



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2025 – 01:03 PM JST

PDB ID : 9KUM / pdb\_00009kum  
Title : Bovine Heart Cytochrome c Oxidase in the Xenon-bound Fully Reduced State  
Authors : Muramoto, K.; Shinzawa-Itoh, K.  
Deposited on : 2024-12-04  
Resolution : 1.80 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 : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

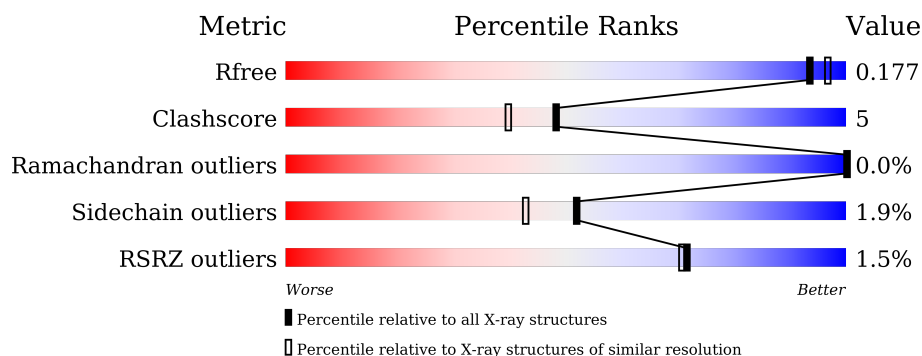
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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.



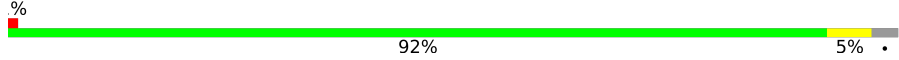




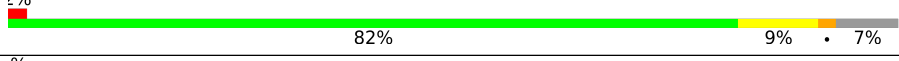

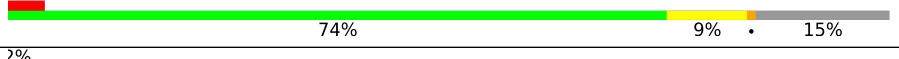


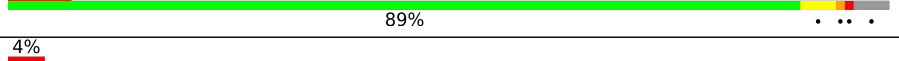


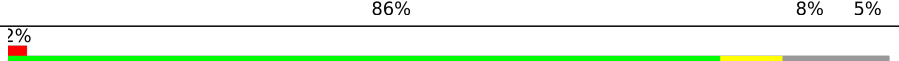
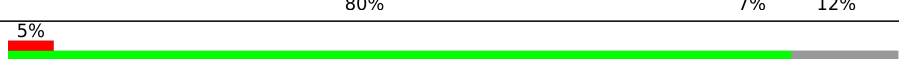
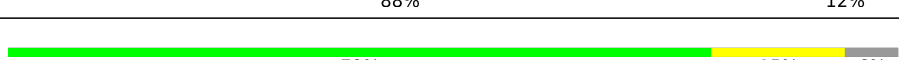
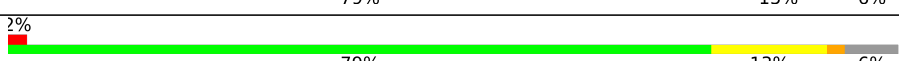
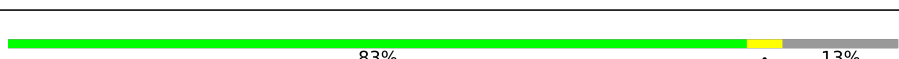


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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	<div> <div style="width: 91%;"></div> <div style="width: 8%;"></div> <div style="width: 1%;"></div> </div> 91% 8% .
1	N	514	<div> <div style="width: 90%;"></div> <div style="width: 9%;"></div> <div style="width: 1%;"></div> </div> 90% 9% .
2	B	227	<div> <div style="width: 4%;"></div> <div style="width: 80%;"></div> <div style="width: 17%;"></div> <div style="width: 1%;"></div> </div> 4% 80% 17% .
2	O	227	<div> <div style="width: 2%;"></div> <div style="width: 82%;"></div> <div style="width: 15%;"></div> <div style="width: 1%;"></div> </div> 2% 82% 15% .
3	C	261	<div> <div style="width: 84%;"></div> <div style="width: 15%;"></div> <div style="width: 1%;"></div> </div> 84% 15% .
3	P	261	<div> <div style="width: 87%;"></div> <div style="width: 11%;"></div> <div style="width: 2%;"></div> </div> 87% 11% .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CDL	C	304	-	-	X	-
19	LFA	P	311	-	-	-	X
22	XE	A	618	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	XE	B	301	-	-	X	-
22	XE	N	621	-	-	X	-
22	XE	O	305	-	-	X	-



## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 33035 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	15	0
			4130	2757	636	696	41			
1	N	513	Total	C	N	O	S	0	15	0
			4130	2757	636	696	41			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	5	0
			1870	1216	288	347	19			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1216	288	347	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	258	Total	C	N	O	S	0	9	0
			2171	1449	342	364	16			
3	P	258	Total	C	N	O	S	0	9	0
			2172	1449	343	364	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	143	Total	C	N	O	S	0	1	0
			1192	776	195	217	4			
4	Q	137	Total	C	N	O	S	0	1	0
			1148	749	188	207	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	102	Total	C	N	O	S	0	0	0
			825	528	139	156	2			
5	R	102	Total	C	N	O	S	0	0	0
			825	528	139	156	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	91	Total	C	N	O	S	0	2	0
			709	441	124	138	6			
6	S	91	Total	C	N	O	S	0	2	0
			709	441	124	138	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	72	Total	C	N	O	S	0	1	0
			606	396	114	95	1			
7	T	72	Total	C	N	O	S	0	1	0
			606	396	114	95	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			
8	U	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			575	375	103	93	4			
9	V	70	Total	C	N	O	S	0	0	0
			575	375	103	93	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	56	Total	C	N	O	S	0	0	0
			441	285	73	80	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	56	Total	C	N	O	S	0	0	0
			441	285	73	80	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

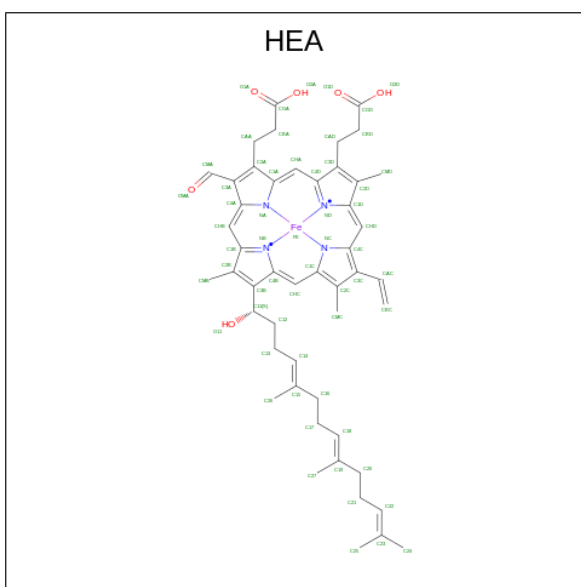
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	44	Total	C	N	O	S	0	0	0
			360	242	59	57	2			
12	Y	44	Total	C	N	O	S	0	0	0
			360	242	59	57	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	40	Total	C	N	O	0	0	0
			311	208	48	55			
13	Z	40	Total	C	N	O	0	0	0
			311	208	48	55			

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



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

- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Cu	0	0
			1	1		
15	N	1	Total	Cu	0	0
			1	1		

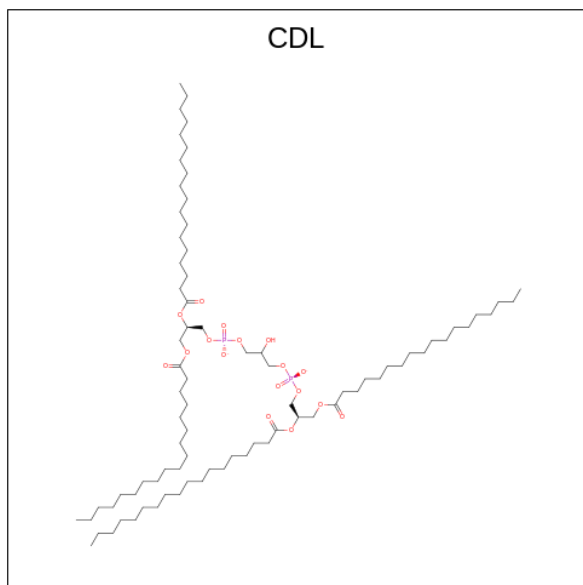
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

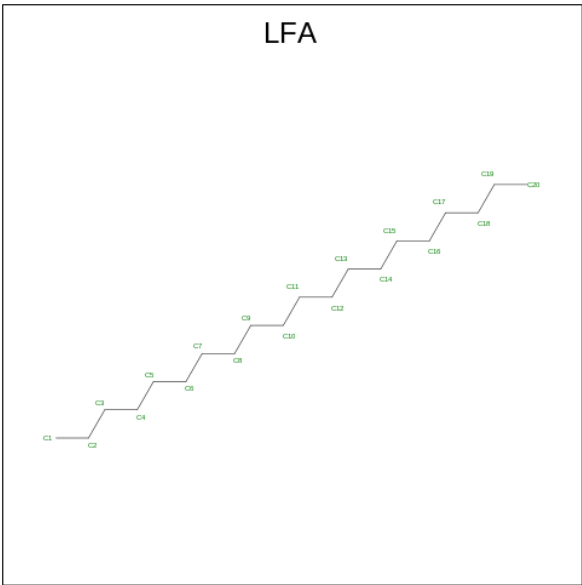
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			64	45	17	2		
18	C	1	Total	C	O	P	0	0
			87	68	17	2		
18	L	1	Total	C	O	P	0	0
			94	75	17	2		
18	N	1	Total	C	O	P	0	0
			64	45	17	2		
18	P	1	Total	C	O	P	0	0
			87	68	17	2		
18	Y	1	Total	C	O	P	0	0
			94	75	17	2		

- Molecule 19 is EICOSANE (CCD ID: LFA) (formula:  $C_{20}H_{42}$ ).



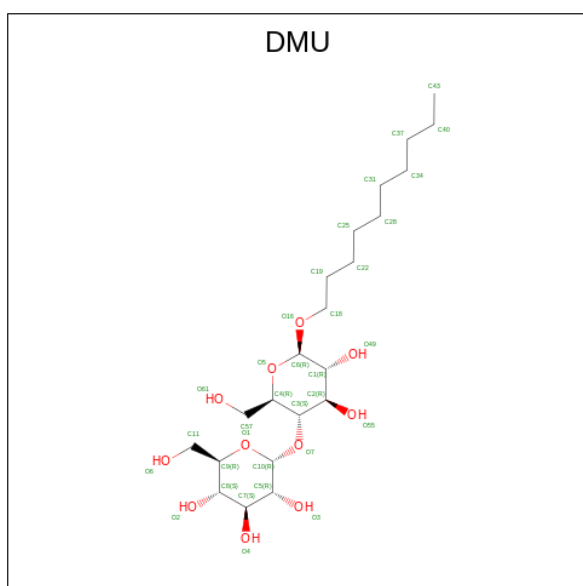
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	C	0	0
			14	14		
19	B	1	Total	C	0	0
			17	17		
19	C	1	Total	C	0	0
			11	11		
19	C	1	Total	C	0	0
			6	6		
19	C	1	Total	C	0	0
			18	18		
19	C	1	Total	C	0	0
			11	11		
19	C	1	Total	C	0	0
			14	14		
19	C	1	Total	C	0	0
			11	11		
19	C	1	Total	C	0	0
			15	15		
19	C	1	Total	C	0	0
			13	13		
19	C	1	Total	C	0	0
			15	15		
19	G	1	Total	C	0	0
			14	14		
19	N	1	Total	C	0	0
			14	14		
19	O	1	Total	C	0	0
			17	17		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	O	1	Total C 11 11	0	0
19	P	1	Total C 15 15	0	0
19	P	1	Total C 11 11	0	0
19	P	1	Total C 6 6	0	0
19	P	1	Total C 18 18	0	0
19	P	1	Total C 11 11	0	0
19	P	1	Total C 11 11	0	0
19	P	1	Total C 15 15	0	0
19	P	1	Total C 13 13	0	0
19	T	1	Total C 14 14	0	0
19	T	1	Total C 14 14	0	0
19	T	1	Total C 11 11	0	0

- Molecule 20 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula:  $C_{22}H_{42}O_{11}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C 7 7	0	0
20	A	1	Total C O 33 22 11	0	0
20	A	1	Total C O 11 10 1	0	0
20	B	1	Total C O 11 10 1	0	0
20	B	1	Total C O 11 10 1	0	0
20	B	1	Total C O 22 16 6	0	0
20	B	1	Total C O 22 16 6	0	0
20	C	1	Total C O 11 10 1	0	0
20	C	1	Total C O 33 22 11	0	0
20	C	1	Total C 7 7	0	0
20	C	1	Total C O 22 16 6	0	0
20	C	1	Total C O 33 22 11	0	0
20	C	1	Total C O 33 22 11	0	0
20	C	1	Total C O 33 22 11	0	0
20	D	1	Total C O 33 22 11	0	0
20	G	1	Total C O 22 16 6	0	0
20	H	1	Total C O 33 22 11	0	0
20	J	1	Total C O 11 10 1	0	0
20	L	1	Total C O 22 16 6	0	0
20	M	1	Total C O 33 22 11	0	0
20	M	1	Total C 8 8	0	0
20	N	1	Total C O 11 10 1	0	0

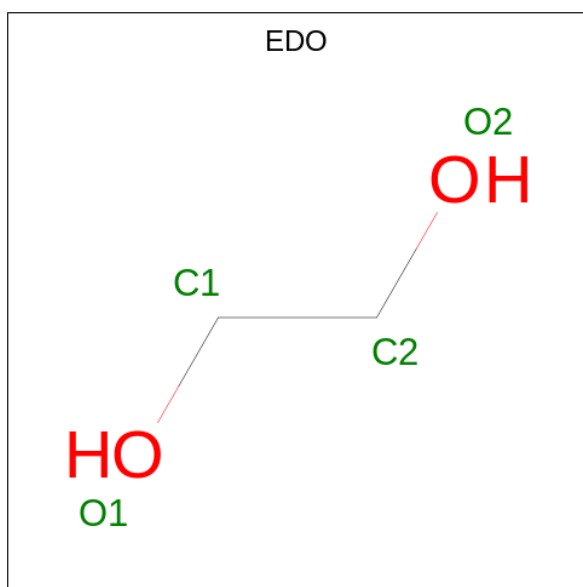
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	N	1	Total C 7 7	0	0
20	N	1	Total C O 33 22 11	0	0
20	O	1	Total C O 22 16 6	0	0
20	O	1	Total C O 11 10 1	0	0
20	O	1	Total C O 11 10 1	0	0
20	O	1	Total C O 22 16 6	0	0
20	P	1	Total C O 11 10 1	0	0
20	P	1	Total C O 33 22 11	0	0
20	P	1	Total C 7 7	0	0
20	P	1	Total C O 22 16 6	0	0
20	P	1	Total C O 33 22 11	0	0
20	P	1	Total C O 33 22 11	0	0
20	P	1	Total C O 33 22 11	0	0
20	Q	1	Total C O 33 22 11	0	0
20	T	1	Total C O 22 16 6	0	0
20	U	1	Total C O 33 22 11	0	0
20	W	1	Total C O 11 10 1	0	0
20	Y	1	Total C O 22 16 6	0	0
20	Z	1	Total C O 33 22 11	0	0
20	Z	1	Total C 8 8	0	0

- Molecule 21 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

- Molecule 22 is XENON (CCD ID: XE) (formula: Xe) (labeled as "Ligand of Interest" by depositor).

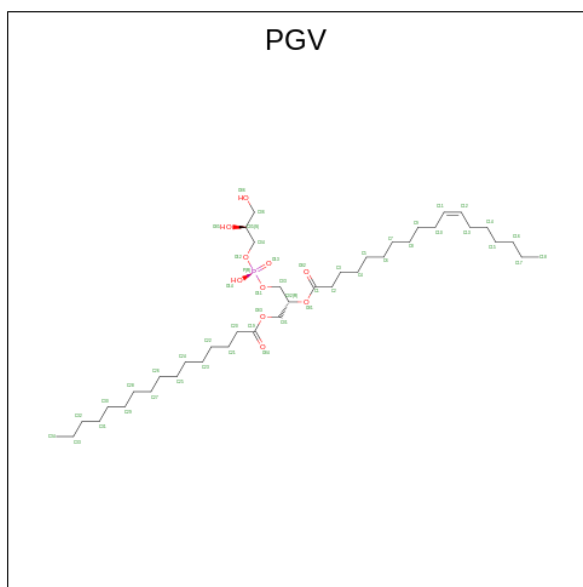
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	6	Total Xe 6 6	0	0
22	B	1	Total Xe 1 1	0	0
22	C	1	Total Xe 1 1	0	0
22	N	6	Total Xe 6 6	0	0

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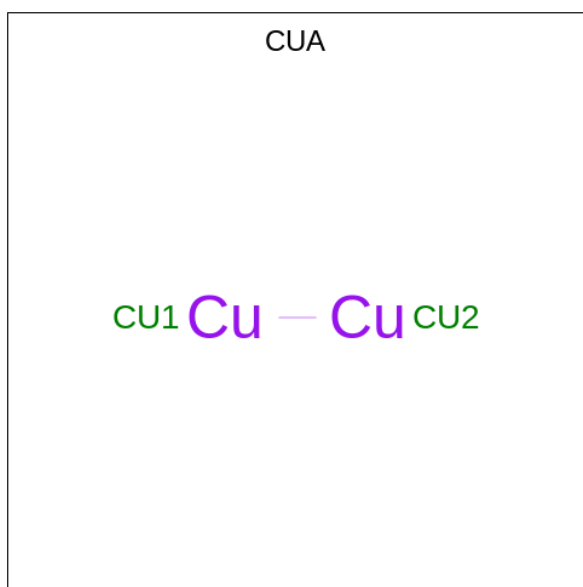
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	O	1	Total	Xe	0	0
			1	1		
22	P	1	Total	Xe	0	0
			1	1		

- Molecule 23 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



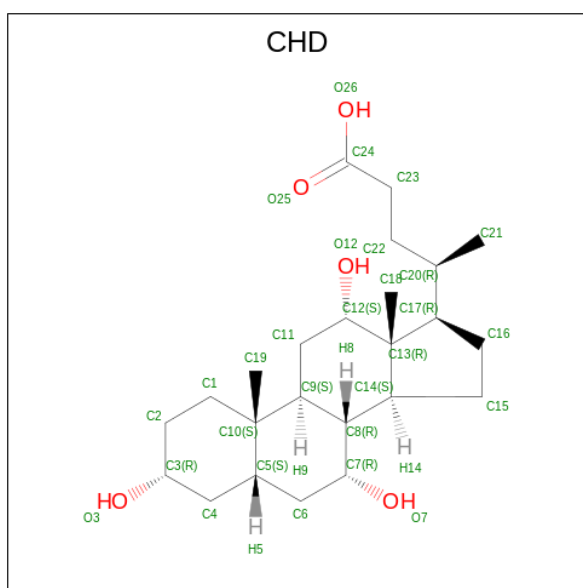
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	O	P	0	0
			51	40	10	1		
23	C	1	Total	C	O	P	0	0
			51	40	10	1		
23	N	1	Total	C	O	P	0	0
			51	40	10	1		
23	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 24 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).



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

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



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

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

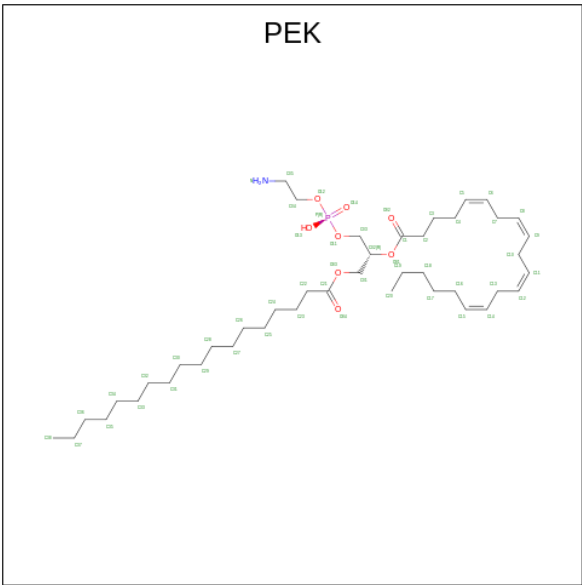
- Molecule 26 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

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

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 28 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	232	Total	O	0	11
			243	243		
29	B	171	Total	O	0	2
			173	173		
29	C	106	Total	O	0	1
			107	107		
29	D	135	Total	O	0	8
			143	143		
29	E	109	Total	O	0	8
			117	117		
29	F	104	Total	O	0	7
			111	111		
29	G	41	Total	O	0	1
			42	42		
29	H	63	Total	O	0	0
			63	63		
29	I	39	Total	O	0	0
			39	39		
29	J	20	Total	O	0	0
			20	20		

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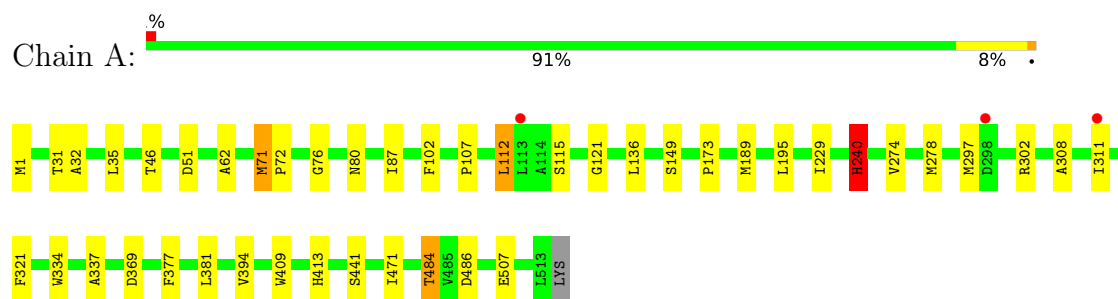
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	K	21	Total 21	O 21	0	0
29	L	26	Total 28	O 28	0	2
29	M	23	Total 23	O 23	0	0
29	N	228	Total 238	O 238	0	10
29	O	145	Total 146	O 146	0	1
29	P	103	Total 104	O 104	0	1
29	Q	81	Total 86	O 86	0	5
29	R	86	Total 93	O 93	0	7
29	S	88	Total 94	O 94	0	6
29	T	36	Total 37	O 37	0	1
29	U	50	Total 50	O 50	0	0
29	V	23	Total 23	O 23	0	0
29	W	14	Total 14	O 14	0	0
29	X	16	Total 16	O 16	0	0
29	Y	23	Total 25	O 25	0	2
29	Z	16	Total 16	O 16	0	0



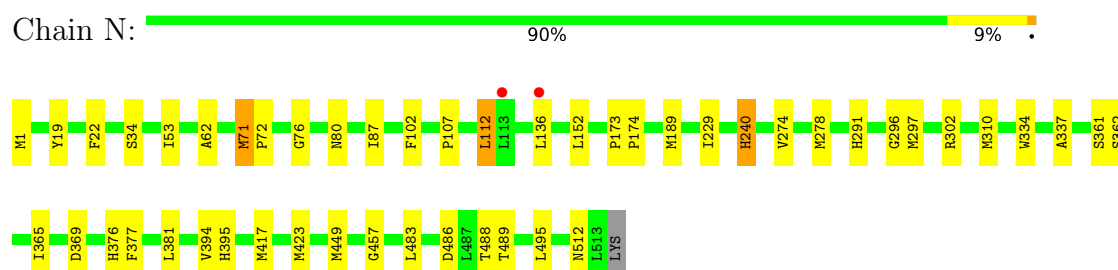
### 3 Residue-property plots [i](#)

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.

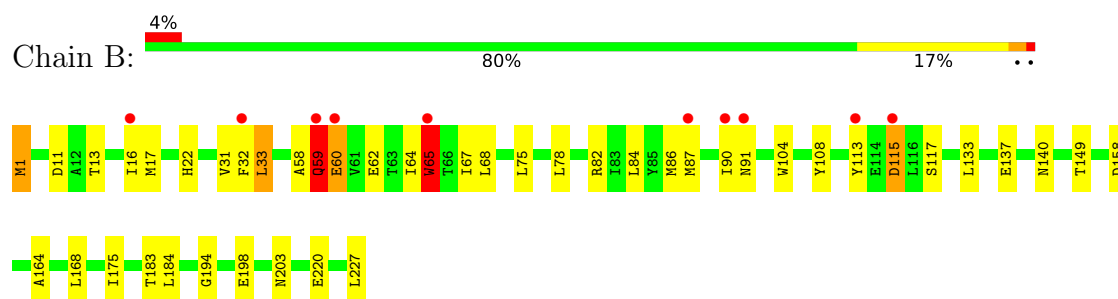
- Molecule 1: Cytochrome c oxidase subunit 1



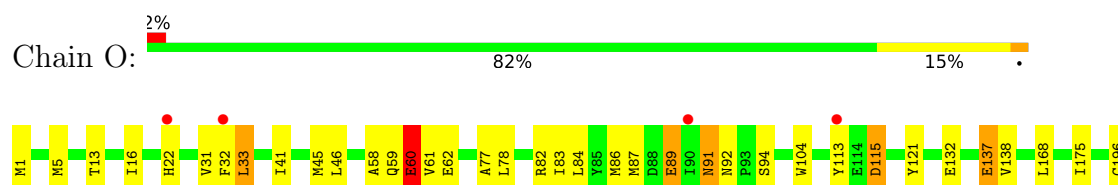
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2





- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 84% 15% .



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 87% 11% .



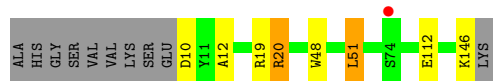
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 92% 5% .



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

Chain Q: 88% 7% .



- Molecule 5: Cytochrome c oxidase subunit 5A

Chain E: 91% 6% .

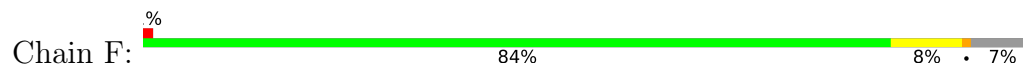


- Molecule 5: Cytochrome c oxidase subunit 5A

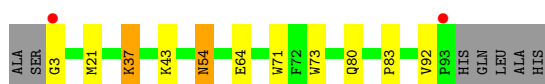
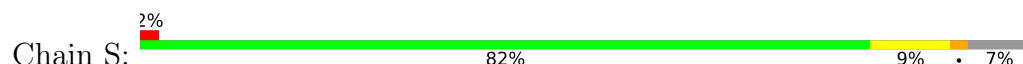
Chain R: 86% 7% 6% .



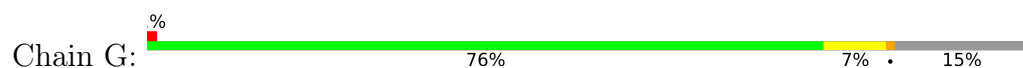
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



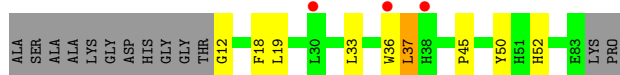
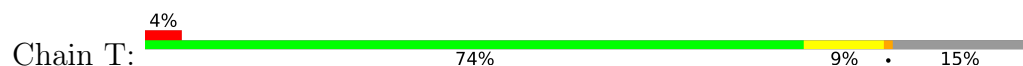
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



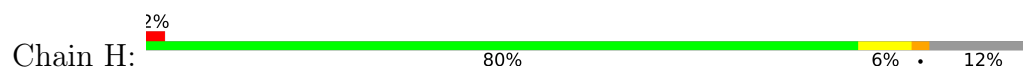
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



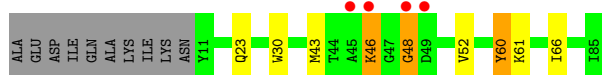
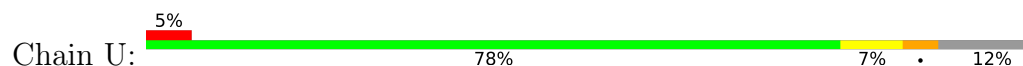
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



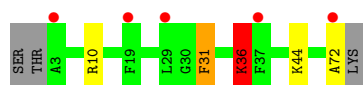
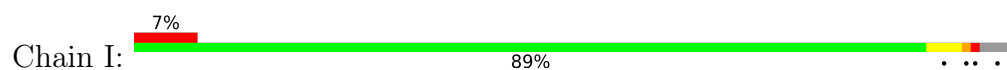
- Molecule 8: Cytochrome c oxidase subunit 6B1



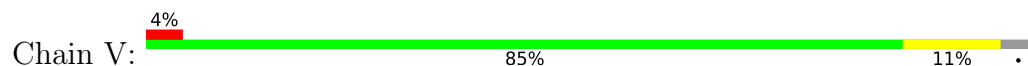
- Molecule 8: Cytochrome c oxidase subunit 6B1



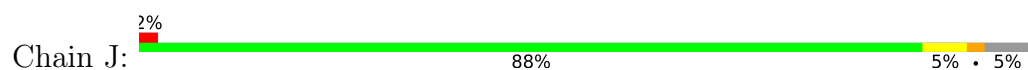
- Molecule 9: Cytochrome c oxidase subunit 6C



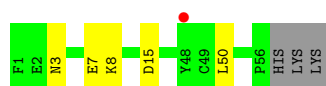
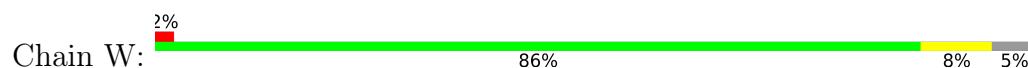
- Molecule 9: Cytochrome c oxidase subunit 6C



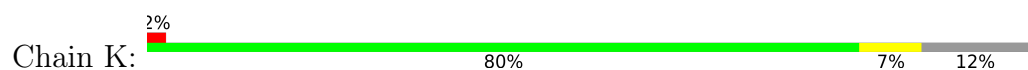
- Molecule 10: Cytochrome c oxidase subunit 7A1



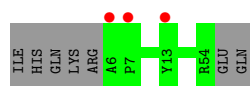
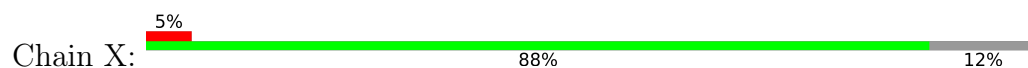
- Molecule 10: Cytochrome c oxidase subunit 7A1



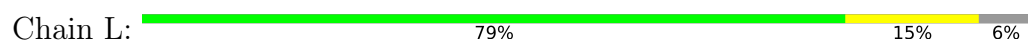
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



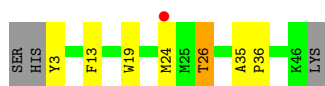
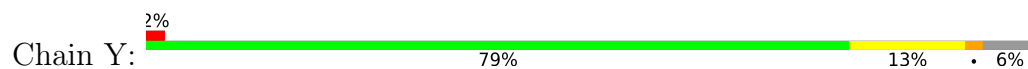
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



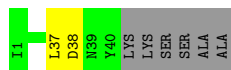
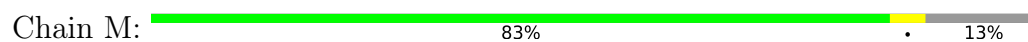
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



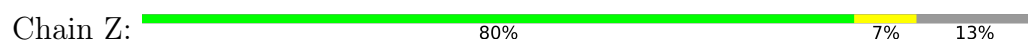
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.50Å 204.70Å 177.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 40.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.80) 100.0 (40.00-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.132 , 0.169 0.146 , 0.177	Depositor DCC
$R_{free}$ test set	30364 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 64.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for l,k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	33035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XE, ZN, FME, UNX, MG, CUA, DMU, CU, NA, EDO, PGV, CHD, PEK, LFA, CDL, HEA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.11	2/4259 (0.0%)	1.21	6/5816 (0.1%)
1	N	1.11	7/4259 (0.2%)	1.22	5/5816 (0.1%)
2	B	1.15	3/1908 (0.2%)	1.31	13/2598 (0.5%)
2	O	1.15	2/1908 (0.1%)	1.27	5/2598 (0.2%)
3	C	1.08	1/2258 (0.0%)	1.17	3/3084 (0.1%)
3	P	1.09	1/2258 (0.0%)	1.19	5/3084 (0.2%)
4	D	1.12	1/1226 (0.1%)	1.25	3/1657 (0.2%)
4	Q	1.12	1/1182 (0.1%)	1.32	3/1598 (0.2%)
5	E	1.14	0/843	1.23	1/1145 (0.1%)
5	R	1.10	0/843	1.31	3/1145 (0.3%)
6	F	1.13	0/724	1.25	0/983
6	S	1.23	2/724 (0.3%)	1.21	0/983
7	G	1.15	1/633 (0.2%)	1.23	0/864
7	T	1.24	2/633 (0.3%)	1.25	0/864
8	H	1.05	1/648 (0.2%)	1.32	0/877
8	U	1.11	0/648	1.34	1/877 (0.1%)
9	I	1.18	2/588 (0.3%)	1.45	3/781 (0.4%)
9	V	1.07	0/588	1.49	2/781 (0.3%)
10	J	1.13	0/451	1.29	1/610 (0.2%)
10	W	1.17	0/451	1.28	1/610 (0.2%)
11	K	1.21	2/398 (0.5%)	1.31	0/546
11	X	1.15	0/398	1.31	0/546
12	L	1.12	1/372 (0.3%)	1.33	3/500 (0.6%)
12	Y	1.06	0/372	1.32	0/500
13	M	1.12	0/321	1.22	0/440
13	Z	1.04	0/321	1.33	0/440
All	All	1.12	29/29214 (0.1%)	1.26	58/39743 (0.1%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	12	GLY	N-CA	-9.17	1.30	1.45
4	D	58	GLU	CD-OE1	7.89	1.40	1.25
7	G	12	GLY	N-CA	-7.61	1.33	1.45
1	N	240	HIS	CE1-NE2	7.19	1.39	1.32
11	K	10	HIS	CE1-NE2	6.95	1.39	1.32
2	O	198	GLU	C-O	6.62	1.31	1.23
1	N	376	HIS	CE1-NE2	6.34	1.38	1.32
4	Q	20	ARG	CD-NE	-6.05	1.37	1.46
12	L	5	GLU	CD-OE2	-5.79	1.14	1.25
1	N	483	LEU	C-O	5.79	1.31	1.24
1	A	189	MET	CG-SD	-5.74	1.66	1.80
3	C	243	HIS	CE1-NE2	5.73	1.38	1.32
2	B	198	GLU	C-O	5.63	1.30	1.23
6	S	64	GLU	C-O	5.60	1.30	1.23
2	B	90	ILE	C-O	5.55	1.29	1.24
1	N	291	HIS	CE1-NE2	5.55	1.38	1.32
9	I	31	PHE	C-O	5.53	1.30	1.24
9	I	72	ALA	C-O	5.48	1.34	1.23
1	N	174	PRO	C-O	-5.48	1.17	1.24
1	N	395	HIS	CE1-NE2	5.47	1.38	1.32
7	T	45	PRO	C-O	-5.42	1.17	1.23
6	S	83	PRO	C-O	-5.31	1.17	1.24
1	N	189	MET	CG-SD	-5.29	1.67	1.80
3	P	204	HIS	CE1-NE2	5.28	1.37	1.32
11	K	41	ASN	N-CA	5.23	1.50	1.46
1	A	413	HIS	CG-ND1	-5.16	1.32	1.38
2	O	60	GLU	CD-OE2	5.12	1.35	1.25
2	B	113	TYR	C-O	-5.07	1.17	1.24
8	H	11	TYR	N-CA	5.07	1.55	1.46

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	HIS	CA-CB-CG	-10.53	103.27	113.80
1	N	240	HIS	CA-CB-CG	-9.88	103.92	113.80
1	A	71	MET	CG-SD-CE	-9.48	80.03	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	72	ALA	CA-C-O	-9.44	104.76	120.80
9	V	72	ALA	CA-C-O	-9.12	105.30	120.80
3	P	230	ASN	CA-CB-CG	-8.87	103.73	112.60
1	N	71	MET	CG-SD-CE	-8.41	82.39	100.90
3	C	80	ARG	CG-CD-NE	-7.92	94.57	112.00
4	D	58	GLU	CB-CG-CD	7.67	125.64	112.60
2	B	59	GLN	CB-CG-CD	7.23	124.89	112.60
2	B	65	TRP	CB-CA-C	7.22	122.77	110.56
4	D	146	LYS	CA-C-O	-7.14	108.66	120.80
2	B	115	ASP	CB-CA-C	6.99	122.67	112.05
4	Q	20	ARG	CG-CD-NE	-6.79	97.06	112.00
5	R	78	HIS	CA-C-N	6.62	130.04	120.38
5	R	78	HIS	C-N-CA	6.62	130.04	120.38
2	B	158	ASP	CA-CB-CG	6.58	119.18	112.60
12	L	25	MET	CA-C-N	6.54	129.37	120.54
12	L	25	MET	C-N-CA	6.54	129.37	120.54
3	P	80	ARG	CG-CD-NE	-6.51	97.67	112.00
1	N	102	PHE	CA-CB-CG	-6.43	107.37	113.80
1	A	102	PHE	CA-CB-CG	-6.24	107.56	113.80
3	C	233	PHE	CA-CB-CG	-6.21	107.59	113.80
10	J	7	GLU	CB-CA-C	6.19	121.37	110.85
2	B	183	THR	CA-CB-OG1	-5.92	100.71	109.60
2	O	89	GLU	CB-CA-C	-5.91	102.53	109.80
2	B	11	ASP	CA-CB-CG	5.90	118.50	112.60
2	B	184	LEU	N-CA-CB	-5.80	100.76	110.80
5	R	80	GLU	CB-CG-CD	5.80	122.46	112.60
9	V	33	THR	CA-CB-OG1	-5.71	101.04	109.60
2	B	82	ARG	CG-CD-NE	-5.69	99.48	112.00
3	P	233	PHE	CA-CB-CG	-5.57	108.23	113.80
9	I	36	LYS	CA-C-N	5.52	127.95	120.44
9	I	36	LYS	C-N-CA	5.52	127.95	120.44
2	B	149	THR	CA-CB-OG1	-5.47	101.39	109.60
10	W	15	ASP	CA-CB-CG	5.45	118.05	112.60
2	O	115	ASP	CB-CA-C	5.35	120.38	112.03
2	O	113	TYR	CB-CA-C	-5.34	100.83	110.23
4	Q	20	ARG	NE-CZ-NH2	-5.33	114.41	119.20
12	L	46	LYS	CA-C-O	-5.31	111.77	120.80
2	O	61	VAL	CA-C-O	-5.27	114.78	120.47
1	N	512	ASN	CB-CA-C	5.26	119.55	110.45
1	A	46	THR	CA-CB-OG1	-5.25	101.72	109.60
3	P	76	GLN	CG-CD-NE2	-5.23	108.56	116.40
1	A	484	THR	CA-CB-OG1	-5.22	101.78	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	66	ILE	CA-C-O	-5.17	115.67	121.05
2	B	64	ILE	CA-C-N	-5.15	114.41	122.65
2	B	64	ILE	C-N-CA	-5.15	114.41	122.65
3	P	122	HIS	CB-CA-C	5.13	115.98	110.65
4	Q	146	LYS	CA-C-O	-5.10	112.13	120.80
1	A	507	GLU	CB-CA-C	5.10	115.66	109.85
2	B	137	GLU	CB-CG-CD	5.10	121.26	112.60
2	O	137	GLU	CB-CG-CD	5.05	121.19	112.60
3	C	76	GLN	CG-CD-NE2	-5.05	108.82	116.40
4	D	20	ARG	NE-CZ-NH2	5.05	123.75	119.20
5	E	108	LYS	CA-C-O	-5.05	112.22	120.80
1	N	240	HIS	N-CA-CB	5.04	116.36	110.42
2	B	64	ILE	N-CA-C	-5.02	105.50	110.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4102	40	0
1	N	4130	0	4102	47	0
2	B	1870	0	1870	33	0
2	O	1870	0	1870	37	0
3	C	2171	0	2080	36	0
3	P	2172	0	2081	22	0
4	D	1192	0	1178	4	0
4	Q	1148	0	1131	5	0
5	E	825	0	823	1	0
5	R	825	0	823	4	0
6	F	709	0	691	9	0
6	S	709	0	691	7	0
7	G	606	0	577	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	T	606	0	577	4	0
8	H	628	0	580	13	0
8	U	628	0	580	10	0
9	I	575	0	584	9	0
9	V	575	0	584	3	0
10	J	441	0	439	5	0
10	W	441	0	439	3	0
11	K	384	0	366	1	0
11	X	384	0	366	0	0
12	L	360	0	360	6	0
12	Y	360	0	360	6	0
13	M	311	0	321	1	0
13	Z	311	0	321	1	0
14	A	120	0	108	4	0
14	N	120	0	108	5	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	64	0	72	0	0
18	C	87	0	124	23	0
18	L	94	0	141	4	0
18	N	64	0	72	2	0
18	P	87	0	124	16	0
18	Y	94	0	141	10	0
19	A	14	0	27	3	0
19	B	17	0	33	1	0
19	C	114	0	207	6	0
19	G	14	0	27	2	0
19	N	14	0	27	5	0
19	O	28	0	54	4	0
19	P	100	0	174	5	0
19	T	39	0	75	2	0
20	A	51	0	76	2	0
20	B	66	0	104	0	0
20	C	172	0	228	3	0
20	D	33	0	41	1	0
20	G	22	0	31	0	0
20	H	33	0	28	1	0
20	J	11	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	L	22	0	31	3	0
20	M	41	0	56	0	0
20	N	51	0	76	0	0
20	O	66	0	104	1	0
20	P	172	0	228	3	0
20	Q	33	0	41	1	0
20	T	22	0	31	2	0
20	U	33	0	21	0	0
20	W	11	0	21	0	0
20	Y	22	0	31	2	0
20	Z	41	0	56	1	0
21	A	12	0	18	0	0
21	B	4	0	6	0	0
21	C	12	0	17	0	0
21	E	12	0	18	0	0
21	F	12	0	18	1	0
21	G	4	0	6	0	0
21	N	20	0	30	0	0
21	O	4	0	6	0	0
21	P	12	0	18	0	0
21	R	12	0	18	0	0
21	S	8	0	12	0	0
21	T	4	0	6	0	0
22	A	6	0	0	5	0
22	B	1	0	0	3	0
22	C	1	0	0	0	0
22	N	6	0	0	4	0
22	O	1	0	0	3	0
22	P	1	0	0	0	0
23	A	51	0	76	0	0
23	C	51	0	76	4	0
23	N	51	0	76	0	0
23	P	51	0	76	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	4	0
25	O	29	0	39	0	0
25	P	58	0	78	4	0
26	C	1	0	0	1	0
26	P	1	0	0	1	0
27	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	S	1	0	0	0	0
28	G	53	0	77	1	0
28	T	53	0	77	2	0
29	A	243	0	0	8	0
29	B	173	0	0	4	0
29	C	107	0	0	6	0
29	D	143	0	0	2	0
29	E	117	0	0	0	0
29	F	111	0	0	1	0
29	G	42	0	0	1	0
29	H	63	0	0	5	0
29	I	39	0	0	3	0
29	J	20	0	0	0	0
29	K	21	0	0	0	0
29	L	28	0	0	1	0
29	M	23	0	0	0	0
29	N	238	0	0	10	0
29	O	146	0	0	1	0
29	P	104	0	0	3	0
29	Q	86	0	0	2	0
29	R	93	0	0	2	0
29	S	94	0	0	1	0
29	T	37	0	0	0	0
29	U	50	0	0	3	0
29	V	23	0	0	0	0
29	W	14	0	0	0	0
29	X	16	0	0	0	0
29	Y	25	0	0	2	0
29	Z	16	0	0	0	0
All	All	33035	0	31500	339	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (339) 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)
19:C:309:LFA:H12	29:H:233:HOH:O	1.32	1.26
1:N:112:LEU:HG	29:N:920:HOH:O	1.09	1.22
1:A:112:LEU:HG	29:A:926:HOH:O	0.97	1.15
3:P:4:GLN:N	29:P:403:HOH:O	1.84	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:274:VAL:HG12	1:N:278[A]:MET:HE2	1.39	1.02
18:L:101:CDL:O1	29:L:220[B]:HOH:O	1.79	0.98
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:HE3	1.44	0.98
20:A:609:DMU:O6	29:A:704:HOH:O	1.83	0.95
4:Q:112:GLU:OE2	29:Q:301:HOH:O	1.86	0.93
8:H:43:MET:HE1	8:U:52:VAL:HG11	1.51	0.90
1:N:417[B]:MET:HE1	29:N:892:HOH:O	1.72	0.90
18:P:305:CDL:H121	18:P:305:CDL:HA62	1.51	0.90
2:B:16[B]:ILE:HG23	29:B:512:HOH:O	1.73	0.88
3:C:245:VAL:C	3:C:246[B]:ASP:CA	2.46	0.88
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.54	0.86
25:P:306:CHD:H162	25:P:306:CHD:H231	1.58	0.86
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.10	0.85
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:HG2	1.57	0.84
29:A:744:HOH:O	3:C:77:LYS:HE3	1.75	0.84
2:B:16[A]:ILE:CG2	2:B:87[A]:MET:HE3	2.09	0.81
3:P:59:ARG:HG3	18:P:305:CDL:HA4	1.64	0.80
2:B:220:GLU:OE1	29:B:402:HOH:O	1.99	0.79
1:A:31:THR:O	1:A:35:LEU:HD23	1.81	0.79
18:P:305:CDL:H121	18:P:305:CDL:CA6	2.11	0.78
18:C:304:CDL:HB21	18:C:304:CDL:HB32	1.64	0.77
2:B:31:VAL:CG2	22:B:301:XE:XE	3.10	0.77
1:N:112:LEU:CG	29:N:920:HOH:O	1.88	0.76
18:C:304:CDL:HA62	18:C:304:CDL:H121	1.66	0.76
18:C:304:CDL:OA5	18:C:304:CDL:OB9	2.02	0.76
9:I:10:ARG:CD	29:I:135:HOH:O	2.34	0.75
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.27	0.74
2:O:89:GLU:O	2:O:91:ASN:OD1	2.05	0.74
2:B:31:VAL:HG22	22:B:301:XE:XE	2.66	0.74
8:H:43:MET:CE	8:U:52:VAL:HG11	2.17	0.73
1:A:112:LEU:O	1:A:112:LEU:HD23	1.89	0.73
1:N:417[B]:MET:CE	29:N:892:HOH:O	2.29	0.73
9:I:10:ARG:HD2	29:I:135:HOH:O	1.87	0.73
2:O:22[B]:HIS:CE1	9:V:44:LYS:HE2	2.24	0.72
1:A:31:THR:O	1:A:35:LEU:CD2	2.37	0.72
25:C:301:CHD:O25	19:C:309:LFA:H13	1.90	0.71
1:A:278[A]:MET:HE1	19:T:101:LFA:H51	1.72	0.71
4:D:42:GLU:OE2	29:D:301:HOH:O	2.08	0.70
26:C:302:UNX:UNK	29:C:500:HOH:O	1.71	0.70
18:C:304:CDL:OB9	18:C:304:CDL:CA3	2.39	0.70
28:T:102:PEK:H71	28:T:102:PEK:H32	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:101:CDL:OB9	18:L:101:CDL:H122	1.92	0.70
2:O:59:GLN:NE2	19:O:303:LFA:H31	2.07	0.70
3:C:33[A]:MET:HE3	3:C:39:SER:OG	1.92	0.70
1:A:112:LEU:HD22	22:A:615:XE:XE	2.70	0.69
8:H:52:VAL:CG1	8:U:46:LYS:HG2	2.22	0.69
3:C:54[A]:MET:HE1	23:C:303:PGV:H141	1.75	0.68
1:N:112:LEU:CD2	29:N:920:HOH:O	2.29	0.68
3:P:149:HIS:NE2	19:P:312:LFA:H11	2.09	0.68
2:B:31:VAL:HG23	22:B:301:XE:XE	2.72	0.67
18:Y:101:CDL:H142	18:Y:101:CDL:OB9	1.94	0.67
7:T:19:LEU:HD23	19:T:101:LFA:H61	1.76	0.67
25:P:306:CHD:H162	25:P:306:CHD:C23	2.25	0.67
6:F:37:LYS:HG2	29:F:294:HOH:O	1.95	0.67
1:A:51:ASP:OD2	1:A:441:SER:OG	2.11	0.66
3:C:33[A]:MET:HE2	3:C:42:LEU:H	1.60	0.66
3:P:50:ASN:ND2	3:P:54[A]:MET:HE2	2.12	0.65
18:C:304:CDL:OB9	18:C:304:CDL:OA4	2.15	0.65
3:C:33[A]:MET:CE	3:C:42:LEU:H	2.09	0.65
1:A:486:ASP:HB3	29:A:907[B]:HOH:O	1.97	0.64
3:P:33[B]:MET:CE	3:P:42:LEU:HD12	2.27	0.64
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:CE	2.23	0.64
2:B:22[B]:HIS:HE1	9:I:44:LYS:HE2	1.57	0.64
2:B:13:THR:HB	2:B:168:LEU:HD23	1.80	0.64
19:P:310:LFA:H41	29:U:213:HOH:O	1.98	0.64
18:Y:101:CDL:H362	18:Y:101:CDL:H711	1.81	0.63
3:C:50:ASN:ND2	3:C:54[A]:MET:HE2	2.13	0.63
18:Y:101:CDL:H711	18:Y:101:CDL:C36	2.29	0.63
26:P:303:UNX:UNK	29:P:501:HOH:O	1.80	0.63
1:A:484:THR:HB	29:D:396:HOH:O	1.98	0.63
19:G:104:LFA:H11	19:N:608:LFA:H12	1.79	0.62
1:A:136[B]:LEU:HD11	29:A:927:HOH:O	1.99	0.62
18:C:304:CDL:H121	18:C:304:CDL:CA6	2.29	0.62
1:N:274:VAL:CG1	1:N:278[A]:MET:HE2	2.23	0.61
2:O:92:ASN:ND2	29:O:402:HOH:O	2.33	0.61
3:C:164:PHE:CD1	25:C:305:CHD:H192	2.35	0.61
2:B:227:LEU:HD21	29:B:486:HOH:O	2.01	0.61
3:C:247:VAL:HG11	19:C:313:LFA:H71	1.82	0.61
12:L:26:THR:HG21	20:L:102:DMU:H26	1.82	0.61
1:N:278[B]:MET:HE1	19:N:608:LFA:H52	1.83	0.61
8:H:23:GLN:CD	29:H:201:HOH:O	2.43	0.61
1:A:278[B]:MET:SD	19:A:607:LFA:H51	2.40	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:ASN:HB3	29:B:535:HOH:O	2.01	0.60
2:B:84:LEU:O	2:B:87[B]:MET:HB2	2.01	0.60
6:F:87[A]:THR:HG22	6:F:89:TYR:CE1	2.36	0.60
14:N:602:HEA:H14	22:N:621:XE:XE	2.79	0.60
3:P:51[B]:MET:HE3	18:P:305:CDL:H873	1.81	0.60
1:N:423[B]:MET:HE2	1:N:457:GLY:N	2.16	0.60
1:N:112:LEU:HD22	22:N:618:XE:XE	2.79	0.60
7:G:34:ASN:O	7:G:38:HIS:HD2	1.85	0.59
2:O:31:VAL:CG2	22:O:305:XE:XE	3.28	0.59
2:O:31:VAL:HG22	22:O:305:XE:XE	2.81	0.58
1:A:274:VAL:HG12	1:A:278[A]:MET:HE2	1.84	0.58
8:H:46:LYS:HE2	8:H:46:LYS:O	2.04	0.58
1:N:362[A]:SER:OG	2:O:87[A]:MET:CE	2.52	0.58
3:P:164:PHE:CD1	25:P:306:CHD:H192	2.39	0.58
18:C:304:CDL:HB21	18:C:304:CDL:CB3	2.32	0.57
2:O:60:GLU:CD	2:O:60:GLU:H	2.11	0.57
29:A:740:HOH:O	6:F:37:LYS:HE3	2.04	0.57
1:A:112:LEU:C	1:A:112:LEU:CD2	2.79	0.56
1:A:278[B]:MET:HE1	19:A:607:LFA:H52	1.87	0.56
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.41	0.56
14:N:602:HEA:H121	22:N:621:XE:XE	2.84	0.56
1:N:53:ILE:HG12	29:N:887:HOH:O	2.06	0.55
1:A:1:FME:HE2	1:A:1:FME:HA	1.88	0.55
3:P:67:PHE:CE2	18:P:305:CDL:O1	2.60	0.55
3:C:33[A]:MET:HE1	3:C:41:THR:HB	1.88	0.55
3:C:67:PHE:CE2	18:C:304:CDL:O1	2.59	0.55
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.87	0.55
6:F:85:CYS:SG	6:F:87[B]:THR:OG1	2.65	0.55
7:G:12:GLY:HA3	29:G:236:HOH:O	2.06	0.55
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.90	0.54
19:P:310:LFA:C4	29:U:213:HOH:O	2.56	0.54
28:T:102:PEK:H32	28:T:102:PEK:C7	2.37	0.54
3:C:226:HIS:HE1	18:C:304:CDL:H111	1.72	0.54
20:P:323:DMU:C2	20:P:323:DMU:O3	2.56	0.54
18:C:304:CDL:H531	18:C:304:CDL:HB4	1.90	0.54
18:P:305:CDL:OB2	10:W:8:LYS:HE3	2.08	0.54
3:C:104:SER:OG	29:C:404:HOH:O	2.18	0.54
3:C:33[B]:MET:HE3	3:C:42:LEU:HD12	1.90	0.53
18:C:304:CDL:OB9	18:C:304:CDL:PA1	2.66	0.53
18:C:304:CDL:H752	10:J:27:THR:HG21	1.89	0.53
1:N:297[B]:MET:SD	1:N:302:ARG:CG	2.96	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:D:201:DMU:H36	20:D:201:DMU:O55	2.09	0.53
18:P:305:CDL:HA62	18:P:305:CDL:C12	2.33	0.53
3:C:258:TRP:CE2	19:C:307:LFA:H32	2.44	0.53
2:O:31:VAL:HG23	22:O:305:XE:XE	2.87	0.53
6:S:54:ASN:HD22	6:S:54:ASN:C	2.17	0.53
2:O:16[A]:ILE:HG21	2:O:87[A]:MET:SD	2.48	0.53
2:B:16[A]:ILE:HD11	2:B:86:MET:HG2	1.92	0.52
4:D:17[B]:VAL:HG22	4:D:19:ARG:HG3	1.92	0.52
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.10	0.52
12:L:26:THR:CG2	20:L:102:DMU:H26	2.39	0.52
18:Y:101:CDL:HB22	18:Y:101:CDL:CA3	2.39	0.52
2:B:1:FME:HE1	2:B:133:LEU:HD22	1.92	0.52
20:P:323:DMU:O3	20:P:323:DMU:O55	2.28	0.52
1:N:112:LEU:HD23	1:N:112:LEU:O	2.10	0.52
14:A:601:HEA:H121	22:A:618:XE:XE	2.88	0.51
4:D:86:MET:HE1	11:K:22:ALA:HB2	1.92	0.51
5:R:90:ARG:NH1	29:R:305:HOH:O	2.40	0.51
1:N:278[B]:MET:SD	19:N:608:LFA:C5	2.99	0.51
1:A:112:LEU:O	1:A:112:LEU:CD2	2.58	0.51
2:O:32[B]:PHE:CD2	9:V:31:PHE:CZ	2.99	0.51
18:C:304:CDL:HB61	18:C:304:CDL:CB2	2.41	0.50
29:C:472[B]:HOH:O	10:J:27:THR:HG22	2.12	0.50
2:B:22[B]:HIS:HE1	9:I:44:LYS:CE	2.24	0.50
2:B:33:LEU:HD13	9:I:31:PHE:CD2	2.46	0.50
1:A:112:LEU:HD23	1:A:112:LEU:C	2.36	0.50
18:C:304:CDL:OA3	18:C:304:CDL:H1	2.02	0.50
8:H:23:GLN:NE2	29:H:201:HOH:O	2.44	0.50
4:D:127:LYS:HD2	29:I:137:HOH:O	2.11	0.50
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.93	0.50
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:CG	2.35	0.49
18:P:305:CDL:HB32	18:P:305:CDL:CB2	2.41	0.49
8:H:23:GLN:HG3	29:H:232:HOH:O	2.13	0.49
18:Y:101:CDL:HB22	18:Y:101:CDL:HA32	1.95	0.49
3:C:180[B]:GLU:HG2	29:C:410:HOH:O	2.12	0.49
3:P:116:TRP:HA	3:P:117:PRO:C	2.37	0.49
8:U:43:MET:O	8:U:48:GLY:N	2.44	0.49
2:O:83:ILE:HG22	2:O:87[A]:MET:HE2	1.94	0.49
18:C:304:CDL:HB22	10:J:8:LYS:HE3	1.95	0.49
1:N:278[B]:MET:SD	19:N:608:LFA:H51	2.52	0.49
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.93	0.49
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16[B]:ILE:HG13	2:B:17:MET:N	2.28	0.48
3:C:38:ASN:ND2	20:C:318:DMU:O4	2.46	0.48
1:N:362[A]:SER:OG	2:O:87[A]:MET:HE2	2.13	0.48
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.43	0.48
1:N:76:GLY:O	1:N:80:ASN:HB2	2.13	0.48
2:O:59:GLN:HE21	19:O:303:LFA:H31	1.77	0.48
18:C:304:CDL:HB4	18:C:304:CDL:C53	2.42	0.48
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.94	0.48
1:N:136[B]:LEU:HD11	29:N:926:HOH:O	2.13	0.48
1:N:423[B]:MET:HA	18:N:607:CDL:H782	1.96	0.48
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.48
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.96	0.48
18:C:304:CDL:C75	10:J:27:THR:HG21	2.44	0.48
8:H:23:GLN:NE2	29:H:203:HOH:O	2.46	0.48
2:O:58:ALA:O	2:O:62:GLU:HG3	2.14	0.47
2:B:22[B]:HIS:CE1	9:I:44:LYS:CE	2.92	0.47
1:N:365:ILE:HD11	29:N:709:HOH:O	2.12	0.47
12:Y:26:THR:HG21	20:Y:102:DMU:H26	1.96	0.47
8:H:52:VAL:HG21	8:U:43:MET:HE1	1.96	0.47
20:C:323:DMU:H10	10:J:53:ALA:HB2	1.97	0.47
1:N:486:ASP:OD2	4:Q:19:ARG:NE	2.47	0.47
3:P:40:MET:O	3:P:44[B]:MET:HG3	2.14	0.47
29:Q:342:HOH:O	5:R:108:LYS:HD3	2.14	0.47
20:P:323:DMU:O3	20:P:323:DMU:H2	2.13	0.47
6:F:84:SER:HB2	21:F:101:EDO:H21	1.97	0.47
12:L:13:PHE:HA	18:L:101:CDL:HB31	1.97	0.47
3:P:247:VAL:HG11	19:P:313:LFA:H71	1.97	0.47
18:Y:101:CDL:OB9	18:Y:101:CDL:H122	2.15	0.47
1:A:321:PHE:CD2	2:B:65:TRP:HB2	2.51	0.46
6:F:92:VAL:HG23	6:F:92:VAL:O	2.15	0.46
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.51	0.46
3:C:37:PHE:CE2	20:C:323:DMU:H13	2.50	0.46
2:B:60:GLU:H	2:B:60:GLU:CD	2.23	0.46
1:N:240:HIS:C	1:N:240:HIS:CD2	2.93	0.46
1:A:486:ASP:CB	29:A:907[B]:HOH:O	2.60	0.46
18:C:304:CDL:HB4	18:C:304:CDL:C52	2.46	0.46
29:P:416:HOH:O	6:S:3:GLY:HA3	2.15	0.46
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.15	0.46
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.96	0.46
3:C:33[B]:MET:HG3	3:C:37:PHE:HB2	1.98	0.46
3:C:51[A]:MET:HE1	23:C:303:PGV:C16	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:34:SER:HB2	14:N:602:HEA:C2B	2.45	0.46
1:N:423[A]:MET:HA	18:N:607:CDL:H782	1.98	0.46
1:A:278[B]:MET:HE3	1:A:278[B]:MET:HB3	1.82	0.46
3:C:160:LEU:HD13	25:C:305:CHD:H181	1.98	0.46
2:O:41:ILE:O	2:O:45:MET:HG2	2.16	0.46
6:S:37:LYS:HG3	29:S:203:HOH:O	2.16	0.46
6:S:92:VAL:O	6:S:92:VAL:HG23	2.16	0.46
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.50	0.46
18:C:304:CDL:C39	18:C:304:CDL:C62	2.94	0.46
18:P:305:CDL:HB32	18:P:305:CDL:HB21	1.97	0.46
18:P:305:CDL:CB2	10:W:8:LYS:HE3	2.46	0.46
14:A:601:HEA:H14	22:A:618:XE:XE	2.94	0.45
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.97	0.45
1:A:297[B]:MET:O	1:A:302:ARG:NH2	2.47	0.45
3:C:116:TRP:HA	3:C:117:PRO:C	2.41	0.45
1:N:377:PHE:O	1:N:381:LEU:HB3	2.16	0.45
2:O:60:GLU:CD	2:O:60:GLU:N	2.73	0.45
3:P:207:HIS:HD2	3:P:241:TYR:OH	2.00	0.45
3:C:59:ARG:HG3	18:C:304:CDL:HA4	1.99	0.45
1:N:302:ARG:HD2	29:N:709:HOH:O	2.17	0.45
1:N:310:MET:HE1	2:O:77:ALA:HB2	1.99	0.45
1:N:362[A]:SER:HA	2:O:87[A]:MET:HE1	1.98	0.45
5:R:46:LYS:NZ	29:R:303:HOH:O	2.49	0.45
1:A:115[A]:SER:O	1:A:121:GLY:HA2	2.17	0.45
19:C:313:LFA:H21	19:C:314:LFA:H71	1.98	0.45
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.99	0.45
8:H:52:VAL:HG12	8:U:46:LYS:CG	2.36	0.44
2:O:59:GLN:NE2	19:O:303:LFA:C3	2.80	0.44
1:A:31:THR:O	1:A:35:LEU:HD22	2.16	0.44
18:C:304:CDL:HB21	18:C:304:CDL:HB61	2.00	0.44
1:A:87:ILE:O	1:A:173:PRO:HD3	2.17	0.44
2:B:58:ALA:O	2:B:62:GLU:HG3	2.16	0.44
3:C:133:ASN:ND2	29:C:407:HOH:O	2.43	0.44
3:C:210:ILE:HD13	23:C:303:PGV:H312	2.00	0.44
3:P:50:ASN:HD22	3:P:51[A]:MET:HE2	1.82	0.44
1:N:278[B]:MET:SD	19:N:608:LFA:H52	2.57	0.44
7:T:50:TYR:HB3	7:T:52:HIS:CE1	2.53	0.44
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.52	0.44
2:B:67:ILE:HD11	19:B:308:LFA:H42	2.00	0.43
12:Y:24:MET:HG3	29:Y:210:HOH:O	2.17	0.43
1:N:361[A]:SER:OG	2:O:84:LEU:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:121:TYR:O	2:O:138:VAL:HA	2.17	0.43
2:O:196:CYS:HB2	2:O:207:MET:HG3	2.00	0.43
8:U:60:TYR:CD1	8:U:60:TYR:C	2.96	0.43
3:C:205:GLY:HA3	28:G:101:PEK:H192	1.99	0.43
1:N:112:LEU:CD2	1:N:112:LEU:C	2.92	0.43
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.18	0.43
29:N:867:HOH:O	4:Q:20:ARG:HG2	2.17	0.43
3:P:226:HIS:HE1	18:P:305:CDL:H111	1.83	0.43
1:A:76:GLY:O	1:A:80:ASN:HB2	2.19	0.43
18:C:304:CDL:H751	18:C:304:CDL:H711	1.99	0.43
18:P:305:CDL:OA3	18:P:305:CDL:H1	2.14	0.43
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	2.01	0.43
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.18	0.43
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.54	0.43
1:A:409:TRP:HB3	1:A:471:ILE:HG12	2.01	0.43
2:B:60:GLU:CD	2:B:60:GLU:N	2.77	0.43
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.54	0.43
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.72	0.43
18:P:305:CDL:HB4	18:P:305:CDL:H521	2.00	0.43
25:P:306:CHD:C23	25:P:306:CHD:C16	2.96	0.43
19:P:310:LFA:C5	29:U:213:HOH:O	2.66	0.43
8:H:22:ASN:ND2	20:H:101:DMU:O3	2.52	0.43
2:O:16[A]:ILE:CD1	2:O:87[A]:MET:HG2	2.40	0.43
2:O:59:GLN:HE22	19:O:303:LFA:C3	2.32	0.43
1:N:449:MET:SD	2:O:5:MET:HG2	2.59	0.42
18:Y:101:CDL:HB22	18:Y:101:CDL:HA31	2.01	0.42
12:L:26:THR:HG21	20:L:102:DMU:C37	2.50	0.42
18:L:101:CDL:C76	18:L:101:CDL:C72	2.97	0.42
1:N:488:THR:HB	1:N:495:LEU:HD13	2.01	0.42
3:P:131:LEU:HD21	20:T:105:DMU:H18	2.02	0.42
3:C:164:PHE:CE1	25:C:305:CHD:H192	2.53	0.42
8:H:60:TYR:CD1	8:H:60:TYR:C	2.97	0.42
1:N:423[B]:MET:HE2	1:N:457:GLY:CA	2.50	0.42
12:Y:19:TRP:CD2	20:Y:102:DMU:H6	2.55	0.42
1:A:71:MET:HE1	1:A:195:LEU:HD21	2.01	0.42
1:A:149:SER:OG	22:A:613:XE:XE	3.15	0.42
2:B:108:TYR:O	2:B:117:SER:HA	2.19	0.42
20:Q:201:DMU:O55	20:Q:201:DMU:H36	2.20	0.42
1:A:278[B]:MET:SD	19:A:607:LFA:C5	3.08	0.42
1:A:377:PHE:O	1:A:381:LEU:HB3	2.20	0.42
18:C:304:CDL:HB61	18:C:304:CDL:HB22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:19:TYR:CD1	1:N:76:GLY:HA3	2.55	0.42
3:C:144[A]:ILE:HD13	3:C:239:ALA:HA	2.02	0.42
13:M:37:LEU:HA	13:M:37:LEU:HD23	1.86	0.42
18:Y:101:CDL:H711	18:Y:101:CDL:H361	2.01	0.42
2:B:16[A]:ILE:HD13	2:B:16[A]:ILE:HA	1.95	0.41
3:C:54[A]:MET:HE1	23:C:303:PGV:C14	2.48	0.41
18:P:305:CDL:CA5	18:P:305:CDL:OA8	2.68	0.41
12:Y:13:PHE:HB3	18:Y:101:CDL:H512	2.02	0.41
7:G:34:ASN:O	7:G:38:HIS:CD2	2.70	0.41
12:Y:3:TYR:N	29:Y:203:HOH:O	2.52	0.41
1:A:240:HIS:CD2	1:A:240:HIS:C	2.98	0.41
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.03	0.41
9:I:36:LYS:HE3	9:I:36:LYS:HA	2.01	0.41
3:P:210:ILE:HG21	23:P:304:PGV:H282	2.02	0.41
7:T:37:LEU:HD12	7:T:37:LEU:HA	1.95	0.41
18:P:305:CDL:H121	18:P:305:CDL:OA8	2.20	0.41
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.55	0.41
3:C:180[A]:GLU:OE2	29:C:405:HOH:O	2.22	0.41
1:N:22:PHE:HA	18:Y:101:CDL:H802	2.02	0.41
2:O:33:LEU:HD13	9:V:31:PHE:CD2	2.55	0.41
1:A:334:TRP:CZ3	20:A:608:DMU:H19	2.56	0.41
29:A:744:HOH:O	3:C:77:LYS:CE	2.52	0.41
1:N:62:ALA:HB2	14:N:602:HEA:HBD1	2.03	0.41
1:N:87:ILE:O	1:N:173:PRO:HD3	2.21	0.41
2:O:82:ARG:HA	20:O:304:DMU:H30	2.02	0.41
3:P:51[B]:MET:HE3	18:P:305:CDL:C87	2.51	0.41
3:P:177:GLN:OE1	3:P:177:GLN:HA	2.21	0.41
1:A:32:ALA:HB3	12:L:36:PRO:HG2	2.03	0.40
1:A:107:PRO:HB3	3:C:25:LEU:HB2	2.02	0.40
22:A:616:XE:XE	12:L:39:ILE:HG21	2.99	0.40
10:W:3:ASN:OD1	10:W:3:ASN:C	2.63	0.40
13:Z:27:LEU:HD22	20:Z:101:DMU:H14	2.03	0.40
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.03	0.40
14:N:602:HEA:C14	22:N:621:XE:XE	3.47	0.40
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	3.09	0.40
2:B:59:GLN:NE2	2:B:59:GLN:O	2.54	0.40
3:C:50:ASN:HD21	3:C:54[A]:MET:HE2	1.85	0.40
3:C:149:HIS:NE2	19:C:312:LFA:H21	2.37	0.40
6:F:21[B]:MET:HE2	6:F:21[B]:MET:HB2	1.91	0.40
1:N:489:THR:HA	6:S:71:TRP:O	2.21	0.40
2:O:82:ARG:O	2:O:86:MET:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:82:TYR:HB3	5:R:83:PRO:HD3	2.02	0.40
1:A:308:ALA:O	1:A:311[B]:ILE:HG12	2.21	0.40
2:O:13:THR:HB	2:O:168:LEU:HD23	2.03	0.40
3:P:127:LEU:HD13	20:T:105:DMU:H10	2.03	0.40
1:A:278[A]:MET:HE1	7:T:18:PHE:CZ	2.55	0.40
7:G:19:LEU:HD23	19:G:104:LFA:H61	2.03	0.40
6:S:21[B]:MET:HE2	6:S:21[B]:MET:HB2	1.88	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	526/514 (102%)	512 (97%)	14 (3%)	0	100	100
1	N	526/514 (102%)	514 (98%)	12 (2%)	0	100	100
2	B	230/227 (101%)	223 (97%)	7 (3%)	0	100	100
2	O	230/227 (101%)	223 (97%)	7 (3%)	0	100	100
3	C	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
3	P	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	136/147 (92%)	132 (97%)	4 (3%)	0	100	100
5	E	100/109 (92%)	100 (100%)	0	0	100	100
5	R	100/109 (92%)	100 (100%)	0	0	100	100
6	F	91/98 (93%)	91 (100%)	0	0	100	100
6	S	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
7	G	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
7	T	71/85 (84%)	69 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
8	U	73/85 (86%)	71 (97%)	1 (1%)	1 (1%)	9	2
9	I	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
9	V	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
10	J	54/59 (92%)	54 (100%)	0	0	100	100
10	W	54/59 (92%)	54 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
12	Y	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
13	M	38/46 (83%)	37 (97%)	1 (3%)	0	100	100
13	Z	38/46 (83%)	37 (97%)	1 (3%)	0	100	100
All	All	3488/3614 (96%)	3417 (98%)	70 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	U	48	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/426 (103%)	438 (100%)	2 (0%)	86	86
1	N	440/426 (103%)	437 (99%)	3 (1%)	81	79
2	B	215/210 (102%)	206 (96%)	9 (4%)	25	13
2	O	215/210 (102%)	209 (97%)	6 (3%)	38	27
3	C	232/226 (103%)	230 (99%)	2 (1%)	75	72
3	P	232/226 (103%)	230 (99%)	2 (1%)	75	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	128/129 (99%)	128 (100%)	0	100	100
4	Q	122/129 (95%)	120 (98%)	2 (2%)	58	50
5	E	89/95 (94%)	89 (100%)	0	100	100
5	R	89/95 (94%)	88 (99%)	1 (1%)	70	65
6	F	78/81 (96%)	75 (96%)	3 (4%)	28	16
6	S	78/81 (96%)	74 (95%)	4 (5%)	20	9
7	G	63/69 (91%)	60 (95%)	3 (5%)	21	10
7	T	63/69 (91%)	60 (95%)	3 (5%)	21	10
8	H	67/75 (89%)	65 (97%)	2 (3%)	36	24
8	U	67/75 (89%)	64 (96%)	3 (4%)	23	11
9	I	55/58 (95%)	54 (98%)	1 (2%)	54	45
9	V	55/58 (95%)	51 (93%)	4 (7%)	11	3
10	J	47/50 (94%)	46 (98%)	1 (2%)	48	38
10	W	47/50 (94%)	45 (96%)	2 (4%)	25	12
11	K	39/46 (85%)	38 (97%)	1 (3%)	41	29
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	37/40 (92%)	37 (100%)	0	100	100
12	Y	37/40 (92%)	36 (97%)	1 (3%)	40	28
13	M	34/38 (90%)	33 (97%)	1 (3%)	37	26
13	Z	34/38 (90%)	32 (94%)	2 (6%)	16	6
All	All	3042/3086 (99%)	2984 (98%)	58 (2%)	52	43

