



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2021 – 11:00 AM JST

PDB ID : 7CP5
Title : Bovine heart cytochrome c oxidase in a catalytic intermediate of E at 1.76 angstrom resolution
Authors : Tsukihara, T.; Shimada, A.
Deposited on : 2020-08-06
Resolution : 1.76 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 2.23.1
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) : 2.23.1

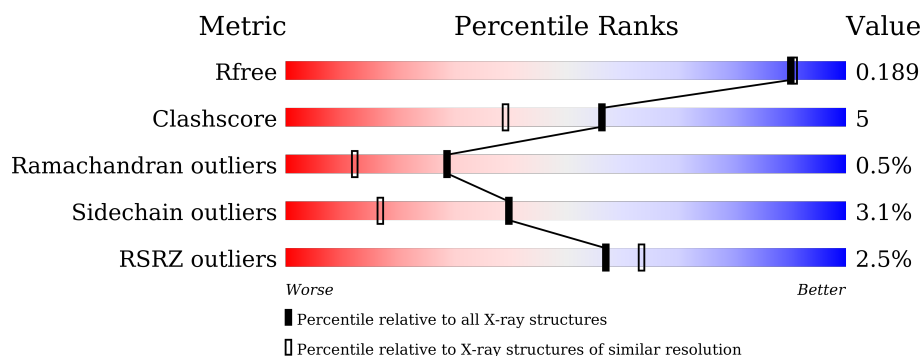
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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>90%</div> <div>9%</div> <div>.</div> </div>
1	N	514	<div> <div>90%</div> <div>10%</div> </div>
2	B	227	<div> <div>83%</div> <div>16%</div> </div>
2	O	227	<div> <div>2%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
3	C	259	<div> <div>92%</div> <div>8%</div> </div>
3	P	259	<div> <div>%</div> <div>88%</div> <div>12%</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	94	
6	S	94	
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	601[C]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	602	X	-	-	-
14	HEA	N	602[A]	X	-	-	-
14	HEA	N	602[B]	X	-	-	-
14	HEA	N	602[C]	X	-	-	-
14	HEA	N	603	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 34258 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	31	0
			4190	2796	644	711	39			
1	N	514	Total	C	N	O	S	0	35	0
			4213	2816	642	713	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	7	0
			1862	1214	281	347	20			
2	O	227	Total	C	N	O	S	0	11	0
			1882	1229	287	345	21			

- 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	12	0
			2167	1451	341	360	15			
3	P	259	Total	C	N	O	S	0	12	0
			2161	1448	341	357	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	3	0
			1211	790	199	218	4			
4	Q	144	Total	C	N	O	S	0	1	0
			1199	781	196	218	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	1	0
			860	549	147	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	94	Total	C	N	O	S	0	5	0
			736	458	128	144	6			
6	S	94	Total	C	N	O	S	0	0	0
			716	444	127	140	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	4	0
			692	448	129	114	1			
7	T	84	Total	C	N	O	S	0	0	0
			672	431	129	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	1	0
			667	420	122	120	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	1	0
			604	391	107	102	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	1	0
			464	299	78	84	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			461	297	78	83	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	3	0
			395	260	65	68	2			
11	X	49	Total	C	N	O	S	0	0	0
			385	250	65	68	2			

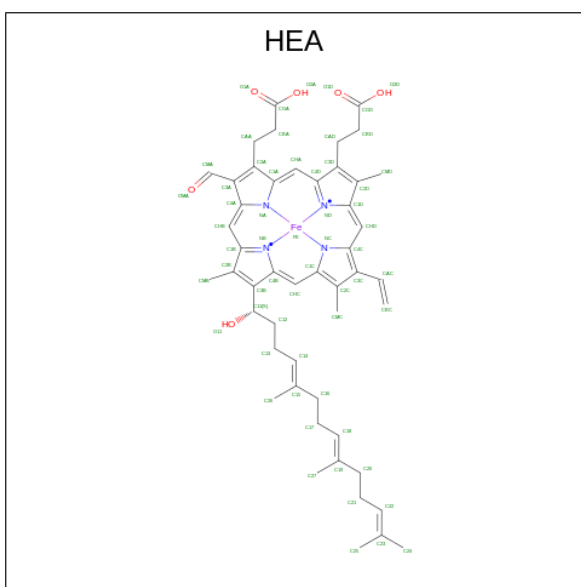
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			384	258	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
			336	223	53	60			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 78	C 66	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 78	C 66	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		

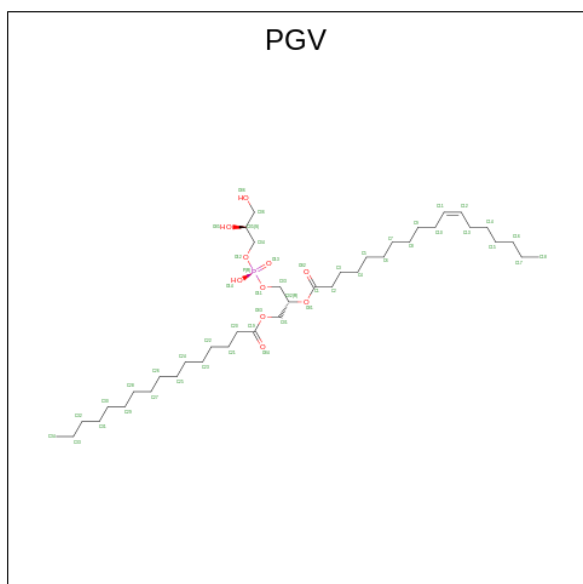
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0
17	P	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).



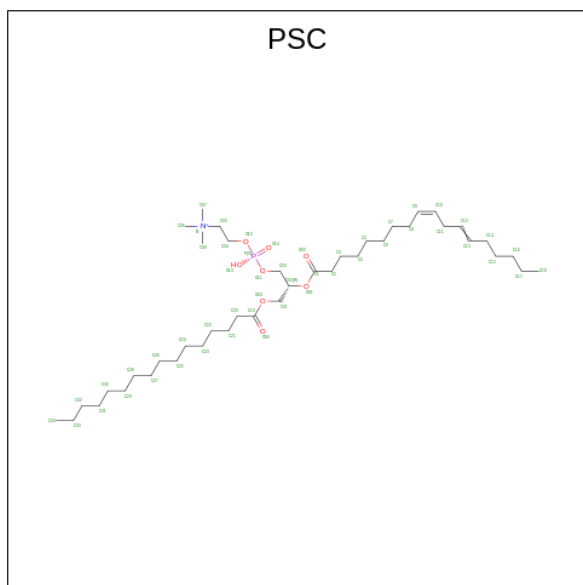
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O 22 21 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 48 37 10 1	0	0
18	C	1	Total C O 28 26 2	0	0
18	G	1	Total C O 32 30 2	0	0
18	N	1	Total C 24 24	0	0
18	N	1	Total C O P 51 40 10 1	0	0

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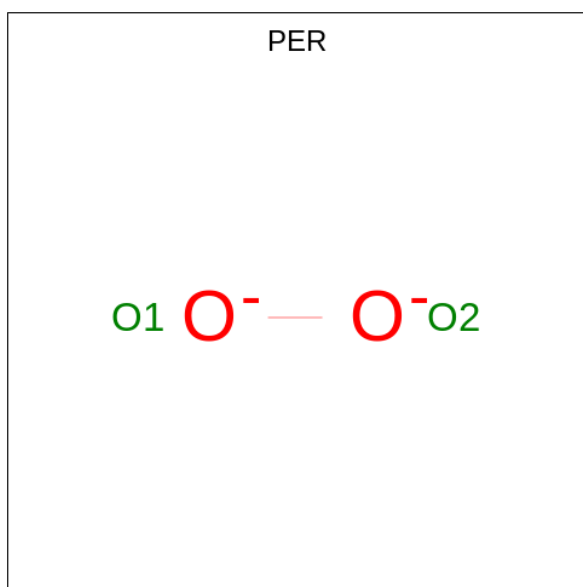
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 19 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



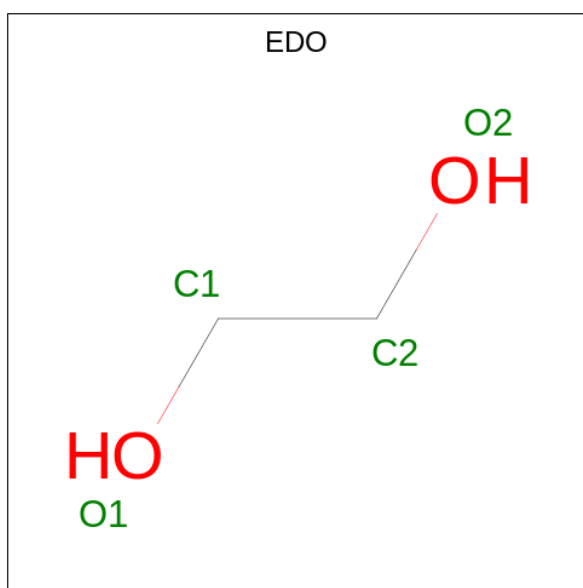
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C			0	0
			27	27				
19	O	1	Total	C	O		0	0
			30	28	2			

- Molecule 20 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



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

- 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	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

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

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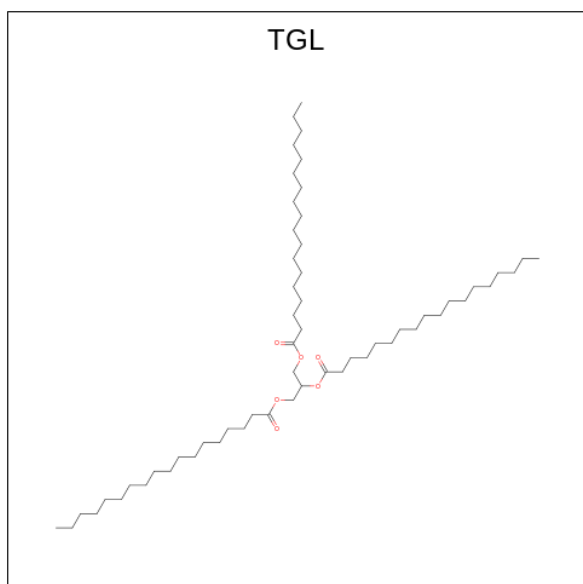
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	O	1	Total C O 4 2 2	0	0
21	O	1	Total C O 4 2 2	0	0
21	O	1	Total C O 4 2 2	0	0
21	P	1	Total C O 4 2 2	0	0
21	P	1	Total C O 4 2 2	0	0
21	P	1	Total C O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

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

- Molecule 22 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



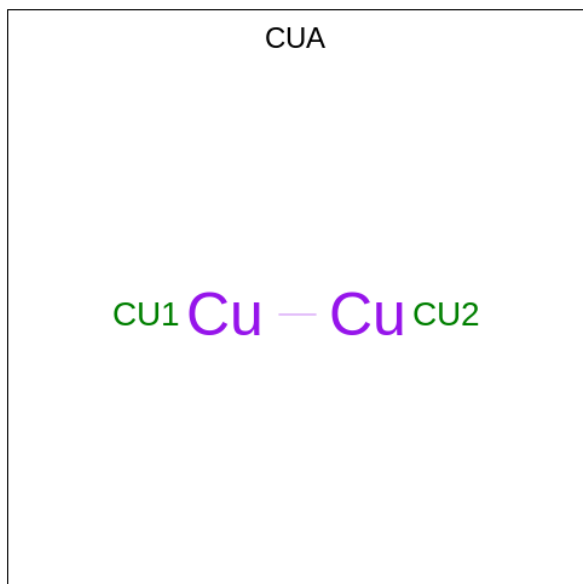
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 49 43 6	0	0
22	D	1	Total C O 57 51 6	0	0
22	L	1	Total C O 56 52 4	0	0
22	N	1	Total C O 63 57 6	0	0
22	N	1	Total C 48 48	0	0

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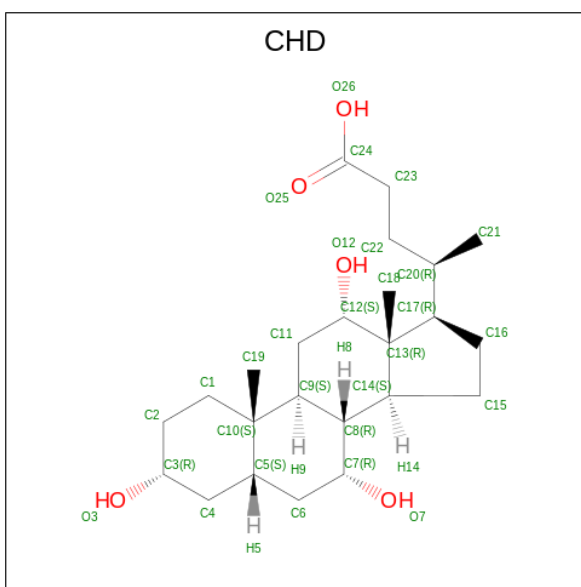
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	N	1	Total	C	O	0	0
			44	39	5		

- Molecule 23 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



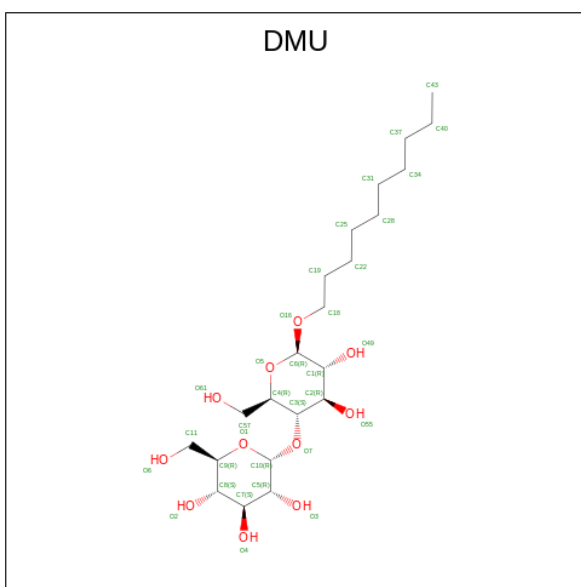
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	B	1	Total	Cu	0	0
			2	2		
23	O	1	Total	Cu	0	0
			2	2		

- Molecule 24 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



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

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



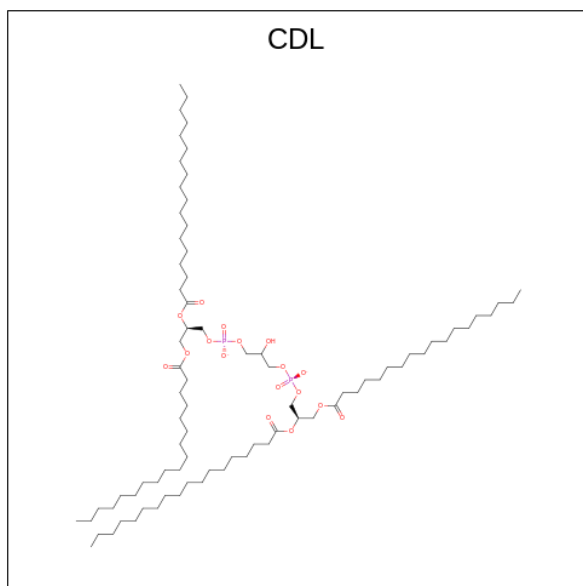
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total 13	C 11	O 2	0	0
25	C	1	Total 21	C 16	O 5	0	0
25	D	1	Total 11	C 10	O 1	0	0
25	D	1	Total 11	C 10	O 1	0	0
25	J	1	Total 11	C 10	O 1	0	0
25	K	1	Total 9	C 9		0	0
25	K	1	Total 10	C 10		0	0
25	K	1	Total 11	C 10	O 1	0	0
25	K	1	Total 9	C 9		0	0
25	K	1	Total 9	C 9		0	0
25	K	1	Total 10	C 10		0	0
25	L	1	Total 21	C 16	O 5	0	0
25	M	1	Total 33	C 22	O 11	0	0
25	O	1	Total 11	C 10	O 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	P	1	Total C O 13 11 2	0	0
25	P	1	Total C O 11 10 1	0	0
25	Q	1	Total C 10 10	0	0
25	W	1	Total C O 11 10 1	0	0
25	X	1	Total C O 11 10 1	0	0
25	X	1	Total C 10 10	0	0
25	X	1	Total C 9 9	0	0
25	X	1	Total C 10 10	0	0
25	Z	1	Total C O 33 22 11	0	0

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



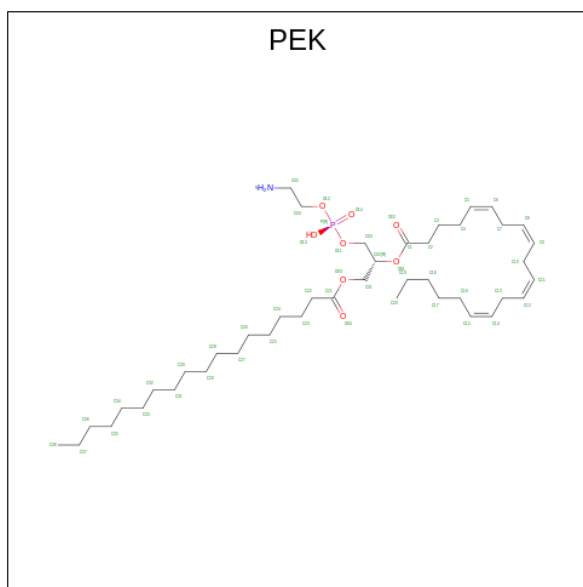
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C O 58 56 2	0	0
26	N	1	Total C O 55 54 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	P	1	Total	C	O	0	0
			61	58	3		
26	T	1	Total	C	O	0	0
			57	54	3		

- Molecule 27 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).

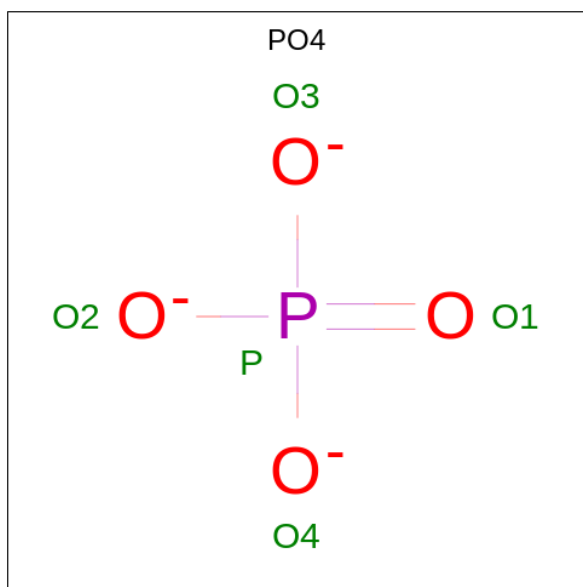


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	C	1	Total	C				0	0
			25	25					
27	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	C	1	Total	C				0	0
			36	36					
27	P	1	Total	C				0	0
			20	20					
27	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	P	1	Total	C				0	0
			34	34					

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	273	Total	O	0	14
			273	273		
30	B	223	Total	O	0	2
			223	223		
30	C	142	Total	O	0	2
			142	142		
30	D	213	Total	O	0	0
			213	213		
30	E	160	Total	O	0	0
			160	160		
30	F	162	Total	O	0	3
			162	162		

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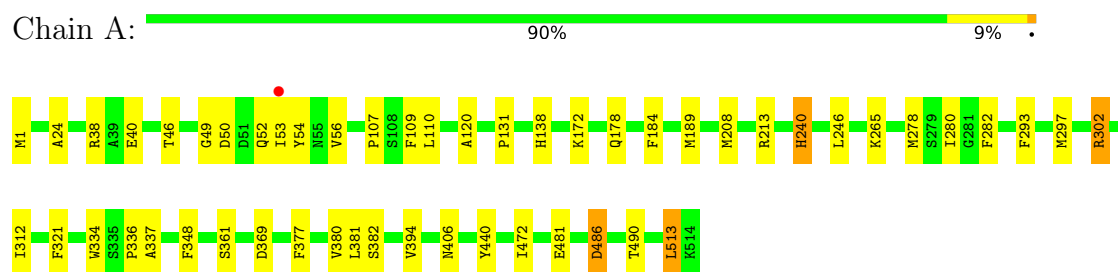
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	G	89	Total 89	O 89	0	0
30	H	94	Total 94	O 94	0	0
30	I	70	Total 70	O 70	0	0
30	J	58	Total 58	O 58	0	0
30	K	44	Total 44	O 44	0	0
30	L	38	Total 38	O 38	0	1
30	M	39	Total 39	O 39	0	0
30	N	273	Total 273	O 273	0	12
30	O	205	Total 205	O 205	0	2
30	P	147	Total 147	O 147	0	0
30	Q	114	Total 114	O 114	0	0
30	R	117	Total 117	O 117	0	0
30	S	141	Total 141	O 141	0	0
30	T	66	Total 66	O 66	0	0
30	U	94	Total 94	O 94	0	0
30	V	72	Total 72	O 72	0	0
30	W	43	Total 43	O 43	0	0
30	X	31	Total 31	O 31	0	0
30	Y	31	Total 31	O 31	0	0
30	Z	29	Total 29	O 29	0	0

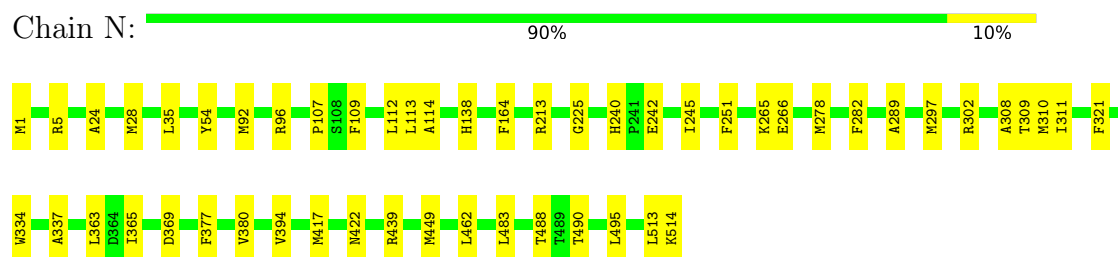
3 Residue-property plots

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.

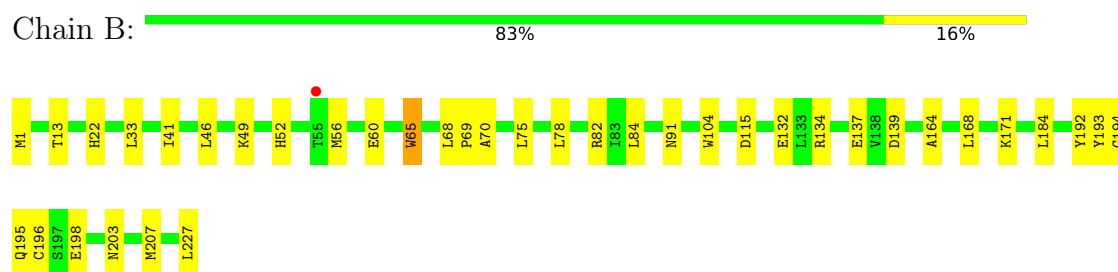
• Molecule 1: Cytochrome c oxidase subunit 1



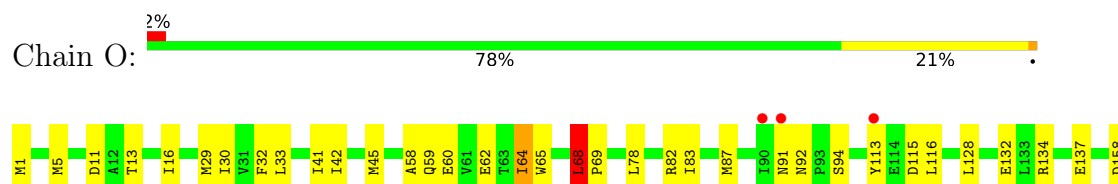
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2

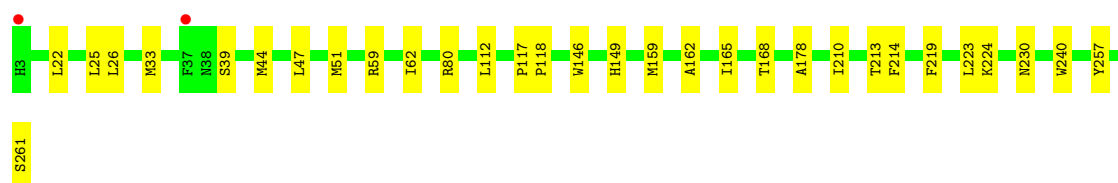
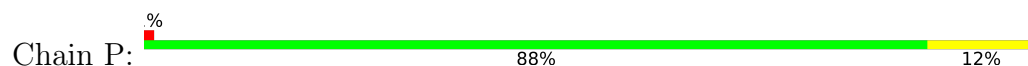




- Molecule 3: Cytochrome c oxidase subunit 3



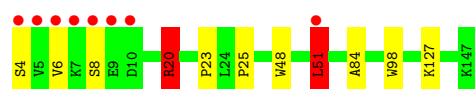
- Molecule 3: Cytochrome c oxidase subunit 3



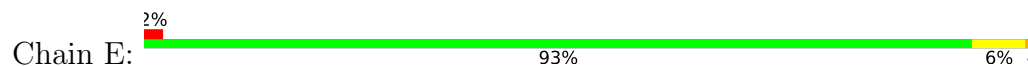
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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



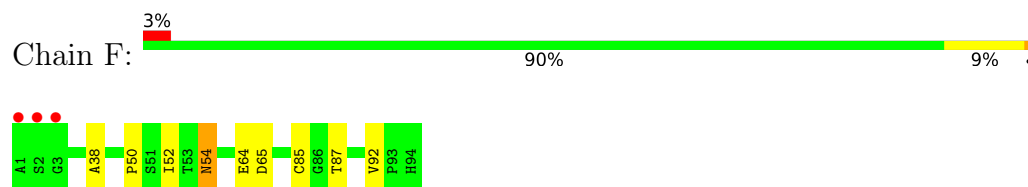
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



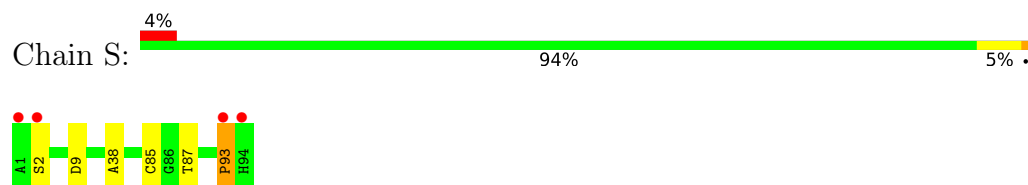
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



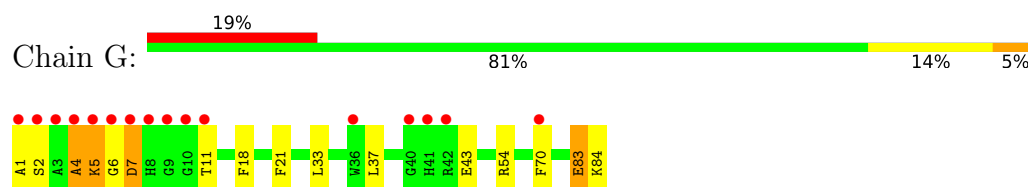
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



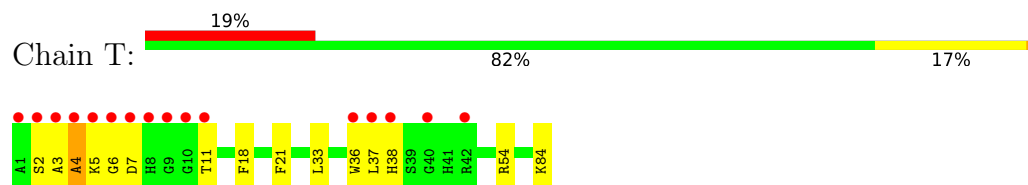
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



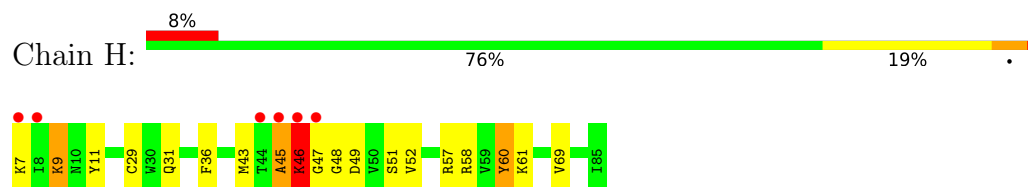
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



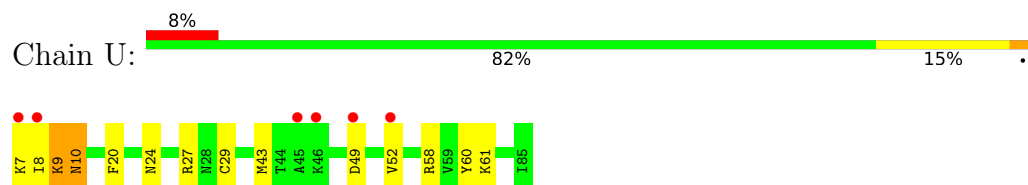
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



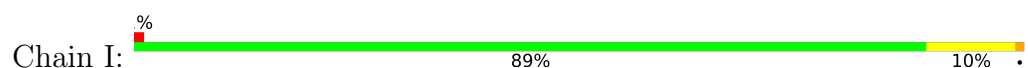
- Molecule 8: Cytochrome c oxidase subunit 6B1

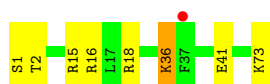


- Molecule 8: Cytochrome c oxidase subunit 6B1

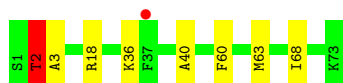
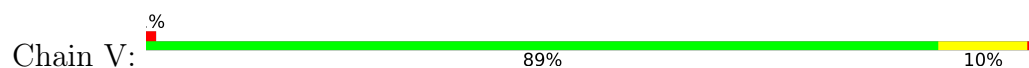


- Molecule 9: Cytochrome c oxidase subunit 6C

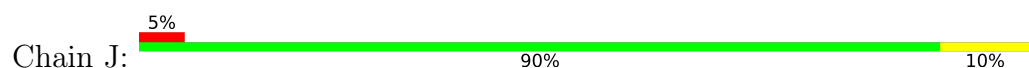




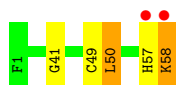
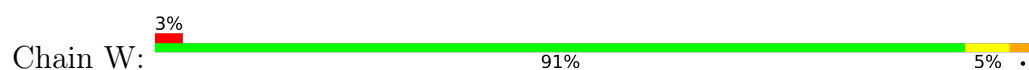
- Molecule 9: Cytochrome c oxidase subunit 6C



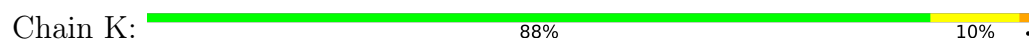
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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



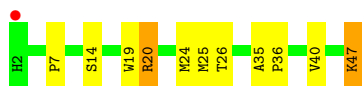
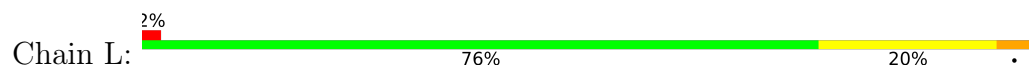
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



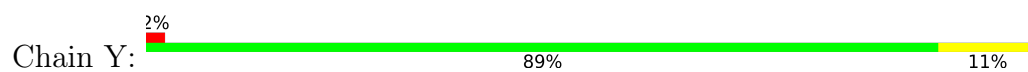
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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



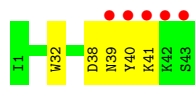
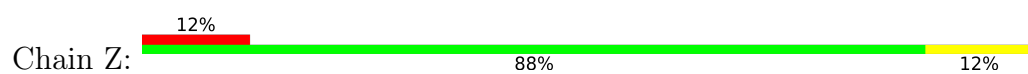
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.59Å 203.22Å 177.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 1.76 135.41 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.91-1.76) 99.8 (135.41-1.76)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 1.76Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.160 , 0.189 0.160 , 0.189	Depositor DCC
R_{free} test set	32242 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.782	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 82.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34258	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: FME, PEK, MG, CDL, SAC, TGL, PGV, PO4, PER, DMU, CHD, HEA, ZN, CUA, NA, PSC, EDO, CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.92	2/4411 (0.0%)	0.89	10/6016 (0.2%)
1	N	0.84	0/4434	0.84	5/6051 (0.1%)
2	B	0.84	3/1920 (0.2%)	0.94	3/2613 (0.1%)
2	O	0.75	1/1966 (0.1%)	0.83	2/2675 (0.1%)
3	C	0.84	2/2296 (0.1%)	0.74	0/3136
3	P	0.77	0/2295	0.73	0/3134
4	D	0.82	0/1259	0.81	2/1698 (0.1%)
4	Q	0.60	0/1236	0.68	3/1668 (0.2%)
5	E	0.80	0/871	0.78	2/1182 (0.2%)
5	R	0.64	0/882	0.73	1/1196 (0.1%)
6	F	0.75	0/771	0.76	0/1047
6	S	0.76	0/732	0.80	0/993
7	G	0.74	0/734	0.83	0/997
7	T	0.64	0/699	0.82	0/950
8	H	0.80	1/690 (0.1%)	0.80	1/932 (0.1%)
8	U	0.72	0/682	0.72	0/921
9	I	0.70	0/614	0.77	1/814 (0.1%)
9	V	0.57	0/605	0.71	0/802
10	J	0.61	0/478	0.63	0/644
10	W	0.55	0/472	0.69	0/636
11	K	0.72	0/420	0.68	0/576
11	X	0.63	0/399	0.62	0/546
12	L	0.84	0/401	0.77	0/537
12	Y	0.76	0/393	0.68	0/526
13	M	0.82	0/346	0.77	0/470
13	Z	0.61	0/345	0.69	0/470
All	All	0.79	9/30351 (0.0%)	0.80	30/41230 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
6	S	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	246[A]	ASP	CB-CG	7.83	1.68	1.51
3	C	246[B]	ASP	CB-CG	7.83	1.68	1.51
2	O	193	TYR	CD2-CE2	6.95	1.49	1.39
1	A	278	MET	CG-SD	-5.85	1.66	1.81
2	B	198	GLU	CD-OE2	-5.23	1.19	1.25
1	A	184	PHE	CG-CD1	5.16	1.46	1.38
2	B	192	TYR	CE1-CZ	5.13	1.45	1.38
2	B	193	TYR	CD2-CE2	5.08	1.47	1.39
8	H	69	VAL	CB-CG1	5.02	1.63	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	MET	CG-SD-CE	-10.35	83.64	100.20
1	A	189	MET	CG-SD-CE	-8.92	85.93	100.20
2	B	82	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	N	310	MET	CG-SD-CE	-6.83	89.28	100.20
4	D	20	ARG	NE-CZ-NH1	-6.81	116.89	120.30
1	N	5	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	302[A]	ARG	NE-CZ-NH1	-6.47	117.07	120.30
1	A	302[B]	ARG	NE-CZ-NH1	-6.47	117.07	120.30
1	A	513	LEU	CA-CB-CG	-6.33	100.75	115.30
4	Q	20	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	N	251	PHE	CB-CG-CD2	-5.95	116.64	120.80
4	D	20	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	A	208	MET	CG-SD-CE	5.93	109.69	100.20
1	N	213	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	O	68	LEU	CB-CG-CD1	-5.84	101.08	111.00
4	Q	20	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	278	MET	CA-CB-CG	-5.61	103.76	113.30
1	A	50[A]	ASP	CB-CG-OD1	5.55	123.29	118.30
1	A	50[B]	ASP	CB-CG-OD1	5.55	123.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	58	ARG	NE-CZ-NH2	-5.51	117.55	120.30
5	E	90	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	B	139	ASP	CB-CG-OD1	5.41	123.17	118.30
4	Q	51	LEU	CA-CB-CG	5.39	127.69	115.30
9	I	16	ARG	NE-CZ-NH2	-5.37	117.61	120.30
5	E	40	ASP	CB-CG-OD1	5.33	123.10	118.30
2	B	134	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	213	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	O	11	ASP	CB-CG-OD1	5.24	123.01	118.30
1	N	96	ARG	NE-CZ-NH2	-5.22	117.69	120.30
5	R	66	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4190	0	4166	46	0
1	N	4213	0	4222	42	0
2	B	1862	0	1881	21	0
2	O	1882	0	1903	28	0
3	C	2167	0	2104	14	0
3	P	2161	0	2106	26	0
4	D	1211	0	1202	12	0
4	Q	1199	0	1192	8	0
5	E	852	0	845	5	0
5	R	860	0	858	3	0
6	F	736	0	726	11	0
6	S	716	0	697	6	0
7	G	692	0	672	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	T	672	0	645	4	0
8	H	667	0	629	8	0
8	U	662	0	623	7	0
9	I	604	0	611	3	0
9	V	601	0	613	4	0
10	J	464	0	464	6	0
10	W	461	0	459	4	0
11	K	395	0	389	7	0
11	X	385	0	366	0	0
12	L	384	0	391	14	0
12	Y	380	0	380	1	0
13	M	336	0	352	4	0
13	Z	335	0	352	2	0
14	A	138	0	111	7	0
14	N	138	0	111	8	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	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	22	0	33	2	0
18	C	127	0	181	5	0
18	G	32	0	51	2	0
18	N	75	0	114	4	0
18	P	51	0	76	2	0
19	A	27	0	48	4	0
19	O	30	0	47	4	0
20	A	2	0	0	1	0
20	N	2	0	0	1	0
21	A	40	0	60	2	0
21	B	16	0	24	0	0
21	C	36	0	54	1	0
21	D	12	0	18	0	0
21	E	12	0	18	0	0
21	F	20	0	29	0	0
21	G	8	0	12	0	0
21	J	8	0	12	1	0
21	L	4	0	6	0	0
21	N	36	0	54	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	O	12	0	18	3	0
21	P	32	0	48	1	0
21	Q	4	0	6	0	0
21	S	20	0	30	1	0
21	T	12	0	18	0	0
21	W	4	0	6	1	0
21	Y	8	0	12	0	0
22	B	49	0	77	1	0
22	D	57	0	95	9	0
22	L	56	0	94	9	0
22	N	155	0	275	14	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	29	0	39	0	0
24	C	29	0	39	0	0
24	G	29	0	39	1	0
24	L	29	0	39	4	0
24	P	29	0	39	0	0
24	Y	29	0	39	1	0
25	C	34	0	51	5	0
25	D	22	0	40	2	0
25	J	11	0	21	2	0
25	K	58	0	110	4	0
25	L	21	0	30	1	0
25	M	33	0	42	2	0
25	O	11	0	21	0	0
25	P	24	0	42	6	0
25	Q	10	0	19	1	0
25	W	11	0	21	1	0
25	X	40	0	74	0	0
25	Z	33	0	42	1	0
26	C	58	0	100	6	0
26	N	55	0	101	3	0
26	P	61	0	104	4	0
26	T	57	0	88	7	0
27	C	114	0	173	8	0
27	P	107	0	163	9	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	273	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	223	0	0	1	0
30	C	142	0	0	1	0
30	D	213	0	0	1	0
30	E	160	0	0	2	0
30	F	162	0	0	4	0
30	G	89	0	0	0	0
30	H	94	0	0	1	0
30	I	70	0	0	2	0
30	J	58	0	0	3	0
30	K	44	0	0	2	0
30	L	38	0	0	1	0
30	M	39	0	0	0	0
30	N	273	0	0	4	0
30	O	205	0	0	3	0
30	P	147	0	0	0	0
30	Q	114	0	0	1	0
30	R	117	0	0	0	0
30	S	141	0	0	3	0
30	T	66	0	0	0	0
30	U	94	0	0	0	0
30	V	72	0	0	1	0
30	W	43	0	0	1	0
30	X	31	0	0	0	0
30	Y	31	0	0	0	0
30	Z	29	0	0	2	0
All	All	34258	0	32062	317	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 5.

