



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2021 – 07:11 PM JST

PDB ID : 5B1B
Title : Bovine heart cytochrome c oxidase in the fully reduced state at 1.6 angstrom resolution
Authors : Yano, N.; Muramoto, K.; Shimada, A.; Takemura, S.; Baba, J.; Fujisawa, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2015-12-01
Resolution : 1.60 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 : 2.23.2
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) : 2.23.2

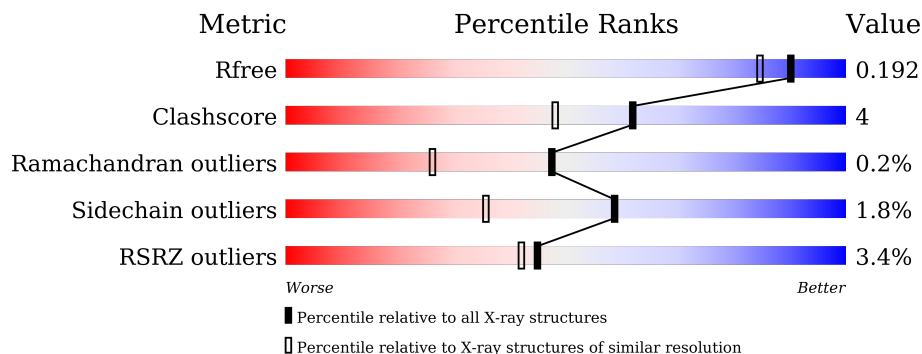
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	N	514	<div> <div>88%</div> <div>12%</div> </div>
2	B	227	<div> <div>%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	O	227	<div> <div>2%</div> <div>85%</div> <div>15%</div> </div>
3	C	259	<div> <div>93%</div> <div>7%</div> </div>
3	P	259	<div> <div>93%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	144	
4	Q	144	
5	E	105	
5	R	105	
6	F	98	
6	S	98	
7	G	84	
7	T	84	
8	H	79	
8	U	79	
9	I	73	
9	V	73	
10	J	58	
10	W	58	
11	K	49	
11	X	49	
12	L	46	
12	Y	46	
13	M	43	
13	Z	43	

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	601[A]	X	-	-	-
14	HEA	N	601[B]	X	-	-	-
14	HEA	N	602	X	-	-	-
23	CHD	J	101	-	-	-	X
24	DMU	D	203	-	-	-	X
24	DMU	K	103	-	-	-	X
24	DMU	X	101	-	-	-	X
25	CDL	P	305	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 34425 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	20	0
			4107	2743	633	689	42			
1	N	514	Total	C	N	O	S	0	21	0
			4107	2742	633	689	43			

- 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	6	0
			1844	1198	283	344	19			
2	O	227	Total	C	N	O	S	0	4	0
			1841	1196	284	343	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	8	0
			2126	1420	337	356	13			
3	P	259	Total	C	N	O	S	0	8	0
			2129	1423	336	355	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	6	0
			1214	792	200	218	4			
4	Q	144	Total	C	N	O	S	0	1	0
			1196	778	196	218	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	1	0
			858	547	147	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	4	0
			758	470	136	147	5			
6	S	98	Total	C	N	O	S	0	1	0
			750	465	134	146	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	S	0	1	0
			677	437	129	110	1			
7	T	84	Total	C	N	O	S	0	3	0
			687	445	130	111	1			

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	1	0
			602	391	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	1	0
			386	252	65	67	2			
11	X	49	Total	C	N	O	S	0	1	0
			386	252	65	67	2			

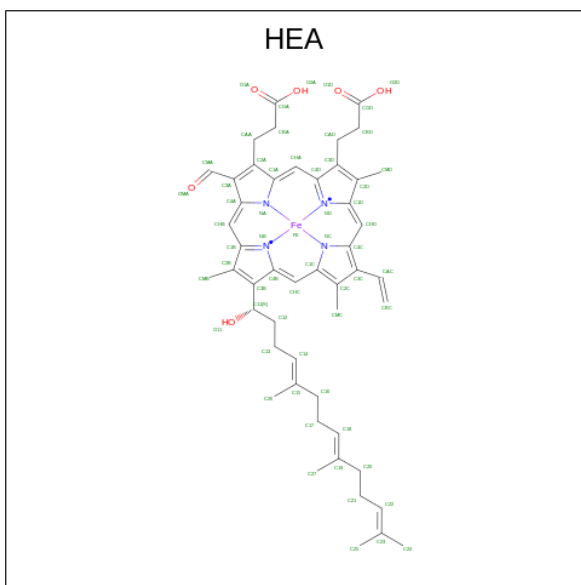
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 70	C 58	Fe 1	N 4	O 7	0	1
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 70	C 58	Fe 1	N 4	O 7	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- 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		

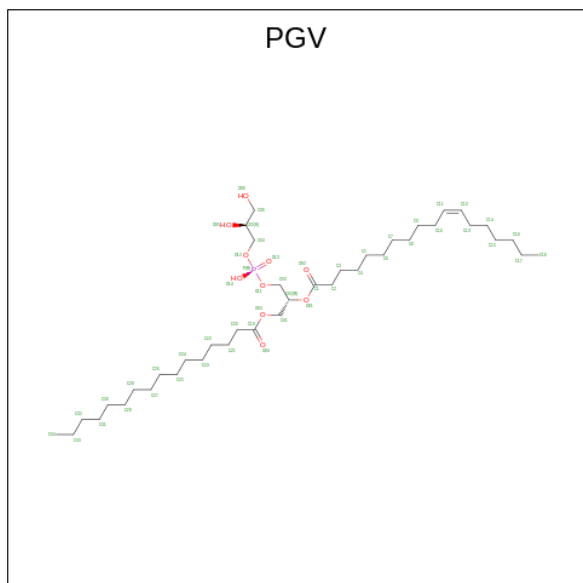
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

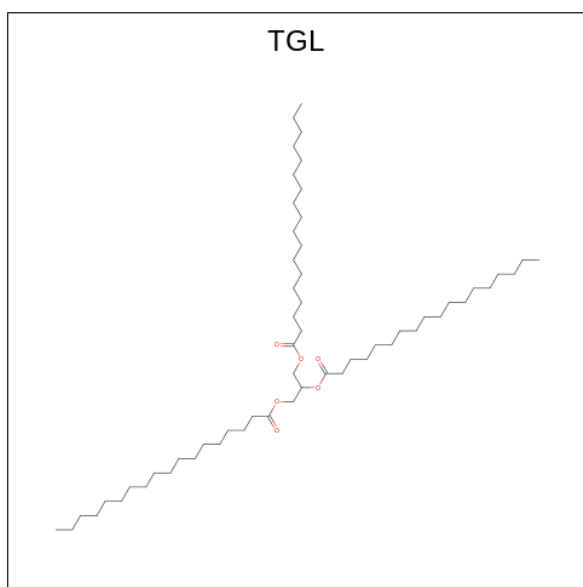
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



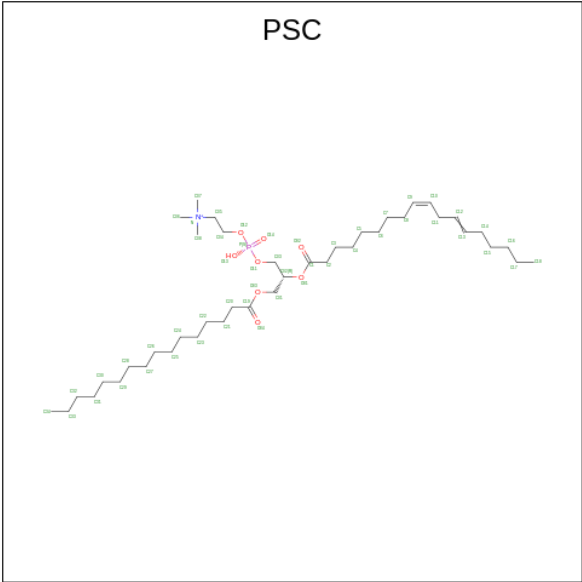
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O P 51 40 10 1	0	0
18	A	1	Total C O 37 34 3	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O 36 34 2	0	0
18	N	1	Total C O 40 36 4	0	0
18	N	1	Total C O P 51 40 10 1	0	0
18	P	1	Total C O 41 37 4	0	0
18	P	1	Total C O P 50 39 10 1	0	0

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



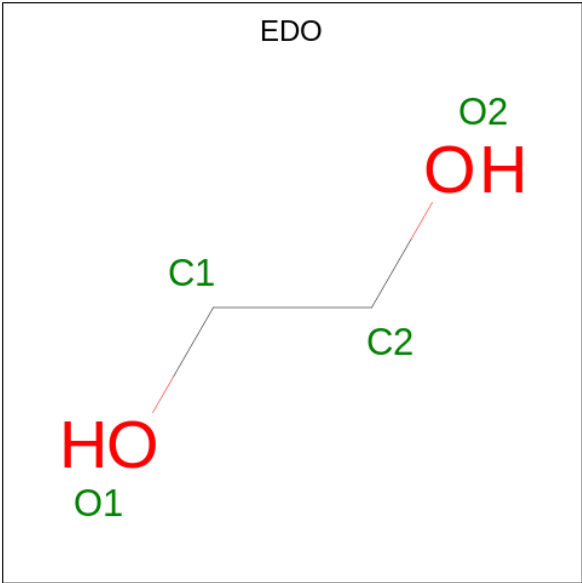
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			62	57	5		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			59	53	6		
19	N	1	Total	C	O	0	0
			57	54	3		
19	O	1	Total	C	O	0	0
			58	52	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYL OXY)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
20	A	1	Total	C	0	0
			25	25		
20	O	1	Total	C	0	0
			24	24		

- 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		

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

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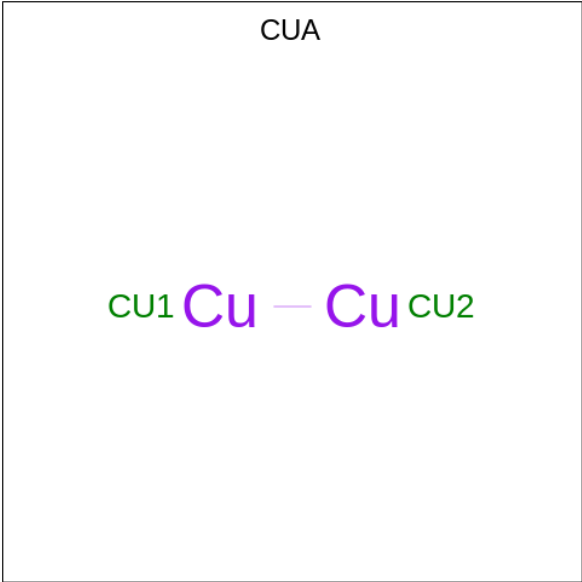
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	J	1	Total 4	C 2	O 2	0	0
21	J	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4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

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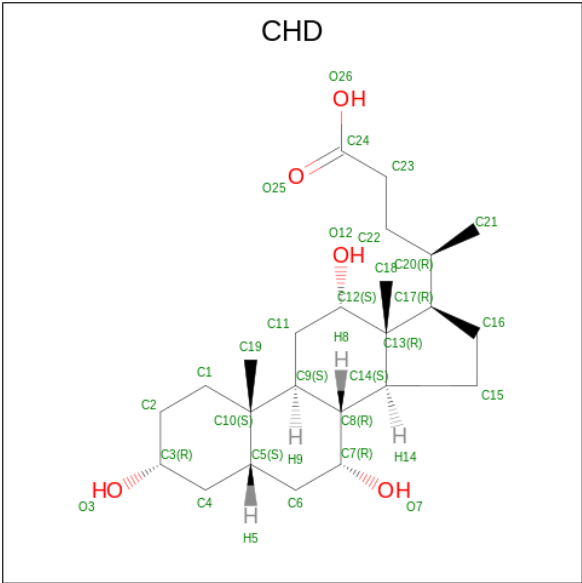
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	O	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	Q	1	Total	C	O	0	0
			4	2	2		
21	Q	1	Total	C	O	0	0
			4	2	2		
21	Q	1	Total	C	O	0	0
			4	2	2		
21	R	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	S	1	Total	C	O	0	0
			4	2	2		
21	T	1	Total	C	O	0	0
			4	2	2		
21	T	1	Total	C	O	0	0
			4	2	2		
21	W	1	Total	C	O	0	0
			4	2	2		
21	W	1	Total	C	O	0	0
			4	2	2		
21	Y	1	Total	C	O	0	0
			4	2	2		

- 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 CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



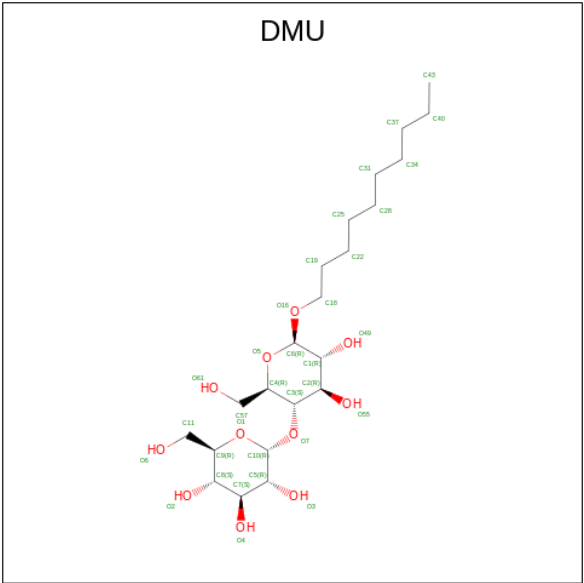
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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

- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



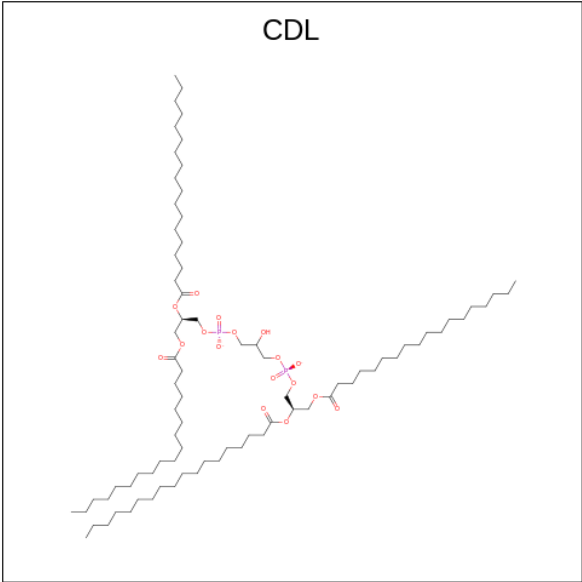
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C		0	0
			9	9			
24	C	1	Total	C	O	0	0
			12	11	1		
24	D	1	Total	C	O	0	0
			12	11	1		
24	D	1	Total	C		0	0
			9	9			
24	J	1	Total	C	O	0	0
			12	10	2		
24	K	1	Total	C	O	0	0
			10	9	1		
24	K	1	Total	C		0	0
			9	9			

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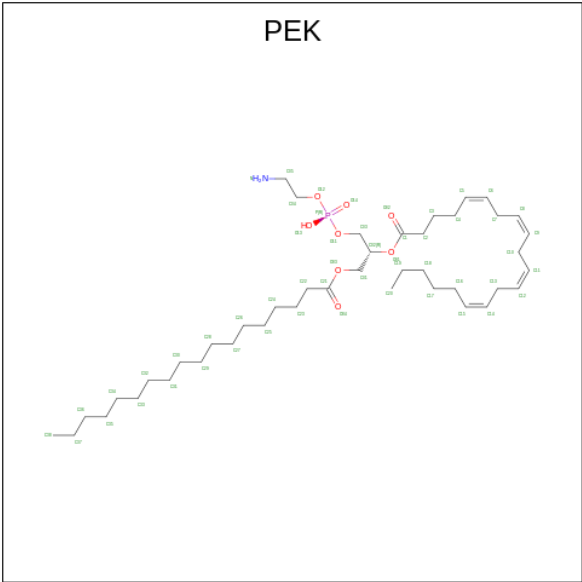
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	K	1	Total C O 33 22 11	0	0
24	K	1	Total C 10 10	0	0
24	K	1	Total C 9 9	0	0
24	K	1	Total C 9 9	0	0
24	L	1	Total C O 21 16 5	0	0
24	M	1	Total C O 33 22 11	0	0
24	O	1	Total C 10 10	0	0
24	P	1	Total C O 33 22 11	0	0
24	P	1	Total C O 11 10 1	0	0
24	W	1	Total C 9 9	0	0
24	X	1	Total C O 33 22 11	0	0
24	X	1	Total C 10 10	0	0
24	X	1	Total C 9 9	0	0
24	X	1	Total C 10 10	0	0
24	X	1	Total C O 11 10 1	0	0
24	Z	1	Total C O 33 22 11	0	0

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total	C	O	0	0
			56	52	4		
25	G	1	Total	C	O	0	0
			64	63	1		
25	P	1	Total	C	O	0	0
			69	65	4		
25	T	1	Total	C	O	0	0
			79	73	6		

- Molecule 26 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).

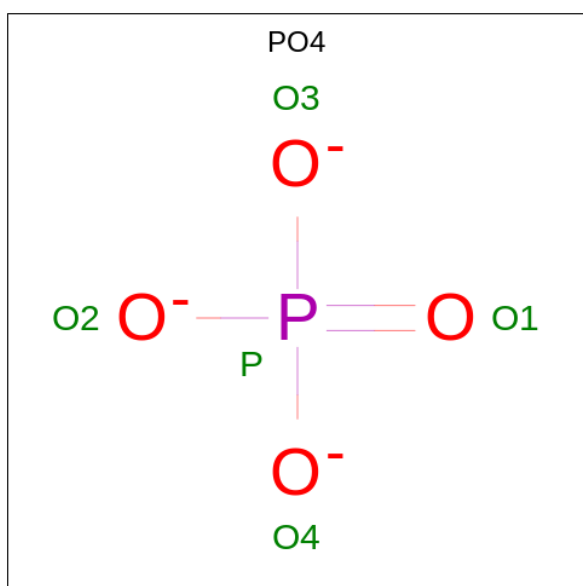


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C 37 37	0	0
26	C	1	Total C 26 26	0	0
26	G	1	Total C N O P 53 43 1 8 1	0	0
26	P	1	Total C 20 20	0	0
26	P	1	Total C N O P 53 43 1 8 1	0	0
26	P	1	Total C O 39 37 2	0	0

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

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

- Molecule 28 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	H	1	Total O P 5 4 1	0	0
28	U	1	Total O P 5 4 1	0	0

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	266	Total O 266 266	0	1
29	B	232	Total O 233 233	0	1
29	C	161	Total O 161 161	0	0
29	D	232	Total O 232 232	0	0
29	E	171	Total O 171 171	0	0
29	F	187	Total O 187 187	0	1
29	G	101	Total O 101 101	0	0
29	H	121	Total O 121 121	0	0
29	I	75	Total O 75 75	0	0
29	J	63	Total O 63 63	0	0
29	K	55	Total O 55 55	0	0
29	L	53	Total O 53 53	0	0
29	M	48	Total O 48 48	0	0
29	N	265	Total O 265 265	0	0
29	O	203	Total O 204 204	0	1
29	P	180	Total O 180 180	0	1
29	Q	133	Total O 133 133	0	0
29	R	148	Total O 148 148	0	0
29	S	174	Total O 174 174	0	0
29	T	84	Total O 84 84	0	0
29	U	103	Total O 103 103	0	0

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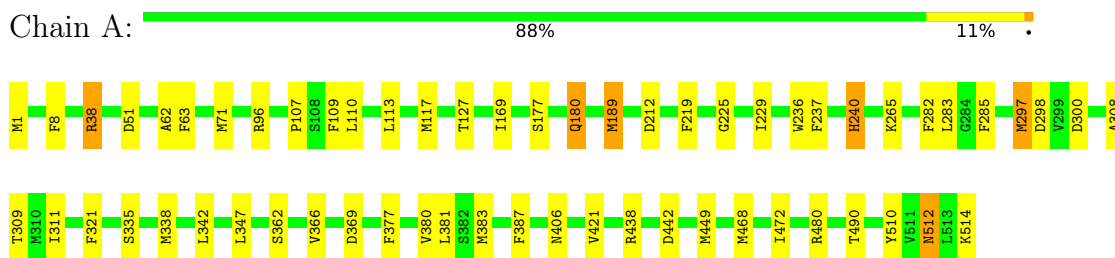
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	V	69	Total 69	O 69	0	0
29	W	66	Total 66	O 66	0	0
29	X	48	Total 48	O 48	0	0
29	Y	35	Total 35	O 35	0	0
29	Z	30	Total 30	O 30	0	0

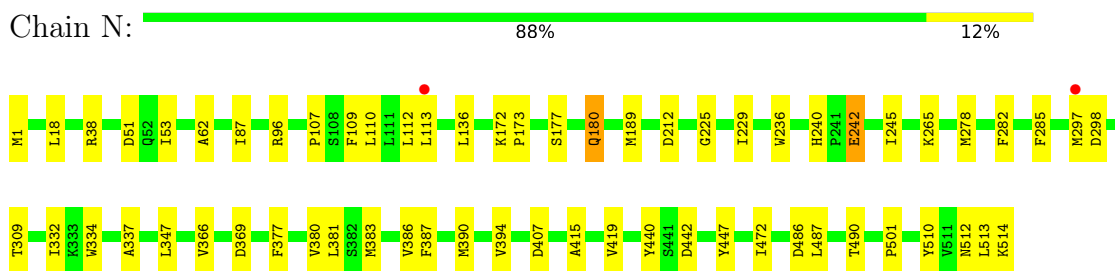
3 Residue-property plots

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

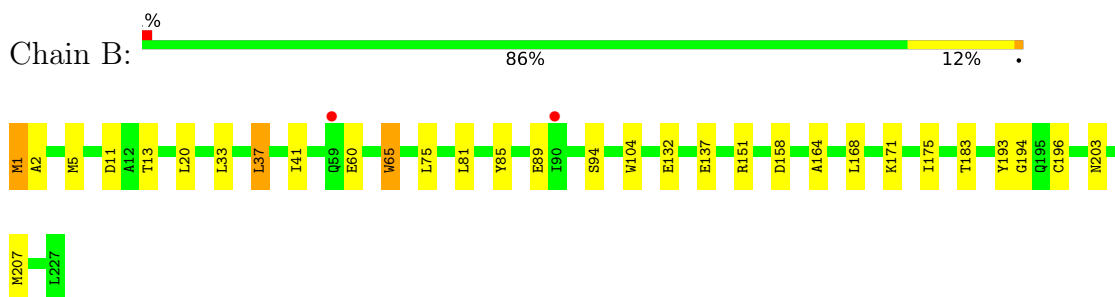
• Molecule 1: Cytochrome c oxidase subunit 1



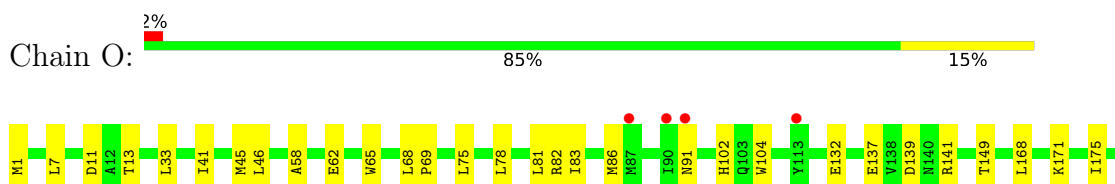
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2





- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 93% 7%



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 93% 7%



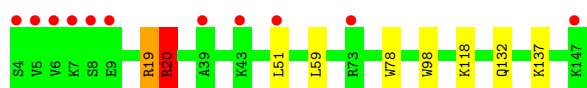
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 90% 9% .



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

Chain Q: 8% 94% 5% ..



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

Chain E: 3% 96% .

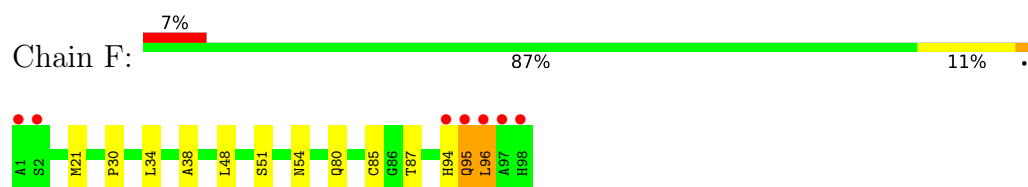


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

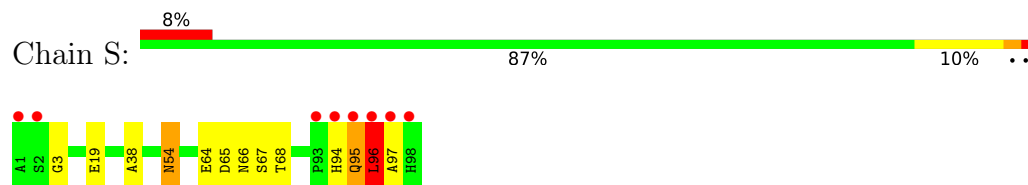
Chain R: 2% 97% .



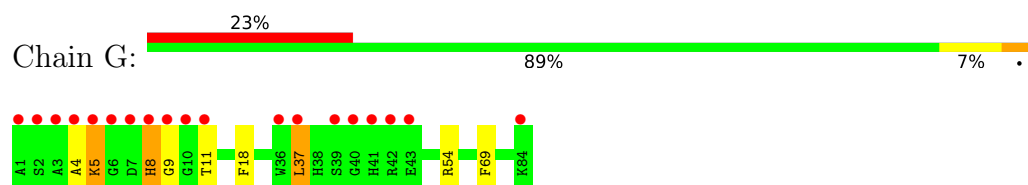
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



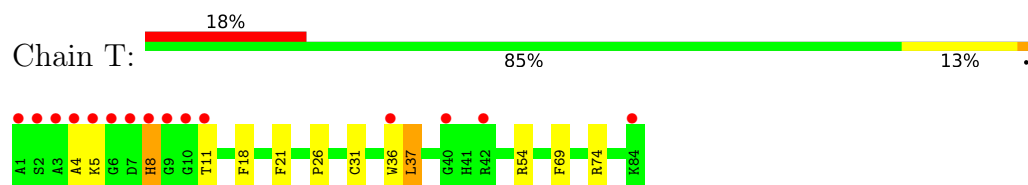
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



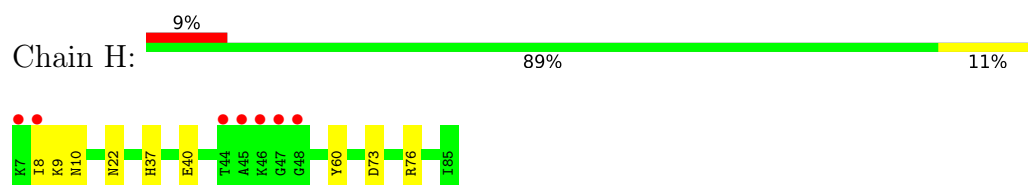
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



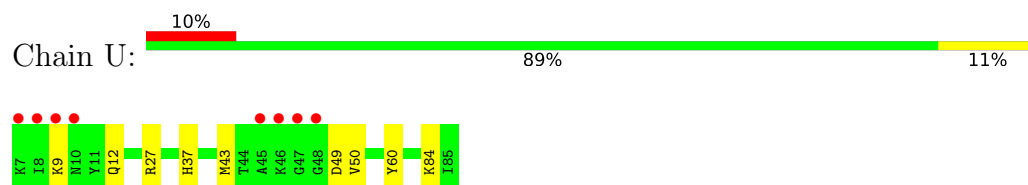
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



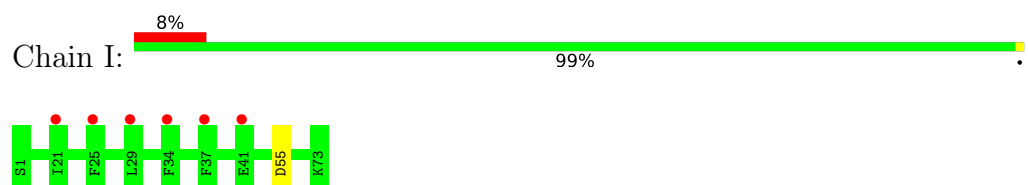
- Molecule 8: Cytochrome c oxidase subunit 6B1



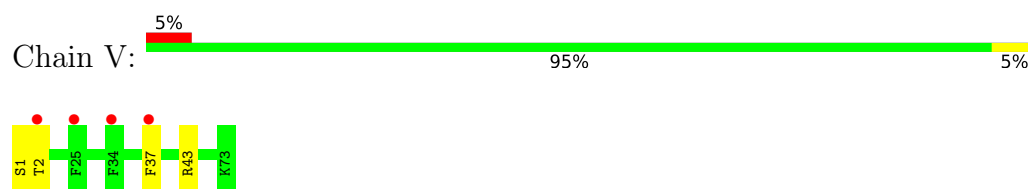
- Molecule 8: Cytochrome c oxidase subunit 6B1



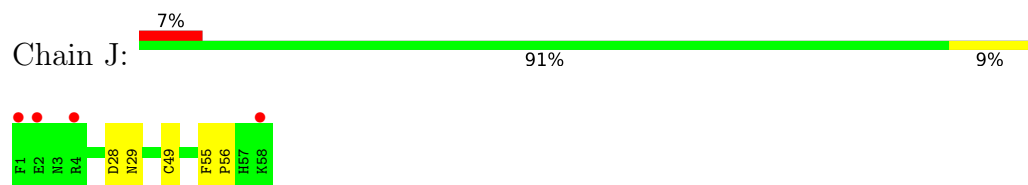
- Molecule 9: Cytochrome c oxidase subunit 6C



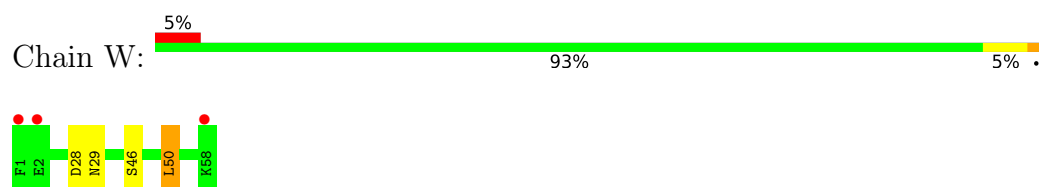
● Molecule 9: Cytochrome c oxidase subunit 6C



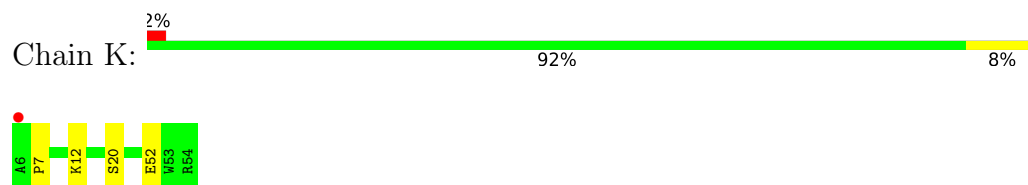
● Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



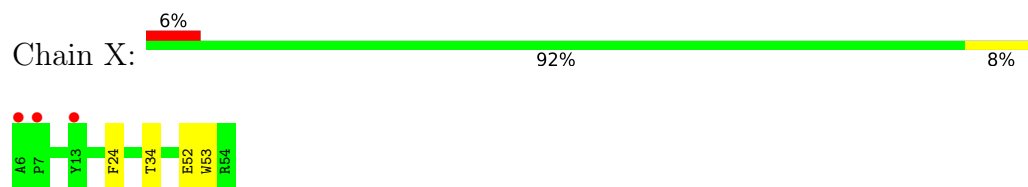
● Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



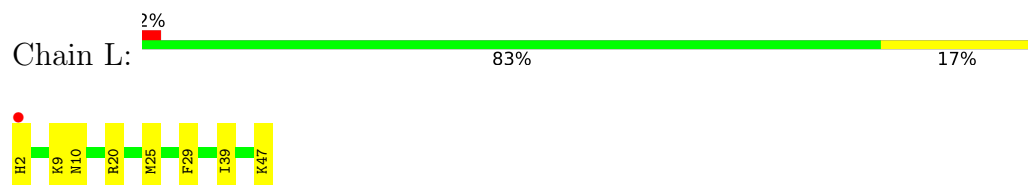
● Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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



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

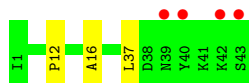


● Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

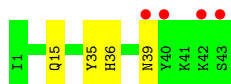
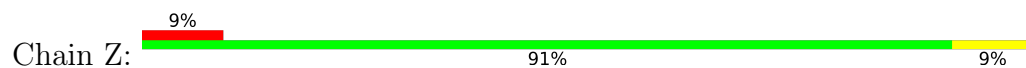




- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



- 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	181.61Å 204.14Å 177.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 1.60 88.98 – 1.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.90-1.60) 96.5 (88.98-1.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.40Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.168 , 0.191 0.169 , 0.192	Depositor DCC
R_{free} test set	61730 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34425	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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: SAC, PEK, HEA, FME, PSC, DMU, PGV, PO4, ZN, CU, TGL, CUA, EDO, NA, CHD, CDL, MG

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	1.07	4/4306 (0.1%)	1.06	20/5877 (0.3%)
1	N	1.01	3/4321 (0.1%)	0.99	13/5896 (0.2%)
2	B	0.96	0/1912	1.00	3/2603 (0.1%)
2	O	0.82	1/1900 (0.1%)	0.92	6/2588 (0.2%)
3	C	0.95	1/2261 (0.0%)	0.89	3/3090 (0.1%)
3	P	0.95	1/2260 (0.0%)	0.89	3/3088 (0.1%)
4	D	0.86	1/1284 (0.1%)	1.19	3/1730 (0.2%)
4	Q	0.65	0/1237	0.72	2/1668 (0.1%)
5	E	0.82	1/882 (0.1%)	0.89	2/1196 (0.2%)
5	R	0.71	0/871	0.71	0/1182
6	F	0.84	0/797	0.89	0/1082
6	S	0.76	0/772	0.82	0/1048
7	G	0.80	0/710	0.80	0/966
7	T	0.70	0/732	0.74	0/997
8	H	0.82	0/682	0.89	2/921 (0.2%)
8	U	0.81	0/682	0.76	0/921
9	I	0.67	0/605	0.73	1/802 (0.1%)
9	V	0.63	0/613	0.71	1/812 (0.1%)
10	J	0.62	0/471	0.72	2/636 (0.3%)
10	W	0.60	0/471	0.71	1/636 (0.2%)
11	K	0.80	0/405	0.75	0/556
11	X	0.61	0/405	0.61	0/556
12	L	1.03	0/393	0.85	0/526
12	Y	0.82	0/393	0.71	0/526
13	M	0.85	0/345	0.83	0/470
13	Z	0.84	1/345 (0.3%)	0.68	0/470
All	All	0.90	13/30055 (0.0%)	0.91	62/40843 (0.2%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Z	35	TYR	CD2-CE2	9.30	1.53	1.39
4	D	20	ARG	CZ-NH1	7.52	1.42	1.33
3	C	102	TYR	CG-CD2	-6.33	1.30	1.39
3	P	153	GLU	CG-CD	6.09	1.61	1.51
5	E	70	VAL	CB-CG1	-5.90	1.40	1.52

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	ARG	NE-CZ-NH1	25.98	133.29	120.30
4	D	20	ARG	NE-CZ-NH2	-22.15	109.23	120.30
1	N	189	MET	CG-SD-CE	-11.60	81.63	100.20
4	Q	20	ARG	NE-CZ-NH1	10.25	125.43	120.30
4	Q	20	ARG	NE-CZ-NH2	-9.69	115.46	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain

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	4107	0	4099	42	0
1	N	4107	0	4086	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1844	0	1850	19	0
2	O	1841	0	1841	17	0
3	C	2126	0	2026	17	0
3	P	2129	0	2043	13	0
4	D	1214	0	1203	11	0
4	Q	1196	0	1180	8	0
5	E	858	0	854	0	0
5	R	852	0	845	1	0
6	F	758	0	736	10	0
6	S	750	0	731	10	0
7	G	677	0	650	8	0
7	T	687	0	657	12	0
8	H	662	0	623	6	0
8	U	662	0	623	4	0
9	I	601	0	613	0	0
9	V	602	0	610	1	0
10	J	460	0	459	5	0
10	W	460	0	459	3	0
11	K	386	0	371	3	0
11	X	386	0	371	3	0
12	L	380	0	380	8	0
12	Y	380	0	380	3	0
13	M	335	0	352	3	0
13	Z	335	0	352	2	0
14	A	130	0	90	7	0
14	N	130	0	90	7	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	88	0	140	6	0
18	C	87	0	136	5	0
18	N	91	0	142	2	0
18	P	91	0	138	2	0
19	A	62	0	110	1	0
19	D	63	0	110	5	0
19	L	59	0	99	6	0
19	N	57	0	103	5	0
19	O	58	0	96	1	0
19	Q	63	0	110	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	25	0	41	3	0
20	O	24	0	40	0	0
21	A	40	0	59	5	0
21	B	16	0	24	2	0
21	C	20	0	30	0	0
21	E	8	0	12	0	0
21	F	20	0	30	3	0
21	G	4	0	6	0	0
21	J	8	0	12	0	0
21	N	52	0	78	4	0
21	O	12	0	18	1	0
21	P	12	0	18	0	0
21	Q	12	0	18	0	0
21	R	4	0	6	0	0
21	S	20	0	30	3	0
21	T	8	0	12	0	0
21	W	8	0	12	0	0
21	Y	4	0	6	0	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	29	0	39	0	0
23	C	29	0	39	0	0
23	G	29	0	39	1	0
23	J	29	0	39	1	0
23	P	58	0	78	1	0
24	C	21	0	38	2	0
24	D	21	0	38	1	0
24	J	12	0	21	0	0
24	K	80	0	127	2	0
24	L	21	0	30	4	0
24	M	33	0	42	0	0
24	O	10	0	19	0	0
24	P	44	0	63	4	0
24	W	9	0	17	0	0
24	X	73	0	116	2	0
24	Z	33	0	42	1	0
25	C	56	0	89	7	0
25	G	64	0	122	9	0
25	P	69	0	121	2	0
25	T	79	0	139	12	0
26	C	63	0	103	3	0
26	G	53	0	77	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	P	112	0	170	11	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	H	5	0	0	0	0
28	U	5	0	0	0	0
29	A	266	0	0	3	0
29	B	233	0	0	1	0
29	C	161	0	0	0	0
29	D	232	0	0	1	0
29	E	171	0	0	0	0
29	F	187	0	0	4	0
29	G	101	0	0	0	0
29	H	121	0	0	2	0
29	I	75	0	0	1	0
29	J	63	0	0	0	0
29	K	55	0	0	0	0
29	L	53	0	0	2	0
29	M	48	0	0	0	0
29	N	265	0	0	4	0
29	O	204	0	0	1	0
29	P	180	0	0	2	0
29	Q	133	0	0	0	0
29	R	148	0	0	0	0
29	S	174	0	0	3	0
29	T	84	0	0	1	0
29	U	103	0	0	2	0
29	V	69	0	0	0	0
29	W	66	0	0	0	0
29	X	48	0	0	0	0
29	Y	35	0	0	1	0
29	Z	30	0	0	0	0
All	All	34425	0	31818	275	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 275 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)
6:S:68:THR:H	21:S:103:EDO:H12	1.43	0.82
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:213:THR:HG23	25:C:303:CDL:H771	1.68	0.74
25:T:101:CDL:H541	25:T:101:CDL:H231	1.72	0.71
7:G:9:GLY:HA3	29:N:707:HOH:O	1.91	0.70