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	A	369	ASP
2	B	33	LEU
2	B	59	GLN
2	B	60	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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Mol	Chain	Res	Type
2	B	115	ASP
3	C	159	MET
3	C	230	ASN
6	F	80	GLN
6	F	87[A]	THR
6	F	87[B]	THR
7	G	33	LEU
7	G	37	LEU
7	G	43	GLU
8	H	46	LYS
8	H	60	TYR
9	I	36	LYS
10	J	7	GLU
11	K	54	ARG
13	M	38	ASP
1	N	112	LEU
1	N	152	LEU
1	N	369	ASP
2	O	33	LEU
2	O	60	GLU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	115	ASP
3	P	159	MET
3	P	230	ASN
4	Q	10	ASP
4	Q	51	LEU
5	R	79	LYS
6	S	37	LYS
6	S	43	LYS
6	S	54	ASN
6	S	80	GLN
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
8	U	46	LYS
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	18	ARG
9	V	29	LEU

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Mol	Chain	Res	Type
9	V	65	LYS
10	W	7	GLU
10	W	50	LEU
12	Y	26	THR
13	Z	13	LYS
13	Z	38	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	52	HIS
2	B	59	GLN
2	B	203	ASN
3	C	38	ASN
3	C	50	ASN
3	C	76	GLN
4	D	119	GLN
5	E	94	ASN
6	F	54	ASN
7	G	38	HIS
8	H	22	ASN
8	H	28	ASN
8	H	32	ASN
8	H	37	HIS
10	J	29	ASN
11	K	35	GLN
2	O	26	HIS
2	O	59	GLN
2	O	92	ASN
2	O	203	ASN
3	P	50	ASN
4	Q	109	HIS
4	Q	119	GLN
4	Q	143	ASN
5	R	94	ASN
6	S	54	ASN
7	T	34	ASN
8	U	12	GLN
8	U	22	ASN
8	U	28	ASN
8	U	32	ASN
8	U	37	HIS

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Mol	Chain	Res	Type
9	V	8	GLN
10	W	29	ASN
11	X	35	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](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	FME	N	1	1	8,9,10	0.81	0	7,9,11	1.48	1 (14%)
1	FME	A	1	1	8,9,10	0.51	0	7,9,11	1.18	0
2	FME	B	1	2	8,9,10	1.04	1 (12%)	7,9,11	1.21	1 (14%)
2	FME	O	1	2	8,9,10	0.68	0	7,9,11	1.25	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	N	1	1	-	4/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-2.65	1.67	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	O-C-CA	-2.65	117.83	124.78
2	B	1	FME	CG-CB-CA	-2.38	106.33	112.95
2	O	1	FME	O-C-CA	-2.34	118.65	124.78

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
1	N	1	FME	CA-CB-CG-SD
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	CB-CG-SD-CE
1	A	1	FME	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
2	B	1	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 147 ligands modelled in this entry, 24 are monoatomic and 2 are unknown - leaving 121 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
19	LFA	C	307	-	10,10,19	0.24	0	9,9,18	0.18	0
21	EDO	N	614	-	3,3,3	0.14	0	2,2,2	0.23	0
19	LFA	O	303	-	10,10,19	0.24	0	9,9,18	0.15	0
21	EDO	N	615	-	3,3,3	0.32	0	2,2,2	0.30	0
19	LFA	P	311	-	10,10,19	0.20	0	9,9,18	0.10	0
21	EDO	P	320	-	3,3,3	0.38	0	2,2,2	0.22	0
25	CHD	P	306	-	32,32,32	0.75	0	51,51,51	1.42	9 (17%)
21	EDO	A	612	-	3,3,3	0.67	0	2,2,2	0.19	0
25	CHD	O	301	-	32,32,32	0.73	0	51,51,51	0.90	1 (1%)
20	DMU	T	105	-	22,22,34	0.77	0	27,27,45	1.55	4 (14%)
25	CHD	P	302	-	32,32,32	0.98	2 (6%)	51,51,51	0.74	2 (3%)
19	LFA	N	608	-	13,13,19	0.37	0	12,12,18	0.27	0
23	PGV	N	622	-	50,50,50	0.86	2 (4%)	53,56,56	1.20	4 (7%)
19	LFA	C	312	-	10,10,19	0.26	0	9,9,18	0.28	0
20	DMU	U	101	-	34,34,34	0.94	2 (5%)	45,45,45	1.47	6 (13%)
19	LFA	P	313	-	14,14,19	0.38	0	13,13,18	0.22	0
21	EDO	S	102	-	3,3,3	0.34	0	2,2,2	0.20	0
14	HEA	N	603	1	57,67,67	1.86	14 (24%)	61,103,103	2.37	23 (37%)
20	DMU	C	306	-	10,10,34	0.40	0	9,9,45	0.56	0
14	HEA	A	602	1	57,67,67	1.86	15 (26%)	61,103,103	2.22	21 (34%)
28	PEK	G	101	-	52,52,52	0.58	1 (1%)	55,57,57	0.67	0
20	DMU	O	309	-	22,22,34	0.75	1 (4%)	27,27,45	1.35	3 (11%)
20	DMU	A	620	-	10,10,34	0.50	0	9,9,45	0.47	0
20	DMU	M	101	-	34,34,34	1.13	2 (5%)	45,45,45	0.98	2 (4%)
20	DMU	N	609	-	6,6,34	0.40	0	5,5,45	0.33	0
21	EDO	B	306	-	3,3,3	0.13	0	2,2,2	0.37	0
20	DMU	M	102	-	7,7,34	0.39	0	6,6,45	0.43	0
19	LFA	P	310	-	17,17,19	0.25	0	16,16,18	0.21	0
19	LFA	C	325	-	14,14,19	0.24	0	13,13,18	0.16	0
21	EDO	R	201	-	3,3,3	0.15	0	2,2,2	0.14	0
20	DMU	C	319	-	34,34,34	0.73	0	45,45,45	1.32	6 (13%)
20	DMU	B	305	-	22,22,34	0.72	0	27,27,45	0.90	1 (3%)
18	CDL	L	101	-	93,93,99	0.45	0	99,105,111	0.63	2 (2%)
28	PEK	T	102	-	52,52,52	0.69	2 (3%)	55,57,57	0.78	2 (3%)
19	LFA	P	308	-	10,10,19	0.22	0	9,9,18	0.23	0
20	DMU	C	315	-	34,34,34	0.86	2 (5%)	45,45,45	1.62	7 (15%)
21	EDO	N	611	-	3,3,3	0.31	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	DMU	A	609	-	34,34,34	1.12	4 (11%)	45,45,45	1.31	8 (17%)
20	DMU	D	201	-	34,34,34	1.31	6 (17%)	45,45,45	1.44	6 (13%)
21	EDO	S	103	-	3,3,3	0.11	0	2,2,2	0.21	0
21	EDO	C	322	-	3,3,3	1.14	0	2,2,2	0.71	0
20	DMU	Z	101	-	34,34,34	0.97	1 (2%)	45,45,45	1.11	5 (11%)
19	LFA	G	104	-	13,13,19	0.57	0	12,12,18	0.26	0
20	DMU	Q	201	-	34,34,34	1.39	6 (17%)	45,45,45	1.63	7 (15%)
20	DMU	G	102	-	22,22,34	0.74	0	27,27,45	1.02	1 (3%)
20	DMU	Z	102	-	7,7,34	0.32	0	6,6,45	0.43	0
20	DMU	B	303	-	10,10,34	0.16	0	9,9,45	0.73	0
24	CUA	B	302	2	0,1,1	-	-	-	-	-
21	EDO	F	103	-	3,3,3	0.24	0	2,2,2	0.29	0
20	DMU	A	608	-	6,6,34	0.59	0	5,5,45	0.27	0
21	EDO	C	321	-	3,3,3	0.42	0	2,2,2	0.15	0
21	EDO	O	310	-	3,3,3	0.14	0	2,2,2	0.26	0
19	LFA	C	313	-	14,14,19	0.29	0	13,13,18	0.39	0
21	EDO	E	203	-	3,3,3	0.11	0	2,2,2	0.03	0
19	LFA	T	103	-	13,13,19	0.27	0	12,12,18	0.17	0
21	EDO	E	202	-	3,3,3	0.15	0	2,2,2	0.12	0
19	LFA	P	309	-	5,5,19	0.27	0	4,4,18	0.10	0
20	DMU	C	317	-	22,22,34	0.84	1 (4%)	27,27,45	1.12	2 (7%)
19	LFA	C	310	-	10,10,19	0.36	0	9,9,18	0.20	0
21	EDO	R	202	-	3,3,3	0.16	0	2,2,2	0.47	0
24	CUA	O	306	2	0,1,1	-	-	-	-	-
20	DMU	P	318	-	34,34,34	1.00	3 (8%)	45,45,45	1.25	2 (4%)
21	EDO	R	203	-	3,3,3	0.50	0	2,2,2	0.40	0
19	LFA	A	607	-	13,13,19	0.29	0	12,12,18	0.20	0
21	EDO	N	612	-	3,3,3	0.37	0	2,2,2	0.16	0
19	LFA	P	312	-	10,10,19	0.19	0	9,9,18	0.23	0
19	LFA	C	311	-	13,13,19	0.27	0	12,12,18	0.21	0
19	LFA	P	314	-	12,12,19	0.27	0	11,11,18	0.35	0
21	EDO	G	103	-	3,3,3	0.16	0	2,2,2	0.05	0
20	DMU	N	610	-	34,34,34	1.52	6 (17%)	45,45,45	1.19	3 (6%)
20	DMU	W	101	-	10,10,34	0.17	0	9,9,45	0.69	0
19	LFA	B	308	-	16,16,19	0.34	0	15,15,18	0.18	0
19	LFA	C	308	-	5,5,19	0.26	0	4,4,18	0.12	0
20	DMU	L	102	-	22,22,34	0.58	0	27,27,45	1.04	1 (3%)
21	EDO	C	320	-	3,3,3	0.10	0	2,2,2	0.16	0
20	DMU	O	307	-	10,10,34	0.23	0	9,9,45	0.56	0
18	CDL	A	606	-	63,63,99	0.54	0	69,75,111	1.10	5 (7%)
20	DMU	P	316	-	6,6,34	0.24	0	5,5,45	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	LFA	T	104	-	10,10,19	0.27	0	9,9,18	0.19	0
23	PGV	P	304	-	50,50,50	0.92	4 (8%)	53,56,56	1.01	4 (7%)
18	CDL	P	305	-	86,86,99	0.65	2 (2%)	92,98,111	1.15	9 (9%)
21	EDO	T	106	-	3,3,3	0.34	0	2,2,2	0.24	0
25	CHD	C	301	-	32,32,32	1.01	3 (9%)	51,51,51	0.78	2 (3%)
14	HEA	N	602	1	57,67,67	1.98	17 (29%)	61,103,103	2.72	26 (42%)
20	DMU	O	304	-	22,22,34	0.94	1 (4%)	27,27,45	1.53	5 (18%)
21	EDO	A	611	-	3,3,3	0.27	0	2,2,2	0.44	0
19	LFA	O	302	-	16,16,19	0.20	0	15,15,18	0.16	0
25	CHD	C	305	-	32,32,32	0.77	0	51,51,51	1.55	7 (13%)
21	EDO	N	613	-	3,3,3	0.38	0	2,2,2	0.15	0
20	DMU	C	323	-	34,34,34	0.86	0	45,45,45	1.24	2 (4%)
18	CDL	C	304	-	86,86,99	0.59	0	92,98,111	1.30	8 (8%)
23	PGV	A	619	-	50,50,50	0.74	2 (4%)	53,56,56	0.97	2 (3%)
23	PGV	C	303	-	50,50,50	0.73	1 (2%)	53,56,56	1.01	3 (5%)
20	DMU	N	601	-	10,10,34	0.55	0	9,9,45	0.50	0
21	EDO	F	104	-	3,3,3	0.23	0	2,2,2	0.13	0
20	DMU	P	315	-	34,34,34	0.75	1 (2%)	45,45,45	1.54	8 (17%)
21	EDO	A	610	-	3,3,3	0.23	0	2,2,2	0.05	0
19	LFA	C	309	-	17,17,19	0.29	0	16,16,18	0.30	0
19	LFA	C	314	-	12,12,19	0.23	0	11,11,18	0.23	0
19	LFA	T	101	-	13,13,19	0.80	0	12,12,18	0.57	0
20	DMU	C	318	-	34,34,34	0.95	3 (8%)	45,45,45	1.25	4 (8%)
21	EDO	E	201	-	3,3,3	0.13	0	2,2,2	0.24	0
21	EDO	P	322	-	3,3,3	0.52	0	2,2,2	0.84	0
20	DMU	P	307	-	10,10,34	0.28	0	9,9,45	0.68	0
21	EDO	P	321	-	3,3,3	0.34	0	2,2,2	0.30	0
19	LFA	P	301	-	14,14,19	0.21	0	13,13,18	0.17	0
20	DMU	O	308	-	10,10,34	0.44	0	9,9,45	0.48	0
20	DMU	Y	102	-	22,22,34	0.76	1 (4%)	27,27,45	1.08	2 (7%)
20	DMU	J	101	-	10,10,34	0.28	0	9,9,45	0.61	0
21	EDO	F	101	-	3,3,3	0.46	0	2,2,2	0.52	0
20	DMU	C	316	-	6,6,34	0.34	0	5,5,45	0.48	0
14	HEA	A	601	1	57,67,67	2.14	16 (28%)	61,103,103	2.57	22 (36%)
20	DMU	B	309	-	22,22,34	0.91	0	27,27,45	1.47	5 (18%)
20	DMU	P	319	-	34,34,34	1.11	3 (8%)	45,45,45	1.31	3 (6%)
20	DMU	P	317	-	22,22,34	0.73	2 (9%)	27,27,45	1.30	4 (14%)
18	CDL	Y	101	-	93,93,99	0.49	0	99,105,111	0.60	0
20	DMU	B	304	-	10,10,34	0.50	0	9,9,45	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CHD	B	307	-	32,32,32	0.90	0	51,51,51	0.77	1 (1%)
18	CDL	N	607	-	63,63,99	0.59	0	69,75,111	1.25	7 (10%)
20	DMU	P	323	-	34,34,34	0.73	1 (2%)	45,45,45	1.51	6 (13%)
20	DMU	H	101	-	34,34,34	1.24	5 (14%)	45,45,45	1.32	5 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LFA	C	307	-	-	4/8/8/17	-
21	EDO	N	614	-	-	0/1/1/1	-
19	LFA	O	303	-	-	3/8/8/17	-
21	EDO	N	615	-	-	0/1/1/1	-
19	LFA	P	311	-	-	6/8/8/17	-
21	EDO	P	320	-	-	1/1/1/1	-
25	CHD	P	306	-	-	8/9/74/74	0/4/4/4
21	EDO	A	612	-	-	0/1/1/1	-
25	CHD	O	301	-	-	2/9/74/74	0/4/4/4
20	DMU	T	105	-	-	8/13/33/59	0/1/1/2
25	CHD	P	302	-	-	2/9/74/74	0/4/4/4
19	LFA	N	608	-	-	3/11/11/17	-
23	PGV	N	622	-	-	10/55/55/55	-
19	LFA	C	312	-	-	3/8/8/17	-
20	DMU	U	101	-	-	7/19/59/59	0/2/2/2
19	LFA	P	313	-	-	7/12/12/17	-
21	EDO	S	102	-	-	0/1/1/1	-
14	HEA	N	603	1	-	5/32/76/76	-
20	DMU	C	306	-	-	2/8/8/59	-
14	HEA	A	602	1	-	7/32/76/76	-
28	PEK	G	101	-	-	17/56/56/56	-
20	DMU	O	309	-	-	2/13/33/59	0/1/1/2
20	DMU	A	620	-	-	3/8/8/59	-
20	DMU	M	101	-	-	4/19/59/59	0/2/2/2
20	DMU	N	609	-	-	3/4/4/59	-
21	EDO	B	306	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	M	102	-	-	3/5/5/59	-
19	LFA	P	310	-	-	9/15/15/17	-
19	LFA	C	325	-	-	9/12/12/17	-
21	EDO	R	201	-	-	1/1/1/1	-
20	DMU	C	319	-	-	11/19/59/59	0/2/2/2
20	DMU	B	305	-	-	7/13/33/59	0/1/1/2
18	CDL	L	101	-	-	51/104/104/110	-
28	PEK	T	102	-	-	21/56/56/56	-
19	LFA	P	308	-	-	3/8/8/17	-
20	DMU	C	315	-	-	14/19/59/59	0/2/2/2
21	EDO	N	611	-	-	0/1/1/1	-
20	DMU	A	609	-	-	8/19/59/59	0/2/2/2
20	DMU	D	201	-	-	10/19/59/59	0/2/2/2
21	EDO	S	103	-	-	0/1/1/1	-
21	EDO	C	322	-	-	1/1/1/1	-
20	DMU	Z	101	-	-	7/19/59/59	0/2/2/2
19	LFA	G	104	-	-	7/11/11/17	-
20	DMU	Q	201	-	-	8/19/59/59	0/2/2/2
20	DMU	G	102	-	-	8/13/33/59	0/1/1/2
20	DMU	Z	102	-	-	3/5/5/59	-
20	DMU	B	303	-	-	5/8/8/59	-
21	EDO	F	103	-	-	0/1/1/1	-
20	DMU	A	608	-	-	3/4/4/59	-
21	EDO	C	321	-	-	0/1/1/1	-
21	EDO	O	310	-	-	0/1/1/1	-
19	LFA	C	313	-	-	3/12/12/17	-
21	EDO	E	203	-	-	0/1/1/1	-
19	LFA	T	103	-	-	4/11/11/17	-
21	EDO	E	202	-	-	0/1/1/1	-
19	LFA	P	309	-	-	0/3/3/17	-
20	DMU	C	317	-	-	10/13/33/59	0/1/1/2
19	LFA	C	310	-	-	7/8/8/17	-
21	EDO	R	202	-	-	0/1/1/1	-
20	DMU	P	318	-	-	12/19/59/59	0/2/2/2
21	EDO	R	203	-	-	1/1/1/1	-
19	LFA	A	607	-	-	3/11/11/17	-
21	EDO	N	612	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LFA	P	312	-	-	3/8/8/17	-
19	LFA	C	311	-	-	6/11/11/17	-
19	LFA	P	314	-	-	3/10/10/17	-
21	EDO	G	103	-	-	0/1/1/1	-
20	DMU	N	610	-	-	5/19/59/59	0/2/2/2
20	DMU	W	101	-	-	4/8/8/59	-
19	LFA	B	308	-	-	7/14/14/17	-
19	LFA	C	308	-	-	1/3/3/17	-
20	DMU	L	102	-	-	11/13/33/59	0/1/1/2
21	EDO	C	320	-	-	0/1/1/1	-
20	DMU	O	307	-	-	5/8/8/59	-
18	CDL	A	606	-	-	37/74/74/110	-
20	DMU	P	316	-	-	3/4/4/59	-
19	LFA	T	104	-	-	4/8/8/17	-
23	PGV	P	304	-	-	12/55/55/55	-
18	CDL	P	305	-	-	50/97/97/110	-
21	EDO	T	106	-	-	0/1/1/1	-
25	CHD	C	301	-	-	2/9/74/74	0/4/4/4
14	HEA	N	602	1	-	2/32/76/76	-
20	DMU	O	304	-	-	4/13/33/59	0/1/1/2
21	EDO	A	611	-	-	1/1/1/1	-
19	LFA	O	302	-	-	6/14/14/17	-
25	CHD	C	305	-	-	8/9/74/74	0/4/4/4
21	EDO	N	613	-	-	0/1/1/1	-
20	DMU	C	323	-	-	4/19/59/59	0/2/2/2
18	CDL	C	304	-	-	54/97/97/110	-
23	PGV	A	619	-	-	7/55/55/55	-
23	PGV	C	303	-	-	12/55/55/55	-
20	DMU	N	601	-	-	4/8/8/59	-
21	EDO	F	104	-	-	1/1/1/1	-
20	DMU	P	315	-	-	7/19/59/59	0/2/2/2
21	EDO	A	610	-	-	0/1/1/1	-
19	LFA	C	309	-	-	9/15/15/17	-
19	LFA	C	314	-	-	3/10/10/17	-
19	LFA	T	101	-	-	5/11/11/17	-
20	DMU	C	318	-	-	12/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	E	201	-	-	0/1/1/1	-
21	EDO	P	322	-	-	1/1/1/1	-
20	DMU	P	307	-	-	4/8/8/59	-
21	EDO	P	321	-	-	0/1/1/1	-
19	LFA	P	301	-	-	7/12/12/17	-
20	DMU	O	308	-	-	3/8/8/59	-
20	DMU	Y	102	-	-	11/13/33/59	0/1/1/2
20	DMU	J	101	-	-	3/8/8/59	-
21	EDO	F	101	-	-	0/1/1/1	-
20	DMU	C	316	-	-	3/4/4/59	-
14	HEA	A	601	1	-	5/32/76/76	-
20	DMU	B	309	-	-	9/13/33/59	0/1/1/2
20	DMU	P	319	-	-	10/19/59/59	0/2/2/2
20	DMU	P	317	-	-	8/13/33/59	0/1/1/2
18	CDL	Y	101	-	-	53/104/104/110	-
20	DMU	B	304	-	-	4/8/8/59	-
25	CHD	B	307	-	-	2/9/74/74	0/4/4/4
18	CDL	N	607	-	-	41/74/74/110	-
20	DMU	P	323	-	-	6/19/59/59	0/2/2/2
20	DMU	H	101	-	-	8/19/59/59	0/2/2/2

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	C3A-C2A	6.13	1.48	1.40
14	N	603	HEA	C3A-C2A	5.09	1.47	1.40
14	N	602	HEA	C1D-ND	-5.04	1.31	1.40
14	A	601	HEA	C1D-ND	-4.95	1.31	1.40
20	N	610	DMU	O16-C6	-4.92	1.31	1.40
14	A	601	HEA	C3C-C2C	4.79	1.47	1.40
14	N	603	HEA	C1D-ND	-4.77	1.32	1.40
14	A	601	HEA	C4B-NB	-4.64	1.32	1.40
14	A	602	HEA	C1D-ND	-4.34	1.32	1.40
14	N	602	HEA	C3A-C2A	4.25	1.46	1.40
14	N	602	HEA	C3C-C2C	4.06	1.46	1.40
14	N	602	HEA	C4B-NB	-3.94	1.33	1.40
14	A	602	HEA	CHD-C1D	3.90	1.45	1.35
14	A	602	HEA	C3B-C2B	3.90	1.43	1.34
14	N	603	HEA	C4B-NB	-3.84	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	C4D-ND	-3.81	1.31	1.38
20	M	101	DMU	O3-C5	-3.76	1.34	1.43
14	N	603	HEA	C3B-C2B	3.75	1.43	1.34
14	N	602	HEA	C3B-C2B	3.74	1.43	1.34
14	A	601	HEA	CHD-C1D	3.71	1.44	1.35
14	A	602	HEA	C1B-NB	-3.70	1.31	1.38
14	N	603	HEA	C4D-ND	-3.59	1.31	1.38
20	Q	201	DMU	O3-C5	-3.54	1.34	1.43
14	A	602	HEA	C4B-NB	-3.52	1.34	1.40
14	A	601	HEA	C3D-C2D	3.47	1.44	1.36
14	N	602	HEA	CHC-C4B	3.45	1.43	1.35
14	N	603	HEA	C3D-C2D	3.40	1.43	1.36
14	A	601	HEA	C3B-C2B	3.39	1.42	1.34
20	Z	101	DMU	O3-C5	-3.38	1.35	1.43
14	N	602	HEA	CHD-C1D	3.34	1.43	1.35
14	N	602	HEA	C4D-ND	-3.33	1.31	1.38
25	P	302	CHD	O26-C24	-3.33	1.19	1.30
14	N	603	HEA	CHD-C1D	3.28	1.43	1.35
20	P	319	DMU	C7-C5	-3.27	1.44	1.52
14	A	602	HEA	C3A-C2A	3.26	1.44	1.40
14	A	601	HEA	CAA-C2A	-3.21	1.46	1.52
23	N	622	PGV	O03-C19	3.16	1.42	1.33
25	C	301	CHD	C22-C23	-3.16	1.42	1.52
20	Q	201	DMU	O5-C6	-3.14	1.33	1.41
20	H	101	DMU	O16-C6	-3.13	1.34	1.40
14	N	602	HEA	C1B-NB	-3.09	1.32	1.38
14	N	603	HEA	CHC-C4B	3.05	1.42	1.35
20	D	201	DMU	O61-C57	3.05	1.55	1.42
23	N	622	PGV	O01-C1	3.00	1.42	1.34
14	N	602	HEA	C3D-C2D	2.99	1.43	1.36
20	C	317	DMU	O16-C6	2.98	1.45	1.40
14	N	603	HEA	C2A-C1A	2.97	1.49	1.42
25	P	302	CHD	C22-C23	-2.97	1.43	1.52
14	A	602	HEA	C3C-C2C	2.96	1.44	1.40
14	A	601	HEA	CHC-C4B	2.95	1.42	1.35
14	N	603	HEA	C1B-NB	-2.94	1.32	1.38
14	N	602	HEA	CAA-C2A	-2.91	1.47	1.52
14	A	601	HEA	C4D-ND	-2.88	1.32	1.38
20	C	318	DMU	O5-C6	-2.84	1.34	1.41
20	A	609	DMU	O7-C10	2.83	1.49	1.41
20	P	319	DMU	C10-C5	-2.82	1.44	1.52
20	C	318	DMU	C7-C5	-2.82	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	T	102	PEK	C23-C22	-2.81	1.41	1.52
14	A	601	HEA	CMC-C2C	-2.79	1.45	1.51
20	N	610	DMU	C6-C1	-2.79	1.44	1.52
20	A	609	DMU	O16-C6	-2.78	1.35	1.40
14	A	601	HEA	C16-C17	-2.76	1.44	1.53
20	P	318	DMU	O5-C6	-2.73	1.34	1.41
14	A	601	HEA	C1B-NB	-2.72	1.33	1.38
14	A	602	HEA	C3D-C2D	2.70	1.42	1.36
20	D	201	DMU	O3-C5	-2.69	1.36	1.43
23	A	619	PGV	O01-C1	2.69	1.41	1.34
14	N	602	HEA	CBA-CGA	2.68	1.56	1.50
20	M	101	DMU	C7-C5	-2.65	1.45	1.52
20	O	309	DMU	C6-C1	-2.65	1.44	1.52
28	G	101	PEK	C23-C22	-2.64	1.42	1.52
20	D	201	DMU	O5-C6	-2.63	1.35	1.41
20	H	101	DMU	O5-C6	-2.63	1.35	1.41
23	P	304	PGV	O03-C19	2.63	1.41	1.33
20	P	318	DMU	C7-C5	-2.63	1.45	1.52
14	A	602	HEA	CBD-CAD	-2.61	1.43	1.52
25	C	301	CHD	O26-C24	-2.60	1.22	1.30
14	A	601	HEA	C12-C11	-2.59	1.48	1.52
14	A	602	HEA	C2A-C1A	2.58	1.48	1.42
20	U	101	DMU	C7-C5	-2.57	1.45	1.52
14	N	602	HEA	C4B-C3B	2.56	1.48	1.44
14	A	602	HEA	CHC-C4B	2.53	1.41	1.35
20	P	318	DMU	O3-C5	2.49	1.48	1.43
20	U	101	DMU	O1-C10	2.47	1.48	1.41
14	N	602	HEA	C2A-C1A	2.45	1.48	1.42
14	N	602	HEA	C16-C17	-2.45	1.45	1.53
20	Q	201	DMU	C10-C5	-2.45	1.45	1.52
20	N	610	DMU	C7-C5	-2.41	1.46	1.52
23	P	304	PGV	O01-C02	-2.38	1.40	1.46
20	D	201	DMU	O16-C6	-2.35	1.36	1.40
23	A	619	PGV	O03-C19	2.33	1.40	1.33
14	N	603	HEA	CMC-C2C	-2.33	1.46	1.51
23	P	304	PGV	O03-C01	-2.32	1.39	1.45
20	C	315	DMU	C7-C5	-2.31	1.46	1.52
20	O	304	DMU	C3-C4	-2.30	1.48	1.53
14	A	601	HEA	C2A-C1A	2.28	1.47	1.42
14	A	602	HEA	C4D-C3D	2.28	1.49	1.45
20	D	201	DMU	O1-C10	2.27	1.47	1.41
14	A	602	HEA	FE-NB	2.27	2.08	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	610	DMU	O5-C6	-2.26	1.36	1.41
20	C	318	DMU	O3-C5	2.26	1.48	1.43
20	P	319	DMU	O3-C5	-2.24	1.37	1.43
20	H	101	DMU	O1-C10	2.22	1.47	1.41
14	N	602	HEA	C1B-C2B	2.22	1.48	1.44
23	C	303	PGV	O01-C1	2.22	1.40	1.34
20	A	609	DMU	C7-C5	-2.21	1.46	1.52
14	N	602	HEA	O11-C11	2.21	1.47	1.42
18	P	305	CDL	C11-CA5	2.20	1.57	1.50
14	N	603	HEA	C1B-C2B	2.20	1.48	1.44
14	A	602	HEA	FE-ND	2.19	2.07	1.96
20	H	101	DMU	C7-C5	-2.18	1.46	1.52
20	A	609	DMU	O3-C5	-2.18	1.37	1.43
20	Q	201	DMU	O1-C10	2.17	1.47	1.41
20	C	315	DMU	C6-C1	-2.17	1.46	1.52
28	T	102	PEK	C2-C1	2.17	1.57	1.50
20	H	101	DMU	O3-C5	2.15	1.48	1.43
25	C	301	CHD	O25-C24	2.14	1.29	1.22
20	P	317	DMU	O16-C6	2.14	1.43	1.40
14	N	603	HEA	FE-ND	2.12	2.07	1.96
20	Q	201	DMU	O16-C6	-2.12	1.36	1.40
20	D	201	DMU	C10-C5	-2.11	1.46	1.52
14	A	601	HEA	O1D-CGD	2.09	1.29	1.22
18	P	305	CDL	C31-CA7	-2.06	1.44	1.50
20	P	323	DMU	C8-C9	-2.05	1.48	1.53
20	P	317	DMU	C3-C4	-2.04	1.48	1.53
20	Y	102	DMU	O16-C6	2.04	1.43	1.40
20	Q	201	DMU	C7-C5	-2.04	1.47	1.52
20	P	315	DMU	O5-C6	-2.03	1.36	1.41
20	N	610	DMU	C10-C5	-2.03	1.46	1.52
14	N	603	HEA	C3C-C2C	2.03	1.43	1.40
20	N	610	DMU	O6-C11	2.00	1.50	1.42
23	P	304	PGV	P-O14	-2.00	1.45	1.55

All (268) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	C3D-C4D-ND	8.06	118.16	110.36
14	A	601	HEA	C3D-C4D-ND	7.02	117.16	110.36
18	C	304	CDL	OA4-PA1-OA5	-6.61	77.03	107.75
20	P	315	DMU	O16-C6-C1	6.37	118.24	108.30
20	Q	201	DMU	O16-C6-C1	6.36	118.23	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	603	HEA	C3D-C4D-ND	6.26	116.42	110.36
18	N	607	CDL	OA6-CA4-CA3	6.08	130.40	108.40
14	A	601	HEA	C2B-C1B-NB	5.92	116.98	109.88
14	A	602	HEA	C2B-C1B-NB	5.81	116.84	109.88
14	N	602	HEA	C2B-C1B-NB	5.78	116.81	109.88
14	A	601	HEA	C13-C12-C11	-5.71	105.76	114.35
20	T	105	DMU	O16-C6-C1	5.69	117.18	108.30
14	A	601	HEA	C2D-C1D-ND	5.62	116.49	109.84
14	N	602	HEA	C3C-C4C-NC	5.60	116.45	109.21
20	C	315	DMU	C6-O5-C4	5.57	124.62	113.69
14	N	602	HEA	C13-C12-C11	-5.48	106.12	114.35
20	C	323	DMU	O16-C6-C1	5.30	116.57	108.30
14	N	602	HEA	C3B-C4B-NB	5.27	116.09	109.84
14	N	602	HEA	C2D-C1D-ND	5.20	116.00	109.84
14	N	603	HEA	C2D-C1D-ND	5.16	115.96	109.84
14	N	603	HEA	C2B-C1B-NB	5.16	116.07	109.88
20	D	201	DMU	O16-C6-C1	5.16	116.36	108.30
14	A	601	HEA	C3B-C4B-NB	5.15	115.94	109.84
20	P	323	DMU	C10-C5-C7	5.14	120.70	110.00
18	A	606	CDL	OA5-PA1-OA3	5.08	128.90	109.07
14	A	602	HEA	C3B-C4B-NB	5.05	115.82	109.84
14	N	603	HEA	C3B-C4B-NB	5.01	115.78	109.84
18	P	305	CDL	OA4-PA1-OA2	-4.98	84.59	107.75
20	P	319	DMU	O16-C6-C1	4.91	115.97	108.30
14	A	601	HEA	C3C-C4C-NC	4.91	115.56	109.21
20	C	315	DMU	O16-C6-C1	4.85	115.87	108.30
20	U	101	DMU	O16-C6-C1	4.81	115.82	108.30
20	B	309	DMU	O16-C6-C1	4.78	115.77	108.30
20	O	304	DMU	O5-C6-C1	4.76	120.43	110.35
14	A	602	HEA	C3D-C4D-ND	4.54	114.76	110.36
14	N	603	HEA	C3C-C4C-NC	4.54	115.08	109.21
14	N	602	HEA	C26-C15-C16	4.54	122.90	115.27
25	C	305	CHD	C14-C13-C12	4.48	111.57	107.40
14	N	602	HEA	C4D-C3D-C2D	-4.41	100.47	106.90
20	C	318	DMU	O16-C6-C1	4.36	115.11	108.30
20	H	101	DMU	O16-C6-C1	4.35	115.09	108.30
14	N	603	HEA	C1D-C2D-C3D	-4.34	102.39	106.96
20	P	318	DMU	O16-C6-C1	4.30	115.02	108.30
14	A	601	HEA	C1B-C2B-C3B	-4.30	101.66	106.80
20	U	101	DMU	C10-C5-C7	4.29	118.94	110.00
25	C	305	CHD	C17-C13-C14	-4.28	95.78	100.09
14	N	603	HEA	CHA-C4D-C3D	-4.27	118.56	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	C1D-C2D-C3D	-4.22	102.52	106.96
25	C	305	CHD	C6-C7-C8	4.17	115.93	111.48
14	A	602	HEA	CHA-C4D-C3D	-4.15	118.74	124.84
14	N	603	HEA	C1B-C2B-C3B	-4.12	101.87	106.80
14	A	602	HEA	C13-C12-C11	-4.12	108.16	114.35
20	U	101	DMU	O3-C5-C10	4.11	120.03	110.05
14	A	601	HEA	C4A-CHB-C1B	4.07	127.93	122.56
14	A	602	HEA	C3C-C4C-NC	4.05	114.45	109.21
18	A	606	CDL	CA4-OA6-CA5	4.05	127.75	117.79
18	C	304	CDL	OA6-CA5-C11	-4.05	102.78	111.50
25	P	306	CHD	C16-C17-C20	3.92	118.22	112.15
20	P	318	DMU	C10-C5-C7	3.91	118.13	110.00
14	N	602	HEA	C1B-C2B-C3B	-3.88	102.17	106.80
20	Z	101	DMU	O16-C6-C1	3.84	114.29	108.30
18	C	304	CDL	OA4-PA1-OA3	3.83	131.18	112.24
20	P	317	DMU	O5-C6-C1	3.78	118.35	110.35
14	N	602	HEA	CHA-C4D-C3D	-3.73	119.35	124.84
25	C	305	CHD	C16-C17-C20	3.71	117.89	112.15
14	A	602	HEA	C1B-C2B-C3B	-3.70	102.37	106.80
23	N	622	PGV	O03-C19-O04	-3.70	114.25	123.59
18	P	305	CDL	OA5-PA1-OA3	3.67	123.42	109.07
20	G	102	DMU	O16-C6-C1	3.66	114.01	108.30
14	A	601	HEA	C4D-C3D-C2D	-3.62	101.63	106.90
20	C	319	DMU	C10-C5-C7	3.60	117.50	110.00
14	A	601	HEA	CHA-C4D-C3D	-3.60	119.55	124.84
23	N	622	PGV	O03-C19-C20	3.59	123.16	111.91
20	C	315	DMU	O5-C6-C1	3.57	117.90	110.35
18	N	607	CDL	CA4-OA6-CA5	3.55	126.54	117.79
20	P	323	DMU	O16-C6-C1	3.55	113.84	108.30
18	P	305	CDL	OA4-PA1-OA5	-3.54	91.31	107.75
14	N	603	HEA	CAD-CBD-CGD	-3.48	106.11	113.60
14	A	602	HEA	CMB-C2B-C1B	3.47	130.32	125.04
18	C	304	CDL	OA5-PA1-OA3	3.46	122.58	109.07
25	P	306	CHD	C6-C7-C8	3.42	115.13	111.48
20	M	101	DMU	O16-C6-C1	3.42	113.64	108.30
14	N	602	HEA	O11-C11-C12	3.39	118.89	109.42
20	P	319	DMU	C10-C5-C7	3.36	117.00	110.00
14	N	602	HEA	C27-C19-C20	3.36	120.92	115.27
14	N	602	HEA	C1D-C2D-C3D	-3.34	103.44	106.96
14	A	602	HEA	C4D-C3D-C2D	-3.34	102.03	106.90
18	L	101	CDL	OB4-PB2-OB2	3.34	123.24	107.75
18	C	304	CDL	OB5-PB2-OB3	3.33	122.08	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	603	HEA	CHB-C1B-C2B	-3.33	119.78	124.98
14	N	603	HEA	C4D-C3D-C2D	-3.32	102.05	106.90
20	N	610	DMU	C10-O1-C9	3.32	120.20	113.69
20	C	319	DMU	O16-C6-C1	3.30	113.46	108.30
20	C	317	DMU	O5-C6-C1	3.29	117.32	110.35
14	N	603	HEA	CMB-C2B-C1B	3.26	130.01	125.04
14	N	602	HEA	CHB-C1B-C2B	-3.25	119.91	124.98
20	L	102	DMU	O5-C6-O16	3.22	117.61	109.97
14	N	603	HEA	CBA-CAA-C2A	-3.21	107.19	112.60
14	N	602	HEA	C1D-ND-C4D	-3.18	101.79	105.07
20	Y	102	DMU	O5-C6-O16	3.16	117.45	109.97
20	O	309	DMU	O5-C6-O16	3.13	117.38	109.97
18	N	607	CDL	OA6-CA4-CA6	-3.12	97.11	108.40
14	A	602	HEA	CAD-CBD-CGD	-3.07	106.99	113.60
20	H	101	DMU	O3-C5-C10	3.04	117.43	110.05
14	A	601	HEA	CHB-C1B-C2B	-3.04	120.23	124.98
20	P	315	DMU	C10-C5-C7	3.03	116.31	110.00
20	C	319	DMU	O3-C5-C10	3.03	117.41	110.05
14	A	602	HEA	C2D-C1D-ND	3.00	113.39	109.84
20	O	304	DMU	O16-C6-C1	3.00	112.98	108.30
20	P	315	DMU	O5-C6-O16	-2.99	102.89	109.97
14	A	601	HEA	C4B-NB-C1B	-2.97	102.00	105.07
14	A	601	HEA	CMC-C2C-C3C	2.95	130.21	124.68
14	A	602	HEA	C4B-C3B-C2B	-2.95	102.37	107.41
18	P	305	CDL	OA4-PA1-OA3	2.94	126.78	112.24
14	A	602	HEA	CHB-C1B-C2B	-2.94	120.39	124.98
20	C	318	DMU	C10-C5-C7	2.93	116.10	110.00
20	Q	201	DMU	C2-C3-C4	-2.91	104.25	110.93
20	H	101	DMU	O5-C6-C1	2.88	116.44	110.35
20	P	319	DMU	O5-C6-C1	2.88	116.44	110.35
18	P	305	CDL	OA6-CA5-C11	-2.87	105.31	111.50
18	P	305	CDL	OB4-PB2-OB3	2.87	126.44	112.24
18	N	607	CDL	OA2-PA1-OA3	-2.86	97.88	109.07
14	A	601	HEA	CAD-CBD-CGD	-2.85	107.46	113.60
18	C	304	CDL	OB6-CB5-C51	2.85	117.64	111.50
20	P	323	DMU	C10-O1-C9	-2.85	108.10	113.69
18	P	305	CDL	OA2-PA1-OA3	2.83	120.13	109.07
20	Q	201	DMU	C11-C9-C8	-2.82	106.39	113.00
14	A	602	HEA	C4B-NB-C1B	-2.82	102.16	105.07
14	N	602	HEA	CHD-C1D-ND	-2.81	120.91	124.38
14	N	602	HEA	C4B-C3B-C2B	-2.80	102.62	107.41
14	A	601	HEA	C1D-ND-C4D	-2.79	102.19	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	303	PGV	O03-C19-O04	-2.79	116.56	123.59
20	A	609	DMU	O3-C5-C10	2.78	116.81	110.05
20	D	201	DMU	C10-O1-C9	2.78	119.14	113.69
20	B	309	DMU	C6-O5-C4	2.76	119.10	113.69
20	C	323	DMU	C10-C5-C7	2.73	115.68	110.00
18	A	606	CDL	OA2-PA1-OA3	-2.71	98.46	109.07
25	P	306	CHD	C17-C13-C14	-2.70	97.37	100.09
20	P	317	DMU	C18-O16-C6	-2.70	109.36	113.84
25	P	306	CHD	C14-C13-C12	2.70	109.92	107.40
14	N	602	HEA	C4B-NB-C1B	-2.67	102.32	105.07
20	D	201	DMU	C10-C5-C7	2.66	115.54	110.00
20	C	315	DMU	O5-C4-C3	2.66	115.36	109.75
14	A	601	HEA	C4D-CHA-C1A	2.66	126.07	122.56
20	O	304	DMU	C6-C1-C2	2.65	115.51	110.00
14	N	603	HEA	C20-C19-C18	-2.64	115.77	121.12
14	N	602	HEA	CMC-C2C-C3C	2.64	129.62	124.68
23	A	619	PGV	O03-C19-O04	-2.64	116.93	123.59
20	C	317	DMU	C18-O16-C6	-2.63	109.48	113.84
23	A	619	PGV	O03-C19-C20	2.63	120.15	111.91
14	N	603	HEA	CMD-C2D-C1D	2.62	129.03	125.04
20	C	315	DMU	C18-O16-C6	-2.59	109.54	113.84
25	P	306	CHD	O7-C7-C6	-2.59	103.53	109.94
14	A	602	HEA	C1D-C2D-C3D	-2.58	104.24	106.96
20	C	318	DMU	C10-O1-C9	-2.58	108.63	113.69
23	P	304	PGV	C27-C26-C25	-2.57	101.40	114.42
18	P	305	CDL	O1-C1-CB2	2.55	118.52	109.56
14	N	603	HEA	CHD-C1D-C2D	-2.55	119.67	126.72
14	N	602	HEA	O2D-CGD-CBD	2.55	122.22	114.03
20	Z	101	DMU	O5-C6-C1	2.55	115.74	110.35
20	N	610	DMU	C7-C8-C9	2.55	114.78	110.24
20	A	609	DMU	O3-C5-C7	2.54	116.23	110.35
20	A	609	DMU	C10-O7-C3	-2.54	111.67	117.96
18	A	606	CDL	OA6-CA4-CA6	2.54	117.58	108.40
20	D	201	DMU	C2-C3-C4	-2.53	105.13	110.93
20	P	315	DMU	O1-C9-C11	2.53	112.72	106.44
18	C	304	CDL	OA7-CA5-C11	2.52	133.55	123.73
20	D	201	DMU	C7-C8-C9	2.51	114.71	110.24
28	T	102	PEK	O01-C1-O02	-2.50	117.65	123.70
20	P	317	DMU	C2-C3-C4	-2.50	105.77	110.24
14	N	603	HEA	C27-C19-C20	2.50	119.48	115.27
25	C	305	CHD	C22-C23-C24	-2.50	105.87	112.51
20	P	323	DMU	O7-C10-O1	-2.50	103.69	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	105	DMU	C18-O16-C6	-2.50	109.70	113.84
20	A	609	DMU	O5-C6-O16	2.50	115.88	109.97
14	N	602	HEA	C4A-CHB-C1B	2.49	125.84	122.56
20	Q	201	DMU	O1-C9-C8	2.48	114.20	109.69
20	T	105	DMU	C57-C4-C3	-2.47	107.21	113.00
20	H	101	DMU	C18-O16-C6	-2.47	109.74	113.84
25	C	301	CHD	C22-C20-C17	-2.46	105.20	110.28
20	Q	201	DMU	C6-O5-C4	-2.45	108.87	113.69
14	N	603	HEA	CAD-C3D-C4D	2.45	128.94	124.66
14	A	601	HEA	CHD-C1D-ND	-2.43	121.37	124.38
23	P	304	PGV	C22-C21-C20	-2.43	104.45	113.19
20	B	309	DMU	C3-C2-C1	-2.42	106.59	110.82
20	O	309	DMU	C57-C4-C3	-2.42	107.34	113.00
14	A	601	HEA	C4B-C3B-C2B	-2.39	103.33	107.41
20	U	101	DMU	O5-C6-O16	2.38	115.62	109.97
20	H	101	DMU	C10-C5-C7	2.38	114.95	110.00
20	B	309	DMU	O5-C6-O16	2.37	115.59	109.97
20	C	315	DMU	C10-C5-C7	2.36	114.92	110.00
20	Q	201	DMU	C10-O1-C9	2.36	118.33	113.69
20	P	323	DMU	O5-C6-C1	2.36	115.34	110.35
20	P	317	DMU	C6-C1-C2	2.34	114.87	110.00
20	C	319	DMU	O3-C5-C7	2.34	115.76	110.35
18	N	607	CDL	OA5-PA1-OA3	2.34	118.19	109.07
14	N	603	HEA	CHC-C4B-C3B	-2.34	119.78	125.80
20	N	610	DMU	O5-C6-C1	2.33	115.28	110.35
18	L	101	CDL	OB5-PB2-OB3	-2.33	99.97	109.07
20	Z	101	DMU	O3-C5-C7	2.33	115.73	110.35
20	B	309	DMU	O5-C6-C1	2.33	115.27	110.35
20	D	201	DMU	O1-C9-C8	2.31	113.89	109.69
14	A	601	HEA	CAD-C3D-C4D	2.31	128.70	124.66
20	U	101	DMU	O4-C7-C5	-2.31	105.01	110.35
20	M	101	DMU	O3-C5-C7	2.31	115.69	110.35
14	N	603	HEA	C4B-C3B-C2B	-2.31	103.47	107.41
14	A	602	HEA	C4A-CHB-C1B	2.30	125.59	122.56
14	N	603	HEA	C4B-NB-C1B	-2.29	102.71	105.07
20	O	304	DMU	C6-O5-C4	2.29	118.18	113.69
20	C	319	DMU	O7-C10-C5	2.29	114.03	108.10
14	N	602	HEA	C26-C15-C14	-2.28	117.82	123.68
20	A	609	DMU	C10-C5-C7	2.28	114.75	110.00
14	N	602	HEA	C4D-CHA-C1A	2.28	125.56	122.56
14	A	601	HEA	C26-C15-C16	2.28	119.10	115.27
20	O	309	DMU	O16-C6-C1	-2.26	104.77	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	N	622	PGV	O01-C1-O02	-2.26	118.23	123.70
23	P	304	PGV	C03-C02-C01	-2.26	106.44	111.79
28	T	102	PEK	O02-C1-C2	2.26	132.54	123.73
20	Z	101	DMU	C10-C5-C7	2.26	114.70	110.00
20	C	319	DMU	O5-C6-C1	2.25	115.11	110.35
20	T	105	DMU	C2-C3-C4	2.24	114.23	110.24
25	P	306	CHD	C22-C23-C24	-2.23	106.58	112.51
20	Y	102	DMU	C57-C4-C3	-2.23	107.77	113.00
14	A	602	HEA	CHD-C1D-C2D	-2.22	120.58	126.72
14	A	602	HEA	CMD-C2D-C1D	2.22	128.42	125.04
23	N	622	PGV	C30-C29-C28	2.21	125.67	114.42
20	P	323	DMU	O1-C9-C8	-2.21	105.68	109.69
14	N	602	HEA	C16-C17-C18	2.20	119.11	111.88
18	N	607	CDL	OA8-CA6-CA4	2.19	114.82	108.43
25	P	306	CHD	C18-C13-C12	-2.19	106.84	109.07
14	N	602	HEA	CHC-C4B-C3B	-2.19	120.17	125.80
18	P	305	CDL	OA7-CA5-C11	2.18	132.22	123.73
20	A	609	DMU	O7-C10-C5	2.17	113.72	108.10
25	B	307	CHD	C1-C2-C3	2.15	113.23	110.47
14	A	601	HEA	C17-C18-C19	-2.15	122.48	127.66
14	A	602	HEA	CBA-CAA-C2A	-2.14	108.99	112.60
20	C	315	DMU	O5-C6-O16	-2.14	104.90	109.97
20	P	315	DMU	O3-C5-C7	2.14	115.30	110.35
14	N	603	HEA	C13-C12-C11	-2.14	111.13	114.35
20	P	315	DMU	C18-O16-C6	-2.14	110.30	113.84
23	C	303	PGV	C29-C28-C27	-2.13	103.61	114.42
18	N	607	CDL	OA6-CA5-C11	-2.12	106.93	111.50
20	O	304	DMU	C57-C4-C3	-2.12	108.04	113.00
25	C	301	CHD	C17-C13-C12	-2.12	115.73	117.67
25	O	301	CHD	C18-C13-C12	-2.11	106.92	109.07
18	C	304	CDL	OB4-PB2-OB3	2.10	122.63	112.24
20	A	609	DMU	O1-C10-C5	-2.10	105.90	110.35
25	P	302	CHD	C22-C20-C17	-2.10	105.95	110.28
25	P	302	CHD	C11-C12-C13	-2.10	109.09	111.24
20	Q	201	DMU	C18-O16-C6	2.09	117.31	113.84
20	P	315	DMU	O5-C6-C1	2.09	114.77	110.35
23	C	303	PGV	C27-C26-C25	-2.09	103.84	114.42
20	U	101	DMU	C10-O7-C3	-2.08	112.81	117.96
25	C	305	CHD	C5-C6-C7	2.07	116.75	114.46
25	C	305	CHD	C16-C17-C13	-2.07	101.52	103.55
20	B	305	DMU	O16-C6-C1	2.07	111.54	108.30
25	P	306	CHD	O25-C24-C23	-2.07	116.43	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	609	DMU	O5-C6-C1	2.06	114.71	110.35
18	A	606	CDL	OB6-CB5-C51	2.06	116.54	110.80
14	N	602	HEA	CMD-C2D-C1D	2.06	128.17	125.04
20	C	318	DMU	O3-C5-C10	2.05	115.02	110.05
14	A	602	HEA	O11-C11-C12	2.03	115.10	109.42
25	P	306	CHD	C18-C13-C14	2.02	114.38	111.21
14	A	602	HEA	CAD-C3D-C2D	2.02	131.63	127.88
23	P	304	PGV	O03-C19-O04	-2.01	118.52	123.59
20	Z	101	DMU	O1-C9-C11	2.01	111.43	106.44
20	P	315	DMU	C6-O5-C4	2.00	117.62	113.69
14	N	603	HEA	C4D-CHA-C1A	2.00	125.20	122.56

There are no chirality outliers.

