
7	G	11	TPO	P-O1P	3.19	1.60	1.50
9	I	1	SAC	CA-N	3.19	1.50	1.46

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	1	SAC	OG-CB-CA	-4.02	100.70	110.97
2	B	1	FME	C-CA-N	-3.44	103.53	109.73
2	B	1	FME	CG-CB-CA	-3.34	103.67	112.95
2	O	1	FME	CG-CB-CA	-3.09	104.35	112.95
1	A	1	FME	CE-SD-CG	3.08	110.99	100.40

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
9	I	1	SAC	C-CA-CB-OG
9	V	1	SAC	C-CA-CB-OG
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 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	3	0
7	T	11	TPO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 131 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 121 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	$\# Z > 2$
24	CHD	P	307	-	29,32,32	1.44	4 (13%)	48,51,51	3.22	23 (47%)
25	DMU	C	309	-	34,34,34	0.88	2 (5%)	45,45,45	2.62	12 (26%)
21	EDO	C	319	-	3,3,3	0.92	0	2,2,2	1.51	0
20	PGV	C	308	-	50,50,50	1.24	2 (4%)	53,56,56	1.35	5 (9%)
21	EDO	S	104	-	3,3,3	0.75	0	2,2,2	1.58	1 (50%)
24	CHD	P	301	-	29,32,32	1.61	6 (20%)	48,51,51	2.22	17 (35%)
21	EDO	A	617	-	3,3,3	0.27	0	2,2,2	1.71	1 (50%)
21	EDO	H	101	-	3,3,3	0.29	0	2,2,2	2.25	2 (100%)
21	EDO	V	101	-	3,3,3	0.41	0	2,2,2	0.43	0
25	DMU	M	102	-	34,34,34	0.60	0	45,45,45	1.42	5 (11%)
21	EDO	N	620	-	3,3,3	0.45	0	2,2,2	1.44	0
21	EDO	D	204	-	3,3,3	0.76	0	2,2,2	0.71	0
14	HEA	N	601	1	44,67,67	1.42	7 (15%)	37,103,103	2.75	18 (48%)
14	HEA	A	601	1	44,67,67	1.51	7 (15%)	37,103,103	3.26	22 (59%)
27	CDL	P	306	-	99,99,99	1.66	19 (19%)	105,111,111	1.55	18 (17%)
21	EDO	E	204	-	3,3,3	0.65	0	2,2,2	0.36	0
27	CDL	T	103	-	99,99,99	1.44	12 (12%)	105,111,111	1.47	19 (18%)
21	EDO	N	618	-	3,3,3	0.78	0	2,2,2	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	N	614	-	3,3,3	0.53	0	2,2,2	0.94	0
21	EDO	T	104	-	3,3,3	1.14	0	2,2,2	0.54	0
19	TGL	N	610	-	62,62,62	1.22	4 (6%)	65,65,65	1.72	11 (16%)
21	EDO	R	201	-	3,3,3	0.36	0	2,2,2	0.92	0
21	EDO	B	303	-	3,3,3	0.80	0	2,2,2	0.32	0
21	EDO	N	613	-	3,3,3	0.66	0	2,2,2	0.48	0
21	EDO	Q	204	-	3,3,3	0.72	0	2,2,2	0.24	0
22	CUA	O	301	2	0,1,1	0.00	-	-		
19	TGL	Y	101	-	62,62,62	1.47	4 (6%)	65,65,65	1.55	11 (16%)
21	EDO	C	314	-	3,3,3	0.71	0	2,2,2	0.60	0
25	DMU	P	310	-	34,34,34	0.78	1 (2%)	45,45,45	2.38	11 (24%)
24	CHD	T	101	-	29,32,32	2.23	12 (41%)	48,51,51	2.00	16 (33%)
28	PEK	P	309	-	52,52,52	1.24	2 (3%)	55,57,57	1.43	6 (10%)
21	EDO	E	202	-	3,3,3	0.54	0	2,2,2	0.89	0
21	EDO	P	314	-	3,3,3	0.55	0	2,2,2	0.65	0
23	PSC	O	302	-	51,51,51	1.28	3 (5%)	57,59,59	1.29	5 (8%)
21	EDO	A	610	-	3,3,3	0.33	0	2,2,2	1.48	0
21	EDO	G	105	-	3,3,3	0.59	0	2,2,2	0.55	0
21	EDO	E	205	-	3,3,3	0.55	0	2,2,2	0.77	0
21	EDO	N	617	-	3,3,3	0.96	0	2,2,2	0.16	0
21	EDO	R	205	-	3,3,3	1.16	0	2,2,2	0.36	0
21	EDO	D	202	-	3,3,3	0.46	0	2,2,2	0.46	0
28	PEK	T	102	-	52,52,52	1.28	2 (3%)	55,57,57	1.49	7 (12%)
21	EDO	U	101	-	3,3,3	0.44	0	2,2,2	0.49	0
20	PGV	N	609	-	50,50,50	1.07	4 (8%)	53,56,56	1.30	4 (7%)
25	DMU	C	310	-	34,34,34	0.97	1 (2%)	45,45,45	2.20	12 (26%)
21	EDO	O	305	-	3,3,3	0.45	0	2,2,2	0.37	0
21	EDO	C	311	-	3,3,3	1.08	0	2,2,2	0.32	0
21	EDO	Q	203	-	3,3,3	1.23	0	2,2,2	1.03	0
28	PEK	G	104	-	52,52,52	1.32	5 (9%)	55,57,57	1.53	6 (10%)
25	DMU	P	308	-	34,34,34	1.10	1 (2%)	45,45,45	1.52	4 (8%)
21	EDO	C	317	-	3,3,3	0.73	0	2,2,2	0.47	0
20	PGV	C	304	-	50,50,50	0.95	2 (4%)	53,56,56	1.53	10 (18%)
21	EDO	N	619	-	3,3,3	0.54	0	2,2,2	0.21	0
21	EDO	R	202	-	3,3,3	0.48	0	2,2,2	1.00	0
21	EDO	C	315	-	3,3,3	1.08	0	2,2,2	1.12	0
24	CHD	C	301	-	29,32,32	1.80	8 (27%)	48,51,51	2.66	17 (35%)
21	EDO	D	206	-	3,3,3	0.32	0	2,2,2	1.19	0
21	EDO	D	203	-	3,3,3	0.29	0	2,2,2	0.69	0
28	PEK	G	101	-	52,52,52	1.05	5 (9%)	55,57,57	1.33	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	TGL	Q	201	-	62,62,62	1.55	4 (6%)	65,65,65	1.45	9 (13%)
20	PGV	A	609	-	50,50,50	1.09	2 (4%)	53,56,56	1.16	5 (9%)
19	TGL	A	608	-	62,62,62	1.32	5 (8%)	65,65,65	2.26	11 (16%)
21	EDO	A	613	-	3,3,3	0.30	0	2,2,2	1.38	0
18	AZI	A	607	14	0,2,2	0.00	-	0,1,1	0.00	-
19	TGL	L	101	-	62,62,62	1.17	3 (4%)	65,65,65	1.76	15 (23%)
28	PEK	P	304	-	52,52,52	1.00	4 (7%)	55,57,57	1.23	5 (9%)
27	CDL	C	305	-	99,99,99	1.55	17 (17%)	105,111,111	1.58	19 (18%)
21	EDO	A	618	-	3,3,3	0.41	0	2,2,2	1.36	0
27	CDL	G	102	-	99,99,99	1.52	15 (15%)	105,111,111	1.51	19 (18%)
21	EDO	A	614	-	3,3,3	3.04	1 (33%)	2,2,2	4.76	1 (50%)
23	PSC	B	302	-	51,51,51	1.44	4 (7%)	57,59,59	1.50	5 (8%)
19	TGL	D	201	-	62,62,62	1.84	5 (8%)	65,65,65	2.30	12 (18%)
21	EDO	S	102	-	3,3,3	1.03	0	2,2,2	0.34	0
21	EDO	E	201	-	3,3,3	0.64	0	2,2,2	0.45	0
21	EDO	A	619	-	3,3,3	0.59	0	2,2,2	0.97	0
18	AZI	N	607	14	0,2,2	0.00	-	0,1,1	0.00	-
21	EDO	F	103	-	3,3,3	0.80	0	2,2,2	0.68	0
21	EDO	P	313	-	3,3,3	0.96	0	2,2,2	0.36	0
25	DMU	P	311	-	34,34,34	0.85	1 (2%)	45,45,45	1.60	8 (17%)
21	EDO	F	104	-	3,3,3	0.34	0	2,2,2	0.33	0
21	EDO	A	612	-	3,3,3	0.95	0	2,2,2	1.36	0
20	PGV	P	302	-	50,50,50	1.16	2 (4%)	53,56,56	1.40	8 (15%)
21	EDO	R	203	-	3,3,3	0.87	0	2,2,2	0.48	0
20	PGV	M	101	-	50,50,50	1.41	4 (8%)	53,56,56	1.61	8 (15%)
24	CHD	G	103	-	29,32,32	1.60	7 (24%)	48,51,51	1.83	16 (33%)
21	EDO	N	616	-	3,3,3	0.57	0	2,2,2	1.31	0
21	EDO	R	204	-	3,3,3	0.26	0	2,2,2	0.45	0
21	EDO	A	620	-	3,3,3	0.33	0	2,2,2	1.09	0
24	CHD	C	306	-	29,32,32	1.19	4 (13%)	48,51,51	3.55	17 (35%)
21	EDO	A	616	-	3,3,3	0.61	0	2,2,2	1.13	0
20	PGV	N	608	-	50,50,50	1.21	2 (4%)	53,56,56	1.34	6 (11%)
20	PGV	P	305	-	50,50,50	1.04	4 (8%)	53,56,56	1.39	7 (13%)
14	HEA	A	602[A]	1,18	44,67,67	1.24	3 (6%)	37,103,103	2.43	15 (40%)
14	HEA	A	602[B]	1,18	44,67,67	1.07	1 (2%)	37,103,103	2.28	13 (35%)
18	AZI	N	606	15	0,2,2	0.00	-	0,1,1	0.00	-
21	EDO	N	611	-	3,3,3	0.48	0	2,2,2	1.43	0
25	DMU	C	302	-	34,34,34	1.16	2 (5%)	45,45,45	1.80	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	C	313	-	3,3,3	0.56	0	2,2,2	0.57	0
21	EDO	C	316	-	3,3,3	0.57	0	2,2,2	0.37	0
21	EDO	C	318	-	3,3,3	0.48	0	2,2,2	0.35	0
21	EDO	N	621	-	3,3,3	0.78	0	2,2,2	0.25	0
21	EDO	P	315	-	3,3,3	0.45	0	2,2,2	0.70	0
21	EDO	D	205	-	3,3,3	0.46	0	2,2,2	1.14	0
21	EDO	E	203	-	3,3,3	0.35	0	2,2,2	1.55	0
21	EDO	A	611	-	3,3,3	0.57	0	2,2,2	1.01	0
21	EDO	A	615	-	3,3,3	1.27	0	2,2,2	0.24	0
21	EDO	O	304	-	3,3,3	0.39	0	2,2,2	1.00	0
21	EDO	P	312	-	3,3,3	0.82	0	2,2,2	1.90	1 (50%)
21	EDO	N	612	-	3,3,3	1.23	0	2,2,2	1.79	1 (50%)
14	HEA	N	602[B]	1,18	44,67,67	1.13	2 (4%)	37,103,103	1.96	14 (37%)
14	HEA	N	602[A]	1,18	44,67,67	1.29	4 (9%)	37,103,103	2.51	16 (43%)
21	EDO	G	106	-	3,3,3	0.99	0	2,2,2	0.58	0
22	CUA	B	301	2	0,1,1	0.00	-	-	-	-
21	EDO	C	312	-	3,3,3	0.36	0	2,2,2	0.60	0
28	PEK	C	307	-	52,52,52	1.21	4 (7%)	55,57,57	1.33	7 (12%)
21	EDO	O	303	-	3,3,3	0.80	0	2,2,2	0.92	0
18	AZI	A	606	15	0,2,2	0.00	-	0,1,1	0.00	-
21	EDO	Q	202	-	3,3,3	0.29	0	2,2,2	1.13	0
21	EDO	N	615	-	3,3,3	1.72	1 (33%)	2,2,2	0.26	0
21	EDO	F	102	-	3,3,3	1.10	0	2,2,2	0.25	0
21	EDO	S	103	-	3,3,3	0.80	0	2,2,2	0.44	0
25	DMU	Z	101	-	34,34,34	0.82	1 (2%)	45,45,45	1.26	5 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHD	P	307	-	-	5/7/74/74	0/4/4/4
25	DMU	C	309	-	-	6/19/59/59	0/2/2/2
21	EDO	C	319	-	-	1/1/1/1	-
20	PGV	C	308	-	-	27/55/55/55	-
21	EDO	S	104	-	-	0/1/1/1	-
24	CHD	P	301	-	-	0/7/74/74	0/4/4/4
21	EDO	A	617	-	-	1/1/1/1	-
21	EDO	H	101	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	V	101	-	-	1/1/1/1	-
25	DMU	M	102	-	-	5/19/59/59	0/2/2/2
21	EDO	N	620	-	-	0/1/1/1	-
21	EDO	D	204	-	-	1/1/1/1	-
14	HEA	A	601	1	2/2/7/16	3/24/76/76	-
27	CDL	P	306	-	-	62/110/110/110	-
21	EDO	E	204	-	-	1/1/1/1	-
27	CDL	T	103	-	-	53/110/110/110	-
21	EDO	N	618	-	-	0/1/1/1	-
21	EDO	N	614	-	-	1/1/1/1	-
21	EDO	T	104	-	-	0/1/1/1	-
19	TGL	N	610	-	-	37/65/65/65	-
21	EDO	R	201	-	-	1/1/1/1	-
21	EDO	B	303	-	-	0/1/1/1	-
21	EDO	N	613	-	-	1/1/1/1	-
21	EDO	Q	204	-	-	0/1/1/1	-
19	TGL	Y	101	-	-	34/65/65/65	-
21	EDO	C	314	-	-	1/1/1/1	-
25	DMU	P	310	-	-	7/19/59/59	0/2/2/2
24	CHD	T	101	-	-	0/7/74/74	0/4/4/4
28	PEK	P	309	-	-	28/56/56/56	-
21	EDO	E	202	-	-	0/1/1/1	-
21	EDO	P	314	-	-	0/1/1/1	-
23	PSC	O	302	-	-	32/55/55/55	-
21	EDO	A	610	-	-	1/1/1/1	-
21	EDO	G	105	-	-	1/1/1/1	-
21	EDO	E	205	-	-	1/1/1/1	-
21	EDO	N	617	-	-	0/1/1/1	-
21	EDO	R	205	-	-	1/1/1/1	-
21	EDO	D	202	-	-	0/1/1/1	-
28	PEK	T	102	-	-	22/56/56/56	-
21	EDO	U	101	-	-	1/1/1/1	-
20	PGV	N	609	-	-	9/55/55/55	-
25	DMU	C	310	-	-	10/19/59/59	0/2/2/2
21	EDO	O	305	-	-	1/1/1/1	-
21	EDO	C	311	-	-	0/1/1/1	-
21	EDO	Q	203	-	-	0/1/1/1	-
28	PEK	G	104	-	-	36/56/56/56	-
25	DMU	P	308	-	-	6/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	C	317	-	-	1/1/1/1	-
20	PGV	C	304	-	-	18/55/55/55	-
21	EDO	N	619	-	-	1/1/1/1	-
21	EDO	R	202	-	-	1/1/1/1	-
21	EDO	C	315	-	-	0/1/1/1	-
24	CHD	C	301	-	-	0/7/74/74	0/4/4/4
21	EDO	D	206	-	-	1/1/1/1	-
21	EDO	D	203	-	-	1/1/1/1	-
28	PEK	G	101	-	-	18/56/56/56	-
19	TGL	Q	201	-	-	39/65/65/65	-
20	PGV	A	609	-	-	8/55/55/55	-
21	EDO	A	611	-	-	1/1/1/1	-
19	TGL	A	608	-	-	39/65/65/65	-
21	EDO	A	613	-	-	1/1/1/1	-
19	TGL	L	101	-	-	43/65/65/65	-
28	PEK	P	304	-	-	16/56/56/56	-
27	CDL	C	305	-	-	66/110/110/110	-
21	EDO	A	618	-	-	0/1/1/1	-
27	CDL	G	102	-	-	58/110/110/110	-
21	EDO	A	614	-	-	1/1/1/1	-
23	PSC	B	302	-	-	30/55/55/55	-
19	TGL	D	201	-	-	41/65/65/65	-
21	EDO	S	102	-	-	0/1/1/1	-
21	EDO	E	201	-	-	0/1/1/1	-
21	EDO	A	619	-	-	1/1/1/1	-
21	EDO	F	103	-	-	0/1/1/1	-
21	EDO	P	313	-	-	0/1/1/1	-
25	DMU	P	311	-	-	13/19/59/59	0/2/2/2
21	EDO	F	104	-	-	0/1/1/1	-
21	EDO	A	612	-	-	1/1/1/1	-
20	PGV	P	302	-	-	25/55/55/55	-
21	EDO	R	203	-	-	0/1/1/1	-
24	CHD	G	103	-	-	0/7/74/74	0/4/4/4
21	EDO	N	616	-	-	0/1/1/1	-
21	EDO	R	204	-	-	1/1/1/1	-
21	EDO	A	620	-	-	0/1/1/1	-
24	CHD	C	306	-	-	4/7/74/74	0/4/4/4
21	EDO	A	616	-	-	1/1/1/1	-
20	PGV	N	608	-	-	27/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	P	305	-	-	9/55/55/55	-
14	HEA	A	602[A]	1,18	3/3/7/16	2/24/76/76	-
14	HEA	A	602[B]	1,18	3/3/7/16	3/24/76/76	-
20	PGV	M	101	-	-	23/55/55/55	-
21	EDO	N	611	-	-	1/1/1/1	-
25	DMU	C	302	-	-	7/19/59/59	0/2/2/2
21	EDO	C	313	-	-	0/1/1/1	-
21	EDO	C	316	-	-	1/1/1/1	-
21	EDO	C	318	-	-	1/1/1/1	-
21	EDO	N	621	-	-	0/1/1/1	-
21	EDO	P	315	-	-	0/1/1/1	-
21	EDO	D	205	-	-	0/1/1/1	-
21	EDO	E	203	-	-	1/1/1/1	-
14	HEA	N	601	1	2/2/7/16	3/24/76/76	-
21	EDO	A	615	-	-	0/1/1/1	-
21	EDO	O	304	-	-	1/1/1/1	-
21	EDO	P	312	-	-	1/1/1/1	-
21	EDO	N	612	-	-	1/1/1/1	-
14	HEA	N	602[B]	1,18	2/2/7/16	4/24/76/76	-
14	HEA	N	602[A]	1,18	2/2/7/16	0/24/76/76	-
21	EDO	G	106	-	-	0/1/1/1	-
21	EDO	C	312	-	-	1/1/1/1	-
28	PEK	C	307	-	-	32/56/56/56	-
21	EDO	O	303	-	-	0/1/1/1	-
21	EDO	Q	202	-	-	0/1/1/1	-
21	EDO	N	615	-	-	0/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
21	EDO	S	103	-	-	1/1/1/1	-
25	DMU	Z	101	-	-	3/19/59/59	0/2/2/2

The worst 5 of 215 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	201	TGL	OB1-CB1	8.49	1.47	1.22
19	Q	201	TGL	OB1-CB1	7.18	1.43	1.22
19	Y	101	TGL	OG2-CB1	6.54	1.52	1.34
19	D	201	TGL	OG1-CA1	6.47	1.52	1.33
19	D	201	TGL	OG2-CB1	6.35	1.52	1.34

The worst 5 of 523 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	306	CHD	C23-C22-C20	-16.50	92.49	114.72
24	P	307	CHD	C23-C22-C20	-11.02	99.88	114.72
19	D	201	TGL	OG2-CB1-CB2	-10.38	89.13	111.50
25	C	310	DMU	O16-C6-C1	9.57	123.24	108.30
25	C	309	DMU	C10-O1-C9	-9.15	95.73	113.69

5 of 14 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	601	HEA	ND
14	A	601	HEA	NB
14	A	602[A]	HEA	ND
14	A	602[A]	HEA	NA
14	A	602[A]	HEA	NB

5 of 949 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	T	102	PEK	C03-O11-P-O13
28	T	102	PEK	C04-O12-P-O14
28	T	102	PEK	O12-C04-C05-N
28	T	102	PEK	O02-C1-O01-C02
28	T	102	PEK	C2-C1-O01-C02

There are no ring outliers.

70 monomers are involved in 436 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	P	307	CHD	4	0
25	C	309	DMU	2	0
20	C	308	PGV	2	0
24	P	301	CHD	2	0
21	A	617	EDO	2	0
21	H	101	EDO	3	0
14	N	601	HEA	7	0
14	A	601	HEA	8	0
27	P	306	CDL	22	0
27	T	103	CDL	25	0
21	N	618	EDO	5	0
19	N	610	TGL	4	0
21	Q	204	EDO	5	0
19	Y	101	TGL	16	0
21	C	314	EDO	1	0

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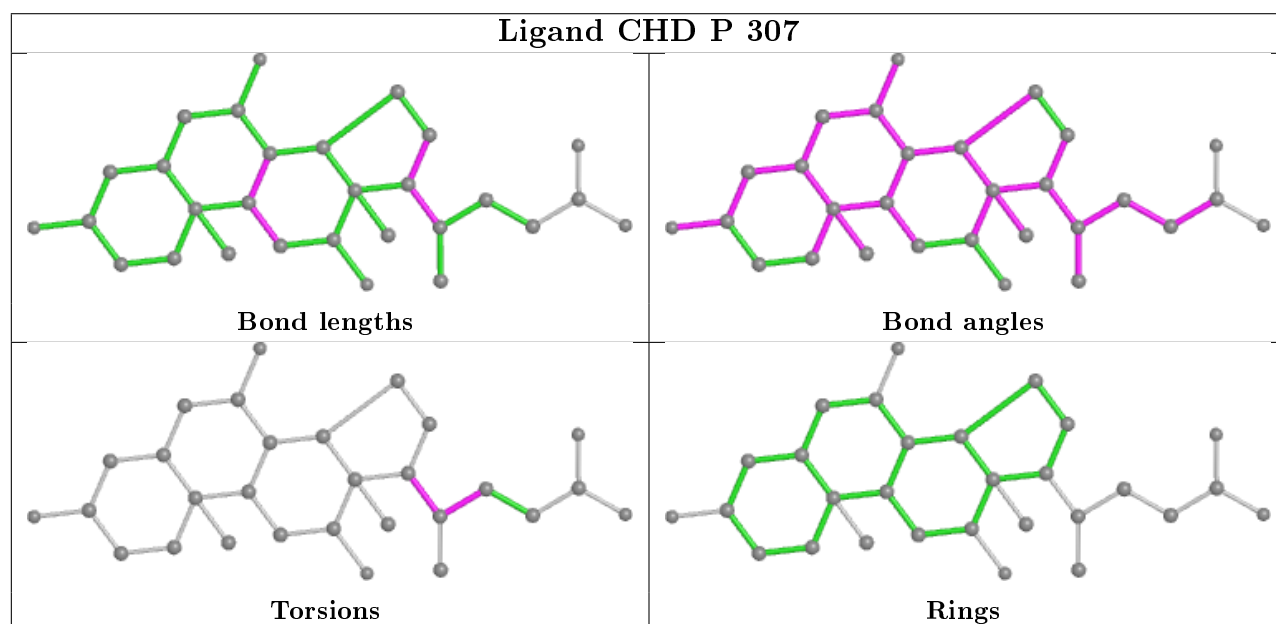
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	310	DMU	2	0
28	P	309	PEK	2	0
23	O	302	PSC	16	0
21	A	610	EDO	1	0
21	G	105	EDO	1	0
21	D	202	EDO	6	0
28	T	102	PEK	10	0
20	N	609	PGV	2	0
25	C	310	DMU	7	0
21	Q	203	EDO	1	0
28	G	104	PEK	14	0
25	P	308	DMU	12	0
21	C	317	EDO	1	0
20	C	304	PGV	2	0
21	D	206	EDO	2	0
21	D	203	EDO	4	0
28	G	101	PEK	9	0
19	Q	201	TGL	12	0
20	A	609	PGV	4	0
19	A	608	TGL	4	0
18	A	607	AZI	6	0
19	L	101	TGL	17	0
28	P	304	PEK	3	0
27	C	305	CDL	26	0
21	A	618	EDO	4	0
27	G	102	CDL	24	0
21	A	614	EDO	7	0
23	B	302	PSC	13	0
19	D	201	TGL	13	0
18	N	607	AZI	6	0
21	F	104	EDO	1	0
21	A	612	EDO	4	0
20	P	302	PGV	10	0
20	M	101	PGV	3	0
24	G	103	CHD	1	0
21	R	204	EDO	3	0
21	A	620	EDO	2	0
24	C	306	CHD	5	0
21	A	616	EDO	1	0
20	N	608	PGV	12	0
20	P	305	PGV	2	0
14	A	602[A]	HEA	6	0