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	532/514 (104%)	517 (97%)	15 (3%)	0	100	100
1	N	534/514 (104%)	522 (98%)	12 (2%)	0	100	100
2	B	231/227 (102%)	226 (98%)	5 (2%)	0	100	100
2	O	229/227 (101%)	222 (97%)	7 (3%)	0	100	100
3	C	265/259 (102%)	260 (98%)	5 (2%)	0	100	100
3	P	265/259 (102%)	260 (98%)	5 (2%)	0	100	100
4	D	148/144 (103%)	145 (98%)	3 (2%)	0	100	100
4	Q	143/144 (99%)	138 (96%)	5 (4%)	0	100	100
5	E	104/105 (99%)	104 (100%)	0	0	100	100
5	R	103/105 (98%)	103 (100%)	0	0	100	100
6	F	100/98 (102%)	95 (95%)	3 (3%)	2 (2%)	7	1
6	S	97/98 (99%)	90 (93%)	4 (4%)	3 (3%)	4	0
7	G	83/84 (99%)	72 (87%)	10 (12%)	1 (1%)	13	2
7	T	85/84 (101%)	75 (88%)	9 (11%)	1 (1%)	13	2
8	H	77/79 (98%)	72 (94%)	4 (5%)	1 (1%)	12	2
8	U	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	V	72/73 (99%)	69 (96%)	3 (4%)	0	100	100
10	J	56/58 (97%)	56 (100%)	0	0	100	100
10	W	56/58 (97%)	56 (100%)	0	0	100	100
11	K	48/49 (98%)	46 (96%)	2 (4%)	0	100	100
11	X	48/49 (98%)	47 (98%)	1 (2%)	0	100	100
12	L	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
13	M	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/43 (95%)	41 (100%)	0	0	100	100
All	All	3594/3558 (101%)	3486 (97%)	100 (3%)	8 (0%)	47	26

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	S	96	LEU
6	F	96	LEU
6	F	95	GLN
6	S	95	GLN
7	G	5	LYS

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	444/426 (104%)	436 (98%)	8 (2%)	59	36
1	N	446/426 (105%)	443 (99%)	3 (1%)	84	73
2	B	216/210 (103%)	209 (97%)	7 (3%)	39	15
2	O	214/210 (102%)	210 (98%)	4 (2%)	57	34
3	C	232/224 (104%)	230 (99%)	2 (1%)	78	65
3	P	232/224 (104%)	230 (99%)	2 (1%)	78	65
4	D	134/128 (105%)	133 (99%)	1 (1%)	84	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Q	129/128 (101%)	127 (98%)	2 (2%)	62	41
5	E	93/92 (101%)	92 (99%)	1 (1%)	73	57
5	R	92/92 (100%)	91 (99%)	1 (1%)	73	57
6	F	85/81 (105%)	84 (99%)	1 (1%)	71	54
6	S	82/81 (101%)	80 (98%)	2 (2%)	49	24
7	G	69/68 (102%)	63 (91%)	6 (9%)	10	1
7	T	71/68 (104%)	64 (90%)	7 (10%)	8	1
8	H	71/71 (100%)	70 (99%)	1 (1%)	67	47
8	U	71/71 (100%)	67 (94%)	4 (6%)	21	5
9	I	57/57 (100%)	57 (100%)	0	100	100
9	V	58/57 (102%)	57 (98%)	1 (2%)	60	38
10	J	49/49 (100%)	49 (100%)	0	100	100
10	W	49/49 (100%)	48 (98%)	1 (2%)	55	31
11	K	40/39 (103%)	40 (100%)	0	100	100
11	X	40/39 (103%)	39 (98%)	1 (2%)	47	22
12	L	39/39 (100%)	37 (95%)	2 (5%)	24	6
12	Y	39/39 (100%)	38 (97%)	1 (3%)	46	21
13	M	37/37 (100%)	37 (100%)	0	100	100
13	Z	37/37 (100%)	37 (100%)	0	100	100
All	All	3126/3042 (103%)	3068 (98%)	58 (2%)	59	34

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	47	LYS
10	W	50	LEU
2	O	217	LYS
9	V	37	PHE
7	T	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
8	U	12	GLN

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Mol	Chain	Res	Type
8	U	23	GLN
11	X	15	ASN
8	H	37	HIS
5	E	94	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FME	B	1	2	8,9,10	2.48	2 (25%)	7,9,11	2.87	3 (42%)
9	SAC	I	1	9	7,8,9	0.64	0	8,9,11	0.79	0
1	FME	A	1	1	8,9,10	0.57	0	7,9,11	1.52	2 (28%)
9	SAC	V	1	9	7,8,9	0.59	0	8,9,11	0.81	0
2	FME	O	1	2	8,9,10	0.95	0	7,9,11	1.05	1 (14%)
1	FME	N	1	1	8,9,10	0.52	0	7,9,11	1.51	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	B	1	2	-	0/7/9/11	-
9	SAC	I	1	9	-	3/7/8/10	-
1	FME	A	1	1	-	5/7/9/11	-
9	SAC	V	1	9	-	3/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CN-N	5.96	1.53	1.33
2	B	1	FME	CG-SD	-2.01	1.70	1.81

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-5.90	113.75	122.82
2	B	1	FME	C-CA-N	3.91	116.80	109.73
1	N	1	FME	O-C-CA	-2.68	117.76	124.78
2	O	1	FME	O-C-CA	-2.31	118.71	124.78
1	N	1	FME	CG-CB-CA	-2.25	106.69	112.95

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	C-CA-N-C1A

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FME	2	0
9	V	1	SAC	1	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 135 ligands modelled in this entry, 8 are monoatomic - leaving 127 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
21	EDO	B	303	-	3,3,3	0.57	0	2,2,2	0.35	0
21	EDO	A	615	-	3,3,3	0.70	0	2,2,2	0.78	0
21	EDO	S	102	-	3,3,3	0.51	0	2,2,2	0.74	0
26	PEK	P	308	-	52,52,52	0.73	2 (3%)	55,57,57	1.53	7 (12%)
24	DMU	C	301	-	8,8,34	0.33	0	7,7,45	0.36	0
19	TGL	D	201	-	62,62,62	1.08	3 (4%)	65,65,65	1.15	6 (9%)
21	EDO	C	311	-	3,3,3	0.70	0	2,2,2	0.23	0
18	PGV	N	606	-	39,39,50	1.09	2 (5%)	40,40,56	1.15	4 (10%)
24	DMU	K	105	-	8,8,34	0.24	0	7,7,45	0.56	0
19	TGL	Q	201	-	62,62,62	1.00	3 (4%)	65,65,65	1.04	6 (9%)
28	PO4	H	101	-	4,4,4	1.10	0	6,6,6	0.48	0
21	EDO	P	313	-	3,3,3	0.82	0	2,2,2	0.44	0
21	EDO	A	612	-	3,3,3	0.64	0	2,2,2	0.24	0
22	CUA	B	301	2	0,1,1	-	-	-	-	-
14	HEA	A	601[B]	-	44,67,67	1.42	6 (13%)	37,103,103	2.38	14 (37%)
21	EDO	N	614	-	3,3,3	0.49	0	2,2,2	0.31	0
21	EDO	A	619	-	3,3,3	1.19	0	2,2,2	0.90	0
18	PGV	A	607	-	32,35,50	0.27	0	30,34,56	0.83	0
14	HEA	N	602	1	44,67,67	1.21	3 (6%)	37,103,103	1.86	6 (16%)
24	DMU	O	304	-	9,9,34	0.22	0	8,8,45	0.47	0
24	DMU	X	101	-	34,34,34	0.42	0	45,45,45	0.80	1 (2%)
24	DMU	D	202	-	11,11,34	0.29	0	10,10,45	0.30	0
18	PGV	A	606	-	50,50,50	0.89	2 (4%)	53,56,56	0.86	1 (1%)
23	CHD	G	103	-	29,32,32	0.86	1 (3%)	48,51,51	1.49	7 (14%)
14	HEA	A	601[A]	-	44,67,67	1.47	7 (15%)	37,103,103	2.19	11 (29%)
21	EDO	J	104	-	3,3,3	0.38	0	2,2,2	0.48	0
18	PGV	N	607	-	50,50,50	1.06	4 (8%)	53,56,56	1.11	4 (7%)
14	HEA	A	602	1	44,67,67	1.42	6 (13%)	37,103,103	1.93	13 (35%)
21	EDO	C	310	-	3,3,3	0.79	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	DMU	P	310	-	10,10,34	0.28	0	9,9,45	0.53	0
21	EDO	N	619	-	3,3,3	0.30	0	2,2,2	1.47	0
21	EDO	N	611	-	3,3,3	0.66	0	2,2,2	0.76	0
24	DMU	K	106	-	8,8,34	0.26	0	7,7,45	0.52	0
24	DMU	C	308	-	11,11,34	0.33	0	10,10,45	0.51	0
21	EDO	N	610	-	3,3,3	1.04	0	2,2,2	0.60	0
21	EDO	C	312	-	3,3,3	0.61	0	2,2,2	0.10	0
26	PEK	G	101	-	52,52,52	0.97	4 (7%)	55,57,57	1.60	8 (14%)
21	EDO	T	103	-	3,3,3	0.42	0	2,2,2	0.51	0
14	HEA	N	601[B]	-	44,67,67	1.34	5 (11%)	37,103,103	2.38	12 (32%)
21	EDO	N	609	-	3,3,3	0.73	0	2,2,2	0.11	0
24	DMU	J	102	-	10,10,34	0.24	0	9,9,45	0.60	0
21	EDO	S	104	-	3,3,3	0.57	0	2,2,2	0.73	0
21	EDO	F	103	-	3,3,3	0.61	0	2,2,2	0.35	0
21	EDO	N	616	-	3,3,3	1.02	0	2,2,2	0.93	0
21	EDO	N	618	-	3,3,3	0.44	0	2,2,2	0.41	0
18	PGV	P	304	-	49,49,50	1.06	4 (8%)	52,55,56	2.06	7 (13%)
21	EDO	A	617	-	3,3,3	0.51	0	2,2,2	0.56	0
21	EDO	B	306	-	3,3,3	0.88	0	2,2,2	0.60	0
24	DMU	K	104	-	8,8,34	0.24	0	7,7,45	0.43	0
21	EDO	N	612	-	3,3,3	0.52	0	2,2,2	0.44	0
21	EDO	O	306	-	3,3,3	0.62	0	2,2,2	0.13	0
21	EDO	N	621	-	3,3,3	0.78	0	2,2,2	0.23	0
24	DMU	X	102	-	9,9,34	0.24	0	8,8,45	0.50	0
21	EDO	F	105	-	3,3,3	0.55	0	2,2,2	0.68	0
19	TGL	O	301	-	56,56,62	1.07	3 (5%)	58,58,65	1.30	5 (8%)
28	PO4	U	101	-	4,4,4	1.02	0	6,6,6	0.35	0
21	EDO	C	313	-	3,3,3	0.66	0	2,2,2	0.48	0
24	DMU	Z	101	-	34,34,34	0.55	1 (2%)	45,45,45	0.83	0
21	EDO	Y	101	-	3,3,3	0.55	0	2,2,2	0.43	0
23	CHD	B	302	-	29,32,32	1.21	3 (10%)	48,51,51	1.84	14 (29%)
19	TGL	L	101	-	58,58,62	1.08	3 (5%)	61,61,65	1.33	8 (13%)
21	EDO	F	102	-	3,3,3	0.67	0	2,2,2	0.51	0
21	EDO	E	201	-	3,3,3	0.57	0	2,2,2	0.46	0
26	PEK	P	301	-	19,19,52	0.23	0	18,18,57	0.52	0
18	PGV	C	302	-	50,50,50	0.81	1 (2%)	53,56,56	0.87	1 (1%)
21	EDO	S	106	-	3,3,3	0.34	0	2,2,2	0.19	0
26	PEK	P	309	-	37,37,52	0.74	1 (2%)	35,36,57	0.83	1 (2%)
26	PEK	C	307	-	24,24,52	0.29	0	22,22,57	0.45	0
21	EDO	N	620	-	3,3,3	0.42	0	2,2,2	0.61	0
21	EDO	O	305	-	3,3,3	0.69	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CDL	P	305	-	66,66,99	1.37	9 (13%)	65,65,111	1.00	1 (1%)
21	EDO	S	105	-	3,3,3	0.67	0	2,2,2	0.53	0
25	CDL	T	101	-	73,76,99	1.34	11 (15%)	73,77,111	1.38	3 (4%)
25	CDL	G	102	-	60,60,99	1.19	8 (13%)	56,56,111	0.77	0
14	HEA	N	601[A]	-	44,67,67	1.24	6 (13%)	37,103,103	2.30	15 (40%)
26	PEK	C	305	-	35,35,52	0.24	0	33,33,57	0.51	0
25	CDL	C	303	-	52,52,99	1.14	5 (9%)	50,50,111	1.06	2 (4%)
21	EDO	Q	203	-	3,3,3	0.34	0	2,2,2	0.73	0
24	DMU	X	103	-	8,8,34	0.27	0	7,7,45	0.50	0
21	EDO	P	311	-	3,3,3	0.57	0	2,2,2	0.30	0
21	EDO	Q	204	-	3,3,3	0.48	0	2,2,2	0.42	0
21	EDO	W	103	-	3,3,3	0.46	0	2,2,2	0.19	0
21	EDO	F	106	-	3,3,3	0.84	0	2,2,2	0.45	0
21	EDO	C	309	-	3,3,3	0.62	0	2,2,2	1.06	0
24	DMU	D	203	-	8,8,34	0.28	0	7,7,45	0.48	0
19	TGL	N	608	-	54,54,62	0.65	1 (1%)	52,52,65	0.79	1 (1%)
21	EDO	A	613	-	3,3,3	0.64	0	2,2,2	0.58	0
21	EDO	O	307	-	3,3,3	0.63	0	2,2,2	0.24	0
21	EDO	Q	202	-	3,3,3	0.53	0	2,2,2	0.13	0
21	EDO	A	610	-	3,3,3	0.93	0	2,2,2	1.20	0
21	EDO	A	618	-	3,3,3	0.38	0	2,2,2	0.60	0
18	PGV	C	306	-	34,34,50	0.93	1 (2%)	33,33,56	1.06	2 (6%)
20	PSC	A	609	-	23,23,51	0.81	1 (4%)	20,21,59	0.77	0
21	EDO	R	201	-	3,3,3	0.81	0	2,2,2	0.42	0
21	EDO	T	102	-	3,3,3	0.64	0	2,2,2	0.28	0
23	CHD	P	306	-	29,32,32	0.70	0	48,51,51	1.39	7 (14%)
24	DMU	K	103	-	34,34,34	0.54	1 (2%)	45,45,45	0.97	2 (4%)
21	EDO	N	613	-	3,3,3	0.65	0	2,2,2	0.40	0
23	CHD	C	304	-	29,32,32	0.98	1 (3%)	48,51,51	1.91	17 (35%)
20	PSC	O	303	-	22,22,51	0.81	1 (4%)	20,20,59	0.85	0
24	DMU	W	101	-	8,8,34	0.21	0	7,7,45	0.51	0
21	EDO	N	617	-	3,3,3	0.49	0	2,2,2	0.21	0
23	CHD	J	101	-	29,32,32	0.61	0	48,51,51	1.27	6 (12%)
21	EDO	A	616	-	3,3,3	0.50	0	2,2,2	0.47	0
22	CUA	O	302	2	0,1,1	-	-	-	-	-
21	EDO	P	312	-	3,3,3	0.33	0	2,2,2	0.75	0
21	EDO	B	305	-	3,3,3	0.63	0	2,2,2	0.37	0
21	EDO	B	304	-	3,3,3	0.61	0	2,2,2	0.64	0
21	EDO	A	614	-	3,3,3	0.84	0	2,2,2	0.81	0
21	EDO	N	615	-	3,3,3	0.53	0	2,2,2	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	DMU	K	102	-	8,8,34	0.26	0	7,7,45	0.48	0
21	EDO	J	103	-	3,3,3	0.59	0	2,2,2	0.16	0
24	DMU	L	102	-	21,21,34	0.50	0	24,25,45	1.13	3 (12%)
24	DMU	K	101	-	8,8,34	0.23	0	7,7,45	0.58	0
24	DMU	P	303	-	34,34,34	0.52	1 (2%)	45,45,45	0.79	0
19	TGL	A	608	-	61,61,62	0.85	2 (3%)	63,63,65	1.23	4 (6%)
21	EDO	S	103	-	3,3,3	0.67	0	2,2,2	0.77	0
21	EDO	W	102	-	3,3,3	0.47	0	2,2,2	1.02	0
24	DMU	X	104	-	9,9,34	0.30	0	8,8,45	0.50	0
24	DMU	M	101	-	34,34,34	0.46	0	45,45,45	1.17	3 (6%)
21	EDO	A	611	-	3,3,3	0.55	0	2,2,2	0.63	0
24	DMU	X	105	-	9,9,34	0.22	0	8,8,45	0.56	0
18	PGV	P	302	-	40,40,50	1.12	2 (5%)	42,42,56	1.45	6 (14%)
21	EDO	E	202	-	3,3,3	0.58	0	2,2,2	0.33	0
21	EDO	G	104	-	3,3,3	0.76	0	2,2,2	0.53	0
21	EDO	F	104	-	3,3,3	0.93	0	2,2,2	0.32	0
23	CHD	P	307	-	29,32,32	0.84	1 (3%)	48,51,51	1.37	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	B	303	-	-	0/1/1/1	-
21	EDO	A	615	-	-	0/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
26	PEK	P	308	-	-	16/56/56/56	-
24	DMU	C	301	-	-	3/6/6/59	-
19	TGL	D	201	-	-	15/65/65/65	-
21	EDO	C	311	-	-	1/1/1/1	-
18	PGV	N	606	-	-	11/39/39/55	-
24	DMU	K	105	-	-	0/6/6/59	-
19	TGL	Q	201	-	-	17/65/65/65	-
21	EDO	P	313	-	-	0/1/1/1	-
21	EDO	A	612	-	-	0/1/1/1	-
14	HEA	A	601[B]	-	3/3/7/16	4/24/76/76	-
21	EDO	N	614	-	-	0/1/1/1	-
21	EDO	A	619	-	-	1/1/1/1	-
18	PGV	A	607	-	-	7/28/31/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	N	602	1	3/3/7/16	3/24/76/76	-
24	DMU	O	304	-	-	2/7/7/59	-
24	DMU	X	101	-	-	1/19/59/59	0/2/2/2
24	DMU	D	202	-	-	5/9/9/59	-
18	PGV	A	606	-	-	7/55/55/55	-
23	CHD	G	103	-	-	0/7/74/74	0/4/4/4
14	HEA	A	601[A]	-	3/3/7/16	2/24/76/76	-
21	EDO	J	104	-	-	0/1/1/1	-
18	PGV	N	607	-	-	4/55/55/55	-
14	HEA	A	602	1	3/3/7/16	2/24/76/76	-
21	EDO	C	310	-	-	0/1/1/1	-
24	DMU	P	310	-	-	0/8/8/59	-
21	EDO	N	619	-	-	1/1/1/1	-
21	EDO	N	611	-	-	0/1/1/1	-
24	DMU	K	106	-	-	1/6/6/59	-
24	DMU	C	308	-	-	0/9/9/59	-
21	EDO	N	610	-	-	0/1/1/1	-
21	EDO	C	312	-	-	0/1/1/1	-
26	PEK	G	101	-	-	14/56/56/56	-
21	EDO	T	103	-	-	0/1/1/1	-
14	HEA	N	601[B]	-	3/3/7/16	4/24/76/76	-
21	EDO	N	609	-	-	0/1/1/1	-
24	DMU	J	102	-	-	2/8/8/59	-
21	EDO	S	104	-	-	0/1/1/1	-
21	EDO	F	103	-	-	0/1/1/1	-
21	EDO	N	616	-	-	0/1/1/1	-
21	EDO	N	618	-	-	0/1/1/1	-
18	PGV	P	304	-	-	9/54/54/55	-
21	EDO	A	617	-	-	0/1/1/1	-
21	EDO	B	306	-	-	0/1/1/1	-
24	DMU	K	104	-	-	1/6/6/59	-
21	EDO	N	612	-	-	0/1/1/1	-
21	EDO	O	306	-	-	0/1/1/1	-
21	EDO	N	621	-	-	0/1/1/1	-
24	DMU	X	102	-	-	1/7/7/59	-
21	EDO	F	105	-	-	0/1/1/1	-
19	TGL	O	301	-	-	14/57/57/65	-
21	EDO	C	313	-	-	0/1/1/1	-
24	DMU	Z	101	-	-	5/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	Y	101	-	-	0/1/1/1	-
23	CHD	B	302	-	-	0/7/74/74	0/4/4/4
19	TGL	L	101	-	-	21/61/61/65	-
21	EDO	F	102	-	-	0/1/1/1	-
21	EDO	E	201	-	-	0/1/1/1	-
26	PEK	P	301	-	-	11/17/17/56	-
18	PGV	C	302	-	-	7/55/55/55	-
21	EDO	S	106	-	-	0/1/1/1	-
26	PEK	P	309	-	-	16/34/34/56	-
26	PEK	C	307	-	-	10/20/20/56	-
21	EDO	N	620	-	-	0/1/1/1	-
21	EDO	O	305	-	-	0/1/1/1	-
25	CDL	P	305	-	-	11/62/62/110	-
21	EDO	S	105	-	-	0/1/1/1	-
25	CDL	T	101	-	-	16/71/73/110	-
25	CDL	G	102	-	-	8/51/52/110	-
14	HEA	N	601[A]	-	3/3/7/16	3/24/76/76	-
26	PEK	C	305	-	-	13/31/31/56	-
25	CDL	C	303	-	-	6/47/47/110	-
21	EDO	Q	203	-	-	0/1/1/1	-
24	DMU	X	103	-	-	1/6/6/59	-
21	EDO	P	311	-	-	0/1/1/1	-
21	EDO	Q	204	-	-	1/1/1/1	-
21	EDO	W	103	-	-	1/1/1/1	-
21	EDO	F	106	-	-	0/1/1/1	-
21	EDO	C	309	-	-	0/1/1/1	-
24	DMU	D	203	-	-	1/6/6/59	-
19	TGL	N	608	-	-	14/48/49/65	-
21	EDO	A	613	-	-	1/1/1/1	-
21	EDO	O	307	-	-	0/1/1/1	-
21	EDO	Q	202	-	-	1/1/1/1	-
21	EDO	A	610	-	-	1/1/1/1	-
21	EDO	A	618	-	-	1/1/1/1	-
18	PGV	C	306	-	-	6/31/31/55	-
20	PSC	A	609	-	-	4/19/19/55	-
21	EDO	R	201	-	-	0/1/1/1	-
21	EDO	T	102	-	-	1/1/1/1	-
23	CHD	P	306	-	-	0/7/74/74	0/4/4/4
24	DMU	K	103	-	-	9/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	N	613	-	-	1/1/1/1	-
23	CHD	C	304	-	-	0/7/74/74	0/4/4/4
20	PSC	O	303	-	-	5/18/18/55	-
24	DMU	W	101	-	-	1/6/6/59	-
21	EDO	N	617	-	-	0/1/1/1	-
23	CHD	J	101	-	-	5/7/74/74	0/4/4/4
21	EDO	A	616	-	-	0/1/1/1	-
21	EDO	P	312	-	-	1/1/1/1	-
21	EDO	B	305	-	-	0/1/1/1	-
21	EDO	B	304	-	-	0/1/1/1	-
21	EDO	A	614	-	-	0/1/1/1	-
21	EDO	N	615	-	-	0/1/1/1	-
24	DMU	K	102	-	-	3/6/6/59	-
21	EDO	J	103	-	-	0/1/1/1	-
24	DMU	L	102	-	-	7/13/29/59	0/1/1/2
24	DMU	K	101	-	-	1/6/6/59	-
24	DMU	P	303	-	-	5/19/59/59	0/2/2/2
19	TGL	A	608	-	-	17/63/63/65	-
21	EDO	S	103	-	-	0/1/1/1	-
21	EDO	W	102	-	-	0/1/1/1	-
24	DMU	X	104	-	-	1/7/7/59	-
24	DMU	M	101	-	-	4/19/59/59	0/2/2/2
21	EDO	A	611	-	-	0/1/1/1	-
24	DMU	X	105	-	-	2/7/7/59	-
18	PGV	P	302	-	-	8/41/41/55	-
21	EDO	E	202	-	-	1/1/1/1	-
21	EDO	G	104	-	-	0/1/1/1	-
21	EDO	F	104	-	-	0/1/1/1	-
23	CHD	P	307	-	-	0/7/74/74	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	306	PGV	O03-C19	5.09	1.48	1.33
25	P	305	CDL	OB6-CB5	4.92	1.47	1.33
25	P	305	CDL	OB8-CB7	4.92	1.47	1.33
19	D	201	TGL	OG3-CC1	4.86	1.47	1.33
14	N	601[B]	HEA	C3B-C11	-4.78	1.49	1.52

The worst 5 of 214 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P	304	PGV	O03-C19-O04	-8.99	100.89	123.59
18	P	304	PGV	O03-C19-C20	7.92	136.76	111.91
14	N	602	HEA	CBD-CAD-C3D	7.24	125.84	112.49
25	T	101	CDL	CB4-OB6-CB5	-6.66	109.31	117.88
14	N	601[B]	HEA	C13-C12-C11	-6.43	104.70	114.35

5 of 18 chirality outliers are listed below:

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

5 of 379 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C14-C15-C16-C17
14	A	601[A]	HEA	C26-C15-C16-C17
14	A	602	HEA	C2D-C3D-CAD-CBD
14	A	602	HEA	C4D-C3D-CAD-CBD
14	N	601[A]	HEA	C14-C15-C16-C17

There are no ring outliers.

51 monomers are involved in 140 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	615	EDO	3	0
26	P	308	PEK	7	0
24	C	301	DMU	2	0
19	D	201	TGL	5	0
18	N	606	PGV	2	0
19	Q	201	TGL	7	0
18	A	607	PGV	4	0
14	N	602	HEA	6	0
18	A	606	PGV	2	0
23	G	103	CHD	1	0
14	A	602	HEA	7	0
24	P	310	DMU	1	0
21	N	611	EDO	1	0
26	G	101	PEK	5	0
14	N	601[B]	HEA	1	0

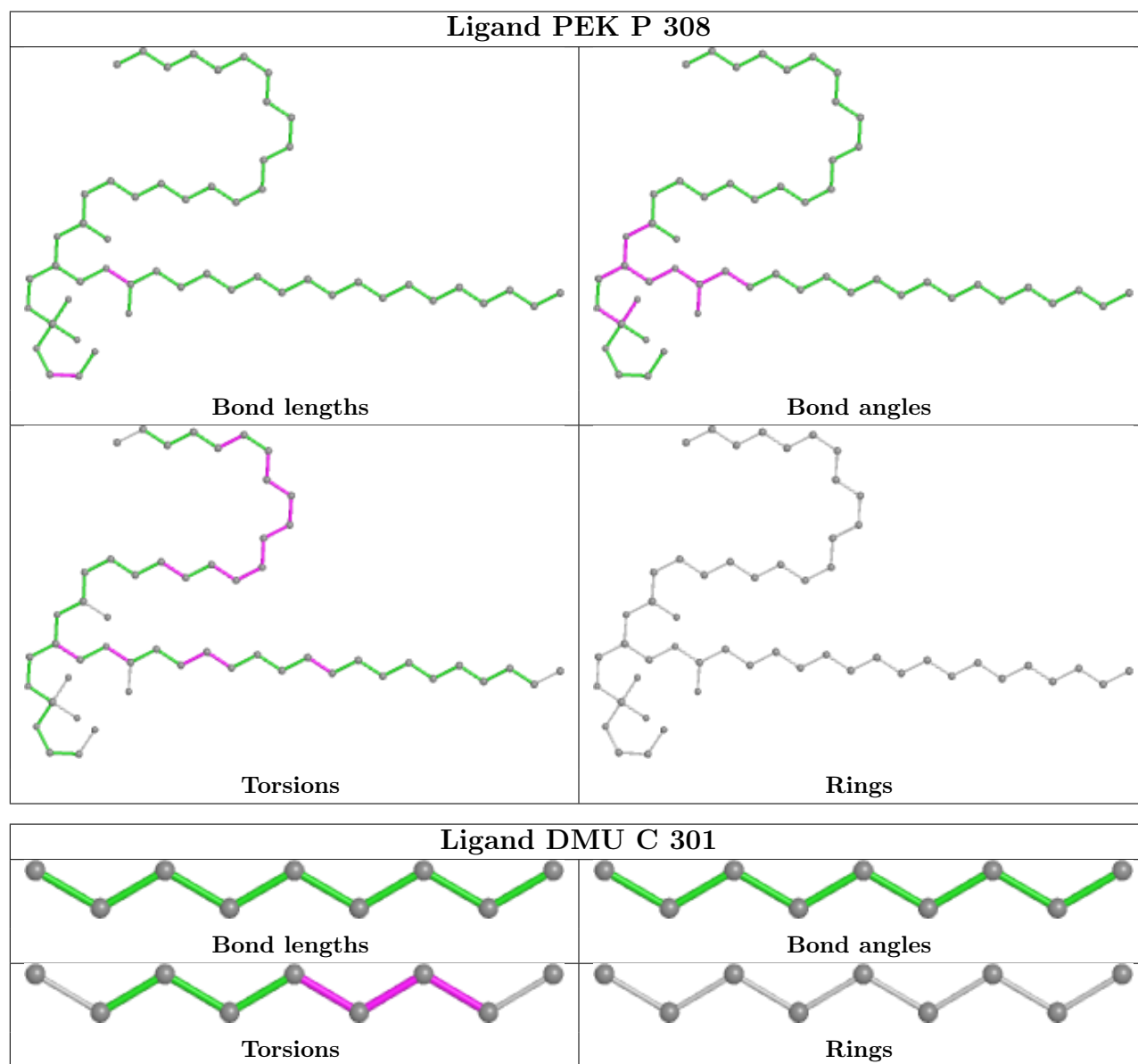
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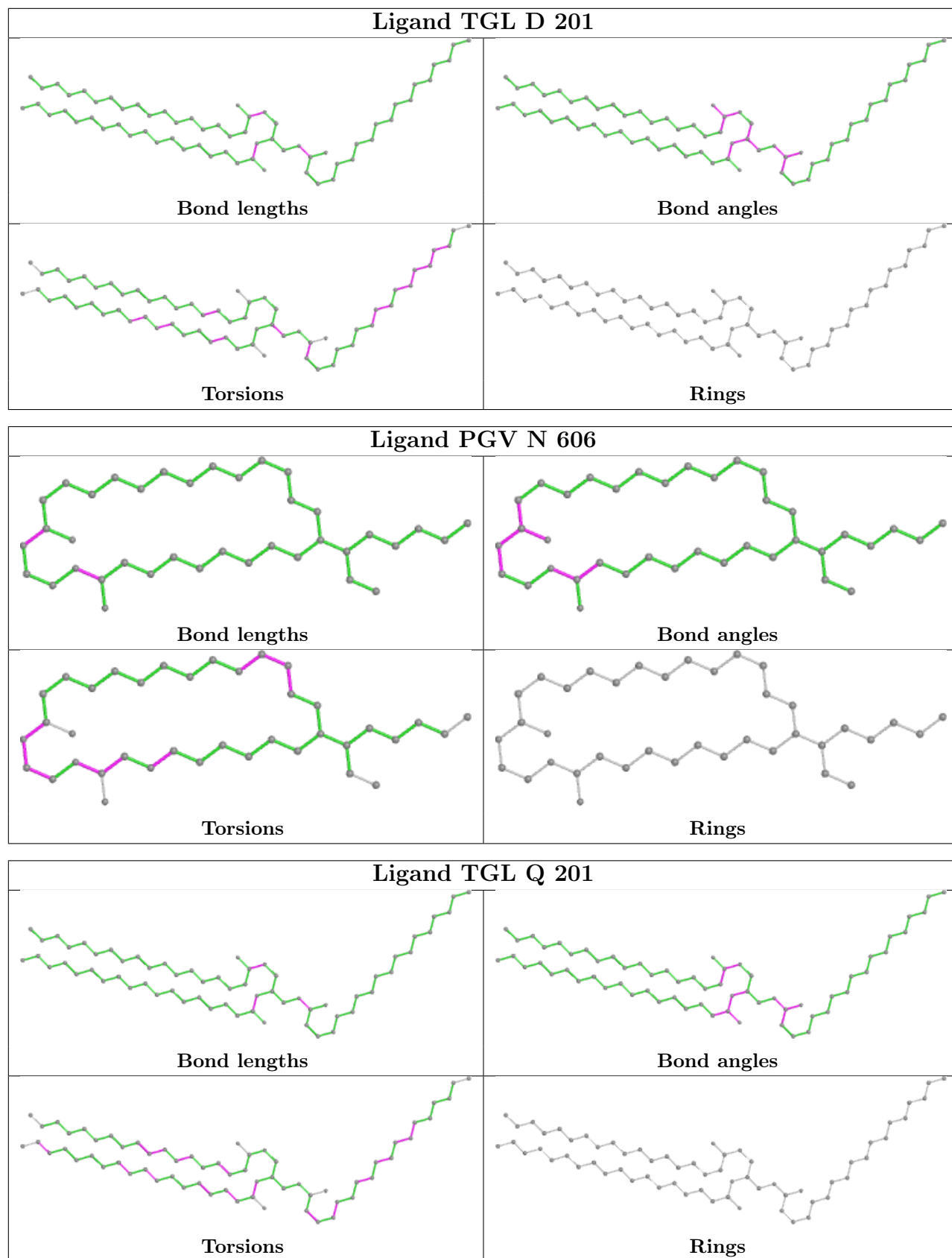
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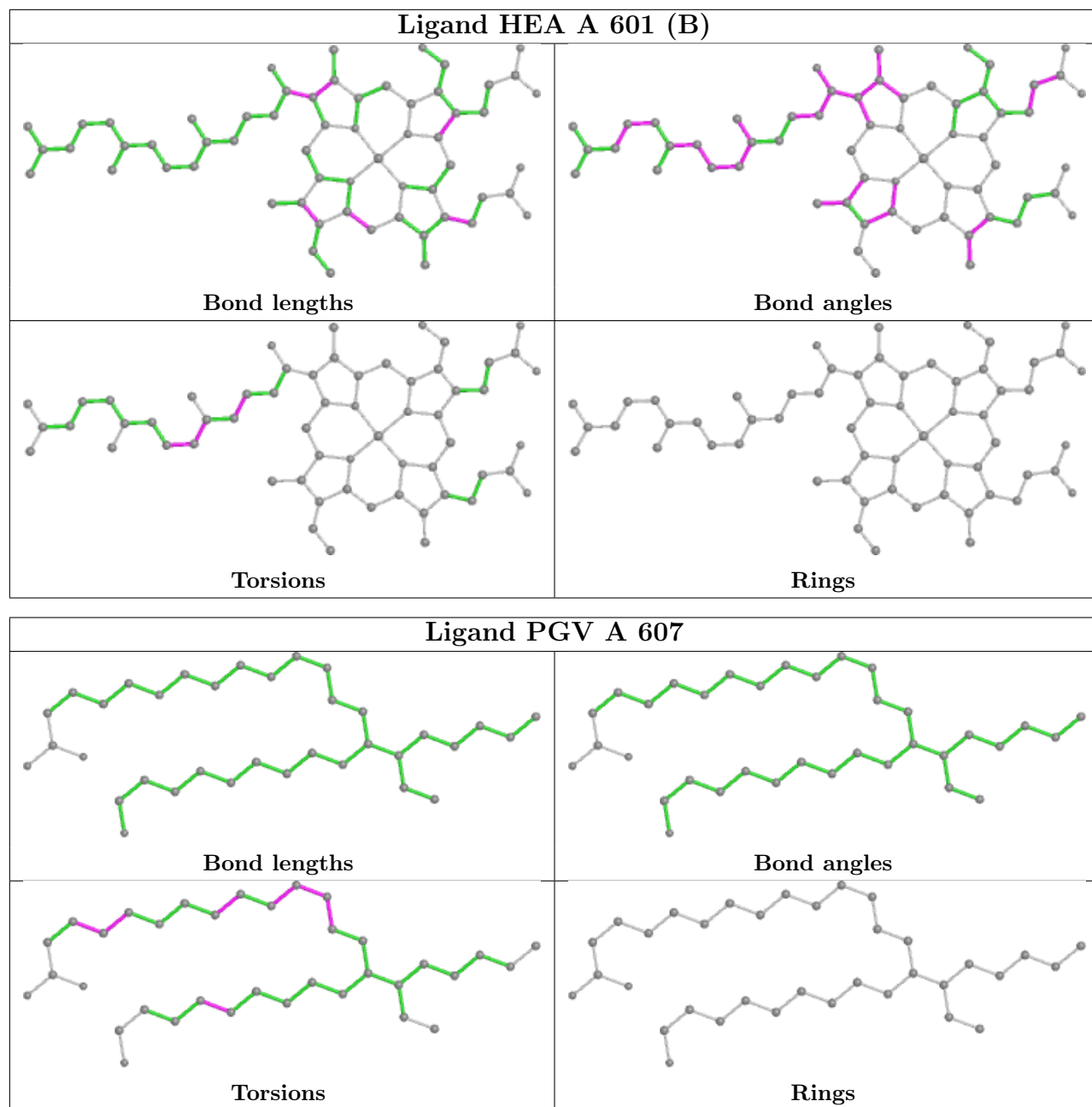
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	F	103	EDO	1	0
18	P	304	PGV	1	0
21	N	621	EDO	2	0
21	F	105	EDO	2	0
19	O	301	TGL	1	0
24	Z	101	DMU	1	0
19	L	101	TGL	6	0
26	P	301	PEK	1	0
18	C	302	PGV	3	0
26	P	309	PEK	3	0
26	C	307	PEK	2	0
25	P	305	CDL	2	0
25	T	101	CDL	12	0
25	G	102	CDL	9	0
26	C	305	PEK	1	0
25	C	303	CDL	7	0
24	X	103	DMU	1	0
24	D	203	DMU	1	0
19	N	608	TGL	5	0
21	O	307	EDO	1	0
21	A	610	EDO	1	0
18	C	306	PGV	2	0
20	A	609	PSC	3	0
23	P	306	CHD	1	0
24	K	103	DMU	2	0
21	N	617	EDO	1	0
23	J	101	CHD	1	0
21	A	616	EDO	2	0
21	B	304	EDO	2	0
21	A	614	EDO	1	0
24	L	102	DMU	4	0
24	P	303	DMU	3	0
19	A	608	TGL	1	0
21	S	103	EDO	3	0
24	X	105	DMU	1	0
18	P	302	PGV	1	0

