



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 06:51 PM JST

PDB ID : 7D5W  
Title : Bovine heart cytochrome c oxidase in a catalytic intermediate of O at 1.84 angstrom resolution  
Authors : Tsukihara, T.; Shimada, A.  
Deposited on : 2020-09-28  
Resolution : 1.84 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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 : 2.36  
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) : 2.36

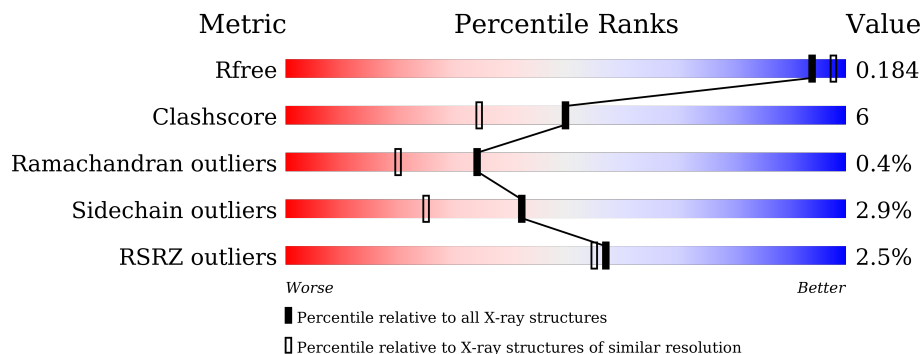
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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.






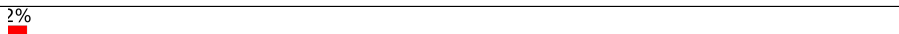
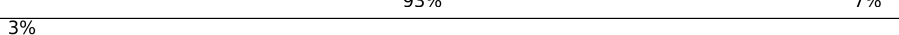




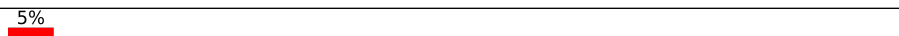
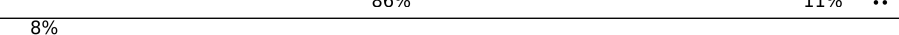

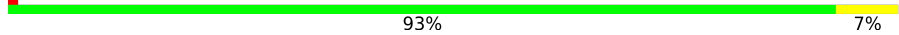


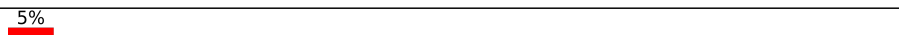


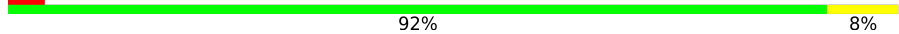

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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  $\geq 3$ , 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	90% 10%
1	N	514	88% 12%
2	B	227	84% 15%
2	O	227	77% 21%
3	C	259	90% 10%
3	P	259	89% 11%

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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
23	DMU	X	104	-	-	-	X
25	CHD	J	101	-	-	-	X
9	SAC	V	1	-	-	-	X

## 2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 34545 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
			Total	C	N	O	S			
1	A	514	Total	C	N	O	S	0	34	0
			4193	2793	646	714	40			
1	N	514	Total	C	N	O	S	0	38	0
			4199	2799	644	714	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	Total	C	N	O	S	0	8	0
			1851	1202	281	347	21			
2	O	227	Total	C	N	O	S	0	12	0
			1872	1217	288	346	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	259	Total	C	N	O	S	0	11	0
			2144	1430	340	359	15			
3	P	259	Total	C	N	O	S	0	11	0
			2143	1431	341	357	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	144	Total	C	N	O	S	0	3	0
			1209	788	199	218	4			
4	Q	144	Total	C	N	O	S	0	1	0
			1197	779	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
			858	547	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
			731	451	129	145	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	5	0
			690	445	130	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
			665	418	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
			605	392	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
			462	297	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
			390	254	65	69	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

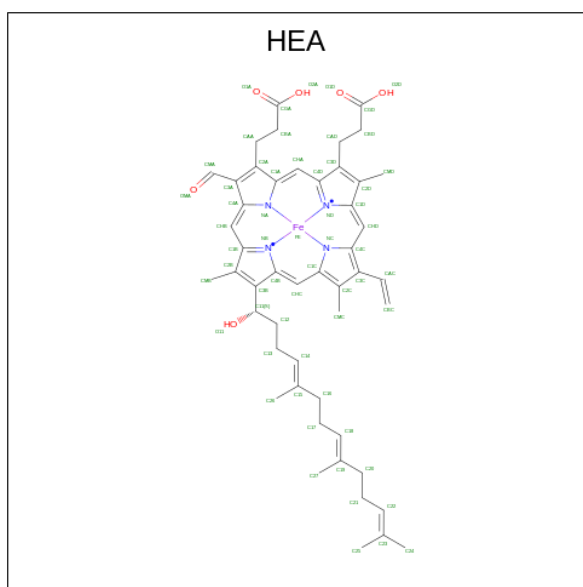
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	2	0
			386	259	64	60	3			
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<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
14	A	1	Total	C	Fe	N	O	0	1
			81	69	1	4	7		
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	1
			81	69	1	4	7		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- 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		

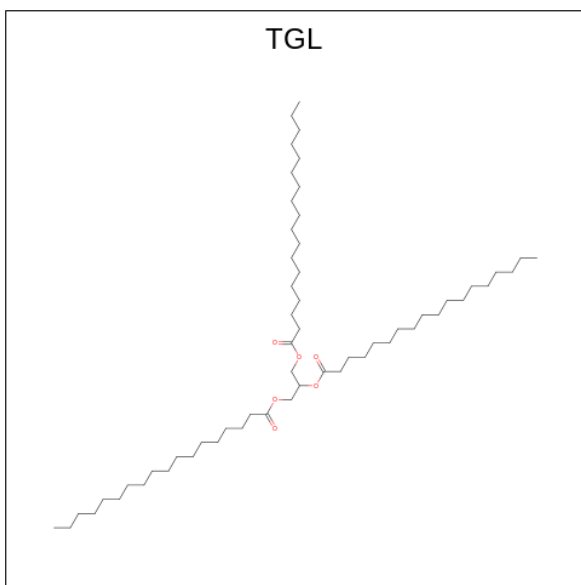
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

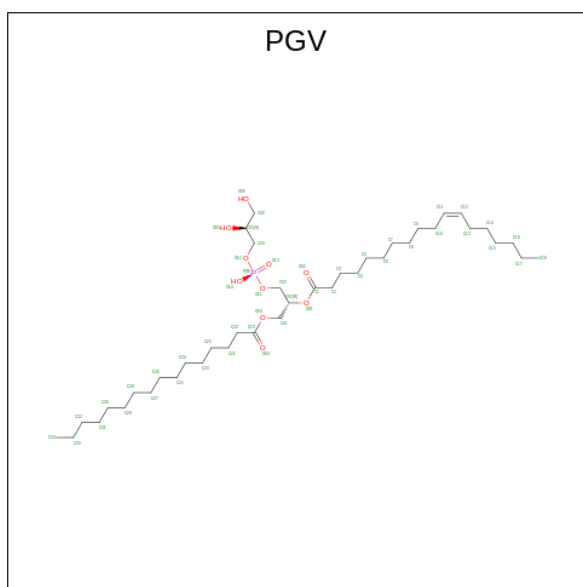
- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O 63 57 6	0	0
18	A	1	Total C O 63 57 6	0	0
18	L	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0
18	N	1	Total C O 55 53 2	0	0
18	N	1	Total C O 55 53 2	0	0

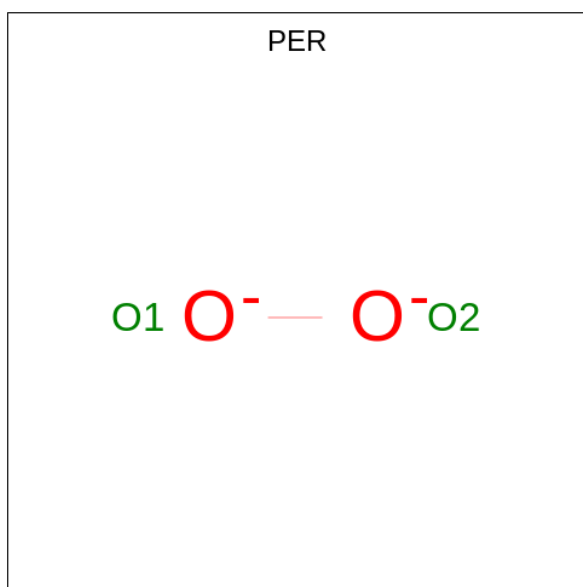
- Molecule 19 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).





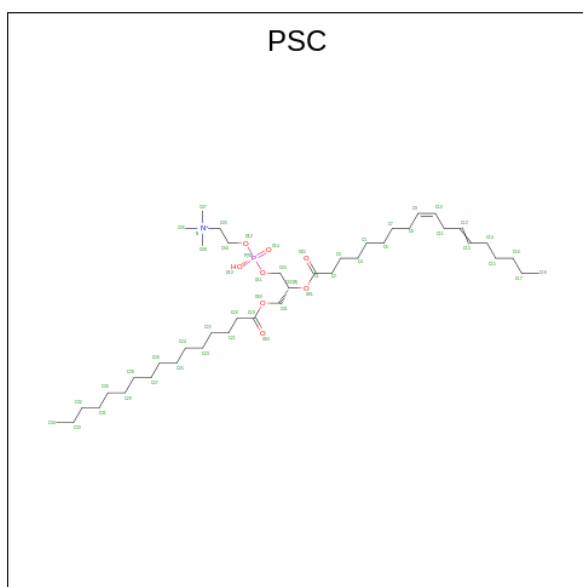
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 34 32 2	0	0
19	A	1	Total C O P 51 40 10 1	0	0
19	C	1	Total C O P 48 37 10 1	0	0
19	C	1	Total C O 36 32 4	0	0
19	N	1	Total C O P 51 40 10 1	0	0
19	N	1	Total C O P 51 40 10 1	0	0
19	P	1	Total C O P 51 40 10 1	0	0
19	P	1	Total C O 31 29 2	0	0

- Molecule 20 is PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



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

- Molecule 21 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: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



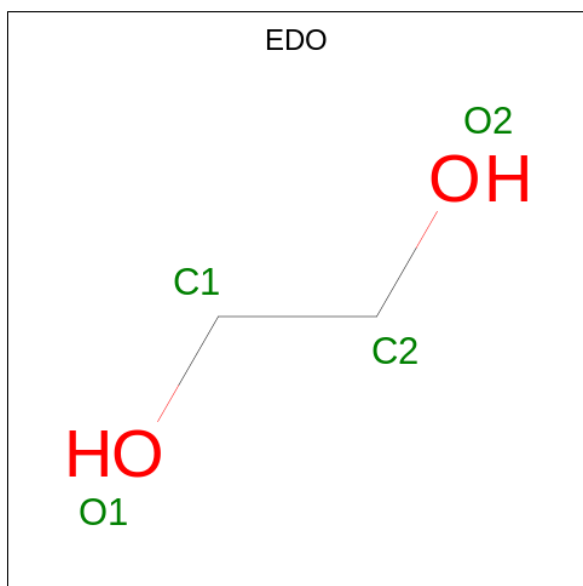
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 25 25	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	O	1	Total	C	O	0	0
			31	29	2		

- Molecule 22 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total 4	C 2	O 2	0	0
22	B	1	Total 4	C 2	O 2	0	0
22	B	1	Total 4	C 2	O 2	0	0
22	B	1	Total 4	C 2	O 2	0	0
22	B	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	C	1	Total 4	C 2	O 2	0	0
22	D	1	Total 4	C 2	O 2	0	0
22	D	1	Total 4	C 2	O 2	0	0
22	D	1	Total 4	C 2	O 2	0	0
22	D	1	Total 4	C 2	O 2	0	0
22	D	1	Total 4	C 2	O 2	0	0
22	E	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	E	1	Total	C	O	0	0
			4	2	2		
22	E	1	Total	C	O	0	0
			4	2	2		
22	F	1	Total	C	O	0	0
			4	2	2		
22	F	1	Total	C	O	0	0
			4	2	2		
22	F	1	Total	C	O	0	0
			4	2	2		
22	F	1	Total	C	O	0	0
			4	2	2		
22	F	1	Total	C	O	0	0
			4	2	2		
22	F	1	Total	C	O	0	0
			4	2	2		
22	F	1	Total	C	O	0	0
			4	2	2		
22	G	1	Total	C	O	0	0
			4	2	2		
22	J	1	Total	C	O	0	0
			4	2	2		
22	J	1	Total	C	O	0	0
			4	2	2		
22	L	1	Total	C	O	0	0
			4	2	2		
22	L	1	Total	C	O	0	0
			4	2	2		
22	M	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		

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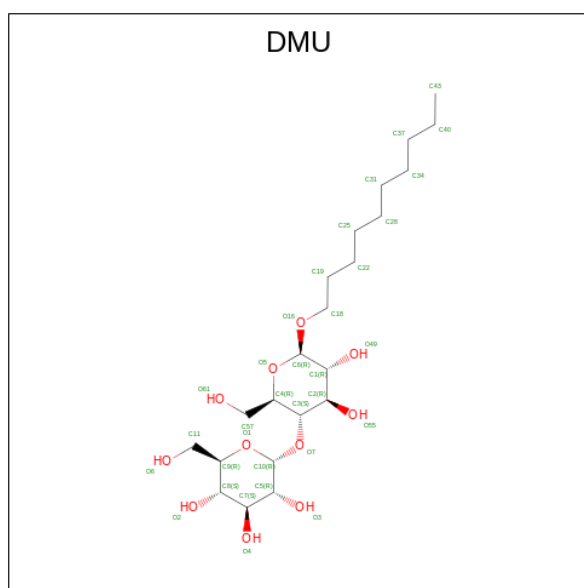
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	O	1	Total 4	C 2	O 2	0	0
22	O	1	Total 4	C 2	O 2	0	0
22	O	1	Total 4	C 2	O 2	0	0
22	P	1	Total 4	C 2	O 2	0	0
22	P	1	Total 4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

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

- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula:  $C_{22}H_{42}O_{11}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 11 10 1	0	0
23	C	1	Total C O 33 22 11	0	0
23	C	1	Total C O 12 11 1	0	0
23	D	1	Total C O 33 22 11	0	0

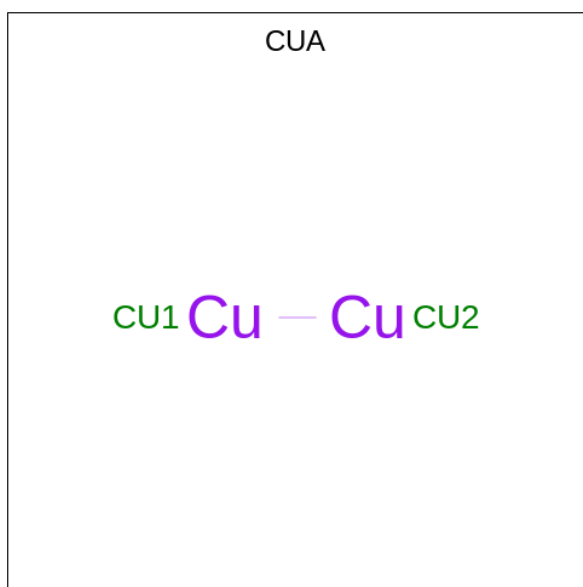
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	D	1	Total C O 11 10 1	0	0
23	J	1	Total C O 11 10 1	0	0
23	K	1	Total C 8 8	0	0
23	K	1	Total C O 11 10 1	0	0
23	K	1	Total C 10 10	0	0
23	K	1	Total C O 11 10 1	0	0
23	K	1	Total C 9 9	0	0
23	L	1	Total C O 21 16 5	0	0
23	M	1	Total C O 33 22 11	0	0
23	O	1	Total C O 13 11 2	0	0
23	P	1	Total C O 33 22 11	0	0
23	P	1	Total C O 21 16 5	0	0
23	P	1	Total C O 32 21 11	0	0
23	Q	1	Total C O 11 10 1	0	0
23	X	1	Total C 10 10	0	0
23	X	1	Total C 9 9	0	0
23	X	1	Total C 9 9	0	0
23	X	1	Total C O 22 16 6	0	0
23	Z	1	Total C O 33 22 11	0	0

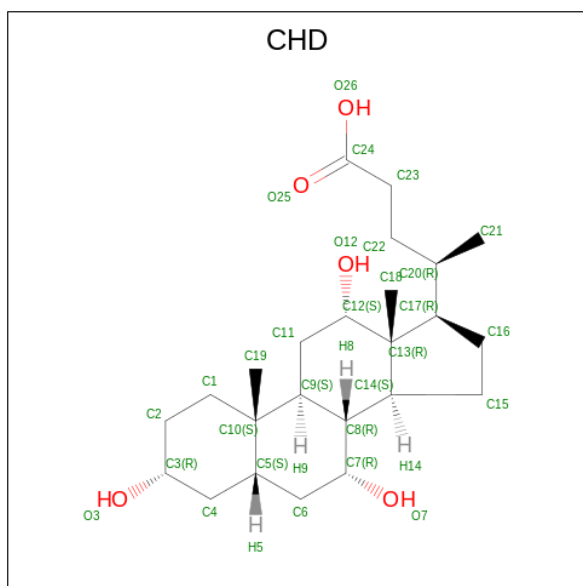
- Molecule 24 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).





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

- Molecule 25 is CHOLIC ACID (three-letter code: CHD) (formula:  $C_{24}H_{40}O_5$ ).



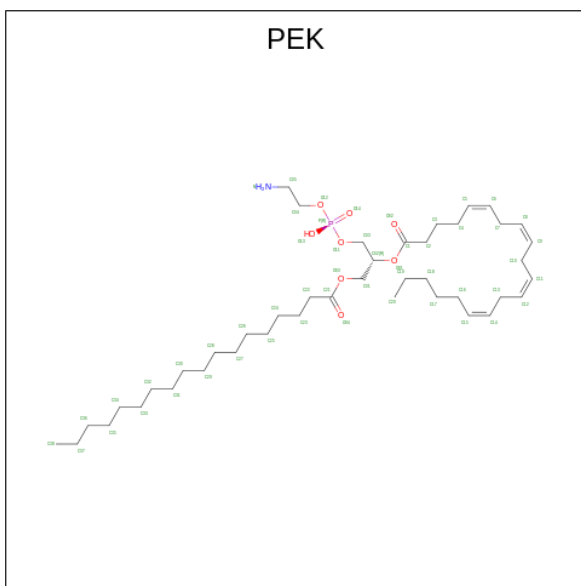
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B	1	Total C O 29 24 5	0	0
25	C	1	Total C O 29 24 5	0	0

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

- Molecule 26 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



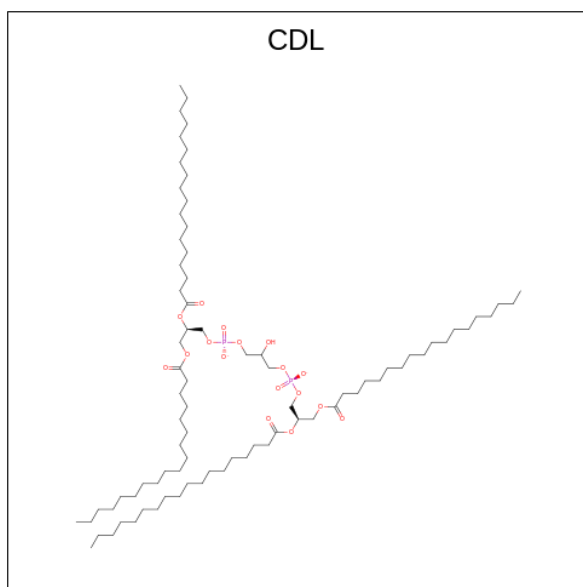
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	C	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
26	C	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	C	1	Total	C				0	0
			36	36					
26	P	1	Total	C	N	O	P	0	0
			38	28	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	P	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	T	1	Total	C	O			0	0
			37	35	2				

- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	C	1	Total	C	O	0	0
			65	61	4		
27	N	1	Total	C	O	0	0
			62	60	2		
27	P	1	Total	C	O	0	0
			68	64	4		
27	T	1	Total	C	O	0	0
			61	59	2		

- 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:  $O_4P$ ).



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	274	Total O 274 274	0	14
30	B	229	Total O 229 229	0	4
30	C	153	Total O 153 153	0	0
30	D	206	Total O 207 207	0	2
30	E	162	Total O 162 162	0	0
30	F	161	Total O 161 161	0	0
30	G	87	Total O 87 87	0	0
30	H	92	Total O 92 92	0	0
30	I	71	Total O 71 71	0	0
30	J	61	Total O 61 61	0	0

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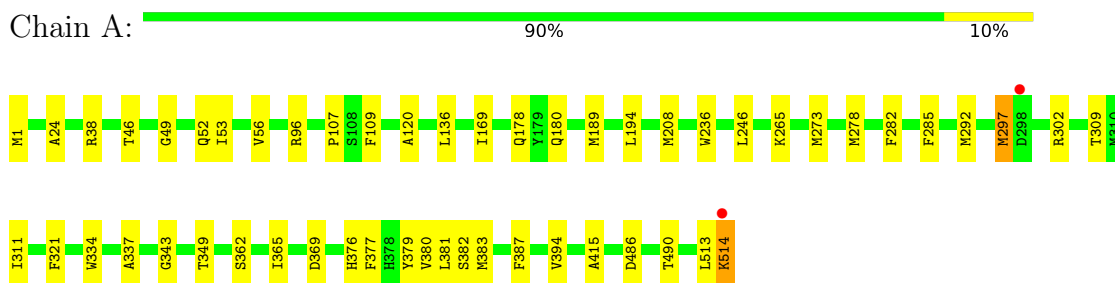
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	45	Total 45	O 45	0	0
30	L	40	Total 40	O 40	0	1
30	M	37	Total 37	O 37	0	0
30	N	282	Total 282	O 282	0	10
30	O	199	Total 199	O 199	0	2
30	P	161	Total 161	O 161	0	3
30	Q	119	Total 119	O 119	0	0
30	R	112	Total 113	O 113	0	1
30	S	141	Total 141	O 141	0	0
30	T	66	Total 66	O 66	0	0
30	U	96	Total 96	O 96	0	0
30	V	65	Total 66	O 66	0	1
30	W	41	Total 41	O 41	0	0
30	X	33	Total 33	O 33	0	0
30	Y	31	Total 31	O 31	0	1
30	Z	28	Total 28	O 28	0	0

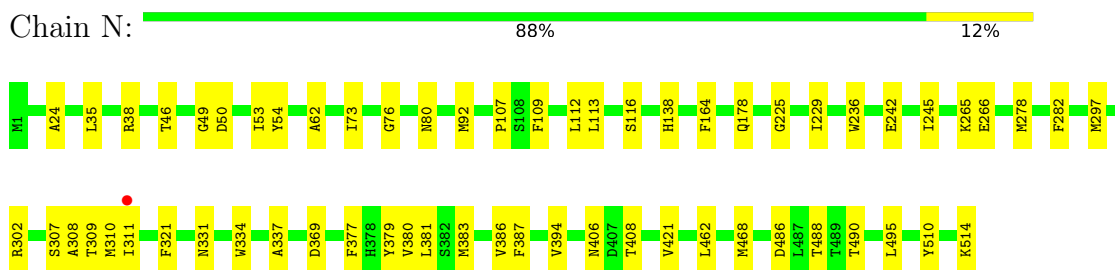
### 3 Residue-property plots [i](#)

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.

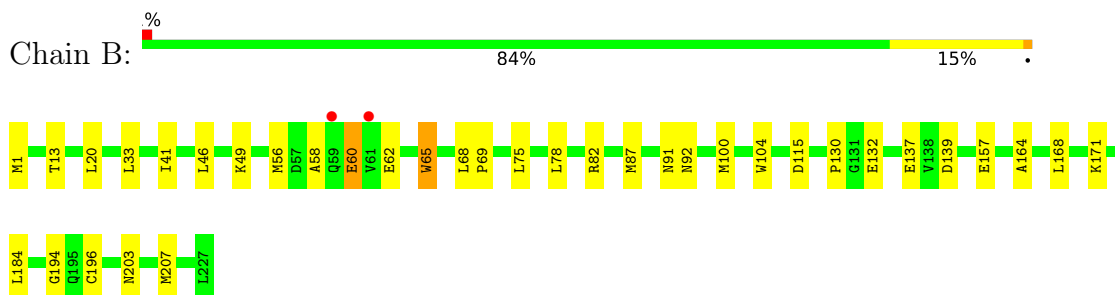
- Molecule 1: Cytochrome c oxidase subunit 1



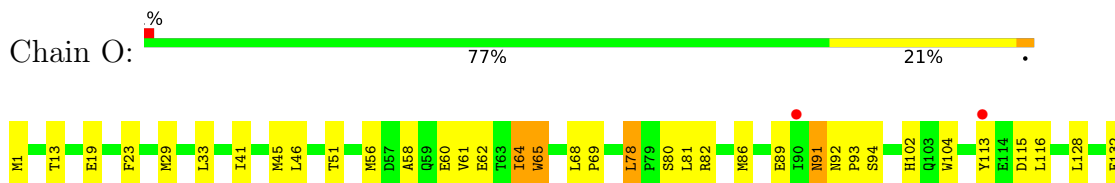
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase subunit 2

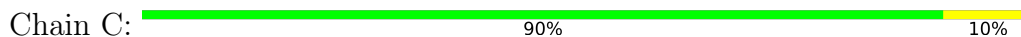


- Molecule 2: Cytochrome c oxidase subunit 2

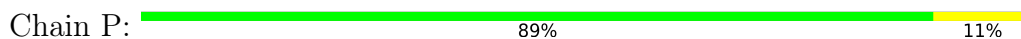




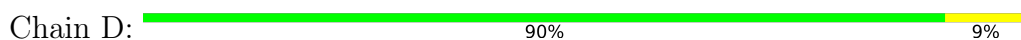
- Molecule 3: Cytochrome c oxidase subunit 3



- Molecule 3: Cytochrome c oxidase subunit 3



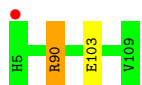
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



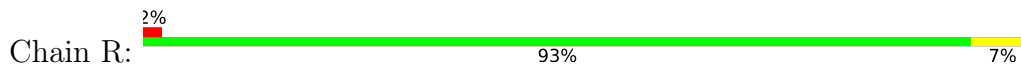
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



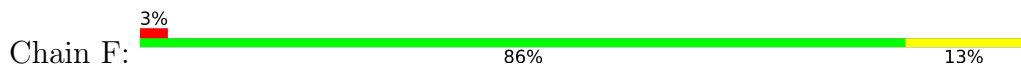
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

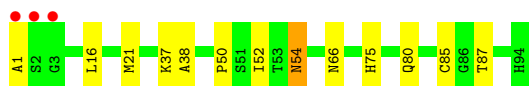


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

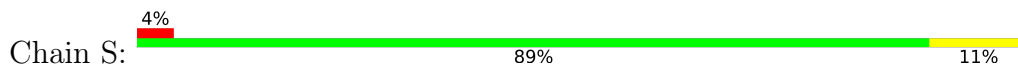


- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

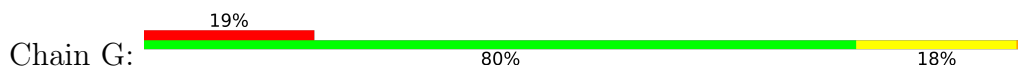




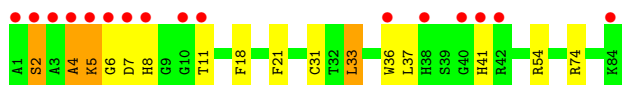
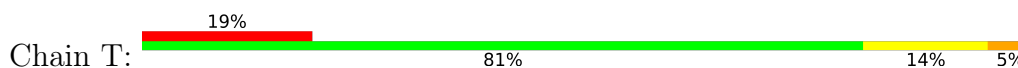
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



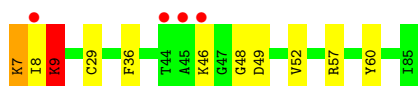
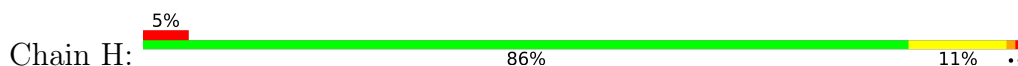
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



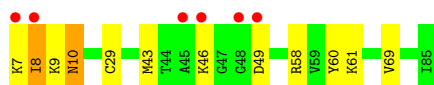
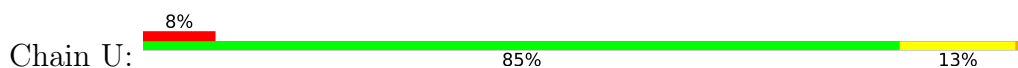
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



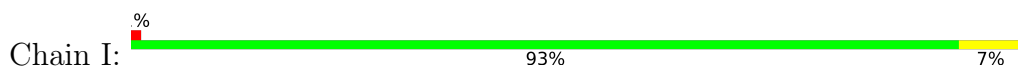
- Molecule 8: Cytochrome c oxidase subunit 6B1



- Molecule 8: Cytochrome c oxidase subunit 6B1

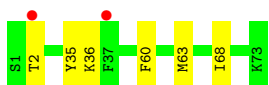


- Molecule 9: Cytochrome c oxidase subunit 6C

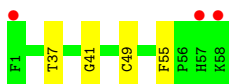
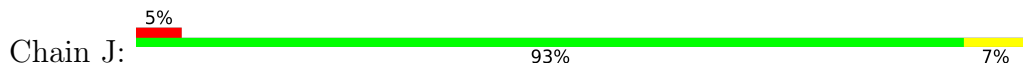


- Molecule 9: Cytochrome c oxidase subunit 6C

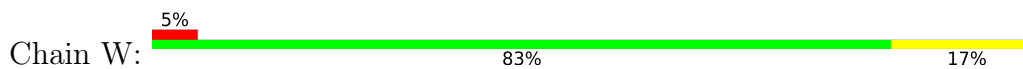




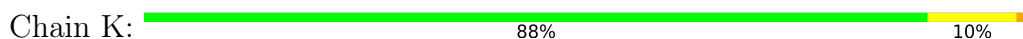
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



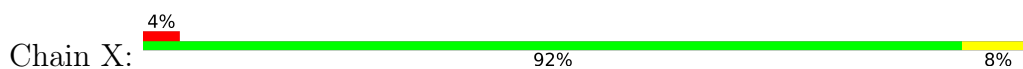
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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



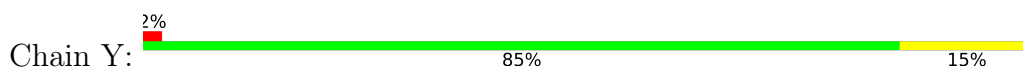
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



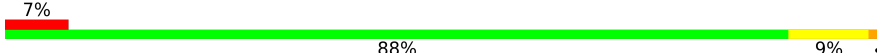
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

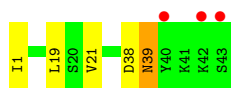


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial




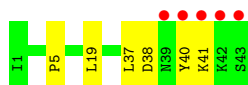
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:  7% 88% 9%



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

Chain Z:  12% 86% 14%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.44Å 203.09Å 177.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 1.84 133.77 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.91-1.84) 99.8 (133.77-1.84)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 1.84Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.154 , 0.184 0.154 , 0.184	Depositor DCC
$R_{free}$ test set	28294 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtrriage
Anisotropy	0.805	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 82.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.007 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	34545	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, PEK, CUA, FME, CDL, PER, PSC, CHD, SAC, PGV, HEA, EDO, NA, MG, TGL, CU, DMU, ZN

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	0.81	0/4432	0.78	3/6043 (0.0%)
1	N	0.76	0/4457	0.74	1/6082 (0.0%)
2	B	0.74	0/1928	0.80	2/2623 (0.1%)
2	O	0.62	0/1973	0.76	2/2686 (0.1%)
3	C	0.73	2/2288 (0.1%)	0.67	0/3125
3	P	0.69	0/2287	0.65	0/3124
4	D	0.68	0/1259	0.68	0/1698
4	Q	0.48	0/1236	0.59	0/1668
5	E	0.62	0/871	0.71	0/1182
5	R	0.52	0/882	0.62	0/1196
6	F	0.67	0/773	0.70	0/1048
6	S	0.68	0/732	0.72	0/993
7	G	0.63	0/743	0.70	0/1009
7	T	0.53	0/699	0.73	1/950 (0.1%)
8	H	0.64	0/690	0.66	0/932
8	U	0.60	1/682 (0.1%)	0.69	0/921
9	I	0.52	0/614	0.63	0/814
9	V	0.48	0/605	0.62	0/802
10	J	0.52	0/478	0.60	0/644
10	W	0.47	0/472	0.59	0/636
11	K	0.57	0/419	0.65	1/574 (0.2%)
11	X	0.50	0/398	0.57	0/544
12	L	0.67	0/409	0.62	0/547
12	Y	0.58	0/393	0.60	0/526
13	M	0.69	0/346	0.66	0/470
13	Z	0.54	0/345	0.60	0/470
All	All	0.68	3/30411 (0.0%)	0.71	10/41307 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	246[A]	ASP	CB-CG	6.16	1.64	1.51
3	C	246[B]	ASP	CB-CG	6.16	1.64	1.51
8	U	69	VAL	CB-CG1	5.04	1.63	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	MET	CG-SD-CE	-7.68	87.90	100.20
1	N	310	MET	CG-SD-CE	-7.37	88.41	100.20
2	O	65[A]	TRP	CA-CB-CG	6.37	125.81	113.70
2	O	65[B]	TRP	CA-CB-CG	6.37	125.81	113.70
1	A	96	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	B	82	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	208	MET	CG-SD-CE	5.55	109.09	100.20
11	K	47	ARG	NE-CZ-NH1	5.41	123.01	120.30
7	T	33	LEU	CA-CB-CG	5.07	126.97	115.30
2	B	139	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	4193	0	4162	51	0
1	N	4199	0	4190	58	0
2	B	1851	0	1858	22	0
2	O	1872	0	1876	29	0
3	C	2144	0	2062	24	0
3	P	2143	0	2069	24	0
4	D	1209	0	1202	14	0
4	Q	1197	0	1188	11	0
5	E	852	0	845	1	0
5	R	858	0	854	5	0
6	F	731	0	709	13	0
6	S	716	0	697	8	0
7	G	690	0	669	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	T	672	0	645	13	0
8	H	665	0	625	6	0
8	U	662	0	623	7	0
9	I	605	0	615	2	0
9	V	601	0	613	5	0
10	J	462	0	460	5	0
10	W	461	0	459	5	0
11	K	390	0	377	6	0
11	X	384	0	366	3	0
12	L	386	0	392	19	0
12	Y	380	0	380	5	0
13	M	336	0	352	7	0
13	Z	335	0	352	5	0
14	A	141	0	115	9	0
14	N	141	0	115	10	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	126	0	220	17	0
18	L	63	0	110	15	0
18	N	173	0	312	11	0
19	A	85	0	136	2	0
19	C	84	0	121	3	0
19	N	102	0	152	4	0
19	P	82	0	130	2	0
20	A	2	0	0	1	0
20	N	2	0	0	1	0
21	A	25	0	44	3	0
21	O	31	0	52	4	0
22	A	44	0	66	5	0
22	B	16	0	24	0	0
22	C	40	0	60	2	0
22	D	20	0	30	5	0
22	E	12	0	18	0	0
22	F	32	0	48	0	0
22	G	4	0	6	0	0
22	J	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	L	8	0	12	0	0
22	M	4	0	6	0	0
22	N	40	0	60	2	0
22	O	12	0	18	0	0
22	P	28	0	42	0	0
22	Q	4	0	6	0	0
22	S	24	0	36	1	0
22	T	12	0	18	0	0
22	W	8	0	12	0	0
22	Y	4	0	6	1	0
23	A	11	0	21	0	0
23	C	45	0	63	3	0
23	D	44	0	63	3	0
23	J	11	0	21	1	0
23	K	49	0	93	2	0
23	L	21	0	30	6	0
23	M	33	0	42	2	0
23	O	13	0	21	0	0
23	P	86	0	109	5	0
23	Q	11	0	21	2	0
23	X	50	0	84	2	0
23	Z	33	0	42	1	0
24	B	2	0	0	0	0
24	O	2	0	0	0	0
25	B	29	0	39	0	0
25	C	58	0	78	2	0
25	G	29	0	39	1	0
25	J	29	0	39	2	0
25	L	29	0	39	2	0
25	P	29	0	39	0	0
25	Y	29	0	39	0	0
26	C	133	0	192	7	0
26	P	90	0	116	2	0
26	T	37	0	59	6	0
27	C	65	0	113	7	0
27	N	62	0	109	5	0
27	P	68	0	119	7	0
27	T	61	0	110	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A	274	0	0	7	0
30	B	229	0	0	1	0
30	C	153	0	0	5	0
30	D	207	0	0	0	0
30	E	162	0	0	0	0
30	F	161	0	0	2	0
30	G	87	0	0	1	0
30	H	92	0	0	0	0
30	I	71	0	0	1	0
30	J	61	0	0	0	0
30	K	45	0	0	0	0
30	L	40	0	0	2	0
30	M	37	0	0	0	0
30	N	282	0	0	7	0
30	O	199	0	0	1	0
30	P	161	0	0	0	0
30	Q	119	0	0	2	0
30	R	113	0	0	1	0
30	S	141	0	0	2	0
30	T	66	0	0	1	0
30	U	96	0	0	1	0
30	V	66	0	0	0	0
30	W	41	0	0	0	0
30	X	33	0	0	0	0
30	Y	31	0	0	0	0
30	Z	28	0	0	0	0
All	All	34545	0	32367	372	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 6.