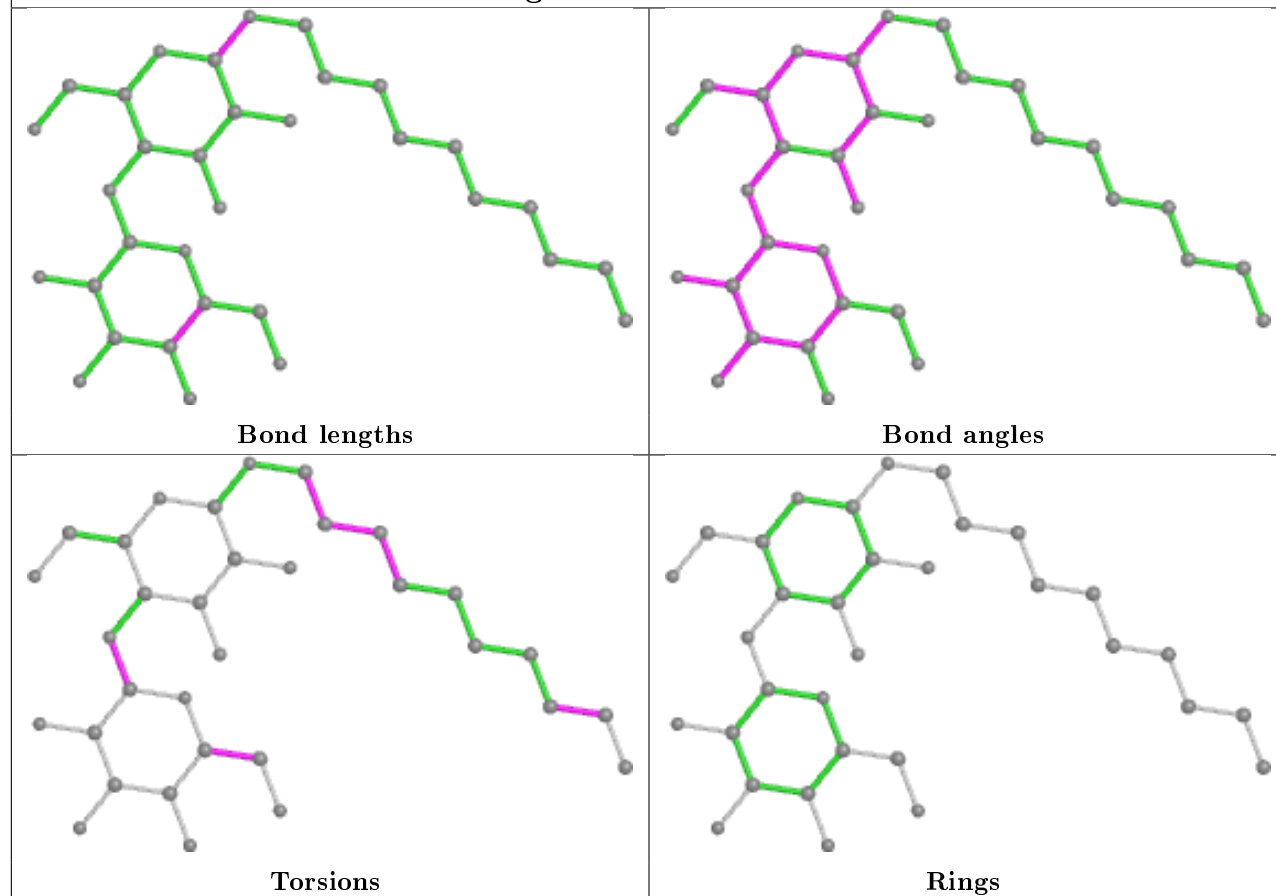
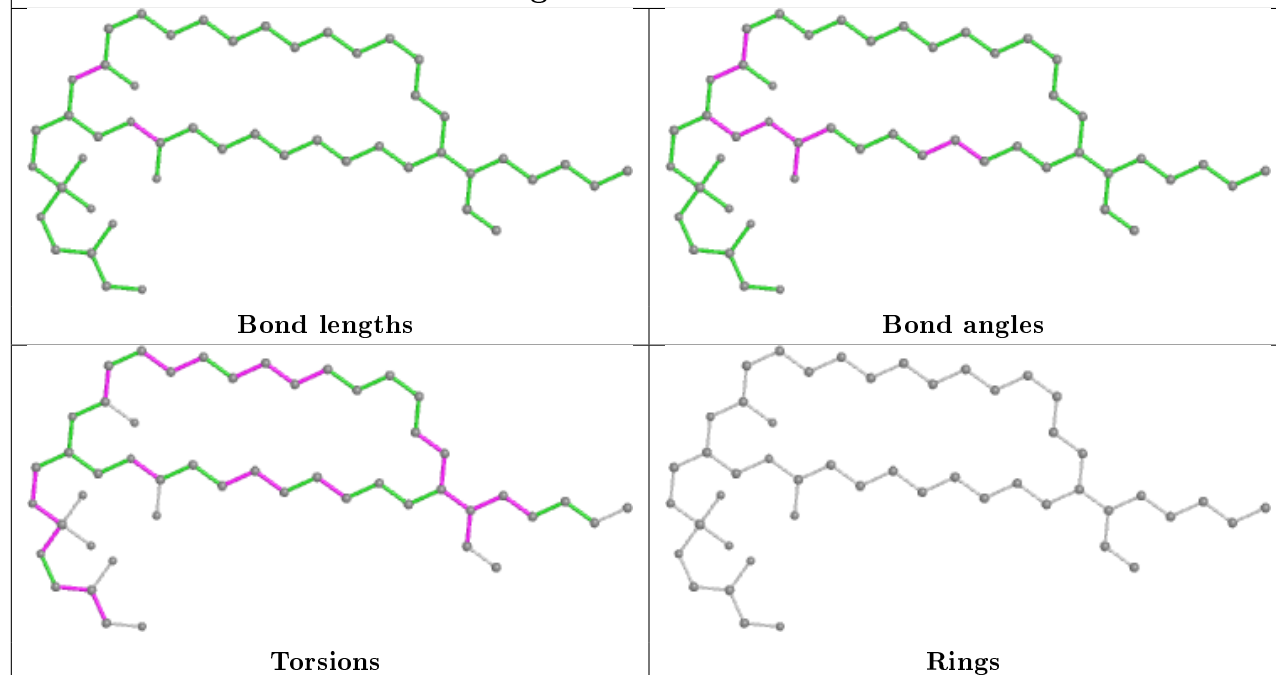
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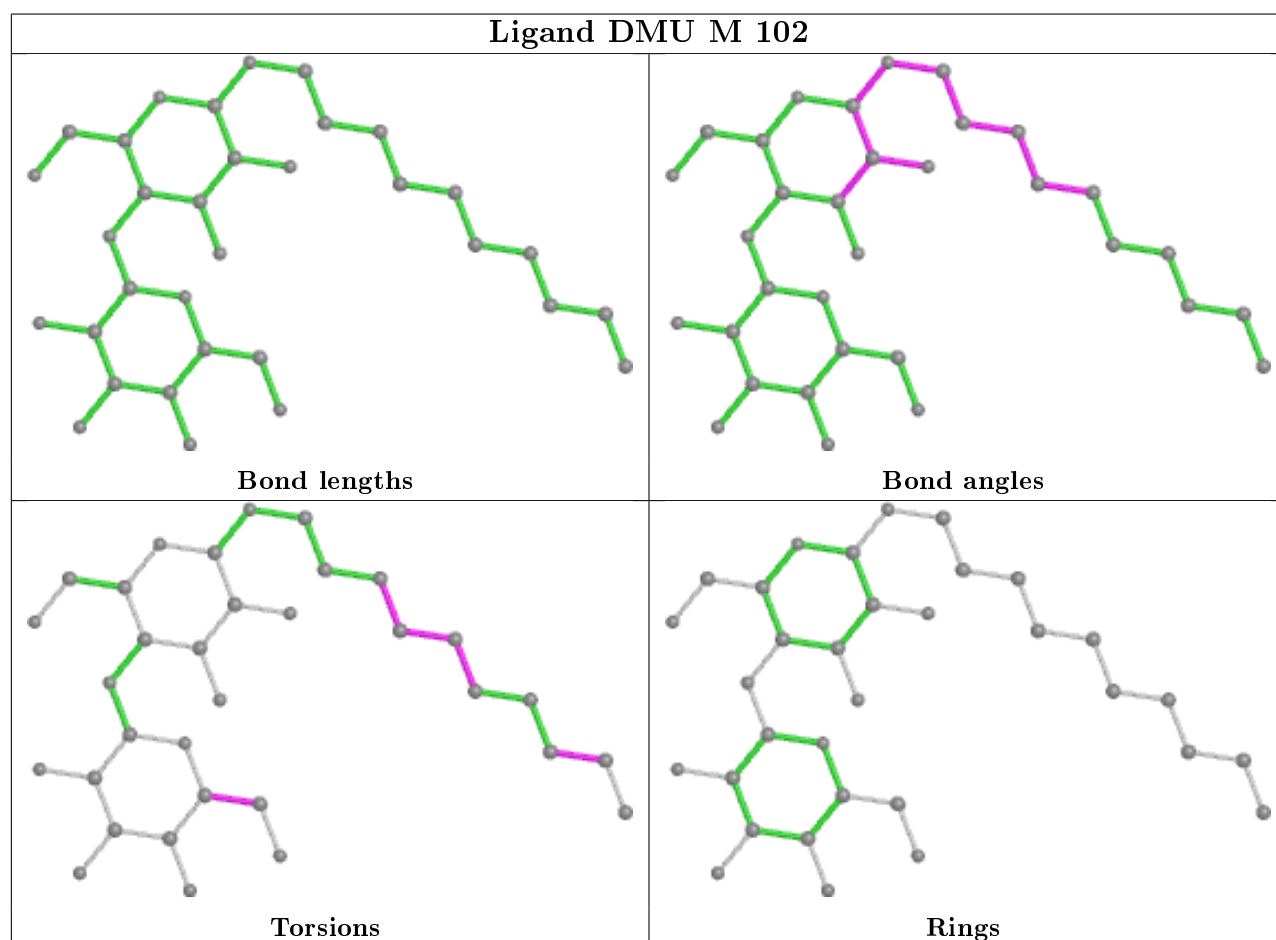
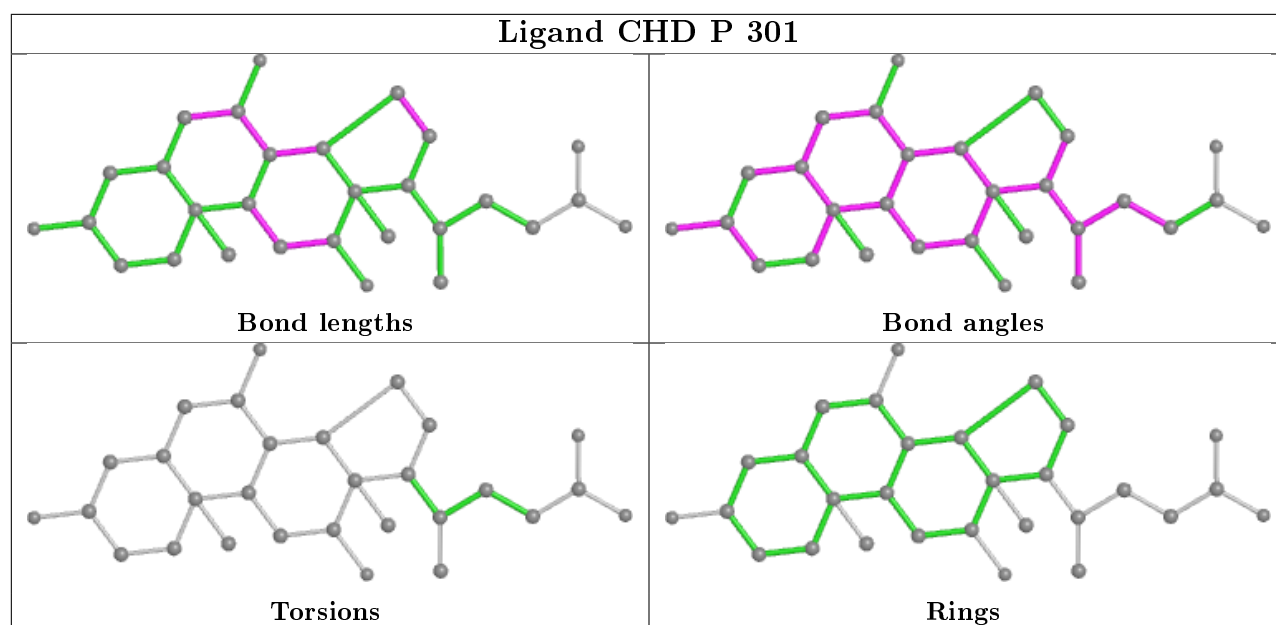
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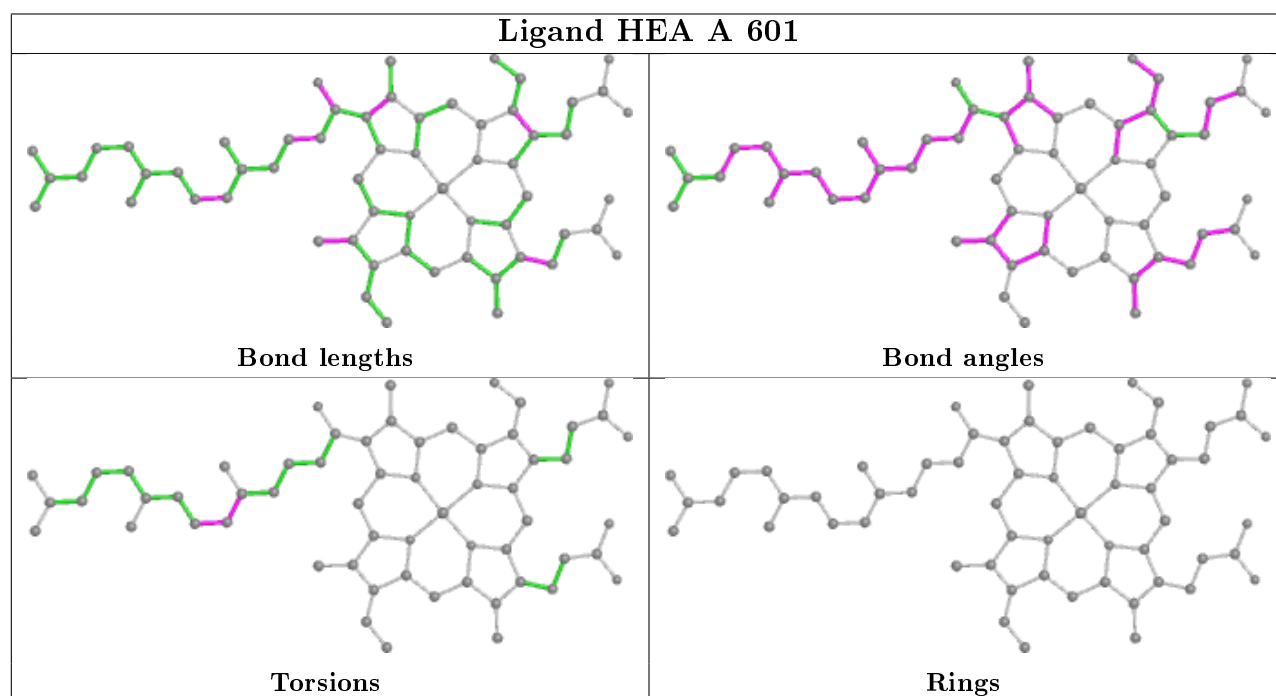
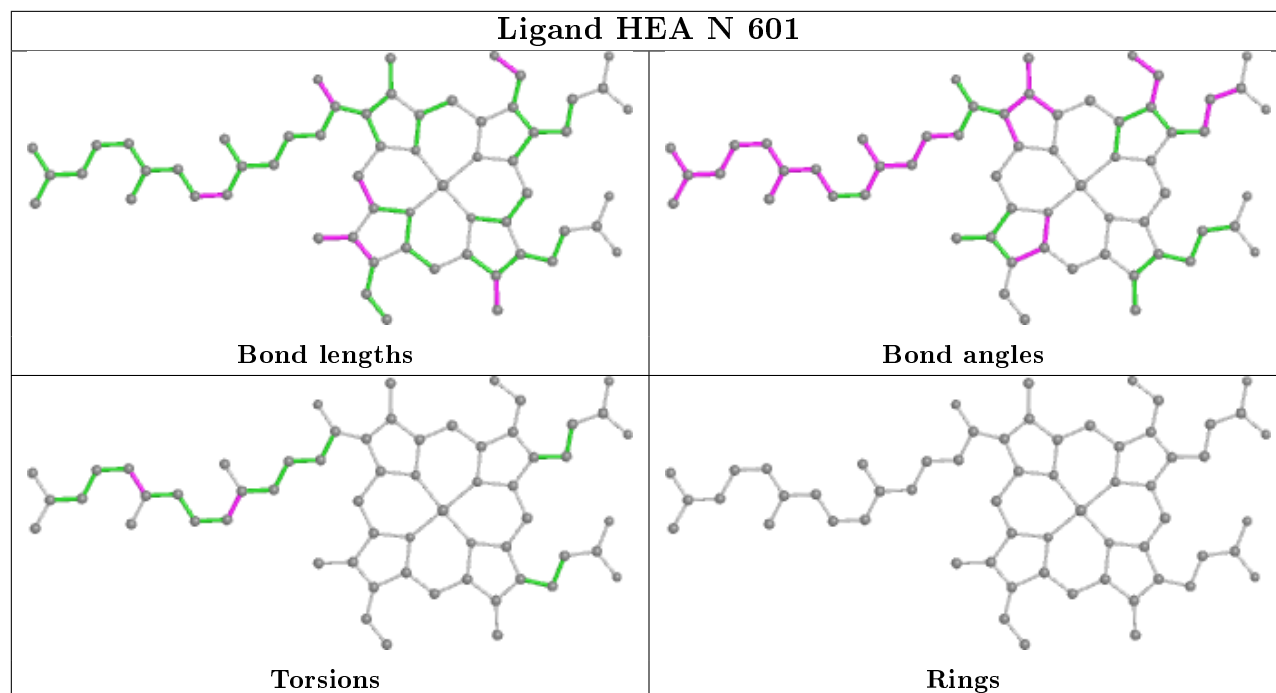
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	602[B]	HEA	11	0
18	N	606	AZI	1	0
25	C	302	DMU	12	0
21	C	313	EDO	1	0
21	N	621	EDO	8	0
21	P	312	EDO	1	0
21	N	612	EDO	2	0
14	N	602[B]	HEA	12	0
14	N	602[A]	HEA	7	0
21	C	312	EDO	1	0
28	C	307	PEK	12	0
18	A	606	AZI	1	0
21	S	103	EDO	3	0

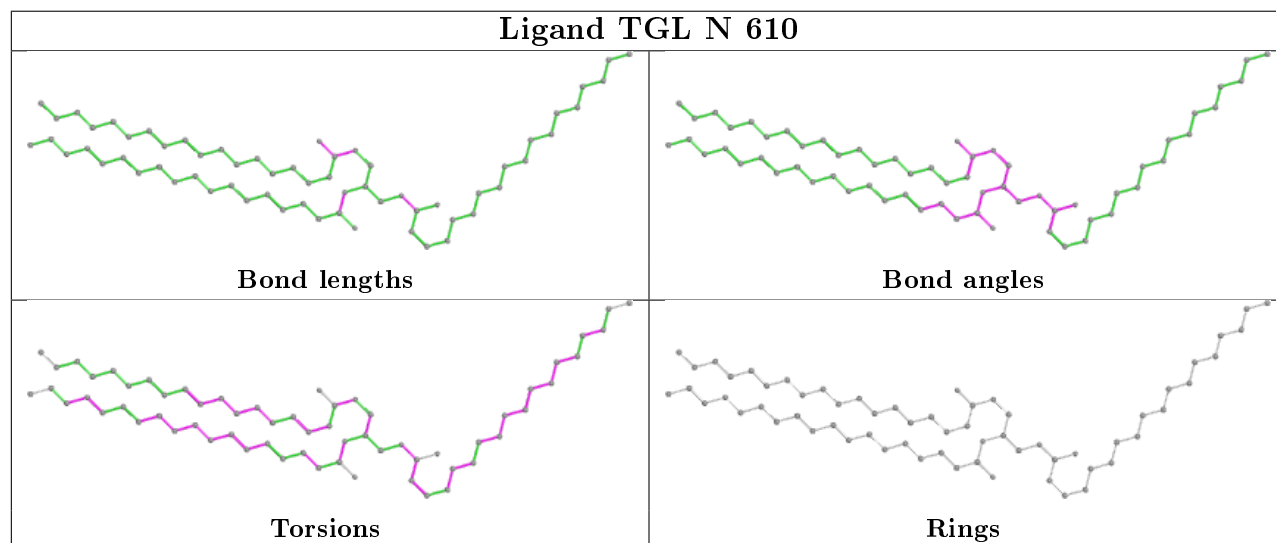
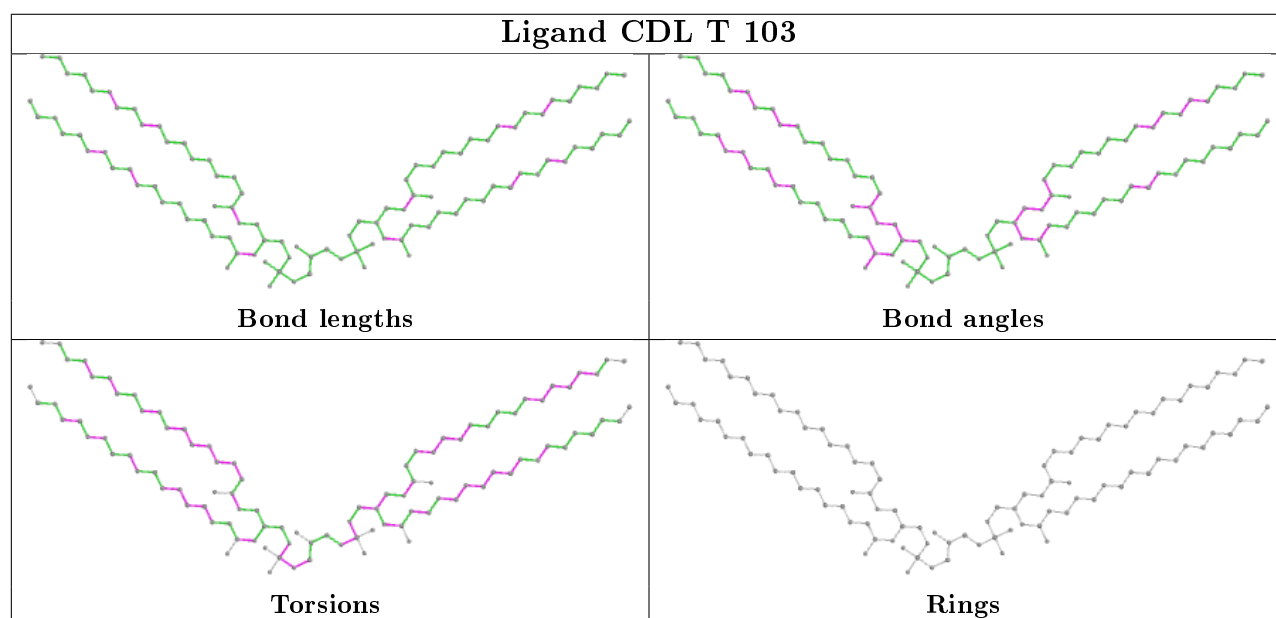
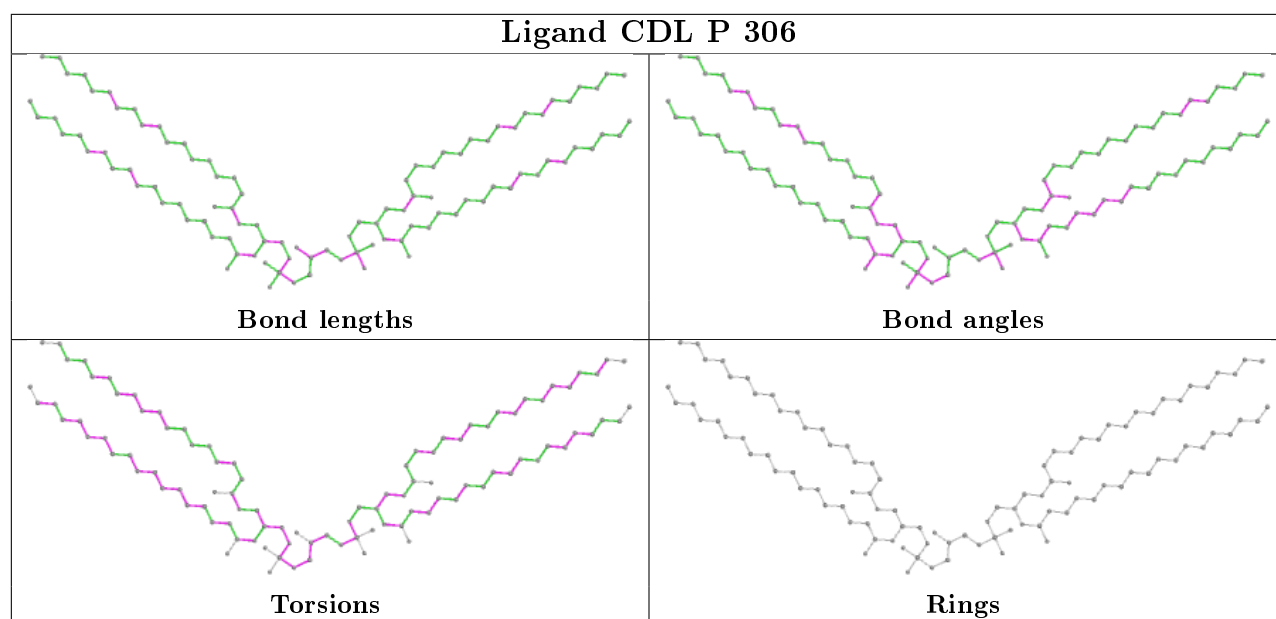
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

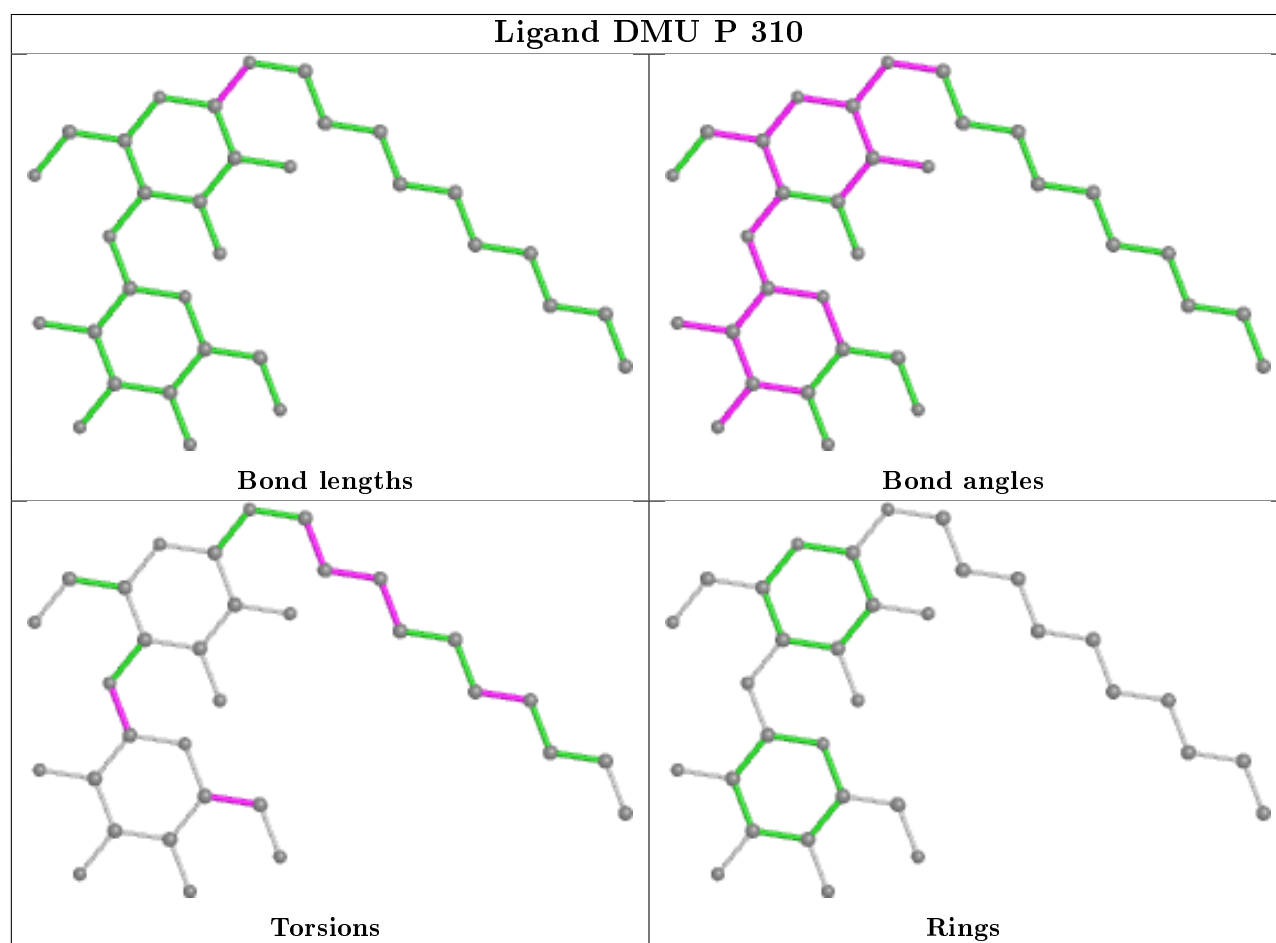
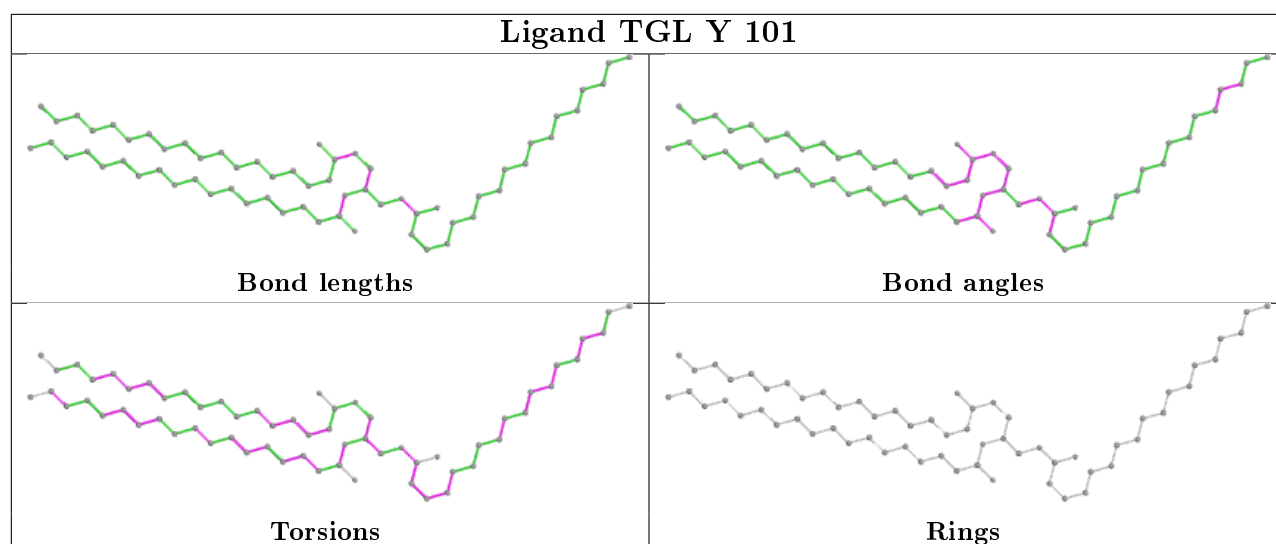


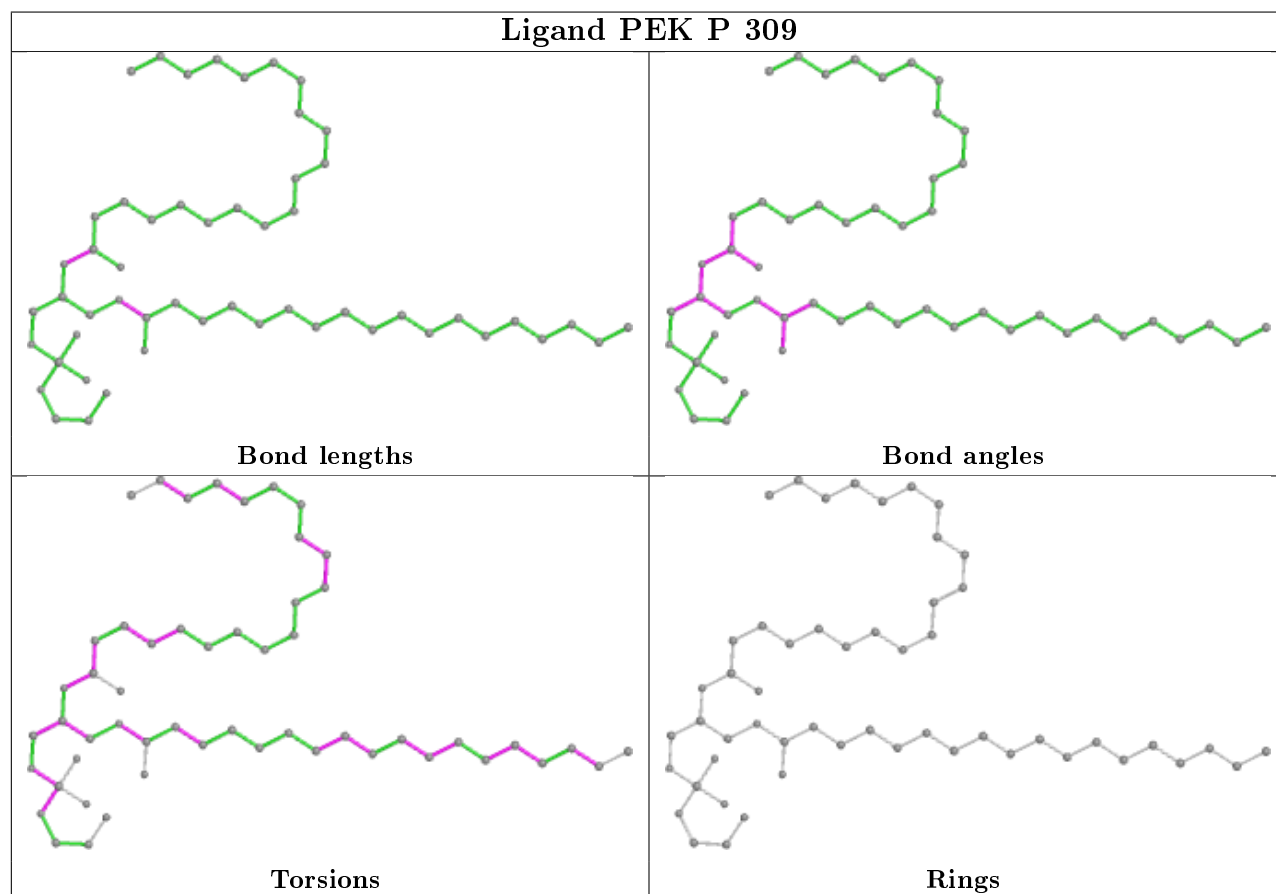
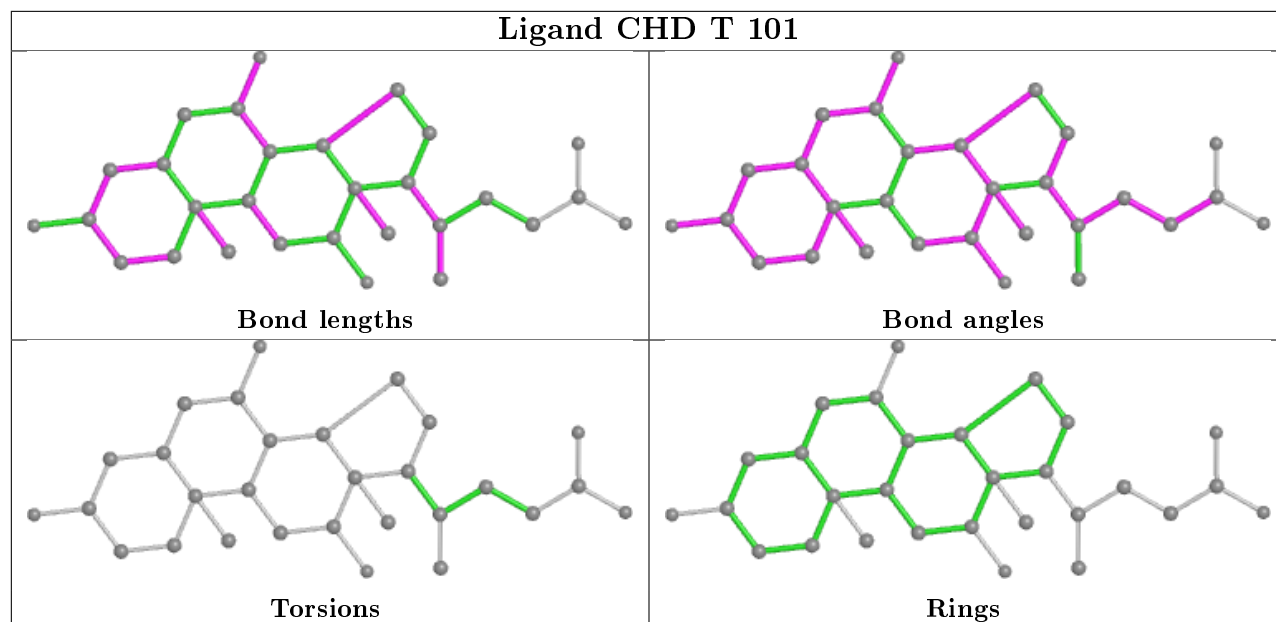
Ligand DMU C 309**Ligand PGV C 308**