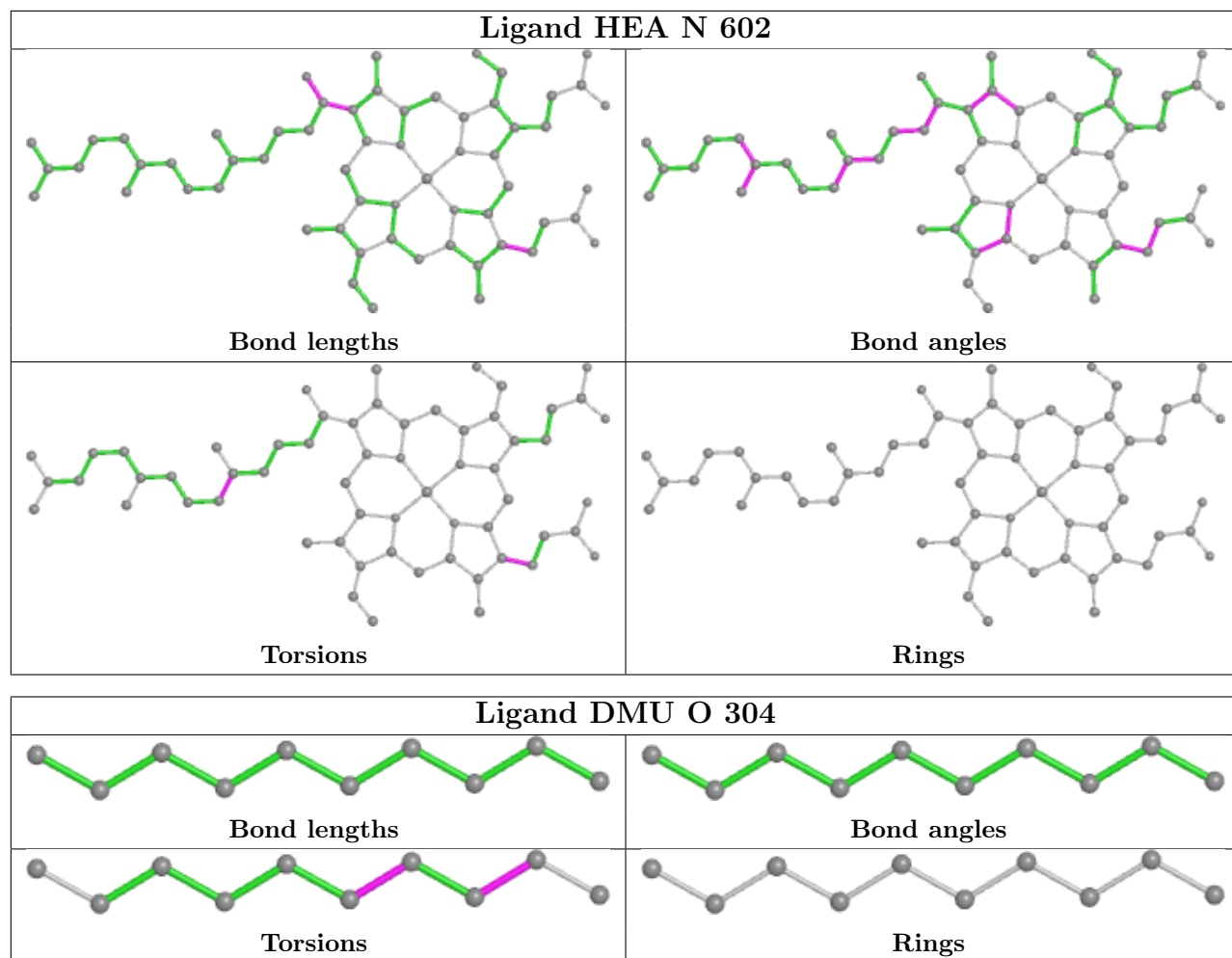
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

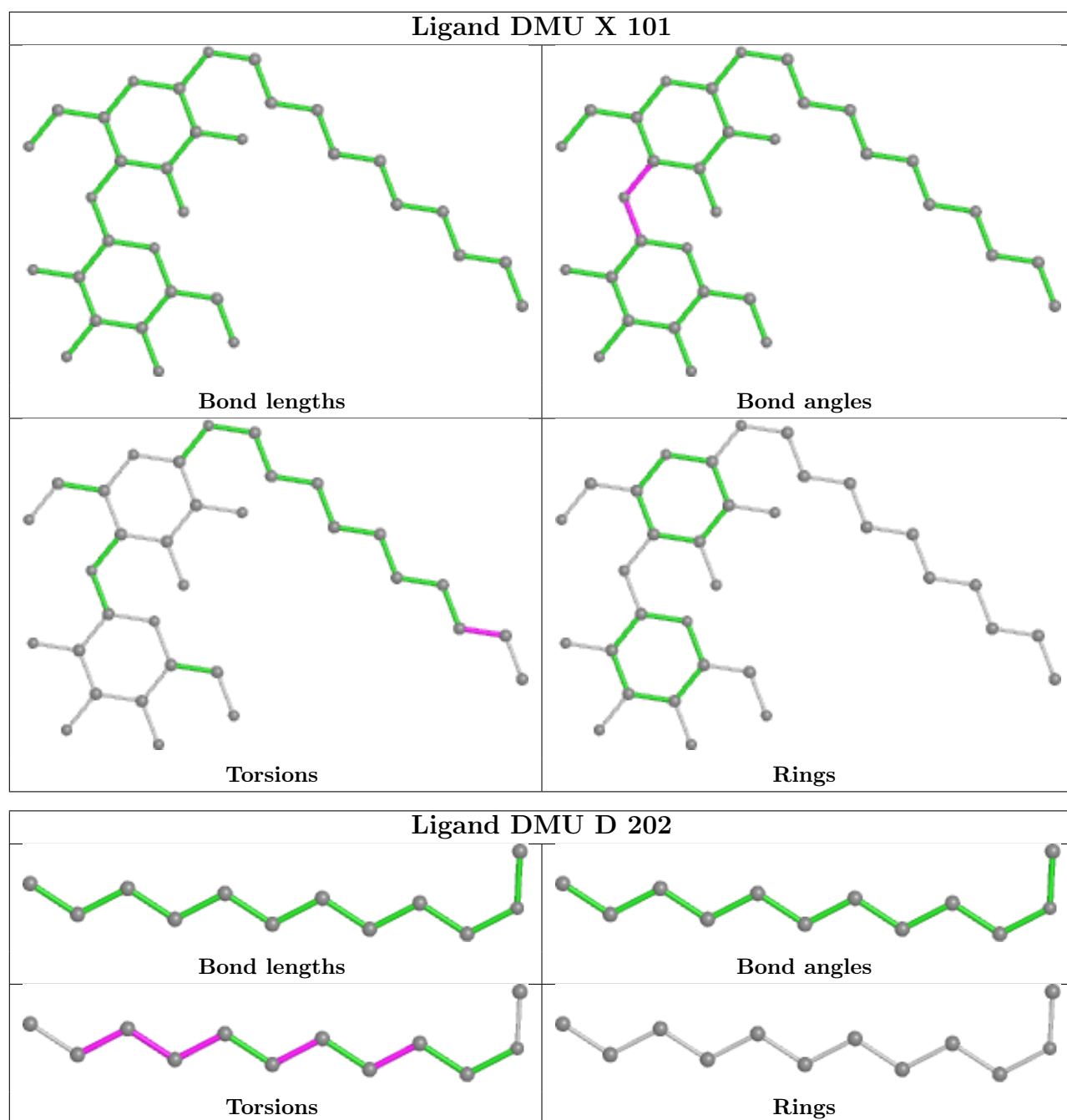
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

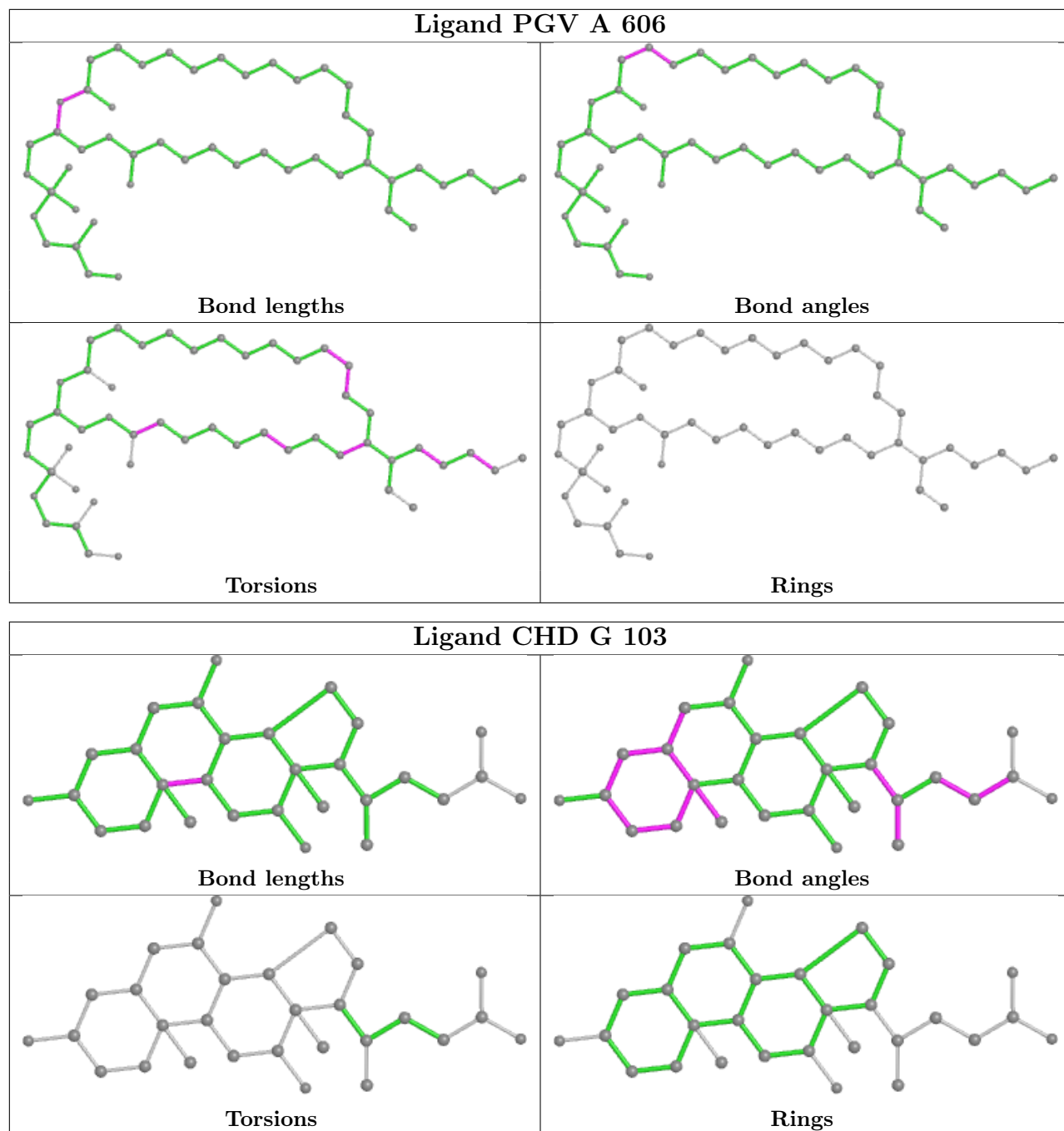


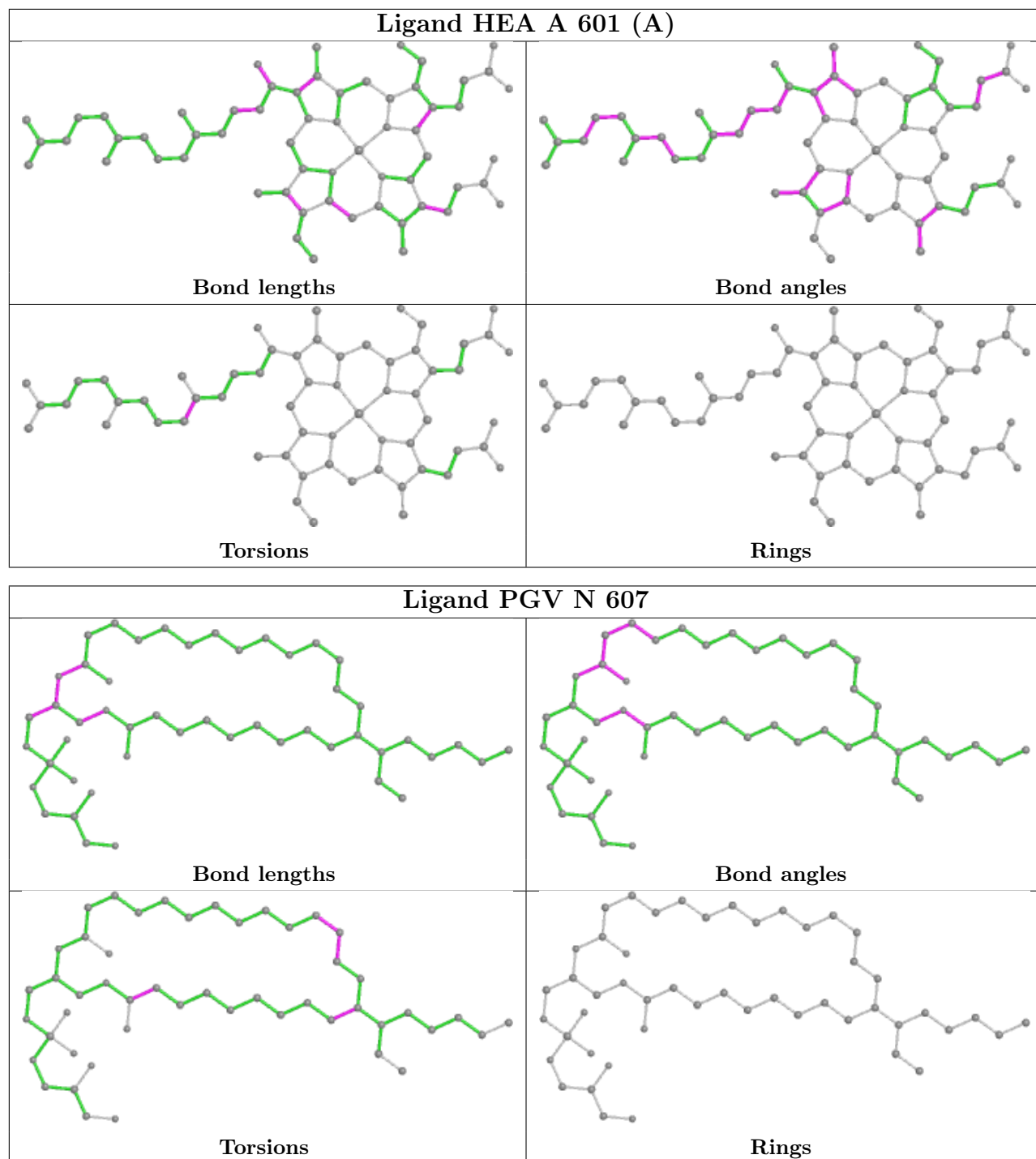


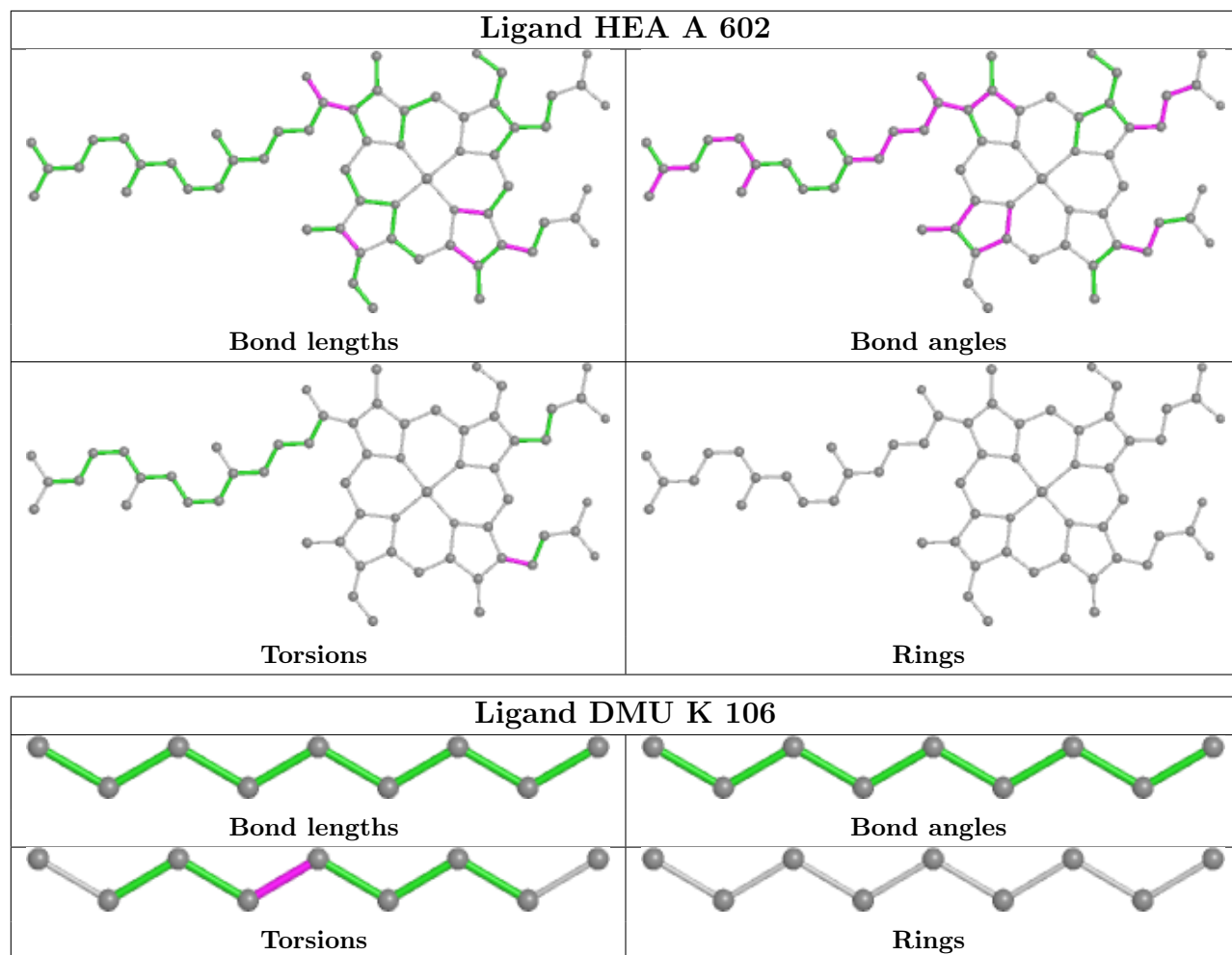


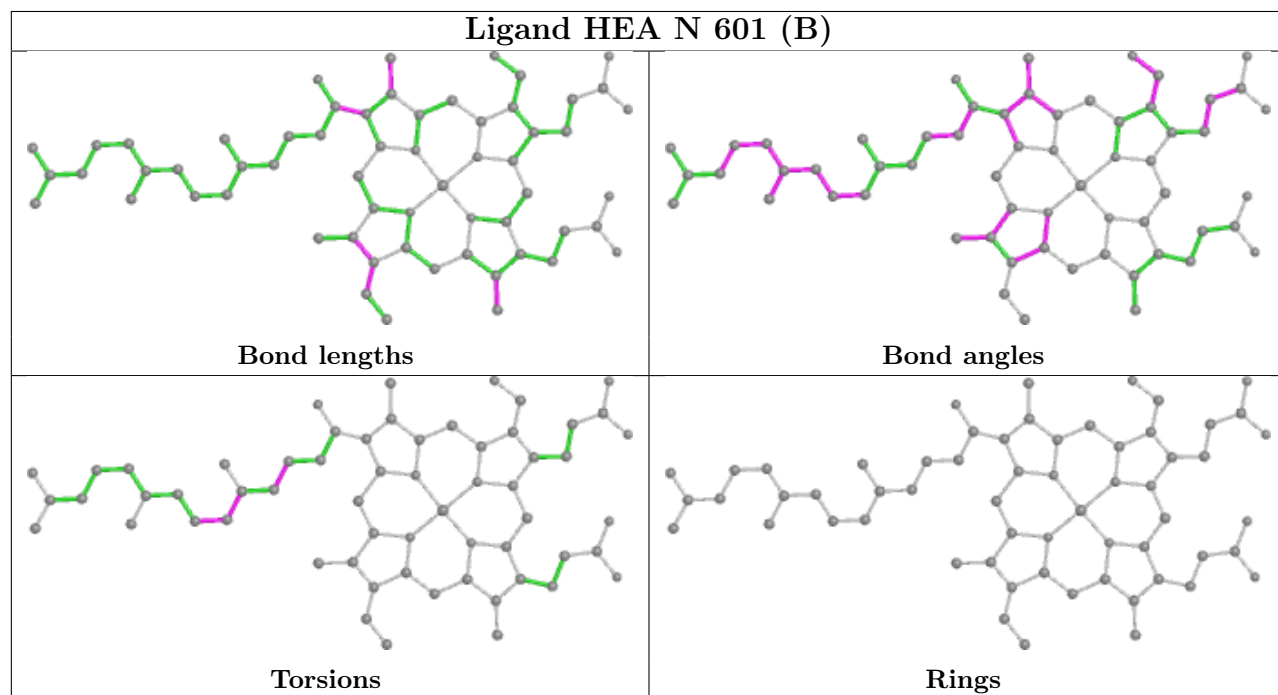
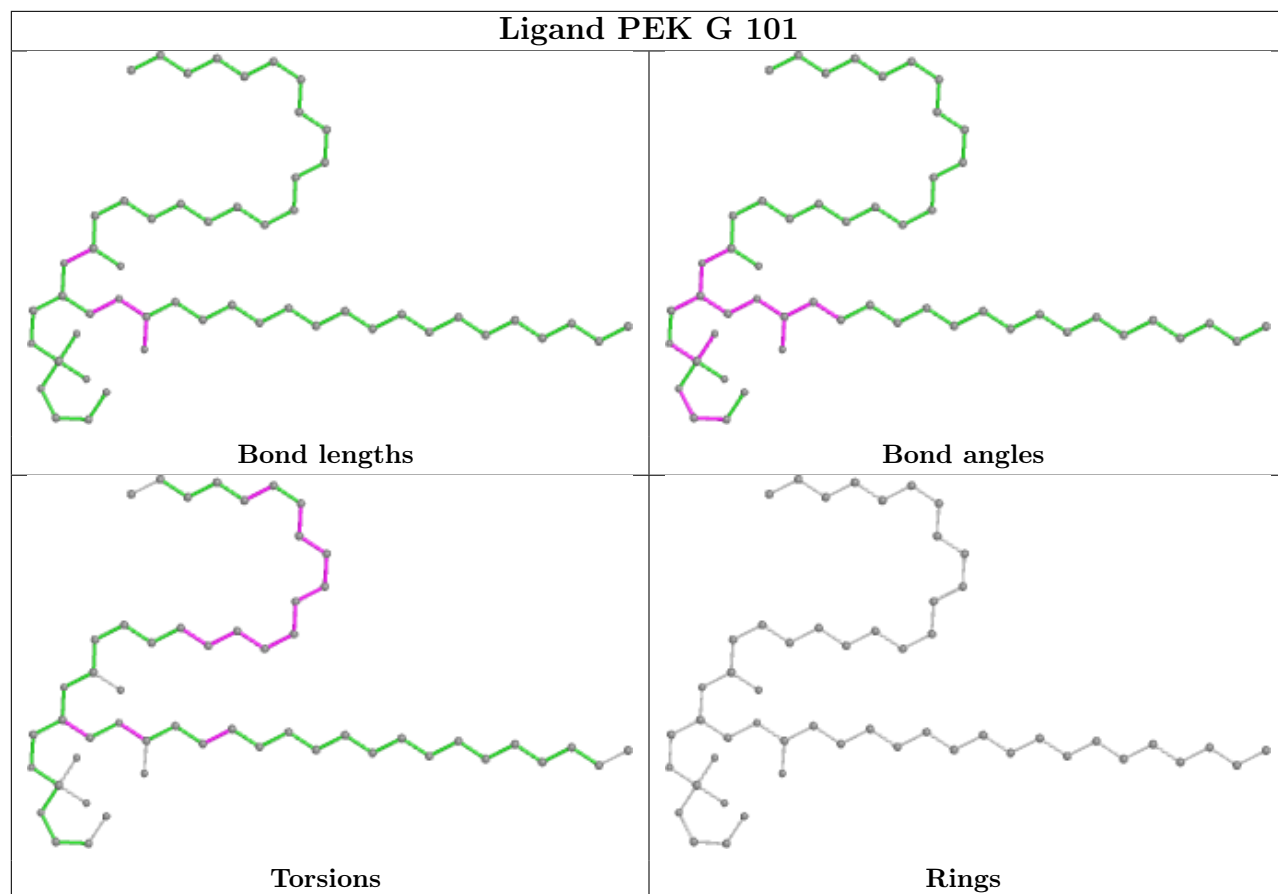


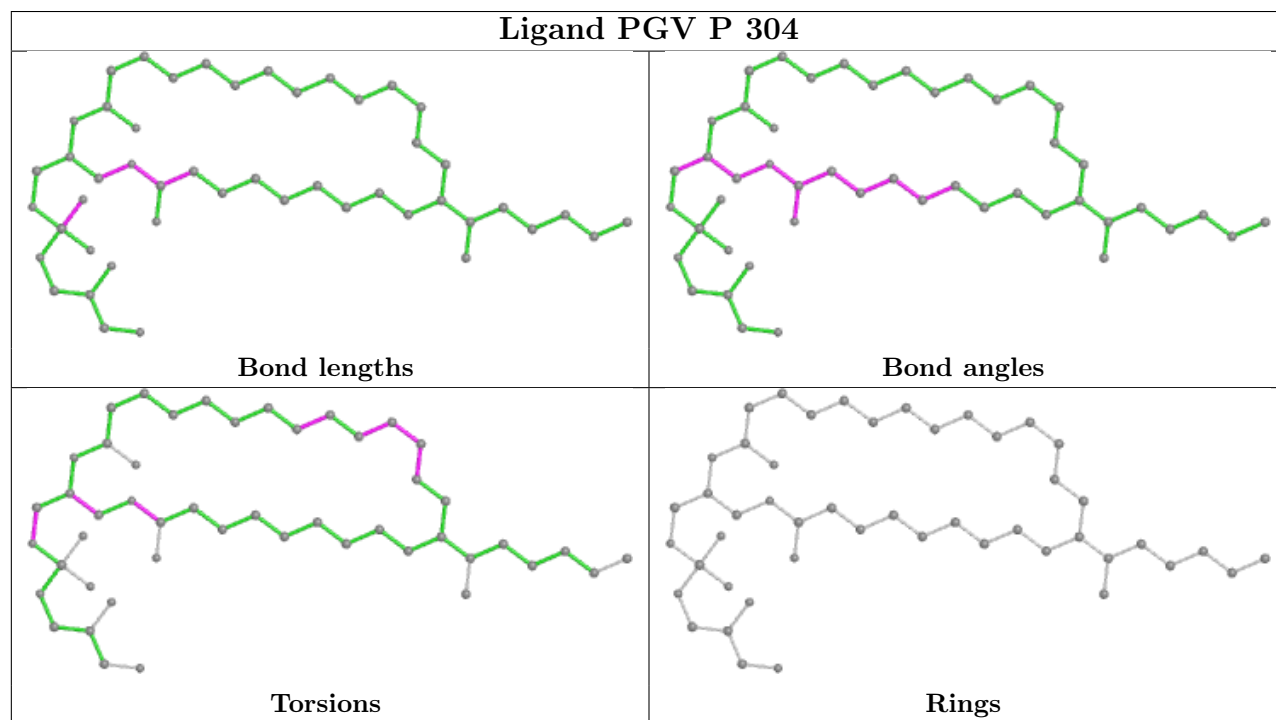
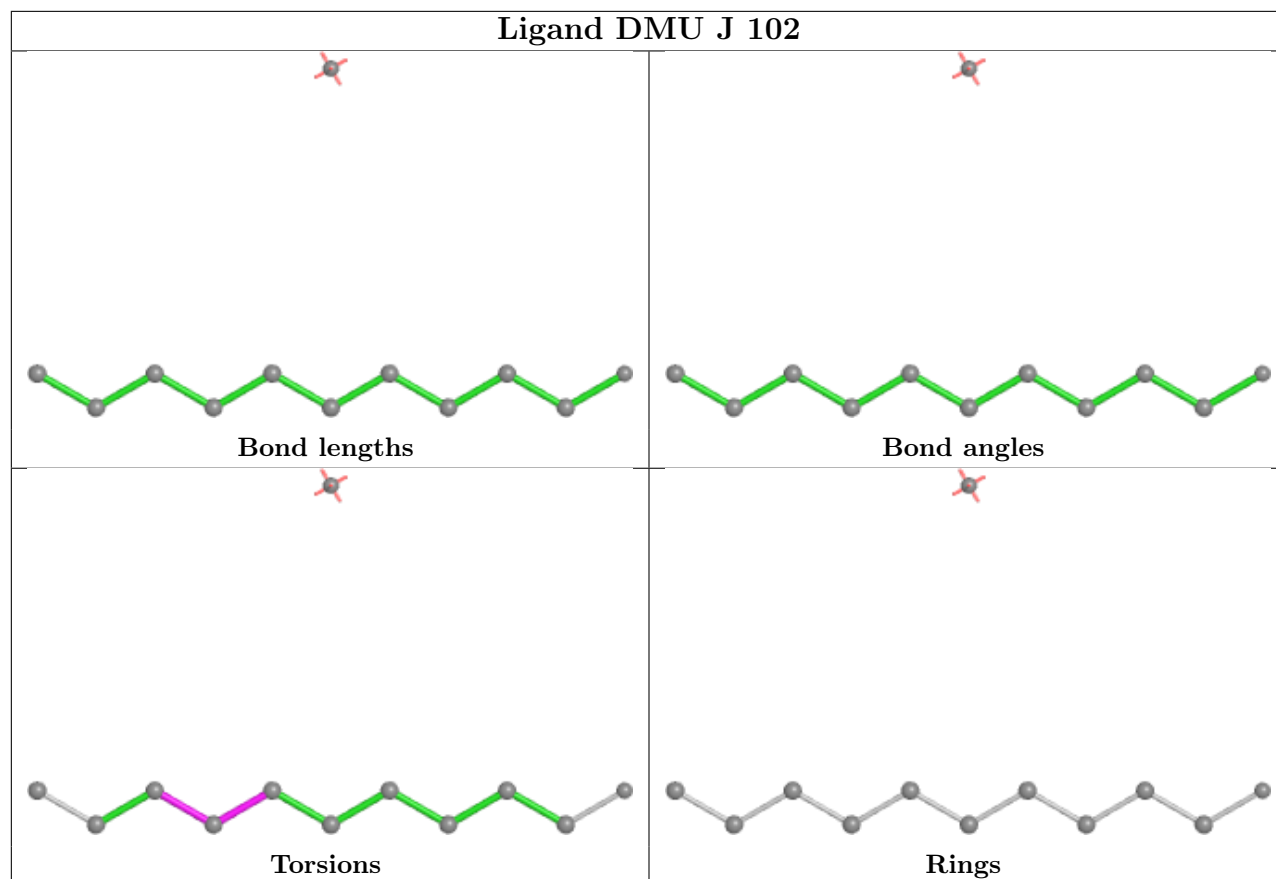


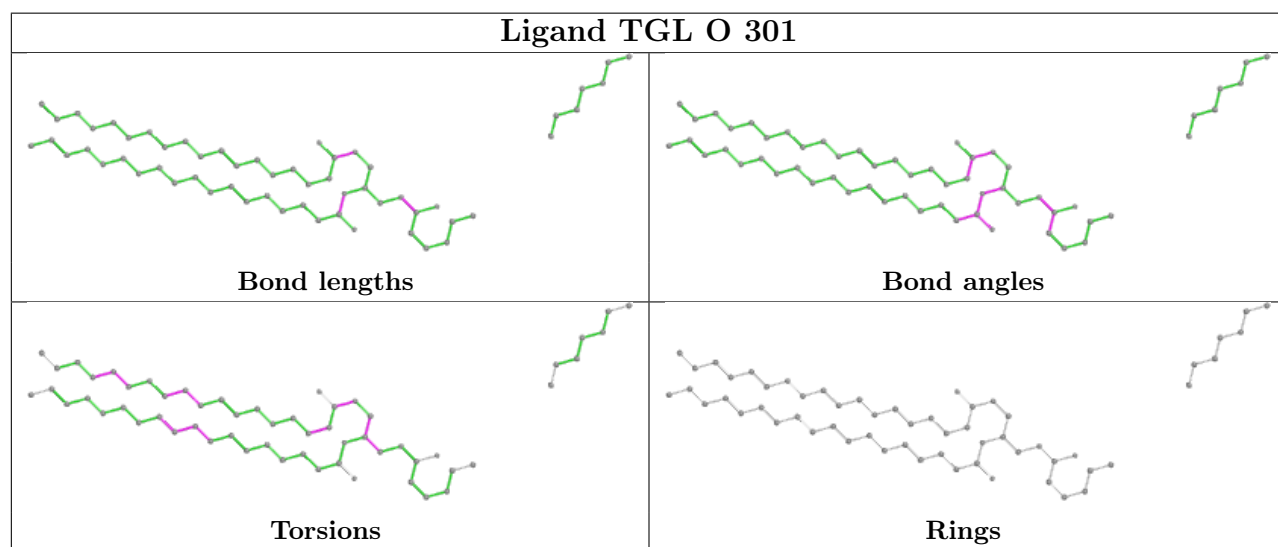
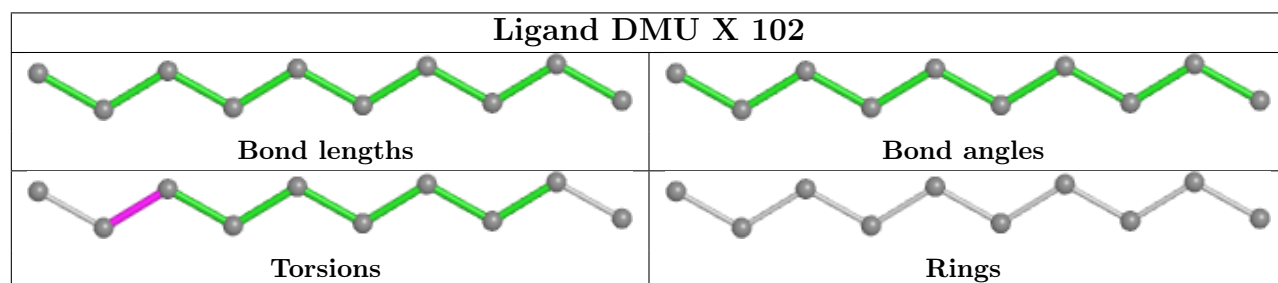
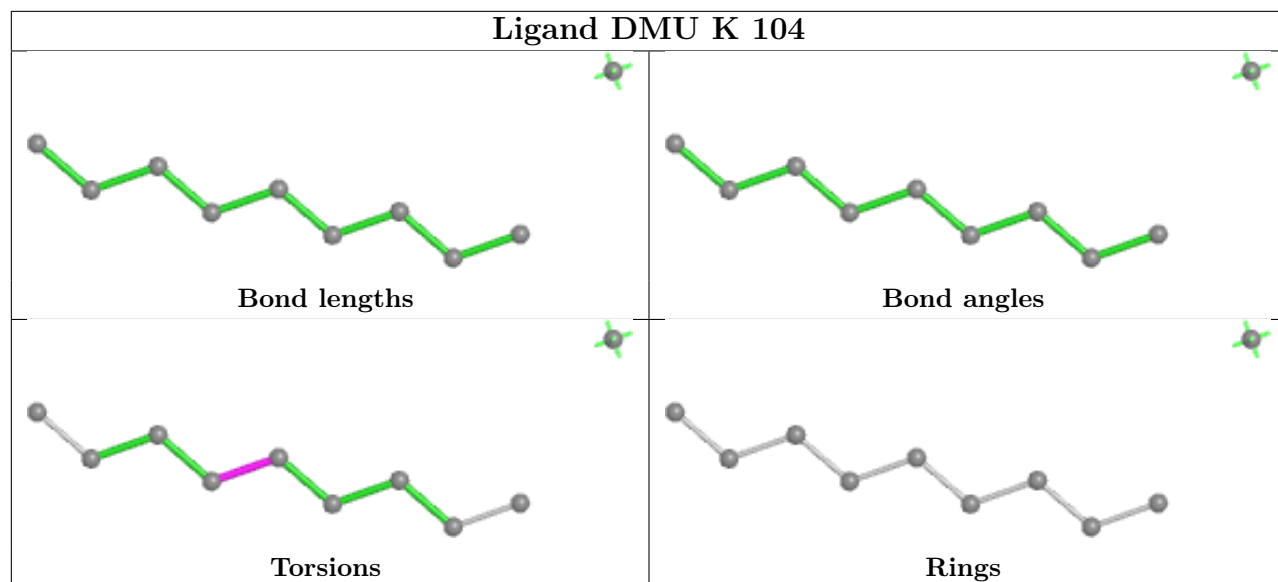