All (806) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	CDL	C1-CA2-OA2-PA1
18	A	606	CDL	CA2-OA2-PA1-OA3
18	A	606	CDL	CB2-OB2-PB2-OB3
18	A	606	CDL	CB3-OB5-PB2-OB3
18	A	606	CDL	CB3-OB5-PB2-OB4
18	A	606	CDL	C51-CB5-OB6-CB4
18	C	304	CDL	O1-C1-CB2-OB2
18	C	304	CDL	C1-CA2-OA2-PA1
18	C	304	CDL	CA3-OA5-PA1-OA2
18	C	304	CDL	CB3-OB5-PB2-OB4
18	C	304	CDL	OB7-CB5-OB6-CB4
18	C	304	CDL	C51-CB5-OB6-CB4
18	L	101	CDL	C11-CA5-OA6-CA4
18	L	101	CDL	CB2-OB2-PB2-OB3
18	N	607	CDL	CA3-OA5-PA1-OA3
18	N	607	CDL	CB2-OB2-PB2-OB3
18	N	607	CDL	CB2-OB2-PB2-OB4
18	N	607	CDL	CB2-OB2-PB2-OB5
18	N	607	CDL	CB3-OB5-PB2-OB2
18	N	607	CDL	CB3-OB5-PB2-OB3
18	N	607	CDL	CB3-OB5-PB2-OB4
18	P	305	CDL	C1-CA2-OA2-PA1
18	P	305	CDL	CA3-OA5-PA1-OA3
18	P	305	CDL	OA7-CA5-OA6-CA4
18	P	305	CDL	C11-CA5-OA6-CA4
18	P	305	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
18	Y	101	CDL	CA2-OA2-PA1-OA3
18	Y	101	CDL	C11-CA5-OA6-CA4
18	Y	101	CDL	CB2-OB2-PB2-OB3
18	Y	101	CDL	OB6-CB4-CB6-OB8
18	Y	101	CDL	C51-CB5-OB6-CB4
20	B	305	DMU	C1-C6-O16-C18
20	B	305	DMU	O5-C6-O16-C18
20	B	309	DMU	O5-C6-O16-C18
20	B	309	DMU	C19-C18-O16-C6
20	C	318	DMU	C1-C6-O16-C18
20	C	318	DMU	O5-C6-O16-C18
20	C	318	DMU	C19-C18-O16-C6
20	D	201	DMU	C19-C18-O16-C6
20	O	304	DMU	C19-C18-O16-C6
20	O	309	DMU	C19-C18-O16-C6
20	P	317	DMU	C19-C18-O16-C6
20	P	318	DMU	C1-C6-O16-C18
20	P	319	DMU	C19-C18-O16-C6
20	Q	201	DMU	O5-C6-O16-C18
20	T	105	DMU	C1-C6-O16-C18
20	U	101	DMU	C1-C6-O16-C18
20	Y	102	DMU	C1-C6-O16-C18
20	Y	102	DMU	C19-C18-O16-C6
25	C	305	CHD	C13-C17-C20-C21
25	C	305	CHD	C13-C17-C20-C22
25	C	305	CHD	C16-C17-C20-C22
25	P	306	CHD	C13-C17-C20-C21
25	P	306	CHD	C16-C17-C20-C22
28	G	101	PEK	C11-C12-C13-C14
28	G	101	PEK	C12-C13-C14-C15
28	T	102	PEK	C11-C12-C13-C14
28	T	102	PEK	C12-C13-C14-C15
20	C	319	DMU	O6-C11-C9-C8
25	C	305	CHD	C16-C17-C20-C21
25	P	306	CHD	C16-C17-C20-C21
20	O	304	DMU	O5-C4-C57-O61
18	A	606	CDL	OB7-CB5-OB6-CB4
18	Y	101	CDL	OA7-CA5-OA6-CA4
18	Y	101	CDL	OB7-CB5-OB6-CB4
18	P	305	CDL	C51-CB5-OB6-CB4
20	C	319	DMU	O5-C4-C57-O61
20	C	319	DMU	O6-C11-C9-O1

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Mol	Chain	Res	Type	Atoms
20	T	105	DMU	O5-C4-C57-O61
25	P	306	CHD	C13-C17-C20-C22
20	C	315	DMU	O6-C11-C9-O1
20	C	315	DMU	O5-C4-C57-O61
19	C	309	LFA	C11-C10-C9-C8
18	L	101	CDL	OA7-CA5-OA6-CA4
20	L	102	DMU	C3-C4-C57-O61
20	P	317	DMU	O5-C4-C57-O61
20	P	318	DMU	O6-C11-C9-O1
18	A	606	CDL	O1-C1-CB2-OB2
18	P	305	CDL	O1-C1-CB2-OB2
18	Y	101	CDL	O1-C1-CB2-OB2
20	P	315	DMU	O5-C4-C57-O61
18	C	304	CDL	C11-CA5-OA6-CA4
20	O	304	DMU	C3-C4-C57-O61
19	C	309	LFA	C12-C13-C14-C15
19	C	325	LFA	C9-C10-C11-C12
19	T	101	LFA	C9-C10-C11-C12
20	U	101	DMU	O5-C4-C57-O61
20	C	319	DMU	C3-C4-C57-O61
20	P	317	DMU	C3-C4-C57-O61
20	T	105	DMU	C3-C4-C57-O61
20	P	319	DMU	O6-C11-C9-O1
20	P	315	DMU	C3-C4-C57-O61
20	N	601	DMU	C19-C22-C25-C28
20	L	102	DMU	O5-C4-C57-O61
20	C	315	DMU	O6-C11-C9-C8
20	P	318	DMU	O5-C6-O16-C18
18	Y	101	CDL	C31-CA7-OA8-CA6
19	P	308	LFA	C7-C8-C9-C10
20	P	319	DMU	C19-C22-C25-C28
20	A	609	DMU	O6-C11-C9-C8
18	A	606	CDL	CA2-C1-CB2-OB2
18	P	305	CDL	CA2-C1-CB2-OB2
18	C	304	CDL	OA7-CA5-OA6-CA4
18	Y	101	CDL	OA9-CA7-OA8-CA6
18	C	304	CDL	C71-CB7-OB8-CB6
18	C	304	CDL	CB5-C51-C52-C53
18	N	607	CDL	C13-C14-C15-C16
20	C	317	DMU	O5-C4-C57-O61
20	C	315	DMU	C3-C4-C57-O61
18	L	101	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
20	Z	101	DMU	O6-C11-C9-O1
18	Y	101	CDL	O1-C1-CA2-OA2
20	Z	101	DMU	O6-C11-C9-C8
18	L	101	CDL	C51-CB5-OB6-CB4
19	P	310	LFA	C11-C10-C9-C8
18	C	304	CDL	CA7-C31-C32-C33
20	D	201	DMU	O6-C11-C9-O1
20	P	319	DMU	O6-C11-C9-C8
18	C	304	CDL	C31-CA7-OA8-CA6
18	N	607	CDL	C31-CA7-OA8-CA6
25	C	305	CHD	C21-C20-C22-C23
28	T	102	PEK	C7-C8-C9-C10
18	L	101	CDL	CA5-C11-C12-C13
18	L	101	CDL	CB7-C71-C72-C73
18	N	607	CDL	CA5-C11-C12-C13
18	P	305	CDL	CB5-C51-C52-C53
18	Y	101	CDL	CA5-C11-C12-C13
20	P	318	DMU	O6-C11-C9-C8
18	N	607	CDL	C51-CB5-OB6-CB4
18	A	606	CDL	CA5-C11-C12-C13
20	G	102	DMU	O16-C18-C19-C22
20	C	317	DMU	O16-C18-C19-C22
20	A	609	DMU	O5-C6-O16-C18
20	T	105	DMU	O5-C6-O16-C18
20	U	101	DMU	O5-C6-O16-C18
20	Y	102	DMU	O5-C6-O16-C18
20	Y	102	DMU	O16-C18-C19-C22
23	C	303	PGV	C28-C29-C30-C31
20	L	102	DMU	O16-C18-C19-C22
20	A	609	DMU	O6-C11-C9-O1
18	C	304	CDL	O1-C1-CA2-OA2
18	L	101	CDL	O1-C1-CA2-OA2
18	N	607	CDL	O1-C1-CB2-OB2
18	L	101	CDL	OB7-CB5-OB6-CB4
18	N	607	CDL	OB7-CB5-OB6-CB4
18	P	305	CDL	C31-CA7-OA8-CA6
18	C	304	CDL	C51-C52-C53-C54
18	N	607	CDL	CA7-C31-C32-C33
25	C	305	CHD	C17-C20-C22-C23
18	C	304	CDL	OA9-CA7-OA8-CA6
18	A	606	CDL	CA3-OA5-PA1-OA2
18	A	606	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
18	A	606	CDL	CB3-OB5-PB2-OB2
18	L	101	CDL	CA2-OA2-PA1-OA5
18	L	101	CDL	CA3-OA5-PA1-OA2
18	L	101	CDL	CB2-OB2-PB2-OB5
18	N	607	CDL	CA3-OA5-PA1-OA2
18	P	305	CDL	CA2-OA2-PA1-OA5
18	P	305	CDL	CA3-OA5-PA1-OA2
18	Y	101	CDL	CB2-OB2-PB2-OB5
18	Y	101	CDL	CB3-OB5-PB2-OB2
20	N	610	DMU	O6-C11-C9-C8
18	C	304	CDL	OB9-CB7-OB8-CB6
18	L	101	CDL	CB2-C1-CA2-OA2
18	Y	101	CDL	CB2-C1-CA2-OA2
18	A	606	CDL	OA7-CA5-OA6-CA4
20	P	319	DMU	C4-C3-O7-C10
19	B	308	LFA	C9-C10-C11-C12
19	G	104	LFA	C11-C10-C9-C8
20	G	102	DMU	C28-C31-C34-C37
20	Z	101	DMU	C22-C25-C28-C31
23	C	303	PGV	C24-C25-C26-C27
18	A	606	CDL	C19-C20-C21-C22
18	N	607	CDL	C31-C32-C33-C34
18	Y	101	CDL	C19-C20-C21-C22
19	O	302	LFA	C5-C6-C7-C8
19	O	302	LFA	C13-C14-C15-C16
20	J	101	DMU	C25-C28-C31-C34
18	N	607	CDL	C73-C74-C75-C76
18	Y	101	CDL	C16-C17-C18-C19
18	Y	101	CDL	C79-C80-C81-C82
19	P	310	LFA	C5-C6-C7-C8
20	B	304	DMU	C19-C22-C25-C28
20	B	309	DMU	C31-C34-C37-C40
23	C	303	PGV	C7-C8-C9-C10
18	Y	101	CDL	C76-C77-C78-C79
20	D	201	DMU	O16-C18-C19-C22
28	T	102	PEK	C22-C23-C24-C25
28	T	102	PEK	C26-C27-C28-C29
18	A	606	CDL	C13-C14-C15-C16
18	C	304	CDL	C22-C23-C24-C25
19	B	308	LFA	C7-C8-C9-C10
28	G	101	PEK	C34-C35-C36-C37
18	P	305	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
19	B	308	LFA	C13-C14-C15-C16
19	P	311	LFA	C7-C8-C9-C10
20	L	102	DMU	C1-C6-O16-C18
18	A	606	CDL	C17-C18-C19-C20
19	G	104	LFA	C3-C4-C5-C6
20	C	317	DMU	C28-C31-C34-C37
20	P	316	DMU	C28-C31-C34-C37
23	A	619	PGV	C14-C15-C16-C17
18	N	607	CDL	C77-C78-C79-C80
18	Y	101	CDL	C13-C14-C15-C16
19	C	309	LFA	C3-C4-C5-C6
20	C	315	DMU	C19-C22-C25-C28
23	N	622	PGV	C29-C30-C31-C32
23	P	304	PGV	C24-C25-C26-C27
28	T	102	PEK	C1-C2-C3-C4
19	P	310	LFA	C4-C5-C6-C7
20	C	316	DMU	C28-C31-C34-C37
20	C	318	DMU	C31-C34-C37-C40
20	G	102	DMU	C25-C28-C31-C34
20	P	319	DMU	C22-C25-C28-C31
20	B	309	DMU	O5-C4-C57-O61
18	Y	101	CDL	C72-C73-C74-C75
20	Z	101	DMU	C28-C31-C34-C37
18	N	607	CDL	C78-C79-C80-C81
19	P	312	LFA	C1-C2-C3-C4
18	C	304	CDL	C35-C36-C37-C38
18	L	101	CDL	C17-C18-C19-C20
18	N	607	CDL	C72-C73-C74-C75
18	N	607	CDL	C76-C77-C78-C79
18	P	305	CDL	C54-C55-C56-C57
19	C	311	LFA	C4-C5-C6-C7
19	P	310	LFA	C13-C14-C15-C16
19	T	103	LFA	C5-C6-C7-C8
20	C	317	DMU	C19-C22-C25-C28
20	P	315	DMU	C28-C31-C34-C37
23	C	303	PGV	C14-C15-C16-C17
23	P	304	PGV	C30-C31-C32-C33
18	L	101	CDL	C36-C37-C38-C39
18	Y	101	CDL	C63-C64-C65-C66
20	L	102	DMU	C31-C34-C37-C40
19	P	301	LFA	C9-C10-C11-C12
19	P	311	LFA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	T	103	LFA	C10-C11-C12-C13
20	M	102	DMU	C31-C34-C37-C40
20	Z	102	DMU	C31-C34-C37-C40
19	C	307	LFA	C3-C4-C5-C6
19	C	309	LFA	C5-C6-C7-C8
19	C	310	LFA	C3-C4-C5-C6
19	C	310	LFA	C6-C7-C8-C9
20	A	608	DMU	C28-C31-C34-C37
20	B	305	DMU	C19-C18-O16-C6
20	C	317	DMU	C19-C18-O16-C6
20	G	102	DMU	C19-C18-O16-C6
18	L	101	CDL	C51-C52-C53-C54
19	O	303	LFA	C2-C3-C4-C5
20	A	609	DMU	C31-C34-C37-C40
18	C	304	CDL	C75-C76-C77-C78
18	P	305	CDL	C53-C54-C55-C56
23	C	303	PGV	C22-C23-C24-C25
18	N	607	CDL	C17-C18-C19-C20
28	T	102	PEK	C32-C33-C34-C35
18	A	606	CDL	C11-CA5-OA6-CA4
19	C	325	LFA	C6-C7-C8-C9
18	L	101	CDL	C34-C35-C36-C37
18	L	101	CDL	C58-C59-C60-C61
18	N	607	CDL	C74-C75-C76-C77
19	C	311	LFA	C10-C11-C12-C13
19	P	301	LFA	C6-C7-C8-C9
19	T	104	LFA	C3-C4-C5-C6
23	C	303	PGV	C13-C14-C15-C16
28	G	101	PEK	C15-C16-C17-C18
18	N	607	CDL	OA9-CA7-OA8-CA6
18	N	607	CDL	O1-C1-CA2-OA2
18	L	101	CDL	C14-C15-C16-C17
20	P	318	DMU	C3-C4-C57-O61
20	U	101	DMU	C3-C4-C57-O61
18	P	305	CDL	C11-C12-C13-C14
19	B	308	LFA	C4-C5-C6-C7
18	C	304	CDL	CB2-C1-CA2-OA2
18	Y	101	CDL	C71-C72-C73-C74
19	T	103	LFA	C4-C5-C6-C7
20	C	315	DMU	C31-C34-C37-C40
20	B	303	DMU	C18-C19-C22-C25
20	J	101	DMU	C18-C19-C22-C25

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Mol	Chain	Res	Type	Atoms
20	A	609	DMU	C3-C4-C57-O61
20	O	308	DMU	C18-C19-C22-C25
19	P	314	LFA	C6-C7-C8-C9
20	A	620	DMU	C22-C25-C28-C31
20	L	102	DMU	C22-C25-C28-C31
20	P	317	DMU	C22-C25-C28-C31
21	P	320	EDO	O1-C1-C2-O2
18	C	304	CDL	C73-C74-C75-C76
19	A	607	LFA	C6-C7-C8-C9
19	C	312	LFA	C1-C2-C3-C4
23	N	622	PGV	C14-C15-C16-C17
18	L	101	CDL	C31-CA7-OA8-CA6
18	P	305	CDL	C57-C58-C59-C60
20	P	323	DMU	C4-C3-O7-C10
19	C	310	LFA	C7-C8-C9-C10
20	M	101	DMU	C25-C28-C31-C34
20	O	309	DMU	C34-C37-C40-C43
18	L	101	CDL	OA9-CA7-OA8-CA6
18	P	305	CDL	OA9-CA7-OA8-CA6
18	L	101	CDL	C37-C38-C39-C40
20	C	317	DMU	C31-C34-C37-C40
20	C	318	DMU	O16-C18-C19-C22
20	P	319	DMU	C2-C3-O7-C10
28	T	102	PEK	C17-C18-C19-C20
23	P	304	PGV	C12-C13-C14-C15
19	C	311	LFA	C3-C4-C5-C6
20	C	315	DMU	C28-C31-C34-C37
20	Y	102	DMU	C18-C19-C22-C25
19	C	311	LFA	C11-C10-C9-C8
19	C	307	LFA	C4-C5-C6-C7
20	N	601	DMU	C25-C28-C31-C34
23	N	622	PGV	C30-C31-C32-C33
23	P	304	PGV	C7-C8-C9-C10
28	G	101	PEK	C28-C29-C30-C31
28	T	102	PEK	C30-C31-C32-C33
19	P	314	LFA	C2-C3-C4-C5
20	C	318	DMU	C19-C22-C25-C28
18	C	304	CDL	C20-C21-C22-C23
19	C	325	LFA	C7-C8-C9-C10
18	P	305	CDL	OA5-CA3-CA4-OA6
18	P	305	CDL	C56-C57-C58-C59
20	Z	101	DMU	C25-C28-C31-C34

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Mol	Chain	Res	Type	Atoms
18	Y	101	CDL	C57-C58-C59-C60
20	H	101	DMU	C19-C22-C25-C28
18	Y	101	CDL	C73-C74-C75-C76
20	A	620	DMU	C19-C22-C25-C28
18	A	606	CDL	OA6-CA4-CA6-OA8
18	N	607	CDL	OA6-CA4-CA6-OA8
19	T	101	LFA	C5-C6-C7-C8
20	C	319	DMU	O16-C18-C19-C22
23	P	304	PGV	C27-C28-C29-C30
20	N	610	DMU	C31-C34-C37-C40
20	P	318	DMU	C4-C3-O7-C10
20	O	307	DMU	C18-C19-C22-C25
20	Y	102	DMU	O5-C4-C57-O61
19	P	312	LFA	C3-C4-C5-C6
20	B	305	DMU	O16-C18-C19-C22
20	B	305	DMU	C31-C34-C37-C40
20	T	105	DMU	C28-C31-C34-C37
20	B	304	DMU	C18-C19-C22-C25
18	A	606	CDL	C78-C79-C80-C81
18	L	101	CDL	C59-C60-C61-C62
18	P	305	CDL	C33-C34-C35-C36
19	P	311	LFA	C2-C3-C4-C5
20	P	315	DMU	O6-C11-C9-O1
19	P	310	LFA	C14-C15-C16-C17
19	P	310	LFA	C3-C4-C5-C6
20	M	101	DMU	C22-C25-C28-C31
20	N	610	DMU	O16-C18-C19-C22
23	N	622	PGV	C23-C24-C25-C26
20	P	317	DMU	C18-C19-C22-C25
20	U	101	DMU	C18-C19-C22-C25
18	Y	101	CDL	CA2-OA2-PA1-OA5
19	P	313	LFA	C9-C10-C11-C12
20	B	309	DMU	C25-C28-C31-C34
20	C	317	DMU	C25-C28-C31-C34
18	C	304	CDL	C23-C24-C25-C26
18	A	606	CDL	C75-C76-C77-C78
19	N	608	LFA	C9-C10-C11-C12
20	Q	201	DMU	C4-C3-O7-C10
20	C	318	DMU	O6-C11-C9-O1
20	A	609	DMU	O5-C4-C57-O61
19	C	309	LFA	C6-C7-C8-C9
19	P	301	LFA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	B	309	DMU	O16-C18-C19-C22
18	N	607	CDL	CA2-C1-CB2-OB2
18	L	101	CDL	C12-C13-C14-C15
18	Y	101	CDL	C12-C13-C14-C15
18	Y	101	CDL	C23-C24-C25-C26
19	N	608	LFA	C7-C8-C9-C10
18	C	304	CDL	C71-C72-C73-C74
18	Y	101	CDL	C59-C60-C61-C62
18	N	607	CDL	CA3-CA4-CA6-OA8
19	T	103	LFA	C3-C4-C5-C6
20	Y	102	DMU	C25-C28-C31-C34
23	C	303	PGV	C25-C26-C27-C28
28	G	101	PEK	C4-C5-C6-C7
18	C	304	CDL	C59-C60-C61-C62
19	C	312	LFA	C5-C6-C7-C8
19	P	308	LFA	C11-C10-C9-C8
20	C	306	DMU	C28-C31-C34-C37
28	G	101	PEK	C17-C18-C19-C20
14	A	602	HEA	C4D-C3D-CAD-CBD
20	P	323	DMU	O1-C10-O7-C3
20	P	318	DMU	O5-C4-C57-O61
20	C	316	DMU	C31-C34-C37-C40
20	N	609	DMU	C34-C37-C40-C43
18	C	304	CDL	C72-C71-CB7-OB8
19	C	310	LFA	C11-C10-C9-C8
20	B	309	DMU	C34-C37-C40-C43
18	L	101	CDL	C21-C22-C23-C24
19	P	301	LFA	C1-C2-C3-C4
20	P	317	DMU	C31-C34-C37-C40
18	L	101	CDL	C84-C85-C86-C87
19	B	308	LFA	C11-C12-C13-C14
19	P	313	LFA	C6-C7-C8-C9
20	Z	101	DMU	C34-C37-C40-C43
23	A	619	PGV	C11-C10-C9-C8
23	N	622	PGV	C11-C10-C9-C8
18	Y	101	CDL	C61-C62-C63-C64
19	C	310	LFA	C5-C6-C7-C8
19	G	104	LFA	C6-C7-C8-C9
20	O	307	DMU	C25-C28-C31-C34
19	O	302	LFA	C9-C10-C11-C12
18	Y	101	CDL	C64-C65-C66-C67
19	P	310	LFA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
18	L	101	CDL	C38-C39-C40-C41
18	L	101	CDL	C80-C81-C82-C83
18	Y	101	CDL	C21-C22-C23-C24
19	N	608	LFA	C6-C7-C8-C9
20	Y	102	DMU	C31-C34-C37-C40
20	L	102	DMU	C34-C37-C40-C43
20	T	105	DMU	C34-C37-C40-C43
18	N	607	CDL	CA3-CA4-OA6-CA5
20	H	101	DMU	O5-C4-C57-O61
20	B	303	DMU	O16-C18-C19-C22
20	O	308	DMU	O16-C18-C19-C22
18	Y	101	CDL	C58-C59-C60-C61
19	C	312	LFA	C11-C10-C9-C8
19	O	302	LFA	C14-C15-C16-C17
20	P	323	DMU	C2-C3-O7-C10
19	O	302	LFA	C11-C12-C13-C14
20	P	318	DMU	C2-C3-O7-C10
18	P	305	CDL	C21-C22-C23-C24
20	A	608	DMU	C25-C28-C31-C34
19	G	104	LFA	C7-C8-C9-C10
20	P	316	DMU	C25-C28-C31-C34
18	A	606	CDL	C20-C21-C22-C23
19	C	314	LFA	C1-C2-C3-C4
19	O	303	LFA	C5-C6-C7-C8
19	P	311	LFA	C11-C10-C9-C8
19	C	309	LFA	C1-C2-C3-C4
23	A	619	PGV	C31-C32-C33-C34
18	P	305	CDL	C73-C74-C75-C76
20	C	318	DMU	C34-C37-C40-C43
20	P	319	DMU	C25-C28-C31-C34
18	C	304	CDL	CB7-C71-C72-C73
20	D	201	DMU	C4-C3-O7-C10
20	B	304	DMU	O16-C18-C19-C22
20	N	601	DMU	O16-C18-C19-C22
20	O	307	DMU	O16-C18-C19-C22
20	P	307	DMU	O16-C18-C19-C22
18	L	101	CDL	C72-C71-CB7-OB8
19	C	313	LFA	C6-C7-C8-C9
20	P	315	DMU	C18-C19-C22-C25
18	N	607	CDL	C20-C21-C22-C23
18	P	305	CDL	C35-C36-C37-C38
18	P	305	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
20	O	308	DMU	C19-C22-C25-C28
20	P	323	DMU	O16-C18-C19-C22
20	Z	102	DMU	C34-C37-C40-C43
20	B	305	DMU	C34-C37-C40-C43
20	C	319	DMU	C22-C25-C28-C31
20	P	307	DMU	C31-C34-C37-C40
19	P	301	LFA	C4-C5-C6-C7
20	O	307	DMU	C22-C25-C28-C31
20	L	102	DMU	C25-C28-C31-C34
18	L	101	CDL	C13-C14-C15-C16
18	P	305	CDL	OA5-CA3-CA4-CA6
20	N	609	DMU	C28-C31-C34-C37
20	A	620	DMU	O16-C18-C19-C22
20	W	101	DMU	O16-C18-C19-C22
28	G	101	PEK	O12-C04-C05-N
18	C	304	CDL	C11-C12-C13-C14
23	N	622	PGV	C31-C32-C33-C34
20	O	304	DMU	C34-C37-C40-C43
28	G	101	PEK	C29-C30-C31-C32
18	A	606	CDL	C12-C13-C14-C15
18	C	304	CDL	C36-C37-C38-C39
18	L	101	CDL	C74-C75-C76-C77
20	N	609	DMU	C25-C28-C31-C34
19	P	310	LFA	C11-C12-C13-C14
19	T	101	LFA	C6-C7-C8-C9
19	T	101	LFA	C3-C4-C5-C6
18	A	606	CDL	C71-CB7-OB8-CB6
20	C	319	DMU	C19-C22-C25-C28
20	H	101	DMU	C28-C31-C34-C37
20	L	102	DMU	C19-C18-O16-C6
18	Y	101	CDL	C52-C53-C54-C55
19	C	308	LFA	C2-C3-C4-C5
19	C	310	LFA	C4-C5-C6-C7
19	C	325	LFA	C12-C13-C14-C15
20	C	318	DMU	C4-C3-O7-C10
23	N	622	PGV	C15-C16-C17-C18
18	L	101	CDL	C76-C77-C78-C79
19	B	308	LFA	C14-C15-C16-C17
19	P	313	LFA	C5-C6-C7-C8
18	C	304	CDL	C12-C11-CA5-OA6
20	C	318	DMU	C2-C3-O7-C10
18	L	101	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
18	P	305	CDL	CB3-CB4-CB6-OB8
18	Y	101	CDL	CB3-CB4-CB6-OB8
20	N	601	DMU	C34-C37-C40-C43
28	T	102	PEK	C4-C5-C6-C7
20	C	316	DMU	C34-C37-C40-C43
19	P	301	LFA	C7-C8-C9-C10
20	P	315	DMU	C19-C22-C25-C28
20	B	303	DMU	C31-C34-C37-C40
20	C	317	DMU	C3-C4-C57-O61
28	G	101	PEK	C6-C7-C8-C9
28	G	101	PEK	C9-C10-C11-C12
28	T	102	PEK	C11-C10-C9-C8
20	P	316	DMU	C31-C34-C37-C40
18	Y	101	CDL	C80-C81-C82-C83
19	C	314	LFA	C11-C10-C9-C8
19	T	104	LFA	C4-C5-C6-C7
20	J	101	DMU	C22-C25-C28-C31
28	T	102	PEK	C2-C3-C4-C5
20	C	319	DMU	C18-C19-C22-C25
20	P	323	DMU	C5-C10-O7-C3
20	Z	102	DMU	C22-C25-C28-C31
28	G	101	PEK	C23-C24-C25-C26
20	B	303	DMU	C22-C25-C28-C31
20	P	318	DMU	C28-C31-C34-C37
20	W	101	DMU	C25-C28-C31-C34
18	N	607	CDL	C32-C33-C34-C35
18	L	101	CDL	OB6-CB4-CB6-OB8
20	P	317	DMU	C19-C22-C25-C28
20	C	317	DMU	O5-C6-O16-C18
18	C	304	CDL	C58-C59-C60-C61
18	N	607	CDL	C18-C19-C20-C21
18	P	305	CDL	C52-C53-C54-C55
19	P	313	LFA	C2-C3-C4-C5
18	C	304	CDL	CA4-CA3-OA5-PA1
23	P	304	PGV	C02-C03-O11-P
19	C	309	LFA	C13-C14-C15-C16
20	T	105	DMU	C25-C28-C31-C34
20	U	101	DMU	C19-C22-C25-C28
19	C	325	LFA	C4-C5-C6-C7
23	P	304	PGV	C11-C12-C13-C14
25	P	306	CHD	C21-C20-C22-C23
20	D	201	DMU	C19-C22-C25-C28

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Mol	Chain	Res	Type	Atoms
19	C	313	LFA	C7-C8-C9-C10
20	P	319	DMU	C34-C37-C40-C43
20	P	323	DMU	C25-C28-C31-C34
18	A	606	CDL	C73-C74-C75-C76
18	Y	101	CDL	C51-C52-C53-C54
20	O	307	DMU	C19-C22-C25-C28
20	P	318	DMU	O16-C18-C19-C22
19	P	314	LFA	C5-C6-C7-C8
20	D	201	DMU	C2-C3-O7-C10
19	C	325	LFA	C5-C6-C7-C8
19	P	311	LFA	C3-C4-C5-C6
19	A	607	LFA	C9-C10-C11-C12
20	P	319	DMU	C28-C31-C34-C37
19	B	308	LFA	C1-C2-C3-C4
20	A	609	DMU	O16-C18-C19-C22
18	P	305	CDL	C13-C14-C15-C16
19	C	313	LFA	C9-C10-C11-C12
20	H	101	DMU	C22-C25-C28-C31
20	C	315	DMU	C25-C28-C31-C34
20	U	101	DMU	C22-C25-C28-C31
20	H	101	DMU	C25-C28-C31-C34
18	P	305	CDL	C75-C76-C77-C78
20	N	610	DMU	O5-C6-O16-C18
18	A	606	CDL	CA3-CA4-CA6-OA8
18	C	304	CDL	CB3-CB4-CB6-OB8
18	Y	101	CDL	CA3-CA4-CA6-OA8
20	H	101	DMU	C18-C19-C22-C25
20	D	201	DMU	O6-C11-C9-C8
20	Q	201	DMU	C2-C3-O7-C10
19	A	607	LFA	C7-C8-C9-C10
20	M	102	DMU	C22-C25-C28-C31
18	A	606	CDL	OB9-CB7-OB8-CB6
18	P	305	CDL	CB4-CB6-OB8-CB7
19	O	302	LFA	C11-C10-C9-C8
23	N	622	PGV	C27-C28-C29-C30
18	P	305	CDL	C77-C78-C79-C80
19	G	104	LFA	C1-C2-C3-C4
20	M	101	DMU	C19-C22-C25-C28
18	Y	101	CDL	C84-C85-C86-C87
19	P	311	LFA	C5-C6-C7-C8
20	C	319	DMU	C28-C31-C34-C37
28	G	101	PEK	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
28	T	102	PEK	C13-C14-C15-C16
19	P	313	LFA	C11-C10-C9-C8
20	Y	102	DMU	C19-C22-C25-C28
18	P	305	CDL	C23-C24-C25-C26
23	P	304	PGV	C22-C23-C24-C25
19	P	313	LFA	C4-C5-C6-C7
20	C	315	DMU	C34-C37-C40-C43
20	C	319	DMU	C31-C34-C37-C40
18	P	305	CDL	CA4-CA3-OA5-PA1
23	C	303	PGV	C02-C03-O11-P
28	G	101	PEK	C26-C27-C28-C29
18	A	606	CDL	CA3-OA5-PA1-OA3
18	A	606	CDL	CB2-OB2-PB2-OB4
18	C	304	CDL	CA3-OA5-PA1-OA3
18	L	101	CDL	CA2-OA2-PA1-OA4
18	L	101	CDL	CA3-OA5-PA1-OA3
18	L	101	CDL	CA3-OA5-PA1-OA4
18	Y	101	CDL	CA2-OA2-PA1-OA4
18	Y	101	CDL	CB2-OB2-PB2-OB4
18	Y	101	CDL	CB3-OB5-PB2-OB3
18	Y	101	CDL	CB3-OB5-PB2-OB4
23	A	619	PGV	C15-C16-C17-C18
19	P	310	LFA	C7-C8-C9-C10
20	P	317	DMU	C28-C31-C34-C37
20	Z	101	DMU	O16-C18-C19-C22
18	L	101	CDL	C19-C20-C21-C22
19	P	312	LFA	C4-C5-C6-C7
18	A	606	CDL	CA7-C31-C32-C33
19	C	314	LFA	C5-C6-C7-C8
18	N	607	CDL	OA5-CA3-CA4-OA6
20	Q	201	DMU	C22-C25-C28-C31
20	C	318	DMU	C5-C10-O7-C3
18	C	304	CDL	C16-C17-C18-C19
18	Y	101	CDL	C32-C33-C34-C35
18	P	305	CDL	CA7-C31-C32-C33
19	C	325	LFA	C10-C11-C12-C13
23	C	303	PGV	C21-C22-C23-C24
18	C	304	CDL	OB6-CB4-CB6-OB8
18	P	305	CDL	OB6-CB4-CB6-OB8
18	Y	101	CDL	OA6-CA4-CA6-OA8
18	C	304	CDL	C79-C80-C81-C82
28	T	102	PEK	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	L	101	CDL	C22-C23-C24-C25
19	C	311	LFA	C5-C6-C7-C8
18	N	607	CDL	C1-CA2-OA2-PA1
20	Y	102	DMU	C34-C37-C40-C43
18	Y	101	CDL	OB9-CB7-OB8-CB6
28	G	101	PEK	C16-C17-C18-C19
20	C	323	DMU	O1-C10-O7-C3
18	P	305	CDL	C14-C15-C16-C17
20	M	102	DMU	C34-C37-C40-C43
19	C	309	LFA	C2-C3-C4-C5
20	H	101	DMU	O6-C11-C9-O1
20	P	307	DMU	C18-C19-C22-C25
20	Q	201	DMU	C28-C31-C34-C37
19	C	307	LFA	C6-C7-C8-C9
18	P	305	CDL	C20-C21-C22-C23
20	D	201	DMU	C25-C28-C31-C34
20	Q	201	DMU	O16-C18-C19-C22
20	B	309	DMU	C18-C19-C22-C25
18	N	607	CDL	C12-C13-C14-C15
20	C	323	DMU	C19-C22-C25-C28
21	R	201	EDO	O1-C1-C2-O2
18	P	305	CDL	C18-C19-C20-C21
20	Q	201	DMU	O5-C4-C57-O61
20	W	101	DMU	C22-C25-C28-C31
20	C	319	DMU	C34-C37-C40-C43
28	T	102	PEK	C23-C24-C25-C26
19	C	309	LFA	C14-C15-C16-C17
20	G	102	DMU	C3-C4-C57-O61
19	G	104	LFA	C5-C6-C7-C8
19	O	303	LFA	C7-C8-C9-C10
20	C	315	DMU	O1-C10-O7-C3
18	A	606	CDL	C52-C51-CB5-OB6
20	M	101	DMU	O16-C18-C19-C22
18	C	304	CDL	C57-C58-C59-C60
20	P	318	DMU	C19-C22-C25-C28
28	G	101	PEK	C25-C26-C27-C28
23	P	304	PGV	C15-C16-C17-C18
18	L	101	CDL	C77-C78-C79-C80
18	N	607	CDL	CB4-CB3-OB5-PB2
18	P	305	CDL	C12-C11-CA5-OA6
18	C	304	CDL	C24-C25-C26-C27
14	A	602	HEA	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
18	P	305	CDL	C71-C72-C73-C74
18	A	606	CDL	CB7-C71-C72-C73
20	C	323	DMU	C5-C10-O7-C3
18	L	101	CDL	C56-C57-C58-C59
20	C	315	DMU	C5-C10-O7-C3
18	L	101	CDL	C15-C16-C17-C18
19	C	325	LFA	C1-C2-C3-C4
18	C	304	CDL	C54-C55-C56-C57
14	N	603	HEA	CAA-CBA-CGA-O1A
18	C	304	CDL	C12-C13-C14-C15
20	B	303	DMU	C34-C37-C40-C43
18	P	305	CDL	C84-C85-C86-C87
18	A	606	CDL	C52-C51-CB5-OB7
18	L	101	CDL	C53-C54-C55-C56
19	C	307	LFA	C11-C10-C9-C8
23	P	304	PGV	C1-C2-C3-C4
23	P	304	PGV	C05-C04-O12-P
14	A	601	HEA	CAD-CBD-CGD-O1D
14	N	602	HEA	CAD-CBD-CGD-O1D
20	C	306	DMU	C31-C34-C37-C40
19	G	104	LFA	C11-C12-C13-C14
20	H	101	DMU	C19-C18-O16-C6
25	B	307	CHD	C22-C23-C24-O26
25	P	306	CHD	C22-C23-C24-O25
21	A	611	EDO	O1-C1-C2-O2
18	Y	101	CDL	CA2-C1-CB2-OB2
18	C	304	CDL	C52-C53-C54-C55
18	L	101	CDL	C75-C76-C77-C78
14	A	602	HEA	CAA-CBA-CGA-O1A
25	B	307	CHD	C22-C23-C24-O25
25	C	305	CHD	C22-C23-C24-O25
18	Y	101	CDL	C71-CB7-OB8-CB6
14	A	602	HEA	CAD-CBD-CGD-O2D
19	C	310	LFA	C1-C2-C3-C4
14	A	602	HEA	CAD-CBD-CGD-O1D
18	P	305	CDL	C19-C20-C21-C22
25	P	306	CHD	C22-C23-C24-O26
20	A	608	DMU	C34-C37-C40-C43
20	B	309	DMU	C28-C31-C34-C37
18	P	305	CDL	C22-C23-C24-C25
23	C	303	PGV	C05-C04-O12-P
14	N	603	HEA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	P	305	CDL	C79-C80-C81-C82
20	B	304	DMU	C28-C31-C34-C37
20	C	315	DMU	C18-C19-C22-C25
18	Y	101	CDL	OA5-CA3-CA4-CA6
20	P	318	DMU	C18-C19-C22-C25
18	P	305	CDL	C72-C73-C74-C75
14	A	601	HEA	CAD-CBD-CGD-O2D
25	O	301	CHD	C22-C23-C24-O25
25	O	301	CHD	C22-C23-C24-O26
18	N	607	CDL	C75-C76-C77-C78
19	T	101	LFA	C11-C10-C9-C8
14	N	603	HEA	CAA-CBA-CGA-O2A
23	C	303	PGV	C27-C28-C29-C30
14	N	603	HEA	CAD-CBD-CGD-O2D
20	D	201	DMU	C28-C31-C34-C37
18	C	304	CDL	CA2-C1-CB2-OB2
14	A	602	HEA	CAA-CBA-CGA-O2A
14	N	602	HEA	CAD-CBD-CGD-O2D
23	A	619	PGV	O03-C19-C20-C21
23	P	304	PGV	C14-C15-C16-C17
20	C	318	DMU	O1-C10-O7-C3
23	C	303	PGV	C23-C24-C25-C26
25	C	305	CHD	C22-C23-C24-O26
18	L	101	CDL	C57-C58-C59-C60
18	N	607	CDL	C19-C20-C21-C22
25	C	301	CHD	C22-C23-C24-O26
20	A	609	DMU	C19-C22-C25-C28
18	Y	101	CDL	OA5-CA3-CA4-OA6
25	P	306	CHD	C20-C22-C23-C24
23	N	622	PGV	O03-C19-C20-C21
25	P	302	CHD	C22-C23-C24-O26
18	C	304	CDL	C83-C84-C85-C86
18	C	304	CDL	C72-C71-CB7-OB9
18	P	305	CDL	C52-C51-CB5-OB6
19	C	311	LFA	C2-C3-C4-C5
20	B	305	DMU	C18-C19-C22-C25
20	G	102	DMU	C34-C37-C40-C43
18	C	304	CDL	C77-C78-C79-C80
18	L	101	CDL	C32-C31-CA7-OA8
18	C	304	CDL	CB2-OB2-PB2-OB5
18	P	305	CDL	C80-C81-C82-C83
18	N	607	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
23	A	619	PGV	C12-C13-C14-C15
25	C	301	CHD	C22-C23-C24-O25
19	T	104	LFA	C6-C7-C8-C9
20	N	610	DMU	O6-C11-C9-O1
18	A	606	CDL	CA3-CA4-OA6-CA5
18	L	101	CDL	C72-C71-CB7-OB9
14	A	602	HEA	C26-C15-C16-C17
25	P	302	CHD	C22-C23-C24-O25
28	T	102	PEK	C2-C1-O01-C02
20	C	315	DMU	C4-C3-O7-C10
20	T	105	DMU	C31-C34-C37-C40
18	C	304	CDL	C13-C14-C15-C16
18	C	304	CDL	C33-C34-C35-C36
21	C	322	EDO	O1-C1-C2-O2
21	R	203	EDO	O1-C1-C2-O2
23	N	622	PGV	C26-C27-C28-C29
20	P	315	DMU	O1-C10-O7-C3
18	N	607	CDL	OA5-CA3-CA4-CA6
18	C	304	CDL	C32-C33-C34-C35
18	A	606	CDL	C32-C31-CA7-OA8
18	Y	101	CDL	C12-C11-CA5-OA6
20	G	102	DMU	O5-C4-C57-O61
18	Y	101	CDL	C53-C54-C55-C56
20	L	102	DMU	C18-C19-C22-C25
20	Y	102	DMU	C22-C25-C28-C31
18	C	304	CDL	C52-C51-CB5-OB6
19	P	308	LFA	C3-C4-C5-C6
18	L	101	CDL	C64-C65-C66-C67
14	A	601	HEA	C26-C15-C16-C17
20	C	323	DMU	C34-C37-C40-C43
18	L	101	CDL	C32-C31-CA7-OA9
18	A	606	CDL	C77-C78-C79-C80
23	A	619	PGV	C26-C27-C28-C29
14	A	601	HEA	CAA-CBA-CGA-O2A
28	T	102	PEK	O02-C1-O01-C02
18	P	305	CDL	C52-C51-CB5-OB7
20	C	315	DMU	C2-C3-O7-C10
18	L	101	CDL	CB2-OB2-PB2-OB4
18	N	607	CDL	C72-C71-CB7-OB9
18	C	304	CDL	OB5-CB3-CB4-CB6
18	A	606	CDL	C32-C31-CA7-OA9
20	C	317	DMU	C22-C25-C28-C31

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Mol	Chain	Res	Type	Atoms
21	F	104	EDO	O1-C1-C2-O2
21	P	322	EDO	O1-C1-C2-O2
28	T	102	PEK	O03-C21-C22-C23
28	T	102	PEK	C3-C4-C5-C6
19	P	313	LFA	C7-C8-C9-C10
14	N	603	HEA	C26-C15-C16-C17
18	Y	101	CDL	C77-C78-C79-C80
28	T	102	PEK	C14-C15-C16-C17
20	W	101	DMU	C18-C19-C22-C25
20	D	201	DMU	C22-C25-C28-C31
20	G	102	DMU	C22-C25-C28-C31
28	T	102	PEK	O01-C1-C2-C3
18	L	101	CDL	OB5-CB3-CB4-OB6
28	G	101	PEK	C22-C23-C24-C25
19	P	301	LFA	C5-C6-C7-C8
20	Q	201	DMU	C19-C18-O16-C6
20	P	307	DMU	C22-C25-C28-C31
20	L	102	DMU	O5-C6-O16-C18
18	C	304	CDL	C82-C83-C84-C85
18	C	304	CDL	C52-C51-CB5-OB7
19	C	325	LFA	C3-C4-C5-C6
19	T	104	LFA	C7-C8-C9-C10
18	P	305	CDL	C72-C71-CB7-OB8
14	A	601	HEA	CAA-CBA-CGA-O1A

There are no ring outliers.

42 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	307	LFA	1	0
19	O	303	LFA	4	0
25	P	306	CHD	4	0
20	T	105	DMU	2	0
19	N	608	LFA	5	0
19	C	312	LFA	1	0
19	P	313	LFA	1	0
28	G	101	PEK	1	0
19	P	310	LFA	3	0
18	L	101	CDL	4	0
28	T	102	PEK	2	0
20	A	609	DMU	1	0
20	D	201	DMU	1	0

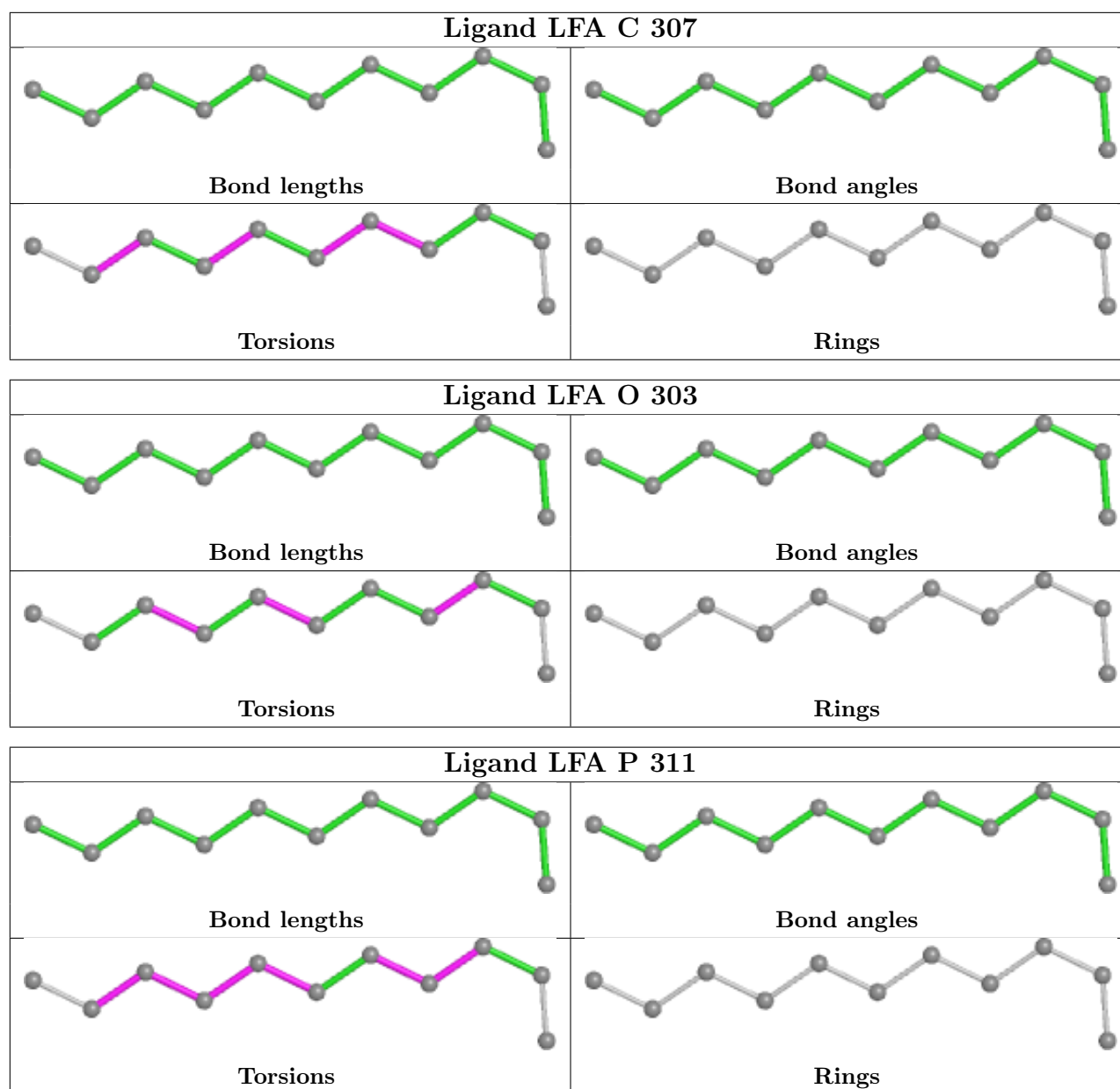
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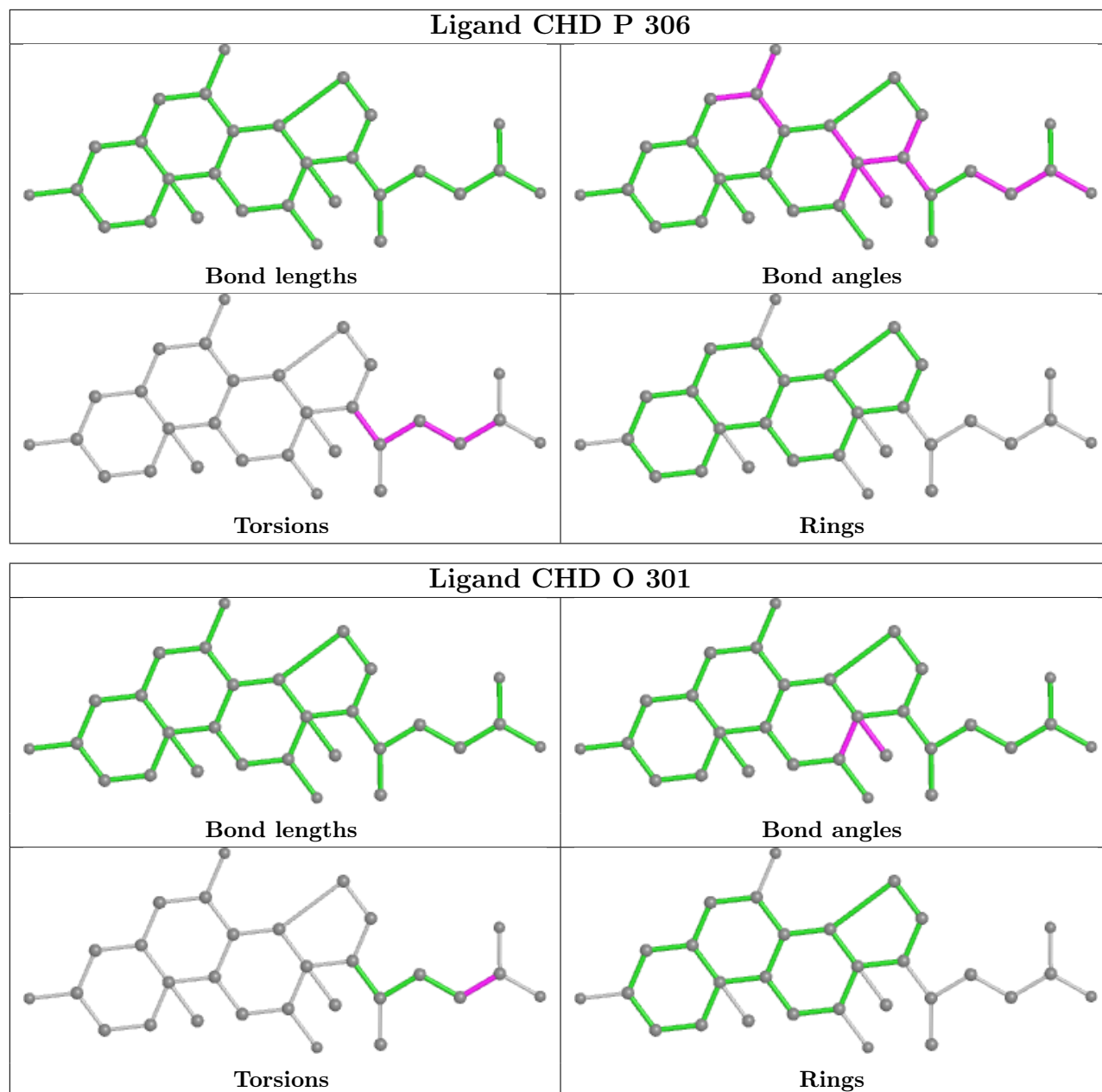


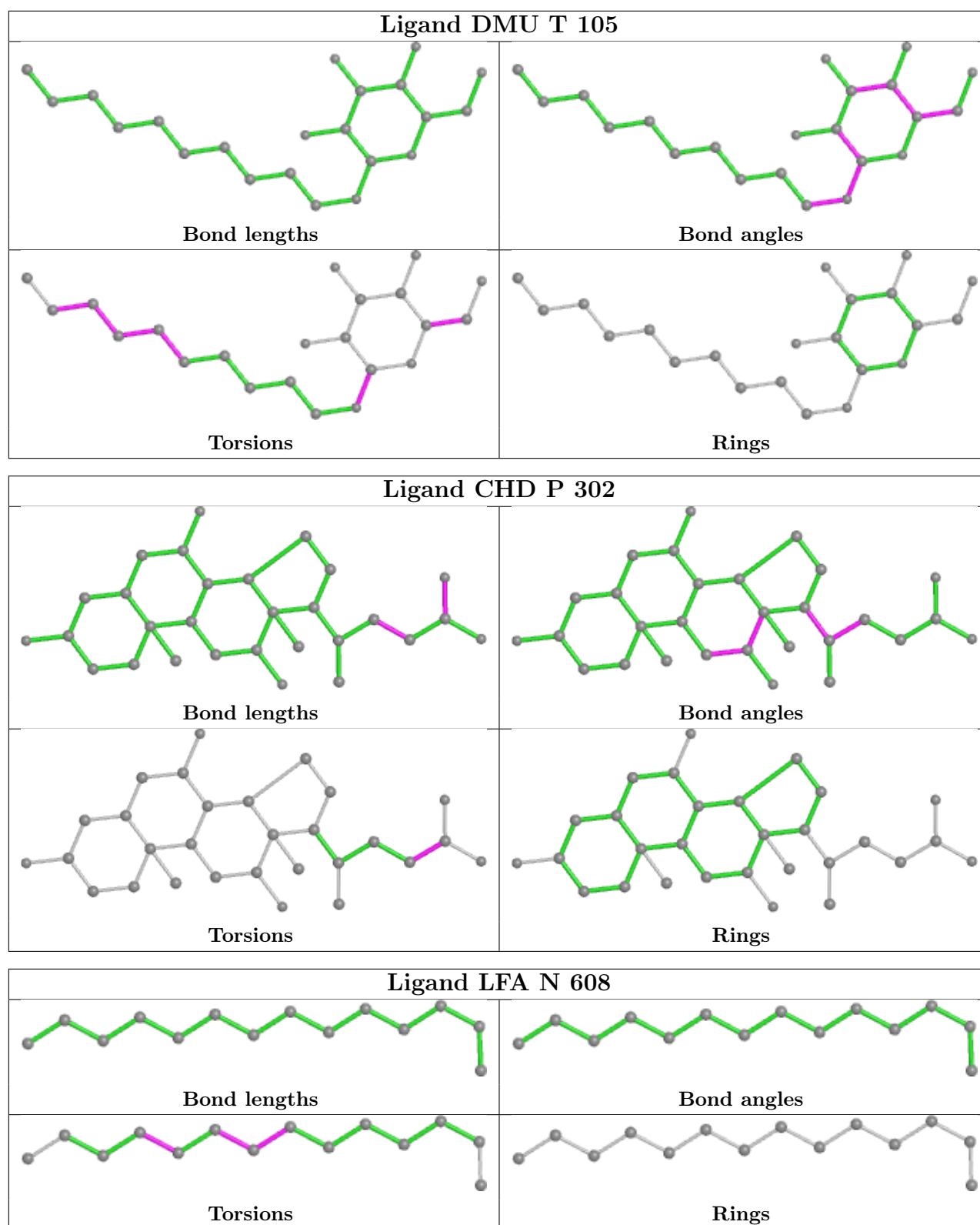
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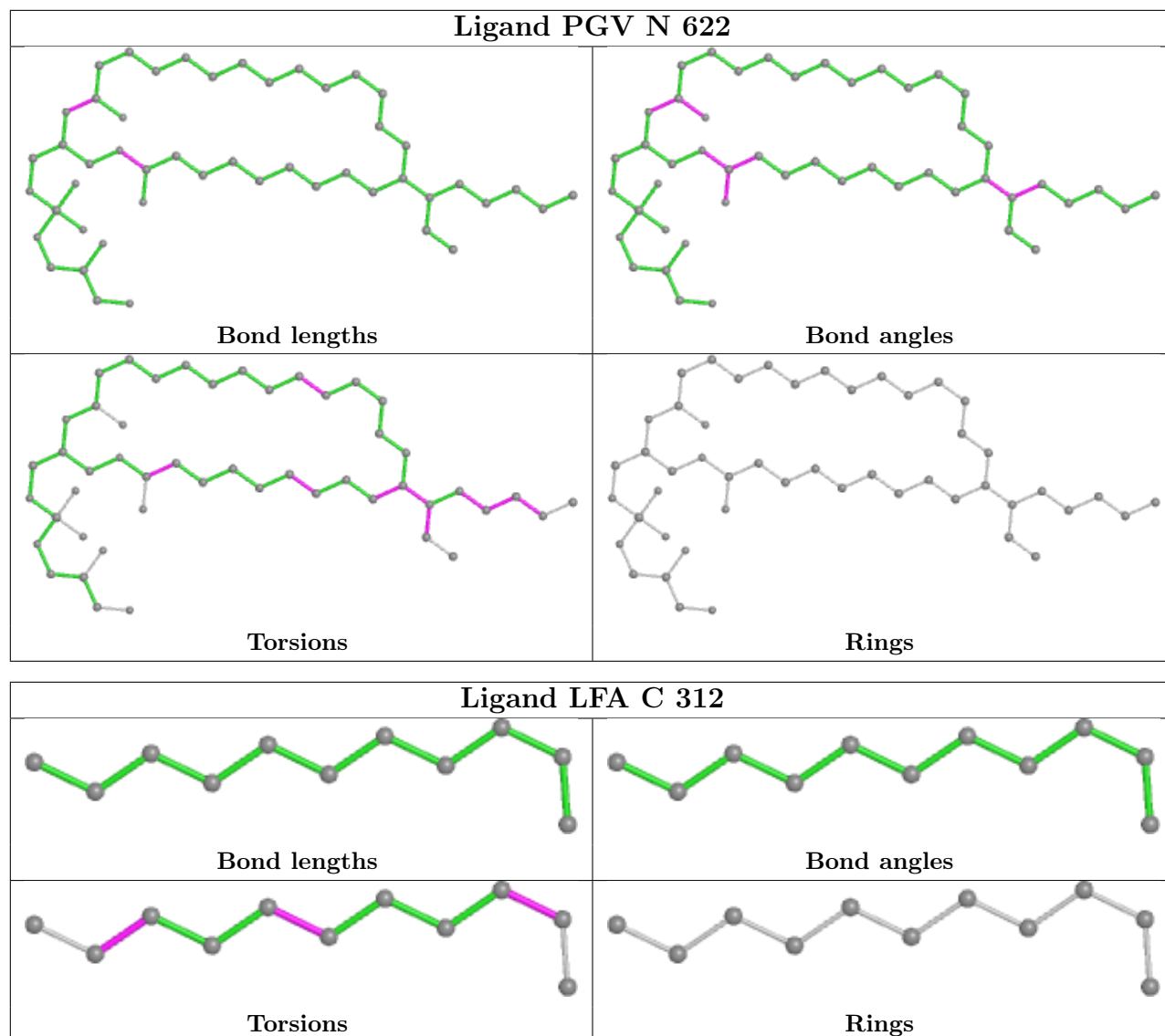
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	Z	101	DMU	1	0
19	G	104	LFA	2	0
20	Q	201	DMU	1	0
20	A	608	DMU	1	0
19	C	313	LFA	2	0
19	A	607	LFA	3	0
19	P	312	LFA	1	0
19	B	308	LFA	1	0
20	L	102	DMU	3	0
23	P	304	PGV	1	0
18	P	305	CDL	16	0
25	C	301	CHD	1	0
14	N	602	HEA	5	0
20	O	304	DMU	1	0
25	C	305	CHD	3	0
20	C	323	DMU	2	0
18	C	304	CDL	23	0
23	C	303	PGV	4	0
19	C	309	LFA	2	0
19	C	314	LFA	1	0
19	T	101	LFA	2	0
20	C	318	DMU	1	0
20	Y	102	DMU	2	0
21	F	101	EDO	1	0
14	A	601	HEA	4	0
18	Y	101	CDL	10	0
18	N	607	CDL	2	0
20	P	323	DMU	3	0
20	H	101	DMU	1	0

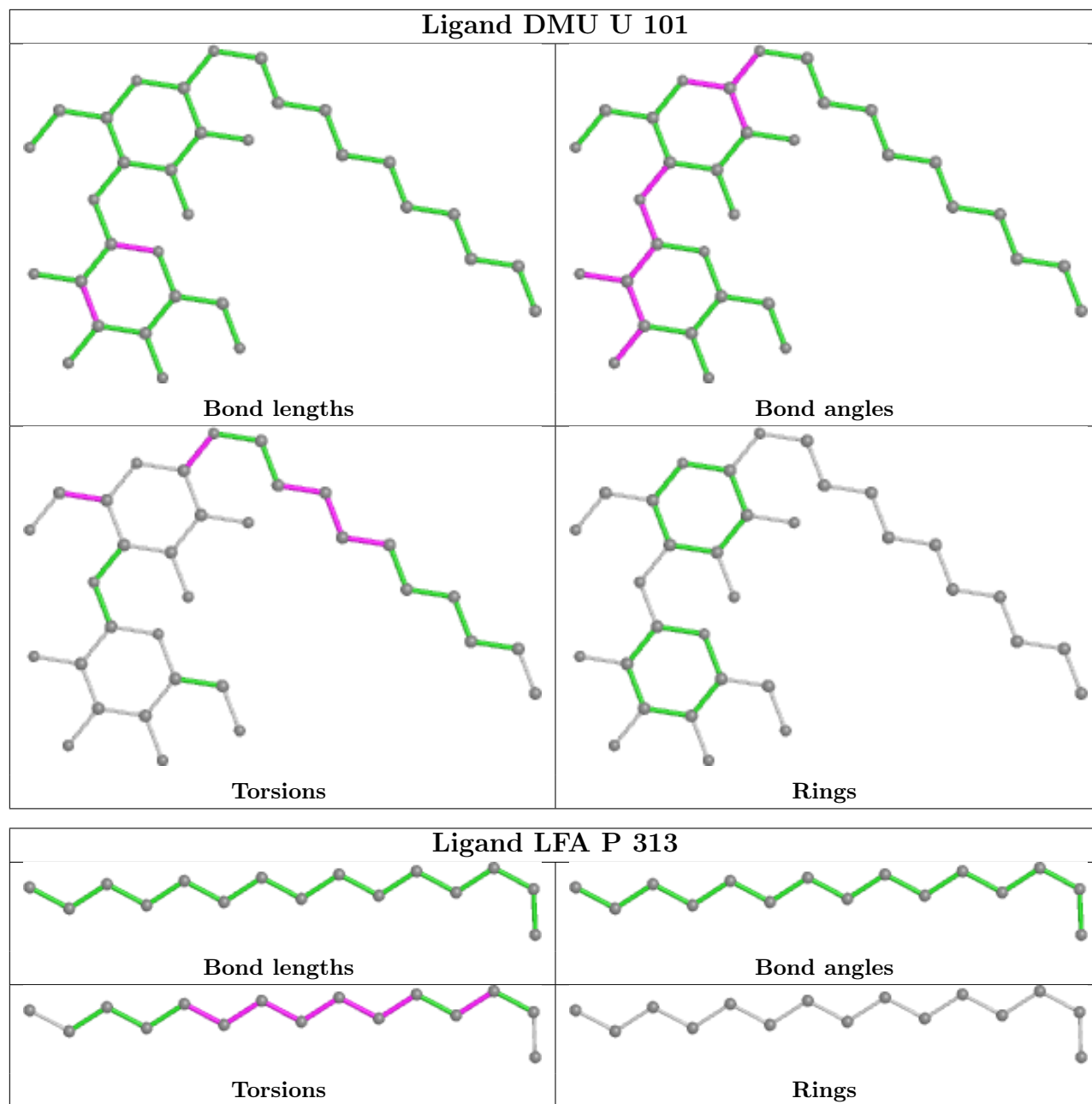
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