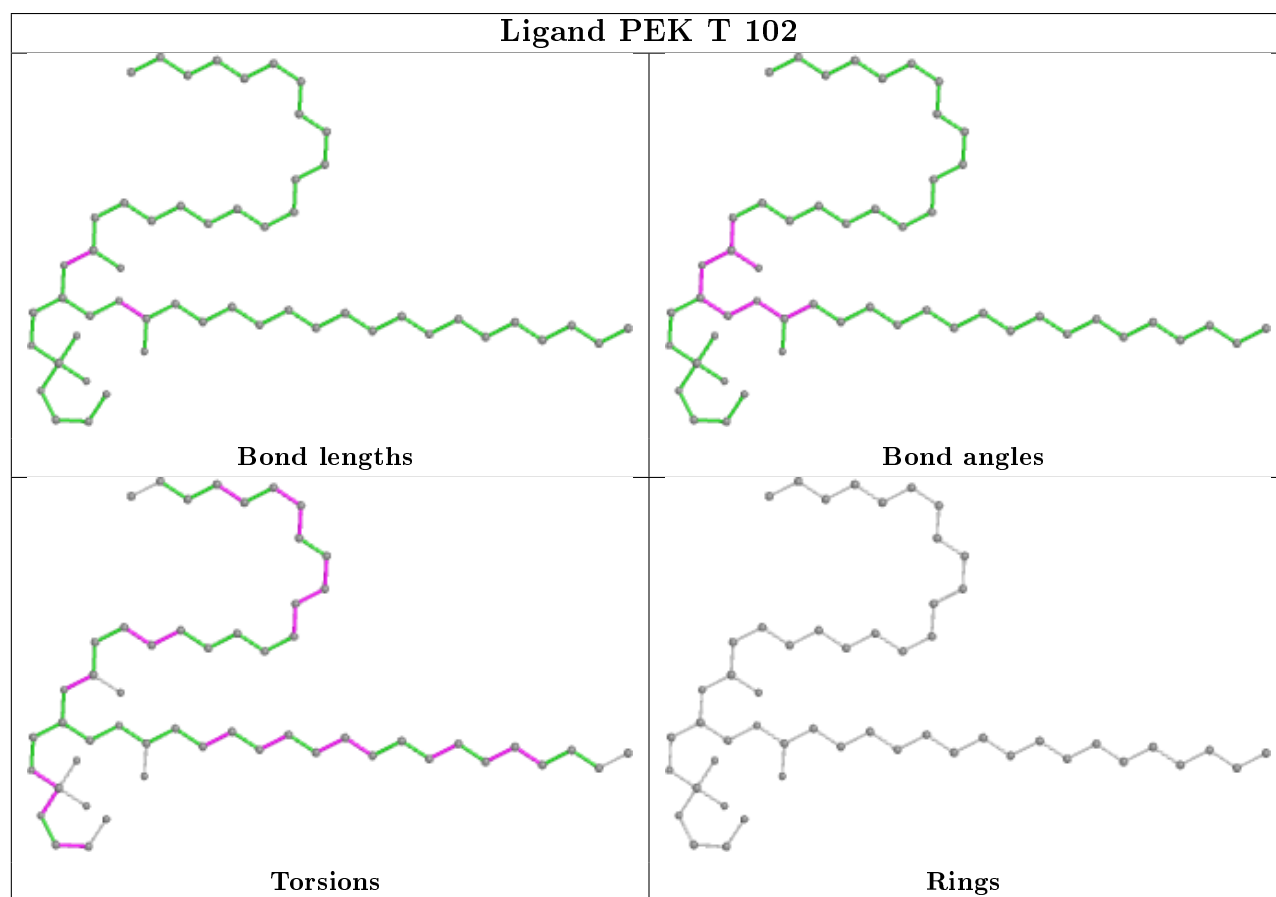
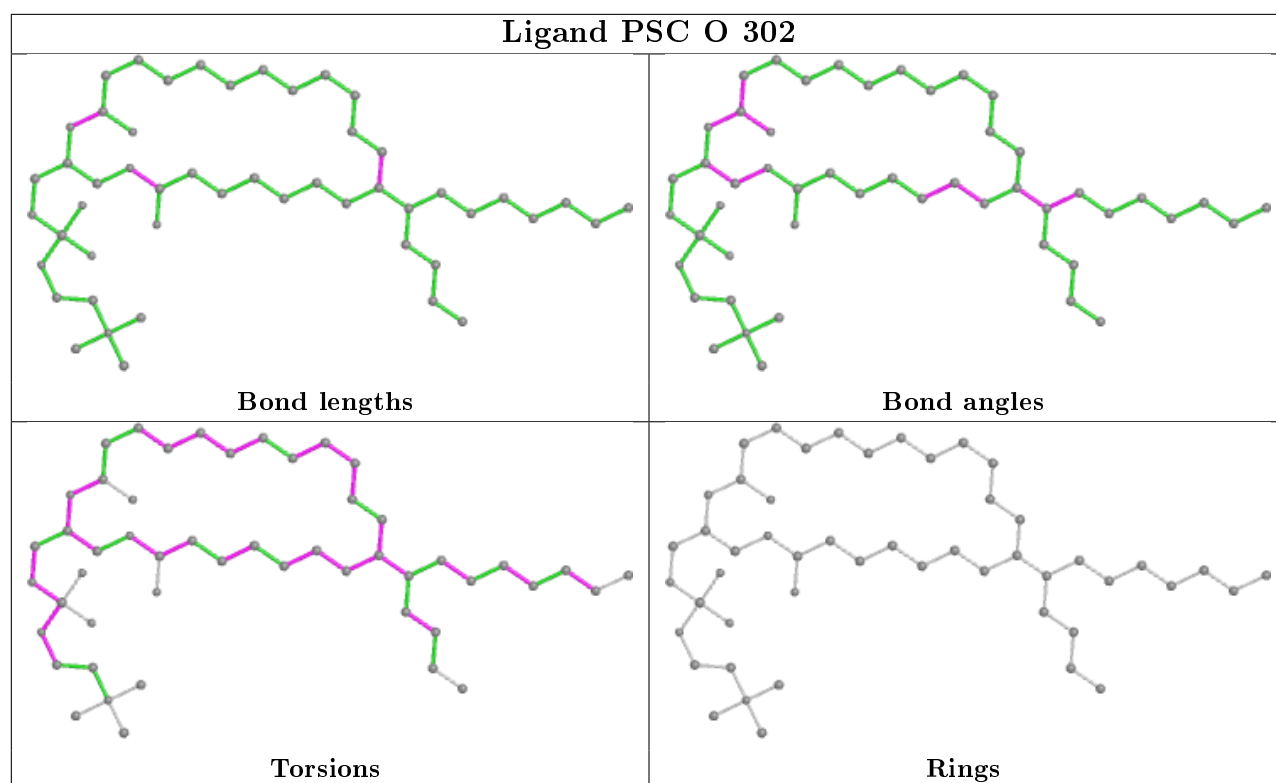


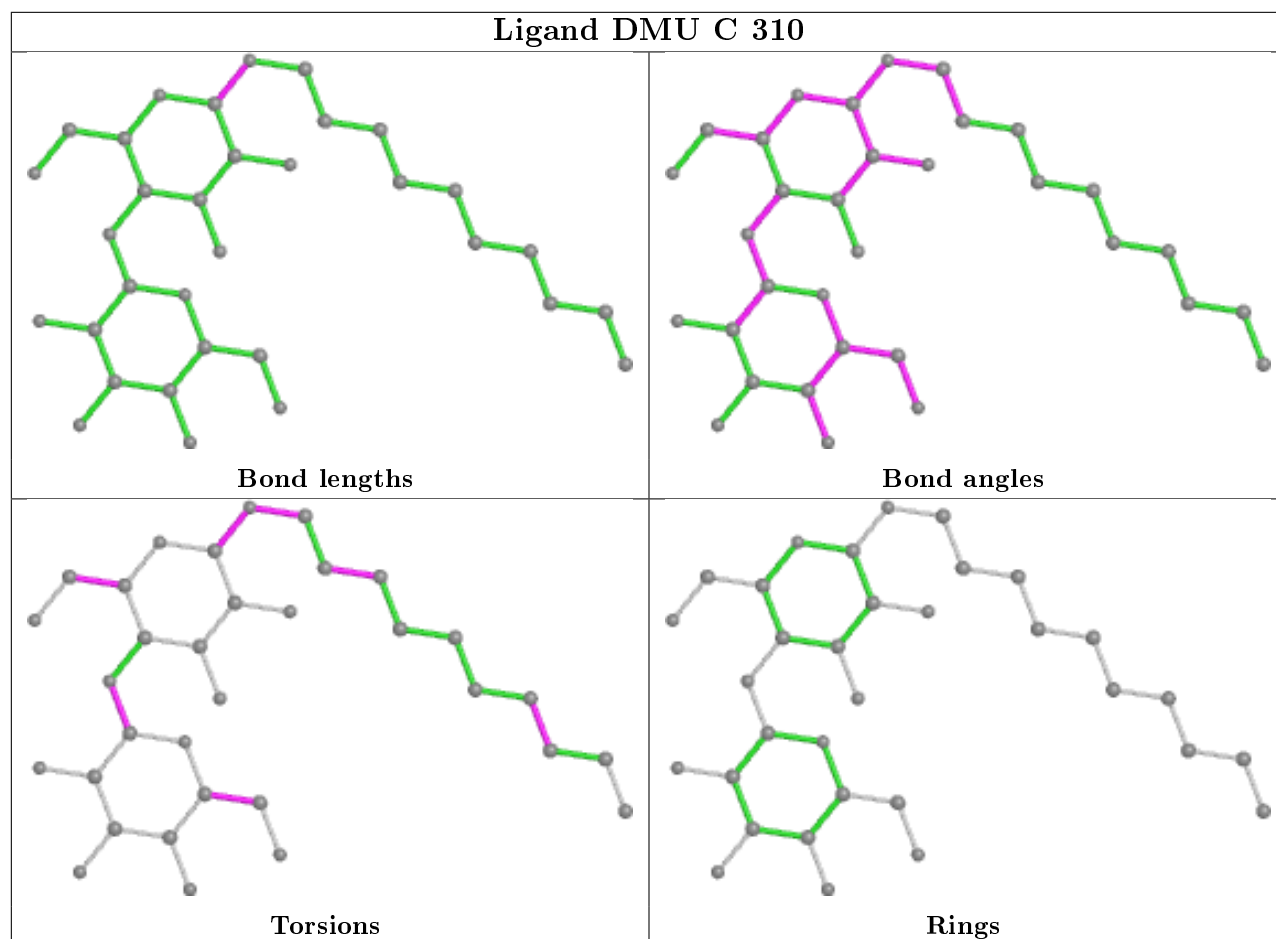
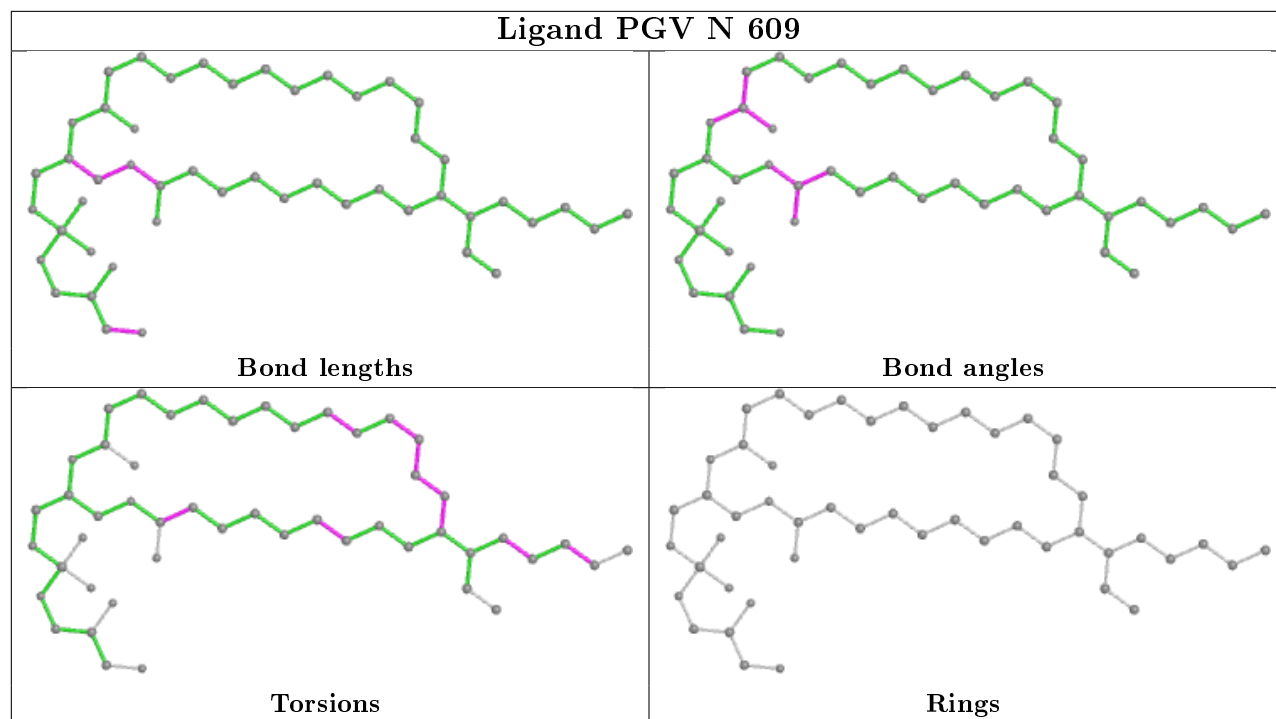


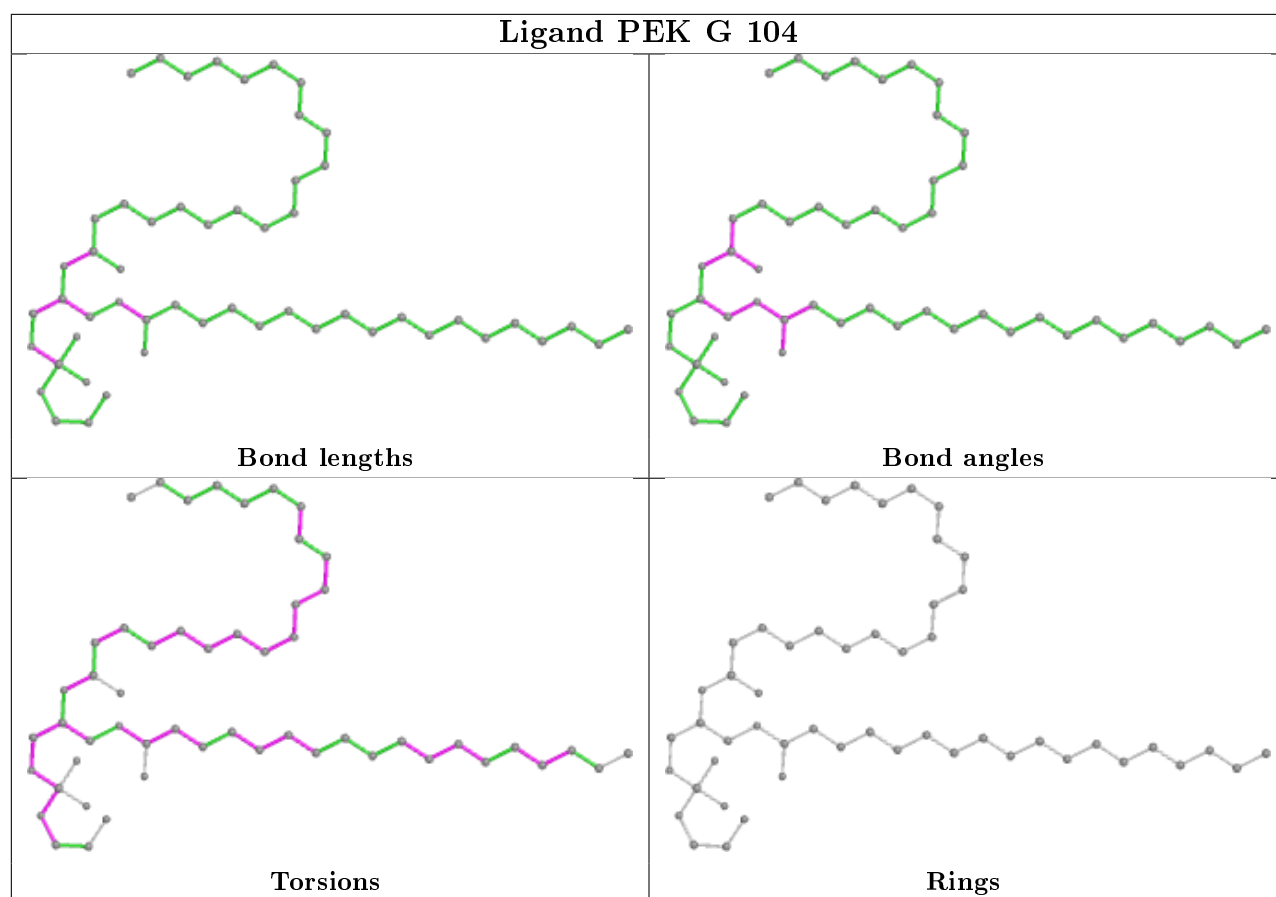




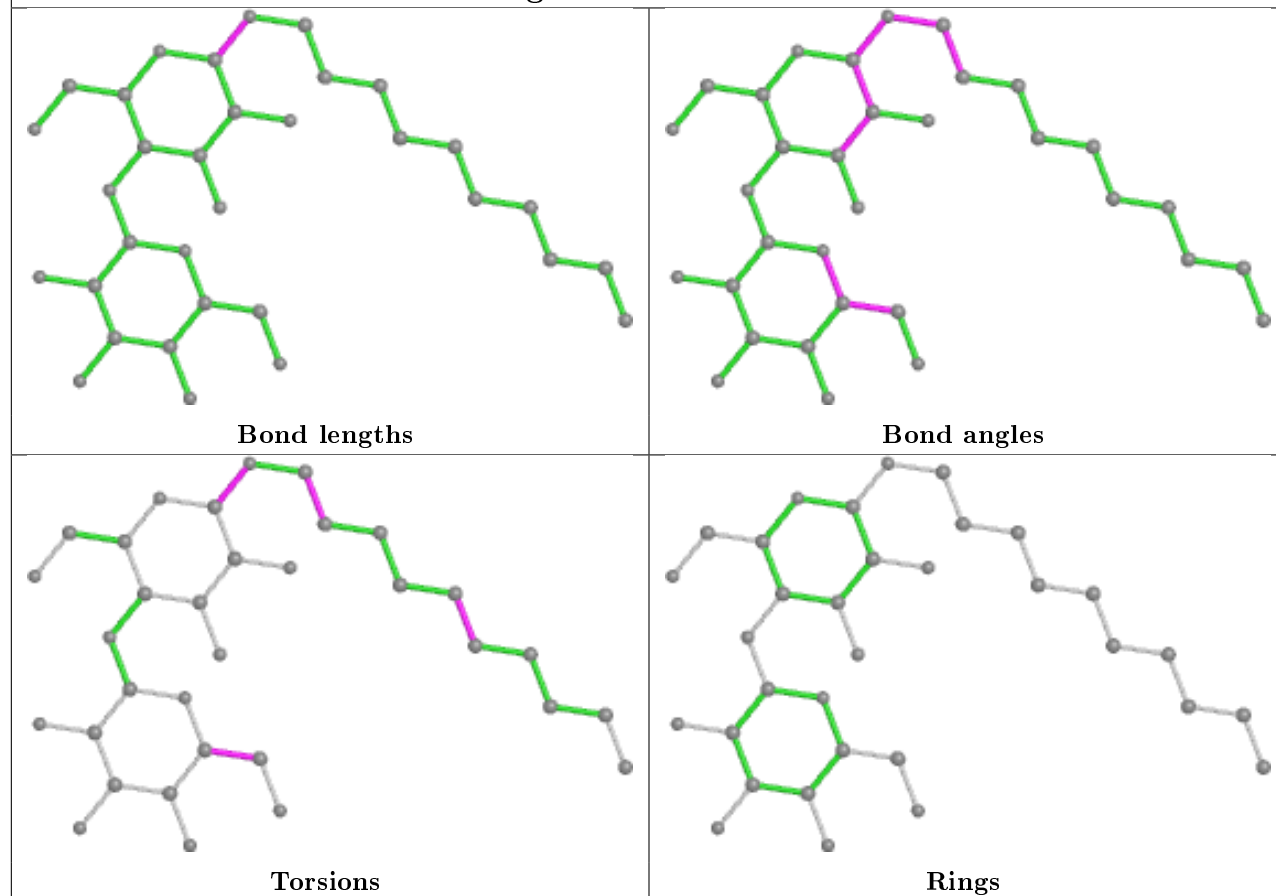




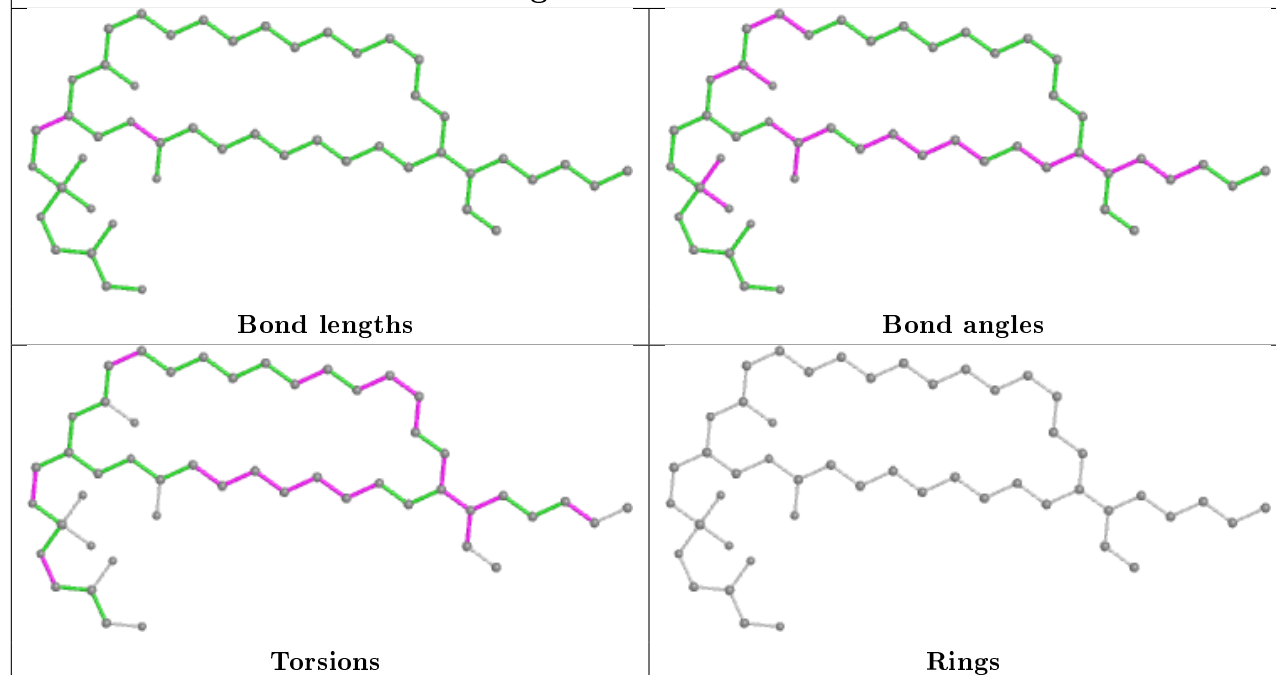


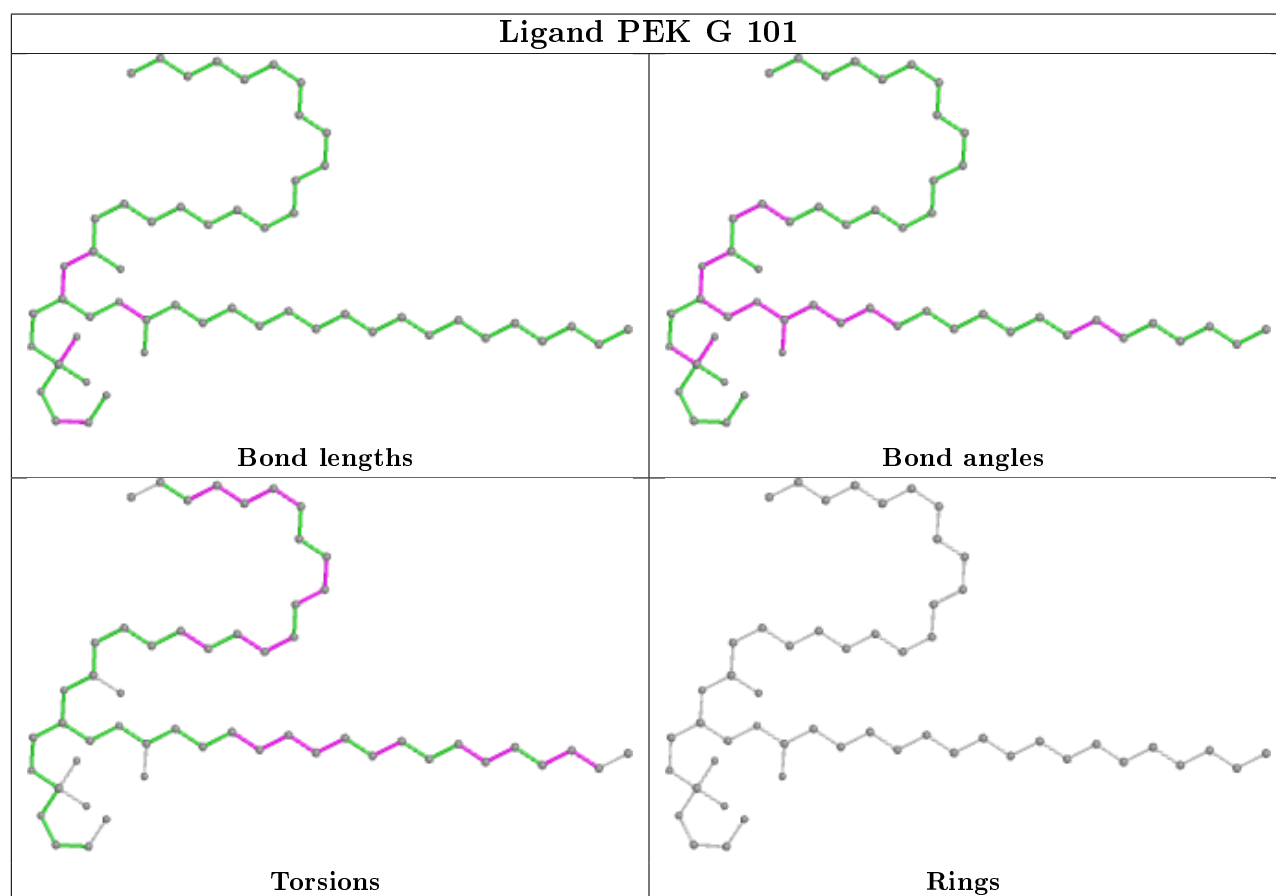
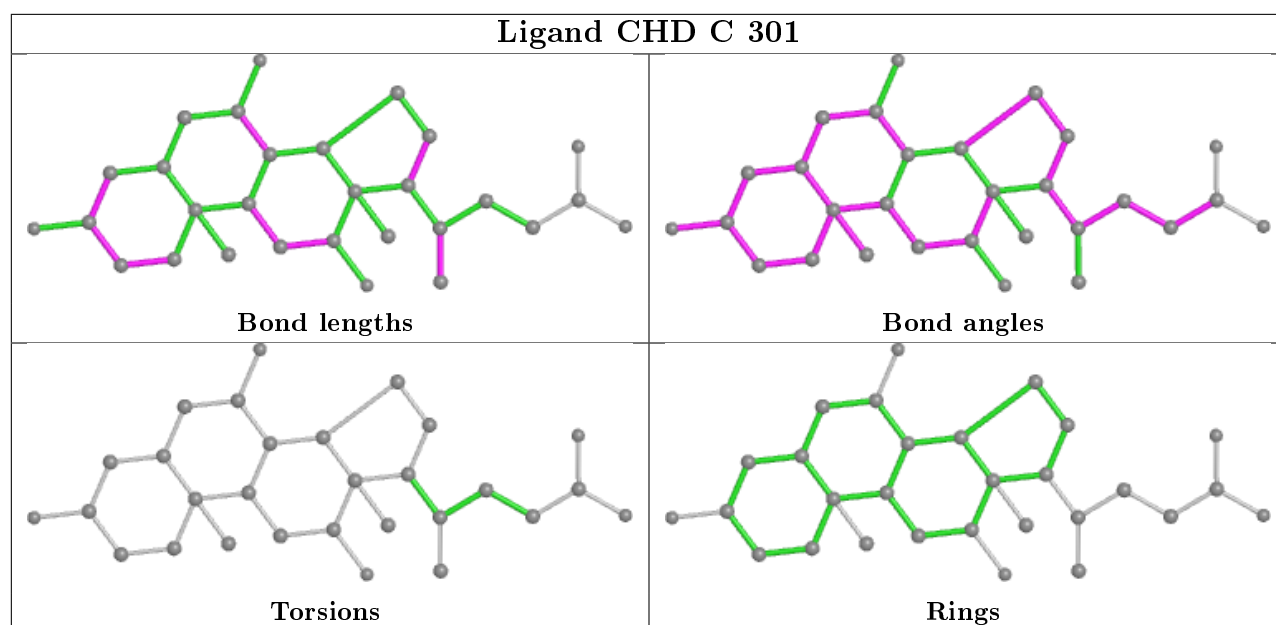