All (372) 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:A:609[A]:PER:O2	20:A:609[A]:PER:O1	1.55	1.24
20:N:611[A]:PER:O2	20:N:611[A]:PER:O1	1.55	1.21
12:L:20:ARG:HH22	18:L:101:TGL:HC52	1.31	0.95
1:N:113:LEU:HB2	18:N:608:TGL:H301	1.58	0.85
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.16	0.85
23:P:308:DMU:H9	10:W:49:CYS:HB3	1.57	0.85
18:A:607:TGL:HB21	4:D:78:TRP:HB3	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178[B]:GLN:NE2	7:T:7:ASP:O	2.10	0.84
8:H:7:LYS:HD2	8:H:8:ILE:HG23	1.63	0.80
12:L:20:ARG:HH12	18:L:101:TGL:HC32	1.46	0.79
1:N:510:TYR:HA	22:N:621:EDO:H12	1.69	0.74
19:A:608:PGV:H311	13:M:19:LEU:HD23	1.71	0.73
12:L:24[B]:MET:HE1	18:L:101:TGL:HC81	1.68	0.73
27:C:308:CDL:H322	27:C:308:CDL:H471	1.70	0.72
13:M:39:ASN:HD22	13:M:39:ASN:H	1.38	0.72
27:T:102:CDL:H531	27:T:102:CDL:H251	1.73	0.71
26:C:304:PEK:H101	26:C:304:PEK:H42	1.72	0.69
1:A:194:LEU:HD11	7:T:4:ALA:HB1	1.75	0.69
12:L:14:SER:H	18:L:101:TGL:HC31	1.58	0.68
3:P:62:ILE:HD12	27:P:307:CDL:H522	1.77	0.67
5:R:80:GLU:N	5:R:80:GLU:OE1	2.28	0.67
27:P:307:CDL:H521	27:P:307:CDL:HB62	1.77	0.67
26:P:304:PEK:H101	26:P:304:PEK:H42	1.76	0.66
12:L:20:ARG:NH2	18:L:101:TGL:HC52	2.06	0.66
18:L:101:TGL:OC1	18:L:101:TGL:HC41	1.95	0.66
19:C:307:PGV:H21	19:C:307:PGV:H71	1.77	0.65
7:T:74:ARG:NH1	30:T:201:HOH:O	2.29	0.65
22:A:616:EDO:H22	30:A:912:HOH:O	1.97	0.65
2:B:100[B]:MET:HG2	2:B:157:GLU:HG3	1.78	0.65
18:A:607:TGL:HC71	2:B:49:LYS:HE3	1.80	0.64
12:L:25:MET:HG2	18:L:101:TGL:HA62	1.79	0.64
3:P:33:MET:HE1	3:P:42:LEU:H	1.62	0.63
1:N:24:ALA:HB2	14:N:602[A]:HEA:H253	1.80	0.63
4:D:4:SER:HB2	22:D:204:EDO:O1	1.97	0.63
3:P:80[B]:ARG:NH2	3:P:236:GLU:OE1	2.31	0.63
3:P:34:TRP:HE1	23:P:316:DMU:H29	1.63	0.61
12:L:2:HIS:CG	12:L:3:TYR:H	2.18	0.61
13:M:39:ASN:H	13:M:39:ASN:ND2	1.99	0.61
1:N:377:PHE:HA	1:N:380[B]:VAL:HG12	1.83	0.61
18:A:606:TGL:H322	18:A:606:TGL:H261	1.83	0.60
1:N:334:TRP:CD1	18:N:609:TGL:HC41	2.36	0.60
1:A:169:ILE:HG23	7:T:8:HIS:O	2.02	0.59
7:G:11:THR:HA	30:N:867:HOH:O	2.02	0.59
18:A:607:TGL:HA31	18:A:607:TGL:HB51	1.83	0.59
18:N:608:TGL:HC51	12:Y:20:ARG:NH2	2.17	0.59
27:T:102:CDL:H781	27:T:102:CDL:H561	1.83	0.59
7:G:37:LEU:HD23	27:N:601:CDL:H381	1.84	0.59
4:D:94:LEU:HB3	23:D:206:DMU:H18	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:1:ALA:HB2	19:P:306:PGV:H342	1.85	0.59
26:C:304:PEK:H14	30:C:535:HOH:O	2.03	0.59
9:I:8:GLN:HG2	30:I:140:HOH:O	2.02	0.59
1:N:514:LYS:OXT	6:S:37:LYS:NZ	2.34	0.59
3:C:203:PHE:CE1	26:C:304:PEK:H9	2.38	0.58
7:G:5:LYS:HB3	1:N:278[B]:MET:HE3	1.84	0.58
1:N:49[B]:GLY:HA3	13:Z:41:LYS:HE3	1.86	0.58
11:X:40:TRP:CD2	23:X:102:DMU:H14	2.38	0.58
2:O:19:GLU:HG3	2:O:86[A]:MET:HE1	1.85	0.58
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.86	0.58
6:F:54[A]:ASN:ND2	30:F:203:HOH:O	2.36	0.58
10:J:55:PHE:CE1	23:L:105:DMU:H29	2.39	0.58
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.85	0.57
1:N:35[B]:LEU:HD23	23:Z:101:DMU:H24	1.86	0.57
1:N:53[B]:ILE:HG12	30:N:895:HOH:O	2.04	0.57
1:N:308:ALA:O	1:N:311[A]:ILE:HG12	2.04	0.57
2:B:130:PRO:HB3	22:D:205:EDO:H21	1.85	0.57
3:C:127:LEU:HD22	27:N:601:CDL:HB61	1.87	0.57
1:N:297[C]:MET:HG2	1:N:302:ARG:HG3	1.85	0.57
1:A:194:LEU:CD1	7:T:4:ALA:HB1	2.35	0.56
3:P:168:THR:HG21	26:T:101:PEK:H12	1.87	0.56
30:C:411:HOH:O	6:F:52:ILE:HD11	2.05	0.56
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.88	0.56
4:Q:20:ARG:HG2	30:Q:386:HOH:O	2.05	0.56
1:A:321[A]:PHE:CD2	2:B:65:TRP:HB2	2.40	0.55
1:A:321[B]:PHE:CD1	21:A:610:PSC:H341	2.41	0.55
21:A:610:PSC:H242	2:B:56:MET:HB3	1.88	0.55
19:N:610:PGV:H311	13:Z:19:LEU:HD23	1.89	0.55
23:D:206:DMU:H29	11:K:36:ILE:HB	1.88	0.55
18:A:607:TGL:HC42	18:A:607:TGL:OG3	2.07	0.55
3:C:156:ARG:HE	25:C:309:CHD:C24	2.20	0.55
1:A:334:TRP:CD1	18:A:607:TGL:HC41	2.42	0.55
27:T:102:CDL:H561	27:T:102:CDL:H761	1.89	0.55
1:N:379:TYR:O	1:N:383[B]:MET:HB2	2.06	0.55
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.89	0.55
1:A:377:PHE:O	1:A:381[B]:LEU:HB3	2.07	0.55
14:N:603:HEA:HMC1	14:N:603:HEA:HBC1	1.89	0.55
2:B:13:THR:HB	2:B:168:LEU:HD23	1.89	0.54
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.90	0.54
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.88	0.54
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:43:MET:HE3	8:U:49:ASP:N	2.23	0.54
19:N:612:PGV:H183	26:P:304:PEK:H342	1.90	0.54
1:N:331[B]:ASN:ND2	4:Q:21:ASP:HB3	2.22	0.53
1:A:278[B]:MET:HB3	7:T:5:LYS:HG2	1.90	0.53
3:C:210:ILE:HG12	19:C:306:PGV:H132	1.90	0.53
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.91	0.53
12:L:24[B]:MET:SD	18:L:101:TGL:HC22	2.48	0.53
1:N:297[C]:MET:CG	1:N:302:ARG:HG3	2.38	0.53
7:T:41:HIS:HB3	7:T:74:ARG:NH2	2.24	0.53
1:N:514:LYS:HD2	30:S:278:HOH:O	2.07	0.53
26:T:101:PEK:H382	27:T:102:CDL:H273	1.91	0.53
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.90	0.53
1:N:113:LEU:HB2	18:N:608:TGL:C32	2.39	0.53
4:Q:6:VAL:HG12	4:Q:7:LYS:H	1.74	0.53
1:A:24:ALA:HB2	14:A:601[A]:HEA:H253	1.91	0.52
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.39	0.52
1:A:349:THR:OG1	1:A:349:THR:CA	2.57	0.52
1:N:488:THR:HB	1:N:495:LEU:HD13	1.91	0.52
4:D:120:THR:HG21	11:K:48[B]:VAL:CG1	2.40	0.52
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.91	0.52
10:J:41:GLY:HA3	23:J:104:DMU:H23	1.90	0.52
4:D:98:TRP:CE2	23:M:101:DMU:H11	2.44	0.52
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.91	0.52
3:C:52:LEU:HD21	27:C:308:CDL:H432	1.92	0.51
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.45	0.51
21:O:302:PSC:H111	21:O:302:PSC:H321	1.92	0.51
1:A:514[A]:LYS:HD2	30:A:731:HOH:O	2.11	0.51
30:A:787:HOH:O	12:L:7:PRO:HG3	2.09	0.51
1:A:379:TYR:O	1:A:383[B]:MET:HB2	2.11	0.51
27:N:601:CDL:H371	2:O:81:LEU:HD12	1.93	0.51
1:A:343:GLY:HA2	18:A:607:TGL:H212	1.93	0.50
1:A:53[A]:ILE:HD11	12:L:40:VAL:HG13	1.93	0.50
10:J:55:PHE:HE1	23:L:105:DMU:H29	1.75	0.50
1:A:377:PHE:HA	1:A:380[B]:VAL:HG12	1.94	0.50
22:A:612:EDO:H22	13:M:1:ILE:H1	1.77	0.50
18:L:101:TGL:CC1	18:L:101:TGL:HC61	2.41	0.50
18:L:101:TGL:CC1	18:L:101:TGL:HG12	2.39	0.50
1:N:297[C]:MET:SD	1:N:302:ARG:HG3	2.51	0.50
2:O:93:PRO:HG3	2:O:151:ARG:HB2	1.91	0.50
1:A:46:THR:HG22	1:A:49[B]:GLY:H	1.77	0.50
26:C:305:PEK:H231	7:G:21:PHE:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:49:ASP:O	8:H:52:VAL:HG22	2.12	0.50
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.93	0.50
8:U:7:LYS:O	8:U:8:ILE:HB	2.11	0.50
3:P:52:LEU:HD21	27:P:307:CDL:H412	1.94	0.50
2:B:87:MET:HE2	30:B:417:HOH:O	2.10	0.50
2:O:78:LEU:O	2:O:82[B]:ARG:HG3	2.12	0.50
3:C:180[B]:GLU:HG3	30:C:416:HOH:O	2.10	0.50
3:C:258:TRP:HZ3	27:N:601:CDL:H651	1.77	0.50
8:U:46:LYS:O	30:U:201:HOH:O	2.19	0.50
21:A:610:PSC:H342	2:B:41:ILE:HD13	1.93	0.49
3:C:37:PHE:CE2	23:C:310:DMU:H13	2.47	0.49
7:T:31:CYS:SG	27:T:102:CDL:H532	2.52	0.49
23:L:105:DMU:H5	30:L:216:HOH:O	2.12	0.49
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.93	0.49
4:Q:65:LYS:HE3	30:Q:410:HOH:O	2.12	0.49
27:T:102:CDL:H781	27:T:102:CDL:C56	2.42	0.49
3:C:180[B]:GLU:HG2	30:C:422:HOH:O	2.11	0.49
11:X:40:TRP:CD1	23:X:102:DMU:H10	2.47	0.49
1:A:311:ILE:CD1	27:T:102:CDL:H441	2.42	0.49
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.48	0.49
1:N:113:LEU:CB	18:N:608:TGL:H301	2.36	0.49
1:A:513:LEU:O	1:A:514[A]:LYS:HB2	2.13	0.49
2:O:58:ALA:O	2:O:62:GLU:HG3	2.13	0.49
3:P:257:TYR:O	3:P:261:SER:HB3	2.12	0.49
1:N:468:MET:HG3	30:N:969:HOH:O	2.11	0.49
12:Y:3:TYR:CE2	22:Y:101:EDO:H21	2.48	0.49
3:P:33:MET:CE	3:P:42:LEU:H	2.25	0.49
2:O:13:THR:HB	2:O:168:LEU:HD23	1.95	0.49
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.94	0.49
3:C:258:TRP:CE3	22:C:315:EDO:H21	2.48	0.49
2:O:56:MET:HB3	21:O:302:PSC:H232	1.94	0.49
4:Q:101:HIS:ND1	23:Q:201:DMU:H6	2.28	0.49
1:N:383[C]:MET:O	1:N:387:PHE:N	2.46	0.48
4:Q:101:HIS:CG	23:Q:201:DMU:H6	2.48	0.48
7:G:7:ASP:O	1:N:178[B]:GLN:NE2	2.46	0.48
25:L:102:CHD:H232	13:M:21:VAL:HG21	1.95	0.48
3:P:41:THR:HA	3:P:44[A]:MET:HE2	1.95	0.48
1:A:381[B]:LEU:HB2	14:A:602:HEA:CAC	2.43	0.48
1:N:46:THR:HG22	1:N:49[B]:GLY:H	1.78	0.48
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.48	0.48
3:P:40:MET:SD	23:P:316:DMU:H6	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:210:ILE:HD13	19:P:305:PGV:H301	1.96	0.48
12:L:24[A]:MET:SD	18:L:101:TGL:H152	2.54	0.48
3:P:34:TRP:CD1	3:P:40:MET:HG2	2.48	0.48
7:G:4:ALA:CB	1:N:282:PHE:HA	2.43	0.48
4:D:120:THR:HG21	11:K:48[B]:VAL:HG11	1.95	0.48
1:A:321[B]:PHE:HB3	2:B:65:TRP:CE3	2.49	0.47
27:P:307:CDL:H161	27:P:307:CDL:H132	1.65	0.47
4:D:4:SER:HB2	22:D:204:EDO:C1	2.45	0.47
8:H:46:LYS:HE3	8:U:7:LYS:HB2	1.96	0.47
10:W:29:ASN:O	10:W:33:ARG:HG3	2.13	0.47
4:Q:126:MET:HG3	4:Q:128:VAL:HG23	1.96	0.47
11:X:24:PHE:O	11:X:28:VAL:HG12	2.15	0.47
18:A:606:TGL:HA72	18:A:606:TGL:H142	1.96	0.47
1:N:406:ASN:HD21	19:N:610:PGV:H21	1.79	0.47
8:H:9:LYS:HA	8:H:9:LYS:HD3	1.38	0.47
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.96	0.47
1:N:486[B]:ASP:OD2	4:Q:19:ARG:NE	2.47	0.47
18:A:606:TGL:H142	18:A:606:TGL:H112	1.43	0.47
8:U:43:MET:HE3	8:U:49:ASP:H	1.80	0.46
11:K:42:PRO:O	11:K:47:ARG:NH2	2.49	0.46
1:N:381[B]:LEU:HB2	14:N:603:HEA:CAC	2.46	0.46
2:O:61:VAL:O	2:O:64[A]:ILE:HG23	2.16	0.46
1:A:273:MET:HE2	30:A:756:HOH:O	2.15	0.46
18:L:101:TGL:H261	18:L:101:TGL:H232	1.71	0.46
3:C:51[A]:MET:SD	27:C:308:CDL:H622	2.56	0.46
6:F:50:PRO:HG2	30:F:265:HOH:O	2.16	0.46
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.50	0.46
3:C:220:PHE:HB2	27:C:308:CDL:H712	1.96	0.46
18:A:606:TGL:H101	18:A:606:TGL:C28	2.46	0.46
1:A:376:HIS:CE1	1:A:380[B]:VAL:HG11	2.50	0.46
1:A:383[C]:MET:O	1:A:387:PHE:N	2.48	0.46
26:C:304:PEK:H221	26:C:304:PEK:H251	1.54	0.46
27:C:308:CDL:H822	27:C:308:CDL:H851	1.66	0.46
2:O:89:GLU:O	2:O:91:ASN:ND2	2.49	0.46
18:N:607:TGL:HB91	18:N:607:TGL:H122	1.72	0.46
30:N:825:HOH:O	3:P:77:LYS:HE3	2.15	0.46
5:R:7:THR:HB	5:R:9:GLU:OE2	2.16	0.46
18:A:607:TGL:HB42	4:D:78:TRP:HA	1.98	0.46
18:N:608:TGL:H222	18:N:608:TGL:HA91	1.54	0.46
27:P:307:CDL:H821	27:P:307:CDL:H851	1.58	0.46
1:A:285:PHE:CE2	7:T:4:ALA:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:THR:HG22	14:A:602:HEA:HMB2	1.99	0.45
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.99	0.45
18:N:607:TGL:H222	18:N:607:TGL:H271	1.99	0.45
14:A:601[B]:HEA:H122	30:A:860:HOH:O	2.17	0.45
8:U:9:LYS:O	8:U:10:ASN:HB2	2.16	0.45
1:A:53[B]:ILE:HG12	30:L:235:HOH:O	2.17	0.45
5:E:90:ARG:NH2	5:E:103:GLU:OE2	2.49	0.45
1:N:408:THR:HB	19:N:610:PGV:H51	1.97	0.45
1:N:35[A]:LEU:HD11	1:N:462:LEU:HB2	1.98	0.45
3:P:224[B]:LYS:HE3	27:P:307:CDL:H131	1.98	0.45
14:A:602:HEA:H243	2:B:69:PRO:HB3	1.99	0.45
1:N:297[C]:MET:SD	1:N:302:ARG:CG	3.05	0.45
1:N:383[A]:MET:HG2	1:N:421:VAL:HG21	1.99	0.45
6:S:22:LEU:HD12	30:S:306:HOH:O	2.15	0.45
2:O:65[B]:TRP:CD1	21:O:302:PSC:H12	2.52	0.45
1:A:285:PHE:CD2	7:T:4:ALA:HB2	2.52	0.45
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.98	0.45
27:C:308:CDL:H662	27:C:308:CDL:H631	1.72	0.44
7:G:9:GLY:HA2	30:N:892:HOH:O	2.17	0.44
7:T:21:PHE:CG	26:T:101:PEK:H222	2.51	0.44
3:C:207:HIS:CE1	19:C:306:PGV:H343	2.52	0.44
2:O:164:ALA:O	2:O:194:GLY:HA3	2.17	0.44
6:S:76:LYS:HE3	6:S:76:LYS:HB3	1.69	0.44
3:C:164:PHE:CD1	25:C:309:CHD:H192	2.52	0.44
3:P:168:THR:HG22	26:T:101:PEK:H14	2.00	0.44
7:T:41:HIS:HB3	7:T:74:ARG:CZ	2.47	0.44
1:A:236:TRP:CH2	14:A:602:HEA:HBD1	2.51	0.44
1:A:334:TRP:CZ3	18:A:607:TGL:HA51	2.52	0.44
22:A:620:EDO:H22	6:F:66:ASN:ND2	2.31	0.44
1:A:311:ILE:HD11	27:T:102:CDL:H421	2.00	0.44
22:C:318:EDO:H11	6:F:16:LEU:HD13	1.99	0.44
12:L:24[B]:MET:CG	18:L:101:TGL:HA22	2.47	0.44
1:N:73:ILE:HD11	14:N:602[C]:HEA:H22	1.98	0.44
14:N:602[C]:HEA:H212	14:N:602[C]:HEA:H271	1.87	0.44
1:N:307:SER:O	1:N:311[A]:ILE:HG23	2.17	0.44
2:O:41:ILE:O	2:O:45:MET:HG2	2.18	0.44
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.52	0.44
1:A:334:TRP:CE3	18:A:607:TGL:HA51	2.53	0.44
13:Z:37:LEU:HD23	13:Z:37:LEU:HA	1.86	0.44
1:N:92:MET:HE1	1:N:164:PHE:CD1	2.52	0.44
1:A:136[B]:LEU:HD11	30:A:962:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:MET:O	1:A:297[B]:MET:HE3	2.17	0.43
26:C:304:PEK:H42	26:C:304:PEK:H72	1.59	0.43
3:P:47:LEU:O	3:P:51[B]:MET:HG2	2.18	0.43
12:L:41:ARG:NH1	23:L:105:DMU:H2	2.33	0.43
3:P:168:THR:CG2	26:T:101:PEK:H12	2.46	0.43
2:B:164:ALA:O	2:B:194:GLY:HA3	2.17	0.43
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.00	0.43
1:N:377:PHE:O	1:N:381[B]:LEU:HB3	2.18	0.43
4:Q:5:VAL:H	13:Z:5:PRO:HD3	1.83	0.43
3:C:158:HIS:CE1	6:F:1:ALA:HB3	2.53	0.43
23:K:101:DMU:H21	23:K:102:DMU:H17	2.00	0.43
12:L:2:HIS:CG	12:L:3:TYR:N	2.85	0.43
1:N:76:GLY:O	1:N:80:ASN:HB2	2.18	0.43
1:A:334:TRP:HZ3	18:A:607:TGL:HA71	1.83	0.43
12:L:41:ARG:HH12	23:L:105:DMU:H2	1.83	0.43
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.54	0.43
3:P:59:ARG:HA	27:P:307:CDL:H522	1.99	0.43
5:R:79:LYS:HD2	5:R:79:LYS:HA	1.89	0.43
6:S:54:ASN:HB2	6:S:76:LYS:HE2	2.00	0.43
10:W:54:SER:O	12:Y:46:LYS:HD3	2.18	0.43
1:A:52[B]:GLN:O	1:A:56:VAL:HG23	2.19	0.43
3:C:37:PHE:CD2	23:C:310:DMU:H13	2.53	0.43
1:N:116:SER:HB3	30:N:834:HOH:O	2.18	0.43
1:A:362[B]:SER:HB2	2:B:20:LEU:HD21	2.01	0.43
22:A:612:EDO:H22	13:M:1:ILE:N	2.34	0.43
12:Y:45:LEU:HD21	13:Z:40:TYR:CD1	2.54	0.43
18:A:607:TGL:HG32	30:A:924:HOH:O	2.18	0.43
6:F:21[B]:MET:HE2	6:F:21[B]:MET:HB2	1.64	0.42
1:N:54[A]:TYR:HB2	30:N:788[A]:HOH:O	2.19	0.42
7:G:5:LYS:HB3	1:N:278[B]:MET:CE	2.49	0.42
1:N:321:PHE:CD1	21:O:302:PSC:H341	2.54	0.42
14:N:603:HEA:H243	2:O:69:PRO:HB3	2.01	0.42
1:A:321[A]:PHE:HB3	2:B:65:TRP:CE3	2.54	0.42
4:D:98:TRP:CD2	23:M:101:DMU:H11	2.54	0.42
23:L:105:DMU:H13	23:L:105:DMU:H18	1.62	0.42
2:B:196:CYS:CB	2:B:207:MET:HG3	2.50	0.42
1:N:266:GLU:OE1	22:S:106:EDO:H11	2.19	0.42
2:O:183:THR:HG22	30:O:567:HOH:O	2.19	0.42
10:W:4:ARG:O	10:W:7:GLU:HG2	2.20	0.42
14:A:601[C]:HEA:H212	14:A:601[C]:HEA:H271	1.69	0.42
3:P:47:LEU:O	3:P:51[A]:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ALA:O	2:B:62:GLU:HG3	2.20	0.42
3:C:58:TRP:HB2	27:C:308:CDL:H552	2.02	0.42
11:K:47:ARG:HG2	11:K:48[A]:VAL:HG23	2.02	0.42
1:N:309:THR:HG22	14:N:603:HEA:HMB2	2.00	0.42
2:O:168:LEU:HD13	2:O:184:LEU:HG	2.01	0.42
5:R:108:LYS:HB3	30:R:298:HOH:O	2.20	0.42
2:B:100[B]:MET:CG	2:B:157:GLU:HG3	2.49	0.42
3:C:244:PHE:HA	26:C:303:PEK:H101	2.01	0.42
4:D:115:TRP:HE3	22:D:205:EDO:H11	1.85	0.42
19:A:611:PGV:H182	3:C:28:THR:HG22	2.02	0.42
12:L:24[B]:MET:SD	18:L:101:TGL:CC2	3.07	0.42
18:N:607:TGL:H311	18:N:607:TGL:H141	1.77	0.42
3:C:158:HIS:HE1	6:F:1:ALA:HB3	1.85	0.41
3:C:191:GLY:HA3	30:G:212:HOH:O	2.19	0.41
12:L:24[B]:MET:HG2	18:L:101:TGL:HA22	2.02	0.41
1:N:112:LEU:HD23	1:N:112:LEU:C	2.40	0.41
1:A:311:ILE:CD1	27:T:102:CDL:H421	2.51	0.41
10:J:37:THR:HG23	25:J:101:CHD:H191	2.02	0.41
25:J:101:CHD:H21	25:J:101:CHD:H9	1.79	0.41
2:O:113:TYR:HD1	8:U:58:ARG:NH2	2.17	0.41
9:V:63:MET:HB3	9:V:68:ILE:CD1	2.50	0.41
3:C:3:HIS:N	30:C:410:HOH:O	2.53	0.41
6:F:75:HIS:H	6:F:80[B]:GLN:HE22	1.68	0.41
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.55	0.41
4:D:19[B]:ARG:NH1	4:D:22:TYR:HB2	2.36	0.41
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.03	0.41
1:N:236:TRP:CH2	14:N:603:HEA:HBD1	2.56	0.41
27:N:601:CDL:H801	27:N:601:CDL:H832	1.77	0.41
1:A:415:ALA:HB1	18:A:607:TGL:H131	2.02	0.41
2:O:102:HIS:O	2:O:104:TRP:HA	2.21	0.41
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.03	0.41
9:V:63:MET:HB3	9:V:68:ILE:HG12	2.02	0.41
1:A:246:LEU:HD13	1:A:381[B]:LEU:HD11	2.02	0.41
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.52	0.41
1:N:225:GLY:HA3	3:P:112:LEU:HD21	2.02	0.41
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.02	0.41
25:L:102:CHD:H183	25:L:102:CHD:H212	2.02	0.41
3:P:165:ILE:HG12	26:T:101:PEK:H11	2.03	0.41
9:V:36:LYS:HE3	9:V:36:LYS:HB3	1.86	0.41
10:W:18:LEU:HB2	10:W:23:LYS:HG3	2.02	0.41
3:C:157:LYS:HE2	3:C:161[B]:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:G:101:CHD:H212	25:G:101:CHD:H12	2.02	0.41
2:O:128:LEU:HD11	2:O:134:ARG:HA	2.02	0.41
23:P:308:DMU:H41	23:P:308:DMU:H36	1.74	0.41
23:P:308:DMU:H29	23:P:308:DMU:H32	2.03	0.41
1:A:120:ALA:HB2	22:A:618:EDO:H12	2.03	0.41
9:I:57:MET:O	9:I:61[B]:GLU:HG2	2.20	0.41
18:A:607:TGL:H132	18:A:607:TGL:H101	1.89	0.40
18:N:608:TGL:HC31	12:Y:13:PHE:HA	2.04	0.40
3:P:207:HIS:HD2	3:P:241:TYR:OH	2.04	0.40
23:C:310:DMU:C22	10:J:49:CYS:HB3	2.51	0.40
4:D:5:VAL:H	22:D:204:EDO:C1	2.35	0.40
1:A:302[B]:ARG:HH22	1:A:365[B]:ILE:HD11	1.86	0.40
12:L:23:ALA:O	12:L:27[A]:LEU:HG	2.21	0.40
1:N:242:GLU:HA	1:N:245:ILE:HD12	2.02	0.40
1:N:331[B]:ASN:ND2	2:O:51:THR:HG21	2.36	0.40
18:N:608:TGL:HC22	18:N:608:TGL:HC52	1.78	0.40
4:D:101:HIS:HB2	23:D:206:DMU:H30	2.03	0.40
11:K:24:PHE:HB2	23:K:103:DMU:H9	2.02	0.40
1:N:50[B]:ASP:CG	1:N:53[B]:ILE:HG13	2.42	0.40
1:N:331[B]:ASN:HD21	4:Q:21:ASP:HB3	1.86	0.40
13:M:39:ASN:ND2	13:M:39:ASN:N	2.68	0.40
1:N:386[B]:VAL:HG21	14:N:602[B]:HEA:H162	2.04	0.40
22:N:620:EDO:H22	6:S:66:ASN:ND2	2.37	0.40
6:S:25:ARG:HE	6:S:25:ARG:HB2	1.68	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	548/514 (107%)	529 (96%)	19 (4%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	553/514 (108%)	534 (97%)	19 (3%)	0	100	100
2	B	233/227 (103%)	227 (97%)	5 (2%)	1 (0%)	34	20
2	O	237/227 (104%)	230 (97%)	5 (2%)	2 (1%)	19	7
3	C	268/259 (104%)	263 (98%)	5 (2%)	0	100	100
3	P	268/259 (104%)	263 (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%)	3 (2%)	2 (1%)	11	3
5	E	103/105 (98%)	102 (99%)	1 (1%)	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%)	90 (98%)	1 (1%)	1 (1%)	14	4
7	G	87/84 (104%)	77 (88%)	8 (9%)	2 (2%)	6	1
7	T	82/84 (98%)	72 (88%)	6 (7%)	4 (5%)	2	0
8	H	78/79 (99%)	73 (94%)	3 (4%)	2 (3%)	5	0
8	U	77/79 (98%)	72 (94%)	3 (4%)	2 (3%)	5	0
9	I	72/73 (99%)	71 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	57/58 (98%)	57 (100%)	0	0	100	100
10	W	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
11	K	50/49 (102%)	49 (98%)	1 (2%)	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	46/46 (100%)	44 (96%)	2 (4%)	0	100	100
12	Y	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
13	M	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
All	All	3640/3550 (102%)	3522 (97%)	102 (3%)	16 (0%)	34	20

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	T	2	SER
8	U	8	ILE

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Mol	Chain	Res	Type
6	S	2	SER
8	H	9	LYS
8	H	48	GLY
2	O	92[A]	ASN
2	O	92[B]	ASN
7	G	3	ALA
7	T	4	ALA
8	U	10	ASN
7	T	5	LYS
4	Q	5	VAL
4	Q	6	VAL
7	T	6	GLY
2	B	92	ASN

### 5.3.2 Protein sidechains [i](#)

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	458/426 (108%)	445 (97%)	13 (3%)	43	26
1	N	463/426 (109%)	459 (99%)	4 (1%)	78	71
2	B	218/210 (104%)	207 (95%)	11 (5%)	24	8
2	O	221/210 (105%)	209 (95%)	12 (5%)	22	7
3	C	235/224 (105%)	230 (98%)	5 (2%)	53	38
3	P	235/224 (105%)	231 (98%)	4 (2%)	60	47
4	D	131/128 (102%)	128 (98%)	3 (2%)	50	34
4	Q	129/128 (101%)	124 (96%)	5 (4%)	32	14
5	E	92/92 (100%)	91 (99%)	1 (1%)	73	64
5	R	93/92 (101%)	93 (100%)	0	100	100
6	F	83/78 (106%)	80 (96%)	3 (4%)	35	17
6	S	78/78 (100%)	78 (100%)	0	100	100
7	G	73/68 (107%)	63 (86%)	10 (14%)	3	0
7	T	68/68 (100%)	61 (90%)	7 (10%)	7	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	72/71 (101%)	68 (94%)	4 (6%)	21	6
8	U	71/71 (100%)	68 (96%)	3 (4%)	30	12
9	I	58/57 (102%)	57 (98%)	1 (2%)	60	47
9	V	57/57 (100%)	56 (98%)	1 (2%)	59	44
10	J	50/49 (102%)	50 (100%)	0	100	100
10	W	49/49 (100%)	47 (96%)	2 (4%)	30	13
11	K	42/39 (108%)	41 (98%)	1 (2%)	49	32
11	X	39/39 (100%)	38 (97%)	1 (3%)	46	29
12	L	41/39 (105%)	40 (98%)	1 (2%)	49	32
12	Y	39/39 (100%)	37 (95%)	2 (5%)	24	8
13	M	37/37 (100%)	35 (95%)	2 (5%)	22	7
13	Z	37/37 (100%)	36 (97%)	1 (3%)	44	28
All	All	3169/3036 (104%)	3072 (97%)	97 (3%)	42	23

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	180	GLN
1	A	297[A]	MET
1	A	297[B]	MET
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
1	A	514[A]	LYS
1	A	514[B]	LYS
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	115[A]	ASP
2	B	115[B]	ASP
2	B	171	LYS
3	C	40	MET
3	C	76	GLN
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	31	LYS
4	D	147	LYS
5	E	90	ARG
6	F	37	LYS
6	F	54[A]	ASN
6	F	54[B]	ASN
7	G	2	SER
7	G	8	HIS
7	G	18	PHE
7	G	33[A]	LEU
7	G	33[B]	LEU
7	G	36	TRP
7	G	37	LEU
7	G	42	ARG
7	G	43	GLU
7	G	54	ARG
8	H	7	LYS
8	H	9	LYS
8	H	29	CYS
8	H	60	TYR
9	I	37	PHE
11	K	54	ARG
12	L	47	LYS
13	M	38	ASP
13	M	39	ASN
1	N	38	ARG
1	N	109	PHE
1	N	138	HIS
1	N	369	ASP
2	O	33	LEU
2	O	64[A]	ILE
2	O	64[B]	ILE
2	O	68	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	225	SER
2	O	226	MET
3	P	3	HIS
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	4	SER
4	Q	7	LYS
4	Q	20	ARG
4	Q	51	LEU
4	Q	58	GLU
7	T	2	SER
7	T	11	THR
7	T	18	PHE
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
7	T	54	ARG
8	U	29	CYS
8	U	60	TYR
8	U	61	LYS
9	V	2	THR
10	W	50	LEU
10	W	58	LYS
11	X	47	ARG
12	Y	2	HIS
12	Y	47	LYS
13	Z	38	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	91	ASN
2	B	181	GLN
4	D	109	HIS
6	F	32	ASN

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Mol	Chain	Res	Type
6	F	94	HIS
13	M	39	ASN
2	O	91	ASN
2	O	195	GLN
3	P	158	HIS
4	Q	101	HIS
4	Q	109	HIS
7	T	8	HIS
8	U	31	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	0.72	0	7,9,11	1.53	2 (28%)
9	SAC	V	1	9	7,8,9	0.60	0	8,9,11	0.80	0
1	FME	N	1	1	8,9,10	0.43	0	7,9,11	1.31	0
2	FME	B	1	2	8,9,10	0.76	0	7,9,11	2.24	1 (14%)
9	SAC	I	1	9	7,8,9	0.63	0	8,9,11	1.02	1 (12%)
1	FME	A	1	1	8,9,10	0.43	0	7,9,11	1.47	2 (28%)

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

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-4.65	100.04	112.95
2	O	1	FME	CG-CB-CA	-3.17	104.15	112.95
1	A	1	FME	C-CA-N	2.40	114.06	109.73
9	I	1	SAC	O-C-CA	-2.16	119.11	124.78
1	A	1	FME	O1-CN-N	-2.12	119.69	125.27
2	O	1	FME	O-C-CA	-2.03	119.45	124.78

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

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 161 ligands modelled in this entry, 10 are monoatomic - leaving 151 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
26	PEK	C	305	-	34,34,52	0.32	0	32,32,57	0.58	0
22	EDO	W	102	-	3,3,3	0.49	0	2,2,2	0.45	0
22	EDO	O	304	-	3,3,3	0.65	0	2,2,2	0.08	0
20	PER	A	609[A]	14,15	0,1,1	-	-	-		
25	CHD	B	302	-	32,32,32	0.86	0	51,51,51	1.39	7 (13%)
23	DMU	A	623	-	10,10,34	0.31	0	9,9,45	0.48	0
23	DMU	X	103	-	8,8,34	0.30	0	7,7,45	0.61	0
23	DMU	K	101	-	7,7,34	0.25	0	6,6,45	0.37	0
18	TGL	A	606	-	62,62,62	1.04	3 (4%)	65,65,65	1.28	5 (7%)
22	EDO	B	306	-	3,3,3	0.57	0	2,2,2	0.32	0
22	EDO	C	320	-	3,3,3	0.71	0	2,2,2	0.45	0
22	EDO	F	104	-	3,3,3	0.58	0	2,2,2	0.33	0
22	EDO	N	620	-	3,3,3	0.58	0	2,2,2	0.15	0
18	TGL	L	101	-	62,62,62	1.12	3 (4%)	65,65,65	1.39	7 (10%)
25	CHD	C	309	-	32,32,32	0.75	0	51,51,51	1.25	6 (11%)
26	PEK	T	101	-	35,35,52	0.86	1 (2%)	34,34,57	1.07	3 (8%)
22	EDO	Q	202	-	3,3,3	0.54	0	2,2,2	0.39	0
27	CDL	N	601	-	58,58,99	1.30	9 (15%)	55,55,111	0.98	4 (7%)
23	DMU	Q	201	-	10,10,34	0.36	0	9,9,45	0.36	0
22	EDO	N	619	-	3,3,3	0.56	0	2,2,2	0.13	0
21	PSC	A	610	-	23,23,51	0.84	1 (4%)	20,21,59	0.79	0
22	EDO	N	622	-	3,3,3	0.75	0	2,2,2	0.28	0
22	EDO	J	103	-	3,3,3	0.36	0	2,2,2	0.76	0
22	EDO	A	614	-	3,3,3	0.45	0	2,2,2	0.28	0
19	PGV	A	611	-	50,50,50	0.90	3 (6%)	53,56,56	1.20	4 (7%)
18	TGL	N	607	-	62,62,62	1.04	3 (4%)	65,65,65	1.20	4 (6%)
22	EDO	C	311	-	3,3,3	0.53	0	2,2,2	0.17	0
22	EDO	B	303	-	3,3,3	0.72	0	2,2,2	0.30	0
22	EDO	P	311	-	3,3,3	0.70	0	2,2,2	0.18	0
19	PGV	P	305	-	50,50,50	0.76	2 (4%)	53,56,56	1.00	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	EDO	C	312	-	3,3,3	0.63	0	2,2,2	0.34	0
22	EDO	W	101	-	3,3,3	0.38	0	2,2,2	0.45	0
24	CUA	B	301	2	0,1,1	-	-	-		
22	EDO	P	309	-	3,3,3	0.53	0	2,2,2	0.21	0
22	EDO	C	313	-	3,3,3	0.80	0	2,2,2	0.35	0
22	EDO	T	105	-	3,3,3	0.62	0	2,2,2	0.32	0
23	DMU	P	317	-	33,33,34	0.73	1 (3%)	44,44,45	1.66	8 (18%)
29	PO4	H	101	-	4,4,4	0.75	0	6,6,6	0.74	0
25	CHD	P	301	-	32,32,32	0.77	0	51,51,51	1.36	10 (19%)
22	EDO	E	203	-	3,3,3	0.46	0	2,2,2	0.40	0
22	EDO	S	103	-	3,3,3	0.59	0	2,2,2	0.12	0
23	DMU	D	207	-	10,10,34	0.33	0	9,9,45	0.57	0
22	EDO	N	613	-	3,3,3	0.63	0	2,2,2	0.64	0
22	EDO	E	201	-	3,3,3	0.56	0	2,2,2	0.25	0
22	EDO	O	303	-	3,3,3	0.76	0	2,2,2	0.48	0
19	PGV	P	306	-	29,29,50	0.99	1 (3%)	28,28,56	0.91	2 (7%)
22	EDO	T	104	-	3,3,3	0.49	0	2,2,2	0.28	0
23	DMU	X	101	-	9,9,34	0.31	0	8,8,45	0.51	0
22	EDO	S	105	-	3,3,3	0.64	0	2,2,2	0.71	0
26	PEK	C	303	-	44,44,52	1.21	2 (4%)	47,49,57	1.41	8 (17%)
19	PGV	C	306	-	47,47,50	0.84	2 (4%)	50,53,56	0.90	3 (6%)
22	EDO	A	621	-	3,3,3	0.61	0	2,2,2	0.51	0
26	PEK	P	304	-	51,51,52	0.77	2 (3%)	54,56,57	1.07	4 (7%)
25	CHD	G	101	-	32,32,32	0.76	1 (3%)	51,51,51	1.13	3 (5%)
22	EDO	A	622	-	3,3,3	0.56	0	2,2,2	0.61	0
22	EDO	D	204	-	3,3,3	0.50	0	2,2,2	0.46	0
22	EDO	F	102	-	3,3,3	0.56	0	2,2,2	0.43	0
23	DMU	K	102	-	10,10,34	0.34	0	9,9,45	0.62	0
22	EDO	J	102	-	3,3,3	0.51	0	2,2,2	0.16	0
22	EDO	D	202	-	3,3,3	0.50	0	2,2,2	0.31	0
22	EDO	B	305	-	3,3,3	0.71	0	2,2,2	0.10	0
25	CHD	J	101	-	32,32,32	0.70	0	51,51,51	2.74	18 (35%)
22	EDO	S	107	-	3,3,3	0.52	0	2,2,2	0.58	0
14	HEA	N	602[A]	-	57,67,67	1.38	8 (14%)	61,103,103	1.90	13 (21%)
22	EDO	S	106	-	3,3,3	0.37	0	2,2,2	0.91	0
22	EDO	A	613	-	3,3,3	0.79	0	2,2,2	0.68	0
22	EDO	F	106	-	3,3,3	0.61	0	2,2,2	0.54	0
22	EDO	F	109	-	3,3,3	0.61	0	2,2,2	0.75	0
23	DMU	K	104	-	10,10,34	0.25	0	9,9,45	0.52	0
25	CHD	Y	102	-	32,32,32	0.67	0	51,51,51	2.19	15 (29%)
22	EDO	A	619	-	3,3,3	0.48	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	EDO	D	201	-	3,3,3	0.57	0	2,2,2	0.29	0
22	EDO	B	304	-	3,3,3	0.40	0	2,2,2	0.53	0
23	DMU	C	310	-	34,34,34	0.55	1 (2%)	45,45,45	1.20	6 (13%)
14	HEA	A	601[A]	-	57,67,67	1.45	9 (15%)	61,103,103	1.98	18 (29%)
27	CDL	T	102	-	57,57,99	1.26	8 (14%)	54,54,111	0.87	1 (1%)
23	DMU	D	206	-	34,34,34	0.70	1 (2%)	45,45,45	1.40	8 (17%)
14	HEA	N	603	1,30,20	57,67,67	1.45	8 (14%)	61,103,103	1.56	16 (26%)
23	DMU	X	104	-	22,22,34	0.57	1 (4%)	27,27,45	0.77	0
23	DMU	Z	101	-	34,34,34	0.46	0	45,45,45	0.82	2 (4%)
22	EDO	N	614	-	3,3,3	0.65	0	2,2,2	0.18	0
22	EDO	A	612	-	3,3,3	0.71	0	2,2,2	0.35	0
27	CDL	C	308	-	62,62,99	1.32	8 (12%)	61,61,111	1.41	11 (18%)
22	EDO	A	618	-	3,3,3	0.75	0	2,2,2	0.29	0
22	EDO	O	305	-	3,3,3	0.55	0	2,2,2	0.11	0
22	EDO	D	205	-	3,3,3	0.37	0	2,2,2	0.39	0
25	CHD	L	102	-	32,32,32	0.67	0	51,51,51	2.42	23 (45%)
26	PEK	C	304	-	51,51,52	0.80	2 (3%)	54,56,57	1.16	4 (7%)
22	EDO	L	103	-	3,3,3	0.24	0	2,2,2	1.02	0
23	DMU	X	102	-	8,8,34	0.29	0	7,7,45	0.48	0
22	EDO	T	103	-	3,3,3	0.73	0	2,2,2	0.36	0
22	EDO	C	318	-	3,3,3	0.56	0	2,2,2	0.35	0
22	EDO	C	314	-	3,3,3	0.34	0	2,2,2	0.67	0
19	PGV	N	610	-	50,50,50	0.96	2 (4%)	53,56,56	1.06	3 (5%)
19	PGV	C	307	-	35,35,50	1.31	2 (5%)	37,37,56	1.95	9 (24%)
22	EDO	N	618	-	3,3,3	0.53	0	2,2,2	0.32	0
21	PSC	O	302	-	27,27,51	0.77	1 (3%)	25,25,59	0.72	1 (4%)
22	EDO	F	108	-	3,3,3	0.48	0	2,2,2	0.37	0
22	EDO	D	203	-	3,3,3	0.50	0	2,2,2	0.22	0
22	EDO	C	317	-	3,3,3	0.54	0	2,2,2	0.15	0
20	PER	N	611[A]	14,15	0,1,1	-	-	-	-	-
22	EDO	N	616	-	3,3,3	0.40	0	2,2,2	0.69	0
27	CDL	P	307	-	65,65,99	1.37	9 (13%)	64,64,111	1.24	6 (9%)
22	EDO	Y	101	-	3,3,3	0.46	0	2,2,2	0.17	0
23	DMU	O	306	-	11,11,34	0.22	0	9,9,45	0.65	0
23	DMU	C	321	-	11,11,34	0.40	0	10,10,45	0.32	0
22	EDO	L	104	-	3,3,3	0.59	0	2,2,2	0.49	0
18	TGL	A	607	-	62,62,62	1.08	3 (4%)	65,65,65	1.11	6 (9%)
22	EDO	A	620	-	3,3,3	0.67	0	2,2,2	0.14	0
22	EDO	M	102	-	3,3,3	0.45	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	EDO	G	102	-	3,3,3	0.83	0	2,2,2	0.50	0
23	DMU	P	316	-	21,21,34	0.61	1 (4%)	24,25,45	0.81	1 (4%)
18	TGL	N	609	-	52,52,62	0.69	1 (1%)	50,50,65	0.69	2 (4%)
23	DMU	P	308	-	34,34,34	0.51	0	45,45,45	1.21	7 (15%)
22	EDO	A	617	-	3,3,3	0.50	0	2,2,2	0.59	0
22	EDO	N	621	-	3,3,3	0.34	0	2,2,2	0.50	0
29	PO4	U	101	-	4,4,4	1.06	0	6,6,6	0.56	0
22	EDO	F	105	-	3,3,3	0.62	0	2,2,2	0.23	0
23	DMU	J	104	-	10,10,34	0.33	0	9,9,45	0.41	0
26	PEK	P	303	-	37,37,52	1.14	2 (5%)	40,42,57	1.27	4 (10%)
22	EDO	N	617	-	3,3,3	0.46	0	2,2,2	0.15	0
23	DMU	L	105	-	21,21,34	0.90	1 (4%)	24,25,45	2.08	5 (20%)
23	DMU	M	101	-	34,34,34	0.44	0	45,45,45	1.03	1 (2%)
22	EDO	P	313	-	3,3,3	0.43	0	2,2,2	0.97	0
22	EDO	P	312	-	3,3,3	0.44	0	2,2,2	0.97	0
23	DMU	K	103	-	9,9,34	0.34	0	8,8,45	0.34	0
24	CUA	O	301	2	0,1,1	-	-	-	-	-
19	PGV	N	612	-	50,50,50	0.89	3 (6%)	53,56,56	1.12	6 (11%)
22	EDO	C	319	-	3,3,3	0.60	0	2,2,2	0.31	0
22	EDO	P	314	-	3,3,3	0.57	0	2,2,2	0.14	0
25	CHD	C	301	-	32,32,32	0.72	0	51,51,51	1.55	9 (17%)
14	HEA	A	602	1,30,20	57,67,67	1.37	7 (12%)	61,103,103	1.79	15 (24%)
18	TGL	N	608	-	52,52,62	0.73	1 (1%)	50,50,65	0.88	2 (4%)
22	EDO	F	107	-	3,3,3	0.50	0	2,2,2	0.38	0
22	EDO	A	616	-	3,3,3	0.45	0	2,2,2	0.50	0
22	EDO	P	310	-	3,3,3	0.54	0	2,2,2	0.19	0
22	EDO	N	615	-	3,3,3	0.54	0	2,2,2	0.34	0
22	EDO	P	315	-	3,3,3	0.53	0	2,2,2	0.13	0
23	DMU	K	105	-	8,8,34	0.30	0	7,7,45	0.57	0
19	PGV	A	608	-	31,31,50	0.41	0	29,29,56	0.58	0
22	EDO	F	103	-	3,3,3	0.47	0	2,2,2	0.52	0
22	EDO	A	615	-	3,3,3	0.68	0	2,2,2	0.98	0
22	EDO	C	315	-	3,3,3	0.56	0	2,2,2	0.18	0
22	EDO	C	316	-	3,3,3	0.38	0	2,2,2	0.35	0
22	EDO	S	102	-	3,3,3	0.77	0	2,2,2	0.72	0
22	EDO	E	202	-	3,3,3	0.45	0	2,2,2	0.12	0
22	EDO	S	104	-	3,3,3	0.49	0	2,2,2	0.77	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
26	PEK	C	305	-	-	13/30/30/56	-
22	EDO	W	102	-	-	1/1/1/1	-
22	EDO	O	304	-	-	0/1/1/1	-
25	CHD	B	302	-	-	2/9/74/74	0/4/4/4
23	DMU	A	623	-	-	0/8/8/59	-
23	DMU	X	103	-	-	0/6/6/59	-
23	DMU	K	101	-	-	1/5/5/59	-
18	TGL	A	606	-	-	37/65/65/65	-
22	EDO	B	306	-	-	0/1/1/1	-
22	EDO	C	320	-	-	1/1/1/1	-
22	EDO	F	104	-	-	0/1/1/1	-
22	EDO	N	620	-	-	0/1/1/1	-
18	TGL	L	101	-	-	39/65/65/65	-
25	CHD	C	309	-	-	5/9/74/74	0/4/4/4
26	PEK	T	101	-	-	14/32/32/56	-
22	EDO	Q	202	-	-	0/1/1/1	-
27	CDL	N	601	-	-	16/51/51/110	-
23	DMU	Q	201	-	-	4/8/8/59	-
22	EDO	N	619	-	-	1/1/1/1	-
21	PSC	A	610	-	-	11/19/19/55	-
22	EDO	N	622	-	-	0/1/1/1	-
22	EDO	J	103	-	-	1/1/1/1	-
22	EDO	A	614	-	-	1/1/1/1	-
19	PGV	A	611	-	-	4/55/55/55	-
18	TGL	N	607	-	-	31/65/65/65	-
22	EDO	C	311	-	-	0/1/1/1	-
22	EDO	B	303	-	-	0/1/1/1	-
22	EDO	P	311	-	-	0/1/1/1	-
19	PGV	P	305	-	-	6/55/55/55	-
22	EDO	C	312	-	-	0/1/1/1	-
22	EDO	W	101	-	-	1/1/1/1	-
22	EDO	P	309	-	-	0/1/1/1	-
22	EDO	C	313	-	-	0/1/1/1	-
22	EDO	T	105	-	-	1/1/1/1	-
23	DMU	P	317	-	-	3/18/58/59	0/2/2/2
25	CHD	P	301	-	-	1/9/74/74	0/4/4/4
22	EDO	E	203	-	-	0/1/1/1	-
22	EDO	S	103	-	-	0/1/1/1	-
23	DMU	D	207	-	-	4/8/8/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	N	613	-	-	0/1/1/1	-
22	EDO	E	201	-	-	0/1/1/1	-
22	EDO	O	303	-	-	0/1/1/1	-
19	PGV	P	306	-	-	5/25/25/55	-
22	EDO	T	104	-	-	1/1/1/1	-
23	DMU	X	101	-	-	2/7/7/59	-
22	EDO	S	105	-	-	0/1/1/1	-
26	PEK	C	303	-	-	19/48/48/56	-
19	PGV	C	306	-	-	13/52/52/55	-
22	EDO	A	621	-	-	0/1/1/1	-
26	PEK	P	304	-	-	10/55/55/56	-
25	CHD	G	101	-	-	2/9/74/74	0/4/4/4
22	EDO	A	622	-	-	0/1/1/1	-
22	EDO	D	204	-	-	1/1/1/1	-
22	EDO	F	102	-	-	0/1/1/1	-
23	DMU	K	102	-	-	4/8/8/59	-
22	EDO	J	102	-	-	1/1/1/1	-
22	EDO	D	202	-	-	1/1/1/1	-
22	EDO	B	305	-	-	0/1/1/1	-
25	CHD	J	101	-	-	7/9/74/74	0/4/4/4
22	EDO	S	107	-	-	0/1/1/1	-
14	HEA	N	602[A]	-	-	4/32/76/76	-
22	EDO	S	106	-	-	1/1/1/1	-
22	EDO	A	613	-	-	0/1/1/1	-
22	EDO	F	106	-	-	0/1/1/1	-
22	EDO	F	109	-	-	0/1/1/1	-
23	DMU	K	104	-	-	3/8/8/59	-
25	CHD	Y	102	-	-	3/9/74/74	0/4/4/4
22	EDO	A	619	-	-	1/1/1/1	-
22	EDO	D	201	-	-	0/1/1/1	-
22	EDO	B	304	-	-	0/1/1/1	-
23	DMU	C	310	-	-	3/19/59/59	0/2/2/2
14	HEA	A	601[A]	-	-	2/32/76/76	-
27	CDL	T	102	-	-	18/50/50/110	-
23	DMU	D	206	-	-	6/19/59/59	0/2/2/2
14	HEA	N	603	1,30,20	-	7/32/76/76	-
23	DMU	X	104	-	-	2/13/33/59	0/1/1/2
23	DMU	Z	101	-	-	7/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	N	614	-	-	0/1/1/1	-
22	EDO	A	612	-	-	1/1/1/1	-
27	CDL	C	308	-	-	17/58/58/110	-
22	EDO	A	618	-	-	1/1/1/1	-
22	EDO	O	305	-	-	0/1/1/1	-
22	EDO	D	205	-	-	1/1/1/1	-
25	CHD	L	102	-	-	5/9/74/74	0/4/4/4
26	PEK	C	304	-	-	17/55/55/56	-
22	EDO	L	103	-	-	1/1/1/1	-
23	DMU	X	102	-	-	2/6/6/59	-
22	EDO	T	103	-	-	0/1/1/1	-
22	EDO	C	318	-	-	0/1/1/1	-
22	EDO	C	314	-	-	0/1/1/1	-
19	PGV	N	610	-	-	14/55/55/55	-
19	PGV	C	307	-	-	16/36/36/55	-
22	EDO	N	618	-	-	1/1/1/1	-
21	PSC	O	302	-	-	5/23/23/55	-
22	EDO	F	108	-	-	1/1/1/1	-
22	EDO	D	203	-	-	0/1/1/1	-
22	EDO	C	317	-	-	0/1/1/1	-
22	EDO	N	616	-	-	0/1/1/1	-
27	CDL	P	307	-	-	27/61/61/110	-
22	EDO	Y	101	-	-	0/1/1/1	-
23	DMU	O	306	-	-	1/8/8/59	-
23	DMU	C	321	-	-	0/9/9/59	-
22	EDO	L	104	-	-	1/1/1/1	-
18	TGL	A	607	-	-	26/65/65/65	-
22	EDO	A	620	-	-	1/1/1/1	-
22	EDO	M	102	-	-	1/1/1/1	-
22	EDO	G	102	-	-	0/1/1/1	-
23	DMU	P	316	-	-	5/13/29/59	0/1/1/2
18	TGL	N	609	-	-	20/47/47/65	-
23	DMU	P	308	-	-	8/19/59/59	0/2/2/2
22	EDO	A	617	-	-	1/1/1/1	-
22	EDO	N	621	-	-	0/1/1/1	-
22	EDO	F	105	-	-	0/1/1/1	-
23	DMU	J	104	-	-	2/8/8/59	-
26	PEK	P	303	-	-	13/41/41/56	-
22	EDO	N	617	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	DMU	L	105	-	-	8/13/29/59	0/1/1/2
23	DMU	M	101	-	-	4/19/59/59	0/2/2/2
22	EDO	P	313	-	-	1/1/1/1	-
22	EDO	P	312	-	-	1/1/1/1	-
23	DMU	K	103	-	-	2/7/7/59	-
19	PGV	N	612	-	-	6/55/55/55	-
22	EDO	C	319	-	-	0/1/1/1	-
22	EDO	P	314	-	-	0/1/1/1	-
25	CHD	C	301	-	-	1/9/74/74	0/4/4/4
14	HEA	A	602	1,30,20	-	6/32/76/76	-
18	TGL	N	608	-	-	22/47/47/65	-
22	EDO	F	107	-	-	0/1/1/1	-
22	EDO	A	616	-	-	0/1/1/1	-
22	EDO	P	310	-	-	0/1/1/1	-
22	EDO	N	615	-	-	0/1/1/1	-
22	EDO	P	315	-	-	0/1/1/1	-
23	DMU	K	105	-	-	0/6/6/59	-
19	PGV	A	608	-	-	9/26/27/55	-
22	EDO	F	103	-	-	0/1/1/1	-
22	EDO	A	615	-	-	0/1/1/1	-
22	EDO	C	315	-	-	0/1/1/1	-
22	EDO	C	316	-	-	0/1/1/1	-
22	EDO	S	102	-	-	0/1/1/1	-
22	EDO	E	202	-	-	1/1/1/1	-
22	EDO	S	104	-	-	0/1/1/1	-

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	307	PGV	O03-C19	5.47	1.49	1.33
26	C	303	PEK	O03-C21	5.28	1.48	1.33
18	L	101	TGL	OG2-CB1	5.01	1.48	1.34
27	N	601	CDL	OB8-CB7	4.91	1.47	1.33
27	P	307	CDL	OB6-CB5	4.82	1.47	1.33
19	P	306	PGV	O03-C19	4.79	1.46	1.30
18	A	607	TGL	OG1-CA1	4.76	1.47	1.33
27	P	307	CDL	OB8-CB7	4.71	1.47	1.33
18	L	101	TGL	OG1-CA1	4.70	1.47	1.33
18	L	101	TGL	OG3-CC1	4.69	1.47	1.33
26	P	303	PEK	O03-C21	4.65	1.46	1.33
18	A	606	TGL	OG1-CA1	4.64	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	303	PEK	O01-C1	4.64	1.47	1.34
27	T	102	CDL	OB8-CB7	4.62	1.46	1.33
18	N	607	TGL	OG2-CB1	4.60	1.47	1.34
18	N	608	TGL	OG3-CC1	4.46	1.47	1.33
18	N	607	TGL	OG1-CA1	4.43	1.46	1.33
19	C	307	PGV	O01-C1	4.42	1.46	1.34
18	A	606	TGL	OG2-CB1	4.39	1.46	1.34
19	N	610	PGV	O03-C19	4.38	1.46	1.33
18	N	609	TGL	OG3-CC1	4.38	1.47	1.33
27	C	308	CDL	OB8-CB7	4.36	1.46	1.33
26	T	101	PEK	O03-C21	4.36	1.46	1.33
27	C	308	CDL	OB6-CB5	4.36	1.46	1.33
26	P	303	PEK	O01-C1	4.34	1.46	1.34
18	A	607	TGL	OG3-CC1	4.32	1.46	1.33
18	A	606	TGL	OG3-CC1	4.32	1.46	1.33
18	N	607	TGL	OG3-CC1	4.24	1.45	1.33
18	A	607	TGL	OG2-CB1	4.17	1.46	1.34
19	N	610	PGV	O01-C1	4.17	1.46	1.34
21	A	610	PSC	C13-C12	3.74	1.53	1.31
21	O	302	PSC	C13-C12	3.72	1.53	1.31
14	A	601[A]	HEA	CHC-C4B	3.67	1.44	1.35
19	A	611	PGV	O01-C1	3.60	1.44	1.34
26	C	304	PEK	O03-C21	3.60	1.43	1.33
14	A	601[A]	HEA	CHD-C1D	3.59	1.44	1.35
27	C	308	CDL	C59-C58	-3.56	1.31	1.51
14	A	602	HEA	CHD-C1D	3.53	1.44	1.35
19	N	612	PGV	O01-C1	3.51	1.44	1.34
14	N	602[A]	HEA	CHC-C4B	3.49	1.43	1.35
27	C	308	CDL	C82-C81	-3.49	1.32	1.51
14	A	602	HEA	CHC-C4B	3.44	1.43	1.35
14	N	602[A]	HEA	CHD-C1D	3.43	1.43	1.35
14	N	603	HEA	CHD-C1D	3.43	1.43	1.35
14	N	603	HEA	CHC-C4B	3.40	1.43	1.35
27	C	308	CDL	C79-C78	-3.36	1.32	1.51
27	P	307	CDL	C82-C81	-3.34	1.32	1.51
27	C	308	CDL	C62-C61	-3.32	1.32	1.51
27	P	307	CDL	C79-C78	-3.26	1.33	1.51
27	T	102	CDL	C62-C61	-3.25	1.33	1.51
27	T	102	CDL	C82-C81	-3.24	1.33	1.51
23	L	105	DMU	O16-C6	3.22	1.45	1.40
26	P	304	PEK	O03-C21	3.22	1.42	1.33
27	T	102	CDL	C59-C58	-3.21	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	P	307	CDL	C59-C58	-3.21	1.33	1.51
27	N	601	CDL	C42-C41	-3.19	1.33	1.51
27	N	601	CDL	C62-C61	-3.18	1.33	1.51
14	N	603	HEA	C4D-C3D	-3.17	1.39	1.45
27	P	307	CDL	C39-C38	-3.17	1.33	1.51
27	P	307	CDL	C42-C41	-3.16	1.33	1.51
27	C	308	CDL	C39-C38	-3.12	1.34	1.51
27	P	307	CDL	C22-C21	-3.11	1.34	1.51
27	C	308	CDL	C42-C41	-3.10	1.34	1.51
14	A	602	HEA	C4D-C3D	-3.09	1.39	1.45
27	T	102	CDL	C79-C78	-3.08	1.34	1.51
27	N	601	CDL	C19-C18	-3.03	1.34	1.51
27	P	307	CDL	C19-C18	-3.02	1.34	1.51
27	T	102	CDL	C19-C18	-3.00	1.34	1.51
27	N	601	CDL	C82-C81	-3.00	1.34	1.51
27	N	601	CDL	C39-C38	-2.96	1.35	1.51
27	T	102	CDL	C22-C21	-2.95	1.35	1.51
14	N	603	HEA	C4B-NB	-2.95	1.35	1.40
27	N	601	CDL	C79-C78	-2.95	1.35	1.51
19	C	306	PGV	O01-C1	2.93	1.42	1.34
26	C	304	PEK	O01-C1	2.89	1.42	1.34
19	A	611	PGV	O03-C19	2.80	1.41	1.33
19	N	612	PGV	O03-C19	2.79	1.41	1.33
14	A	601[A]	HEA	C4D-C3D	-2.71	1.40	1.45
14	N	602[A]	HEA	C4B-NB	-2.67	1.35	1.40
14	A	601[A]	HEA	CAD-C3D	2.66	1.58	1.51
14	A	602	HEA	O11-C11	2.61	1.48	1.42
23	D	206	DMU	O16-C6	2.57	1.44	1.40
27	N	601	CDL	C58-C59	-2.56	1.33	1.51
14	N	603	HEA	O11-C11	2.54	1.48	1.42
23	P	317	DMU	O16-C6	2.52	1.44	1.40
19	P	305	PGV	O03-C19	2.51	1.40	1.33
19	P	305	PGV	O01-C1	2.51	1.41	1.34
14	N	602[A]	HEA	C1D-ND	-2.50	1.36	1.40
14	N	603	HEA	C4B-C3B	-2.49	1.40	1.44
27	T	102	CDL	C41-C42	-2.48	1.34	1.51
14	A	601[A]	HEA	C4B-NB	-2.42	1.36	1.40
19	C	306	PGV	O03-C19	2.42	1.40	1.33
26	P	304	PEK	O01-C1	2.39	1.41	1.34
27	N	601	CDL	C22-C21	-2.37	1.34	1.51
14	N	603	HEA	C1D-ND	-2.36	1.36	1.40
14	N	603	HEA	CBA-CGA	2.34	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	310	DMU	O16-C6	2.28	1.44	1.40
19	A	611	PGV	O01-C02	-2.27	1.40	1.46
19	N	612	PGV	O01-C02	-2.26	1.40	1.46
14	A	601[A]	HEA	C4B-C3B	-2.23	1.40	1.44
14	A	601[A]	HEA	CBD-CGD	2.22	1.55	1.50
14	A	602	HEA	CBA-CGA	2.22	1.55	1.50
14	N	602[A]	HEA	CBD-CGD	2.21	1.55	1.50
14	N	602[A]	HEA	O2D-CGD	-2.18	1.23	1.30
14	N	602[A]	HEA	O11-C11	2.16	1.47	1.42
23	X	104	DMU	O16-C6	2.15	1.43	1.40
14	A	602	HEA	C4B-C3B	-2.14	1.41	1.44
25	G	101	CHD	O7-C7	2.09	1.47	1.43
23	P	316	DMU	O16-C6	2.06	1.43	1.40
14	A	602	HEA	CMC-C2C	2.05	1.55	1.51
14	A	601[A]	HEA	CBA-CGA	2.01	1.55	1.50
14	N	602[A]	HEA	C1B-C2B	-2.01	1.40	1.44
14	A	601[A]	HEA	CMC-C2C	2.00	1.55	1.51