All (317) 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)
20:N:610[A]:PER:O2	20:N:610[A]:PER:O1	1.54	1.25
20:A:608[A]:PER:O2	20:A:608[A]:PER:O1	1.55	1.25
1:N:311[A]:ILE:HG22	26:N:601:CDL:H441	1.58	0.85
3:P:224[B]:LYS:HE2	26:P:304:CDL:H131	1.62	0.82
1:A:406:ASN:HD21	18:A:606:PGV:H22	1.47	0.79
12:L:20:ARG:HH21	22:L:103:TGL:HC32	1.47	0.79
12:L:20:ARG:HH22	22:L:103:TGL:HC72	1.49	0.78
19:A:607:PSC:H242	2:B:56:MET:HB3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:62:ILE:HD12	26:P:304:CDL:H522	1.65	0.77
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.67	0.76
21:O:305:EDO:H21	8:U:24:ASN:HD21	1.49	0.75
3:C:213:THR:HG23	26:C:305:CDL:H771	1.69	0.74
3:P:33[A]:MET:HG2	25:P:309:DMU:H12	1.70	0.73
3:P:59:ARG:HG3	26:P:304:CDL:H512	1.71	0.72
10:W:41:GLY:HA3	25:W:101:DMU:H23	1.71	0.71
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.31	0.70
6:F:54[A]:ASN:ND2	30:F:201:HOH:O	2.24	0.70
7:G:1:ALA:HB2	18:G:102:PGV:H342	1.74	0.70
1:A:302[B]:ARG:NH1	30:A:701:HOH:O	2.25	0.68
11:K:22:ALA:O	11:K:26[B]:VAL:HG22	1.93	0.68
6:S:85:CYS:SG	6:S:87:THR:HG23	2.34	0.68
3:P:33[A]:MET:SD	25:P:309:DMU:H8	2.34	0.67
1:A:321[A]:PHE:CD2	2:B:65:TRP:HB2	2.29	0.66
14:N:603:HEA:HMC1	14:N:603:HEA:HBC1	1.78	0.65
8:U:7:LYS:O	8:U:9:LYS:N	2.26	0.65
25:P:309:DMU:H11	10:W:49:CYS:HB3	1.79	0.64
25:K:104:DMU:H20	25:K:106:DMU:H11	1.79	0.64
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.80	0.64
25:C:310:DMU:H11	10:J:49:CYS:HB3	1.78	0.63
27:C:307:PEK:H101	27:C:307:PEK:H42	1.79	0.63
12:L:14:SER:H	22:L:103:TGL:HC31	1.63	0.63
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.81	0.63
1:N:113:LEU:HB2	22:N:612:TGL:H301	1.80	0.62
9:I:36:LYS:O	9:I:41:GLU:HB2	1.99	0.62
1:N:289:ALA:HB1	1:N:297[C]:MET:HE1	1.81	0.62
3:P:213:THR:HG23	26:P:304:CDL:H772	1.82	0.62
22:N:609:TGL:H312	22:N:609:TGL:H201	1.81	0.62
27:P:306:PEK:H101	27:P:306:PEK:H42	1.80	0.62
4:D:4:SER:HB2	30:D:363:HOH:O	1.99	0.62
12:L:20:ARG:NH2	22:L:103:TGL:HC52	2.16	0.61
3:P:33[A]:MET:HG2	25:P:309:DMU:C25	2.30	0.61
24:L:102:CHD:H232	13:M:21:VAL:HG21	1.83	0.60
26:T:101:CDL:H602	26:T:101:CDL:H782	1.83	0.60
3:C:51[A]:MET:SD	26:C:305:CDL:H622	2.42	0.60
19:A:607:PSC:H222	2:B:52:HIS:HE1	1.68	0.58
6:F:92[A]:VAL:HG21	30:F:345:HOH:O	2.03	0.58
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.85	0.57
4:D:78:TRP:CA	22:D:202:TGL:HB32	2.35	0.57
3:C:165:ILE:HG12	27:C:309:PEK:H9	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.87	0.57
22:N:611:TGL:HA32	22:N:611:TGL:HB51	1.87	0.57
1:N:24:ALA:HB2	14:N:602[A]:HEA:H253	1.87	0.56
22:N:611:TGL:H232	2:O:42:ILE:HG21	1.86	0.56
4:Q:98:TRP:HB2	25:Q:201:DMU:H18	1.86	0.56
9:V:63:MET:HB3	9:V:68:ILE:HG12	1.88	0.56
1:A:282:PHE:HA	7:T:4:ALA:CB	2.34	0.56
10:W:57:HIS:O	10:W:58:LYS:HB3	2.05	0.56
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.88	0.56
30:C:408:HOH:O	6:F:52:ILE:HD11	2.06	0.56
1:N:113:LEU:HB2	22:N:612:TGL:H322	1.87	0.55
3:P:33[B]:MET:SD	25:P:309:DMU:H8	2.46	0.55
3:P:168:THR:HG22	27:P:308:PEK:H14	1.87	0.55
1:A:381[B]:LEU:HB2	14:A:602:HEA:CAC	2.37	0.55
1:A:334:TRP:HZ3	22:D:202:TGL:HA72	1.72	0.55
1:N:35[A]:LEU:HD11	1:N:462:LEU:HB2	1.88	0.55
30:N:918:HOH:O	4:Q:20:ARG:HG2	2.07	0.55
1:N:297[C]:MET:SD	1:N:302:ARG:HG2	2.47	0.55
26:T:101:CDL:H601	26:T:101:CDL:H762	1.88	0.54
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.37	0.54
2:B:22:HIS:HB3	30:I:154:HOH:O	2.07	0.54
26:T:101:CDL:H752	26:T:101:CDL:H212	1.89	0.54
1:A:24:ALA:HB2	14:A:601[A]:HEA:H253	1.89	0.54
1:A:377:PHE:O	1:A:381[B]:LEU:HB3	2.07	0.54
22:D:202:TGL:HA41	22:D:202:TGL:HB52	1.89	0.53
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.90	0.53
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.90	0.53
8:H:49:ASP:O	8:H:52:VAL:HG22	2.09	0.53
4:D:94:LEU:HB3	25:D:201:DMU:H18	1.91	0.53
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.91	0.53
30:A:732:HOH:O	12:L:7:PRO:HG3	2.09	0.53
7:G:83[B]:GLU:HB3	7:G:84:LYS:HG2	1.90	0.52
1:A:40:GLU:HG2	1:A:54[B]:TYR:CD1	2.44	0.52
10:J:55:PHE:HE1	25:L:101:DMU:H29	1.73	0.52
2:O:64[A]:ILE:HD11	19:O:303:PSC:H141	1.91	0.52
4:D:78:TRP:HA	22:D:202:TGL:HB32	1.91	0.52
1:N:112:LEU:HD23	1:N:112:LEU:C	2.30	0.52
11:K:12:LYS:NZ	30:K:201:HOH:O	2.42	0.52
10:J:4:ARG:NH1	30:J:202:HOH:O	2.43	0.52
5:R:80:GLU:OE1	5:R:80:GLU:N	2.43	0.52
2:O:60[A]:GLU:OE2	30:O:401:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302[B]:ARG:HE	2:B:84:LEU:HD11	1.75	0.52
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:HD3	2.10	0.52
12:L:47:LYS:HA	12:L:47:LYS:HE3	1.92	0.51
2:O:29[B]:MET:HE3	2:O:30:ILE:HG13	1.93	0.51
8:U:43:MET:HE3	8:U:49:ASP:N	2.24	0.51
4:D:78:TRP:HB3	22:D:202:TGL:HB32	1.92	0.51
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.92	0.51
1:A:52[B]:GLN:O	1:A:56:VAL:HG23	2.10	0.51
2:B:164:ALA:O	2:B:194:GLY:HA3	2.10	0.51
3:P:178:ALA:HB2	27:P:306:PEK:H202	1.92	0.51
1:A:334:TRP:CZ3	22:D:202:TGL:HA52	2.46	0.51
1:N:334:TRP:CE3	22:N:611:TGL:HA31	2.46	0.51
11:K:26[B]:VAL:HG23	30:K:223:HOH:O	2.10	0.51
12:L:35:ALA:HB3	12:L:36:PRO:HD3	1.92	0.50
26:C:305:CDL:H642	18:C:308:PGV:H12	1.94	0.50
12:L:26:THR:HG23	13:M:25:SER:HB3	1.92	0.50
25:K:102:DMU:H18	25:K:105:DMU:H13	1.94	0.50
1:A:53[A]:ILE:HD11	12:L:40:VAL:HG13	1.92	0.50
7:G:83[A]:GLU:HB2	7:G:84:LYS:HG2	1.94	0.50
1:A:348:PHE:CE1	1:A:380[B]:VAL:HG22	2.47	0.49
22:N:611:TGL:HA92	22:N:611:TGL:H231	1.92	0.49
1:N:514:LYS:HG2	6:S:38:ALA:CB	2.42	0.49
3:P:165:ILE:HG12	27:P:308:PEK:H11	1.95	0.49
12:L:24:MET:HG3	30:L:221:HOH:O	2.11	0.49
3:C:210:ILE:HG12	18:C:308:PGV:H132	1.94	0.49
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.95	0.49
3:P:80[A]:ARG:HG2	3:P:240:TRP:HH2	1.77	0.49
1:A:246:LEU:HD13	1:A:381[B]:LEU:HD11	1.95	0.49
1:A:472:ILE:HG21	22:L:103:TGL:HA91	1.95	0.49
3:C:99:TRP:CZ3	18:C:311:PGV:H271	2.48	0.49
13:Z:41:LYS:HE2	30:Z:201:HOH:O	2.12	0.49
12:L:25:MET:HG2	22:L:103:TGL:HA62	1.95	0.49
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.47	0.48
30:N:790:HOH:O	21:O:305:EDO:H11	2.12	0.48
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.95	0.48
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.95	0.48
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.95	0.48
7:G:4:ALA:CB	1:N:282:PHE:HA	2.43	0.48
12:L:26:THR:HG23	13:M:25:SER:CB	2.43	0.48
5:E:90:ARG:HD2	30:E:402:HOH:O	2.13	0.48
26:T:101:CDL:H762	26:T:101:CDL:C60	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:78:TRP:CB	22:D:202:TGL:HB32	2.44	0.48
22:N:609:TGL:H222	22:N:609:TGL:H271	1.95	0.48
14:N:603:HEA:H243	2:O:69:PRO:HB3	1.94	0.48
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.40	0.48
22:L:103:TGL:HA92	22:L:103:TGL:H221	1.68	0.48
1:A:302[B]:ARG:CZ	1:A:361[B]:SER:OG	2.62	0.47
5:E:94:ASN:HB3	30:E:427:HOH:O	2.14	0.47
6:F:50:PRO:HG2	30:F:277:HOH:O	2.15	0.47
26:T:101:CDL:H212	26:T:101:CDL:H732	1.96	0.47
26:C:305:CDL:H851	26:C:305:CDL:H822	1.50	0.47
8:U:9:LYS:HB3	8:U:10:ASN:H	1.48	0.47
1:A:321[A]:PHE:HB3	2:B:65:TRP:CE3	2.49	0.47
22:B:301:TGL:H142	22:B:301:TGL:H112	1.33	0.47
8:H:45:ALA:O	8:H:47:GLY:N	2.47	0.47
1:N:297[C]:MET:CG	1:N:302:ARG:HG3	2.45	0.47
1:N:309:THR:HG22	14:N:603:HEA:HMB2	1.96	0.47
2:O:68:LEU:HD23	19:O:303:PSC:H171	1.97	0.47
1:A:131:PRO:HB3	21:A:613:EDO:H12	1.97	0.47
25:D:201:DMU:H26	25:M:101:DMU:H8	1.97	0.47
9:V:36:LYS:HD2	9:V:40:ALA:HB3	1.96	0.46
3:C:90[B]:GLU:OE2	18:C:301:PGV:H321	2.15	0.46
18:N:608:PGV:H183	27:P:306:PEK:H342	1.96	0.46
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.77	0.46
3:C:58:TRP:HB2	26:C:305:CDL:H551	1.97	0.46
1:N:242:GLU:HA	1:N:245:ILE:HD12	1.96	0.46
1:N:514:LYS:HD2	30:S:270:HOH:O	2.16	0.46
18:N:607:PGV:H11	4:Q:84:ALA:CB	2.45	0.46
22:N:609:TGL:HC42	22:N:609:TGL:H152	1.97	0.46
2:O:13:THR:HB	2:O:168:LEU:HD23	1.96	0.46
4:Q:4:SER:N	30:Q:304:HOH:O	2.47	0.46
3:P:47:LEU:O	3:P:51[B]:MET:HG2	2.16	0.46
2:O:164:ALA:O	2:O:194:GLY:HA3	2.15	0.46
2:B:70:ALA:HB1	26:T:101:CDL:H441	1.98	0.46
18:G:102:PGV:H71	18:G:102:PGV:H42	1.60	0.46
8:H:9:LYS:HD2	8:H:11:TYR:HB2	1.98	0.46
19:A:607:PSC:H231	19:A:607:PSC:H262	1.75	0.45
6:S:87:THR:HG22	30:S:333:HOH:O	2.16	0.45
4:D:98:TRP:CE2	25:M:101:DMU:H11	2.51	0.45
11:K:26[A]:VAL:HG13	25:K:101:DMU:H11	1.98	0.45
24:Y:101:CHD:H112	24:Y:101:CHD:H12A	1.51	0.45
4:D:19[B]:ARG:HH11	4:D:21:ASP:CG	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.52	0.45
3:P:210:ILE:HG23	18:P:307:PGV:H91	1.99	0.45
21:J:103:EDO:H12	30:J:215:HOH:O	2.15	0.45
3:P:257:TYR:O	3:P:261:SER:HB3	2.16	0.45
19:A:607:PSC:H342	2:B:41:ILE:HD13	1.99	0.45
21:C:320:EDO:H21	30:J:204:HOH:O	2.16	0.45
1:N:514:LYS:HG2	6:S:38:ALA:HB2	1.98	0.45
22:N:611:TGL:H231	22:N:611:TGL:CA9	2.47	0.45
1:A:321[A]:PHE:CE2	2:B:65:TRP:HB2	2.52	0.45
5:E:6:GLU:OE1	5:E:14:ARG:NH2	2.46	0.45
1:N:488:THR:HB	1:N:495:LEU:HD13	1.99	0.44
3:P:80[A]:ARG:HG2	3:P:240:TRP:CH2	2.51	0.44
22:D:202:TGL:OG3	22:D:202:TGL:HC42	2.18	0.44
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.99	0.44
2:O:113:TYR:HD1	8:U:58:ARG:HH22	1.66	0.44
22:L:103:TGL:CC1	22:L:103:TGL:HC61	2.48	0.44
6:F:92[A]:VAL:HG23	30:F:205:HOH:O	2.17	0.44
1:N:92:MET:HE1	1:N:164:PHE:CD1	2.52	0.44
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.99	0.44
25:P:303:DMU:H25	25:P:303:DMU:H18	1.63	0.44
8:H:60:TYR:CD1	8:H:60:TYR:C	2.91	0.44
10:J:41:GLY:HA3	25:J:101:DMU:H23	2.00	0.44
22:N:609:TGL:HB32	22:N:609:TGL:HB61	1.88	0.43
3:P:33[B]:MET:HG2	3:P:39:SER:HB3	2.00	0.43
3:C:33:MET:HE3	25:C:310:DMU:O16	2.19	0.43
26:N:601:CDL:H582	26:N:601:CDL:H771	2.00	0.43
1:A:46:THR:HG22	1:A:49[B]:GLY:H	1.82	0.43
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.99	0.43
1:A:481:GLU:HB2	13:M:4:LYS:HD2	2.00	0.43
2:O:83:ILE:O	2:O:87:MET:HG3	2.18	0.43
1:A:406:ASN:ND2	18:A:606:PGV:H22	2.26	0.43
10:J:45:TYR:OH	25:J:101:DMU:H7	2.18	0.43
8:H:31:GLN:NE2	30:H:201:HOH:O	2.37	0.43
11:K:54:ARG:HE	11:K:54:ARG:HB3	1.54	0.43
2:O:82[C]:ARG:HD3	30:O:402:HOH:O	2.17	0.43
9:V:2:THR:HB	9:V:3:ALA:H	1.63	0.43
27:C:307:PEK:H041	7:G:70[B]:PHE:HB2	2.00	0.43
3:P:22:LEU:O	3:P:26:LEU:HG	2.18	0.43
1:N:225:GLY:HA3	3:P:112:LEU:HD21	2.01	0.43
1:N:365:ILE:HD11	30:N:708:HOH:O	2.19	0.43
1:A:293:PHE:O	1:A:302[B]:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:266:GLU:OE1	21:S:106:EDO:H11	2.18	0.43
1:N:308:ALA:O	1:N:311[A]:ILE:HG12	2.19	0.43
2:B:227:LEU:HD21	30:B:501:HOH:O	2.19	0.42
24:L:102:CHD:H183	24:L:102:CHD:H212	2.01	0.42
3:C:99:TRP:CE2	18:C:311:PGV:H232	2.55	0.42
25:C:303:DMU:H23	27:C:307:PEK:H282	2.01	0.42
1:N:309:THR:CG2	14:N:603:HEA:HMB2	2.49	0.42
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	2.01	0.42
5:R:6:GLU:HB2	5:R:10:GLU:HB2	2.00	0.42
8:H:43:MET:HE3	8:H:49:ASP:N	2.34	0.42
18:N:608:PGV:H343	27:P:306:PEK:C37	2.49	0.42
1:A:120:ALA:HB2	21:A:615:EDO:H12	2.01	0.42
2:B:13:THR:HB	2:B:168:LEU:HD23	2.02	0.42
2:B:132:GLU:HB3	2:B:137:GLU:HG3	2.00	0.42
1:N:449:MET:SD	2:O:5:MET:HG2	2.59	0.42
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.54	0.42
18:P:307:PGV:H131	18:P:307:PGV:H101	1.66	0.42
12:Y:26:THR:HA	30:Z:211:HOH:O	2.19	0.42
1:A:110:LEU:HD21	25:C:310:DMU:H24	2.01	0.42
3:P:168:THR:HG21	27:P:308:PEK:H12	2.00	0.42
6:F:64:GLU:O	6:F:65:ASP:HB2	2.20	0.42
9:I:36:LYS:HE2	9:I:36:LYS:HB2	1.68	0.42
24:L:102:CHD:H8	24:L:102:CHD:H182	1.84	0.42
19:O:303:PSC:H302	19:O:303:PSC:H111	2.02	0.42
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.73	0.42
1:A:336:PRO:HB2	1:A:394[B]:VAL:HG11	2.01	0.42
2:B:49:LYS:HE3	22:D:202:TGL:HC71	2.02	0.42
4:D:19[B]:ARG:NE	4:D:21:ASP:OD1	2.47	0.42
1:N:439:ARG:HD3	2:O:199:ILE:HB	2.01	0.42
1:A:302[A]:ARG:HH11	1:A:302[A]:ARG:HD2	1.61	0.42
27:C:307:PEK:H221	27:C:307:PEK:H251	1.82	0.42
6:S:9:ASP:OD2	30:S:201:HOH:O	2.22	0.42
2:O:41:ILE:O	2:O:45:MET:HG2	2.20	0.41
2:O:58:ALA:O	2:O:62:GLU:HG3	2.21	0.41
3:C:59:ARG:HA	26:C:305:CDL:H512	2.02	0.41
1:N:114:ALA:HA	10:W:50:LEU:HD21	2.02	0.41
14:A:602:HEA:H243	2:B:69:PRO:HB3	2.03	0.41
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.54	0.41
1:N:321:PHE:HB3	2:O:65[A]:TRP:CE3	2.54	0.41
2:O:218:TYR:HB3	30:O:436:HOH:O	2.20	0.41
19:O:303:PSC:H262	19:O:303:PSC:H291	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:84:LYS:HE2	7:T:84:LYS:HB2	1.88	0.41
1:A:302[B]:ARG:HH21	2:B:84:LEU:CD1	2.33	0.41
7:G:5:LYS:HB3	1:N:278[B]:MET:HE3	2.01	0.41
1:N:28:MET:CE	14:N:602[C]:HEA:H271	2.50	0.41
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.55	0.41
26:T:101:CDL:OB6	26:T:101:CDL:H151	2.20	0.41
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.19	0.41
1:N:35[B]:LEU:HD22	1:N:462:LEU:HD22	2.02	0.41
3:P:219:PHE:CE2	3:P:223[A]:LEU:HD11	2.56	0.41
27:P:308:PEK:H222	7:T:21:PHE:CG	2.55	0.41
1:A:280:ILE:HG23	1:A:312[A]:ILE:HD11	2.02	0.41
14:A:601[A]:HEA:H211	14:A:601[A]:HEA:H271	1.85	0.41
5:E:6:GLU:H	5:E:6:GLU:HG2	1.55	0.41
1:N:54[A]:TYR:HB2	30:N:756[A]:HOH:O	2.19	0.41
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.21	0.41
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.56	0.41
9:I:73:LYS:HE2	30:I:163:HOH:O	2.20	0.41
1:A:240:HIS:CD2	1:A:240:HIS:C	2.94	0.41
8:H:46:LYS:HG2	8:U:52:VAL:HA	2.01	0.41
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.94	0.41
3:C:161[A]:GLN:NE2	27:C:309:PEK:H41	2.36	0.41
25:C:310:DMU:H4	10:J:52:TRP:CZ2	2.56	0.41
24:G:101:CHD:H212	24:G:101:CHD:H12	2.02	0.41
12:L:19:TRP:CD2	24:L:102:CHD:O12	2.74	0.41
1:N:380[A]:VAL:HG21	14:N:603:HEA:C3C	2.51	0.41
1:N:422:ASN:HB3	22:N:609:TGL:H221	2.03	0.41
22:N:609:TGL:HB72	2:O:32[A]:PHE:CE2	2.56	0.41
5:R:43:PRO:HB2	5:R:48:ILE:HD11	2.03	0.41
27:C:309:PEK:H221	7:G:21:PHE:CD1	2.56	0.41
21:W:102:EDO:H12	30:W:204:HOH:O	2.21	0.41
4:Q:127:LYS:HD2	30:V:153:HOH:O	2.21	0.40
8:U:20:PHE:HE1	8:U:27:ARG:HG2	1.85	0.40
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.18	0.40
18:N:608:PGV:H343	27:P:306:PEK:H381	2.03	0.40
2:O:206:PHE:CE1	21:O:306:EDO:H21	2.55	0.40
11:K:40:TRP:CD2	25:K:103:DMU:H14	2.57	0.40
3:P:117:PRO:HA	3:P:118:PRO:HD3	1.94	0.40
14:A:601[C]:HEA:H212	14:A:601[C]:HEA:H271	1.86	0.40
3:C:117:PRO:HA	3:C:118:PRO:HD3	1.98	0.40
27:C:309:PEK:C37	26:N:601:CDL:H273	2.52	0.40
4:D:120:THR:HG21	11:K:48[B]:VAL:CG1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:108:LYS:HE2	5:E:108:LYS:HB2	1.85	0.40
3:P:149:HIS:NE2	21:P:310:EDO:H12	2.36	0.40
12:L:20:ARG:HH22	22:L:103:TGL:HC52	1.82	0.40
1:N:35[B]:LEU:HD23	25:Z:101:DMU:H24	2.04	0.40
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	2.01	0.40
22:N:612:TGL:H222	22:N:612:TGL:HA91	1.71	0.40

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	545/514 (106%)	530 (97%)	15 (3%)	0	100	100
1	N	550/514 (107%)	538 (98%)	12 (2%)	0	100	100
2	B	232/227 (102%)	227 (98%)	5 (2%)	0	100	100
2	O	236/227 (104%)	229 (97%)	6 (2%)	1 (0%)	34	17
3	C	269/259 (104%)	264 (98%)	5 (2%)	0	100	100
3	P	269/259 (104%)	264 (98%)	5 (2%)	0	100	100
4	D	145/144 (101%)	142 (98%)	3 (2%)	0	100	100
4	Q	143/144 (99%)	138 (96%)	5 (4%)	0	100	100
5	E	103/105 (98%)	103 (100%)	0	0	100	100
5	R	104/105 (99%)	103 (99%)	1 (1%)	0	100	100
6	F	97/94 (103%)	95 (98%)	2 (2%)	0	100	100
6	S	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
7	G	86/84 (102%)	77 (90%)	4 (5%)	5 (6%)	1	0
7	T	82/84 (98%)	72 (88%)	5 (6%)	5 (6%)	1	0
8	H	78/79 (99%)	70 (90%)	5 (6%)	3 (4%)	3	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	U	77/79 (98%)	72 (94%)	4 (5%)	1 (1%)	12	2
9	I	72/73 (99%)	71 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	68 (96%)	2 (3%)	1 (1%)	11	2
10	J	57/58 (98%)	56 (98%)	1 (2%)	0	100	100
10	W	56/58 (97%)	56 (100%)	0	0	100	100
11	K	50/49 (102%)	48 (96%)	2 (4%)	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	45/46 (98%)	43 (96%)	2 (4%)	0	100	100
12	Y	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
13	M	41/43 (95%)	41 (100%)	0	0	100	100
13	Z	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
All	All	3632/3550 (102%)	3525 (97%)	91 (2%)	16 (0%)	29	17

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	37	LEU
7	T	4	ALA
7	T	5	LYS
8	U	8	ILE
8	H	46	LYS
7	T	3	ALA
7	G	5	LYS
7	T	7	ASP
8	H	45	ALA
9	V	2	THR
7	T	6	GLY
8	H	48	GLY
2	O	92	ASN
7	G	6	GLY

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	456/426 (107%)	447 (98%)	9 (2%)	55	34
1	N	460/426 (108%)	454 (99%)	6 (1%)	69	54
2	B	217/210 (103%)	206 (95%)	11 (5%)	24	6
2	O	221/210 (105%)	206 (93%)	15 (7%)	16	3
3	C	236/224 (105%)	232 (98%)	4 (2%)	60	42
3	P	236/224 (105%)	233 (99%)	3 (1%)	69	54
4	D	131/128 (102%)	129 (98%)	2 (2%)	65	49
4	Q	129/128 (101%)	126 (98%)	3 (2%)	50	28
5	E	92/92 (100%)	91 (99%)	1 (1%)	73	60
5	R	93/92 (101%)	93 (100%)	0	100	100
6	F	83/78 (106%)	81 (98%)	2 (2%)	49	26
6	S	78/78 (100%)	76 (97%)	2 (3%)	46	23
7	G	72/68 (106%)	62 (86%)	10 (14%)	3	0
7	T	68/68 (100%)	60 (88%)	8 (12%)	5	0
8	H	72/71 (101%)	65 (90%)	7 (10%)	8	1
8	U	71/71 (100%)	66 (93%)	5 (7%)	15	2
9	I	58/57 (102%)	54 (93%)	4 (7%)	15	2
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	13
10	J	50/49 (102%)	50 (100%)	0	100	100
10	W	49/49 (100%)	47 (96%)	2 (4%)	30	10
11	K	42/39 (108%)	41 (98%)	1 (2%)	49	26
11	X	39/39 (100%)	39 (100%)	0	100	100
12	L	40/39 (103%)	38 (95%)	2 (5%)	24	6
12	Y	39/39 (100%)	35 (90%)	4 (10%)	7	1
13	M	37/37 (100%)	37 (100%)	0	100	100
13	Z	37/37 (100%)	35 (95%)	2 (5%)	22	5
All	All	3163/3036 (104%)	3058 (97%)	105 (3%)	40	15

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	369	ASP
1	A	382[A]	SER
1	A	382[B]	SER
1	A	382[C]	SER
1	A	486[A]	ASP
1	A	486[B]	ASP
2	B	33	LEU
2	B	60[A]	GLU
2	B	60[B]	GLU
2	B	65	TRP
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115[A]	ASP
2	B	115[B]	ASP
2	B	171	LYS
3	C	40	MET
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	74	SER
4	D	147	LYS
5	E	70	VAL
6	F	54[A]	ASN
6	F	54[B]	ASN
7	G	2	SER
7	G	7	ASP
7	G	11	THR
7	G	18	PHE
7	G	33[A]	LEU
7	G	33[B]	LEU
7	G	43	GLU
7	G	54	ARG
7	G	83[A]	GLU
7	G	83[B]	GLU
8	H	7	LYS
8	H	9	LYS
8	H	29	CYS
8	H	46	LYS

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Mol	Chain	Res	Type
8	H	51	SER
8	H	60	TYR
8	H	61	LYS
9	I	2	THR
9	I	15	ARG
9	I	18	ARG
9	I	36	LYS
11	K	54	ARG
12	L	20	ARG
12	L	47	LYS
1	N	109	PHE
1	N	138	HIS
1	N	363	LEU
1	N	369	ASP
1	N	417[A]	MET
1	N	417[B]	MET
2	O	33	LEU
2	O	59	GLN
2	O	64[A]	ILE
2	O	64[B]	ILE
2	O	68	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	115	ASP
2	O	158	ASP
2	O	171	LYS
2	O	223	SER
2	O	225	SER
2	O	226	MET
2	O	227	LEU
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	20	ARG
4	Q	51	LEU
6	S	2	SER
6	S	93	PRO
7	T	2	SER
7	T	11	THR
7	T	18	PHE

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Mol	Chain	Res	Type
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
7	T	38	HIS
7	T	54	ARG
8	U	9	LYS
8	U	10	ASN
8	U	29	CYS
8	U	60	TYR
8	U	61	LYS
9	V	2	THR
9	V	18	ARG
10	W	50	LEU
10	W	58	LYS
12	Y	2	HIS
12	Y	20	ARG
12	Y	46	LYS
12	Y	47	LYS
13	Z	38	ASP
13	Z	39	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
2	B	10	GLN
4	D	109	HIS
6	F	94	HIS
2	O	195	GLN
4	Q	101	HIS
4	Q	109	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	O	1	2	8,9,10	0.80	0	7,9,11	1.54	2 (28%)
1	FME	A	1	1	8,9,10	0.47	0	7,9,11	1.26	1 (14%)
2	FME	B	1	2	8,9,10	1.01	1 (12%)	7,9,11	1.86	2 (28%)
9	SAC	V	1	9	7,8,9	0.61	0	8,9,11	0.90	0
9	SAC	I	1	9	7,8,9	0.68	0	8,9,11	1.42	1 (12%)
1	FME	N	1	1	8,9,10	0.56	0	7,9,11	1.47	1 (14%)

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	O	1	2	-	0/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
9	SAC	V	1	9	-	4/7/8/10	-
9	SAC	I	1	9	-	2/7/8/10	-
1	FME	N	1	1	-	3/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-2.03	1.70	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-3.36	103.62	112.95
2	O	1	FME	CG-CB-CA	-2.67	105.52	112.95
1	N	1	FME	O-C-CA	-2.67	117.79	124.78
9	I	1	SAC	CA-N-C1A	-2.58	118.38	123.15
2	B	1	FME	C-CA-N	-2.46	105.29	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	O1-CN-N	-2.27	119.30	125.27
1	A	1	FME	C-CA-N	2.12	113.55	109.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 150 ligands modelled in this entry, 10 are monoatomic - leaving 140 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
27	PEK	C	306	-	23,23,52	0.39	0	21,21,57	0.42	0
21	EDO	D	205	-	3,3,3	0.67	0	2,2,2	0.24	0
25	DMU	X	101	-	9,9,34	0.41	0	8,8,45	0.44	0
21	EDO	T	103	-	3,3,3	0.49	0	2,2,2	0.34	0
21	EDO	A	616	-	3,3,3	0.47	0	2,2,2	0.42	0
21	EDO	B	305	-	3,3,3	0.41	0	2,2,2	0.78	0
21	EDO	A	615	-	3,3,3	0.76	0	2,2,2	0.25	0
27	PEK	P	306	-	52,52,52	0.75	2 (3%)	55,57,57	1.09	4 (7%)
21	EDO	J	103	-	3,3,3	0.34	0	2,2,2	0.58	0
21	EDO	C	312	-	3,3,3	0.47	0	2,2,2	0.14	0
21	EDO	S	105	-	3,3,3	0.78	0	2,2,2	0.53	0
21	EDO	F	104	-	3,3,3	0.58	0	2,2,2	0.68	0
25	DMU	X	103	-	8,8,34	0.40	0	7,7,45	0.53	0
18	PGV	C	311	-	26,26,50	1.17	1 (3%)	25,25,56	2.06	5 (20%)
21	EDO	N	616	-	3,3,3	0.47	0	2,2,2	0.50	0
21	EDO	P	314	-	3,3,3	0.44	0	2,2,2	0.87	0
22	TGL	N	612	-	43,43,62	1.18	2 (4%)	45,45,65	1.60	8 (17%)
27	PEK	C	309	-	34,34,52	0.35	0	32,32,57	0.62	0
25	DMU	X	102	-	9,9,34	0.39	0	8,8,45	0.37	0
25	DMU	P	303	-	11,11,34	0.43	0	10,10,45	0.37	0
25	DMU	L	101	-	21,21,34	0.66	1 (4%)	24,25,45	2.46	6 (25%)
21	EDO	P	316	-	3,3,3	0.58	0	2,2,2	0.42	0
22	TGL	D	202	-	56,56,62	1.17	3 (5%)	59,59,65	1.13	5 (8%)
21	EDO	P	310	-	3,3,3	0.61	0	2,2,2	0.15	0
21	EDO	P	313	-	3,3,3	0.80	0	2,2,2	0.15	0
20	PER	A	608[A]	15,14	0,1,1	0.00	-	-		
20	PER	N	610[A]	15,14	0,1,1	0.00	-	-		
21	EDO	P	315	-	3,3,3	0.40	0	2,2,2	1.15	0
18	PGV	P	307	-	50,50,50	0.69	2 (4%)	53,56,56	1.09	5 (9%)
25	DMU	X	104	-	9,9,34	0.46	0	8,8,45	0.18	0
22	TGL	B	301	-	47,47,62	1.16	3 (6%)	50,50,65	1.47	5 (10%)
26	CDL	N	601	-	51,51,99	1.20	8 (15%)	47,47,111	0.88	1 (2%)
25	DMU	J	101	-	10,10,34	0.36	0	9,9,45	0.39	0
21	EDO	A	613	-	3,3,3	0.51	0	2,2,2	0.26	0
18	PGV	C	301	-	50,50,50	0.94	4 (8%)	53,56,56	1.21	4 (7%)
21	EDO	B	307	-	3,3,3	0.64	0	2,2,2	0.25	0
14	HEA	A	601[C]	-	44,58,67	1.28	3 (6%)	37,91,103	3.97	15 (40%)
18	PGV	N	608	-	50,50,50	0.90	4 (8%)	53,56,56	1.24	5 (9%)
25	DMU	K	101	-	8,8,34	0.28	0	7,7,45	0.59	0
21	EDO	O	305	-	3,3,3	0.56	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	A	618	-	3,3,3	0.70	0	2,2,2	0.78	0
22	TGL	L	103	-	53,53,62	0.74	1 (1%)	51,51,65	1.08	3 (5%)
24	CHD	B	303	-	29,32,32	0.92	1 (3%)	48,51,51	1.64	10 (20%)
21	EDO	P	311	-	3,3,3	0.46	0	2,2,2	0.31	0
24	CHD	Y	101	-	29,32,32	0.73	0	48,51,51	2.40	18 (37%)
21	EDO	S	103	-	3,3,3	0.63	0	2,2,2	0.06	0
21	EDO	C	320	-	3,3,3	0.68	0	2,2,2	0.53	0
14	HEA	A	601[A]	-	44,67,67	1.17	2 (4%)	37,103,103	2.39	15 (40%)
21	EDO	T	104	-	3,3,3	0.72	0	2,2,2	0.41	0
27	PEK	P	308	-	32,32,52	0.43	0	29,30,57	0.57	0
27	PEK	C	307	-	52,52,52	0.84	2 (3%)	55,57,57	1.07	3 (5%)
21	EDO	F	103	-	3,3,3	0.63	0	2,2,2	0.17	0
21	EDO	B	304	-	3,3,3	0.63	0	2,2,2	0.34	0
25	DMU	Q	201	-	9,9,34	0.45	0	8,8,45	0.22	0
29	PO4	U	101	-	4,4,4	1.14	0	6,6,6	0.76	0
21	EDO	Y	102	-	3,3,3	0.46	0	2,2,2	0.21	0
27	PEK	P	305	-	19,19,52	0.30	0	18,18,57	0.57	0
25	DMU	K	104	-	8,8,34	0.53	0	7,7,45	0.25	0
21	EDO	F	102	-	3,3,3	0.98	0	2,2,2	0.54	0
24	CHD	G	101	-	29,32,32	0.84	0	48,51,51	1.34	7 (14%)
25	DMU	D	201	-	10,10,34	0.33	0	9,9,45	0.41	0
21	EDO	N	618	-	3,3,3	0.50	0	2,2,2	0.36	0
21	EDO	B	306	-	3,3,3	0.82	0	2,2,2	0.33	0
25	DMU	P	309	-	10,10,34	0.33	0	9,9,45	0.55	0
21	EDO	G	103	-	3,3,3	0.62	0	2,2,2	0.55	0
14	HEA	N	603	20,1,30	44,67,67	1.13	3 (6%)	37,103,103	1.81	9 (24%)
25	DMU	K	106	-	9,9,34	0.28	0	8,8,45	0.32	0
26	CDL	C	305	-	54,54,99	1.04	5 (9%)	50,50,111	1.12	5 (10%)
21	EDO	W	102	-	3,3,3	0.34	0	2,2,2	0.24	0
21	EDO	A	609	-	3,3,3	0.57	0	2,2,2	0.60	0
25	DMU	O	302	-	10,10,34	0.20	0	9,9,45	0.72	0
25	DMU	D	203	-	9,9,34	0.36	0	8,8,45	0.55	0
21	EDO	N	619	-	3,3,3	0.74	0	2,2,2	0.18	0
21	EDO	E	201	-	3,3,3	0.54	0	2,2,2	0.38	0
26	CDL	P	304	-	57,57,99	1.22	7 (12%)	54,54,111	1.05	4 (7%)
21	EDO	D	206	-	3,3,3	0.56	0	2,2,2	0.13	0
24	CHD	P	301	-	29,32,32	0.68	0	48,51,51	1.58	9 (18%)
21	EDO	E	202	-	3,3,3	0.43	0	2,2,2	0.32	0
14	HEA	A	602	20,1,30	44,67,67	1.17	4 (9%)	37,103,103	2.00	10 (27%)
21	EDO	N	617	-	3,3,3	0.51	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	S	106	-	3,3,3	0.43	0	2,2,2	0.79	0
26	CDL	T	101	-	52,53,99	1.34	8 (15%)	49,51,111	1.21	4 (8%)
22	TGL	N	609	-	62,62,62	1.13	3 (4%)	65,65,65	1.07	4 (6%)
21	EDO	O	306	-	3,3,3	0.49	0	2,2,2	0.09	0
21	EDO	Y	103	-	3,3,3	0.50	0	2,2,2	0.71	0
18	PGV	N	607	-	22,22,50	0.36	0	20,20,56	0.52	0
14	HEA	N	602[A]	-	44,67,67	0.83	1 (2%)	37,103,103	1.90	13 (35%)
21	EDO	C	317	-	3,3,3	0.62	0	2,2,2	0.18	0
25	DMU	K	105	-	8,8,34	0.24	0	7,7,45	0.61	0
21	EDO	P	312	-	3,3,3	0.58	0	2,2,2	0.28	0
18	PGV	C	308	-	47,47,50	0.84	1 (2%)	50,53,56	0.93	3 (6%)
18	PGV	A	606	-	20,20,50	0.51	0	18,18,56	0.78	0
25	DMU	K	102	-	9,9,34	0.27	0	8,8,45	0.46	0
25	DMU	M	101	-	34,34,34	0.57	0	45,45,45	1.28	4 (8%)
21	EDO	N	615	-	3,3,3	0.58	0	2,2,2	0.12	0
21	EDO	C	316	-	3,3,3	0.40	0	2,2,2	0.36	0
21	EDO	S	104	-	3,3,3	0.50	0	2,2,2	0.23	0
22	TGL	N	611	-	45,45,62	0.36	0	42,42,65	0.44	0
21	EDO	F	106	-	3,3,3	0.68	0	2,2,2	0.76	0
18	PGV	G	102	-	30,30,50	0.98	1 (3%)	28,29,56	1.48	3 (10%)
23	CUA	O	301	2	0,1,1	0.00	-	-		
21	EDO	L	104	-	3,3,3	0.53	0	2,2,2	0.76	0
21	EDO	T	102	-	3,3,3	0.65	0	2,2,2	0.77	0
21	EDO	N	613	-	3,3,3	0.81	0	2,2,2	0.75	0
25	DMU	Z	101	-	34,34,34	0.51	0	45,45,45	1.03	2 (4%)
21	EDO	A	610	-	3,3,3	0.49	0	2,2,2	0.28	0
21	EDO	F	105	-	3,3,3	0.58	0	2,2,2	0.36	0
21	EDO	G	104	-	3,3,3	0.62	0	2,2,2	0.16	0
25	DMU	C	310	-	21,21,34	0.88	1 (4%)	24,25,45	1.35	3 (12%)
21	EDO	P	317	-	3,3,3	0.55	0	2,2,2	0.17	0
21	EDO	Q	202	-	3,3,3	0.46	0	2,2,2	0.64	0
21	EDO	A	614	-	3,3,3	0.48	0	2,2,2	0.48	0
24	CHD	C	304	-	29,32,32	0.78	0	48,51,51	1.57	7 (14%)
14	HEA	N	602[C]	-	44,58,67	3.53	1 (2%)	37,91,103	4.75	16 (43%)
21	EDO	A	611	-	3,3,3	0.81	0	2,2,2	0.53	0
25	DMU	W	101	-	10,10,34	0.38	0	9,9,45	0.54	0
21	EDO	N	614	-	3,3,3	0.79	0	2,2,2	0.35	0
21	EDO	J	102	-	3,3,3	0.53	0	2,2,2	0.37	0
25	DMU	C	303	-	12,12,34	0.54	0	10,11,45	0.35	0
25	DMU	K	103	-	10,10,34	0.40	0	9,9,45	0.48	0
21	EDO	C	319	-	3,3,3	0.60	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	N	621	-	3,3,3	0.56	0	2,2,2	0.09	0
23	CUA	B	302	2	0,1,1	0.00	-	-		
21	EDO	S	102	-	3,3,3	0.80	0	2,2,2	0.74	0
21	EDO	A	617	-	3,3,3	0.62	0	2,2,2	0.13	0
21	EDO	D	204	-	3,3,3	0.57	0	2,2,2	0.13	0
21	EDO	C	315	-	3,3,3	0.39	0	2,2,2	1.06	0
21	EDO	N	620	-	3,3,3	0.76	0	2,2,2	0.34	0
19	PSC	A	607	-	25,25,51	0.81	1 (4%)	22,23,59	0.93	0
21	EDO	C	313	-	3,3,3	0.70	0	2,2,2	0.61	0
21	EDO	C	314	-	3,3,3	0.84	0	2,2,2	0.40	0
21	EDO	A	612	-	3,3,3	0.79	0	2,2,2	0.67	0
21	EDO	C	318	-	3,3,3	0.56	0	2,2,2	0.49	0
24	CHD	L	102	-	29,32,32	0.72	0	48,51,51	2.87	20 (41%)
29	PO4	H	101	-	4,4,4	0.77	0	6,6,6	0.66	0
21	EDO	E	203	-	3,3,3	0.57	0	2,2,2	0.27	0
19	PSC	O	303	-	25,28,51	0.79	1 (4%)	23,27,59	0.95	1 (4%)
21	EDO	O	304	-	3,3,3	0.66	0	2,2,2	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PEK	C	306	-	-	9/19/19/56	-
21	EDO	D	205	-	-	1/1/1/1	-
25	DMU	X	101	-	-	0/7/7/59	-
21	EDO	T	103	-	-	0/1/1/1	-
21	EDO	A	616	-	-	0/1/1/1	-
21	EDO	B	305	-	-	0/1/1/1	-
21	EDO	A	615	-	-	1/1/1/1	-
27	PEK	P	306	-	-	14/56/56/56	-
21	EDO	J	103	-	-	1/1/1/1	-
21	EDO	C	312	-	-	0/1/1/1	-
21	EDO	S	105	-	-	0/1/1/1	-
21	EDO	F	104	-	-	0/1/1/1	-
25	DMU	X	103	-	-	1/6/6/59	-
18	PGV	C	311	-	-	10/23/23/55	-
21	EDO	N	616	-	-	0/1/1/1	-
21	EDO	P	314	-	-	0/1/1/1	-
22	TGL	N	612	-	-	26/45/45/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PEK	C	309	-	-	15/30/30/56	-
25	DMU	X	102	-	-	2/7/7/59	-
25	DMU	P	303	-	-	4/9/9/59	-
25	DMU	L	101	-	-	4/13/29/59	0/1/1/2
21	EDO	P	316	-	-	0/1/1/1	-
22	TGL	D	202	-	-	32/59/59/65	-
21	EDO	P	310	-	-	1/1/1/1	-
21	EDO	P	313	-	-	0/1/1/1	-
21	EDO	P	315	-	-	1/1/1/1	-
18	PGV	P	307	-	-	6/55/55/55	-
25	DMU	X	104	-	-	0/7/7/59	-
22	TGL	B	301	-	-	29/50/50/65	-
26	CDL	N	601	-	-	17/42/43/110	-
25	DMU	J	101	-	-	6/8/8/59	-
21	EDO	A	613	-	-	1/1/1/1	-
18	PGV	C	301	-	-	8/55/55/55	-
21	EDO	B	307	-	-	0/1/1/1	-
14	HEA	A	601[C]	-	3/3/5/16	4/24/60/76	-
18	PGV	N	608	-	-	9/55/55/55	-
25	DMU	K	101	-	-	0/6/6/59	-
21	EDO	O	305	-	-	1/1/1/1	-
21	EDO	A	618	-	-	0/1/1/1	-
22	TGL	L	103	-	-	24/47/48/65	-
24	CHD	B	303	-	-	0/7/74/74	0/4/4/4
14	HEA	A	601[B]	-	3/3/5/16	-	-
21	EDO	P	311	-	-	1/1/1/1	-
24	CHD	Y	101	-	-	4/7/74/74	0/4/4/4
21	EDO	S	103	-	-	0/1/1/1	-
21	EDO	C	320	-	-	1/1/1/1	-
14	HEA	A	601[A]	-	3/3/7/16	2/24/76/76	-
21	EDO	T	104	-	-	1/1/1/1	-
27	PEK	P	308	-	-	12/28/28/56	-
27	PEK	C	307	-	-	15/56/56/56	-
21	EDO	F	103	-	-	0/1/1/1	-
21	EDO	B	304	-	-	0/1/1/1	-
25	DMU	Q	201	-	-	4/7/7/59	-
21	EDO	Y	102	-	-	0/1/1/1	-
27	PEK	P	305	-	-	10/17/17/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DMU	K	104	-	-	2/6/6/59	-
21	EDO	F	102	-	-	0/1/1/1	-
24	CHD	G	101	-	-	0/7/74/74	0/4/4/4
25	DMU	D	201	-	-	3/8/8/59	-
21	EDO	N	618	-	-	0/1/1/1	-
21	EDO	B	306	-	-	0/1/1/1	-
25	DMU	P	309	-	-	2/8/8/59	-
21	EDO	G	103	-	-	0/1/1/1	-
14	HEA	N	603	20,1,30	3/3/7/16	0/24/76/76	-
25	DMU	K	106	-	-	3/7/7/59	-
26	CDL	C	305	-	-	14/45/46/110	-
21	EDO	W	102	-	-	1/1/1/1	-
21	EDO	A	609	-	-	0/1/1/1	-
25	DMU	O	302	-	-	3/8/8/59	-
25	DMU	D	203	-	-	2/7/7/59	-
21	EDO	N	619	-	-	1/1/1/1	-
21	EDO	E	201	-	-	0/1/1/1	-
26	CDL	P	304	-	-	17/49/50/110	-
21	EDO	D	206	-	-	0/1/1/1	-
24	CHD	P	301	-	-	0/7/74/74	0/4/4/4
21	EDO	E	202	-	-	1/1/1/1	-
14	HEA	A	602	20,1,30	3/3/7/16	0/24/76/76	-
21	EDO	N	617	-	-	0/1/1/1	-
21	EDO	S	106	-	-	0/1/1/1	-
26	CDL	T	101	-	-	21/47/47/110	-
22	TGL	N	609	-	-	34/65/65/65	-
21	EDO	O	306	-	-	0/1/1/1	-
21	EDO	Y	103	-	-	1/1/1/1	-
18	PGV	N	607	-	-	5/18/18/55	-
14	HEA	N	602[A]	-	3/3/7/16	0/24/76/76	-
21	EDO	C	317	-	-	0/1/1/1	-
25	DMU	K	105	-	-	4/6/6/59	-
21	EDO	P	312	-	-	0/1/1/1	-
18	PGV	C	308	-	-	10/52/52/55	-
18	PGV	A	606	-	-	3/15/16/55	-
25	DMU	K	102	-	-	3/7/7/59	-
25	DMU	M	101	-	-	3/19/59/59	0/2/2/2
21	EDO	N	615	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	C	316	-	-	0/1/1/1	-
21	EDO	S	104	-	-	0/1/1/1	-
22	TGL	N	611	-	-	20/39/39/65	-
21	EDO	F	106	-	-	0/1/1/1	-
18	PGV	G	102	-	-	7/27/27/55	-
21	EDO	L	104	-	-	1/1/1/1	-
21	EDO	T	102	-	-	0/1/1/1	-
21	EDO	N	613	-	-	0/1/1/1	-
25	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
21	EDO	A	610	-	-	1/1/1/1	-
21	EDO	F	105	-	-	0/1/1/1	-
21	EDO	G	104	-	-	1/1/1/1	-
25	DMU	C	310	-	-	5/13/29/59	0/1/1/2
21	EDO	P	317	-	-	0/1/1/1	-
21	EDO	Q	202	-	-	0/1/1/1	-
21	EDO	A	614	-	-	1/1/1/1	-
24	CHD	C	304	-	-	0/7/74/74	0/4/4/4
14	HEA	N	602[C]	-	3/3/5/16	7/24/60/76	-
21	EDO	A	611	-	-	0/1/1/1	-
25	DMU	W	101	-	-	1/8/8/59	-
21	EDO	N	614	-	-	0/1/1/1	-
21	EDO	J	102	-	-	1/1/1/1	-
25	DMU	C	303	-	-	2/9/10/59	-
25	DMU	K	103	-	-	6/8/8/59	-
21	EDO	C	319	-	-	0/1/1/1	-
14	HEA	N	602[B]	-	3/3/5/16	-	-
21	EDO	N	621	-	-	0/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
21	EDO	A	617	-	-	0/1/1/1	-
21	EDO	D	204	-	-	0/1/1/1	-
21	EDO	C	315	-	-	0/1/1/1	-
21	EDO	N	620	-	-	0/1/1/1	-
19	PSC	A	607	-	-	10/21/21/55	-
21	EDO	C	313	-	-	0/1/1/1	-
21	EDO	C	314	-	-	0/1/1/1	-
21	EDO	A	612	-	-	0/1/1/1	-
21	EDO	C	318	-	-	0/1/1/1	-
24	CHD	L	102	-	-	6/7/74/74	0/4/4/4
21	EDO	E	203	-	-	1/1/1/1	-
19	PSC	O	303	-	-	7/22/24/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	O	304	-	-	0/1/1/1	-

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602[C]	HEA	C18-C19	22.89	1.87	1.33
22	N	612	TGL	OG2-CB1	5.58	1.50	1.34
18	C	311	PGV	O03-C19	5.52	1.49	1.33
22	N	609	TGL	OG2-CB1	5.12	1.48	1.34
22	D	202	TGL	OG1-CA1	4.92	1.47	1.33
18	G	102	PGV	O03-C19	4.81	1.48	1.33
26	T	101	CDL	OB8-CB7	4.79	1.47	1.33
22	N	609	TGL	OG3-CC1	4.70	1.47	1.33
22	B	301	TGL	OG1-CA1	4.59	1.46	1.33
26	P	304	CDL	OB8-CB7	4.52	1.47	1.33
22	N	609	TGL	OG1-CA1	4.52	1.46	1.33
22	L	103	TGL	OG1-CA1	4.44	1.47	1.33
22	D	202	TGL	OG3-CC1	4.37	1.46	1.33
22	N	612	TGL	OG1-CA1	4.35	1.46	1.33
14	A	601[A]	HEA	CAD-C3D	4.22	1.58	1.52
14	A	601[C]	HEA	CAD-C3D	4.22	1.58	1.52
22	B	301	TGL	OG3-CC1	4.18	1.45	1.33
22	D	202	TGL	OG2-CB1	4.00	1.45	1.34
22	B	301	TGL	OG2-CB1	3.95	1.45	1.34
14	A	601[C]	HEA	C18-C19	3.89	1.42	1.33
19	A	607	PSC	C13-C12	3.77	1.53	1.31
19	O	303	PSC	C13-C12	3.70	1.53	1.31
18	C	301	PGV	O01-C1	3.58	1.44	1.34
27	P	306	PEK	O03-C21	3.56	1.43	1.33
27	C	307	PEK	O03-C21	3.45	1.43	1.33
26	C	305	CDL	C59-C58	-3.38	1.32	1.51
26	C	305	CDL	C82-C81	-3.27	1.33	1.51
26	P	304	CDL	C82-C81	-3.24	1.33	1.51
26	T	101	CDL	C79-C78	-3.20	1.33	1.51
18	N	608	PGV	O01-C1	3.19	1.43	1.34
26	P	304	CDL	C19-C18	-3.19	1.33	1.51
26	P	304	CDL	C39-C38	-3.19	1.33	1.51
27	C	307	PEK	O01-C1	3.17	1.43	1.34
26	N	601	CDL	C62-C61	-3.16	1.33	1.51
26	C	305	CDL	C62-C61	-3.16	1.33	1.51
26	N	601	CDL	C42-C41	-3.15	1.33	1.51
26	N	601	CDL	C82-C81	-3.15	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	101	CDL	C82-C81	-3.13	1.34	1.51
26	P	304	CDL	C59-C58	-3.13	1.34	1.51
26	P	304	CDL	C79-C78	-3.13	1.34	1.51
14	A	602	HEA	O11-C11	3.11	1.49	1.42
26	C	305	CDL	C79-C78	-3.10	1.34	1.51
14	A	602	HEA	C3C-C2C	-3.07	1.36	1.40
26	N	601	CDL	C22-C21	-3.06	1.34	1.51
26	P	304	CDL	C42-C41	-3.05	1.34	1.51
26	N	601	CDL	C19-C18	-3.03	1.34	1.51
25	C	310	DMU	O16-C6	3.03	1.45	1.40
26	T	101	CDL	C62-C61	-3.02	1.34	1.51
26	T	101	CDL	C42-C41	-3.01	1.34	1.51
26	T	101	CDL	C19-C18	-2.98	1.34	1.51
18	C	308	PGV	O01-C1	2.97	1.42	1.34
26	N	601	CDL	C79-C78	-2.96	1.34	1.51
14	A	602	HEA	CMC-C2C	2.96	1.57	1.51
26	T	101	CDL	C22-C21	-2.89	1.35	1.51
18	N	608	PGV	O03-C19	2.81	1.41	1.33
14	N	603	HEA	CAD-C3D	2.70	1.56	1.52
26	N	601	CDL	C58-C59	-2.54	1.33	1.51
14	N	603	HEA	C3A-C2A	-2.53	1.36	1.40
26	C	305	CDL	C39-C38	-2.53	1.33	1.51
26	N	601	CDL	C38-C39	-2.49	1.34	1.51
14	N	603	HEA	O11-C11	2.43	1.48	1.42
18	N	608	PGV	O01-C02	-2.41	1.40	1.46
18	C	301	PGV	O01-C02	-2.38	1.40	1.46
26	T	101	CDL	C58-C59	-2.32	1.35	1.51
25	L	101	DMU	O16-C6	2.24	1.44	1.40
14	A	602	HEA	C18-C19	2.24	1.38	1.33
18	C	301	PGV	O03-C19	2.18	1.39	1.33
24	B	303	CHD	O7-C7	2.12	1.47	1.43
14	A	601[A]	HEA	C3C-C2C	-2.11	1.37	1.40
14	A	601[C]	HEA	C3C-C2C	-2.11	1.37	1.40
18	C	301	PGV	C03-C02	2.10	1.57	1.50
27	P	306	PEK	O01-C1	2.06	1.40	1.34
14	N	602[A]	HEA	O11-C11	2.04	1.47	1.42
18	P	307	PGV	O01-C1	2.04	1.40	1.34
18	P	307	PGV	O03-C19	2.01	1.39	1.33
18	N	608	PGV	C03-C02	2.01	1.56	1.50