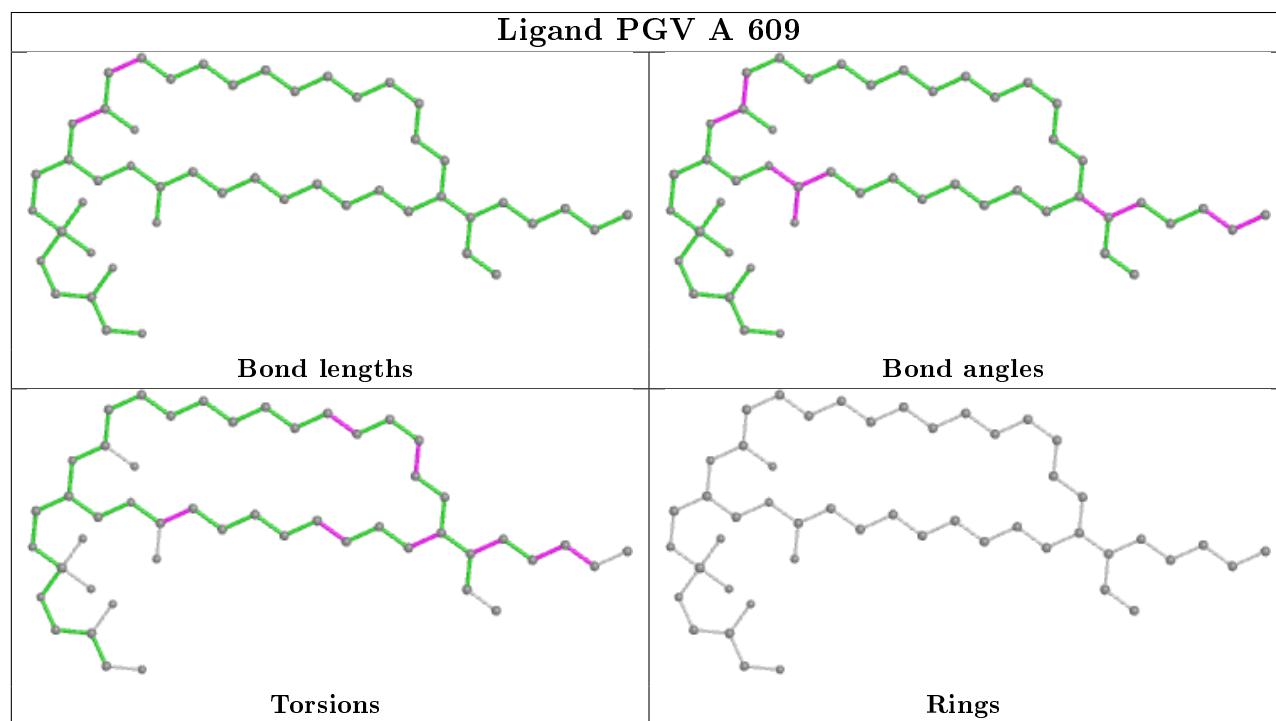
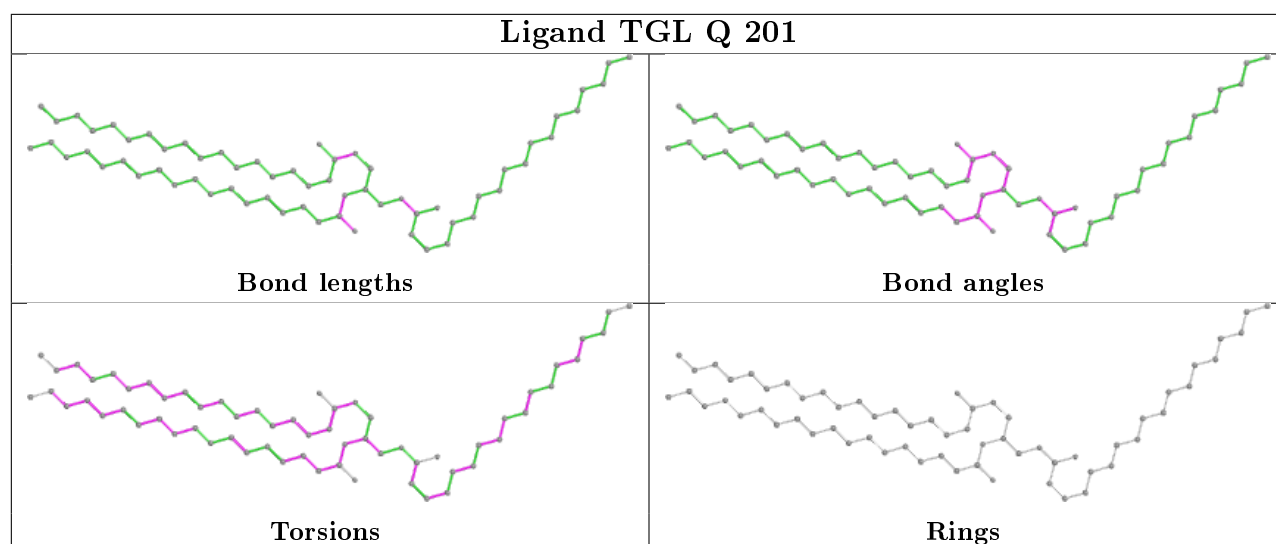
Ligand DMU P 308

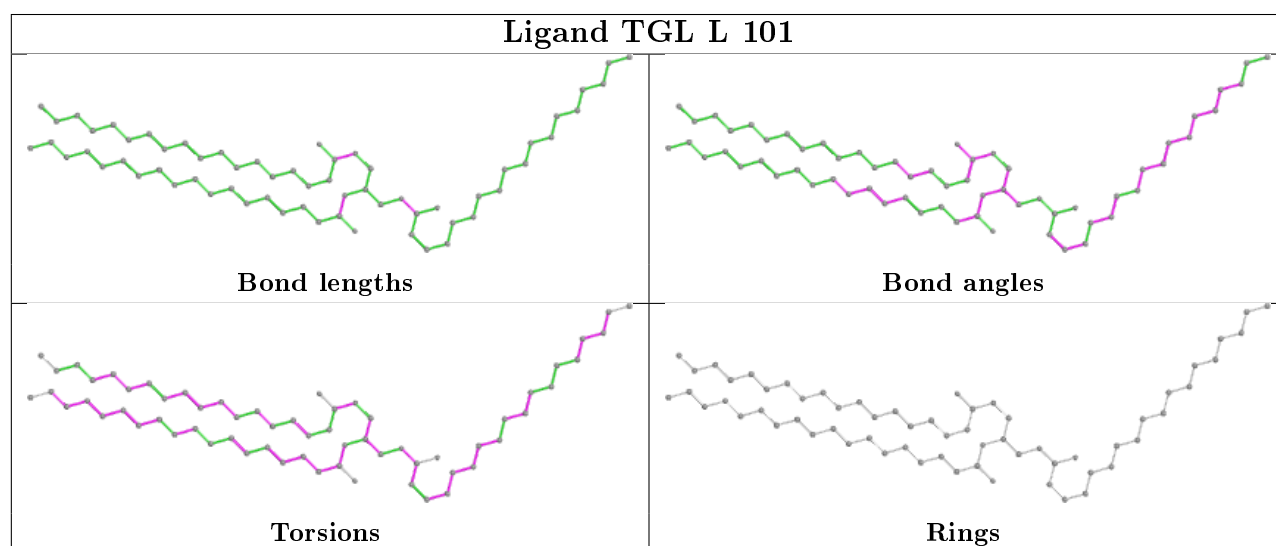
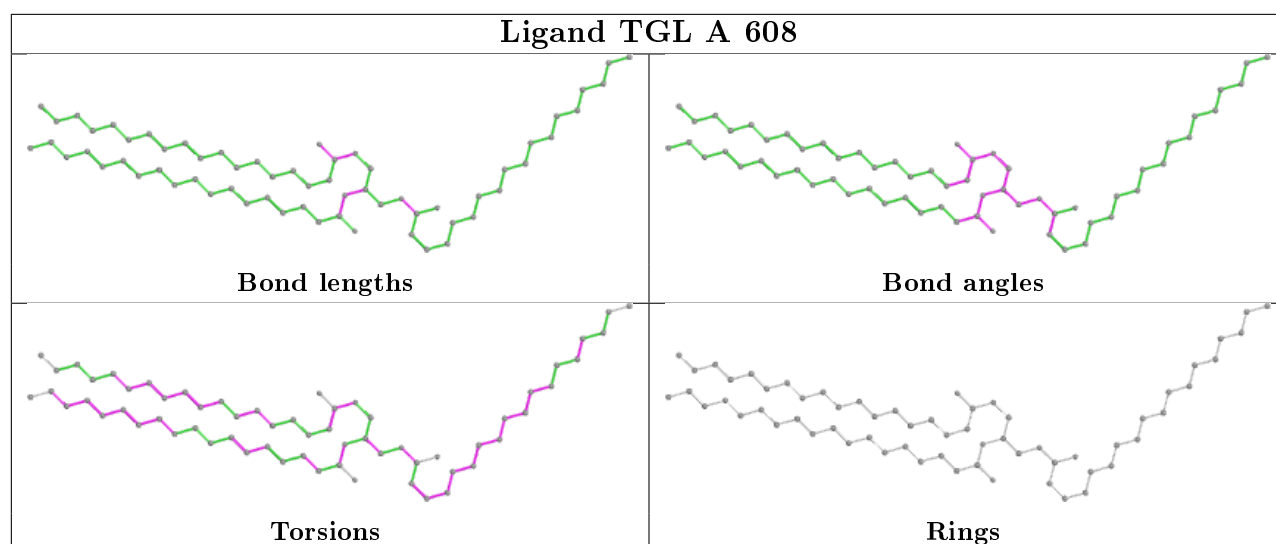


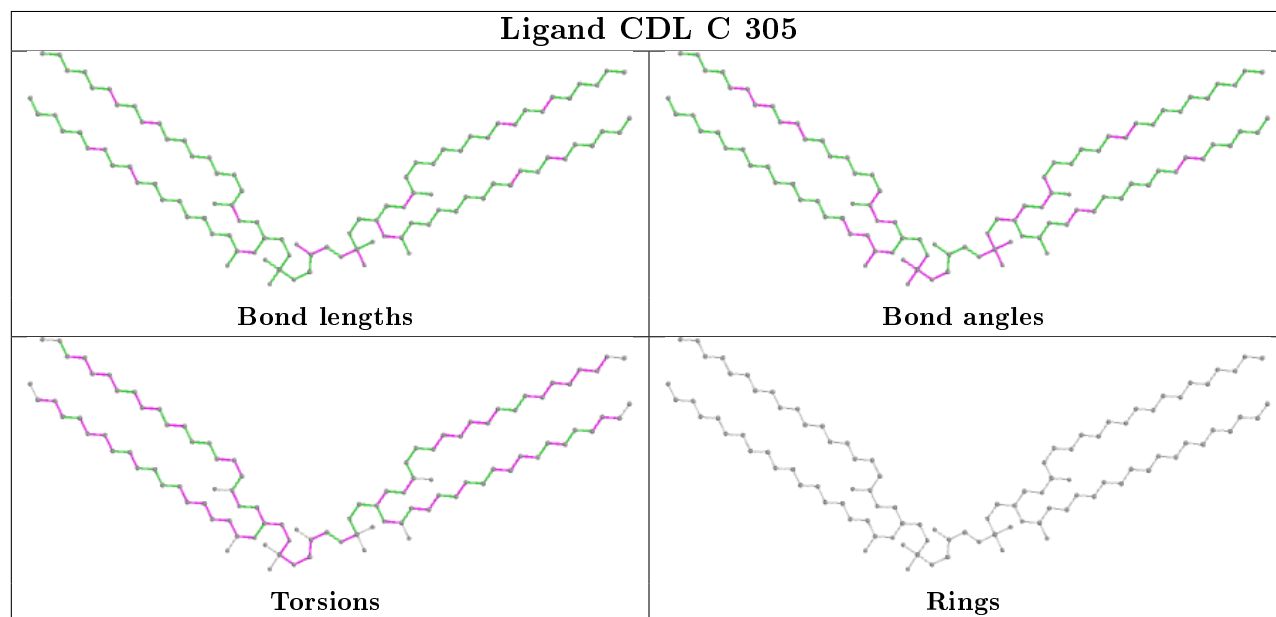
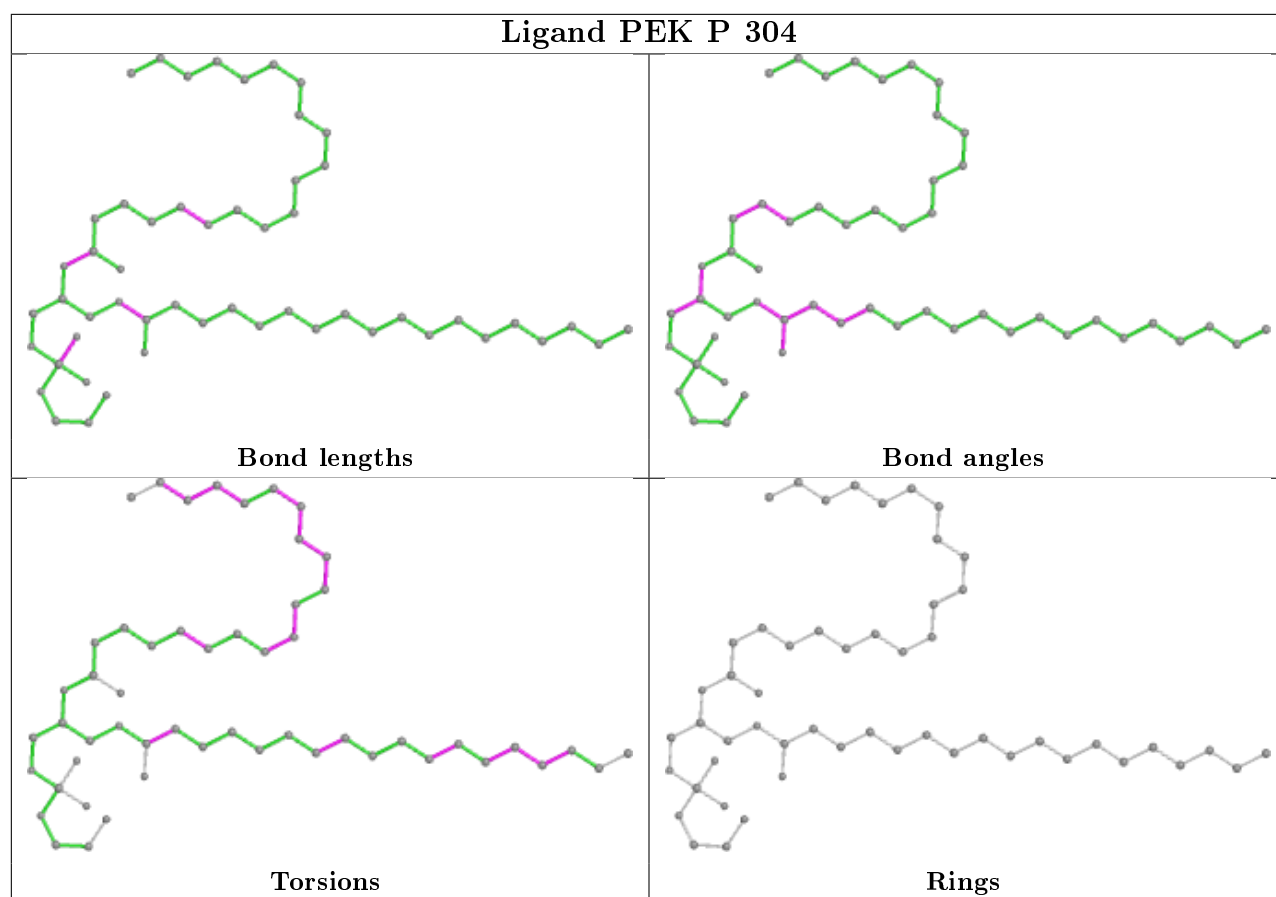
Ligand PGV C 304

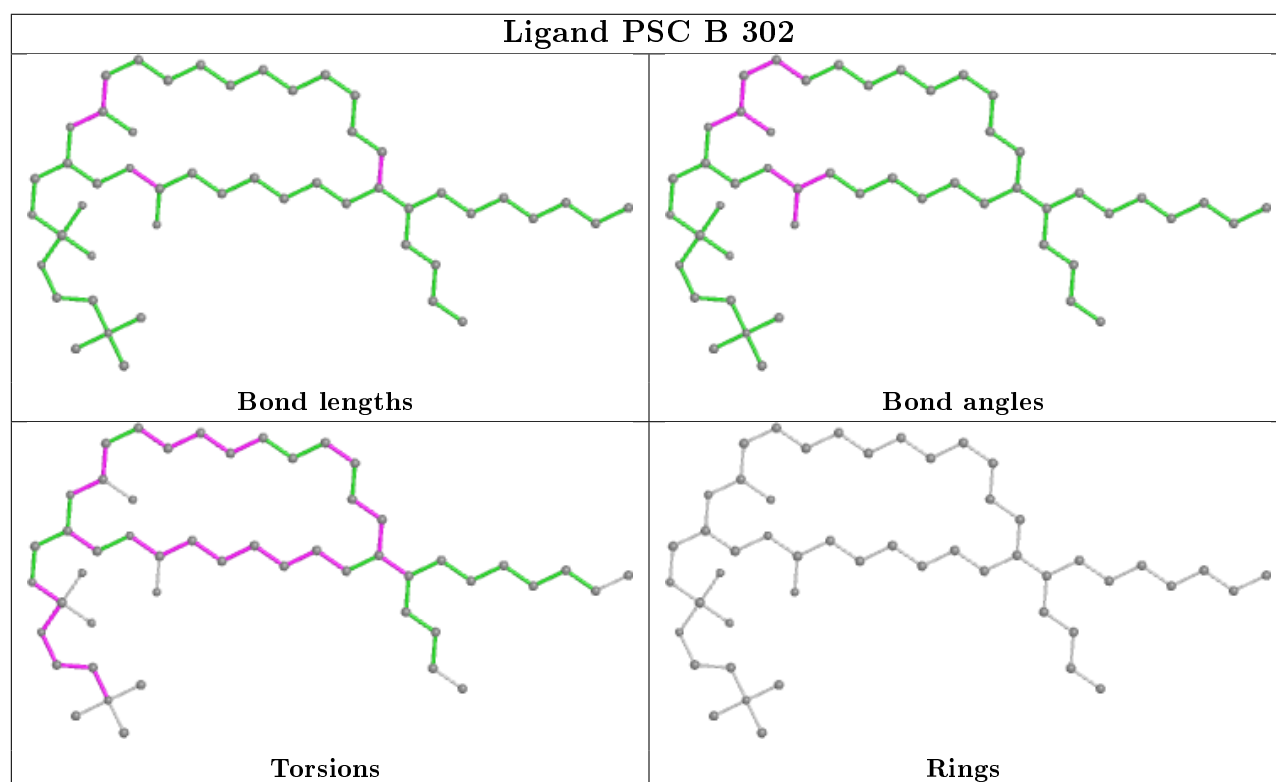
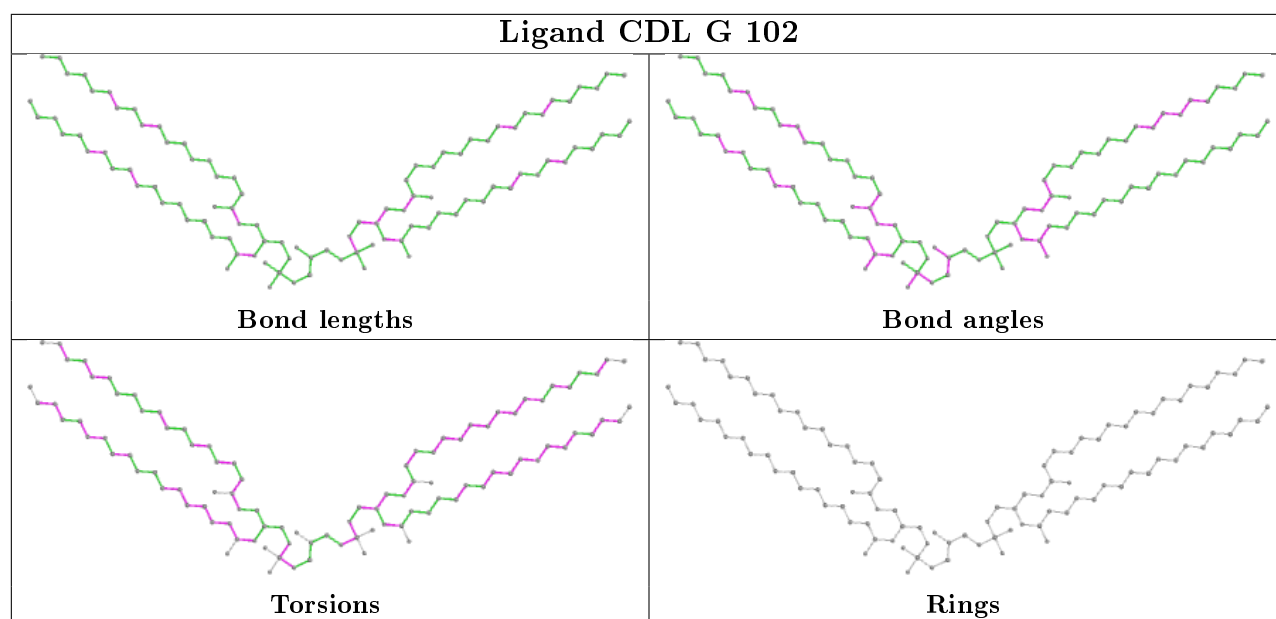


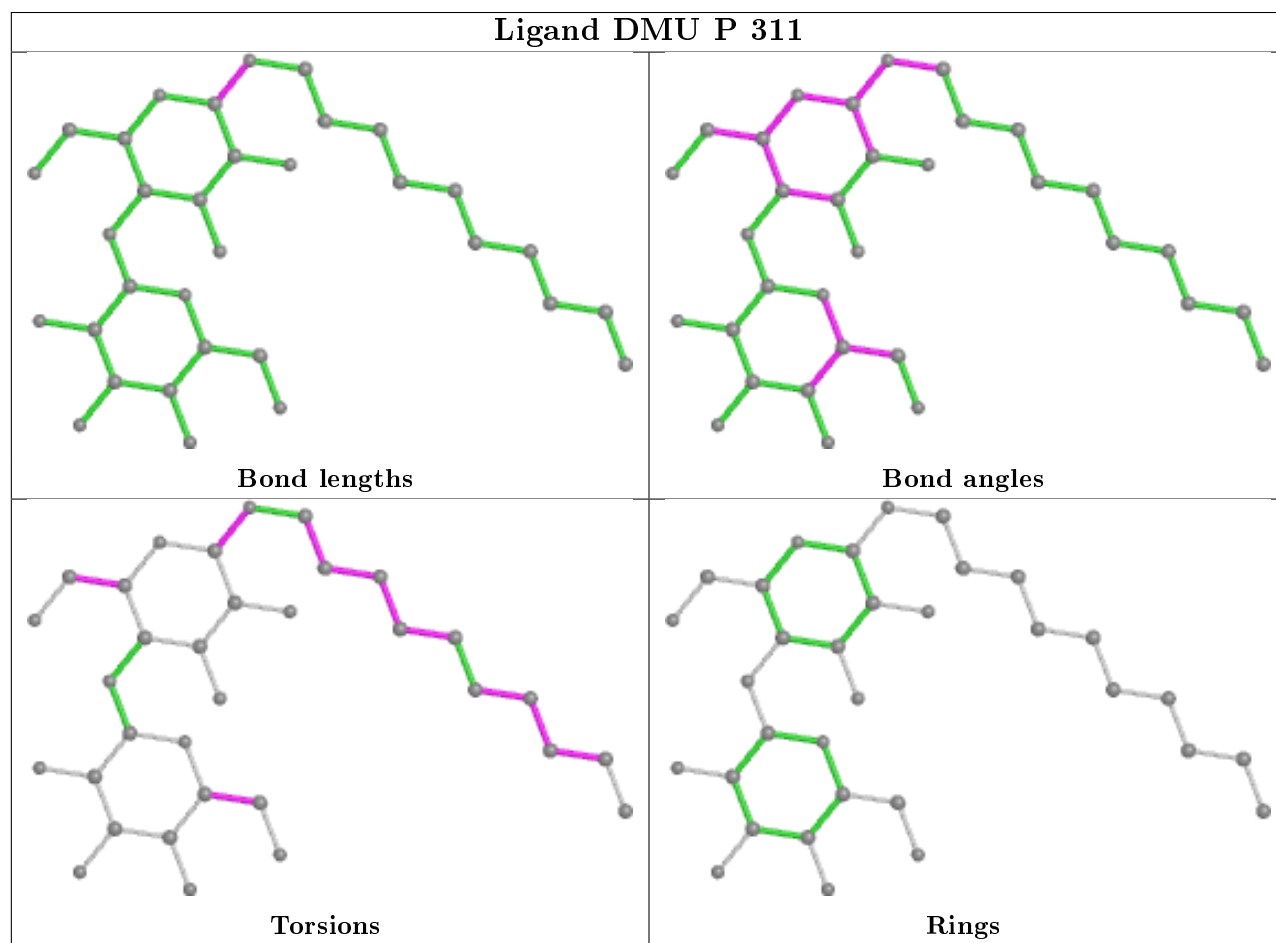
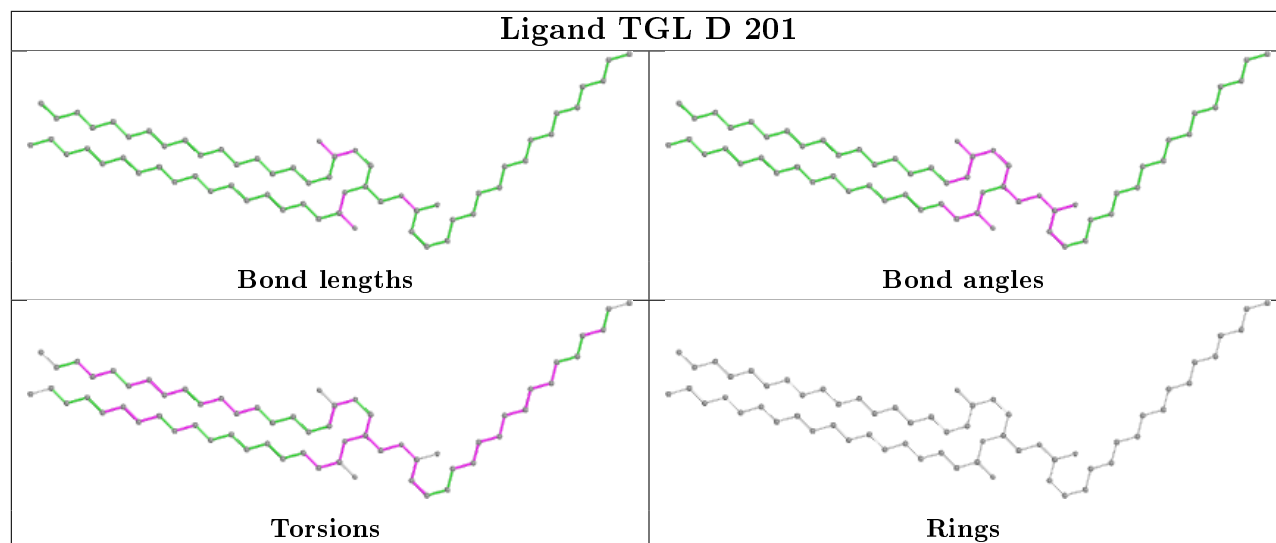


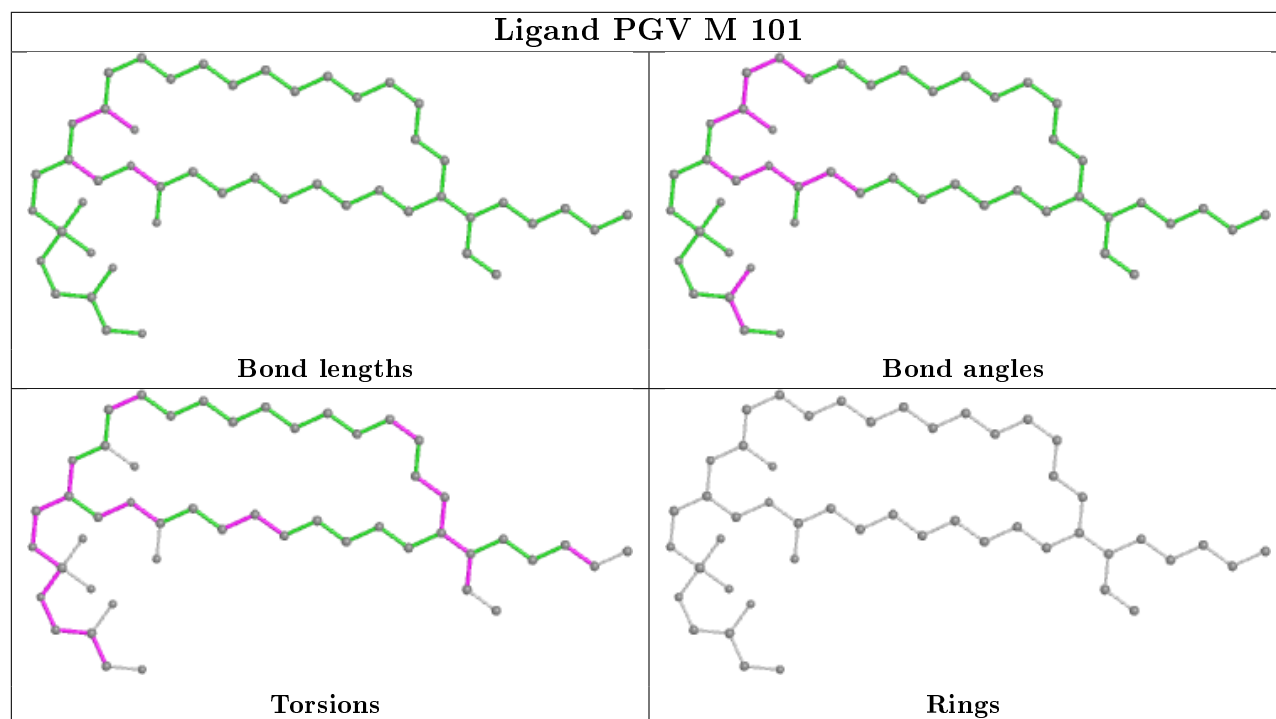
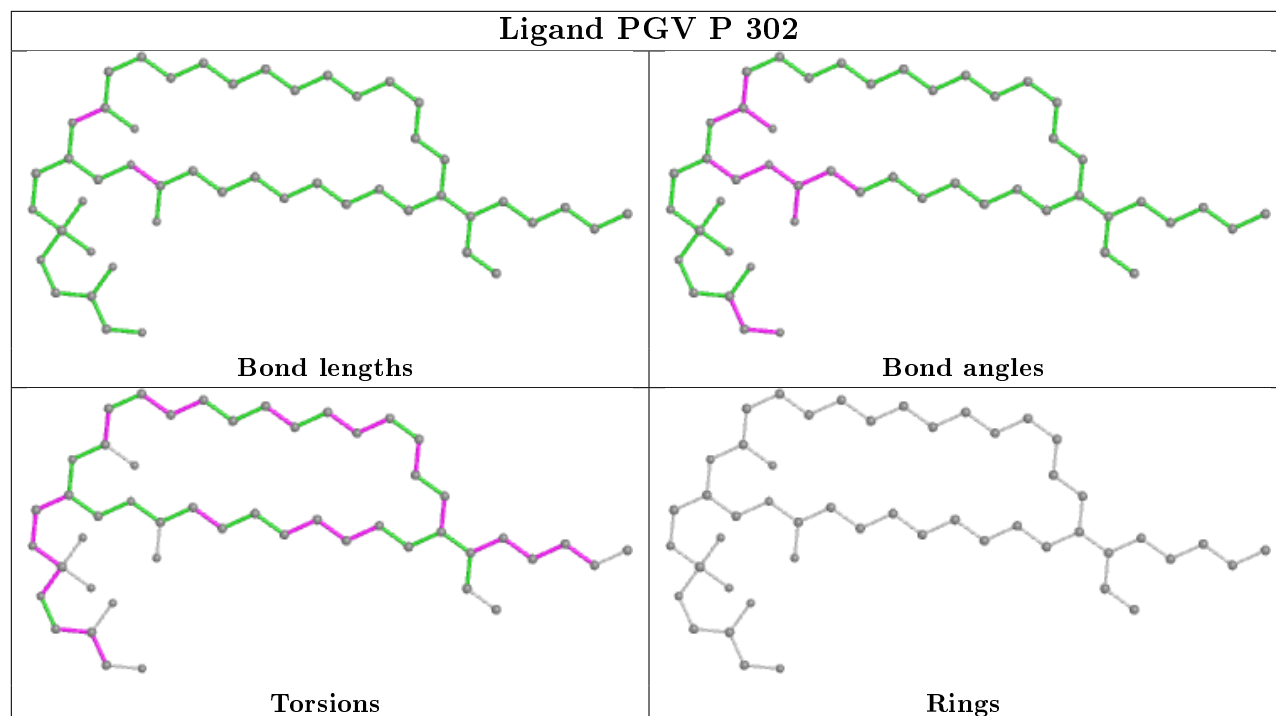