All (291) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	101	CHD	C10-C9-C8	7.54	119.92	111.82
25	J	101	CHD	C14-C8-C9	-7.45	99.48	109.71
25	J	101	CHD	C14-C8-C7	7.39	121.60	111.81
14	N	602[A]	HEA	C13-C12-C11	-7.03	103.78	114.35
18	A	606	TGL	OG2-CB1-CB2	6.40	125.30	111.50
19	C	307	PGV	O03-C19-C20	6.11	131.09	111.91
18	N	607	TGL	OG2-CB1-CB2	5.95	124.33	111.50
19	C	307	PGV	O01-C1-C2	5.68	123.75	111.50
25	L	102	CHD	C4-C5-C10	5.65	118.66	112.66
25	Y	102	CHD	C1-C10-C5	5.65	116.12	107.77
14	A	601[A]	HEA	C13-C12-C11	-5.54	106.02	114.35
25	L	102	CHD	C21-C20-C17	5.39	121.17	112.92
23	L	105	DMU	C18-O16-C6	5.33	122.67	113.84
25	J	101	CHD	C14-C13-C12	5.27	112.31	107.40
25	Y	102	CHD	C9-C11-C12	-5.19	107.44	114.30
25	C	301	CHD	C18-C13-C12	5.16	114.32	109.07
25	J	101	CHD	C9-C11-C12	-4.92	107.81	114.30
23	L	105	DMU	O5-C6-O16	4.73	121.18	109.97
26	P	303	PEK	O03-C21-C22	4.73	123.79	111.38
25	Y	102	CHD	C6-C5-C4	-4.66	105.82	111.19
23	P	317	DMU	C10-O1-C9	4.63	122.77	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	102	CHD	C14-C8-C7	4.57	117.87	111.81
27	P	307	CDL	OB8-CB7-C71	4.55	126.19	111.91
25	J	101	CHD	C22-C20-C17	4.53	119.65	110.28
14	N	602[A]	HEA	C3D-C4D-ND	4.52	114.73	110.36
25	Y	102	CHD	C21-C20-C17	4.48	119.78	112.92
25	L	102	CHD	C5-C4-C3	4.46	119.30	112.76
26	C	303	PEK	O03-C21-C22	4.43	125.82	111.91
25	L	102	CHD	C10-C9-C8	4.40	116.55	111.82
25	L	102	CHD	C13-C17-C20	4.38	124.72	119.50
26	C	303	PEK	O01-C1-C2	4.37	120.92	111.50
18	L	101	TGL	OG2-CB1-CB2	4.36	120.89	111.50
19	C	307	PGV	C01-O03-C19	4.33	133.16	117.12
14	A	601[A]	HEA	C3D-C4D-ND	4.23	114.45	110.36
25	J	101	CHD	C13-C17-C20	4.21	124.53	119.50
25	L	102	CHD	C17-C13-C12	-4.16	113.86	117.67
14	A	602	HEA	CAD-CBD-CGD	-4.15	104.67	113.60
25	J	101	CHD	C9-C10-C5	4.12	114.37	108.58
19	N	610	PGV	C02-O01-C1	-4.12	107.65	117.79
25	L	102	CHD	C11-C9-C10	-4.03	109.57	113.73
14	N	602[A]	HEA	C26-C15-C16	3.97	121.96	115.27
14	A	601[A]	HEA	C2B-C1B-NB	3.97	114.63	109.88
25	B	302	CHD	C6-C5-C4	-3.95	106.65	111.19
23	L	105	DMU	C3-C4-C57	-3.92	105.72	112.60
25	Y	102	CHD	C19-C10-C1	-3.90	101.98	108.26
27	C	308	CDL	C52-C51-CB5	-3.79	99.83	113.62
14	A	601[A]	HEA	C2D-C1D-ND	3.75	114.28	109.84
18	L	101	TGL	OG1-CA1-CA2	3.70	123.53	111.91
23	L	105	DMU	O5-C4-C57	3.68	112.73	106.83
27	C	308	CDL	OB8-CB7-C71	3.67	123.41	111.91
23	M	101	DMU	C18-O16-C6	-3.66	107.77	113.84
25	L	102	CHD	C6-C5-C4	-3.66	106.98	111.19
23	P	317	DMU	C10-C5-C7	3.60	117.49	110.00
18	L	101	TGL	CC3-CC2-CC1	3.59	126.66	113.62
18	A	607	TGL	OG3-CC1-CC2	3.56	123.09	111.91
19	A	611	PGV	O03-C19-O04	-3.55	114.63	123.59
14	N	602[A]	HEA	C1D-ND-C4D	-3.55	101.41	105.07
19	C	307	PGV	O03-C19-O04	-3.54	114.65	123.59
25	J	101	CHD	C18-C13-C14	-3.53	105.69	111.21
25	J	101	CHD	C1-C10-C9	-3.52	105.81	111.35
18	A	607	TGL	OG1-CA1-CA2	3.49	122.87	111.91
26	T	101	PEK	O03-C21-C22	3.49	126.02	112.23
25	Y	102	CHD	C14-C13-C12	3.48	110.64	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602[A]	HEA	C2D-C1D-ND	3.47	113.95	109.84
25	C	301	CHD	C1-C2-C3	-3.47	106.02	110.47
25	L	102	CHD	C14-C13-C12	3.46	110.62	107.40
23	P	317	DMU	C6-C1-C2	3.46	117.20	110.00
14	N	602[A]	HEA	C2B-C1B-NB	3.45	114.01	109.88
18	A	606	TGL	CB3-CB2-CB1	-3.44	101.09	113.62
14	A	602	HEA	C2B-C1B-NB	3.39	113.94	109.88
14	A	601[A]	HEA	C1D-ND-C4D	-3.38	101.58	105.07
25	C	301	CHD	C22-C20-C17	-3.38	103.31	110.28
27	C	308	CDL	OB6-CB5-C51	3.37	122.50	111.91
25	Y	102	CHD	C4-C3-C2	-3.37	106.53	110.55
23	P	317	DMU	O1-C9-C8	3.36	115.79	109.69
23	D	206	DMU	C6-O5-C4	3.36	120.28	113.69
23	P	308	DMU	C18-O16-C6	-3.33	108.32	113.84
14	A	602	HEA	C3B-C4B-NB	3.33	113.78	109.84
26	P	303	PEK	O01-C1-C2	3.33	118.67	111.50
14	A	601[A]	HEA	O1A-CGA-CBA	-3.30	112.50	123.08
23	P	317	DMU	O16-C6-C1	3.29	113.44	108.30
19	A	611	PGV	O03-C19-C20	3.28	122.20	111.91
27	P	307	CDL	OB8-CB7-OB9	-3.28	115.32	123.59
25	G	101	CHD	C6-C5-C4	-3.26	107.43	111.19
25	J	101	CHD	C15-C14-C8	3.26	122.89	118.33
14	A	601[A]	HEA	CHA-C4D-C3D	-3.25	120.06	124.84
14	A	602	HEA	C20-C19-C18	-3.22	114.59	121.12
23	P	317	DMU	O1-C10-C5	3.22	117.16	110.35
25	B	302	CHD	C13-C17-C20	-3.21	115.66	119.50
25	J	101	CHD	C5-C6-C7	-3.21	110.92	114.46
14	A	601[A]	HEA	O2A-CGA-CBA	3.21	124.33	114.03
18	A	607	TGL	OG3-CC1-OC1	-3.20	115.51	123.59
19	P	305	PGV	O01-C1-O02	-3.19	115.98	123.70
18	L	101	TGL	CG3-CG2-CG1	-3.14	104.36	111.79
14	A	601[A]	HEA	C1B-C2B-C3B	-3.13	103.06	106.80
25	Y	102	CHD	C10-C9-C8	3.12	115.17	111.82
19	N	612	PGV	O03-C19-O04	-3.12	115.73	123.59
14	A	602	HEA	C4B-NB-C1B	-3.11	101.86	105.07
27	C	308	CDL	C61-C60-C59	-3.11	98.64	114.42
14	A	602	HEA	C13-C12-C11	-3.11	109.68	114.35
14	A	601[A]	HEA	CAA-CBA-CGA	-3.10	105.07	113.76
14	A	602	HEA	C1D-C2D-C3D	-3.05	103.75	106.96
25	L	102	CHD	C1-C10-C5	3.03	112.24	107.77
26	C	304	PEK	O03-C21-C22	3.01	121.37	111.91
14	A	602	HEA	CBA-CAA-C2A	-3.00	107.54	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602[A]	HEA	C16-C15-C14	-2.99	115.06	121.12
25	L	102	CHD	C14-C8-C7	2.98	115.76	111.81
18	L	101	TGL	OG3-CC1-OC1	-2.95	116.14	123.59
25	L	102	CHD	C1-C10-C9	-2.93	106.74	111.35
23	D	206	DMU	C10-O1-C9	2.93	119.44	113.69
19	N	610	PGV	O01-C1-C2	2.89	117.74	111.50
14	N	602[A]	HEA	O2A-CGA-CBA	2.89	123.32	114.03
25	L	102	CHD	C9-C10-C5	2.87	112.61	108.58
23	C	310	DMU	C8-C7-C5	2.86	115.81	110.82
26	T	101	PEK	C01-O03-C21	2.84	125.45	116.11
27	N	601	CDL	CB6-OB8-CB7	2.84	126.08	116.92
23	D	206	DMU	C11-C9-C8	-2.80	106.44	113.00
25	B	302	CHD	C16-C17-C13	2.79	106.29	103.55
14	N	603	HEA	C13-C12-C11	-2.79	110.16	114.35
27	T	102	CDL	OB8-CB7-C71	2.79	120.65	111.91
27	P	307	CDL	OB6-CB5-C51	2.78	120.64	111.91
14	A	601[A]	HEA	C4A-CHB-C1B	2.77	126.22	122.56
25	C	309	CHD	C11-C9-C10	-2.77	110.87	113.73
23	P	317	DMU	O7-C10-C5	2.76	115.25	108.10
19	N	610	PGV	O03-C19-C20	2.75	120.55	111.91
25	C	301	CHD	C18-C13-C17	-2.75	106.91	111.21
14	N	602[A]	HEA	CAD-C3D-C2D	2.74	132.98	127.88
25	L	102	CHD	C18-C13-C14	-2.74	106.93	111.21
14	A	602	HEA	C27-C19-C20	2.73	119.87	115.27
14	N	603	HEA	CHB-C1B-C2B	-2.73	120.72	124.98
18	A	606	TGL	OG3-CC1-CC2	2.71	120.42	111.91
23	D	206	DMU	O1-C9-C8	2.71	114.61	109.69
25	B	302	CHD	C19-C10-C5	-2.70	105.78	110.36
19	C	307	PGV	O01-C1-O02	-2.69	117.19	123.70
27	C	308	CDL	OB8-CB7-OB9	-2.69	116.79	123.59
19	P	306	PGV	O03-C19-O04	-2.69	116.60	123.30
25	J	101	CHD	C13-C14-C8	-2.69	111.31	114.74
25	C	309	CHD	C19-C10-C9	-2.67	107.50	111.18
23	P	308	DMU	O7-C3-C2	2.67	114.38	107.28
25	P	301	CHD	C22-C20-C17	-2.67	104.78	110.28
26	C	303	PEK	C01-O03-C21	2.66	126.97	117.12
18	L	101	TGL	OG1-CG1-CG2	2.66	116.17	108.43
25	Y	102	CHD	C13-C17-C20	2.65	122.65	119.50
25	P	301	CHD	C22-C23-C24	-2.64	105.50	112.51
25	P	301	CHD	C11-C9-C10	-2.63	111.02	113.73
18	A	606	TGL	OG1-CA1-CA2	2.63	120.15	111.91
25	L	102	CHD	C11-C12-C13	2.62	113.94	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	P	306	PGV	O03-C19-C20	2.62	122.45	114.03
14	N	603	HEA	O2A-CGA-CBA	2.62	122.44	114.03
14	A	602	HEA	C2D-C1D-ND	2.62	112.94	109.84
23	L	105	DMU	O5-C6-C1	-2.61	104.81	110.35
19	N	612	PGV	O03-C19-C20	2.60	120.08	111.91
14	N	602[A]	HEA	C3C-C4C-NC	2.60	112.57	109.21
26	C	303	PEK	O03-C21-O04	-2.59	117.06	123.59
14	N	602[A]	HEA	CAA-CBA-CGA	-2.58	106.52	113.76
18	N	608	TGL	OG3-CC1-OC1	-2.57	115.08	123.14
14	N	602[A]	HEA	C1B-C2B-C3B	-2.57	103.73	106.80
18	N	607	TGL	OG1-CA1-CA2	2.57	119.96	111.91
14	A	601[A]	HEA	C4B-NB-C1B	-2.56	102.43	105.07
25	J	101	CHD	C6-C5-C4	-2.55	108.26	111.19
25	P	301	CHD	C6-C5-C10	-2.54	109.96	112.66
14	A	601[A]	HEA	CHB-C1B-NB	-2.54	121.67	124.43
26	P	304	PEK	C8-C7-C6	-2.52	99.63	112.02
14	N	603	HEA	C3B-C4B-NB	2.51	112.81	109.84
23	D	206	DMU	C10-C5-C7	2.51	115.22	110.00
19	C	307	PGV	C21-C20-C19	-2.50	104.52	113.62
25	Y	102	CHD	C15-C14-C8	2.50	121.83	118.33
23	C	310	DMU	C10-C5-C7	2.48	115.15	110.00
26	T	101	PEK	O03-C21-O04	-2.47	115.40	123.14
25	L	102	CHD	O25-C24-C23	-2.47	115.15	123.08
26	P	303	PEK	C01-O03-C21	2.46	126.24	117.12
25	B	302	CHD	C11-C9-C10	-2.46	111.19	113.73
26	P	304	PEK	O03-C21-C22	2.45	119.60	111.91
19	C	307	PGV	O04-C19-C20	-2.45	114.17	123.73
18	A	607	TGL	OG2-CB1-CB2	2.44	116.77	111.50
25	Y	102	CHD	C2-C1-C10	2.44	116.96	112.78
26	P	303	PEK	O03-C21-O04	-2.44	117.44	123.59
14	A	602	HEA	C13-C14-C15	-2.43	121.82	127.66
26	C	303	PEK	O01-C1-O02	-2.42	117.84	123.70
26	C	303	PEK	O03-C01-C02	2.42	115.48	108.43
19	A	611	PGV	C32-C31-C30	-2.42	102.15	114.42
23	D	206	DMU	C7-C8-C9	2.42	114.55	110.24
18	N	607	TGL	OG3-CC1-CC2	2.41	119.46	111.91
19	C	306	PGV	O03-C19-O04	-2.40	117.53	123.59
27	C	308	CDL	C77-C76-C75	-2.40	102.25	114.42
18	N	609	TGL	OG3-CC1-CC2	2.40	121.71	112.23
25	J	101	CHD	O7-C7-C8	2.40	114.78	109.43
23	C	310	DMU	C7-C8-C9	2.39	114.51	110.24
25	P	301	CHD	O12-C12-C13	-2.39	106.98	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	608	TGL	OG3-CC1-CC2	2.39	121.67	112.23
14	N	603	HEA	C2B-C1B-NB	2.38	112.74	109.88
19	N	612	PGV	O01-C02-C01	-2.38	99.77	108.40
14	N	603	HEA	C1D-C2D-C3D	-2.38	104.45	106.96
27	C	308	CDL	C80-C79-C78	2.38	126.51	114.42
27	P	307	CDL	C83-C82-C81	2.37	126.45	114.42
25	C	301	CHD	C4-C5-C10	-2.37	110.14	112.66
14	N	603	HEA	C3C-C4C-NC	2.37	112.27	109.21
25	Y	102	CHD	C16-C17-C13	-2.37	101.23	103.55
14	N	603	HEA	CAD-CBD-CGD	-2.37	108.51	113.60
14	N	603	HEA	C27-C19-C20	2.36	119.25	115.27
14	A	601[A]	HEA	C1D-C2D-C3D	-2.36	104.47	106.96
25	J	101	CHD	C11-C9-C8	-2.36	107.42	110.88
23	C	310	DMU	C10-O1-C9	-2.35	109.07	113.69
23	P	308	DMU	C1-C2-C3	-2.35	104.31	109.68
25	L	102	CHD	C15-C14-C8	2.35	121.61	118.33
25	L	102	CHD	C14-C8-C9	-2.35	106.49	109.71
14	A	602	HEA	C26-C15-C16	2.35	119.22	115.27
26	C	303	PEK	C2-C3-C4	2.34	117.40	113.23
14	A	601[A]	HEA	C26-C15-C16	2.34	119.20	115.27
27	C	308	CDL	C81-C80-C79	-2.33	102.60	114.42
19	N	612	PGV	C01-O03-C19	-2.33	108.50	117.12
25	C	301	CHD	C5-C4-C3	-2.32	109.34	112.76
23	C	310	DMU	O7-C10-C5	2.31	114.09	108.10
14	A	601[A]	HEA	C13-C14-C15	-2.31	122.10	127.66
14	A	601[A]	HEA	C3C-C4C-NC	2.31	112.19	109.21
25	G	101	CHD	C18-C13-C12	-2.30	106.72	109.07
23	Z	101	DMU	O1-C9-C8	2.29	113.86	109.69
23	P	317	DMU	C1-C2-C3	2.28	114.90	109.68
23	P	308	DMU	C10-C5-C7	2.27	114.72	110.00
26	P	304	PEK	C3-C2-C1	-2.26	105.39	113.62
25	C	309	CHD	C14-C8-C9	-2.26	106.61	109.71
25	P	301	CHD	C18-C13-C12	2.26	111.37	109.07
18	A	607	TGL	CG3-CG2-CG1	-2.26	106.45	111.79
25	P	301	CHD	C18-C13-C17	-2.25	107.69	111.21
25	C	301	CHD	C11-C9-C10	-2.24	111.41	113.73
27	N	601	CDL	C40-C39-C38	2.24	125.80	114.42
26	C	304	PEK	O03-C21-O04	-2.24	117.94	123.59
26	C	304	PEK	C3-C2-C1	-2.23	105.50	113.62
14	N	603	HEA	C13-C14-C15	-2.23	122.29	127.66
27	C	308	CDL	C62-C61-C60	2.23	125.74	114.42
19	A	611	PGV	O01-C1-C2	2.22	116.29	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	307	PGV	C02-O01-C1	-2.22	115.02	117.88
25	C	301	CHD	C19-C10-C1	-2.22	104.68	108.26
27	C	308	CDL	CB4-OB6-CB5	-2.22	109.75	116.92
23	D	206	DMU	O16-C6-C1	2.21	111.76	108.30
25	L	102	CHD	C18-C13-C12	2.21	111.31	109.07
27	P	307	CDL	OB8-CB6-CB4	2.20	115.12	108.61
19	N	612	PGV	O01-C1-C2	2.20	116.25	111.50
25	G	101	CHD	C13-C14-C8	-2.19	111.95	114.74
14	A	602	HEA	C16-C15-C14	-2.18	116.71	121.12
26	C	303	PEK	C02-O01-C1	-2.17	112.44	117.79
14	N	603	HEA	C2D-C1D-ND	2.17	112.41	109.84
18	L	101	TGL	OG3-CC1-CC2	2.17	118.71	111.91
25	L	102	CHD	C22-C20-C17	-2.16	105.82	110.28
18	N	607	TGL	OG2-CB1-OB1	-2.15	118.49	123.70
14	A	602	HEA	CMB-C2B-C1B	2.15	128.31	125.04
14	N	603	HEA	CHA-C4D-C3D	-2.15	121.68	124.84
25	P	301	CHD	C5-C4-C3	-2.14	109.61	112.76
19	N	612	PGV	C9-C10-C11	-2.14	100.17	112.43
25	J	101	CHD	C16-C17-C20	2.12	115.43	112.15
25	Y	102	CHD	O7-C7-C8	2.12	114.17	109.43
25	L	102	CHD	C22-C23-C24	-2.12	106.89	112.51
14	N	603	HEA	CBA-CAA-C2A	-2.11	109.04	112.60
26	P	304	PEK	O03-C21-O04	-2.11	118.27	123.59
25	Y	102	CHD	C21-C20-C22	-2.10	107.07	110.36
14	N	603	HEA	CMB-C2B-C1B	2.10	128.23	125.04
23	P	308	DMU	C7-C8-C9	2.09	113.97	110.24
25	J	101	CHD	C23-C22-C20	-2.09	110.70	114.52
23	P	316	DMU	C3-C2-C1	2.09	113.72	110.69
25	L	102	CHD	C13-C14-C8	-2.08	112.08	114.74
14	N	602[A]	HEA	O1A-CGA-CBA	-2.08	116.40	123.08
19	C	307	PGV	C03-C02-C01	-2.07	106.67	112.63
25	P	301	CHD	C21-C20-C22	-2.07	107.12	110.36
25	B	302	CHD	O26-C24-C23	2.06	120.66	114.03
25	L	102	CHD	O7-C7-C8	2.06	114.03	109.43
14	N	603	HEA	C21-C22-C23	-2.06	120.70	127.75
25	B	302	CHD	C13-C14-C8	-2.06	112.11	114.74
23	C	310	DMU	C18-O16-C6	2.06	117.25	113.84
18	N	609	TGL	CG3-OG3-CC1	2.05	122.88	116.11
18	A	606	TGL	OB1-CB1-CB2	-2.05	115.72	123.73
27	N	601	CDL	C44-C43-C42	-2.05	104.03	114.42
27	N	601	CDL	C19-C18-C17	2.04	124.80	114.42
25	C	309	CHD	C1-C10-C5	2.04	110.79	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	206	DMU	O61-C57-C4	2.04	118.29	111.29
19	C	306	PGV	O03-C19-C20	2.04	118.31	111.91
26	C	304	PEK	O01-C1-C2	2.04	115.89	111.50
23	P	308	DMU	C6-O5-C4	2.04	117.69	113.69
25	C	309	CHD	C17-C13-C14	2.03	102.14	100.09
23	P	308	DMU	O1-C10-C5	2.03	114.65	110.35
27	P	307	CDL	OB6-CB4-CB6	-2.03	102.61	108.61
19	C	306	PGV	O03-C01-C02	-2.03	102.53	108.43
14	N	603	HEA	O1A-CGA-CBA	-2.02	116.58	123.08
23	Z	101	DMU	C10-O7-C3	-2.02	112.96	117.96
25	P	301	CHD	C16-C17-C20	-2.02	109.02	112.15
25	C	301	CHD	O12-C12-C13	-2.02	107.62	111.03
27	C	308	CDL	C84-C83-C82	-2.02	104.17	114.42
21	O	302	PSC	C14-C13-C12	-2.02	109.25	124.73
14	A	601[A]	HEA	CMC-C2C-C3C	2.01	128.45	124.68
25	C	309	CHD	C5-C6-C7	2.01	116.68	114.46
14	A	602	HEA	C21-C20-C19	2.01	119.58	112.98
18	A	607	TGL	OG1-CA1-OA1	-2.00	118.54	123.59

There are no chirality outliers.

All (570) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	607	TGL	OB1-CB1-OG2-CG2
18	L	101	TGL	CB2-CB1-OG2-CG2
18	L	101	TGL	OB1-CB1-OG2-CG2
18	N	609	TGL	CC2-CC1-OG3-CG3
19	A	608	PGV	C1-C2-C3-C4
19	C	307	PGV	O04-C19-O03-C01
19	C	307	PGV	C20-C19-O03-C01
19	N	610	PGV	C04-O12-P-O13
19	N	610	PGV	O04-C19-O03-C01
19	N	610	PGV	C20-C19-O03-C01
21	A	610	PSC	C7-C8-C9-C10
21	A	610	PSC	C11-C10-C9-C8
22	W	101	EDO	O1-C1-C2-O2
23	L	105	DMU	C3-C4-C57-O61
23	L	105	DMU	O5-C4-C57-O61
23	L	105	DMU	O5-C6-O16-C18
25	J	101	CHD	C13-C17-C20-C22
25	J	101	CHD	C16-C17-C20-C21
25	J	101	CHD	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
25	L	102	CHD	C20-C22-C23-C24
26	C	305	PEK	C4-C5-C6-C7
26	C	305	PEK	C13-C14-C15-C16
26	P	303	PEK	O04-C21-O03-C01
26	P	303	PEK	C22-C21-O03-C01
26	P	303	PEK	C5-C6-C7-C8
26	P	304	PEK	C7-C8-C9-C10
26	T	101	PEK	C6-C7-C8-C9
26	T	101	PEK	C11-C12-C13-C14
26	C	303	PEK	O04-C21-O03-C01
26	T	101	PEK	O04-C21-O03-C01
26	T	101	PEK	C22-C21-O03-C01
26	C	303	PEK	C22-C21-O03-C01
23	D	206	DMU	C3-C4-C57-O61
18	N	609	TGL	OC1-CC1-OG3-CG3
25	L	102	CHD	C13-C17-C20-C21
25	L	102	CHD	C16-C17-C20-C22
18	A	607	TGL	CB2-CB1-OG2-CG2
25	L	102	CHD	C16-C17-C20-C21
25	L	102	CHD	C13-C17-C20-C22
19	A	608	PGV	C10-C11-C12-C13
26	C	303	PEK	C4-C5-C6-C7
26	C	303	PEK	C7-C8-C9-C10
19	N	610	PGV	C2-C1-O01-C02
26	P	303	PEK	C2-C1-O01-C02
18	A	606	TGL	C22-C23-C24-C25
25	J	101	CHD	C21-C20-C22-C23
18	N	608	TGL	C16-C15-CC9-CC8
27	C	308	CDL	C37-C38-C39-C40
23	D	206	DMU	O5-C4-C57-O61
25	J	101	CHD	C13-C17-C20-C21
23	P	308	DMU	O6-C11-C9-O1
19	N	610	PGV	O02-C1-O01-C02
26	P	303	PEK	O02-C1-O01-C02
27	C	308	CDL	OB6-CB4-CB6-OB8
18	A	606	TGL	C11-C12-C13-C14
27	P	307	CDL	C20-C21-C22-C23
18	L	101	TGL	CC1-CC2-CC3-CC4
25	J	101	CHD	C17-C20-C22-C23
26	C	303	PEK	O02-C1-O01-C02
25	C	309	CHD	C17-C20-C22-C23
27	P	307	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
25	C	309	CHD	C21-C20-C22-C23
26	C	303	PEK	C2-C1-O01-C02
19	P	305	PGV	C10-C11-C12-C13
26	C	305	PEK	C10-C11-C12-C13
26	P	304	PEK	C4-C5-C6-C7
26	P	304	PEK	C10-C11-C12-C13
27	N	601	CDL	C80-C81-C82-C83
27	P	307	CDL	C82-C83-C84-C85
18	L	101	TGL	C23-C24-C25-C26
26	C	304	PEK	C22-C23-C24-C25
18	L	101	TGL	CA9-C20-C21-C22
23	C	310	DMU	O16-C18-C19-C22
23	L	105	DMU	O16-C18-C19-C22
19	N	610	PGV	O12-C04-C05-O05
19	P	306	PGV	C10-C11-C12-C13
26	C	304	PEK	C7-C8-C9-C10
26	P	303	PEK	C4-C5-C6-C7
26	T	101	PEK	C13-C14-C15-C16
23	P	308	DMU	C19-C22-C25-C28
19	N	610	PGV	C04-O12-P-O11
23	D	206	DMU	C22-C25-C28-C31
19	C	307	PGV	O02-C1-O01-C02
23	P	308	DMU	O6-C11-C9-C8
27	C	308	CDL	C51-CB5-OB6-CB4
23	Z	101	DMU	O16-C18-C19-C22
18	L	101	TGL	C19-C33-C34-C35
18	N	607	TGL	CB9-C10-C11-C12
23	K	102	DMU	C31-C34-C37-C40
26	C	303	PEK	C22-C23-C24-C25
19	C	307	PGV	C2-C1-O01-C02
18	A	606	TGL	C12-C13-C14-C29
18	L	101	TGL	C21-C22-C23-C24
19	C	307	PGV	C24-C25-C26-C27
23	K	103	DMU	C22-C25-C28-C31
23	M	101	DMU	C19-C22-C25-C28
26	C	304	PEK	C23-C24-C25-C26
23	K	103	DMU	C25-C28-C31-C34
23	X	104	DMU	O16-C18-C19-C22
27	P	307	CDL	C37-C38-C39-C40
27	T	102	CDL	C79-C80-C81-C82
18	A	607	TGL	C19-C33-C34-C35
19	C	306	PGV	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
27	N	601	CDL	C37-C38-C39-C40
19	C	306	PGV	C10-C11-C12-C13
18	A	606	TGL	CA5-CA6-CA7-CA8
18	A	607	TGL	CC5-CC6-CC7-CC8
18	L	101	TGL	CA5-CA6-CA7-CA8
18	N	607	TGL	C24-C25-C26-C27
19	C	307	PGV	C4-C5-C6-C7
27	C	308	CDL	C77-C78-C79-C80
18	N	608	TGL	C19-C33-C34-C35
27	T	102	CDL	C60-C61-C62-C63
18	A	607	TGL	CC7-CC8-CC9-C15
18	N	607	TGL	CB3-CB4-CB5-CB6
18	N	609	TGL	CC9-C15-C16-C17
18	A	606	TGL	CC7-CC8-CC9-C15
18	A	606	TGL	C17-C18-C19-C33
18	A	607	TGL	CA9-C20-C21-C22
18	L	101	TGL	CB6-CB7-CB8-CB9
18	L	101	TGL	C11-C10-CB9-CB8
19	P	305	PGV	C7-C8-C9-C10
27	P	307	CDL	C77-C78-C79-C80
27	T	102	CDL	C82-C83-C84-C85
18	A	607	TGL	CB9-C10-C11-C12
19	C	306	PGV	C20-C21-C22-C23
23	P	308	DMU	C4-C3-O7-C10
18	N	607	TGL	OB1-CB1-OG2-CG2
23	K	104	DMU	C25-C28-C31-C34
27	P	307	CDL	CB5-C51-C52-C53
18	A	607	TGL	CB4-CB5-CB6-CB7
18	N	608	TGL	CC3-CC4-CC5-CC6
18	N	609	TGL	C22-C23-C24-C25
21	A	610	PSC	C28-C29-C30-C31
27	P	307	CDL	C41-C42-C43-C44
18	N	609	TGL	CA6-CA7-CA8-CA9
23	L	105	DMU	C25-C28-C31-C34
23	P	316	DMU	O16-C18-C19-C22
23	P	316	DMU	C31-C34-C37-C40
27	N	601	CDL	C40-C41-C42-C43
18	A	606	TGL	C21-C20-CA9-CA8
18	N	607	TGL	C19-C33-C34-C35
18	N	608	TGL	C22-C23-C24-C25
19	P	305	PGV	C30-C31-C32-C33
27	N	601	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
18	L	101	TGL	C13-C14-C29-C30
23	Z	101	DMU	C28-C31-C34-C37
23	L	105	DMU	C19-C18-O16-C6
23	C	310	DMU	C18-C19-C22-C25
21	O	302	PSC	C11-C10-C9-C8
18	A	607	TGL	CC9-C15-C16-C17
18	N	608	TGL	C21-C22-C23-C24
27	T	102	CDL	C20-C21-C22-C23
27	C	308	CDL	OB7-CB5-OB6-CB4
23	P	308	DMU	C2-C3-O7-C10
23	Z	101	DMU	O6-C11-C9-C8
18	L	101	TGL	C18-C19-C33-C34
19	C	306	PGV	C19-C20-C21-C22
27	P	307	CDL	C57-C58-C59-C60
19	N	610	PGV	O12-C04-C05-C06
18	N	607	TGL	C10-C11-C12-C13
18	N	608	TGL	C21-C20-CA9-CA8
18	N	609	TGL	CA9-C20-C21-C22
18	N	607	TGL	CC5-CC6-CC7-CC8
27	T	102	CDL	C40-C41-C42-C43
22	A	612	EDO	O1-C1-C2-O2
22	D	204	EDO	O1-C1-C2-O2
22	J	103	EDO	O1-C1-C2-O2
22	L	103	EDO	O1-C1-C2-O2
22	L	104	EDO	O1-C1-C2-O2
22	N	619	EDO	O1-C1-C2-O2
18	N	608	TGL	CB9-C10-C11-C12
19	C	306	PGV	C27-C28-C29-C30
23	Z	101	DMU	C25-C28-C31-C34
27	N	601	CDL	C17-C18-C19-C20
18	A	606	TGL	CB2-CB1-OG2-CG2
18	N	607	TGL	CB2-CB1-OG2-CG2
18	A	607	TGL	C16-C17-C18-C19
27	N	601	CDL	C33-C34-C35-C36
23	D	206	DMU	C18-C19-C22-C25
27	P	307	CDL	CB6-CB4-OB6-CB5
23	L	105	DMU	C34-C37-C40-C43
27	C	308	CDL	C55-C56-C57-C58
27	N	601	CDL	C77-C78-C79-C80
18	N	607	TGL	C17-C18-C19-C33
18	A	606	TGL	CB1-CB2-CB3-CB4
27	P	307	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
25	C	309	CHD	C20-C22-C23-C24
18	N	607	TGL	C20-C21-C22-C23
18	N	609	TGL	CC4-CC5-CC6-CC7
18	N	609	TGL	C23-C24-C25-C26
18	N	607	TGL	CB1-CB2-CB3-CB4
18	N	607	TGL	C14-C29-C30-C31
18	N	608	TGL	CB4-CB5-CB6-CB7
27	C	308	CDL	C59-C60-C61-C62
27	P	307	CDL	C36-C37-C38-C39
18	A	607	TGL	C20-C21-C22-C23
23	Z	101	DMU	C22-C25-C28-C31
18	N	609	TGL	CC5-CC6-CC7-CC8
18	N	607	TGL	CA4-CA5-CA6-CA7
27	N	601	CDL	C42-C43-C44-C45
21	O	302	PSC	C29-C30-C31-C32
18	L	101	TGL	C15-C16-C17-C18
18	N	607	TGL	C23-C24-C25-C26
18	N	609	TGL	CA4-CA5-CA6-CA7
19	P	306	PGV	C28-C29-C30-C31
19	A	608	PGV	C11-C10-C9-C8
18	A	606	TGL	CB9-C10-C11-C12
18	N	607	TGL	CB7-CB8-CB9-C10
19	N	610	PGV	C10-C11-C12-C13
26	T	101	PEK	C10-C11-C12-C13
18	A	606	TGL	CC5-CC6-CC7-CC8
19	C	306	PGV	C28-C29-C30-C31
23	Q	201	DMU	C18-C19-C22-C25
27	P	307	CDL	OB7-CB5-OB6-CB4
18	A	606	TGL	OB1-CB1-OG2-CG2
18	A	606	TGL	C21-C22-C23-C24
27	N	601	CDL	C43-C44-C45-C46
18	L	101	TGL	CC3-CC4-CC5-CC6
18	A	606	TGL	CC1-CC2-CC3-CC4
23	Q	201	DMU	C19-C22-C25-C28
23	D	207	DMU	O16-C18-C19-C22
21	A	610	PSC	C29-C30-C31-C32
18	A	606	TGL	C16-C17-C18-C19
19	A	608	PGV	C4-C5-C6-C7
23	O	306	DMU	C25-C28-C31-C34
18	A	606	TGL	C18-C19-C33-C34
18	L	101	TGL	OG1-CG1-CG2-CG3
19	C	307	PGV	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	N	609	TGL	CC6-CC7-CC8-CC9
23	M	101	DMU	C22-C25-C28-C31
19	N	612	PGV	C25-C26-C27-C28
27	P	307	CDL	C81-C82-C83-C84
18	N	609	TGL	C11-C10-CB9-CB8
19	C	307	PGV	C23-C24-C25-C26
23	P	316	DMU	C28-C31-C34-C37
18	L	101	TGL	OG1-CA1-CA2-CA3
23	P	308	DMU	O5-C6-O16-C18
18	N	608	TGL	C29-C30-C31-C32
18	N	608	TGL	CA3-CA4-CA5-CA6
18	A	606	TGL	CA2-CA1-OG1-CG1
23	Z	101	DMU	C34-C37-C40-C43
27	P	307	CDL	C40-C41-C42-C43
18	L	101	TGL	CC5-CC6-CC7-CC8
23	K	104	DMU	C28-C31-C34-C37
27	N	601	CDL	C20-C21-C22-C23
19	A	608	PGV	C21-C22-C23-C24
19	P	305	PGV	C31-C32-C33-C34
18	A	606	TGL	CB4-CB5-CB6-CB7
22	J	102	EDO	O1-C1-C2-O2
22	P	313	EDO	O1-C1-C2-O2
18	N	608	TGL	C12-C13-C14-C29
18	A	607	TGL	CC3-CC4-CC5-CC6
23	M	101	DMU	C28-C31-C34-C37
27	P	307	CDL	C73-C74-C75-C76
18	N	607	TGL	CB4-CB5-CB6-CB7
23	D	207	DMU	C25-C28-C31-C34
26	C	305	PEK	C25-C26-C27-C28
27	P	307	CDL	C53-C54-C55-C56
23	L	105	DMU	C22-C25-C28-C31
18	A	606	TGL	CC2-CC1-OG3-CG3
18	A	607	TGL	CC2-CC1-OG3-CG3
27	C	308	CDL	C58-C59-C60-C61
27	N	601	CDL	C81-C82-C83-C84
19	C	307	PGV	C3-C4-C5-C6
18	A	606	TGL	CA2-CA3-CA4-CA5
18	L	101	TGL	CA2-CA1-OG1-CG1
25	Y	102	CHD	C13-C17-C20-C21
26	T	101	PEK	C29-C30-C31-C32
27	T	102	CDL	C80-C81-C82-C83
18	A	606	TGL	CA1-CA2-CA3-CA4

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Mol	Chain	Res	Type	Atoms
18	L	101	TGL	CB4-CB5-CB6-CB7
18	N	607	TGL	C16-C15-CC9-CC8
19	C	307	PGV	C13-C14-C15-C16
18	L	101	TGL	C21-C20-CA9-CA8
23	P	308	DMU	O16-C18-C19-C22
18	N	608	TGL	CA2-CA3-CA4-CA5
19	A	611	PGV	C10-C11-C12-C13
26	C	304	PEK	C10-C11-C12-C13
26	P	304	PEK	C13-C14-C15-C16
27	T	102	CDL	C78-C79-C80-C81
26	C	304	PEK	O03-C21-C22-C23
18	N	607	TGL	CA7-CA8-CA9-C20
18	N	607	TGL	CC6-CC7-CC8-CC9
27	C	308	CDL	C36-C37-C38-C39
18	N	609	TGL	CA5-CA6-CA7-CA8
18	A	607	TGL	C16-C15-CC9-CC8
21	A	610	PSC	C9-C10-C11-C12
21	A	610	PSC	C10-C11-C12-C13
21	O	302	PSC	C9-C10-C11-C12
21	O	302	PSC	C10-C11-C12-C13
26	C	303	PEK	C5-C6-C7-C8
26	C	303	PEK	C6-C7-C8-C9
26	C	303	PEK	C11-C10-C9-C8
26	C	303	PEK	C9-C10-C11-C12
26	C	303	PEK	C11-C12-C13-C14
26	C	303	PEK	C12-C13-C14-C15
26	C	304	PEK	C6-C7-C8-C9
26	C	304	PEK	C9-C10-C11-C12
26	C	304	PEK	C12-C13-C14-C15
26	C	305	PEK	C5-C6-C7-C8
26	C	305	PEK	C6-C7-C8-C9
26	C	305	PEK	C11-C10-C9-C8
26	C	305	PEK	C9-C10-C11-C12
26	C	305	PEK	C11-C12-C13-C14
26	C	305	PEK	C12-C13-C14-C15
26	P	303	PEK	C6-C7-C8-C9
26	P	303	PEK	C11-C10-C9-C8
26	P	303	PEK	C11-C12-C13-C14
26	P	303	PEK	C12-C13-C14-C15
26	P	304	PEK	C9-C10-C11-C12
26	P	304	PEK	C12-C13-C14-C15
26	T	101	PEK	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
26	T	101	PEK	C9-C10-C11-C12
26	T	101	PEK	C12-C13-C14-C15
18	A	606	TGL	OA1-CA1-OG1-CG1
27	T	102	CDL	C71-CB7-OB8-CB6
18	A	606	TGL	C13-C14-C29-C30
23	Q	201	DMU	C28-C31-C34-C37
27	C	308	CDL	C64-C65-C66-C67
18	L	101	TGL	CC4-CC5-CC6-CC7
19	P	305	PGV	C24-C25-C26-C27
27	T	102	CDL	C43-C44-C45-C46
22	A	614	EDO	O1-C1-C2-O2
22	A	619	EDO	O1-C1-C2-O2
22	A	620	EDO	O1-C1-C2-O2
19	C	307	PGV	C6-C7-C8-C9
18	N	608	TGL	C33-C34-C35-C36
18	L	101	TGL	C10-C11-C12-C13
18	A	607	TGL	CA6-CA7-CA8-CA9
18	L	101	TGL	CB3-CB4-CB5-CB6
18	N	607	TGL	C21-C20-CA9-CA8
23	D	206	DMU	C34-C37-C40-C43
18	A	607	TGL	C18-C19-C33-C34
26	P	304	PEK	C22-C23-C24-C25
18	N	608	TGL	C11-C12-C13-C14
19	A	608	PGV	C2-C3-C4-C5
21	A	610	PSC	C26-C27-C28-C29
27	N	601	CDL	C62-C63-C64-C65
18	N	607	TGL	CA2-CA3-CA4-CA5
18	N	608	TGL	CA9-C20-C21-C22
18	L	101	TGL	OA1-CA1-OG1-CG1
19	P	305	PGV	C02-C03-O11-P
27	T	102	CDL	OB9-CB7-OB8-CB6
18	A	606	TGL	C20-C21-C22-C23
18	N	608	TGL	C10-C11-C12-C13
18	N	609	TGL	CA7-CA8-CA9-C20
18	L	101	TGL	C24-C25-C26-C27
18	A	607	TGL	OG1-CG1-CG2-OG2
18	L	101	TGL	OG2-CG2-CG3-OG3
18	A	607	TGL	OC1-CC1-OG3-CG3
18	A	606	TGL	OC1-CC1-OG3-CG3
21	A	610	PSC	C27-C28-C29-C30
18	A	607	TGL	CB1-CB2-CB3-CB4
26	C	303	PEK	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
23	M	101	DMU	C25-C28-C31-C34
19	C	306	PGV	C02-C03-O11-P
19	N	610	PGV	C04-O12-P-O14
26	T	101	PEK	C5-C6-C7-C8
19	P	306	PGV	C7-C8-C9-C10
26	P	304	PEK	O12-C04-C05-N
22	F	108	EDO	O1-C1-C2-O2
23	P	317	DMU	C18-C19-C22-C25
26	T	101	PEK	C28-C29-C30-C31
26	C	304	PEK	C16-C17-C18-C19
19	N	612	PGV	C27-C28-C29-C30
27	C	308	CDL	C76-C77-C78-C79
18	L	101	TGL	CA6-CA7-CA8-CA9
23	X	102	DMU	C34-C37-C40-C43
18	A	607	TGL	CB3-CB4-CB5-CB6
18	L	101	TGL	CG1-CG2-CG3-OG3
18	N	607	TGL	C13-C14-C29-C30
18	N	607	TGL	CG1-CG2-CG3-OG3
18	L	101	TGL	OG1-CG1-CG2-OG2
18	N	607	TGL	OG2-CG2-CG3-OG3
27	P	307	CDL	C42-C43-C44-C45
27	P	307	CDL	C13-C14-C15-C16
18	L	101	TGL	CC2-CC3-CC4-CC5
26	C	304	PEK	C26-C27-C28-C29
27	N	601	CDL	C36-C37-C38-C39
19	C	306	PGV	C22-C23-C24-C25
18	L	101	TGL	C11-C12-C13-C14
23	K	102	DMU	C28-C31-C34-C37
23	K	101	DMU	C34-C37-C40-C43
23	D	207	DMU	C28-C31-C34-C37
18	L	101	TGL	C17-C18-C19-C33
19	N	610	PGV	C01-C02-O01-C1
27	P	307	CDL	C72-C73-C74-C75
18	N	607	TGL	C16-C17-C18-C19
23	X	101	DMU	C28-C31-C34-C37
18	L	101	TGL	CA1-CA2-CA3-CA4
22	A	617	EDO	O1-C1-C2-O2
22	A	618	EDO	O1-C1-C2-O2
22	C	320	EDO	O1-C1-C2-O2
22	E	202	EDO	O1-C1-C2-O2
23	J	104	DMU	C28-C31-C34-C37
19	A	611	PGV	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	P	317	DMU	C1-C6-O16-C18
19	C	306	PGV	C26-C27-C28-C29
18	A	606	TGL	C19-C33-C34-C35
23	K	102	DMU	C22-C25-C28-C31
25	Y	102	CHD	C16-C17-C20-C22
27	T	102	CDL	CB3-CB4-CB6-OB8
27	P	307	CDL	C17-C18-C19-C20
23	P	308	DMU	C25-C28-C31-C34
27	P	307	CDL	C12-C13-C14-C15
18	L	101	TGL	C22-C23-C24-C25
27	C	308	CDL	C38-C39-C40-C41
18	N	609	TGL	C20-C21-C22-C23
19	C	307	PGV	C11-C12-C13-C14
26	C	305	PEK	C3-C4-C5-C6
14	A	602	HEA	CAA-CBA-CGA-O1A
19	N	612	PGV	C26-C27-C28-C29
23	D	207	DMU	C18-C19-C22-C25
14	A	602	HEA	C2D-C3D-CAD-CBD
27	C	308	CDL	C41-C42-C43-C44
25	G	101	CHD	C22-C23-C24-O26
19	C	307	PGV	C22-C23-C24-C25
23	Q	201	DMU	C31-C34-C37-C40
18	N	608	TGL	CB6-CB7-CB8-CB9
14	N	603	HEA	CAA-CBA-CGA-O1A
23	X	102	DMU	C22-C25-C28-C31
25	Y	102	CHD	C16-C17-C20-C21
26	T	101	PEK	C32-C33-C34-C35
18	N	607	TGL	CA6-CA7-CA8-CA9
18	L	101	TGL	OA1-CA1-CA2-CA3
27	P	307	CDL	C78-C79-C80-C81
19	A	608	PGV	C11-C12-C13-C14
19	C	306	PGV	C11-C12-C13-C14
21	A	610	PSC	C12-C13-C14-C15
23	D	206	DMU	C28-C31-C34-C37
18	N	607	TGL	CA3-CA4-CA5-CA6
18	A	606	TGL	CA7-CA8-CA9-C20
14	A	602	HEA	CAD-CBD-CGD-O2D
23	Z	101	DMU	O6-C11-C9-O1
18	A	607	TGL	OG1-CG1-CG2-CG3
25	P	301	CHD	C22-C23-C24-O25
19	N	612	PGV	C11-C12-C13-C14
26	C	304	PEK	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	P	317	DMU	O5-C6-O16-C18
25	B	302	CHD	C22-C23-C24-O25
25	G	101	CHD	C22-C23-C24-O25
18	N	607	TGL	C15-C16-C17-C18
14	N	603	HEA	CAD-CBD-CGD-O1D
21	A	610	PSC	C30-C31-C32-C33
14	A	602	HEA	CAD-CBD-CGD-O1D
27	N	601	CDL	C72-C73-C74-C75
26	C	304	PEK	C11-C12-C13-C14
26	P	303	PEK	C9-C10-C11-C12
26	P	304	PEK	C11-C12-C13-C14
18	L	101	TGL	CC6-CC7-CC8-CC9
14	N	603	HEA	CAD-CBD-CGD-O2D
25	B	302	CHD	C22-C23-C24-O26
27	T	102	CDL	C59-C60-C61-C62
23	X	104	DMU	O5-C4-C57-O61
14	N	603	HEA	CAA-CBA-CGA-O2A
18	N	608	TGL	C18-C19-C33-C34
19	C	306	PGV	C24-C25-C26-C27
27	N	601	CDL	C31-C32-C33-C34
25	J	101	CHD	C22-C23-C24-O26
18	N	609	TGL	CC3-CC4-CC5-CC6
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
23	P	316	DMU	C34-C37-C40-C43
14	A	602	HEA	CAA-CBA-CGA-O2A
18	A	607	TGL	C24-C25-C26-C27
19	C	306	PGV	C1-C2-C3-C4
27	C	308	CDL	CB6-CB4-OB6-CB5
22	M	102	EDO	O1-C1-C2-O2
22	T	105	EDO	O1-C1-C2-O2
23	C	310	DMU	C28-C31-C34-C37
27	P	307	CDL	C43-C44-C45-C46
23	K	104	DMU	C18-C19-C22-C25
19	A	608	PGV	C22-C23-C24-C25
14	N	603	HEA	C26-C15-C16-C17
19	A	611	PGV	O03-C19-C20-C21
18	N	608	TGL	CC2-CC3-CC4-CC5
19	C	306	PGV	C9-C10-C11-C12
19	C	307	PGV	C9-C10-C11-C12
26	C	305	PEK	C14-C15-C16-C17
27	P	307	CDL	C52-C53-C54-C55
18	N	607	TGL	CC2-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
26	C	304	PEK	O12-C04-C05-N
26	P	304	PEK	C14-C15-C16-C17
18	A	606	TGL	OG2-CG2-CG3-OG3
14	N	602[A]	HEA	CAD-CBD-CGD-O1D
26	P	303	PEK	C14-C15-C16-C17
18	A	606	TGL	OG3-CC1-CC2-CC3
27	N	601	CDL	OB9-CB7-OB8-CB6
18	A	607	TGL	CB5-CB6-CB7-CB8
25	C	309	CHD	C22-C23-C24-O26
19	C	307	PGV	O01-C1-C2-C3
19	N	610	PGV	C9-C10-C11-C12
19	N	610	PGV	C11-C12-C13-C14
21	O	302	PSC	C12-C13-C14-C15
26	C	304	PEK	C14-C15-C16-C17
19	A	611	PGV	C26-C27-C28-C29
27	T	102	CDL	C55-C56-C57-C58
23	P	316	DMU	C19-C18-O16-C6
18	N	608	TGL	CB3-CB4-CB5-CB6
26	C	304	PEK	C34-C35-C36-C37
27	C	308	CDL	C40-C41-C42-C43
26	C	303	PEK	O03-C21-C22-C23
18	A	606	TGL	OG1-CA1-CA2-CA3
27	P	307	CDL	C58-C59-C60-C61
26	P	303	PEK	C3-C4-C5-C6
19	N	612	PGV	O03-C19-C20-C21
21	A	610	PSC	C23-C24-C25-C26
27	T	102	CDL	C17-C18-C19-C20
14	N	603	HEA	C4D-C3D-CAD-CBD
22	D	205	EDO	O1-C1-C2-O2
22	N	618	EDO	O1-C1-C2-O2
22	P	312	EDO	O1-C1-C2-O2
22	S	106	EDO	O1-C1-C2-O2
22	T	104	EDO	O1-C1-C2-O2
25	C	301	CHD	C22-C23-C24-O25
25	C	309	CHD	C22-C23-C24-O25
18	L	101	TGL	CB7-CB8-CB9-C10
27	T	102	CDL	C24-C25-C26-C27
19	P	306	PGV	C29-C30-C31-C32
14	N	602[A]	HEA	CAD-CBD-CGD-O2D
27	C	308	CDL	C56-C57-C58-C59
14	N	602[A]	HEA	CAA-CBA-CGA-O1A
14	N	603	HEA	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
18	N	607	TGL	C22-C23-C24-C25
19	A	608	PGV	C9-C10-C11-C12
26	T	101	PEK	C14-C15-C16-C17
18	A	607	TGL	C15-C16-C17-C18
27	P	307	CDL	C52-C51-CB5-OB6
26	C	305	PEK	C33-C34-C35-C36
18	N	609	TGL	C11-C12-C13-C14
18	N	608	TGL	C24-C25-C26-C27
27	T	102	CDL	C72-C71-CB7-OB8
26	C	303	PEK	C23-C24-C25-C26
18	N	608	TGL	CC5-CC6-CC7-CC8
18	A	606	TGL	OC1-CC1-CC2-CC3
27	P	307	CDL	C52-C51-CB5-OB7
18	A	606	TGL	CG1-CG2-CG3-OG3
26	C	303	PEK	O04-C21-C22-C23
18	N	609	TGL	C16-C15-CC9-CC8
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
23	J	104	DMU	C18-C19-C22-C25
18	A	606	TGL	C24-C25-C26-C27
26	C	303	PEK	C03-O11-P-O13
26	C	303	PEK	C03-O11-P-O14
18	A	606	TGL	OG1-CG1-CG2-OG2
18	L	101	TGL	CA4-CA5-CA6-CA7
27	C	308	CDL	C34-C35-C36-C37
18	A	606	TGL	OA1-CA1-CA2-CA3
26	C	304	PEK	O04-C21-C22-C23
19	C	307	PGV	O02-C1-C2-C3
22	D	202	EDO	O1-C1-C2-O2
22	W	102	EDO	O1-C1-C2-O2
18	N	609	TGL	C10-C11-C12-C13
18	A	607	TGL	CA7-CA8-CA9-C20
19	N	610	PGV	O03-C19-C20-C21
27	T	102	CDL	C57-C58-C59-C60
26	C	304	PEK	C30-C31-C32-C33
18	A	606	TGL	C29-C30-C31-C32
19	N	612	PGV	O04-C19-C20-C21
27	T	102	CDL	C72-C71-CB7-OB9
18	L	101	TGL	C14-C29-C30-C31
18	N	607	TGL	OG3-CC1-CC2-CC3
19	P	306	PGV	C9-C10-C11-C12
18	N	609	TGL	C13-C14-C29-C30
14	A	602	HEA	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
23	X	101	DMU	C19-C22-C25-C28
14	N	602[A]	HEA	CAA-CBA-CGA-O2A
23	K	102	DMU	O16-C18-C19-C22
18	A	606	TGL	C25-C26-C27-C28
18	A	607	TGL	OG3-CC1-CC2-CC3

There are no ring outliers.