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602[C]	HEA	C20-C19-C18	18.57	158.70	121.12
14	N	602[C]	HEA	C27-C19-C18	-17.43	78.95	123.68
14	A	601[C]	HEA	C20-C19-C18	13.27	147.98	121.12
14	A	601[C]	HEA	C27-C19-C18	-12.76	90.94	123.68
14	A	601[C]	HEA	C13-C12-C11	-9.41	100.21	114.35
24	L	102	CHD	C6-C5-C4	-8.48	101.43	111.19
14	N	602[C]	HEA	C13-C12-C11	-7.29	103.39	114.35
25	L	101	DMU	O16-C6-C1	7.20	119.54	108.30
24	L	102	CHD	C10-C9-C8	7.14	119.48	111.82
18	C	311	PGV	O03-C19-C20	6.85	133.42	111.91
22	B	301	TGL	OG2-CB1-CB2	6.38	125.25	111.50
14	A	601[A]	HEA	C26-C15-C16	6.32	125.90	115.27
22	N	612	TGL	OG2-CB1-CB2	6.01	124.46	111.50
24	Y	101	CHD	C14-C8-C7	5.98	119.74	111.81
24	C	304	CHD	C18-C13-C12	5.61	114.78	109.07
25	L	101	DMU	C6-O5-C4	-5.48	107.06	113.13
24	Y	101	CHD	C1-C10-C5	5.24	115.52	107.77
14	A	601[A]	HEA	CAA-CBA-CGA	-5.20	103.94	112.67
14	A	601[C]	HEA	CAA-CBA-CGA	-5.20	103.94	112.67
24	L	102	CHD	C21-C20-C17	5.16	120.82	112.92
25	L	101	DMU	C18-O16-C6	5.16	122.39	113.84
14	N	603	HEA	CAD-CBD-CGD	-5.14	104.05	112.67
18	C	311	PGV	C01-O03-C19	5.03	133.17	116.92
14	A	602	HEA	C27-C19-C20	5.02	123.71	115.27
24	L	102	CHD	C11-C9-C10	-4.99	108.58	113.73
14	A	602	HEA	CAD-CBD-CGD	-4.86	104.52	112.67
24	Y	101	CHD	C21-C20-C17	4.78	120.23	112.92
24	L	102	CHD	C17-C13-C12	-4.72	113.36	117.67
18	G	102	PGV	O03-C19-C20	4.37	129.52	112.23
14	A	601[A]	HEA	C27-C19-C20	4.37	122.62	115.27
24	P	301	CHD	C21-C20-C22	-4.29	103.64	110.36
18	C	311	PGV	O03-C19-O04	-4.28	112.80	123.59
14	N	602[C]	HEA	C27-C19-C20	4.21	122.34	115.27
22	N	609	TGL	OG2-CB1-CB2	4.17	120.48	111.50
14	A	602	HEA	C26-C15-C16	4.16	122.28	115.27
14	A	601[A]	HEA	C1B-C2B-C3B	-4.15	104.11	107.00
14	A	601[C]	HEA	C1B-C2B-C3B	-4.15	104.11	107.00
24	Y	101	CHD	C19-C10-C1	-4.14	101.59	108.26
24	L	102	CHD	C14-C8-C7	4.05	117.17	111.81
14	A	601[A]	HEA	C13-C12-C11	-4.03	108.29	114.35
24	L	102	CHD	C13-C17-C20	3.98	124.24	119.50
24	Y	101	CHD	C10-C9-C8	3.96	116.07	111.82
18	C	301	PGV	O03-C19-C20	3.95	124.29	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	M	101	DMU	C18-O16-C6	-3.91	107.36	113.84
22	B	301	TGL	OG1-CA1-CA2	3.90	121.60	111.38
24	L	102	CHD	C1-C10-C9	-3.89	105.24	111.35
24	B	303	CHD	C19-C10-C1	-3.86	102.04	108.26
18	C	301	PGV	O03-C19-O04	-3.86	113.85	123.59
14	N	602[A]	HEA	C13-C12-C11	-3.85	108.57	114.35
14	A	601[C]	HEA	C25-C23-C24	3.83	123.06	114.60
24	Y	101	CHD	C9-C11-C12	-3.82	109.26	114.30
24	Y	101	CHD	C4-C3-C2	-3.74	106.09	110.55
14	A	602	HEA	C20-C19-C18	-3.68	113.66	121.12
26	T	101	CDL	OB6-CB5-C51	3.66	123.27	109.74
24	Y	101	CHD	C16-C17-C13	-3.64	99.98	103.55
24	P	301	CHD	O12-C12-C13	-3.62	104.91	111.03
14	A	601[A]	HEA	C16-C15-C14	-3.62	113.79	121.12
24	L	102	CHD	C15-C14-C8	3.54	123.28	118.33
24	C	304	CHD	C1-C2-C3	-3.52	105.94	110.47
18	N	608	PGV	O03-C19-O04	-3.51	114.73	123.59
14	A	602	HEA	C1B-C2B-C3B	-3.51	104.56	107.00
18	G	102	PGV	C01-O03-C19	3.48	127.58	116.11
24	L	102	CHD	C9-C10-C5	3.48	113.47	108.58
24	B	303	CHD	C11-C9-C10	-3.48	110.14	113.73
24	L	102	CHD	C18-C13-C14	-3.47	105.78	111.21
22	B	301	TGL	CB3-CB2-CB1	-3.45	101.07	113.62
25	M	101	DMU	C28-C25-C22	-3.45	96.94	114.42
14	N	603	HEA	C16-C15-C14	-3.44	114.15	121.12
24	B	303	CHD	C4-C5-C10	-3.43	109.01	112.66
25	C	310	DMU	O5-C4-C57	3.43	112.32	106.83
22	D	202	TGL	CG2-OG2-CB1	-3.42	109.38	117.79
14	N	602[A]	HEA	CMB-C2B-C3B	3.40	131.34	124.69
14	N	602[C]	HEA	CMB-C2B-C3B	3.40	131.34	124.69
14	N	603	HEA	C13-C12-C11	-3.39	109.26	114.35
18	G	102	PGV	O03-C19-O04	-3.38	112.54	123.14
22	D	202	TGL	OG3-CC1-OC1	-3.38	115.06	123.59
26	P	304	CDL	OB8-CB7-C71	3.36	125.52	112.23
14	N	602[A]	HEA	C1B-C2B-C3B	-3.36	104.66	107.00
14	N	602[C]	HEA	C1B-C2B-C3B	-3.36	104.66	107.00
22	N	612	TGL	OG1-CA1-CA2	3.33	122.37	111.91
22	D	202	TGL	OG3-CC1-CC2	3.32	122.31	111.91
24	Y	101	CHD	C21-C20-C22	-3.31	105.18	110.36
25	Z	101	DMU	O1-C9-C8	3.30	115.69	109.69
22	N	612	TGL	CG2-OG2-CB1	3.26	125.83	117.79
14	A	601[A]	HEA	CMB-C2B-C3B	3.25	131.05	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601[C]	HEA	CMB-C2B-C3B	3.25	131.05	124.69
24	Y	101	CHD	C15-C14-C8	3.25	122.88	118.33
22	L	103	TGL	OG3-CC1-CC2	3.25	124.23	109.94
14	N	602[A]	HEA	C26-C15-C16	3.23	120.71	115.27
14	A	601[C]	HEA	C17-C18-C19	3.21	135.39	127.66
14	N	603	HEA	CBD-CAD-C3D	3.19	118.38	112.49
24	L	102	CHD	C11-C12-C13	3.14	114.47	111.24
14	A	601[C]	HEA	C26-C15-C16	3.13	120.53	115.27
24	L	102	CHD	C13-C14-C8	-3.09	110.80	114.74
24	L	102	CHD	C18-C13-C12	3.08	112.20	109.07
18	P	307	PGV	O01-C1-O02	-3.08	116.27	123.70
24	Y	101	CHD	C9-C8-C7	-3.08	108.20	111.88
24	Y	101	CHD	C2-C1-C10	3.07	118.05	112.78
24	Y	101	CHD	C14-C13-C12	3.07	110.26	107.40
24	L	102	CHD	C14-C8-C9	-3.06	105.51	109.71
25	L	101	DMU	O5-C6-O16	3.05	117.19	109.97
14	A	602	HEA	C16-C15-C14	-3.04	114.97	121.12
25	L	101	DMU	O5-C4-C57	3.02	111.67	106.83
22	D	202	TGL	OG1-CA1-CA2	3.01	121.37	111.91
25	M	101	DMU	O16-C6-C1	3.00	112.99	108.30
14	N	603	HEA	C27-C19-C20	2.98	120.28	115.27
18	N	608	PGV	O01-C1-O02	-2.96	116.54	123.70
24	B	303	CHD	C16-C17-C13	2.96	106.45	103.55
14	N	602[A]	HEA	CMB-C2B-C1B	-2.94	123.94	128.46
14	N	602[C]	HEA	CMB-C2B-C1B	-2.94	123.94	128.46
22	N	609	TGL	OG3-CC1-CC2	2.93	121.11	111.91
24	L	102	CHD	C22-C23-C24	-2.93	107.30	113.59
14	N	603	HEA	C3C-C4C-NC	2.91	112.98	109.21
24	P	301	CHD	C22-C20-C17	-2.89	104.31	110.28
24	Y	101	CHD	C6-C5-C4	-2.87	107.89	111.19
14	A	601[A]	HEA	C20-C19-C18	-2.86	115.32	121.12
18	N	608	PGV	C9-C10-C11	-2.86	96.04	112.43
14	N	602[A]	HEA	C27-C19-C20	2.86	120.08	115.27
24	C	304	CHD	C22-C20-C17	-2.85	104.40	110.28
14	A	601[C]	HEA	C13-C14-C15	-2.83	120.84	127.66
14	N	603	HEA	C26-C15-C16	2.83	120.03	115.27
14	A	601[C]	HEA	C25-C23-C22	-2.79	114.58	122.65
14	N	602[C]	HEA	C26-C15-C16	2.77	119.94	115.27
24	L	102	CHD	C1-C2-C3	2.77	114.02	110.47
24	C	304	CHD	C6-C7-C8	-2.76	108.53	111.48
14	N	602[C]	HEA	C13-C14-C15	-2.76	121.02	127.66
14	N	602[A]	HEA	CAA-CBA-CGA	-2.75	108.05	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602[C]	HEA	CAA-CBA-CGA	-2.75	108.05	112.67
14	N	602[A]	HEA	C3C-C4C-NC	2.75	112.77	109.21
14	N	602[C]	HEA	C3C-C4C-NC	2.75	112.77	109.21
14	N	602[A]	HEA	OMA-CMA-C3A	-2.75	118.92	124.91
14	N	602[C]	HEA	OMA-CMA-C3A	-2.75	118.92	124.91
22	N	612	TGL	OG2-CB1-OB1	-2.74	117.08	123.70
14	N	602[A]	HEA	C12-C11-C3B	2.74	119.76	112.56
24	B	303	CHD	C13-C14-C8	-2.74	111.24	114.74
26	T	101	CDL	OB8-CB7-C71	2.73	120.47	111.91
18	C	301	PGV	O01-C1-C2	2.72	117.36	111.50
24	B	303	CHD	O3-C3-C4	-2.67	104.53	109.85
24	G	101	CHD	C4-C5-C10	-2.65	109.85	112.66
26	C	305	CDL	C83-C82-C81	2.63	127.76	114.42
24	Y	101	CHD	C15-C14-C13	-2.62	100.99	103.55
24	B	303	CHD	C19-C10-C5	-2.61	105.93	110.36
24	Y	101	CHD	C11-C9-C10	-2.60	111.04	113.73
24	B	303	CHD	C15-C14-C13	2.59	106.09	103.55
27	P	306	PEK	C8-C7-C6	-2.57	99.39	112.02
14	A	601[A]	HEA	C21-C20-C19	-2.57	104.54	112.98
27	P	306	PEK	C3-C2-C1	-2.55	104.34	113.62
18	C	311	PGV	O04-C19-C20	-2.55	113.77	123.73
24	P	301	CHD	C6-C7-C8	-2.55	108.76	111.48
24	P	301	CHD	C16-C17-C20	-2.55	108.20	112.15
24	G	101	CHD	C17-C13-C12	2.53	119.97	117.67
26	P	304	CDL	OB8-CB7-OB9	-2.53	115.22	123.14
14	A	602	HEA	C3C-C4C-NC	2.52	112.47	109.21
27	C	307	PEK	O03-C21-C22	2.52	119.82	111.91
18	N	608	PGV	O03-C19-C20	2.52	119.81	111.91
24	C	304	CHD	O12-C12-C13	-2.51	106.78	111.03
27	P	306	PEK	O11-P-O14	-2.51	99.25	109.07
24	P	301	CHD	C18-C13-C17	-2.50	107.30	111.21
22	N	609	TGL	OG1-CA1-CA2	2.50	119.75	111.91
14	A	601[C]	HEA	C26-C15-C14	-2.50	117.28	123.68
25	C	310	DMU	O16-C18-C19	2.49	118.30	109.56
18	P	307	PGV	C03-C02-C01	-2.49	105.90	111.79
26	C	305	CDL	C80-C79-C78	2.49	127.06	114.42
18	C	308	PGV	C21-C20-C19	-2.49	104.58	113.62
18	P	307	PGV	O03-C19-O04	-2.48	117.33	123.59
26	T	101	CDL	C43-C42-C41	2.48	126.99	114.42
24	P	301	CHD	C11-C9-C10	-2.47	111.17	113.73
26	N	601	CDL	C19-C18-C17	2.47	126.94	114.42
26	C	305	CDL	C61-C60-C59	-2.45	101.97	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	CMB-C2B-C1B	2.43	132.20	128.46
14	A	601[A]	HEA	CMB-C2B-C1B	-2.43	124.72	128.46
14	A	601[C]	HEA	CMB-C2B-C1B	-2.43	124.72	128.46
18	C	311	PGV	C21-C20-C19	-2.42	104.81	113.62
24	P	301	CHD	C22-C23-C24	-2.42	108.40	113.59
14	N	602[C]	HEA	C17-C18-C19	-2.41	121.85	127.66
22	N	612	TGL	OG1-CA1-OA1	-2.40	117.52	123.59
24	G	101	CHD	C1-C10-C5	2.40	111.32	107.77
22	L	103	TGL	CG1-OG1-CA1	2.37	123.93	116.11
22	N	612	TGL	OG1-CG1-CG2	2.37	115.34	108.43
18	N	608	PGV	C01-O03-C19	-2.36	108.37	117.12
14	N	602[C]	HEA	C25-C23-C24	2.36	119.81	114.60
24	G	101	CHD	C9-C10-C5	2.35	111.88	108.58
22	B	301	TGL	OG3-CC1-CC2	2.34	119.24	111.91
24	L	102	CHD	C5-C6-C7	2.33	117.04	114.46
14	N	603	HEA	C1B-C2B-C3B	-2.32	105.38	107.00
26	P	304	CDL	C54-C53-C52	-2.28	102.83	114.42
14	A	602	HEA	CBD-CAD-C3D	2.28	116.69	112.49
18	P	307	PGV	O03-C01-C02	-2.26	101.86	108.43
24	G	101	CHD	C19-C10-C1	-2.26	104.62	108.26
26	P	304	CDL	C59-C58-C57	2.25	125.84	114.42
19	O	303	PSC	C14-C13-C12	-2.24	107.50	124.73
14	A	602	HEA	C13-C12-C11	-2.24	110.98	114.35
27	C	307	PEK	C02-O01-C1	-2.23	112.31	117.79
24	L	102	CHD	C4-C5-C10	2.21	115.00	112.66
26	C	305	CDL	OB8-CB7-C71	2.21	119.64	109.94
22	B	301	TGL	OB1-CB1-CB2	-2.20	115.16	123.73
14	N	602[A]	HEA	C25-C23-C22	-2.19	116.32	122.65
27	P	306	PEK	O03-C21-C22	2.19	118.78	111.91
24	C	304	CHD	C18-C13-C14	-2.19	107.79	111.21
14	A	601[A]	HEA	C21-C22-C23	-2.18	120.30	127.75
27	C	307	PEK	C3-C2-C1	-2.17	105.73	113.62
22	N	609	TGL	CG3-CG2-CG1	-2.17	106.66	111.79
14	N	602[C]	HEA	C16-C17-C18	-2.16	104.80	111.88
14	A	601[A]	HEA	C25-C23-C22	-2.15	116.42	122.65
14	A	601[C]	HEA	C12-C13-C14	-2.15	106.57	112.23
25	Z	101	DMU	O1-C9-C11	2.13	111.74	106.44
18	C	308	PGV	O03-C19-O04	-2.13	118.22	123.59
24	Y	101	CHD	O7-C7-C8	2.13	114.18	109.43
25	L	101	DMU	O16-C18-C19	-2.12	102.13	109.56
22	N	612	TGL	C26-C25-C24	-2.12	103.66	114.42
22	L	103	TGL	OG1-CA1-CA2	2.11	120.58	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	301	CHD	C1-C2-C3	-2.11	107.76	110.47
24	Y	101	CHD	C13-C17-C20	2.11	122.01	119.50
25	M	101	DMU	O7-C10-C5	2.09	113.52	108.10
25	C	310	DMU	C22-C19-C18	-2.07	104.32	113.49
18	C	308	PGV	O12-P-O13	-2.07	100.98	109.07
24	L	102	CHD	C5-C4-C3	2.07	115.79	112.76
14	A	601[A]	HEA	O11-C11-C3B	-2.06	106.06	112.00
14	A	601[A]	HEA	C25-C23-C24	2.05	119.14	114.60
24	G	101	CHD	C13-C14-C8	-2.05	112.12	114.74
26	C	305	CDL	C52-C51-CB5	-2.05	105.14	114.26
26	T	101	CDL	OB8-CB6-CB4	2.05	114.29	108.38
14	N	603	HEA	CMC-C2C-C1C	-2.05	125.32	128.46
24	B	303	CHD	C19-C10-C9	2.04	114.00	111.18
18	P	307	PGV	C22-C21-C20	-2.04	105.85	113.19
24	C	304	CHD	C5-C6-C7	2.04	116.71	114.46
22	N	612	TGL	CA7-CA6-CA5	-2.04	104.08	114.42
14	N	602[A]	HEA	CMC-C2C-C3C	2.03	128.48	124.68
14	N	602[C]	HEA	CMC-C2C-C3C	2.03	128.48	124.68
14	N	602[A]	HEA	O11-C11-C3B	-2.03	106.15	112.00
24	G	101	CHD	O3-C3-C4	-2.02	105.83	109.85
18	C	301	PGV	O01-C02-C01	-2.02	101.10	108.40
14	A	601[A]	HEA	C4B-C3B-C2B	-2.01	105.46	106.87
14	A	601[C]	HEA	C4B-C3B-C2B	-2.01	105.46	106.87
22	D	202	TGL	CB3-CB2-CB1	2.01	120.92	113.62
24	B	303	CHD	C1-C10-C5	2.00	110.73	107.77

All (24) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
14	N	602[A]	HEA	ND
14	N	602[A]	HEA	NA
14	N	602[B]	HEA	NB
14	N	602[B]	HEA	ND
14	N	602[B]	HEA	NA
14	N	602[C]	HEA	NB
14	N	602[C]	HEA	ND
14	N	602[C]	HEA	NA
14	N	603	HEA	NB
14	N	603	HEA	ND
14	N	603	HEA	NA

All (493) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[C]	HEA	C11-C12-C13-C14
14	N	602[C]	HEA	C14-C15-C16-C17
14	N	602[C]	HEA	C26-C15-C16-C17
14	N	602[C]	HEA	C17-C18-C19-C20
18	A	606	PGV	C1-C2-C3-C4
18	C	311	PGV	O04-C19-O03-C01
18	C	311	PGV	C20-C19-O03-C01
18	G	102	PGV	O04-C19-O03-C01
18	G	102	PGV	C20-C19-O03-C01
18	G	102	PGV	C11-C12-C13-C14
19	A	607	PSC	C7-C8-C9-C10
19	O	303	PSC	C10-C11-C12-C13
22	D	202	TGL	OB1-CB1-OG2-CG2
22	N	612	TGL	OB1-CB1-OG2-CG2
22	N	612	TGL	OG2-CG2-CG3-OG3
26	C	305	CDL	CB5-C51-C52-C53
26	T	101	CDL	OB6-CB4-CB6-OB8
27	C	306	PEK	C4-C5-C6-C7
27	C	306	PEK	C7-C8-C9-C10
27	C	306	PEK	C11-C10-C9-C8
27	P	306	PEK	C11-C12-C13-C14
24	L	102	CHD	C16-C17-C20-C21
24	L	102	CHD	C13-C17-C20-C21
24	L	102	CHD	C16-C17-C20-C22
24	L	102	CHD	C13-C17-C20-C22
22	D	202	TGL	CB2-CB1-OG2-CG2
22	N	612	TGL	CB2-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
27	C	307	PEK	C7-C8-C9-C10
27	C	309	PEK	C4-C5-C6-C7
27	C	309	PEK	C13-C14-C15-C16
14	A	601[C]	HEA	C17-C18-C19-C27
14	N	602[C]	HEA	C17-C18-C19-C27
22	L	103	TGL	CA2-CA1-OG1-CG1
22	N	609	TGL	CA4-CA5-CA6-CA7
24	Y	101	CHD	C13-C17-C20-C21
22	D	202	TGL	CG2-CG1-OG1-CA1
22	N	612	TGL	CA2-CA1-OG1-CG1
22	B	301	TGL	C11-C12-C13-C14
25	Z	101	DMU	O6-C11-C9-O1
22	L	103	TGL	OA1-CA1-OG1-CG1
24	Y	101	CHD	C16-C17-C20-C22
22	L	103	TGL	CC1-CC2-CC3-CC4
22	N	612	TGL	OA1-CA1-OG1-CG1
22	N	609	TGL	CB9-C10-C11-C12
14	N	602[C]	HEA	C15-C16-C17-C18
26	N	601	CDL	C40-C41-C42-C43
26	P	304	CDL	C40-C41-C42-C43
18	C	311	PGV	O03-C01-C02-C03
22	N	609	TGL	CB3-CB4-CB5-CB6
24	L	102	CHD	C20-C22-C23-C24
22	N	609	TGL	C14-C29-C30-C31
25	Z	101	DMU	O6-C11-C9-C8
22	N	611	TGL	C20-C21-C22-C23
22	L	103	TGL	C23-C24-C25-C26
26	P	304	CDL	C82-C83-C84-C85
18	C	308	PGV	C10-C11-C12-C13
18	N	608	PGV	C10-C11-C12-C13
27	P	305	PEK	C4-C5-C6-C7
22	B	301	TGL	CB1-CB2-CB3-CB4
22	L	103	TGL	CA9-C20-C21-C22
25	C	303	DMU	O16-C18-C19-C22
25	C	310	DMU	O16-C18-C19-C22
26	N	601	CDL	C80-C81-C82-C83
27	P	306	PEK	C16-C17-C18-C19
22	D	202	TGL	C21-C22-C23-C24
25	Z	101	DMU	O16-C18-C19-C22
22	N	612	TGL	C12-C13-C14-C29
26	P	304	CDL	C57-C58-C59-C60
22	L	103	TGL	CB3-CB4-CB5-CB6

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Mol	Chain	Res	Type	Atoms
22	N	609	TGL	CC5-CC6-CC7-CC8
22	N	611	TGL	C21-C22-C23-C24
26	T	101	CDL	C58-C59-C60-C61
22	L	103	TGL	CA5-CA6-CA7-CA8
25	L	101	DMU	C28-C31-C34-C37
18	G	102	PGV	C28-C29-C30-C31
22	B	301	TGL	CC7-CC8-CC9-C15
25	K	105	DMU	C31-C34-C37-C40
27	P	308	PEK	C13-C14-C15-C16
22	D	202	TGL	CB3-CB4-CB5-CB6
22	N	612	TGL	C21-C22-C23-C24
22	N	609	TGL	CB4-CB5-CB6-CB7
25	L	101	DMU	C1-C6-O16-C18
18	C	308	PGV	C7-C8-C9-C10
18	N	607	PGV	C4-C5-C6-C7
22	L	103	TGL	C21-C22-C23-C24
22	N	612	TGL	CB4-CB5-CB6-CB7
22	B	301	TGL	CB9-C10-C11-C12
22	N	609	TGL	C13-C14-C29-C30
22	N	609	TGL	C24-C25-C26-C27
22	N	611	TGL	CC5-CC6-CC7-CC8
22	N	611	TGL	CC9-C15-C16-C17
22	N	612	TGL	CA2-CA3-CA4-CA5
22	N	612	TGL	CB3-CB4-CB5-CB6
25	K	102	DMU	C28-C31-C34-C37
25	K	103	DMU	C31-C34-C37-C40
25	M	101	DMU	C19-C22-C25-C28
25	Z	101	DMU	C22-C25-C28-C31
26	C	305	CDL	C52-C53-C54-C55
26	C	305	CDL	C58-C59-C60-C61
27	C	307	PEK	C28-C29-C30-C31
19	A	607	PSC	C27-C28-C29-C30
22	N	611	TGL	C11-C10-CB9-CB8
25	K	104	DMU	C25-C28-C31-C34
26	P	304	CDL	C81-C82-C83-C84
22	L	103	TGL	CB5-CB6-CB7-CB8
26	C	305	CDL	C62-C63-C64-C65
22	D	202	TGL	CC6-CC7-CC8-CC9
22	N	611	TGL	CA4-CA5-CA6-CA7
22	N	611	TGL	CB5-CB6-CB7-CB8
26	T	101	CDL	C79-C80-C81-C82
19	A	607	PSC	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
22	D	202	TGL	CC2-CC3-CC4-CC5
22	L	103	TGL	C11-C10-CB9-CB8
25	Z	101	DMU	C25-C28-C31-C34
22	B	301	TGL	C13-C14-C29-C30
22	B	301	TGL	C17-C18-C19-C33
22	D	202	TGL	C16-C17-C18-C19
22	N	612	TGL	CA3-CA4-CA5-CA6
18	C	311	PGV	C6-C7-C8-C9
25	K	104	DMU	C22-C25-C28-C31
26	T	101	CDL	C72-C73-C74-C75
26	T	101	CDL	C73-C74-C75-C76
27	C	309	PEK	C22-C23-C24-C25
22	D	202	TGL	C20-C21-C22-C23
22	N	609	TGL	C10-C11-C12-C13
25	L	101	DMU	C25-C28-C31-C34
18	C	308	PGV	C28-C29-C30-C31
25	C	303	DMU	C19-C22-C25-C28
22	L	103	TGL	C21-C20-CA9-CA8
22	B	301	TGL	OG1-CG1-CG2-CG3
19	A	607	PSC	C11-C10-C9-C8
22	L	103	TGL	CC4-CC5-CC6-CC7
22	B	301	TGL	CC5-CC6-CC7-CC8
27	C	307	PEK	C23-C24-C25-C26
22	D	202	TGL	CA9-C20-C21-C22
22	N	612	TGL	C22-C23-C24-C25
26	P	304	CDL	C12-C13-C14-C15
25	P	303	DMU	C31-C34-C37-C40
26	C	305	CDL	C80-C81-C82-C83
26	P	304	CDL	C73-C74-C75-C76
22	N	609	TGL	C21-C20-CA9-CA8
25	W	101	DMU	C18-C19-C22-C25
18	G	102	PGV	C7-C8-C9-C10
26	T	101	CDL	C42-C43-C44-C45
26	T	101	CDL	C74-C75-C76-C77
19	O	303	PSC	C5-C6-C7-C8
21	D	205	EDO	O1-C1-C2-O2
21	E	203	EDO	O1-C1-C2-O2
21	P	310	EDO	O1-C1-C2-O2
21	W	102	EDO	O1-C1-C2-O2
22	B	301	TGL	CB4-CB5-CB6-CB7
26	C	305	CDL	C63-C64-C65-C66
22	N	609	TGL	CB2-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
22	D	202	TGL	CC9-C15-C16-C17
26	N	601	CDL	C23-C24-C25-C26
26	P	304	CDL	C15-C16-C17-C18
22	N	612	TGL	CB5-CB6-CB7-CB8
24	Y	101	CHD	C16-C17-C20-C21
22	N	609	TGL	C11-C10-CB9-CB8
22	N	611	TGL	CA7-CA8-CA9-C20
25	P	303	DMU	C34-C37-C40-C43
22	N	609	TGL	OB1-CB1-OG2-CG2
22	D	202	TGL	CA2-CA1-OG1-CG1
22	N	609	TGL	CC2-CC1-OG3-CG3
22	N	609	TGL	CB7-CB8-CB9-C10
22	D	202	TGL	CB4-CB5-CB6-CB7
18	N	608	PGV	C25-C26-C27-C28
22	N	609	TGL	C20-C21-C22-C23
26	T	101	CDL	C60-C61-C62-C63
18	C	308	PGV	C19-C20-C21-C22
22	N	611	TGL	CA5-CA6-CA7-CA8
18	C	311	PGV	C23-C24-C25-C26
22	N	612	TGL	C21-C20-CA9-CA8
22	D	202	TGL	CA3-CA4-CA5-CA6
22	N	611	TGL	CB4-CB5-CB6-CB7
22	B	301	TGL	C16-C17-C18-C19
22	N	612	TGL	CB7-CB8-CB9-C10
22	B	301	TGL	OG1-CG1-CG2-OG2
22	N	611	TGL	C19-C33-C34-C35
27	P	306	PEK	C15-C16-C17-C18
22	L	103	TGL	CC6-CC7-CC8-CC9
26	P	304	CDL	C36-C37-C38-C39
18	C	301	PGV	C10-C11-C12-C13
25	J	101	DMU	C18-C19-C22-C25
26	P	304	CDL	C37-C38-C39-C40
25	O	302	DMU	C28-C31-C34-C37
22	N	612	TGL	C11-C12-C13-C14
25	K	106	DMU	C31-C34-C37-C40
25	X	102	DMU	C34-C37-C40-C43
26	T	101	CDL	C21-C22-C23-C24
27	P	308	PEK	C28-C29-C30-C31
19	A	607	PSC	C26-C27-C28-C29
18	A	606	PGV	C11-C10-C9-C8
18	P	307	PGV	C11-C10-C9-C8
22	L	103	TGL	C18-C19-C33-C34

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Mol	Chain	Res	Type	Atoms
22	D	202	TGL	CA7-CA8-CA9-C20
22	D	202	TGL	OA1-CA1-OG1-CG1
22	B	301	TGL	C12-C13-C14-C29
25	J	101	DMU	C28-C31-C34-C37
22	D	202	TGL	OG1-CG1-CG2-CG3
22	N	612	TGL	OG1-CG1-CG2-CG3
25	O	302	DMU	C25-C28-C31-C34
25	L	101	DMU	C34-C37-C40-C43
25	M	101	DMU	C22-C25-C28-C31
22	N	609	TGL	CB6-CB7-CB8-CB9
25	K	102	DMU	C18-C19-C22-C25
25	K	105	DMU	C34-C37-C40-C43
26	T	101	CDL	C57-C58-C59-C60
22	N	611	TGL	CC2-CC3-CC4-CC5
26	T	101	CDL	C22-C23-C24-C25
22	N	609	TGL	C15-C16-C17-C18
22	N	609	TGL	OC1-CC1-OG3-CG3
25	K	105	DMU	C22-C25-C28-C31
26	T	101	CDL	C82-C83-C84-C85
22	N	612	TGL	C24-C25-C26-C27
25	D	203	DMU	C25-C28-C31-C34
22	N	612	TGL	CA1-CA2-CA3-CA4
27	P	306	PEK	C17-C18-C19-C20
22	L	103	TGL	CC2-CC3-CC4-CC5
22	N	609	TGL	C16-C15-CC9-CC8
25	J	101	DMU	O16-C18-C19-C22
14	N	602[C]	HEA	C11-C12-C13-C14
22	L	103	TGL	C11-C12-C13-C14
26	T	101	CDL	C71-C72-C73-C74
22	B	301	TGL	CC2-CC1-OG3-CG3
27	P	306	PEK	C4-C5-C6-C7
27	P	306	PEK	C13-C14-C15-C16
25	J	101	DMU	C22-C25-C28-C31
21	P	315	EDO	O1-C1-C2-O2
25	K	106	DMU	C22-C25-C28-C31
26	N	601	CDL	C14-C15-C16-C17
25	O	302	DMU	C34-C37-C40-C43
22	B	301	TGL	OB1-CB1-OG2-CG2
22	N	609	TGL	C23-C24-C25-C26
18	N	607	PGV	C2-C3-C4-C5
26	N	601	CDL	C13-C14-C15-C16
27	P	308	PEK	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	T	101	CDL	C39-C40-C41-C42
18	C	301	PGV	C31-C32-C33-C34
18	G	102	PGV	C4-C5-C6-C7
25	Z	101	DMU	C34-C37-C40-C43
25	K	103	DMU	C34-C37-C40-C43
18	N	607	PGV	C11-C10-C9-C8
27	C	307	PEK	C17-C18-C19-C20
26	T	101	CDL	CB3-CB4-CB6-OB8
26	N	601	CDL	C58-C59-C60-C61
18	C	311	PGV	C10-C11-C12-C13
27	C	307	PEK	C10-C11-C12-C13
27	P	306	PEK	C7-C8-C9-C10
22	B	301	TGL	C15-C16-C17-C18
25	C	310	DMU	C18-C19-C22-C25
14	A	601[A]	HEA	C27-C19-C20-C21
22	B	301	TGL	CC2-CC3-CC4-CC5
22	B	301	TGL	C18-C19-C33-C34
22	N	609	TGL	CA2-CA3-CA4-CA5
22	N	612	TGL	CB2-CB3-CB4-CB5
25	K	103	DMU	C28-C31-C34-C37
19	A	607	PSC	C9-C10-C11-C12
19	A	607	PSC	C10-C11-C12-C13
19	O	303	PSC	C9-C10-C11-C12
27	C	306	PEK	C5-C6-C7-C8
27	C	306	PEK	C6-C7-C8-C9
27	C	306	PEK	C9-C10-C11-C12
27	C	306	PEK	C11-C12-C13-C14
27	C	306	PEK	C12-C13-C14-C15
27	C	307	PEK	C6-C7-C8-C9
27	C	307	PEK	C9-C10-C11-C12
27	C	307	PEK	C11-C12-C13-C14
27	C	307	PEK	C12-C13-C14-C15
27	C	309	PEK	C5-C6-C7-C8
27	C	309	PEK	C6-C7-C8-C9
27	C	309	PEK	C11-C10-C9-C8
27	C	309	PEK	C9-C10-C11-C12
27	C	309	PEK	C11-C12-C13-C14
27	C	309	PEK	C12-C13-C14-C15
27	P	305	PEK	C5-C6-C7-C8
27	P	305	PEK	C11-C10-C9-C8
27	P	305	PEK	C11-C12-C13-C14
27	P	305	PEK	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
27	P	306	PEK	C9-C10-C11-C12
27	P	308	PEK	C5-C6-C7-C8
27	P	308	PEK	C6-C7-C8-C9
27	P	308	PEK	C11-C10-C9-C8
27	P	308	PEK	C9-C10-C11-C12
27	P	308	PEK	C11-C12-C13-C14
25	K	103	DMU	C22-C25-C28-C31
26	P	304	CDL	C58-C59-C60-C61
22	N	612	TGL	CG1-CG2-CG3-OG3
25	C	310	DMU	C22-C25-C28-C31
22	B	301	TGL	C10-C11-C12-C13
22	N	611	TGL	CA9-C20-C21-C22
26	T	101	CDL	C16-C17-C18-C19
25	Q	201	DMU	C19-C22-C25-C28
21	C	320	EDO	O1-C1-C2-O2
21	J	103	EDO	O1-C1-C2-O2
22	B	301	TGL	CB2-CB1-OG2-CG2
25	D	201	DMU	C34-C37-C40-C43
26	T	101	CDL	C80-C81-C82-C83
22	D	202	TGL	CC7-CC8-CC9-C15
25	Q	201	DMU	C28-C31-C34-C37
27	P	308	PEK	C3-C4-C5-C6
27	P	308	PEK	C29-C30-C31-C32
18	N	607	PGV	C10-C11-C12-C13
25	K	106	DMU	C28-C31-C34-C37
26	N	601	CDL	C81-C82-C83-C84
22	N	609	TGL	CB5-CB6-CB7-CB8
24	Y	101	CHD	C13-C17-C20-C22
22	D	202	TGL	C19-C33-C34-C35
22	N	612	TGL	C11-C10-CB9-CB8
25	K	105	DMU	C28-C31-C34-C37
22	N	609	TGL	C29-C30-C31-C32
25	K	103	DMU	C19-C22-C25-C28
26	P	304	CDL	C77-C78-C79-C80
22	B	301	TGL	OC1-CC1-OG3-CG3
22	B	301	TGL	CC9-C15-C16-C17
22	B	301	TGL	CC4-CC5-CC6-CC7
18	C	311	PGV	C24-C25-C26-C27
26	N	601	CDL	C37-C38-C39-C40
26	N	601	CDL	C20-C21-C22-C23
25	P	309	DMU	C28-C31-C34-C37
26	N	601	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
27	C	307	PEK	C26-C27-C28-C29
18	C	308	PGV	C27-C28-C29-C30
25	C	310	DMU	C3-C4-C57-O61
25	P	303	DMU	C28-C31-C34-C37
22	N	609	TGL	C12-C13-C14-C29
22	N	611	TGL	C15-C16-C17-C18
18	C	308	PGV	C02-C03-O11-P
18	P	307	PGV	C02-C03-O11-P
26	N	601	CDL	C60-C61-C62-C63
18	C	308	PGV	C1-C2-C3-C4
22	D	202	TGL	CA1-CA2-CA3-CA4
25	D	201	DMU	C22-C25-C28-C31
25	Q	201	DMU	C18-C19-C22-C25
22	D	202	TGL	OG1-CG1-CG2-OG2
22	D	202	TGL	CB7-CB8-CB9-C10
22	N	609	TGL	C17-C18-C19-C33
25	K	102	DMU	C34-C37-C40-C43
22	D	202	TGL	OG3-CC1-CC2-CC3
26	N	601	CDL	C57-C58-C59-C60
22	N	609	TGL	CC6-CC7-CC8-CC9
25	M	101	DMU	C25-C28-C31-C34
27	C	307	PEK	C4-C5-C6-C7
26	T	101	CDL	C18-C19-C20-C21
26	T	101	CDL	C41-C42-C43-C44
25	K	103	DMU	C18-C19-C22-C25
22	L	103	TGL	CC3-CC4-CC5-CC6
25	P	309	DMU	O16-C18-C19-C22
22	B	301	TGL	CC3-CC4-CC5-CC6
22	N	609	TGL	OG3-CC1-CC2-CC3
19	O	303	PSC	C26-C27-C28-C29
26	P	304	CDL	C44-C45-C46-C47
22	L	103	TGL	CC9-C15-C16-C17
26	N	601	CDL	C19-C20-C21-C22
21	A	610	EDO	O1-C1-C2-O2
21	A	615	EDO	O1-C1-C2-O2
21	L	104	EDO	O1-C1-C2-O2
21	N	619	EDO	O1-C1-C2-O2
21	T	104	EDO	O1-C1-C2-O2
22	L	103	TGL	OG1-CA1-CA2-CA3
25	D	203	DMU	C28-C31-C34-C37
19	A	607	PSC	C12-C13-C14-C15
27	C	309	PEK	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
22	N	612	TGL	OG1-CG1-CG2-OG2
18	N	608	PGV	C20-C21-C22-C23
22	D	202	TGL	CG1-CG2-CG3-OG3
22	N	612	TGL	CB6-CB7-CB8-CB9
25	J	101	DMU	C25-C28-C31-C34
26	N	601	CDL	C17-C18-C19-C20
25	J	101	DMU	C19-C22-C25-C28
19	O	303	PSC	C11-C10-C9-C8
18	C	301	PGV	C29-C30-C31-C32
22	L	103	TGL	CA3-CA4-CA5-CA6
26	N	601	CDL	C61-C62-C63-C64
27	C	307	PEK	C27-C28-C29-C30
26	P	304	CDL	C78-C79-C80-C81
27	C	307	PEK	O03-C21-C22-C23
18	P	307	PGV	C7-C8-C9-C10
22	D	202	TGL	CC5-CC6-CC7-CC8
27	C	306	PEK	C2-C3-C4-C5
24	L	102	CHD	C17-C20-C22-C23
25	Q	201	DMU	C31-C34-C37-C40
26	C	305	CDL	C78-C79-C80-C81
18	C	301	PGV	C11-C12-C13-C14
18	C	308	PGV	C11-C12-C13-C14
27	P	305	PEK	C3-C4-C5-C6
26	P	304	CDL	C72-C73-C74-C75
22	N	609	TGL	C16-C17-C18-C19
21	A	614	EDO	O1-C1-C2-O2
26	P	304	CDL	CB7-C71-C72-C73
26	C	305	CDL	C60-C61-C62-C63
18	N	608	PGV	C29-C30-C31-C32
14	A	601[C]	HEA	C26-C15-C16-C17
25	X	103	DMU	C28-C31-C34-C37
18	C	301	PGV	C23-C24-C25-C26
18	C	308	PGV	C9-C10-C11-C12
18	N	607	PGV	C9-C10-C11-C12
27	C	307	PEK	C14-C15-C16-C17
22	B	301	TGL	OG1-CA1-CA2-CA3
22	L	103	TGL	CC7-CC8-CC9-C15
27	P	305	PEK	C6-C7-C8-C9
27	P	305	PEK	C9-C10-C11-C12
27	P	306	PEK	C6-C7-C8-C9
27	P	306	PEK	C12-C13-C14-C15
27	P	308	PEK	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	N	611	TGL	CC6-CC7-CC8-CC9
26	T	101	CDL	C77-C78-C79-C80
22	N	612	TGL	CB9-C10-C11-C12
22	B	301	TGL	C19-C33-C34-C35
27	P	306	PEK	C22-C23-C24-C25
22	D	202	TGL	C22-C23-C24-C25
27	P	305	PEK	C7-C8-C9-C10
14	N	602[C]	HEA	C19-C20-C21-C22
22	N	609	TGL	OA1-CA1-OG1-CG1
26	N	601	CDL	C16-C17-C18-C19
18	A	606	PGV	C9-C10-C11-C12
27	P	305	PEK	C14-C15-C16-C17
26	P	304	CDL	C41-C42-C43-C44
21	A	613	EDO	O1-C1-C2-O2
21	E	202	EDO	O1-C1-C2-O2
21	O	305	EDO	O1-C1-C2-O2
26	C	305	CDL	C61-C62-C63-C64
22	B	301	TGL	CB5-CB6-CB7-CB8
22	N	609	TGL	CA9-C20-C21-C22
26	C	305	CDL	C57-C58-C59-C60
27	C	309	PEK	C28-C29-C30-C31
22	D	202	TGL	CC1-CC2-CC3-CC4
22	N	609	TGL	C22-C23-C24-C25
18	C	301	PGV	O03-C19-C20-C21
22	D	202	TGL	CB9-C10-C11-C12
18	C	311	PGV	C9-C10-C11-C12
19	O	303	PSC	C12-C13-C14-C15
18	C	301	PGV	C26-C27-C28-C29
19	A	607	PSC	C25-C26-C27-C28
27	P	306	PEK	O12-C04-C05-N
27	C	309	PEK	C33-C34-C35-C36
22	B	301	TGL	OG2-CG2-CG3-OG3
26	N	601	CDL	C15-C16-C17-C18
22	D	202	TGL	CC3-CC4-CC5-CC6
22	N	609	TGL	CA2-CA1-OG1-CG1
18	C	311	PGV	C11-C12-C13-C14
18	N	608	PGV	C11-C12-C13-C14
27	P	308	PEK	C14-C15-C16-C17
18	N	608	PGV	O03-C19-C20-C21
14	A	601[A]	HEA	C18-C19-C20-C21
26	C	305	CDL	C13-C14-C15-C16
18	C	308	PGV	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
18	G	102	PGV	C9-C10-C11-C12
27	C	309	PEK	C14-C15-C16-C17
22	L	103	TGL	C33-C34-C35-C36
26	T	101	CDL	CB3-CB4-OB6-CB5
26	C	305	CDL	C37-C38-C39-C40
18	P	307	PGV	C11-C12-C13-C14
27	C	307	PEK	C22-C23-C24-C25
22	L	103	TGL	C19-C33-C34-C35
25	C	310	DMU	C28-C31-C34-C37
25	D	201	DMU	C25-C28-C31-C34
21	G	104	EDO	O1-C1-C2-O2
21	J	102	EDO	O1-C1-C2-O2
21	P	311	EDO	O1-C1-C2-O2
21	Y	103	EDO	O1-C1-C2-O2
22	N	611	TGL	CB3-CB4-CB5-CB6
22	D	202	TGL	OG2-CG2-CG3-OG3
22	N	609	TGL	OG2-CG2-CG3-OG3
18	N	608	PGV	C27-C28-C29-C30
18	N	608	PGV	C9-C10-C11-C12
27	C	309	PEK	C25-C26-C27-C28
27	C	309	PEK	C23-C24-C25-C26
22	D	202	TGL	CB5-CB6-CB7-CB8
22	N	611	TGL	CC3-CC4-CC5-CC6
27	P	306	PEK	C14-C15-C16-C17
26	C	305	CDL	C31-C32-C33-C34
22	N	611	TGL	C18-C19-C33-C34
18	C	301	PGV	C11-C10-C9-C8
18	P	307	PGV	C13-C14-C15-C16
22	L	103	TGL	CA1-CA2-CA3-CA4
22	N	611	TGL	C16-C15-CC9-CC8
27	P	306	PEK	C26-C27-C28-C29
18	N	608	PGV	O04-C19-C20-C21
19	O	303	PSC	C15-C16-C17-C18
25	P	303	DMU	C19-C18-O16-C6
19	A	607	PSC	C24-C25-C26-C27
22	N	612	TGL	OG1-CA1-CA2-CA3
22	B	301	TGL	C11-C10-CB9-CB8
25	X	102	DMU	C25-C28-C31-C34
22	N	611	TGL	CC4-CC5-CC6-CC7
18	P	307	PGV	C05-C04-O12-P
14	A	601[C]	HEA	C14-C15-C16-C17
22	D	202	TGL	OG1-CA1-CA2-CA3

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Mol	Chain	Res	Type	Atoms
22	B	301	TGL	C29-C30-C31-C32
26	C	305	CDL	C53-C54-C55-C56
18	C	311	PGV	C20-C21-C22-C23
26	P	304	CDL	C17-C18-C19-C20

There are no ring outliers.