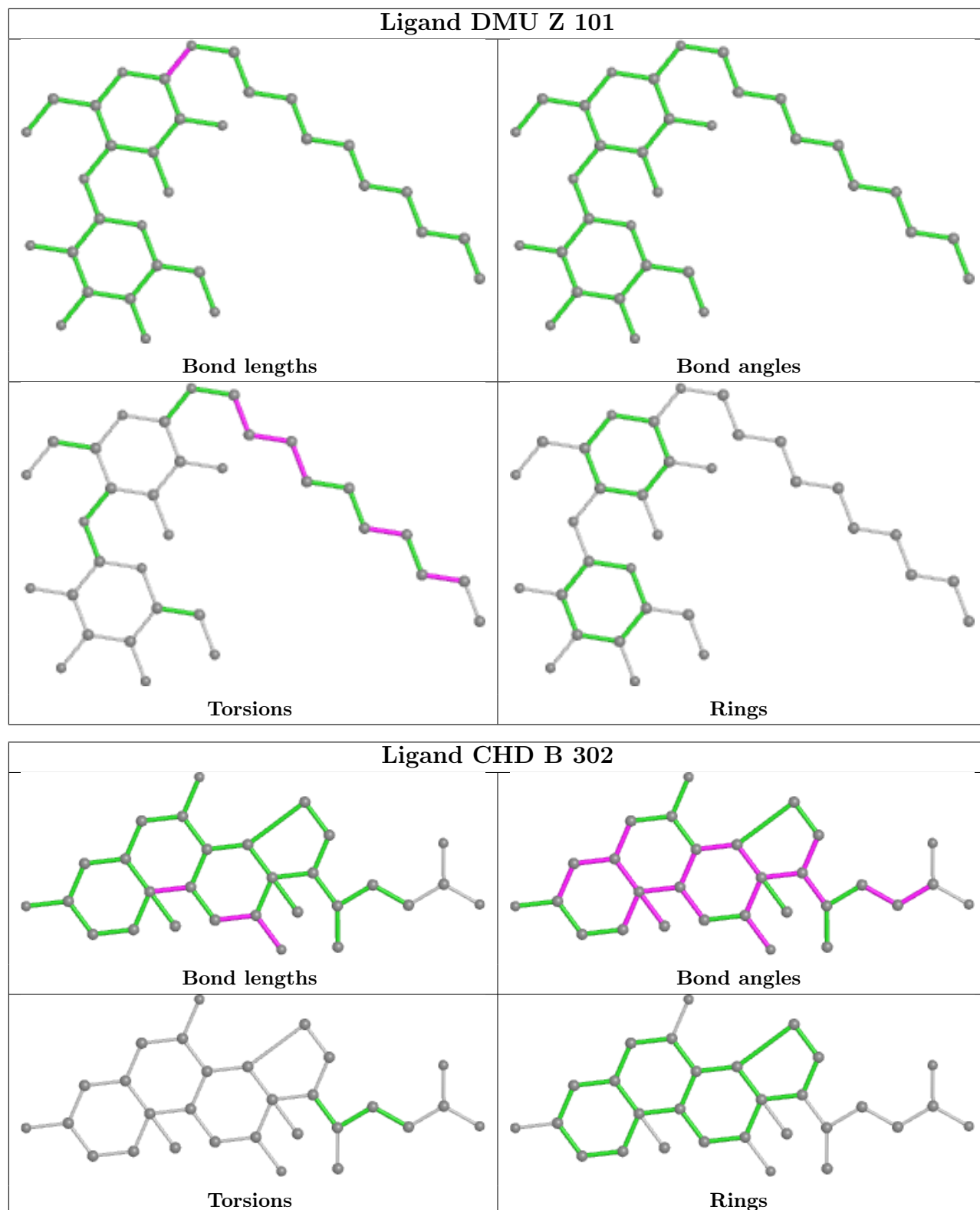


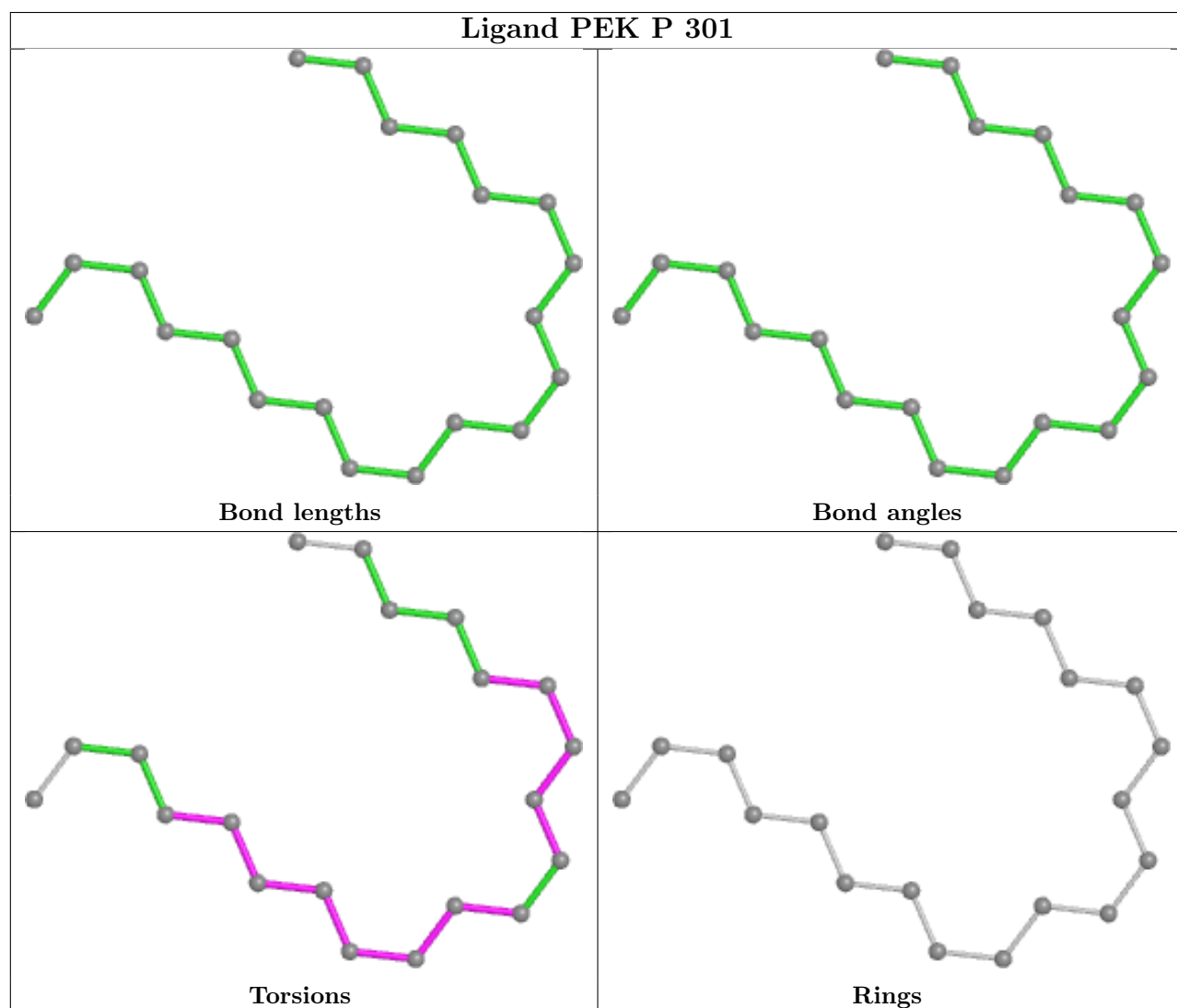
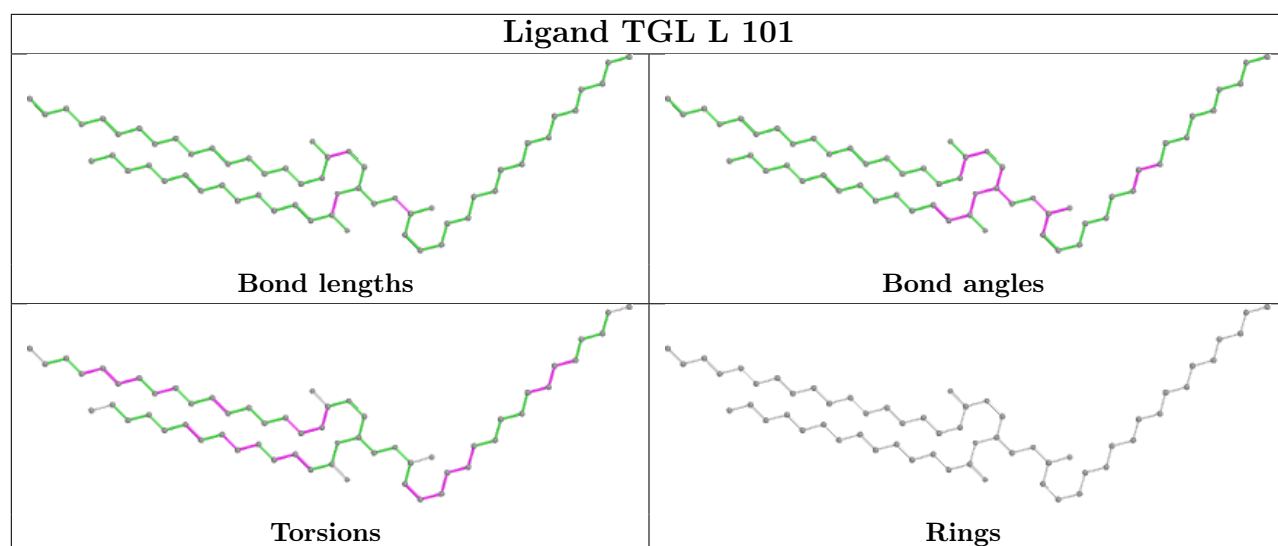


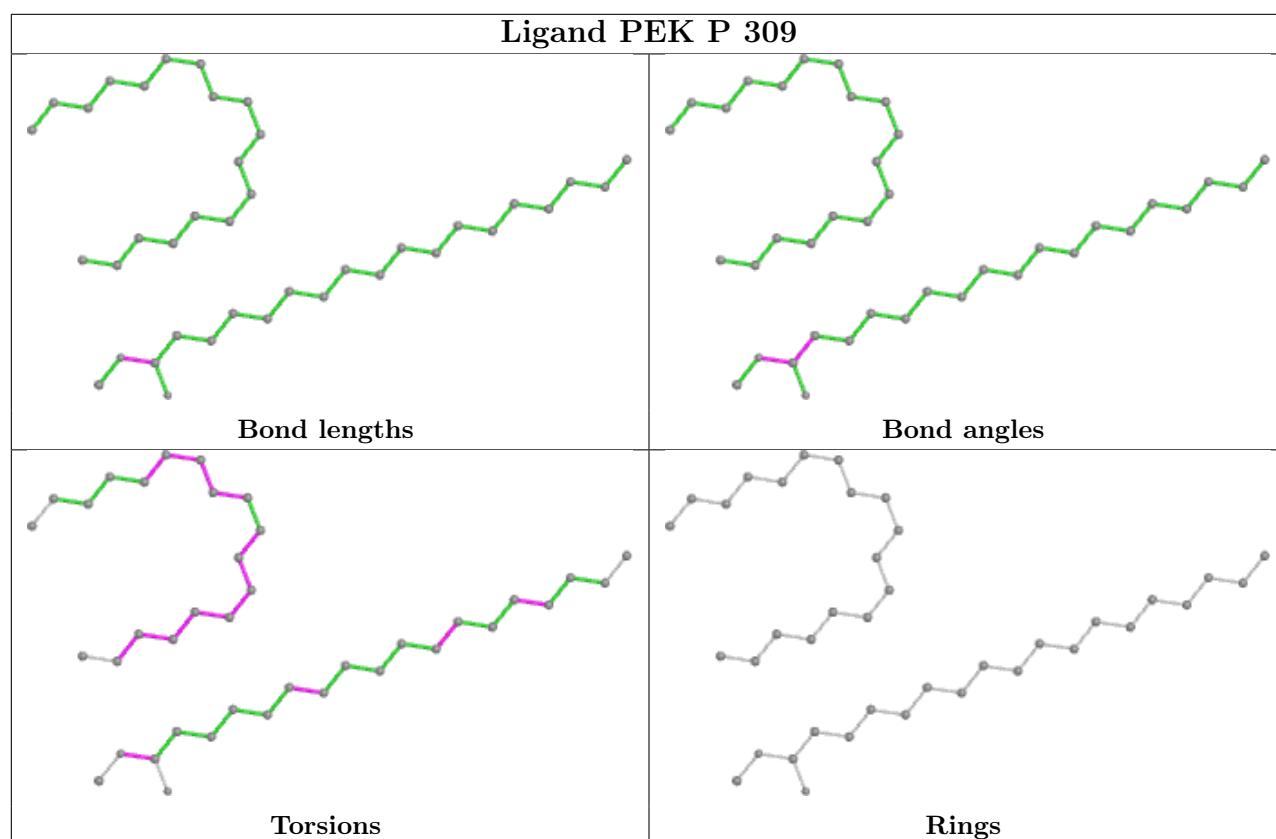
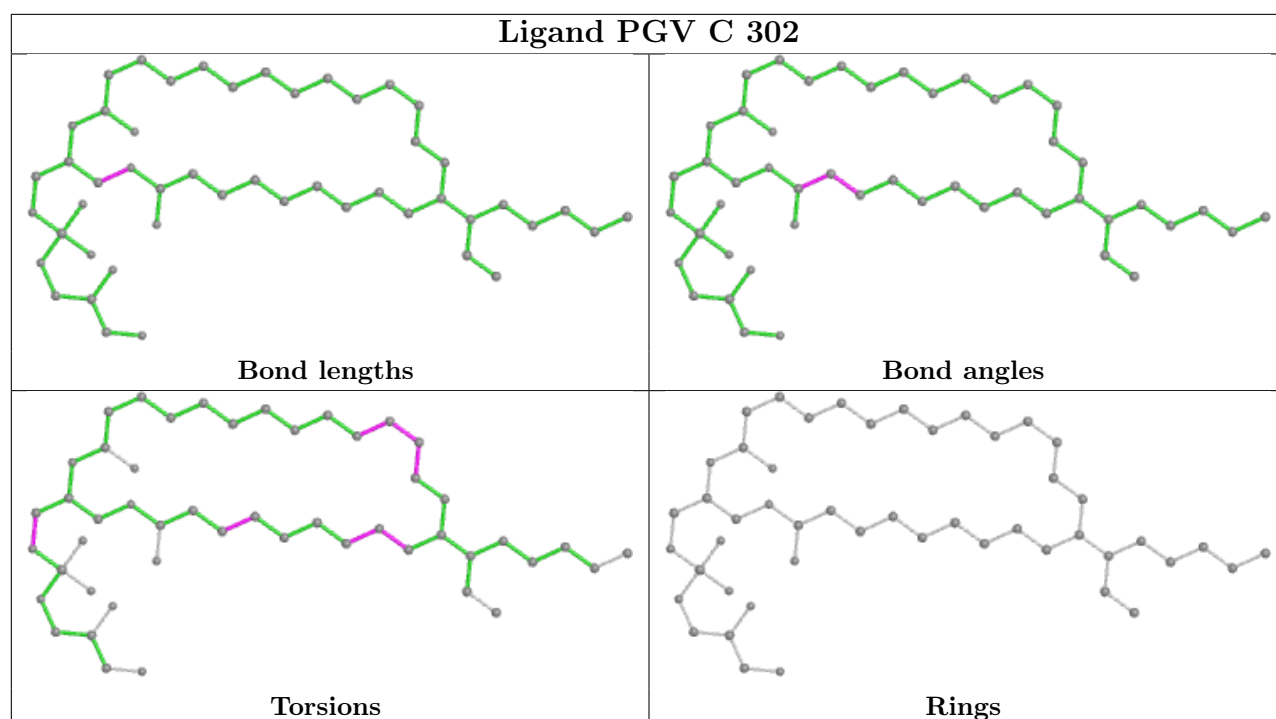


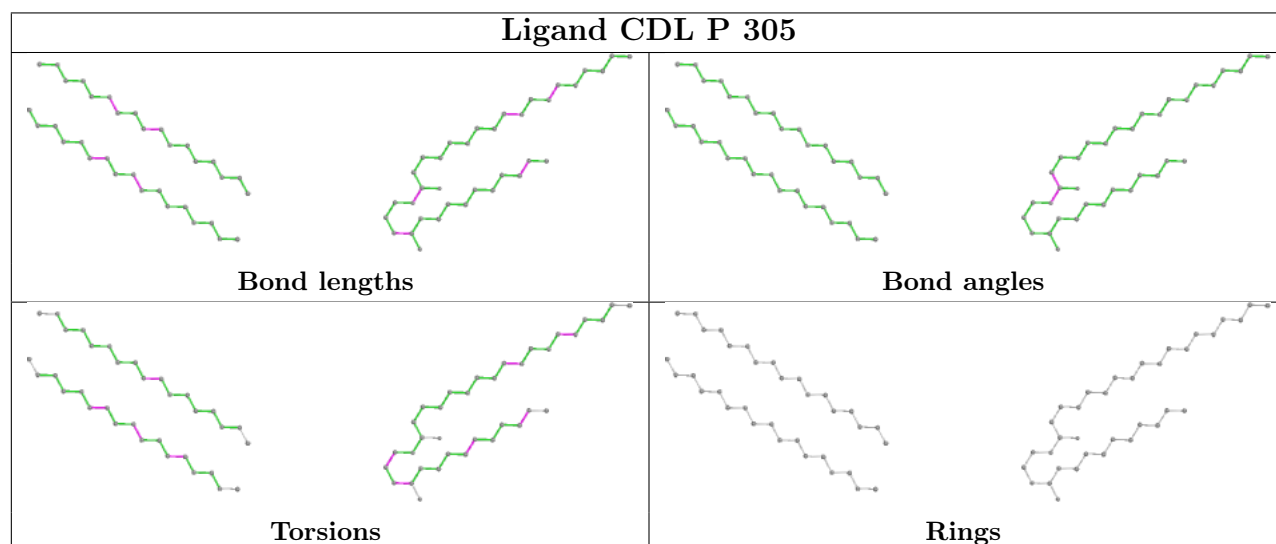
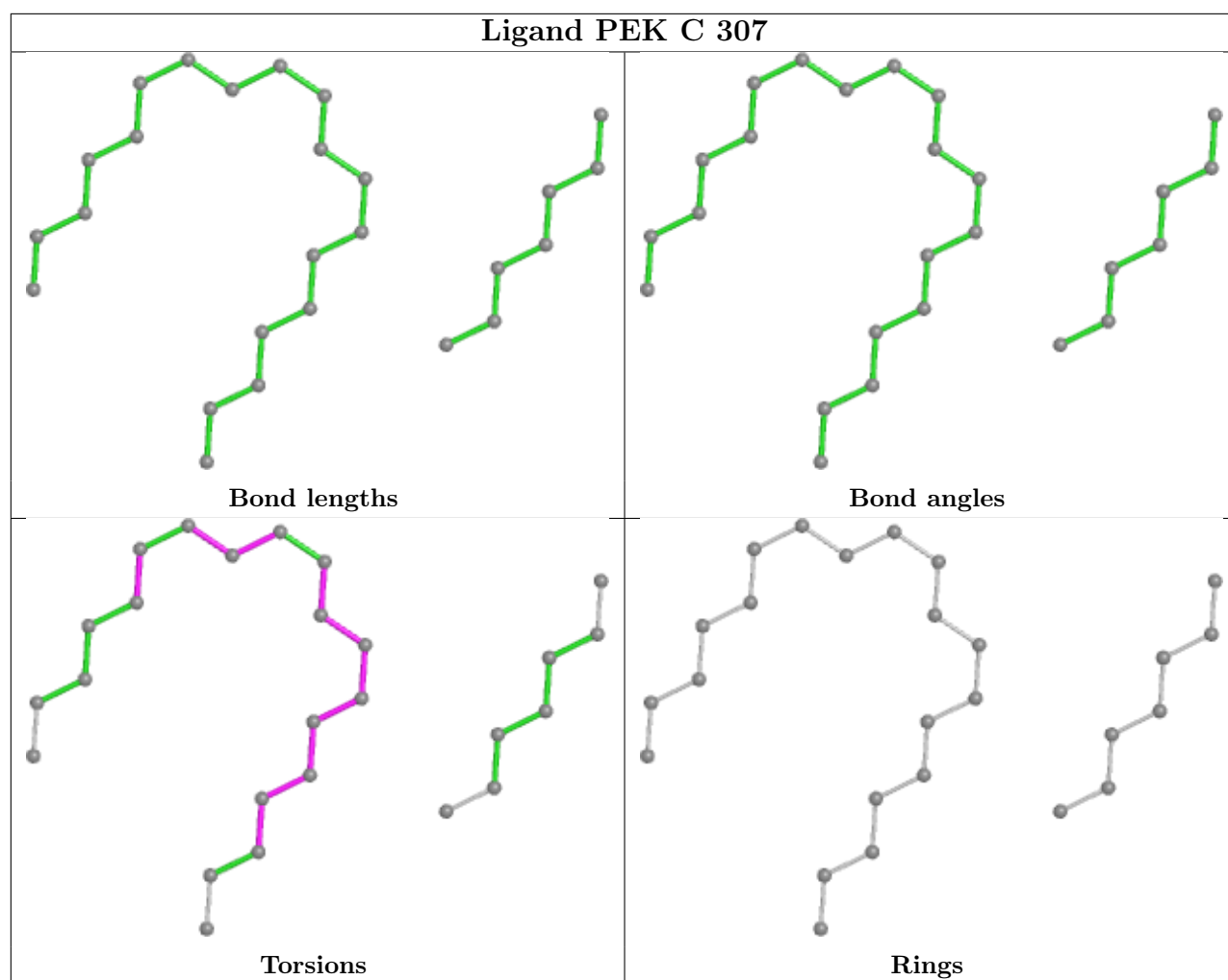


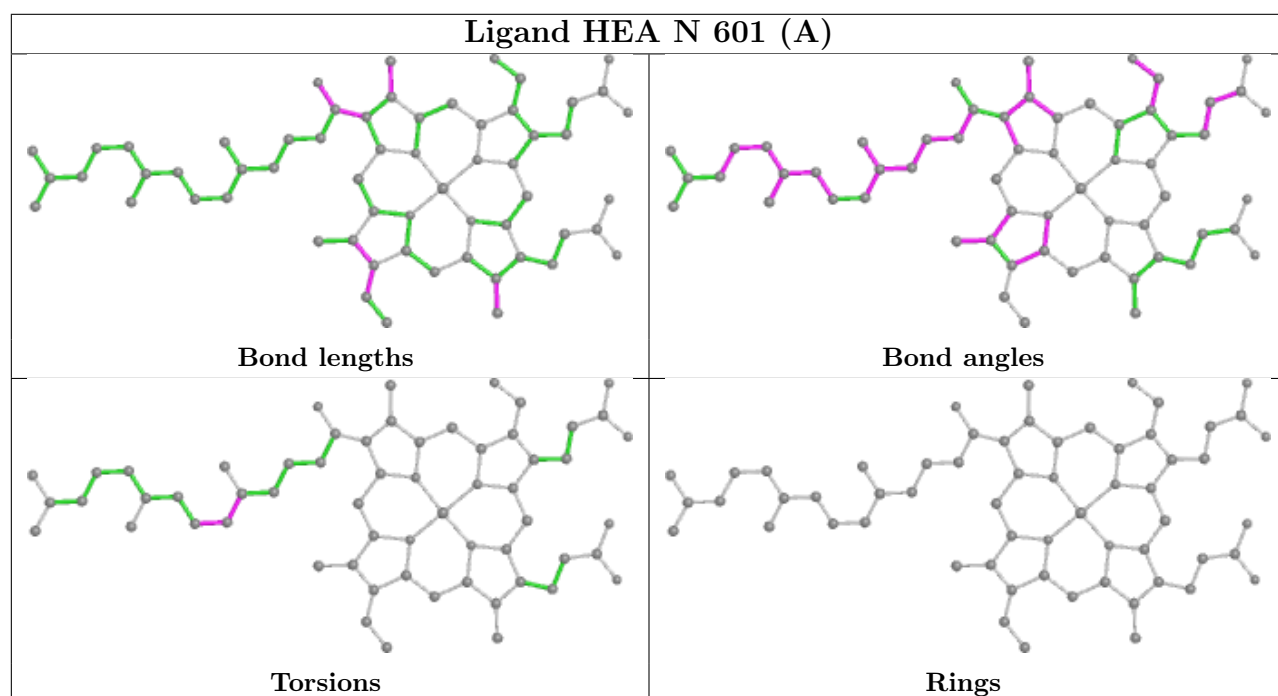
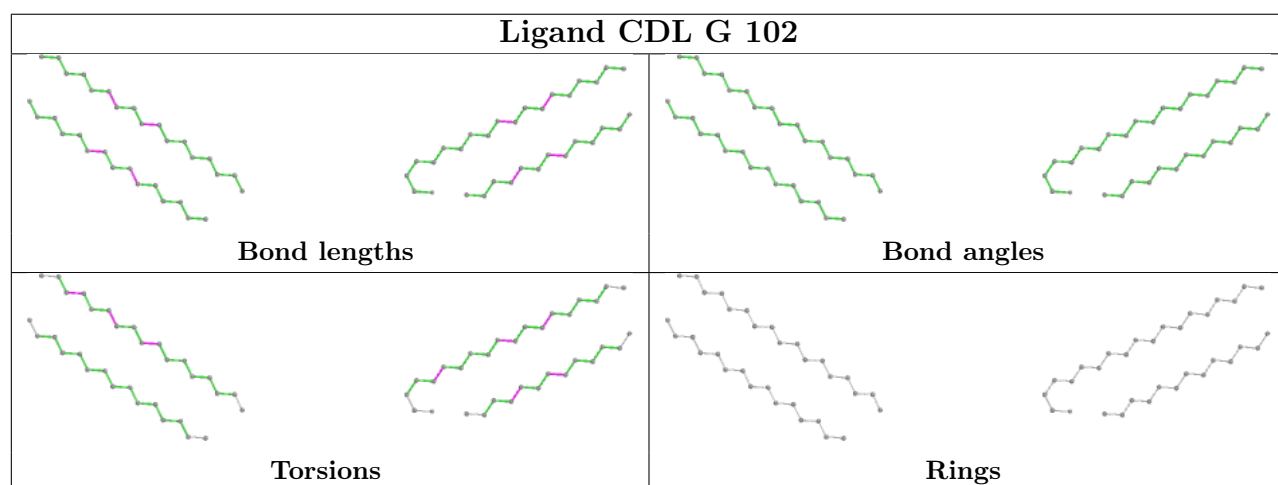
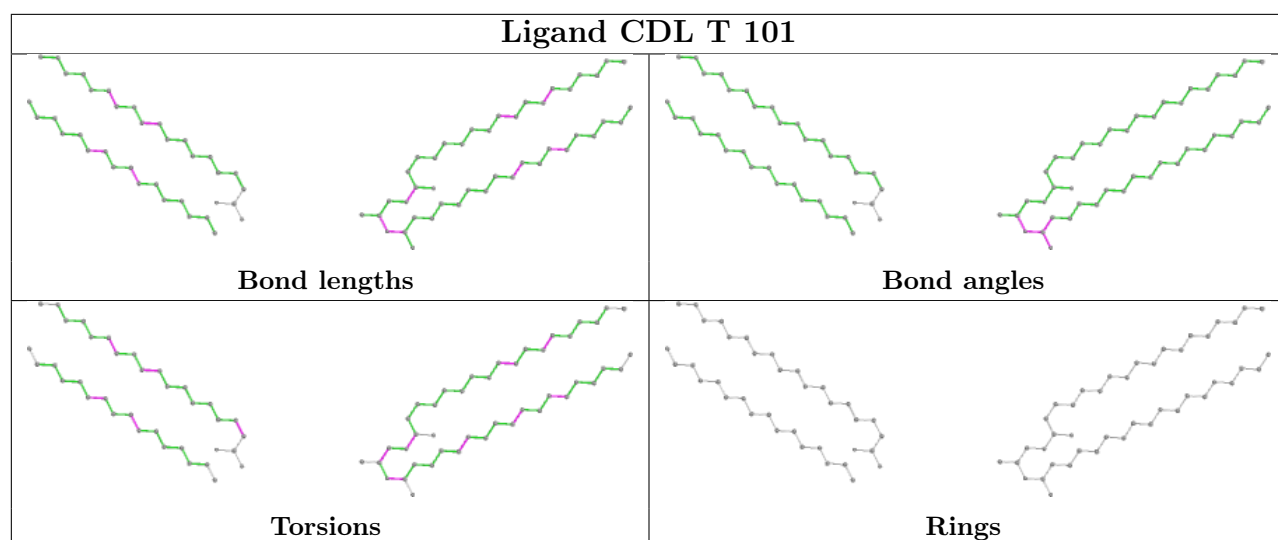


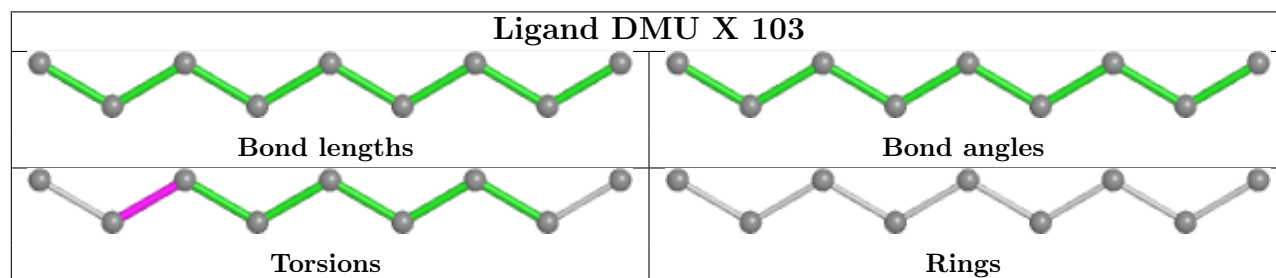
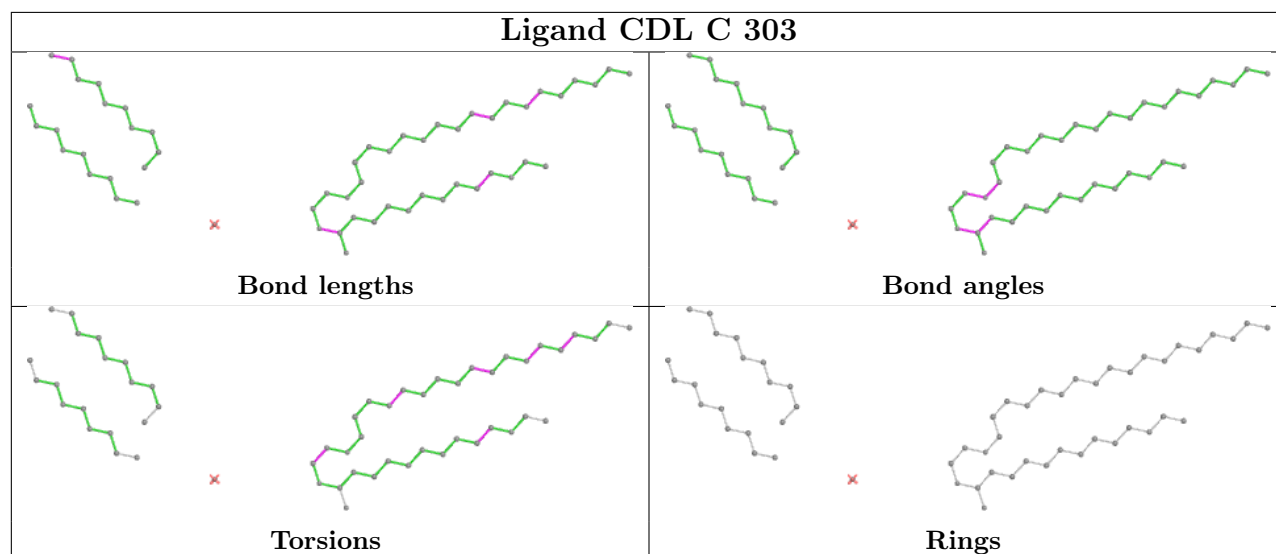
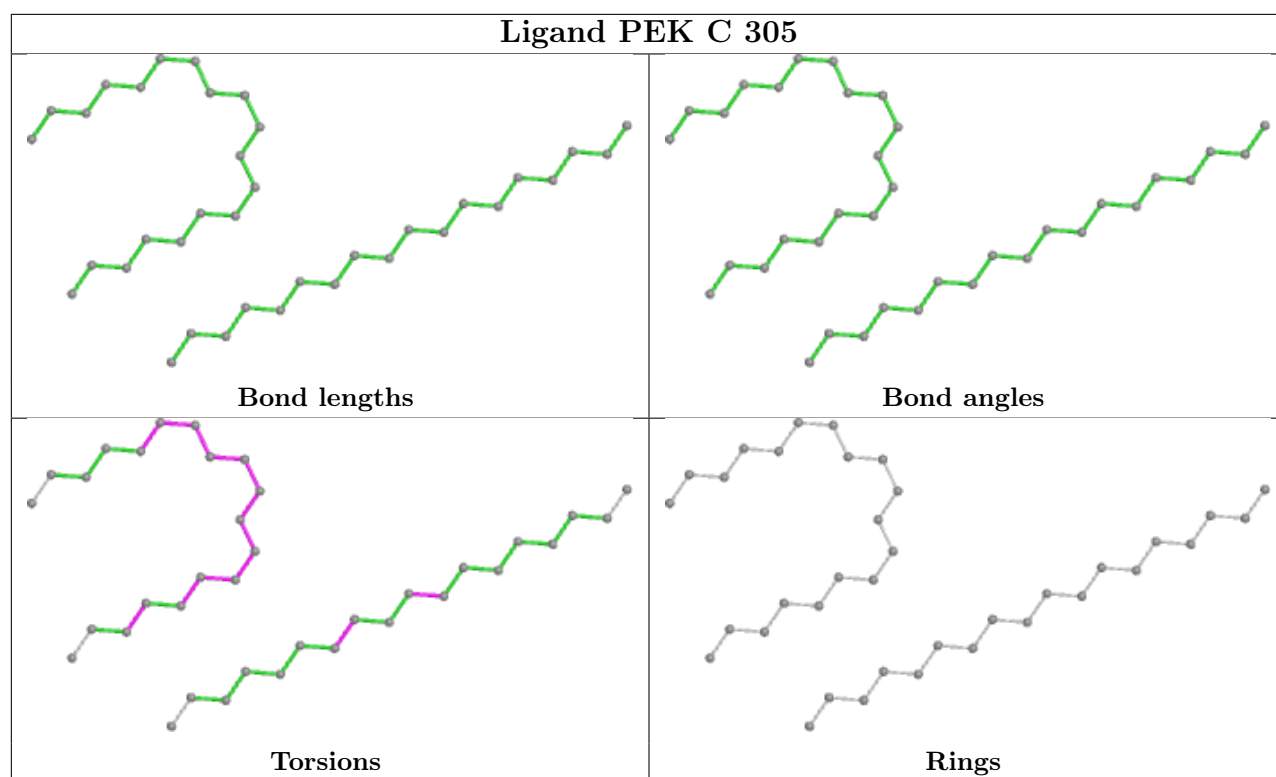


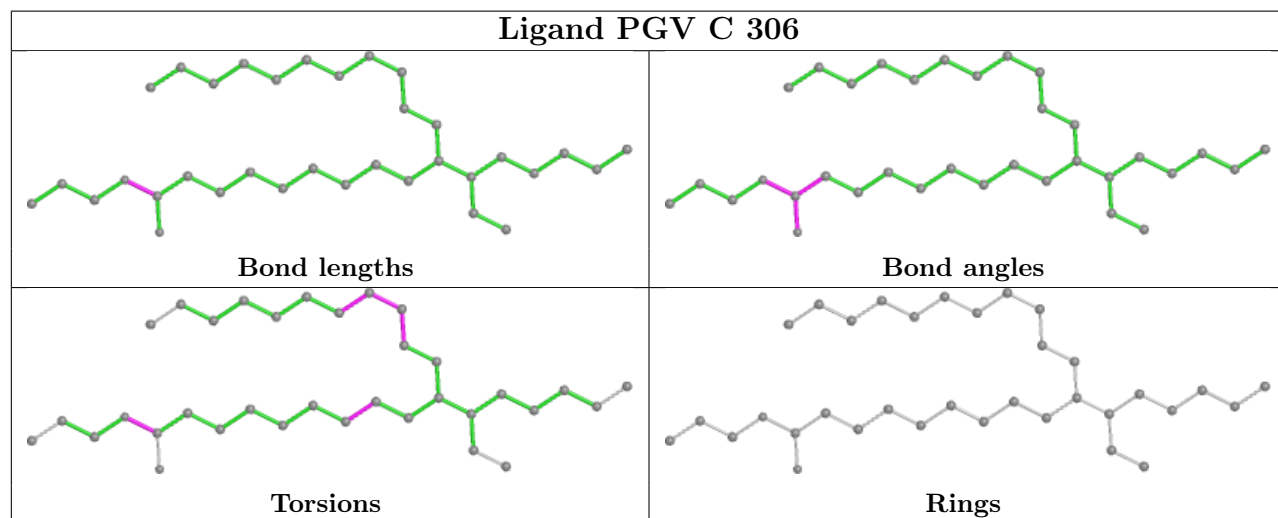
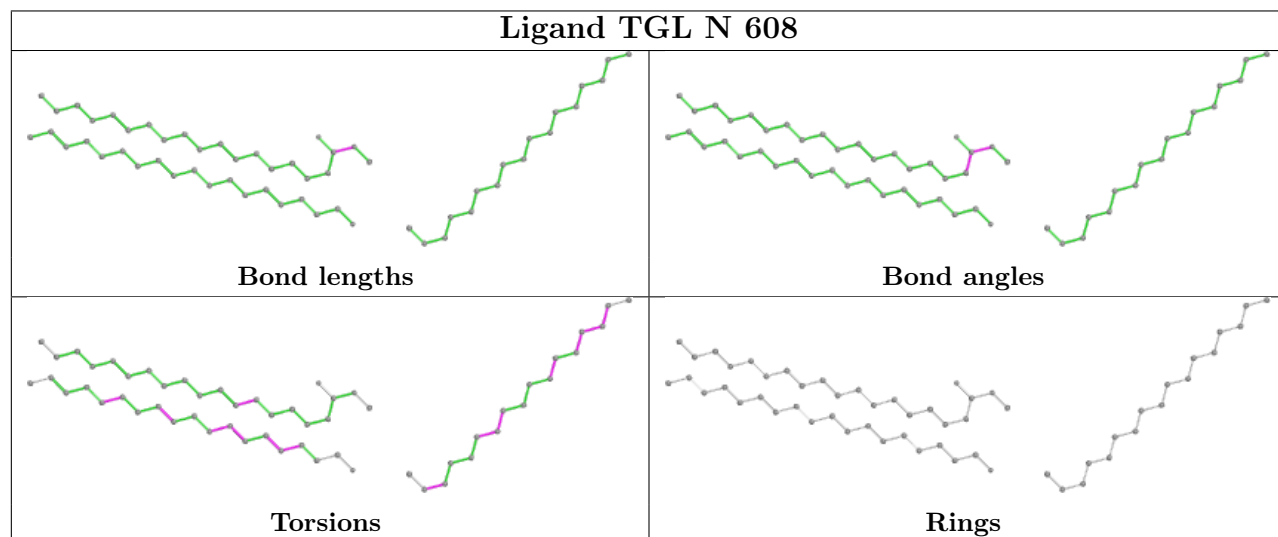
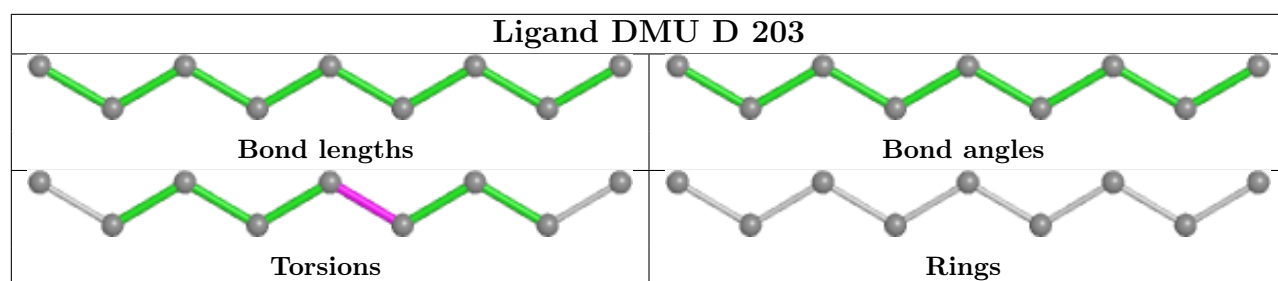