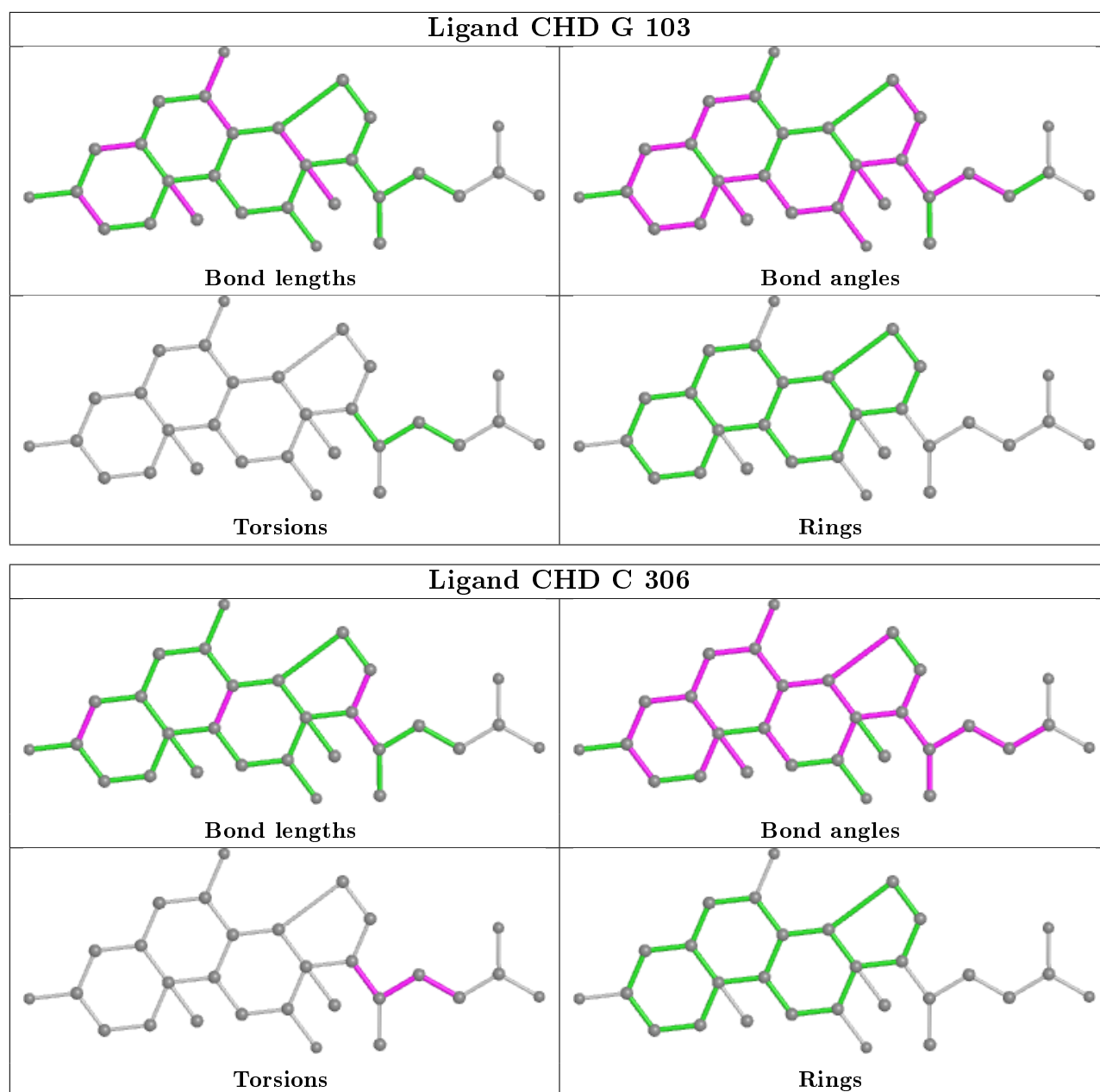


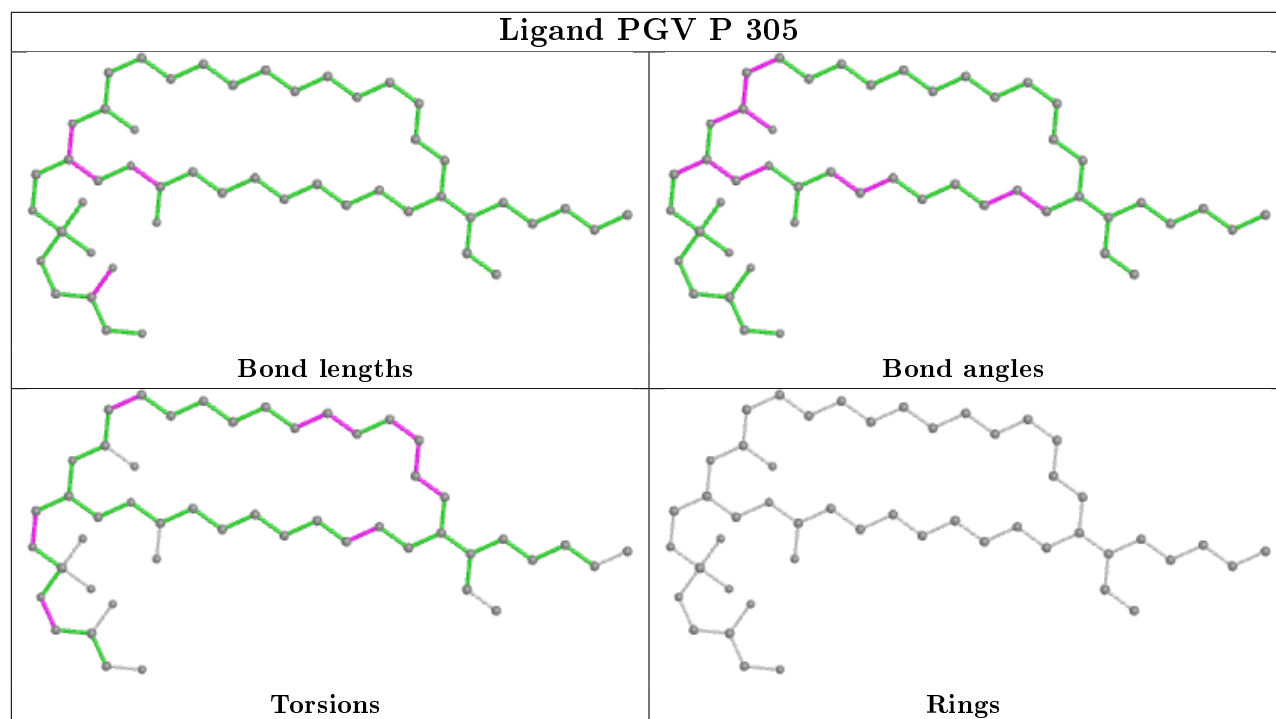
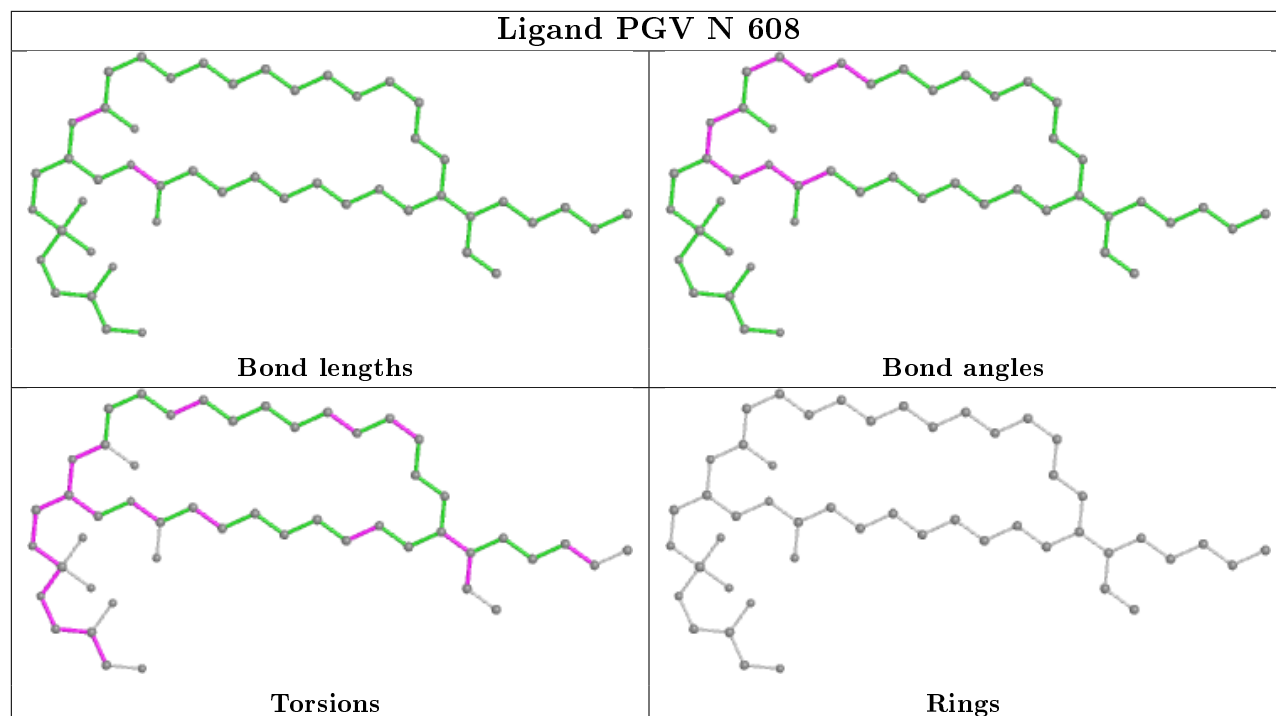


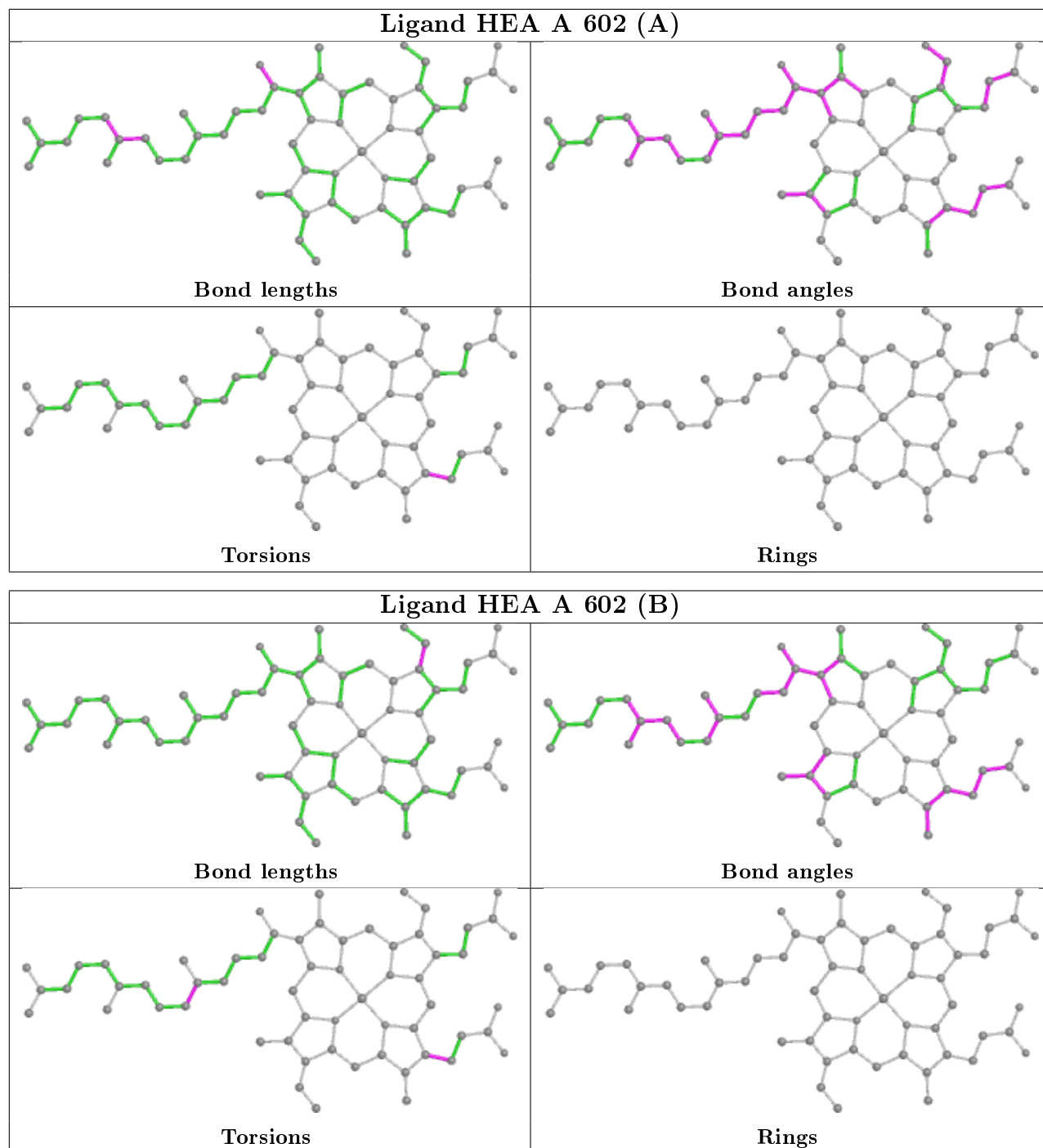


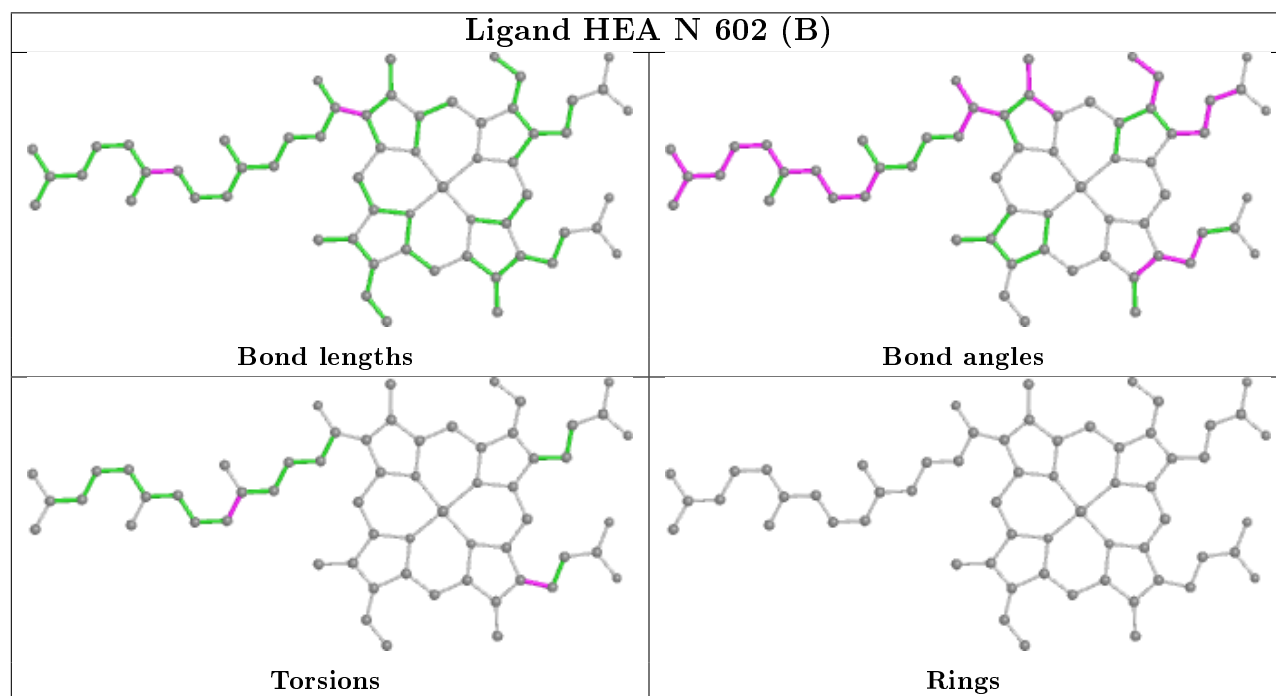
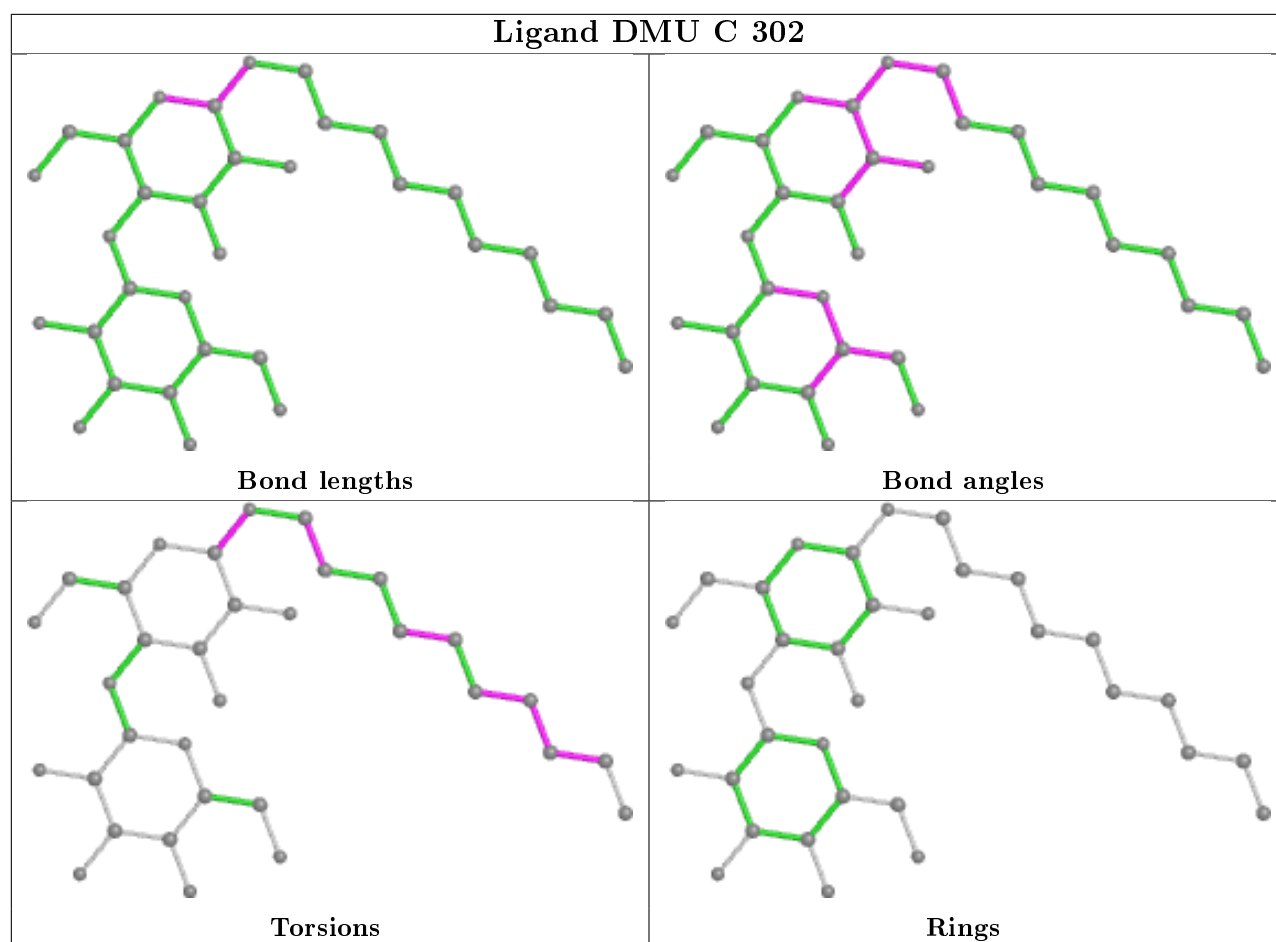