62 monomers are involved in 144 short contacts:

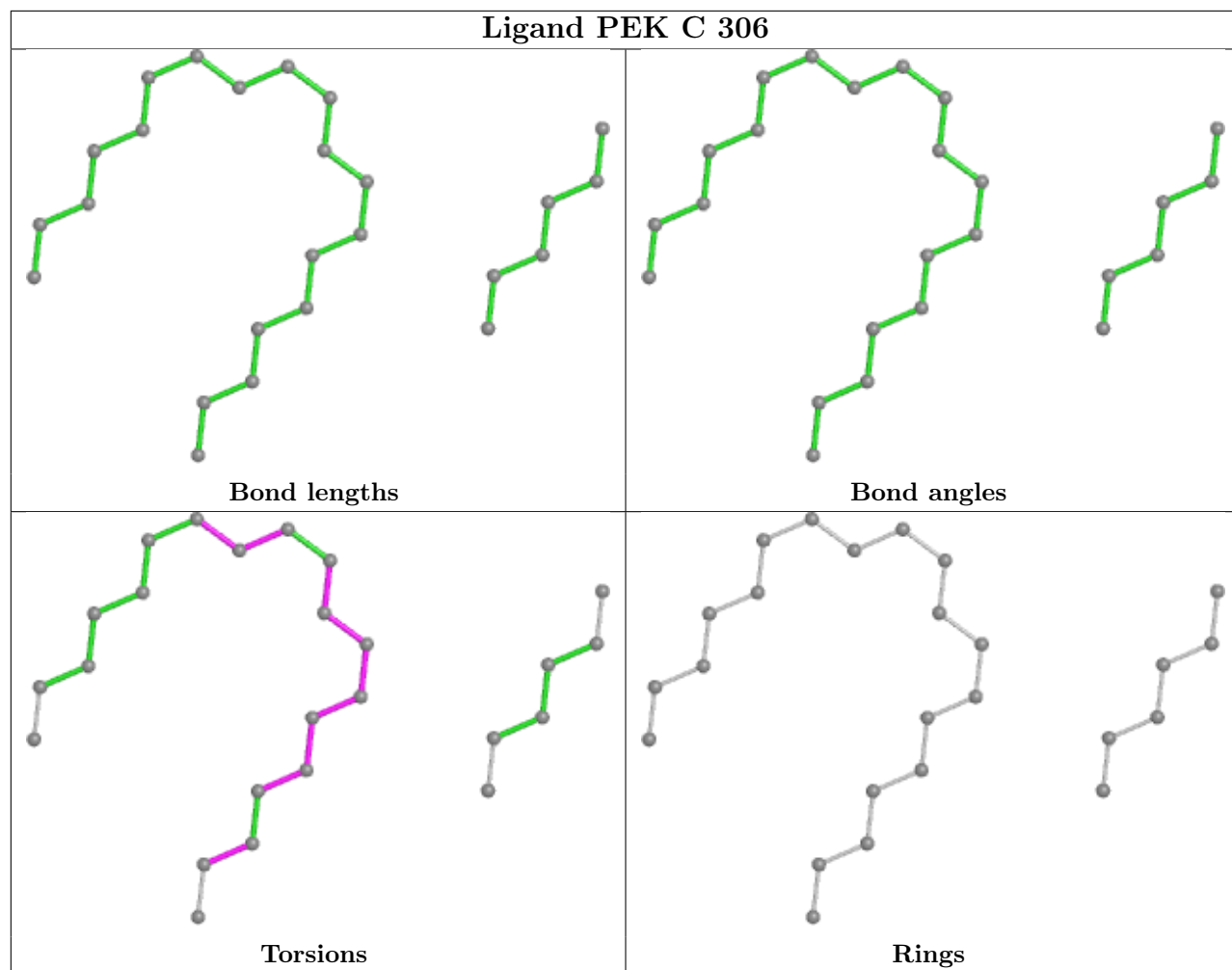
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	615	EDO	1	0
27	P	306	PEK	5	0
21	J	103	EDO	1	0
18	C	311	PGV	2	0
22	N	612	TGL	3	0
27	C	309	PEK	4	0
25	P	303	DMU	1	0
25	L	101	DMU	1	0
22	D	202	TGL	9	0
21	P	310	EDO	1	0
20	A	608[A]	PER	1	0
20	N	610[A]	PER	1	0
18	P	307	PGV	2	0
22	B	301	TGL	1	0
26	N	601	CDL	3	0
25	J	101	DMU	2	0
21	A	613	EDO	1	0
18	C	301	PGV	1	0
14	A	601[C]	HEA	1	0
18	N	608	PGV	3	0
25	K	101	DMU	1	0
21	O	305	EDO	2	0
22	L	103	TGL	9	0
14	A	601[B]	HEA	1	0
24	Y	101	CHD	1	0
21	C	320	EDO	1	0
14	A	601[A]	HEA	2	0
27	P	308	PEK	4	0
27	C	307	PEK	4	0
25	Q	201	DMU	1	0
25	K	104	DMU	1	0
24	G	101	CHD	1	0
25	D	201	DMU	2	0

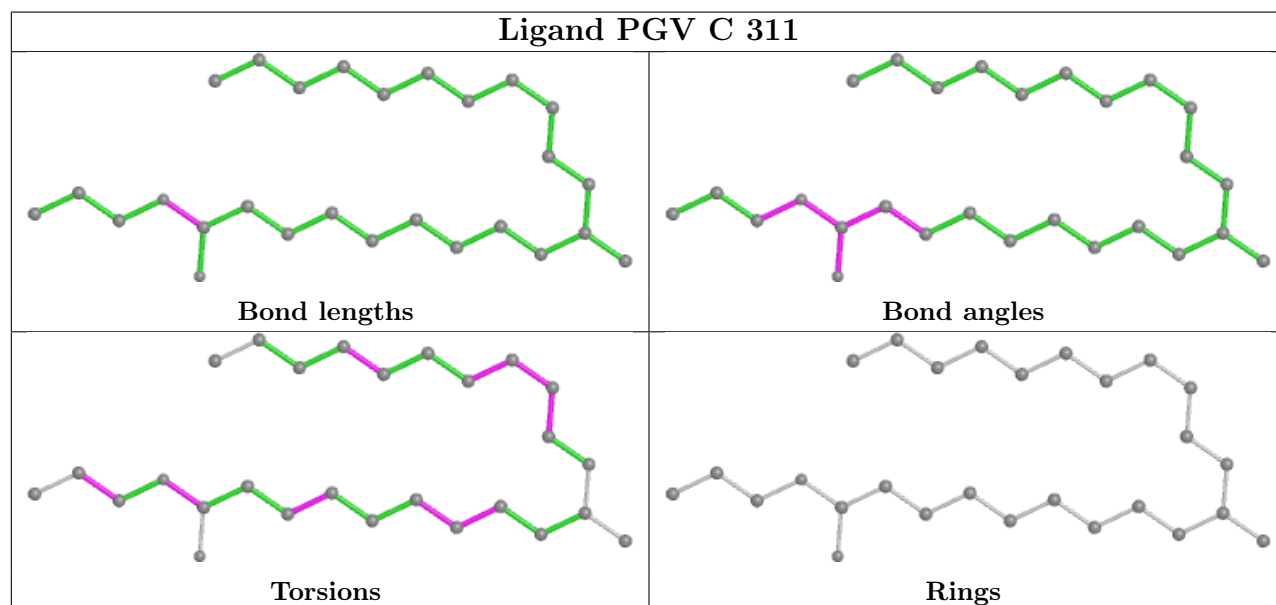
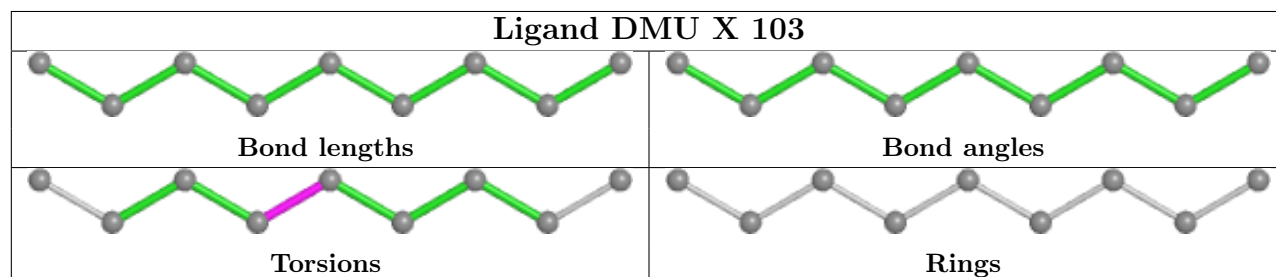
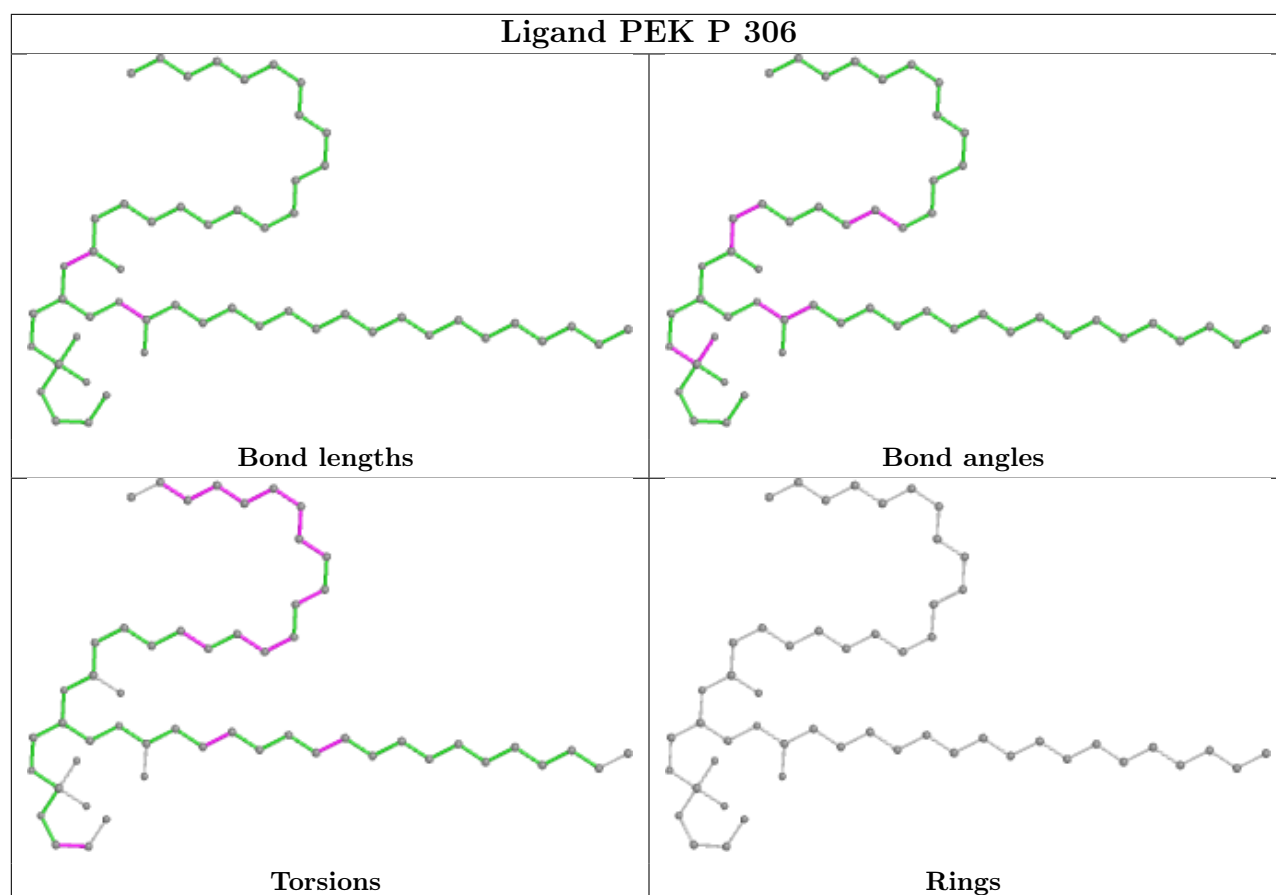
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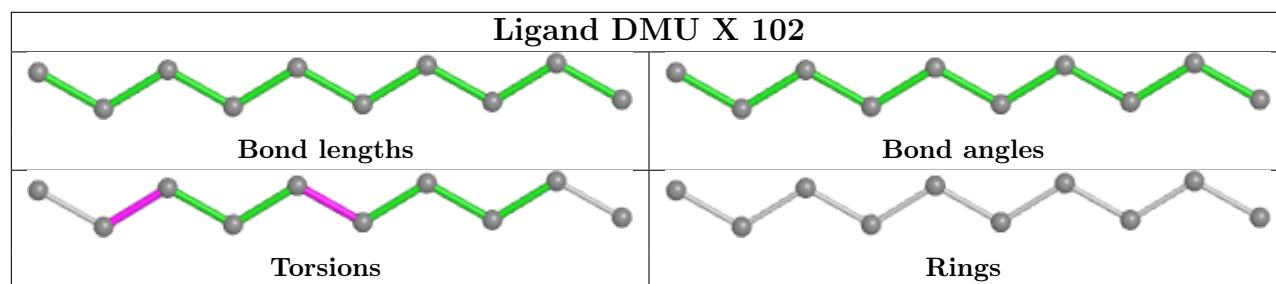
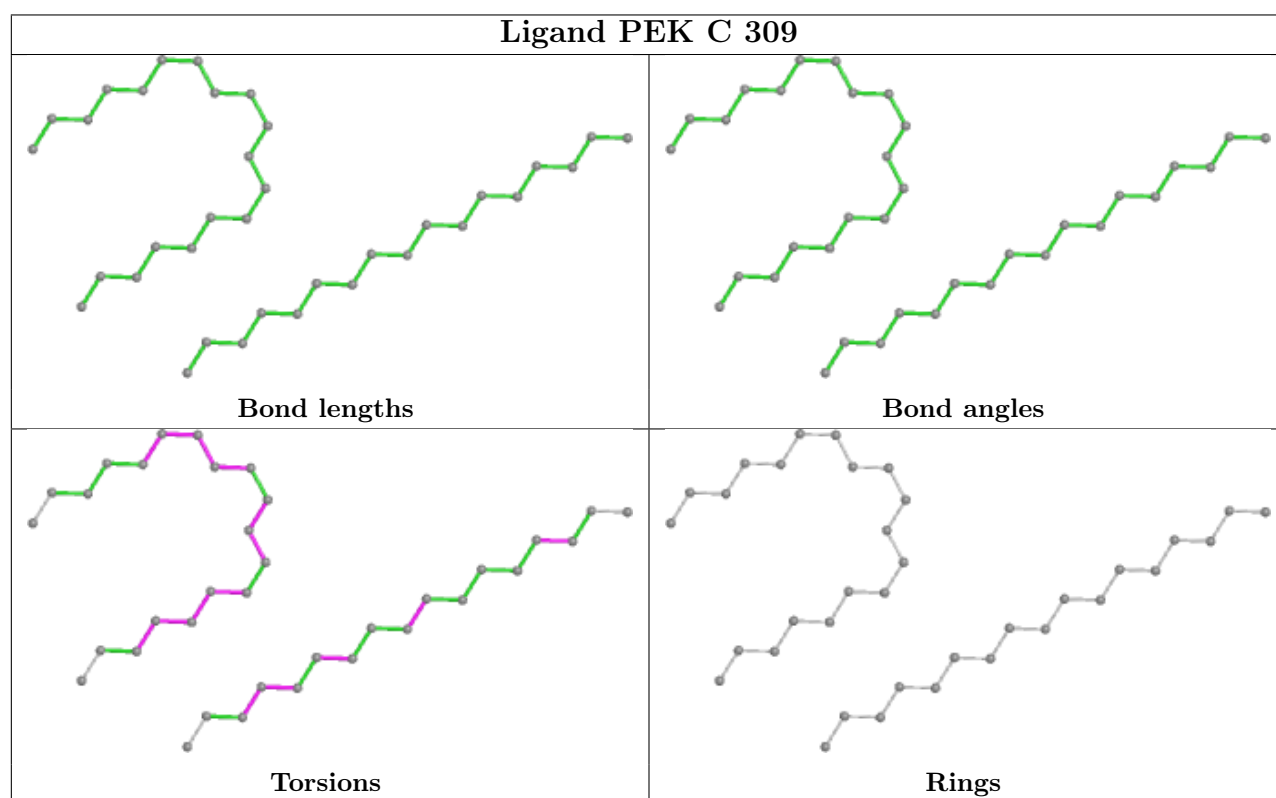
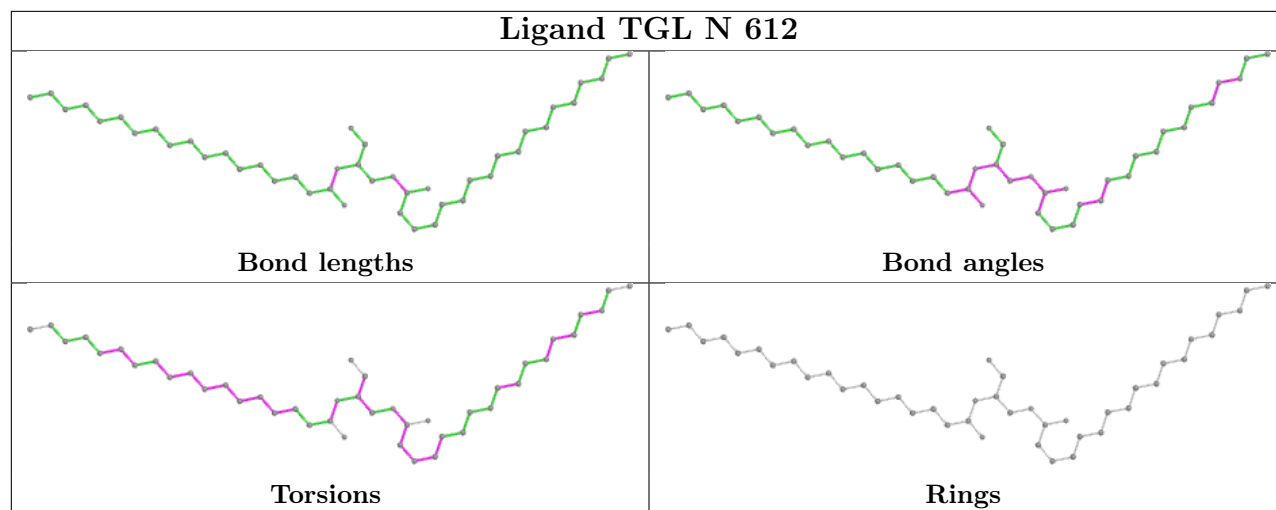
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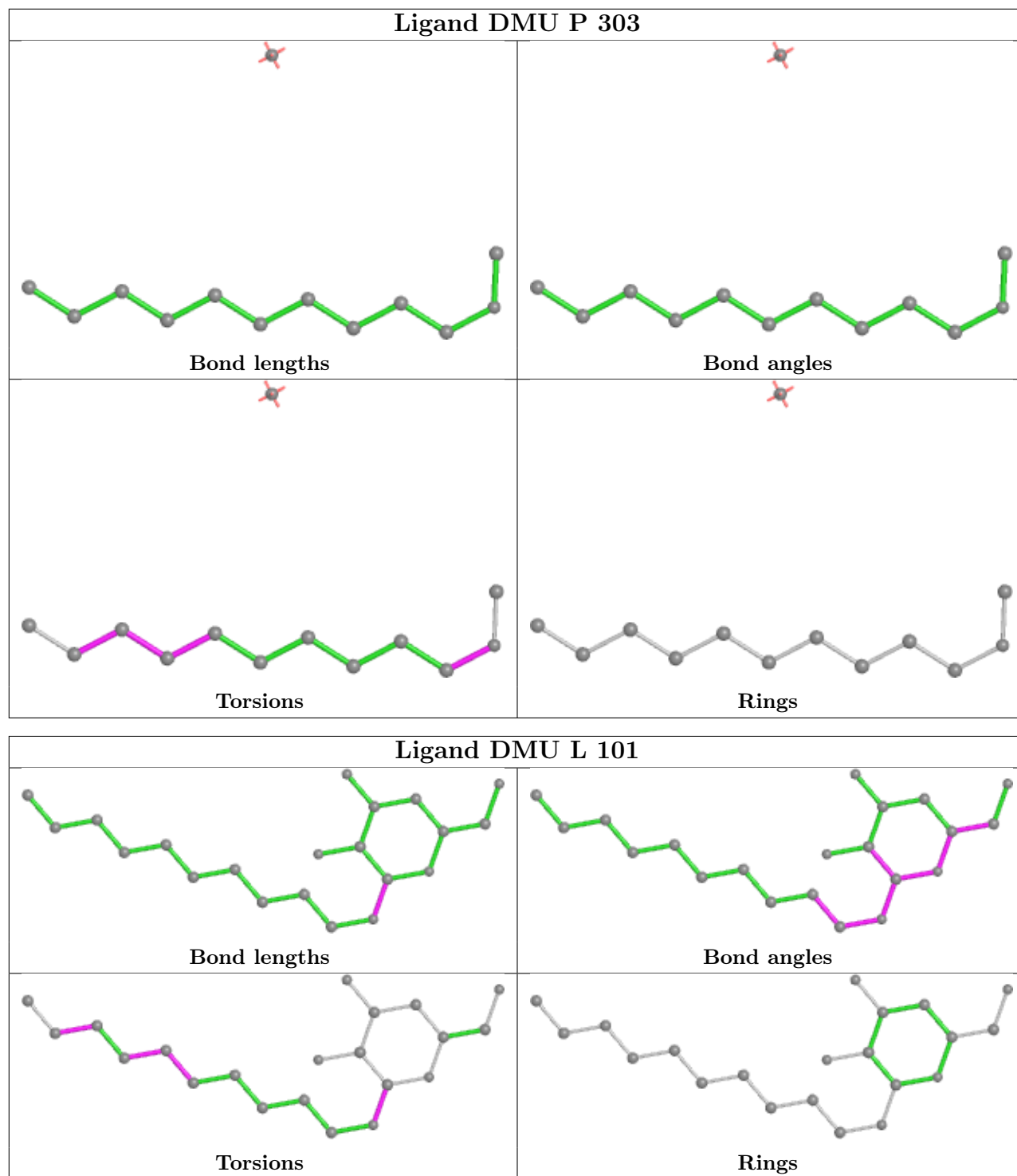
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	309	DMU	5	0
14	N	603	HEA	5	0
25	K	106	DMU	1	0
26	C	305	CDL	6	0
21	W	102	EDO	1	0
26	P	304	CDL	4	0
14	A	602	HEA	3	0
21	S	106	EDO	1	0
26	T	101	CDL	7	0
22	N	609	TGL	6	0
21	O	306	EDO	1	0
18	N	607	PGV	1	0
14	N	602[A]	HEA	2	0
25	K	105	DMU	1	0
18	C	308	PGV	2	0
18	A	606	PGV	2	0
25	K	102	DMU	1	0
25	M	101	DMU	2	0
22	N	611	TGL	5	0
18	G	102	PGV	2	0
25	Z	101	DMU	1	0
25	C	310	DMU	4	0
14	N	602[C]	HEA	1	0
25	W	101	DMU	1	0
25	C	303	DMU	1	0
25	K	103	DMU	1	0
19	A	607	PSC	4	0
24	L	102	CHD	4	0
19	O	303	PSC	4	0

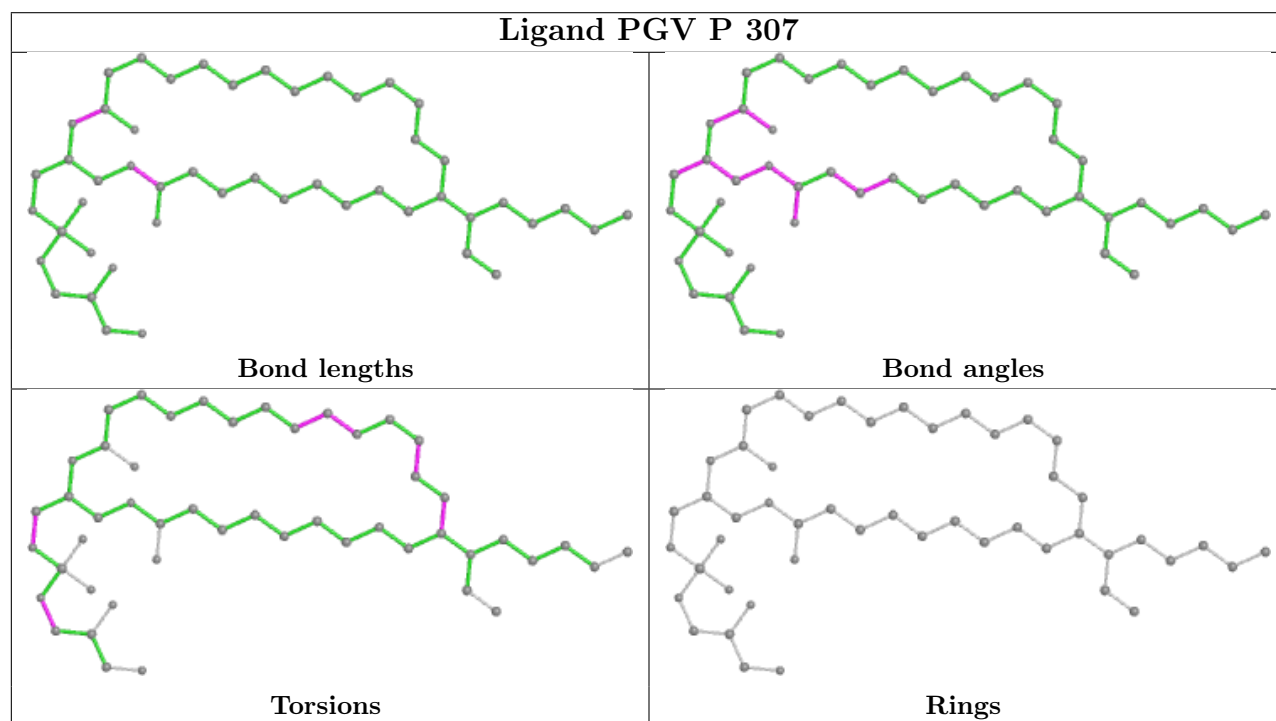
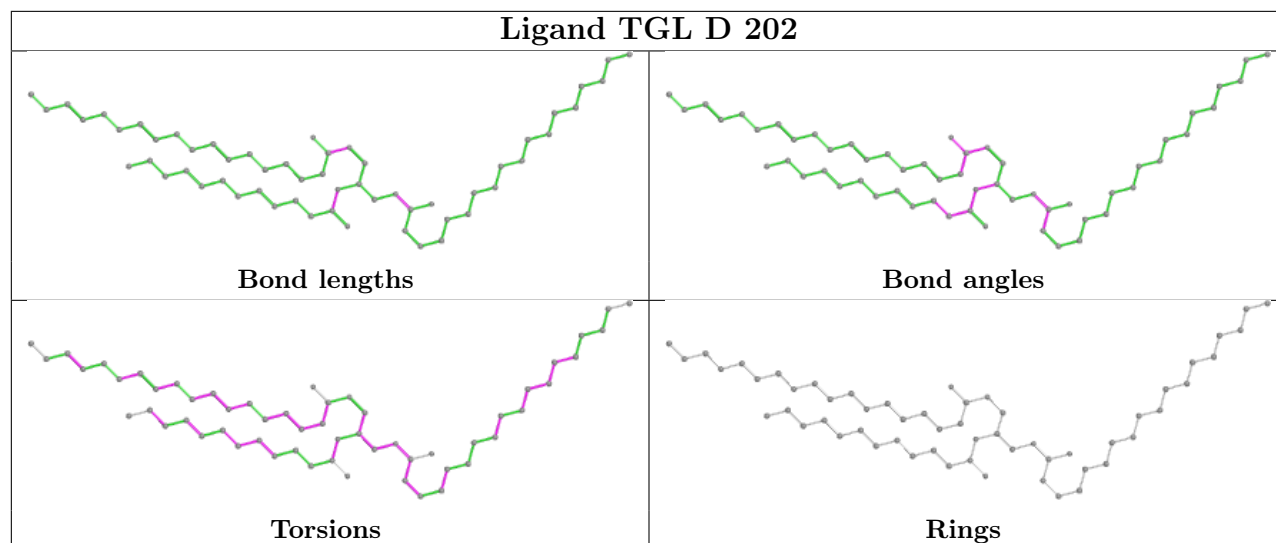
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

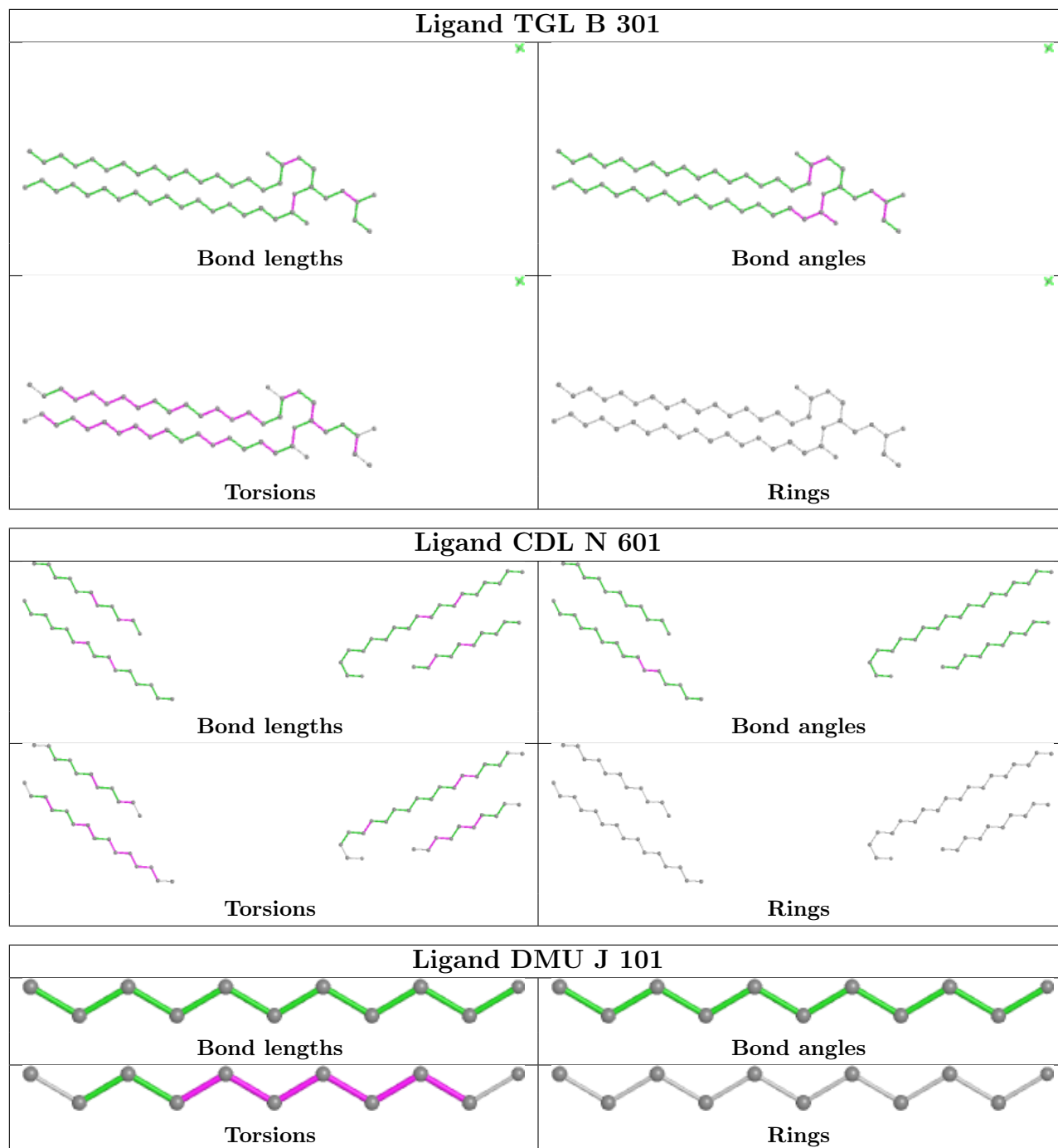


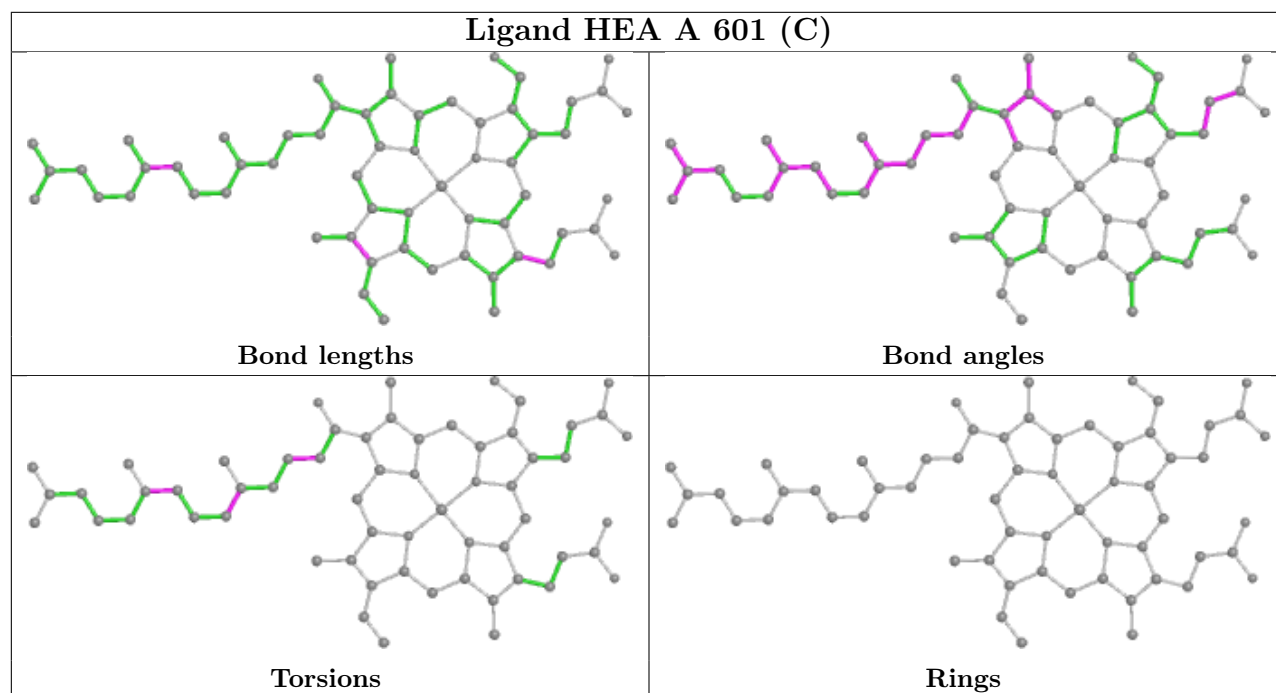
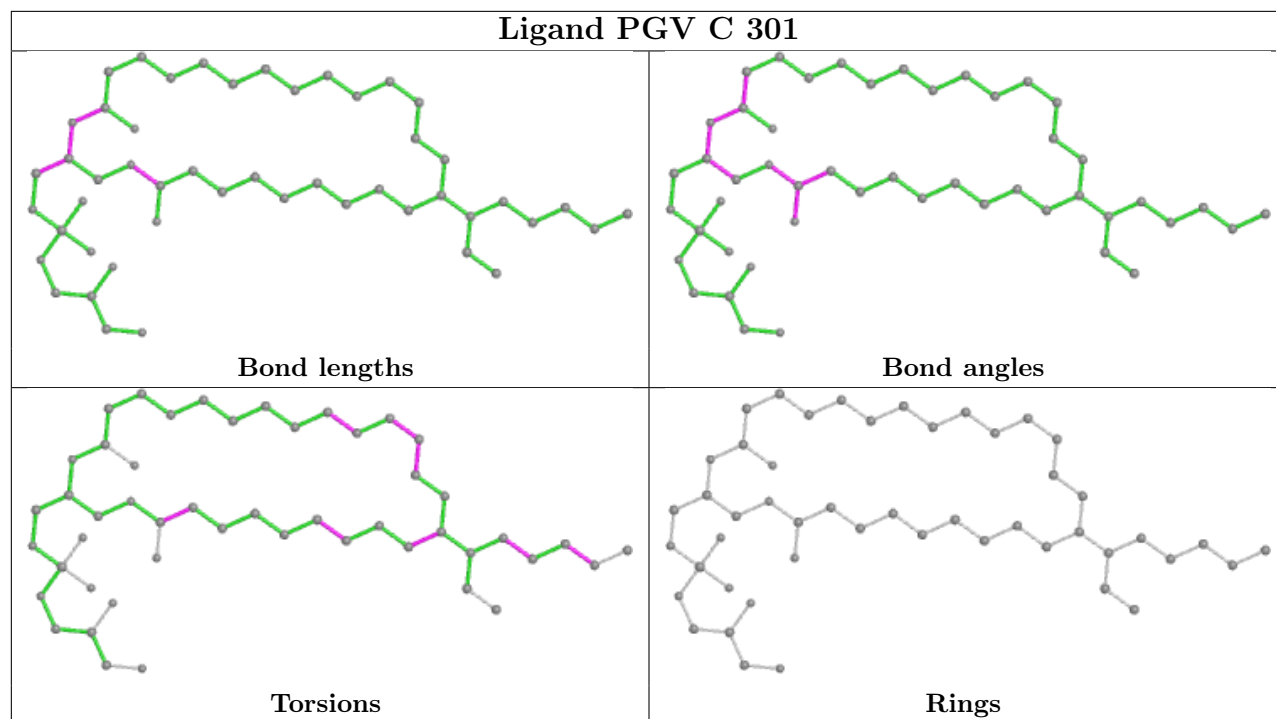


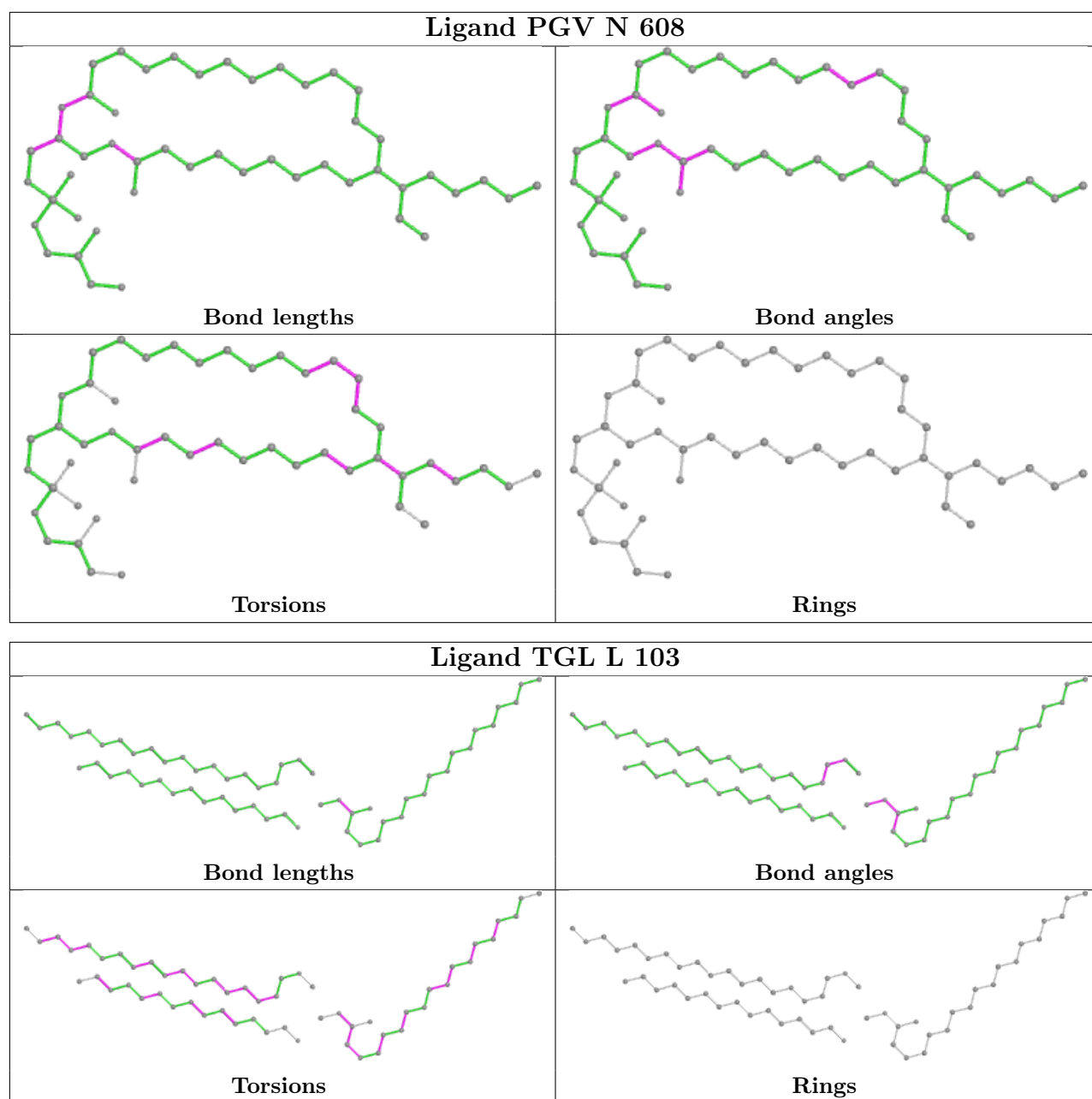


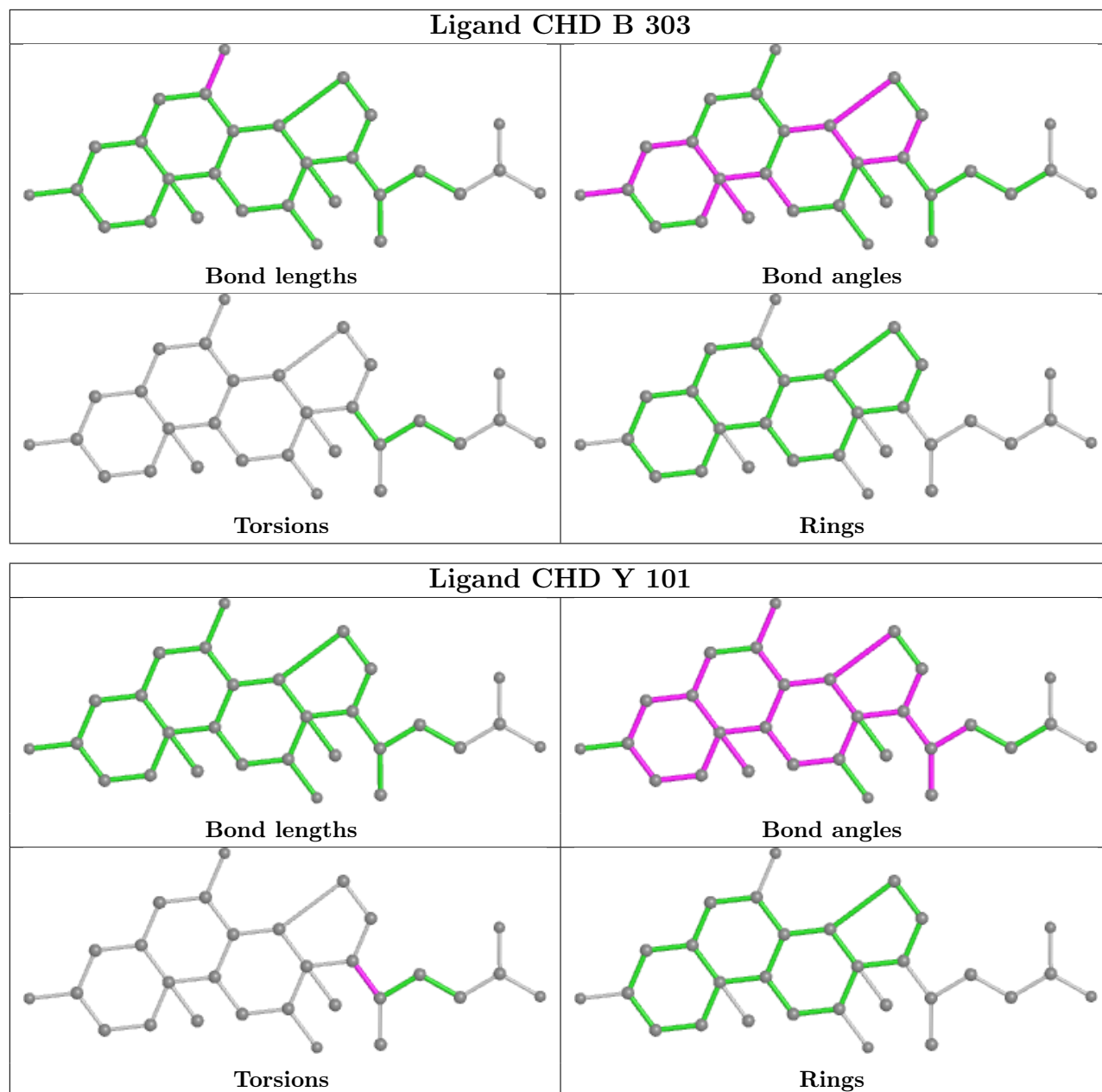


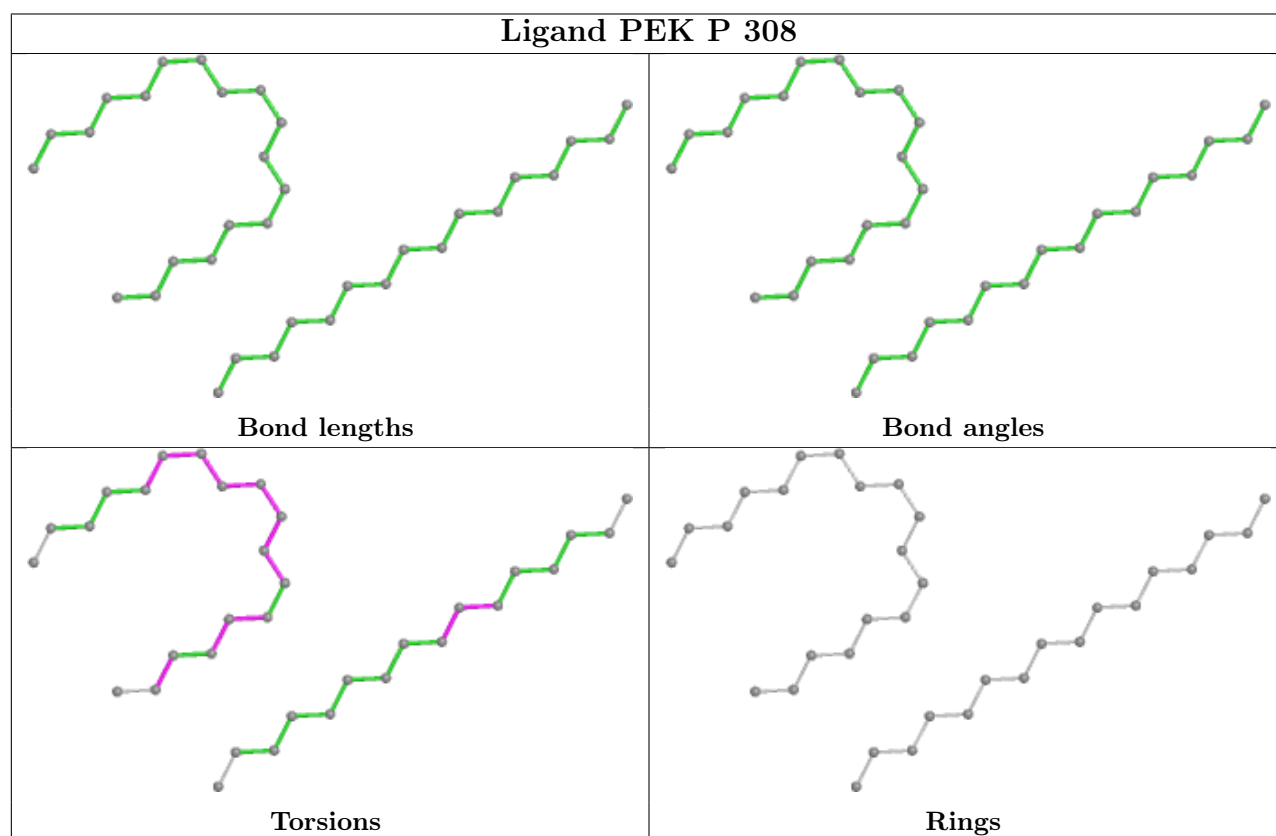
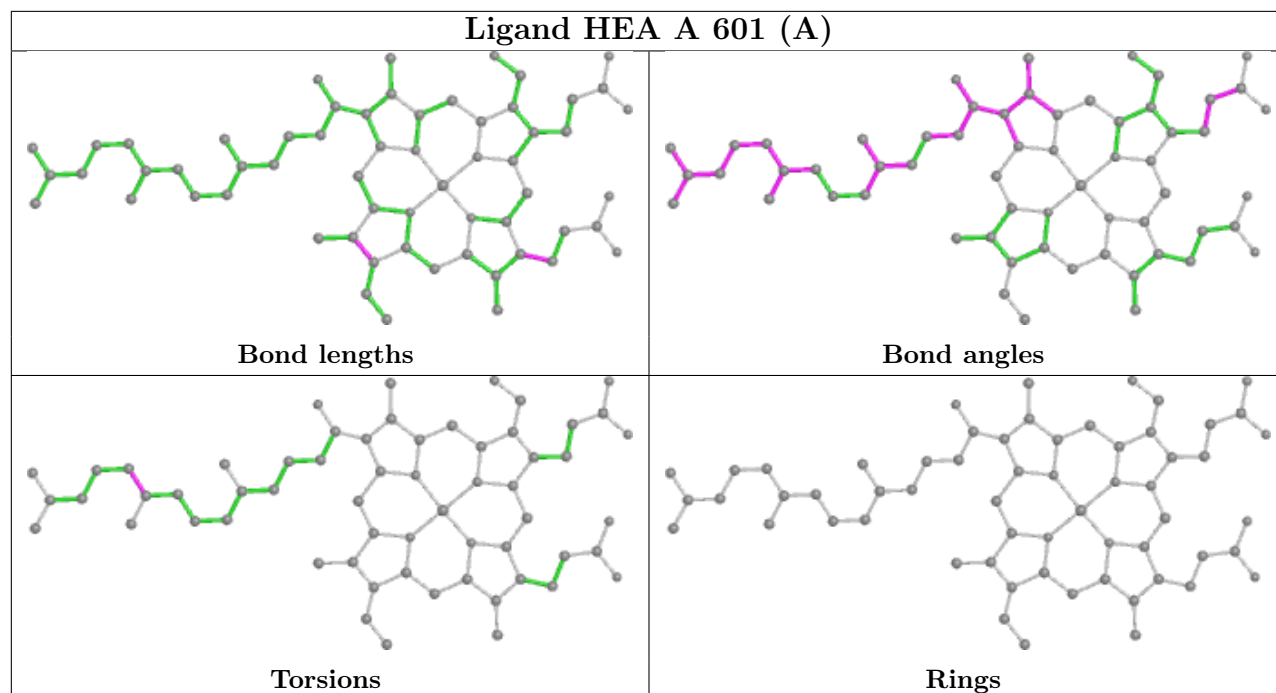