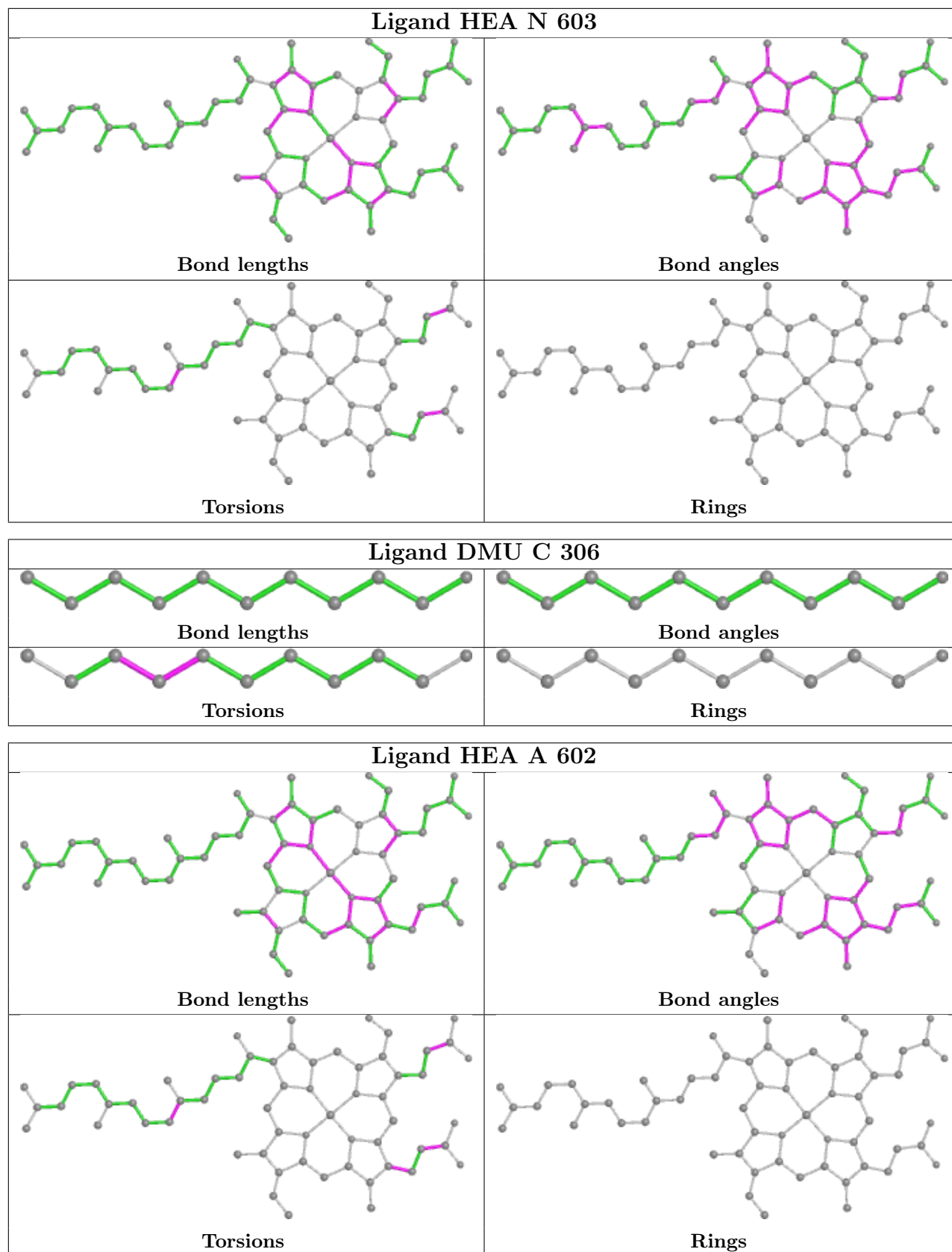


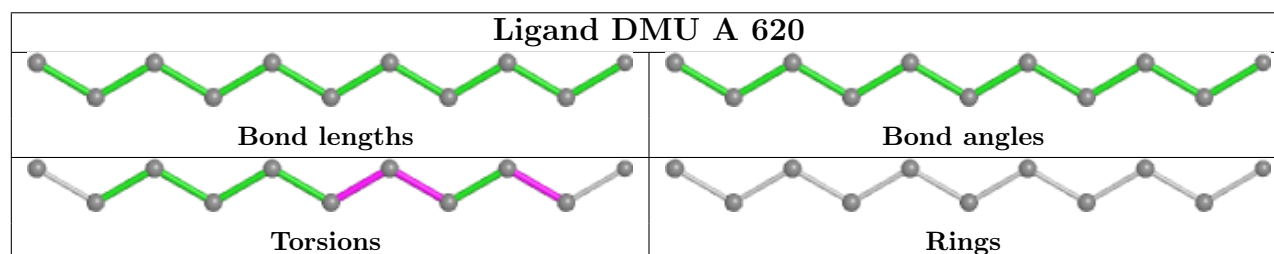
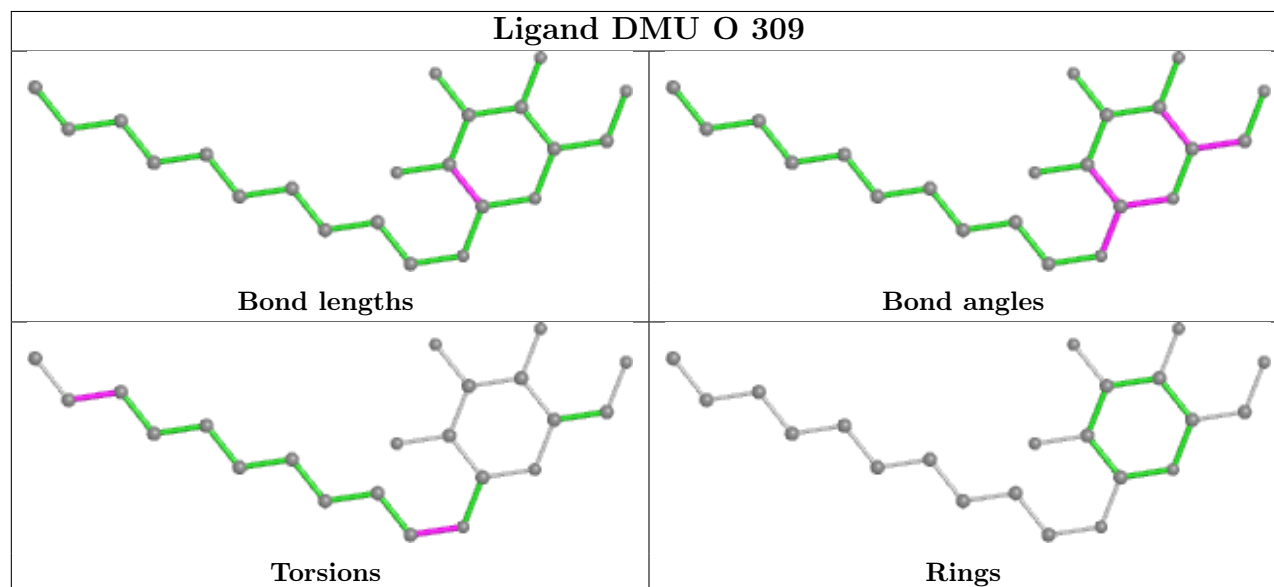
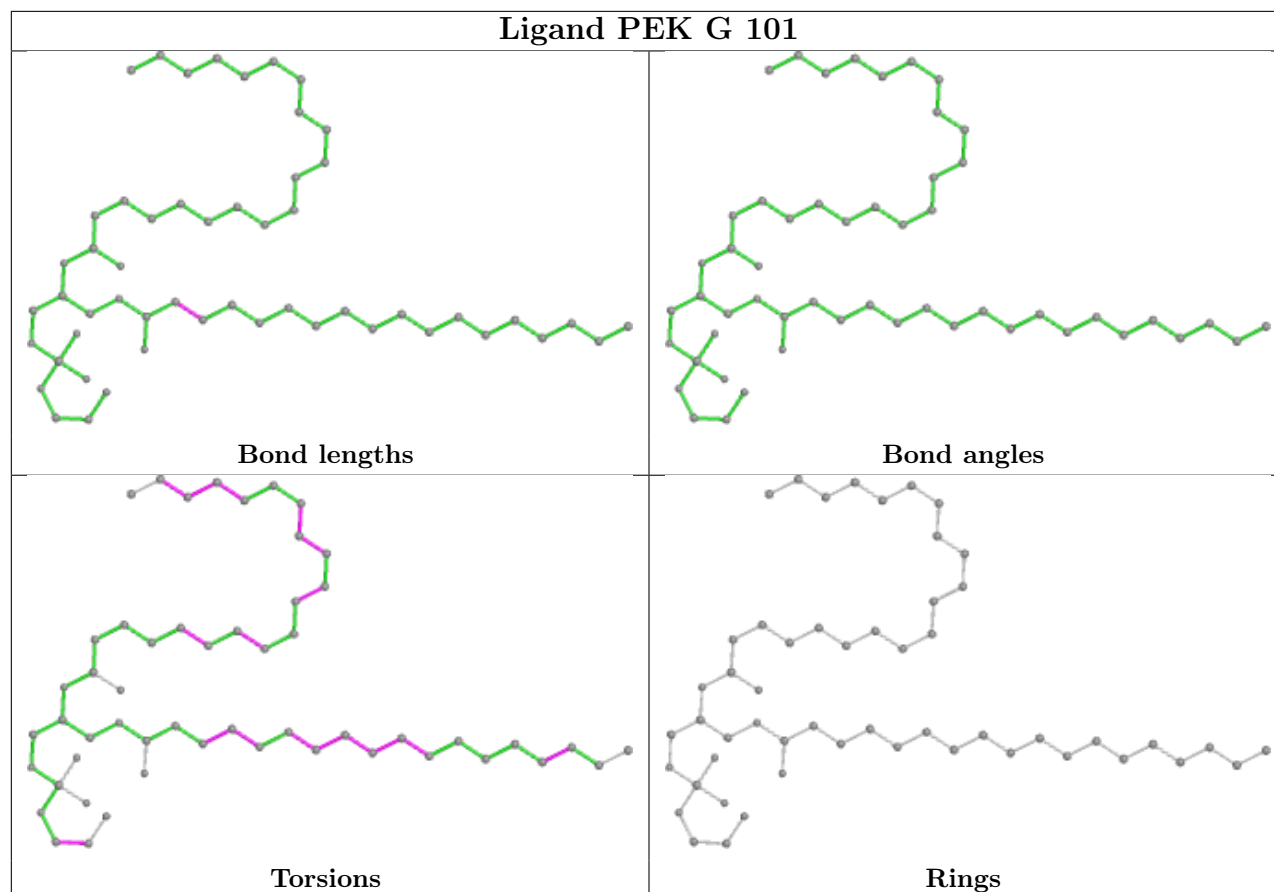




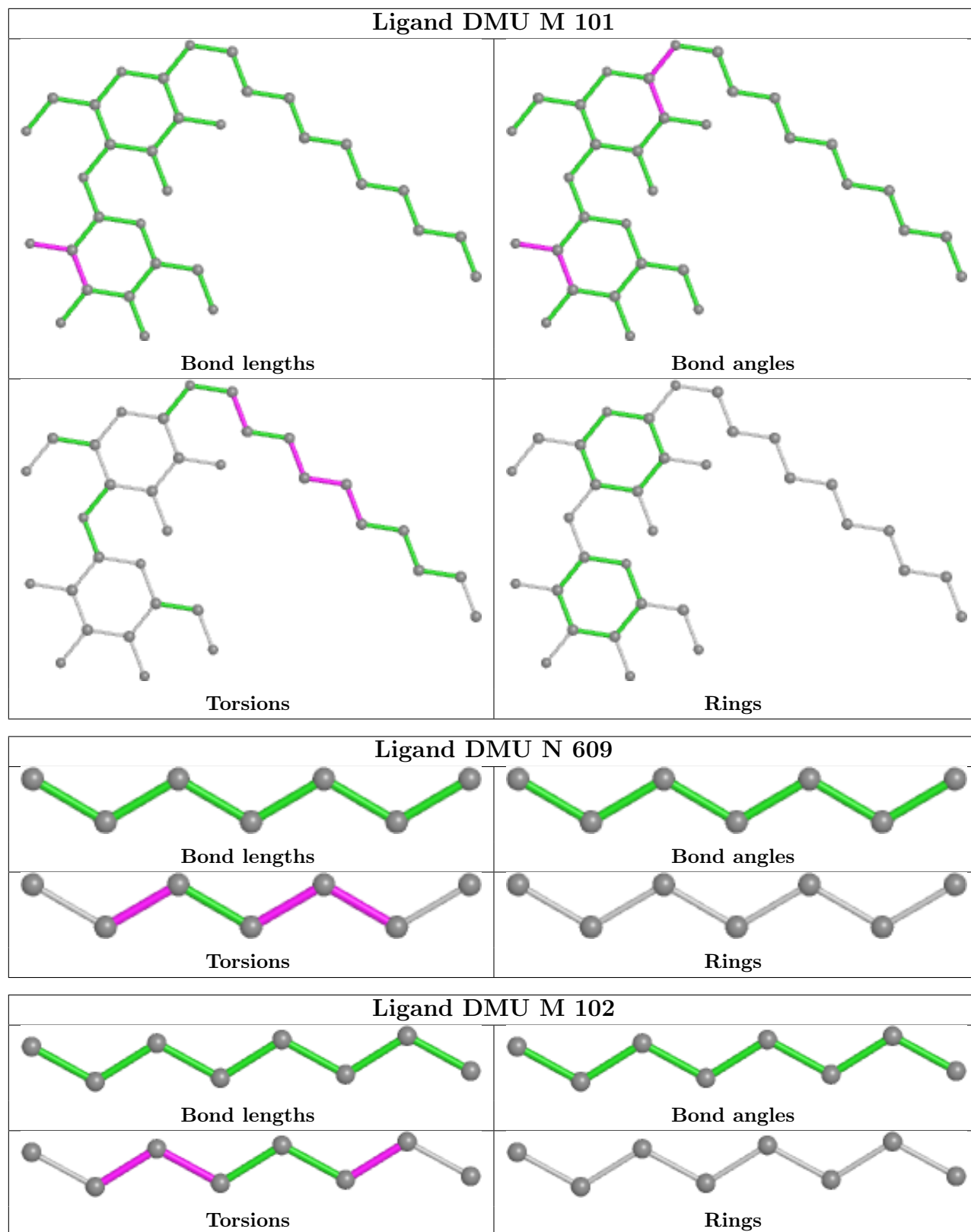


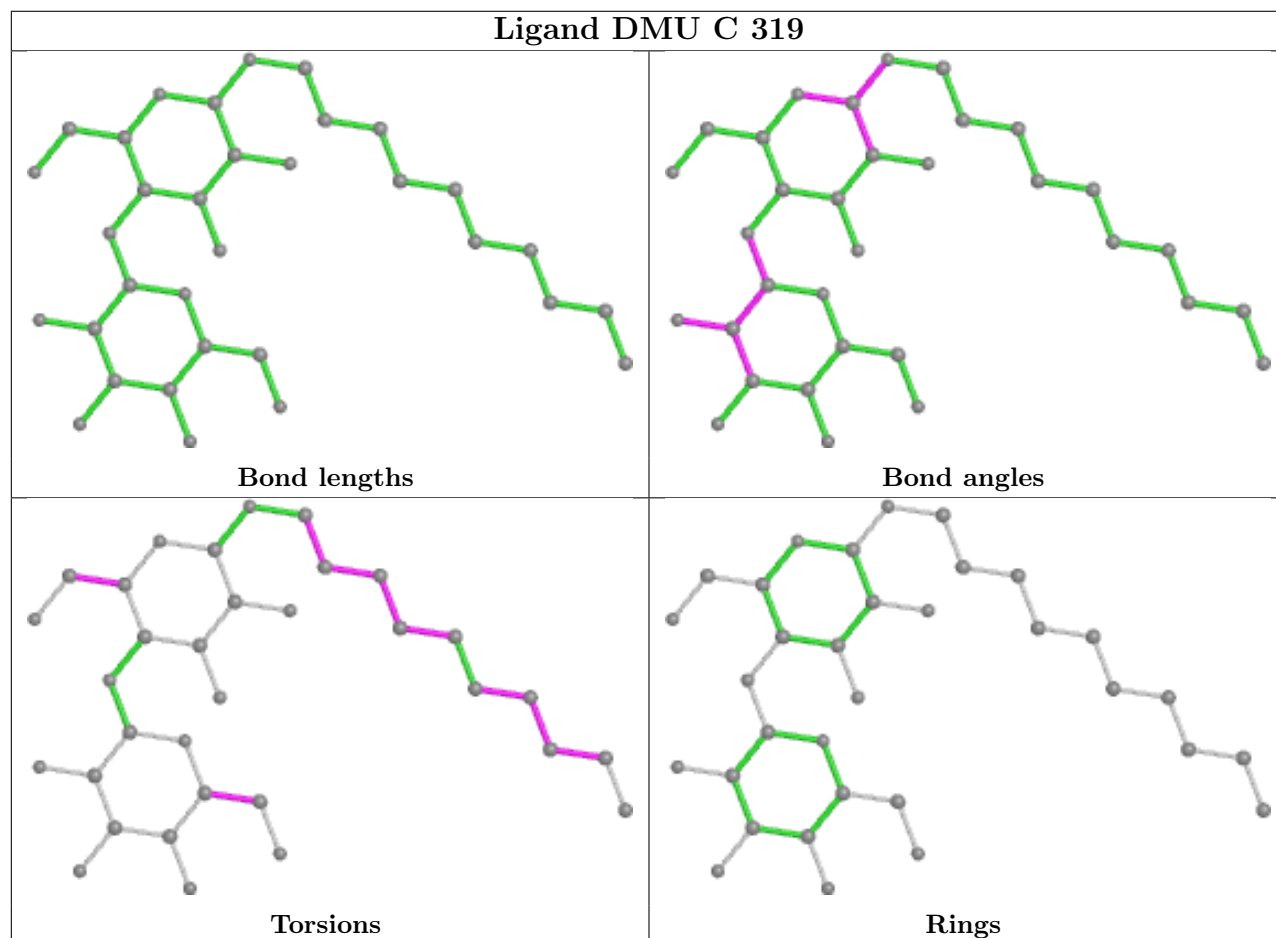
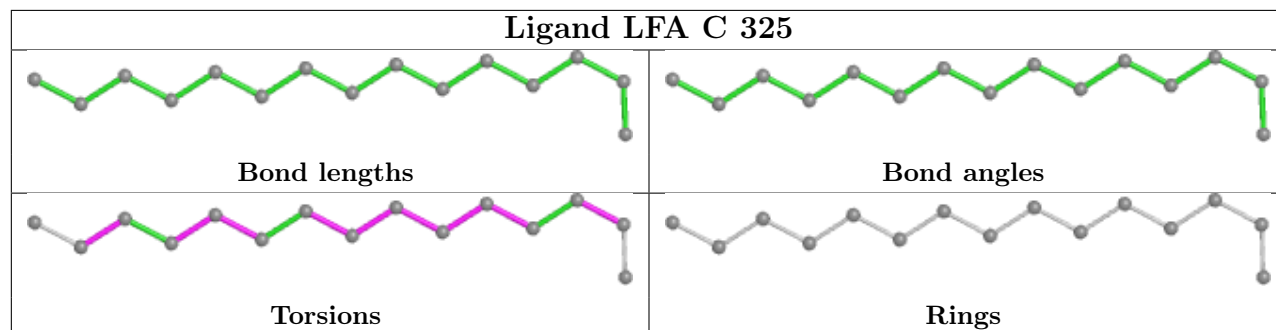
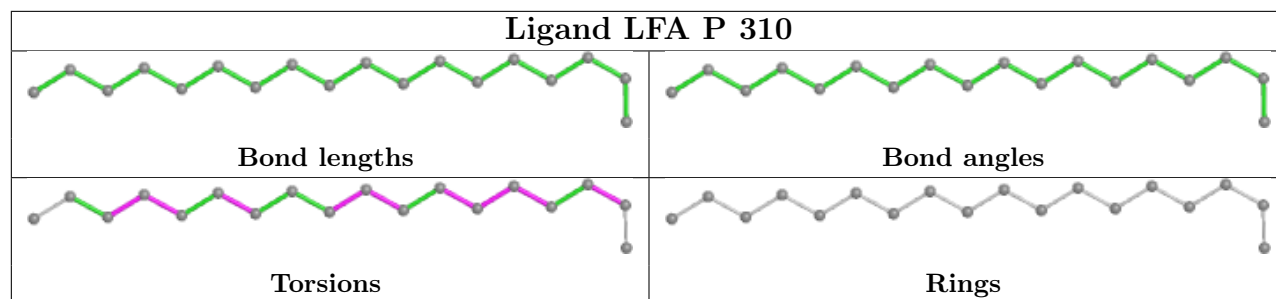


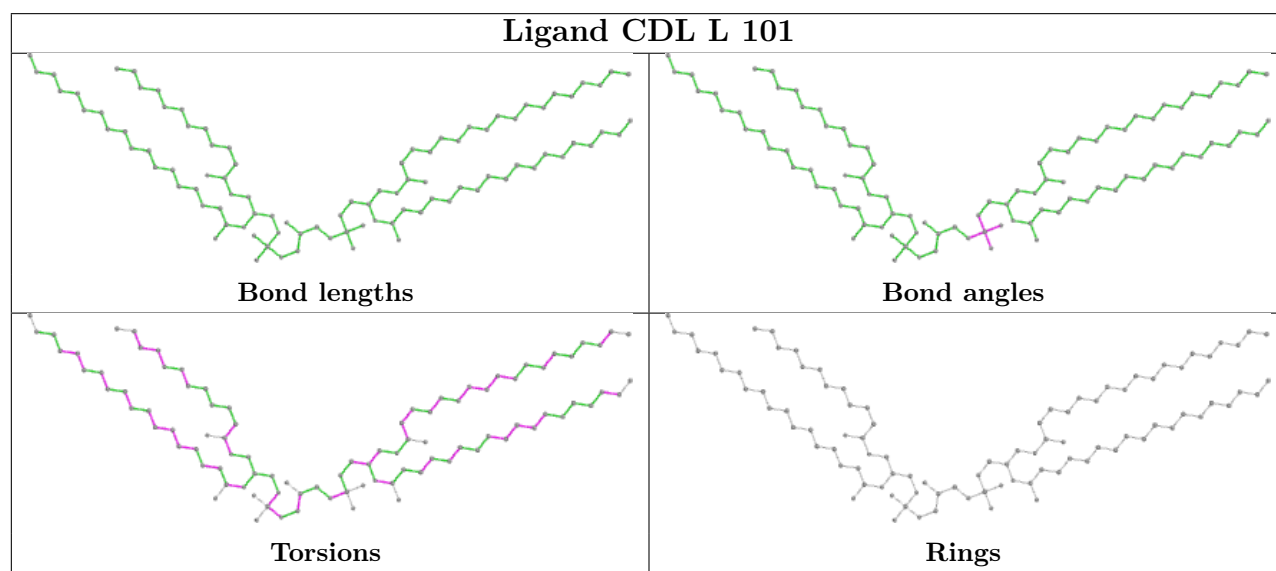
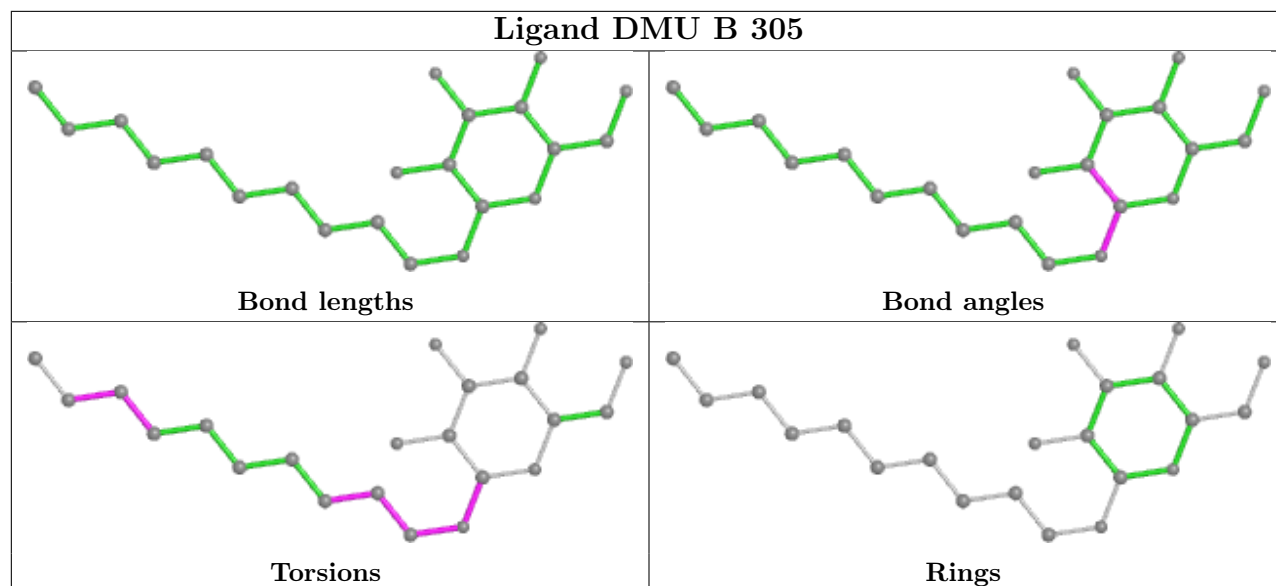


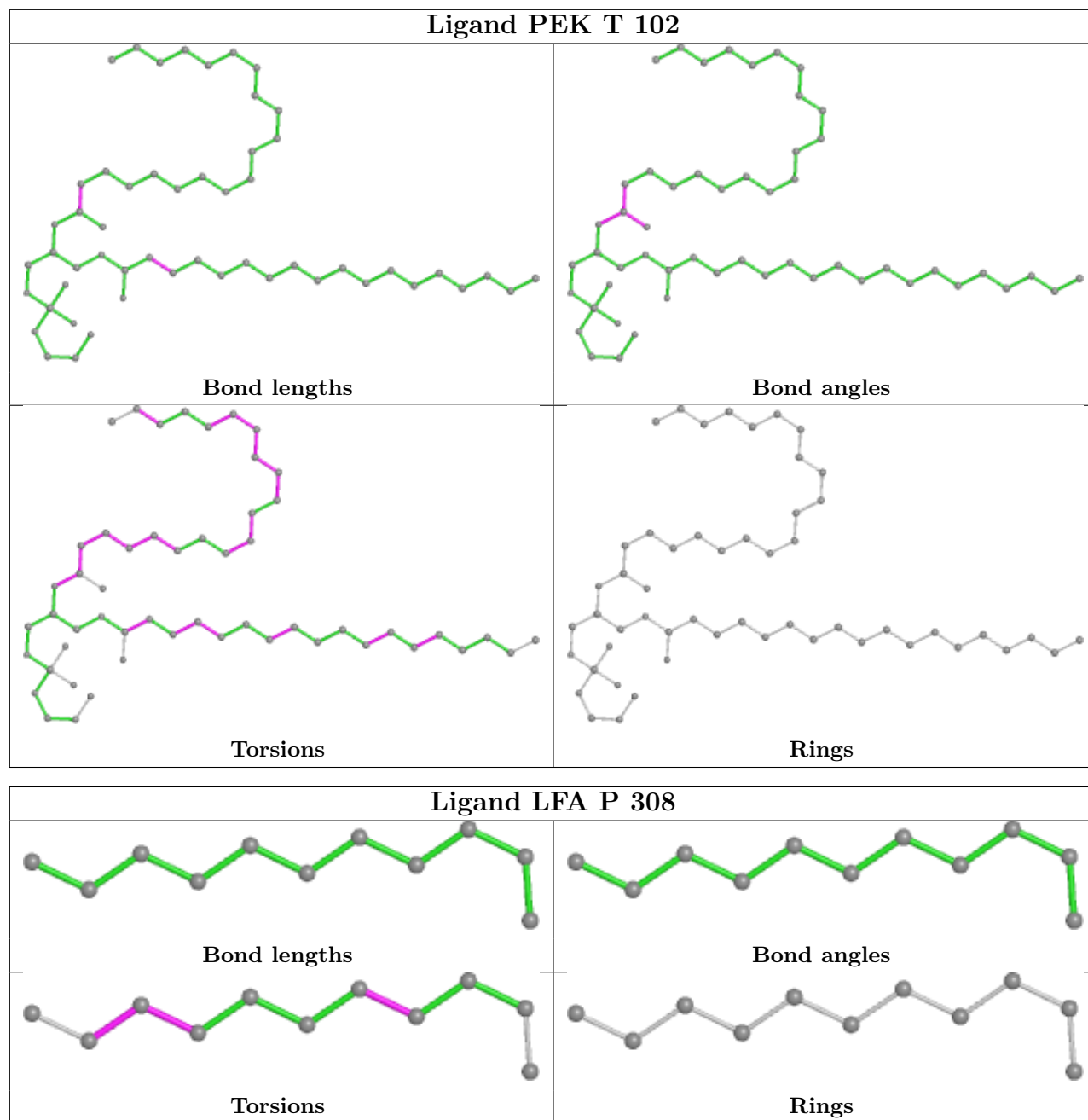


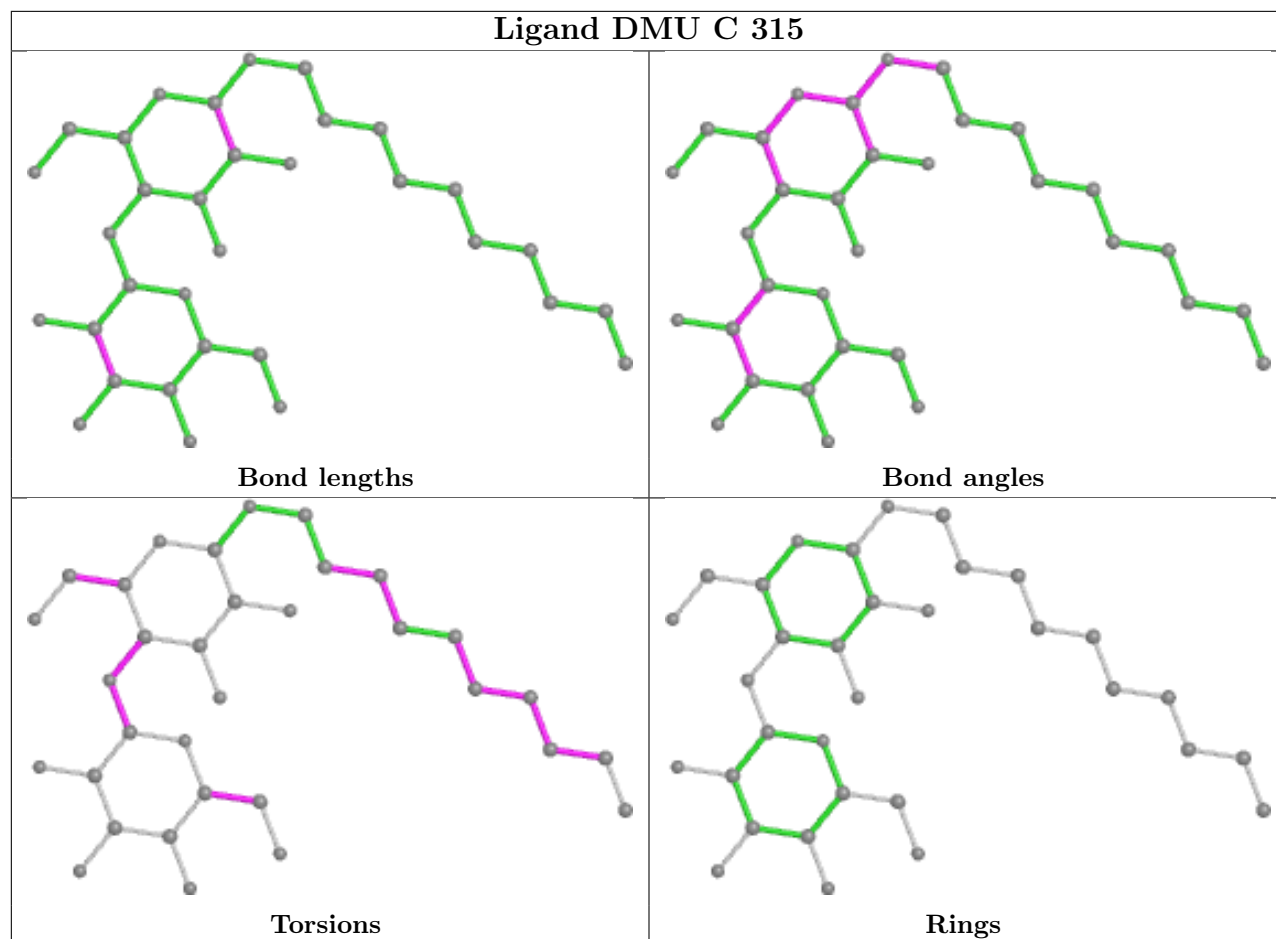


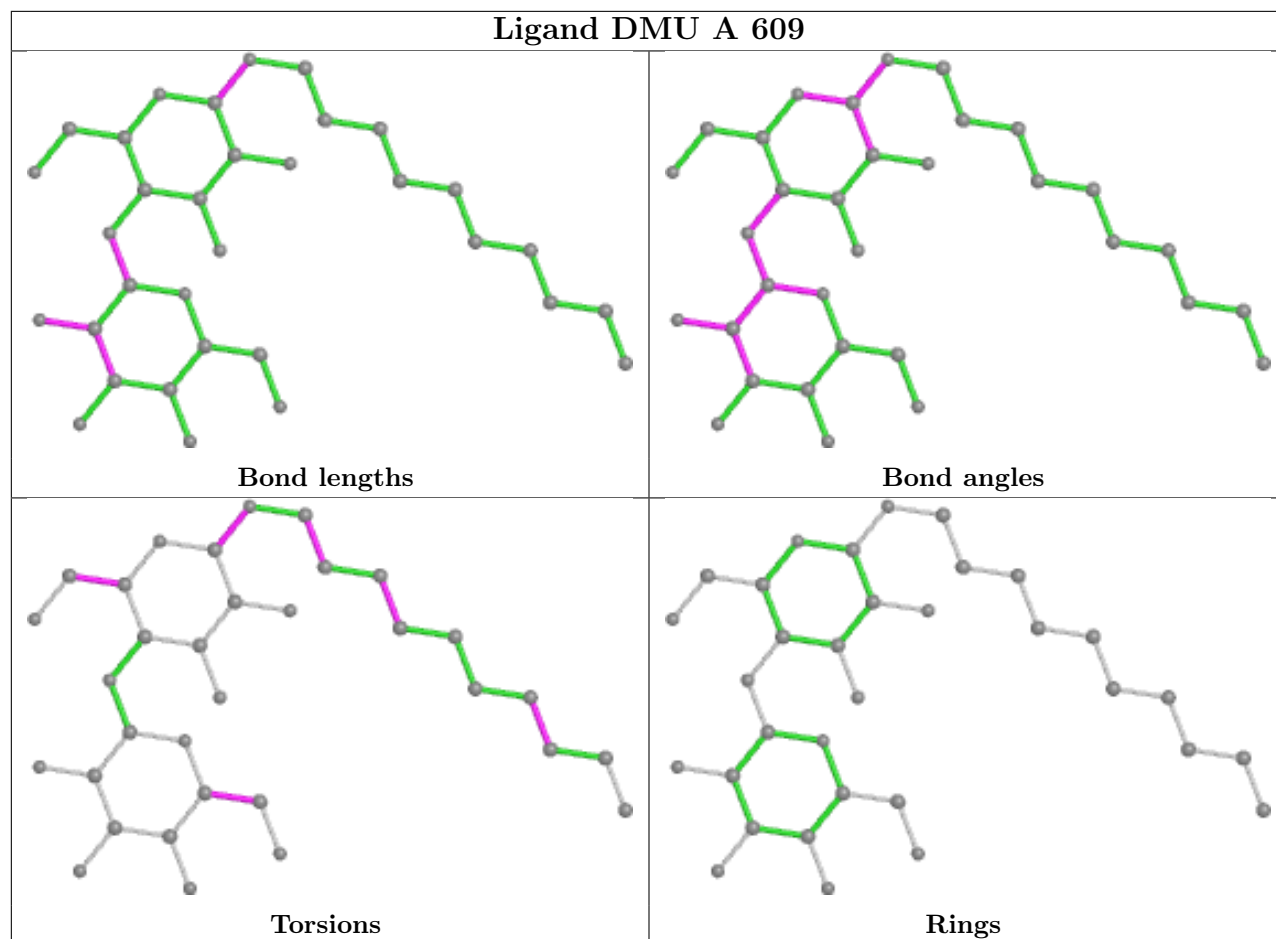


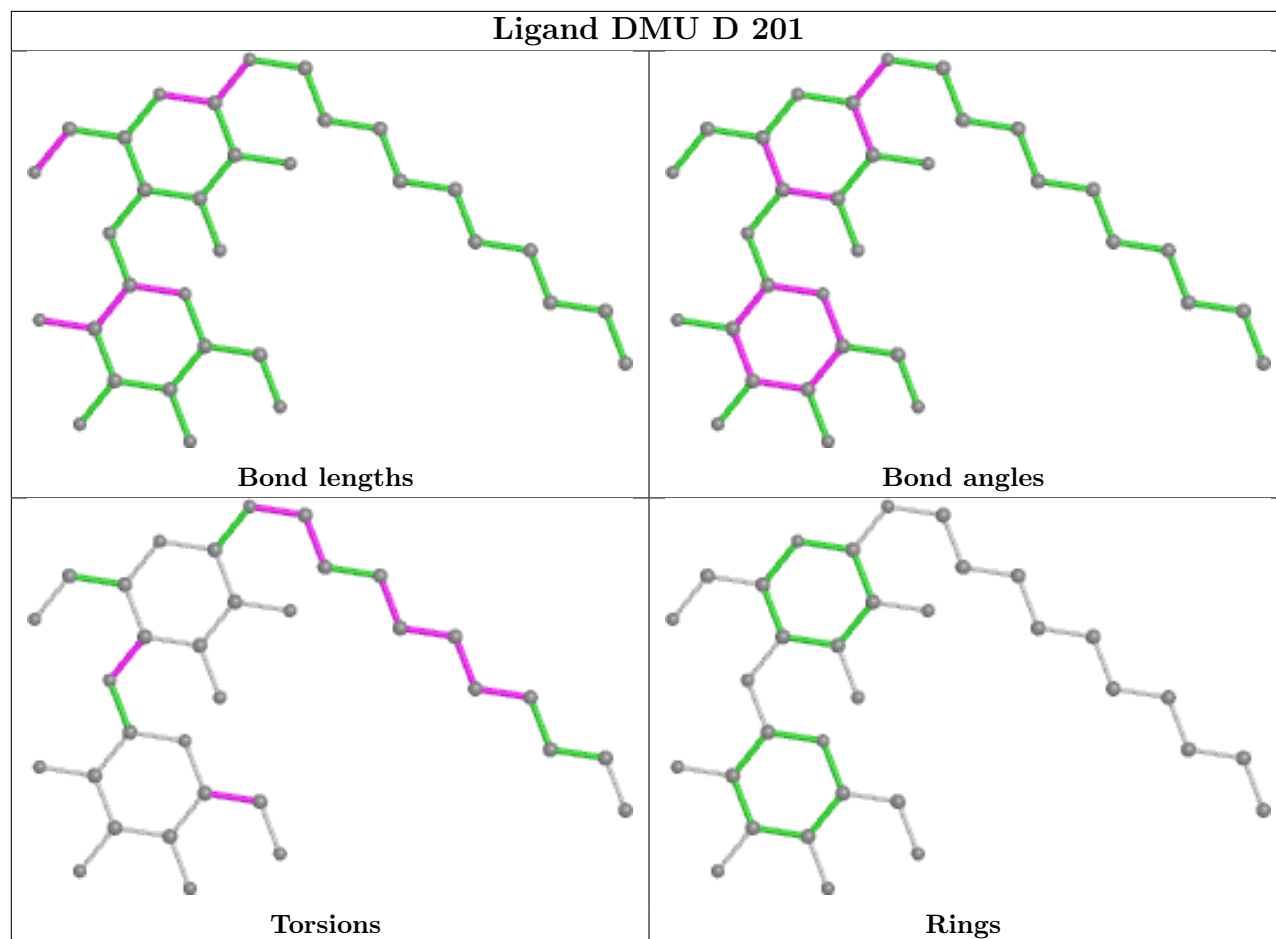


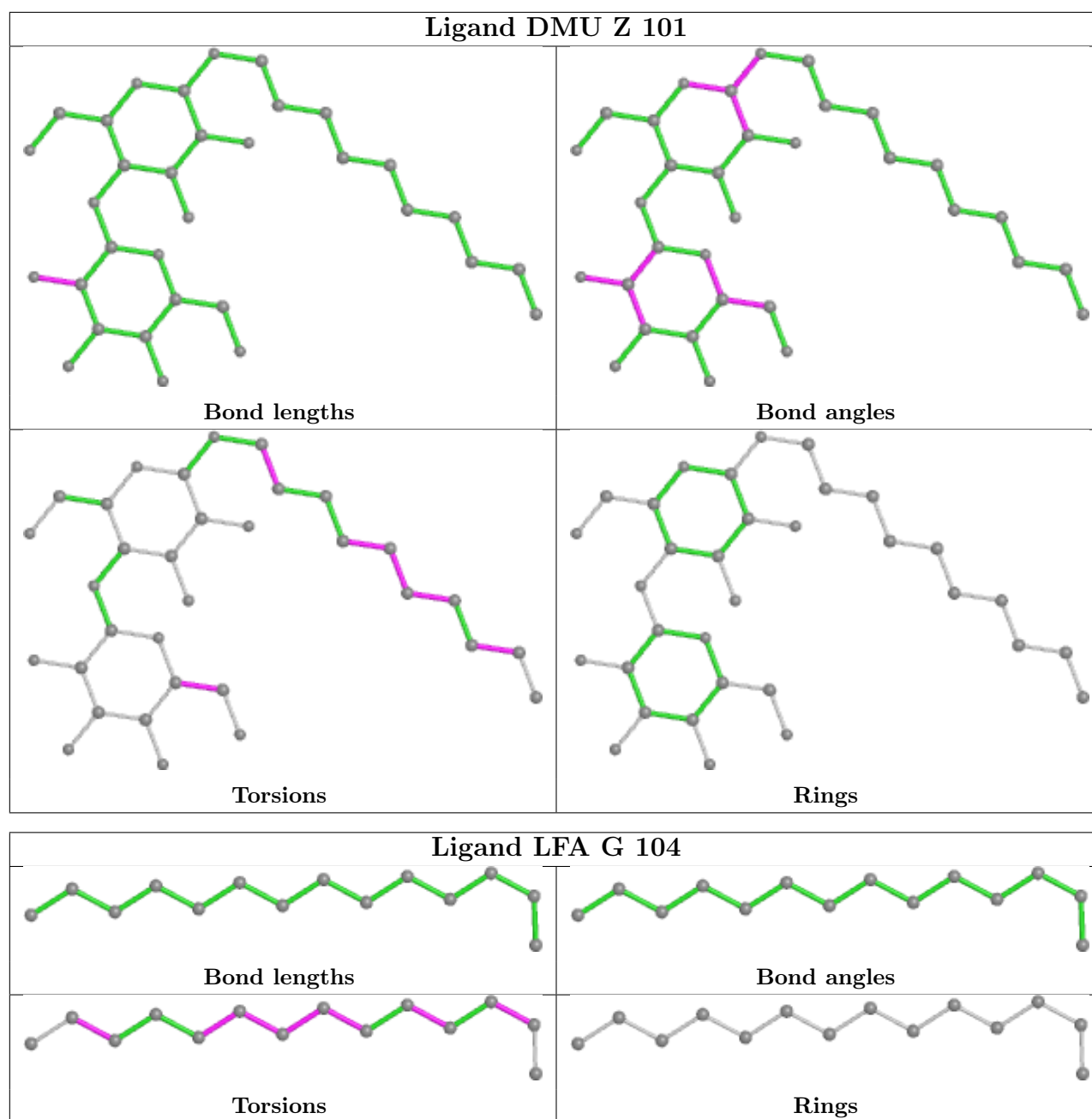




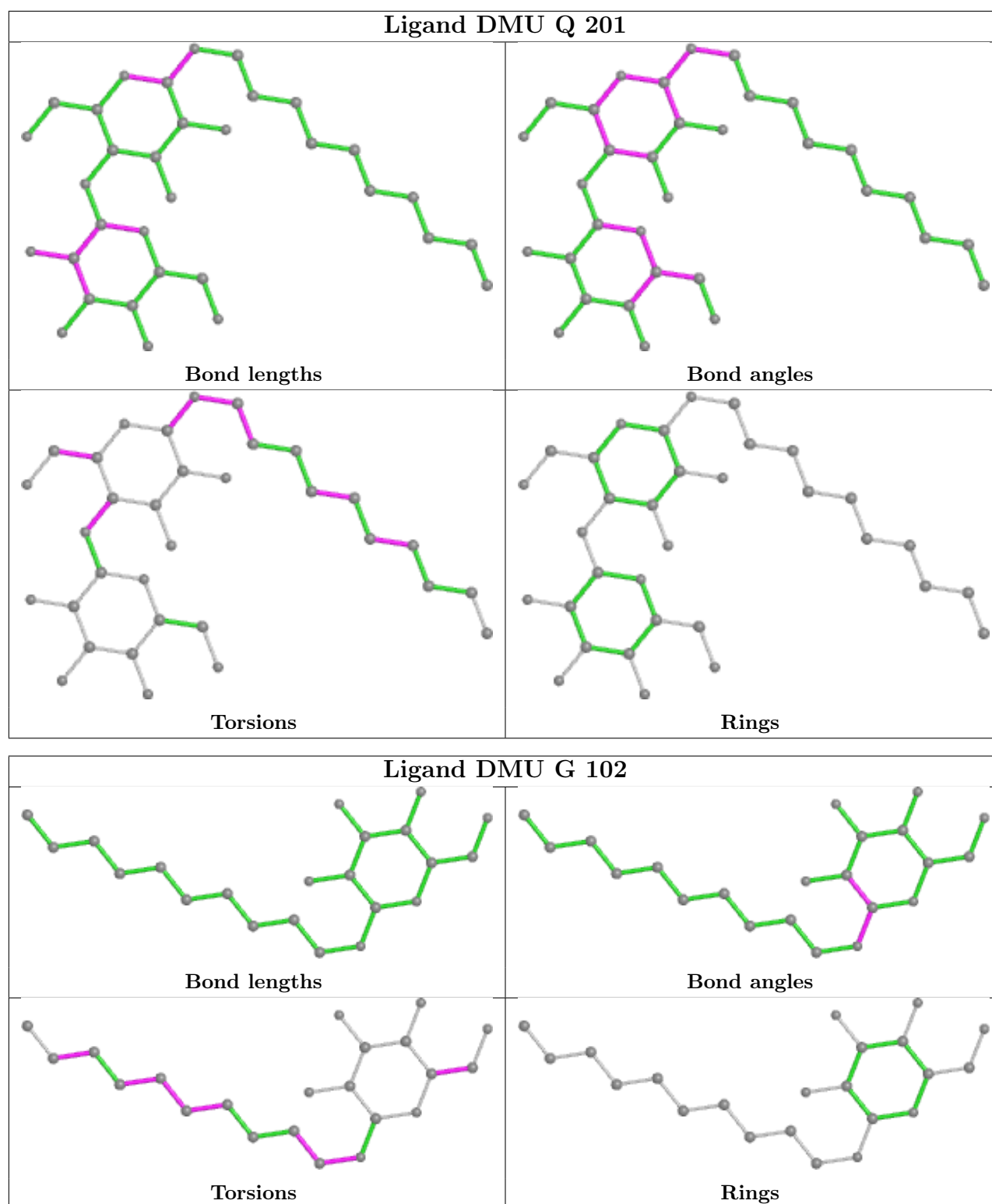


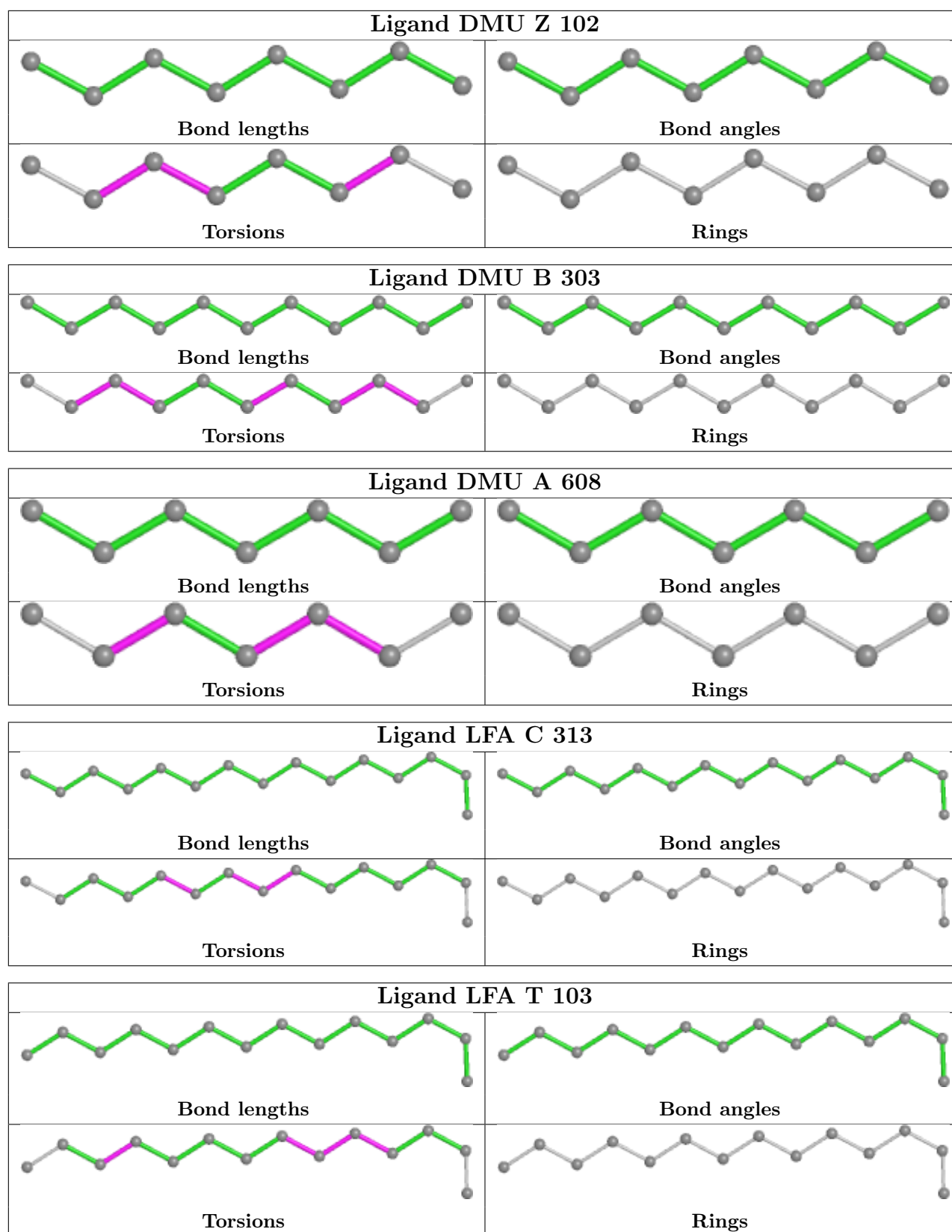


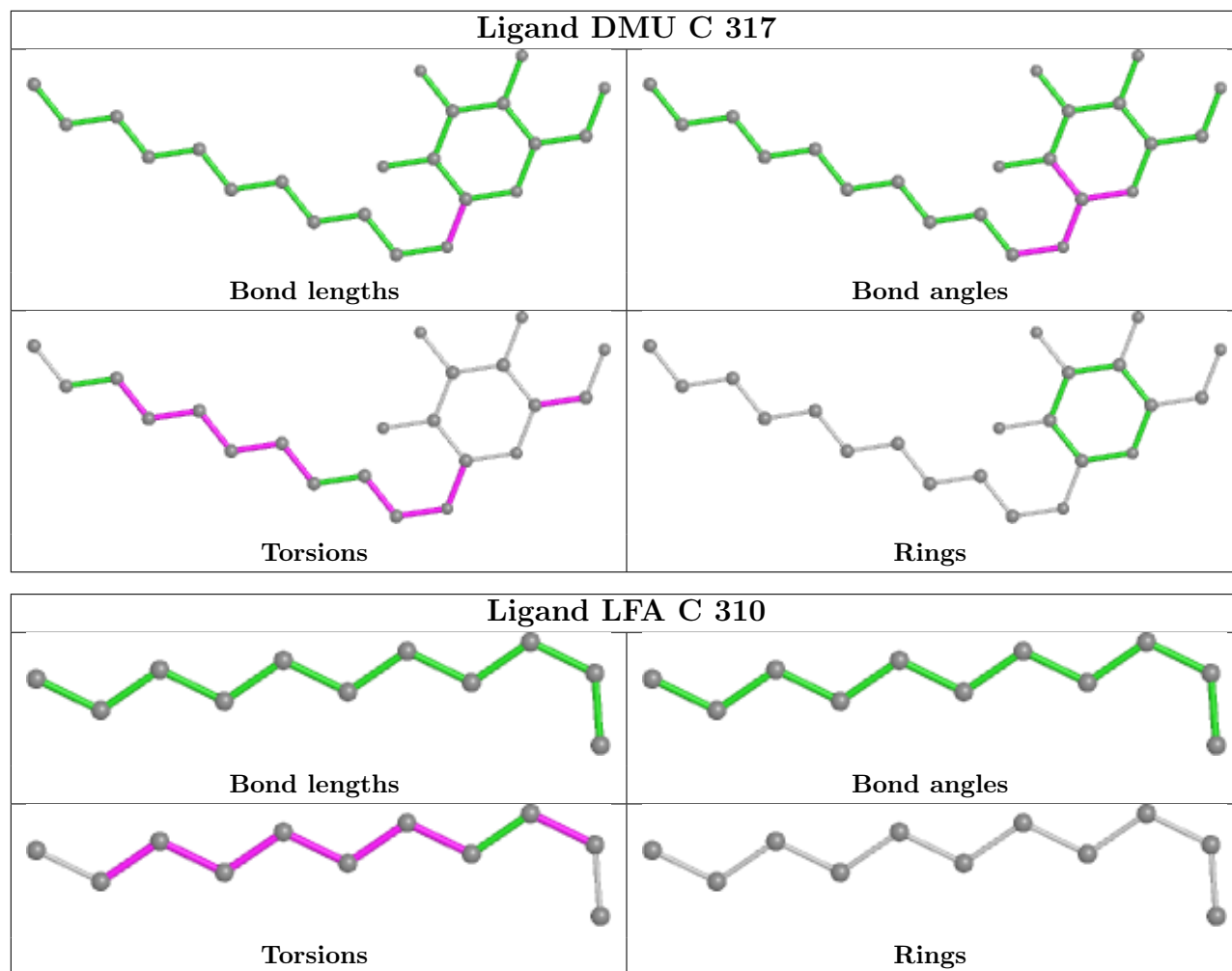


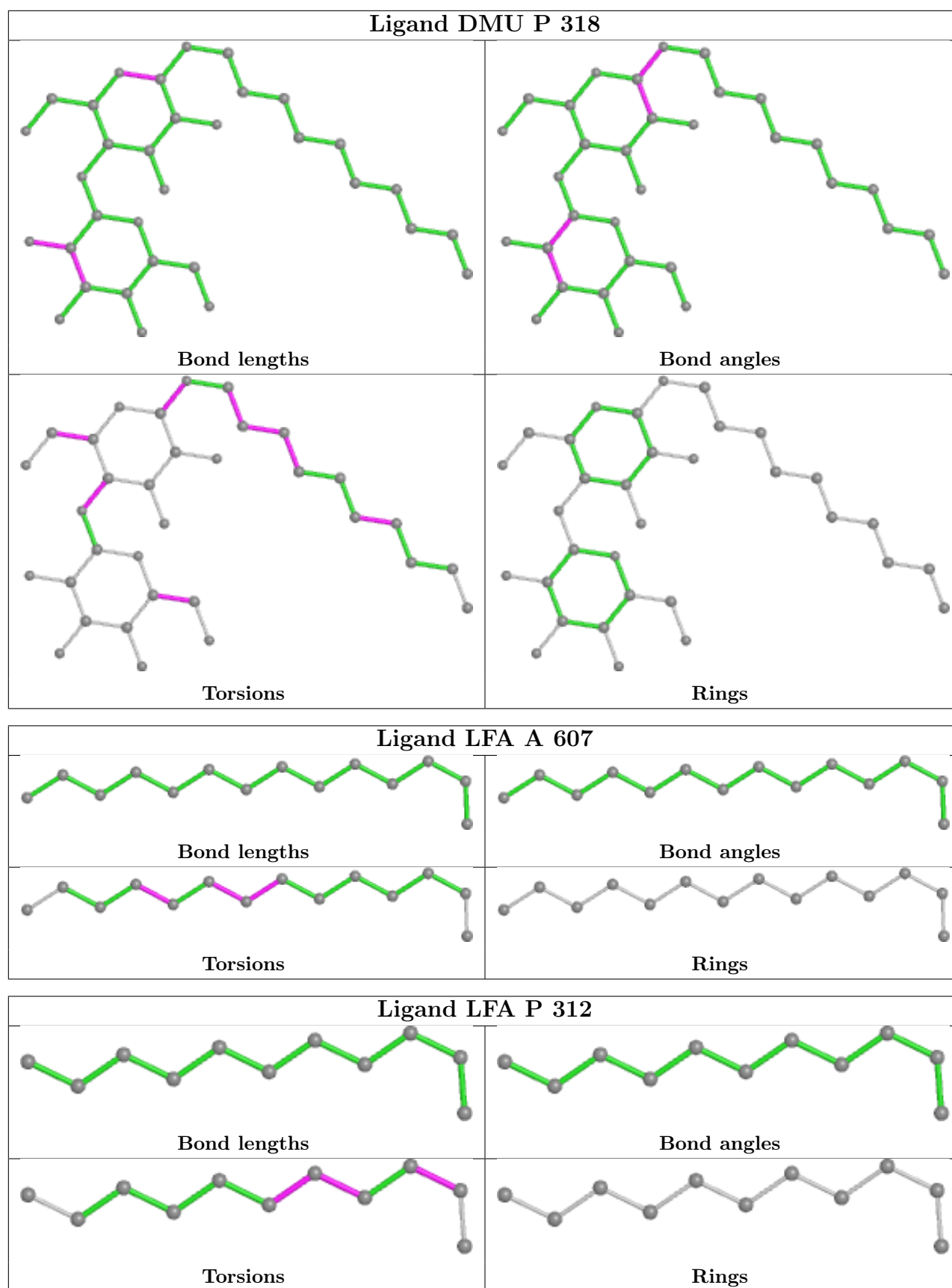


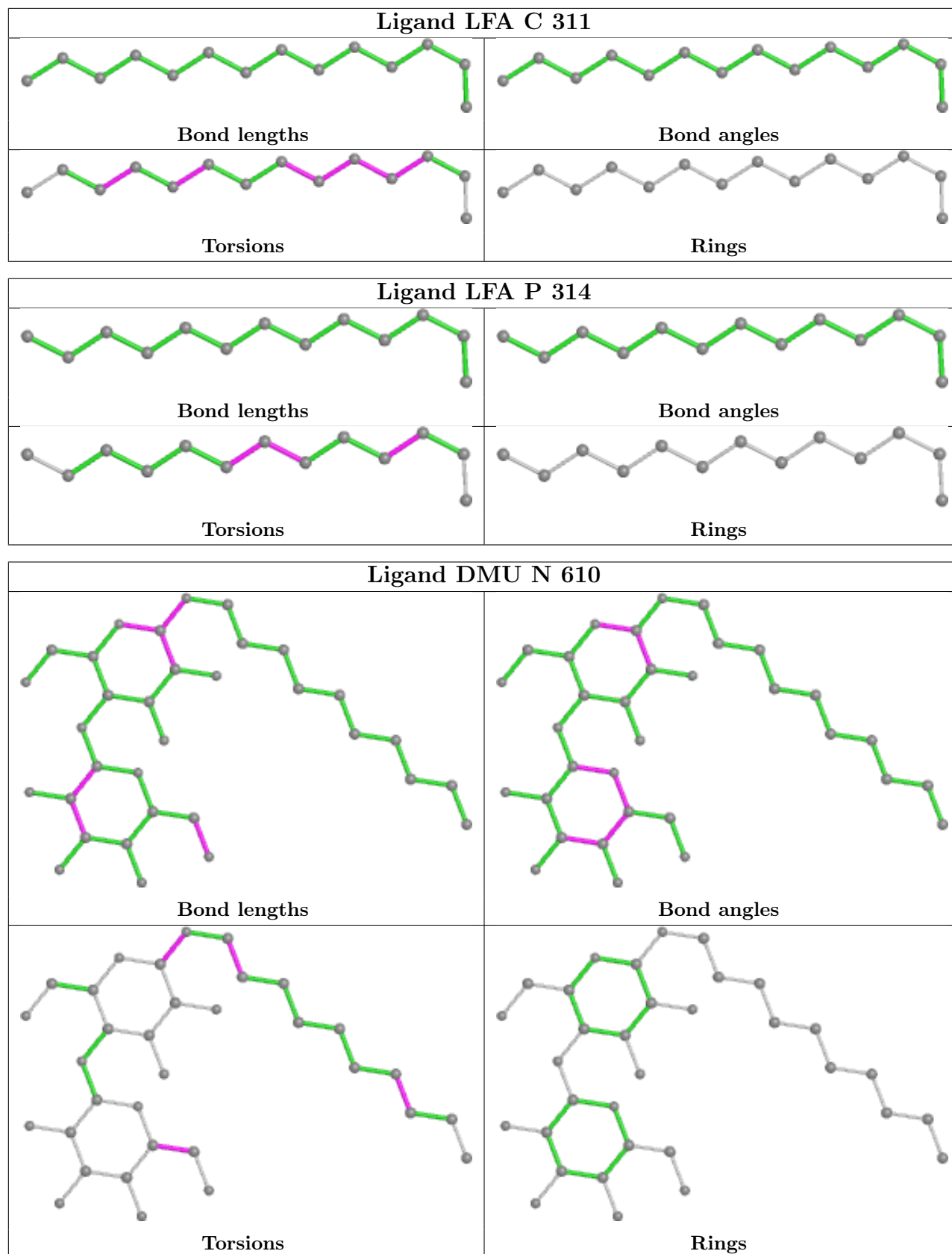


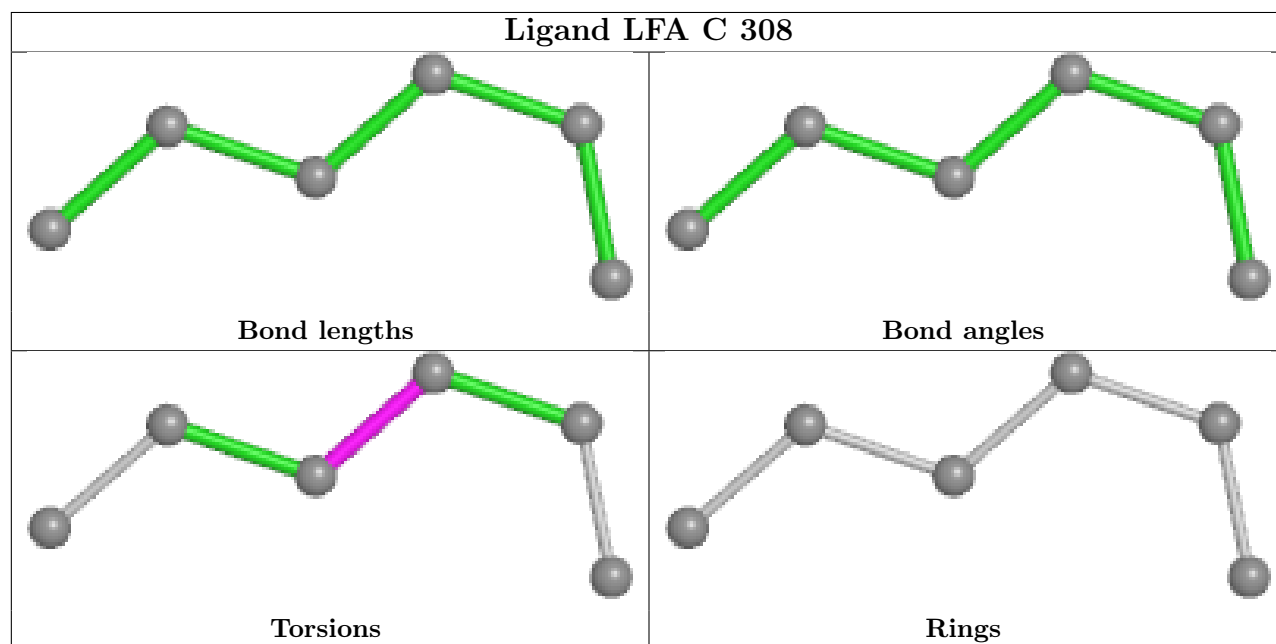
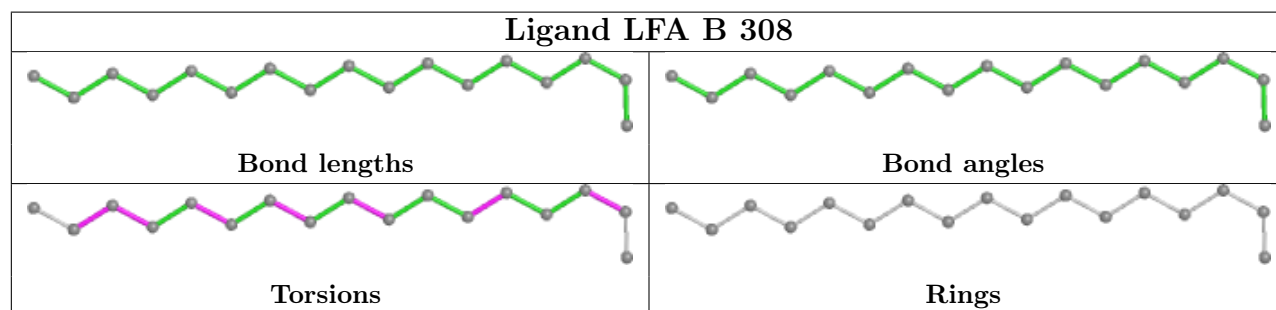
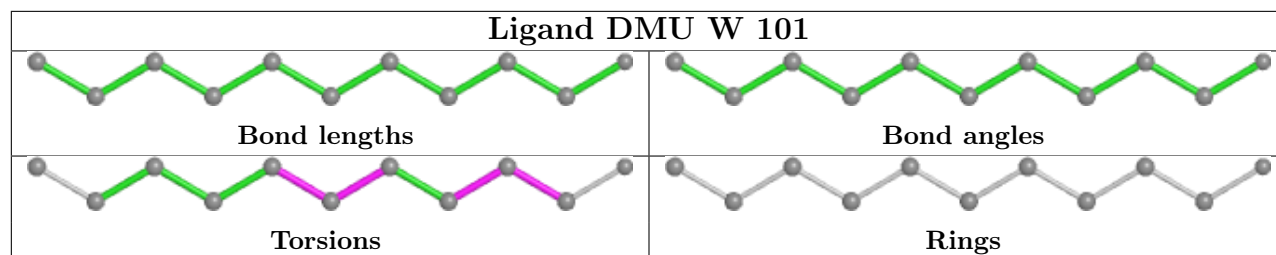