60 monomers are involved in 168 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	305	PEK	1	0
20	A	609[A]	PER	1	0
23	K	101	DMU	1	0
18	A	606	TGL	4	0
22	N	620	EDO	1	0
18	L	101	TGL	15	0
25	C	309	CHD	2	0
26	T	101	PEK	6	0
27	N	601	CDL	5	0
23	Q	201	DMU	2	0
21	A	610	PSC	3	0
19	A	611	PGV	1	0
18	N	607	TGL	3	0
19	P	305	PGV	1	0
19	P	306	PGV	1	0
26	C	303	PEK	1	0
19	C	306	PGV	2	0
26	P	304	PEK	2	0
25	G	101	CHD	1	0
22	D	204	EDO	3	0
23	K	102	DMU	1	0
25	J	101	CHD	2	0
14	N	602[A]	HEA	2	0
22	S	106	EDO	1	0
23	C	310	DMU	3	0
14	A	601[A]	HEA	2	0
27	T	102	CDL	9	0
23	D	206	DMU	3	0
14	N	603	HEA	5	0
23	Z	101	DMU	1	0
22	A	612	EDO	2	0
27	C	308	CDL	7	0

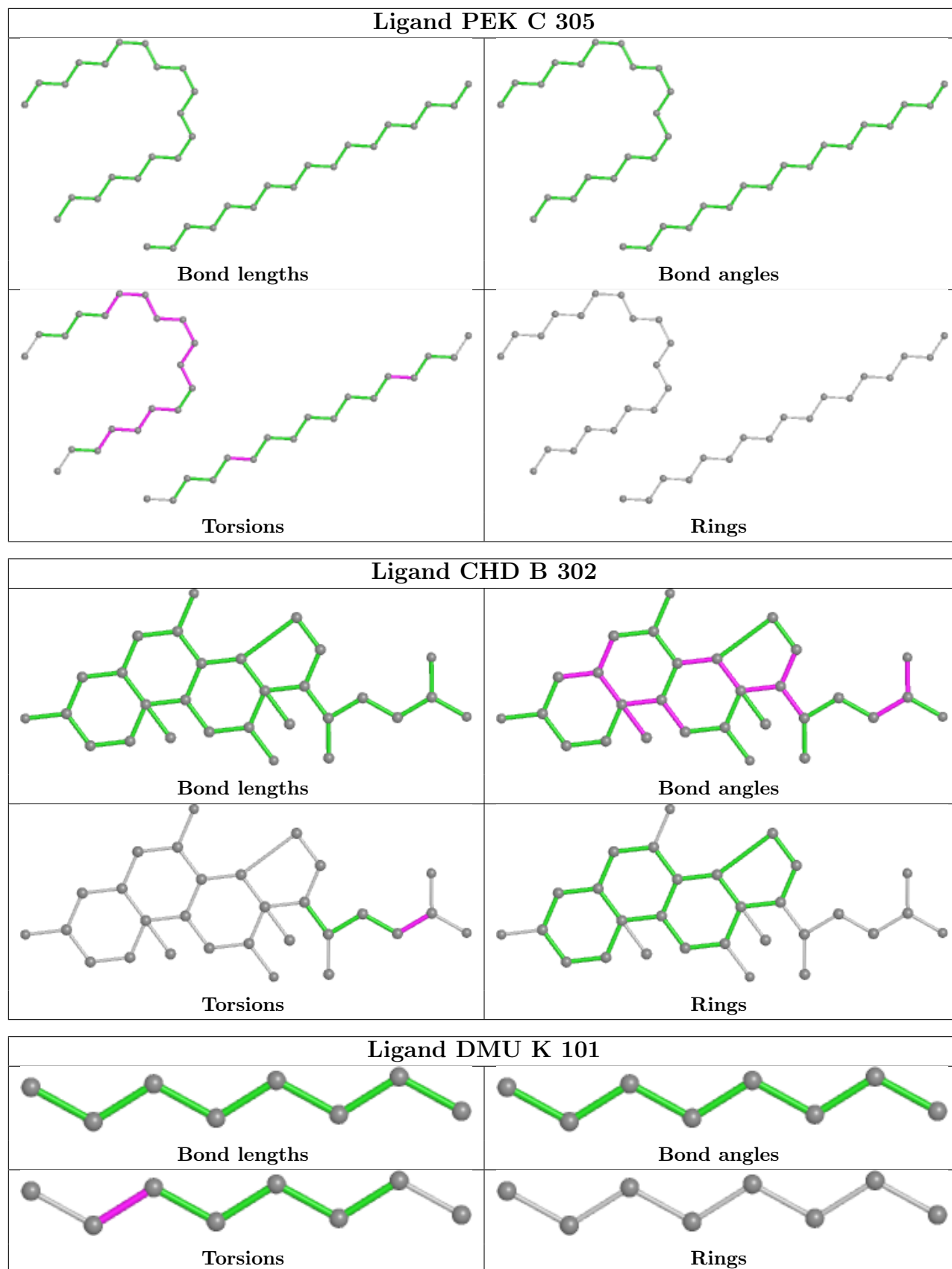
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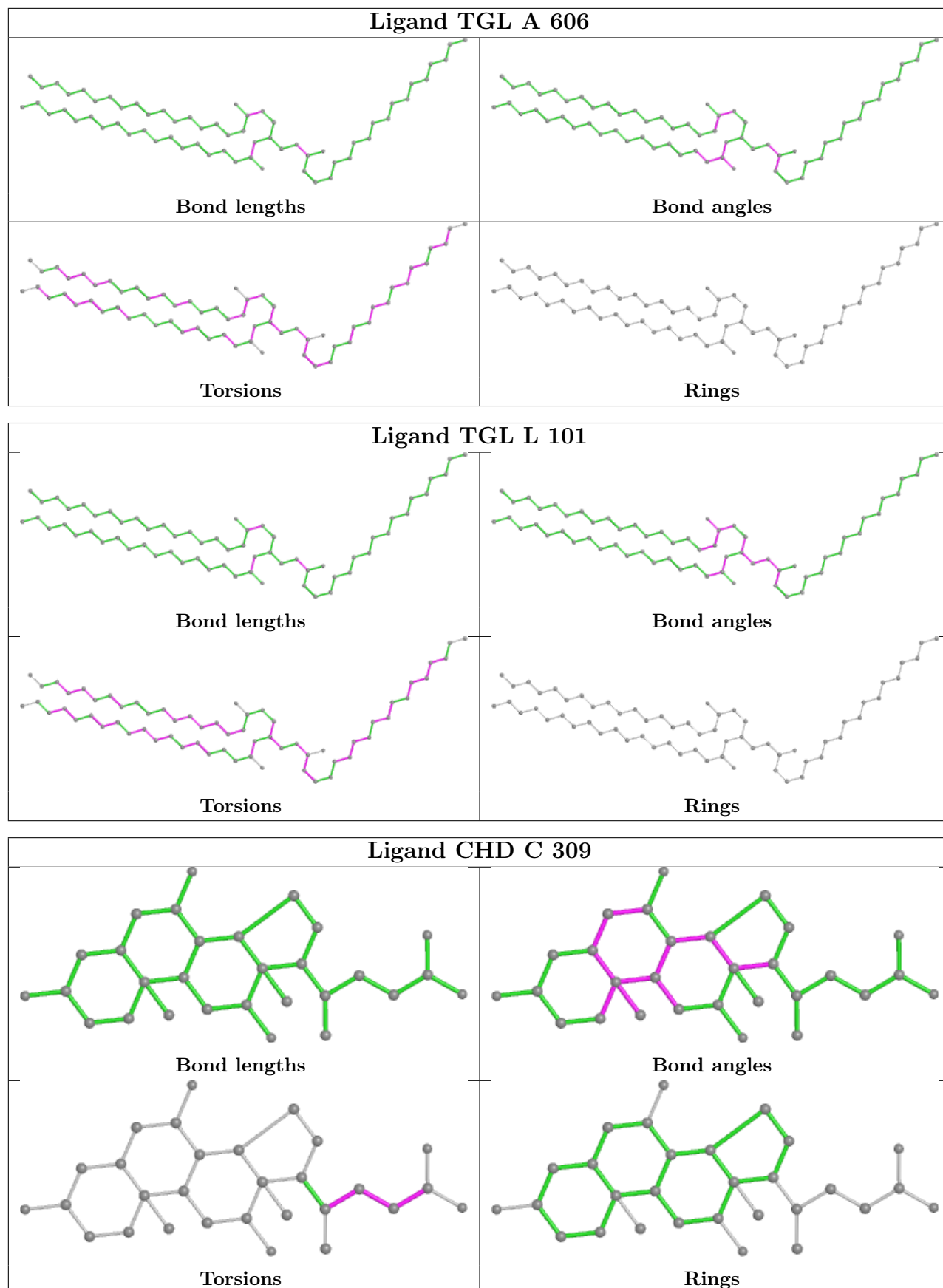


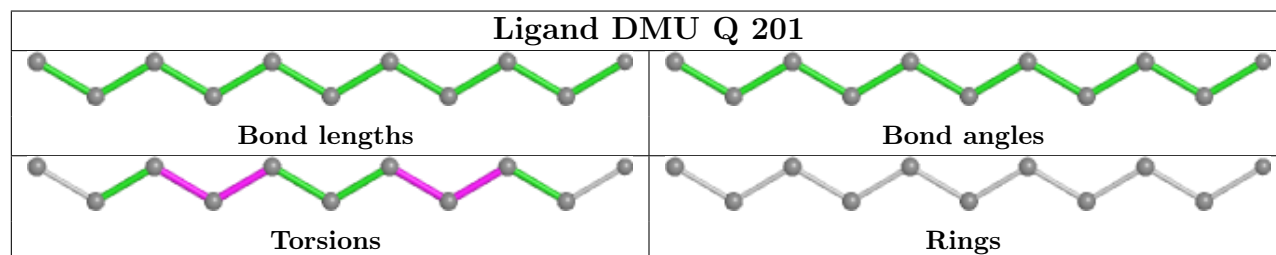
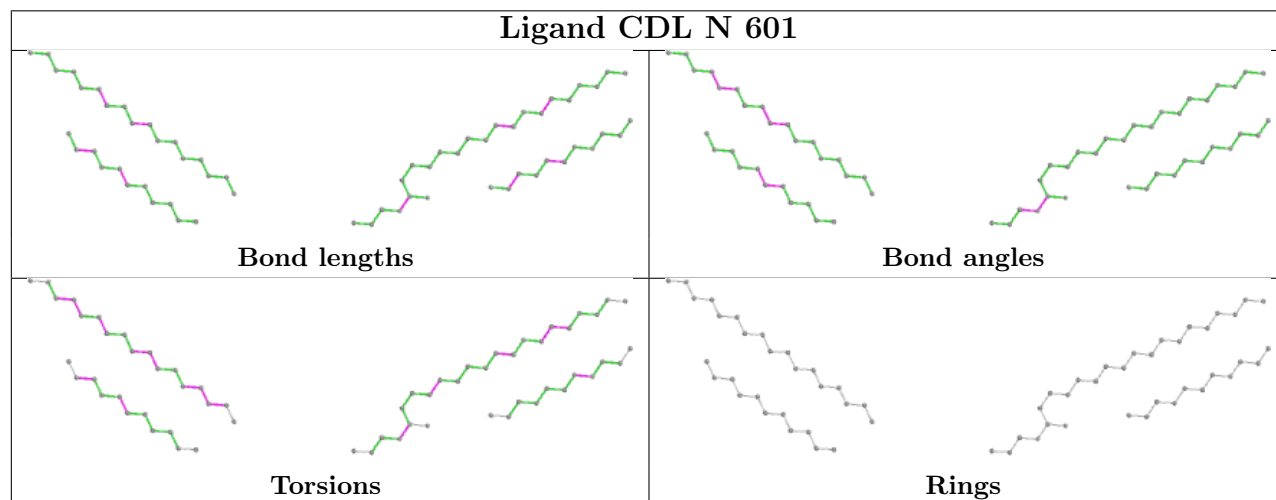
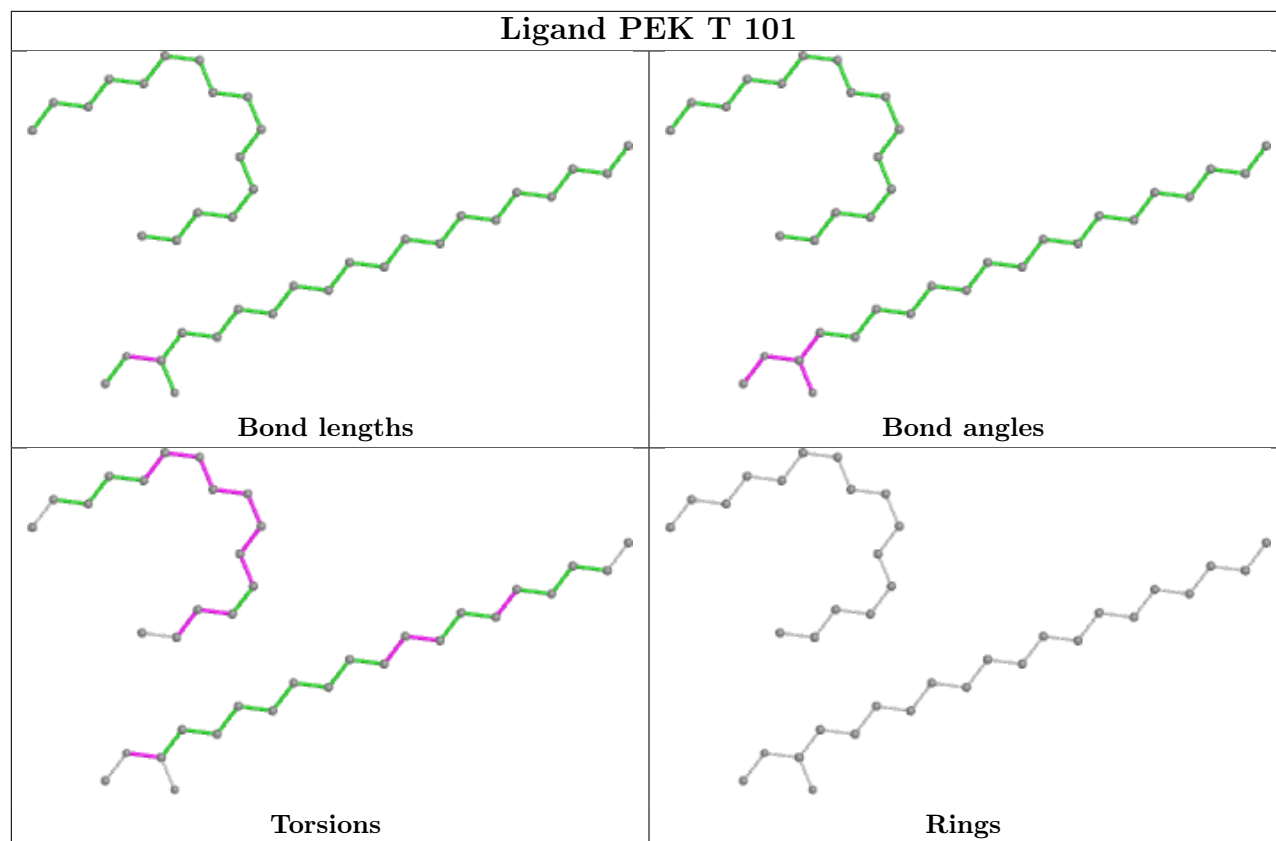
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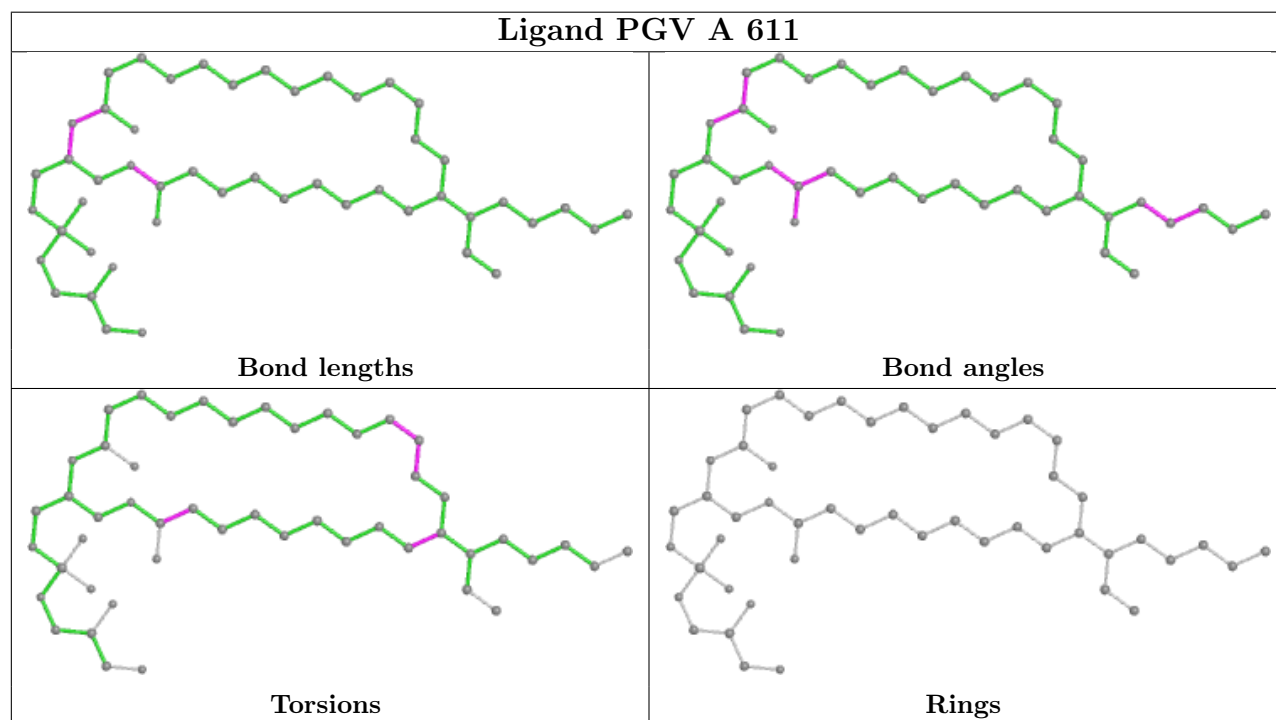
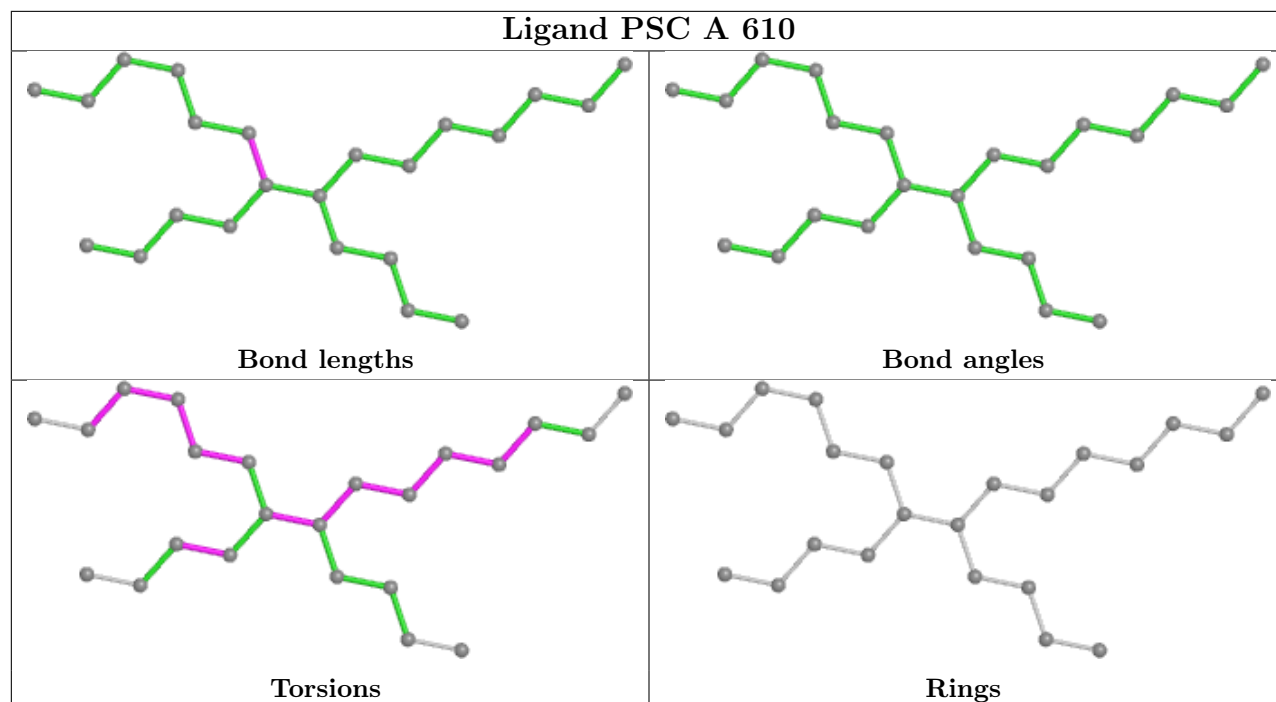
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	618	EDO	1	0
22	D	205	EDO	2	0
25	L	102	CHD	2	0
26	C	304	PEK	5	0
23	X	102	DMU	2	0
22	C	318	EDO	1	0
19	N	610	PGV	3	0
19	C	307	PGV	1	0
21	O	302	PSC	4	0
20	N	611[A]	PER	1	0
27	P	307	CDL	7	0
22	Y	101	EDO	1	0
18	A	607	TGL	13	0
22	A	620	EDO	1	0
23	P	316	DMU	2	0
18	N	609	TGL	1	0
23	P	308	DMU	3	0
22	N	621	EDO	1	0
23	J	104	DMU	1	0
23	L	105	DMU	6	0
23	M	101	DMU	2	0
23	K	103	DMU	1	0
19	N	612	PGV	1	0
14	A	602	HEA	5	0
18	N	608	TGL	7	0
22	A	616	EDO	1	0
19	A	608	PGV	1	0
22	C	315	EDO	1	0

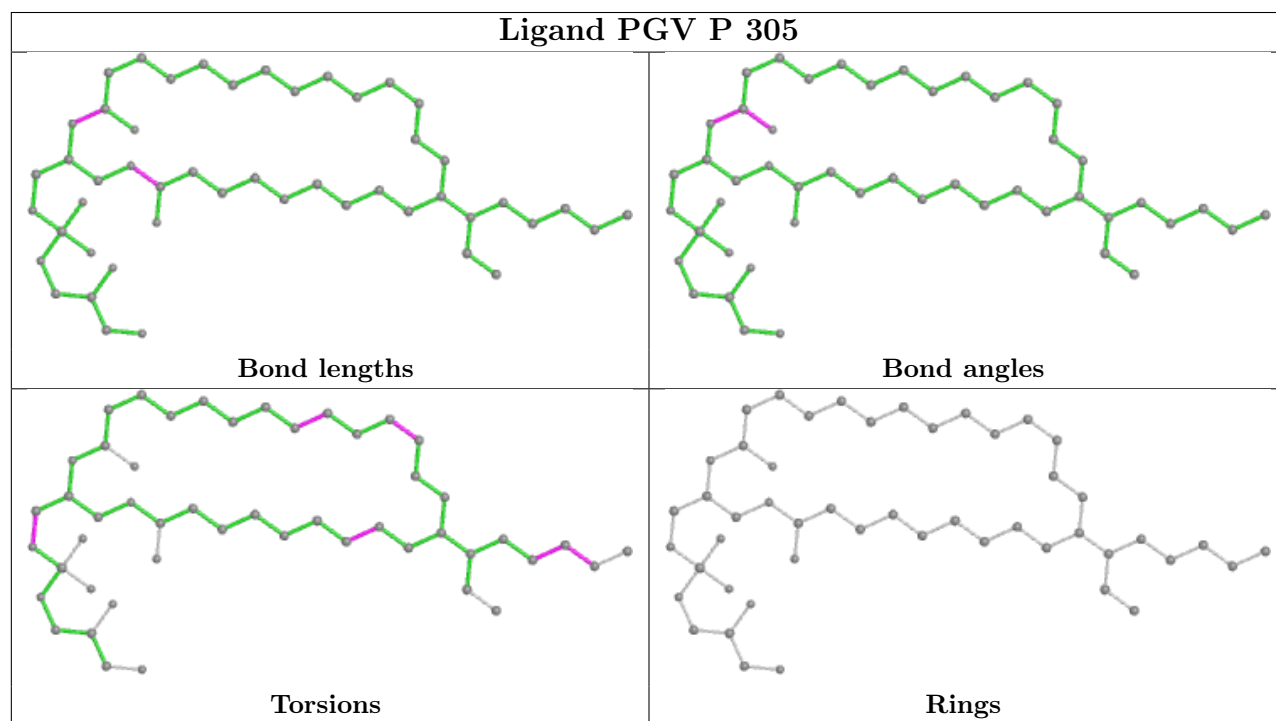
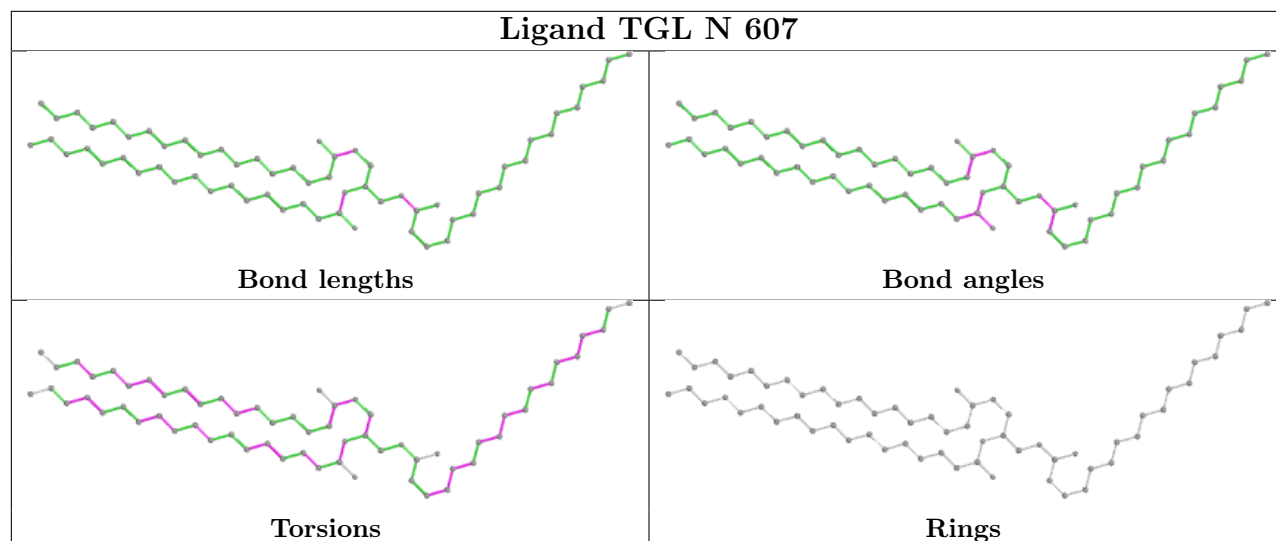
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

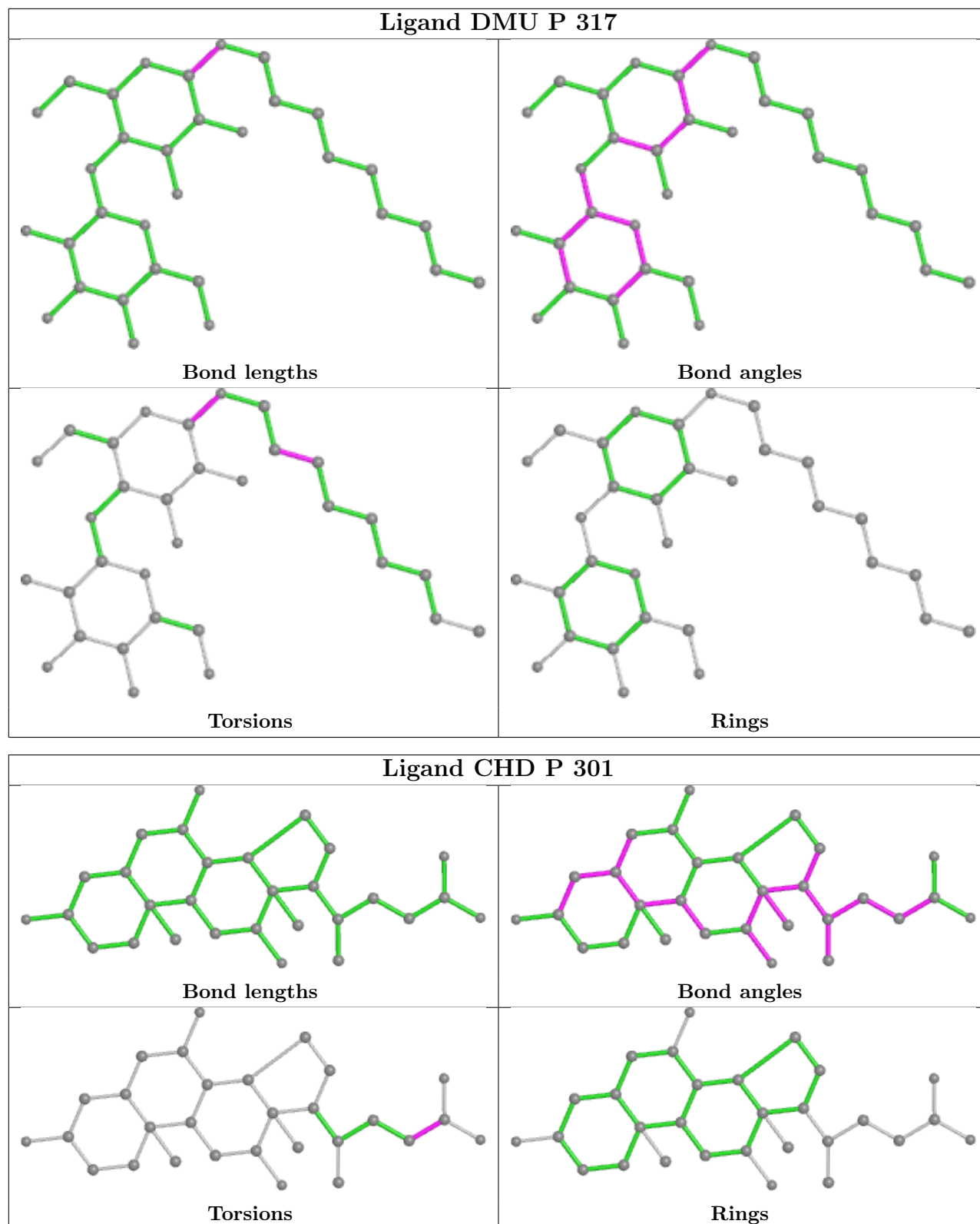


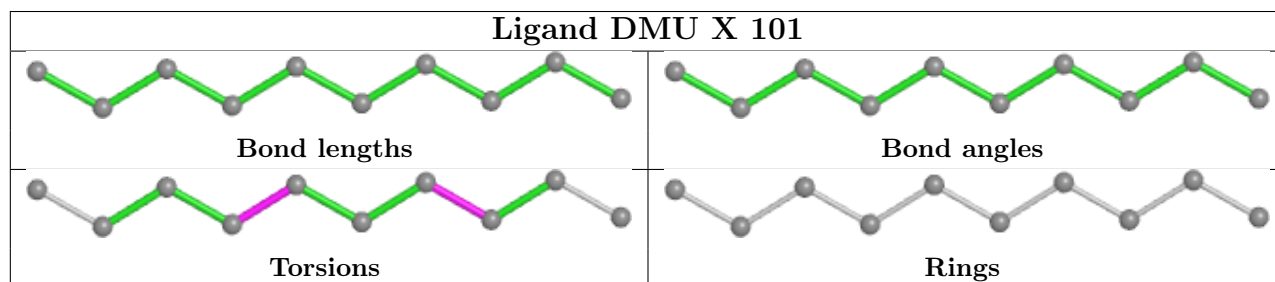
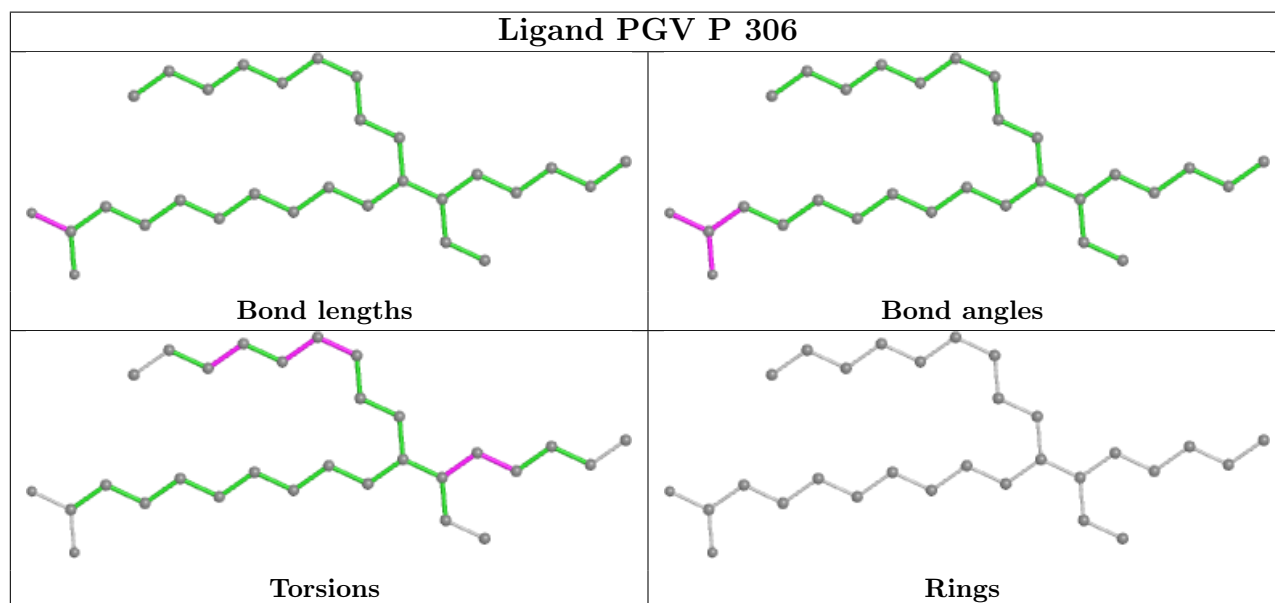
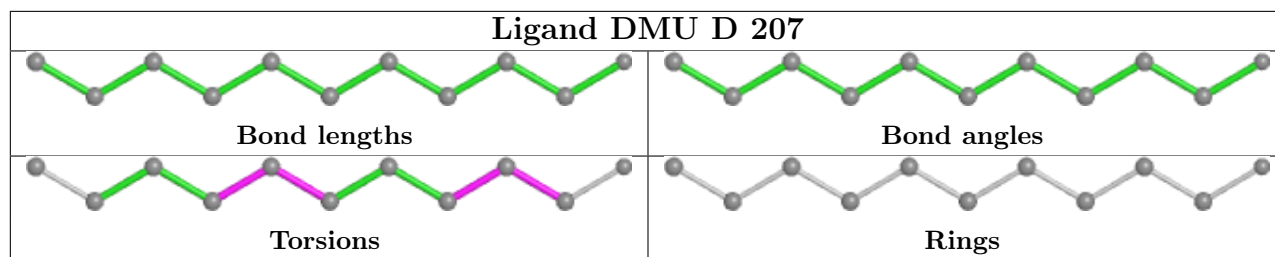




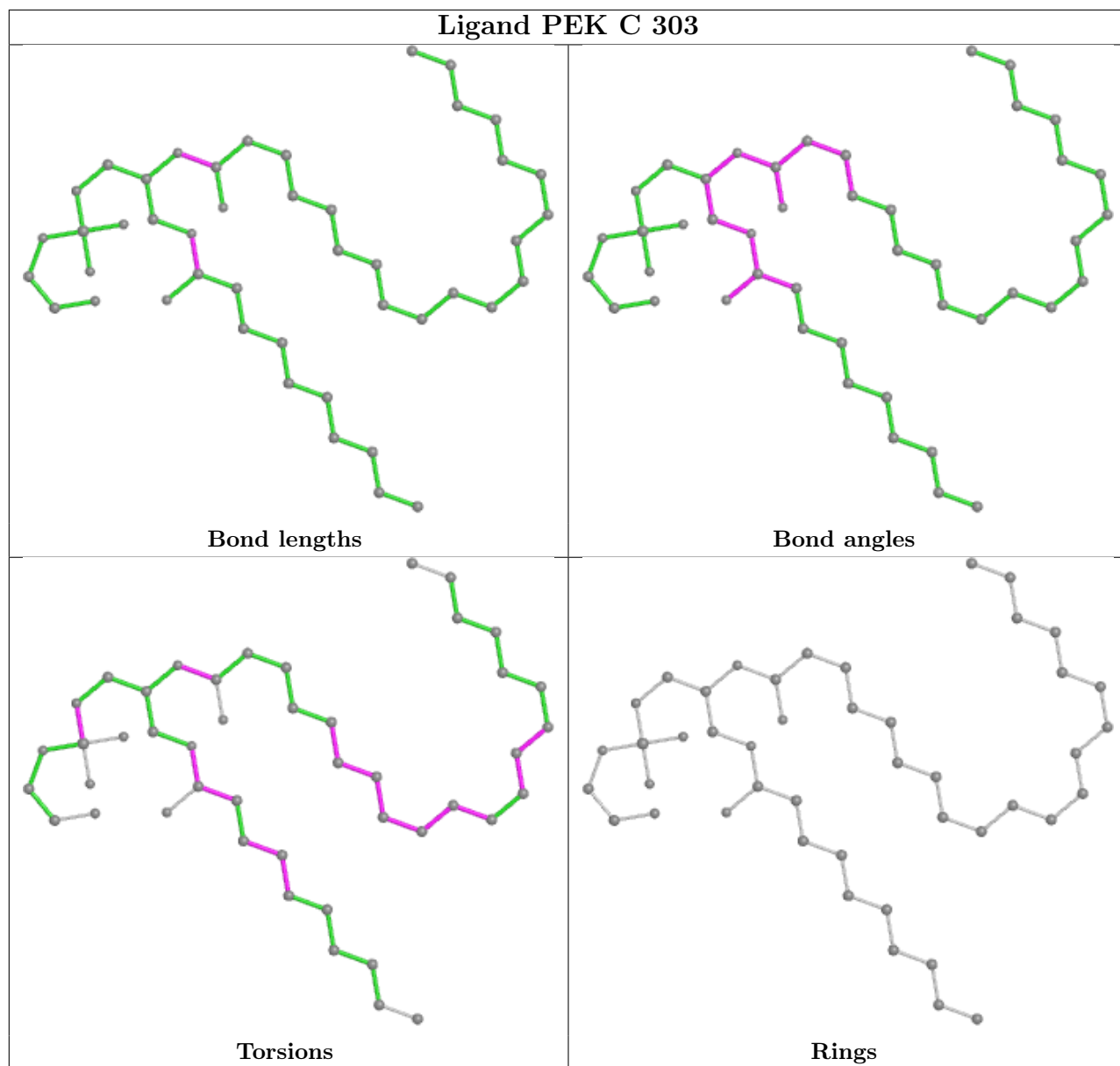


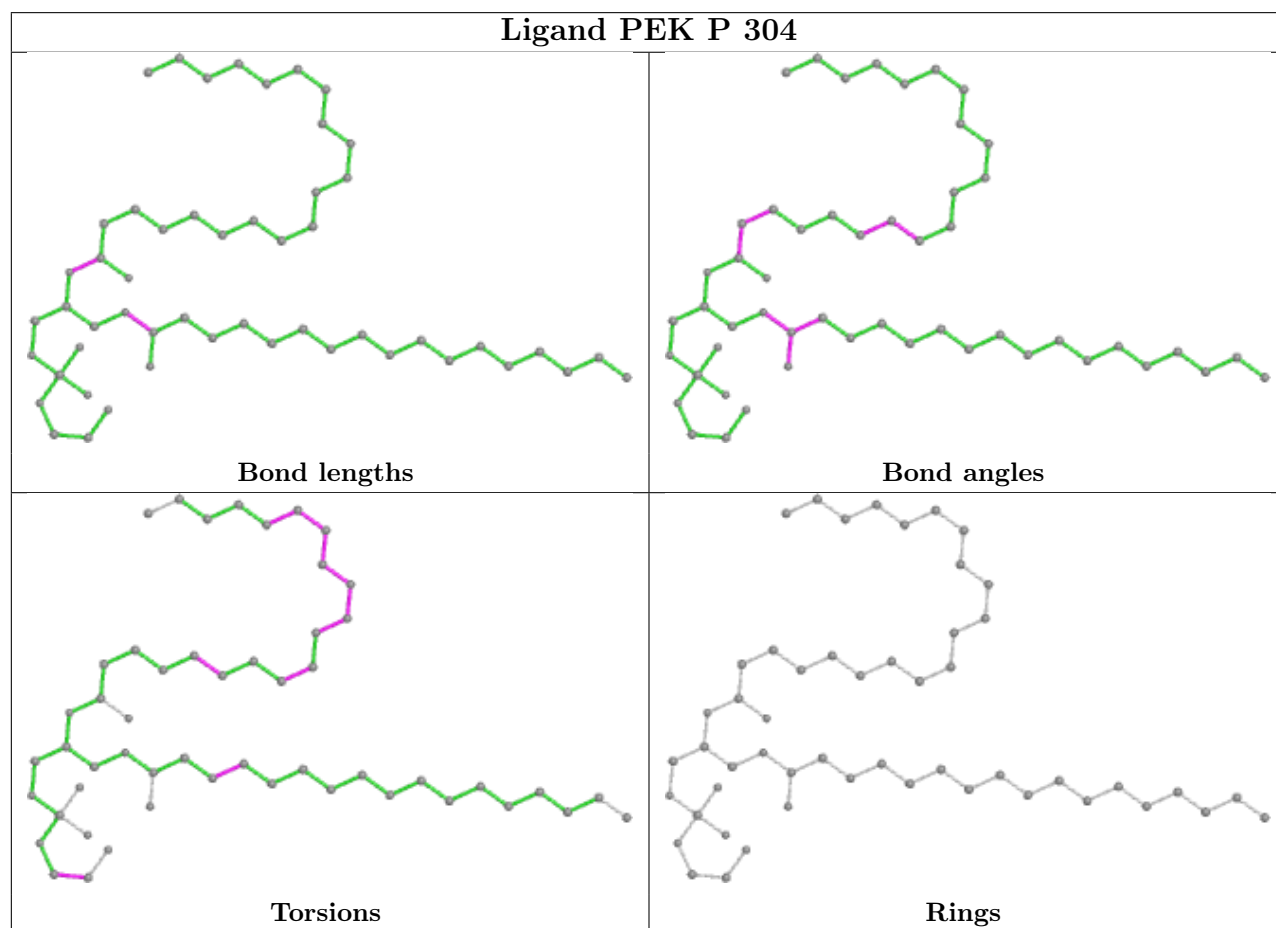
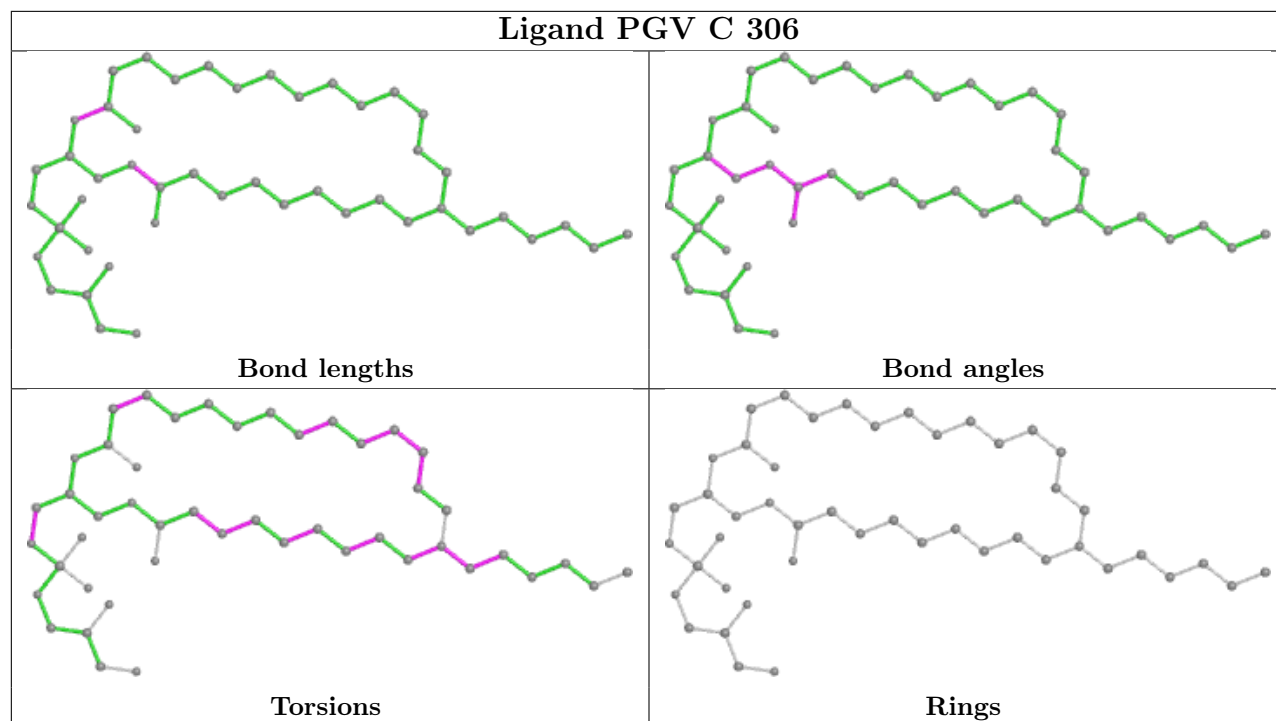