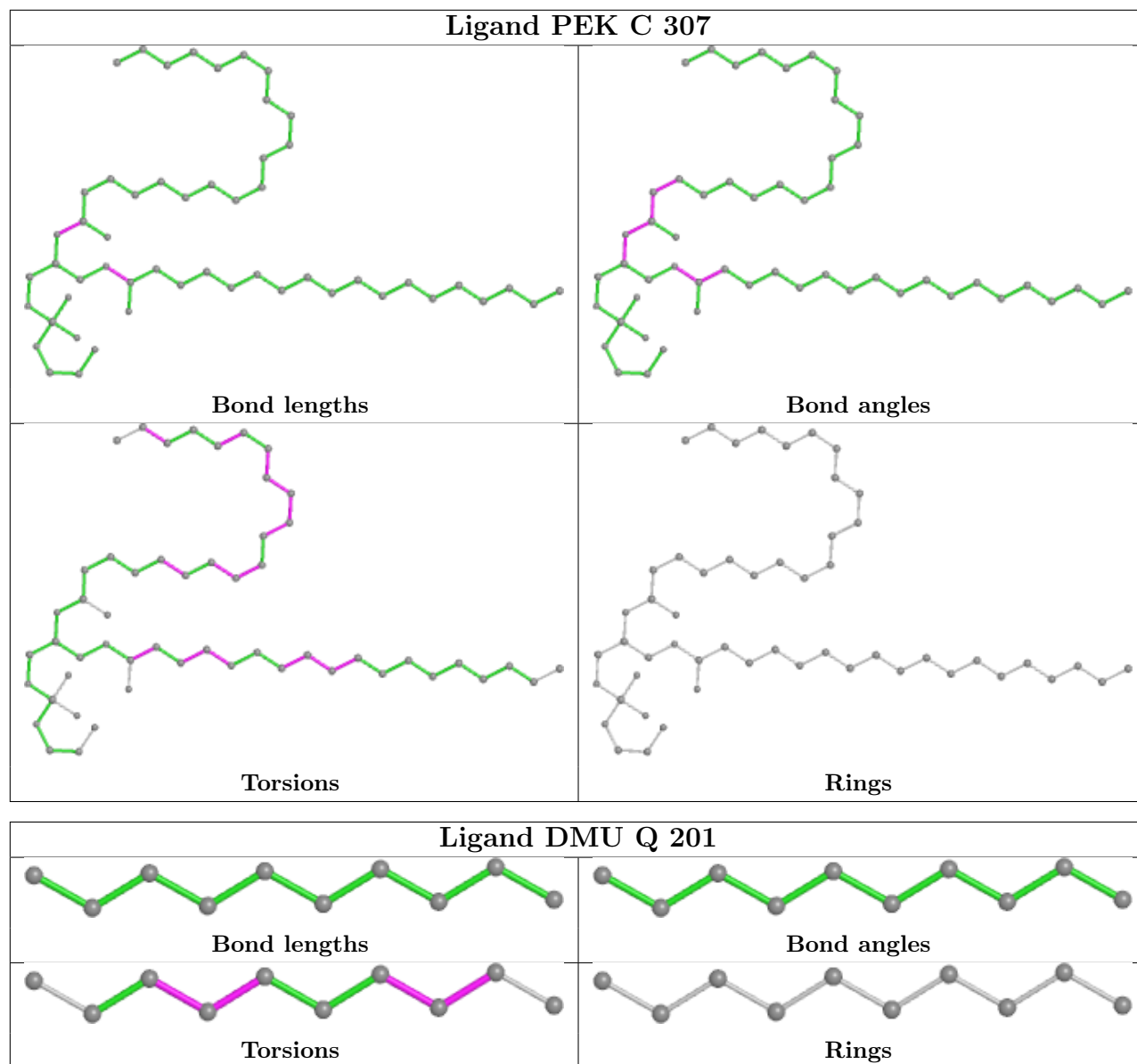


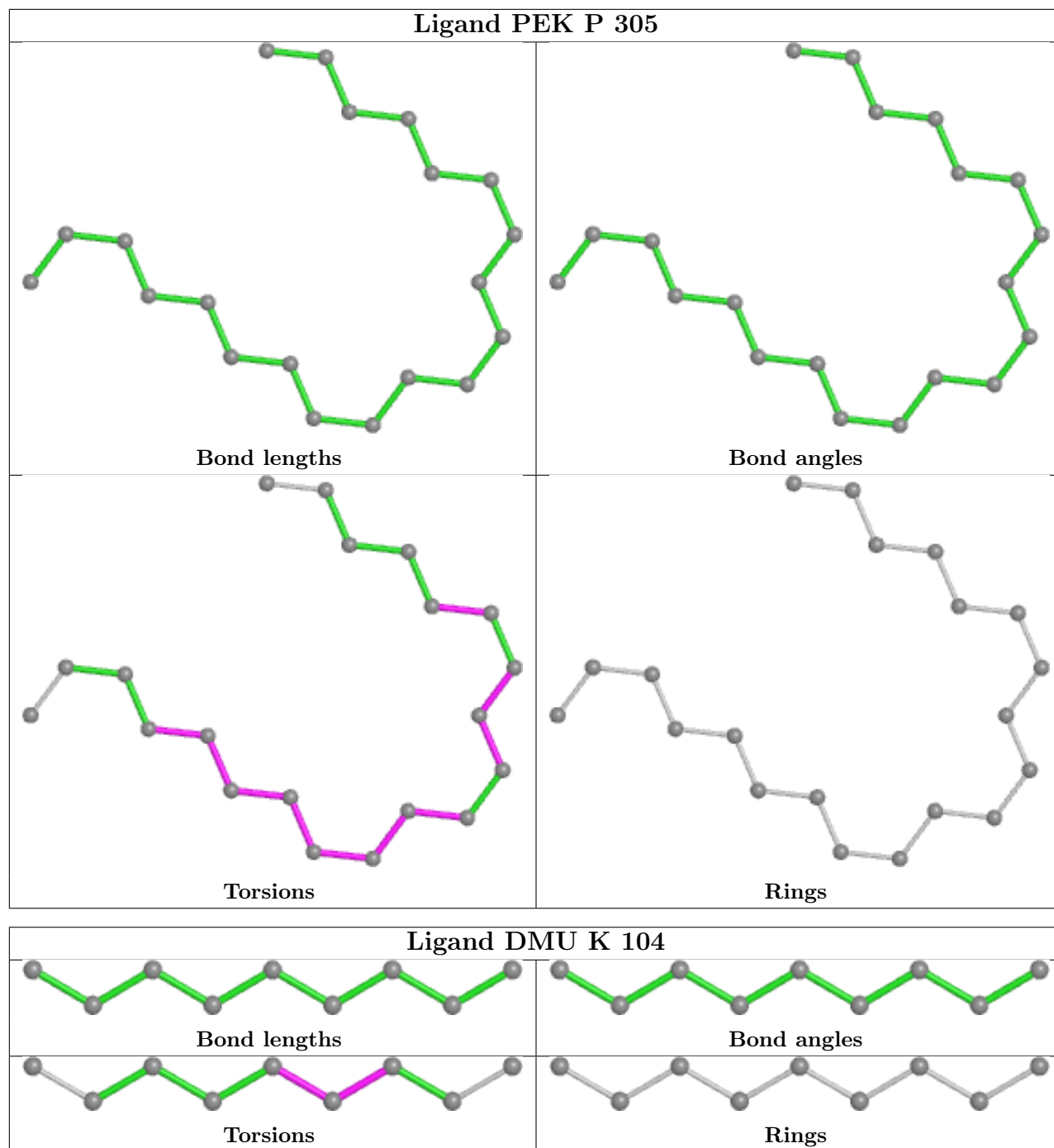


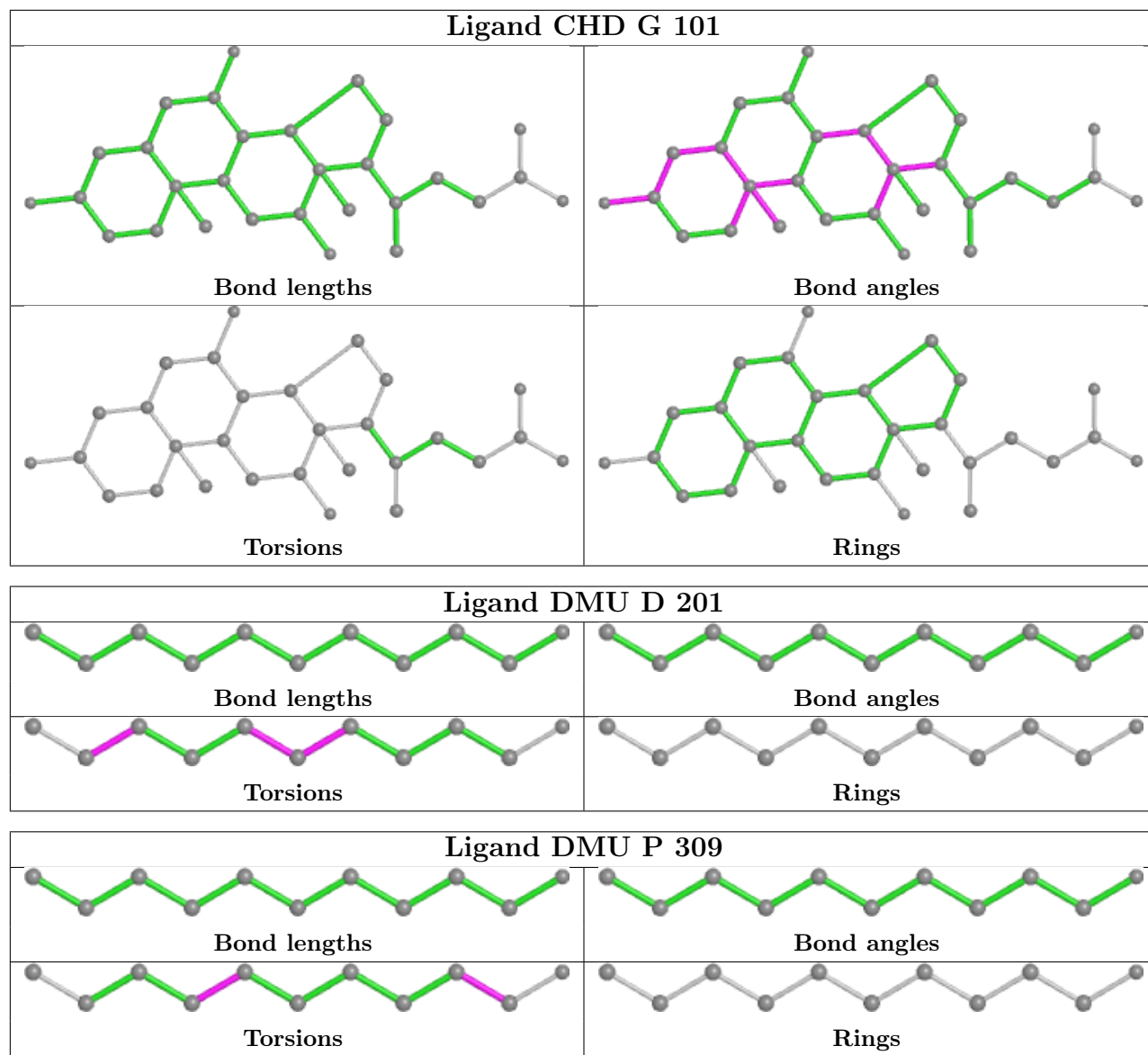


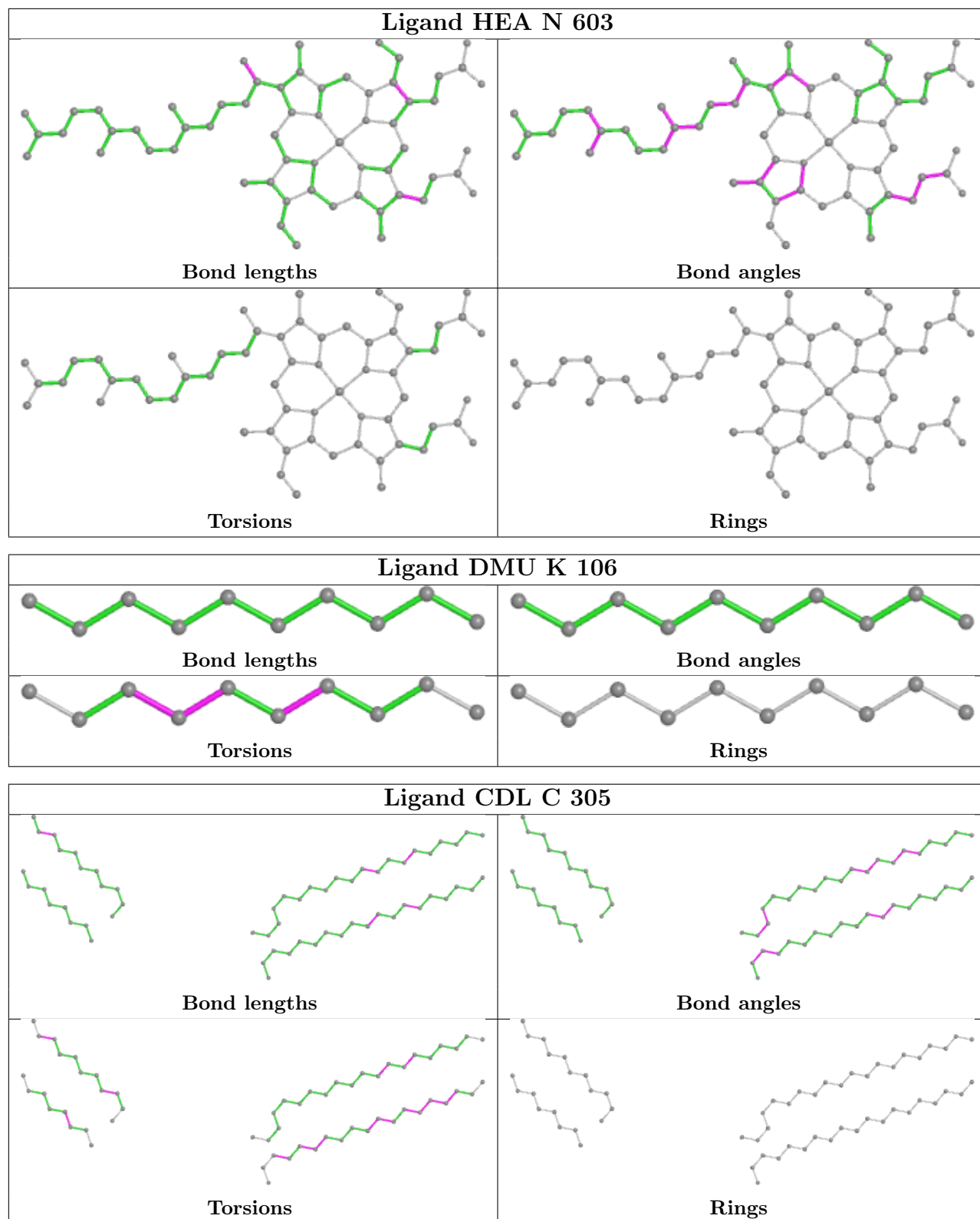


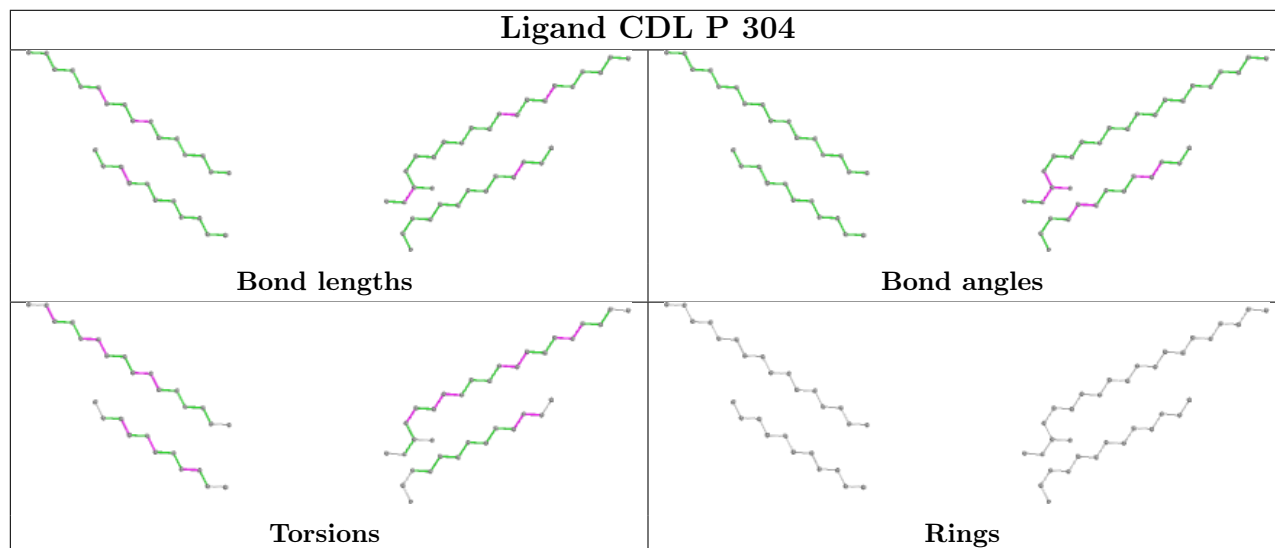
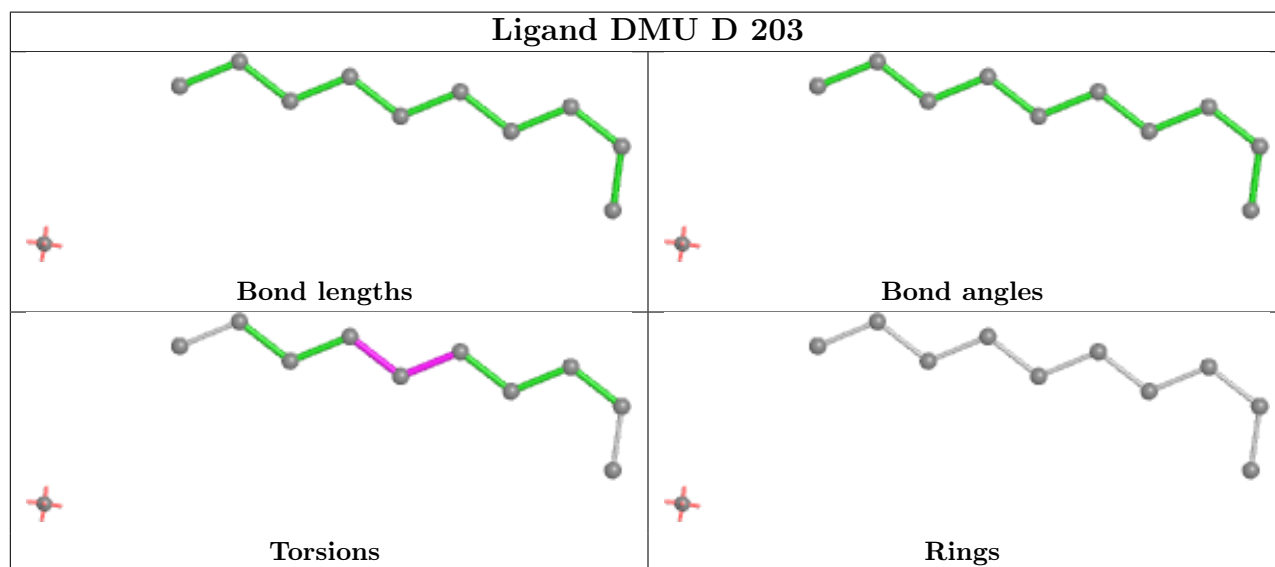
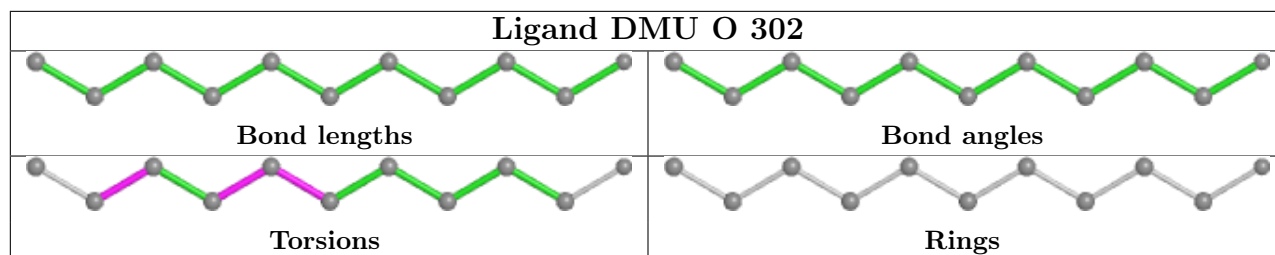


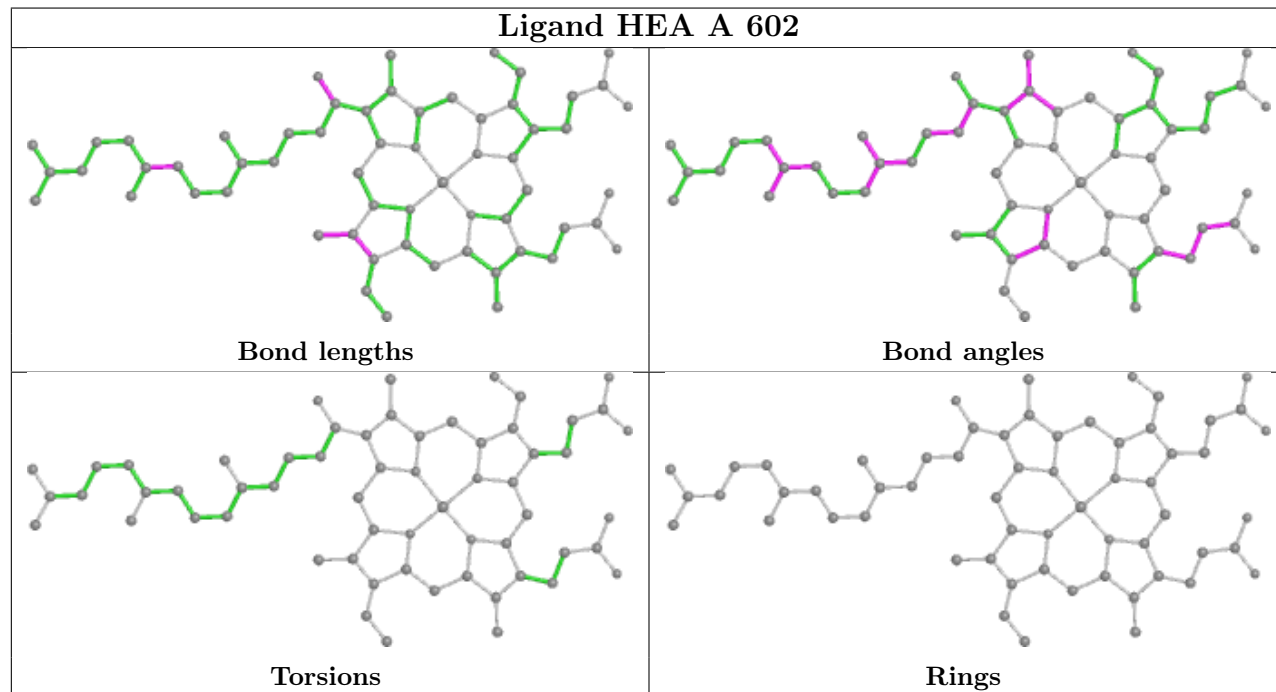
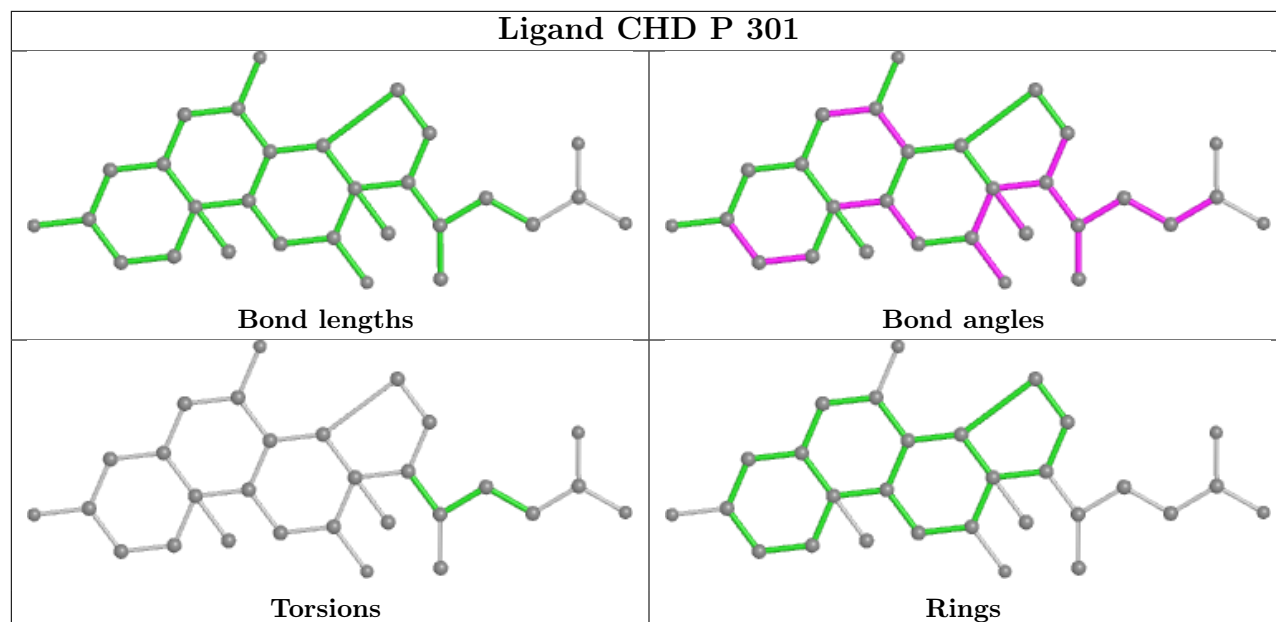


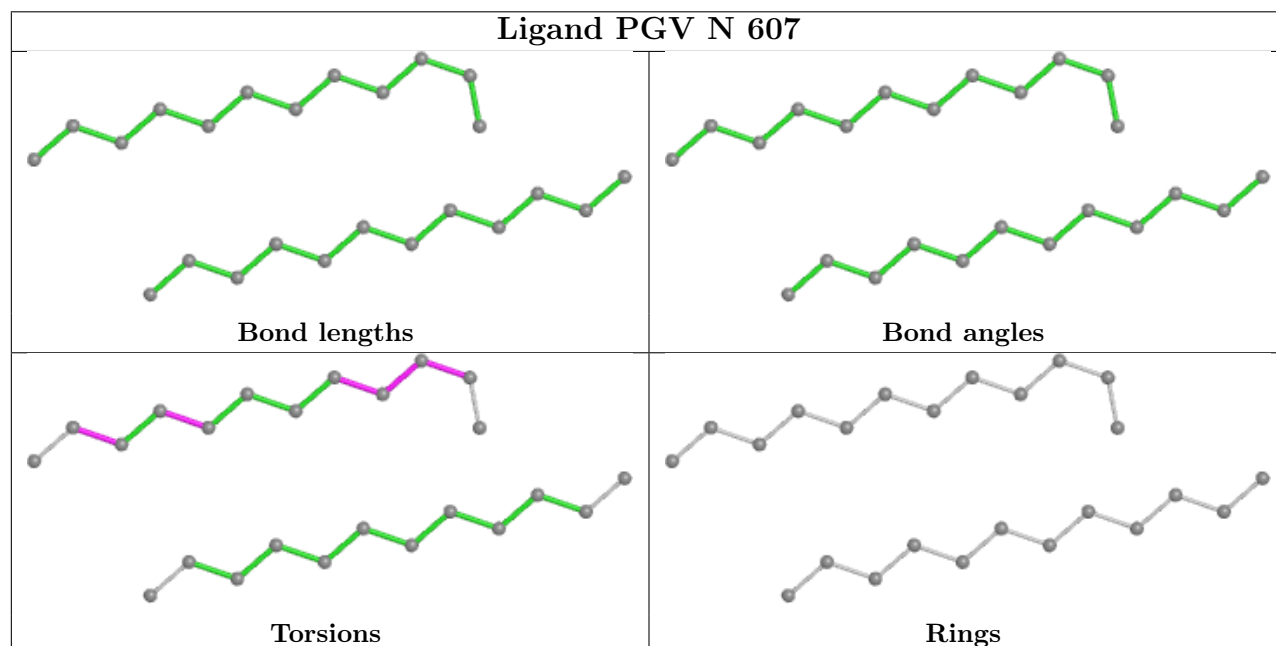
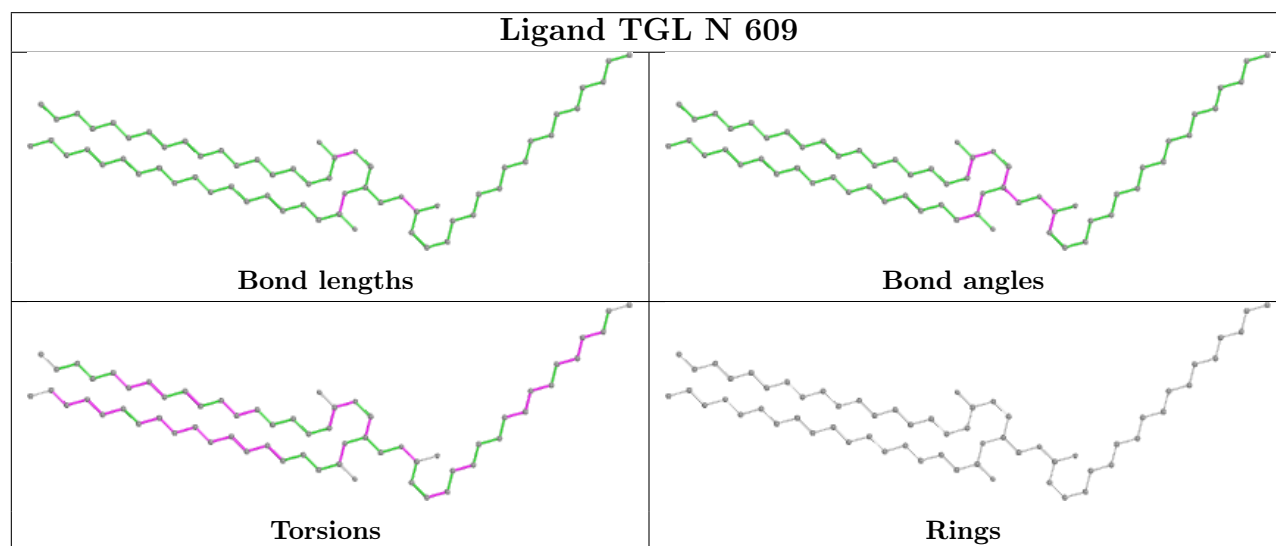
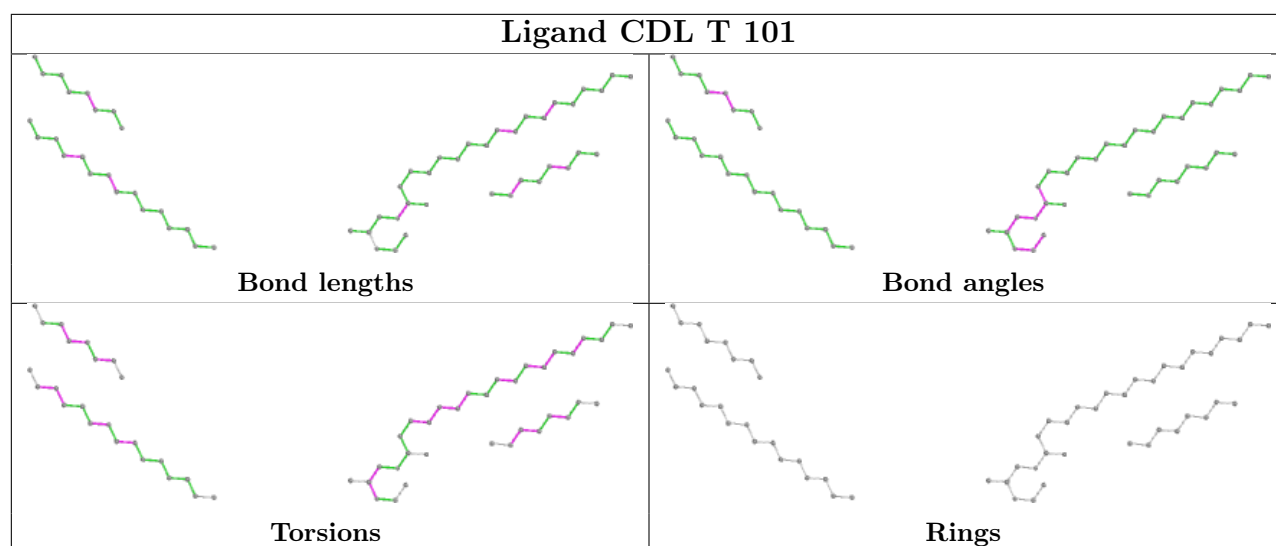


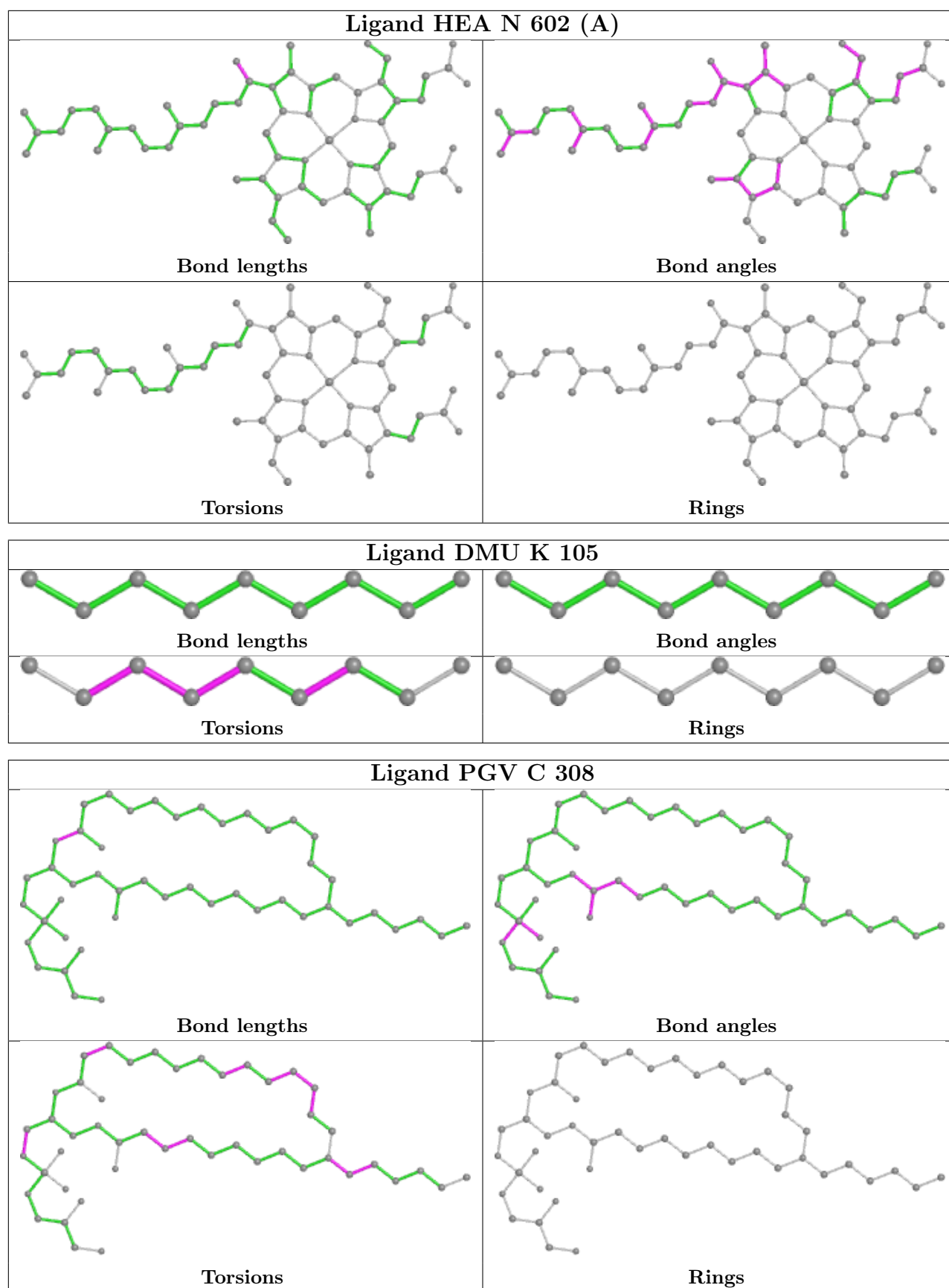


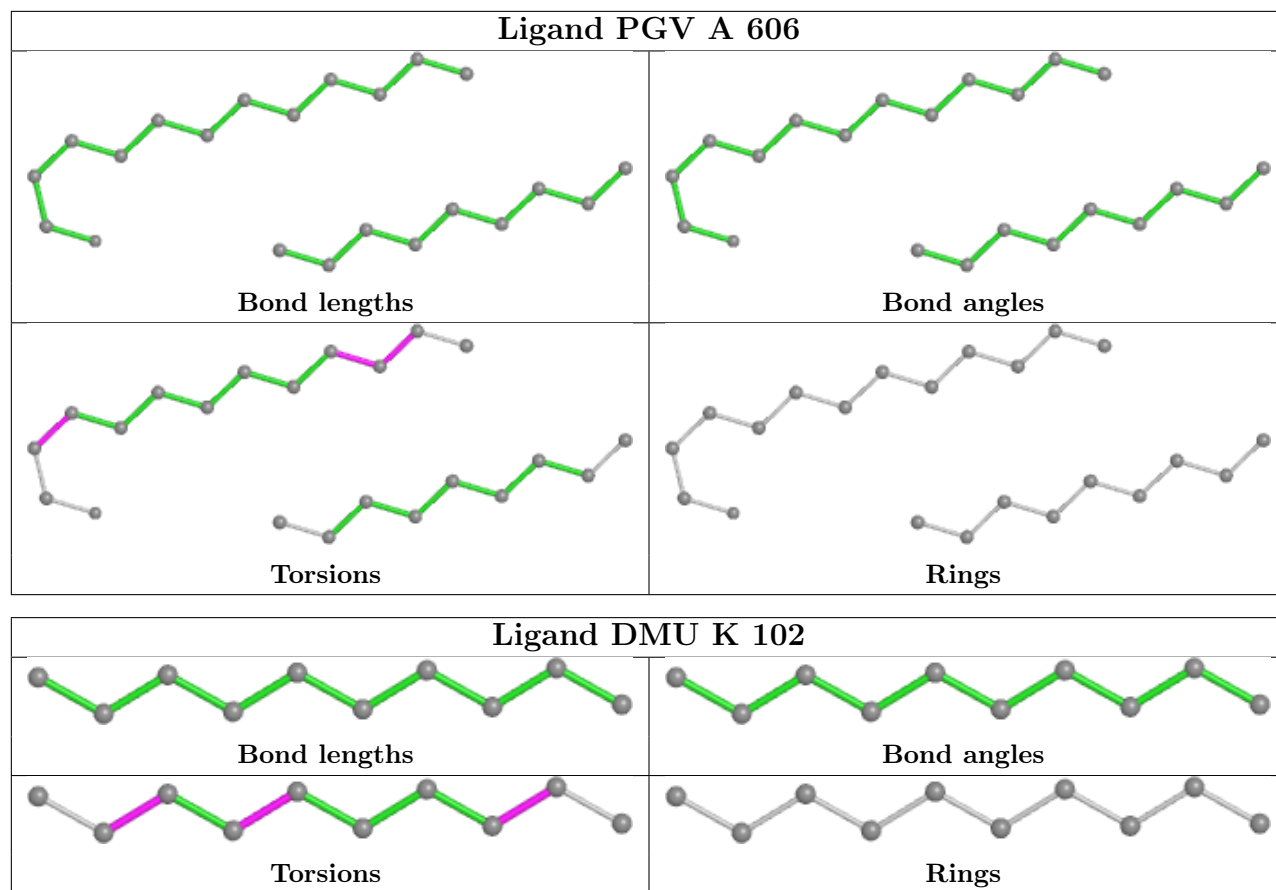


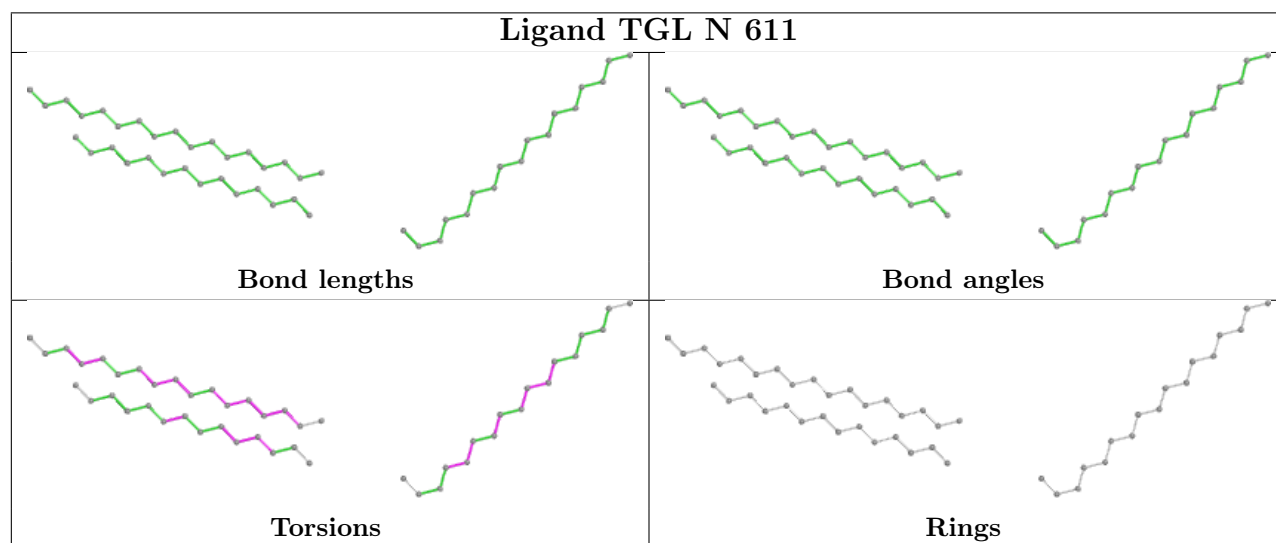
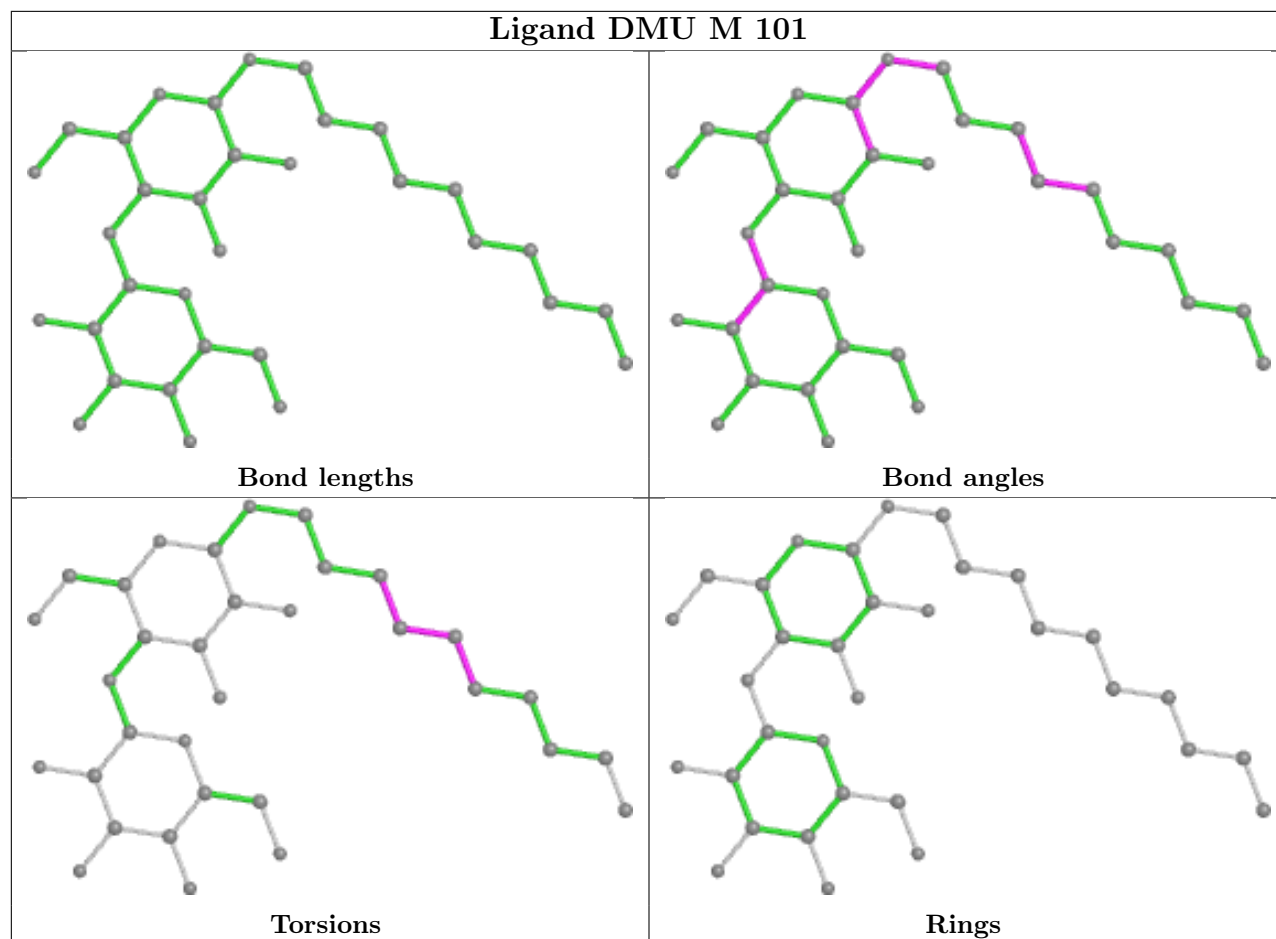