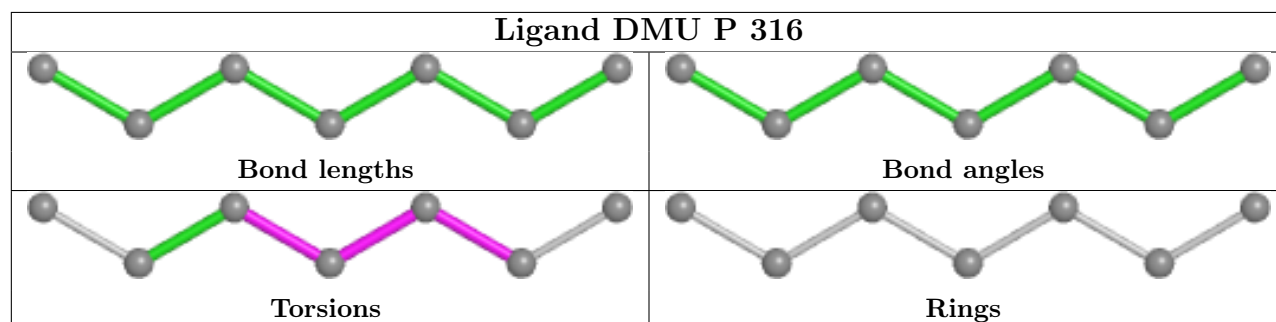
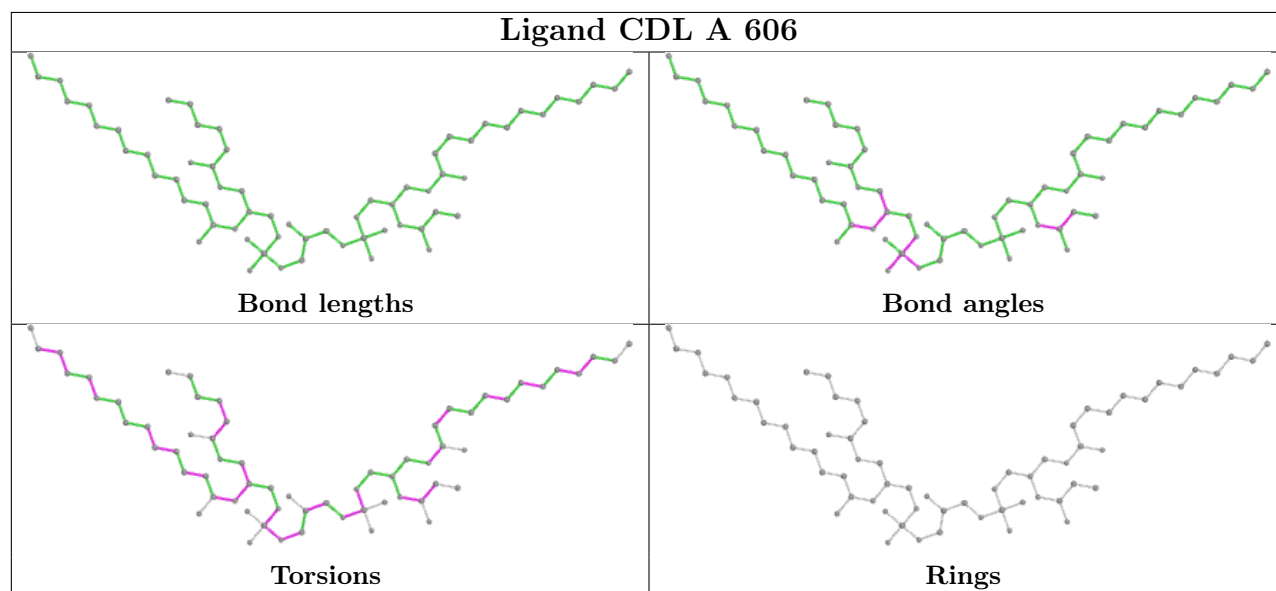
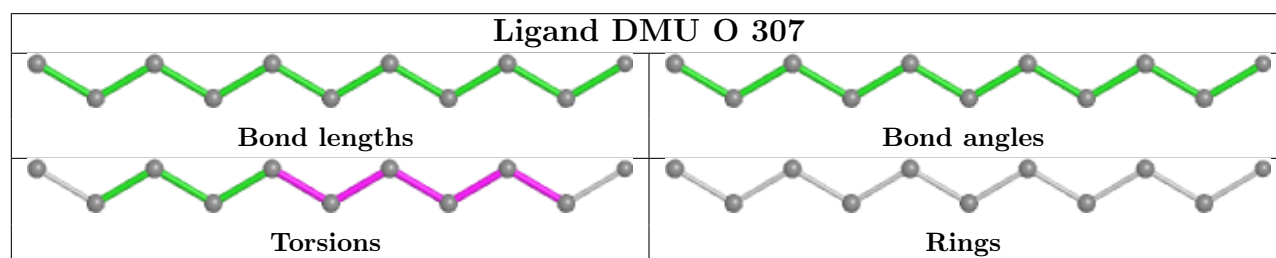
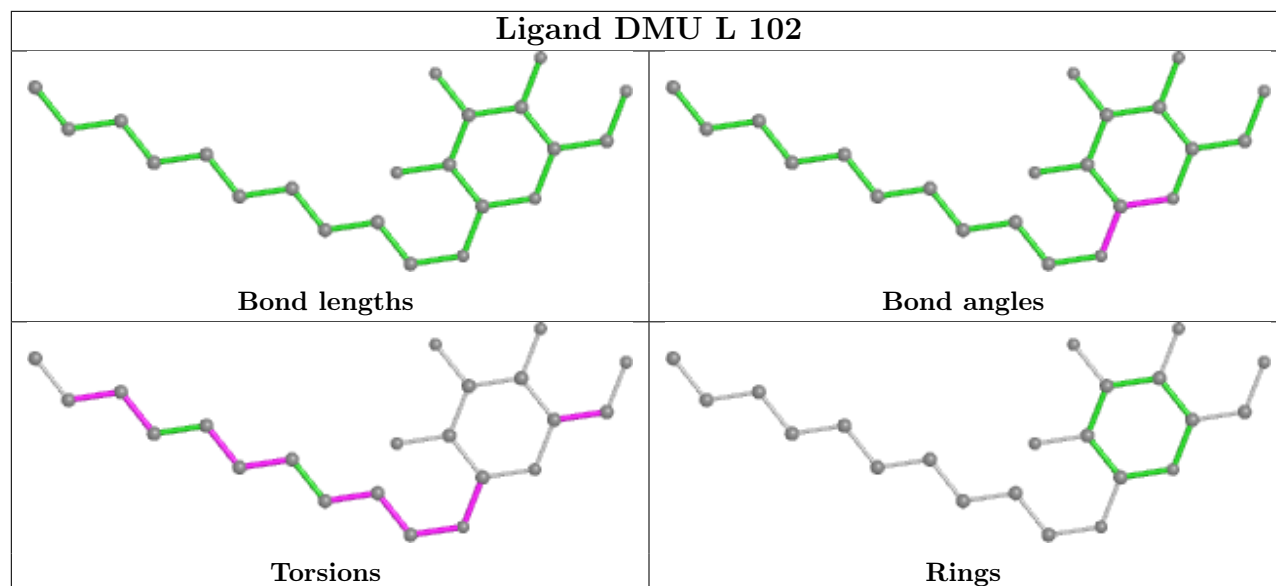


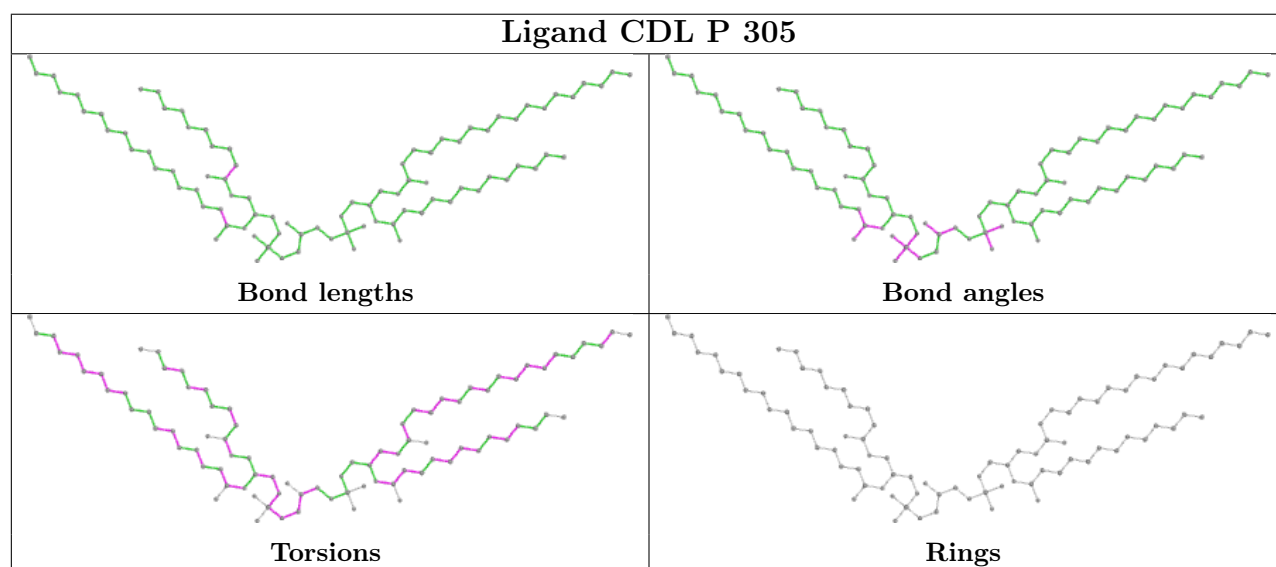
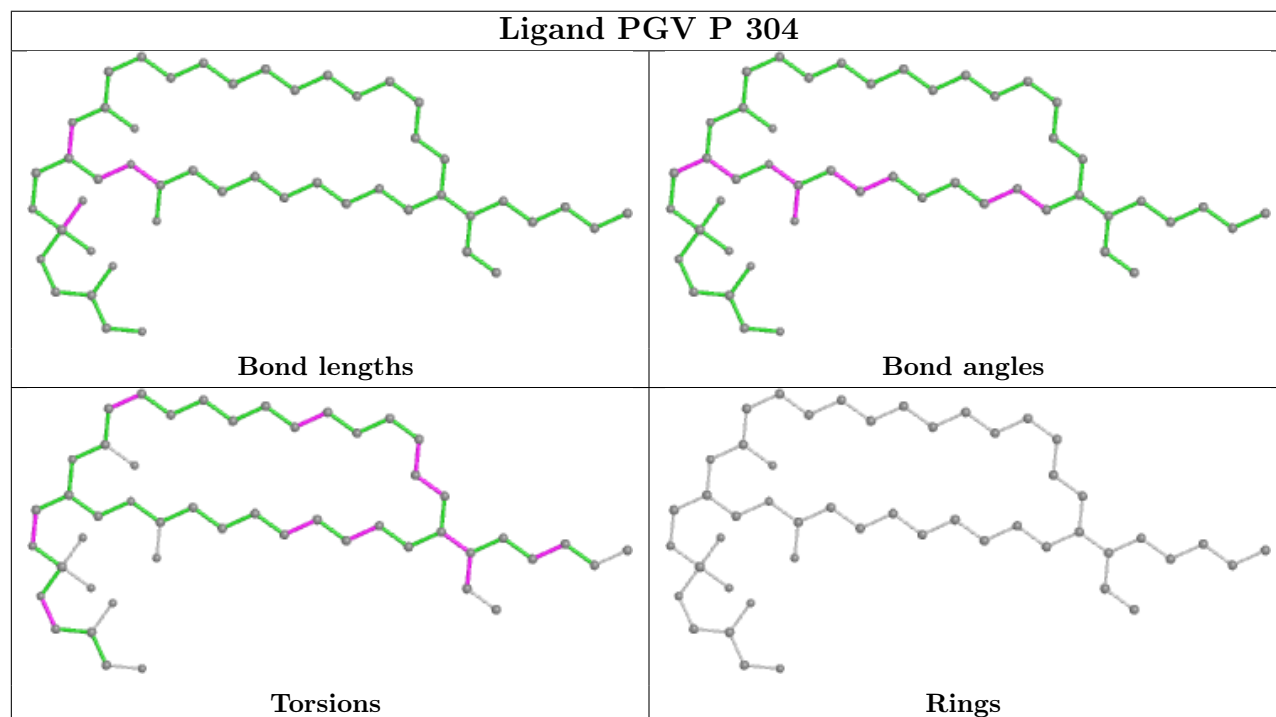
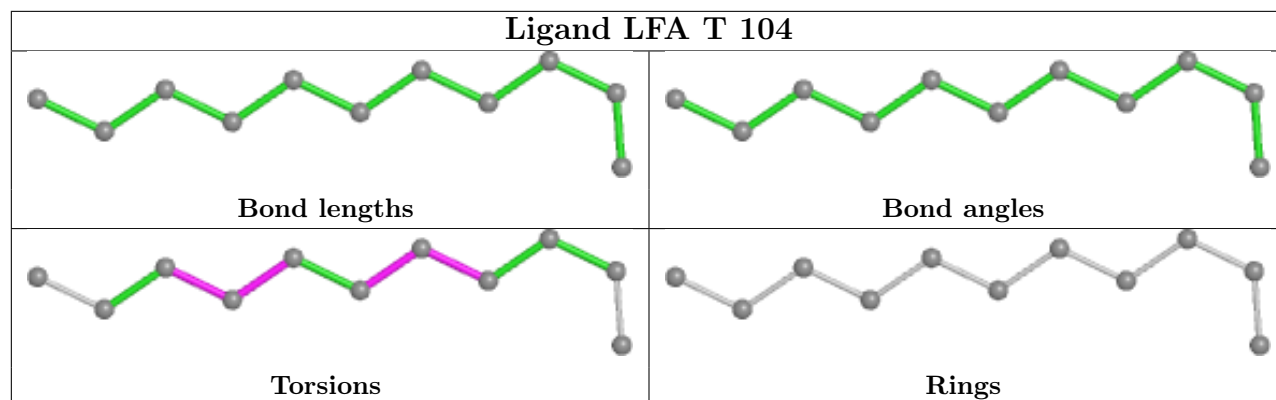




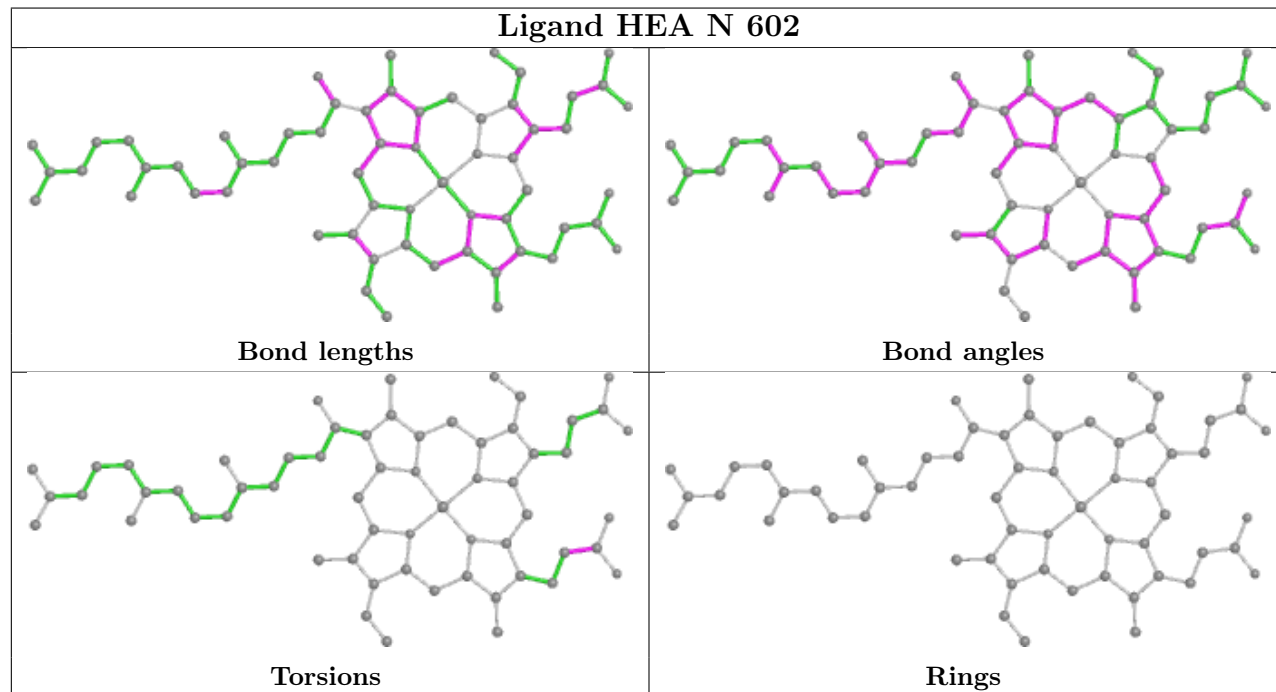
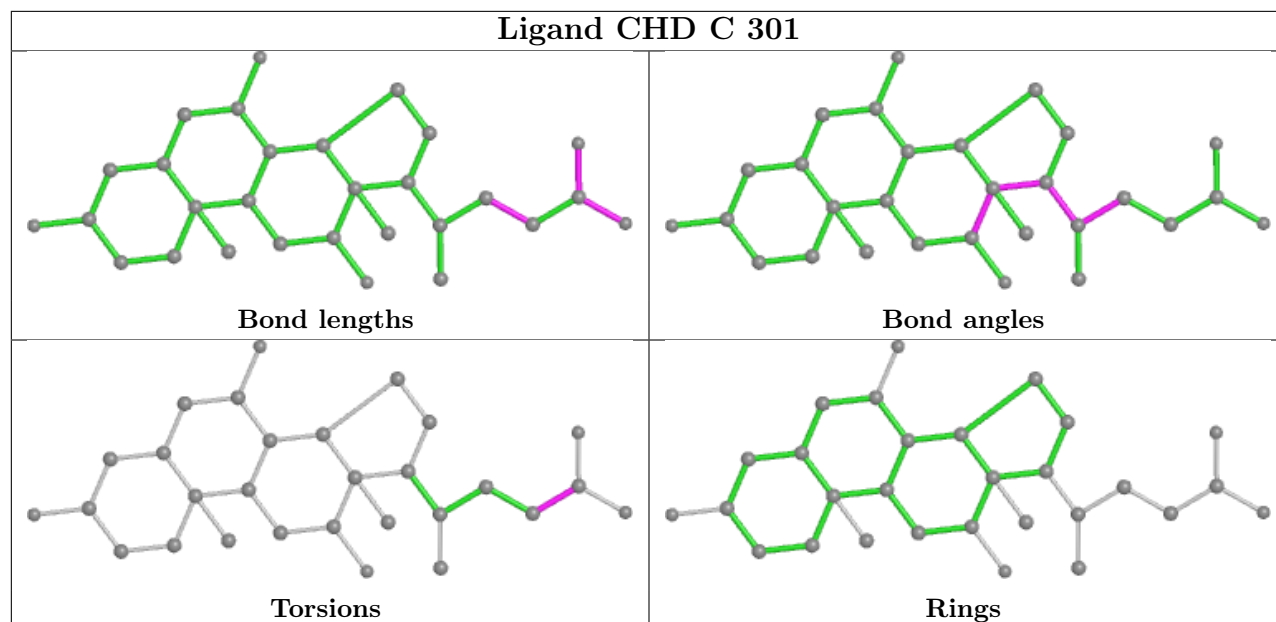


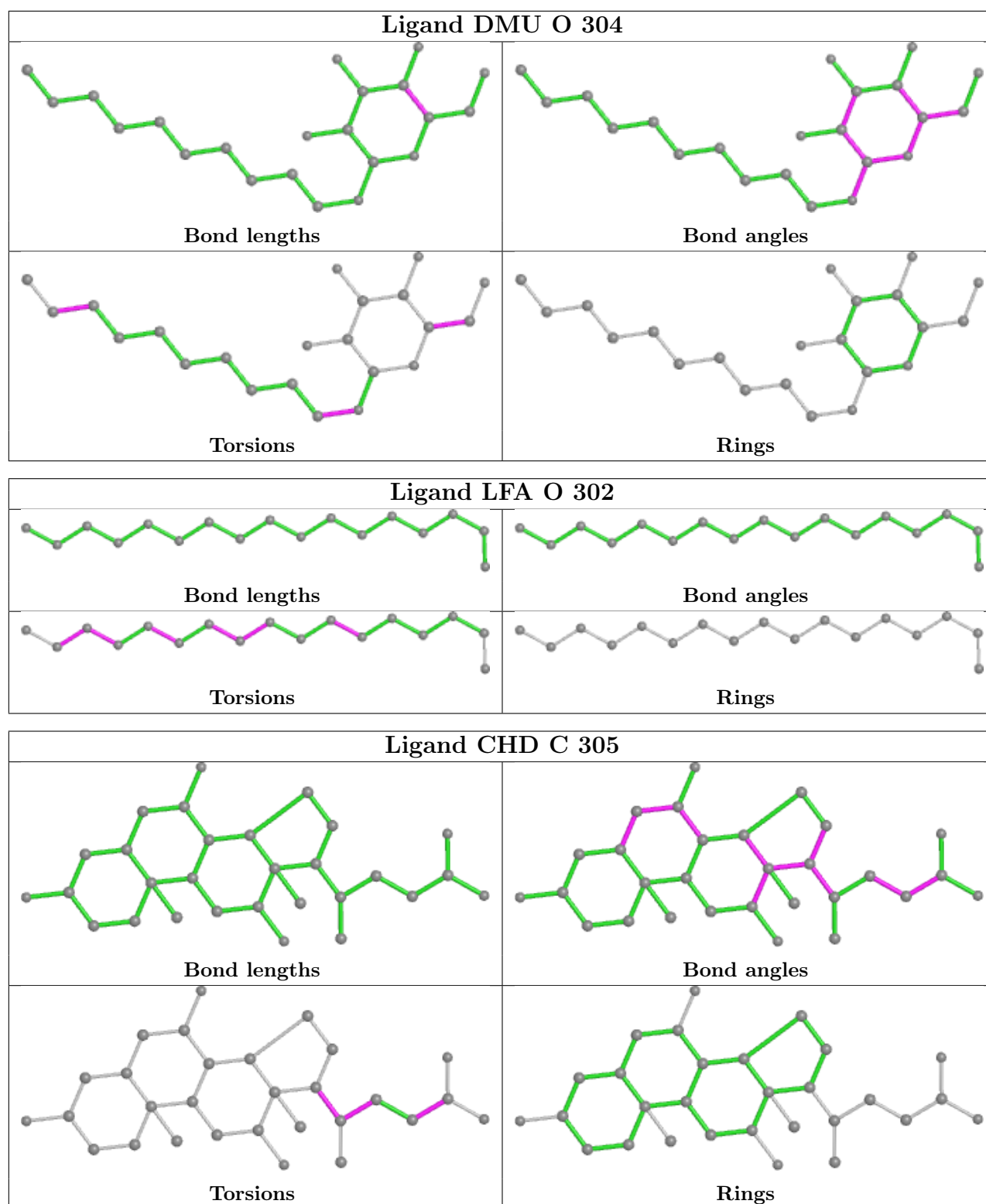


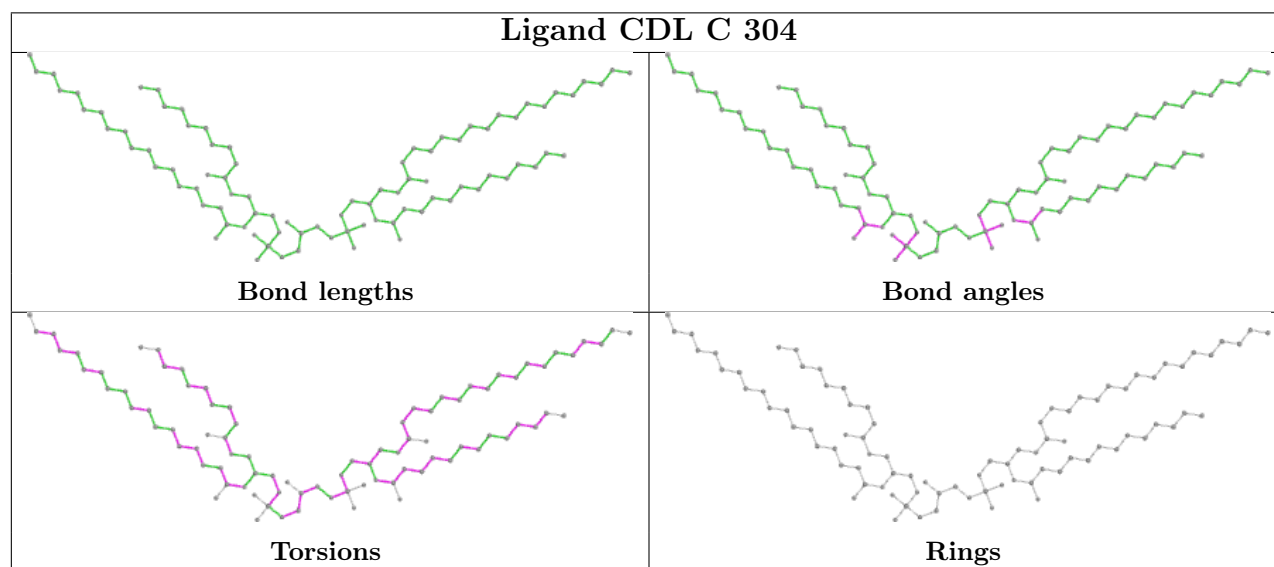
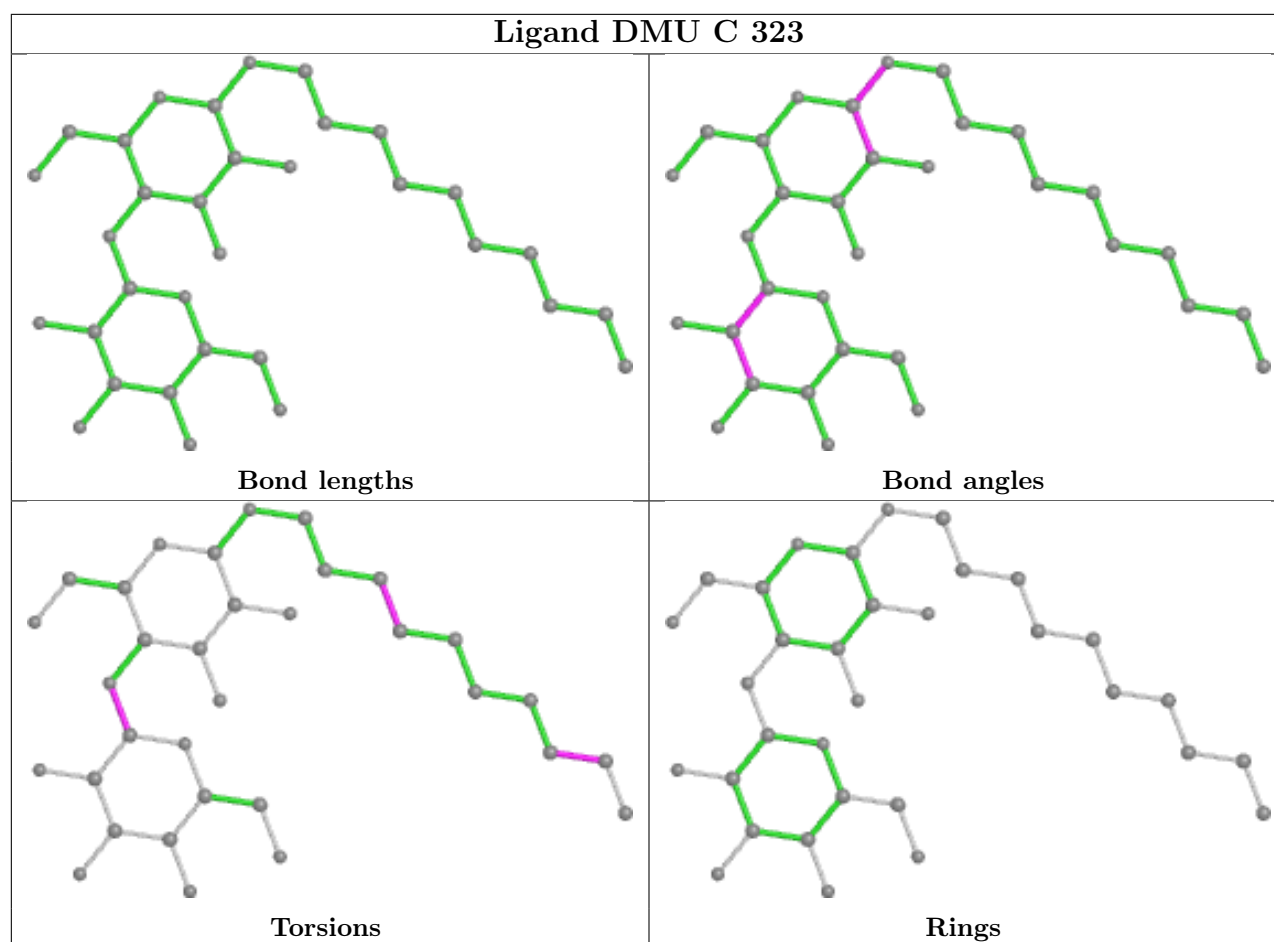


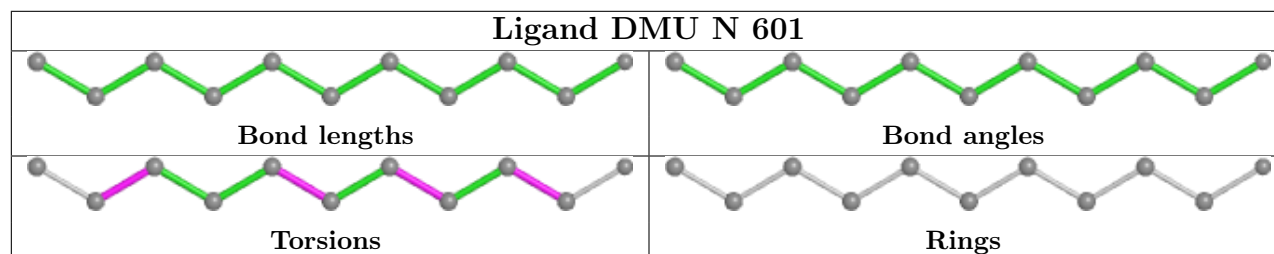
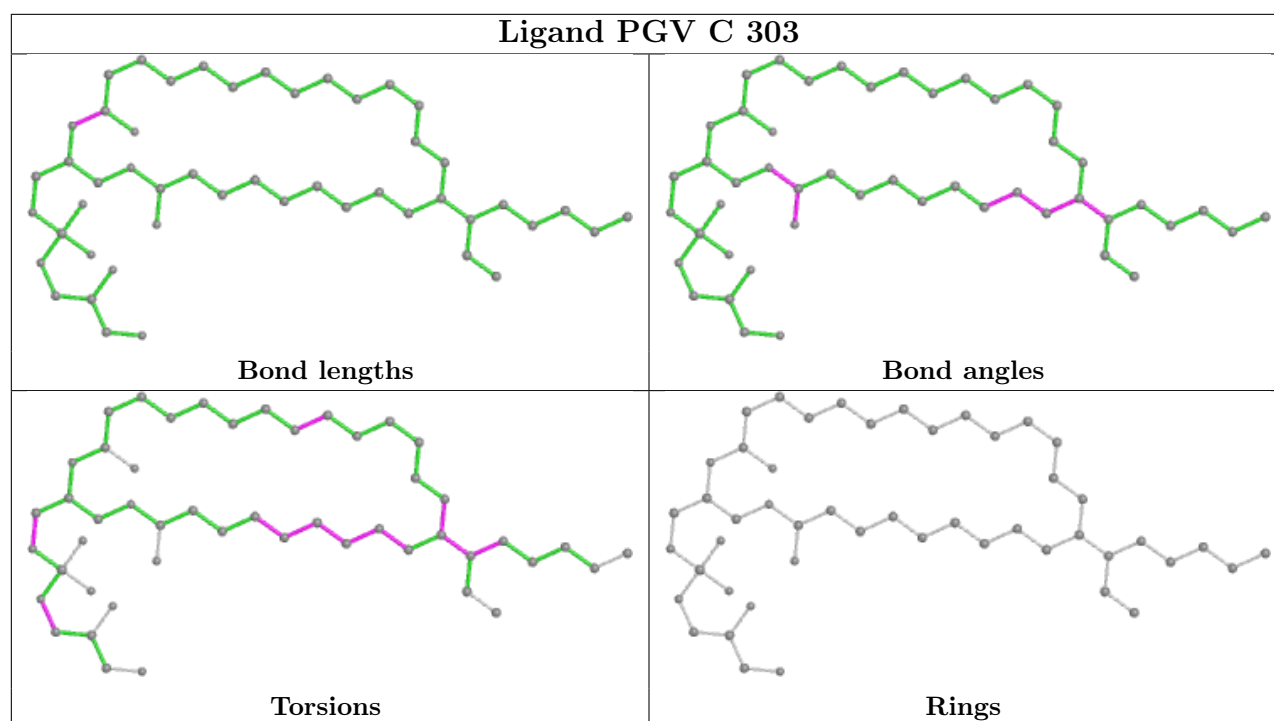
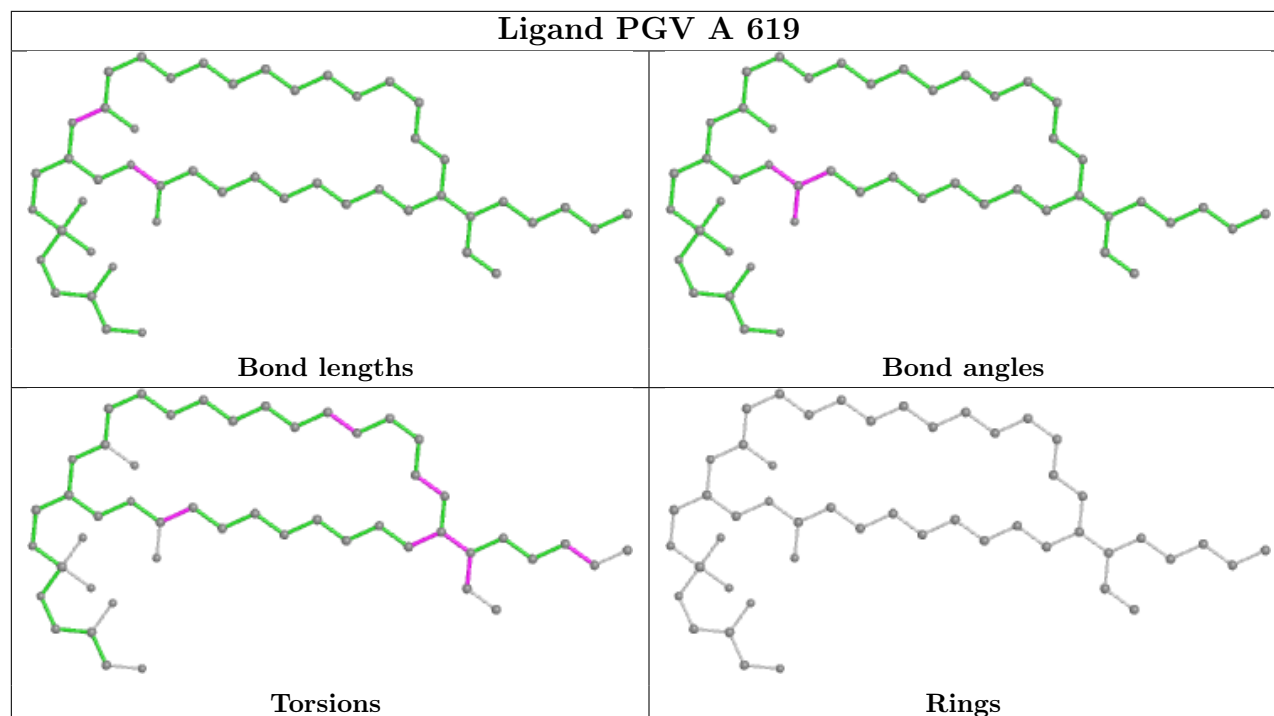


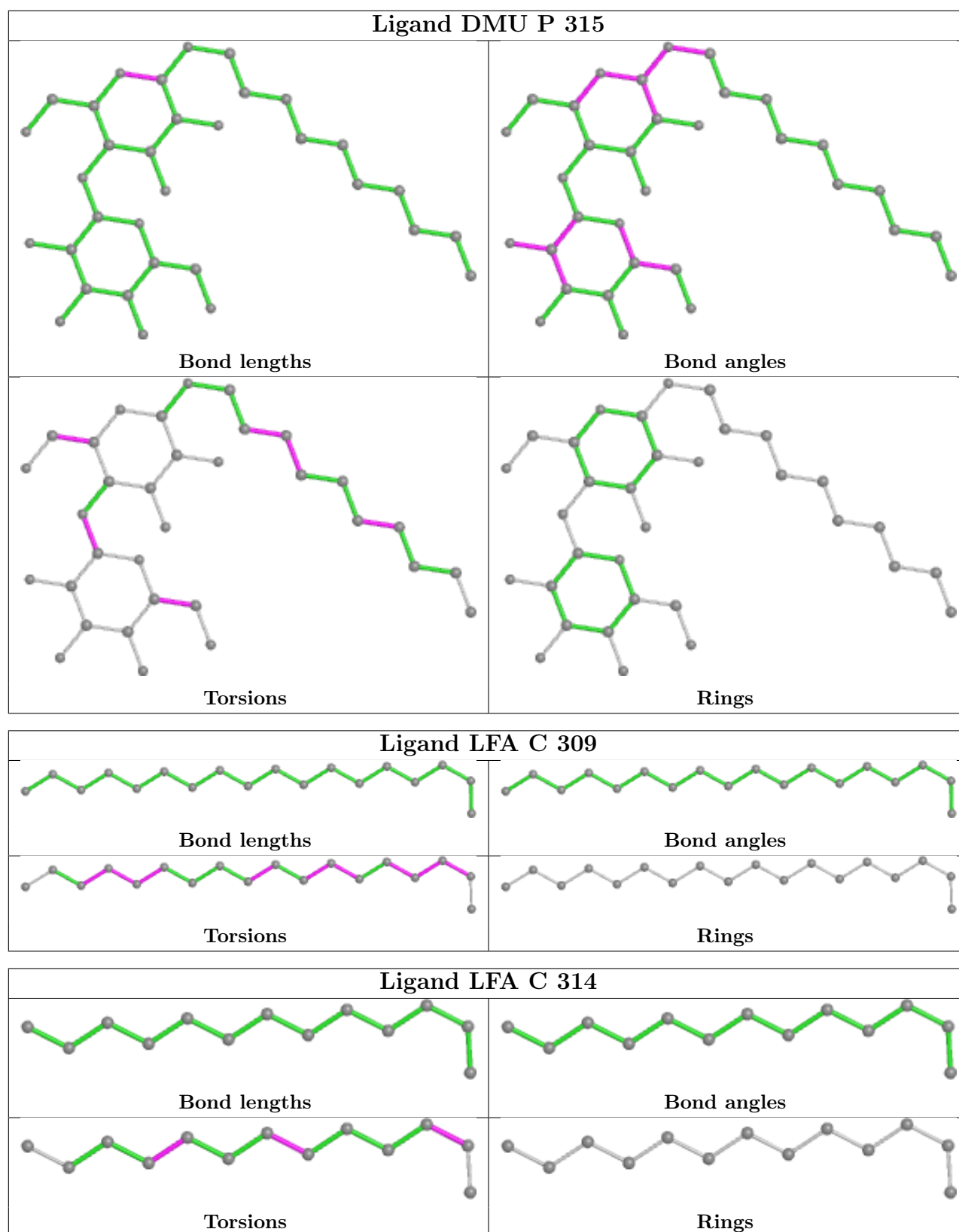


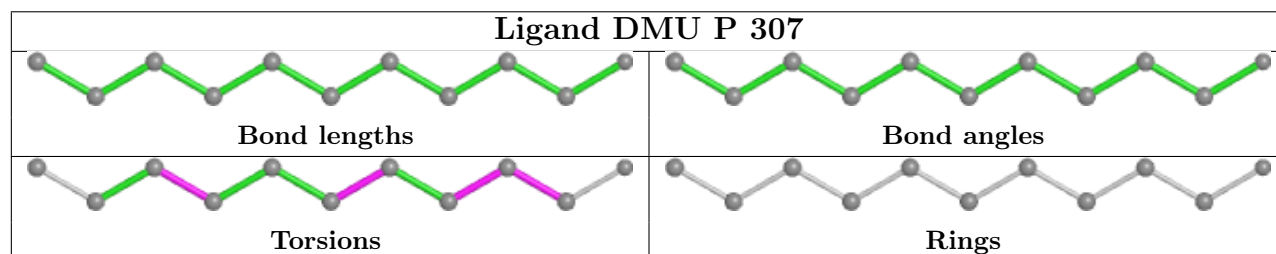
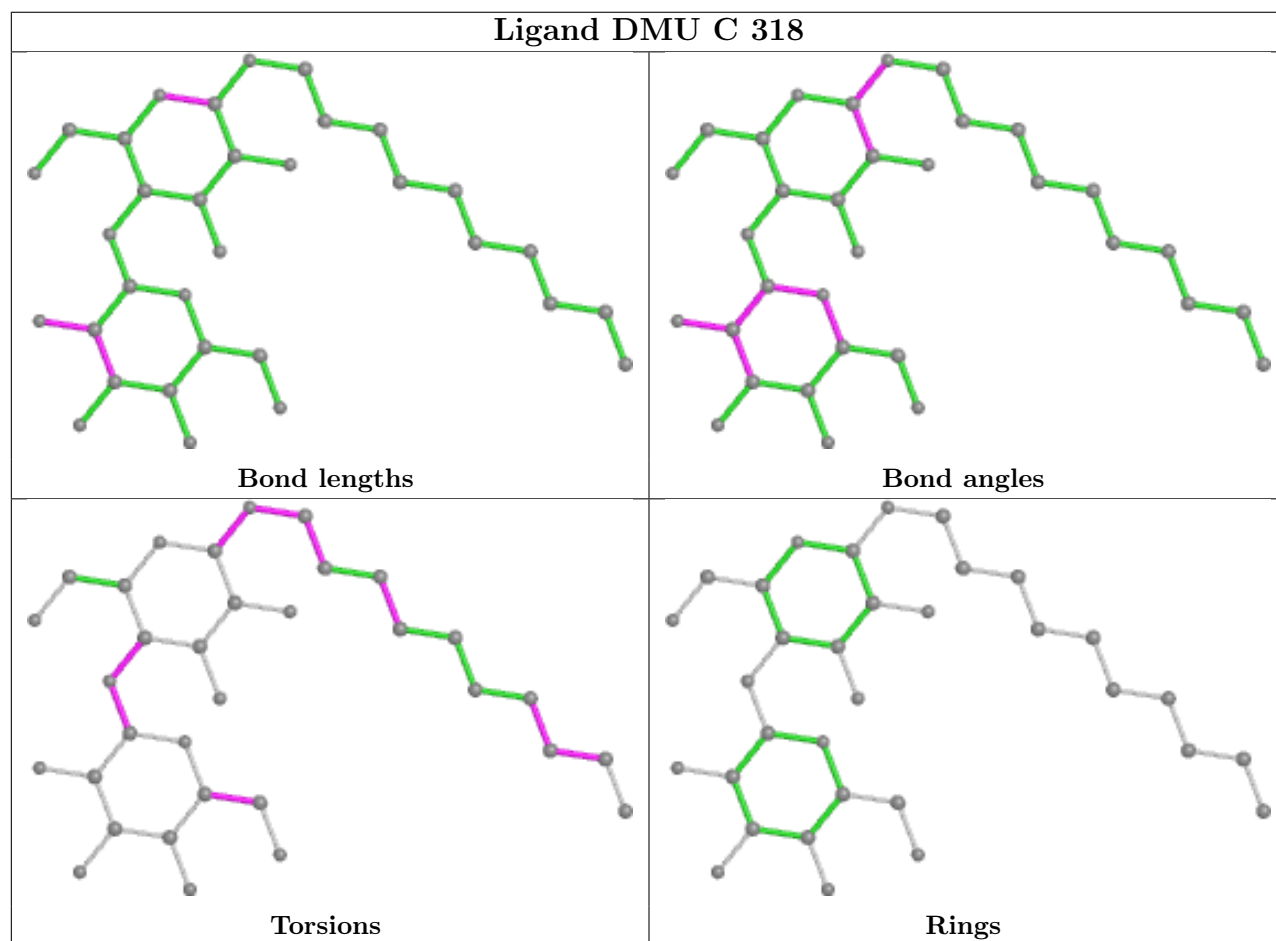
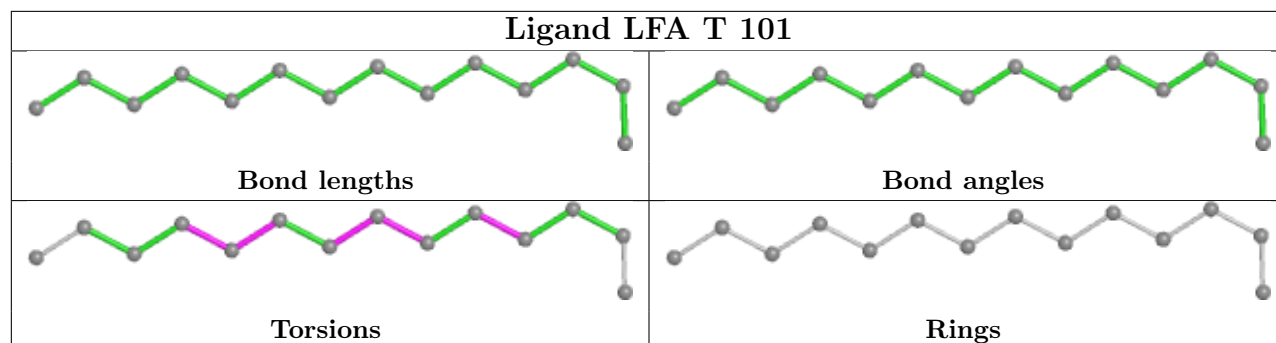


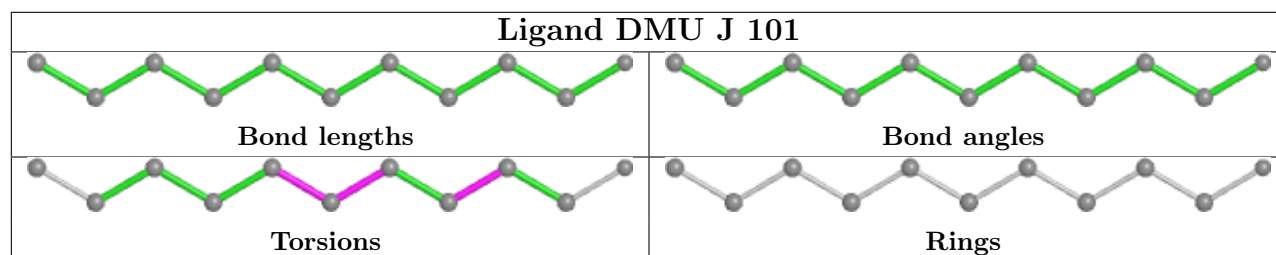
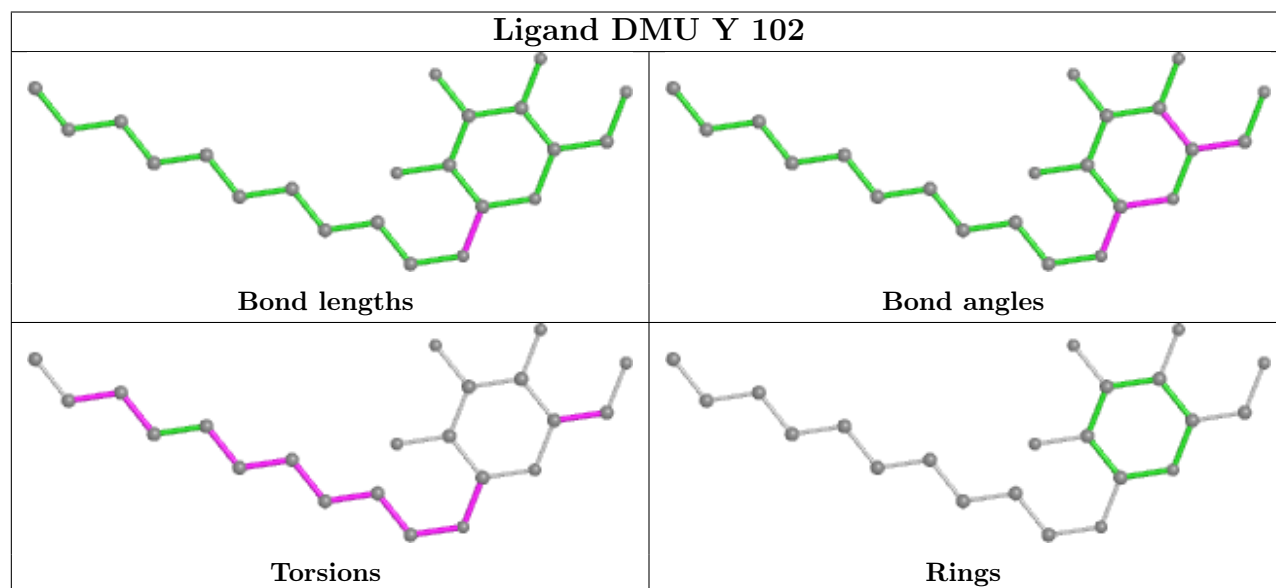
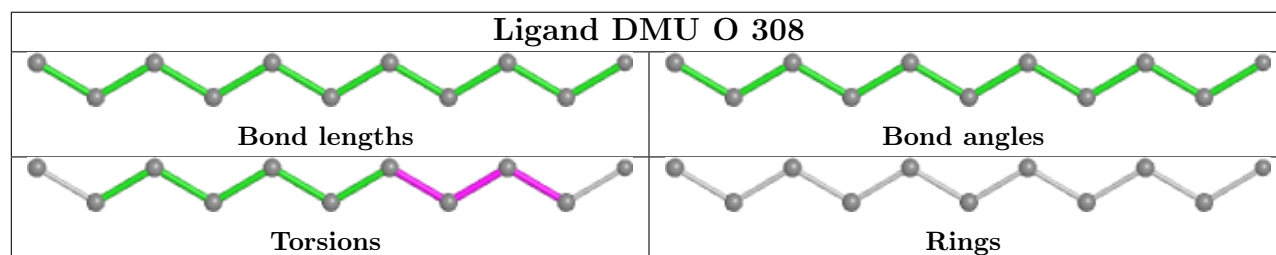
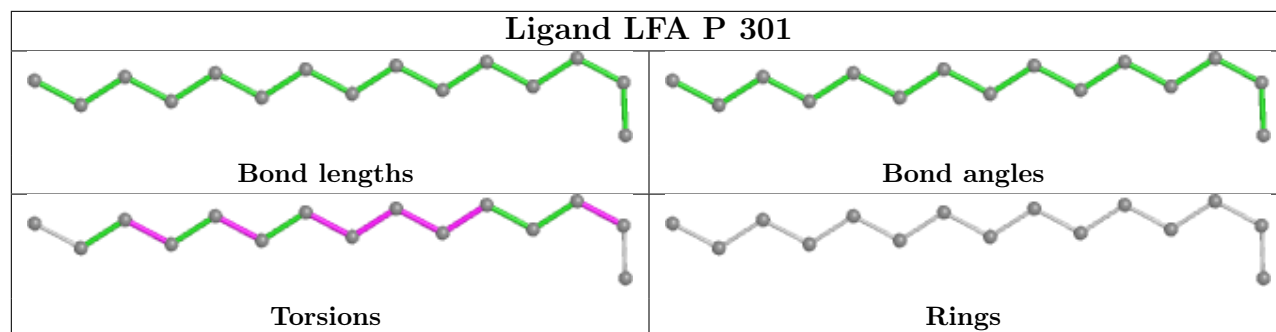


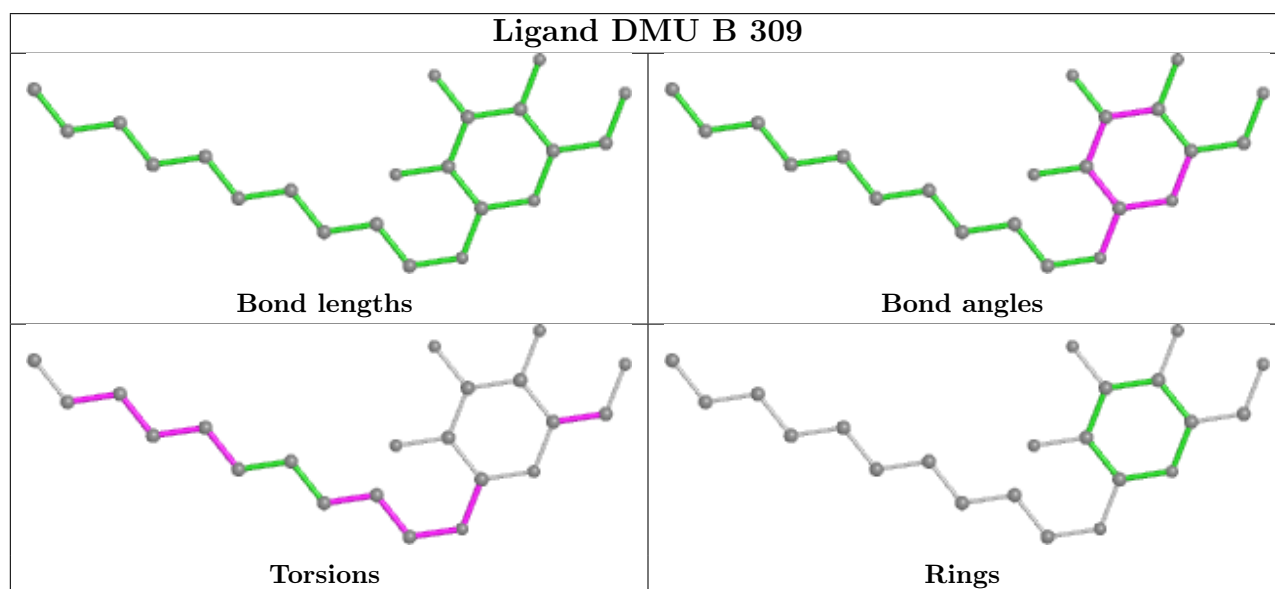
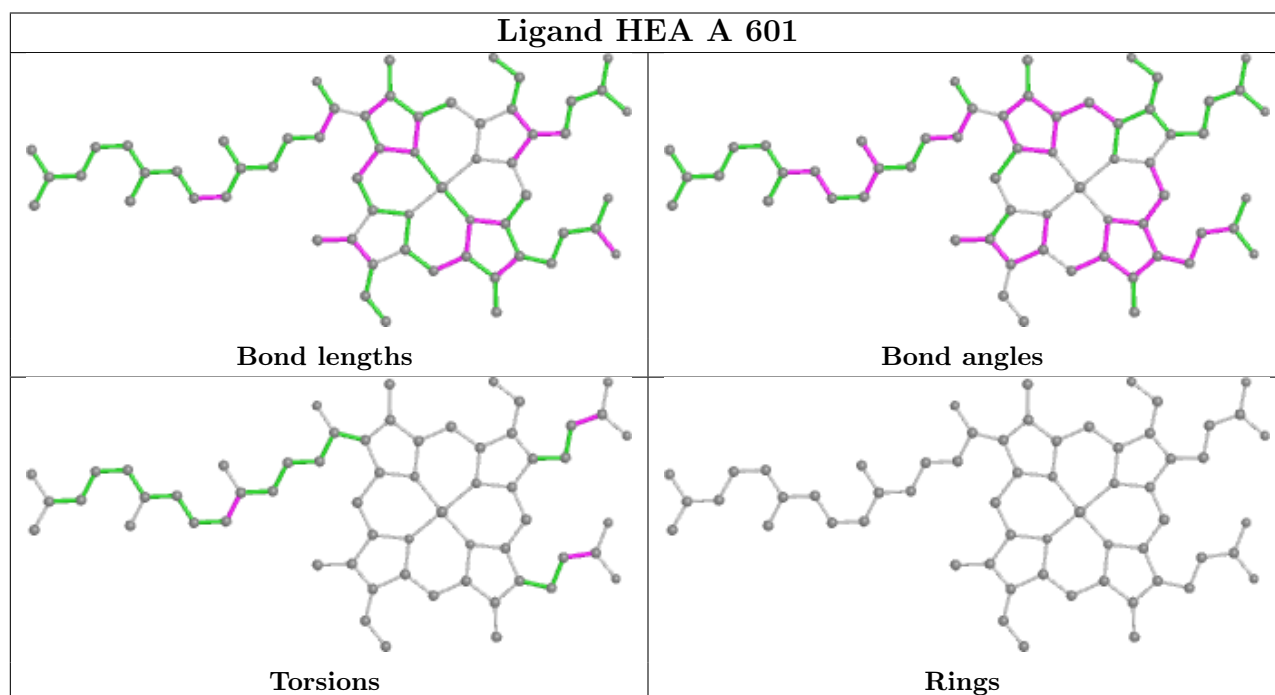
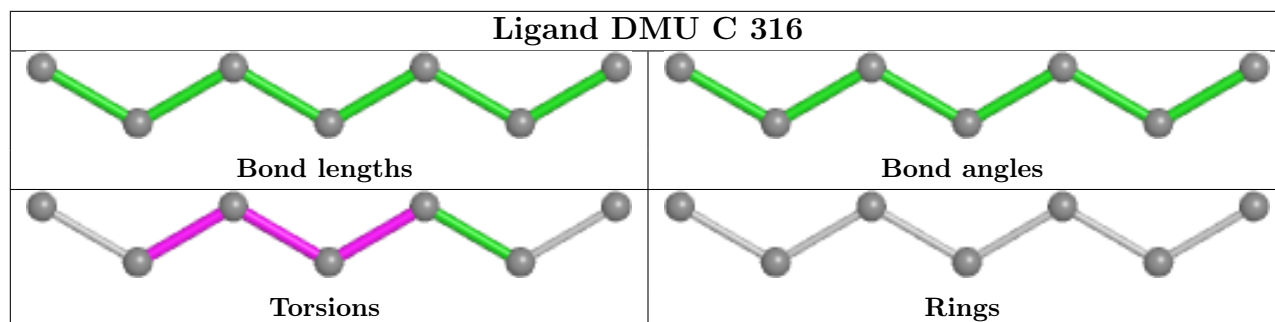