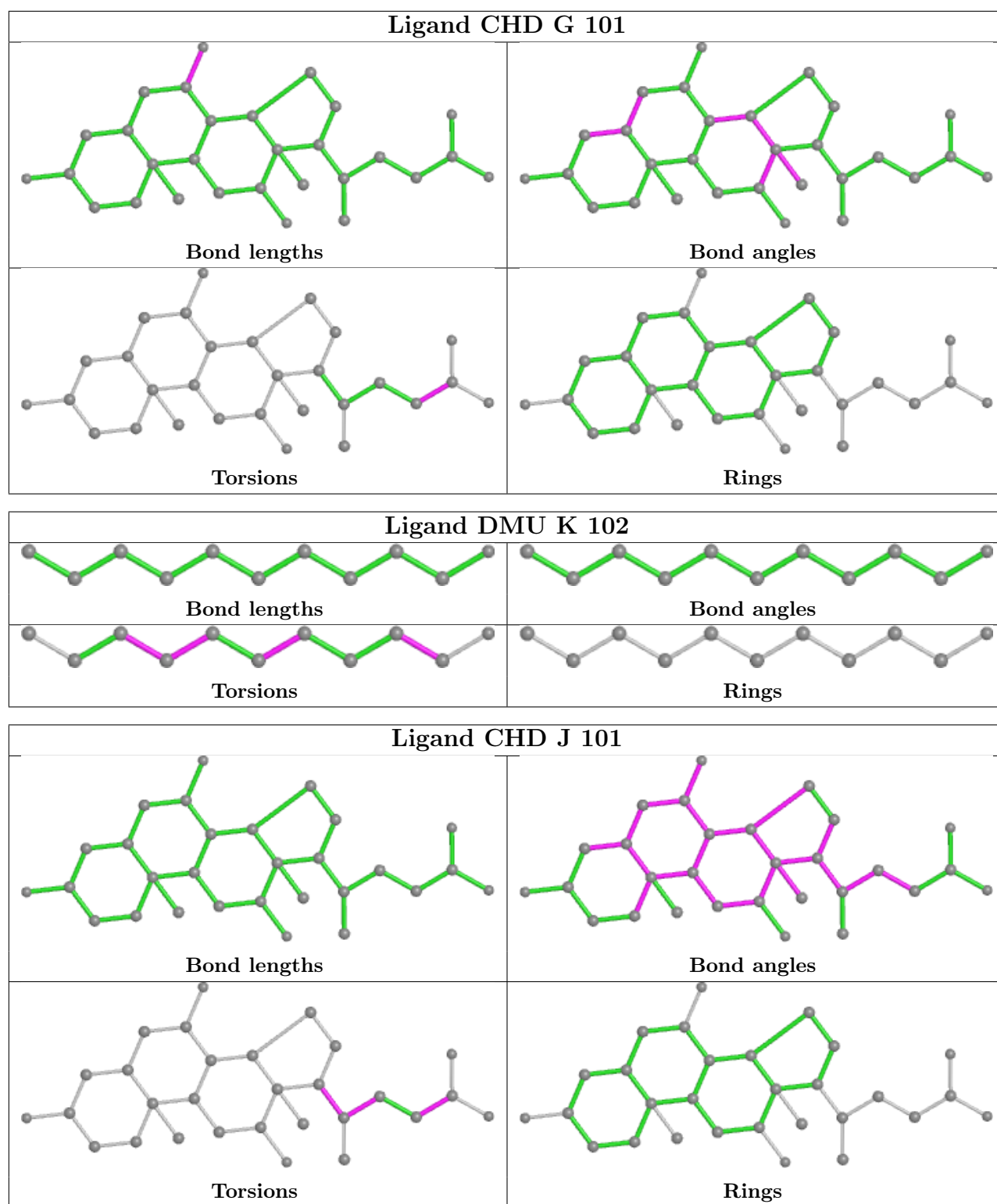


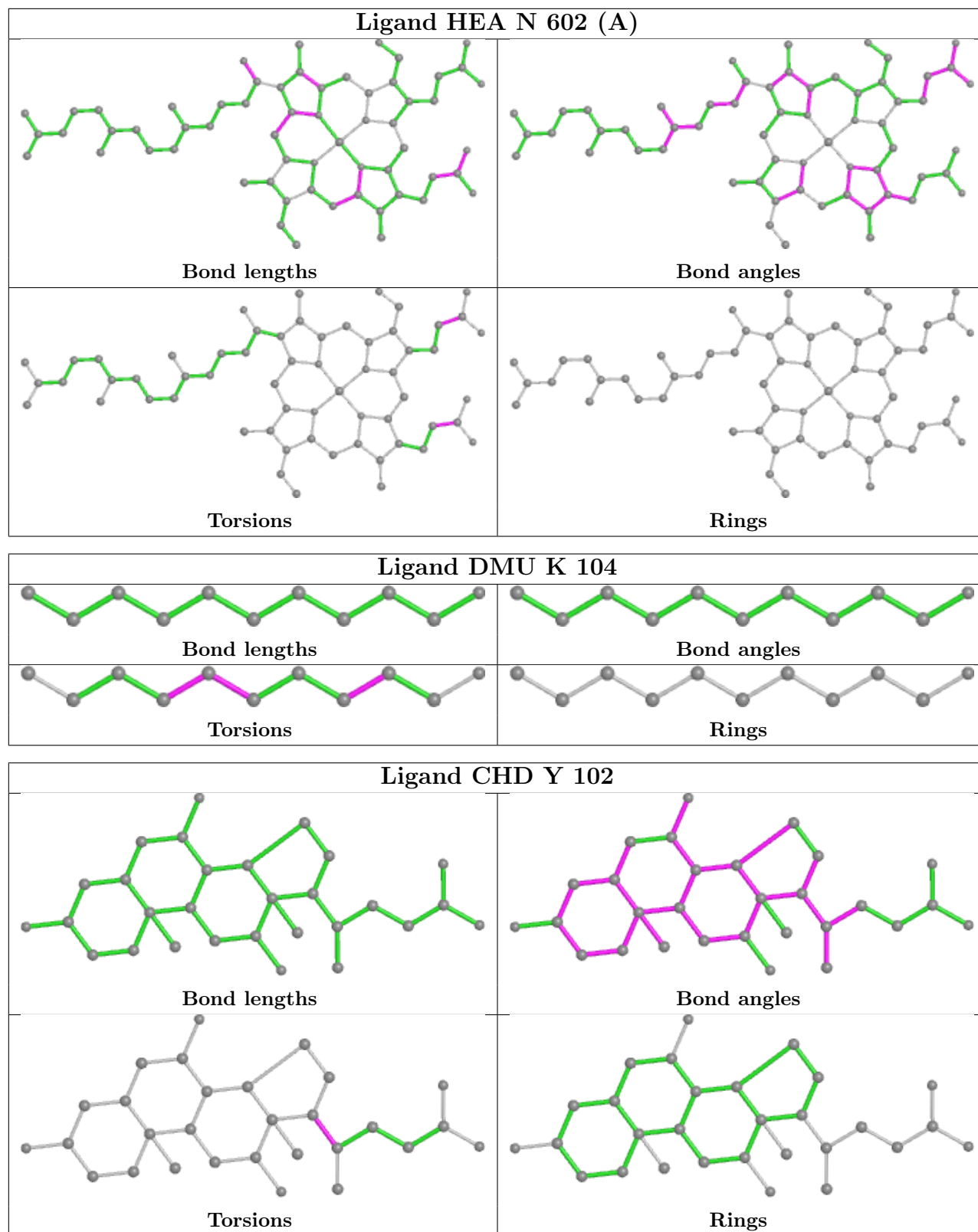


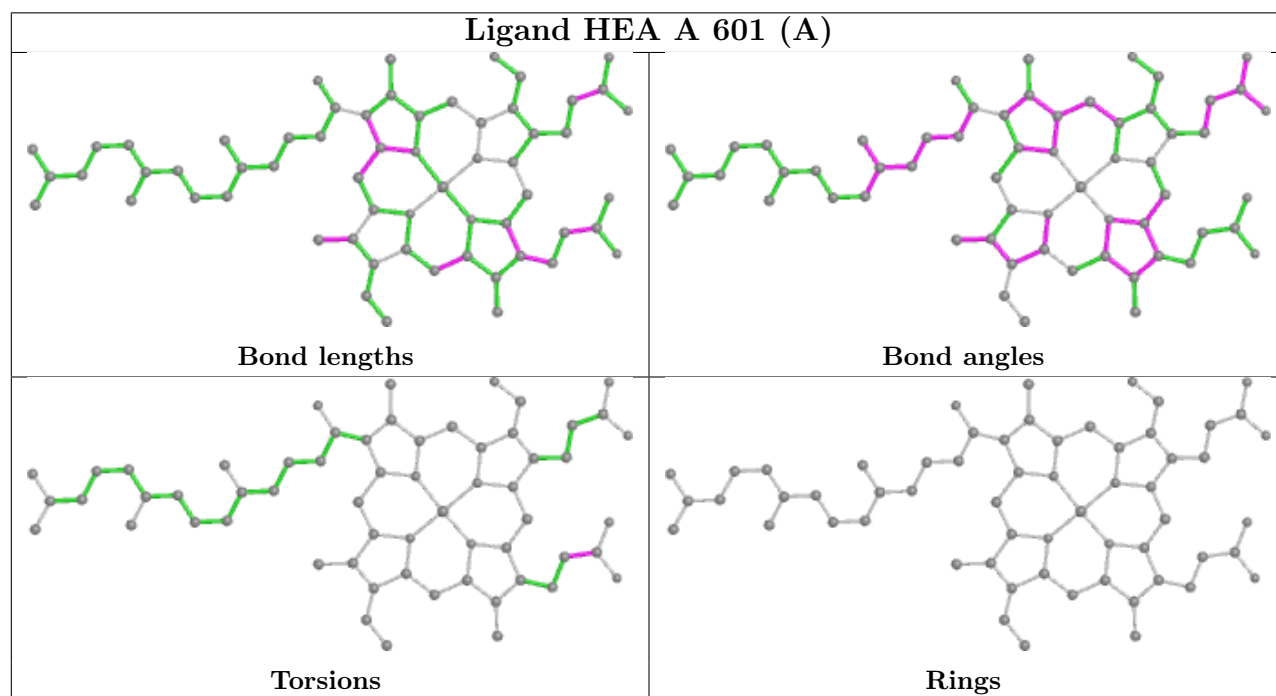
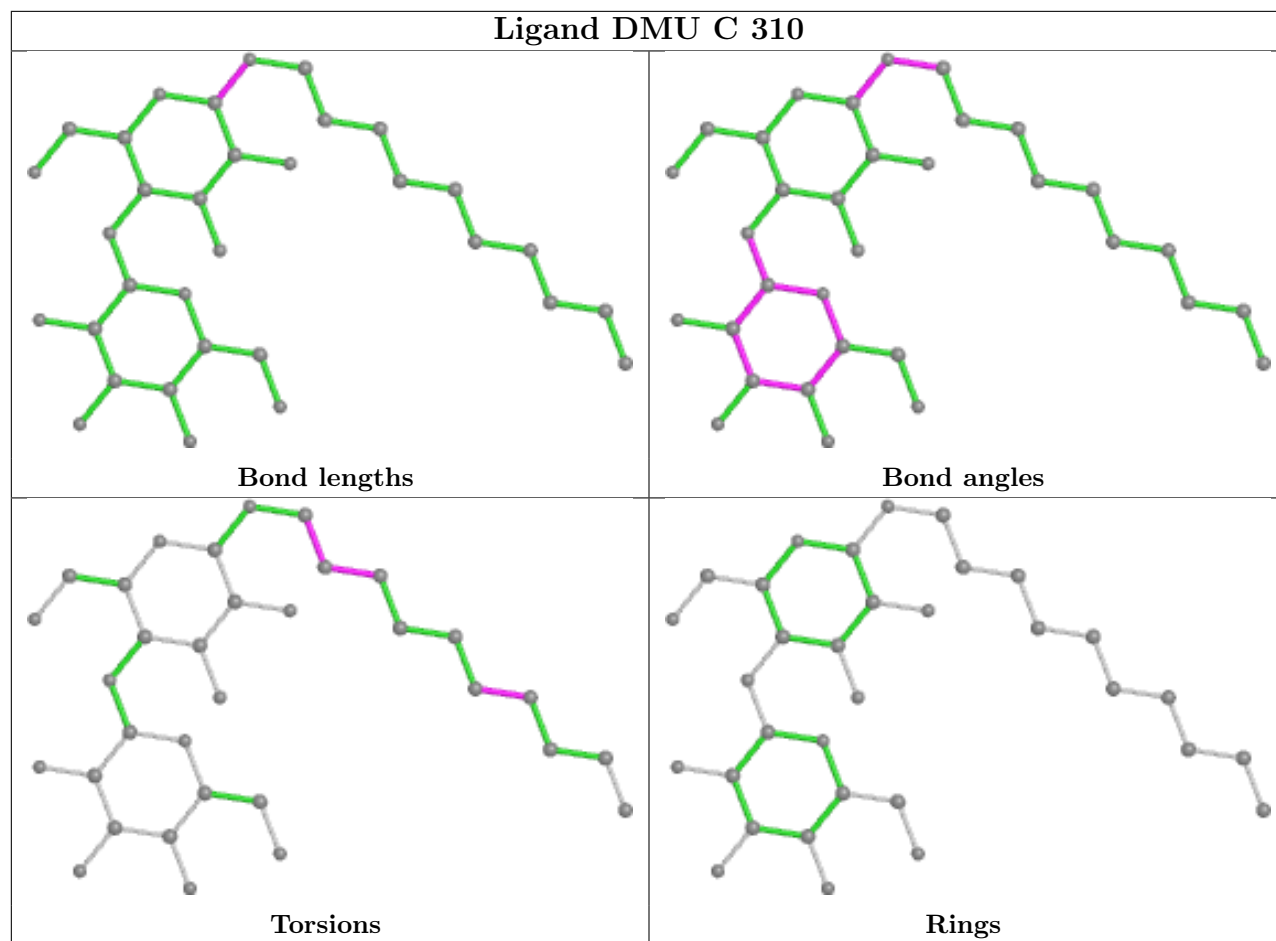


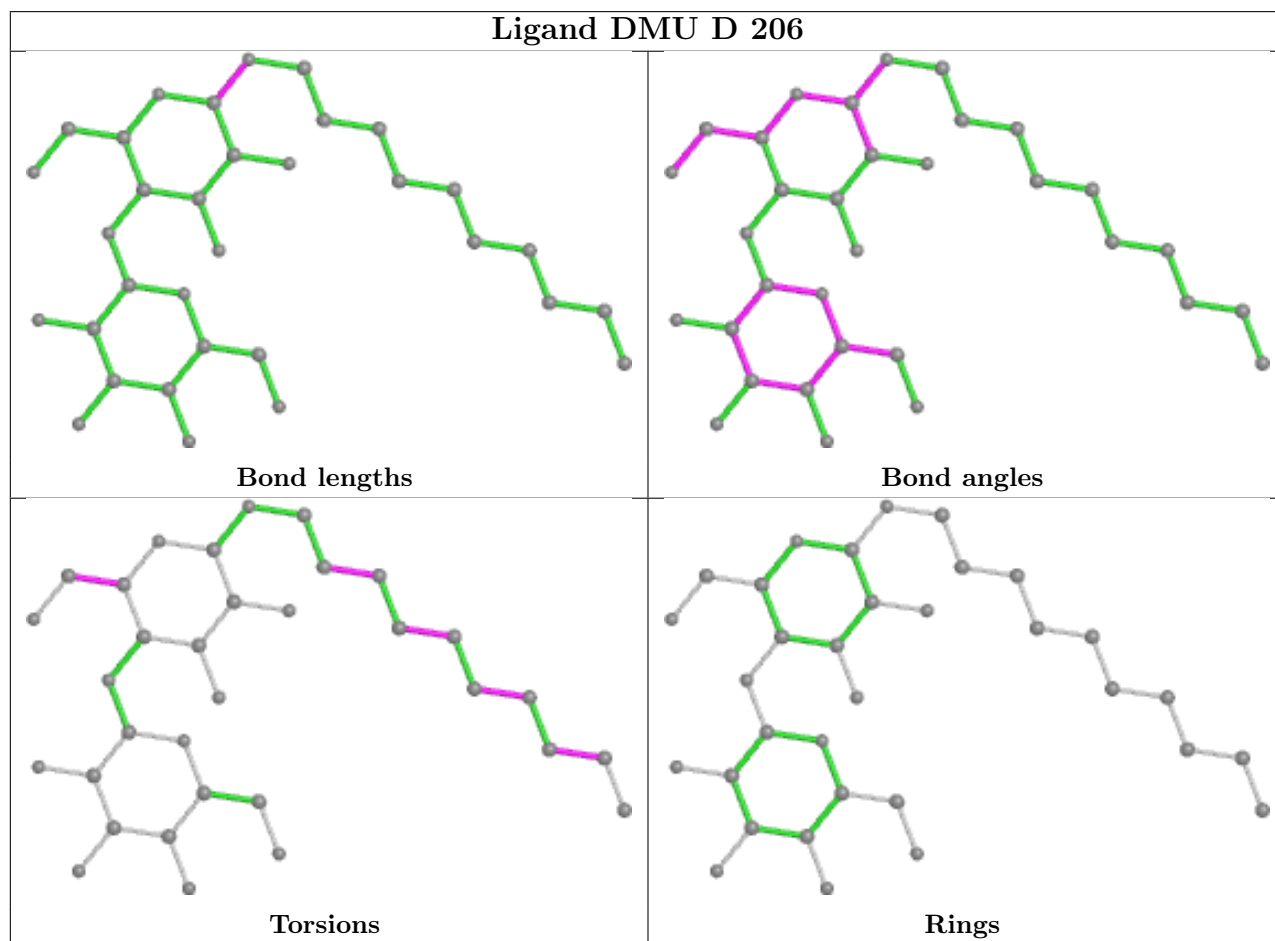
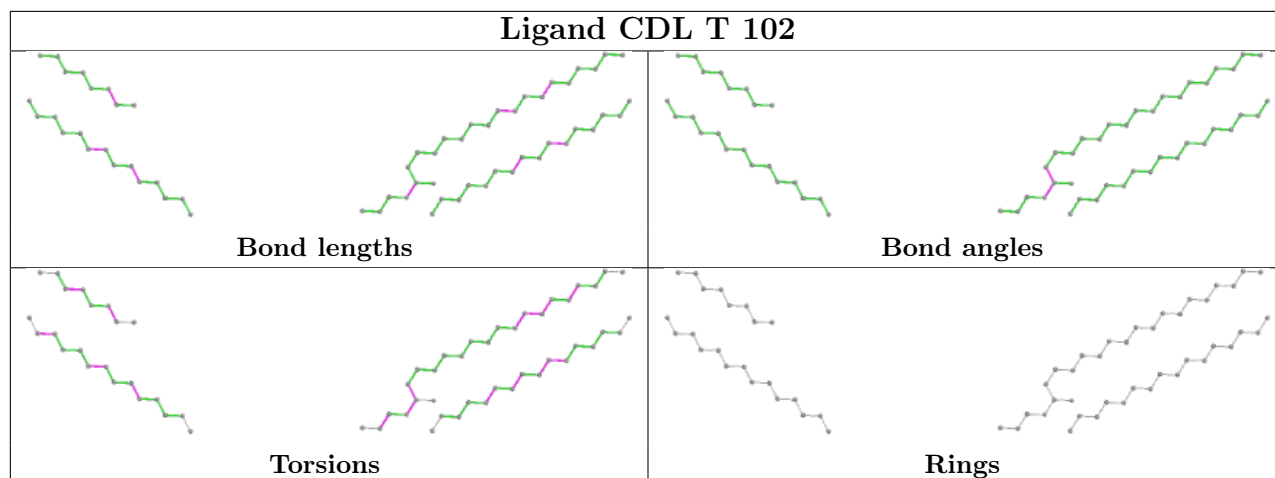


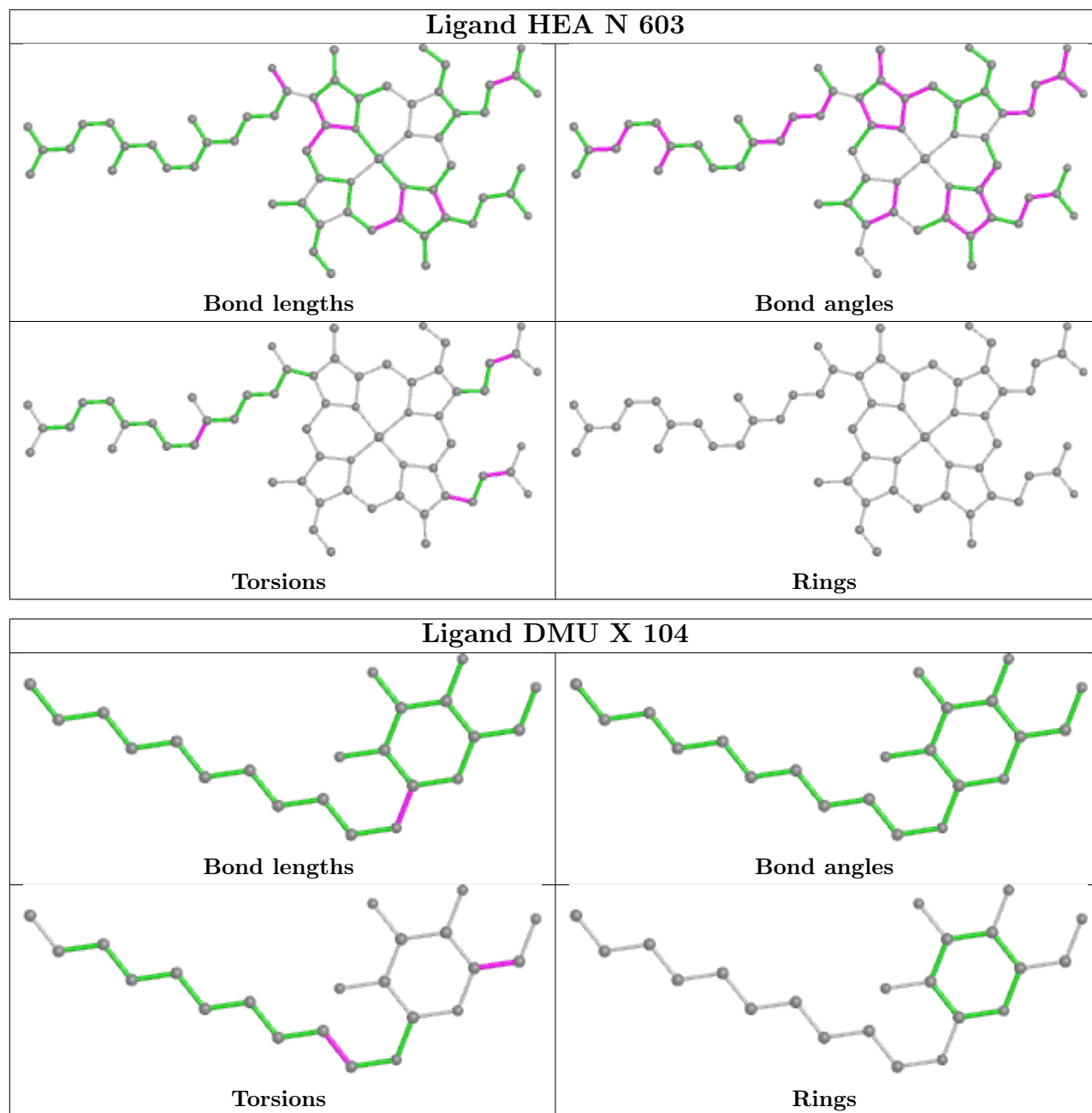


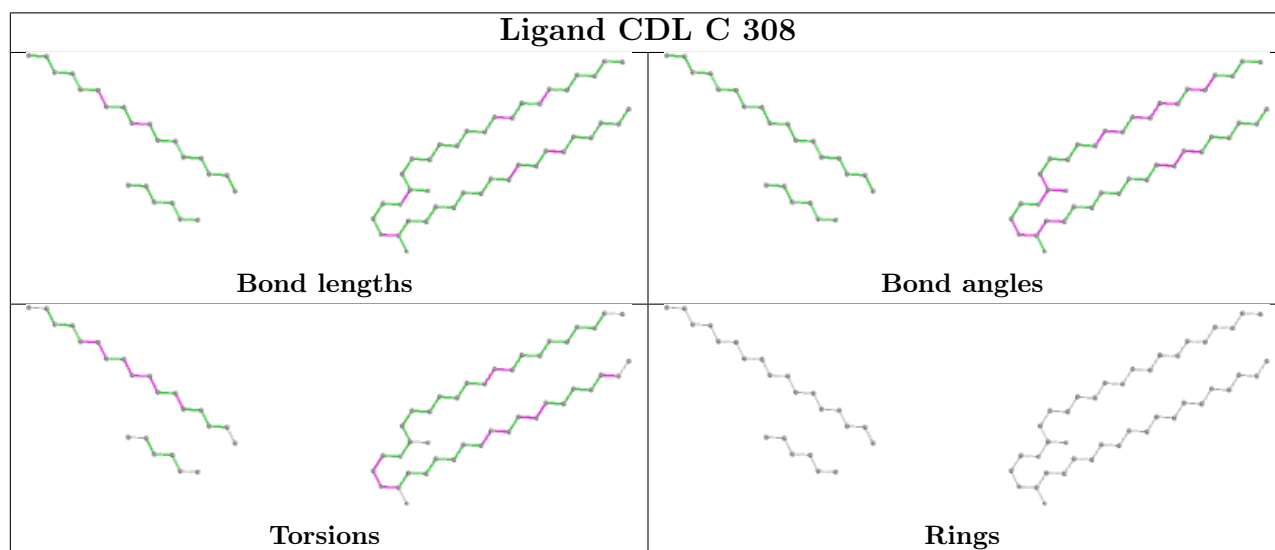
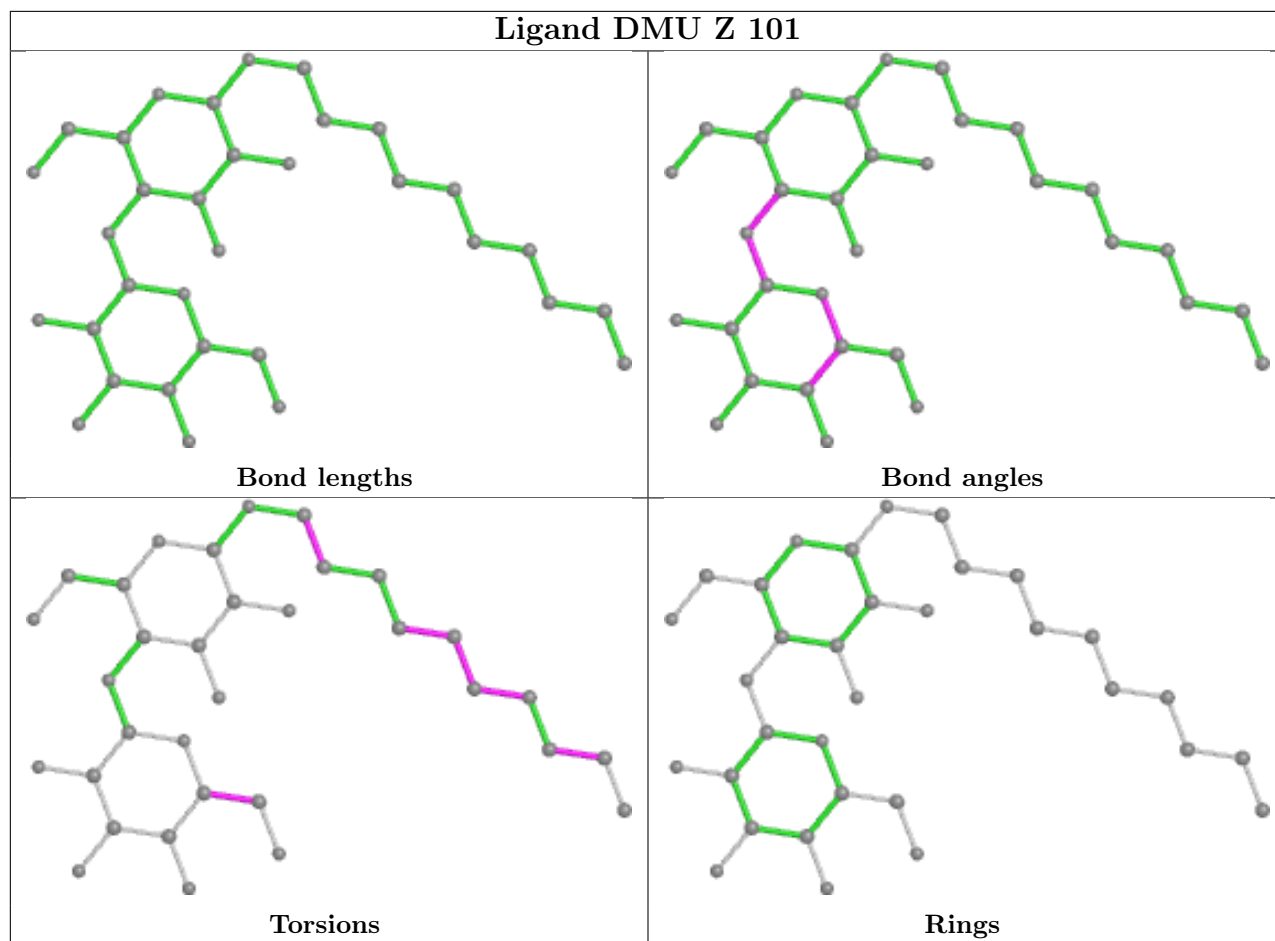




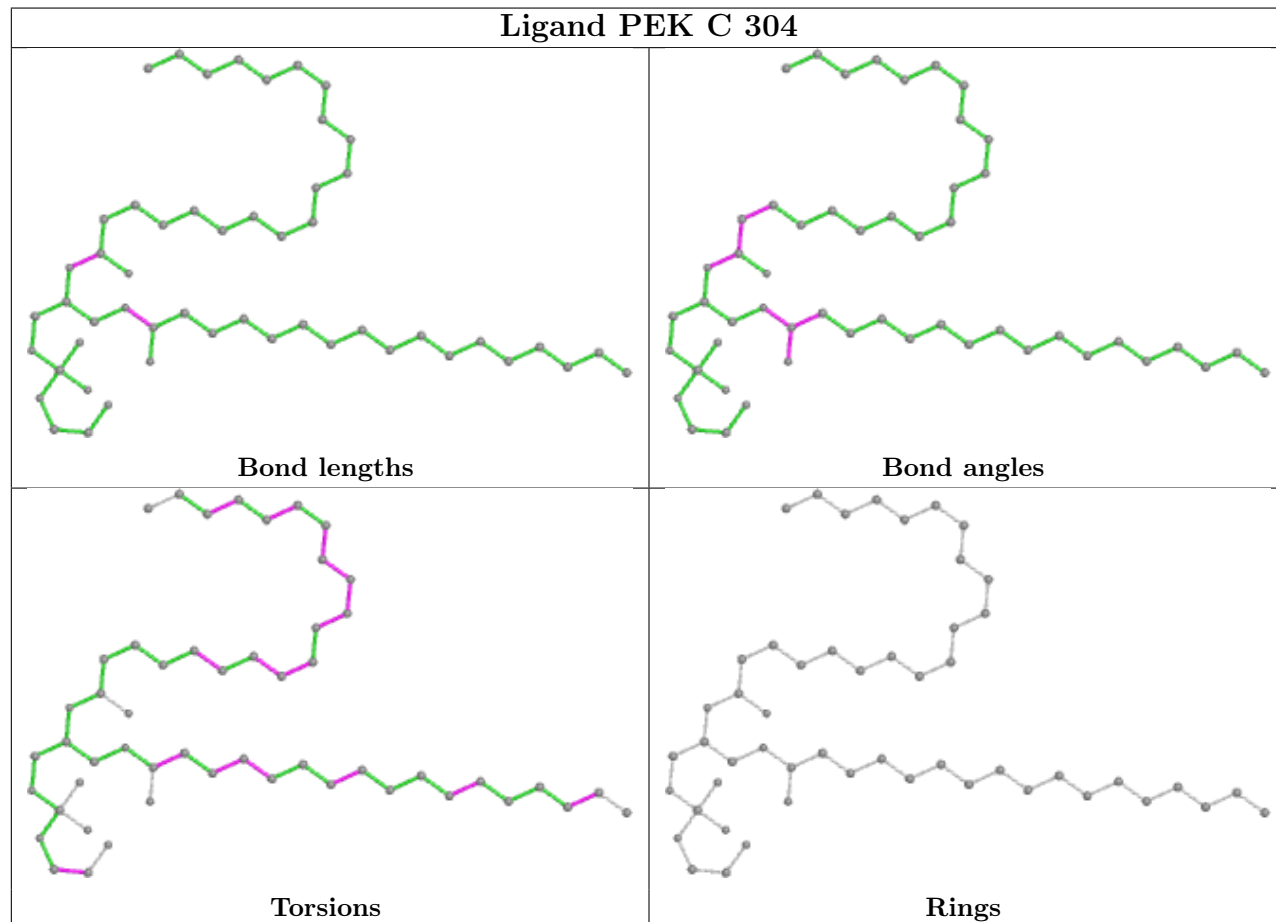
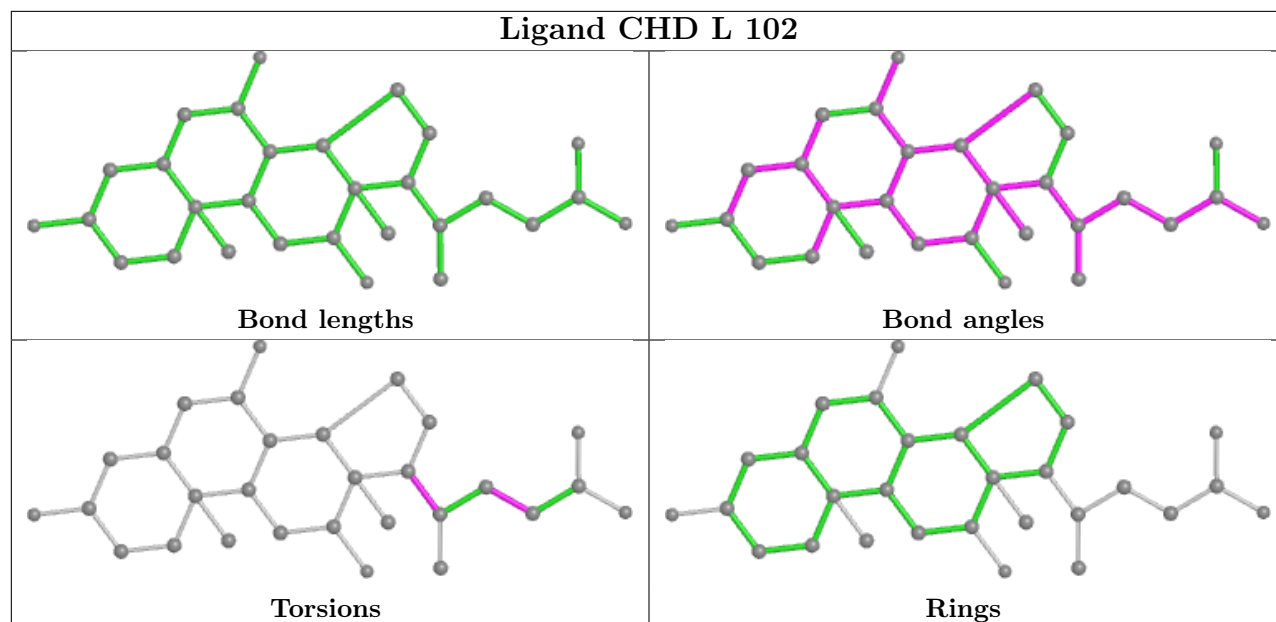


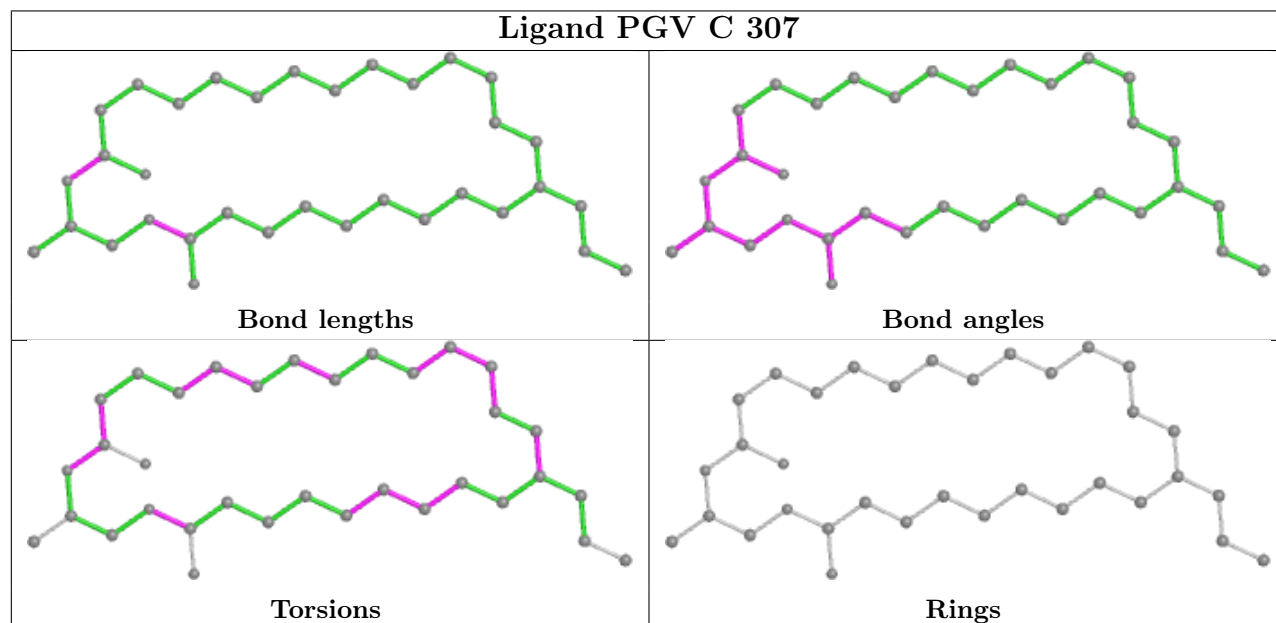
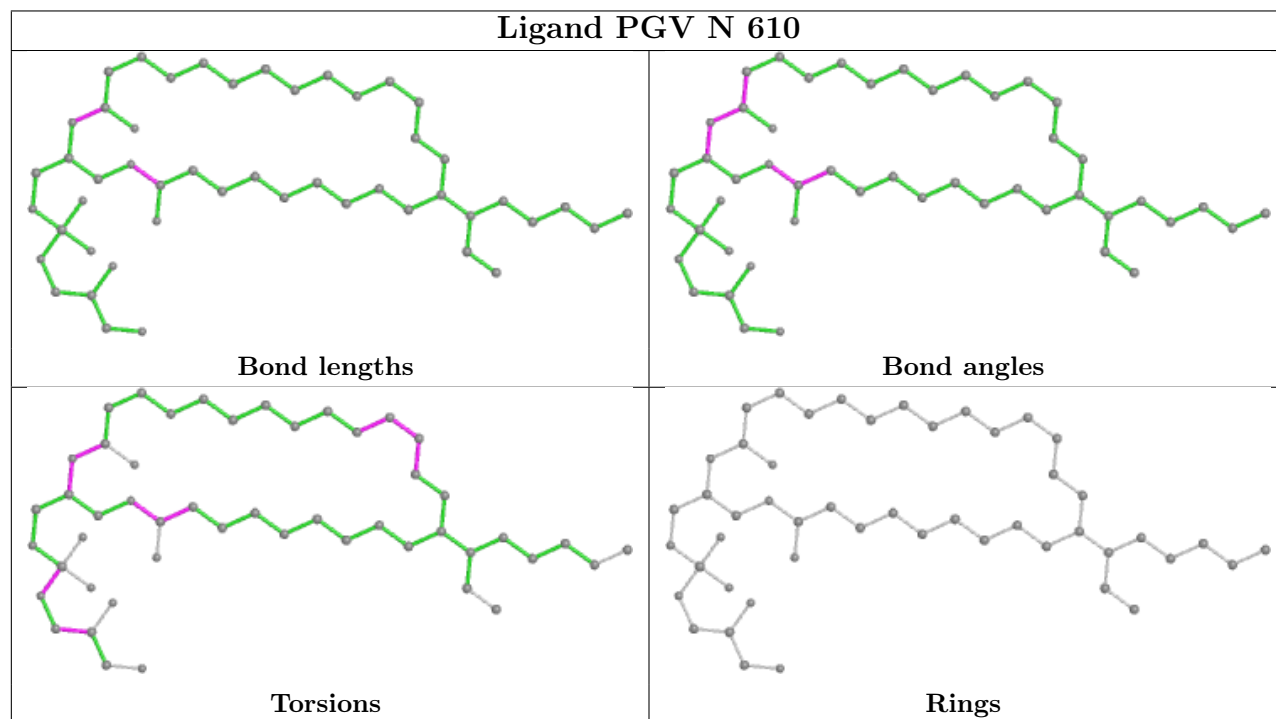
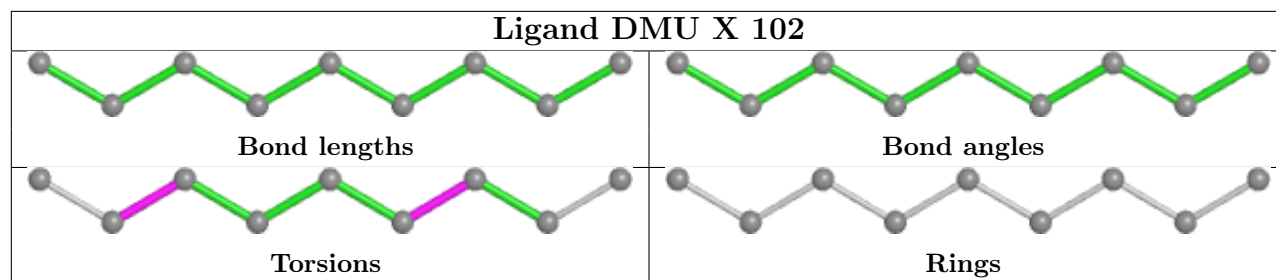


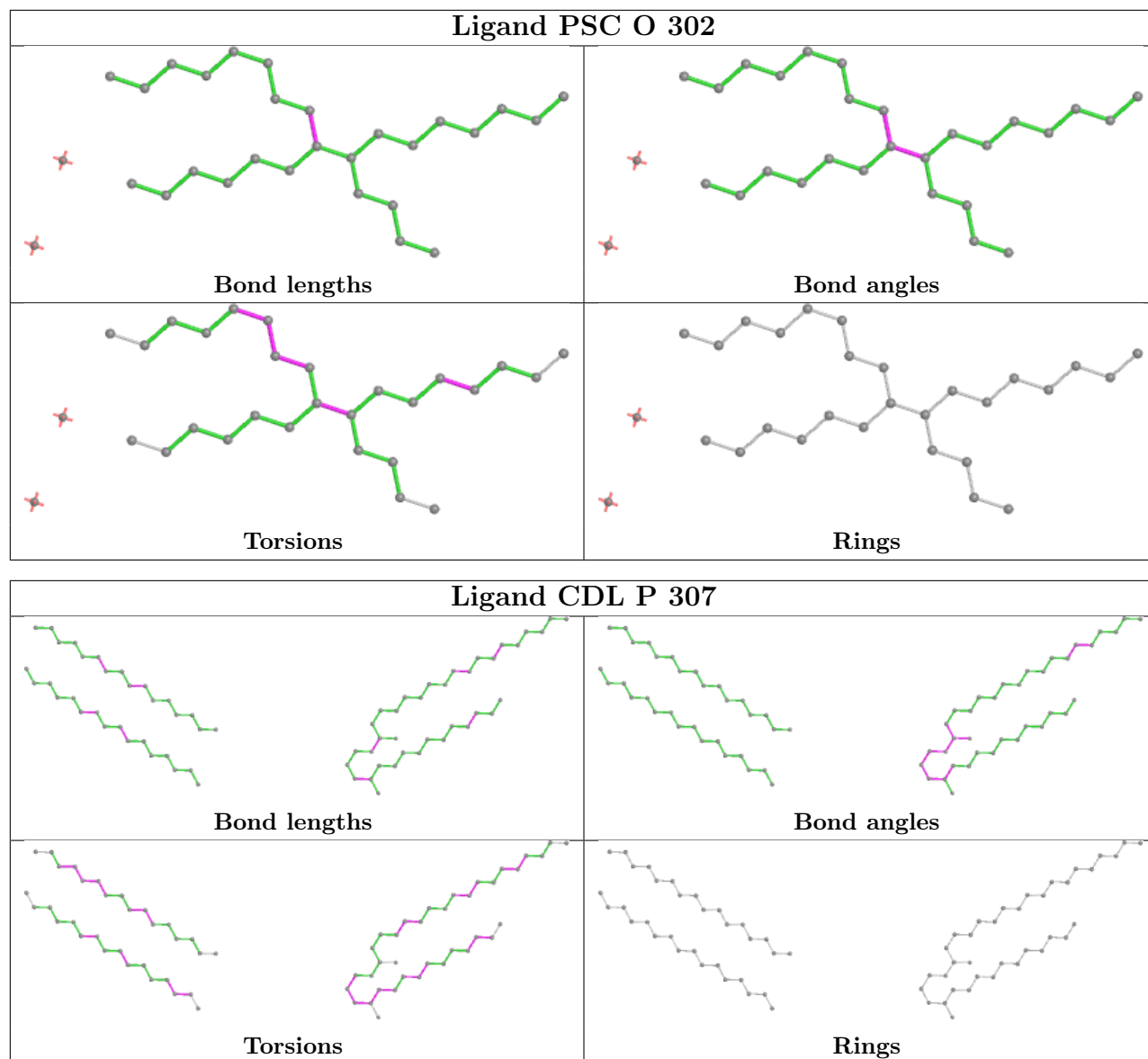


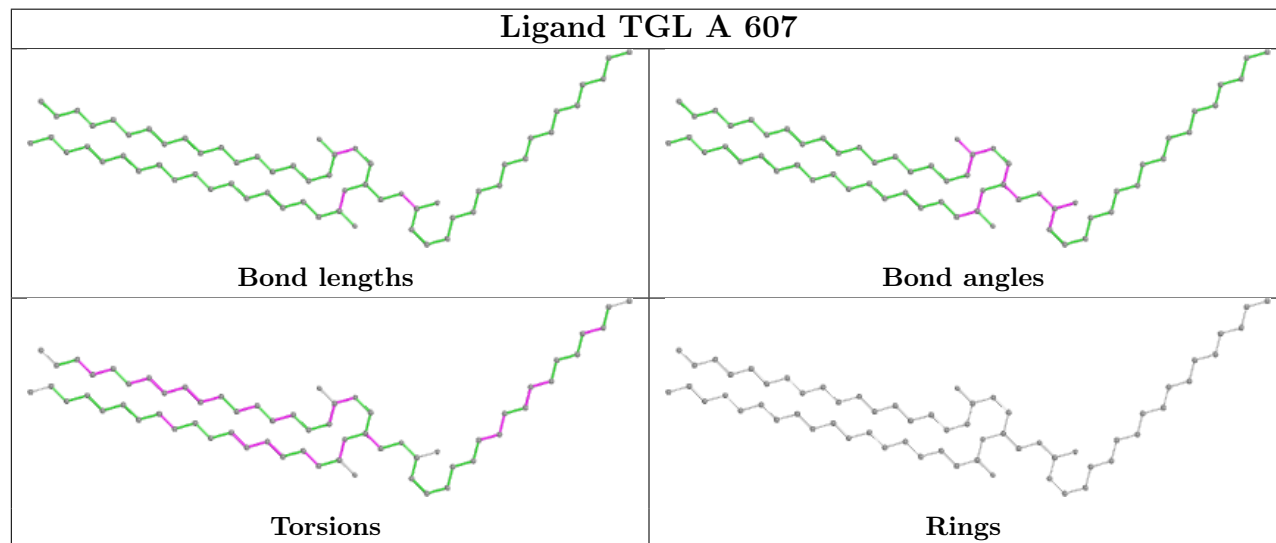
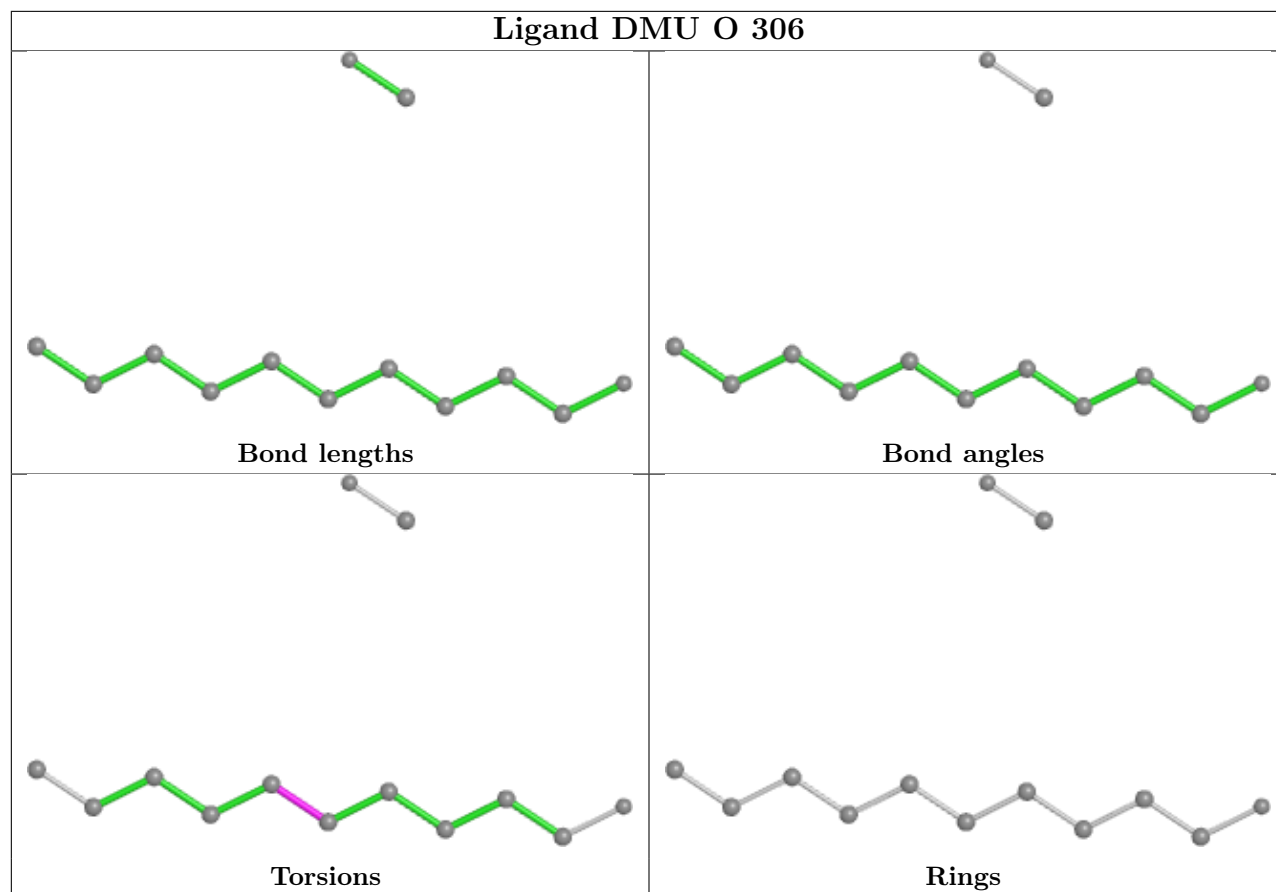