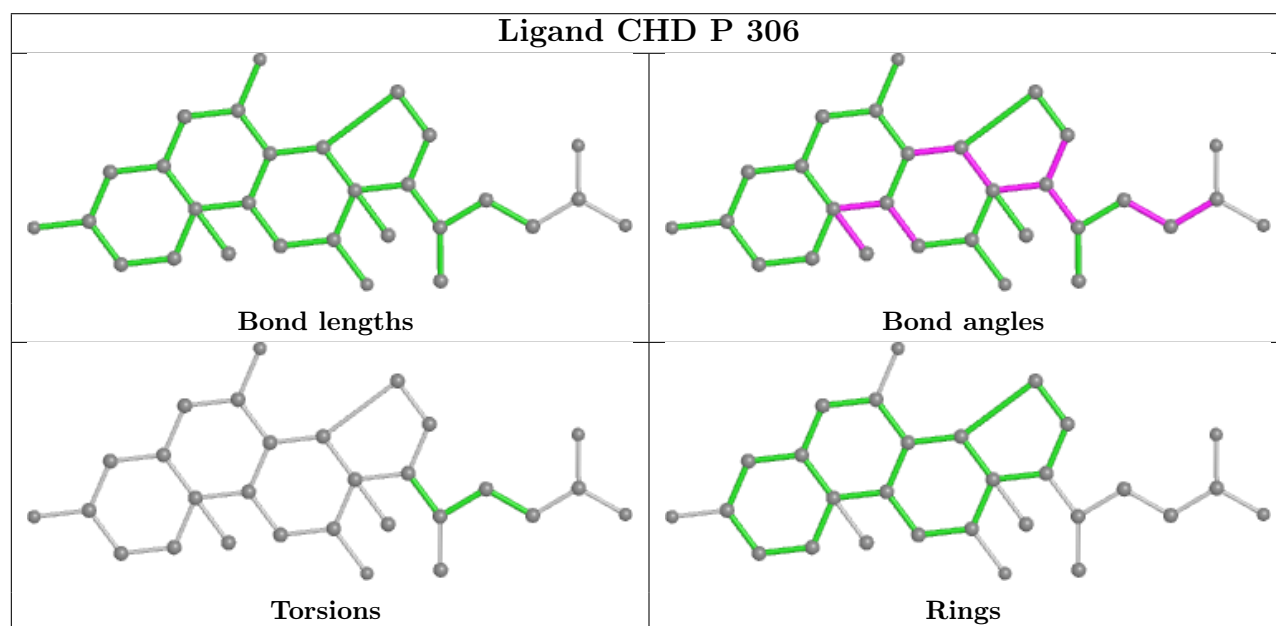
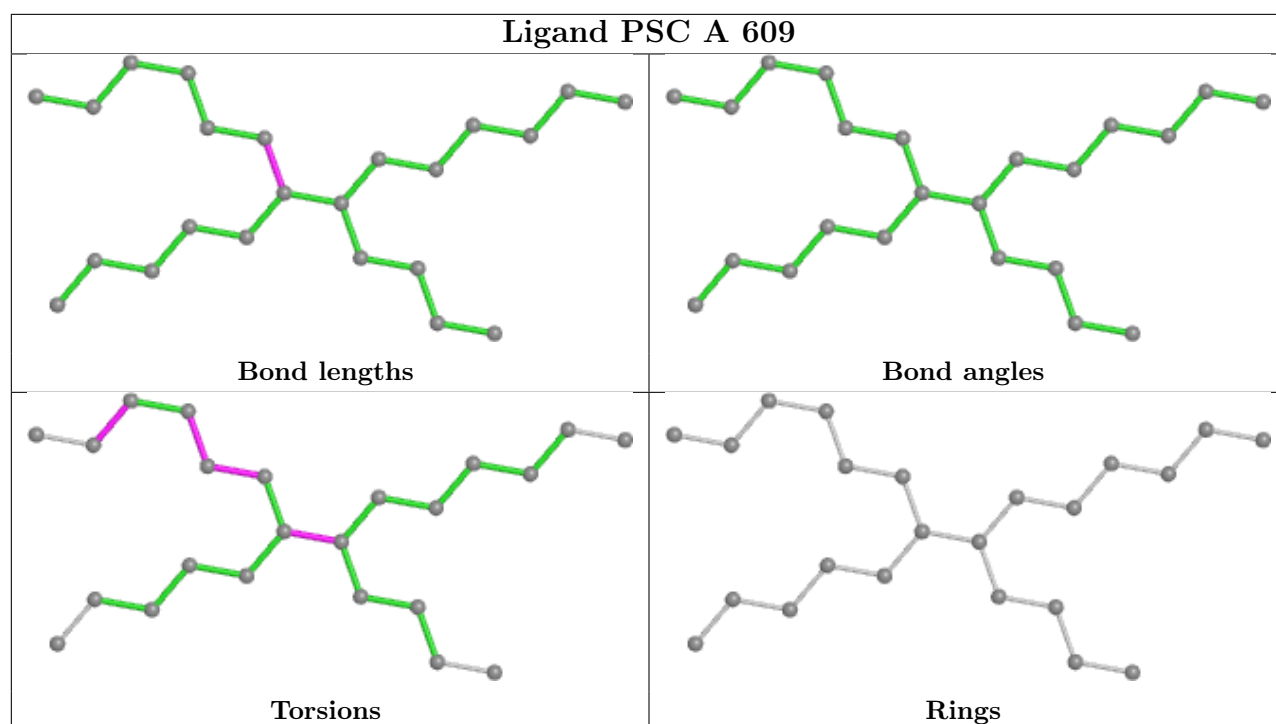




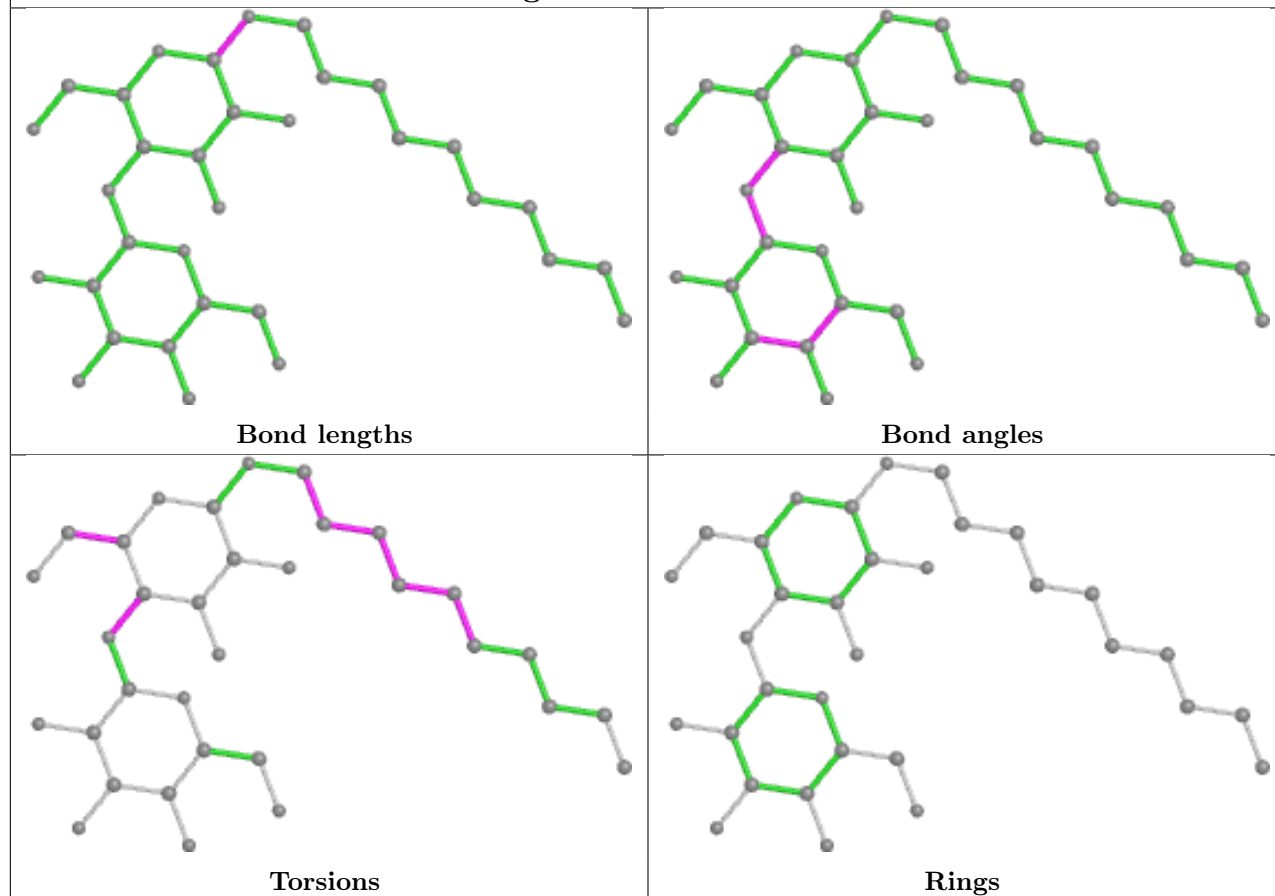




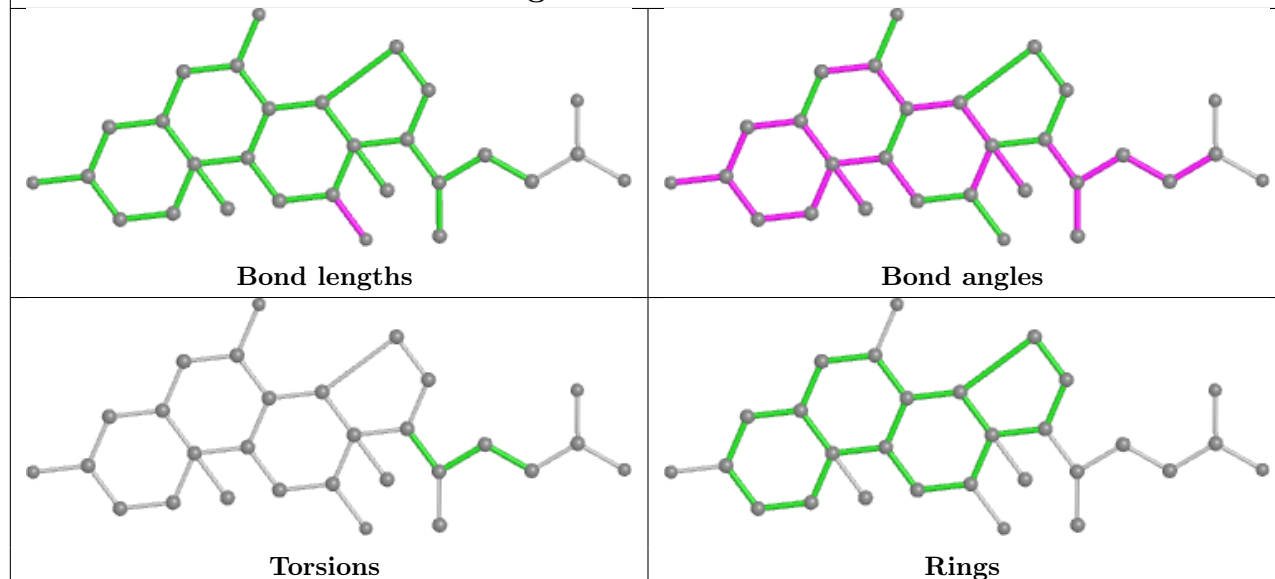




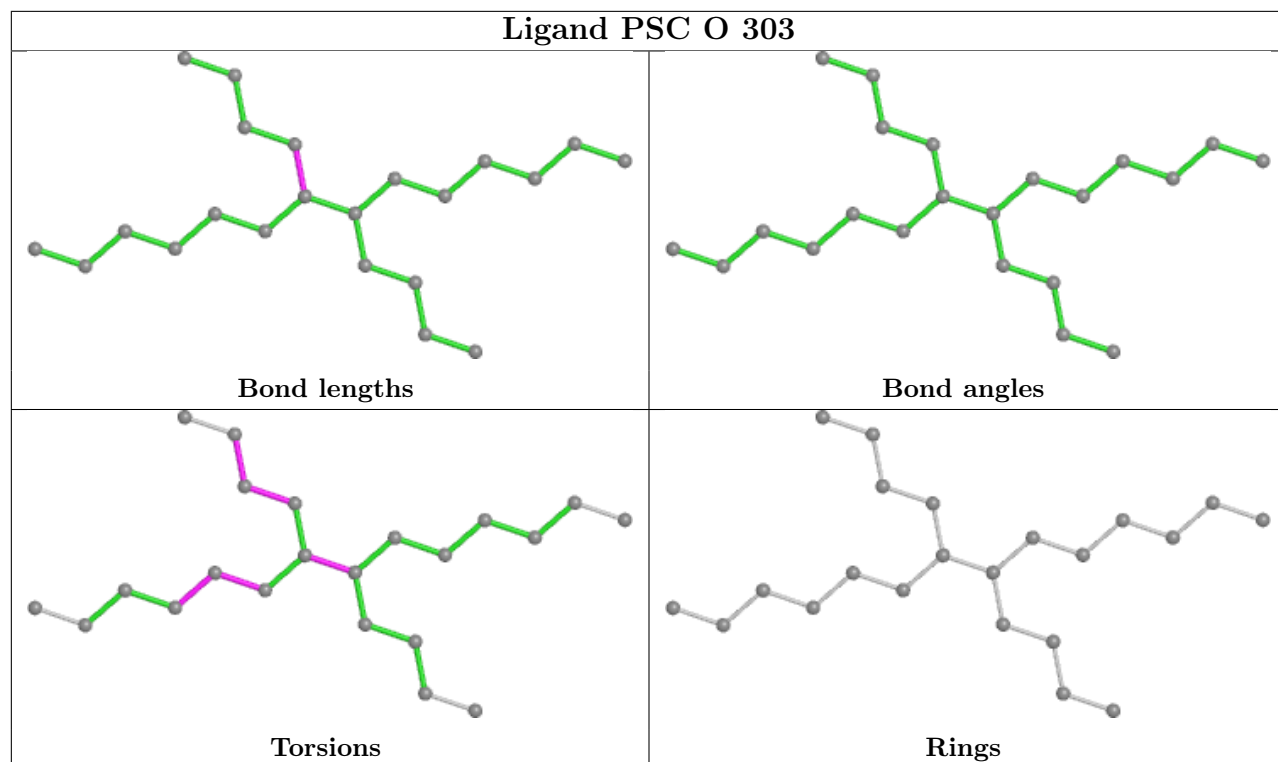
Ligand DMU K 103



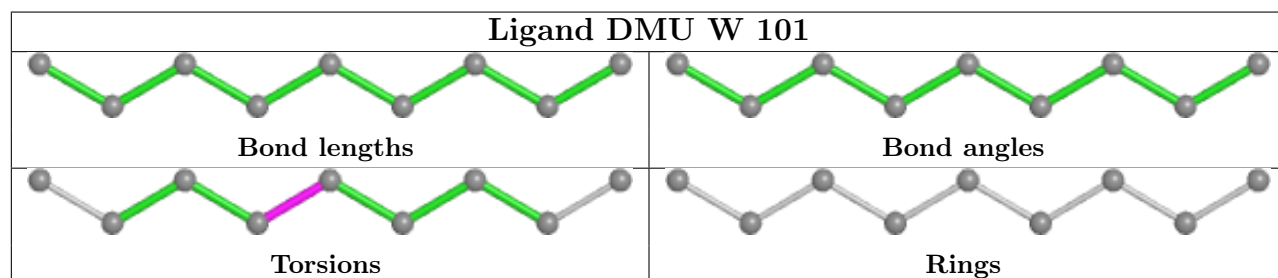
Ligand CHD C 304



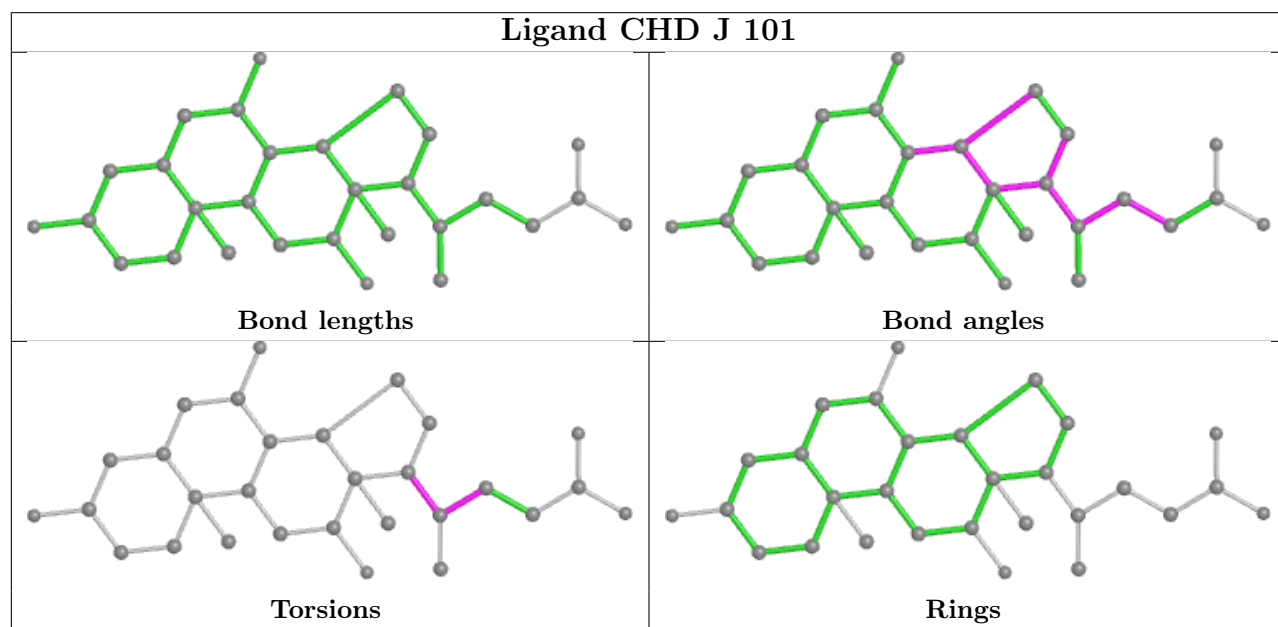
Ligand PSC O 303

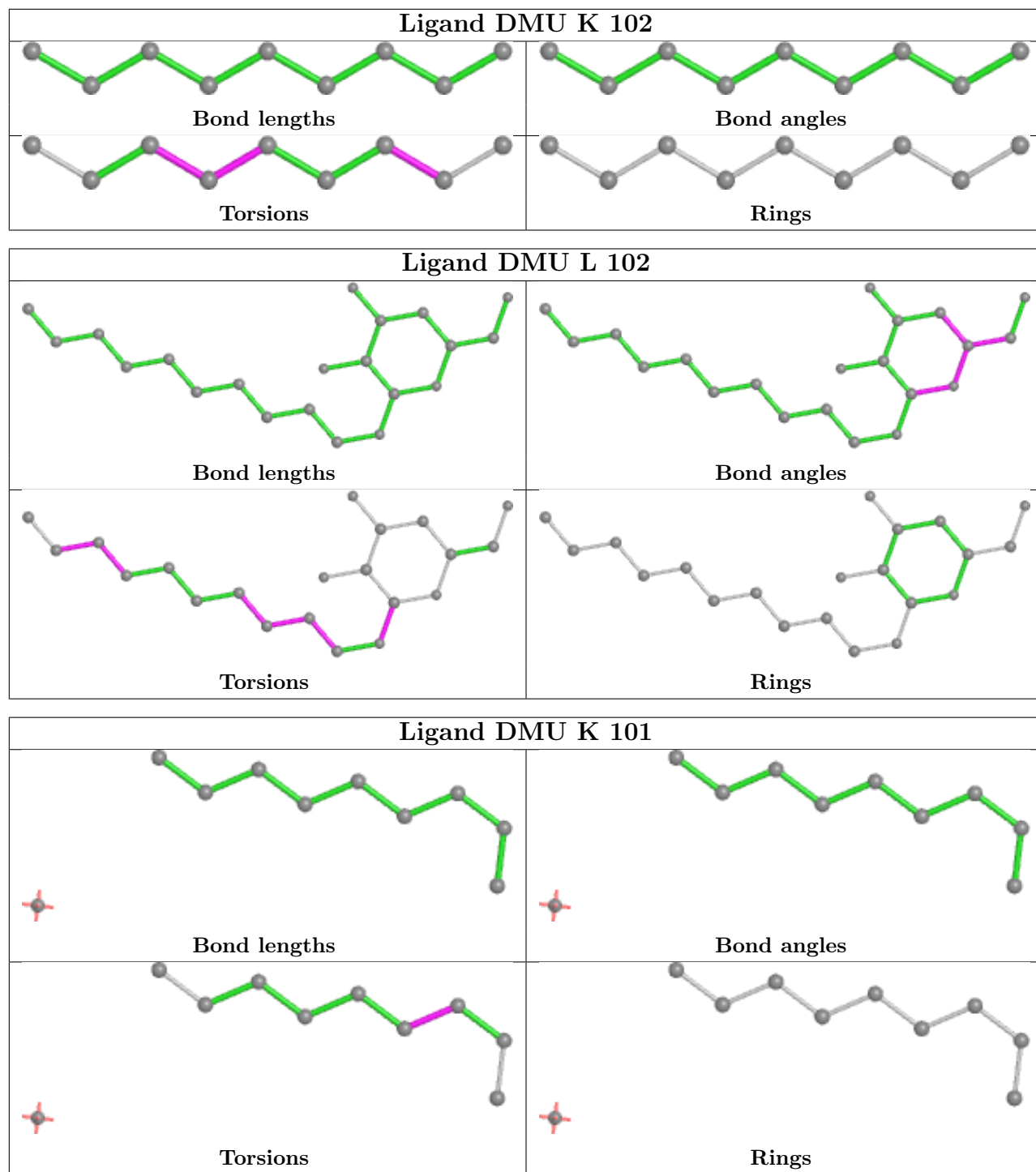


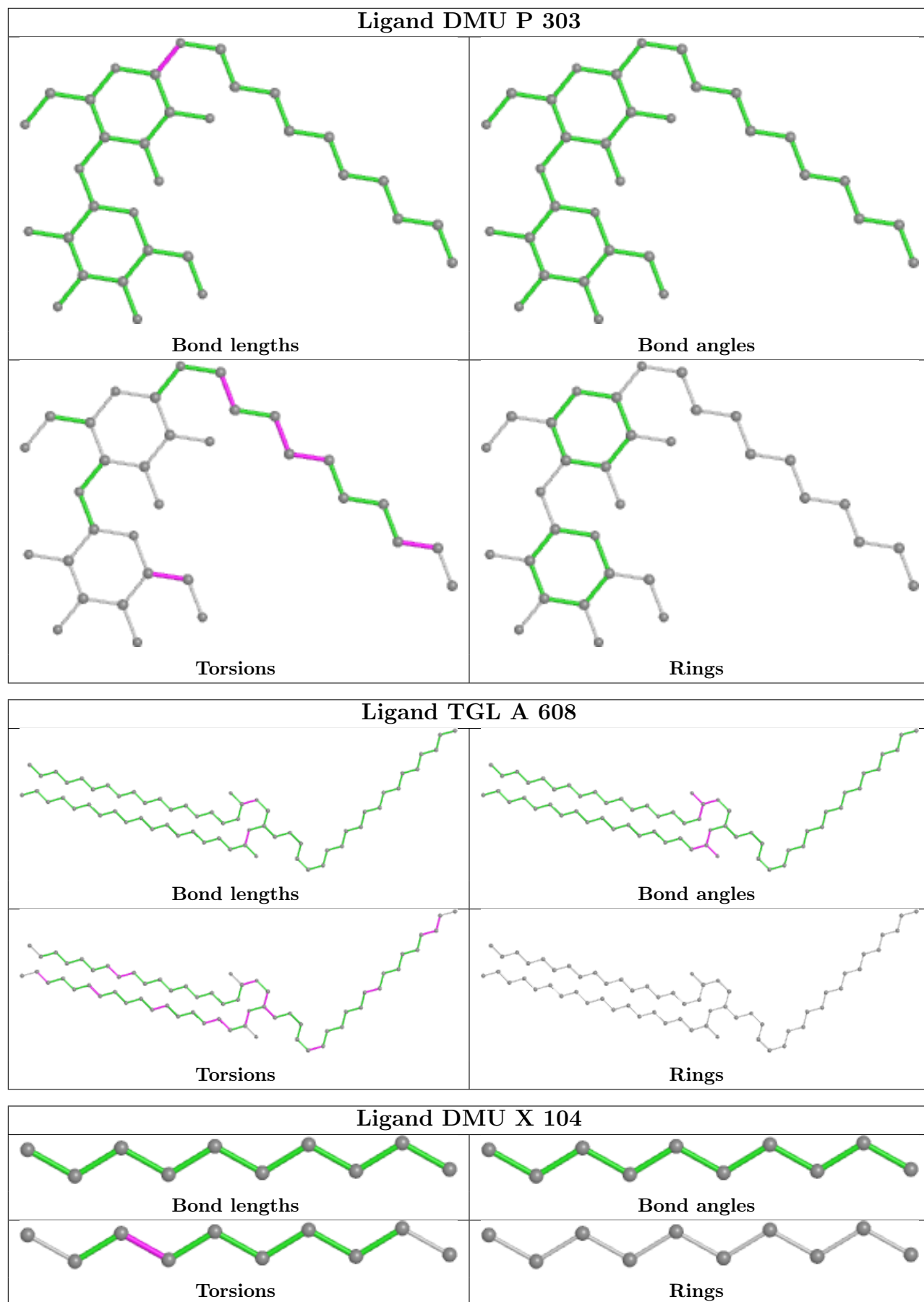
Ligand DMU W 101

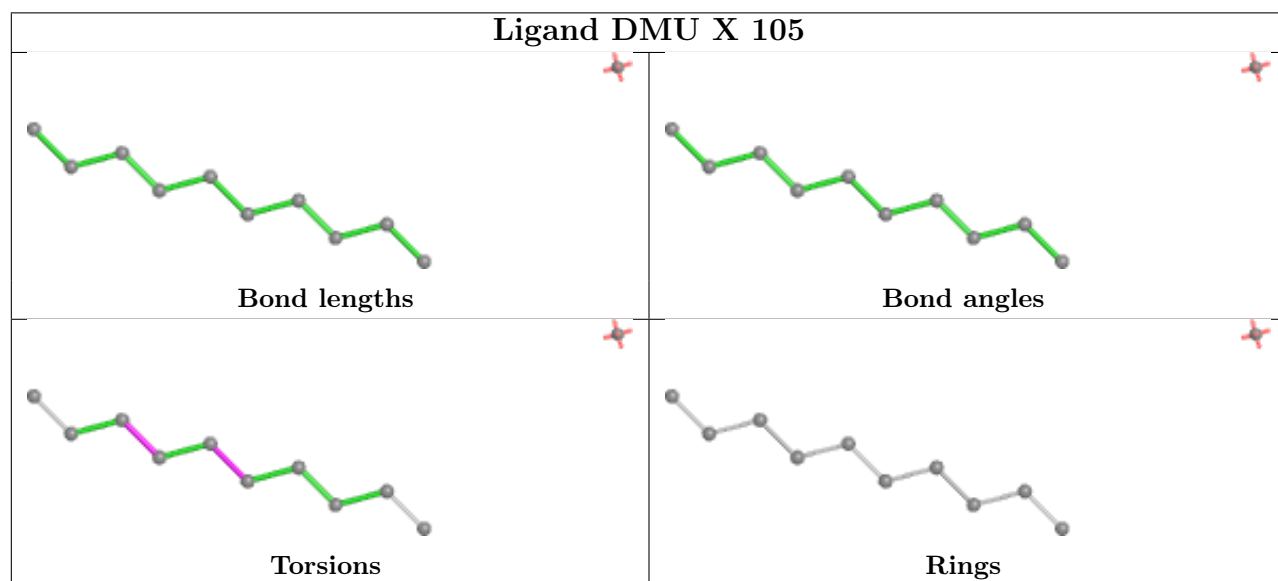
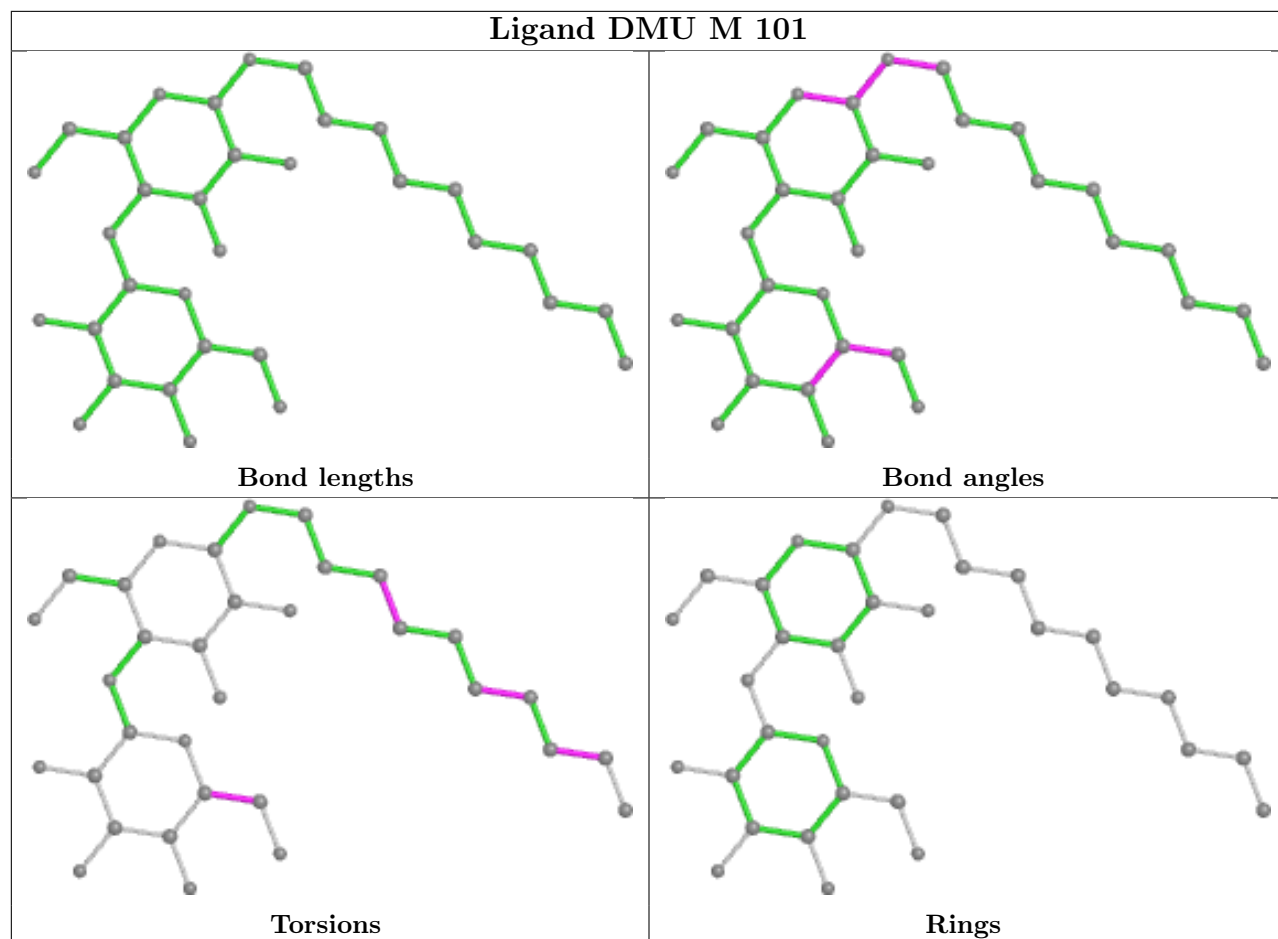


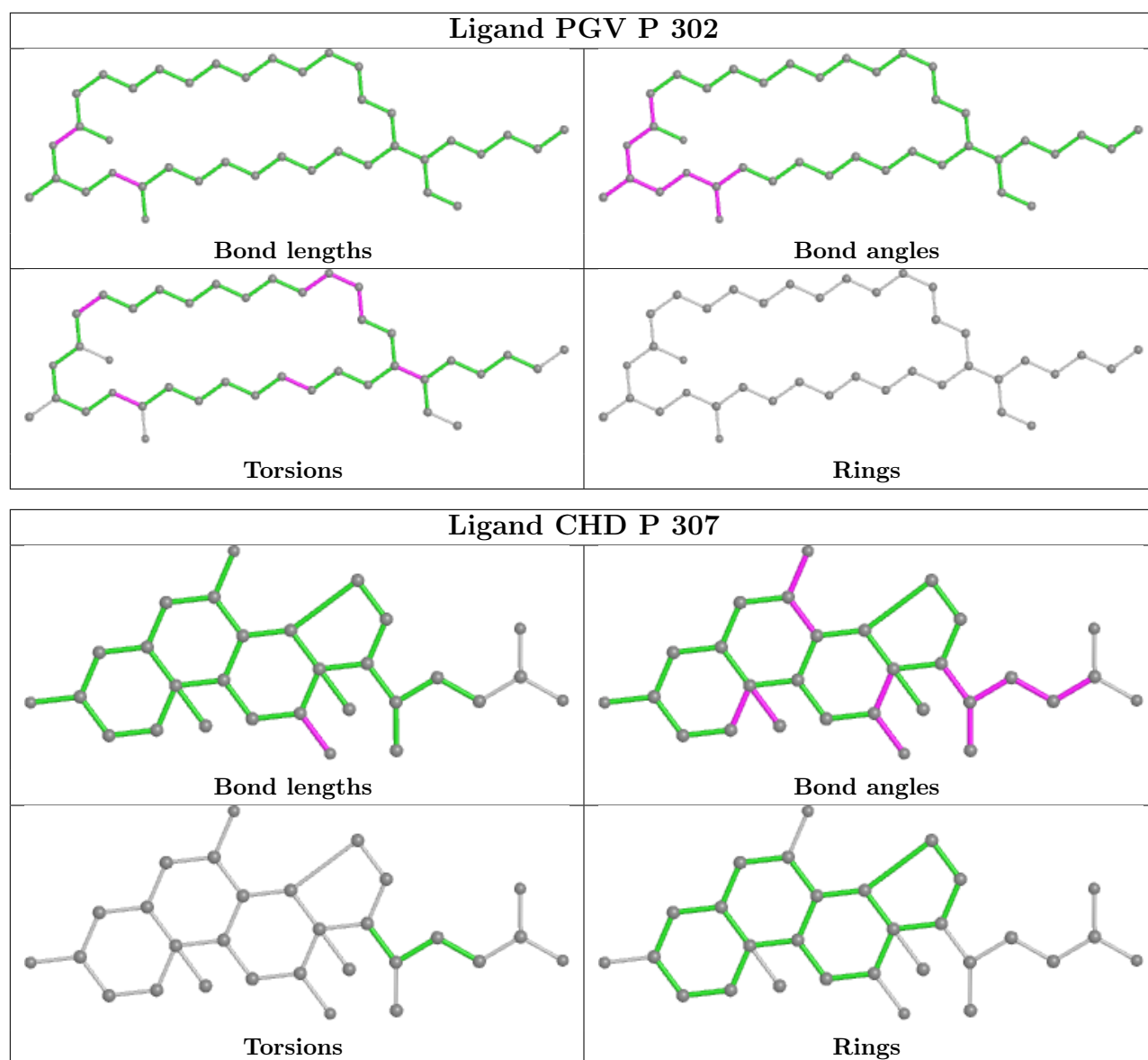
Ligand CHD J 101











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%)	-0.62	0 100 100	16, 20, 29, 79	0
1	N	513/514 (99%)	-0.55	2 (0%) 92 92	18, 23, 33, 82	0
2	B	226/227 (99%)	-0.54	2 (0%) 84 84	19, 28, 57, 115	0
2	O	226/227 (99%)	-0.47	4 (1%) 68 67	24, 33, 77, 129	0
3	C	259/259 (100%)	-0.85	0 100 100	18, 24, 41, 82	0
3	P	259/259 (100%)	-0.80	1 (0%) 92 92	19, 25, 40, 87	0
4	D	144/144 (100%)	-0.74	1 (0%) 87 87	22, 30, 53, 94	0
4	Q	144/144 (100%)	0.65	11 (7%) 13 12	28, 44, 92, 221	0
5	E	105/105 (100%)	-0.65	3 (2%) 51 49	23, 30, 62, 164	0
5	R	105/105 (100%)	-0.25	2 (1%) 66 65	26, 36, 79, 178	0
6	F	98/98 (100%)	-0.06	7 (7%) 16 14	20, 30, 118, 222	0
6	S	98/98 (100%)	0.01	8 (8%) 11 10	20, 29, 143, 247	0
7	G	84/84 (100%)	1.06	19 (22%) 0 0	23, 32, 149, 231	0
7	T	84/84 (100%)	0.88	15 (17%) 1 1	21, 34, 132, 230	0
8	H	79/79 (100%)	0.12	7 (8%) 9 8	24, 34, 153, 180	0
8	U	79/79 (100%)	0.19	8 (10%) 7 5	29, 39, 141, 209	0
9	I	72/73 (98%)	0.16	6 (8%) 11 10	26, 41, 76, 101	0
9	V	72/73 (98%)	0.25	4 (5%) 24 22	27, 50, 95, 229	0
10	J	58/58 (100%)	0.37	4 (6%) 16 15	25, 34, 92, 143	0
10	W	58/58 (100%)	-0.14	3 (5%) 27 24	25, 36, 99, 164	0
11	K	49/49 (100%)	-0.36	1 (2%) 65 64	26, 34, 60, 64	0
11	X	49/49 (100%)	0.68	3 (6%) 21 19	34, 44, 91, 111	0
12	L	46/46 (100%)	-0.82	1 (2%) 62 60	21, 25, 53, 114	0
12	Y	46/46 (100%)	-0.59	1 (2%) 62 60	25, 32, 73, 145	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/43 (100%)	-0.40	4 (9%) 8 7	22, 26, 75, 150	0
13	Z	43/43 (100%)	-0.09	4 (9%) 8 7	30, 35, 128, 256	0
All	All	3552/3558 (99%)	-0.34	121 (3%) 45 42	16, 28, 76, 256	0