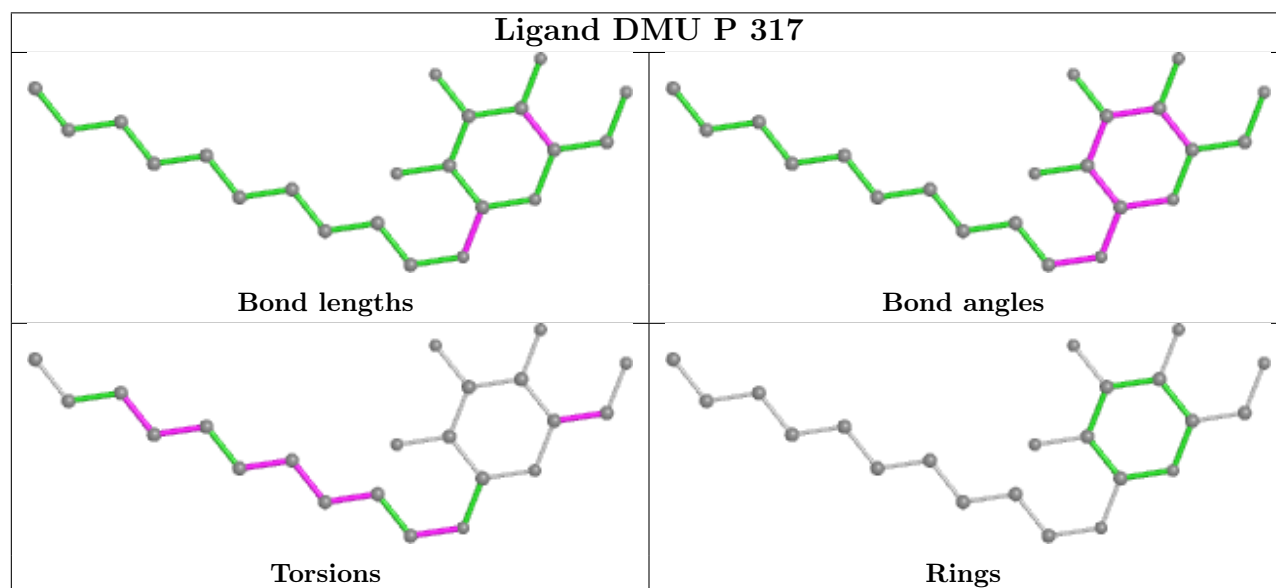
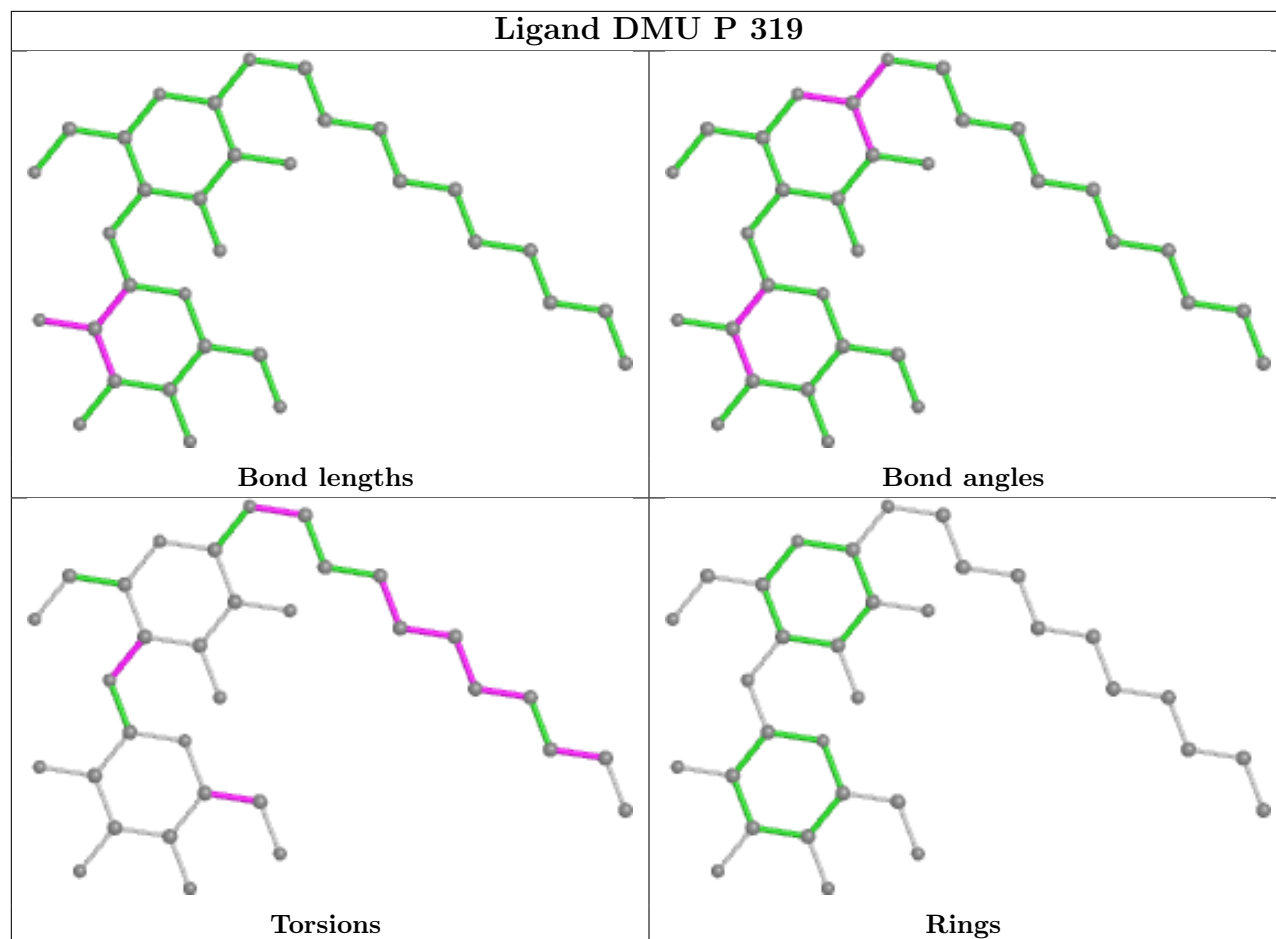


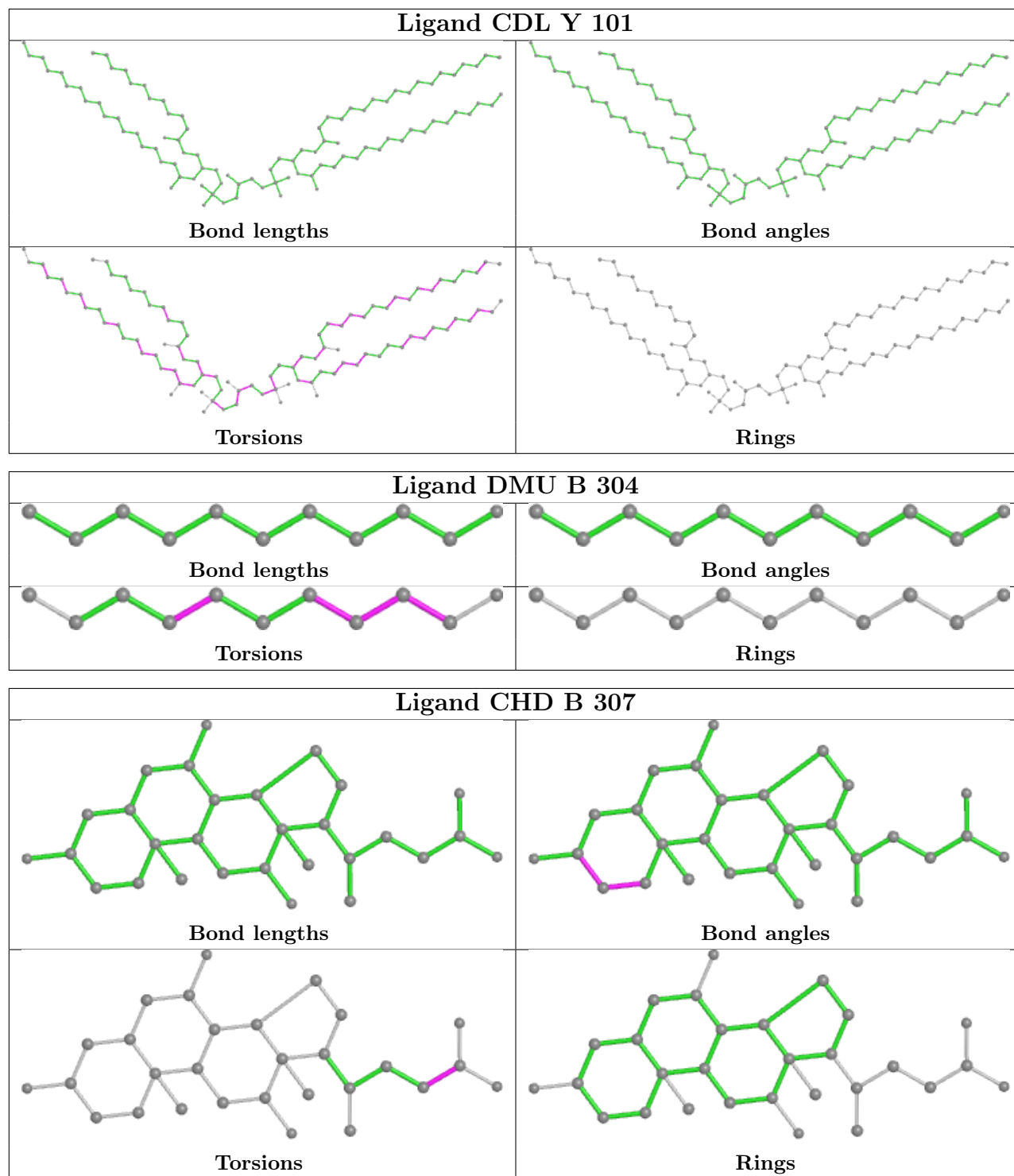


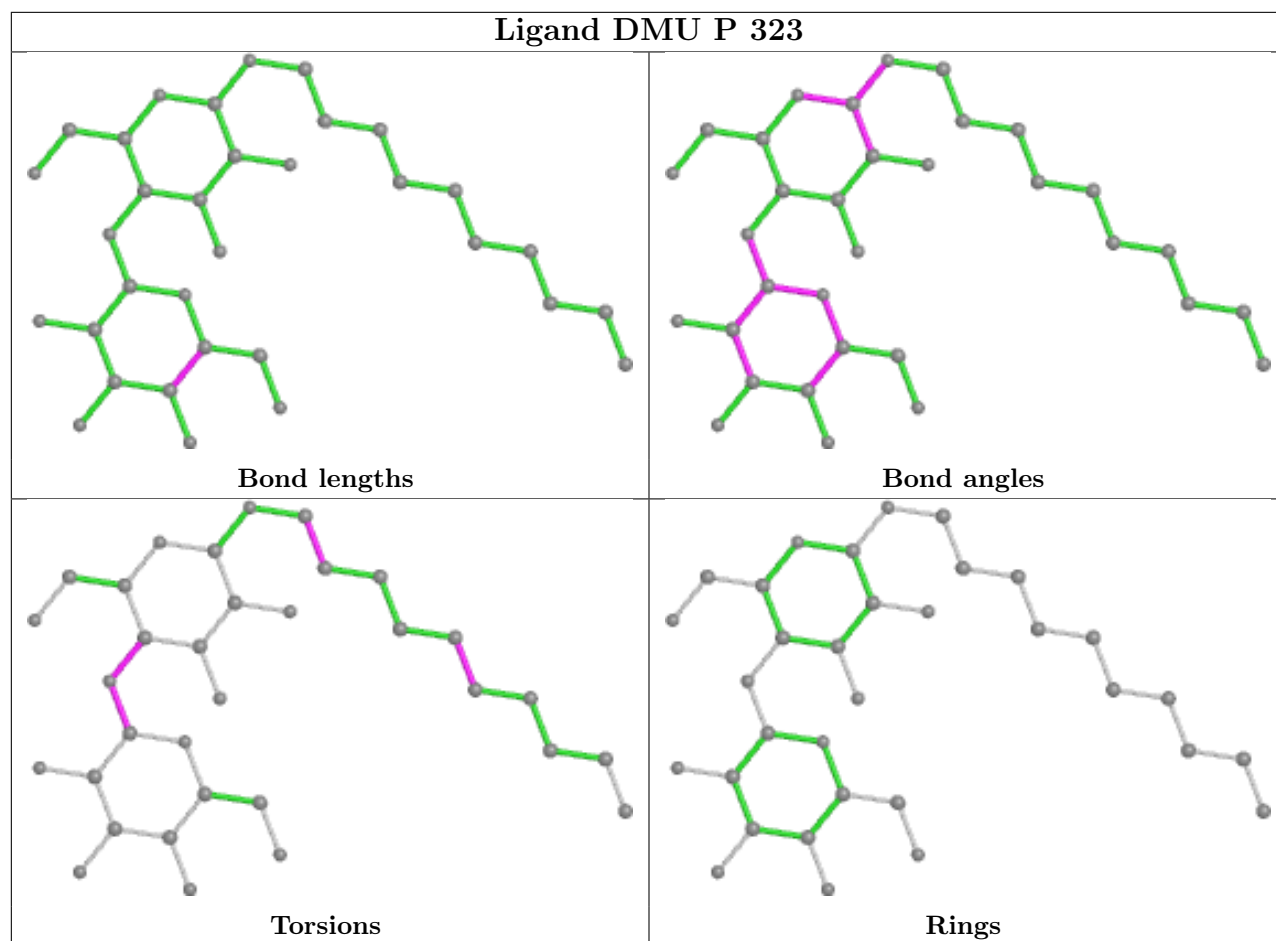
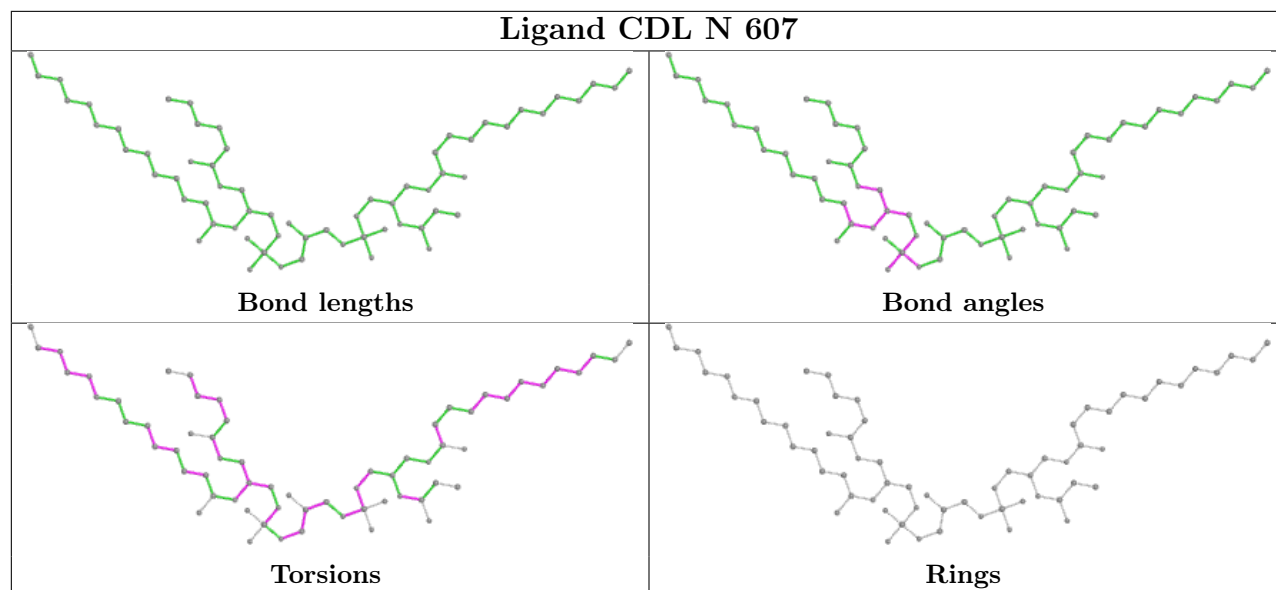


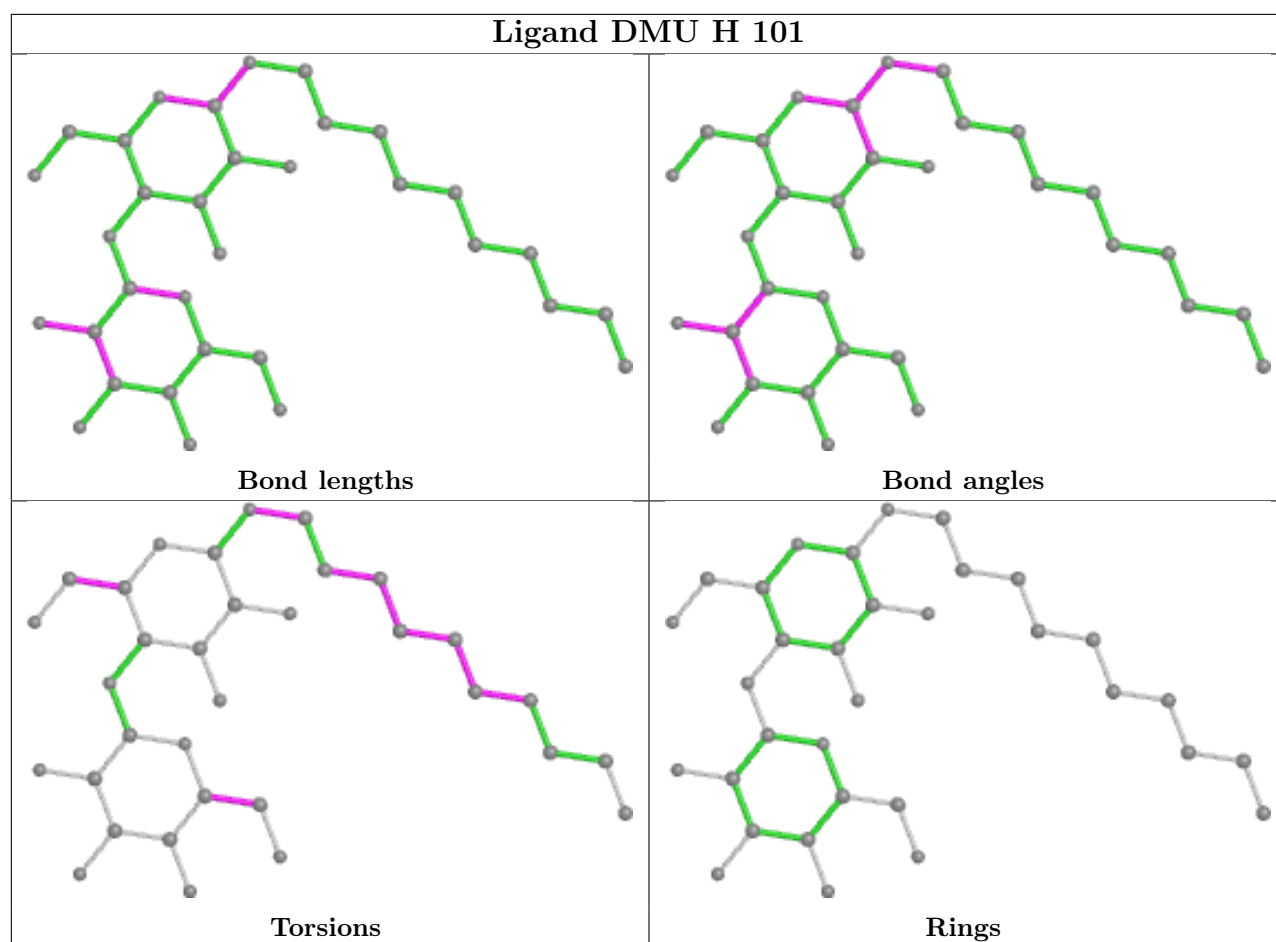












## 5.7 Other polymers [i](#)

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	512/514 (99%)	-0.41	3 (0%) 85 85	17, 36, 44, 58	15 (2%)
1	N	512/514 (99%)	-0.37	2 (0%) 89 88	18, 37, 45, 60	15 (2%)
2	B	226/227 (99%)	-0.00	10 (4%) 39 37	23, 43, 62, 81	5 (2%)
2	O	226/227 (99%)	-0.05	4 (1%) 67 66	24, 46, 67, 91	5 (2%)
3	C	258/261 (98%)	-0.32	1 (0%) 89 88	18, 39, 49, 62	9 (3%)
3	P	258/261 (98%)	-0.37	1 (0%) 89 88	18, 39, 49, 66	9 (3%)
4	D	143/147 (97%)	-0.12	2 (1%) 73 72	20, 46, 62, 75	1 (0%)
4	Q	137/147 (93%)	0.08	1 (0%) 84 84	24, 53, 75, 87	1 (0%)
5	E	102/109 (93%)	-0.36	0 100 100	37, 44, 58, 72	0
5	R	102/109 (93%)	-0.20	1 (0%) 79 78	41, 51, 65, 80	0
6	F	91/98 (92%)	-0.15	1 (1%) 77 77	21, 44, 63, 74	2 (2%)
6	S	91/98 (92%)	-0.11	2 (2%) 62 60	20, 43, 63, 73	2 (2%)
7	G	72/85 (84%)	0.06	1 (1%) 73 72	23, 46, 77, 93	1 (1%)
7	T	72/85 (84%)	0.15	3 (4%) 41 38	22, 46, 71, 96	1 (1%)
8	H	75/85 (88%)	0.11	2 (2%) 56 54	40, 48, 86, 109	0
8	U	75/85 (88%)	0.18	4 (5%) 33 30	42, 50, 89, 106	0
9	I	70/73 (95%)	0.32	5 (7%) 23 20	41, 53, 72, 90	0
9	V	70/73 (95%)	0.26	3 (4%) 40 37	41, 58, 74, 97	0
10	J	56/59 (94%)	0.06	1 (1%) 67 66	40, 49, 70, 79	0
10	W	56/59 (94%)	0.11	1 (1%) 67 66	40, 50, 69, 85	0
11	K	49/56 (87%)	0.19	1 (2%) 64 63	44, 50, 65, 76	0
11	X	49/56 (87%)	0.44	3 (6%) 28 26	47, 56, 70, 94	0
12	L	44/47 (93%)	-0.20	0 100 100	38, 41, 53, 60	0
12	Y	44/47 (93%)	-0.08	1 (2%) 61 59	40, 46, 59, 62	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	40/46 (86%)	0.02	0 100 100	39, 43, 61, 73	0
13	Z	40/46 (86%)	0.27	0 100 100	45, 51, 71, 81	0
All	All	3470/3614 (96%)	-0.16	53 (1%) 71 71	17, 42, 65, 109	66 (1%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	36	TRP	6.2
8	U	48	GLY	4.7
11	X	6	ALA	4.6
2	O	90	ILE	4.5
2	B	87[A]	MET	4.5
2	O	113	TYR	4.1
8	H	45	ALA	3.8
4	D	5	VAL	3.8
6	S	3	GLY	3.7
2	B	59	GLN	3.6
6	S	93	PRO	3.5
9	I	3	ALA	3.4
4	D	4	SER	3.3
6	F	3	GLY	3.3
2	B	90	ILE	3.2
9	V	72	ALA	3.2
2	B	91	ASN	3.2
11	K	6	ALA	3.2
2	B	60	GLU	3.1
1	N	113[A]	LEU	3.1
2	O	32[A]	PHE	3.0
8	U	45	ALA	2.9
1	A	113[A]	LEU	2.8
11	X	7	PRO	2.8
10	J	1	PHE	2.8
8	U	49	ASP	2.8
9	I	72	ALA	2.7
3	C	38	ASN	2.7
8	H	48	GLY	2.6
7	T	38	HIS	2.5
5	R	108	LYS	2.5
1	N	136[A]	LEU	2.5
7	G	35	SER	2.5
9	V	3	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
9	I	37	PHE	2.5
9	V	37	PHE	2.5
2	B	113	TYR	2.4
3	P	37	PHE	2.4
2	B	16[A]	ILE	2.4
2	B	65	TRP	2.4
7	T	30	LEU	2.3
2	B	32[A]	PHE	2.3
12	Y	24	MET	2.3
2	B	115	ASP	2.3
4	Q	74	SER	2.3
11	X	13	TYR	2.2
1	A	311[A]	ILE	2.2
10	W	48	TYR	2.1
2	O	22[A]	HIS	2.1
9	I	19	PHE	2.1
8	U	46	LYS	2.1
9	I	29	LEU	2.0
1	A	298[A]	ASP	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
1	FME	A	1	10/11	0.93	0.14	45,52,85,90	0
1	FME	N	1	10/11	0.94	0.14	45,55,79,88	0
2	FME	B	1	10/11	0.97	0.09	39,44,54,74	0
2	FME	O	1	10/11	0.97	0.10	43,46,54,74	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
20	DMU	C	317	22/33	0.69	0.32	43,59,67,83	22
20	DMU	P	317	22/33	0.73	0.33	43,60,71,90	22
21	EDO	P	322	4/4	0.77	0.35	37,37,41,46	4
20	DMU	A	608	7/33	0.78	0.39	49,55,63,66	7
19	LFA	P	311	11/20	0.78	0.42	47,64,77,82	11
19	LFA	C	312	11/20	0.79	0.33	41,48,63,68	11
20	DMU	N	601	11/33	0.81	0.37	49,57,64,67	11
20	DMU	N	609	7/33	0.81	0.40	52,59,63,67	7
19	LFA	P	309	6/20	0.81	0.42	43,49,52,52	6
19	LFA	C	311	14/20	0.81	0.38	40,58,68,70	14
25	CHD	P	306	29/29	0.81	0.17	63,76,95,106	0
20	DMU	C	315	33/33	0.82	0.35	44,56,70,74	33
20	DMU	O	304	22/33	0.83	0.29	55,69,82,88	22
20	DMU	C	318	33/33	0.83	0.31	41,56,72,84	33
19	LFA	P	312	11/20	0.83	0.31	45,51,62,70	11
19	LFA	C	325	15/20	0.83	0.40	51,54,68,69	15
20	DMU	P	319	33/33	0.84	0.25	49,71,83,86	33
21	EDO	A	611	4/4	0.84	0.31	39,47,47,48	4
19	LFA	P	308	11/20	0.84	0.31	47,50,55,57	11
19	LFA	G	104	14/20	0.84	0.29	38,51,57,60	14
20	DMU	P	318	33/33	0.85	0.29	44,55,64,71	33
19	LFA	C	310	11/20	0.85	0.34	50,65,76,77	11
19	LFA	C	308	6/20	0.85	0.41	39,46,55,56	6
20	DMU	B	309	22/33	0.85	0.31	50,71,80,84	22
25	CHD	C	305	29/29	0.85	0.14	66,76,97,106	0
20	DMU	M	102	8/33	0.85	0.24	46,48,51,66	8
19	LFA	C	314	13/20	0.86	0.27	52,56,68,68	13
20	DMU	C	319	33/33	0.86	0.23	45,68,75,76	33
20	DMU	A	620	11/33	0.86	0.34	40,56,63,63	11
20	DMU	P	323	33/33	0.86	0.17	44,56,86,97	33
21	EDO	A	610	4/4	0.86	0.21	32,35,36,37	4
19	LFA	B	308	17/20	0.86	0.29	41,56,67,71	17
21	EDO	N	612	4/4	0.86	0.24	41,42,46,48	4
19	LFA	C	313	15/20	0.86	0.25	42,51,69,71	15
20	DMU	N	610	33/33	0.86	0.23	40,57,80,86	33
19	LFA	O	302	17/20	0.86	0.29	43,56,69,71	17
20	DMU	C	323	33/33	0.87	0.17	44,57,75,83	33
19	LFA	O	303	11/20	0.87	0.31	44,58,69,72	11
18	CDL	P	305	87/100	0.87	0.20	49,82,119,134	0
18	CDL	Y	101	94/100	0.87	0.17	51,81,123,135	0
21	EDO	C	322	4/4	0.87	0.30	38,40,42,43	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
18	CDL	A	606	64/100	0.87	0.17	49,80,105,115	0
18	CDL	N	607	64/100	0.87	0.18	55,82,107,129	0
21	EDO	R	203	4/4	0.87	0.24	42,43,48,53	4
19	LFA	T	101	14/20	0.87	0.26	38,47,62,62	14
19	LFA	T	104	11/20	0.87	0.29	47,56,73,76	11
20	DMU	B	303	11/33	0.88	0.31	41,50,62,67	11
20	DMU	P	315	33/33	0.88	0.27	45,54,64,68	33
20	DMU	W	101	11/33	0.88	0.30	59,65,74,77	11
20	DMU	Y	102	22/33	0.88	0.36	53,63,77,79	22
20	DMU	H	101	33/33	0.88	0.24	38,49,64,69	33
19	LFA	P	301	15/20	0.88	0.31	43,55,60,66	15
20	DMU	A	609	33/33	0.89	0.21	39,53,66,70	33
19	LFA	P	314	13/20	0.89	0.24	46,53,69,72	13
19	LFA	C	309	18/20	0.89	0.21	37,45,56,58	18
19	LFA	T	103	14/20	0.89	0.30	40,59,67,69	14
21	EDO	E	201	4/4	0.89	0.27	44,49,49,54	4
20	DMU	L	102	22/33	0.89	0.32	50,57,71,75	22
18	CDL	C	304	87/100	0.89	0.17	48,77,111,122	0
20	DMU	C	316	7/33	0.89	0.24	51,54,56,61	7
20	DMU	Q	201	33/33	0.89	0.20	44,56,65,75	33
19	LFA	A	607	14/20	0.89	0.25	38,46,68,69	14
19	LFA	P	310	18/20	0.90	0.23	38,48,57,58	18
20	DMU	T	105	22/33	0.90	0.23	41,54,70,71	22
21	EDO	C	320	4/4	0.90	0.29	52,52,60,71	4
20	DMU	D	201	33/33	0.90	0.17	31,48,60,68	33
20	DMU	G	102	22/33	0.90	0.26	41,58,63,66	22
20	DMU	J	101	11/33	0.91	0.30	54,60,66,85	11
19	LFA	P	313	15/20	0.91	0.19	41,50,56,64	15
20	DMU	U	101	33/33	0.91	0.22	36,48,63,67	33
20	DMU	B	305	22/33	0.91	0.20	41,61,69,87	22
18	CDL	L	101	94/100	0.91	0.14	46,79,108,122	0
26	UNX	P	303	1/1	0.91	0.24	53,53,53,53	0
19	LFA	N	608	14/20	0.92	0.21	36,45,60,60	14
21	EDO	P	320	4/4	0.92	0.23	48,53,57,73	4
19	LFA	C	307	11/20	0.92	0.26	46,50,60,61	11
20	DMU	B	304	11/33	0.92	0.25	34,58,64,68	11
20	DMU	O	307	11/33	0.92	0.27	42,47,59,65	11
20	DMU	O	309	22/33	0.92	0.19	39,55,60,65	22
21	EDO	E	203	4/4	0.92	0.25	36,41,43,45	4
20	DMU	Z	101	33/33	0.93	0.09	54,59,73,78	0
20	DMU	P	307	11/33	0.93	0.26	49,52,62,62	11
21	EDO	E	202	4/4	0.93	0.26	36,39,39,41	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	DMU	C	306	11/33	0.93	0.21	51,57,63,68	11
21	EDO	F	103	4/4	0.93	0.16	27,28,33,36	4
20	DMU	P	316	7/33	0.93	0.20	51,58,66,67	7
21	EDO	N	611	4/4	0.94	0.15	32,34,36,38	4
20	DMU	O	308	11/33	0.94	0.23	38,53,61,62	11
20	DMU	Z	102	8/33	0.94	0.20	50,54,57,59	8
21	EDO	A	612	4/4	0.94	0.20	31,32,33,33	4
21	EDO	F	101	4/4	0.95	0.19	41,47,51,53	4
21	EDO	R	201	4/4	0.95	0.30	59,65,71,75	4
20	DMU	M	101	33/33	0.95	0.08	48,54,65,74	0
22	XE	A	618	1/1	0.95	0.10	46,46,46,46	1
22	XE	N	621	1/1	0.95	0.12	47,47,47,47	1
25	CHD	C	301	29/29	0.95	0.07	35,40,43,46	0
21	EDO	N	613	4/4	0.95	0.20	33,34,36,36	4
21	EDO	N	615	4/4	0.95	0.19	33,35,36,40	4
26	UNX	C	302	1/1	0.95	0.17	53,53,53,53	0
21	EDO	G	103	4/4	0.95	0.15	40,41,42,43	4
25	CHD	P	302	29/29	0.96	0.07	35,39,45,47	0
21	EDO	O	310	4/4	0.96	0.11	38,39,39,41	4
28	PEK	G	101	53/53	0.96	0.12	39,58,93,122	0
28	PEK	T	102	53/53	0.96	0.12	38,59,88,99	0
25	CHD	B	307	29/29	0.97	0.06	35,38,42,48	0
21	EDO	S	102	4/4	0.97	0.09	26,29,32,34	4
21	EDO	T	106	4/4	0.97	0.12	39,39,40,44	4
25	CHD	O	301	29/29	0.97	0.06	34,38,41,48	0
21	EDO	C	321	4/4	0.97	0.18	39,41,42,45	4
22	XE	N	618	1/1	0.97	0.06	51,51,51,51	1
21	EDO	N	614	4/4	0.97	0.16	39,40,41,42	4
23	PGV	A	619	51/51	0.97	0.09	33,43,79,93	0
23	PGV	C	303	51/51	0.97	0.09	36,44,100,111	0
23	PGV	N	622	51/51	0.97	0.09	35,45,72,76	0
22	XE	A	615	1/1	0.98	0.06	52,52,52,52	1
22	XE	A	616	1/1	0.98	0.05	48,48,48,48	1
17	NA	A	605	1/1	0.98	0.12	41,41,41,41	0
21	EDO	R	202	4/4	0.98	0.16	38,41,41,42	4
22	XE	N	619	1/1	0.98	0.07	50,50,50,50	1
21	EDO	B	306	4/4	0.98	0.08	32,35,36,38	4
21	EDO	P	321	4/4	0.98	0.14	38,39,42,44	4
21	EDO	S	103	4/4	0.98	0.09	33,40,41,42	4
21	EDO	F	104	4/4	0.98	0.11	37,40,40,41	4
23	PGV	P	304	51/51	0.98	0.08	34,45,80,108	0
17	NA	N	606	1/1	0.99	0.11	45,45,45,45	0

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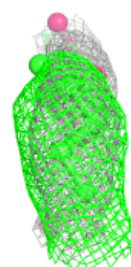
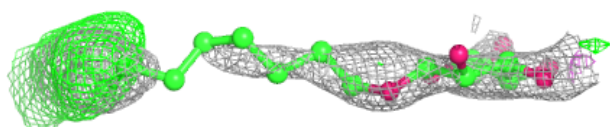
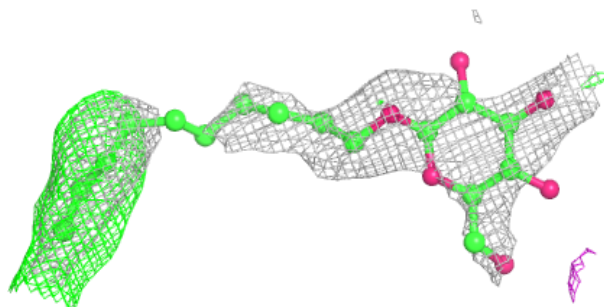
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	HEA	A	602	60/60	0.99	0.05	30,34,40,46	0
22	XE	C	324	1/1	0.99	0.04	53,53,53,53	1
14	HEA	N	602	60/60	0.99	0.05	32,36,48,59	0
14	HEA	N	603	60/60	0.99	0.05	32,35,42,50	0
14	HEA	A	601	60/60	0.99	0.05	30,34,46,54	0
22	XE	P	324	1/1	0.99	0.05	53,53,53,53	1
22	XE	B	301	1/1	1.00	0.24	56,56,56,56	1
15	CU	A	603	1/1	1.00	0.01	33,33,33,33	0
24	CUA	B	302	2/2	1.00	0.03	35,35,35,36	0
24	CUA	O	306	2/2	1.00	0.02	37,37,37,38	0
22	XE	N	616	1/1	1.00	0.14	48,48,48,48	0
22	XE	N	617	1/1	1.00	0.19	47,47,47,47	0
22	XE	A	613	1/1	1.00	0.15	48,48,48,48	0
22	XE	A	614	1/1	1.00	0.15	45,45,45,45	1
22	XE	N	620	1/1	1.00	0.07	54,54,54,54	1
15	CU	N	604	1/1	1.00	0.02	34,34,34,34	0
22	XE	O	305	1/1	1.00	0.17	52,52,52,52	1
16	MG	A	604	1/1	1.00	0.03	35,35,35,35	0
27	ZN	F	102	1/1	1.00	0.01	39,39,39,39	0
27	ZN	S	101	1/1	1.00	0.01	39,39,39,39	0
22	XE	A	617	1/1	1.00	0.04	51,51,51,51	1
16	MG	N	605	1/1	1.00	0.01	36,36,36,36	0

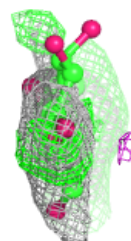
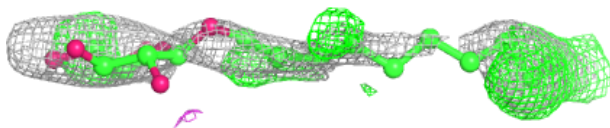
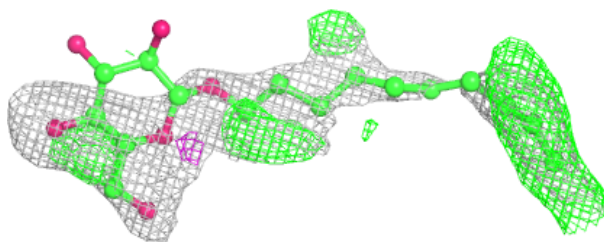
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DMU C 317:**

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

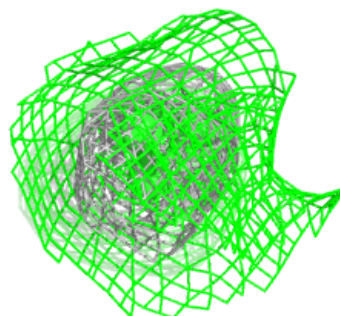
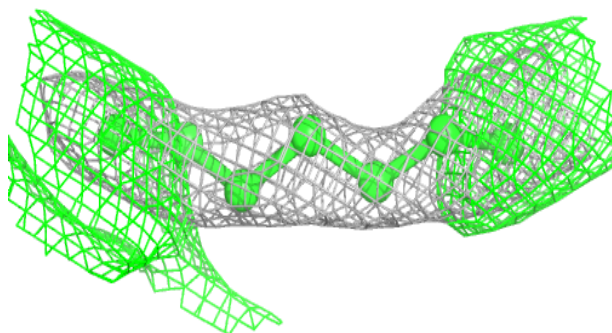
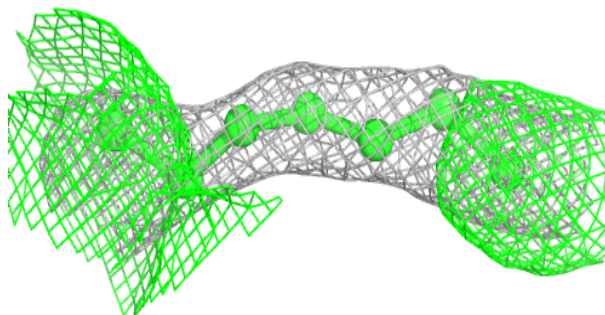
**Electron density around DMU P 317:**

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

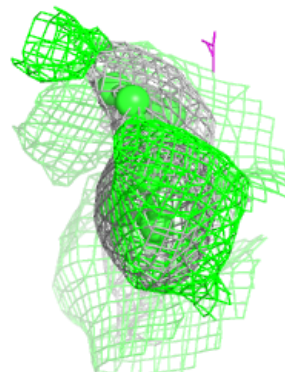
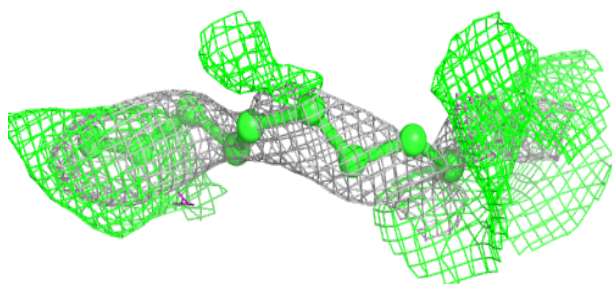
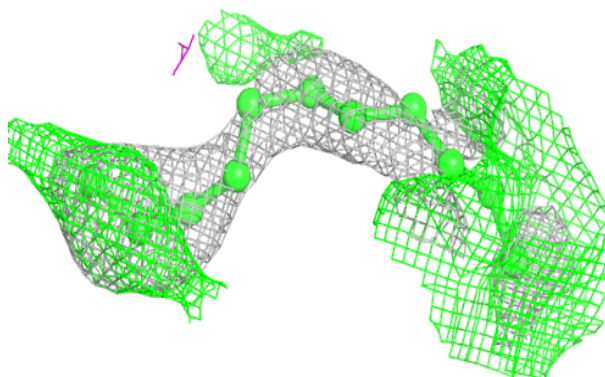


**Electron density around DMU A 608:**

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

**Electron density around LFA P 311:**

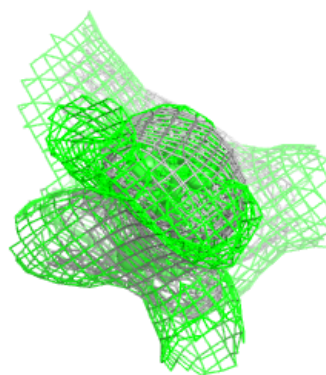
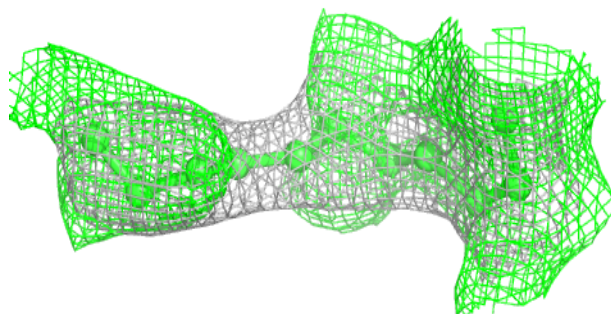
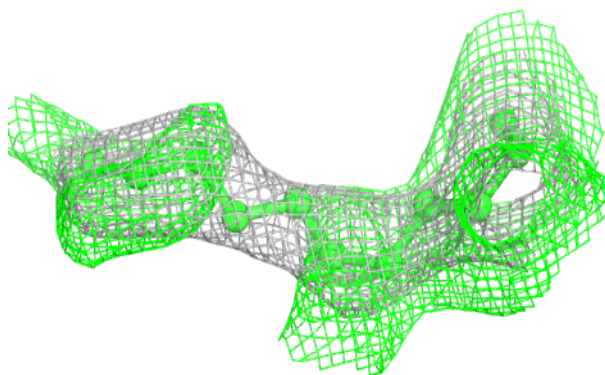
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



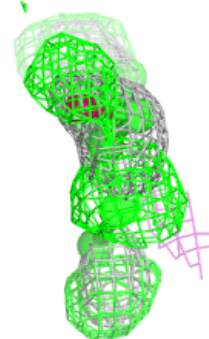
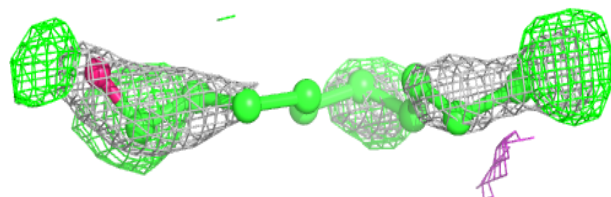
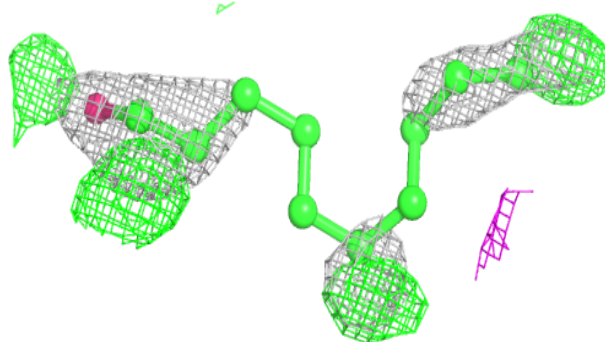


**Electron density around LFA C 312:**

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

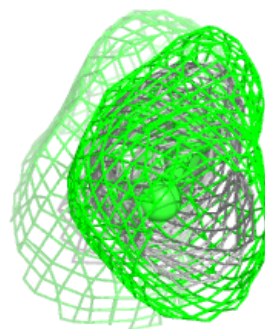
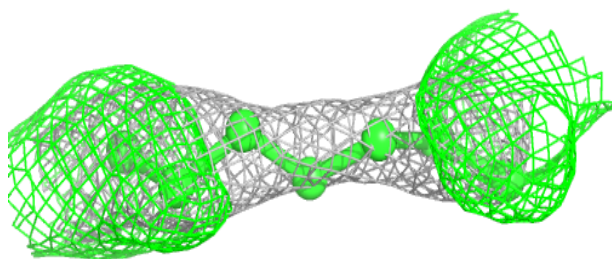
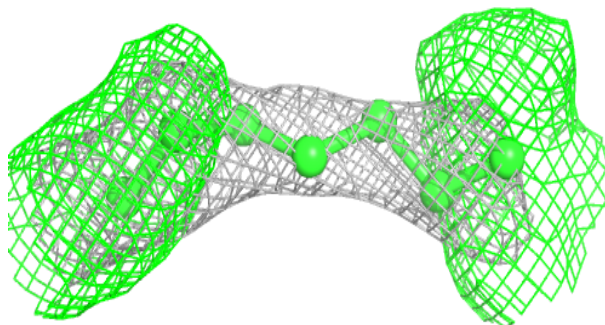
**Electron density around DMU N 601:**

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

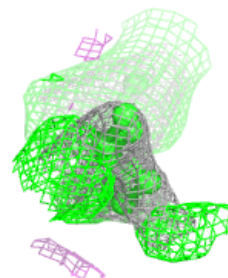
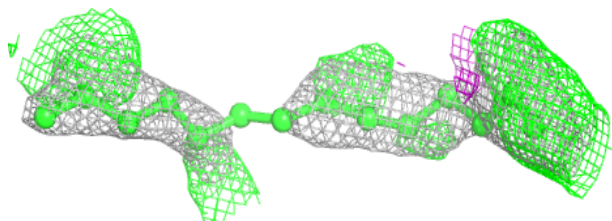
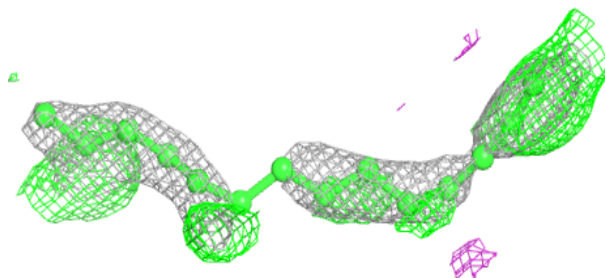


**Electron density around DMU N 609:**

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

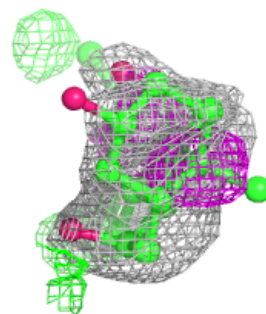
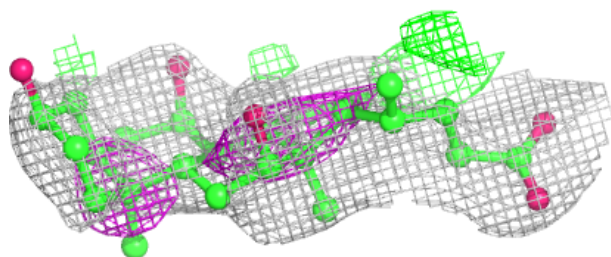
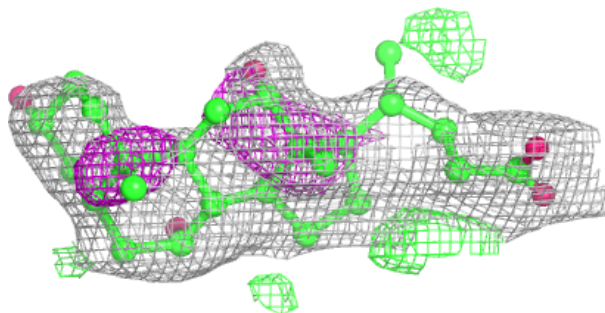
**Electron density around LFA C 311:**

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

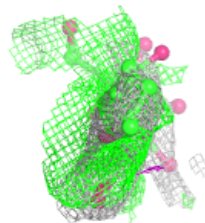
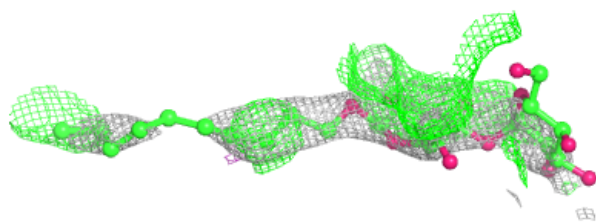
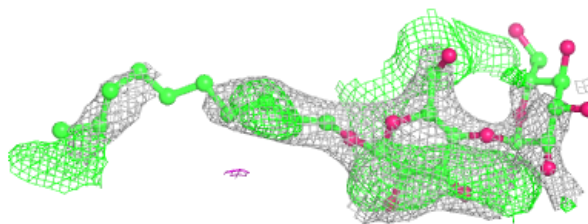


**Electron density around CHD P 306:**

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

**Electron density around DMU C 315:**

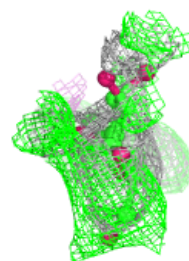
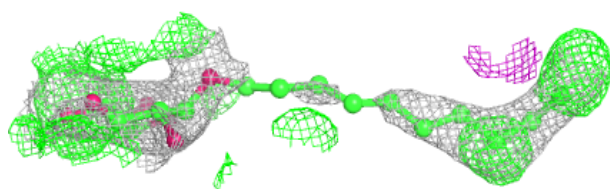
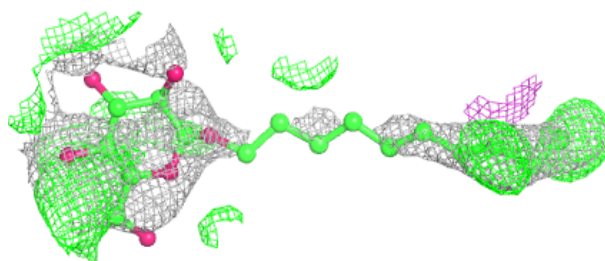
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



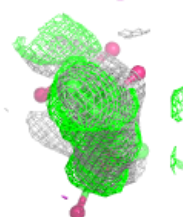
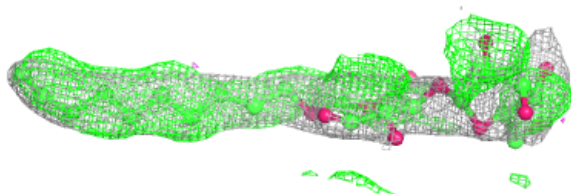
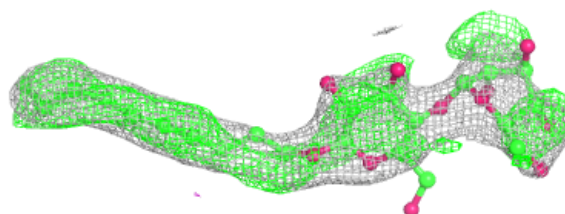


**Electron density around DMU O 304:**

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

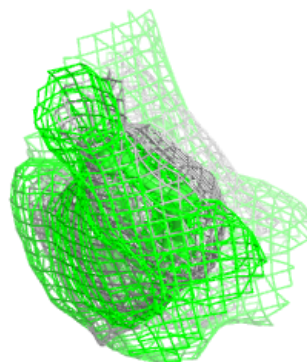
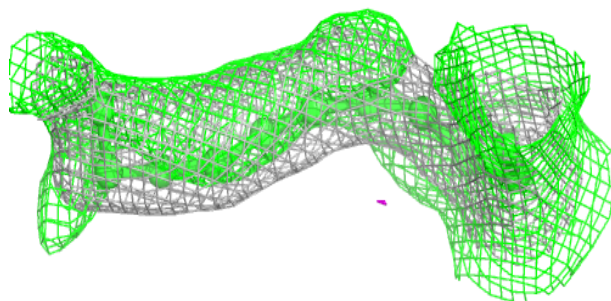
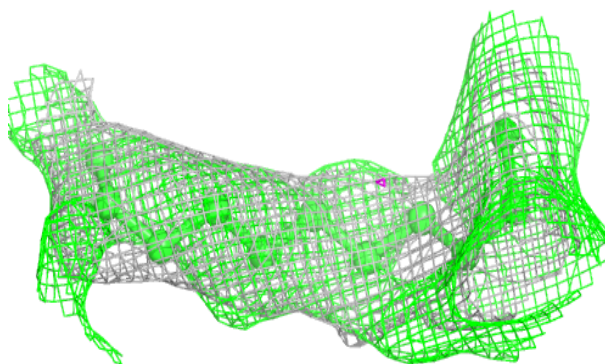
**Electron density around DMU C 318:**

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

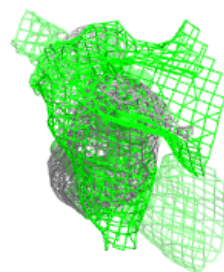
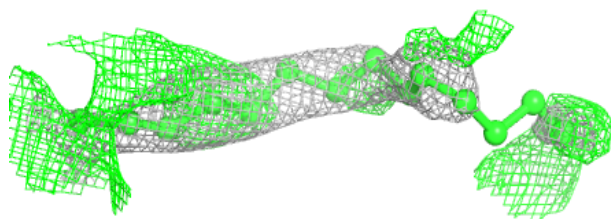
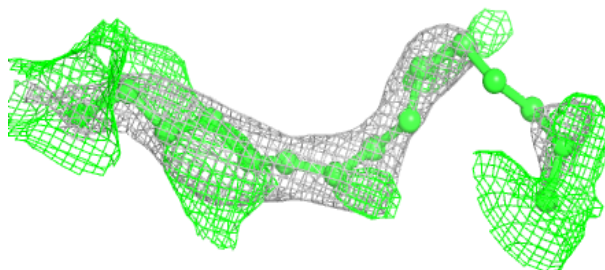


**Electron density around LFA P 312:**

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

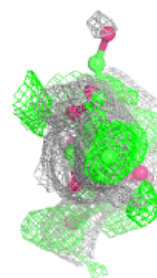
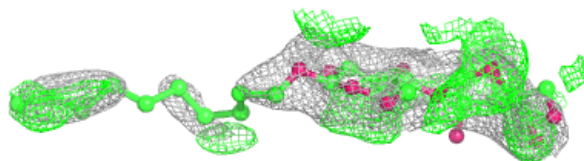
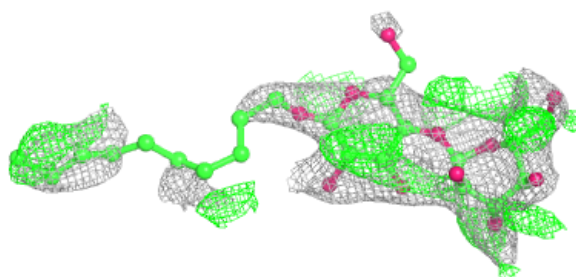
**Electron density around LFA C 325:**

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

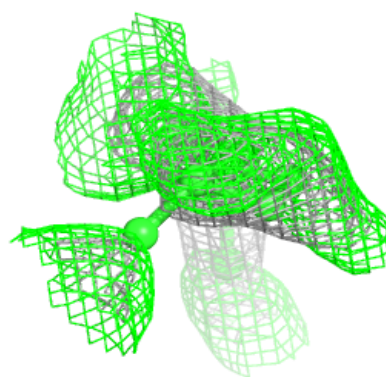
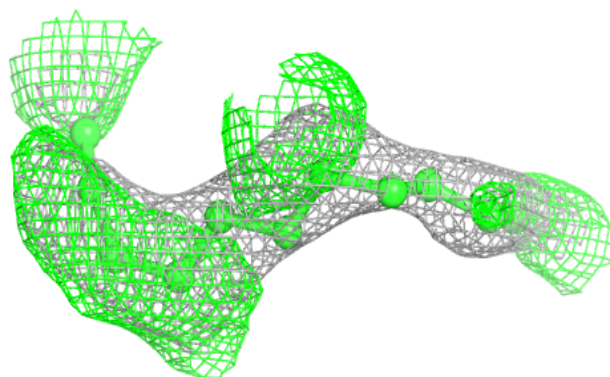
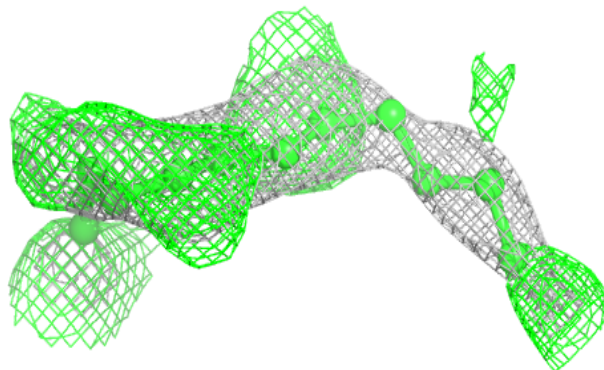


**Electron density around DMU P 319:**

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

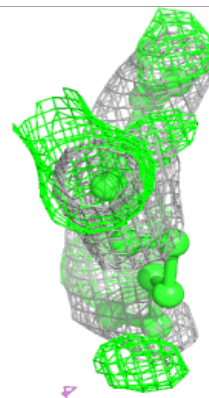
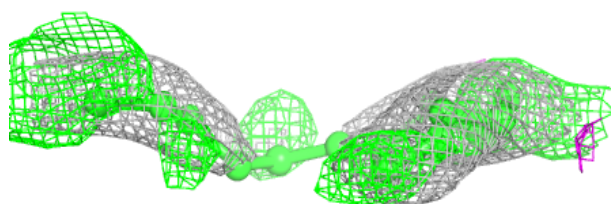
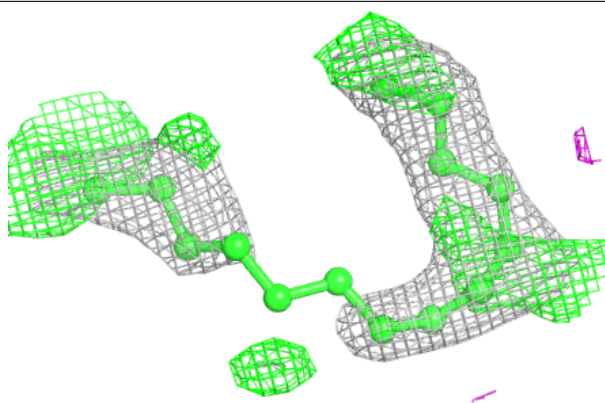
**Electron density around LFA P 308:**