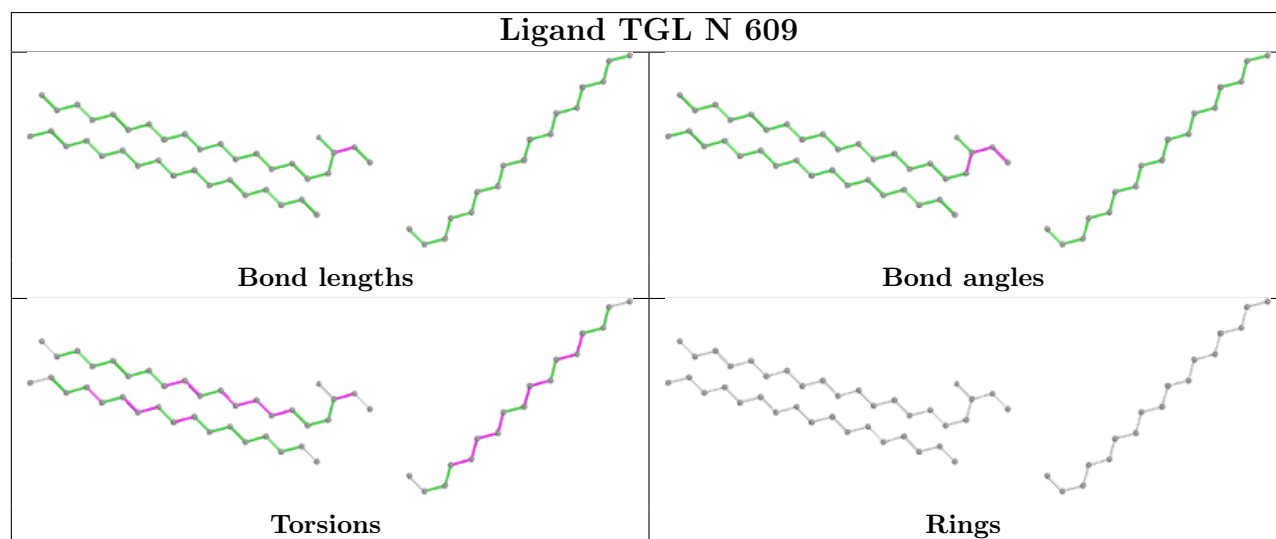
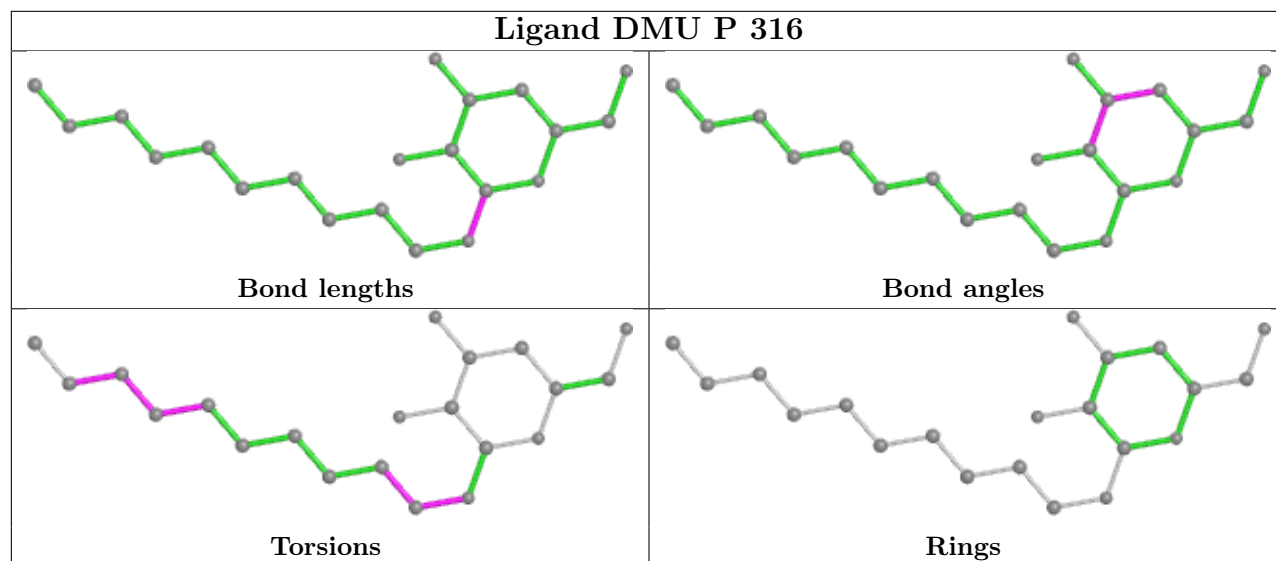


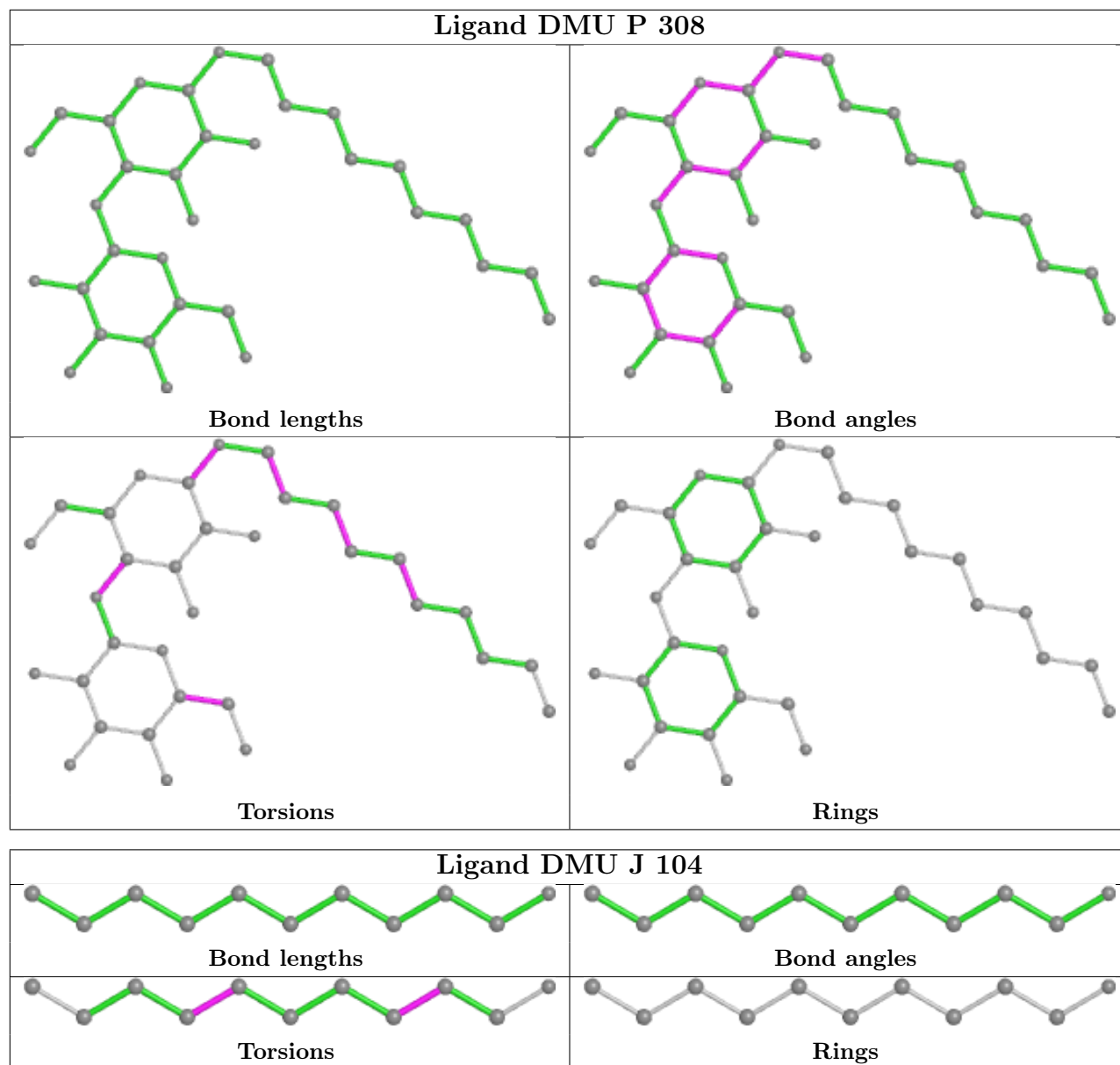


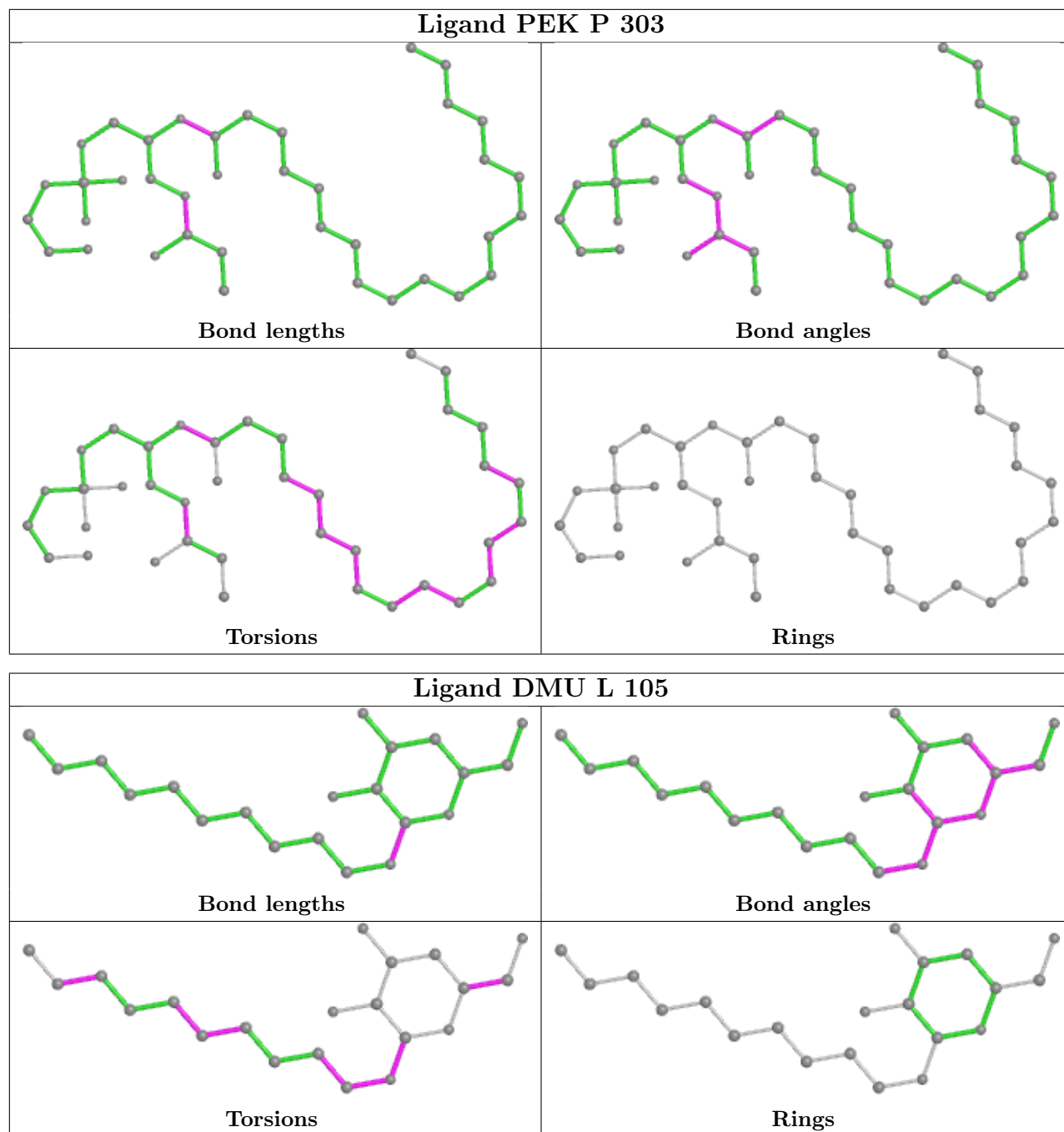


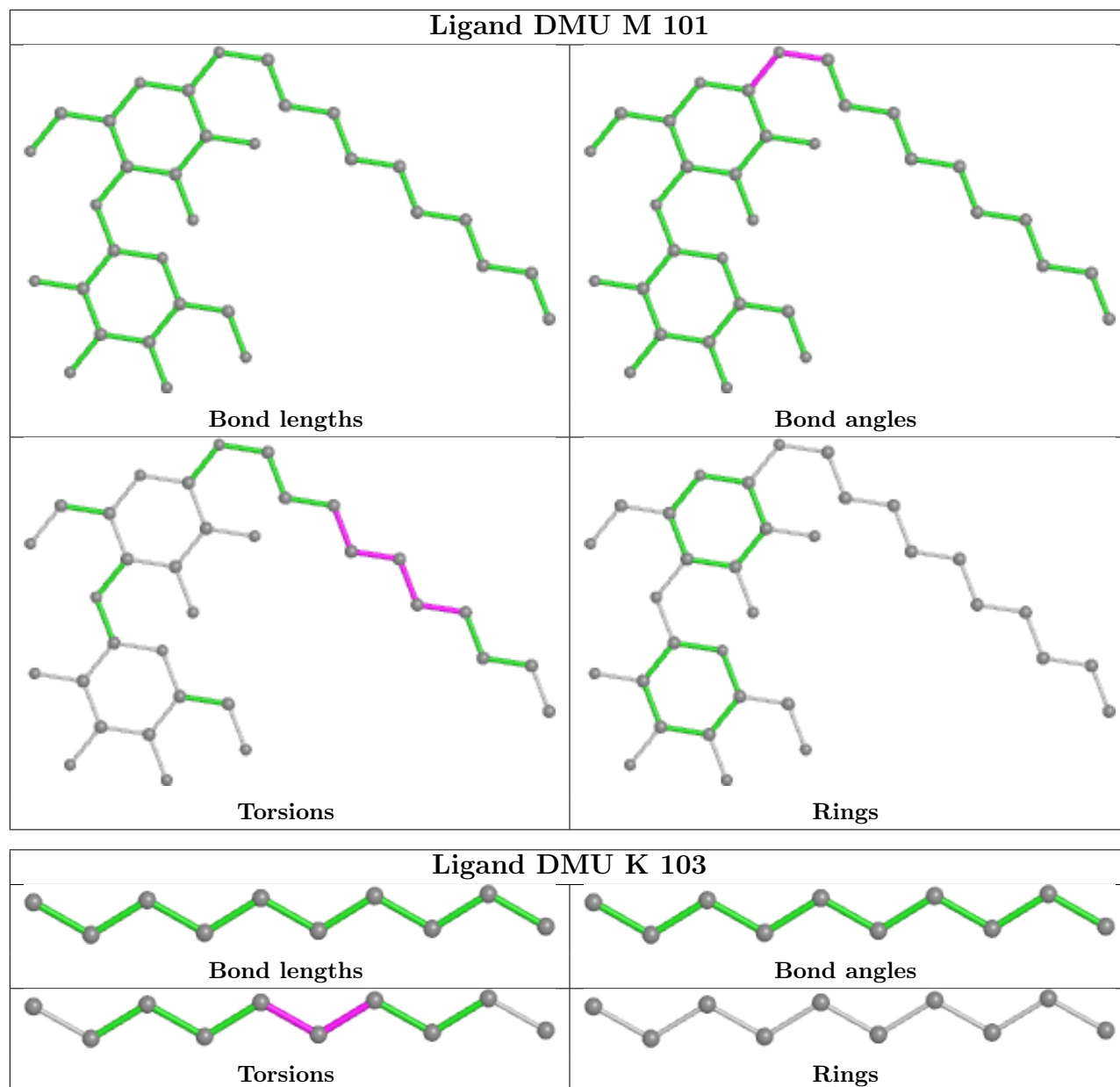




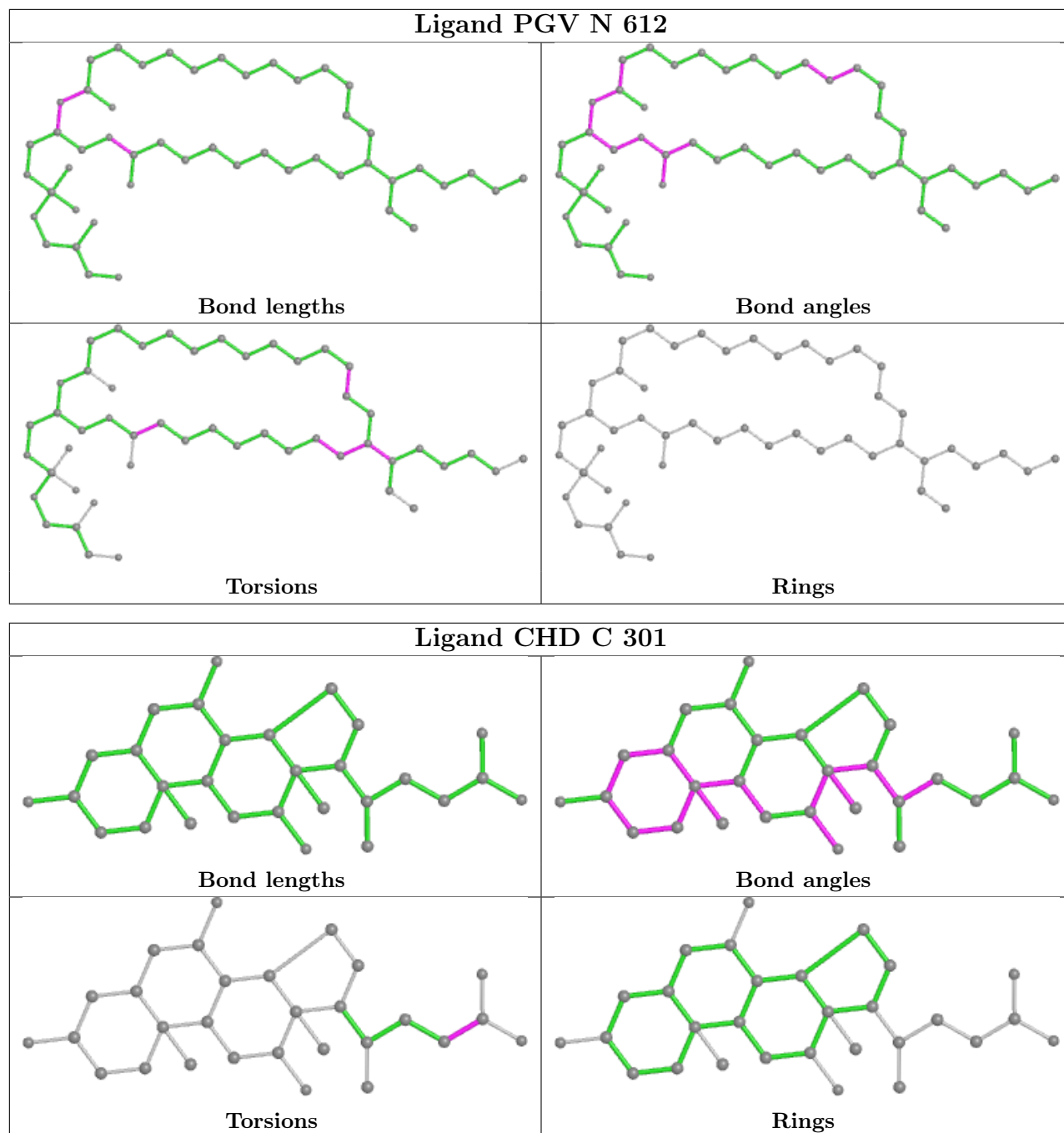


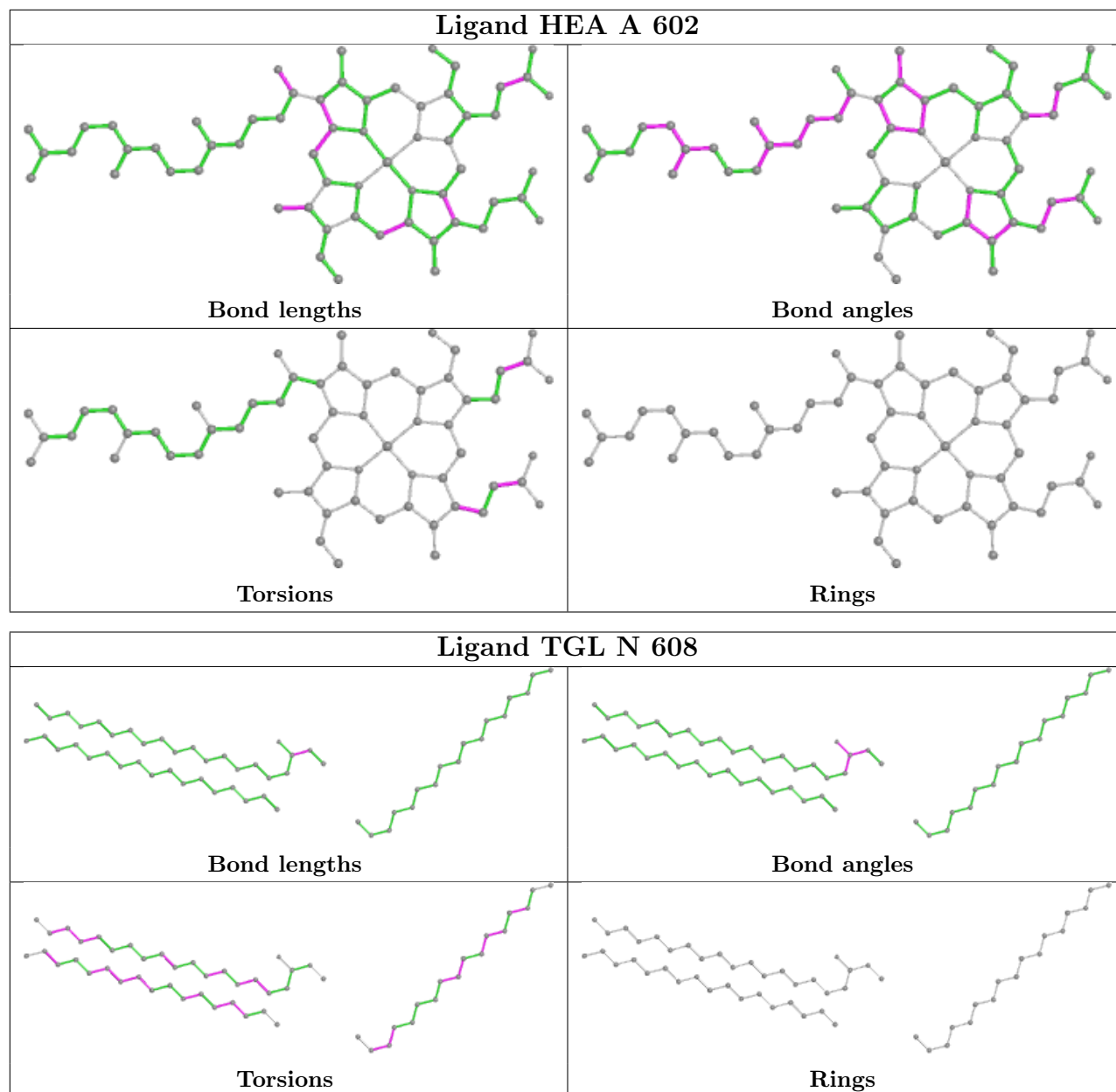


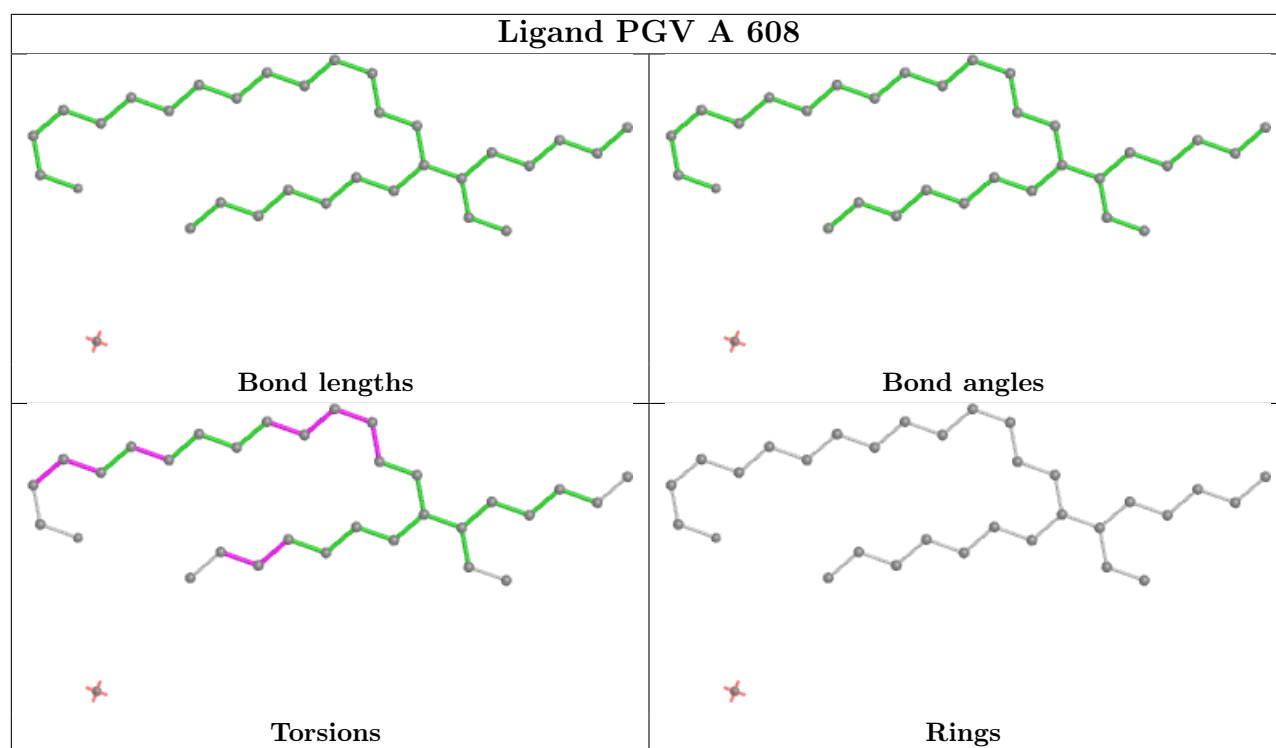












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	-0.12	2 (0%) 92 92	19, 24, 33, 82	0
1	N	513/514 (99%)	-0.13	1 (0%) 95 94	19, 26, 35, 80	0
2	B	226/227 (99%)	-0.10	2 (0%) 84 84	22, 32, 61, 110	0
2	O	226/227 (99%)	-0.13	2 (0%) 84 84	25, 36, 73, 115	0
3	C	259/259 (100%)	-0.15	0 100 100	21, 27, 40, 93	0
3	P	259/259 (100%)	-0.13	0 100 100	21, 28, 43, 90	0
4	D	144/144 (100%)	-0.28	0 100 100	25, 34, 56, 93	0
4	Q	144/144 (100%)	0.34	7 (4%) 29 27	31, 48, 96, 243	0
5	E	105/105 (100%)	-0.26	1 (0%) 82 82	27, 33, 69, 156	0
5	R	105/105 (100%)	-0.17	2 (1%) 66 65	29, 42, 77, 169	0
6	F	94/94 (100%)	-0.05	3 (3%) 47 44	23, 34, 65, 130	0
6	S	94/94 (100%)	-0.02	4 (4%) 35 32	22, 31, 66, 125	0
7	G	84/84 (100%)	0.88	16 (19%) 1 1	25, 35, 140, 183	0
7	T	84/84 (100%)	0.73	16 (19%) 1 1	25, 39, 127, 194	0
8	H	79/79 (100%)	0.15	4 (5%) 28 25	26, 38, 112, 179	0
8	U	79/79 (100%)	0.16	6 (7%) 13 12	31, 42, 117, 215	0
9	I	72/73 (98%)	0.14	1 (1%) 75 75	30, 48, 86, 102	0
9	V	72/73 (98%)	0.17	2 (2%) 53 51	29, 55, 95, 161	0
10	J	58/58 (100%)	0.17	3 (5%) 27 24	27, 38, 88, 175	0
10	W	58/58 (100%)	0.04	3 (5%) 27 24	28, 39, 86, 171	0
11	K	49/49 (100%)	-0.11	0 100 100	30, 38, 59, 72	0
11	X	49/49 (100%)	0.10	2 (4%) 37 34	36, 47, 86, 100	0
12	L	46/46 (100%)	-0.18	1 (2%) 62 60	25, 30, 56, 105	0
12	Y	46/46 (100%)	-0.19	1 (2%) 62 60	28, 36, 74, 133	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/43 (100%)	-0.03	3 (6%) 16 14	25, 30, 86, 141	0
13	Z	43/43 (100%)	0.09	5 (11%) 4 4	33, 38, 122, 190	0
All	All	3544/3550 (99%)	-0.03	87 (2%) 57 55	19, 31, 77, 243	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	4	SER	17.4
10	J	58	LYS	13.6
6	F	1	ALA	13.1
4	Q	6	VAL	12.9
4	Q	5	VAL	12.0
7	G	3	ALA	9.0
7	T	3	ALA	8.3
7	T	10	GLY	8.2
7	G	11	THR	7.9
7	G	8	HIS	7.8
7	T	8	HIS	7.8
4	Q	7	LYS	7.6
6	S	1	ALA	7.0
5	R	5	HIS	6.5
10	W	58	LYS	6.4
7	G	9	GLY	5.9
4	Q	8	SER	5.8
7	G	6	GLY	5.8
8	H	8	ILE	5.8
8	U	45	ALA	5.4
8	U	8	ILE	5.4
7	T	11	THR	5.3
7	G	7	ASP	5.3
7	T	2	SER	4.9
9	V	37	PHE	4.7
9	I	37	PHE	4.5
7	G	42	ARG	4.4
7	G	2	SER	4.2
7	T	5	LYS	4.1
8	H	45	ALA	4.1
7	T	1	ALA	4.0
7	T	7	ASP	3.9
7	G	36	TRP	3.9
6	S	2	SER	3.9

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Mol	Chain	Res	Type	RSRZ
8	U	7	LYS	3.9
7	T	36	TRP	3.7
7	G	10	GLY	3.7
13	Z	43	SER	3.6
10	J	1	PHE	3.5
13	Z	42	LYS	3.5
7	T	4	ALA	3.2
11	X	6	ALA	3.2
7	G	5	LYS	3.2
10	J	57	HIS	3.1
7	G	37	LEU	3.0
13	M	42	LYS	2.9
7	T	40	GLY	2.9
13	M	40	TYR	2.9
7	T	84	LYS	2.9
6	F	2	SER	2.8
2	O	113	TYR	2.8
10	W	57	HIS	2.8
7	G	4	ALA	2.6
2	O	90	ILE	2.6
7	G	40	GLY	2.6
8	H	46	LYS	2.6
13	Z	41	LYS	2.6
2	B	59	GLN	2.6
7	T	6	GLY	2.5
9	V	2	THR	2.5
8	U	48	GLY	2.5
13	M	43	SER	2.4
13	Z	40	TYR	2.4
12	Y	47	LYS	2.4
6	S	94	HIS	2.4
8	U	46	LYS	2.4
7	T	42	ARG	2.3
7	T	38	HIS	2.3
7	G	41	HIS	2.3
6	S	93	PRO	2.3
1	A	514[A]	LYS	2.2
5	R	109	VAL	2.2
8	U	49	ASP	2.2
1	N	311[A]	ILE	2.2
4	Q	72	ASN	2.2
7	G	1	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
13	Z	39	ASN	2.2
10	W	1	PHE	2.2
2	B	61	VAL	2.2
11	X	7	PRO	2.1
5	E	5	HIS	2.1
7	T	41	HIS	2.1
12	L	2	HIS	2.1
1	A	298[A]	ASP	2.1
6	F	3	GLY	2.0
4	Q	51	LEU	2.0
8	H	44	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
9	SAC	V	1	9/10	0.19	0.53	201,217,238,247	0
9	SAC	I	1	9/10	0.73	0.32	129,147,176,183	0
1	FME	N	1	10/11	0.95	0.10	36,45,97,109	0
2	FME	B	1	10/11	0.96	0.11	28,31,40,126	0
1	FME	A	1	10/11	0.96	0.10	37,51,85,99	0
2	FME	O	1	10/11	0.97	0.12	31,36,44,111	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
23	DMU	X	102	9/33	0.52	0.31	65,70,82,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
27	CDL	N	601	62/100	0.52	0.35	44,76,103,117	0
22	EDO	P	310	4/4	0.54	0.17	71,72,75,80	0
23	DMU	X	104	22/33	0.56	0.43	58,94,150,157	0
22	EDO	A	618	4/4	0.58	0.26	52,59,65,85	0
23	DMU	A	623	11/33	0.64	0.37	62,76,106,114	0
22	EDO	F	105	4/4	0.66	0.18	56,58,67,70	0
22	EDO	C	315	4/4	0.66	0.23	65,78,87,99	0
25	CHD	J	101	29/29	0.68	0.41	50,120,146,151	0
23	DMU	L	105	21/33	0.68	0.20	54,80,107,120	0
23	DMU	D	207	11/33	0.69	0.33	58,81,115,120	0
23	DMU	P	317	32/33	0.69	0.22	52,107,133,136	0
23	DMU	Q	201	11/33	0.70	0.22	49,70,93,95	0
22	EDO	C	317	4/4	0.71	0.18	60,67,70,80	0
23	DMU	K	103	10/33	0.73	0.26	62,75,106,112	0
26	PEK	C	303	45/53	0.73	0.33	44,95,175,209	0
23	DMU	D	206	33/33	0.73	0.23	46,95,141,151	0
27	CDL	T	102	61/100	0.74	0.27	42,77,110,117	0
26	PEK	P	303	38/53	0.75	0.25	49,79,163,172	0
23	DMU	P	308	33/33	0.76	0.29	37,102,137,160	0
26	PEK	C	305	36/53	0.77	0.23	42,76,101,118	0
22	EDO	O	305	4/4	0.77	0.19	49,61,62,105	0
25	CHD	Y	102	29/29	0.78	0.24	56,91,135,152	0
23	DMU	K	102	11/33	0.78	0.24	55,70,95,105	0
23	DMU	X	103	9/33	0.78	0.23	56,62,103,104	0
22	EDO	T	104	4/4	0.78	0.26	56,73,98,107	0
22	EDO	P	315	4/4	0.78	0.17	66,95,100,113	0
25	CHD	L	102	29/29	0.78	0.30	51,95,117,134	0
22	EDO	C	311	4/4	0.79	0.16	44,65,68,73	0
22	EDO	C	320	4/4	0.79	0.35	33,68,70,73	0
18	TGL	N	609	55/63	0.79	0.21	46,72,112,119	0
22	EDO	N	620	4/4	0.80	0.20	52,52,53,80	0
19	PGV	P	306	31/51	0.80	0.25	32,72,96,109	0
21	PSC	O	302	31/52	0.80	0.23	36,62,106,153	0
26	PEK	T	101	37/53	0.80	0.26	43,75,105,131	0
22	EDO	A	612	4/4	0.80	0.24	51,51,71,101	0
22	EDO	L	103	4/4	0.80	0.22	42,49,64,119	0
23	DMU	P	316	21/33	0.81	0.17	51,81,126,136	0
22	EDO	A	617	4/4	0.81	0.27	57,70,72,73	0
22	EDO	L	104	4/4	0.81	0.24	50,51,79,128	0
25	CHD	C	309	29/29	0.83	0.27	47,86,113,140	0
22	EDO	P	314	4/4	0.83	0.14	37,53,55,74	0
21	PSC	A	610	25/52	0.83	0.22	44,70,88,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
19	PGV	N	610	51/51	0.83	0.28	40,83,151,204	0
18	TGL	A	607	63/63	0.83	0.21	32,68,117,128	0
19	PGV	A	608	34/51	0.84	0.23	32,57,110,126	0
18	TGL	N	608	55/63	0.84	0.20	38,64,110,123	0
22	EDO	A	620	4/4	0.84	0.19	44,52,61,82	0
18	TGL	L	101	63/63	0.85	0.21	25,60,114,165	0
18	TGL	N	607	63/63	0.85	0.24	40,79,108,125	0
23	DMU	O	306	13/33	0.85	0.19	45,66,128,139	0
27	CDL	C	308	65/100	0.85	0.24	37,69,123,156	0
19	PGV	C	307	36/51	0.85	0.25	41,74,140,164	0
18	TGL	A	606	63/63	0.85	0.17	39,72,108,119	0
22	EDO	N	619	4/4	0.86	0.15	40,78,80,94	0
22	EDO	F	102	4/4	0.86	0.11	33,36,53,121	0
27	CDL	P	307	68/100	0.86	0.24	39,76,127,157	0
23	DMU	C	310	33/33	0.86	0.24	35,81,151,167	0
22	EDO	B	305	4/4	0.87	0.14	28,36,44,63	0
22	EDO	P	309	4/4	0.87	0.18	60,63,63,69	0
23	DMU	K	104	11/33	0.87	0.20	50,68,100,112	0
23	DMU	J	104	11/33	0.87	0.17	49,60,84,99	0
22	EDO	J	103	4/4	0.88	0.26	59,62,62,75	0
22	EDO	C	319	4/4	0.88	0.25	43,47,61,111	0
22	EDO	F	103	4/4	0.88	0.14	44,51,53,59	0
22	EDO	C	313	4/4	0.88	0.14	30,39,40,49	0
23	DMU	C	321	12/33	0.89	0.13	51,66,84,89	0
23	DMU	X	101	10/33	0.89	0.15	41,60,84,103	0
22	EDO	W	101	4/4	0.89	0.18	54,56,71,77	0
22	EDO	S	104	4/4	0.89	0.13	44,46,48,54	0
22	EDO	A	614	4/4	0.89	0.19	51,61,65,80	0
23	DMU	Z	101	33/33	0.89	0.11	37,47,68,72	0
22	EDO	C	312	4/4	0.90	0.12	32,33,33,82	0
22	EDO	M	102	4/4	0.90	0.33	68,86,88,93	0
22	EDO	C	316	4/4	0.90	0.13	49,55,70,77	0
23	DMU	K	101	8/33	0.90	0.18	48,63,77,85	0
22	EDO	D	205	4/4	0.90	0.33	53,58,59,61	0
22	EDO	A	616	4/4	0.90	0.32	31,40,42,78	0
22	EDO	P	313	4/4	0.91	0.18	49,54,61,76	0
23	DMU	M	101	33/33	0.91	0.11	35,41,54,65	0
22	EDO	B	306	4/4	0.92	0.15	38,47,48,48	0
22	EDO	Q	202	4/4	0.92	0.17	41,46,48,52	0
22	EDO	J	102	4/4	0.92	0.17	48,48,91,98	0
22	EDO	D	201	4/4	0.92	0.21	39,49,70,82	0
22	EDO	P	311	4/4	0.92	0.13	33,37,37,44	0

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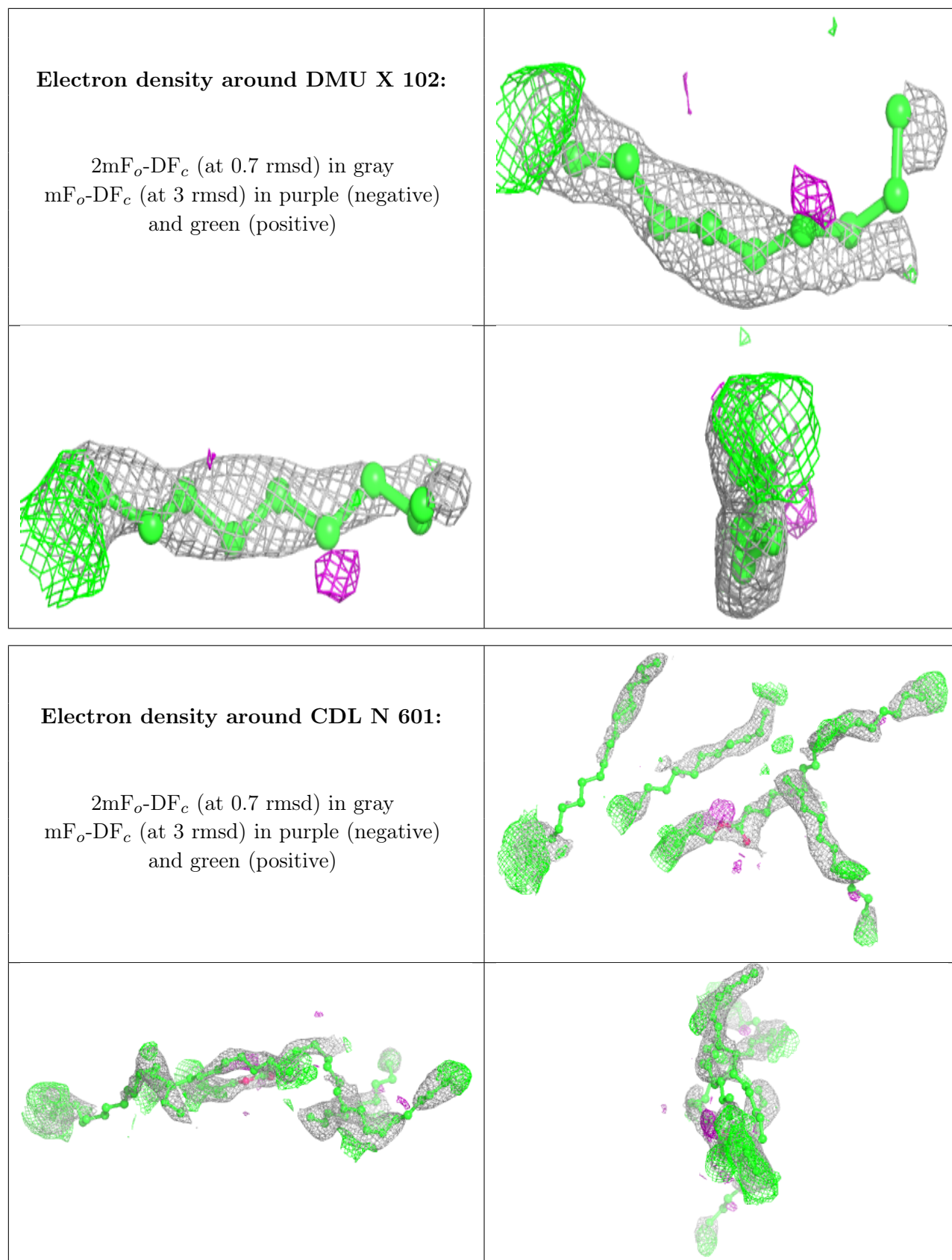
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	EDO	W	102	4/4	0.92	0.24	46,63,67,113	0
22	EDO	D	204	4/4	0.92	0.32	41,43,50,59	0
22	EDO	O	304	4/4	0.92	0.13	46,46,48,52	0
29	PO4	U	101	5/5	0.92	0.20	51,53,120,124	0
22	EDO	N	622	4/4	0.93	0.18	30,34,50,92	0
22	EDO	N	614	4/4	0.93	0.11	38,39,40,40	0
22	EDO	F	109	4/4	0.93	0.19	35,36,71,71	0
22	EDO	A	621	4/4	0.93	0.17	37,40,40,52	0
23	DMU	K	105	9/33	0.93	0.16	38,52,70,105	0
22	EDO	F	108	4/4	0.94	0.16	37,42,79,101	0
22	EDO	S	106	4/4	0.94	0.14	37,52,72,76	0
22	EDO	C	318	4/4	0.94	0.20	40,60,68,94	0
17	NA	C	302	1/1	0.94	0.09	36,36,36,36	0
22	EDO	E	203	4/4	0.94	0.12	49,49,49,75	0
22	EDO	Y	101	4/4	0.94	0.15	48,51,53,64	0
22	EDO	A	622	4/4	0.95	0.22	32,37,42,42	0
22	EDO	N	615	4/4	0.95	0.09	38,41,42,58	0
22	EDO	T	103	4/4	0.95	0.11	30,30,38,40	0
25	CHD	C	301	29/29	0.95	0.09	26,29,39,44	0
22	EDO	N	616	4/4	0.95	0.16	33,40,44,86	0
22	EDO	T	105	4/4	0.95	0.15	37,48,58,62	0
22	EDO	F	107	4/4	0.95	0.15	45,50,81,119	0
25	CHD	P	301	29/29	0.95	0.09	26,30,35,44	0
22	EDO	C	314	4/4	0.95	0.18	31,35,53,60	0
20	PER	A	609[A]	2/2	0.96	0.12	20,20,20,24	2
22	EDO	A	615	4/4	0.96	0.11	26,26,28,33	0
25	CHD	G	101	29/29	0.96	0.10	20,26,34,40	0
19	PGV	N	612	51/51	0.96	0.13	24,31,73,93	0
22	EDO	D	203	4/4	0.96	0.14	37,40,57,68	0
26	PEK	P	304	52/53	0.96	0.13	28,43,96,117	0
22	EDO	N	613	4/4	0.97	0.10	24,27,28,32	0
17	NA	P	302	1/1	0.97	0.10	38,38,38,38	0
22	EDO	P	312	4/4	0.97	0.11	28,39,39,57	0
16	MG	A	604	1/1	0.97	0.06	18,18,18,18	0
20	PER	N	611[A]	2/2	0.97	0.15	20,20,20,31	2
22	EDO	G	102	4/4	0.97	0.07	25,32,32,34	0
26	PEK	C	304	52/53	0.97	0.13	25,42,97,111	0
19	PGV	A	611	51/51	0.97	0.13	19,30,73,90	0
22	EDO	S	103	4/4	0.97	0.08	32,33,43,43	0
22	EDO	N	621	4/4	0.97	0.29	39,41,43,116	0
22	EDO	S	105	4/4	0.97	0.14	29,31,32,32	0
22	EDO	B	304	4/4	0.97	0.14	33,43,55,80	0

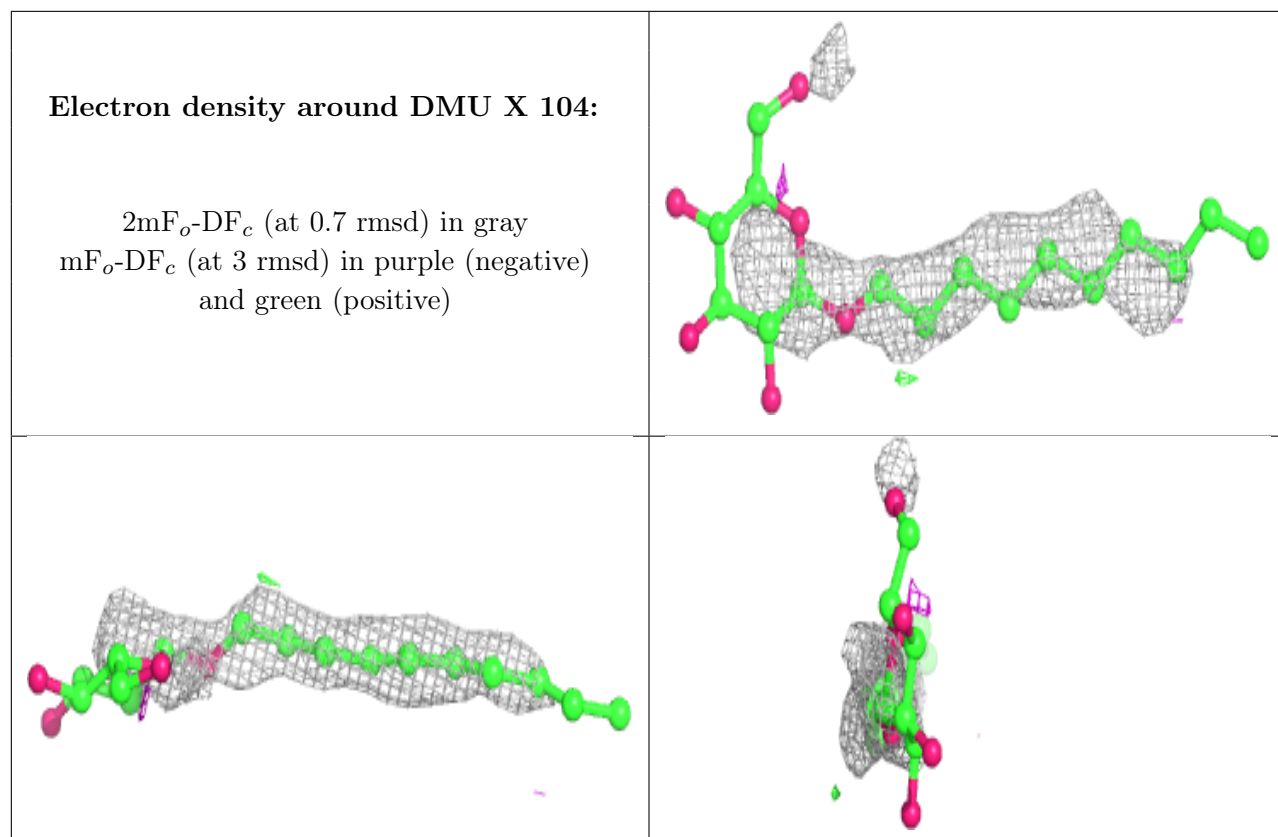
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
19	PGV	P	305	51/51	0.97	0.14	22,31,87,120	0
25	CHD	B	302	29/29	0.97	0.09	21,27,36,50	0
22	EDO	D	202	4/4	0.97	0.15	43,43,57,86	0
29	PO4	H	101	5/5	0.97	0.22	62,62,77,101	0
22	EDO	F	106	4/4	0.97	0.11	30,31,32,32	0
14	HEA	A	602	60/60	0.98	0.10	16,21,30,37	0
22	EDO	E	201	4/4	0.98	0.13	38,39,40,40	0
22	EDO	E	202	4/4	0.98	0.11	37,37,41,43	0
14	HEA	N	602[A]	60/60	0.98	0.12	18,24,38,44	18
14	HEA	N	602[B]	54/60	0.98	0.12	15,24,33,40	12
22	EDO	S	102	4/4	0.98	0.12	20,22,22,24	0
14	HEA	N	602[C]	51/60	0.98	0.12	16,24,28,33	9
22	EDO	N	617	4/4	0.98	0.12	20,26,28,31	0
22	EDO	N	618	4/4	0.98	0.16	29,42,46,46	0
22	EDO	A	619	4/4	0.98	0.12	28,42,71,95	0
22	EDO	S	107	4/4	0.98	0.18	28,45,48,62	0
14	HEA	N	603	60/60	0.98	0.10	18,23,28,37	0
14	HEA	A	601[A]	60/60	0.98	0.13	17,21,40,61	18
14	HEA	A	601[B]	54/60	0.98	0.13	9,20,29,45	12
22	EDO	O	303	4/4	0.98	0.11	25,29,30,31	0
22	EDO	B	303	4/4	0.98	0.09	21,25,26,32	0
17	NA	N	606	1/1	0.98	0.07	30,30,30,30	0
19	PGV	C	306	48/51	0.98	0.13	21,28,66,92	0
22	EDO	A	613	4/4	0.98	0.14	21,24,30,30	0
14	HEA	A	601[C]	51/60	0.98	0.13	9,20,24,40	9
16	MG	N	605	1/1	0.99	0.05	21,21,21,21	0
28	ZN	S	101	1/1	0.99	0.11	25,25,25,25	0
17	NA	A	605	1/1	0.99	0.08	24,24,24,24	0
22	EDO	F	104	4/4	0.99	0.13	22,24,25,27	0
15	CU	A	603	1/1	1.00	0.15	23,23,23,23	0
28	ZN	F	101	1/1	1.00	0.11	26,26,26,26	0
24	CUA	B	301	2/2	1.00	0.13	22,22,22,23	0
24	CUA	O	301	2/2	1.00	0.12	26,26,26,26	0
15	CU	N	604	1/1	1.00	0.14	24,24,24,24	0

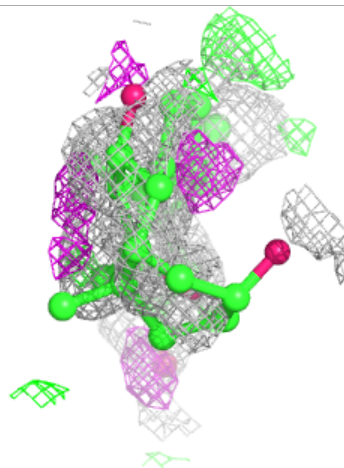
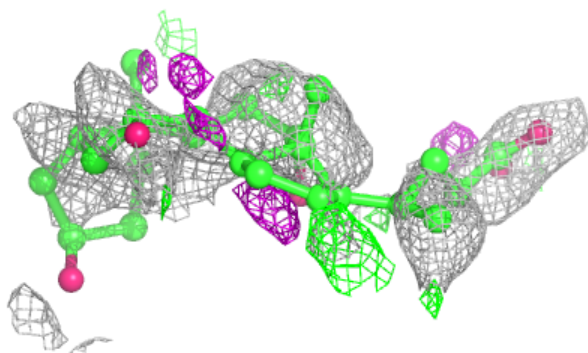
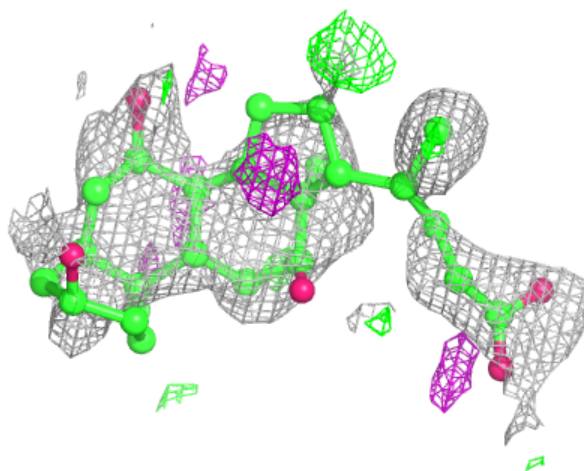
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