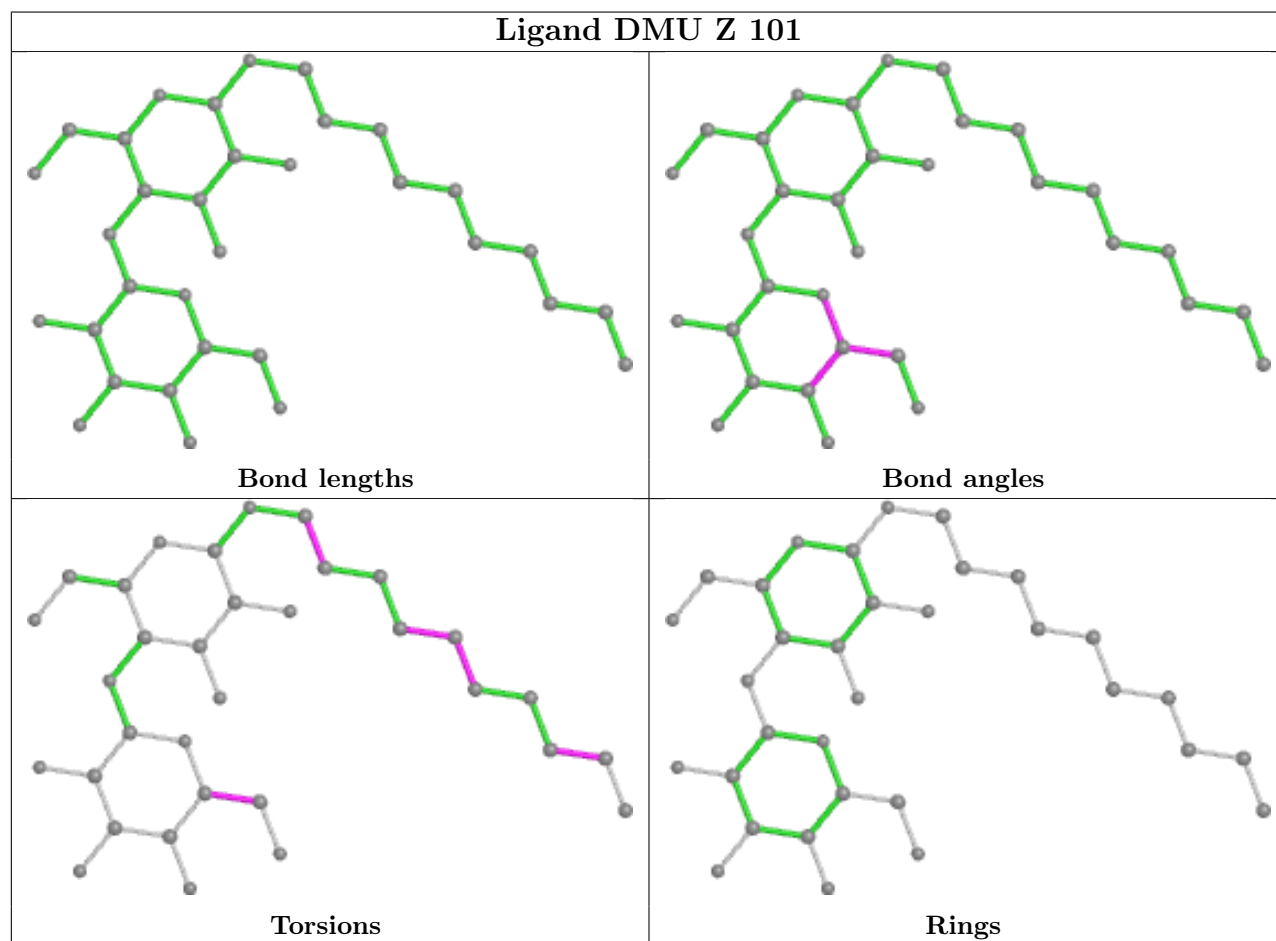
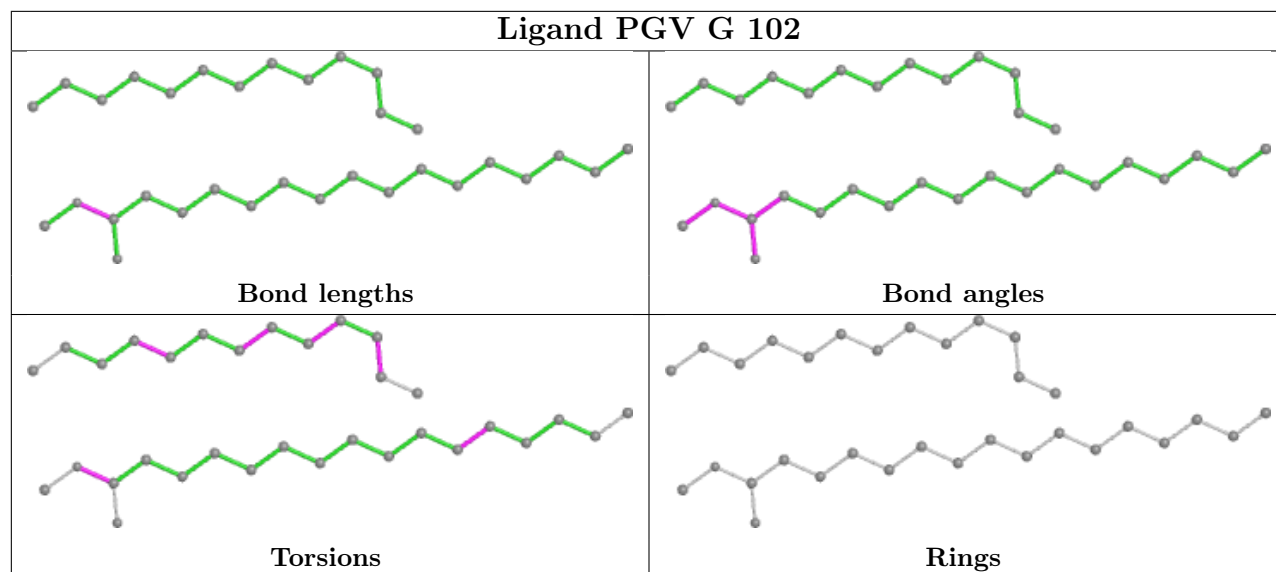


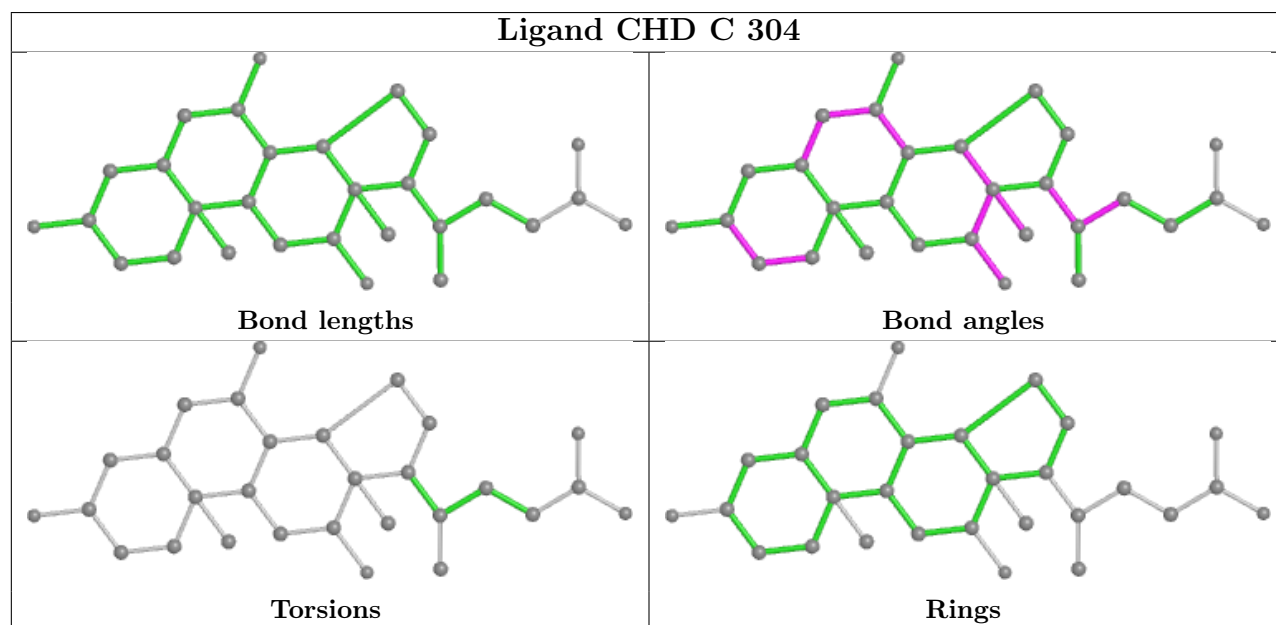
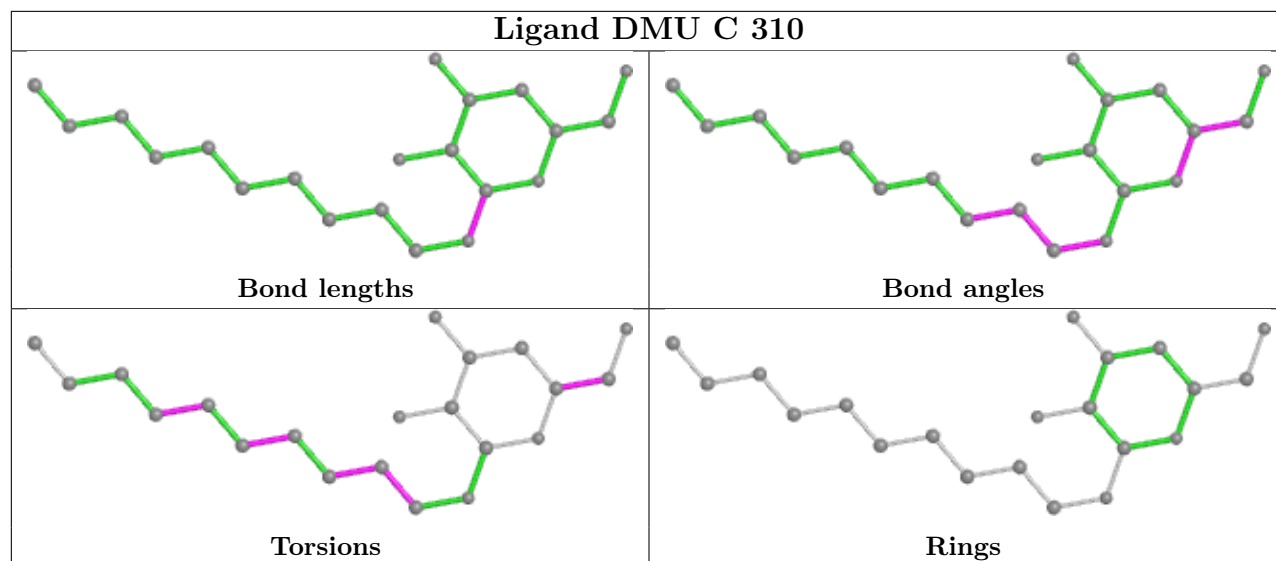


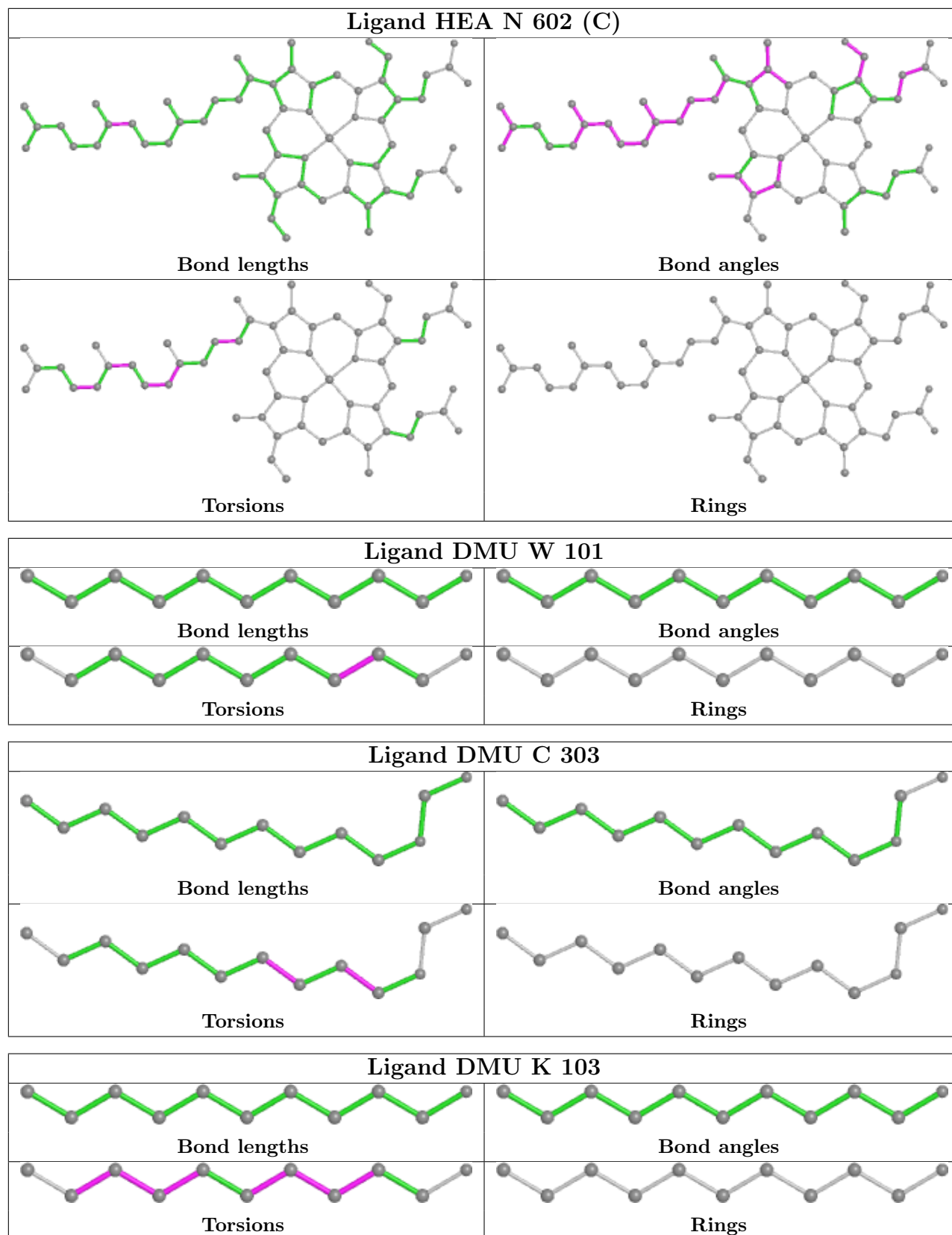




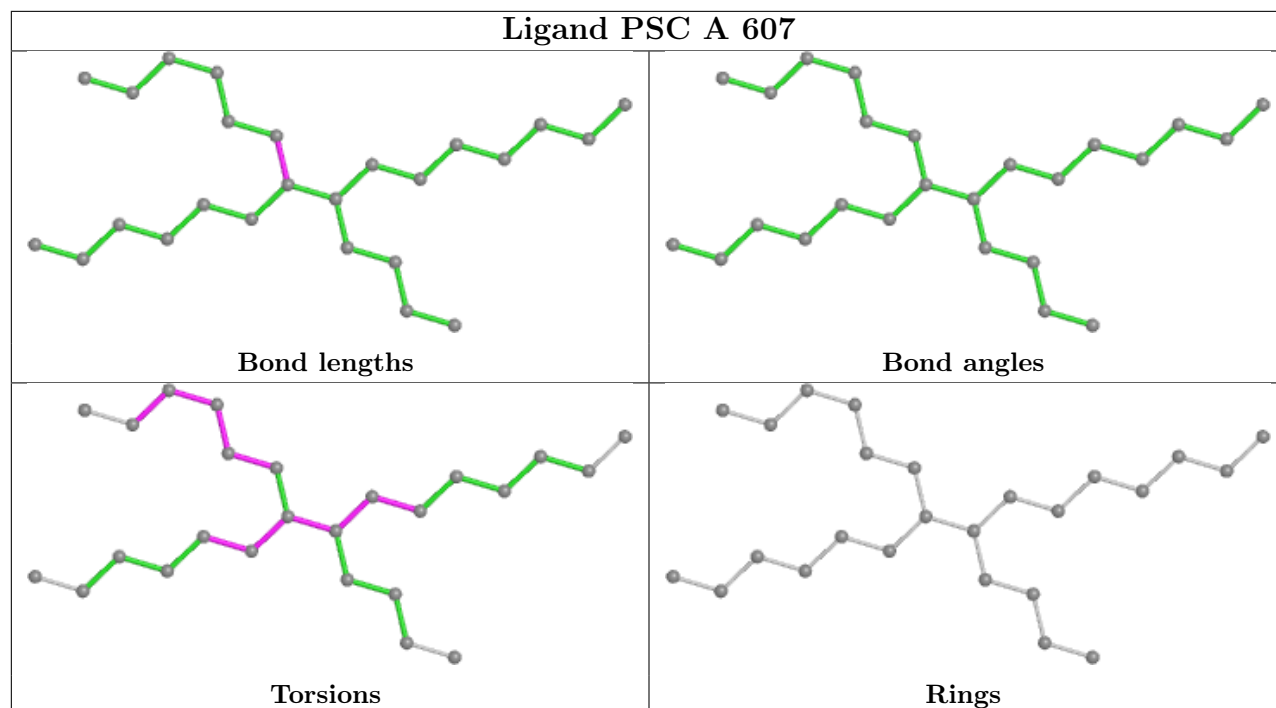




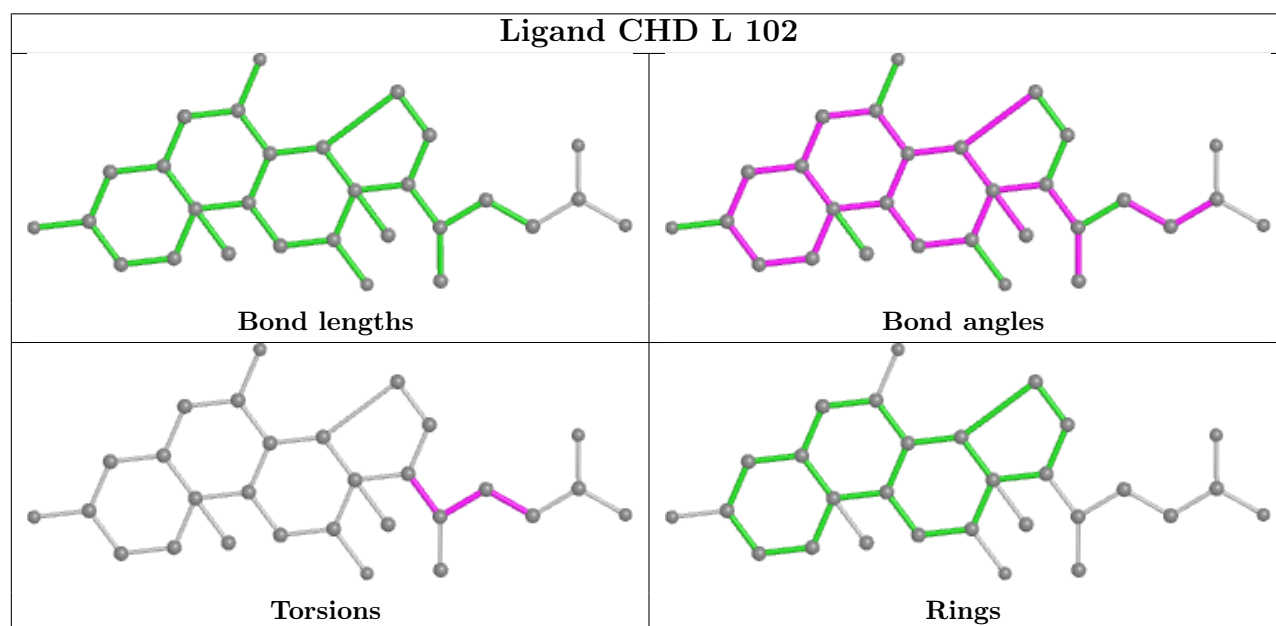


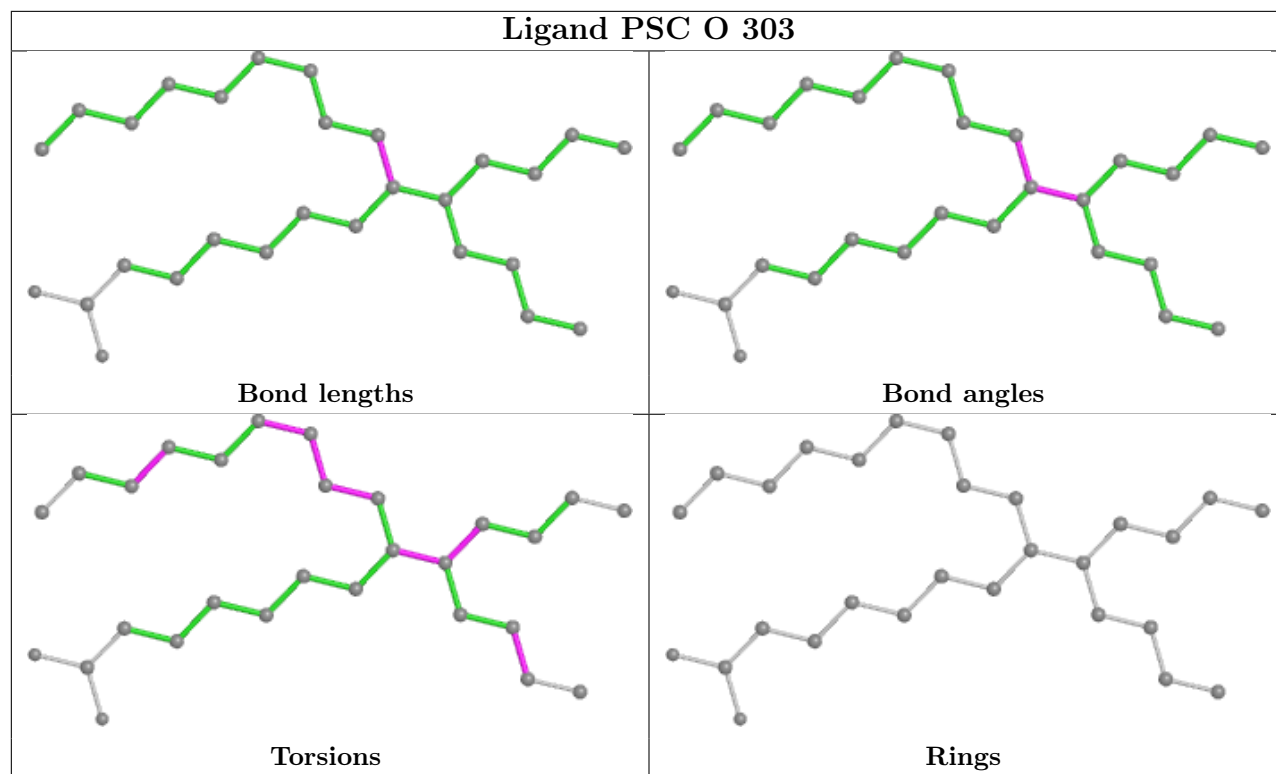


Ligand PSC A 607



Ligand CHD L 102





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%)	-0.01	1 (0%) 95 96	20, 24, 32, 88	0
1	N	513/514 (99%)	-0.04	0 100 100	21, 27, 36, 89	0
2	B	226/227 (99%)	-0.10	1 (0%) 92 94	21, 30, 60, 105	0
2	O	226/227 (99%)	-0.03	4 (1%) 68 76	24, 34, 75, 148	0
3	C	259/259 (100%)	-0.05	0 100 100	21, 27, 41, 105	0
3	P	259/259 (100%)	-0.02	2 (0%) 86 90	22, 28, 46, 111	0
4	D	144/144 (100%)	-0.22	0 100 100	25, 31, 57, 97	0
4	Q	144/144 (100%)	0.99	8 (5%) 24 30	30, 46, 101, 215	0
5	E	105/105 (100%)	-0.16	2 (1%) 66 74	25, 32, 66, 157	0
5	R	105/105 (100%)	-0.01	2 (1%) 66 74	29, 41, 78, 155	0
6	F	94/94 (100%)	0.02	3 (3%) 47 54	23, 33, 66, 148	0
6	S	94/94 (100%)	0.07	4 (4%) 35 41	23, 32, 73, 159	0
7	G	84/84 (100%)	0.74	16 (19%) 1 1	25, 36, 137, 156	0
7	T	84/84 (100%)	1.00	16 (19%) 1 1	25, 38, 137, 184	0
8	H	79/79 (100%)	0.30	6 (7%) 13 18	26, 36, 116, 171	0
8	U	79/79 (100%)	0.24	6 (7%) 13 18	30, 40, 117, 216	0
9	I	72/73 (98%)	0.14	1 (1%) 75 82	29, 45, 77, 103	0
9	V	72/73 (98%)	0.22	1 (1%) 75 82	30, 52, 96, 146	0
10	J	58/58 (100%)	0.26	3 (5%) 27 33	27, 38, 93, 172	0
10	W	58/58 (100%)	0.22	2 (3%) 45 51	29, 42, 92, 152	0
11	K	49/49 (100%)	-0.04	0 100 100	29, 37, 59, 79	0
11	X	49/49 (100%)	0.33	2 (4%) 37 44	36, 48, 98, 113	0
12	L	46/46 (100%)	-0.11	1 (2%) 62 69	25, 29, 57, 111	0
12	Y	46/46 (100%)	0.05	1 (2%) 62 69	29, 36, 85, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/43 (100%)	0.06	2 (4%) 31 37	25, 29, 95, 126	0
13	Z	43/43 (100%)	0.32	5 (11%) 4 6	32, 37, 110, 225	0
All	All	3544/3550 (99%)	0.08	89 (2%) 57 63	20, 31, 78, 225	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	37.3
4	Q	4	SER	35.1
4	Q	6	VAL	23.4
4	Q	8	SER	15.8
7	T	3	ALA	14.7
8	H	8	ILE	10.7
7	T	8	HIS	10.3
7	T	7	ASP	9.7
4	Q	9	GLU	9.6
4	Q	7	LYS	9.1
6	F	1	ALA	8.2
10	J	58	LYS	8.0
6	S	1	ALA	8.0
7	G	8	HIS	7.1
10	W	58	LYS	7.0
5	R	5	HIS	7.0
6	F	2	SER	6.8
7	G	3	ALA	6.7
13	Z	43	SER	6.1
6	S	2	SER	6.0
9	I	37	PHE	5.8
8	U	45	ALA	5.6
7	T	6	GLY	5.4
5	E	5	HIS	5.2
7	T	10	GLY	5.0
4	Q	10	ASP	4.9
8	H	46	LYS	4.9
7	T	2	SER	4.6
7	G	7	ASP	4.5
7	G	6	GLY	4.5
7	G	10	GLY	4.5
12	Y	47	LYS	4.5
10	J	1	PHE	4.4
7	G	36	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
7	T	36	TRP	4.3
8	U	8	ILE	4.3
7	G	42	ARG	4.2
7	G	2	SER	4.2
13	Z	42	LYS	4.1
2	O	90	ILE	4.1
7	T	40	GLY	4.0
2	O	91	ASN	4.0
7	T	9	GLY	3.7
8	H	47	GLY	3.7
7	T	5	LYS	3.7
7	G	40	GLY	3.6
7	T	42	ARG	3.5
7	G	5	LYS	3.5
7	T	11	THR	3.4
11	X	6	ALA	3.3
6	S	94	HIS	3.3
5	R	109	VAL	3.3
7	G	4	ALA	3.3
8	H	44	THR	3.2
7	T	1	ALA	3.1
7	G	9	GLY	3.1
13	Z	39	ASN	2.9
12	L	2	HIS	2.9
11	X	7	PRO	2.9
8	H	7	LYS	2.9
7	G	70[A]	PHE	2.9
7	G	11	THR	2.8
13	Z	40	TYR	2.8
3	P	37	PHE	2.7
7	T	38	HIS	2.7
4	Q	51	LEU	2.7
10	J	57	HIS	2.6
13	M	40	TYR	2.6
7	T	4	ALA	2.6
9	V	37	PHE	2.5
13	Z	41	LYS	2.5
3	P	3	HIS	2.4
8	U	49	ASP	2.4
2	O	227	LEU	2.3
7	T	37	LEU	2.3
13	M	43	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	53[A]	ILE	2.3
8	U	46	LYS	2.3
6	F	3	GLY	2.3
7	G	41	HIS	2.2
2	O	113	TYR	2.2
7	G	1	ALA	2.2
8	U	52	VAL	2.1
5	E	109	VAL	2.1
8	U	7	LYS	2.1
10	W	57	HIS	2.1
6	S	93	PRO	2.1
8	H	45	ALA	2.1
2	B	55	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.25	0.34	113,156,190,197	0
9	SAC	I	1	9/10	0.82	0.23	112,134,180,200	0
1	FME	N	1	10/11	0.94	0.14	38,42,98,131	0
2	FME	B	1	10/11	0.97	0.12	27,28,38,142	0
1	FME	A	1	10/11	0.97	0.09	35,49,83,103	0
2	FME	O	1	10/11	0.98	0.09	31,34,42,112	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	DMU	X	102	10/33	0.38	0.33	62,71,99,116	0
25	DMU	D	203	11/33	0.60	0.32	52,74,124,137	0
21	EDO	C	312	4/4	0.63	0.19	48,71,72,75	0
26	CDL	T	101	57/100	0.66	0.25	42,72,104,149	0
21	EDO	N	619	4/4	0.68	0.24	51,52,54,67	0
21	EDO	A	615	4/4	0.68	0.18	49,58,60,64	0
21	EDO	P	312	4/4	0.69	0.15	67,72,73,77	0
25	DMU	K	104	9/33	0.69	0.27	49,70,113,125	0
25	DMU	X	104	10/33	0.74	0.27	62,84,90,92	0
25	DMU	Q	201	10/33	0.74	0.16	52,62,68,111	0
21	EDO	F	103	4/4	0.75	0.16	50,61,64,82	0
25	DMU	P	309	11/33	0.76	0.30	42,58,101,104	0
21	EDO	P	316	4/4	0.77	0.15	39,56,66,82	0
22	TGL	N	611	48/63	0.77	0.18	48,68,120,134	0
24	CHD	Y	101	29/29	0.77	0.27	56,95,143,158	0
21	EDO	P	310	4/4	0.77	0.10	46,60,67,75	0
21	EDO	C	317	4/4	0.77	0.13	55,56,72,75	0
26	CDL	N	601	55/100	0.78	0.28	51,69,104,118	0
25	DMU	X	103	9/33	0.78	0.30	55,62,94,101	0
21	EDO	P	311	4/4	0.80	0.14	62,62,65,73	0
27	PEK	C	309	36/53	0.80	0.23	42,75,110,130	0
27	PEK	P	308	34/53	0.80	0.25	37,70,117,134	0
18	PGV	C	311	28/51	0.81	0.19	41,66,117,126	0
21	EDO	P	317	4/4	0.81	0.11	57,90,97,106	0
25	DMU	L	101	21/33	0.81	0.17	42,81,114,129	0
18	PGV	G	102	32/51	0.81	0.20	39,72,108,130	0
22	TGL	N	612	44/63	0.81	0.23	41,59,127,197	0
27	PEK	P	305	20/53	0.81	0.17	47,56,95,96	0
21	EDO	C	313	4/4	0.81	0.12	30,32,33,94	0
25	DMU	X	101	11/33	0.82	0.16	43,59,104,225	0
21	EDO	C	320	4/4	0.82	0.24	32,56,75,112	0
25	DMU	K	102	10/33	0.82	0.21	46,69,87,103	0
18	PGV	N	607	24/51	0.83	0.19	41,53,106,166	0
27	PEK	C	306	25/53	0.83	0.22	41,57,96,119	0
21	EDO	L	104	4/4	0.83	0.20	50,51,77,148	0
22	TGL	D	202	57/63	0.83	0.16	32,65,134,156	0
25	DMU	K	105	9/33	0.83	0.34	72,75,92,107	0
22	TGL	B	301	49/63	0.84	0.15	38,61,98,147	0
24	CHD	L	102	29/29	0.84	0.30	51,100,145,177	0
21	EDO	G	104	4/4	0.84	0.14	33,77,87,92	0
21	EDO	A	609	4/4	0.84	0.14	34,38,47,146	0
25	DMU	O	302	11/33	0.84	0.20	54,58,104,111	0
25	DMU	P	303	13/33	0.84	0.14	53,62,94,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	DMU	C	303	13/33	0.85	0.11	53,63,88,92	0
26	CDL	C	305	58/100	0.85	0.18	44,65,131,156	0
21	EDO	Q	202	4/4	0.85	0.14	43,50,52,56	0
25	DMU	W	101	11/33	0.85	0.20	51,59,82,111	0
22	TGL	L	103	56/63	0.86	0.17	28,56,121,139	0
25	DMU	K	103	11/33	0.86	0.23	50,70,100,120	0
25	DMU	J	101	11/33	0.86	0.17	49,58,81,102	0
25	DMU	C	310	21/33	0.87	0.18	29,58,111,142	0
22	TGL	N	609	63/63	0.87	0.18	40,72,117,154	0
21	EDO	D	204	4/4	0.87	0.22	37,47,79,85	0
21	EDO	A	614	4/4	0.87	0.21	55,66,70,75	0
26	CDL	P	304	61/100	0.88	0.18	37,69,128,196	0
21	EDO	C	314	4/4	0.88	0.14	32,39,42,44	0
19	PSC	O	303	30/52	0.89	0.16	37,59,103,106	0
21	EDO	O	306	4/4	0.89	0.15	48,63,79,92	0
25	DMU	D	201	11/33	0.89	0.14	44,69,79,88	0
21	EDO	B	306	4/4	0.90	0.12	29,35,41,55	0
25	DMU	K	106	10/33	0.90	0.19	52,65,91,120	0
21	EDO	T	103	4/4	0.90	0.23	43,65,78,97	0
21	EDO	N	621	4/4	0.90	0.10	46,52,52,62	0
21	EDO	J	102	4/4	0.91	0.30	52,52,100,116	0
25	DMU	K	101	9/33	0.91	0.14	41,52,77,94	0
19	PSC	A	607	27/52	0.91	0.18	36,66,100,129	0
18	PGV	A	606	22/51	0.91	0.14	31,45,70,94	0
21	EDO	T	104	4/4	0.91	0.22	39,49,54,71	0
29	PO4	U	101	5/5	0.91	0.17	47,54,128,200	0
25	DMU	Z	101	33/33	0.92	0.10	38,46,79,84	0
21	EDO	O	305	4/4	0.92	0.31	42,46,51,95	0
21	EDO	N	620	4/4	0.92	0.17	33,34,66,104	0
21	EDO	W	102	4/4	0.92	0.19	47,57,68,111	0
21	EDO	S	104	4/4	0.92	0.20	40,56,58,88	0
21	EDO	S	106	4/4	0.93	0.17	39,47,67,81	0
21	EDO	A	610	4/4	0.93	0.13	39,48,53,70	0
21	EDO	C	316	4/4	0.93	0.11	53,56,61,69	0
21	EDO	J	103	4/4	0.93	0.20	51,52,72,74	0
25	DMU	M	101	33/33	0.93	0.10	31,40,53,69	0
21	EDO	B	307	4/4	0.93	0.16	34,45,46,48	0
21	EDO	A	617	4/4	0.94	0.25	37,39,46,63	0
21	EDO	C	318	4/4	0.94	0.20	40,60,63,111	0
21	EDO	P	315	4/4	0.94	0.15	53,58,63,73	0
21	EDO	F	106	4/4	0.94	0.19	35,38,76,104	0
21	EDO	N	616	4/4	0.94	0.21	33,41,44,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CHD	C	304	29/29	0.94	0.09	26,29,35,41	0
21	EDO	Y	103	4/4	0.94	0.31	46,59,90,134	0
21	EDO	A	618	4/4	0.94	0.16	33,34,39,87	0
21	EDO	N	614	4/4	0.95	0.10	37,38,39,44	0
21	EDO	C	319	4/4	0.95	0.29	43,53,61,115	0
17	NA	P	302	1/1	0.95	0.10	30,30,30,30	0
21	EDO	A	612	4/4	0.95	0.15	28,31,32,38	0
21	EDO	T	102	4/4	0.95	0.13	31,32,37,40	0
21	EDO	P	313	4/4	0.95	0.18	34,37,39,39	0
21	EDO	E	203	4/4	0.95	0.12	42,45,54,117	0
21	EDO	A	613	4/4	0.95	0.15	28,39,46,48	0
24	CHD	G	101	29/29	0.95	0.09	21,26,35,42	0
21	EDO	Y	102	4/4	0.95	0.20	48,57,57,83	0
24	CHD	P	301	29/29	0.95	0.08	24,29,35,40	0
21	EDO	D	205	4/4	0.96	0.13	44,45,46,101	0
18	PGV	N	608	51/51	0.96	0.13	23,34,69,80	0
21	EDO	P	314	4/4	0.96	0.10	30,35,40,62	0
21	EDO	S	105	4/4	0.96	0.10	31,31,31,33	0
27	PEK	P	306	53/53	0.96	0.11	28,41,84,122	0
21	EDO	N	617	4/4	0.96	0.10	22,29,30,32	0
21	EDO	O	304	4/4	0.96	0.08	30,31,32,32	0
21	EDO	C	315	4/4	0.97	0.15	28,35,50,72	0
21	EDO	G	103	4/4	0.97	0.08	30,31,35,35	0
21	EDO	A	616	4/4	0.97	0.11	30,42,68,94	0
24	CHD	B	303	29/29	0.97	0.08	21,26,31,46	0
18	PGV	C	301	51/51	0.97	0.11	22,32,67,80	0
21	EDO	D	206	4/4	0.97	0.11	36,38,58,71	0
21	EDO	E	201	4/4	0.97	0.09	37,38,38,39	0
21	EDO	N	613	4/4	0.97	0.11	28,29,29,32	0
21	EDO	E	202	4/4	0.97	0.09	31,38,43,45	0
27	PEK	C	307	53/53	0.97	0.12	26,42,102,136	0
21	EDO	N	615	4/4	0.97	0.16	37,40,41,67	0
20	PER	A	608[A]	2/2	0.97	0.12	23,23,23,23	2
20	PER	N	610[A]	2/2	0.97	0.09	28,28,28,28	2
21	EDO	N	618	4/4	0.97	0.15	31,41,43,47	0
29	PO4	H	101	5/5	0.97	0.18	56,61,94,161	0
21	EDO	F	105	4/4	0.97	0.14	39,44,64,96	0
14	HEA	N	602[A]	60/60	0.98	0.11	20,25,38,46	17
14	HEA	N	602[B]	52/60	0.98	0.11	16,24,33,47	9
14	HEA	N	602[C]	52/60	0.98	0.11	20,24,40,52	9
18	PGV	P	307	51/51	0.98	0.12	23,32,97,138	0
14	HEA	N	603	60/60	0.98	0.09	19,23,29,38	0

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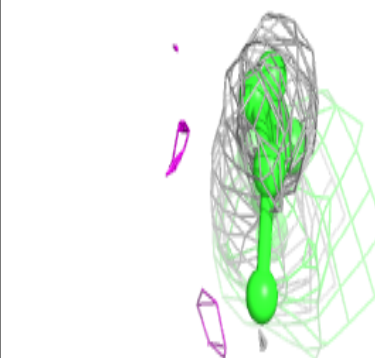
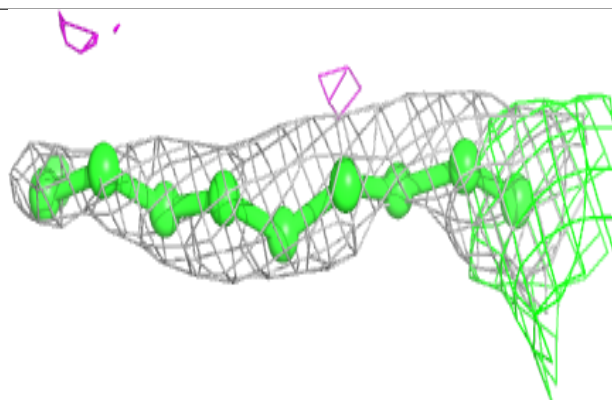
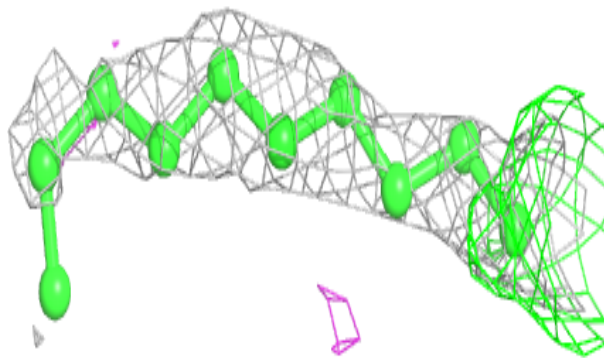
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	EDO	B	304	4/4	0.98	0.10	24,25,27,29	0
21	EDO	B	305	4/4	0.98	0.13	32,34,45,103	0
16	MG	A	604	1/1	0.98	0.04	19,19,19,19	0
17	NA	C	302	1/1	0.98	0.08	31,31,31,31	0
14	HEA	A	601[A]	60/60	0.98	0.11	17,21,33,63	17
21	EDO	S	102	4/4	0.98	0.15	23,25,25,25	0
21	EDO	S	103	4/4	0.98	0.07	32,33,38,41	0
14	HEA	A	601[B]	52/60	0.98	0.11	10,20,27,55	9
21	EDO	F	104	4/4	0.98	0.15	30,30,31,32	0
14	HEA	A	601[C]	52/60	0.98	0.11	17,21,31,57	9
18	PGV	C	308	48/51	0.98	0.11	22,29,71,88	0
14	HEA	A	602	60/60	0.98	0.09	18,22,28,38	0
16	MG	N	605	1/1	0.99	0.04	21,21,21,21	0
21	EDO	F	102	4/4	0.99	0.10	24,25,26,27	0
17	NA	N	606	1/1	0.99	0.07	28,28,28,28	0
21	EDO	A	611	4/4	0.99	0.10	22,24,27,28	0
17	NA	A	605	1/1	0.99	0.06	24,24,24,24	0
15	CU	A	603	1/1	1.00	0.13	22,22,22,22	0
23	CUA	B	302	2/2	1.00	0.13	22,22,22,22	0
28	ZN	F	101	1/1	1.00	0.09	25,25,25,25	0
28	ZN	S	101	1/1	1.00	0.10	26,26,26,26	0
23	CUA	O	301	2/2	1.00	0.10	26,26,26,26	0
15	CU	N	604	1/1	1.00	0.12	24,24,24,24	0

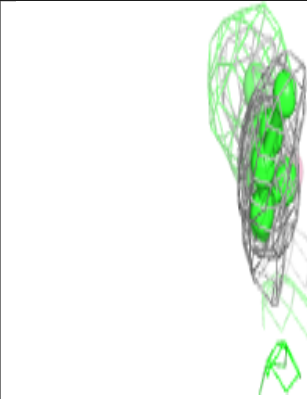
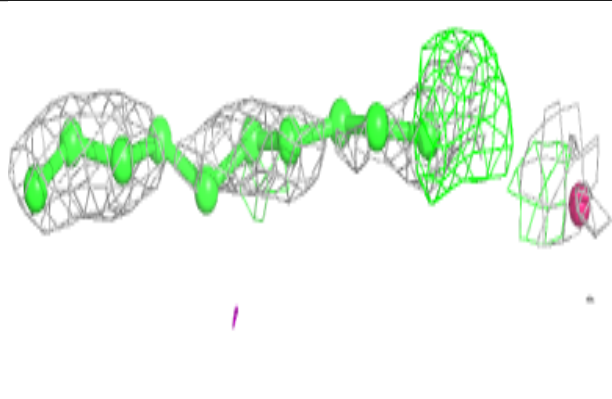
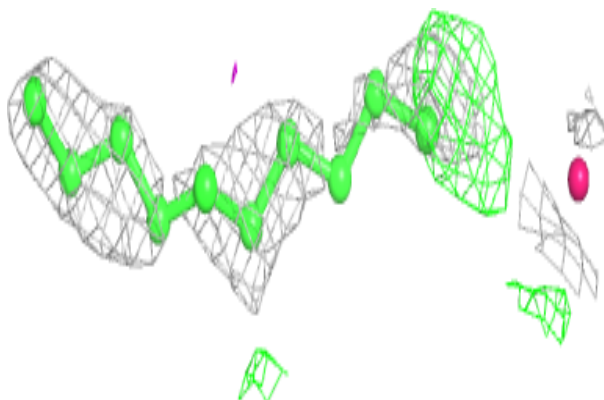
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU X 102:

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

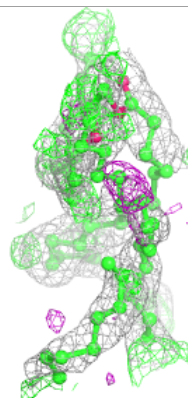
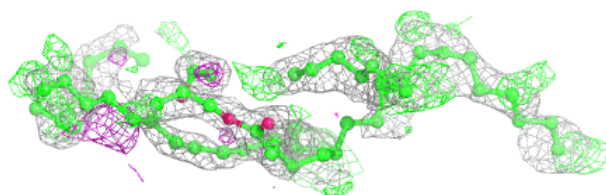
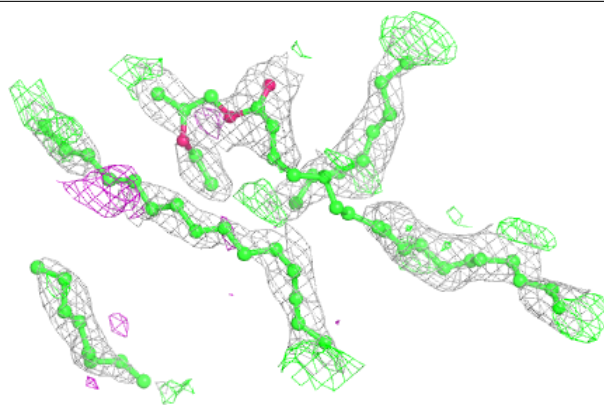
**Electron density around DMU D 203:**

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

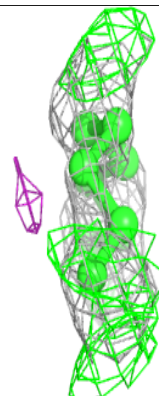
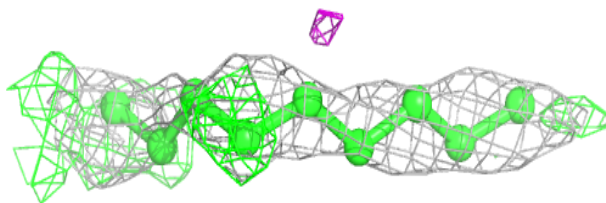
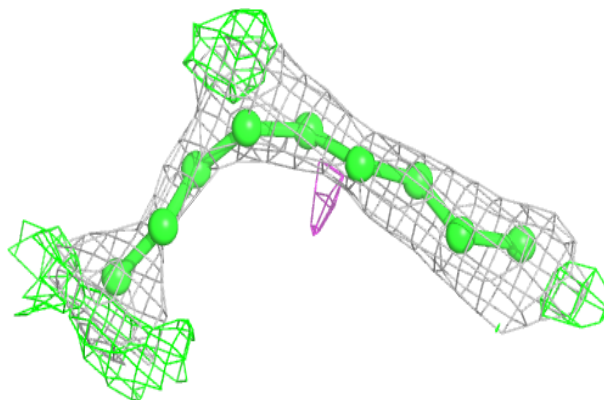