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	4	SER	40.0
4	Q	6	VAL	32.2
6	S	97	ALA	29.3
7	G	2	SER	21.5
4	Q	5	VAL	18.3

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	0.26	0.64	178,202,219,230	0
9	SAC	I	1	9/10	0.73	0.21	102,127,159,160	0
1	FME	N	1	10/11	0.95	0.11	31,37,74,75	0
2	FME	B	1	10/11	0.95	0.10	17,27,59,100	0
1	FME	A	1	10/11	0.96	0.07	31,42,90,117	0
2	FME	O	1	10/11	0.98	0.05	30,34,37,88	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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
24	DMU	D	203	9/33	0.24	0.62	67,73,89,108	0
24	DMU	X	103	9/33	0.30	0.25	71,75,93,95	0
24	DMU	K	103	33/33	0.48	0.50	53,116,180,196	0
24	DMU	X	101	33/33	0.48	0.49	56,111,187,198	0
23	CHD	J	101	29/29	0.48	0.64	59,123,157,161	0
24	DMU	X	104	10/33	0.56	0.33	60,65,106,130	0
25	CDL	G	102	64/100	0.57	0.37	50,77,106,116	0
26	PEK	C	305	37/53	0.62	0.27	41,67,97,107	0
24	DMU	J	102	12/33	0.63	0.21	51,62,91,111	0
25	CDL	T	101	79/100	0.65	0.32	49,80,113,135	0
21	EDO	W	103	4/4	0.66	0.16	55,62,82,96	0
26	PEK	P	309	39/53	0.66	0.32	36,74,102,104	0
21	EDO	C	309	4/4	0.67	0.30	44,49,70,77	0
21	EDO	N	621	4/4	0.67	0.14	40,55,66,68	0
23	CHD	P	306	29/29	0.68	0.34	59,87,115,124	0
26	PEK	P	301	20/53	0.70	0.23	41,52,86,90	0
25	CDL	P	305	69/100	0.72	0.42	41,76,134,145	0
18	PGV	P	302	41/51	0.73	0.31	46,78,111,124	0
24	DMU	W	101	9/33	0.74	0.22	61,64,72,87	0
24	DMU	K	104	10/33	0.74	0.30	46,68,94,156	0
21	EDO	N	612	4/4	0.75	0.17	44,59,71,81	0
21	EDO	C	311	4/4	0.76	0.31	31,70,77,85	0
21	EDO	C	312	4/4	0.76	0.24	38,70,75,119	0
24	DMU	P	303	33/33	0.76	0.18	46,92,140,148	0
25	CDL	C	303	56/100	0.76	0.34	37,62,94,99	0
19	TGL	D	201	63/63	0.76	0.25	30,73,104,130	0
18	PGV	C	306	36/51	0.77	0.33	35,74,108,121	0
24	DMU	L	102	21/33	0.78	0.21	46,81,117,144	0
26	PEK	C	307	26/53	0.78	0.25	40,56,95,102	0
19	TGL	L	101	59/63	0.79	0.22	26,59,112,149	0
19	TGL	N	608	57/63	0.79	0.25	37,67,99,118	0
19	TGL	O	301	58/63	0.79	0.28	46,69,105,116	0
21	EDO	Y	101	4/4	0.79	0.16	43,48,52,89	0
20	PSC	A	609	25/52	0.80	0.23	44,68,88,93	0
19	TGL	Q	201	63/63	0.80	0.23	41,73,102,123	0
24	DMU	C	308	12/33	0.81	0.15	55,59,89,91	0
24	DMU	X	105	11/33	0.81	0.46	49,80,93,110	0
24	DMU	K	102	9/33	0.82	0.41	59,68,90,92	0
21	EDO	Q	203	4/4	0.82	0.14	33,38,60,65	0
20	PSC	O	303	24/52	0.83	0.22	35,62,98,102	0
21	EDO	R	201	4/4	0.83	0.07	43,47,48,52	0
24	DMU	K	105	9/33	0.83	0.58	59,82,91,107	0
21	EDO	N	617	4/4	0.84	0.14	40,72,73,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	DMU	X	102	10/33	0.84	0.20	48,60,96,115	0
21	EDO	S	102	4/4	0.84	0.11	40,42,47,64	0
21	EDO	J	103	4/4	0.84	0.18	60,61,61,99	0
24	DMU	P	310	11/33	0.84	0.18	47,64,82,98	0
24	DMU	Z	101	33/33	0.84	0.17	35,46,65,75	0
19	TGL	A	608	62/63	0.84	0.20	36,70,100,112	0
18	PGV	N	606	40/51	0.85	0.27	37,69,127,133	0
18	PGV	A	607	37/51	0.86	0.21	33,60,113,122	0
24	DMU	K	101	10/33	0.86	0.25	43,70,82,180	0
21	EDO	B	304	4/4	0.86	0.20	50,51,53,97	0
21	EDO	A	617	4/4	0.87	0.10	35,40,42,43	0
21	EDO	T	102	4/4	0.87	0.17	36,52,64,76	0
21	EDO	W	102	4/4	0.87	0.10	39,55,67,102	0
28	PO4	U	101	5/5	0.87	0.52	72,73,93,94	5
21	EDO	A	613	4/4	0.88	0.11	32,34,37,41	0
24	DMU	M	101	33/33	0.88	0.11	31,36,67,74	0
24	DMU	D	202	12/33	0.89	0.17	43,67,98,130	0
24	DMU	O	304	10/33	0.89	0.12	41,49,79,82	0
24	DMU	C	301	9/33	0.89	0.13	25,44,63,71	0
21	EDO	B	306	4/4	0.89	0.13	27,39,40,47	0
21	EDO	S	103	4/4	0.90	0.16	28,55,84,92	0
21	EDO	O	307	4/4	0.90	0.17	31,64,82,96	0
24	DMU	K	106	9/33	0.90	0.12	36,50,95,95	0
28	PO4	H	101	5/5	0.90	0.44	57,64,83,100	5
21	EDO	F	105	4/4	0.90	0.16	29,42,54,61	0
21	EDO	N	609	4/4	0.91	0.13	36,36,41,47	0
21	EDO	A	615	4/4	0.91	0.23	36,37,51,110	0
21	EDO	F	102	4/4	0.91	0.13	42,45,57,87	0
21	EDO	A	619	4/4	0.92	0.16	25,30,35,41	0
21	EDO	B	305	4/4	0.92	0.13	32,43,44,54	0
21	EDO	S	106	4/4	0.92	0.14	29,57,60,67	0
21	EDO	N	619	4/4	0.93	0.12	29,40,56,95	0
21	EDO	T	103	4/4	0.93	0.16	52,69,83,104	0
21	EDO	F	104	4/4	0.93	0.09	30,33,35,44	0
21	EDO	N	613	4/4	0.93	0.07	33,38,40,69	0
21	EDO	F	103	4/4	0.93	0.09	33,39,61,104	0
21	EDO	P	313	4/4	0.94	0.07	31,34,37,39	0
23	CHD	P	307	29/29	0.94	0.08	22,27,31,36	0
21	EDO	J	104	4/4	0.94	0.22	39,44,62,104	0
21	EDO	P	311	4/4	0.94	0.09	26,28,38,61	0
21	EDO	P	312	4/4	0.94	0.10	47,57,60,67	0
21	EDO	N	610	4/4	0.95	0.06	30,32,32,33	0

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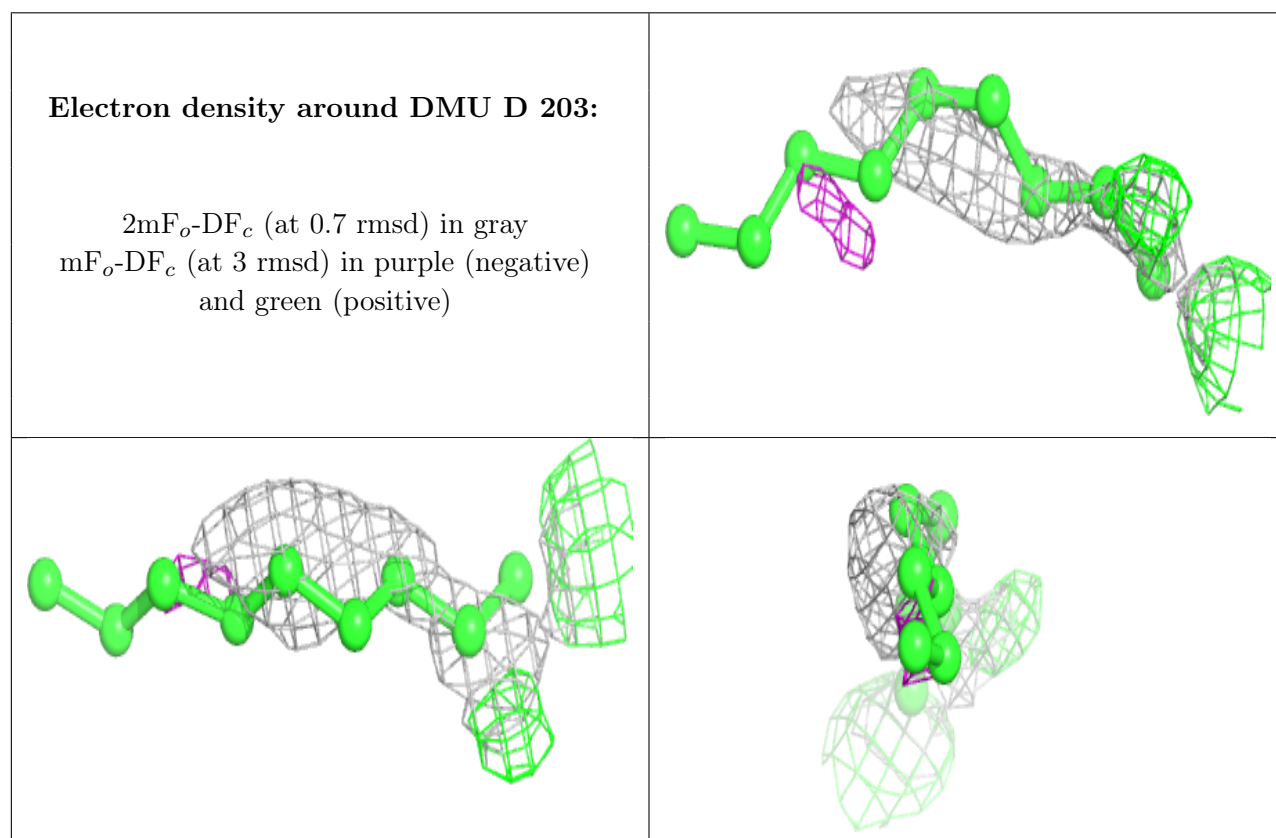
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	EDO	G	104	4/4	0.95	0.06	27,29,33,35	0
26	PEK	G	101	53/53	0.95	0.15	23,42,90,126	0
21	EDO	Q	204	4/4	0.95	0.13	49,51,59,60	0
21	EDO	A	612	4/4	0.95	0.10	30,34,72,79	0
23	CHD	B	302	29/29	0.95	0.07	20,24,28,37	0
23	CHD	C	304	29/29	0.95	0.08	22,26,31,32	0
21	EDO	N	611	4/4	0.96	0.09	27,36,42,77	0
21	EDO	C	313	4/4	0.96	0.10	27,28,38,68	0
21	EDO	E	201	4/4	0.96	0.07	33,35,35,36	0
21	EDO	N	614	4/4	0.96	0.08	28,30,58,80	0
21	EDO	N	615	4/4	0.96	0.10	25,34,70,102	0
21	EDO	E	202	4/4	0.96	0.09	33,36,38,41	0
23	CHD	G	103	29/29	0.96	0.06	20,23,27,34	0
17	NA	N	605	1/1	0.96	0.05	27,27,27,27	0
26	PEK	P	308	53/53	0.96	0.11	26,43,95,124	0
21	EDO	A	610	4/4	0.96	0.08	28,28,35,77	0
21	EDO	O	306	4/4	0.96	0.09	37,37,40,43	0
21	EDO	A	614	4/4	0.96	0.06	22,23,25,26	0
21	EDO	S	105	4/4	0.97	0.05	30,32,35,35	0
21	EDO	Q	202	4/4	0.97	0.07	26,33,55,56	0
21	EDO	N	616	4/4	0.97	0.07	22,23,24,26	0
21	EDO	A	616	4/4	0.97	0.08	26,33,34,42	0
21	EDO	C	310	4/4	0.97	0.06	28,30,31,34	0
18	PGV	P	304	50/51	0.97	0.08	19,30,70,100	0
21	EDO	O	305	4/4	0.97	0.06	28,28,29,32	0
21	EDO	S	104	4/4	0.97	0.06	20,21,21,22	0
21	EDO	B	303	4/4	0.98	0.04	21,23,23,26	0
21	EDO	A	611	4/4	0.98	0.12	19,20,20,25	0
14	HEA	N	602	60/60	0.98	0.07	16,20,28,30	0
17	NA	A	605	1/1	0.98	0.04	22,22,22,22	0
18	PGV	N	607	51/51	0.98	0.08	20,25,70,93	0
14	HEA	N	601[A]	60/60	0.98	0.07	19,22,34,44	10
18	PGV	A	606	51/51	0.98	0.08	18,24,66,83	0
21	EDO	N	618	4/4	0.98	0.06	29,37,44,45	0
14	HEA	N	601[B]	60/60	0.98	0.07	12,22,35,46	10
21	EDO	N	620	4/4	0.98	0.10	21,24,24,28	0
21	EDO	A	618	4/4	0.98	0.10	28,35,67,106	0
18	PGV	C	302	51/51	0.98	0.08	19,26,75,97	0
21	EDO	F	106	4/4	0.99	0.04	19,20,20,22	0
16	MG	A	604	1/1	0.99	0.04	17,17,17,17	0
16	MG	N	604	1/1	0.99	0.04	20,20,20,20	0
14	HEA	A	601[A]	60/60	0.99	0.07	15,18,28,40	10

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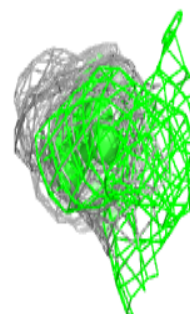
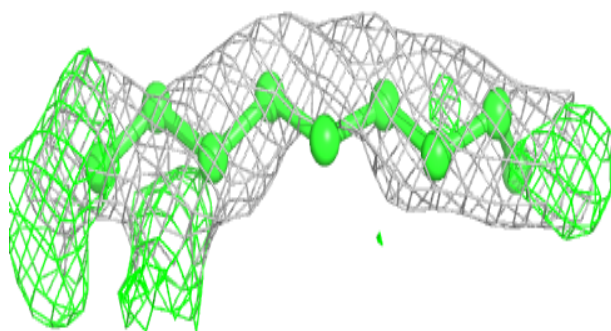
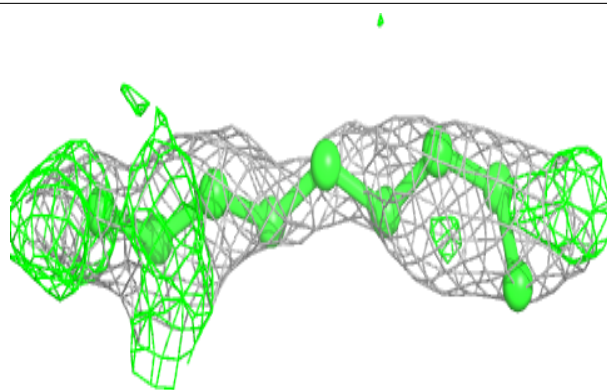
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	ZN	S	101	1/1	0.99	0.03	24,24,24,24	0
14	HEA	A	601[B]	60/60	0.99	0.07	10,18,32,53	10
14	HEA	A	602	60/60	0.99	0.06	15,18,26,31	0
22	CUA	B	301	2/2	1.00	0.05	20,20,20,20	0
27	ZN	F	101	1/1	1.00	0.02	23,23,23,23	0
22	CUA	O	302	2/2	1.00	0.05	24,24,24,25	0
15	CU	A	603	1/1	1.00	0.06	17,17,17,17	0
15	CU	N	603	1/1	1.00	0.06	20,20,20,20	0

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

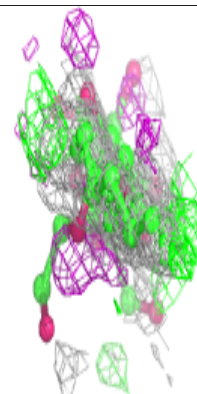
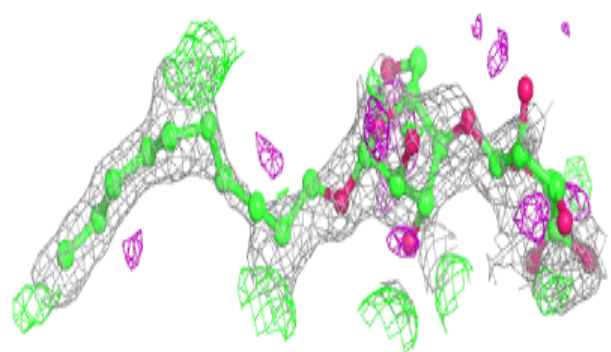
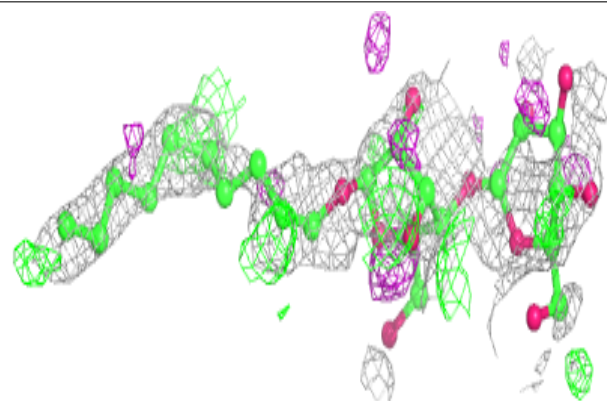


Electron density around DMU X 103:

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

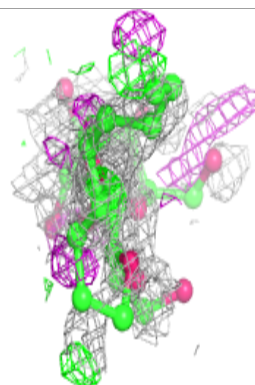
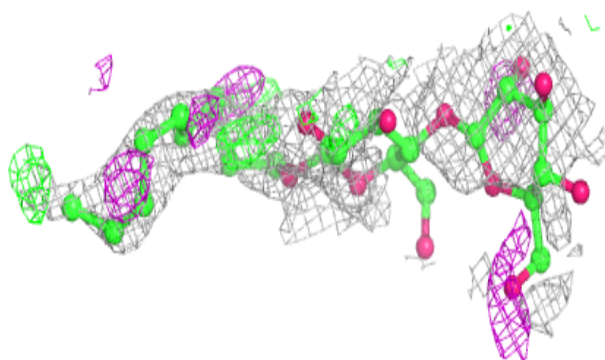
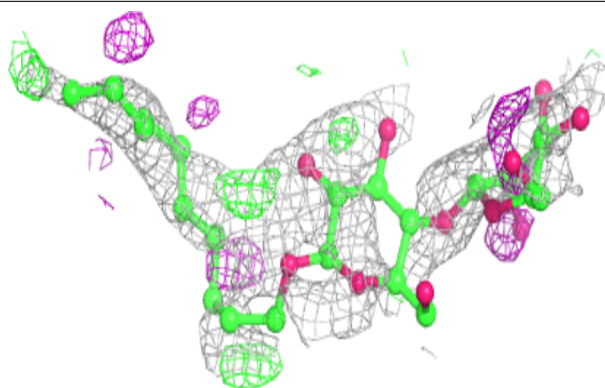
**Electron density around DMU K 103:**

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

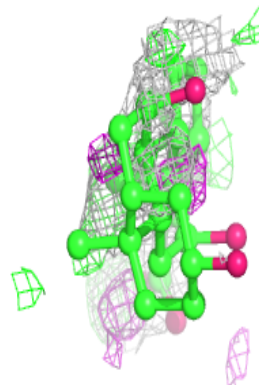
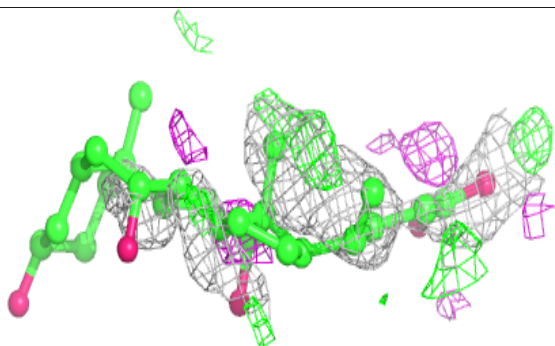
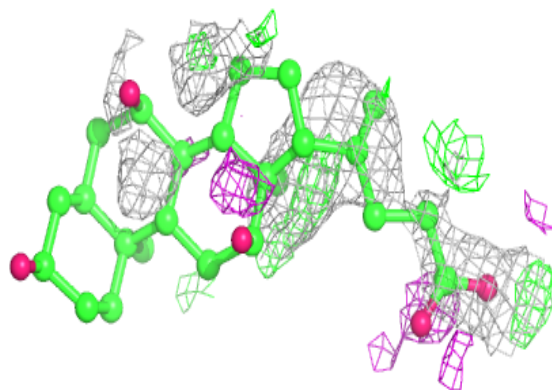


Electron density around DMU X 101:

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

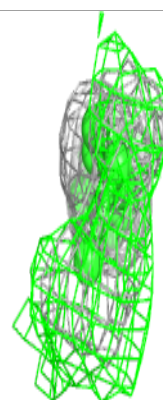
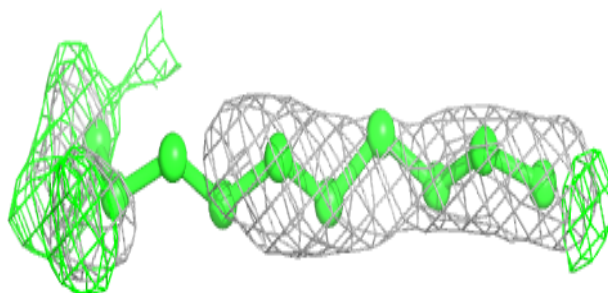
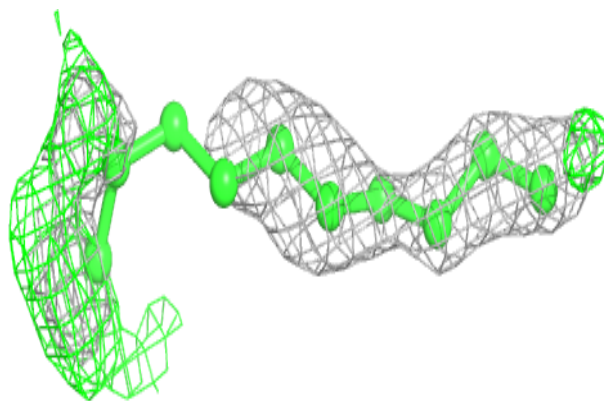
**Electron density around CHD J 101:**

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

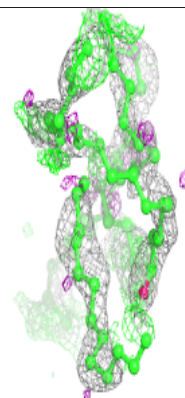
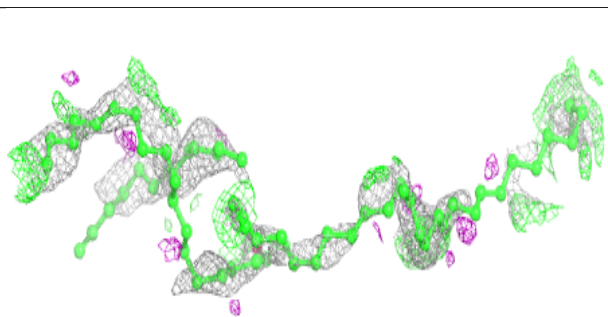
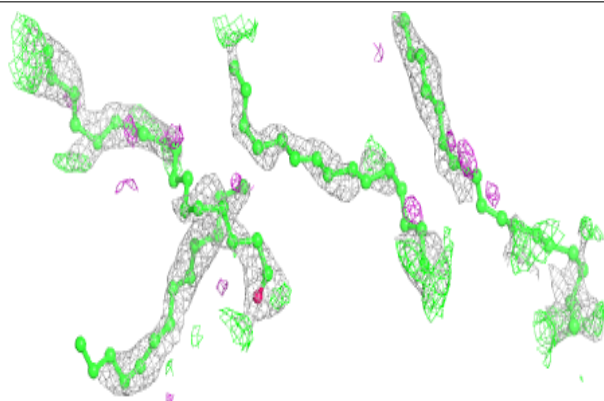


Electron density around DMU X 104:

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

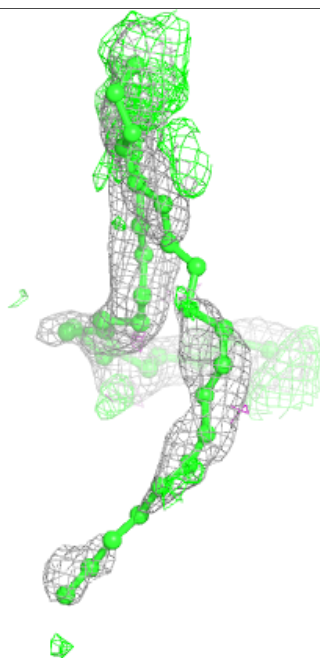
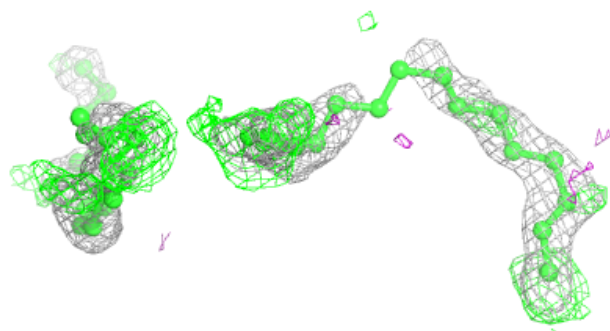
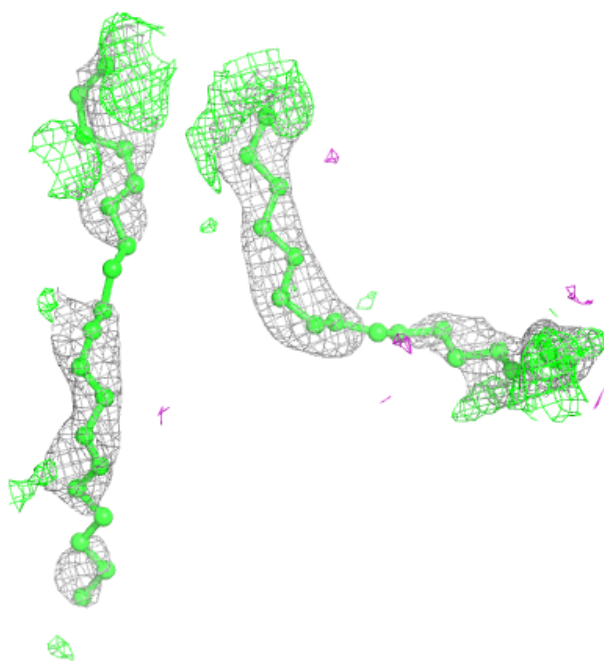
**Electron density around CDL G 102:**

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



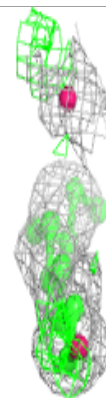
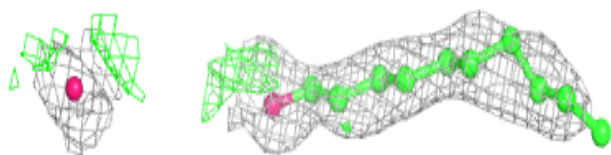
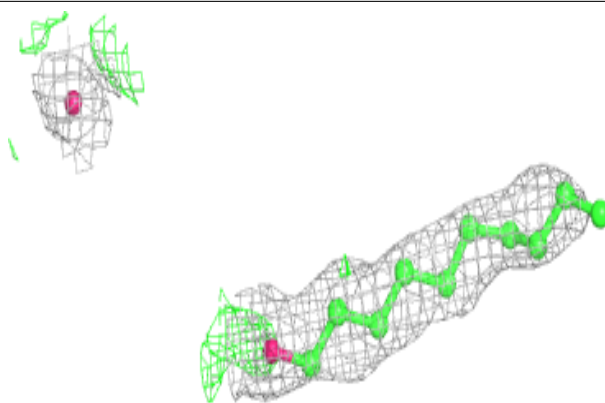
Electron density around PEK C 305:

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

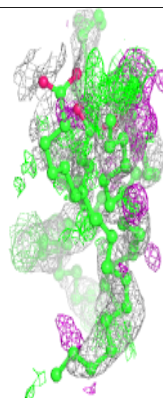
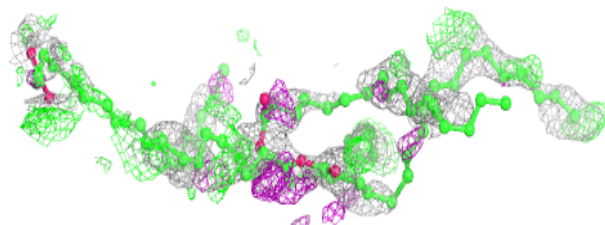
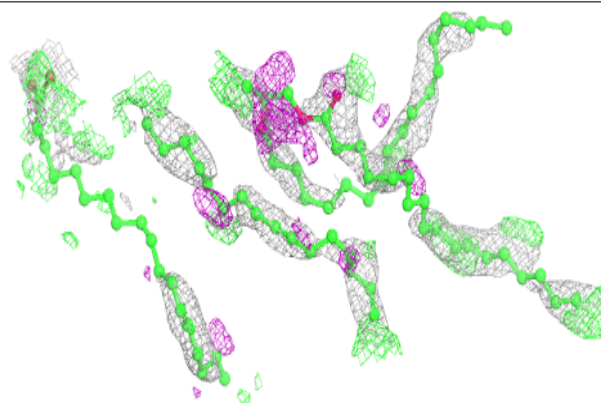


Electron density around DMU J 102:

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

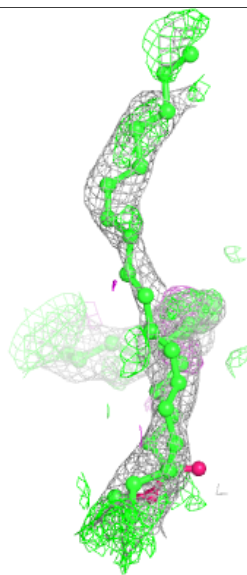
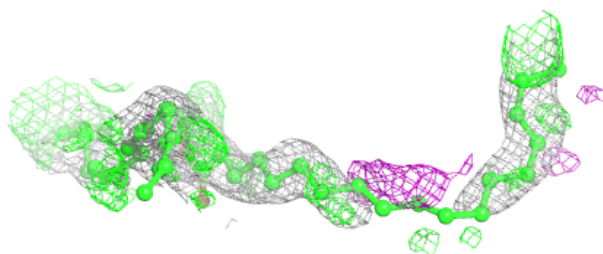
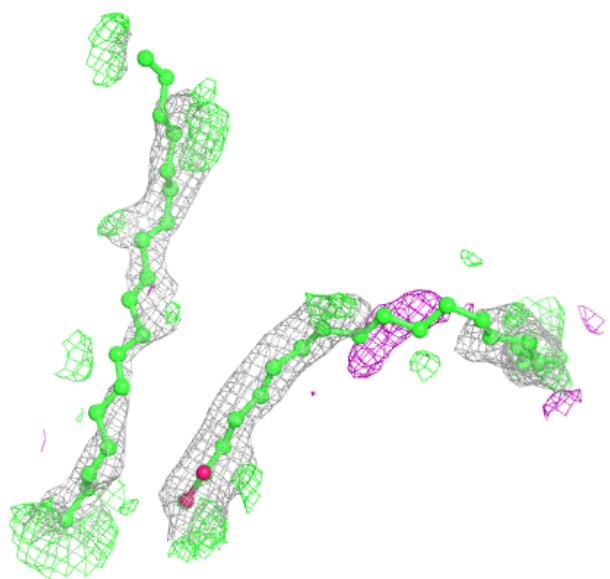
**Electron density around CDL T 101:**

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



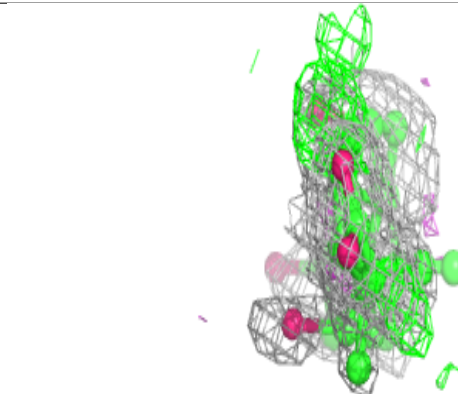
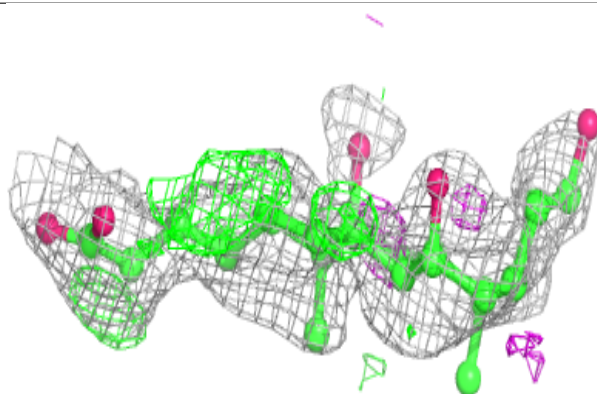
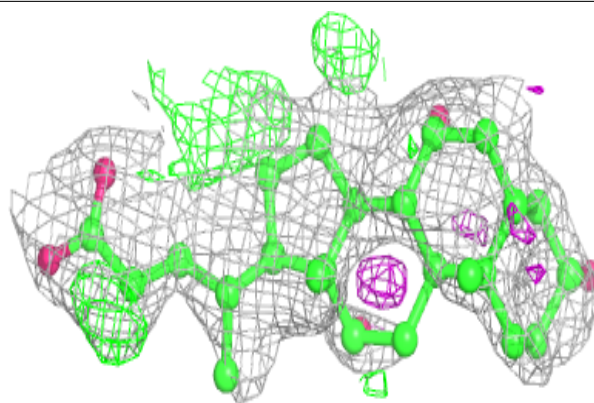
Electron density around PEK P 309:

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

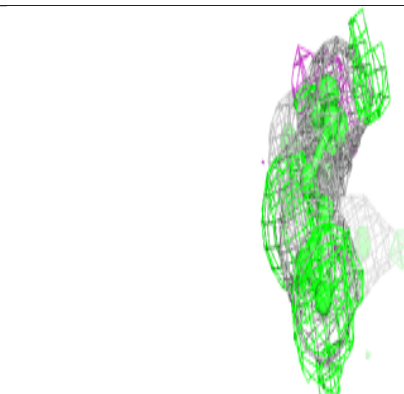
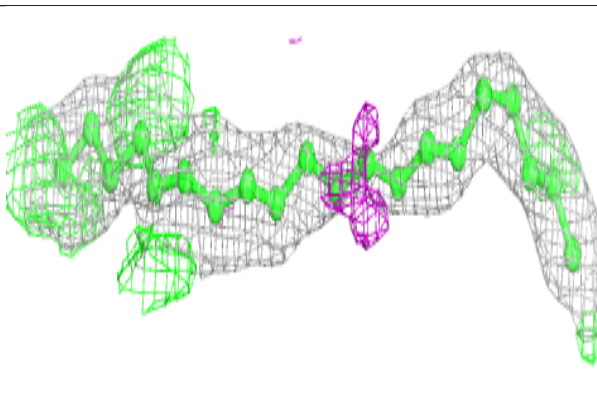
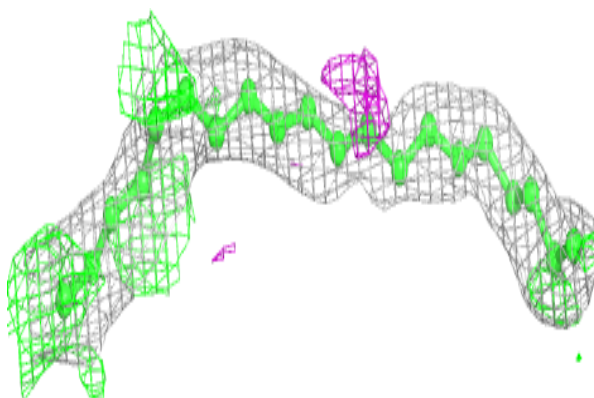


Electron density around CHD P 306:

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

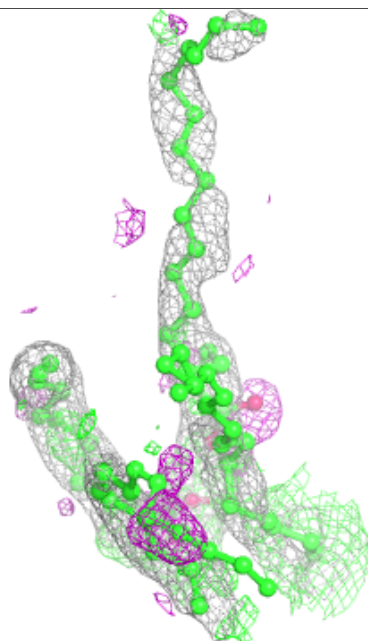
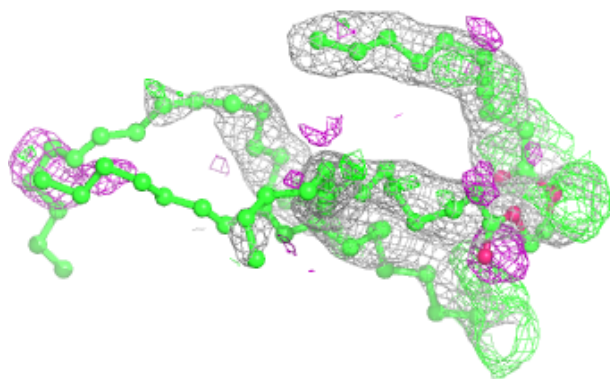
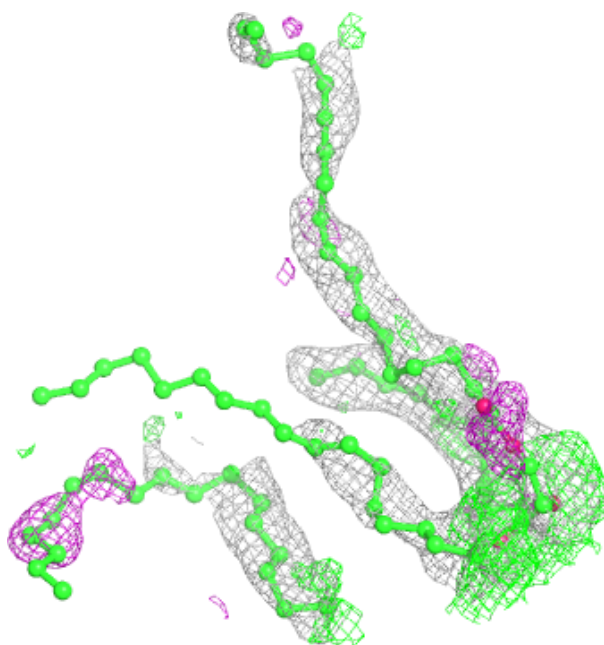
**Electron density around PEK P 301:**

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



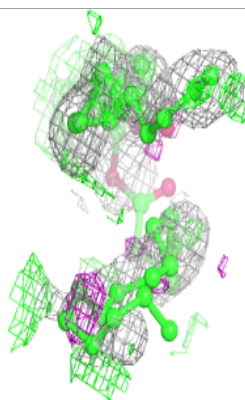
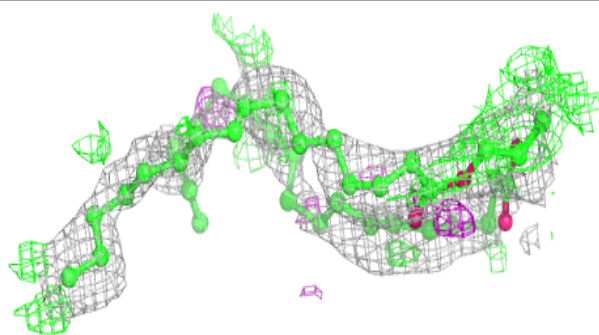
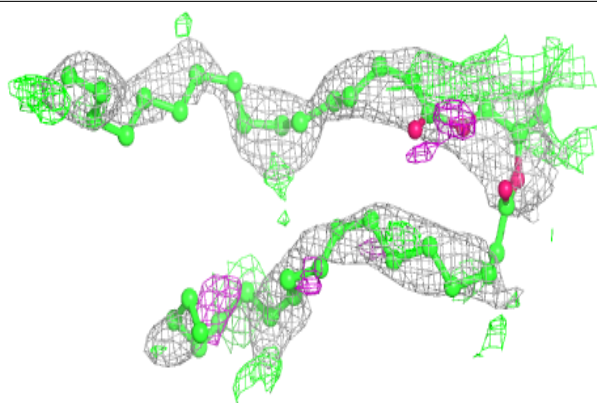
Electron density around CDL P 305:

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

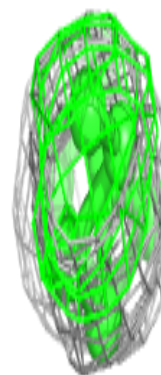
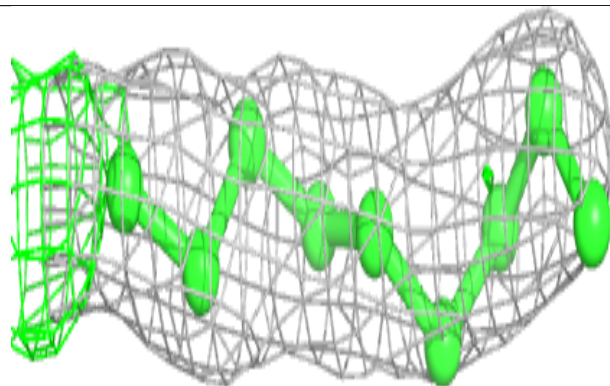
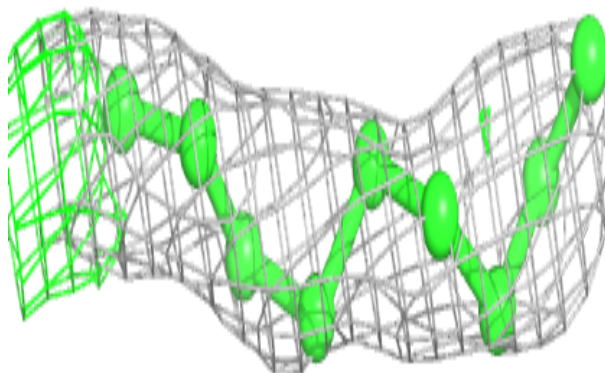


Electron density around PGV P 302:

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

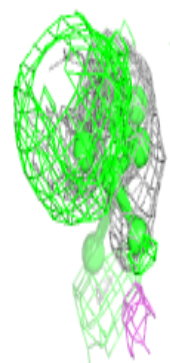
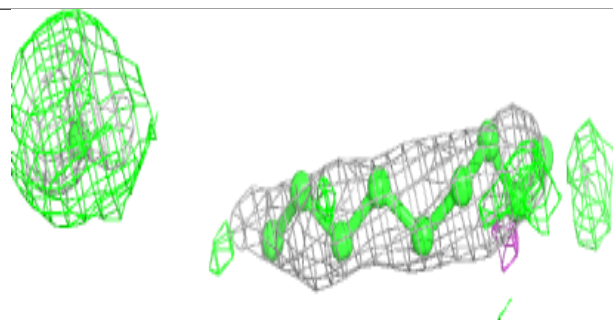
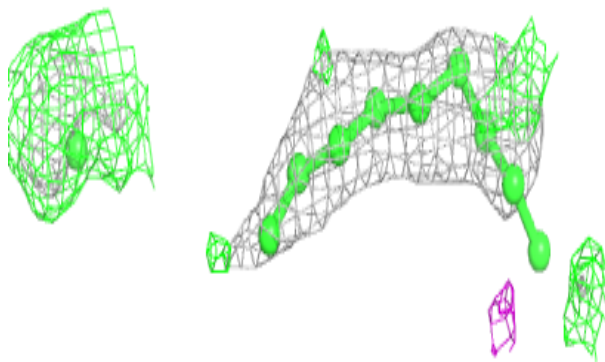
**Electron density around DMU W 101:**

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

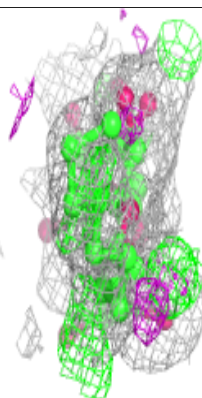
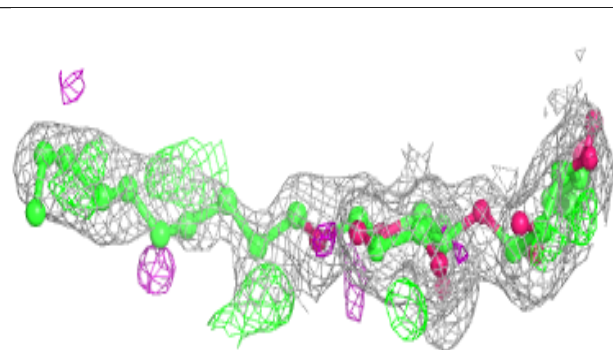
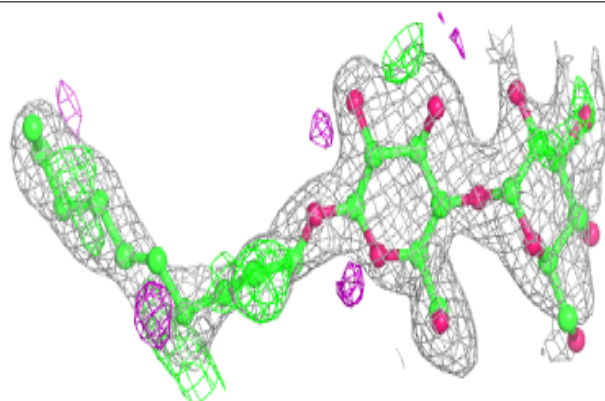


Electron density around DMU K 104:

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

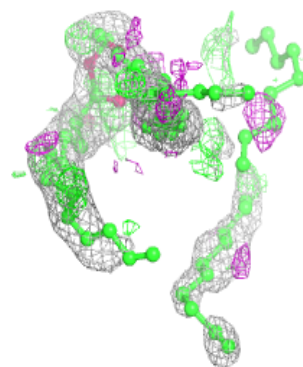
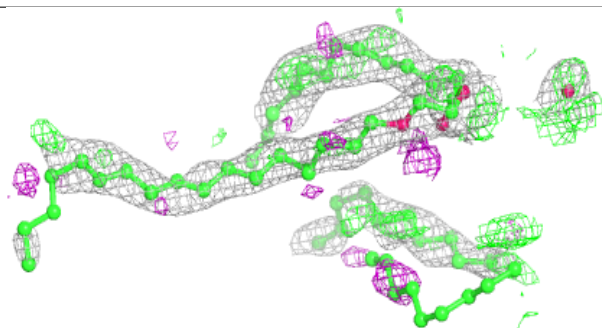
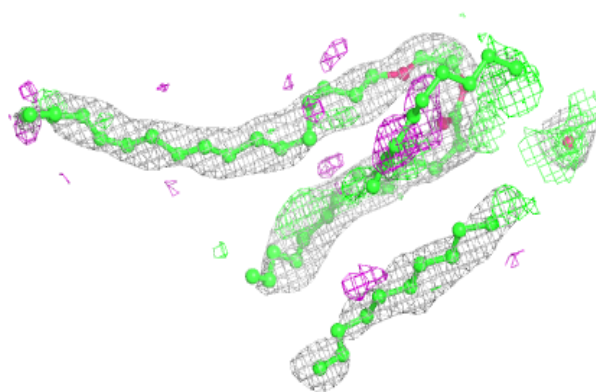
**Electron density around DMU P 303:**

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

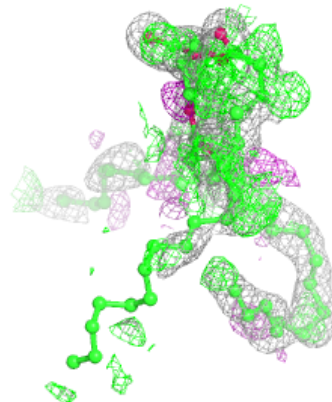
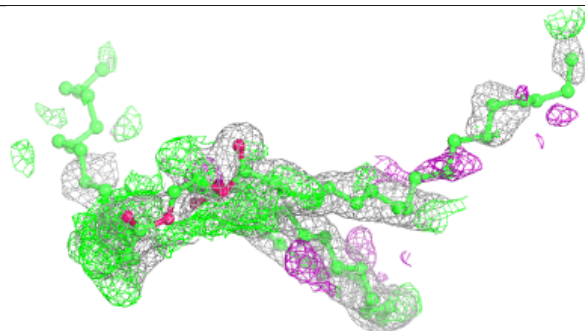
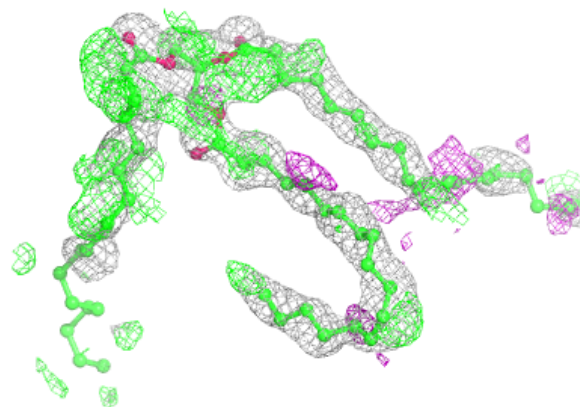


Electron density around CDL C 303:

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

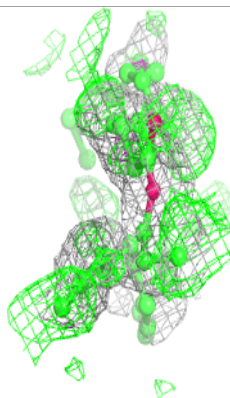
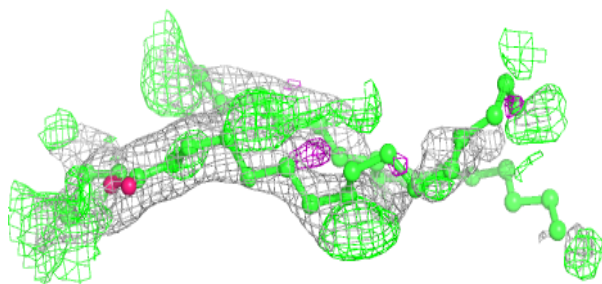
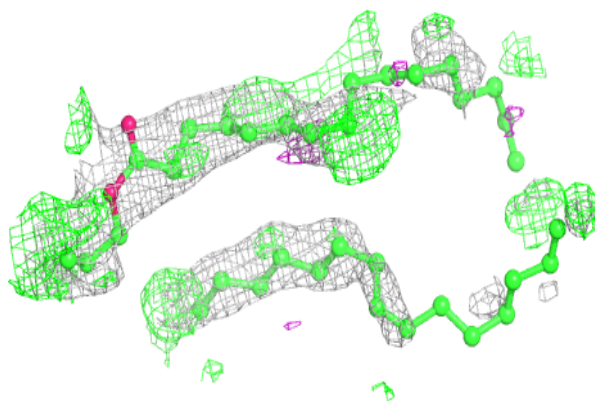
**Electron density around TGL D 201:**

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

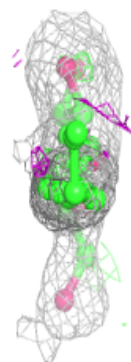
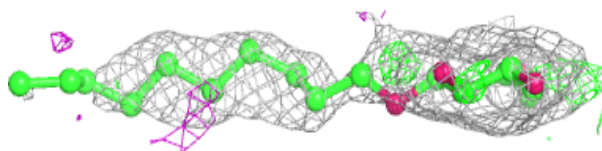
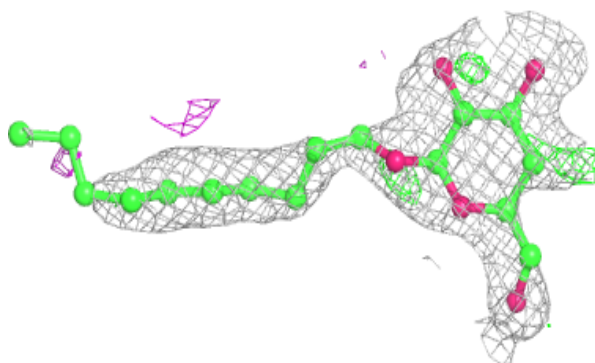


Electron density around PGV C 306:

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

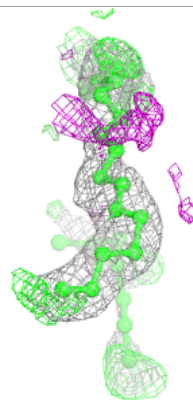
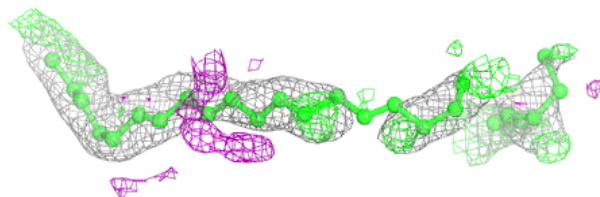
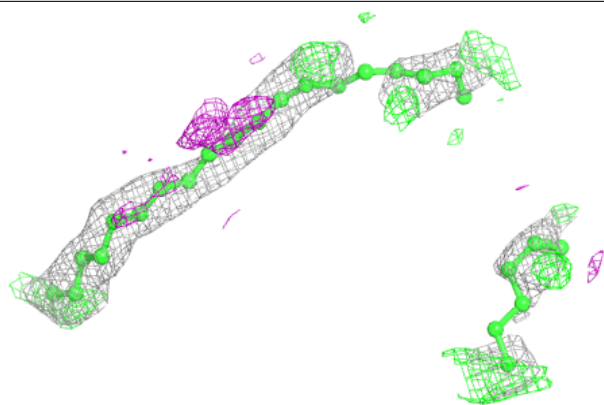
**Electron density around DMU L 102:**

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



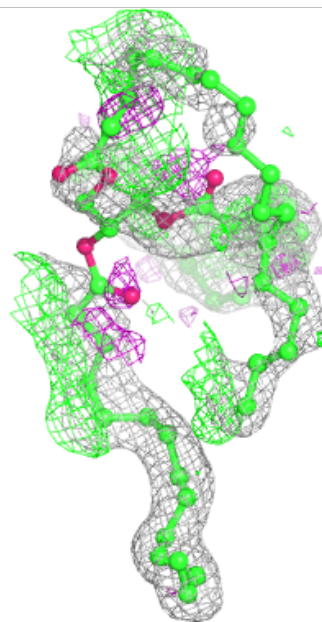
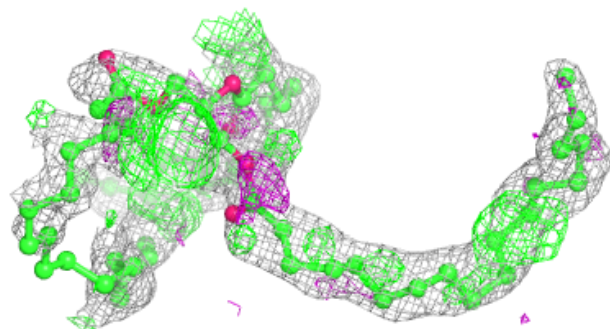
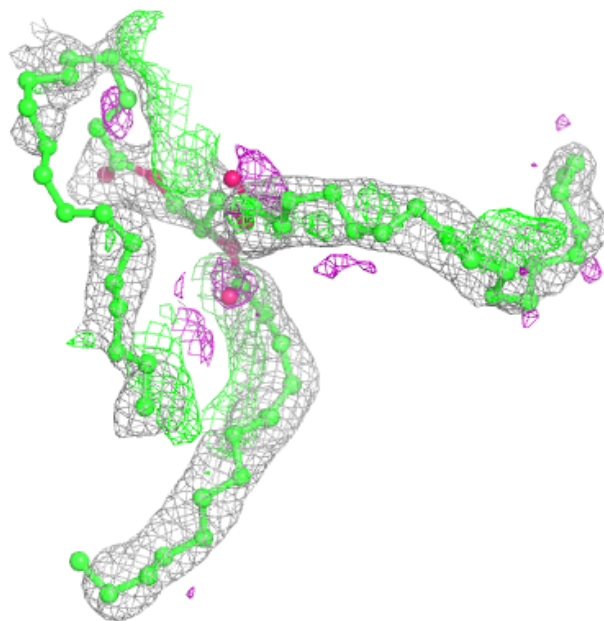
Electron density around PEK C 307:

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



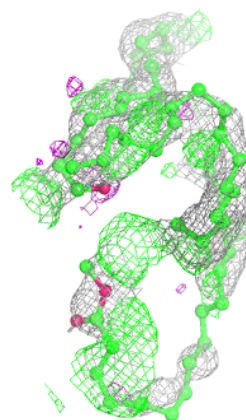
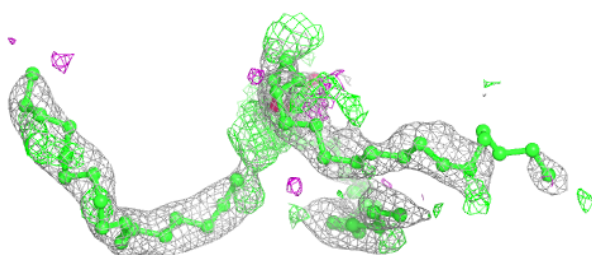
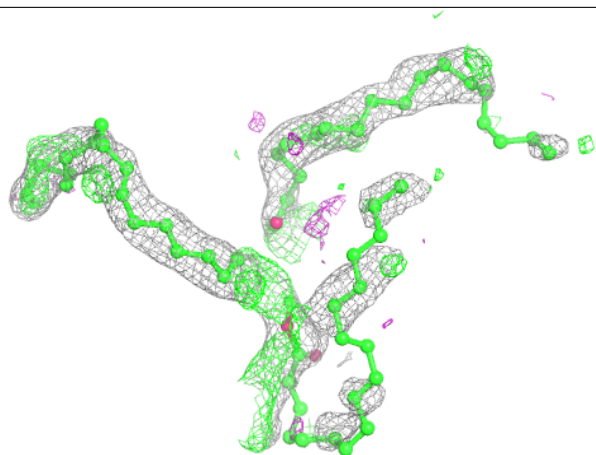
Electron density around TGL L 101:

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

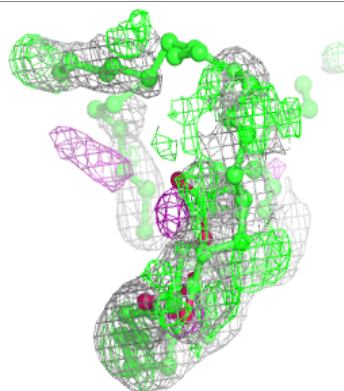
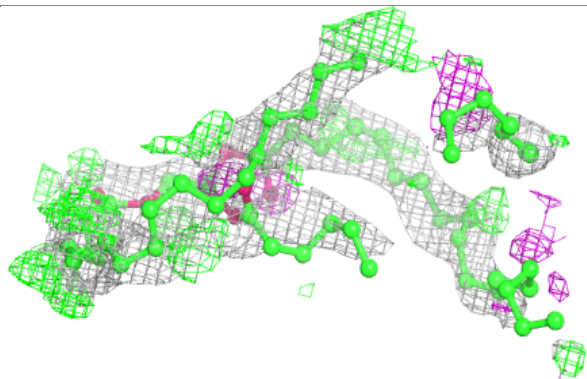
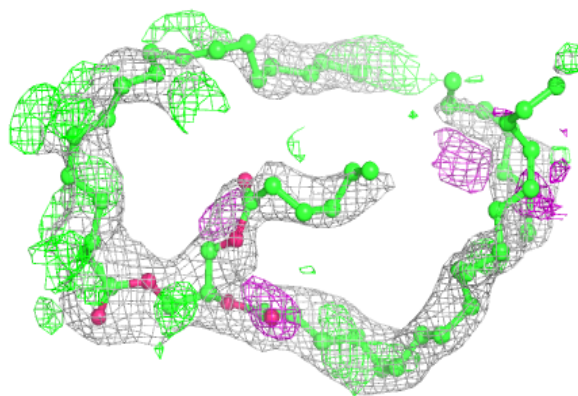


Electron density around TGL N 608:

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

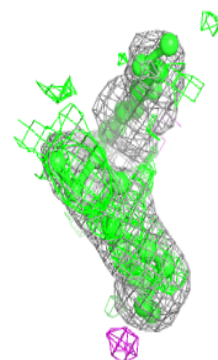
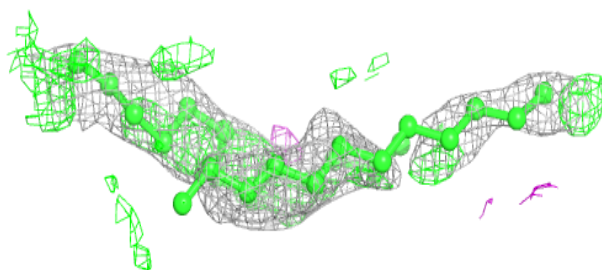
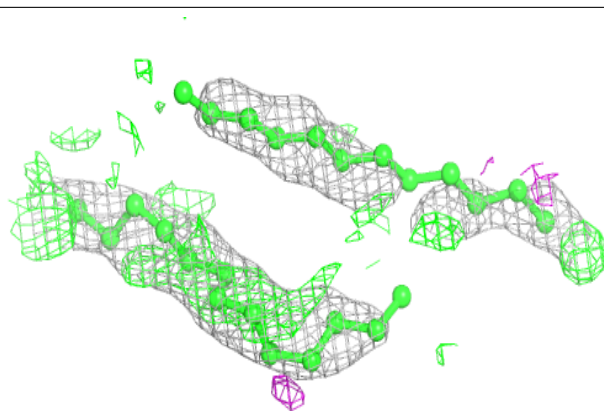
**Electron density around TGL O 301:**

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

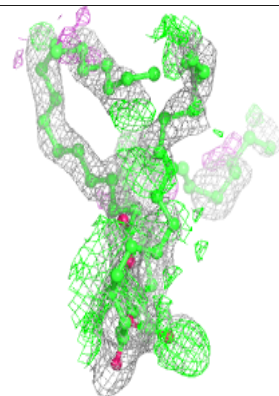
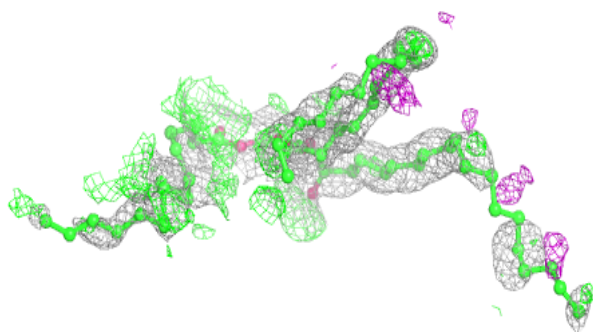
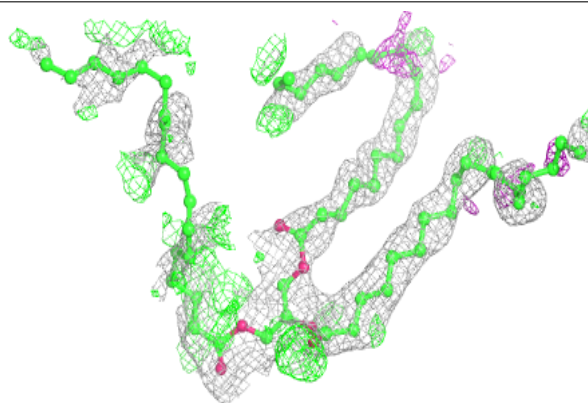


Electron density around PSC A 609:

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

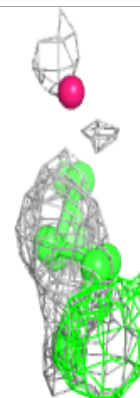
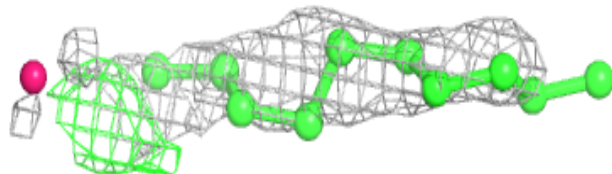
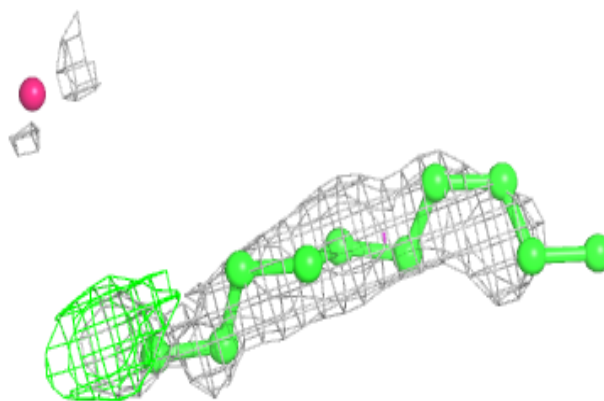
**Electron density around TGL Q 201:**

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

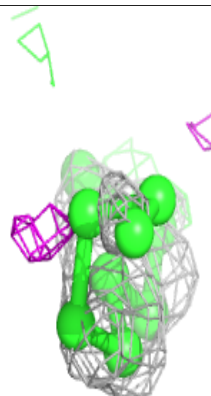
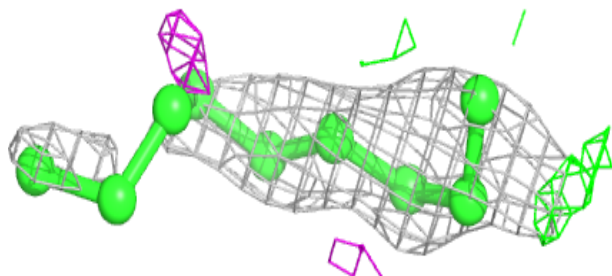
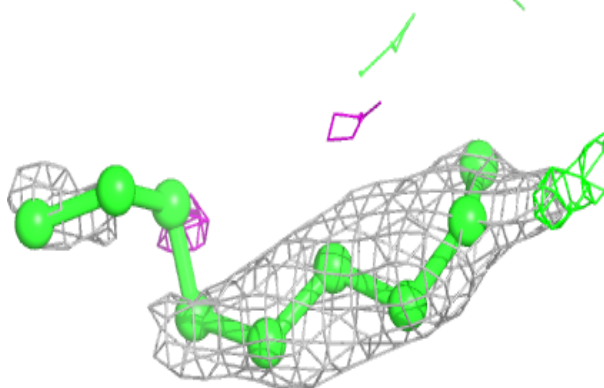


Electron density around DMU X 105:

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

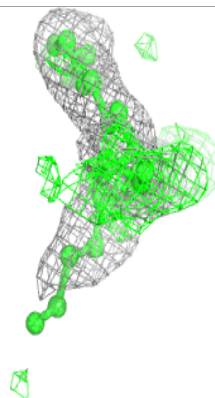
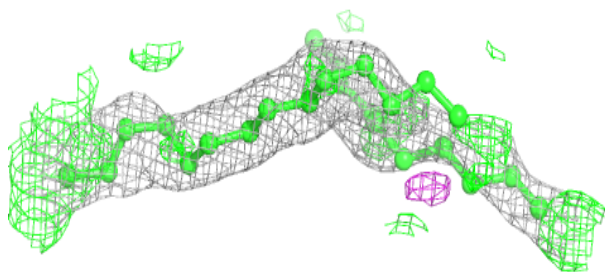
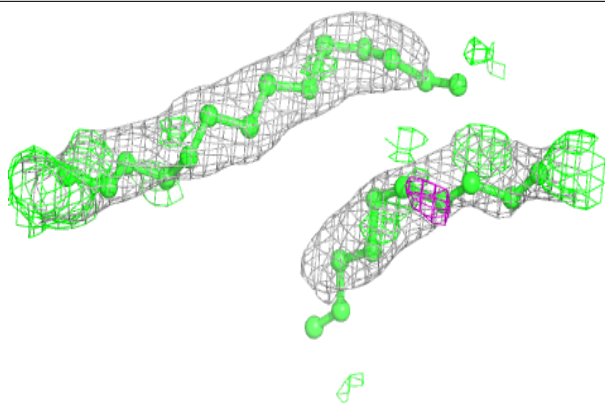
**Electron density around DMU K 102:**

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

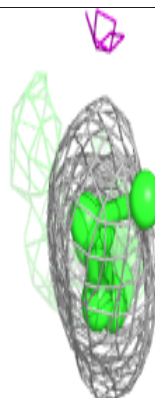
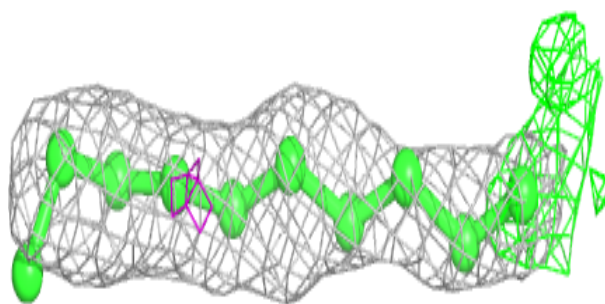
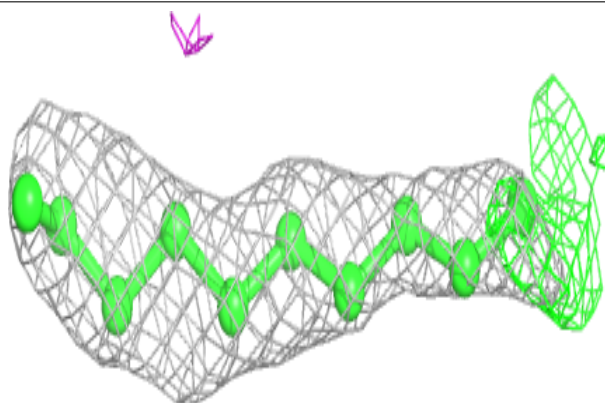


Electron density around PSC O 303:

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

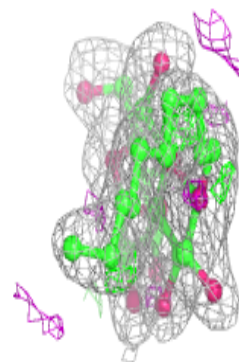
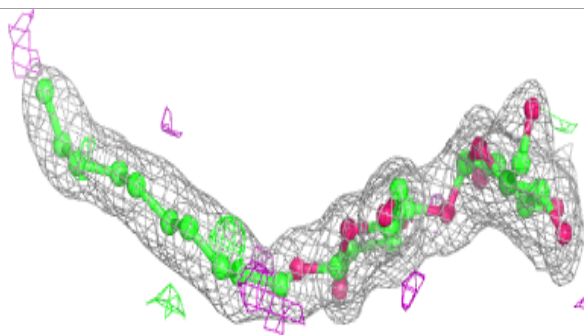
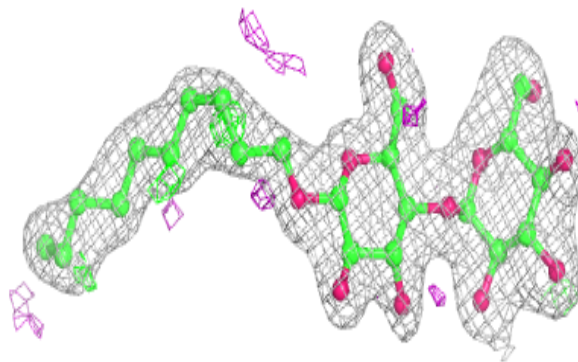
**Electron density around DMU X 102:**

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

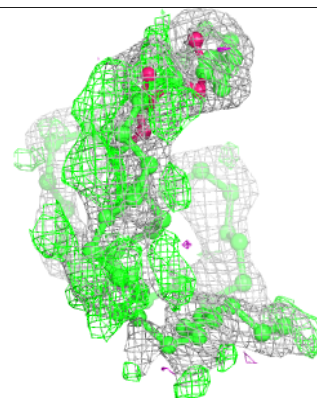
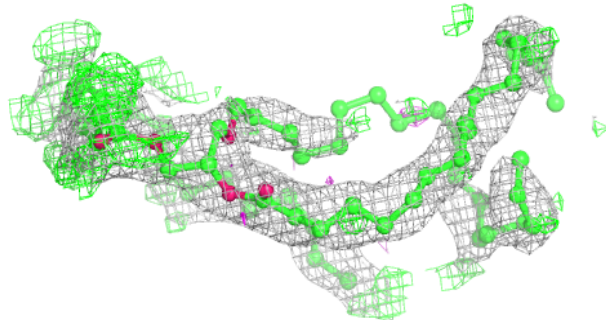
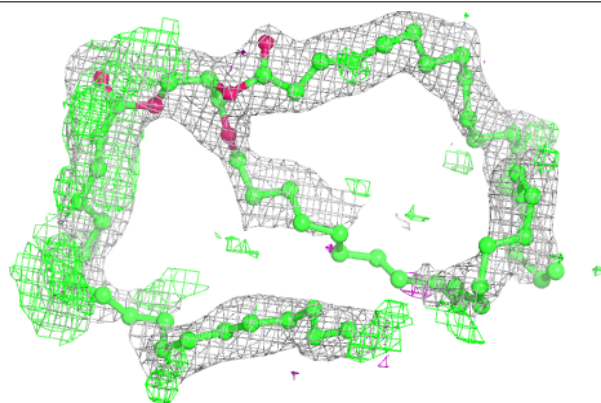


Electron density around DMU Z 101:

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

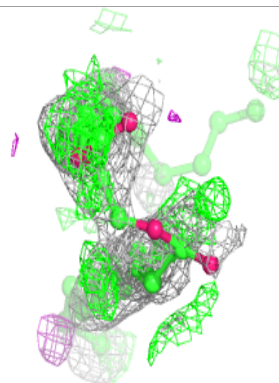
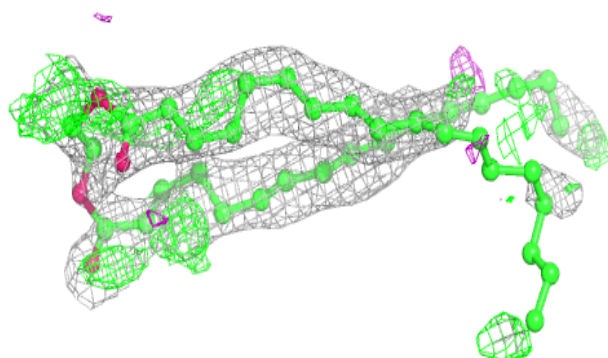
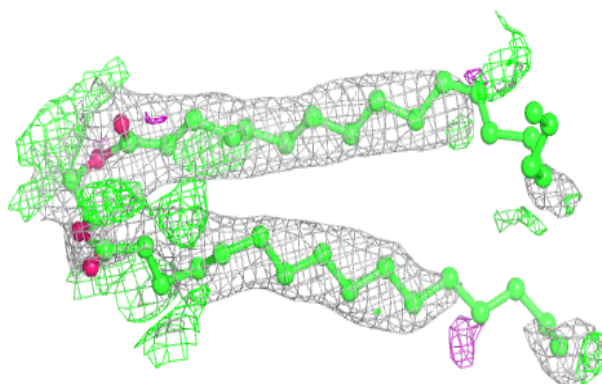
**Electron density around TGL A 608:**