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

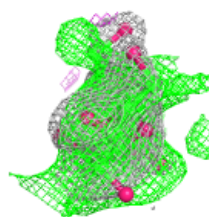
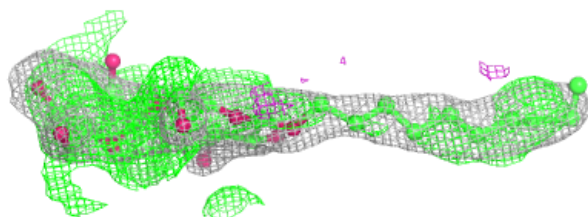
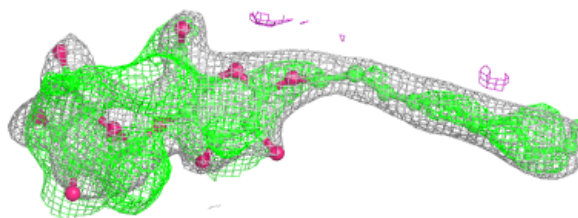


**Electron density around LFA G 104:**

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

**Electron density around DMU P 318:**

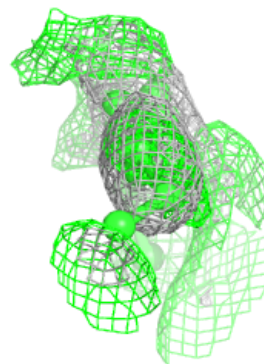
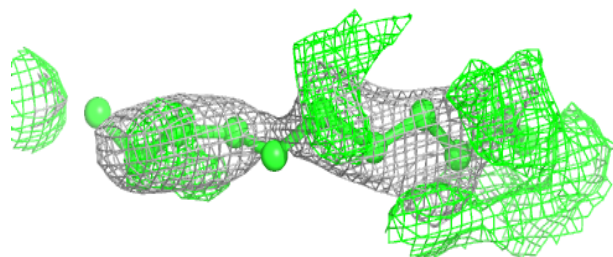
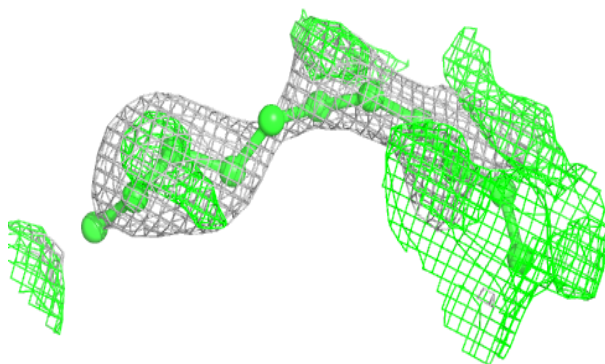
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



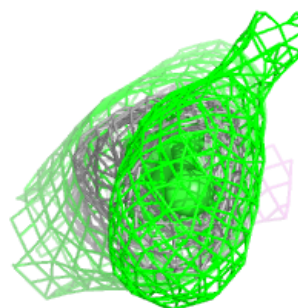
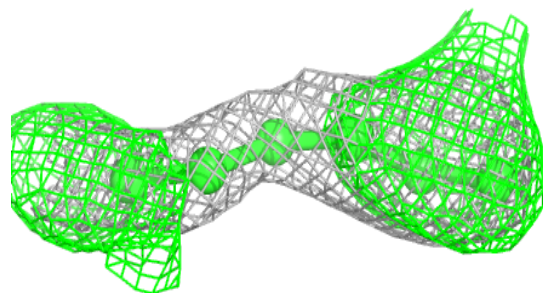
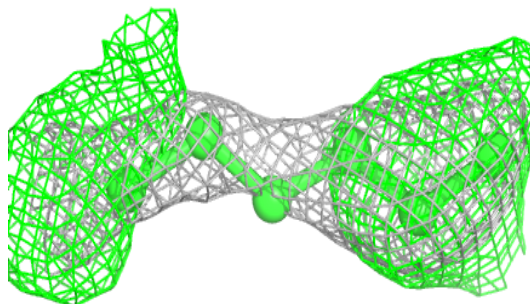


**Electron density around LFA C 310:**

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

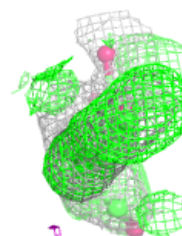
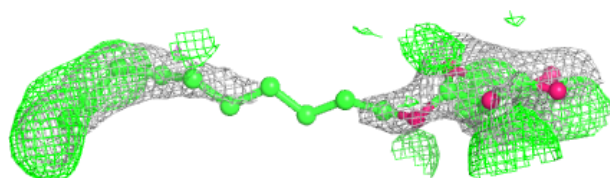
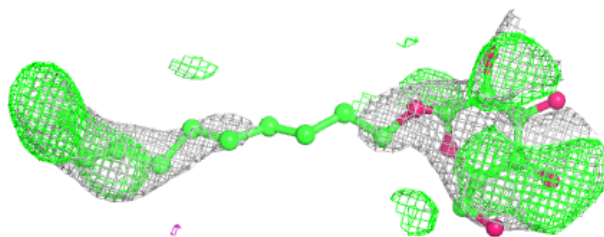
**Electron density around LFA C 308:**

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

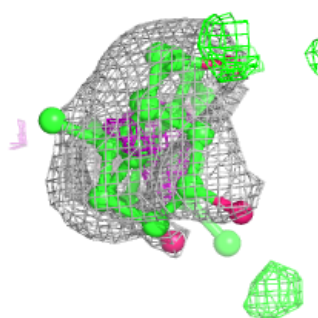
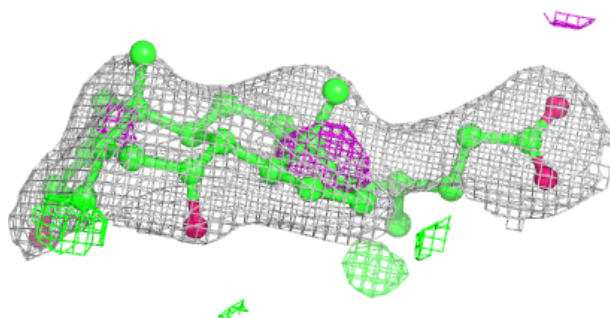
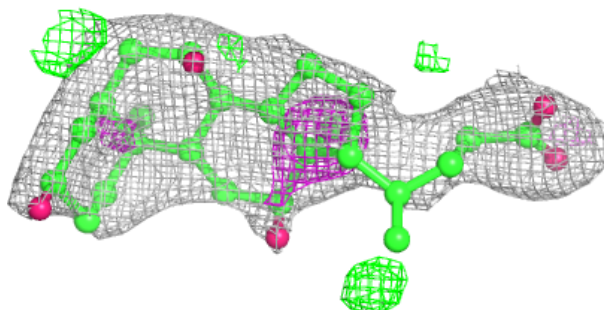


**Electron density around DMU B 309:**

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

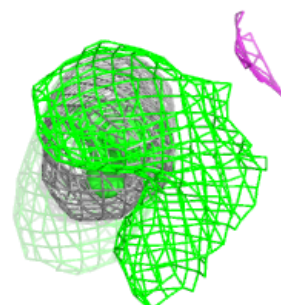
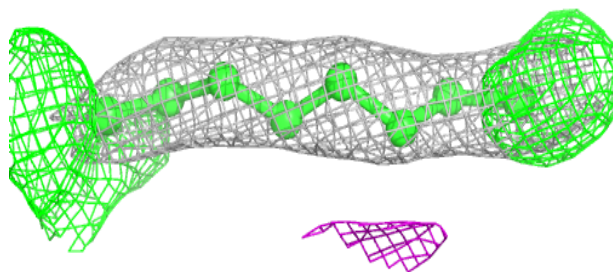
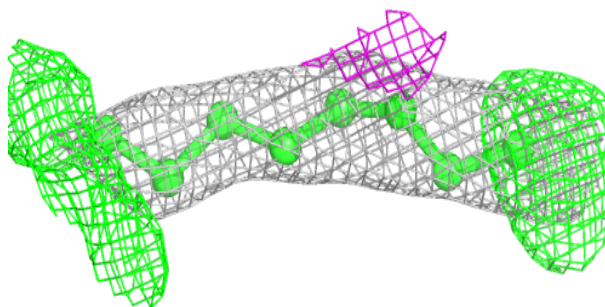
**Electron density around CHD C 305:**

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

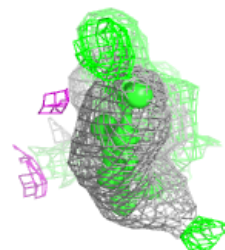
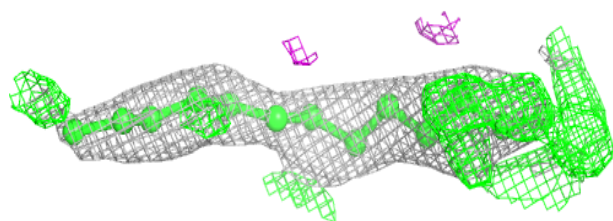
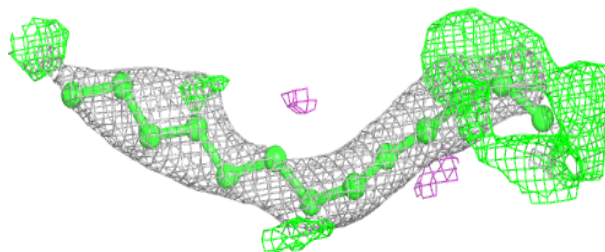


**Electron density around DMU M 102:**

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

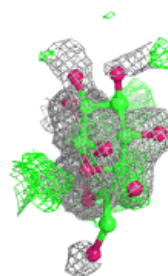
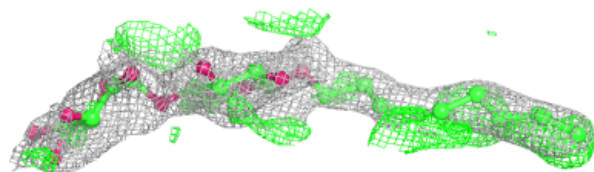
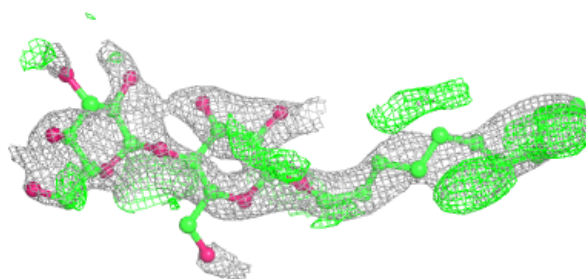
**Electron density around LFA C 314:**

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

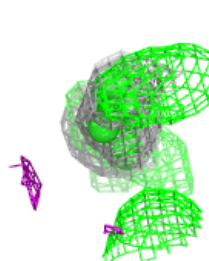
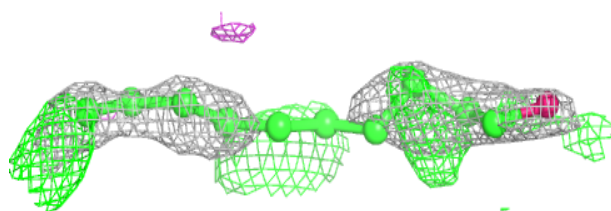
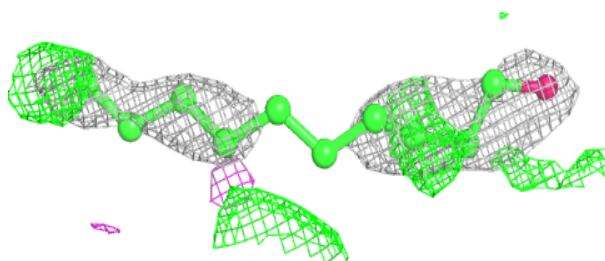


**Electron density around DMU C 319:**

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

**Electron density around DMU A 620:**

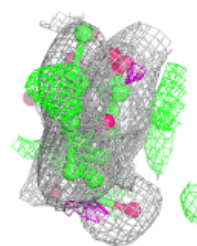
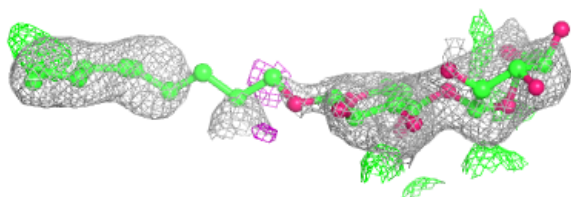
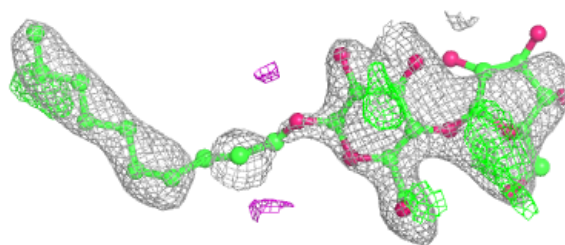
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



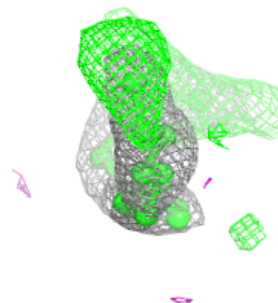
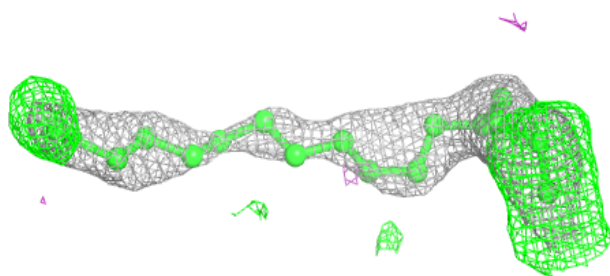
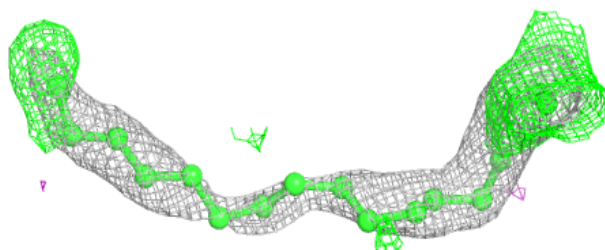


**Electron density around DMU P 323:**

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

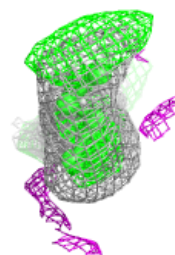
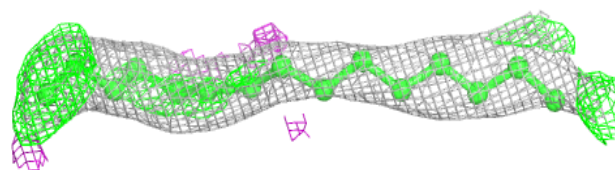
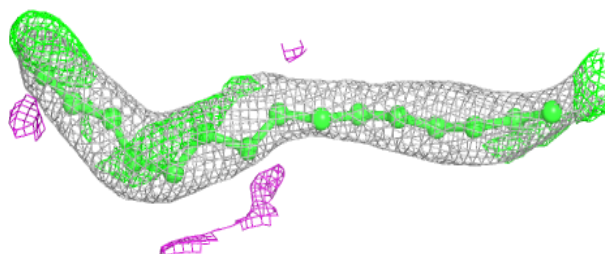
**Electron density around LFA B 308:**

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

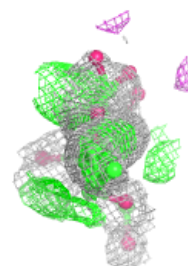
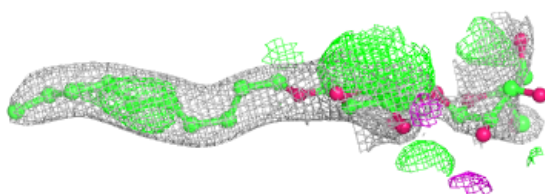
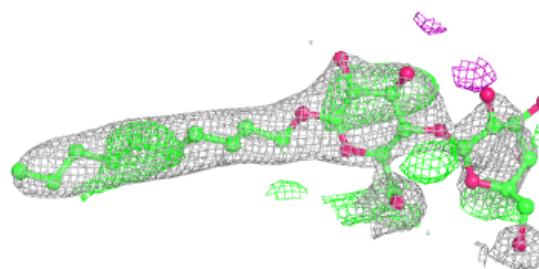


**Electron density around LFA C 313:**

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

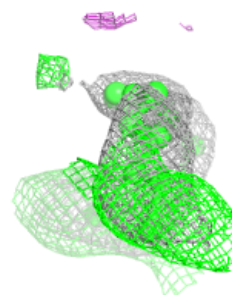
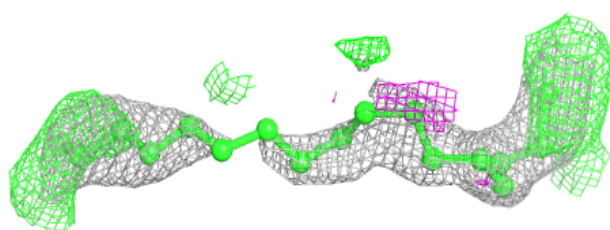
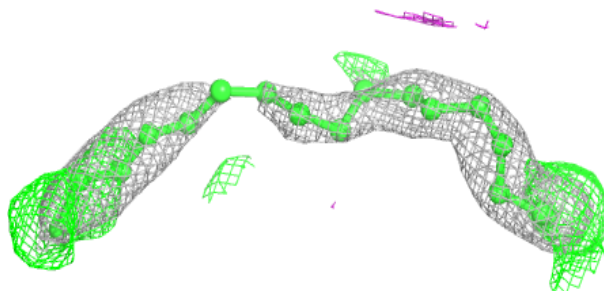
**Electron density around DMU N 610:**

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

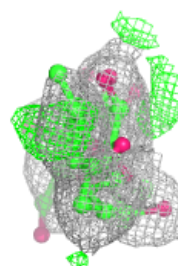
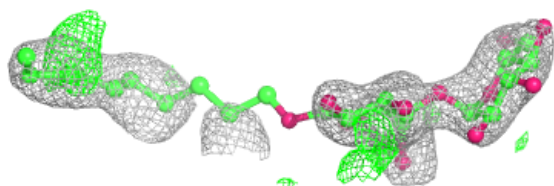
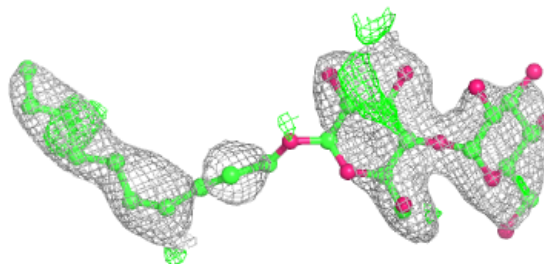


**Electron density around LFA O 302:**

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

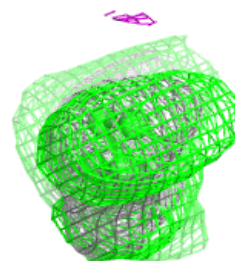
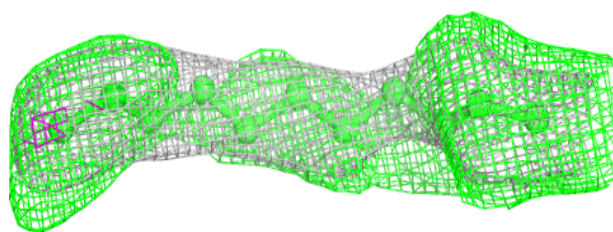
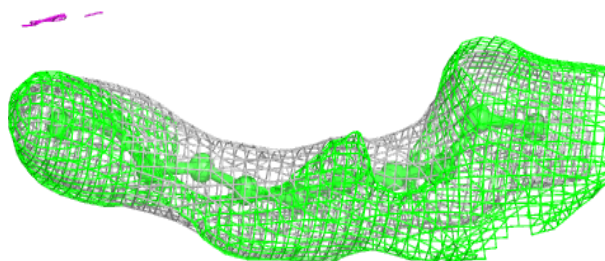
**Electron density around DMU C 323:**

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

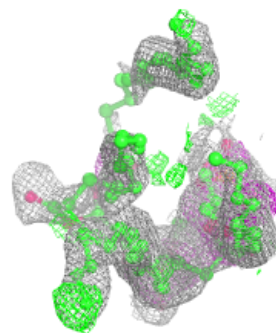
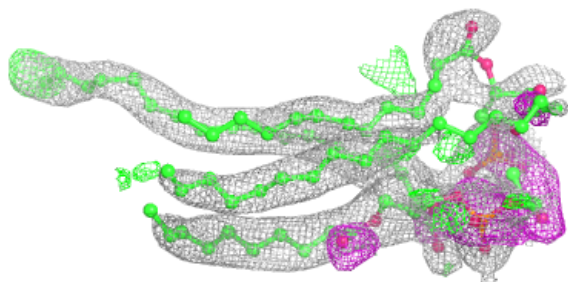
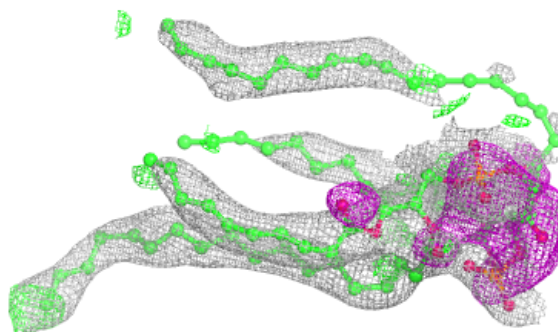


**Electron density around LFA O 303:**

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

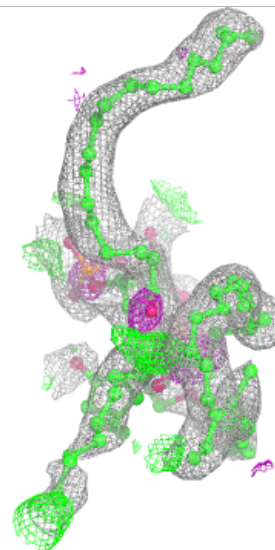
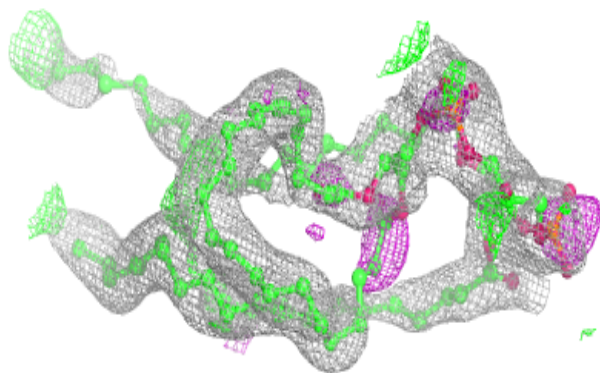
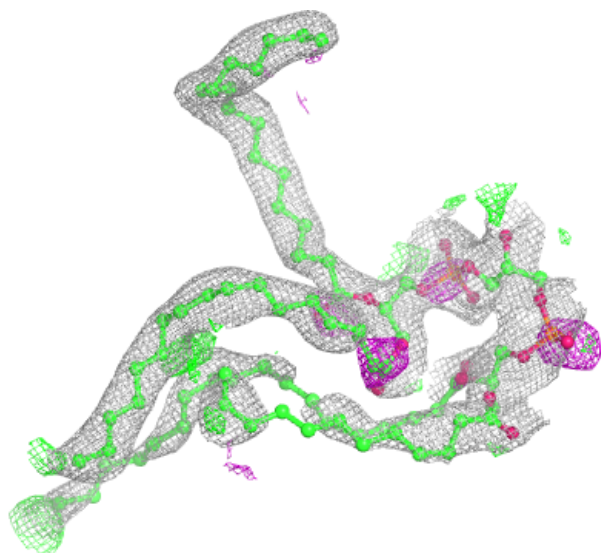
**Electron density around CDL P 305:**

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



**Electron density around CDL Y 101:**

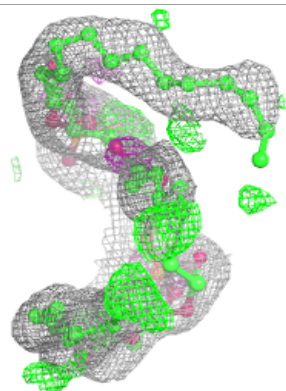
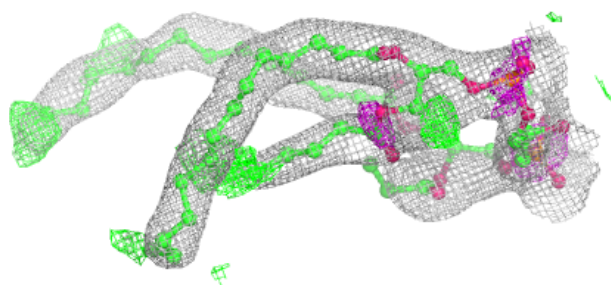
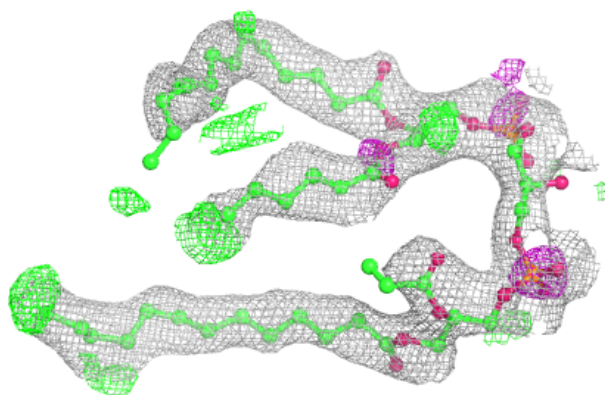
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



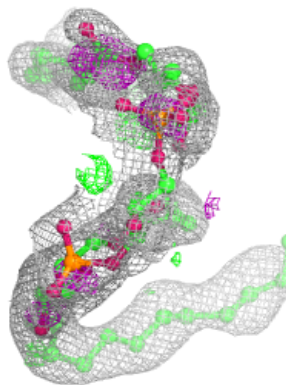
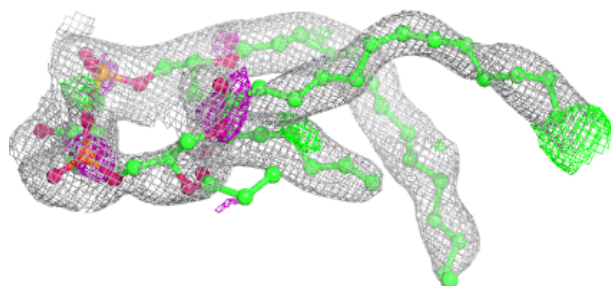
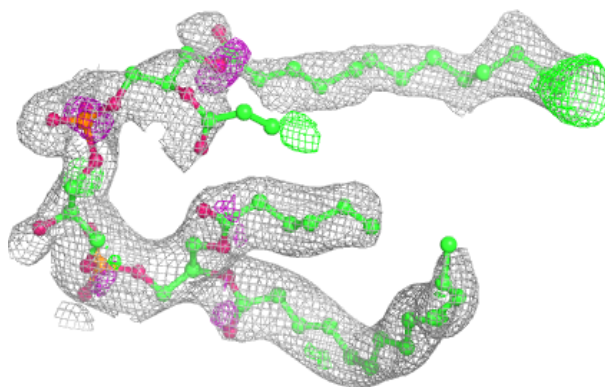


**Electron density around CDL A 606:**

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

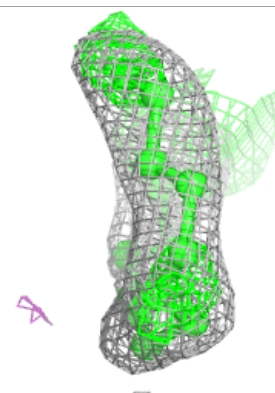
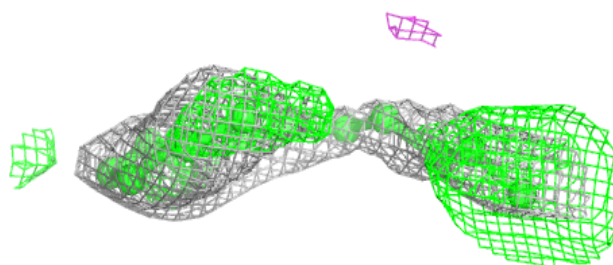
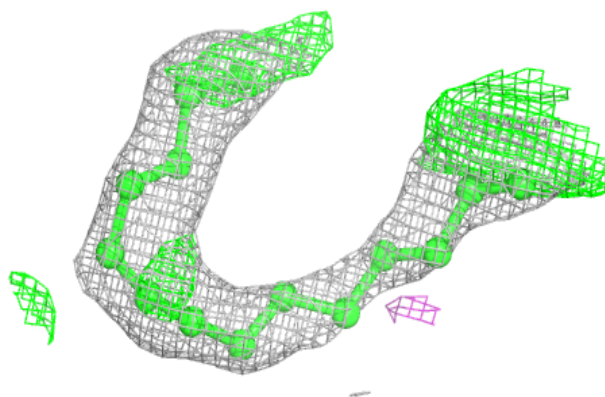
**Electron density around CDL N 607:**

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

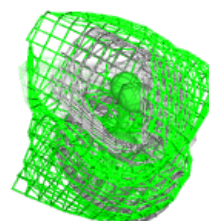
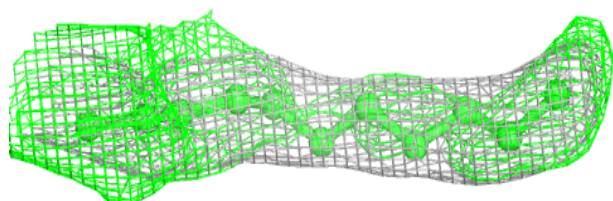
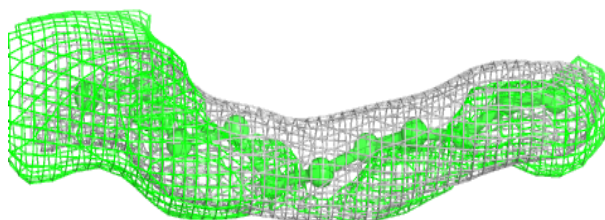


**Electron density around LFA T 101:**

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

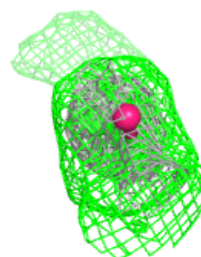
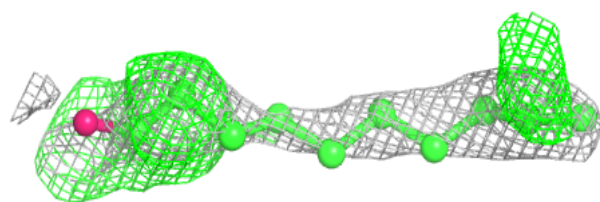
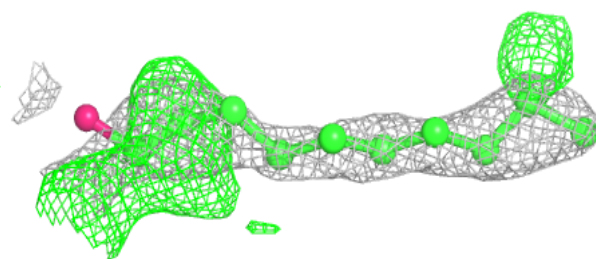
**Electron density around LFA T 104:**

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

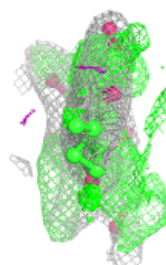
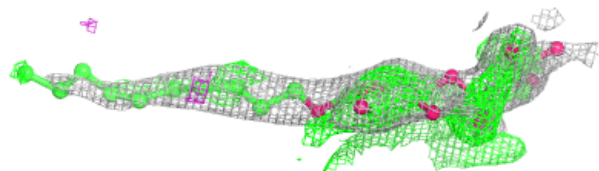
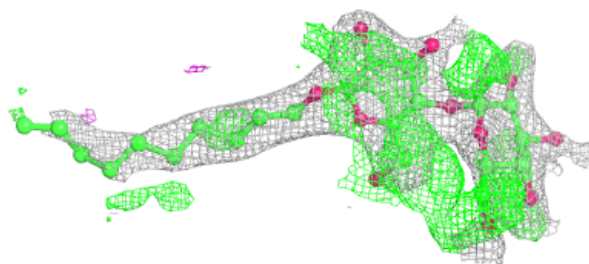


**Electron density around DMU B 303:**

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

**Electron density around DMU P 315:**

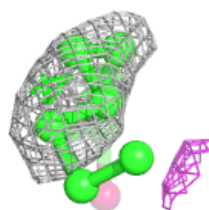
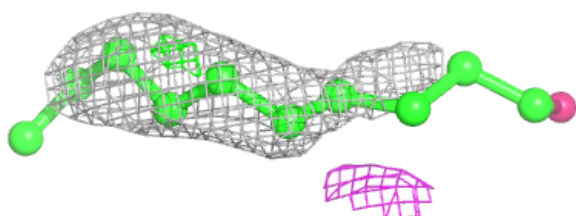
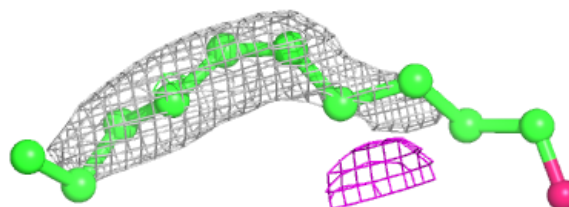
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



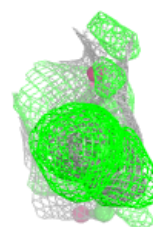
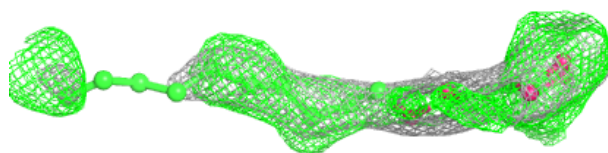
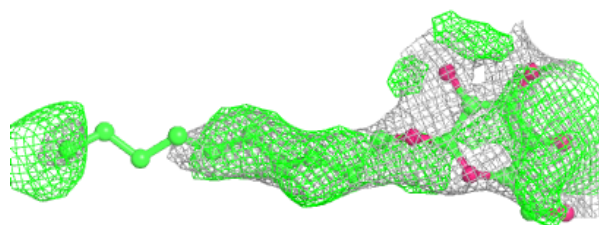


**Electron density around DMU W 101:**

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

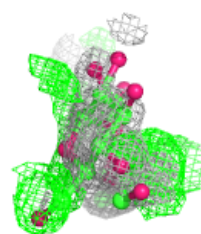
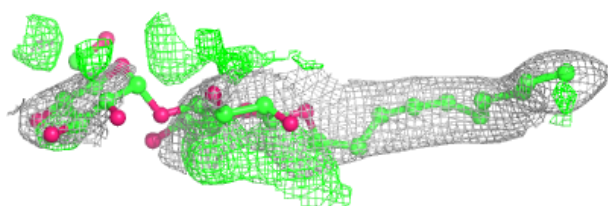
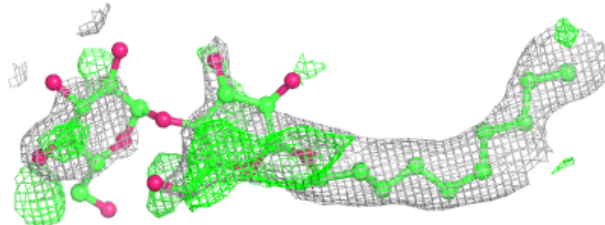
**Electron density around DMU Y 102:**

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

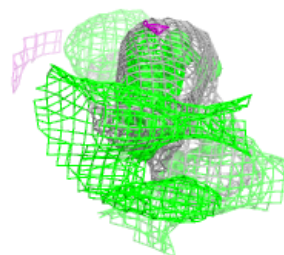
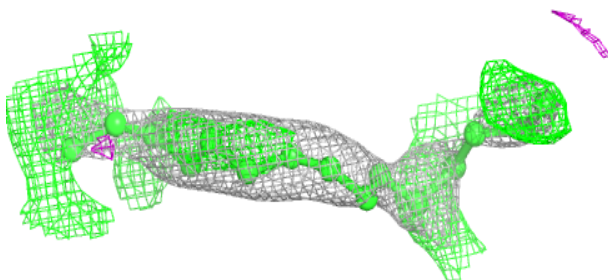
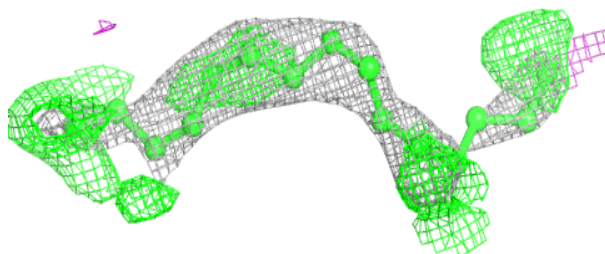


**Electron density around DMU H 101:**

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

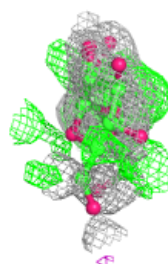
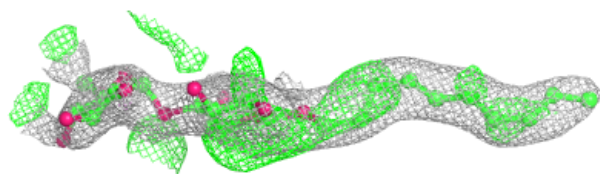
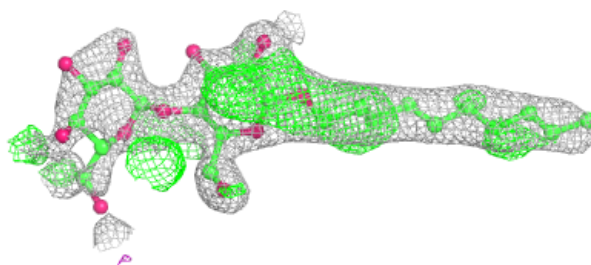
**Electron density around LFA P 301:**

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

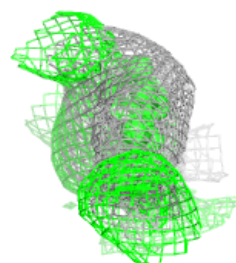
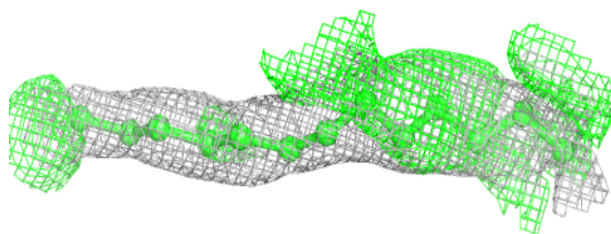
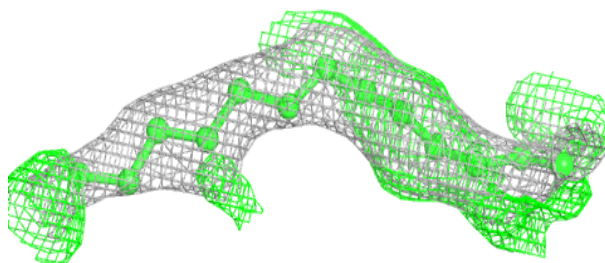


**Electron density around DMU A 609:**

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

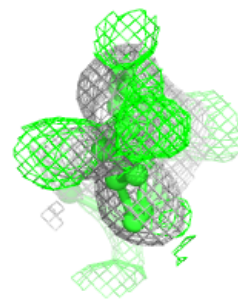
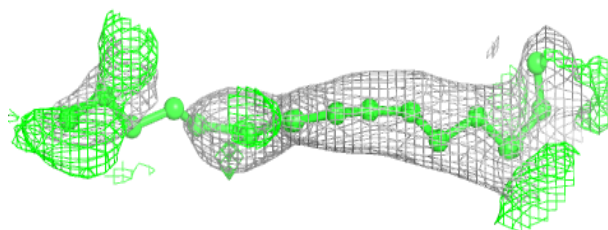
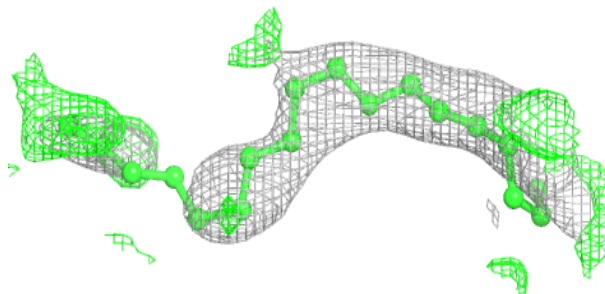
**Electron density around LFA P 314:**

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

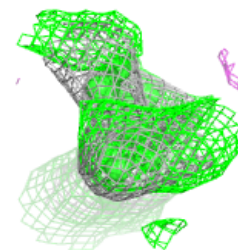
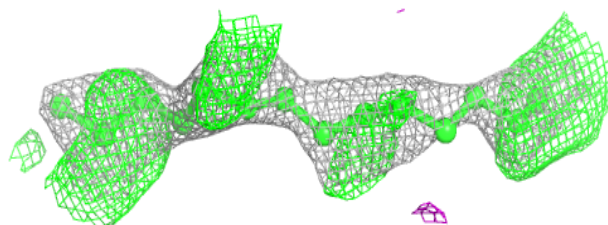
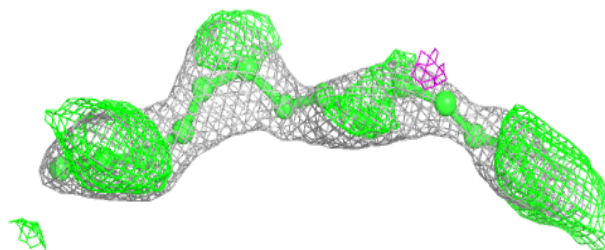


**Electron density around LFA C 309:**

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

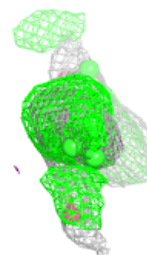
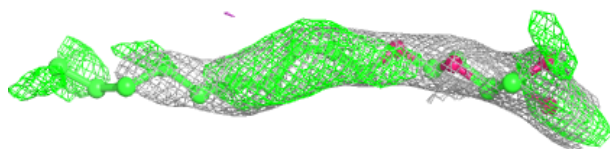
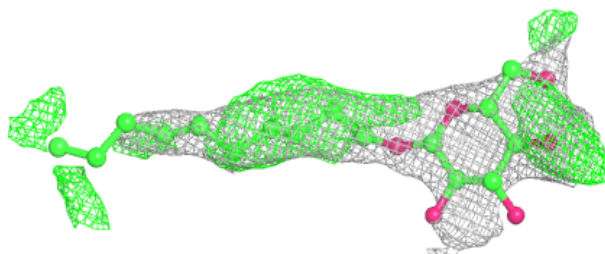
**Electron density around LFA T 103:**

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

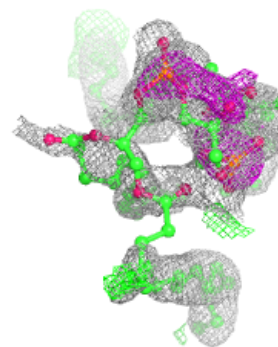
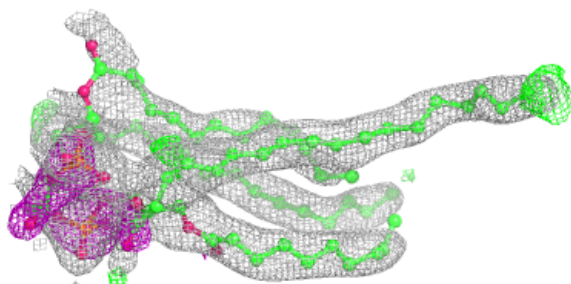
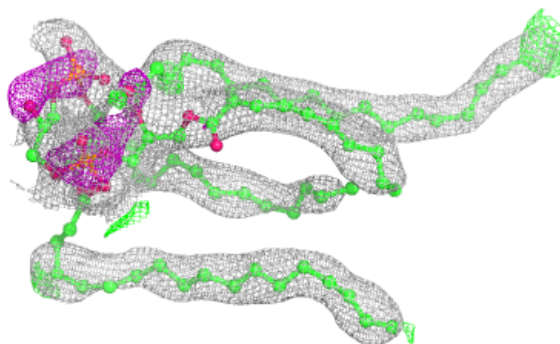


**Electron density around DMU L 102:**

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

**Electron density around CDL C 304:**

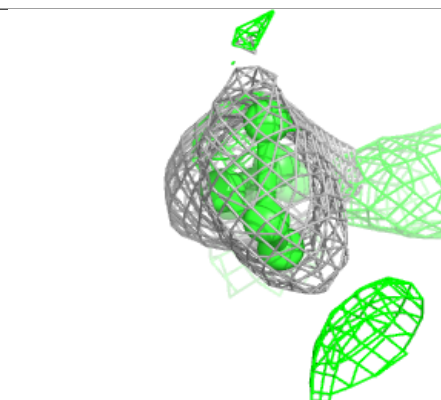
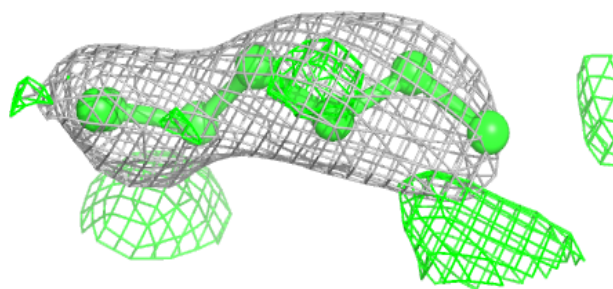
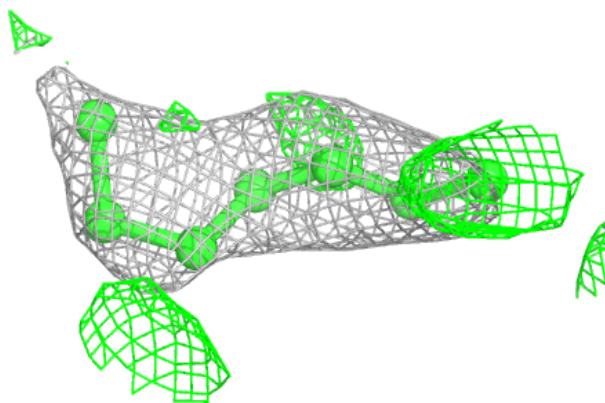
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



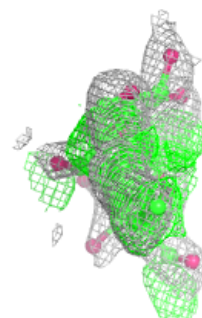
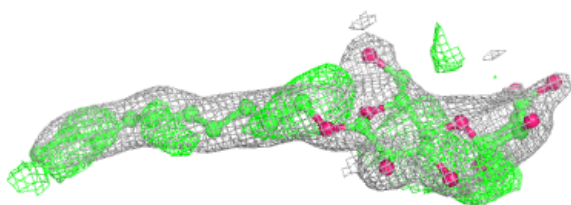
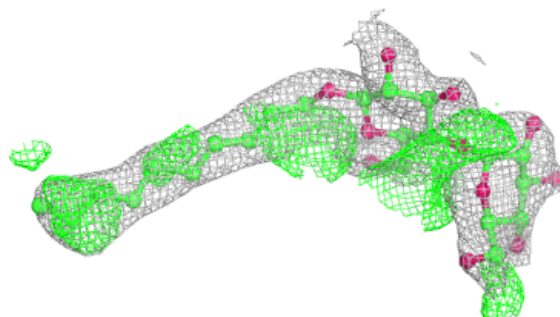


**Electron density around DMU C 316:**

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

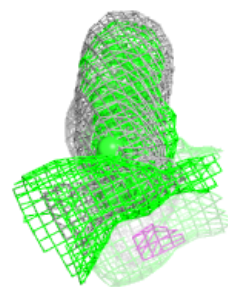
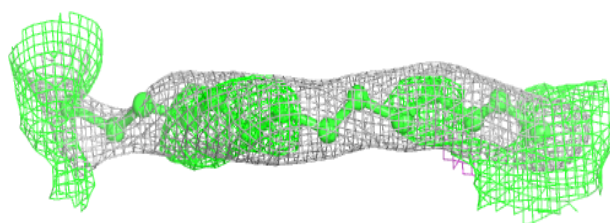
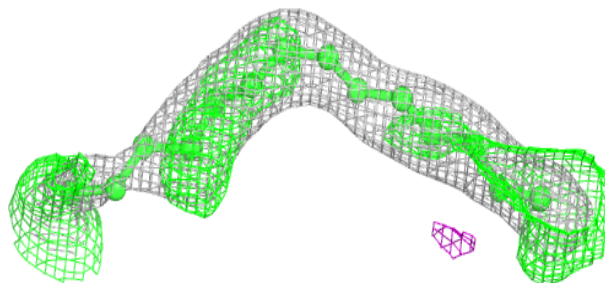
**Electron density around DMU Q 201:**

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

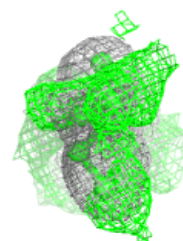
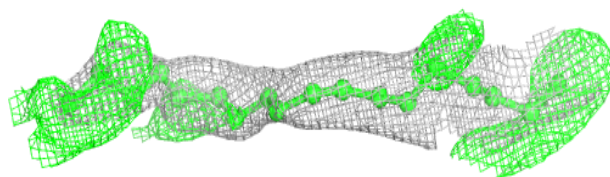
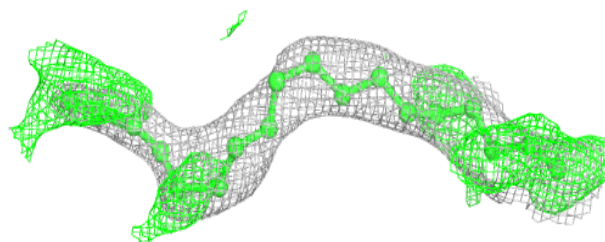


**Electron density around LFA A 607:**

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

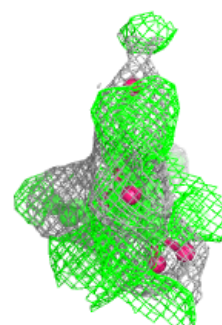
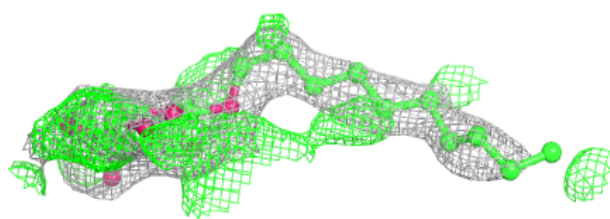
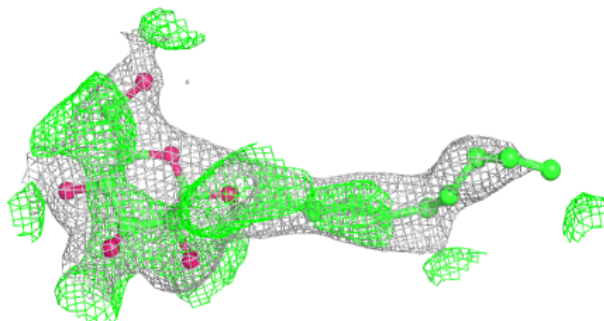
**Electron density around LFA P 310:**

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

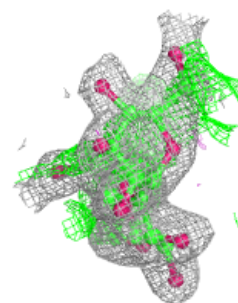
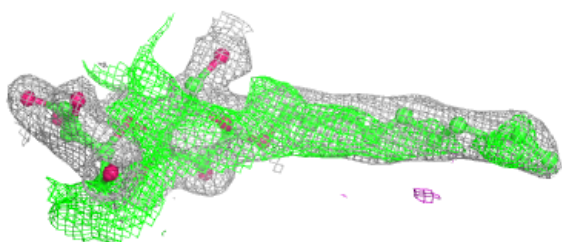
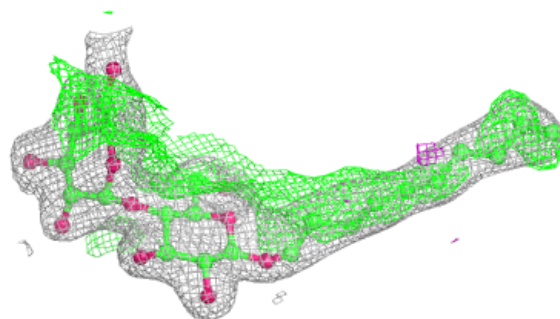


**Electron density around DMU T 105:**

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

**Electron density around DMU D 201:**

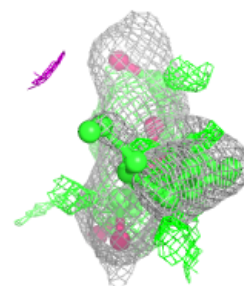
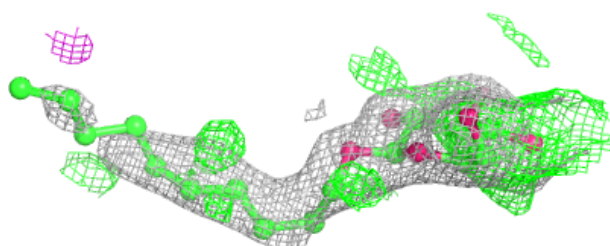
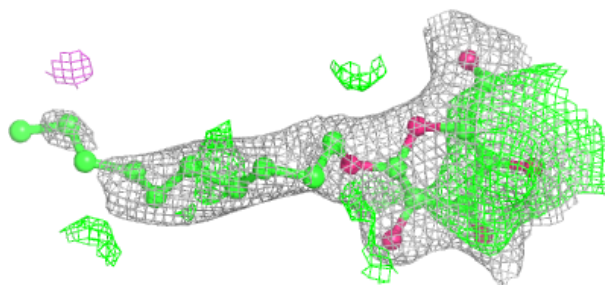
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



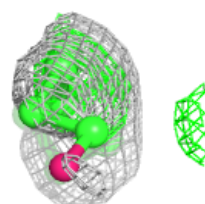
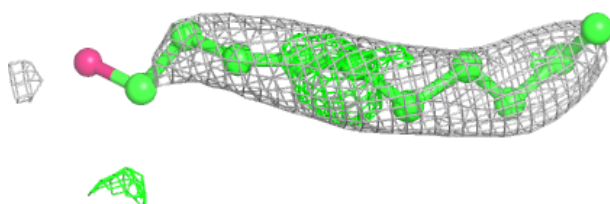
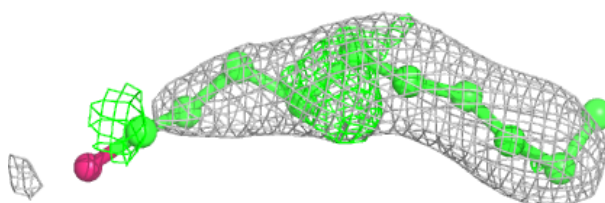


**Electron density around DMU G 102:**

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

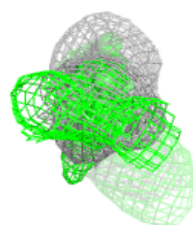
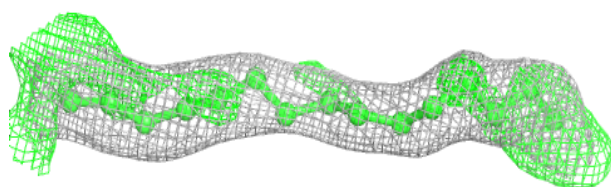
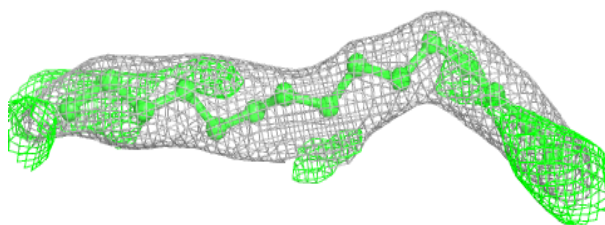
**Electron density around DMU J 101:**

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

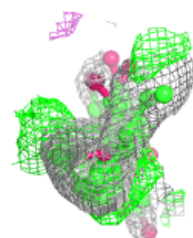
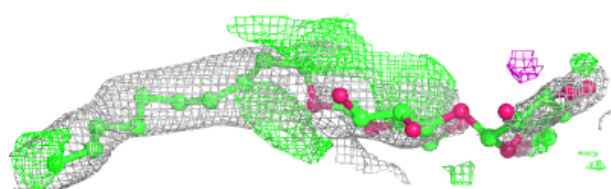
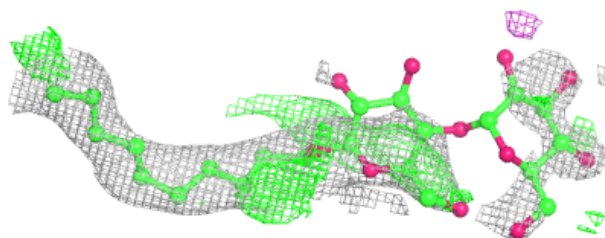


**Electron density around LFA P 313:**

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

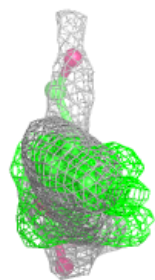
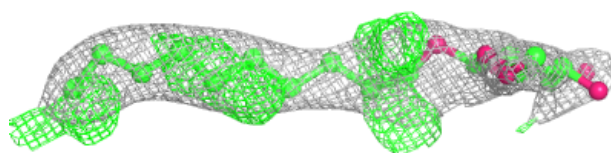
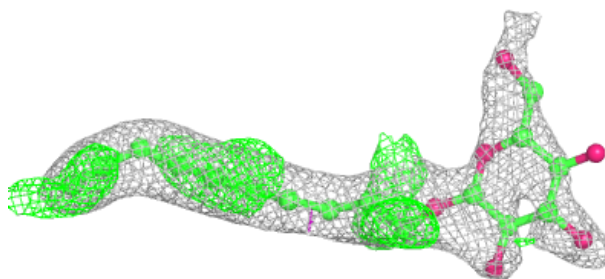
**Electron density around DMU U 101:**

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



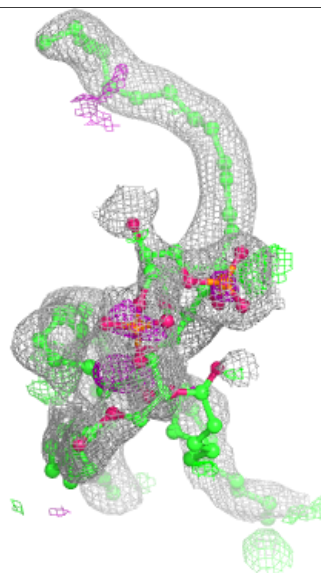
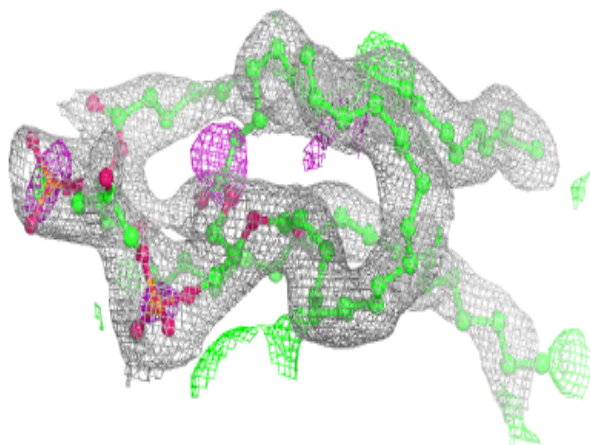
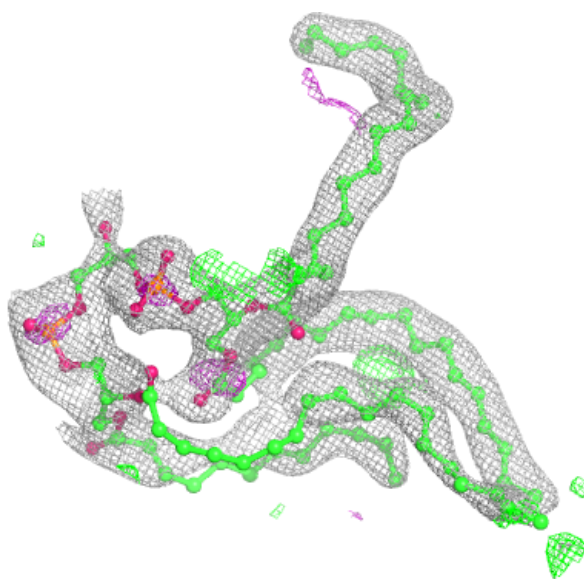
**Electron density around DMU B 305:**

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



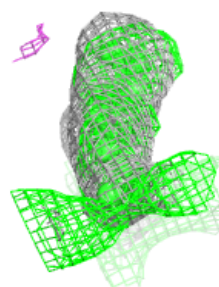
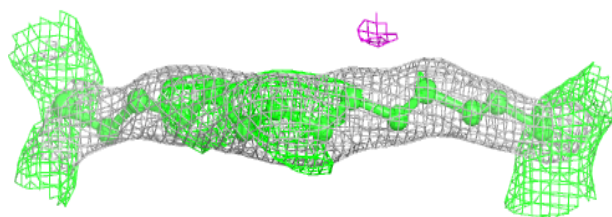
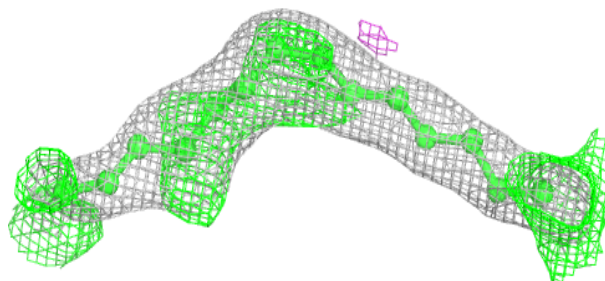
**Electron density around CDL L 101:**