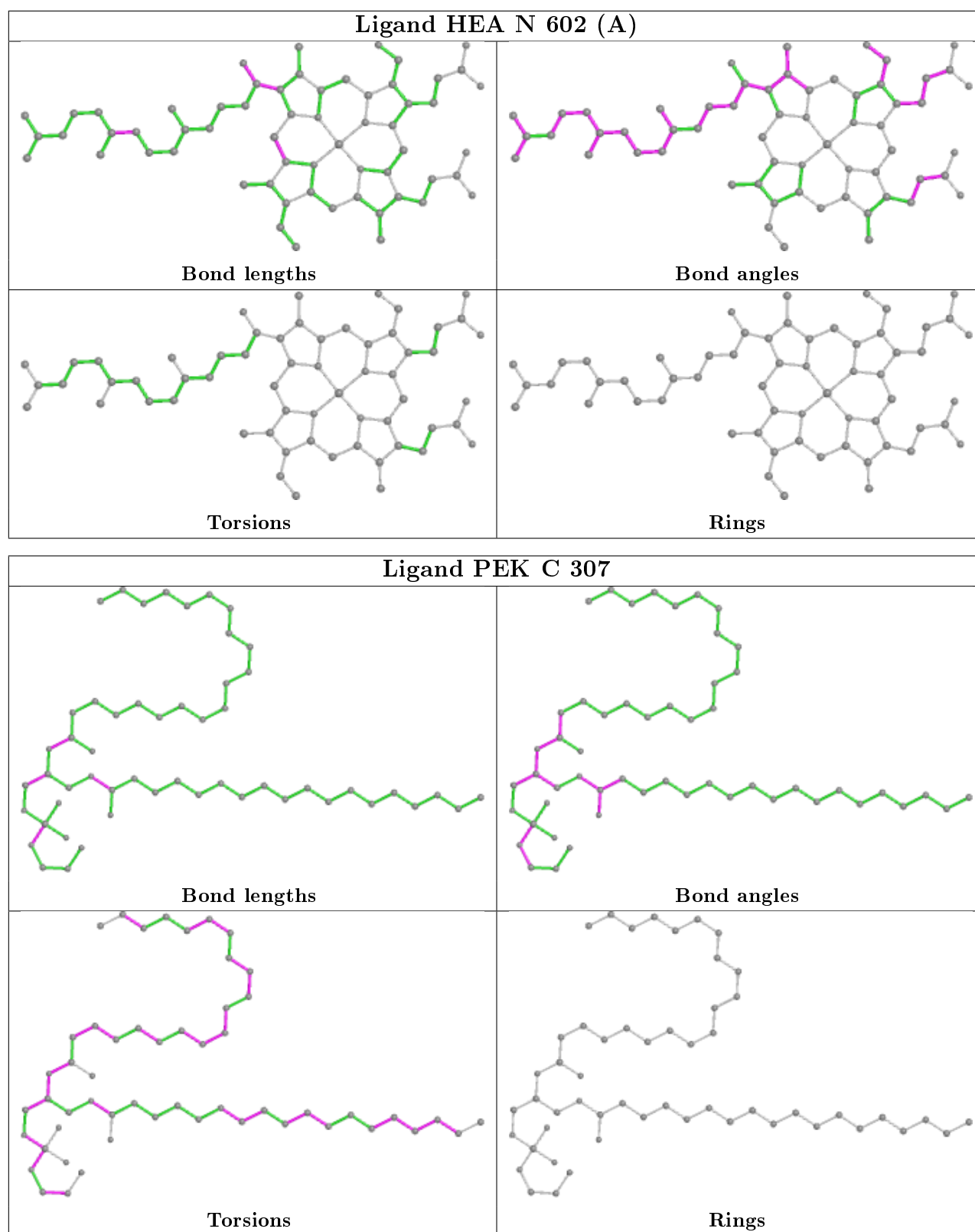


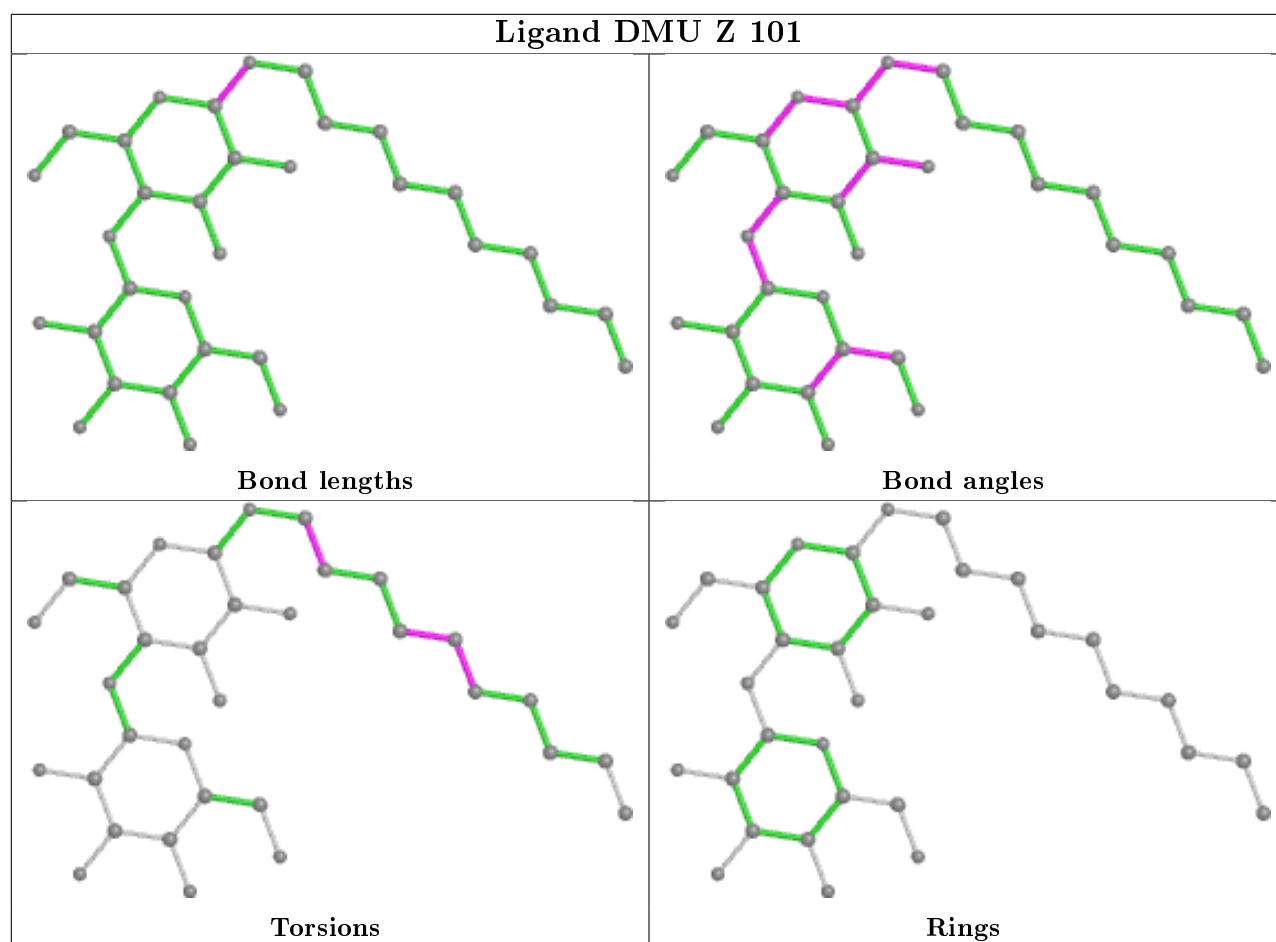












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	0.04	0 100 100	20, 25, 33, 69	0
1	N	513/514 (99%)	-0.09	1 (0%) 95 94	22, 30, 40, 72	0
2	B	226/227 (99%)	-0.04	3 (1%) 77 78	23, 33, 53, 77	0
2	O	226/227 (99%)	-0.02	3 (1%) 77 78	29, 40, 65, 85	0
3	C	259/261 (99%)	-0.03	0 100 100	22, 29, 41, 79	0
3	P	259/261 (99%)	-0.05	3 (1%) 79 79	24, 30, 42, 65	0
4	D	144/147 (97%)	-0.16	2 (1%) 75 76	25, 34, 55, 77	0
4	Q	144/147 (97%)	0.46	9 (6%) 20 19	35, 48, 74, 125	0
5	E	105/109 (96%)	-0.17	2 (1%) 66 66	26, 33, 57, 116	0
5	R	105/109 (96%)	-0.13	2 (1%) 66 66	32, 41, 60, 113	0
6	F	98/98 (100%)	0.36	7 (7%) 16 15	25, 37, 93, 130	0
6	S	98/98 (100%)	0.54	8 (8%) 11 11	25, 37, 91, 133	0
7	G	83/85 (97%)	0.87	14 (16%) 1 1	28, 38, 109, 137	0
7	T	83/85 (97%)	0.85	16 (19%) 1 1	27, 40, 97, 133	0
8	H	79/85 (92%)	0.23	7 (8%) 9 9	30, 41, 90, 95	0
8	U	79/85 (92%)	0.41	6 (7%) 13 13	35, 45, 96, 124	0
9	I	72/73 (98%)	0.36	5 (6%) 16 16	31, 44, 75, 89	0
9	V	72/73 (98%)	0.45	5 (6%) 16 16	31, 53, 77, 99	0
10	J	58/59 (98%)	0.29	4 (6%) 16 16	29, 39, 65, 120	0
10	W	58/59 (98%)	0.21	2 (3%) 45 42	33, 44, 70, 110	0
11	K	49/56 (87%)	-0.04	0 100 100	33, 40, 55, 60	0
11	X	49/56 (87%)	0.35	4 (8%) 11 11	42, 50, 70, 78	0
12	L	46/47 (97%)	-0.01	1 (2%) 62 61	26, 32, 50, 85	0
12	Y	46/47 (97%)	0.04	1 (2%) 62 61	33, 41, 58, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.10	1 (2%) 60 59	27, 31, 66, 101	0
13	Z	43/46 (93%)	0.42	4 (9%) 8 8	39, 44, 76, 115	0
All	All	3550/3614 (98%)	0.10	110 (3%) 49 47	20, 34, 66, 137	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	16.0
7	G	10	GLY	15.2
4	Q	6	VAL	13.4
6	S	1	ALA	12.6
4	Q	5	VAL	10.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.27	0.44	113,119,130,131	0
7	TPO	G	11	11/12	0.36	0.39	91,100,118,123	0
7	TPO	T	11	11/12	0.37	0.43	104,118,157,157	0
9	SAC	I	1	9/10	0.84	0.25	64,73,78,78	0
1	FME	A	1	10/11	0.96	0.12	36,45,72,87	0
1	FME	N	1	10/11	0.97	0.13	41,50,72,76	0
2	FME	O	1	10/11	0.98	0.11	37,39,48,60	0
2	FME	B	1	10/11	0.99	0.13	29,30,41,66	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	EDO	C	318	4/4	0.45	0.83	74,101,105,116	0
21	EDO	Q	204	4/4	0.61	0.21	64,68,71,77	0
28	PEK	T	102	53/53	0.66	0.34	52,89,154,154	0
21	EDO	D	204	4/4	0.66	0.42	59,71,80,85	0
27	CDL	T	103	100/100	0.68	0.24	52,89,137,160	0
27	CDL	G	102	100/100	0.70	0.25	53,89,128,159	0
28	PEK	C	307	53/53	0.70	0.27	47,77,139,164	0
27	CDL	P	306	100/100	0.71	0.28	39,84,113,122	0
23	PSC	B	302	52/52	0.71	0.27	40,78,152,157	0
28	PEK	P	309	53/53	0.74	0.28	42,74,121,135	0
28	PEK	G	104	53/53	0.75	0.26	48,77,135,152	0
19	TGL	Q	201	63/63	0.75	0.21	48,73,95,107	0
20	PGV	C	308	51/51	0.76	0.23	44,78,123,132	0
21	EDO	Q	203	4/4	0.76	0.27	52,54,57,67	0
21	EDO	S	103	4/4	0.76	0.29	61,68,69,70	0
25	DMU	C	302	33/33	0.77	0.28	32,72,98,105	0
23	PSC	O	302	52/52	0.77	0.27	42,78,156,162	0
21	EDO	N	611	4/4	0.78	0.18	65,65,66,69	0
21	EDO	C	317	4/4	0.78	0.39	59,74,76,85	0
25	DMU	C	309	33/33	0.78	0.24	55,75,100,104	0
21	EDO	C	312	4/4	0.78	0.14	79,82,85,92	0
25	DMU	C	310	33/33	0.78	0.22	53,80,105,115	0
25	DMU	P	308	33/33	0.78	0.30	45,74,113,121	0
25	DMU	P	310	33/33	0.79	0.24	59,76,103,104	0
25	DMU	P	311	33/33	0.79	0.21	62,82,105,108	0
27	CDL	C	305	100/100	0.80	0.23	37,77,110,115	0
19	TGL	Y	101	63/63	0.80	0.23	41,74,110,136	0
24	CHD	P	307	29/29	0.81	0.25	53,67,73,77	0
20	PGV	P	302	51/51	0.82	0.23	48,76,122,137	0
19	TGL	D	201	63/63	0.83	0.18	33,61,85,90	0
24	CHD	C	306	29/29	0.83	0.28	49,64,71,73	0
21	EDO	A	616	4/4	0.83	0.21	47,50,53,66	0
20	PGV	N	608	51/51	0.83	0.26	47,78,115,127	0
19	TGL	L	101	63/63	0.83	0.21	32,59,93,112	0
21	EDO	R	204	4/4	0.84	0.35	52,55,58,60	0
21	EDO	A	619	4/4	0.84	0.19	55,58,58,60	0
21	EDO	C	314	4/4	0.84	0.25	55,65,65,66	0
21	EDO	O	305	4/4	0.84	0.14	72,74,75,82	0
20	PGV	M	101	51/51	0.84	0.23	31,63,99,110	0
25	DMU	Z	101	33/33	0.84	0.17	47,56,73,77	0
21	EDO	N	618	4/4	0.85	0.23	42,43,51,55	0
19	TGL	N	610	63/63	0.86	0.19	48,74,101,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	EDO	A	615	4/4	0.86	0.17	41,42,45,45	0
21	EDO	C	315	4/4	0.86	0.17	35,45,47,50	0
21	EDO	A	611	4/4	0.87	0.17	46,60,61,62	0
21	EDO	G	105	4/4	0.87	0.34	51,62,74,87	0
21	EDO	C	313	4/4	0.87	0.16	56,60,64,81	0
25	DMU	M	102	33/33	0.88	0.12	39,47,56,66	0
21	EDO	C	316	4/4	0.88	0.17	61,63,71,83	0
19	TGL	A	608	63/63	0.89	0.17	40,74,96,112	0
21	EDO	P	315	4/4	0.89	0.26	46,54,57,72	0
21	EDO	E	203	4/4	0.89	0.25	48,52,54,60	0
21	EDO	U	101	4/4	0.89	0.14	62,65,66,72	0
21	EDO	A	617	4/4	0.90	0.29	44,66,70,75	0
26	UNX	C	303	1/1	0.90	0.14	30,30,30,30	0
21	EDO	H	101	4/4	0.90	0.12	51,57,59,66	0
26	UNX	P	303	1/1	0.91	0.18	29,29,29,29	0
21	EDO	D	203	4/4	0.91	0.28	54,54,66,72	0
21	EDO	O	304	4/4	0.91	0.22	61,62,65,76	0
21	EDO	V	101	4/4	0.91	0.22	63,67,68,70	0
21	EDO	A	613	4/4	0.92	0.17	59,63,69,80	0
21	EDO	D	202	4/4	0.92	0.48	39,45,50,65	0
21	EDO	P	312	4/4	0.92	0.13	32,33,45,52	0
21	EDO	D	206	4/4	0.92	0.17	49,59,60,73	0
21	EDO	N	614	4/4	0.92	0.17	58,61,62,72	0
21	EDO	R	201	4/4	0.92	0.18	56,62,64,83	0
21	EDO	R	205	4/4	0.92	0.19	42,49,53,53	0
21	EDO	R	202	4/4	0.92	0.17	49,58,63,63	0
21	EDO	E	201	4/4	0.93	0.11	41,41,47,56	0
21	EDO	P	314	4/4	0.93	0.26	48,56,63,65	0
21	EDO	A	614	4/4	0.93	0.17	19,25,27,39	0
21	EDO	F	104	4/4	0.93	0.25	47,48,53,55	0
21	EDO	N	612	4/4	0.93	0.24	30,37,45,57	0
21	EDO	N	621	4/4	0.94	0.17	40,45,52,57	0
21	EDO	S	104	4/4	0.94	0.23	39,54,65,66	0
21	EDO	E	205	4/4	0.94	0.13	52,55,58,67	0
21	EDO	R	203	4/4	0.95	0.09	44,44,46,46	0
28	PEK	P	304	53/53	0.95	0.14	29,47,85,94	0
24	CHD	C	301	29/29	0.95	0.09	27,31,34,38	0
21	EDO	A	620	4/4	0.95	0.34	45,45,48,65	0
21	EDO	A	618	4/4	0.95	0.43	43,51,65,69	0
21	EDO	N	617	4/4	0.95	0.13	41,42,44,52	0
21	EDO	Q	202	4/4	0.95	0.12	58,58,64,64	0
21	EDO	N	615	4/4	0.95	0.11	33,33,39,43	0

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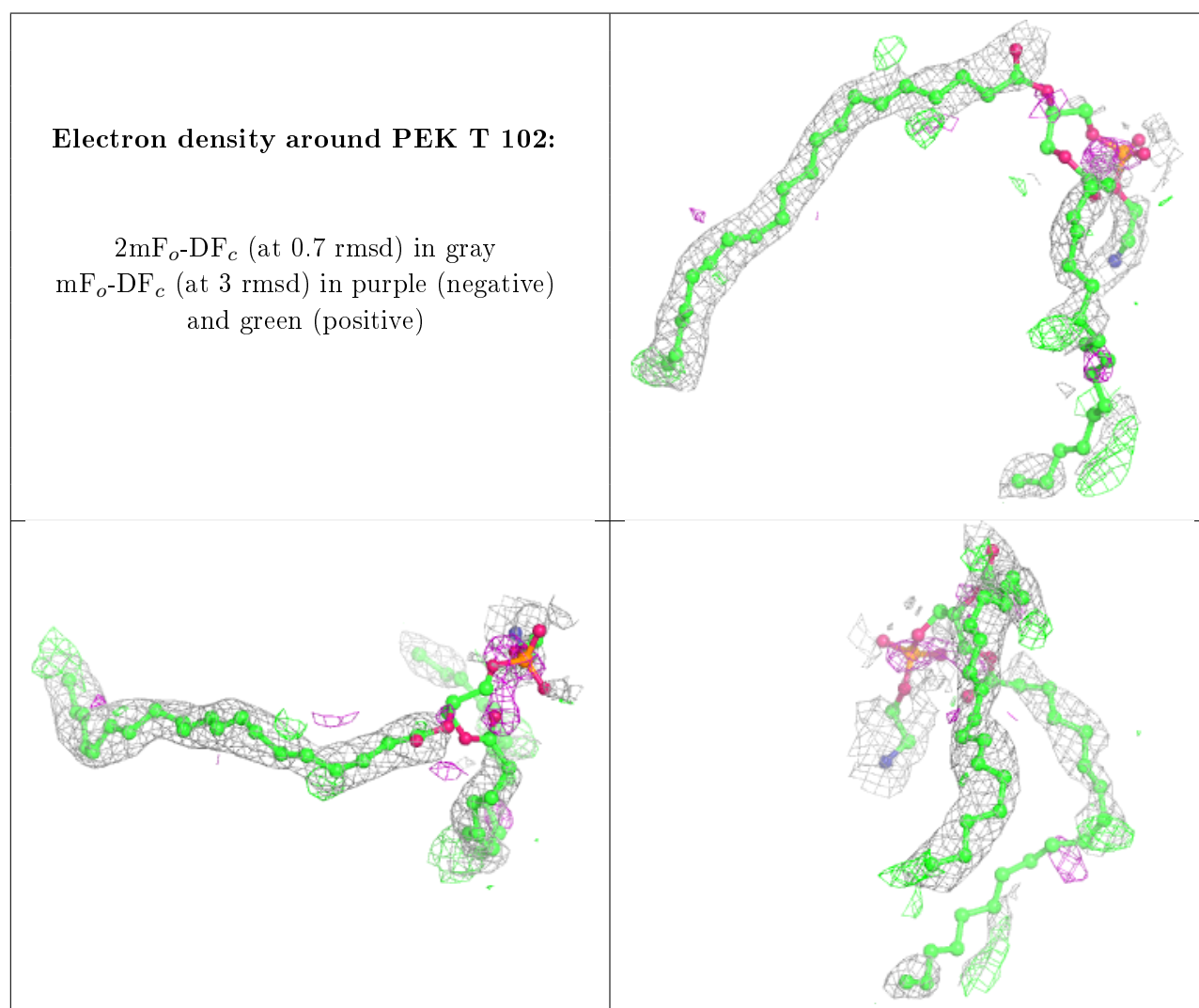
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	MG	N	604	1/1	0.95	0.08	31,31,31,31	0
21	EDO	C	319	4/4	0.95	0.23	32,42,46,58	0
21	EDO	T	104	4/4	0.96	0.14	34,36,39,42	0
21	EDO	N	619	4/4	0.96	0.15	45,46,55,56	0
21	EDO	E	204	4/4	0.96	0.10	37,39,42,46	0
21	EDO	A	612	4/4	0.96	0.17	31,32,37,74	0
21	EDO	G	106	4/4	0.96	0.10	29,34,38,40	0
24	CHD	P	301	29/29	0.96	0.08	27,32,36,40	0
18	AZI	N	607	3/3	0.97	0.18	32,32,34,38	0
20	PGV	A	609	51/51	0.97	0.12	23,32,62,65	0
21	EDO	N	620	4/4	0.97	0.17	42,55,55,65	0
21	EDO	F	103	4/4	0.97	0.10	36,37,37,39	0
20	PGV	C	304	51/51	0.97	0.13	26,32,80,91	0
21	EDO	N	613	4/4	0.97	0.15	36,44,45,49	0
28	PEK	G	101	53/53	0.97	0.14	27,44,79,97	0
20	PGV	N	609	51/51	0.97	0.12	27,35,62,66	0
14	HEA	N	601	60/60	0.98	0.11	25,28,48,50	0
20	PGV	P	305	51/51	0.98	0.12	26,35,72,76	0
14	HEA	A	602[A]	60/60	0.98	0.14	18,22,25,27	60
14	HEA	A	602[B]	60/60	0.98	0.14	18,22,33,37	60
21	EDO	P	313	4/4	0.98	0.15	41,42,43,46	0
14	HEA	N	602[B]	60/60	0.98	0.15	21,26,39,42	60
14	HEA	N	602[A]	60/60	0.98	0.15	21,25,29,31	60
24	CHD	G	103	29/29	0.98	0.09	26,30,33,38	0
21	EDO	N	616	4/4	0.98	0.11	26,31,33,35	0
21	EDO	B	303	4/4	0.98	0.11	28,28,34,34	0
21	EDO	C	311	4/4	0.98	0.09	38,39,39,41	0
21	EDO	O	303	4/4	0.98	0.14	37,37,37,38	0
21	EDO	A	610	4/4	0.98	0.13	36,38,39,45	0
18	AZI	A	607	3/3	0.98	0.17	30,30,31,34	0
21	EDO	D	205	4/4	0.98	0.14	35,36,53,55	0
24	CHD	T	101	29/29	0.98	0.10	26,28,31,39	0
17	NA	N	605	1/1	0.99	0.07	35,35,35,35	0
17	NA	A	605	1/1	0.99	0.10	28,28,28,28	0
21	EDO	S	102	4/4	0.99	0.13	28,29,30,31	0
21	EDO	E	202	4/4	0.99	0.15	37,39,43,45	0
22	CUA	O	301	2/2	0.99	0.14	31,31,31,32	0
18	AZI	A	606	3/3	0.99	0.15	28,28,28,28	0
21	EDO	F	102	4/4	0.99	0.10	24,25,26,28	0
16	MG	A	604	1/1	0.99	0.09	24,24,24,24	0
14	HEA	A	601	60/60	0.99	0.12	19,23,45,45	0
15	CU	N	603	1/1	1.00	0.16	28,28,28,28	0

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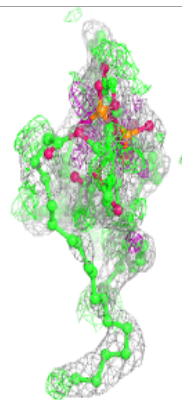
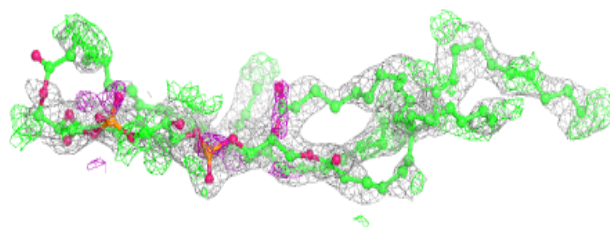
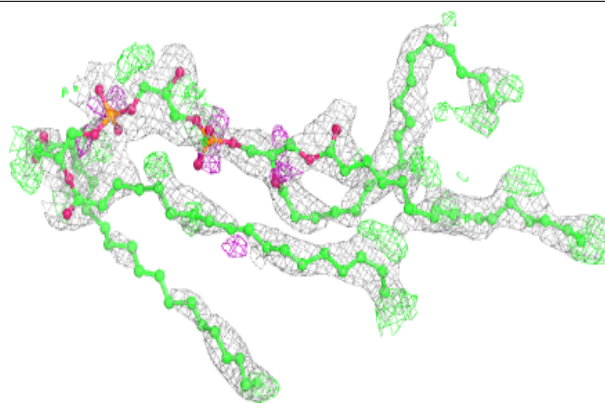
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	CU	A	603	1/1	1.00	0.15	25,25,25,25	0
29	ZN	F	101	1/1	1.00	0.14	30,30,30,30	0
22	CUA	B	301	2/2	1.00	0.17	25,25,25,26	0
29	ZN	S	101	1/1	1.00	0.13	32,32,32,32	0
18	AZI	N	606	3/3	1.00	0.13	33,33,34,35	0

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

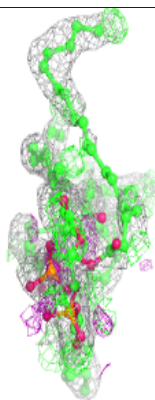
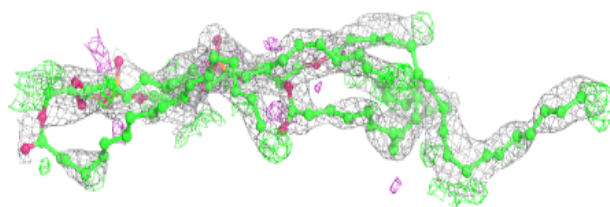
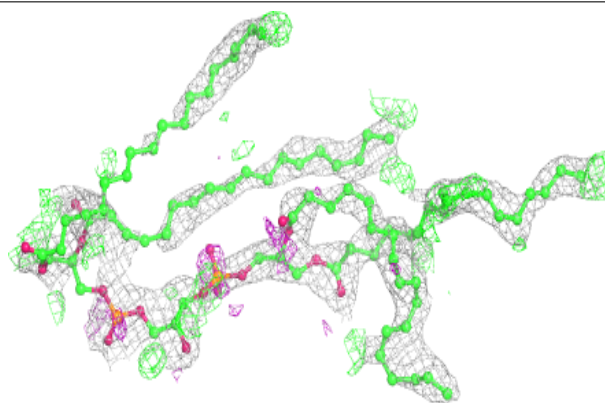


Electron density around CDL T 103:

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

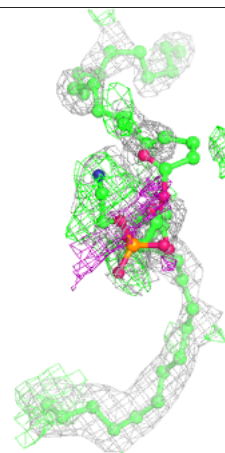
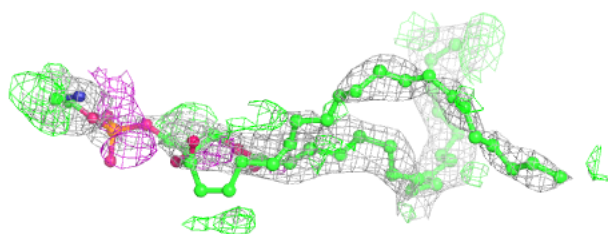
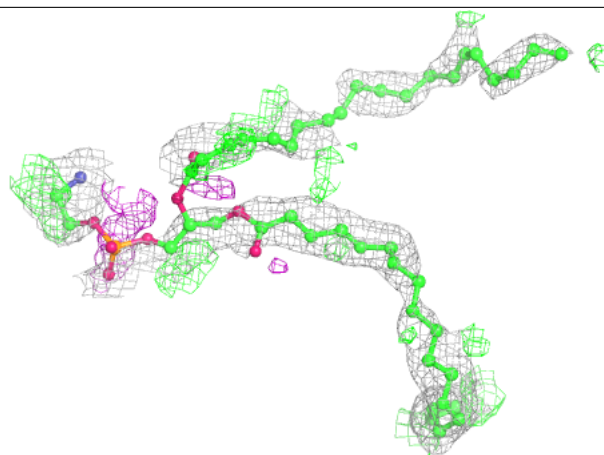
**Electron density around CDL G 102:**

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



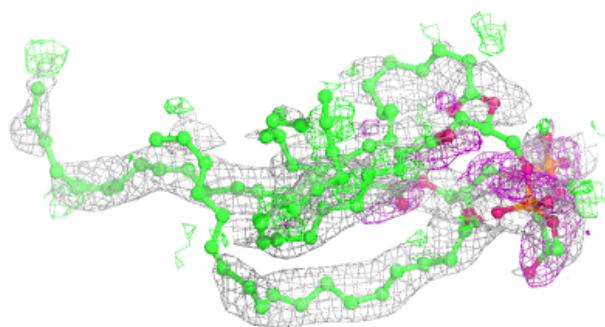
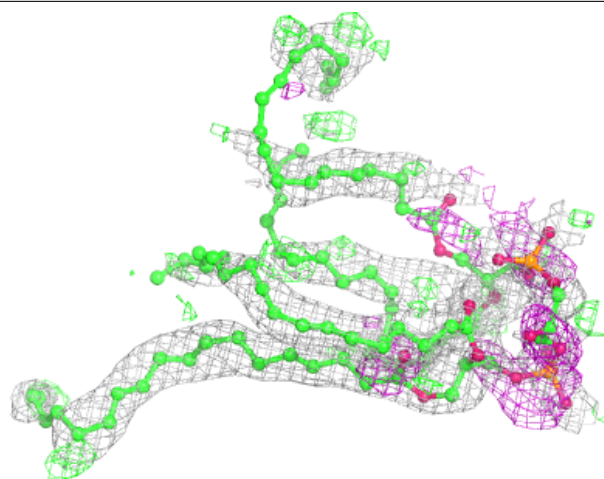
Electron density around PEK C 307:

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



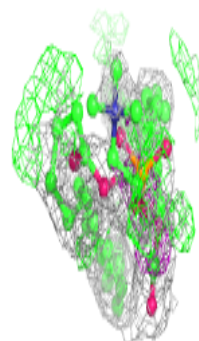
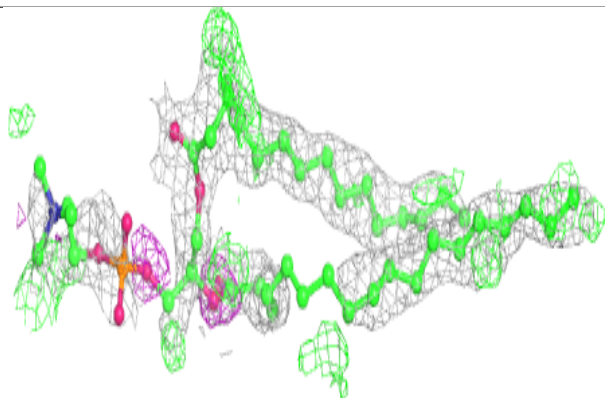
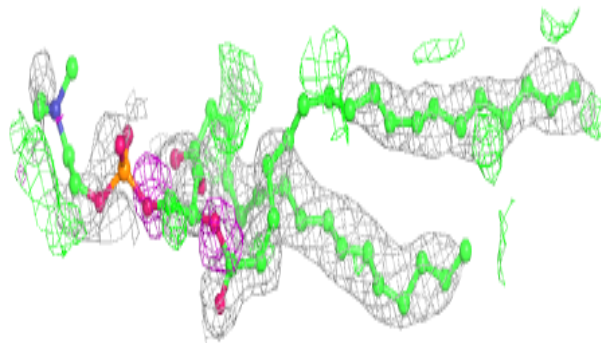
Electron density around CDL P 306:

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

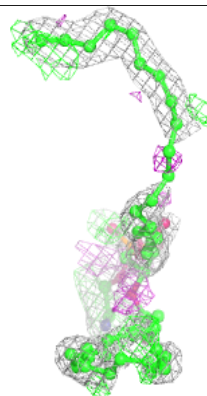
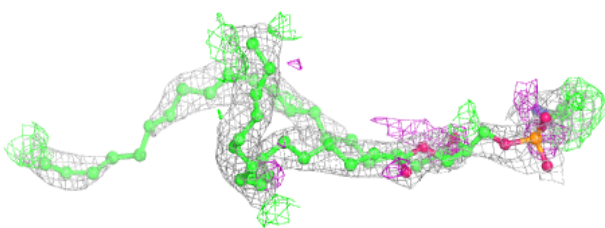
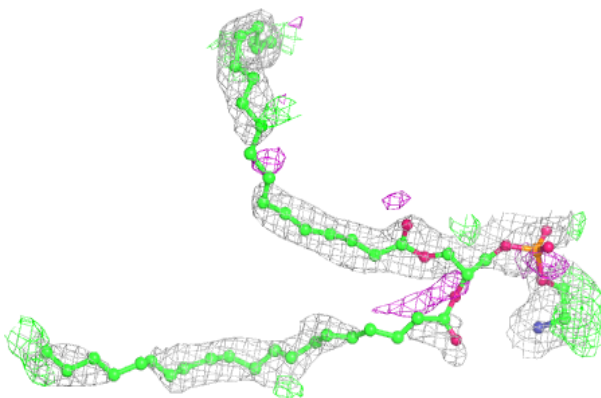


Electron density around PSC B 302:

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

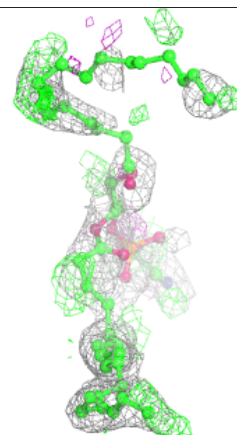
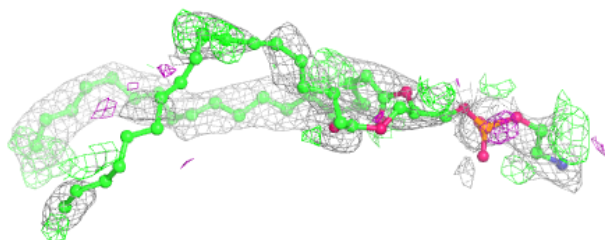
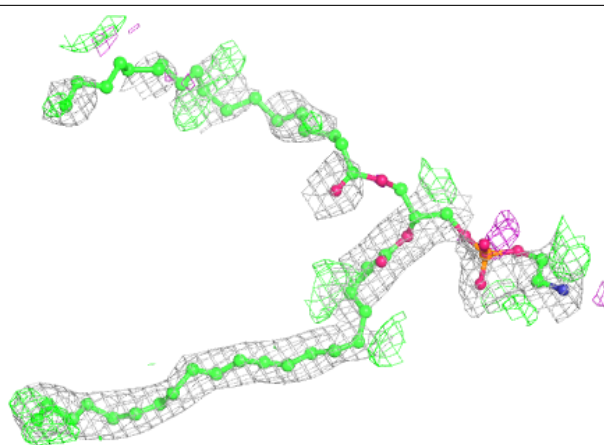
**Electron density around PEK P 309:**

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

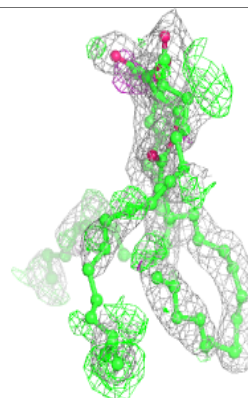
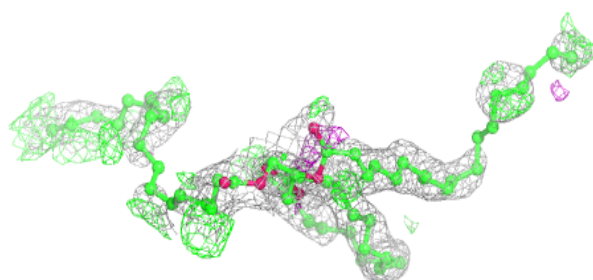
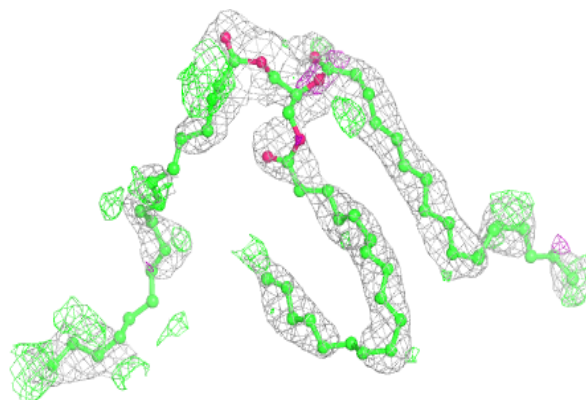


Electron density around PEK G 104:

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

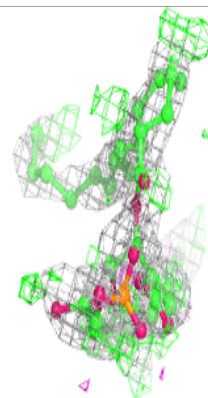
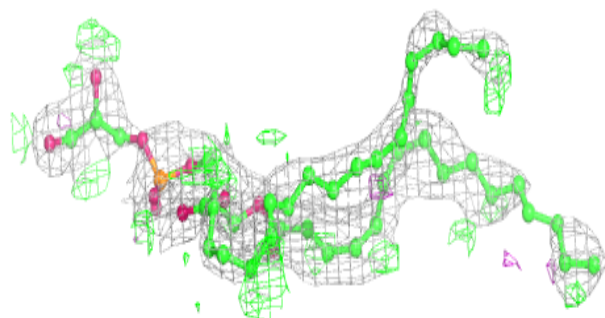
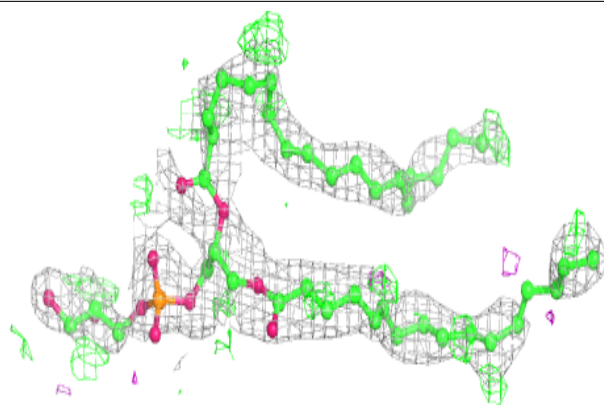
**Electron density around TGL Q 201:**

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

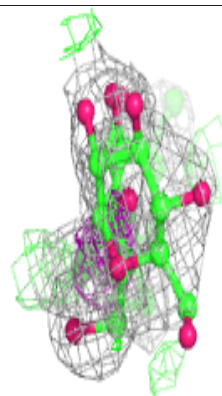
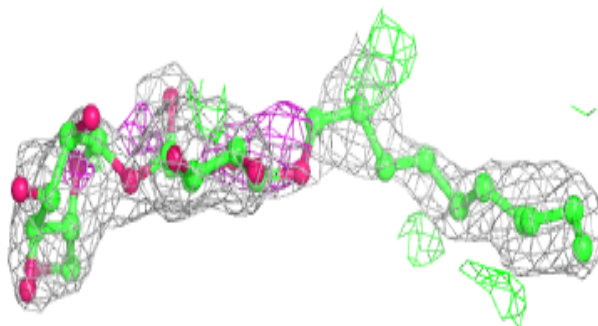
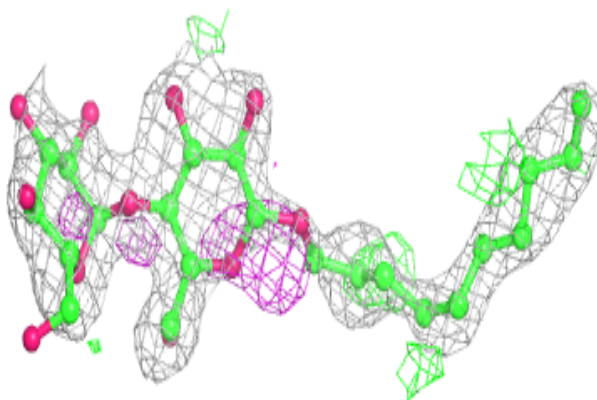


Electron density around PGV C 308:

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

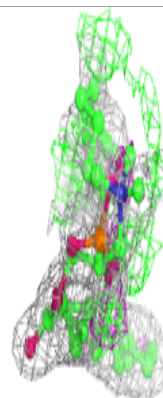
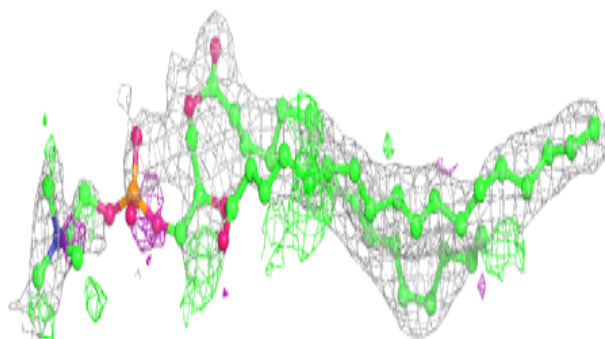
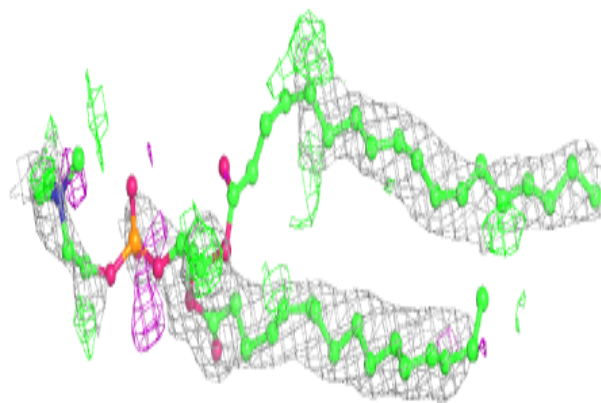
**Electron density around DMU C 302:**

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

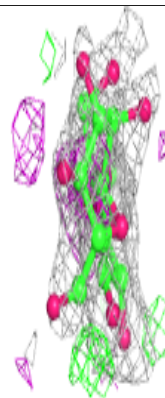
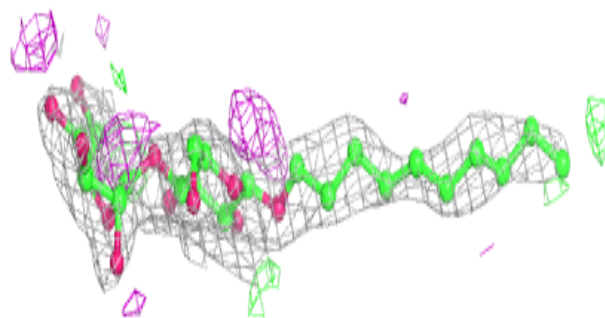
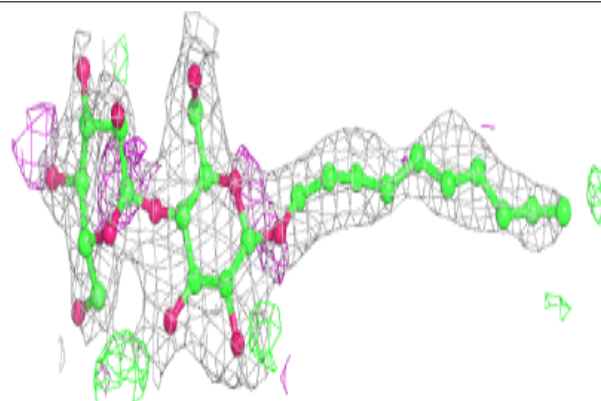


Electron density around PSC O 302:

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

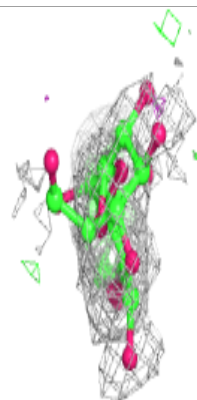
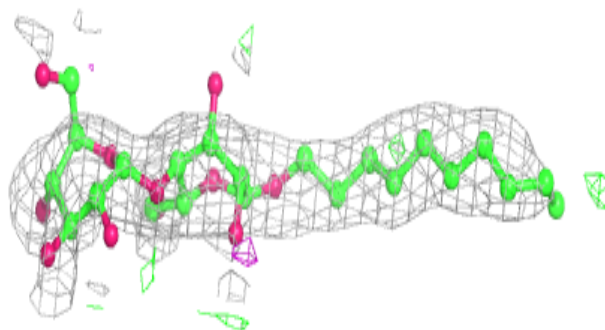
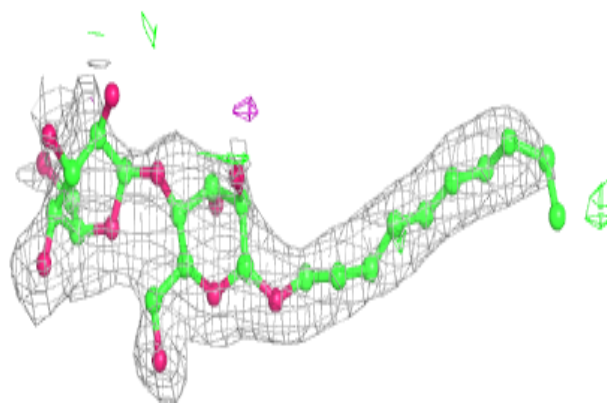
**Electron density around DMU C 309:**

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

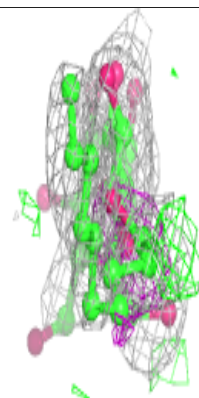
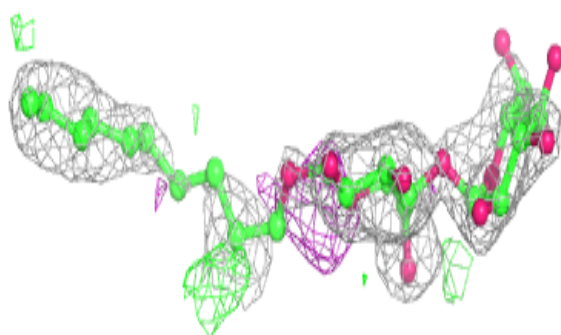
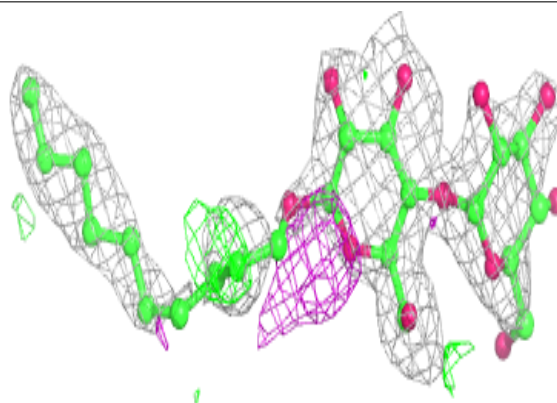


Electron density around DMU C 310:

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

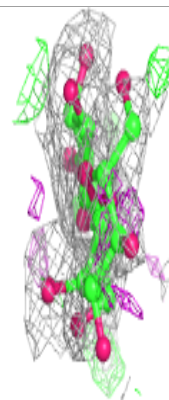
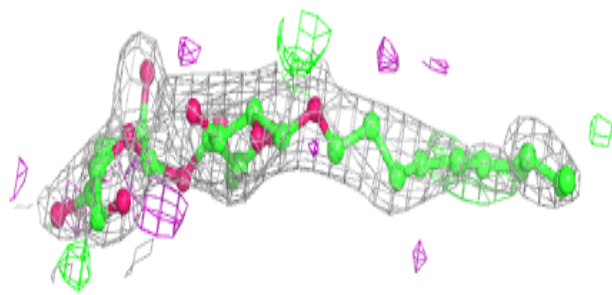
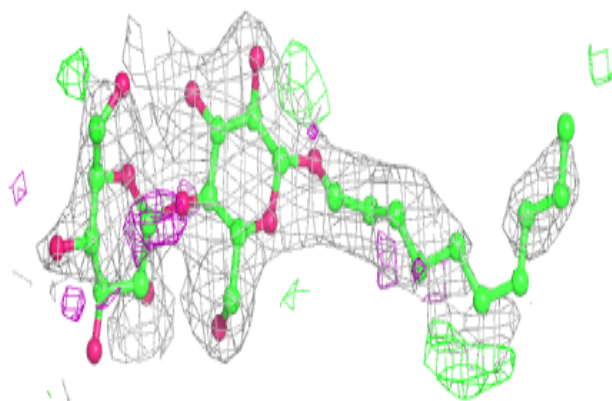
**Electron density around DMU P 308:**

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

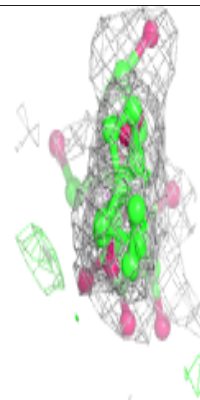
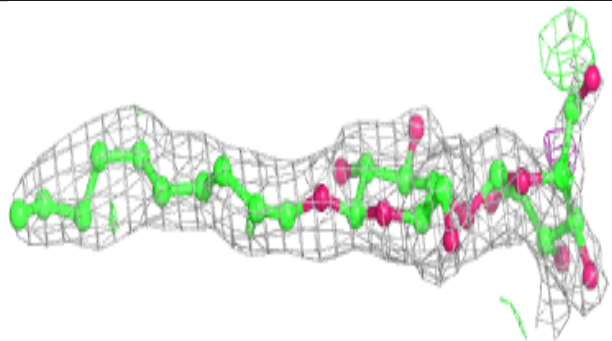
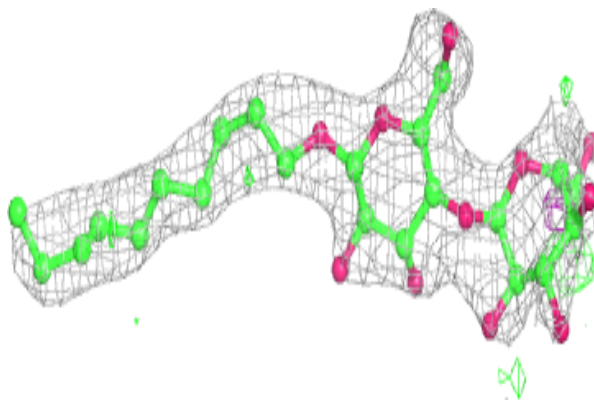


Electron density around DMU P 310:

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

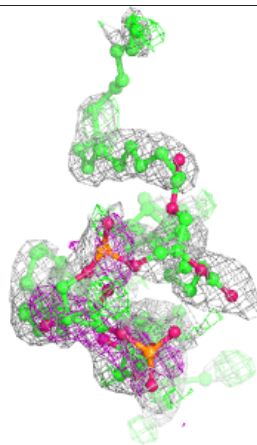
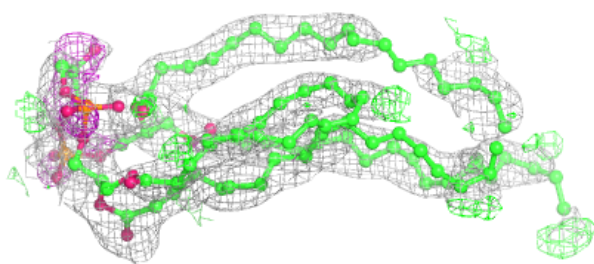
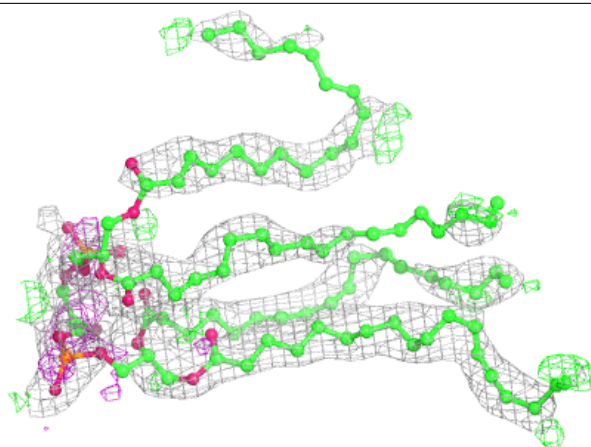
**Electron density around DMU P 311:**

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



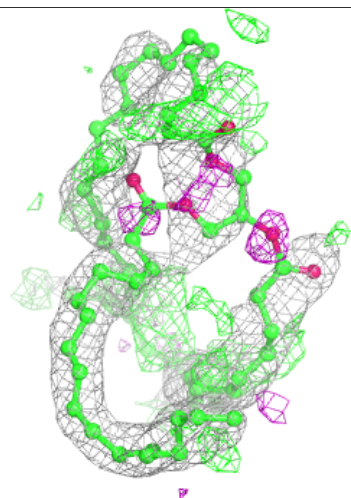
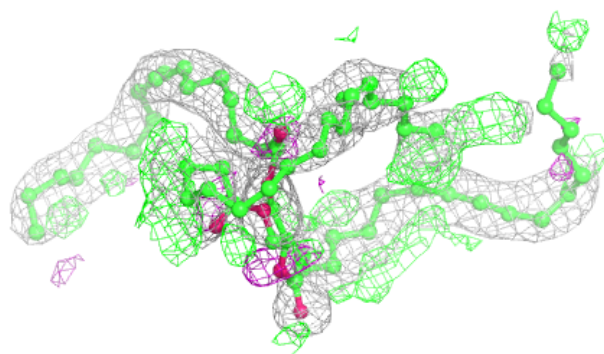
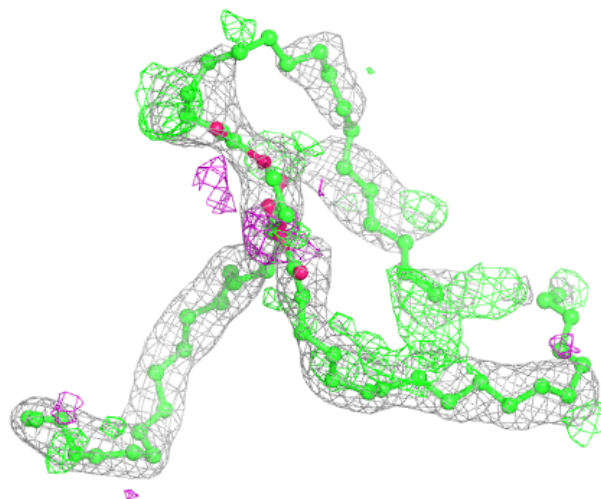
Electron density around CDL C 305:

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



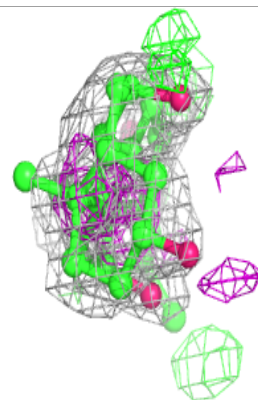
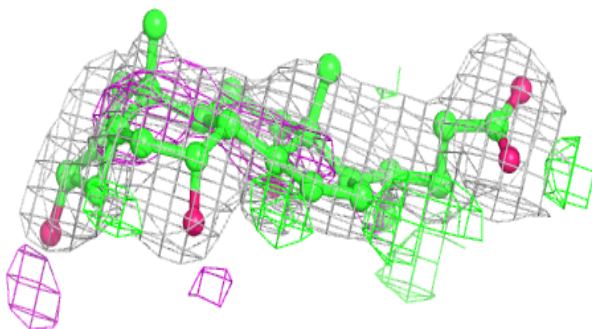
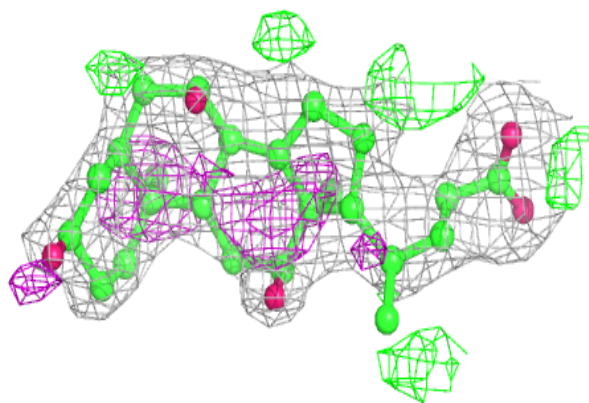
Electron density around TGL Y 101:

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

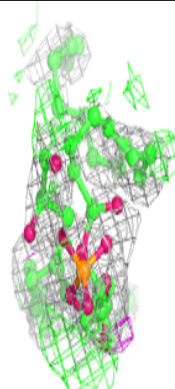
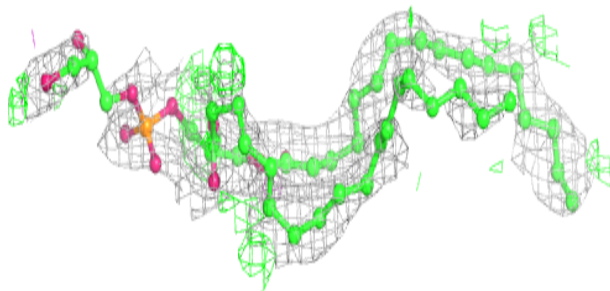
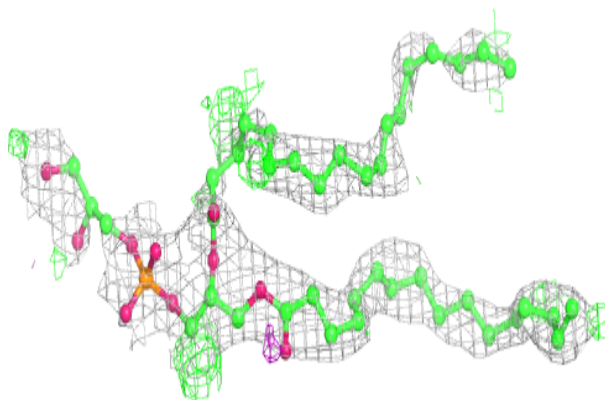


Electron density around CHD P 307:

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

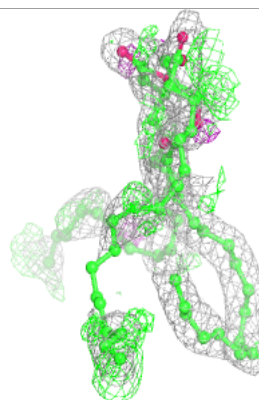
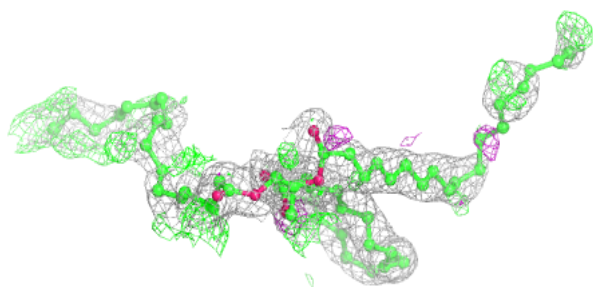
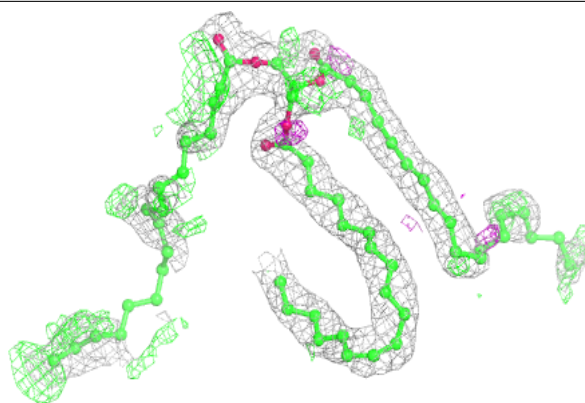
**Electron density around PGV P 302:**

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

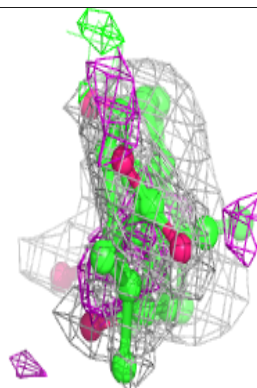
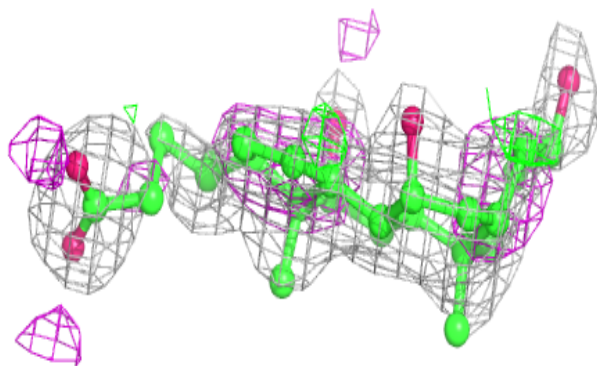
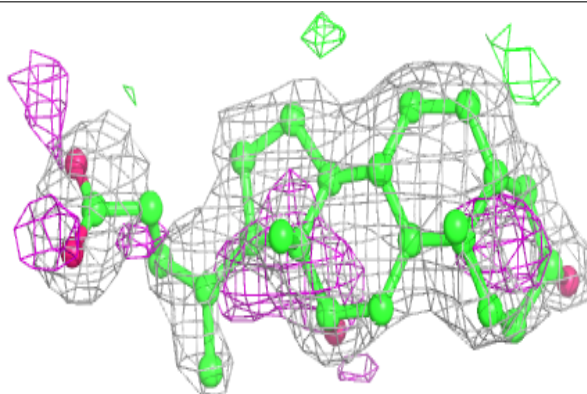


Electron density around TGL D 201:

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

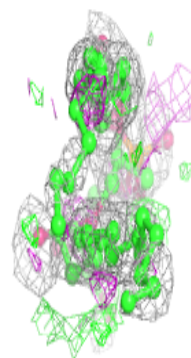
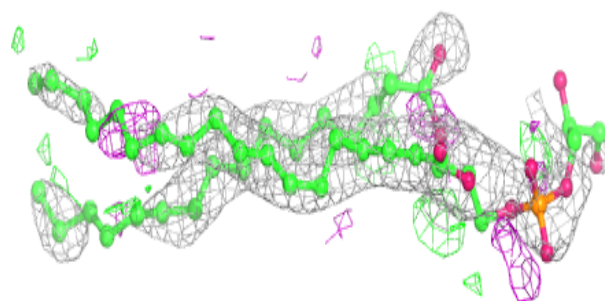
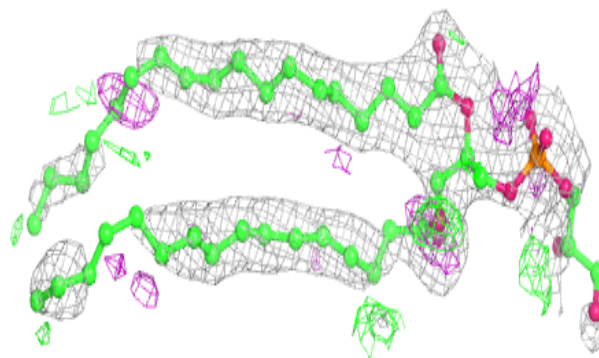
**Electron density around CHD C 306:**

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



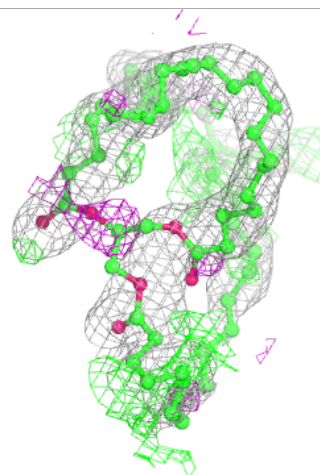
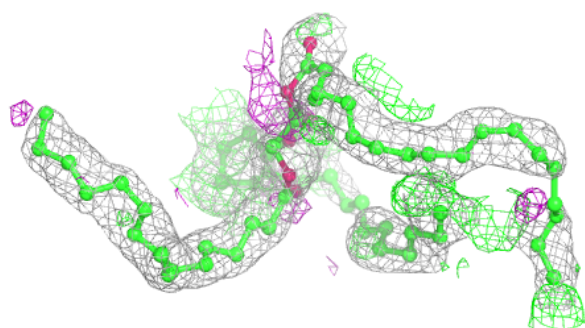
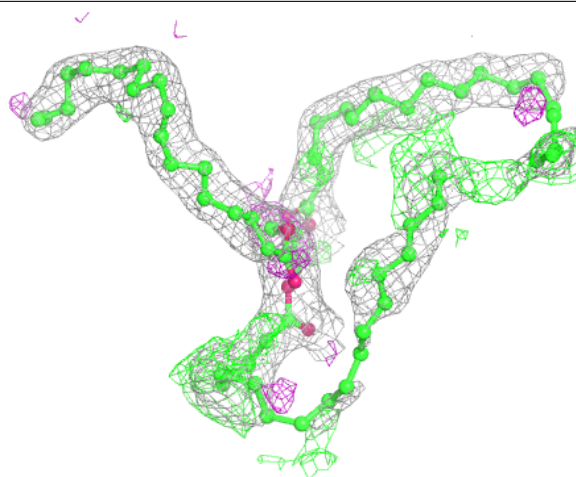
Electron density around PGV N 608:

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



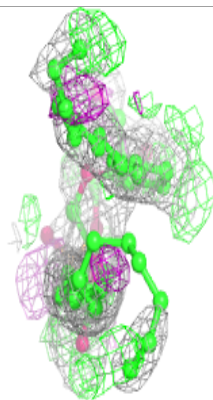
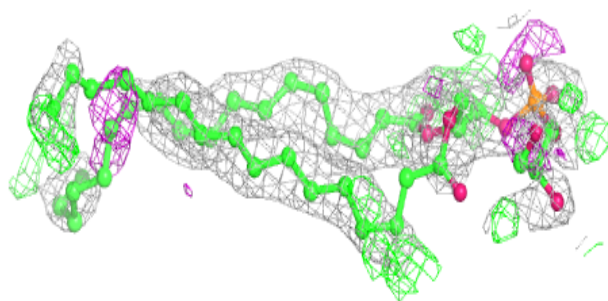
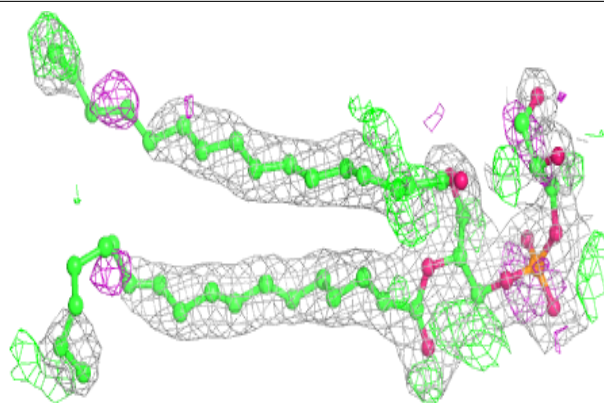
Electron density around TGL L 101:

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

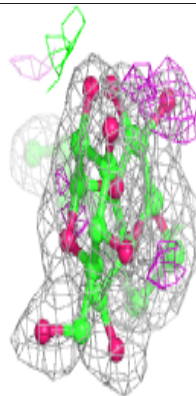
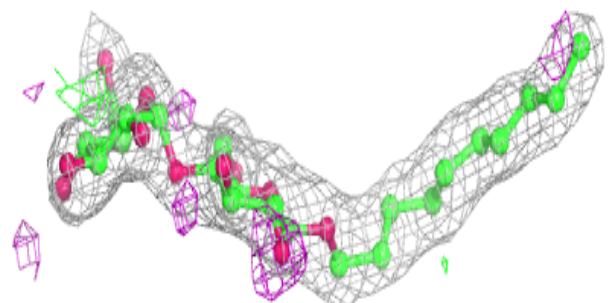
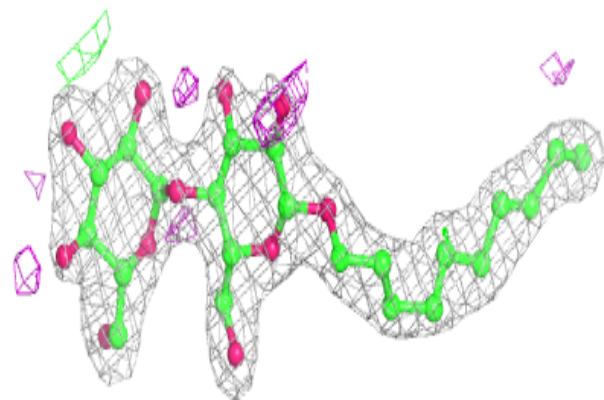


Electron density around PGV M 101:

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

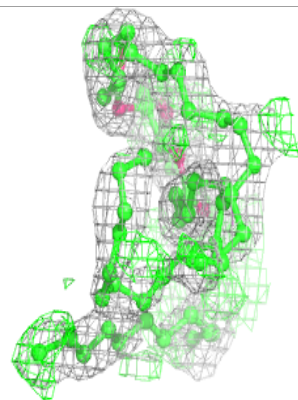
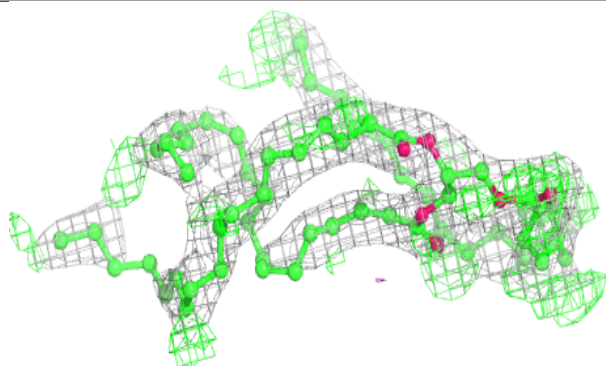
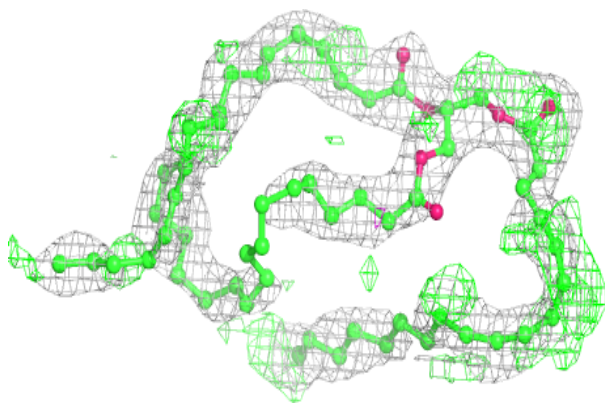
**Electron density around DMU Z 101:**