Electron density around CDL T 101:

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

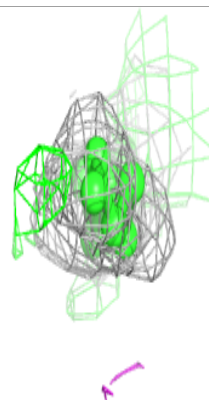
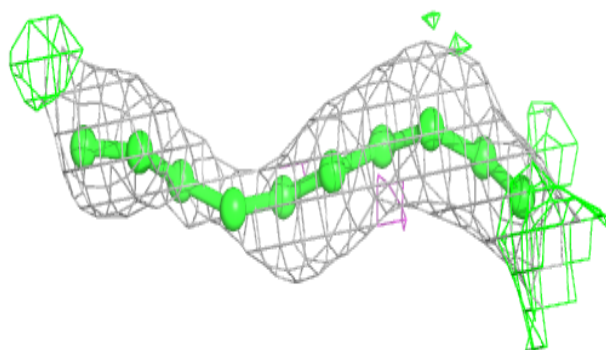
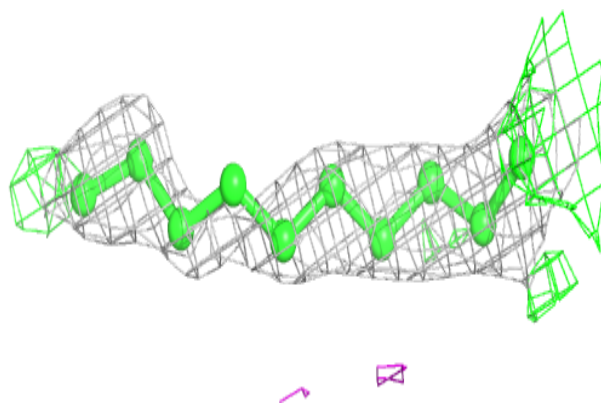
**Electron density around DMU K 104:**

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

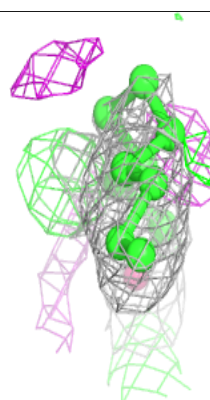
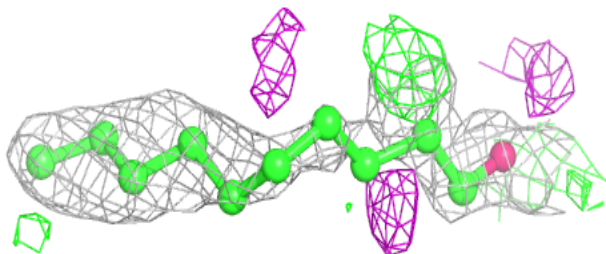
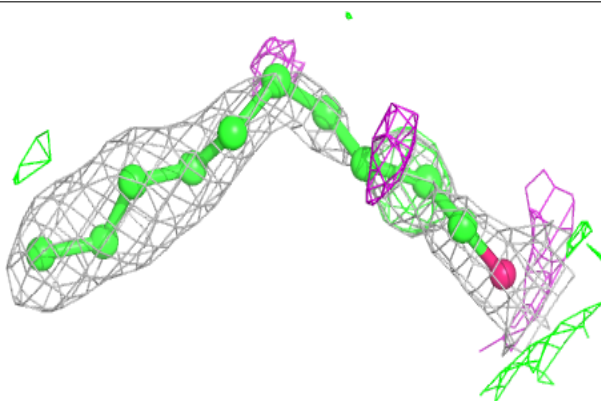


Electron density around DMU Q 201:

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

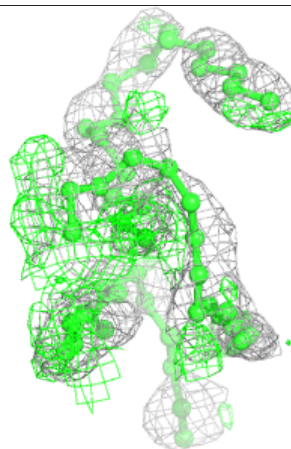
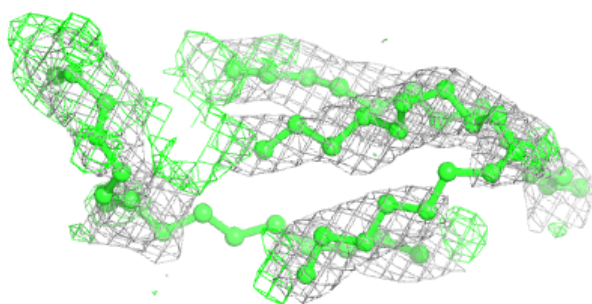
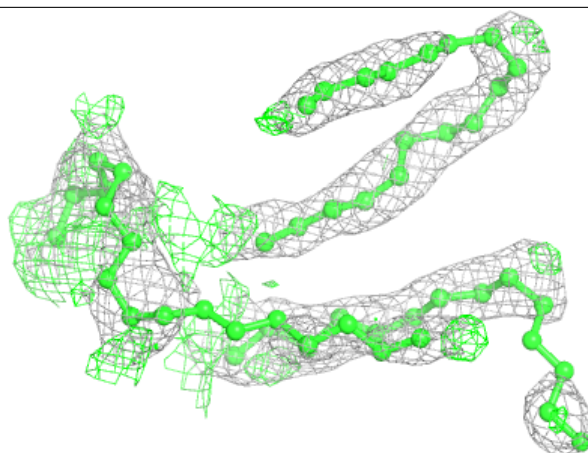
**Electron density around DMU P 309:**

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

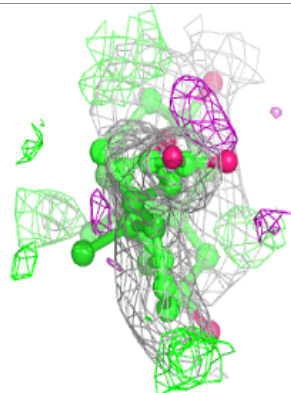
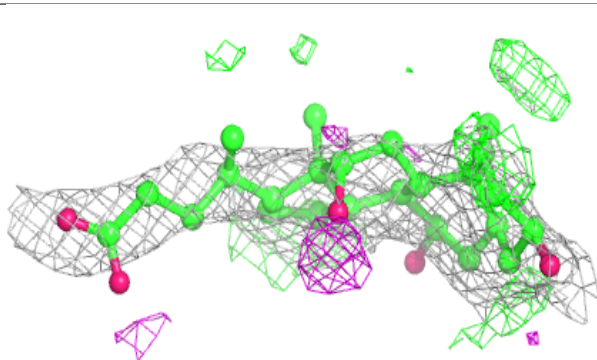
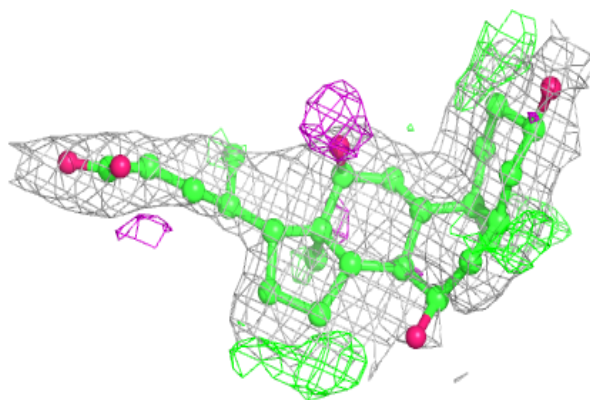


Electron density around TGL N 611:

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

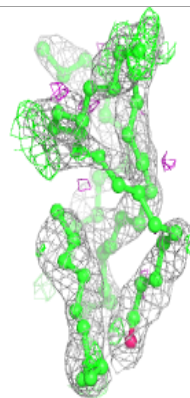
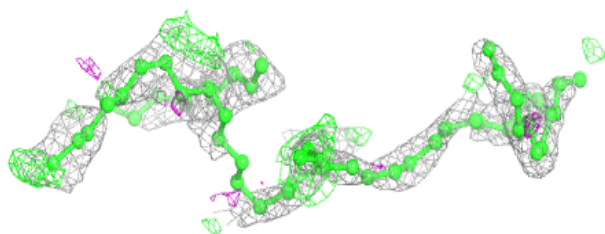
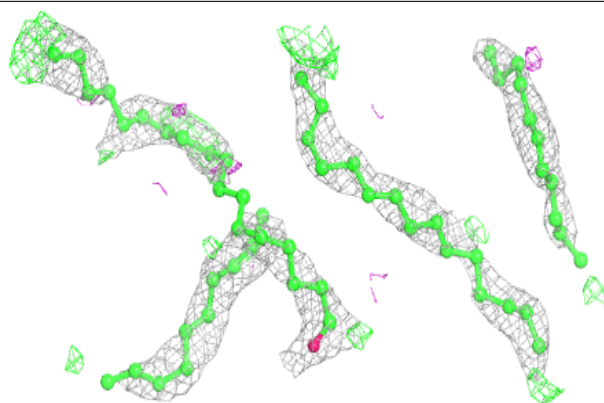
**Electron density around CHD Y 101:**

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

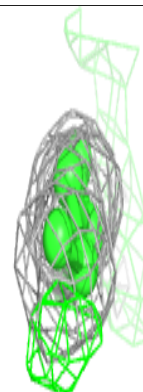
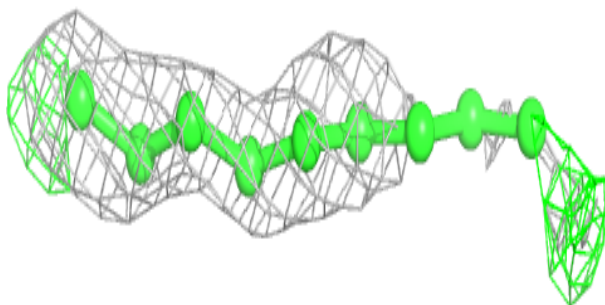
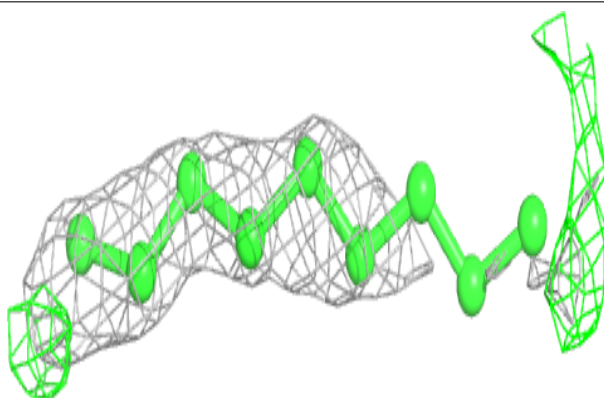


Electron density around CDL N 601:

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

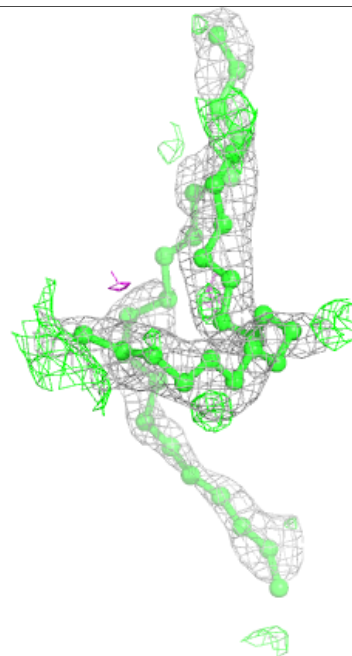
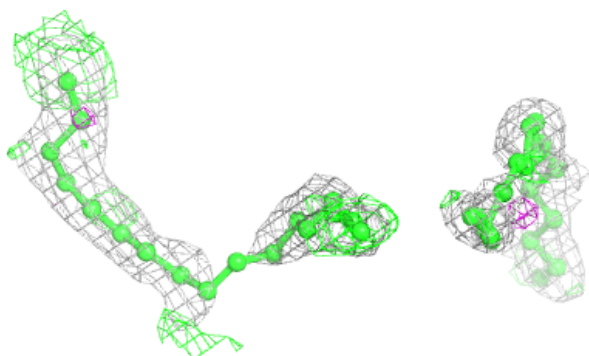
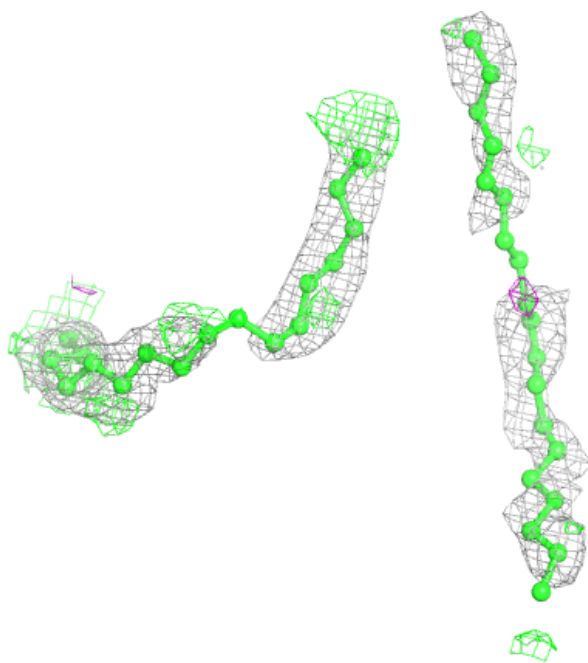
**Electron density around DMU X 103:**

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



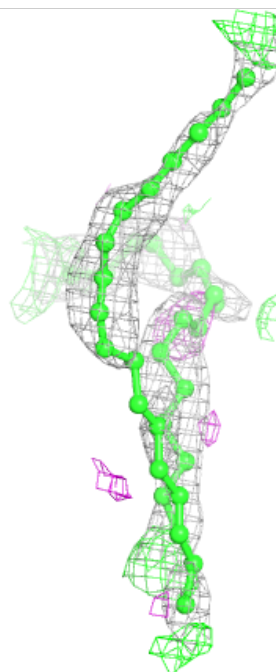
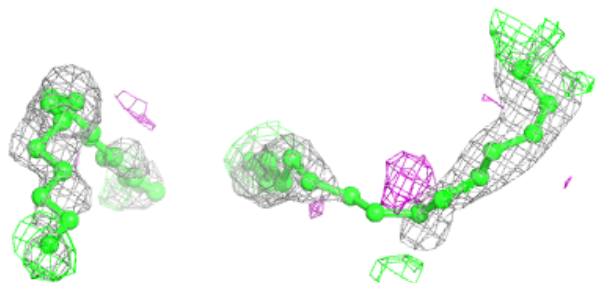
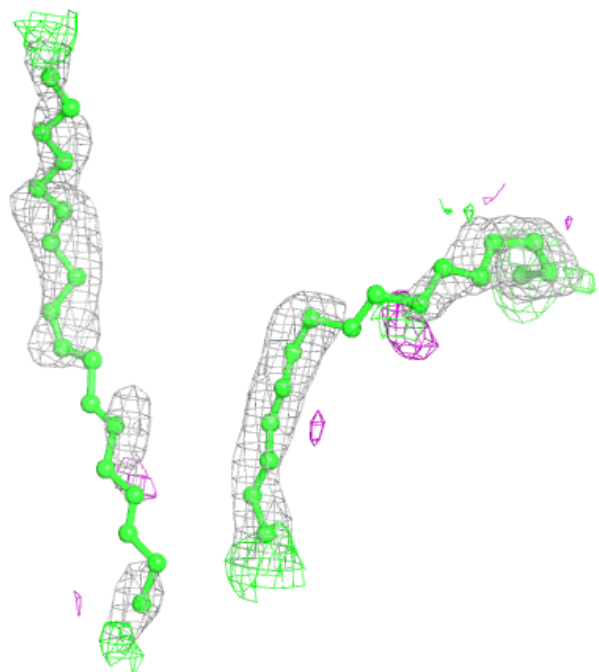
Electron density around PEK C 309:

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



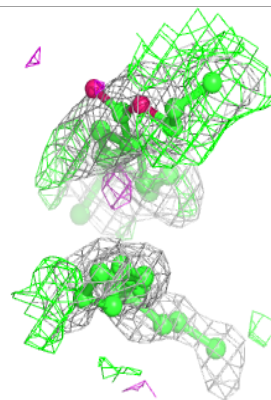
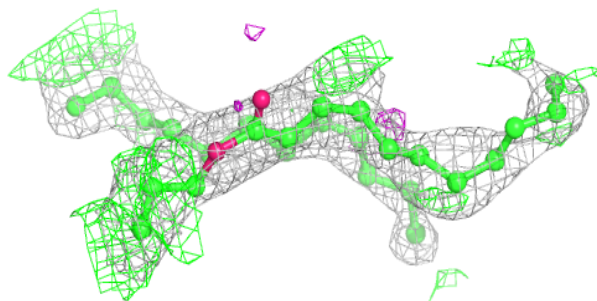
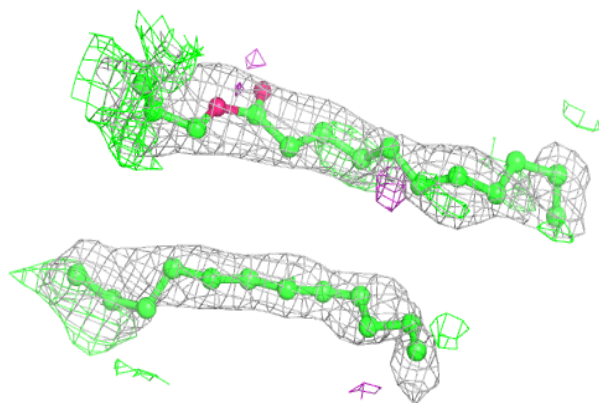
Electron density around PEK P 308:

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

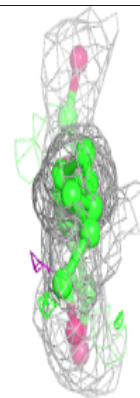
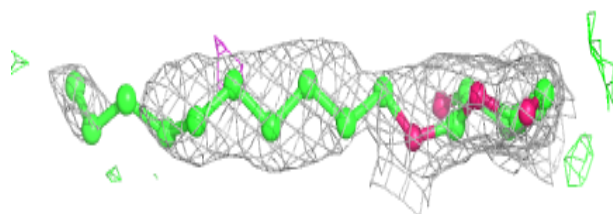
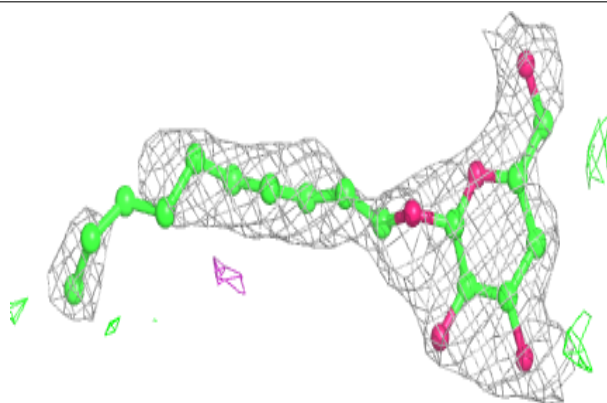


Electron density around PGV C 311:

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

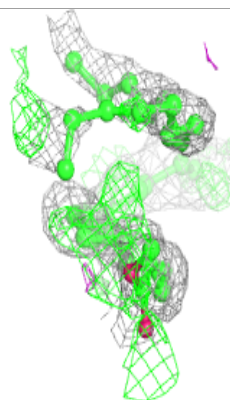
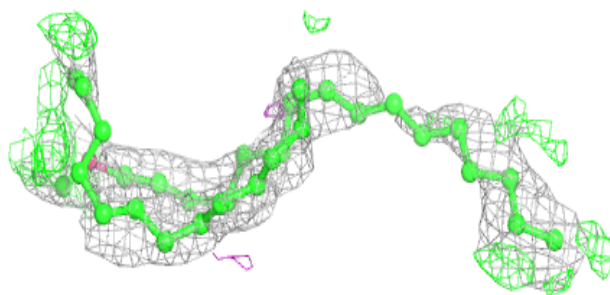
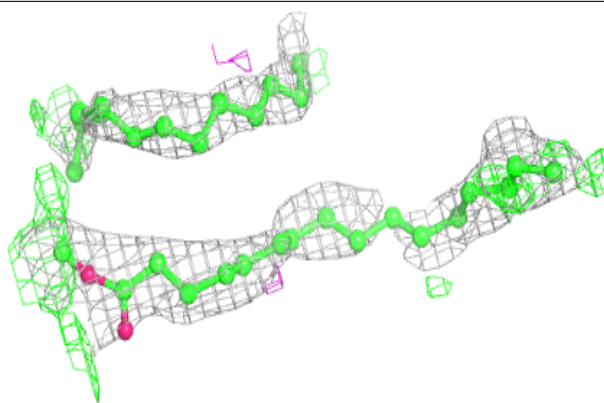
**Electron density around DMU L 101:**

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

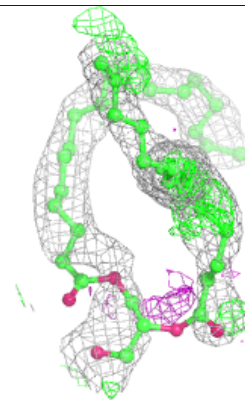
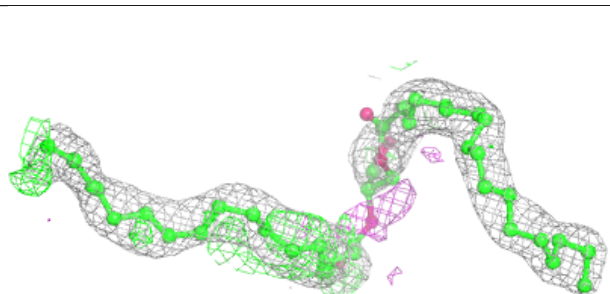
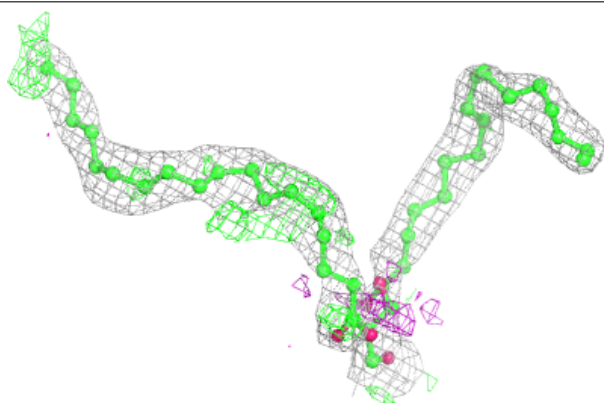


Electron density around PGV G 102:

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

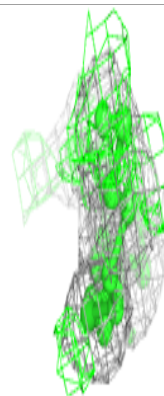
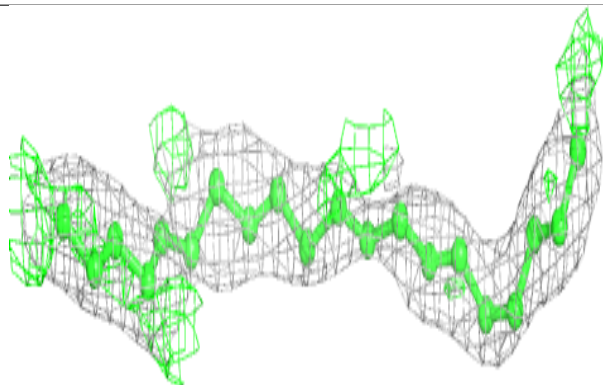
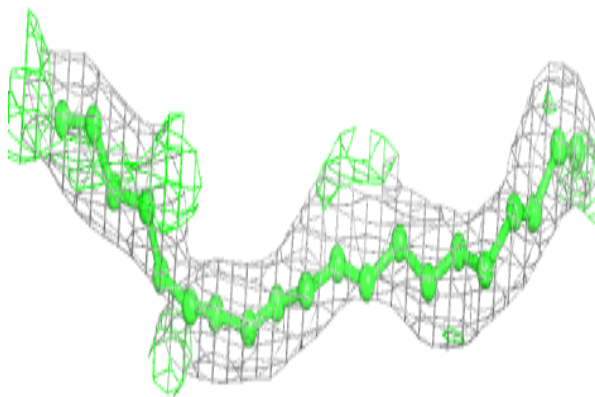
**Electron density around TGL N 612:**

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

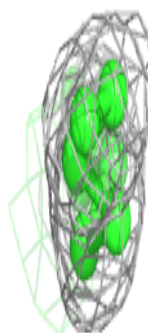
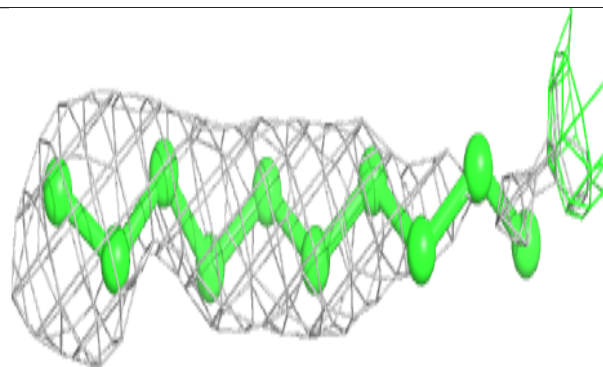
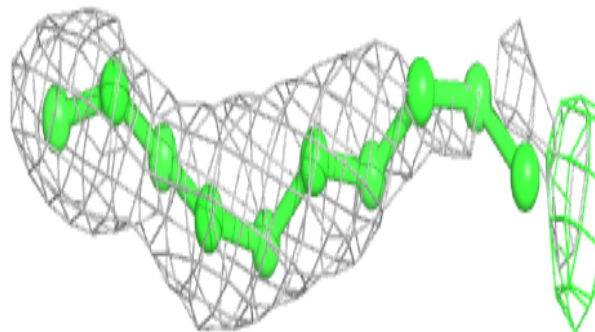


Electron density around PEK P 305:

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

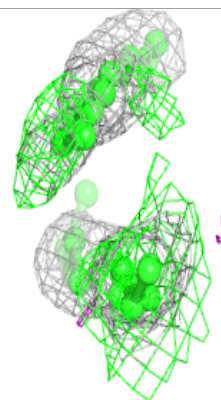
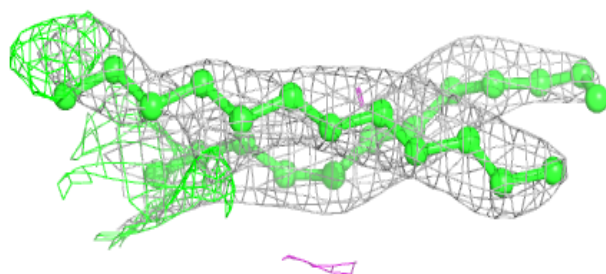
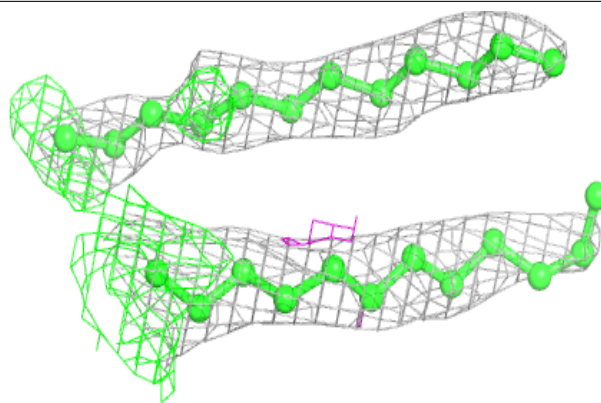
**Electron density around DMU K 102:**

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

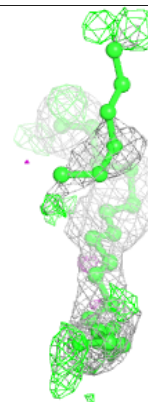
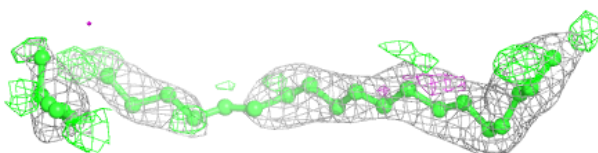
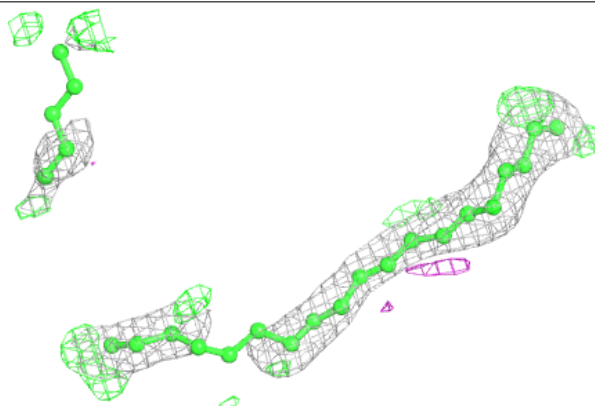


Electron density around PGV N 607:

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

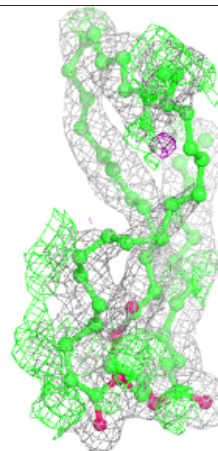
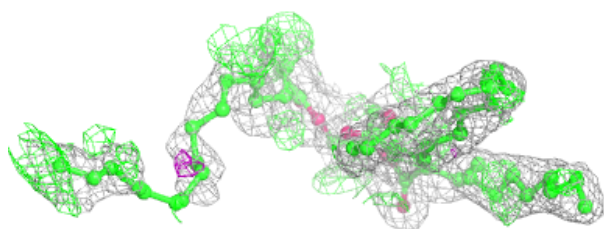
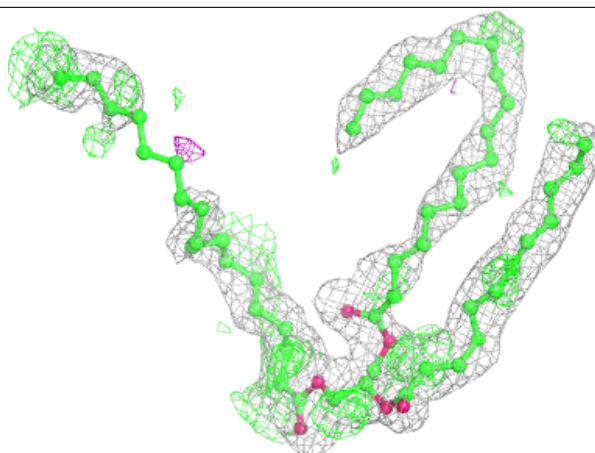
**Electron density around PEK C 306:**

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

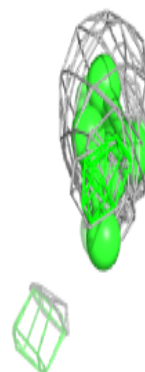
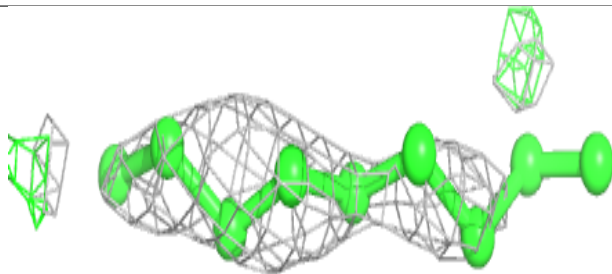
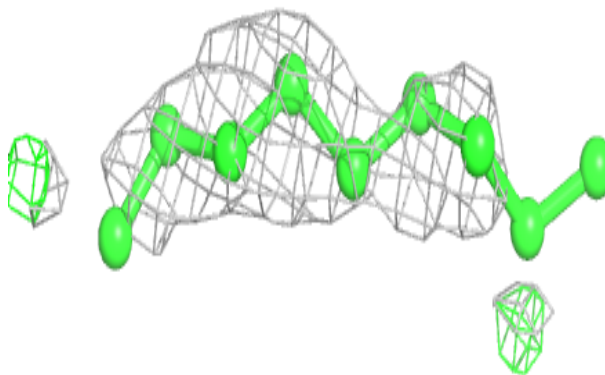


Electron density around TGL D 202:

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

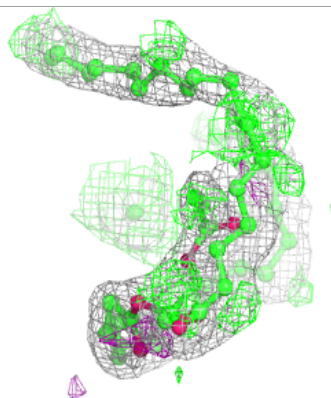
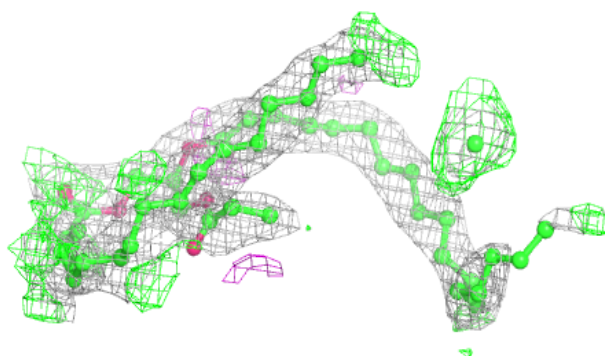
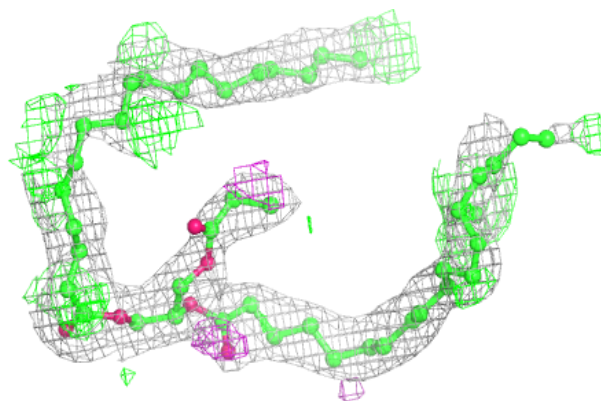
**Electron density around DMU K 105:**

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

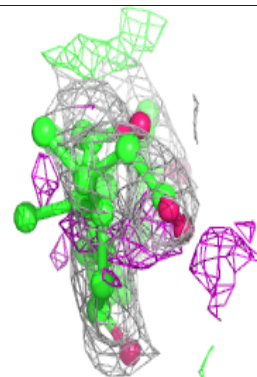
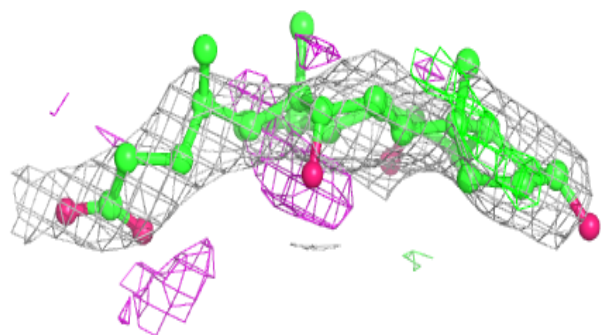
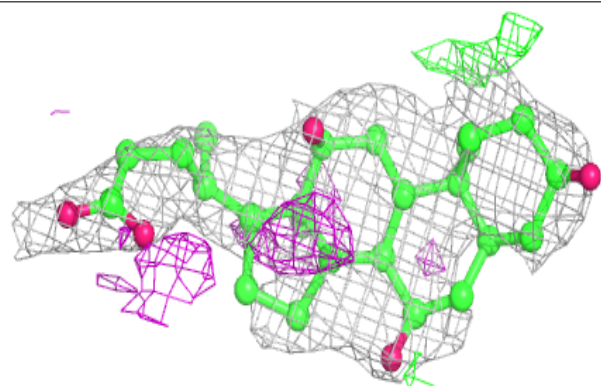


Electron density around TGL B 301:

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

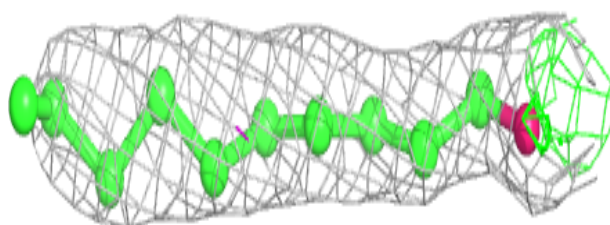
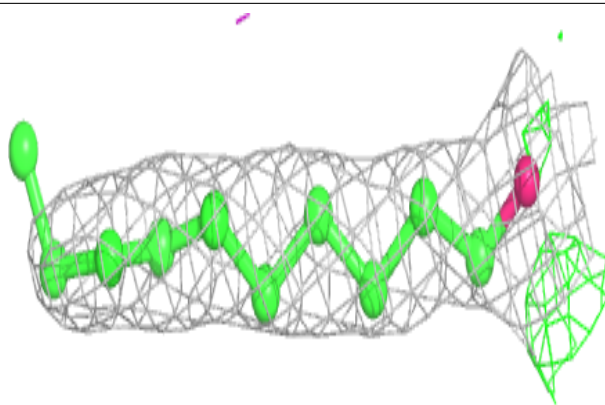
**Electron density around CHD L 102:**

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

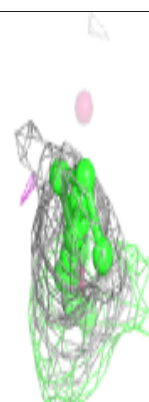
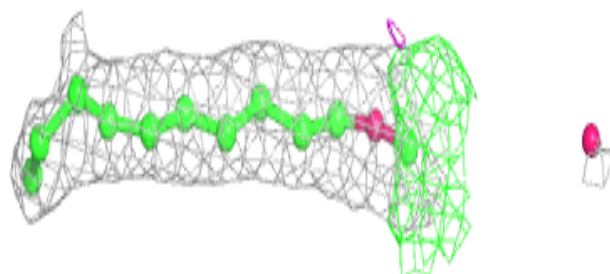
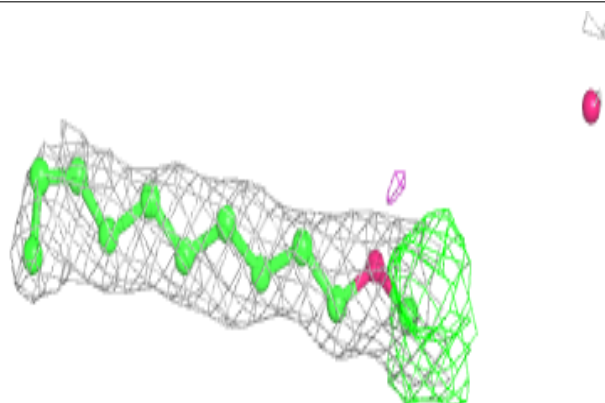


Electron density around DMU O 302:

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

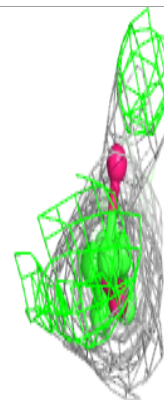
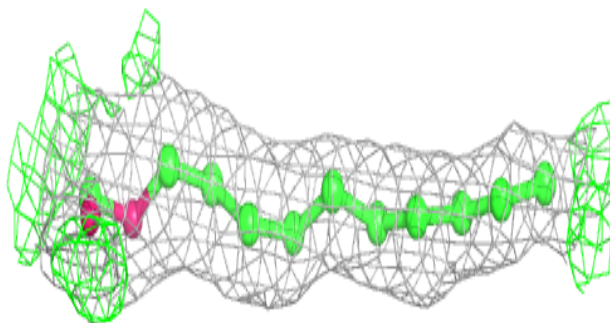
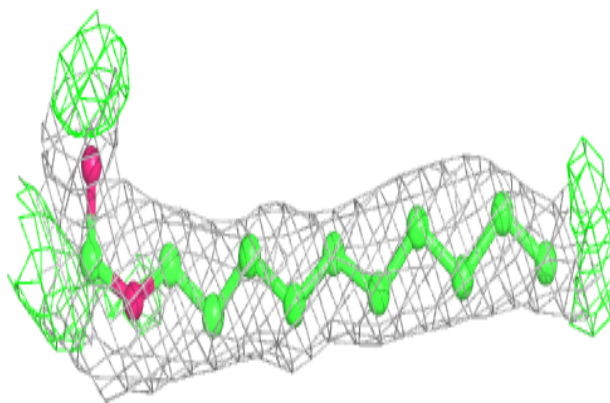
**Electron density around DMU P 303:**

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

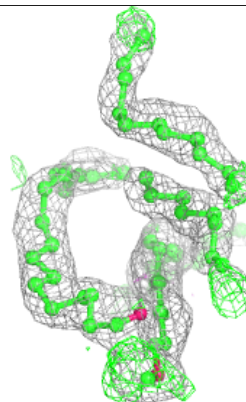
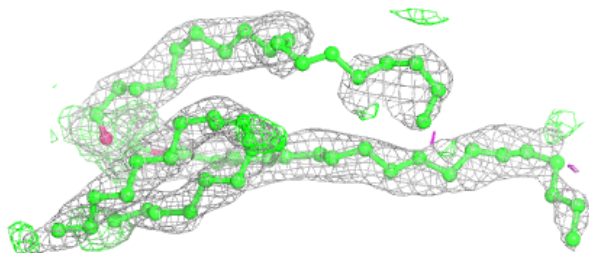
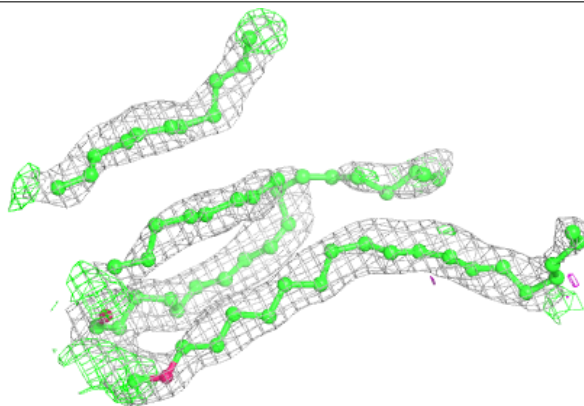


Electron density around DMU C 303:

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

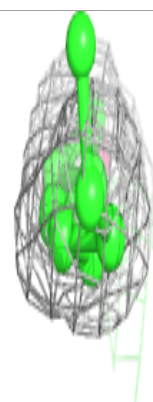
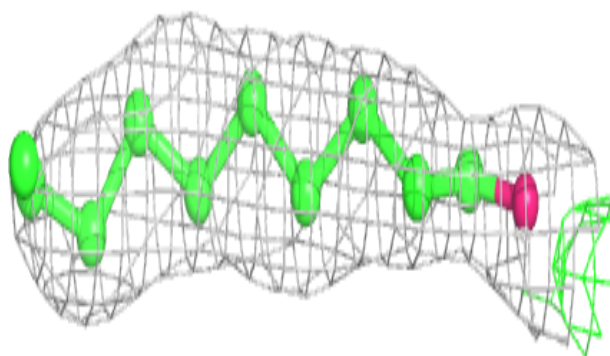
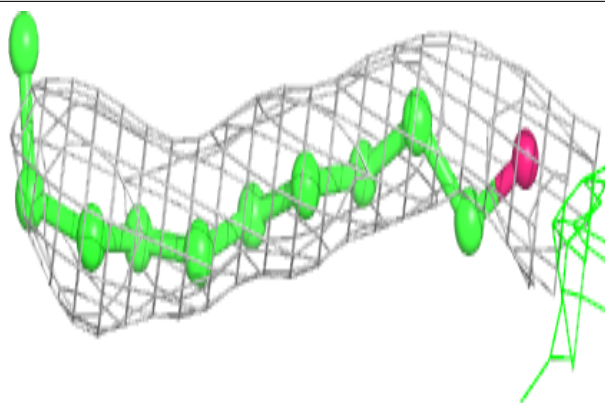
**Electron density around CDL C 305:**

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



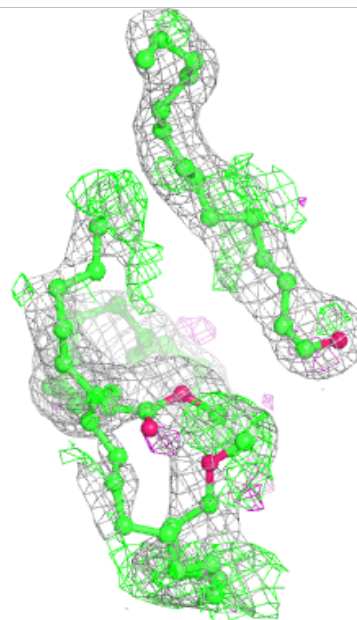
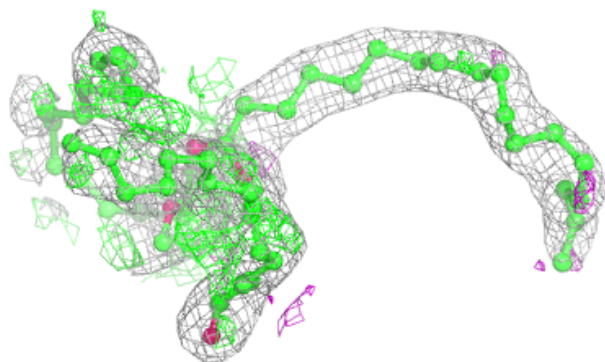
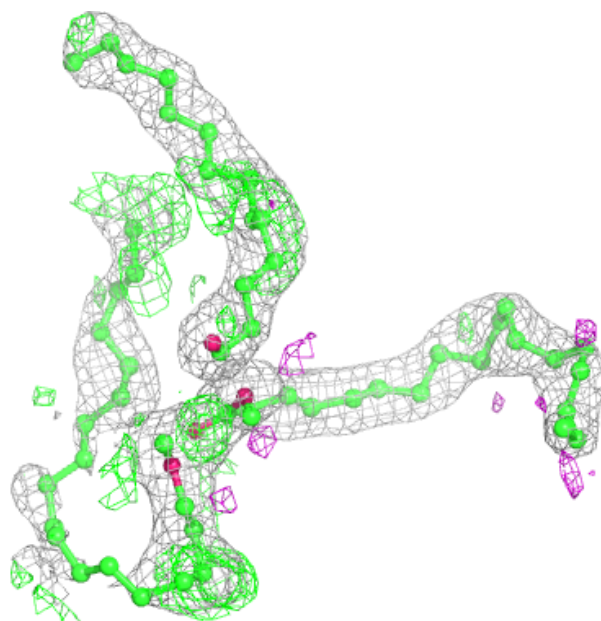
Electron density around DMU W 101:

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



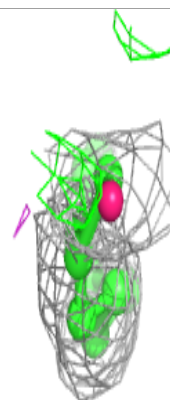
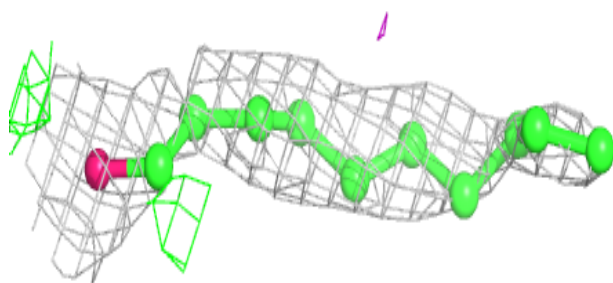
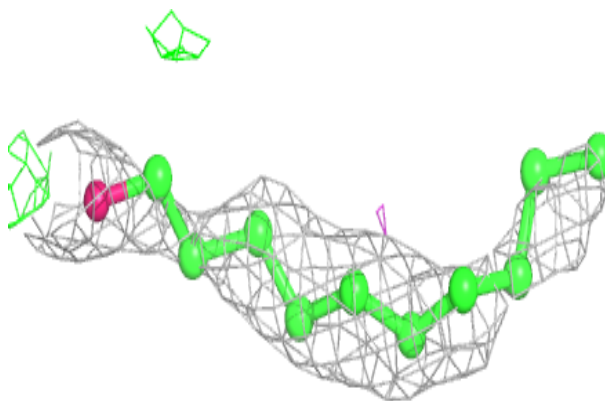
Electron density around TGL L 103:

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

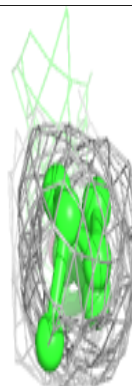
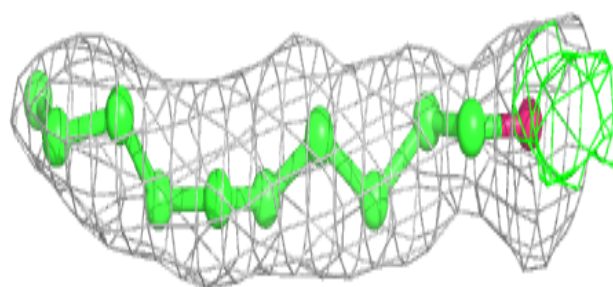
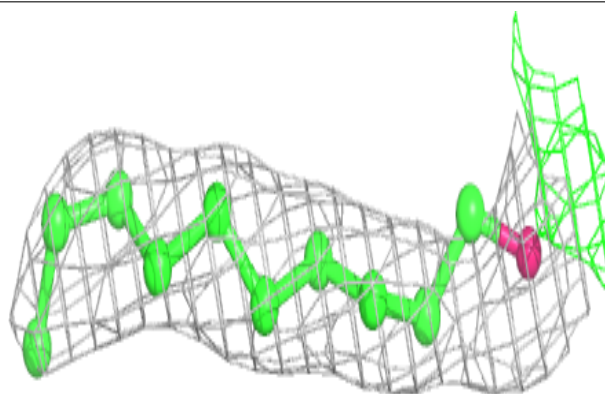


Electron density around DMU K 103:

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

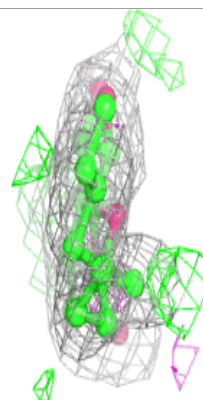
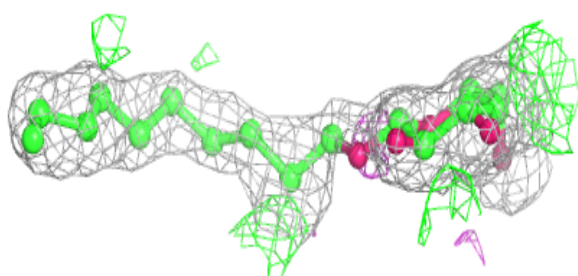
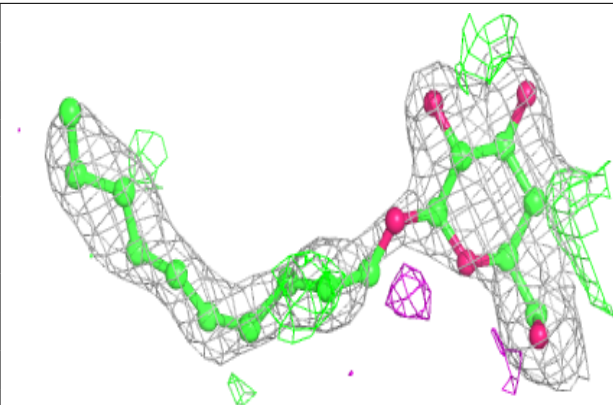
**Electron density around DMU J 101:**

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

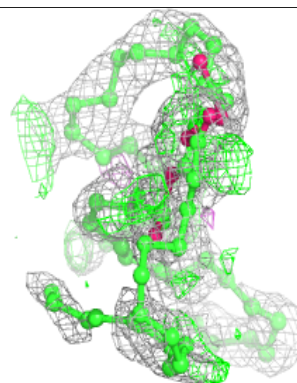
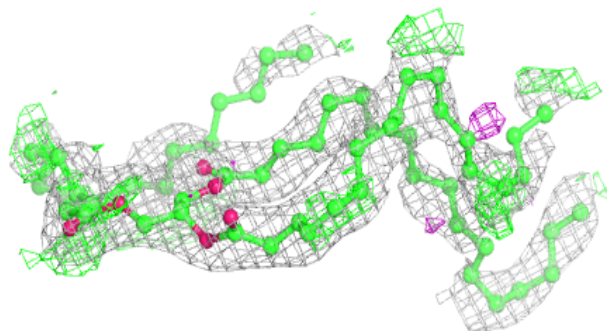
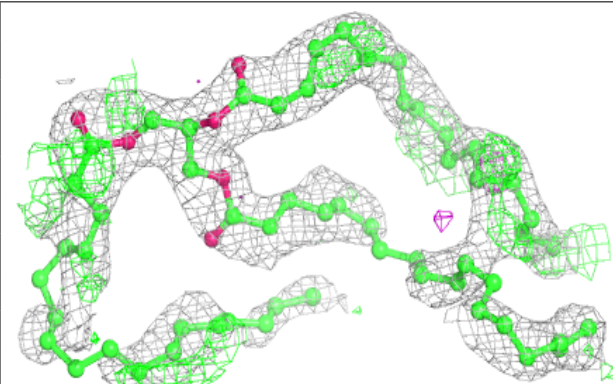


Electron density around DMU C 310:

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

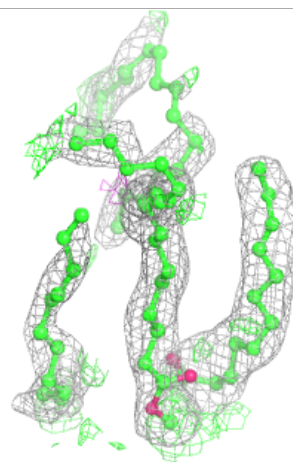
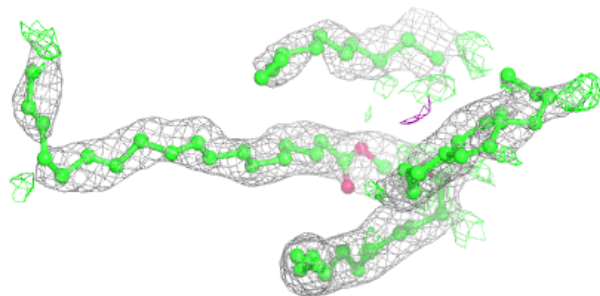
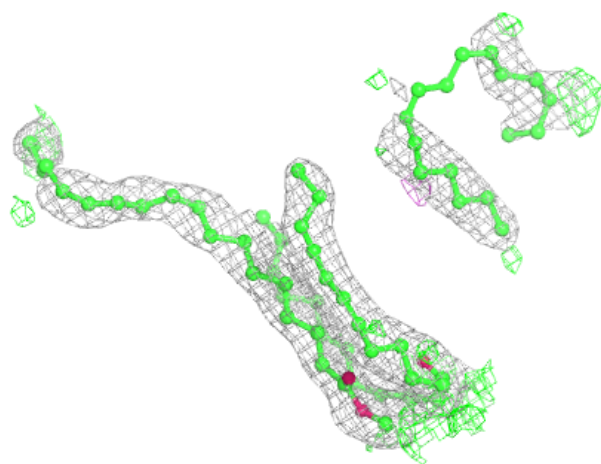
**Electron density around TGL N 609:**

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



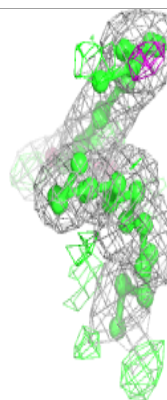
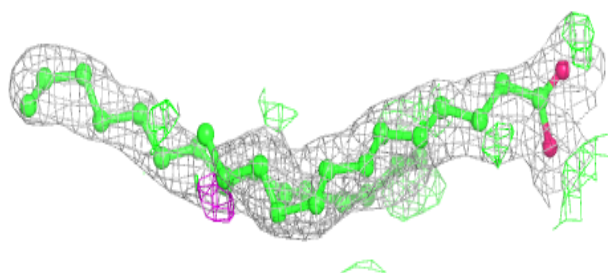
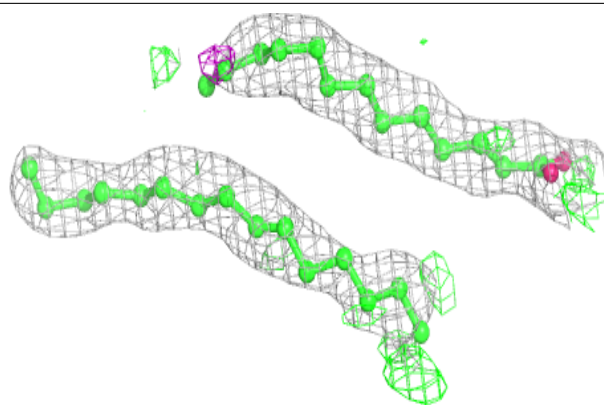
Electron density around CDL P 304:

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

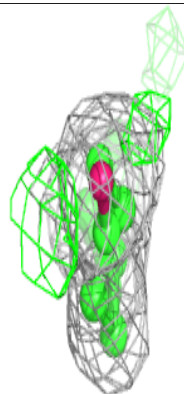
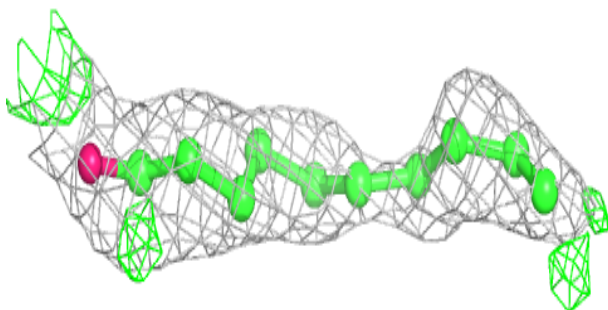
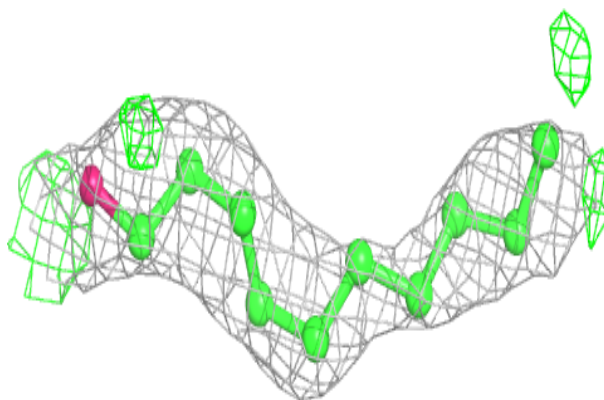


Electron density around PSC O 303:

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

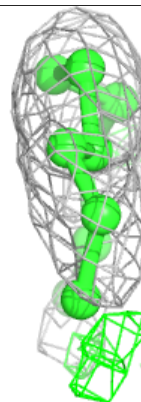
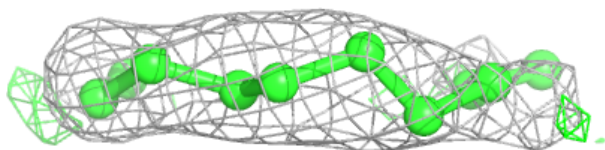
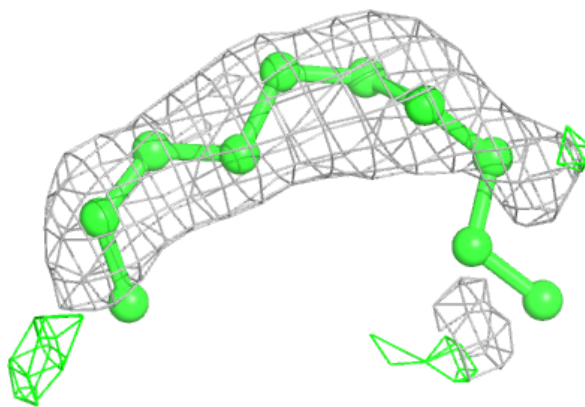
**Electron density around DMU D 201:**

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

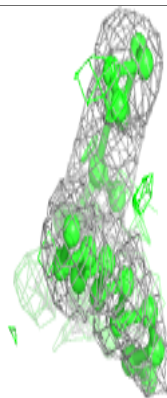
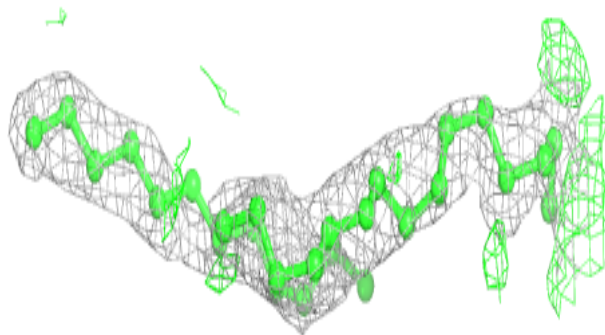
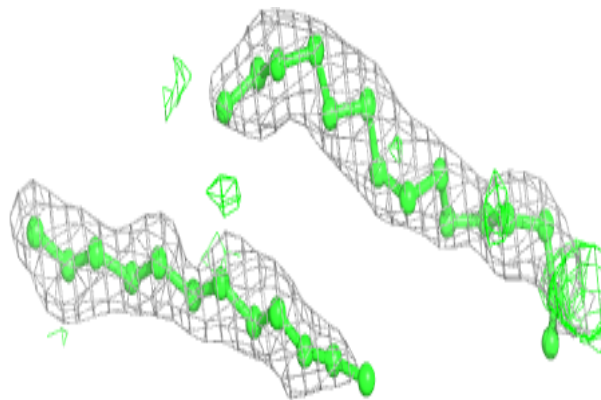


Electron density around DMU K 106:

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

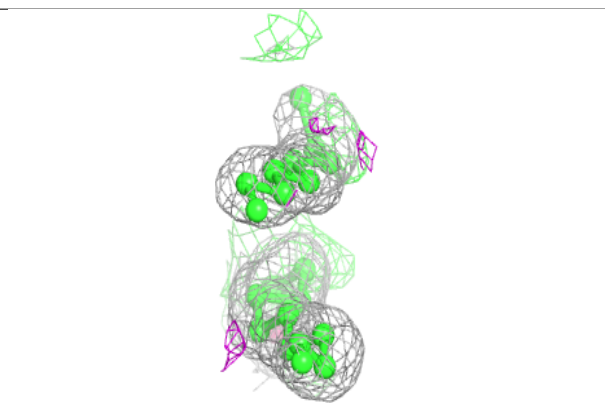
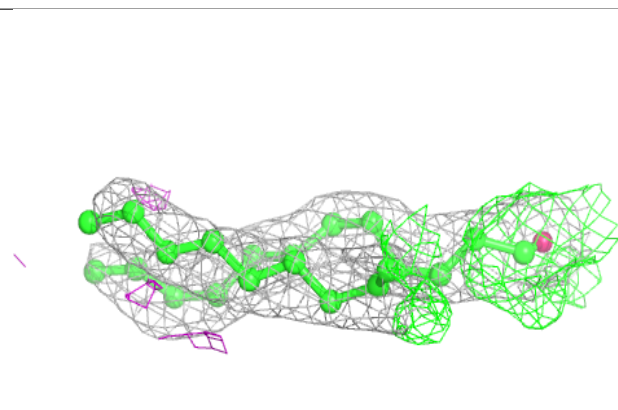
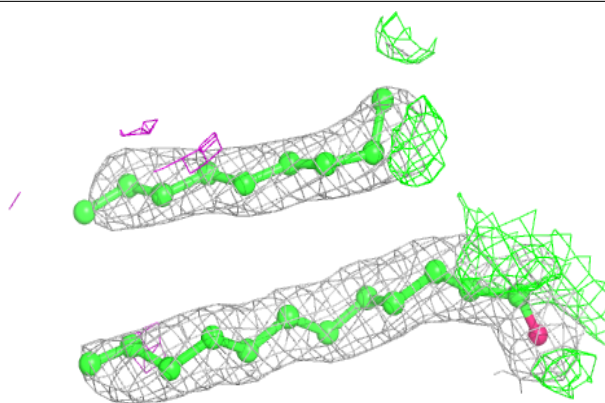
**Electron density around PSC A 607:**

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

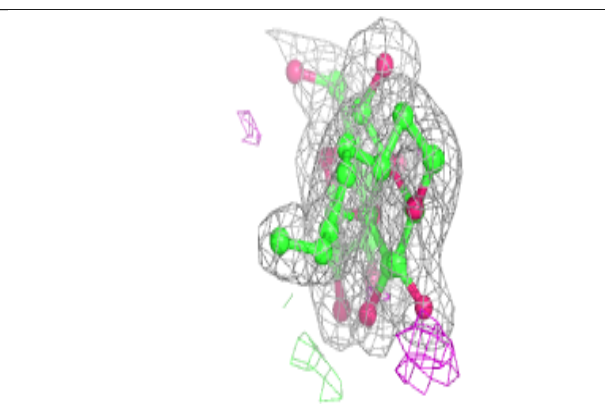
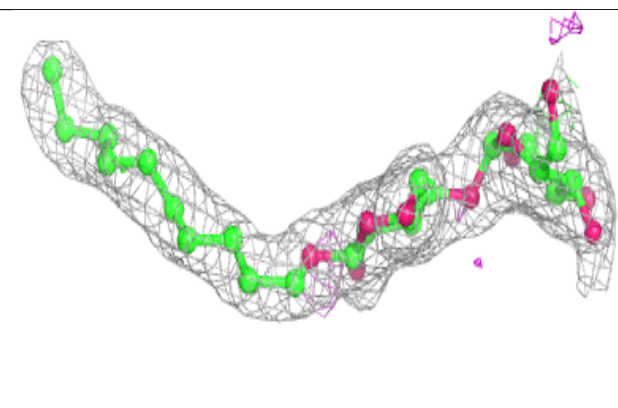
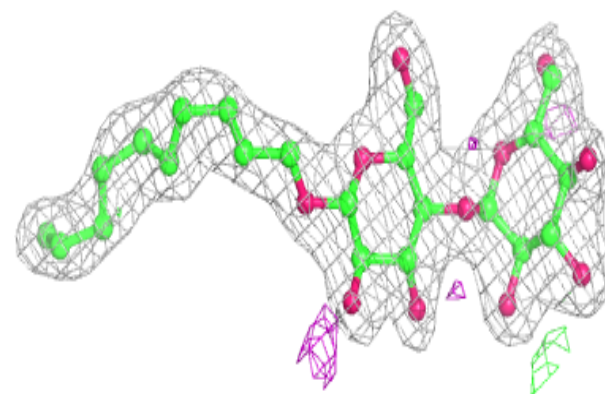


Electron density around PGV A 606:

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

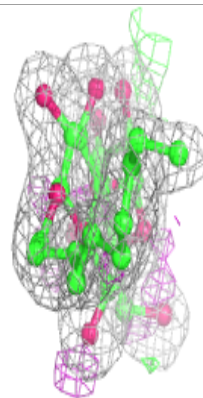
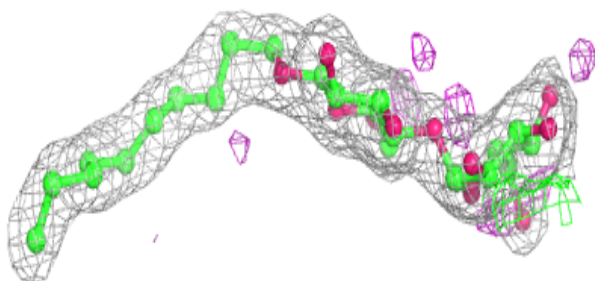
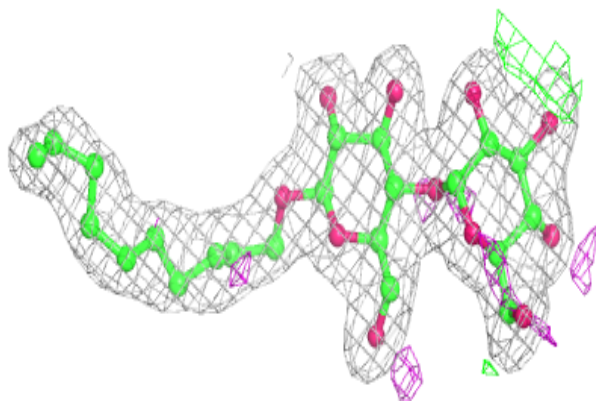
**Electron density around DMU Z 101:**

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

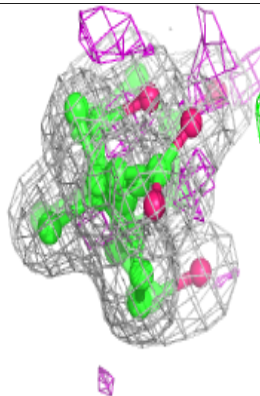
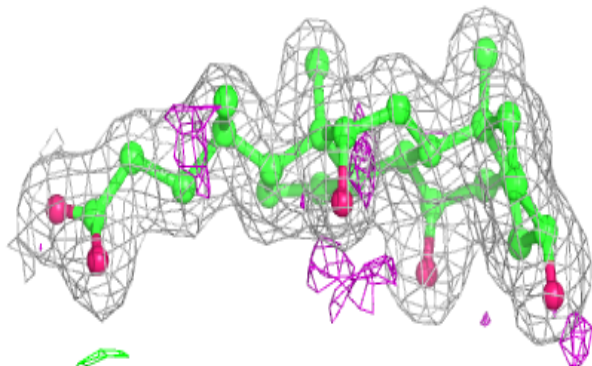
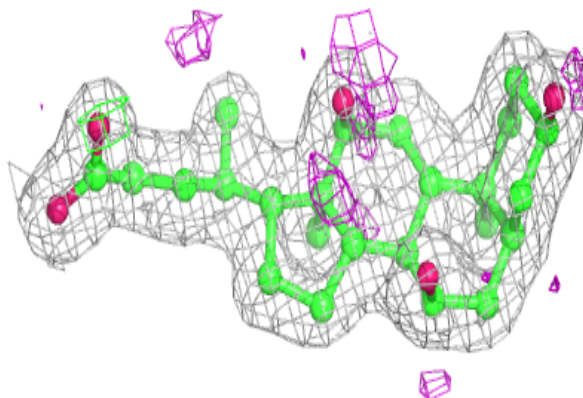


Electron density around DMU M 101:

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

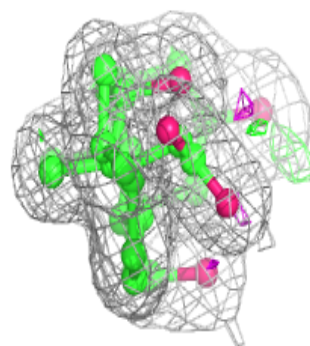
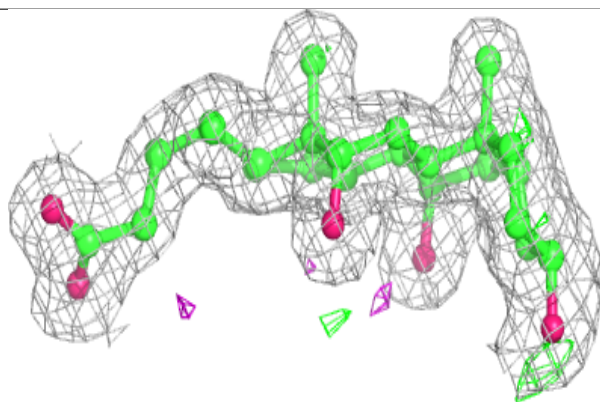
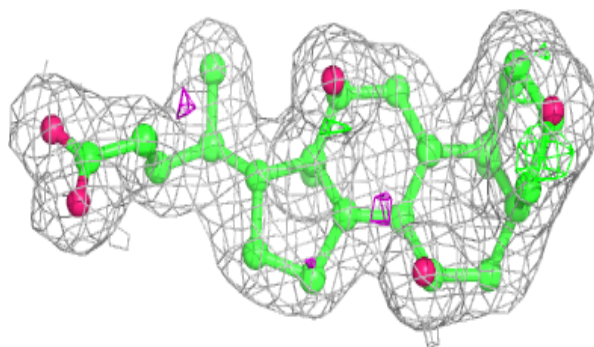
**Electron density around CHD C 304:**

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

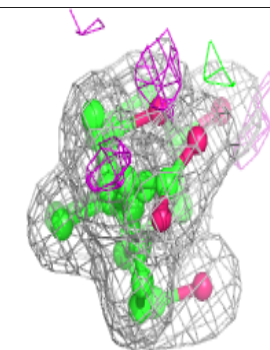
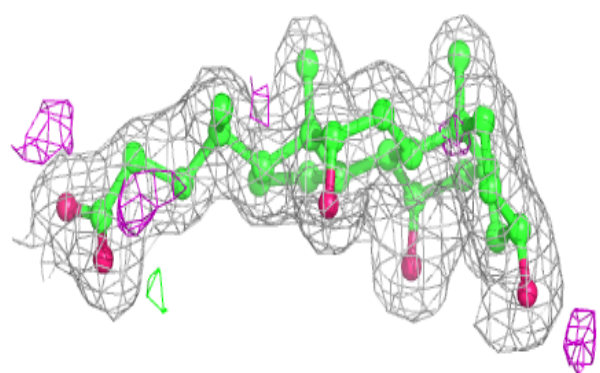
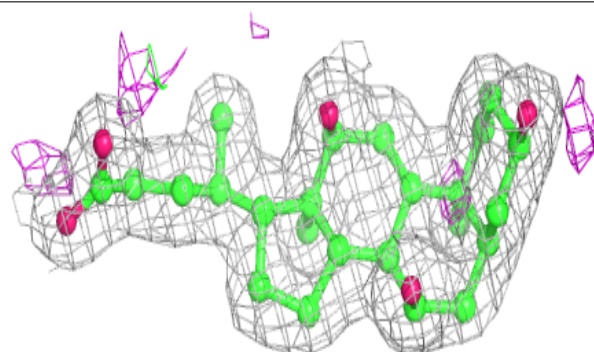


Electron density around CHD G 101:

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

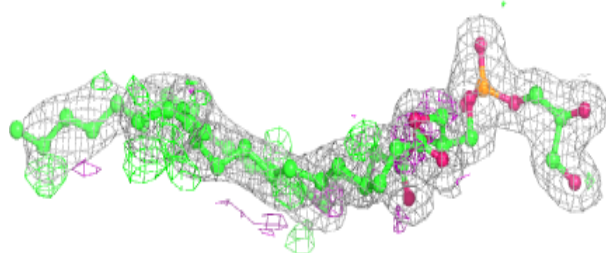
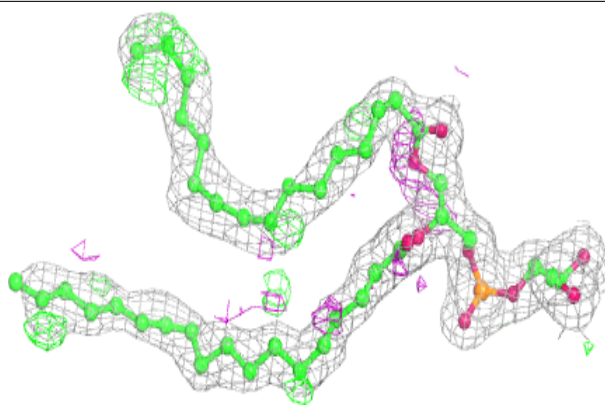
**Electron density around CHD P 301:**

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

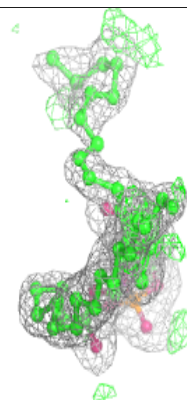
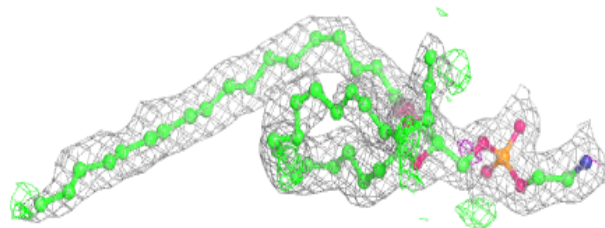
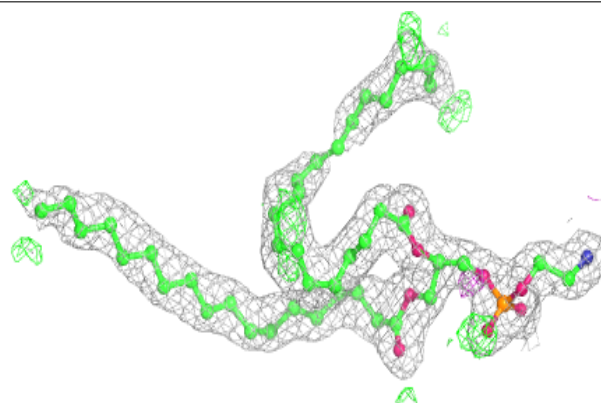


Electron density around PGV N 608:

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

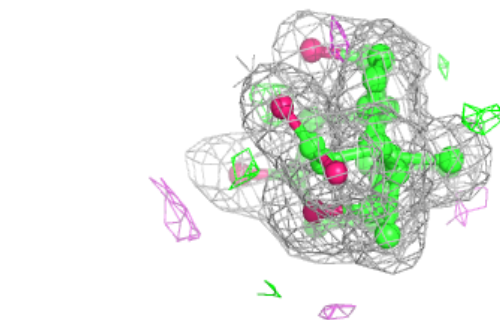
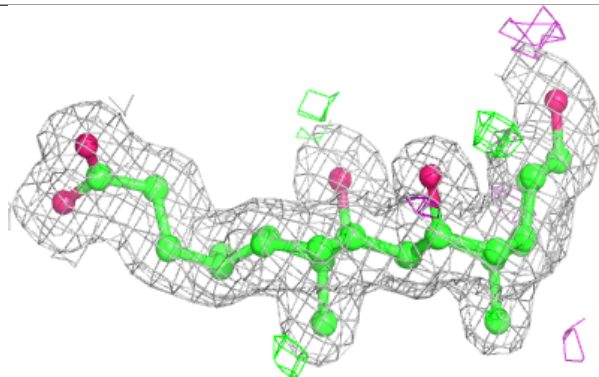
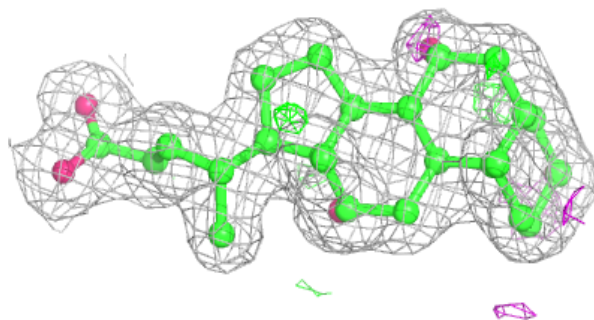
**Electron density around PEK P 306:**

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

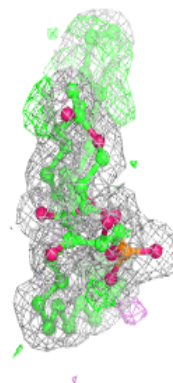
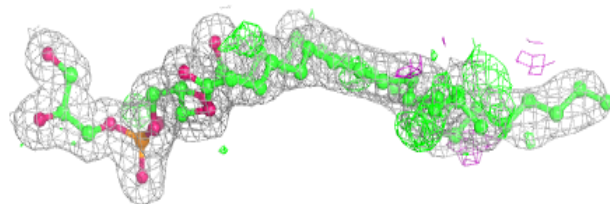
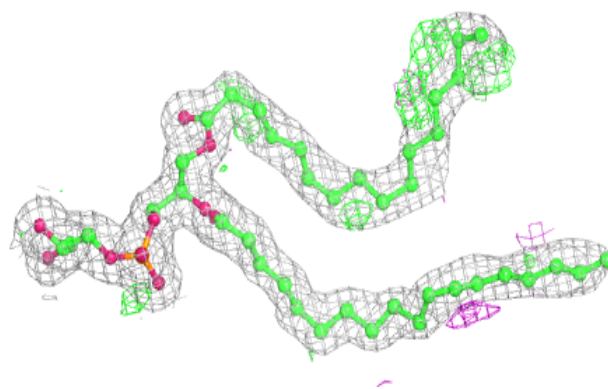


Electron density around CHD B 303:

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

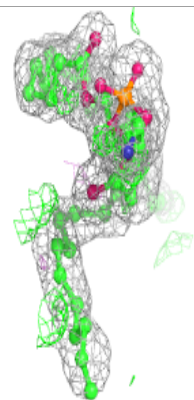
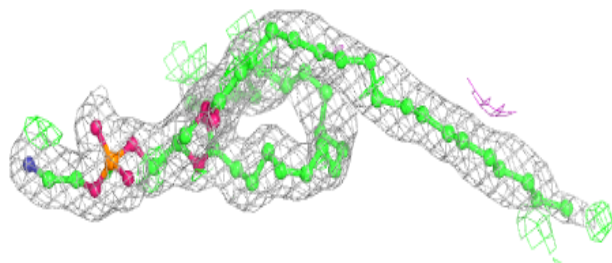
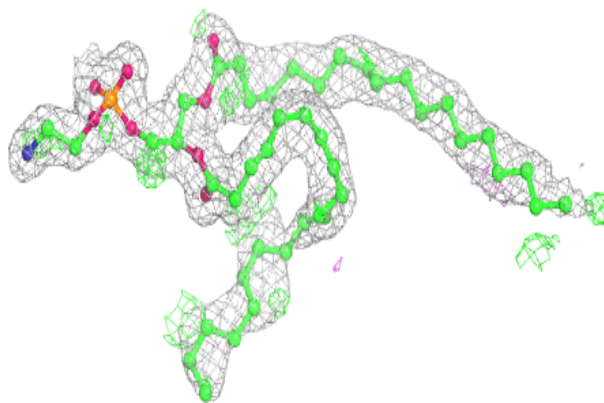
**Electron density around PGV C 301:**

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

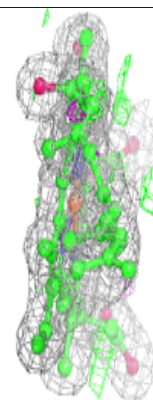
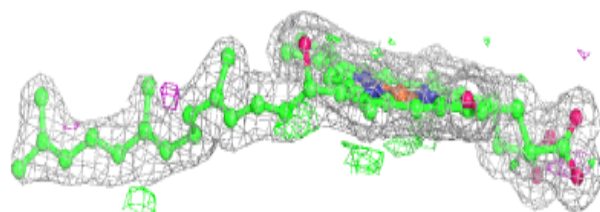
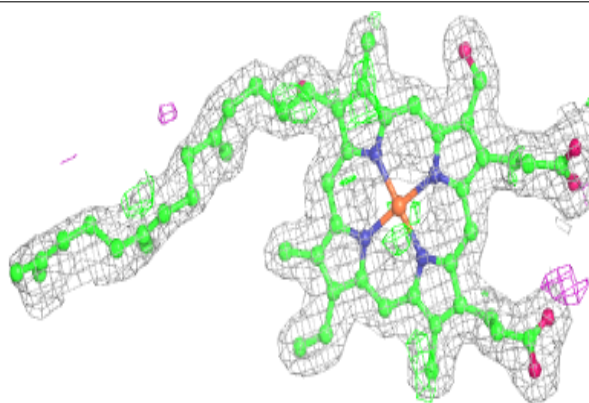


Electron density around PEK C 307:

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

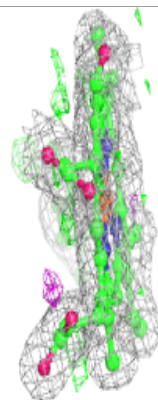
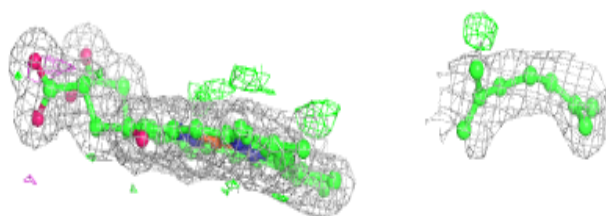
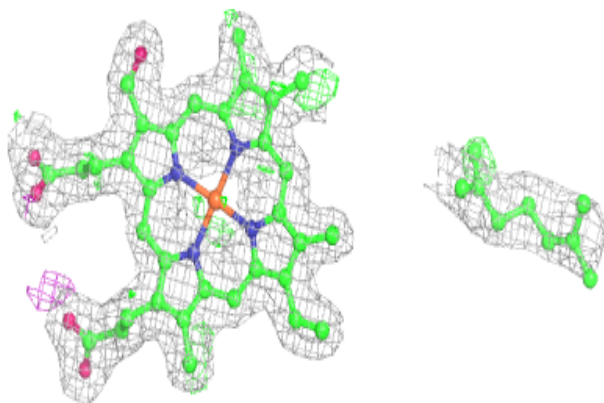
**Electron density around HEA N 602 (A):**

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

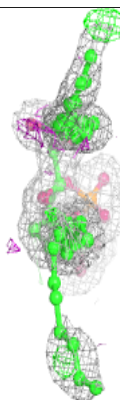
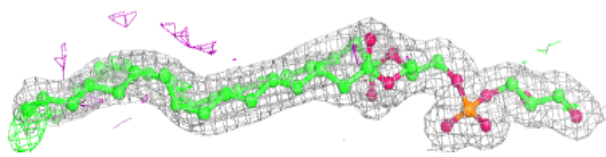
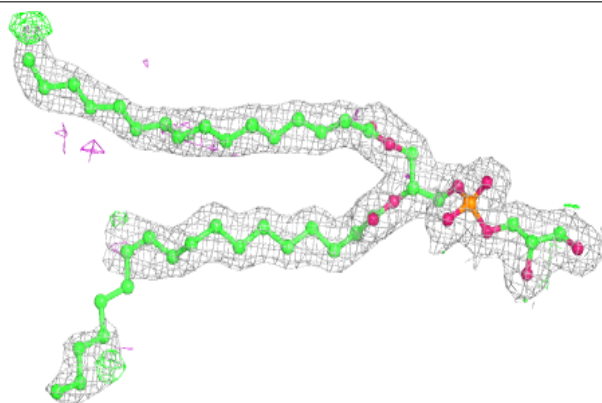


Electron density around HEA N 602 (C):

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

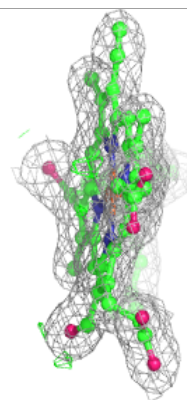
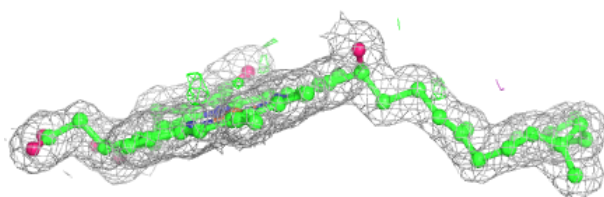
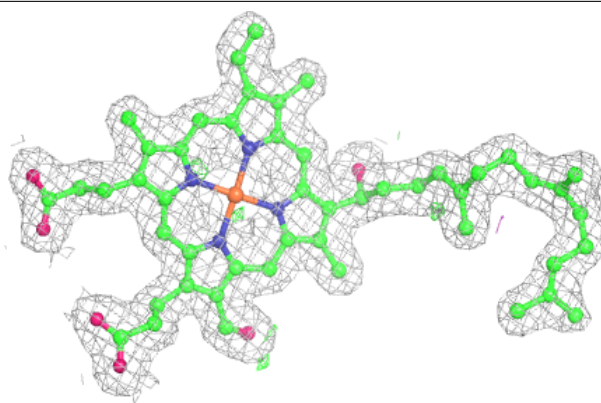
**Electron density around PGV P 307:**

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

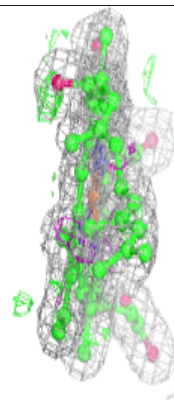
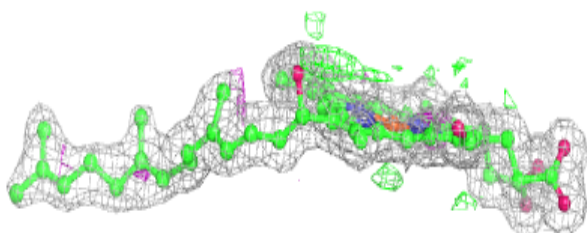
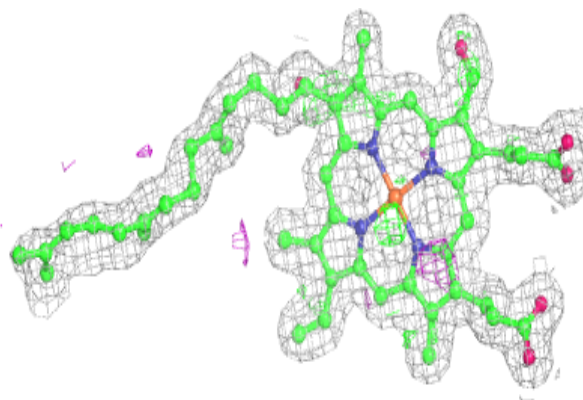


Electron density around HEA N 603:

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

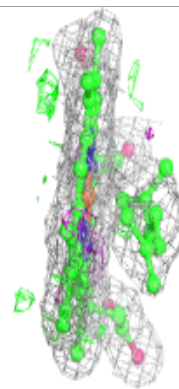
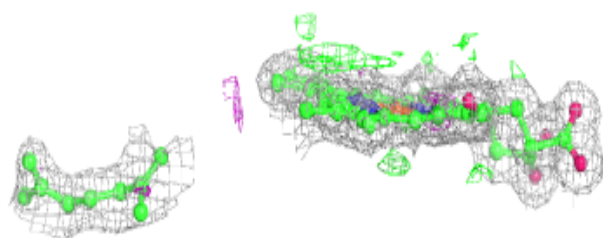
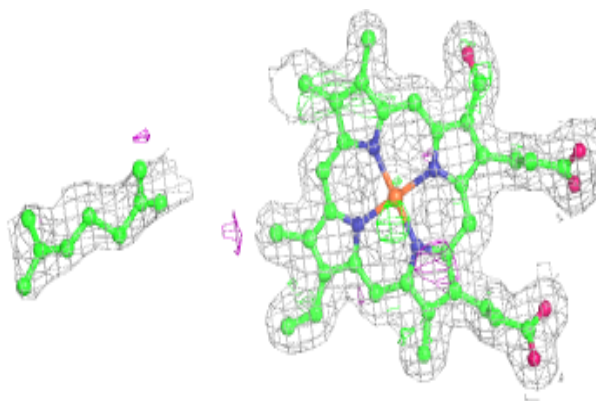
**Electron density around HEA A 601 (A):**

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

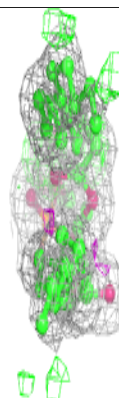
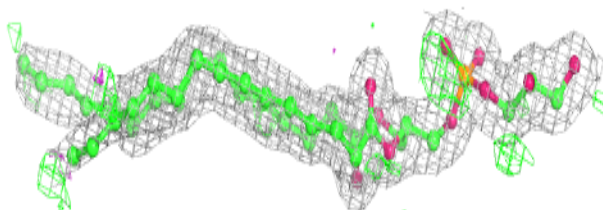
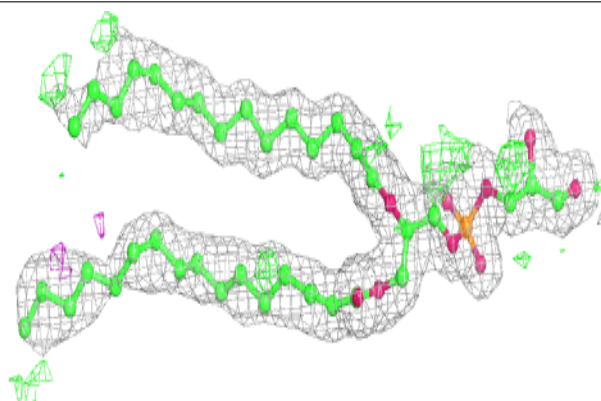


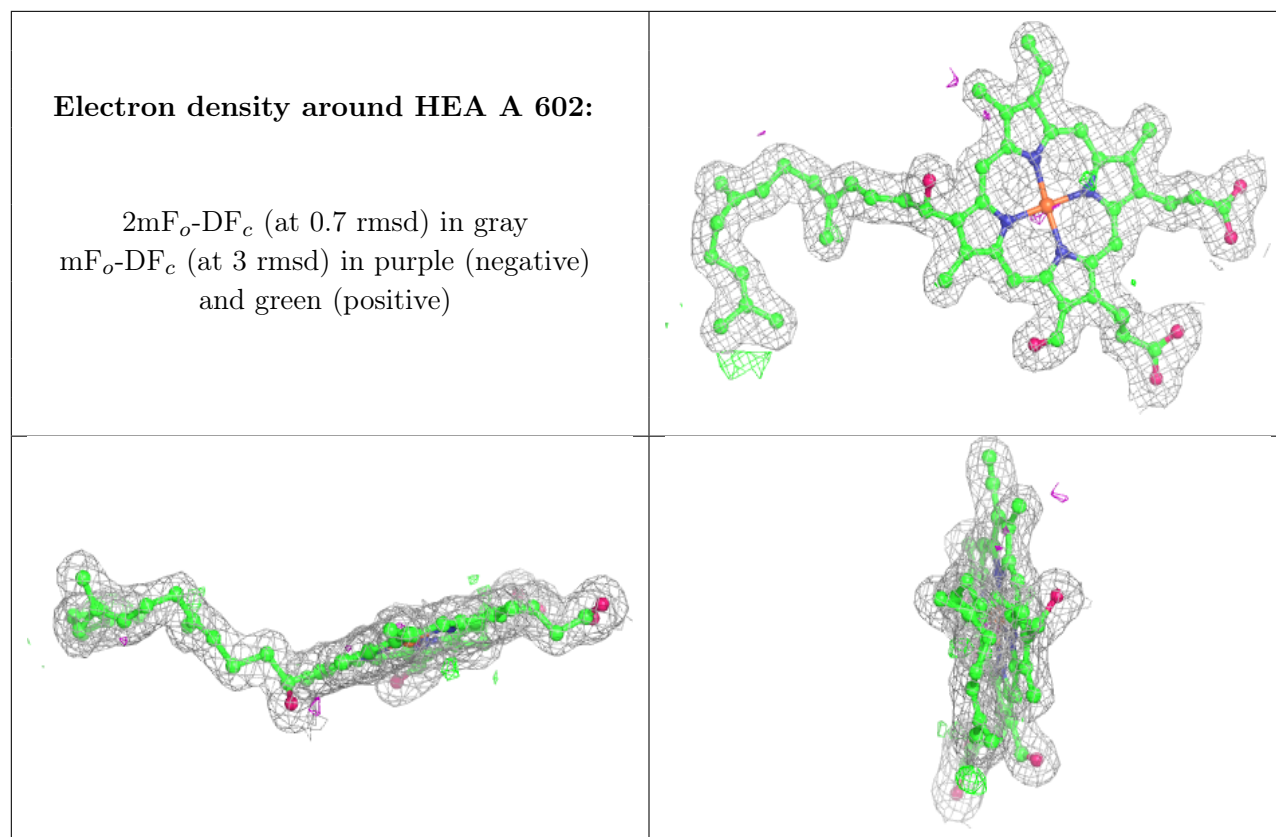
Electron density around HEA A 601 (C):

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

**Electron density around PGV C 308:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.