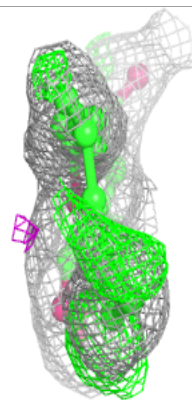
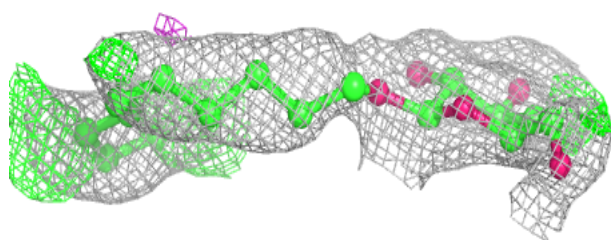
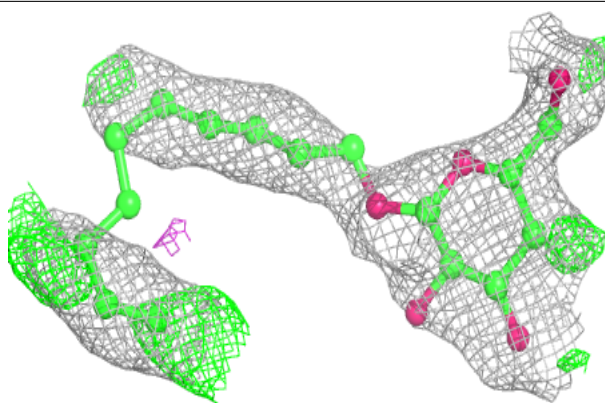
**Electron density around CHD J 101:**

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

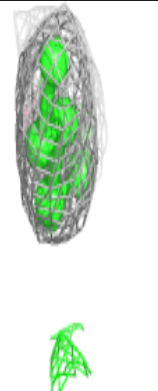
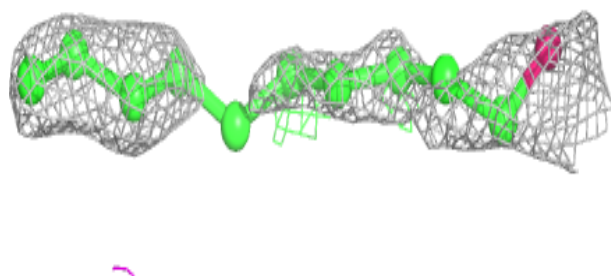
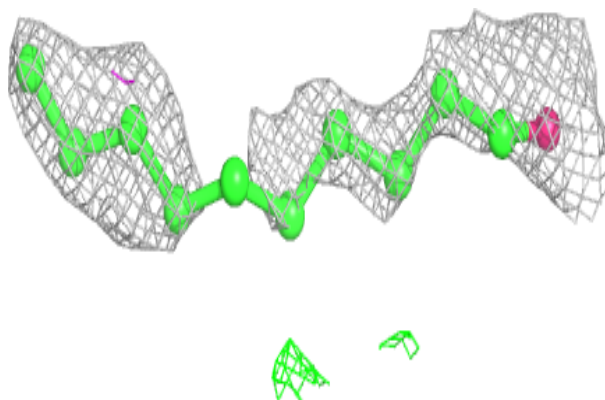


**Electron density around DMU L 105:**

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

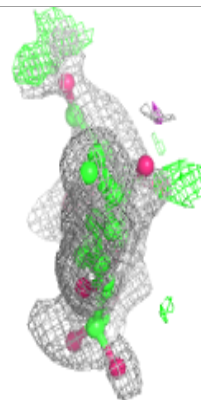
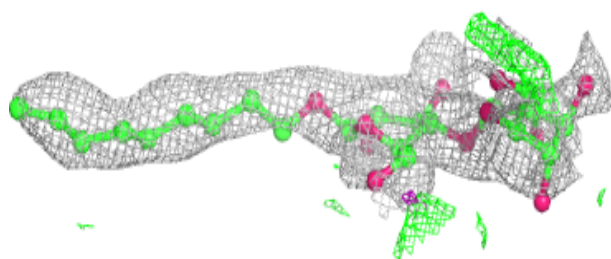
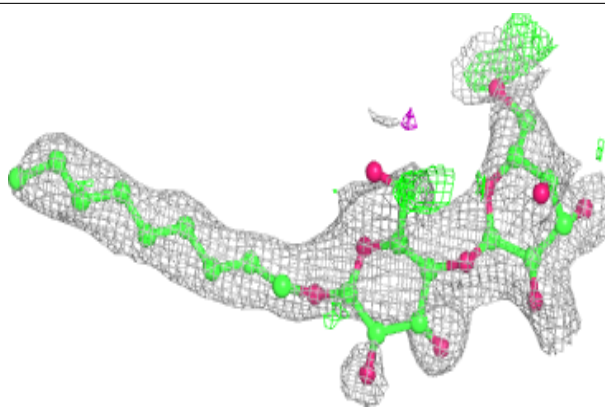
**Electron density around DMU D 207:**

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

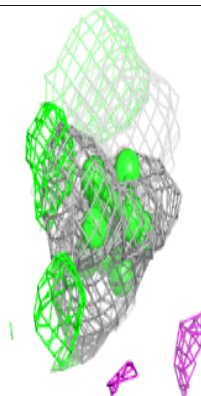
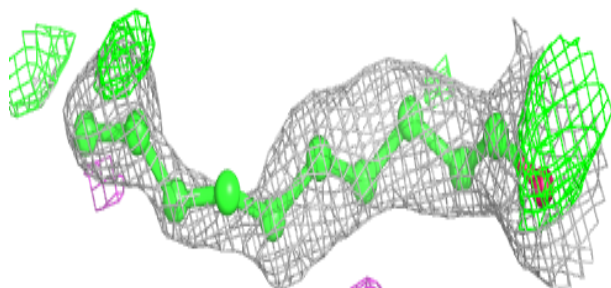
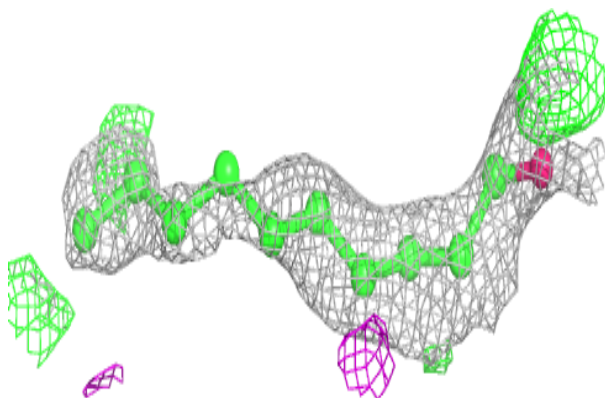


**Electron density around DMU P 317:**

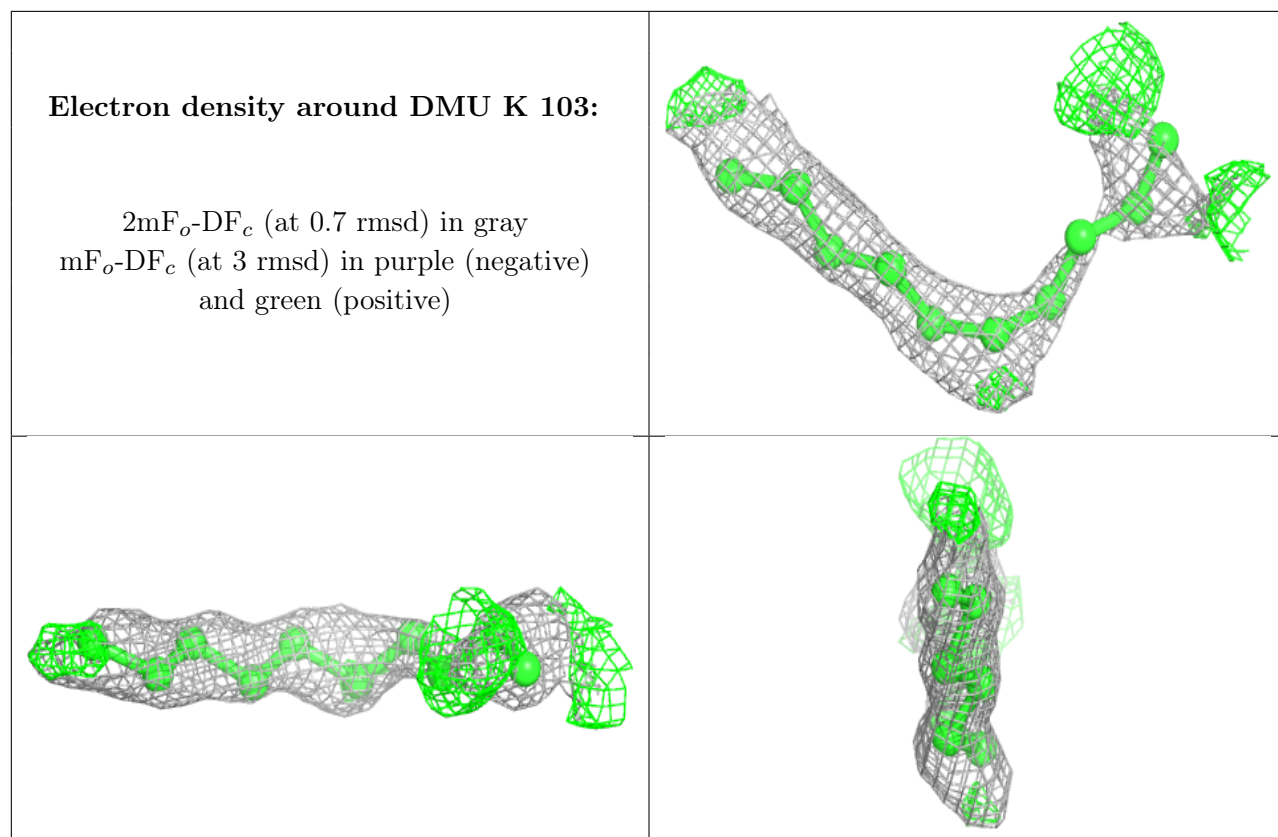
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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)

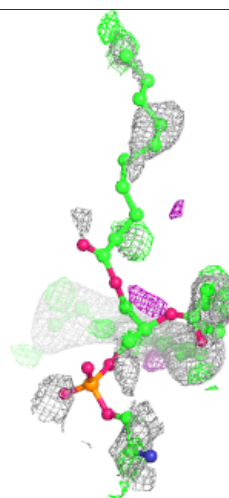
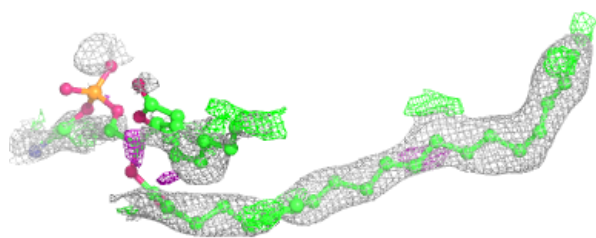
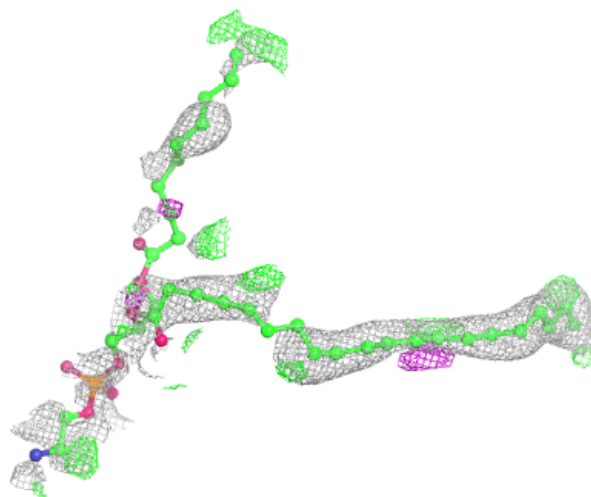






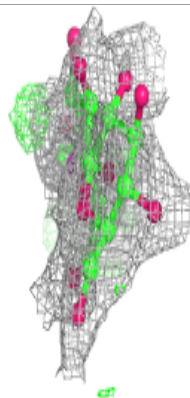
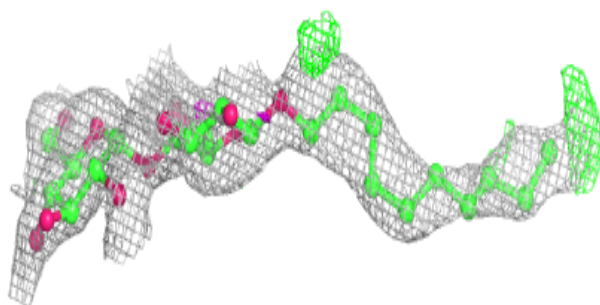
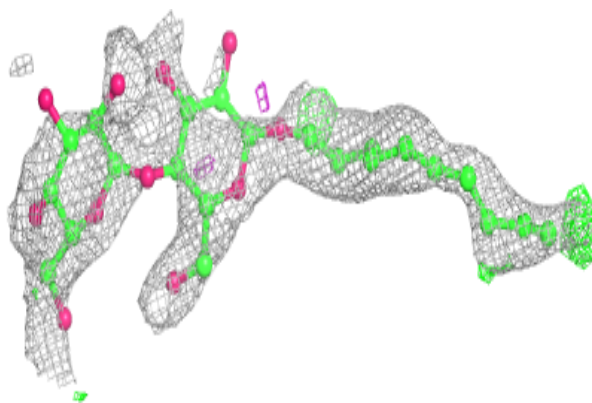
**Electron density around PEK C 303:**

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

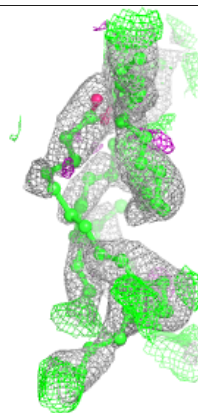
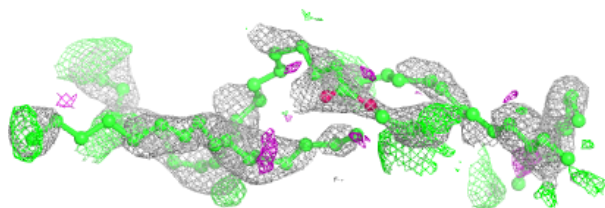
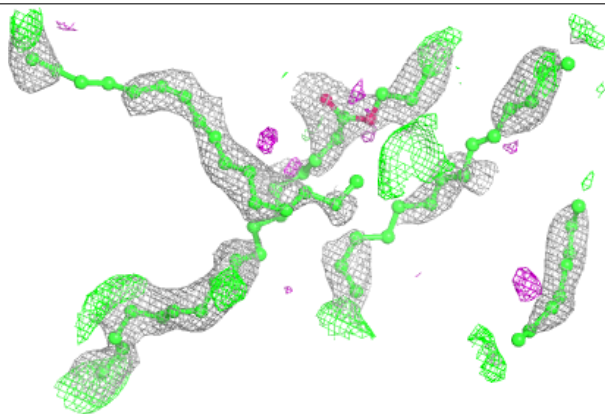


**Electron density around DMU D 206:**

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

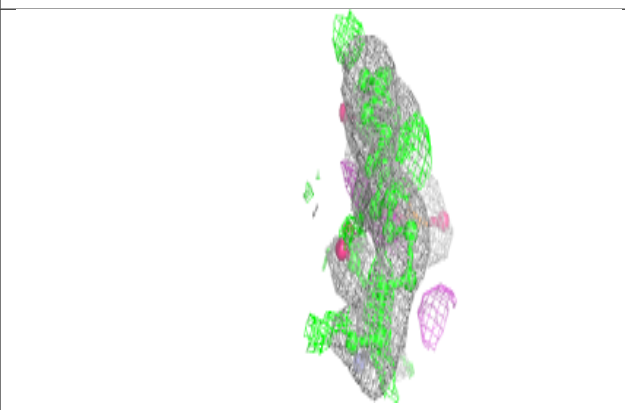
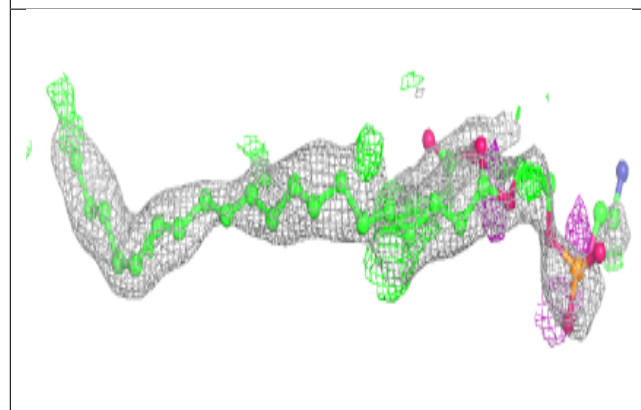
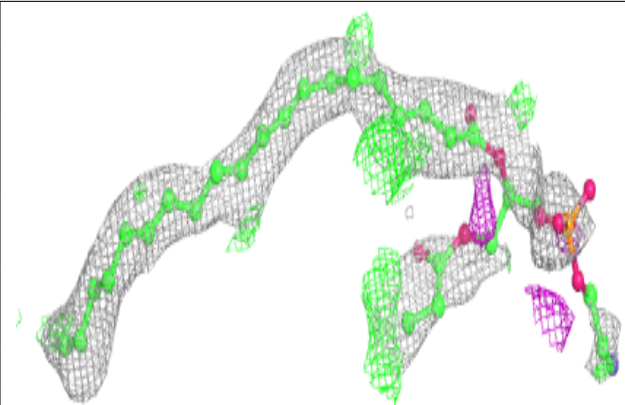
**Electron density around CDL T 102:**

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

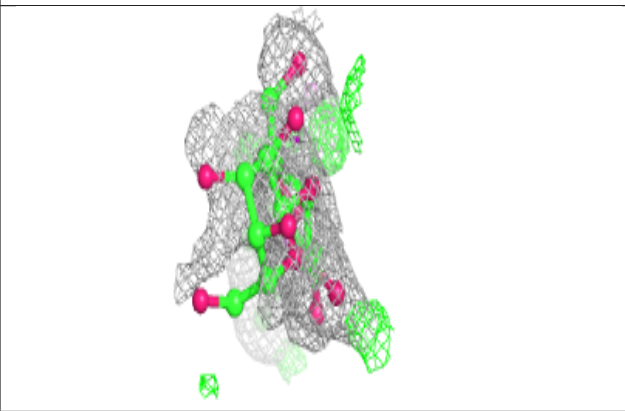
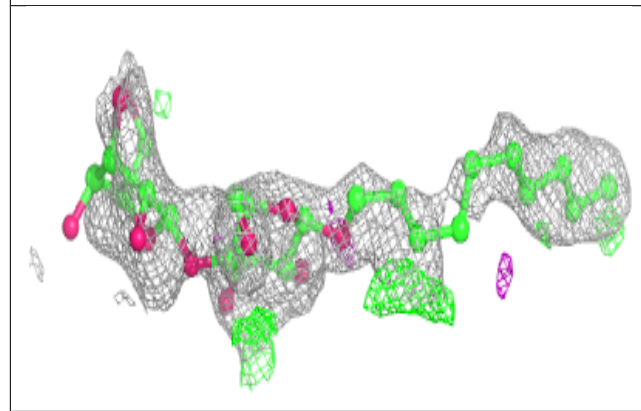
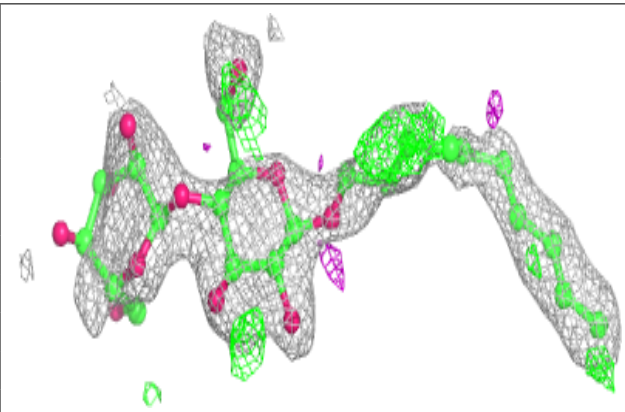


**Electron density around PEK P 303:**

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

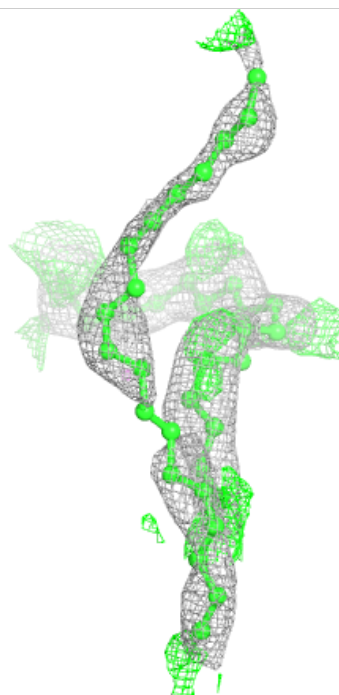
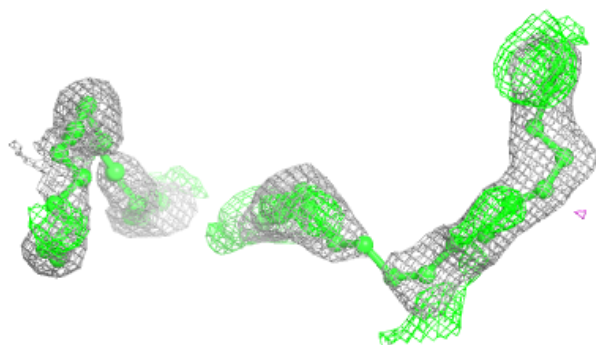
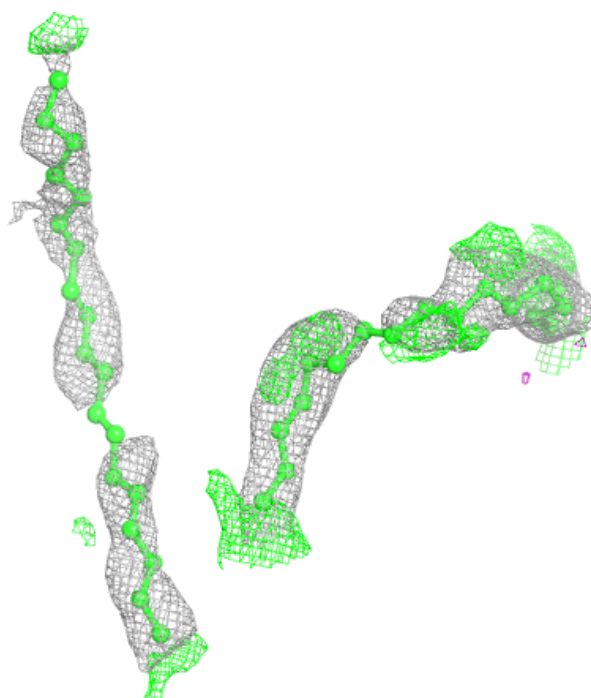
**Electron density around DMU P 308:**

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



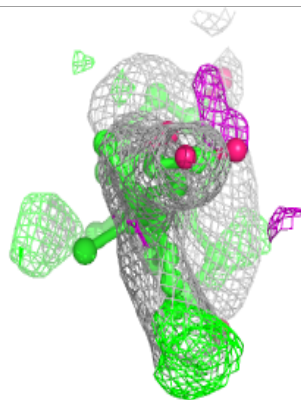
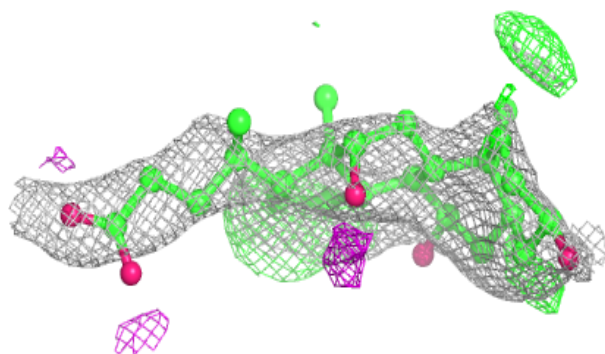
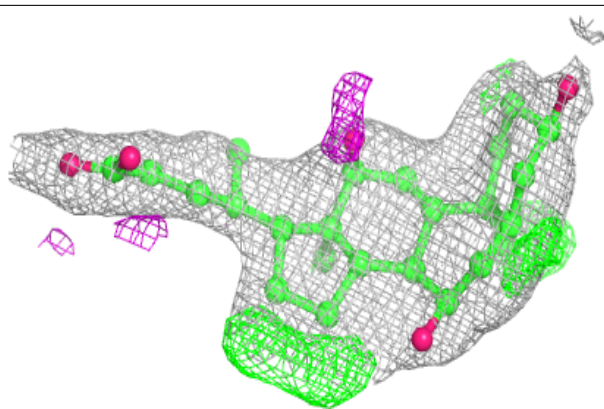
**Electron density around PEK C 305:**

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

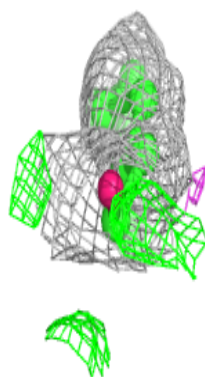
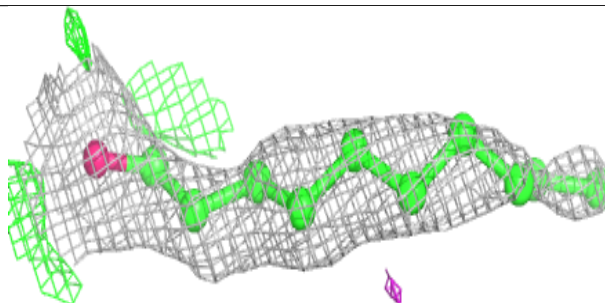
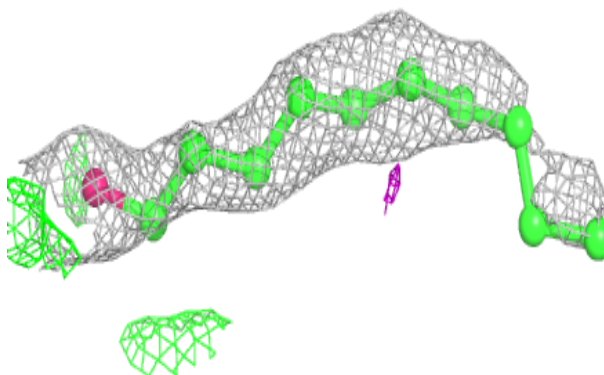


**Electron density around CHD Y 102:**

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

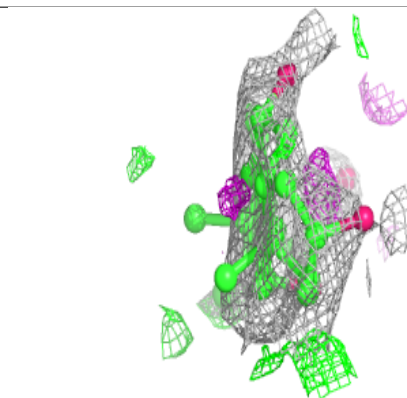
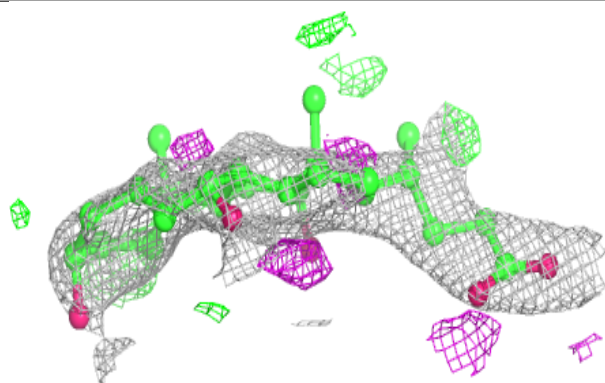
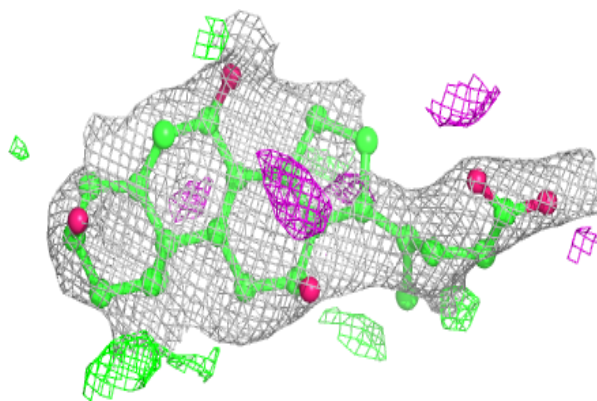
**Electron density around DMU K 102:**

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

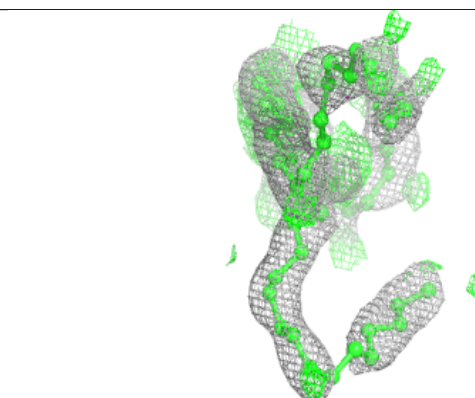
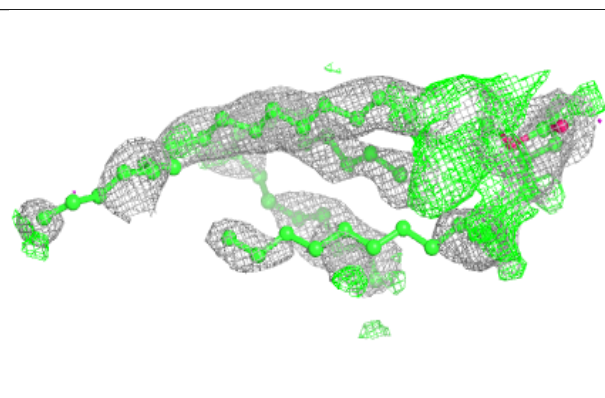
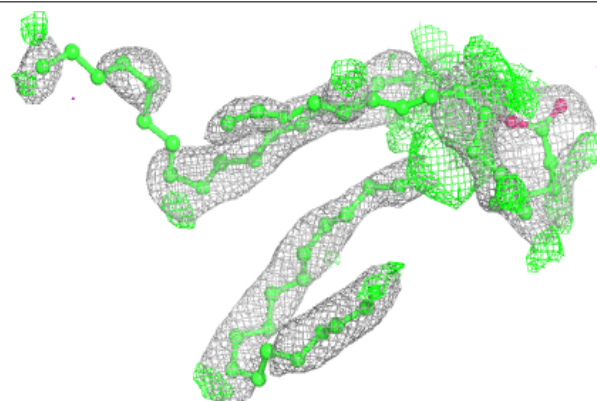


**Electron density around CHD L 102:**

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

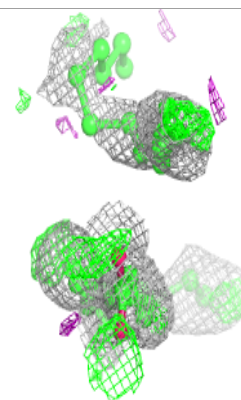
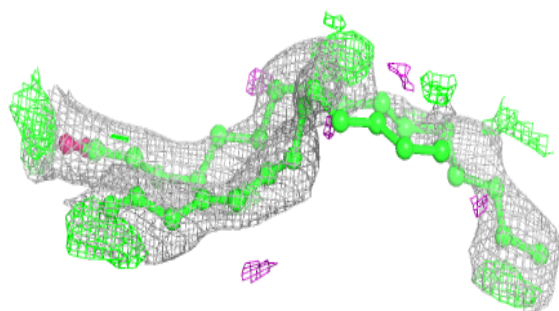
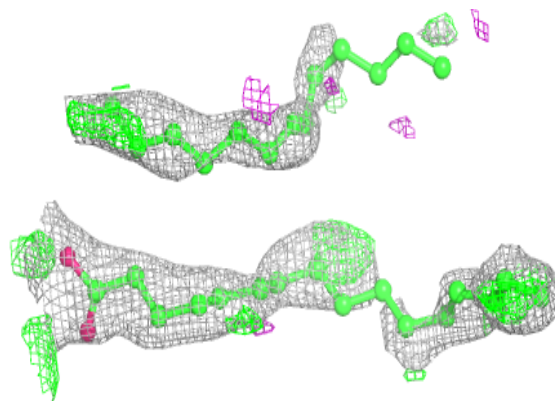
**Electron density around TGL N 609:**

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

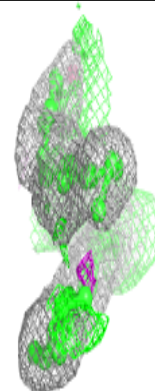
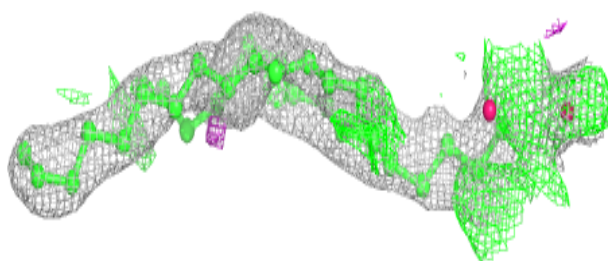
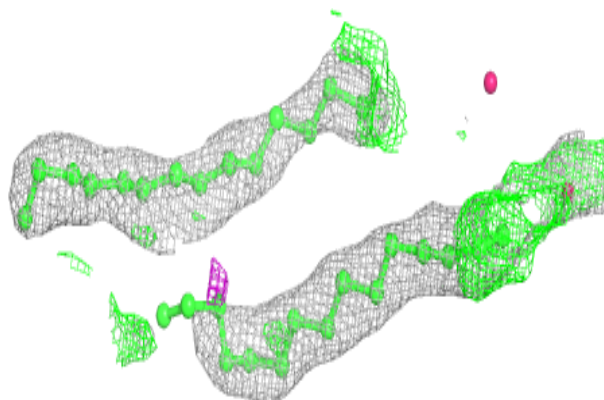


**Electron density around PGV P 306:**

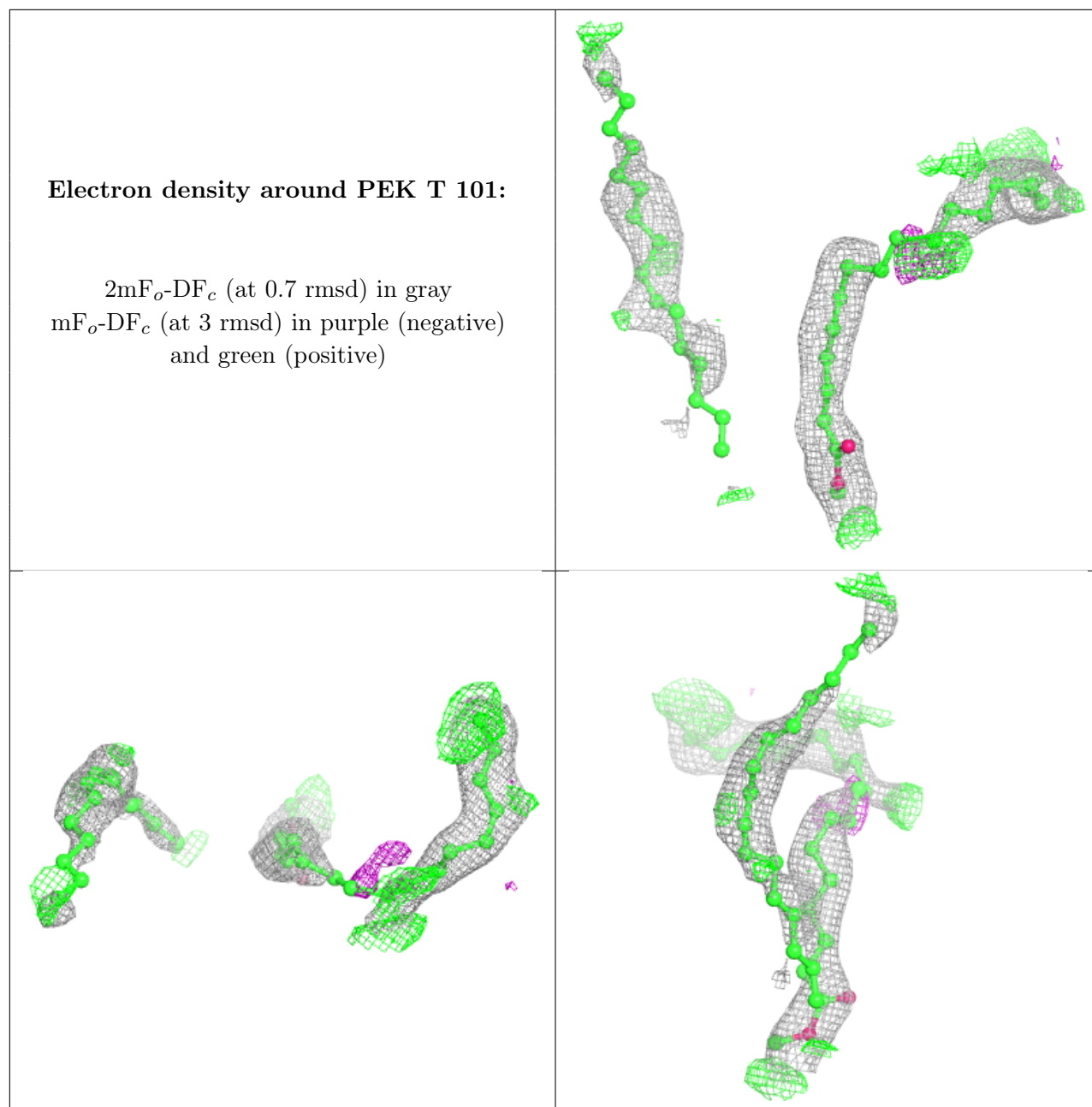
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PSC 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)

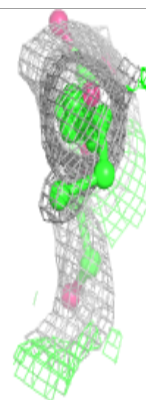
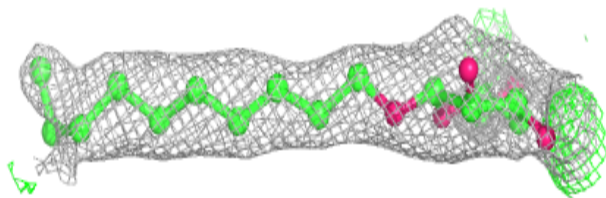
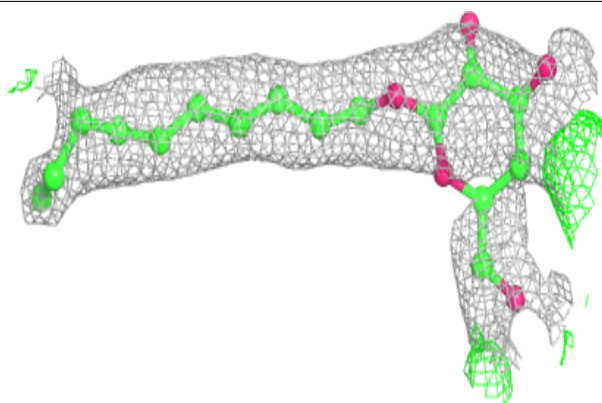




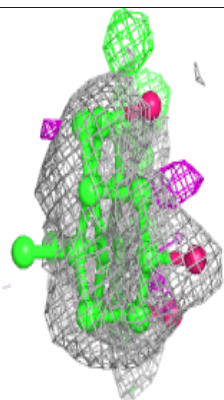
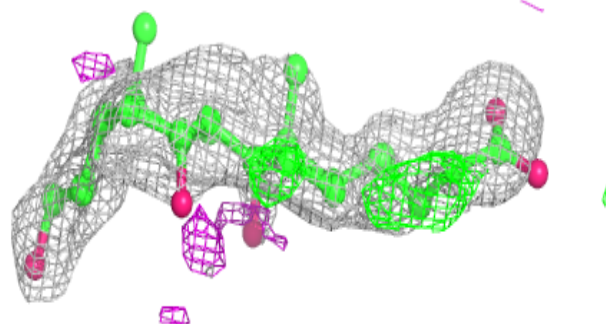
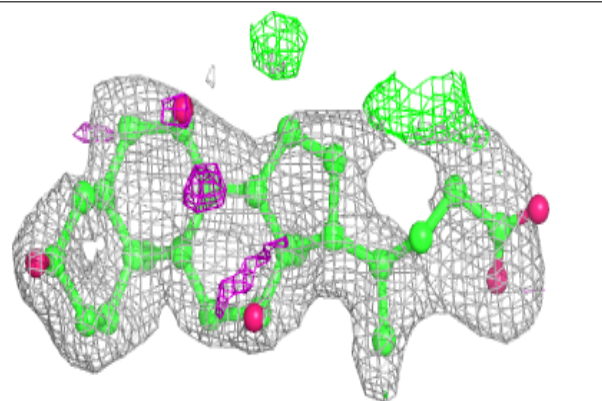


**Electron density around DMU P 316:**

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

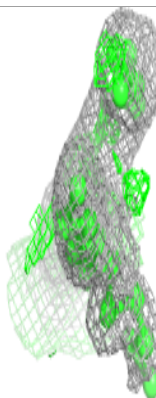
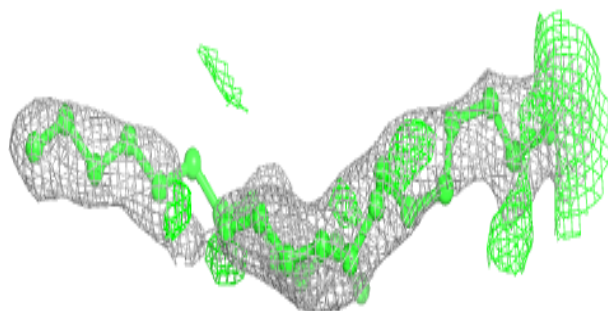
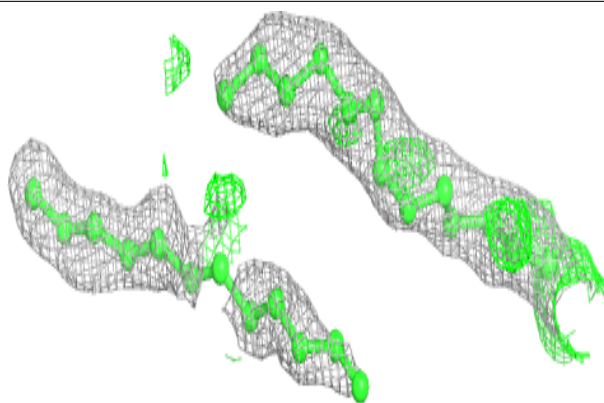
**Electron density around CHD C 309:**

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

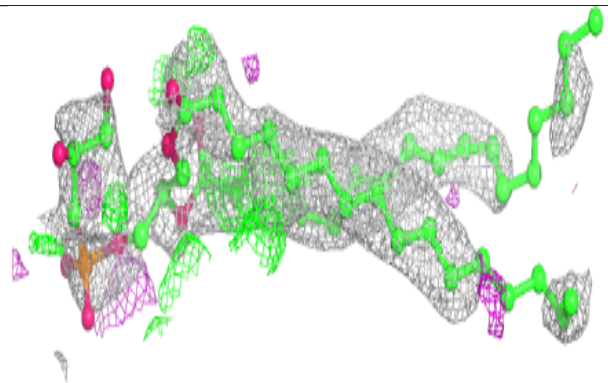
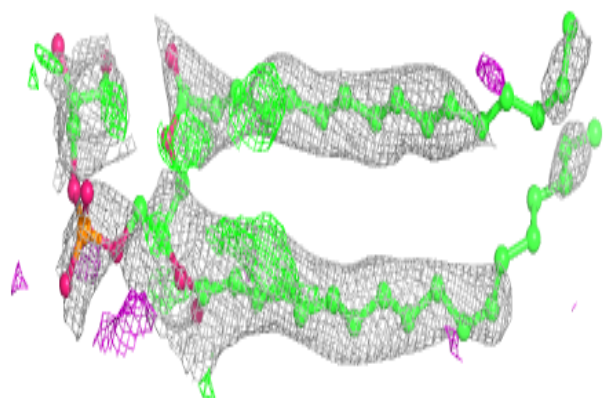


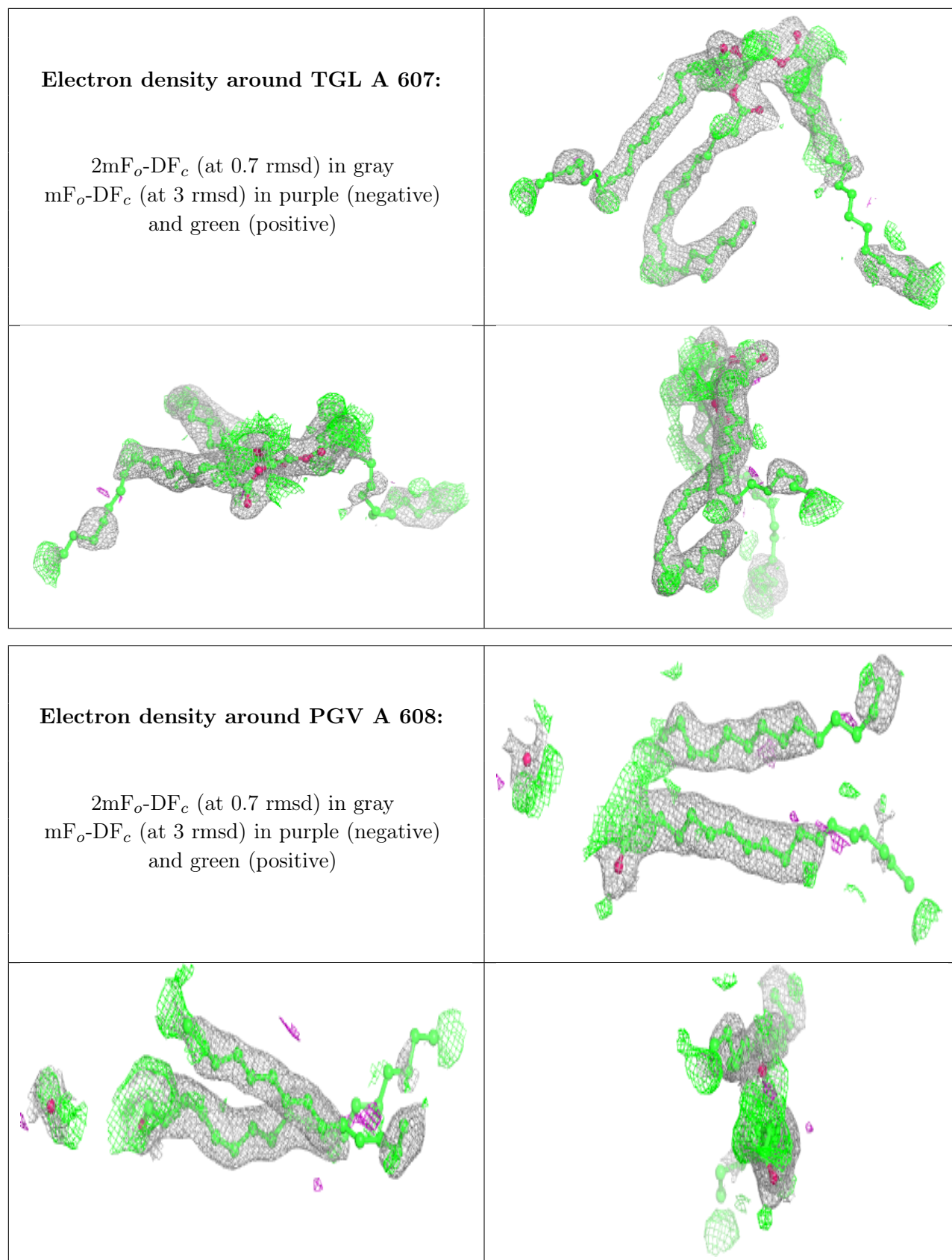
**Electron density around PSC A 610:**

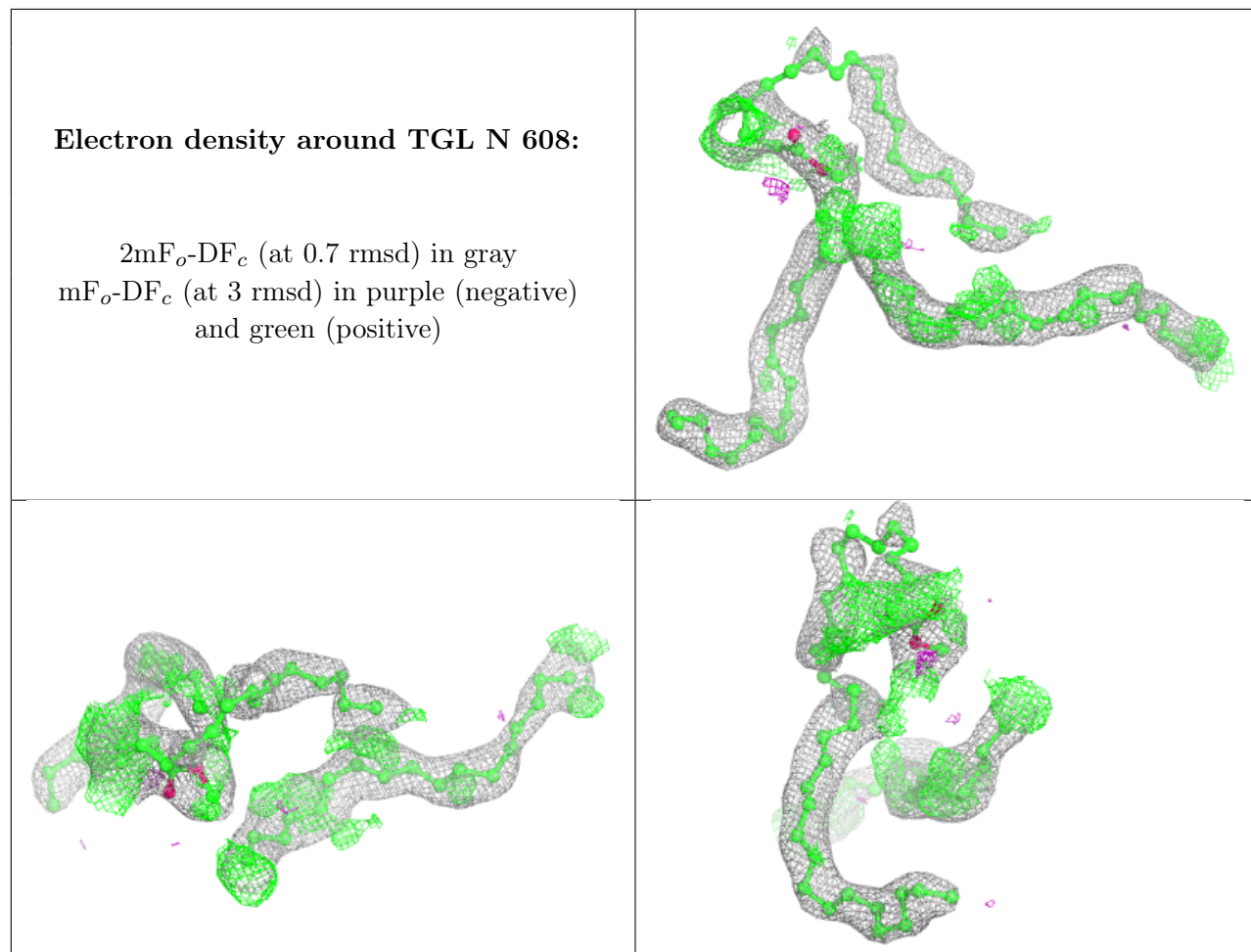
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PGV N 610:**