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

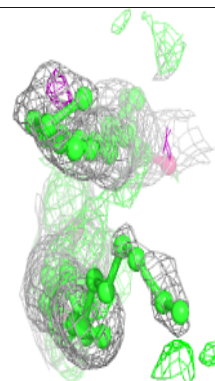
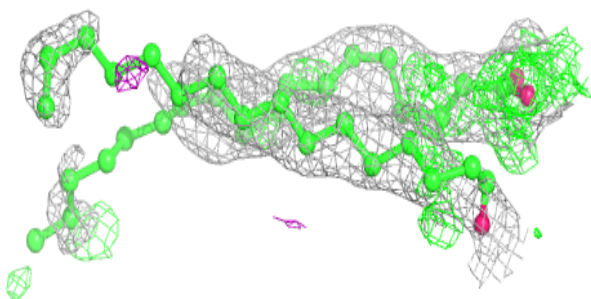
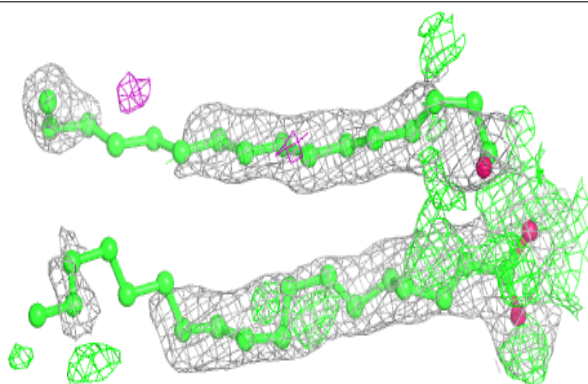


Electron density around PGV N 606:

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

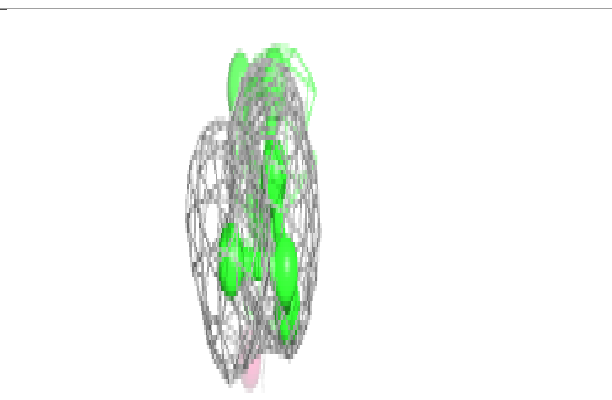
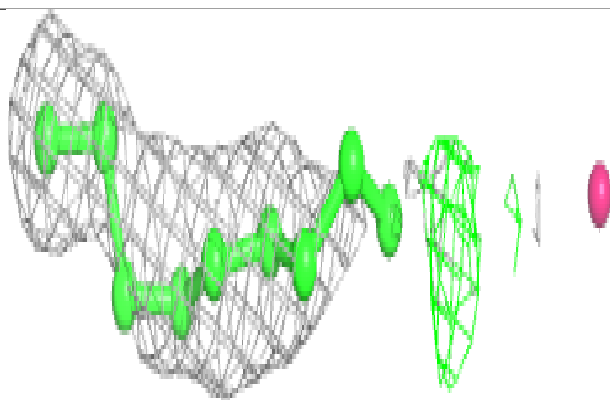
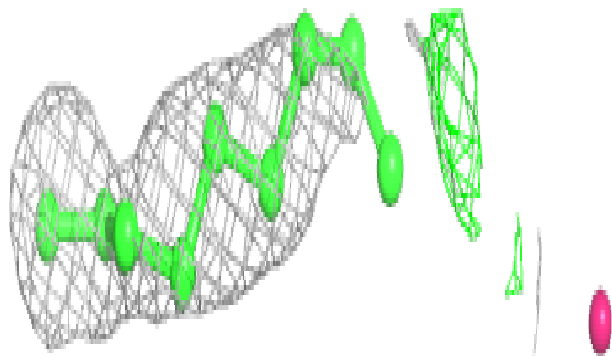
**Electron density around PGV A 607:**

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

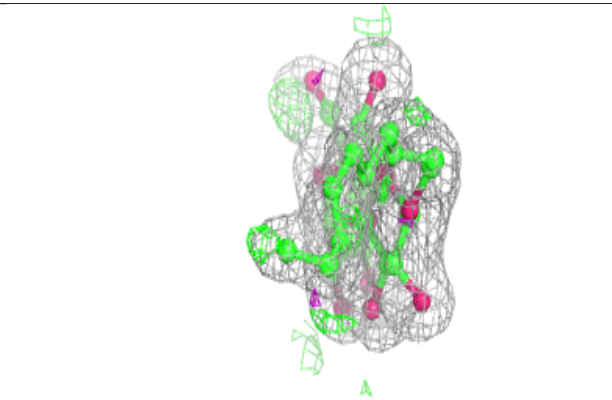
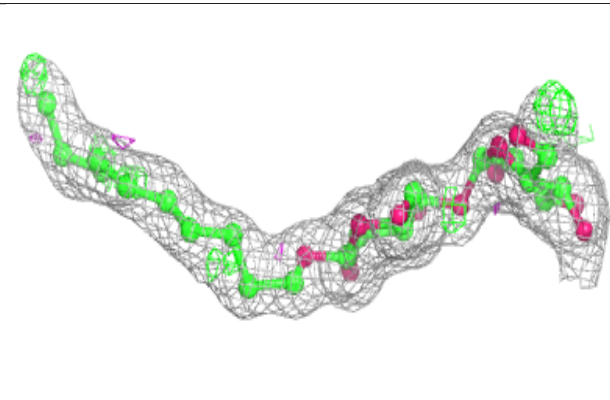
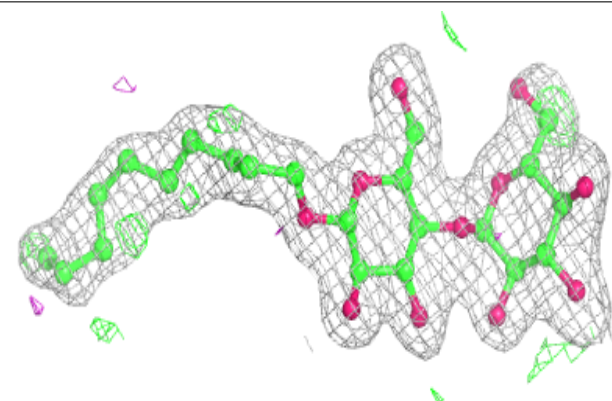


Electron density around DMU K 101:

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

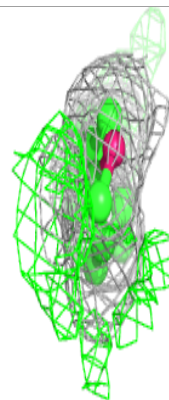
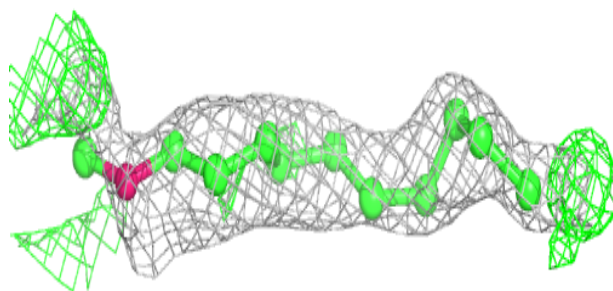
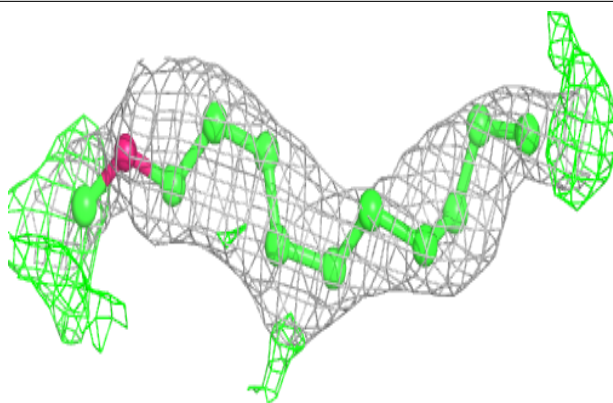
**Electron density around DMU M 101:**

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

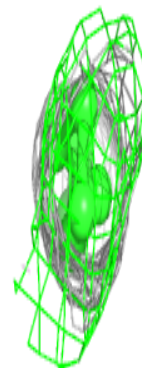
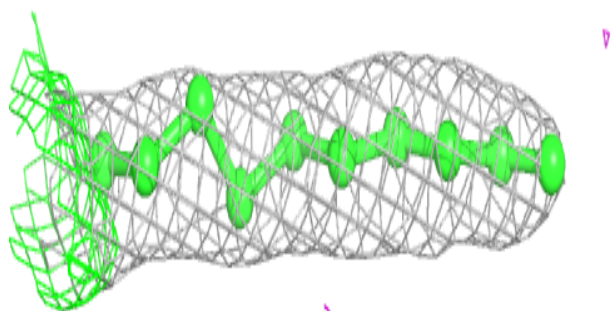
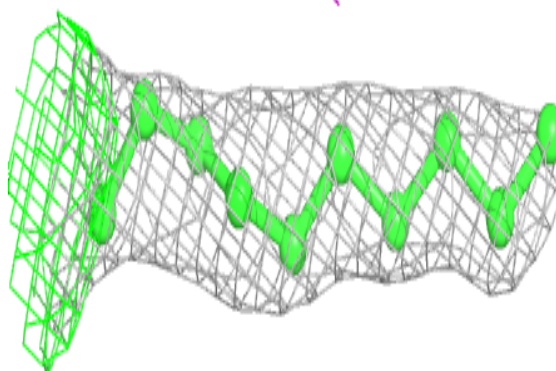


Electron density around DMU D 202:

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

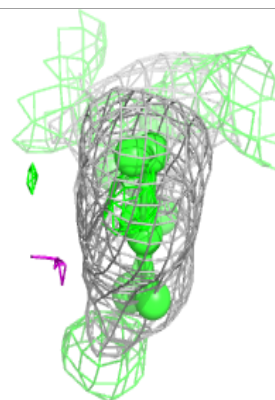
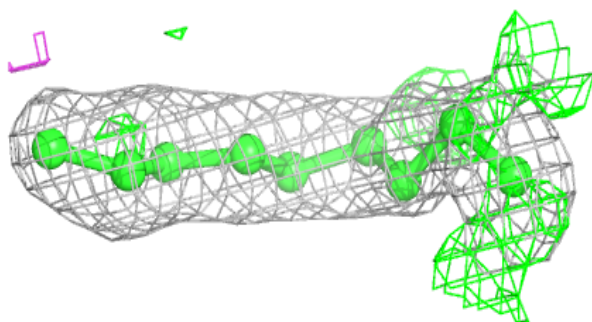
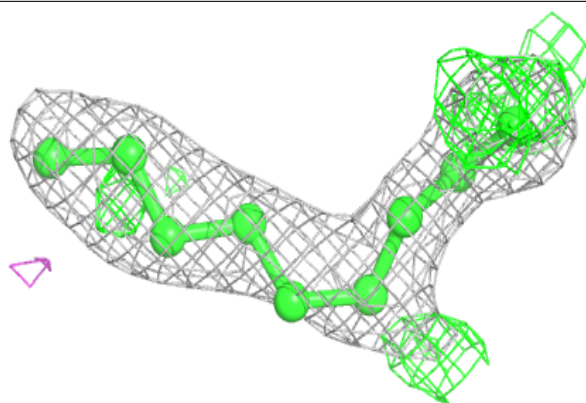
**Electron density around DMU O 304:**

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

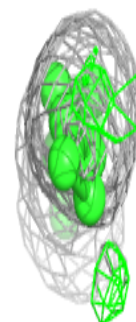
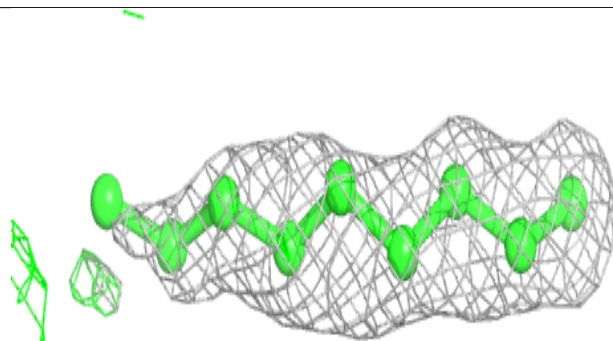
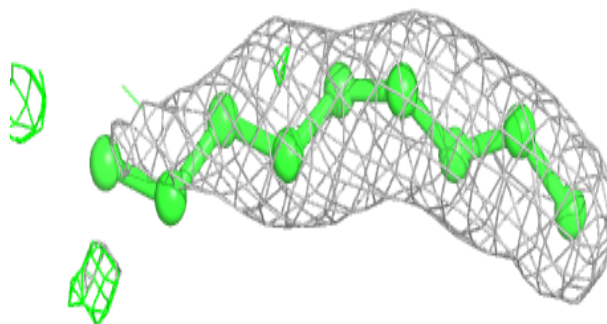


Electron density around DMU C 301:

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

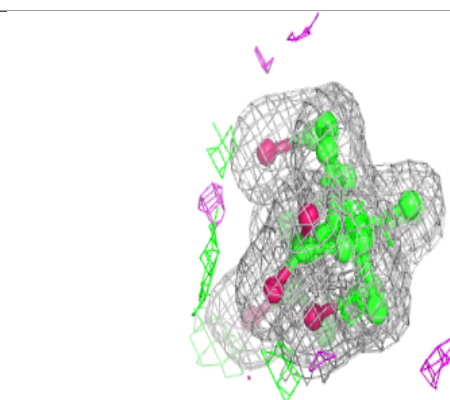
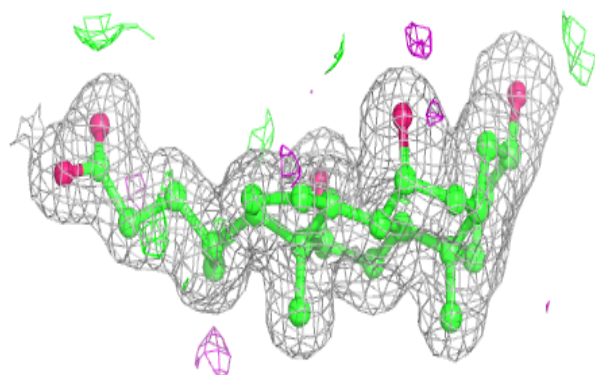
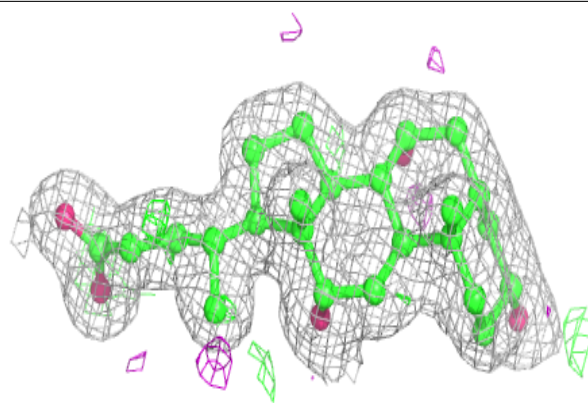
**Electron density around DMU K 106:**

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

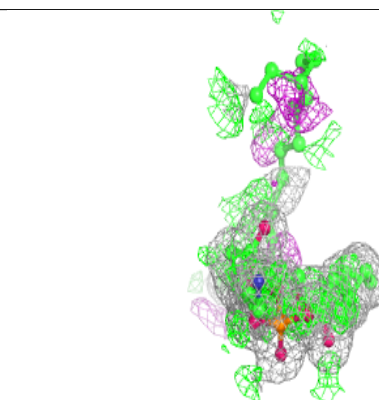
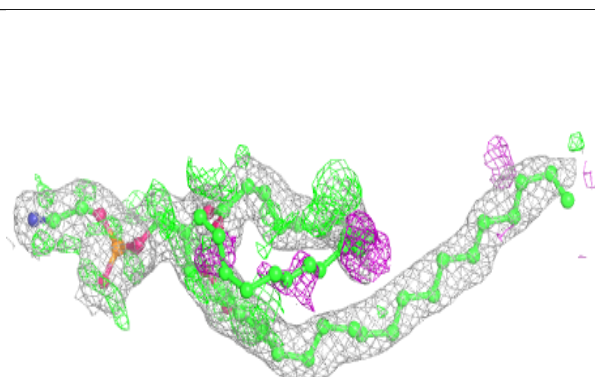
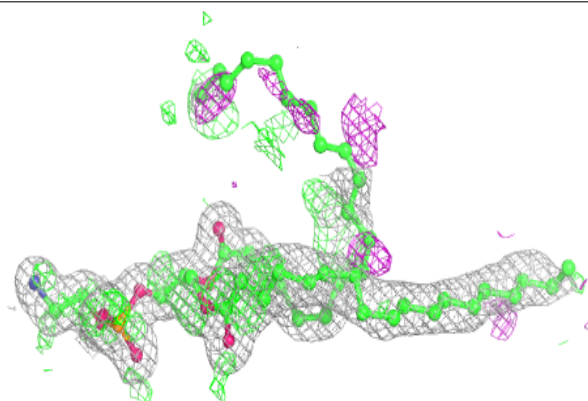


Electron density around CHD P 307:

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

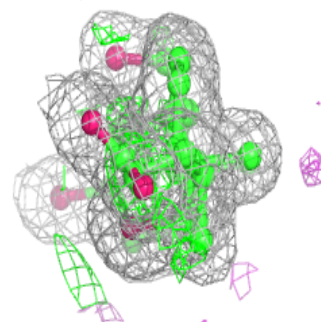
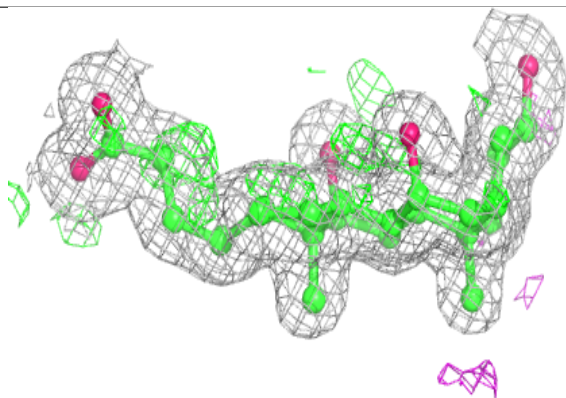
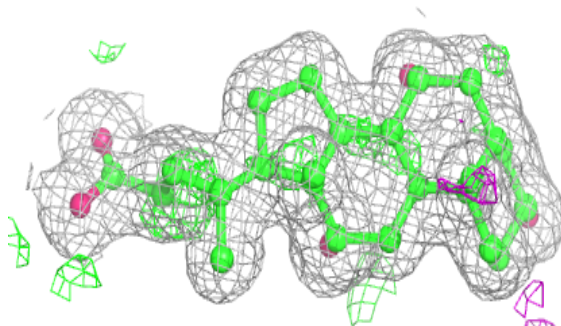
**Electron density around PEK G 101:**

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

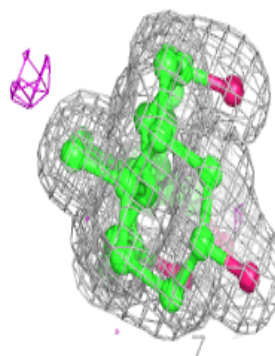
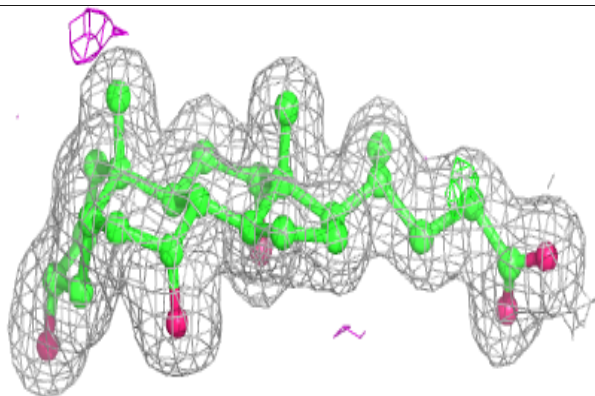
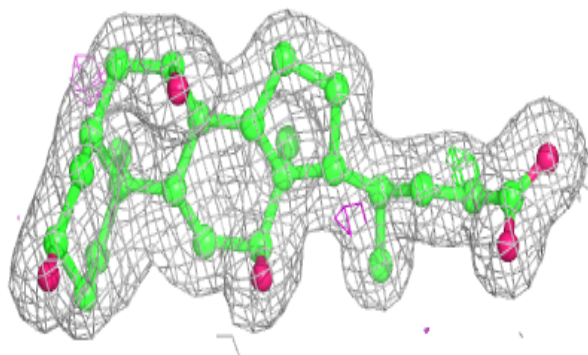


Electron density around CHD B 302:

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

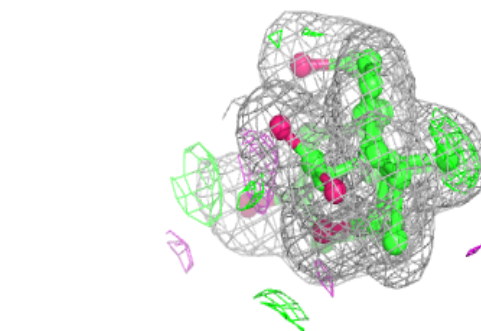
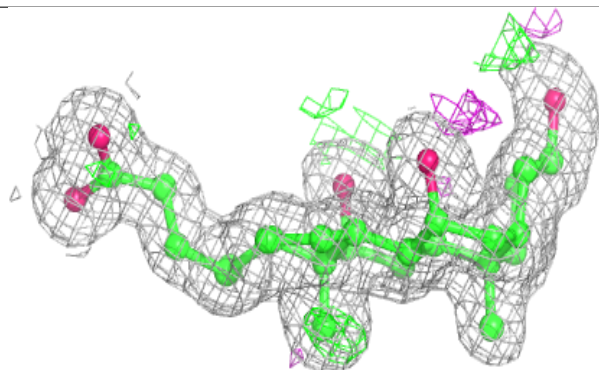
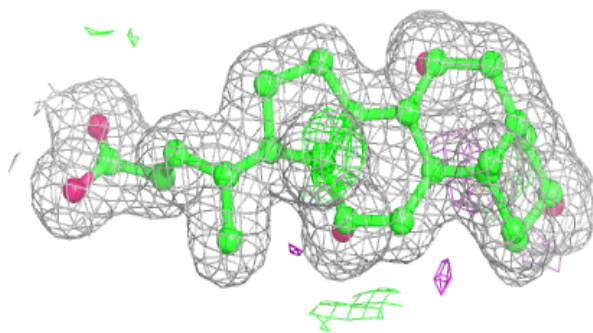
**Electron density around CHD C 304:**

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

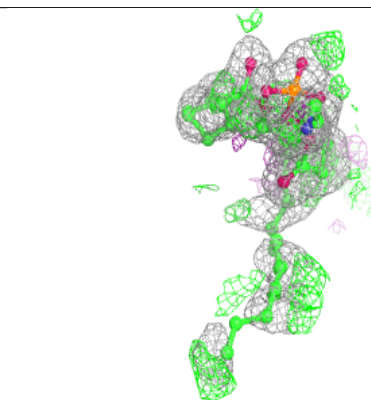
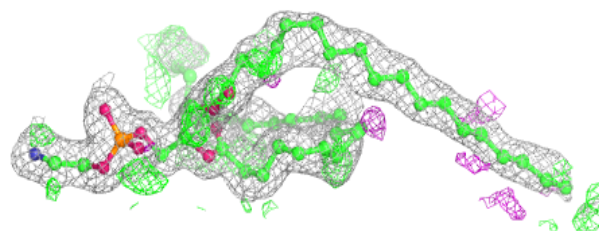
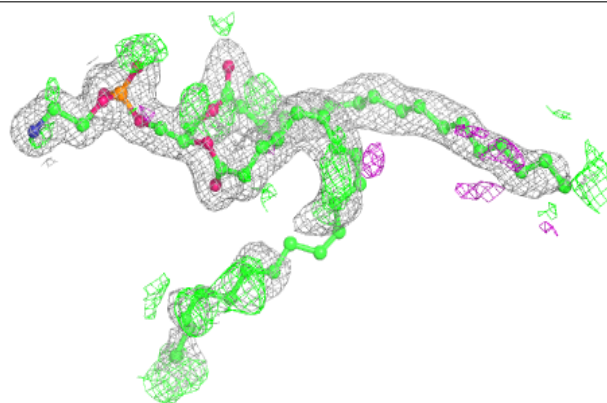


Electron density around CHD G 103:

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

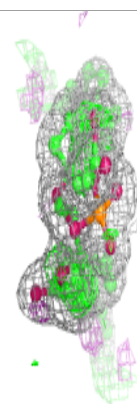
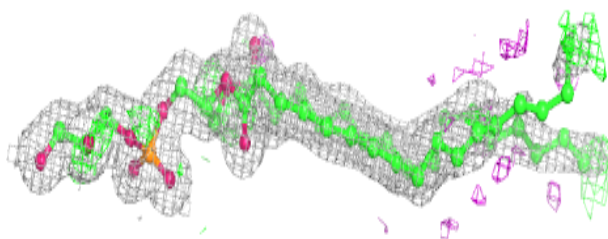
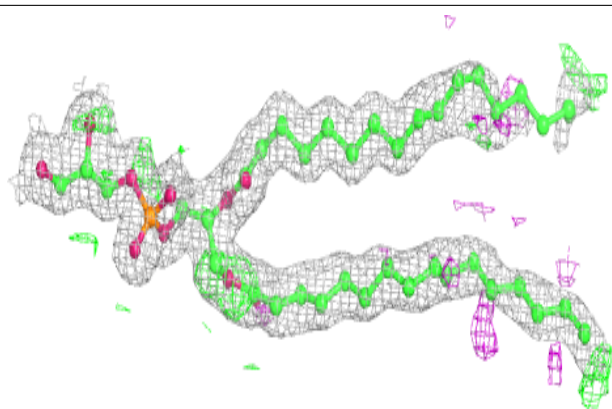
**Electron density around PEK P 308:**

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

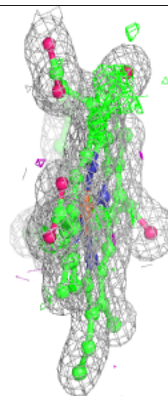
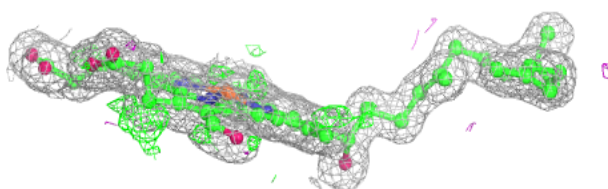
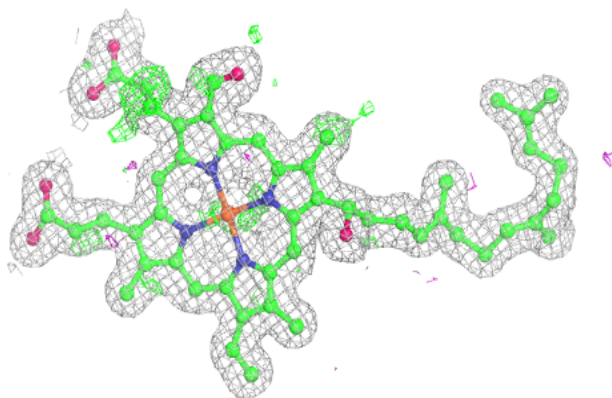


Electron density around PGV P 304:

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

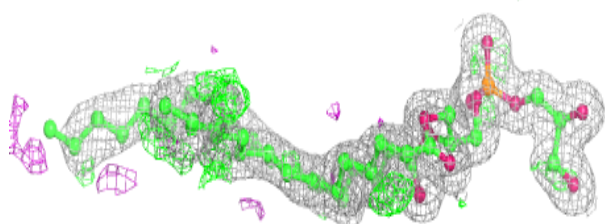
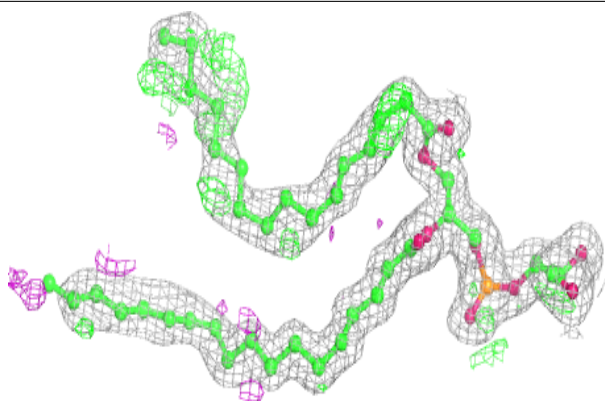
**Electron density around HEA N 602:**

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

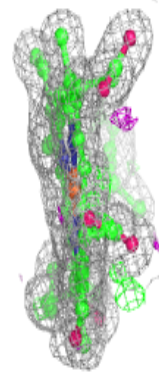
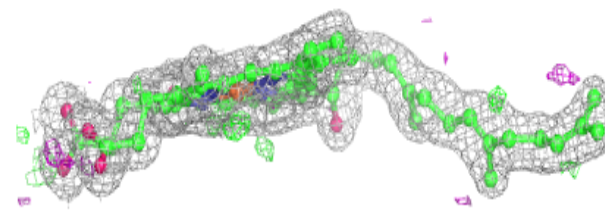
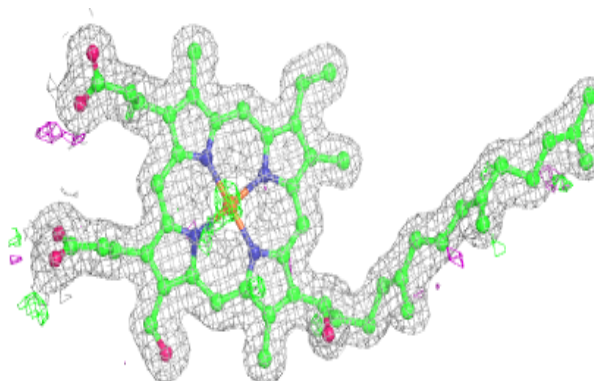


Electron density around PGV N 607:

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

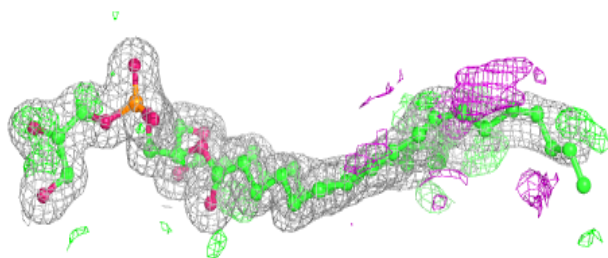
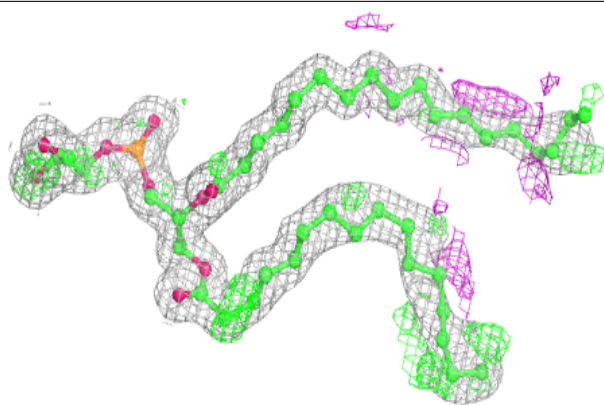
**Electron density around HEA N 601 (A):**

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

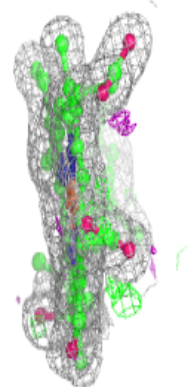
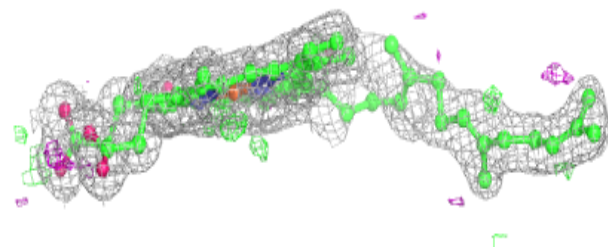
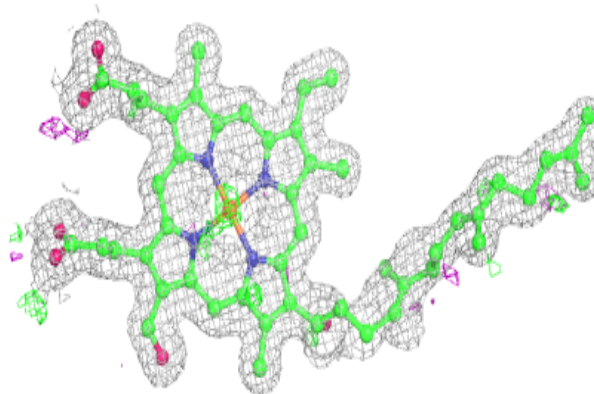


Electron density around PGV A 606:

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

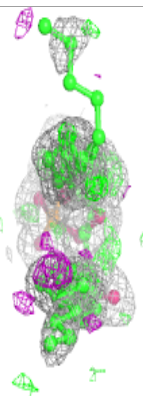
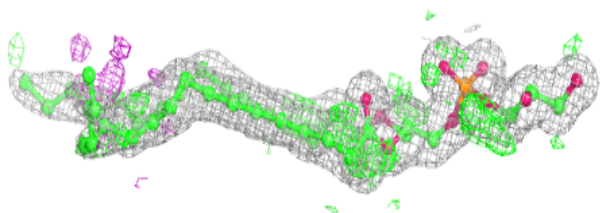
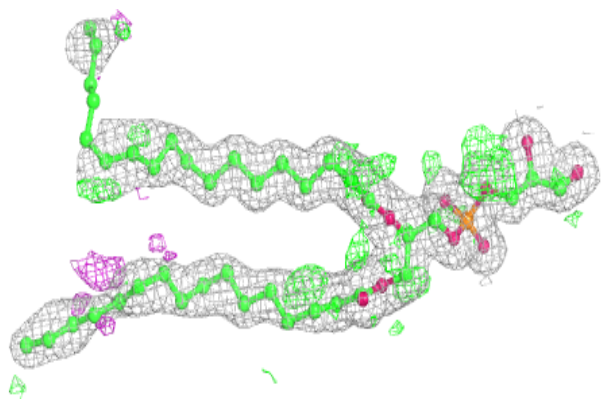
**Electron density around HEA N 601 (B):**

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

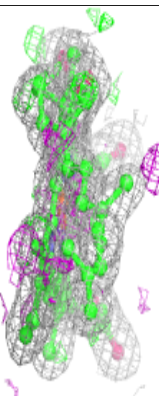
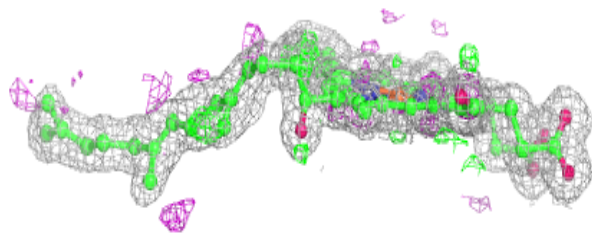
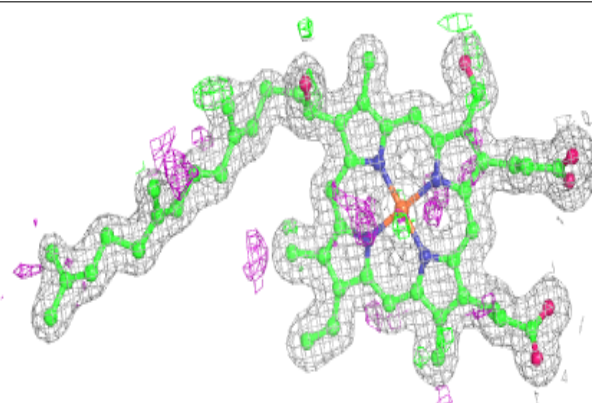


Electron density around PGV C 302:

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

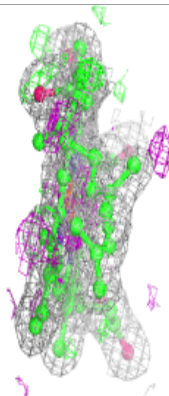
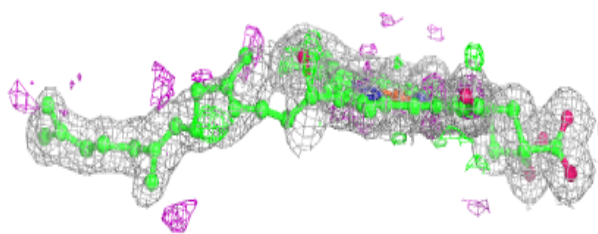
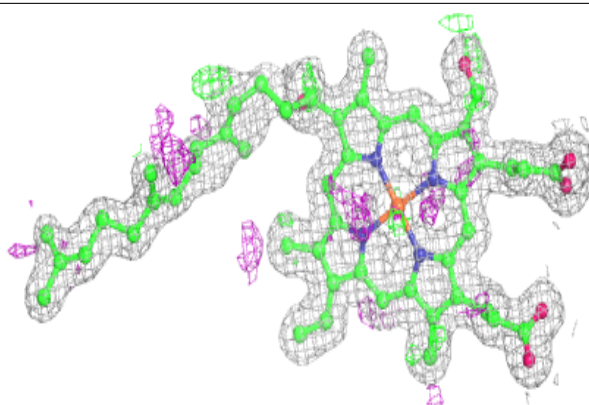
**Electron density around HEA A 601 (A):**

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

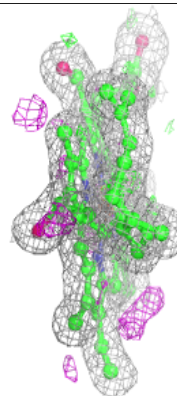
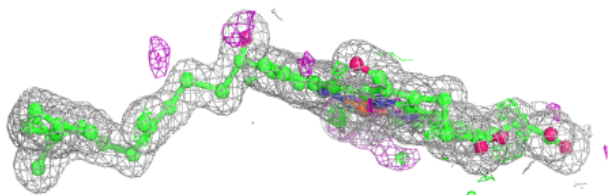
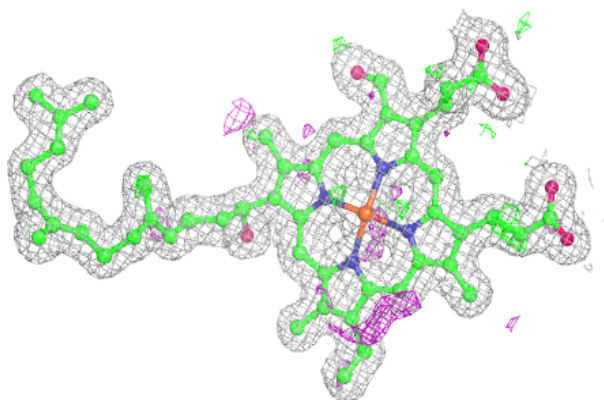


Electron density around HEA A 601 (B):

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

**Electron density around HEA A 602:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.