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

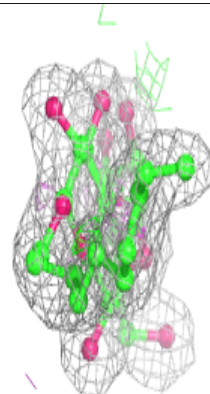
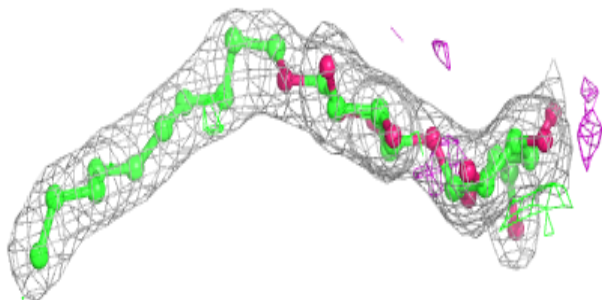
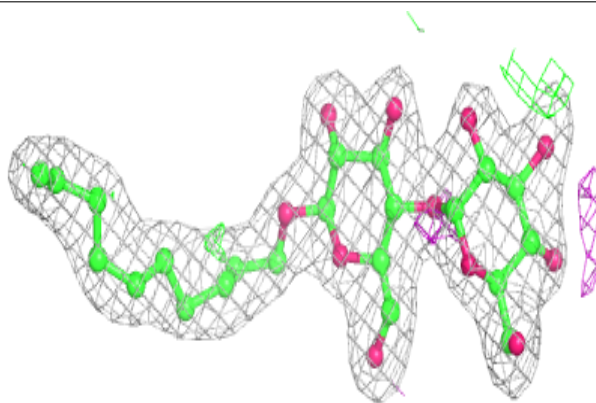


Electron density around TGL N 610:

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

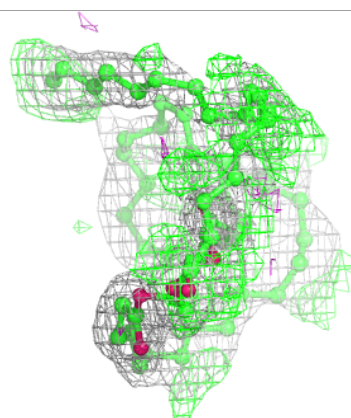
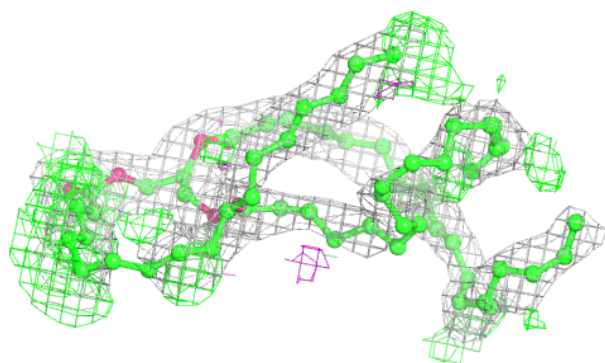
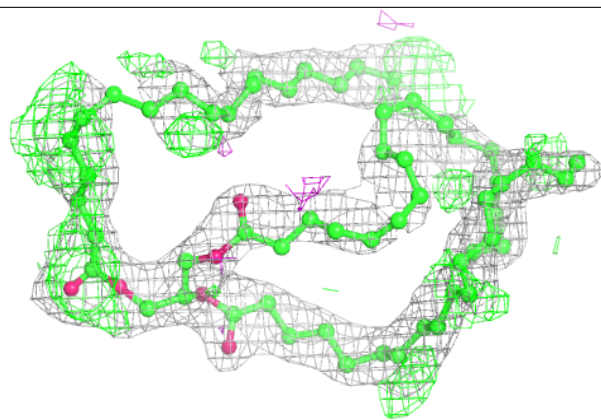
**Electron density around DMU M 102:**

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

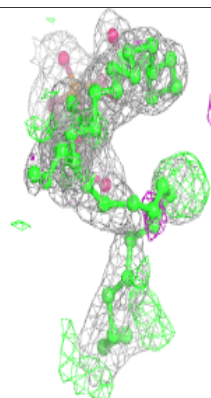
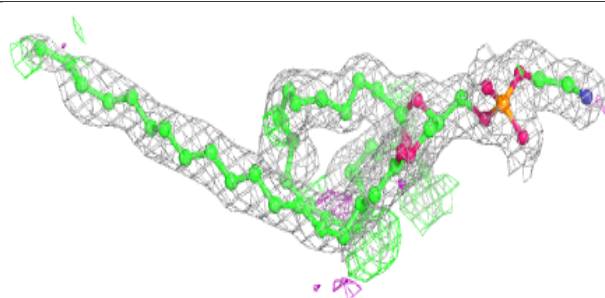
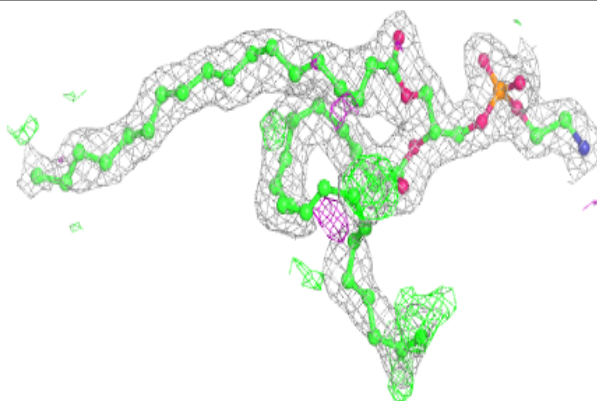


Electron density around TGL A 608:

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

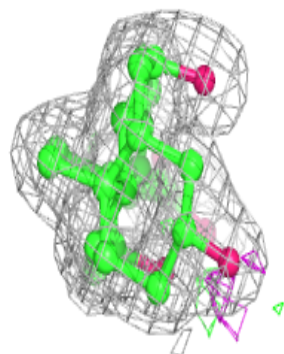
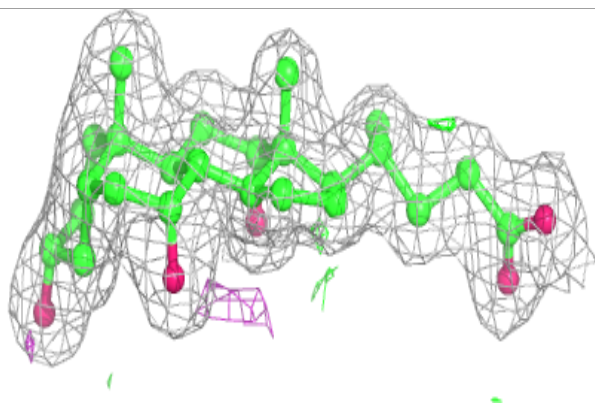
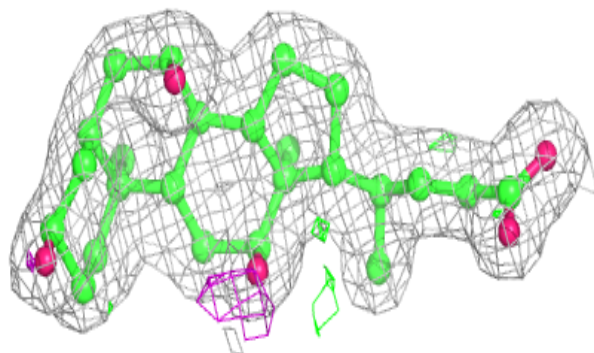
**Electron density around PEK P 304:**

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

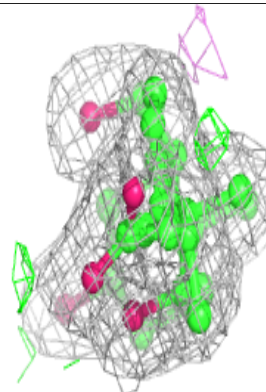
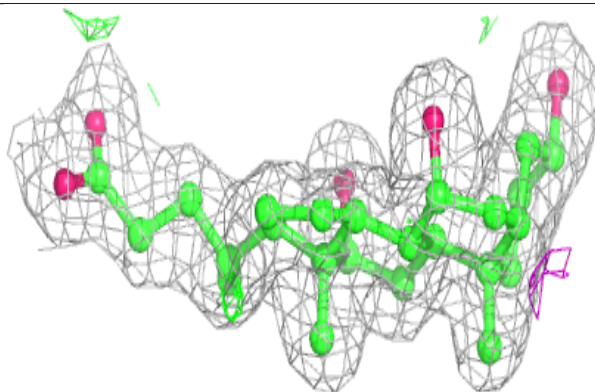
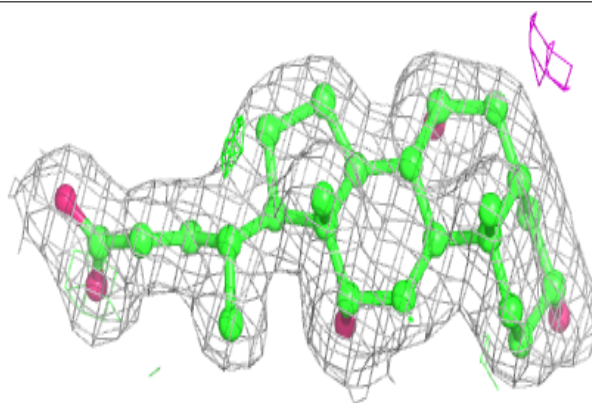


Electron density around CHD C 301:

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

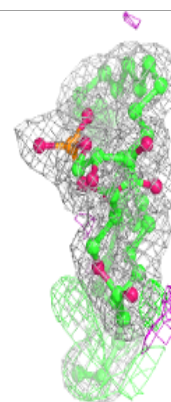
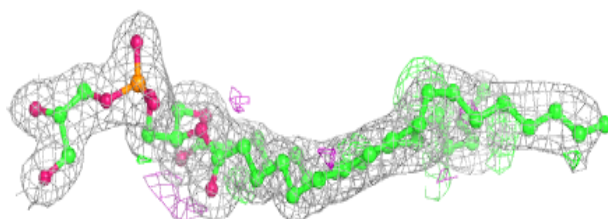
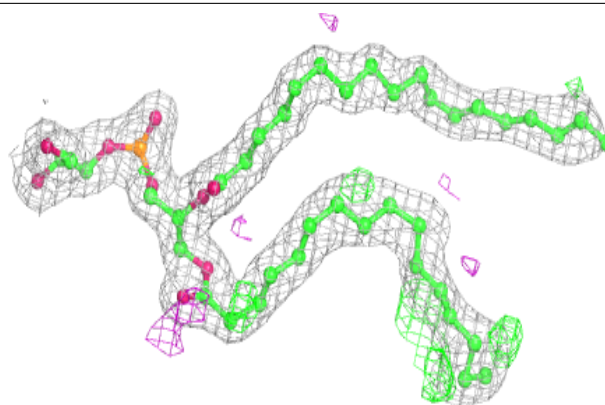
**Electron density around CHD P 301:**

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

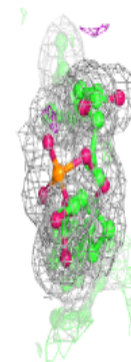
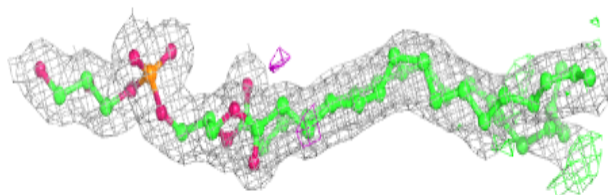
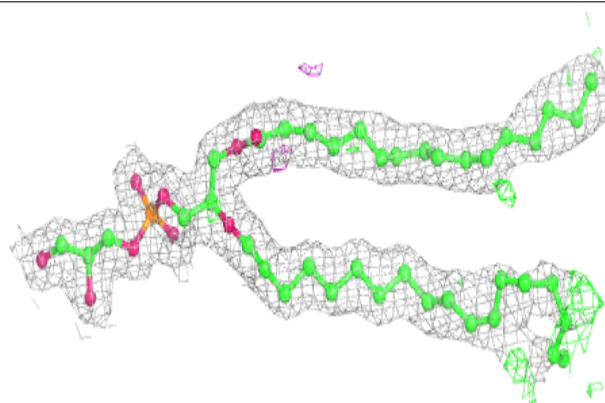


Electron density around PGV A 609:

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

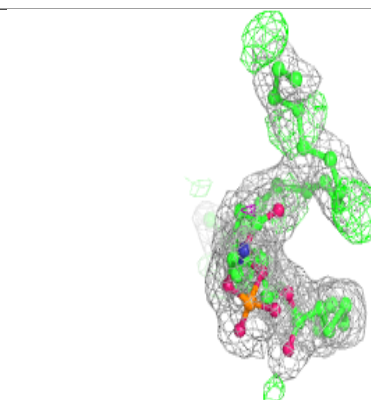
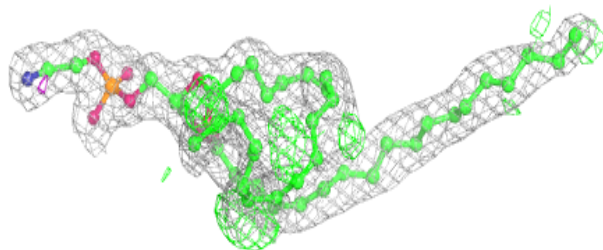
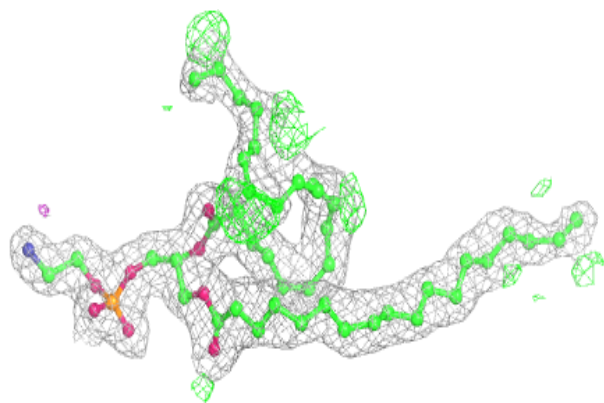
**Electron density around PGV C 304:**

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

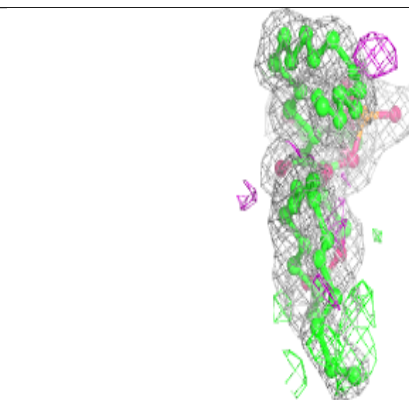
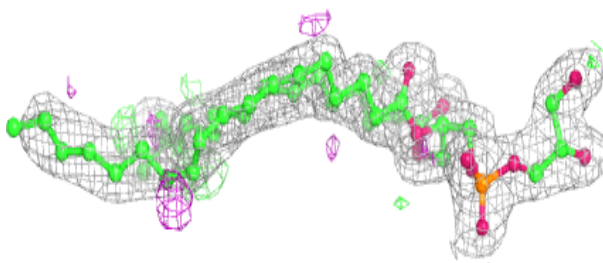
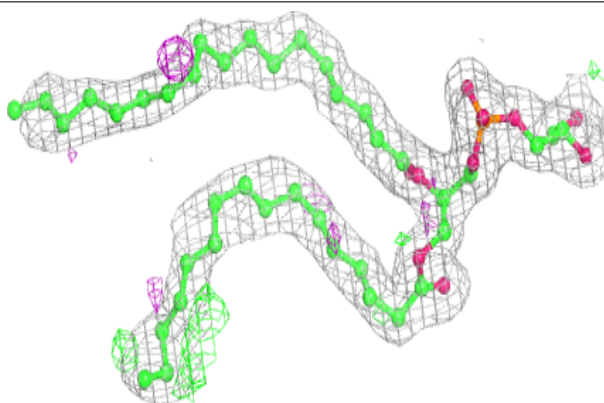


Electron density around PEK G 101:

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

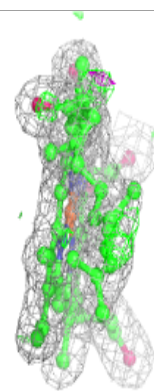
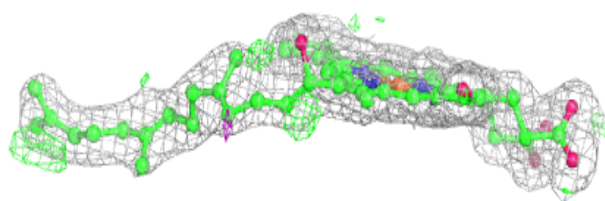
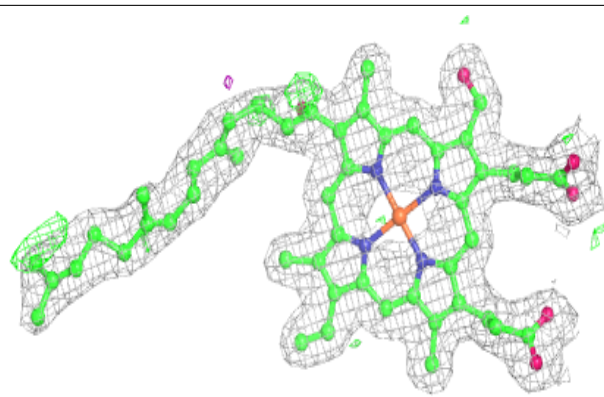
**Electron density around PGV N 609:**

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

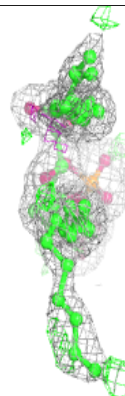
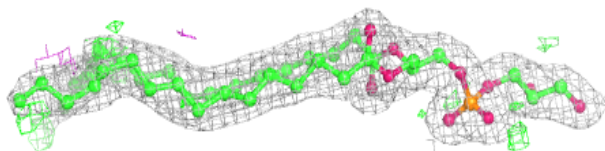
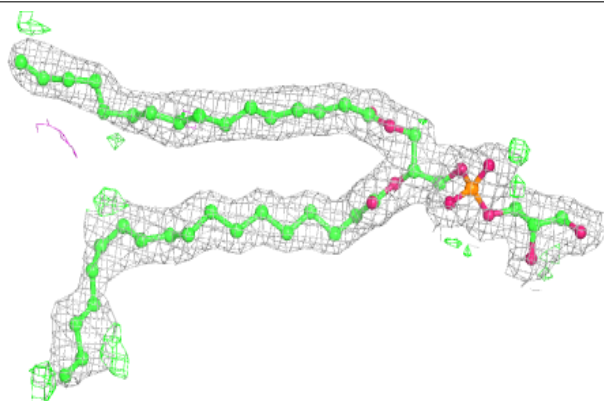


Electron density around HEA N 601:

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

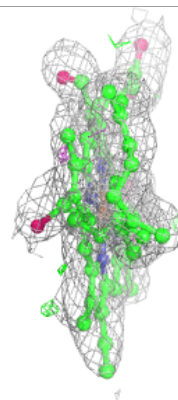
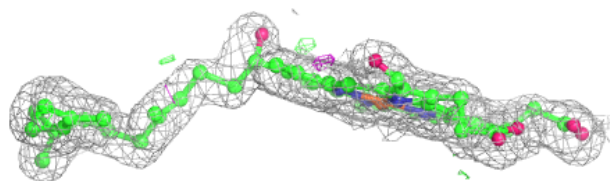
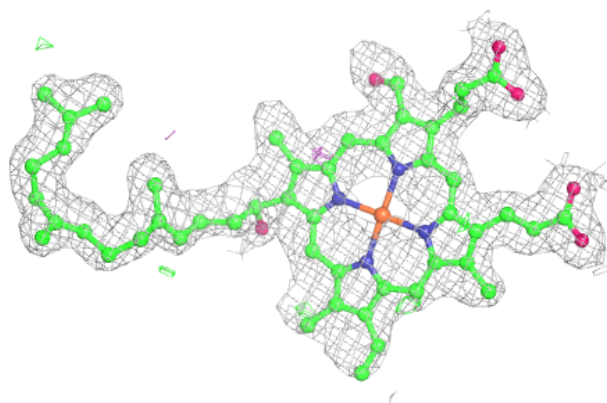
**Electron density around PGV P 305:**

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

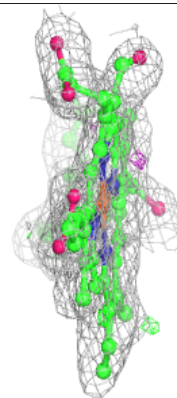
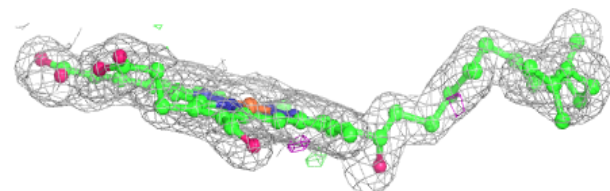
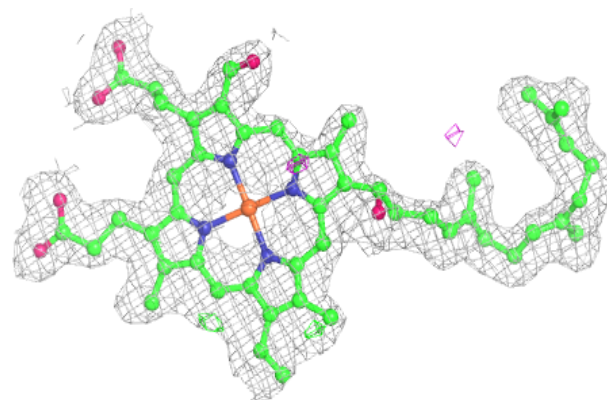


Electron density around HEA A 602 (A):

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

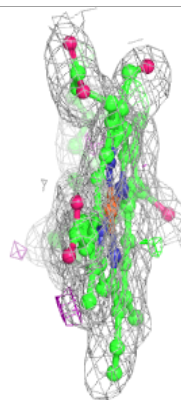
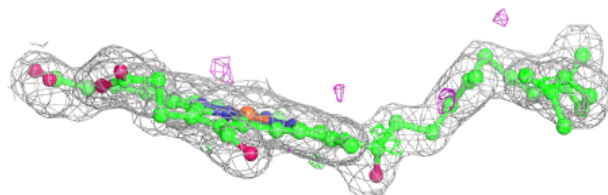
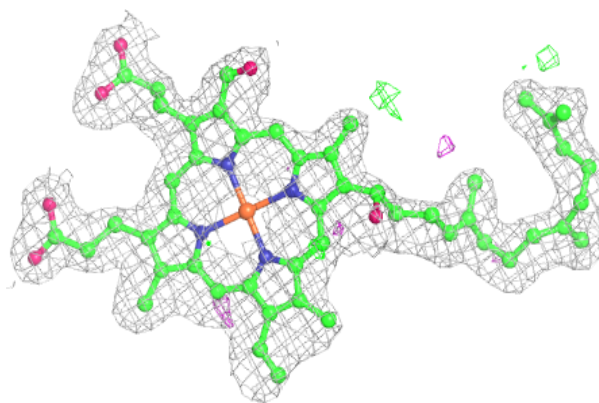
**Electron density around HEA A 602 (B):**

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

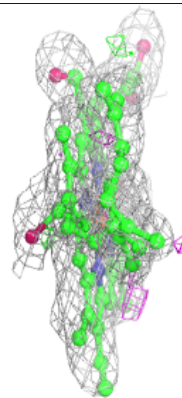
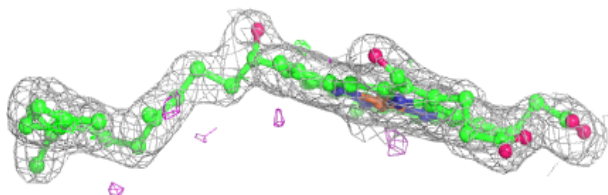
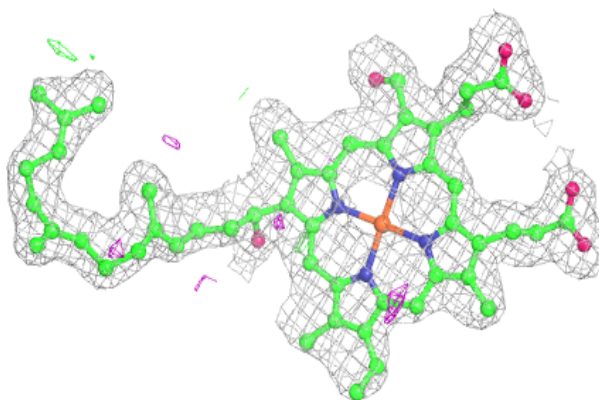


Electron density around HEA N 602 (B):

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

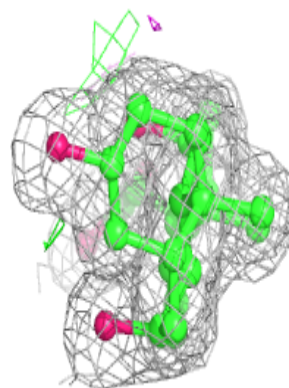
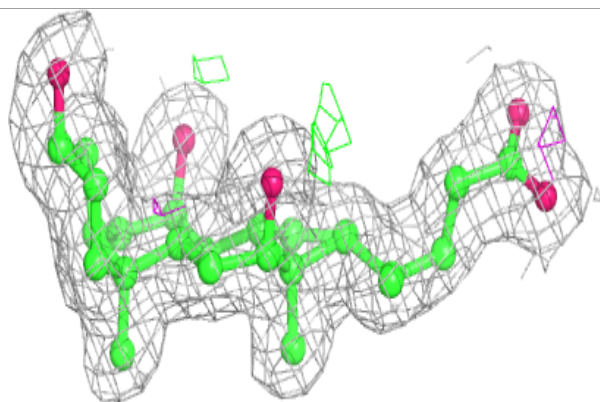
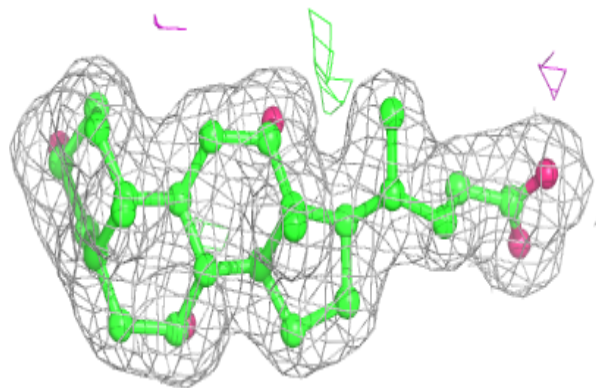
**Electron density around HEA N 602 (A):**

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

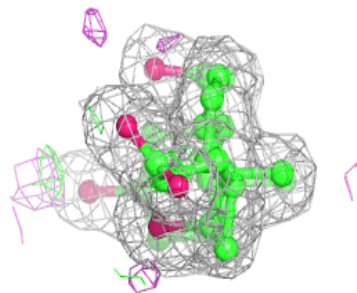
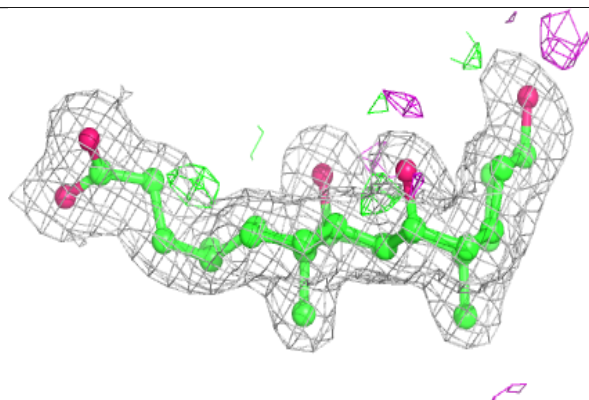
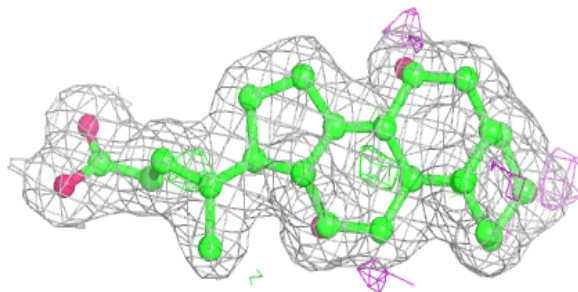


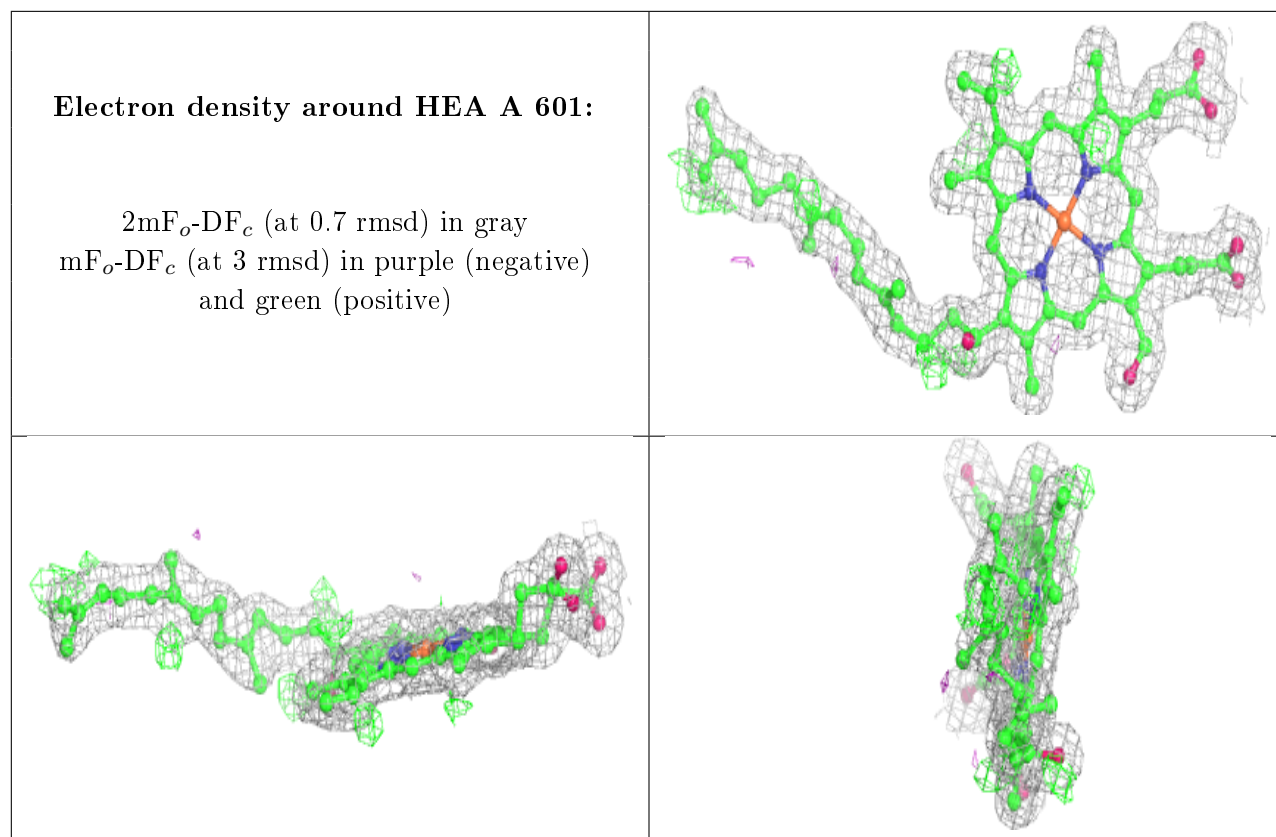
Electron density around CHD G 103:

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

**Electron density around CHD 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.