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

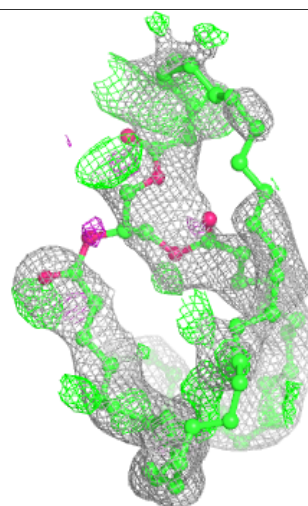
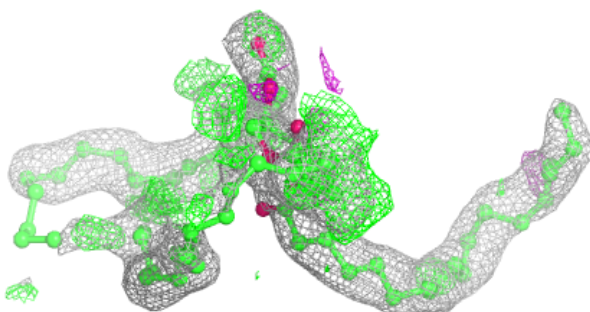
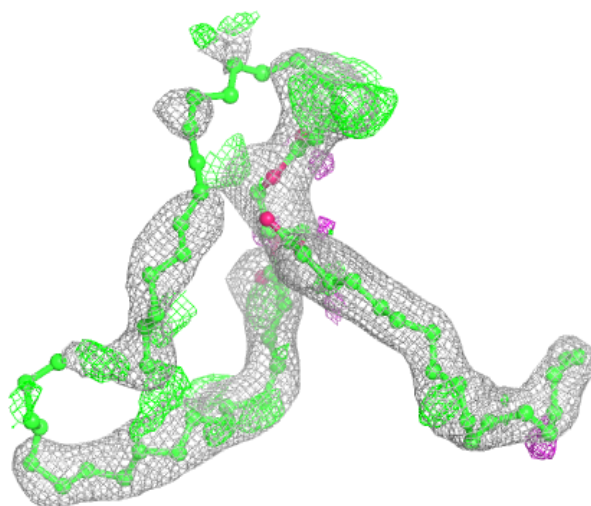


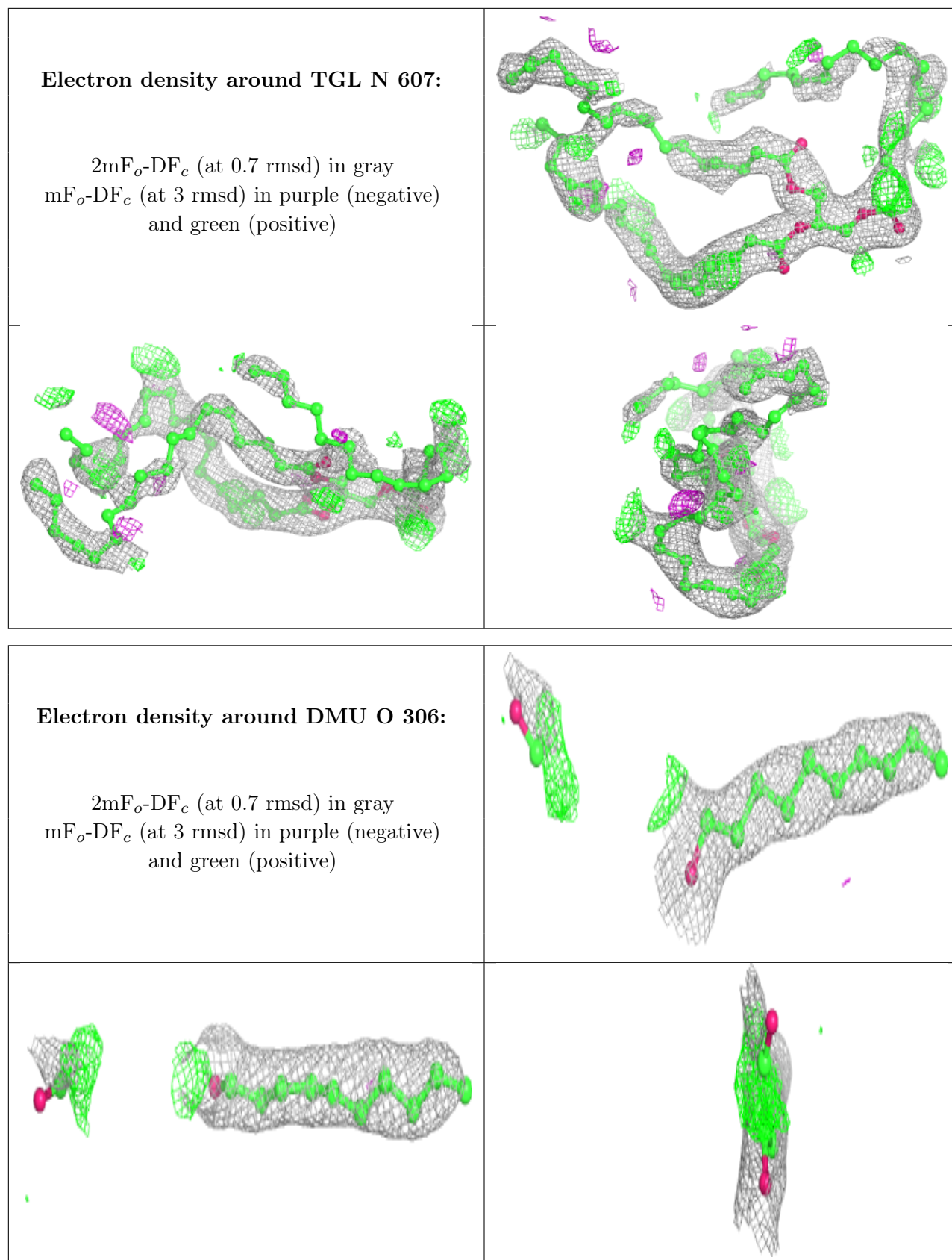




**Electron density around TGL L 101:**

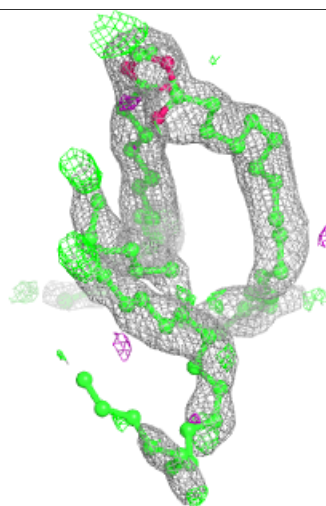
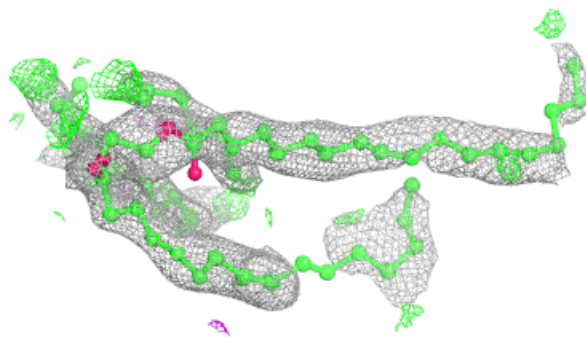
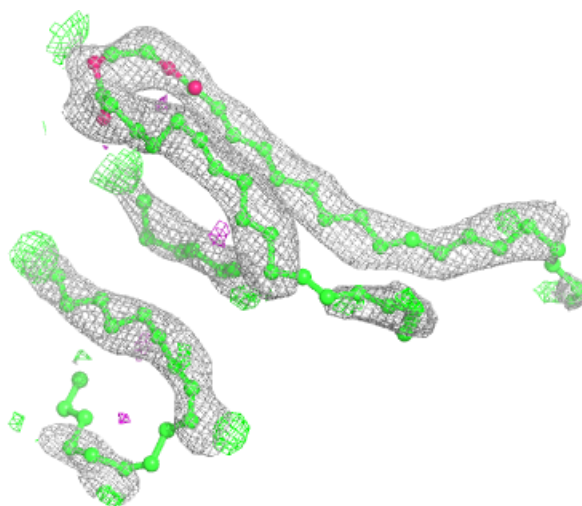
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CDL C 308:**

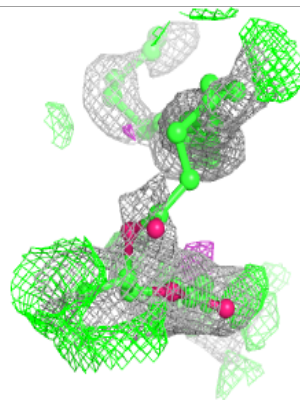
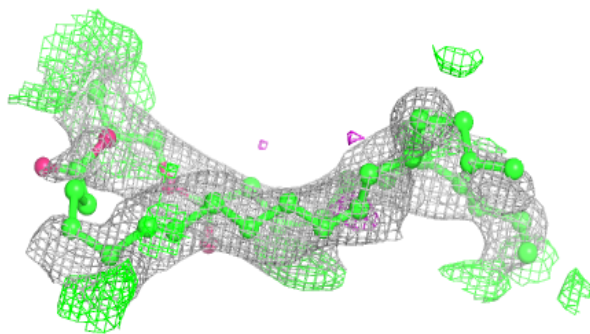
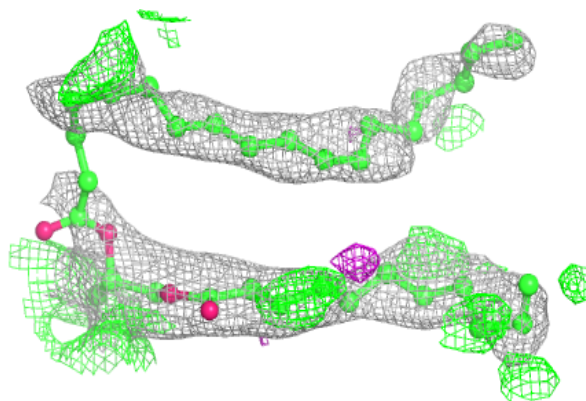
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



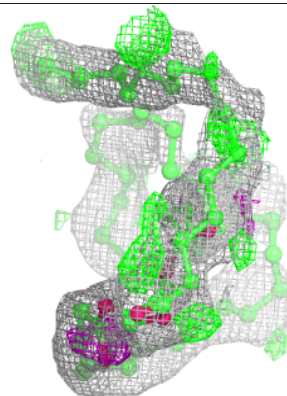
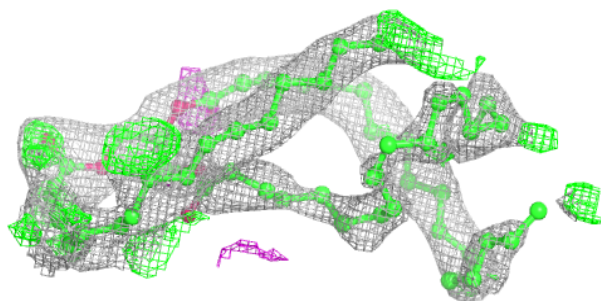
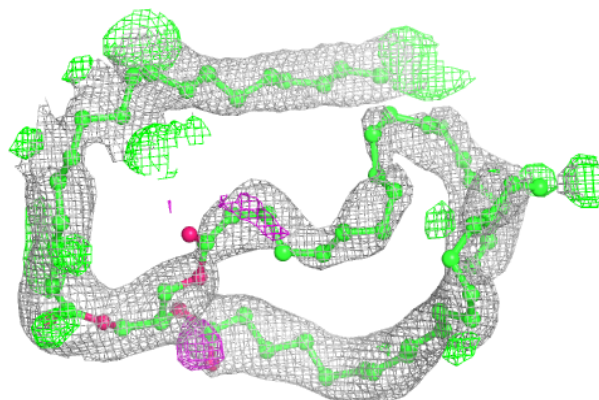


**Electron density around PGV C 307:**

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

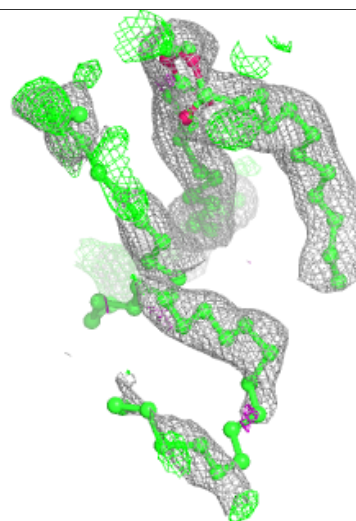
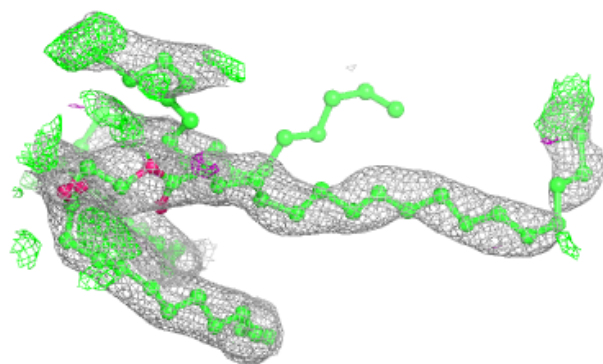
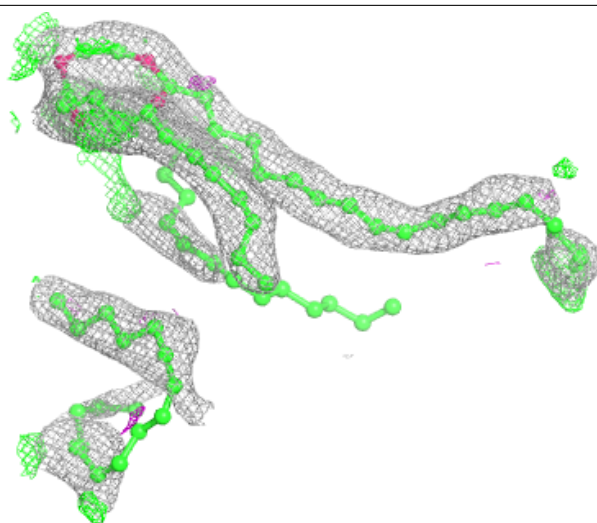
**Electron density around TGL A 606:**

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



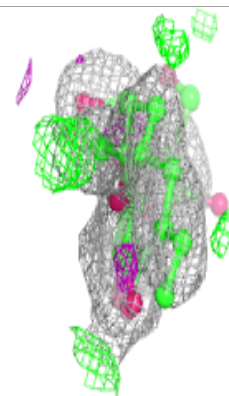
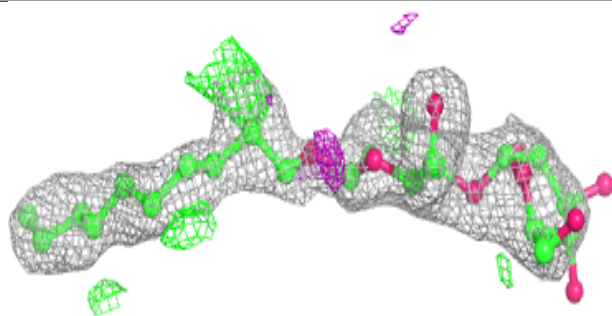
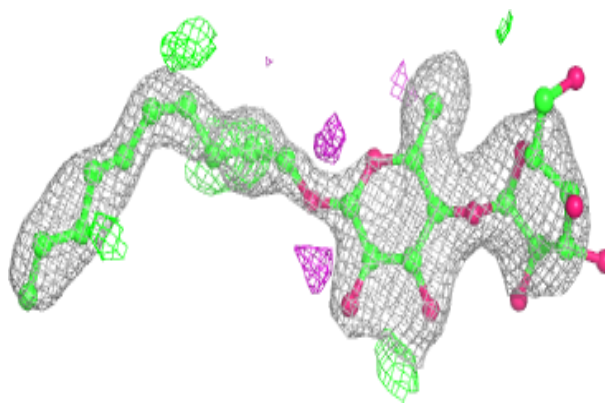
**Electron density around CDL P 307:**

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

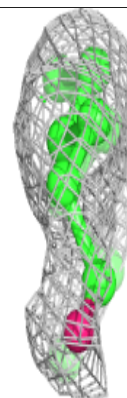
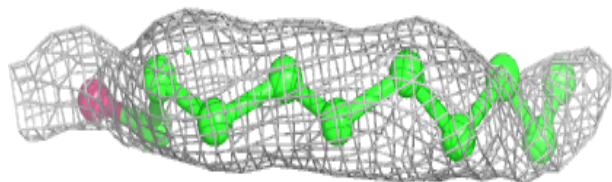
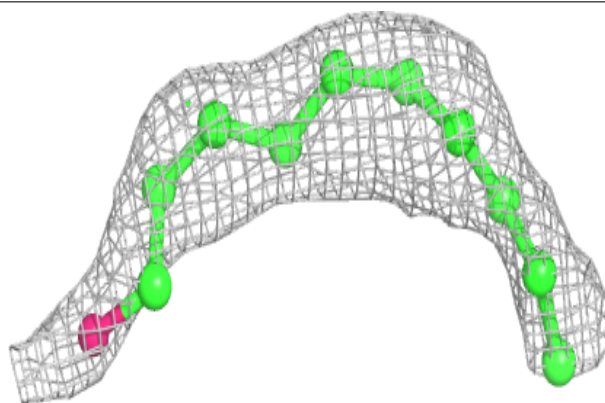


**Electron density around DMU C 310:**

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

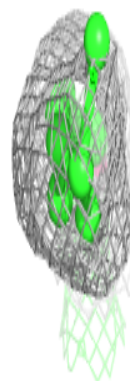
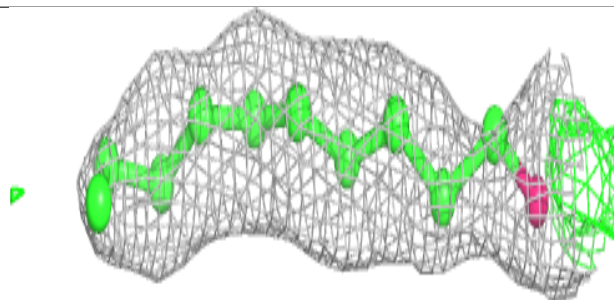
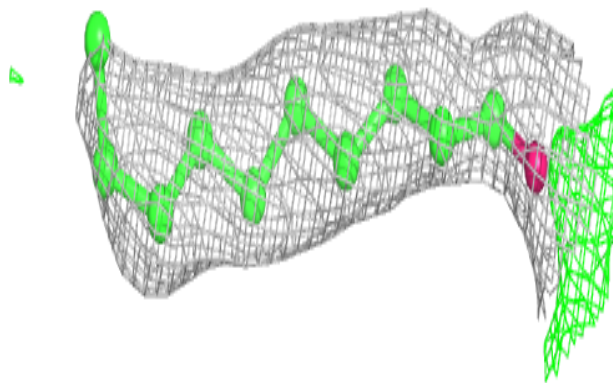
**Electron density around DMU K 104:**

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

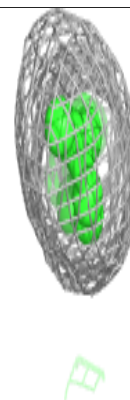
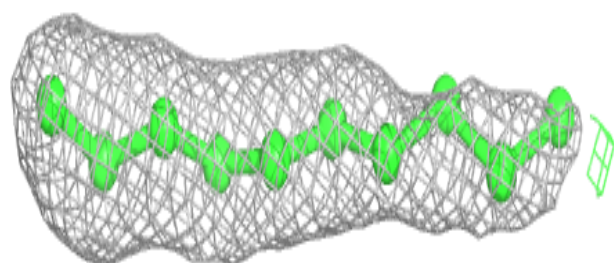
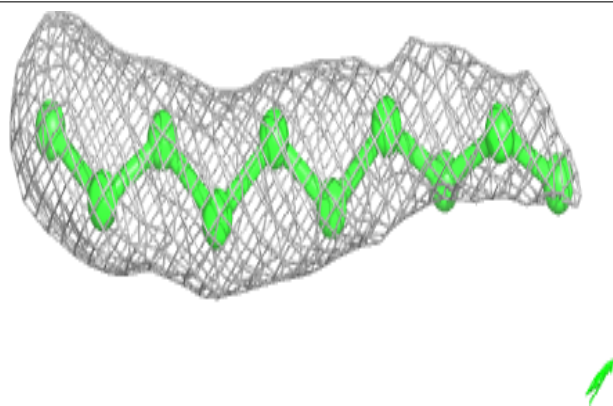


**Electron density around DMU J 104:**

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

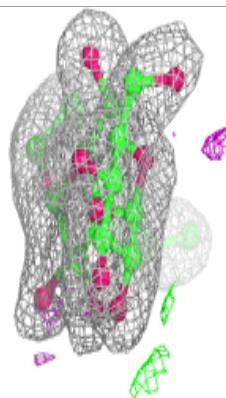
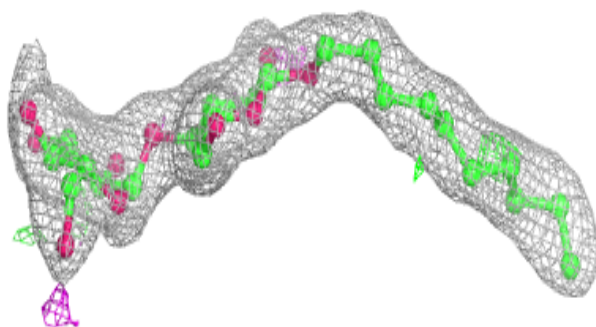
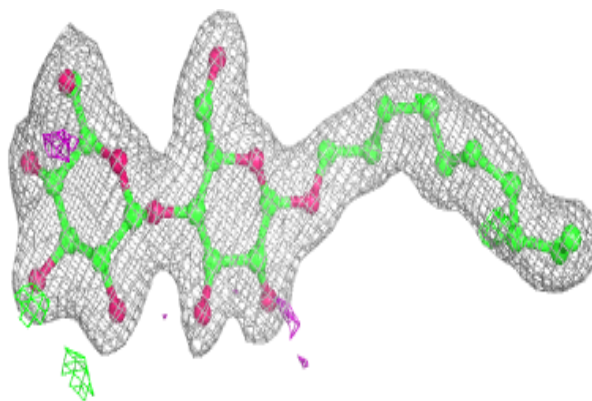
**Electron density around DMU X 101:**

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

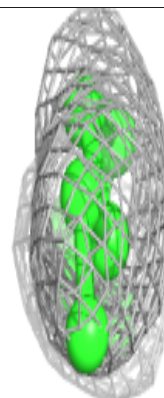
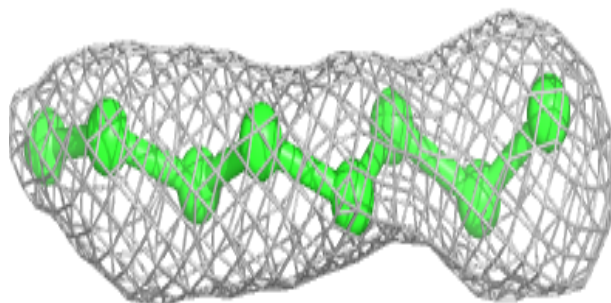
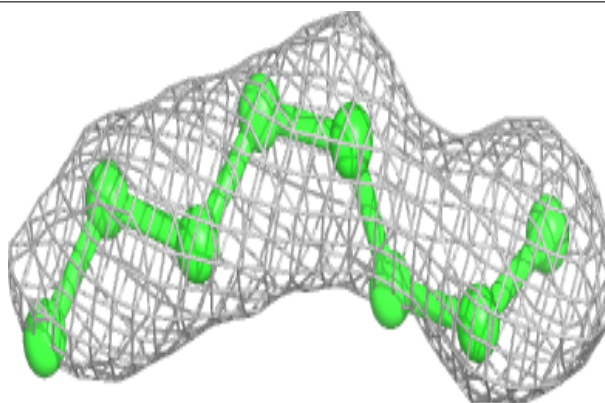


**Electron density around DMU Z 101:**

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

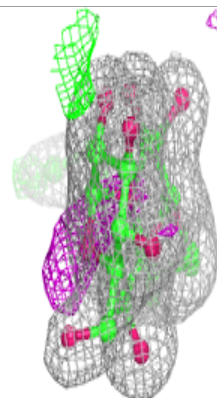
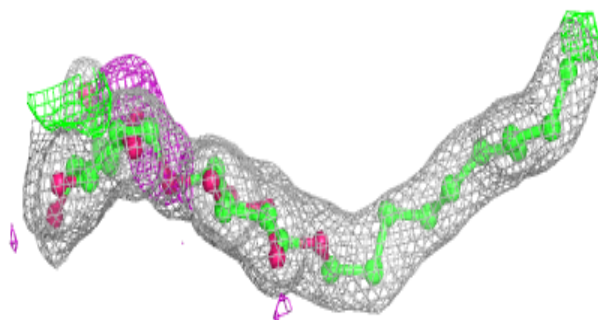
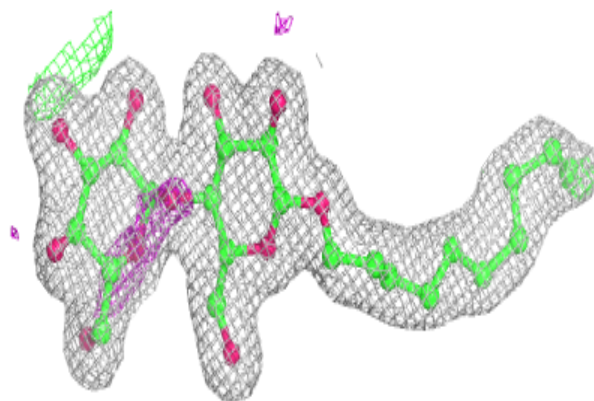
**Electron density around DMU K 101:**

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

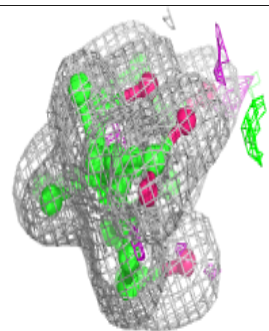
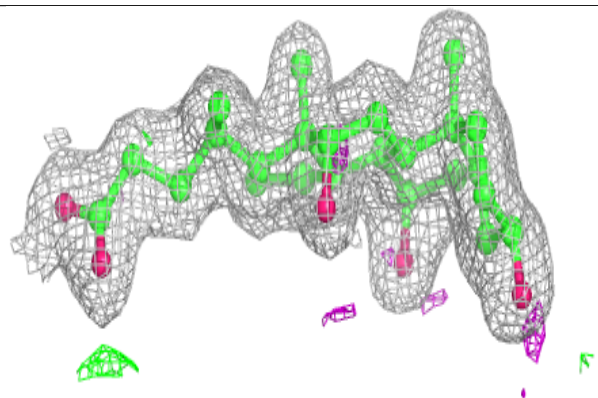
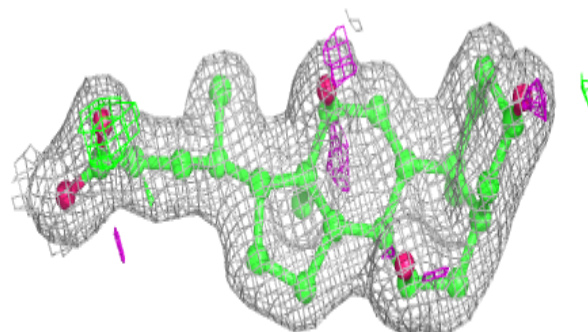


**Electron density around DMU M 101:**

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

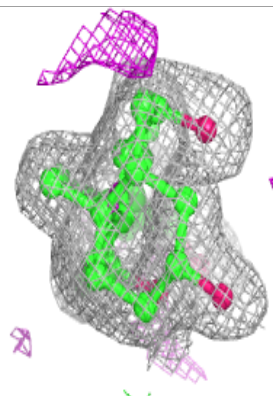
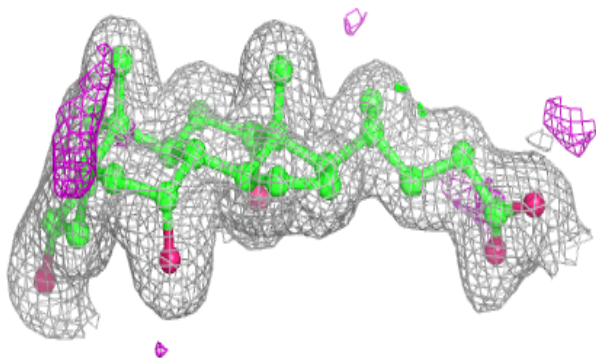
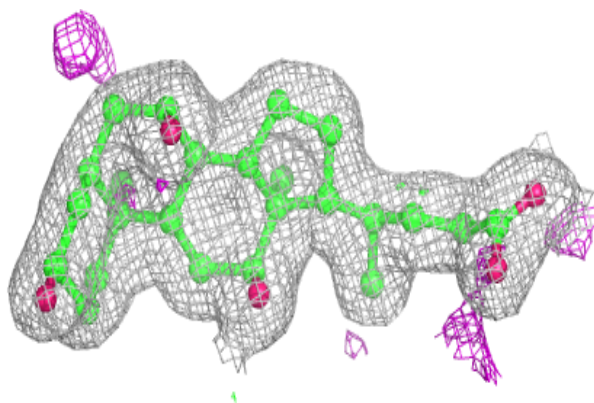
**Electron density around CHD C 301:**

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

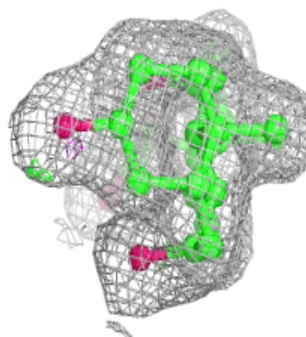
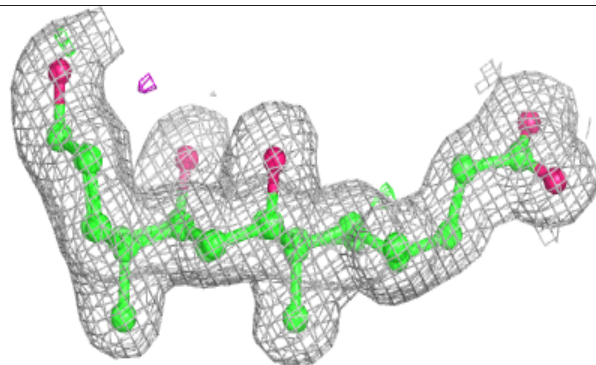
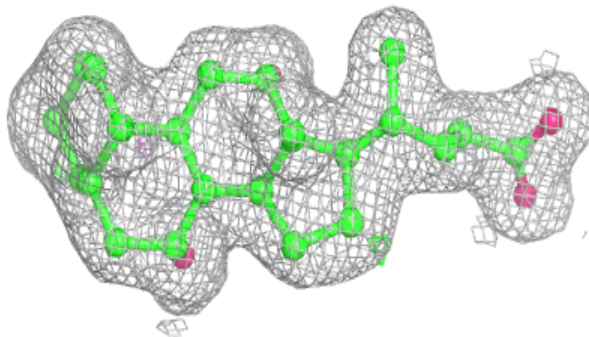


**Electron density around CHD P 301:**

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

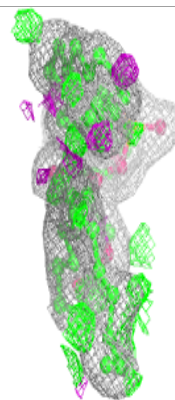
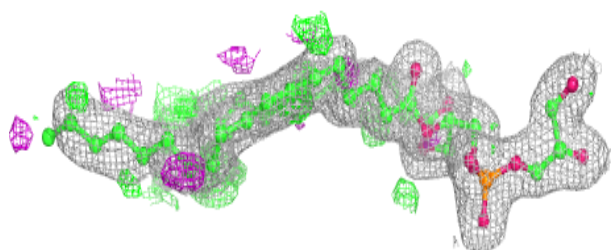
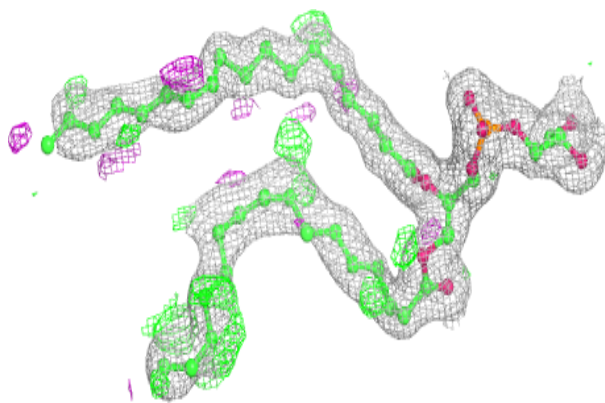
**Electron density around CHD G 101:**

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

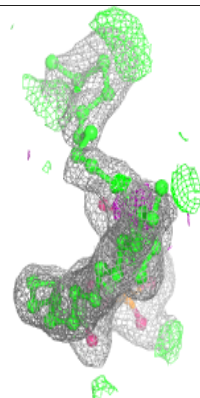
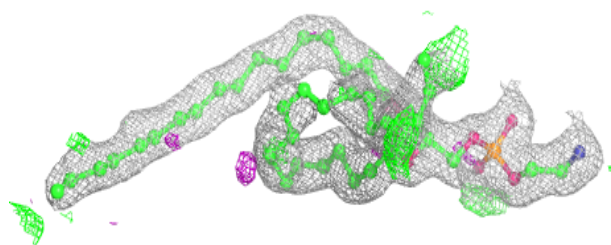
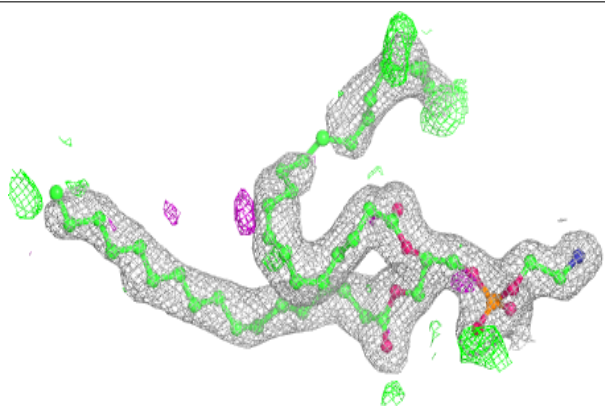


**Electron density around PGV N 612:**

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

**Electron density around PEK P 304:**

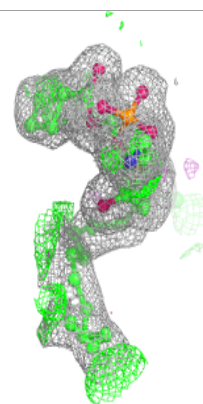
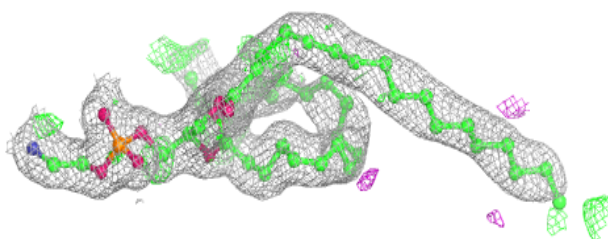
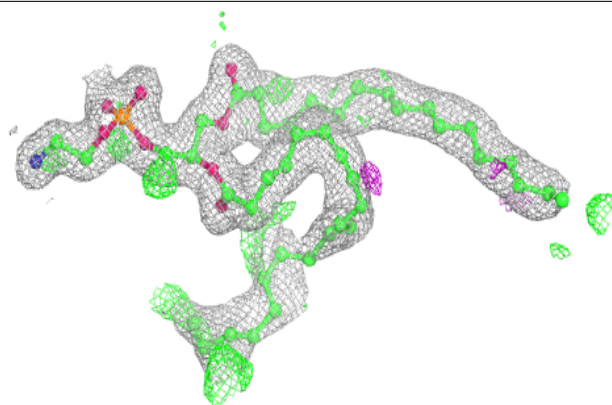
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



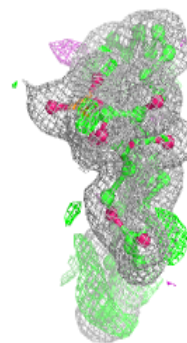
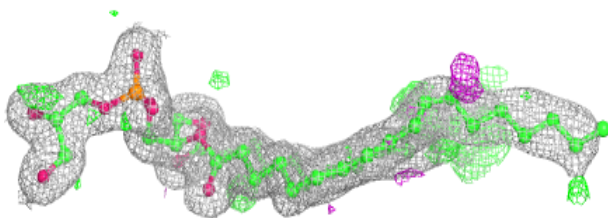
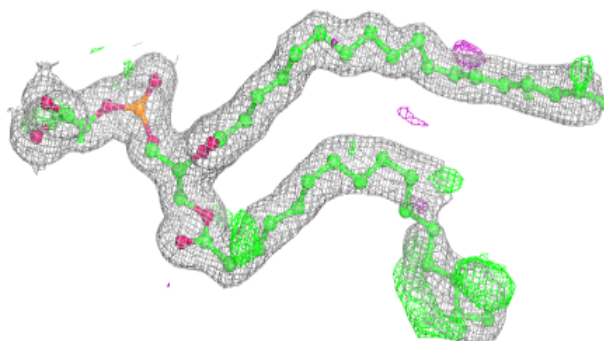


**Electron density around PEK C 304:**

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

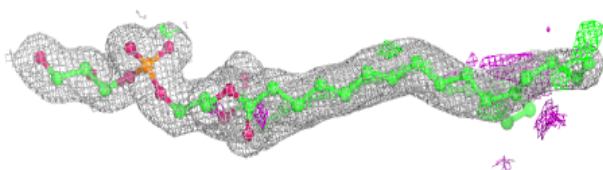
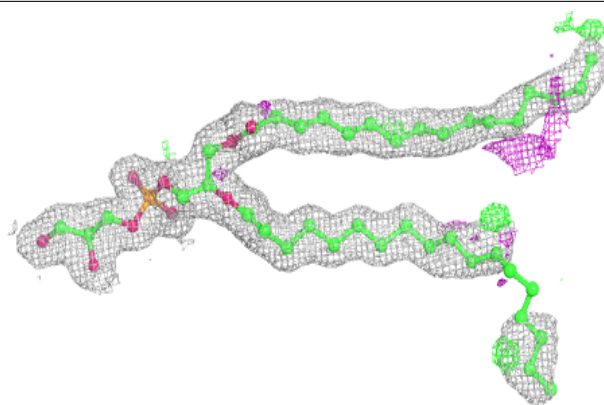
**Electron density around PGV A 611:**

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

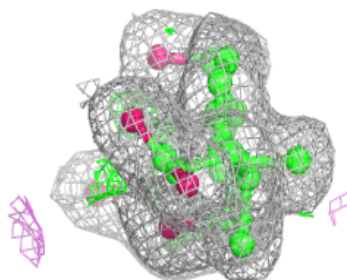
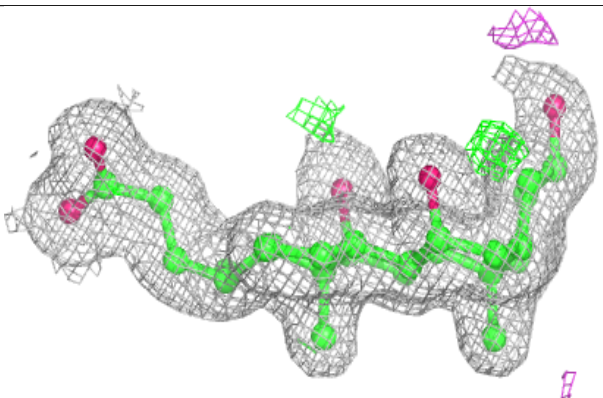
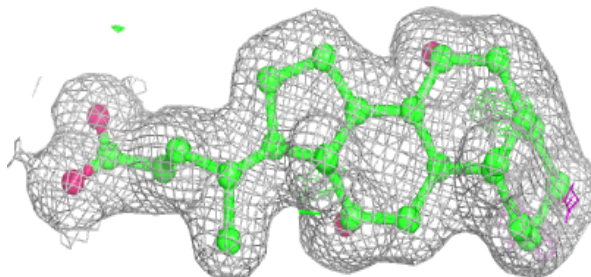


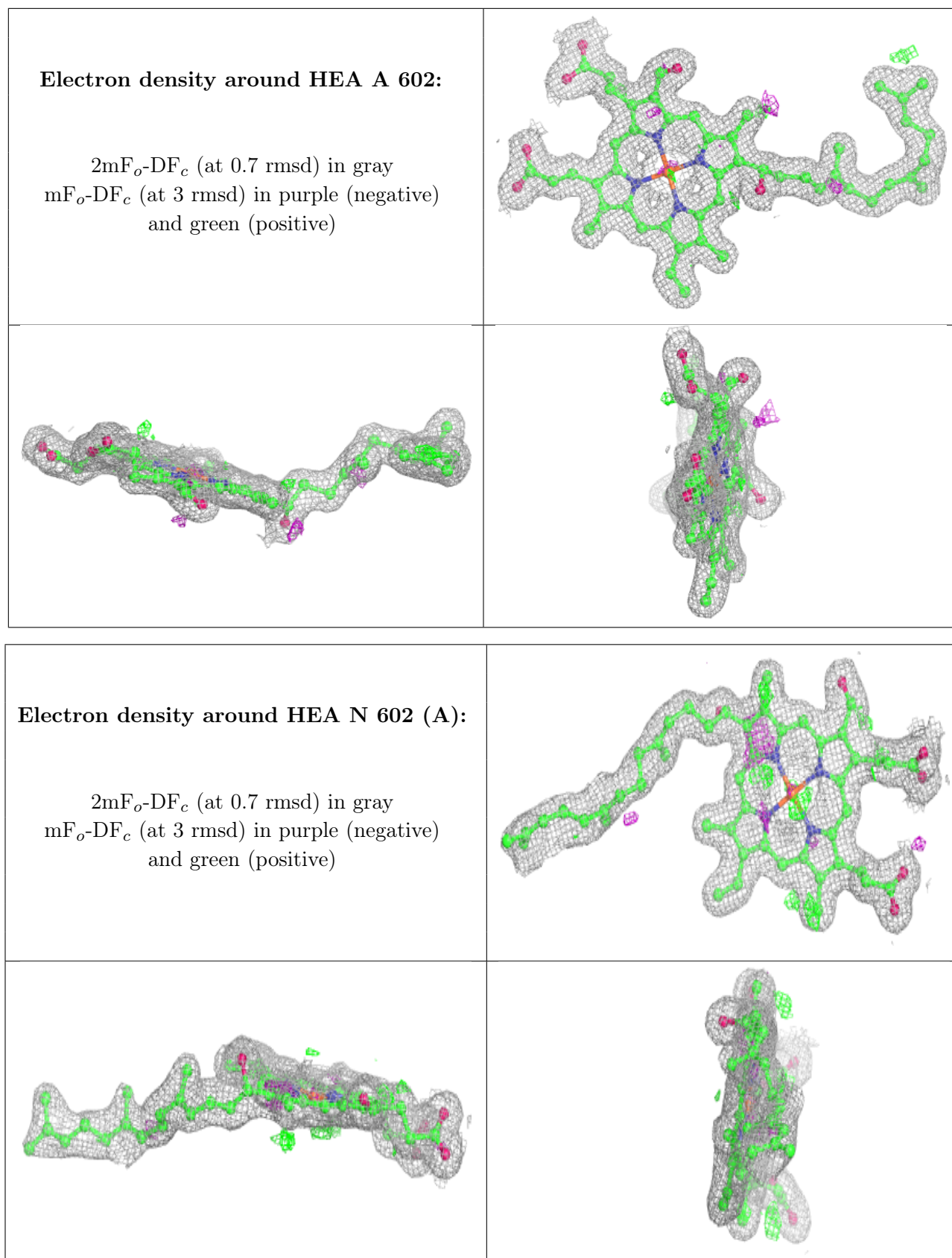
**Electron density around PGV P 305:**

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

**Electron density around CHD B 302:**

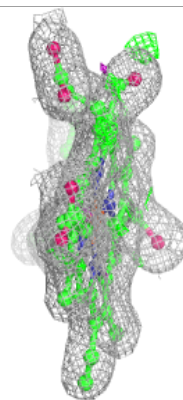
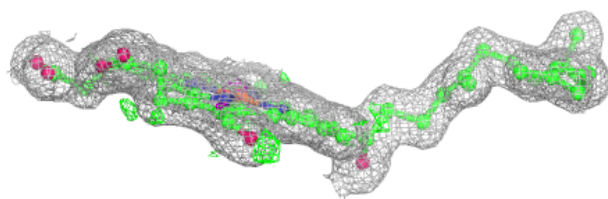
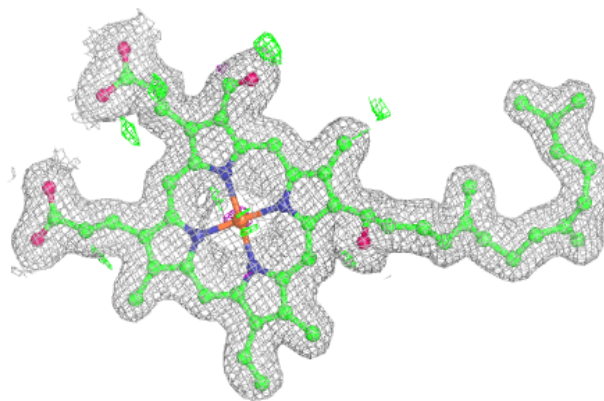
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



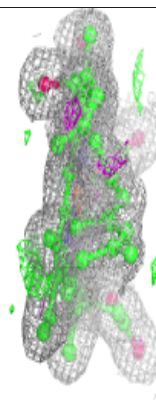
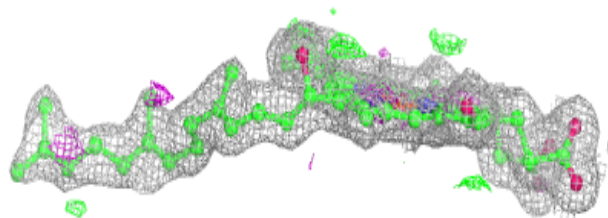
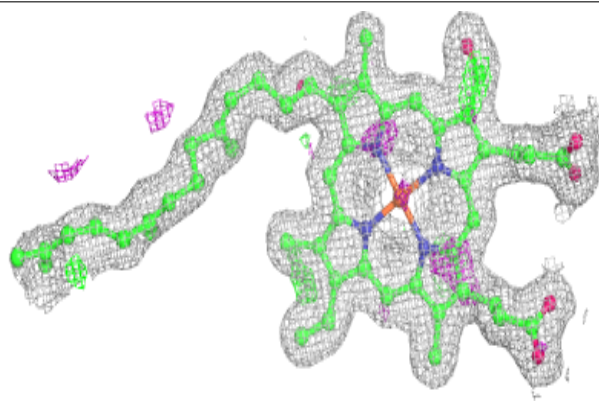


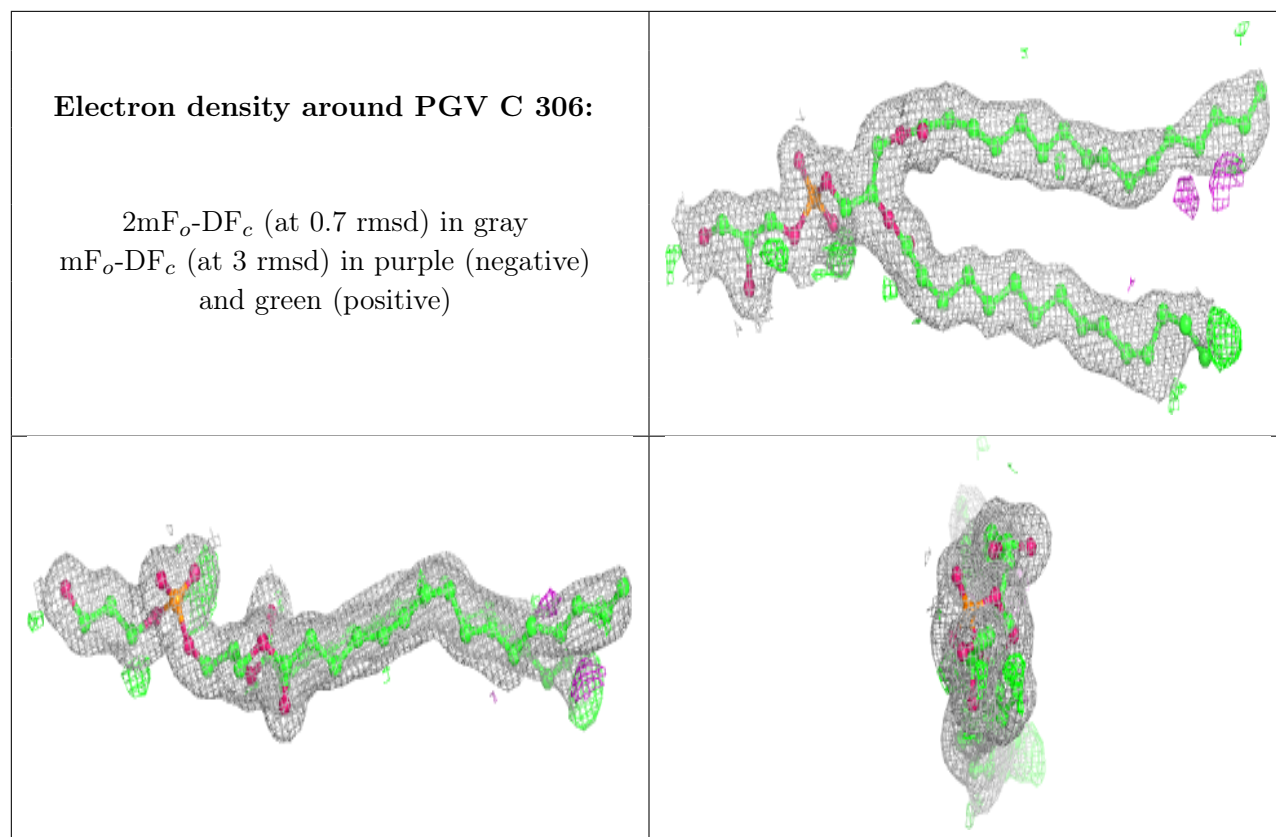
**Electron density around HEA N 603:**

$2mF_o-DF_c$  (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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.