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

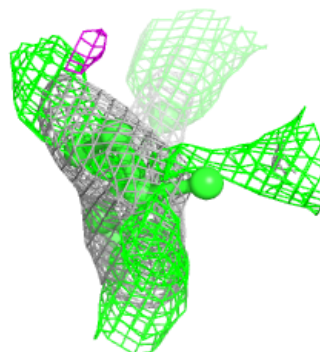
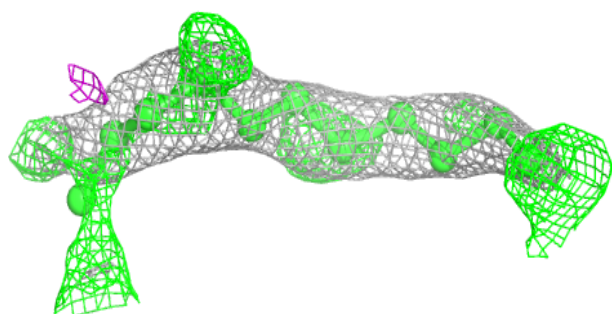
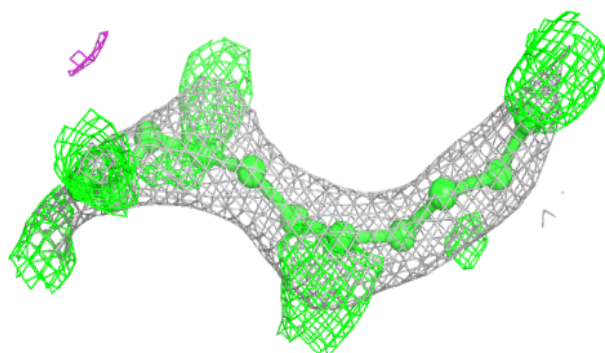


**Electron density around LFA N 608:**

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

**Electron density around LFA C 307:**

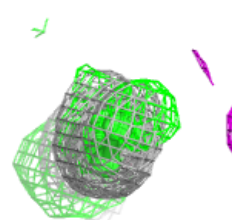
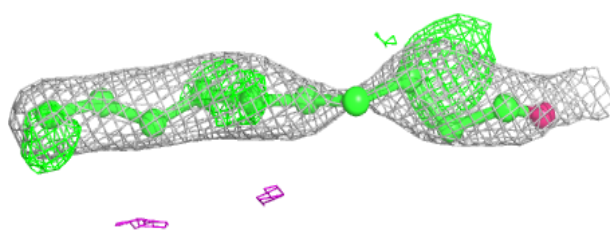
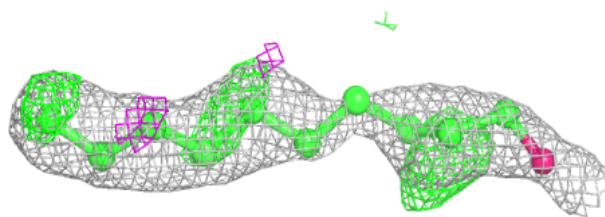
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



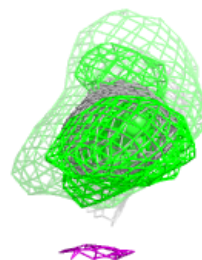
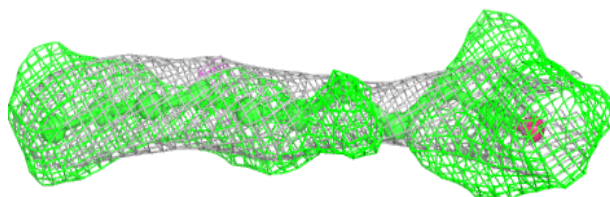
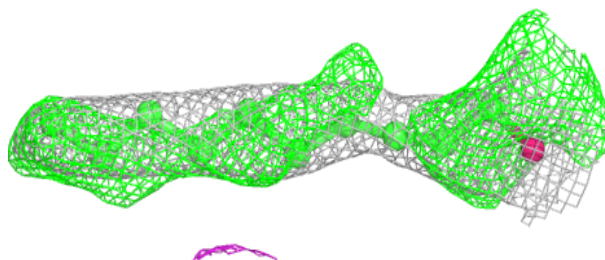


**Electron density around DMU B 304:**

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

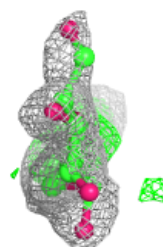
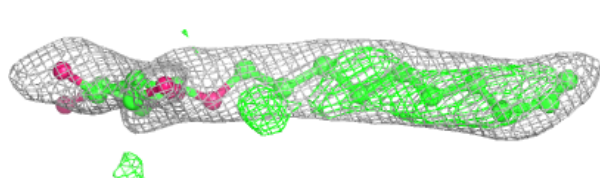
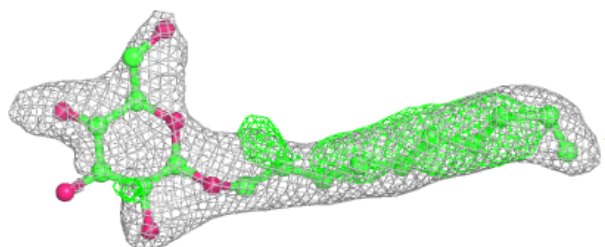
**Electron density around DMU O 307:**

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

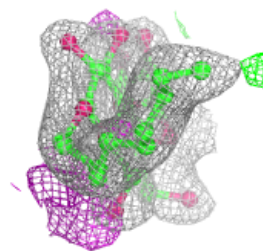
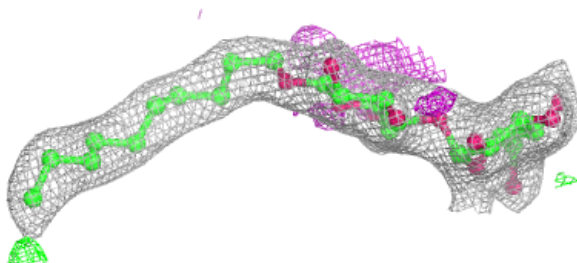
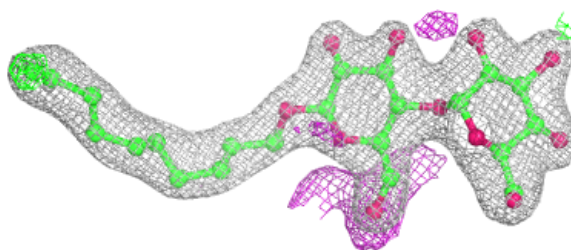


**Electron density around DMU O 309:**

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

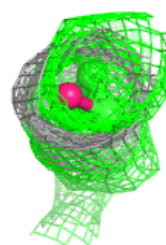
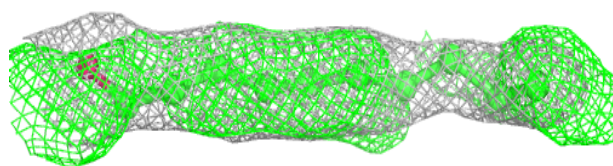
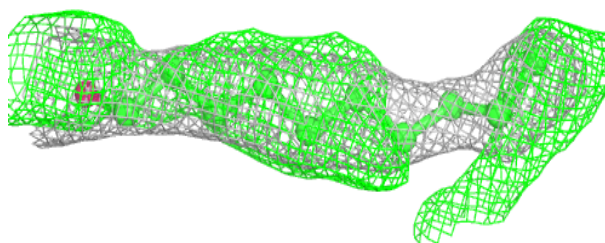
**Electron density around DMU Z 101:**

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

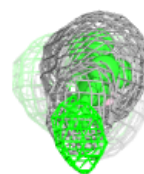
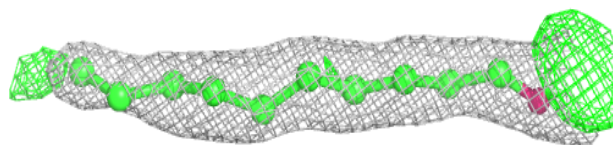
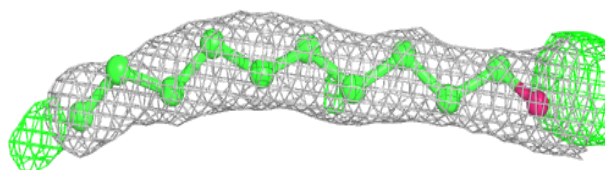


**Electron density around DMU P 307:**

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

**Electron density around DMU C 306:**

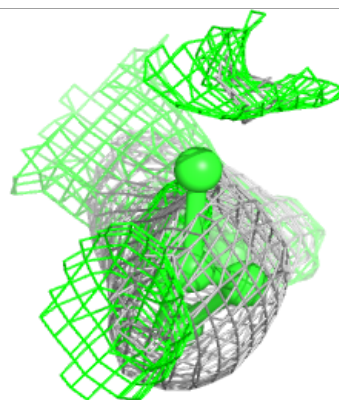
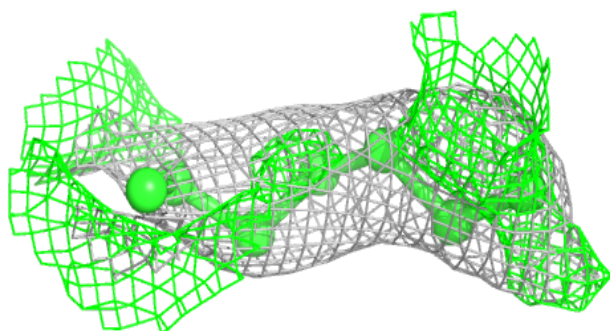
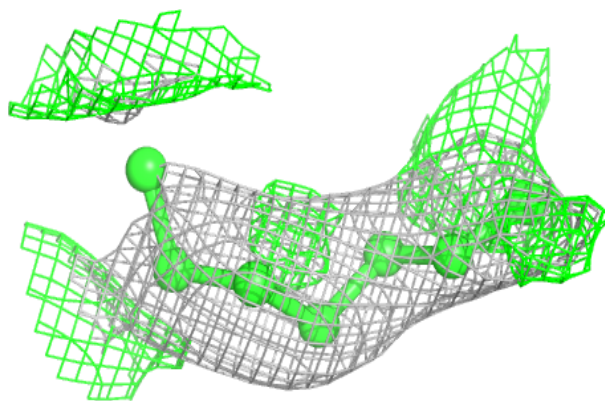
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



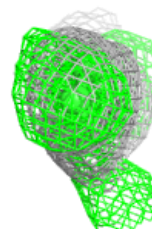
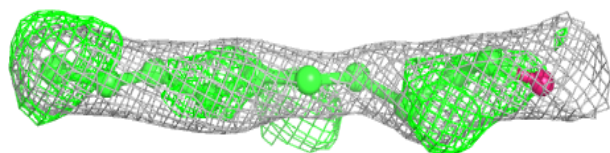
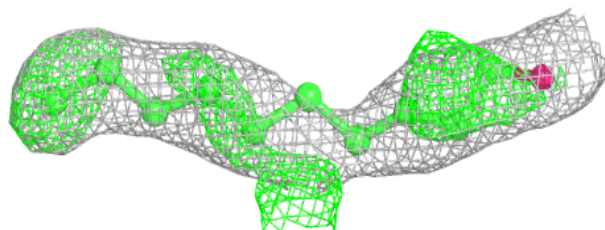


**Electron density around DMU P 316:**

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

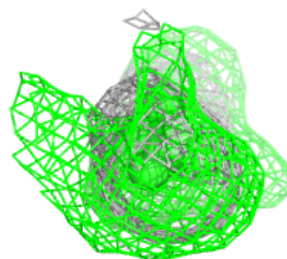
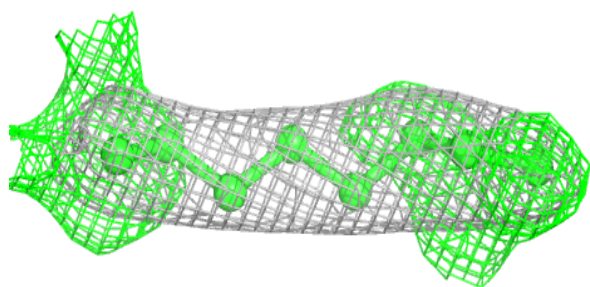
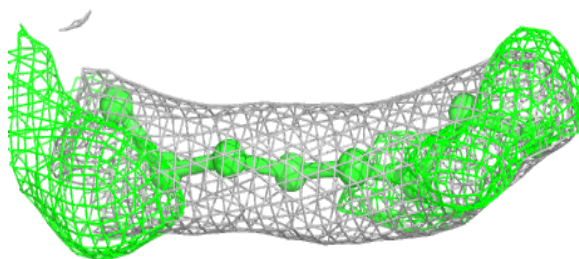
**Electron density around DMU O 308:**

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

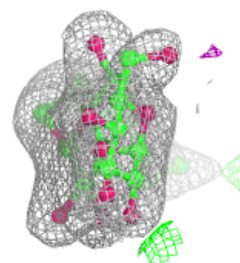
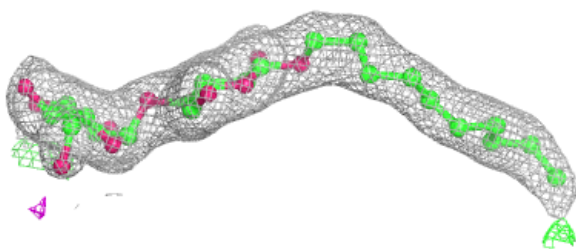
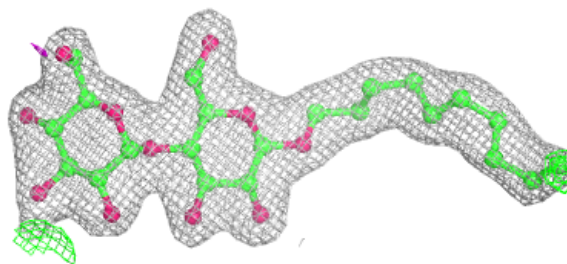


**Electron density around DMU Z 102:**

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

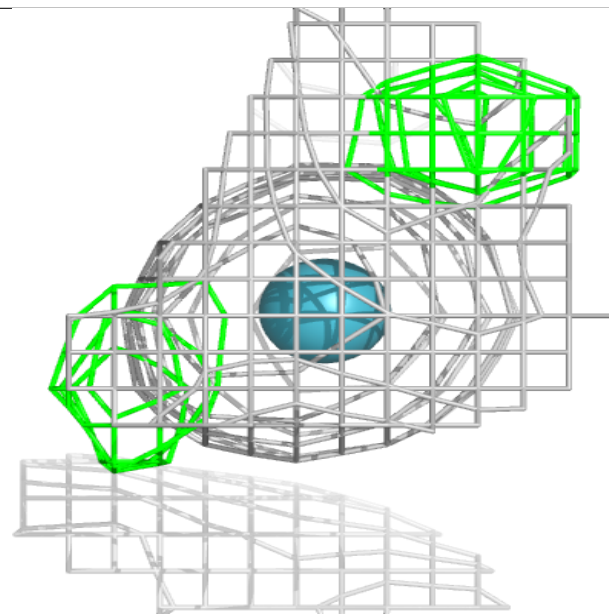
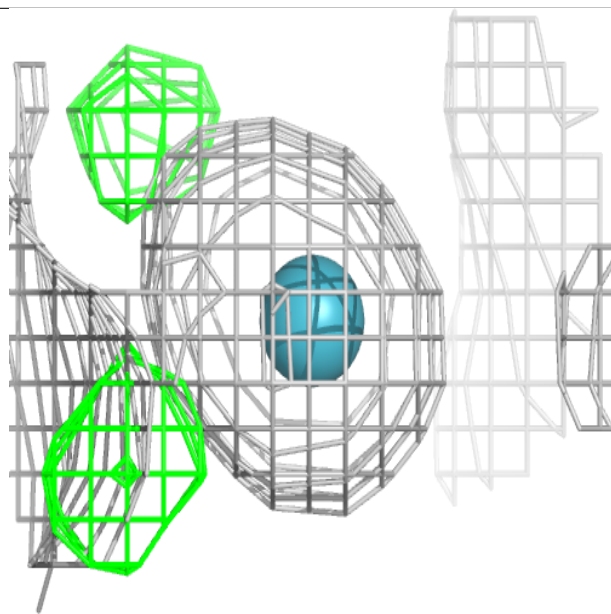
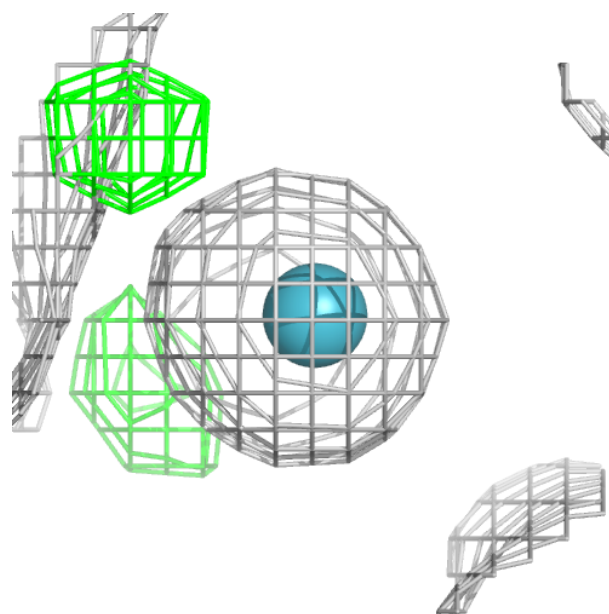
**Electron density around DMU M 101:**

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



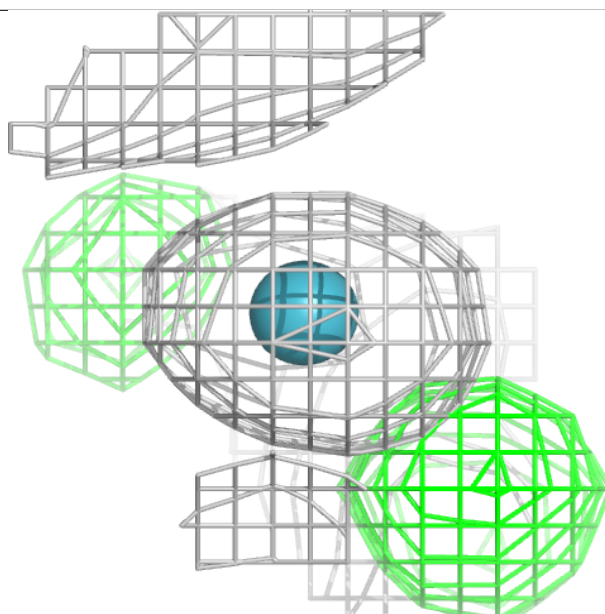
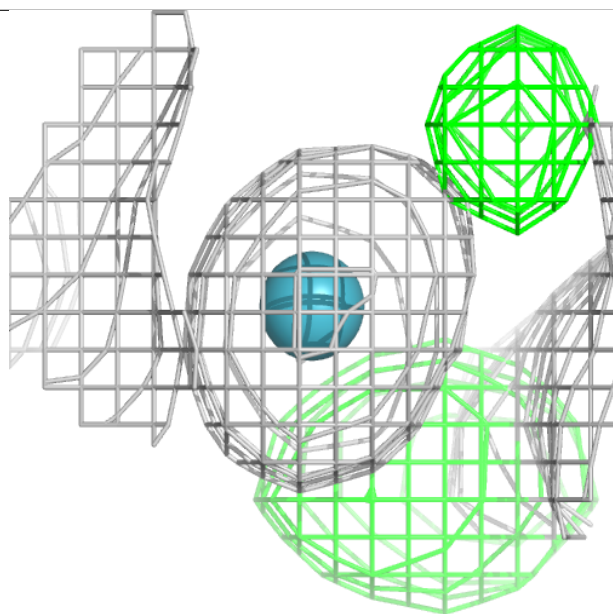
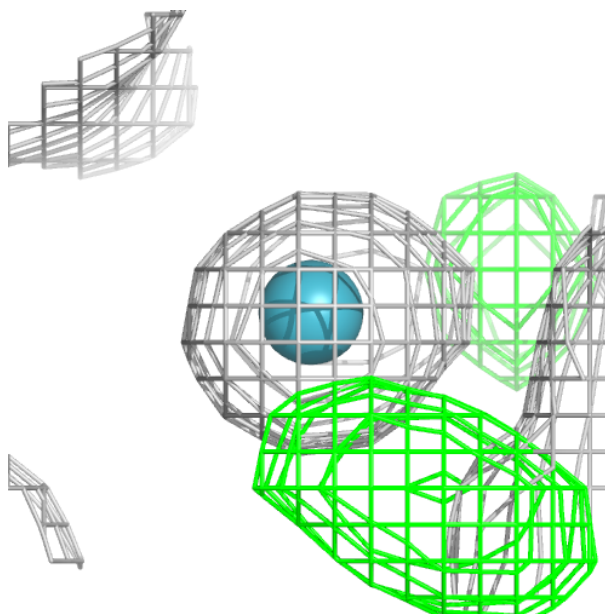
**Electron density around XE A 618:**

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



**Electron density around XE N 621:**

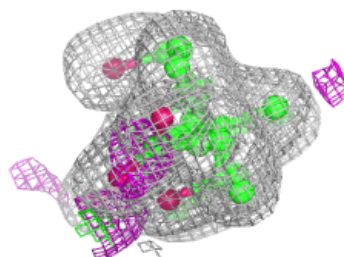
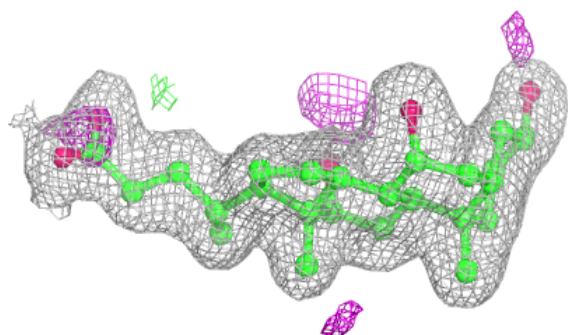
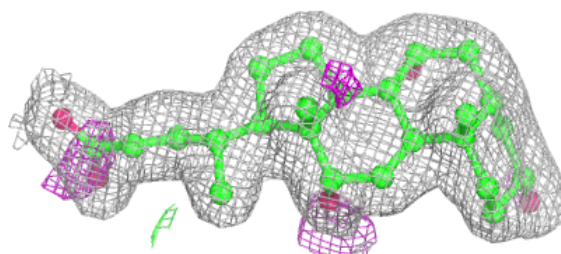
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



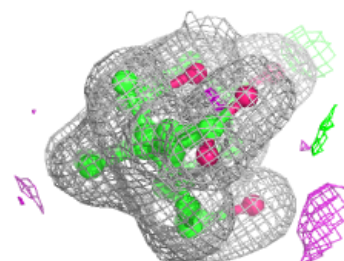
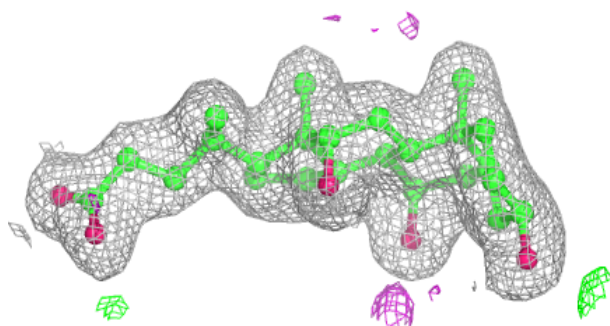
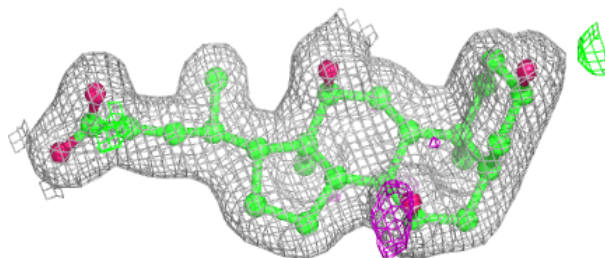


**Electron density around CHD C 301:**

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

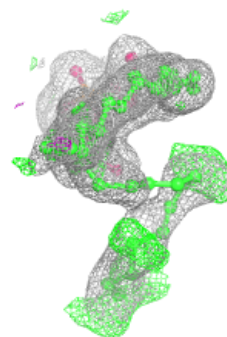
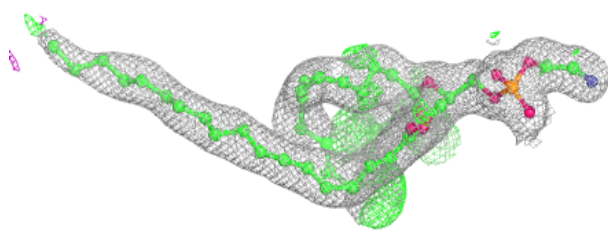
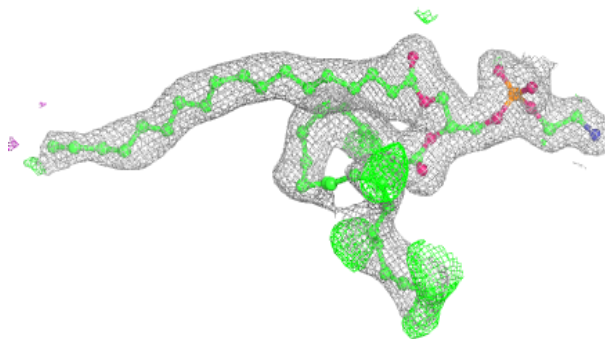
**Electron density around CHD P 302:**

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

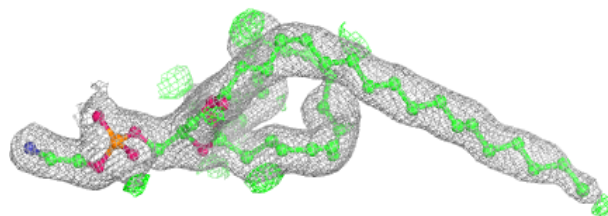
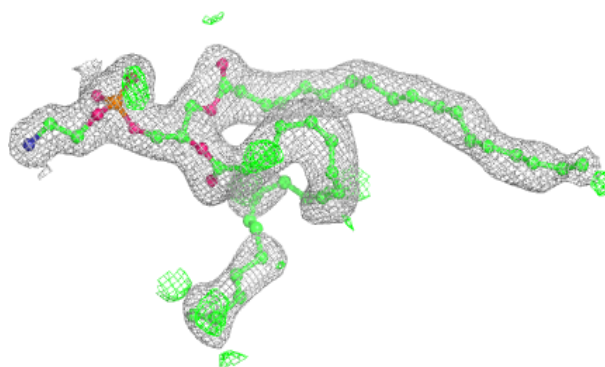


**Electron density around PEK G 101:**

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

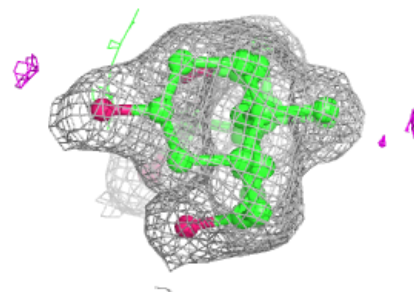
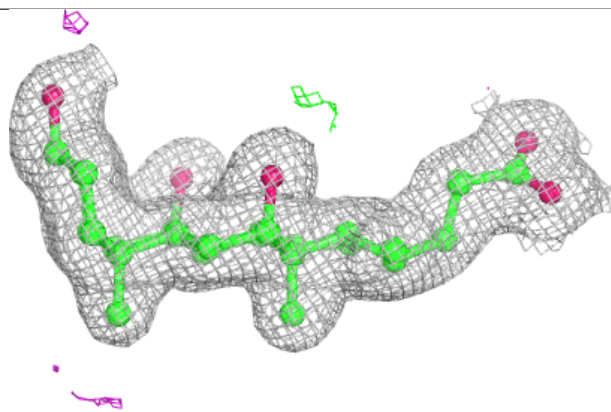
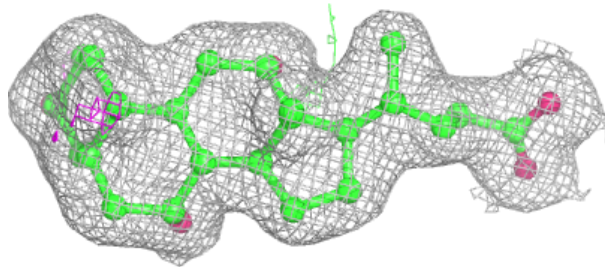
**Electron density around PEK T 102:**

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

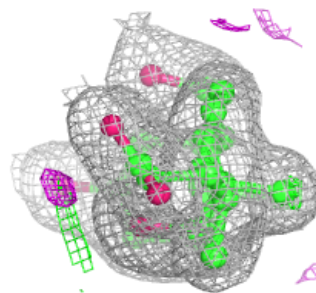
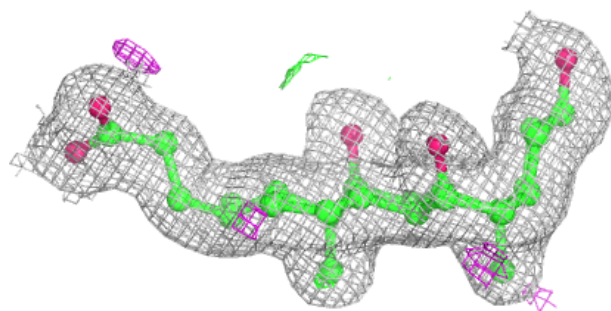
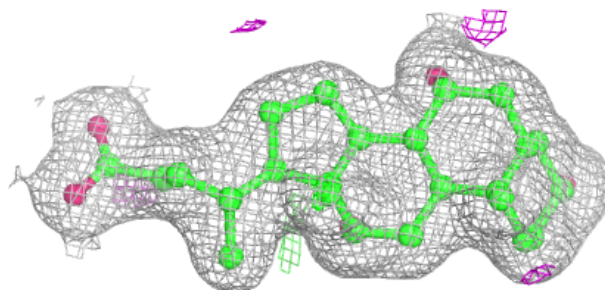


**Electron density around CHD B 307:**

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

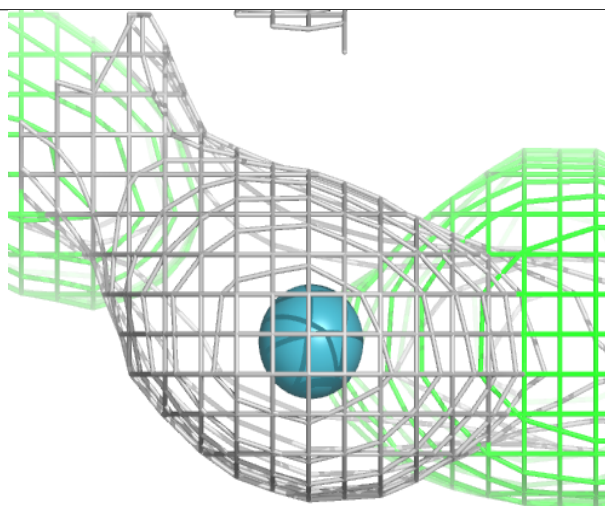
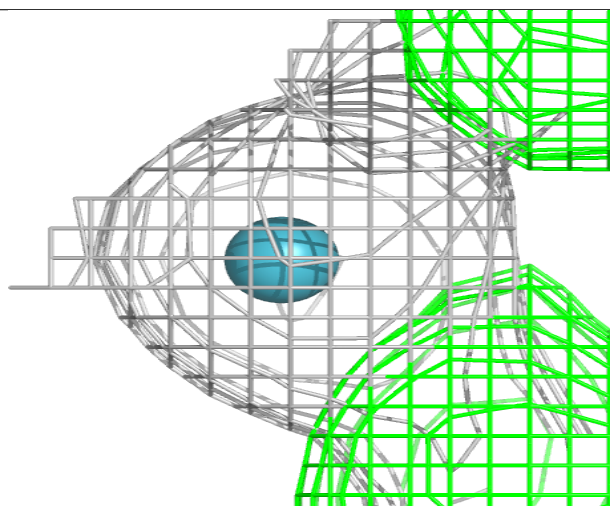
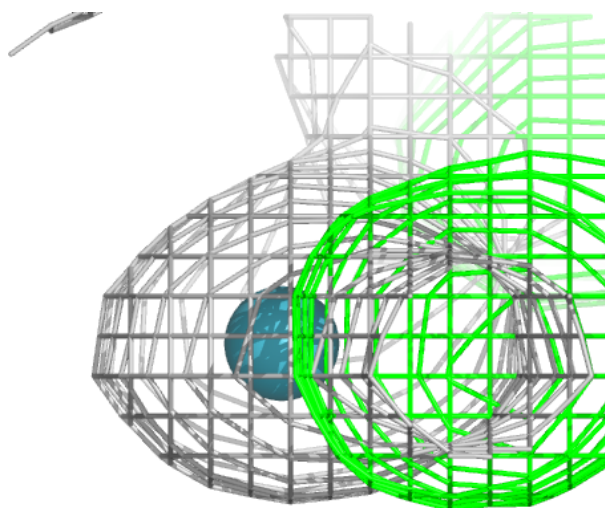
**Electron density around CHD O 301:**

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



**Electron density around XE N 618:**

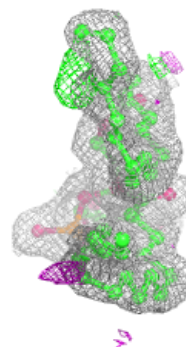
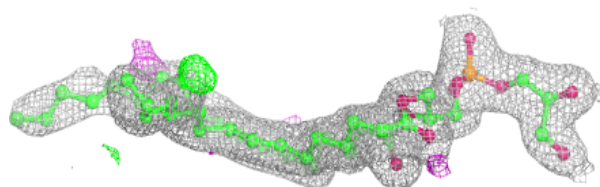
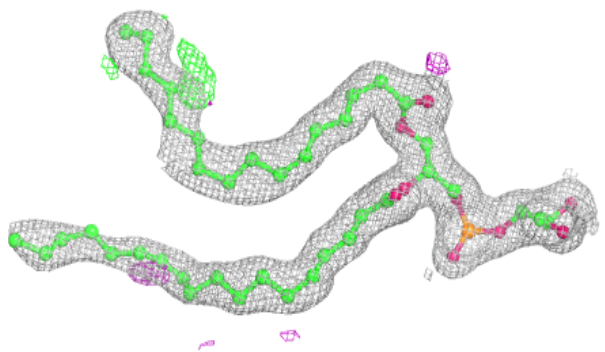
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



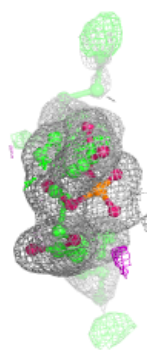
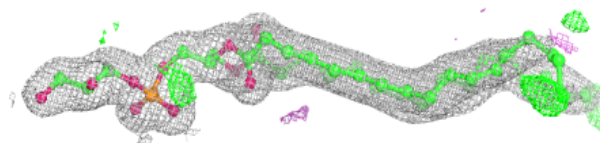
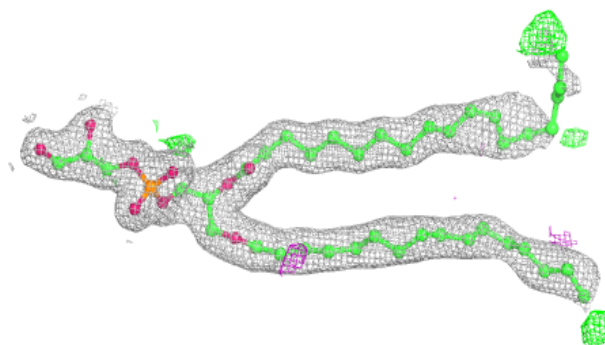


**Electron density around PGV A 619:**

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

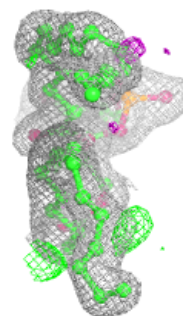
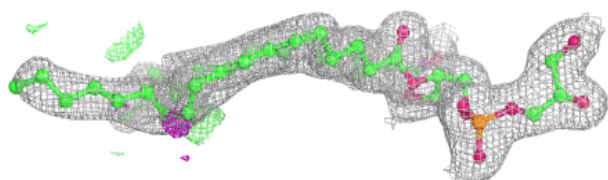
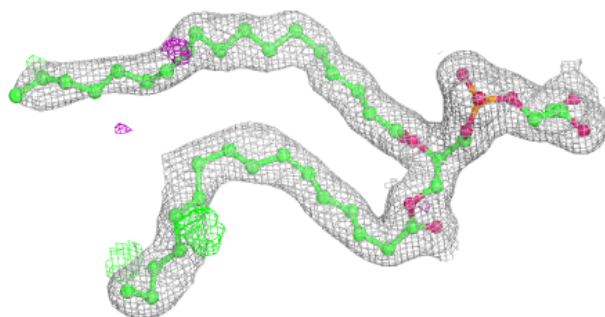
**Electron density around PGV C 303:**

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



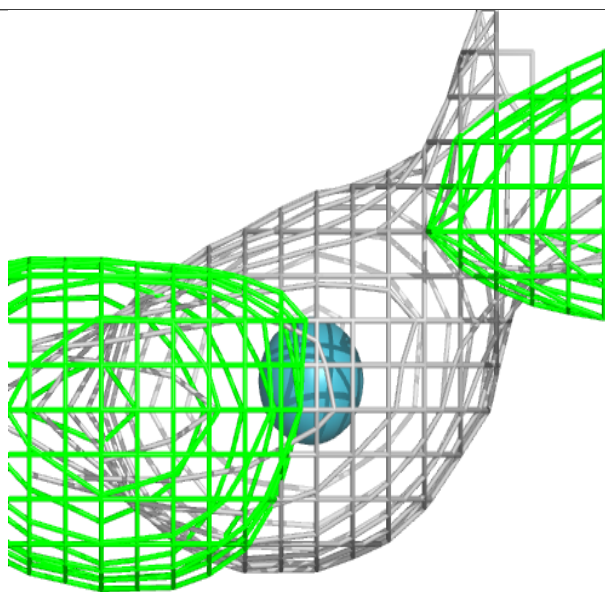
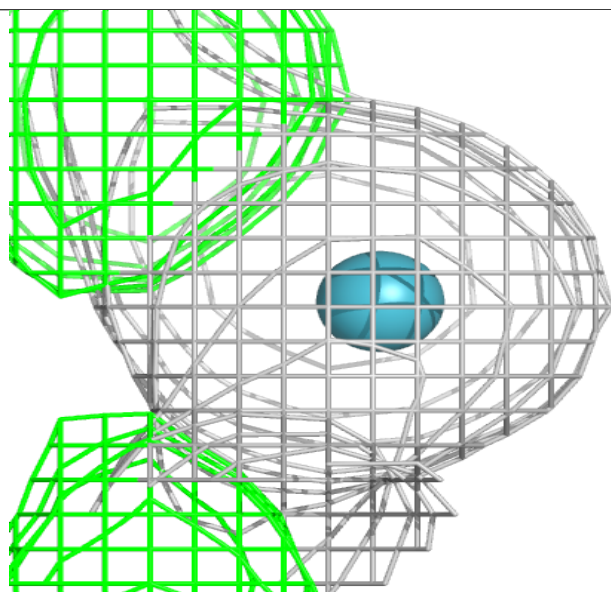
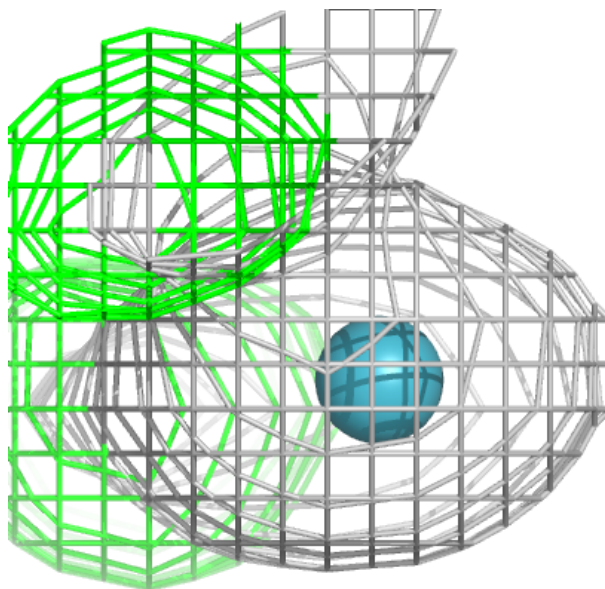
**Electron density around PGV N 622:**

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



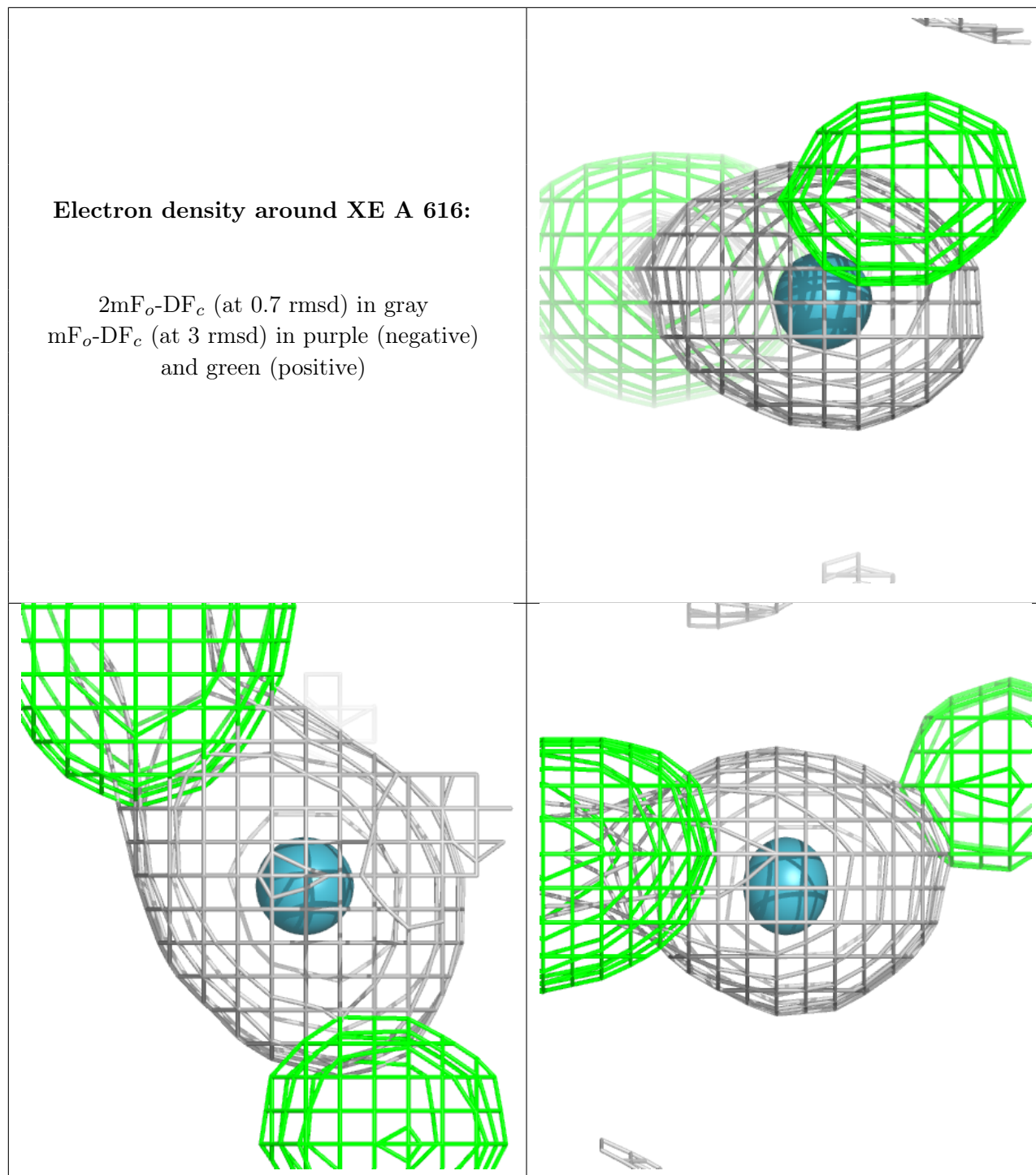
**Electron density around XE A 615:**

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



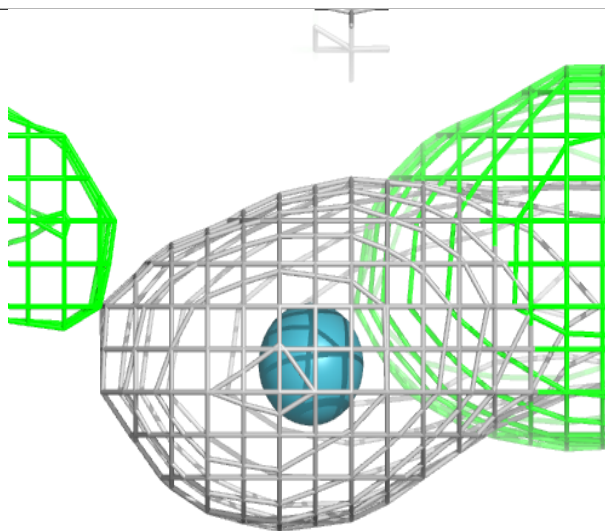
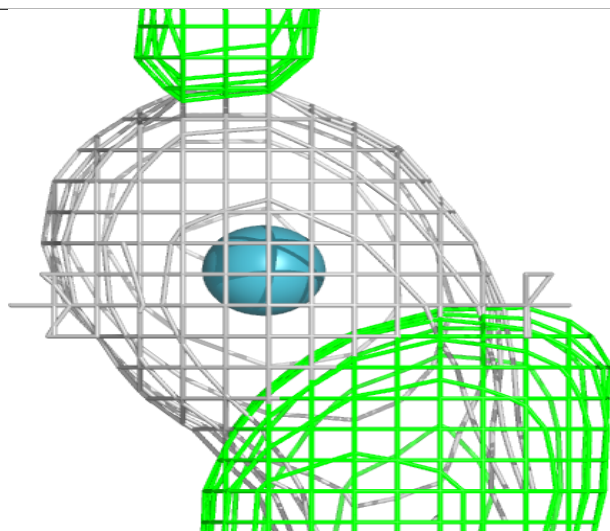
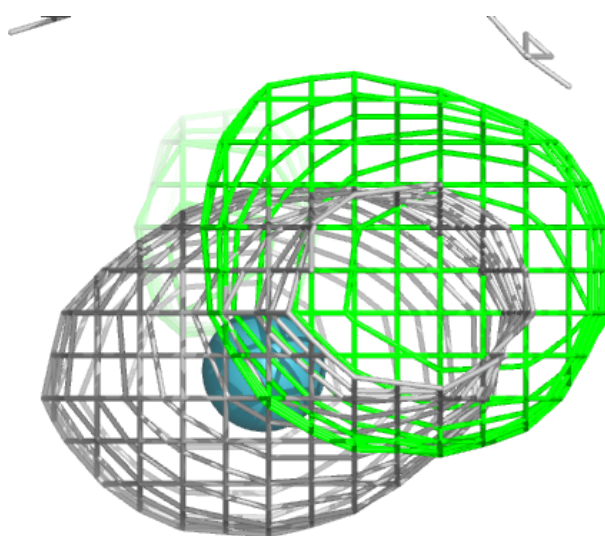
**Electron density around XE A 616:**

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



**Electron density around XE N 619:**

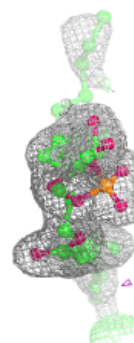
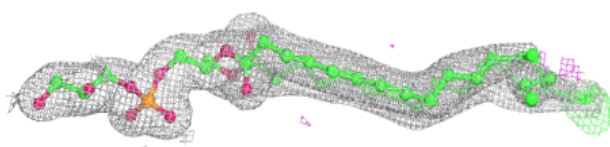
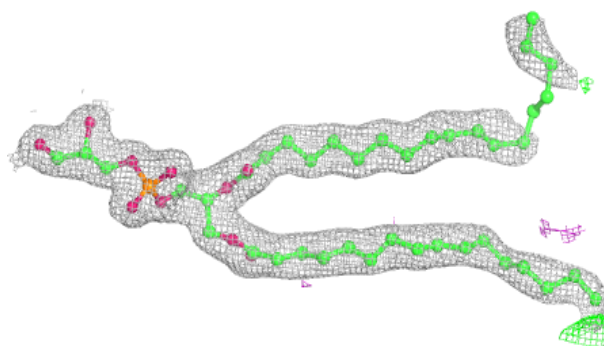
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



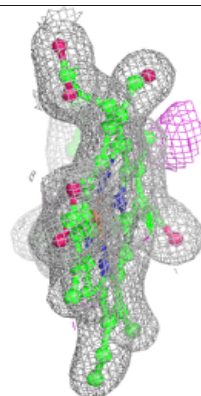
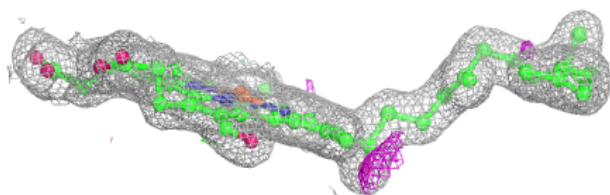
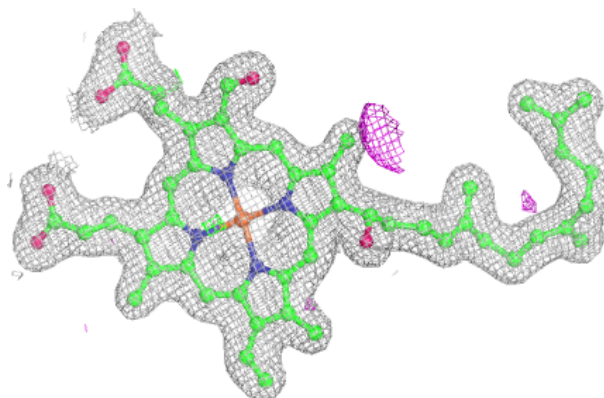


**Electron density around PGV P 304:**

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

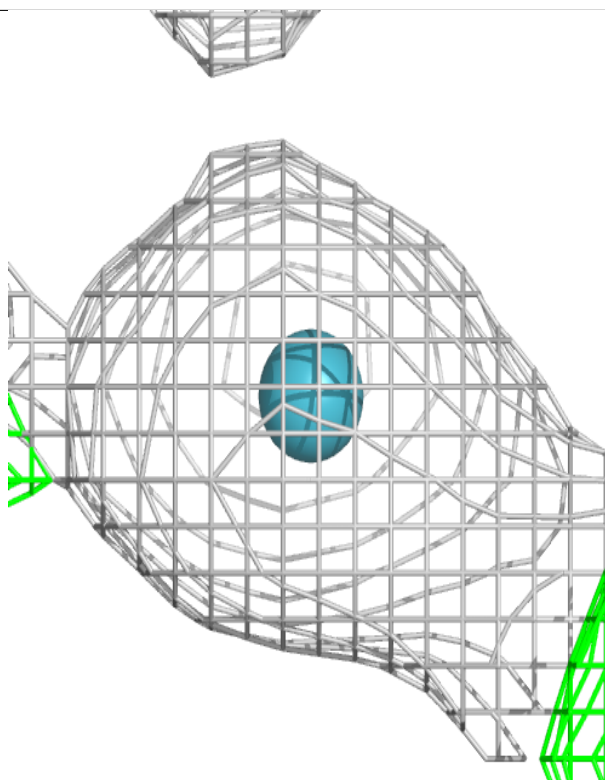
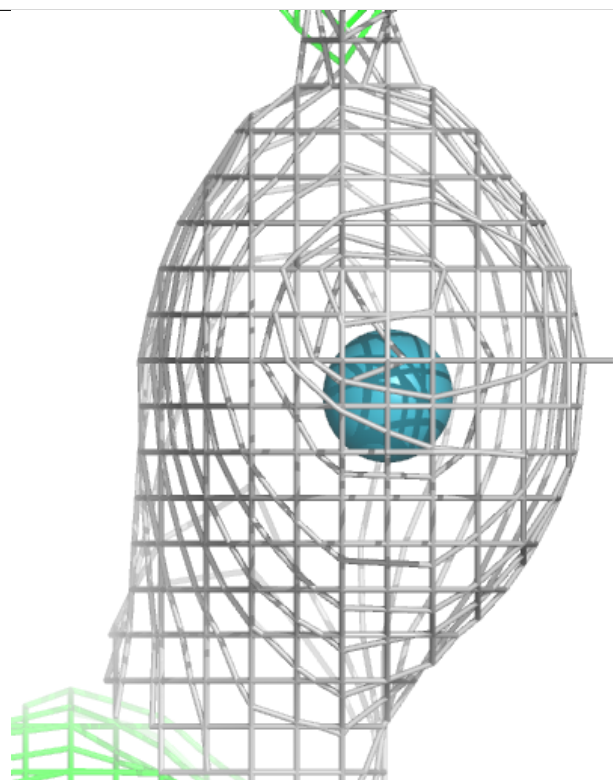
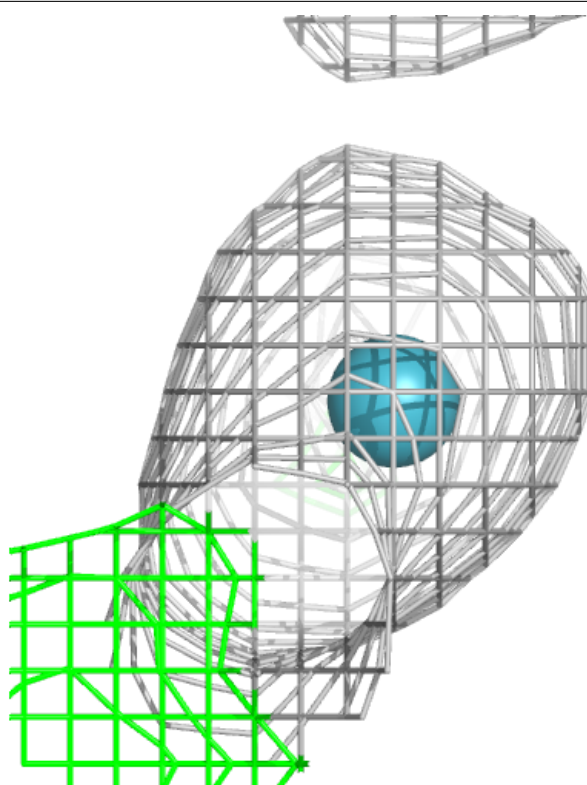
**Electron density around HEA A 602:**

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



**Electron density around XE C 324:**

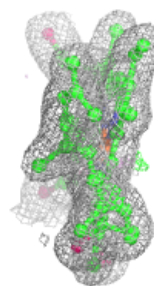
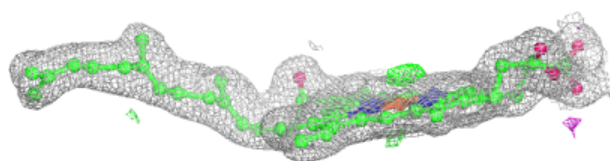
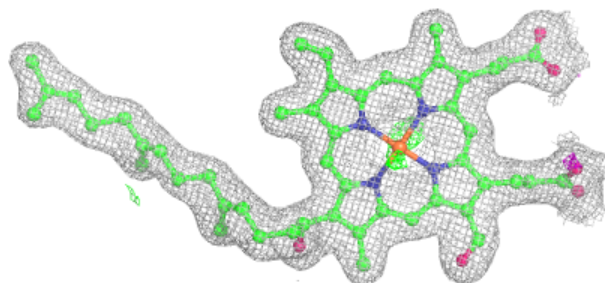
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



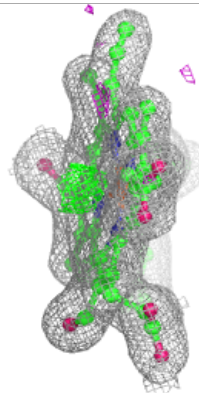
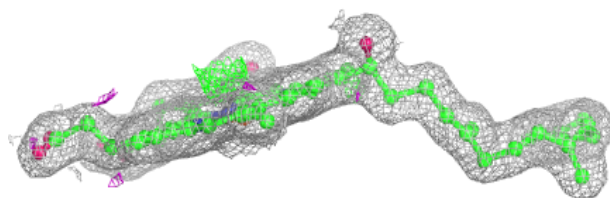
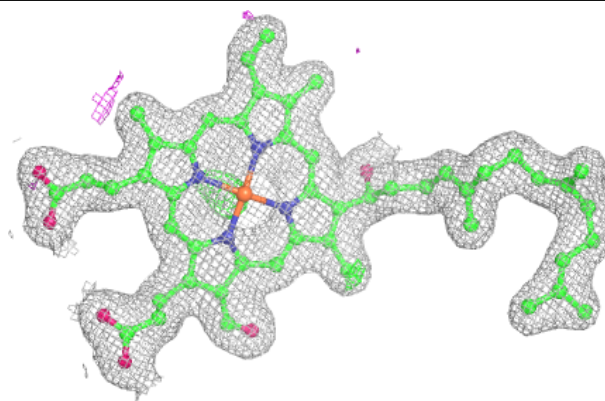


**Electron density around HEA N 602:**

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

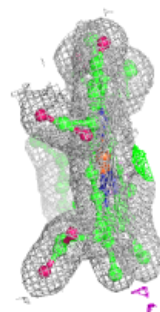
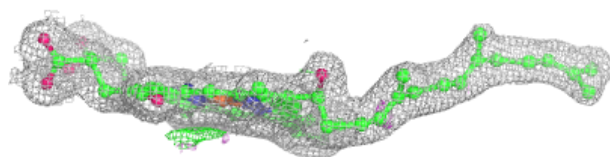
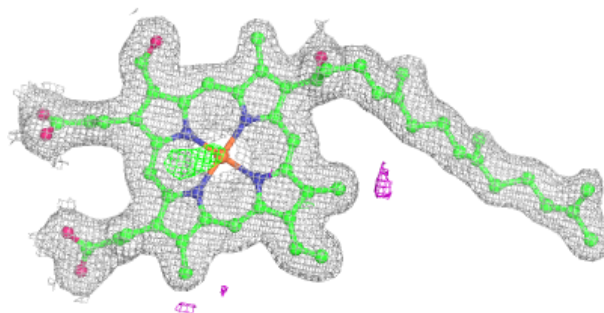
**Electron density around HEA N 603:**

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



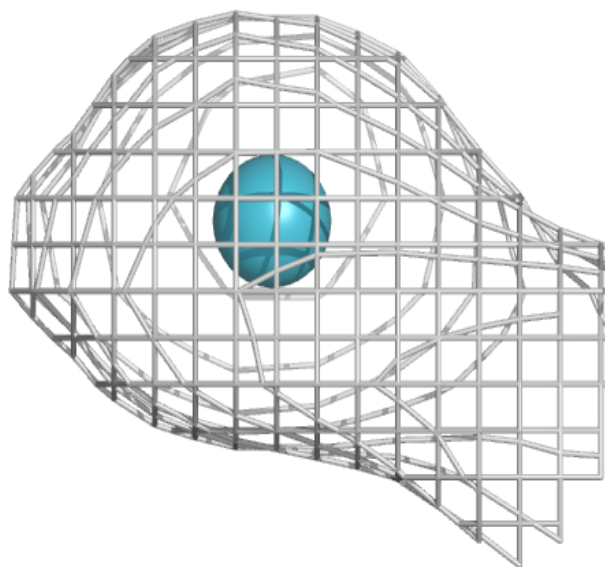
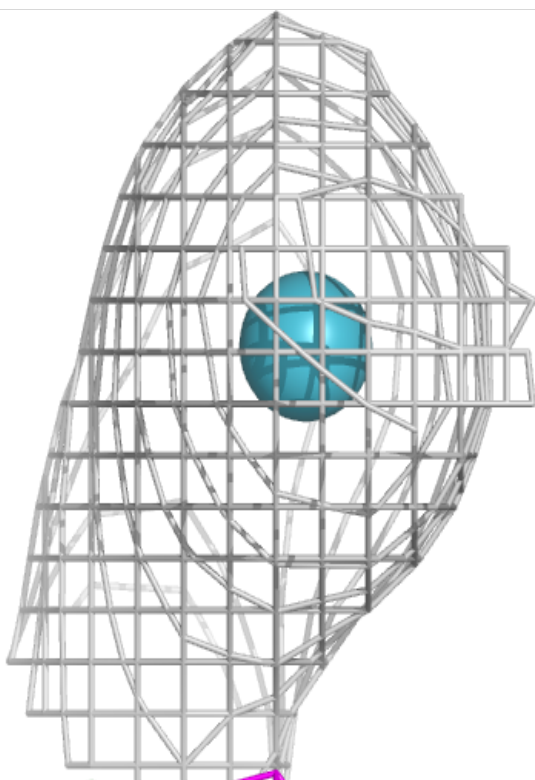
**Electron density around HEA A 601:**

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



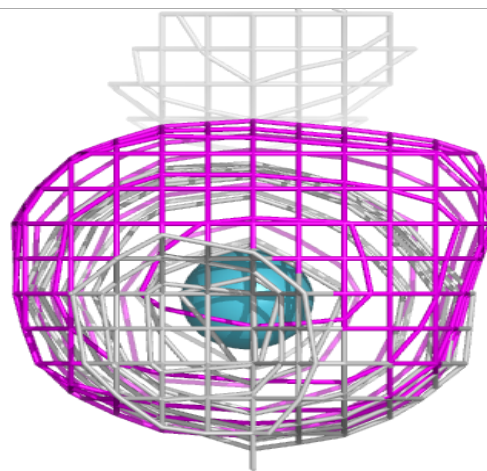
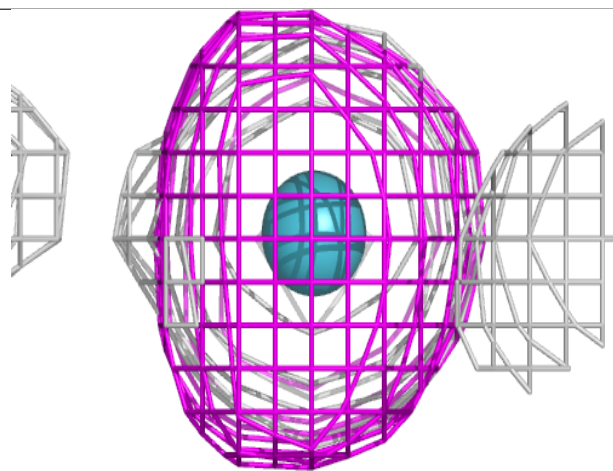
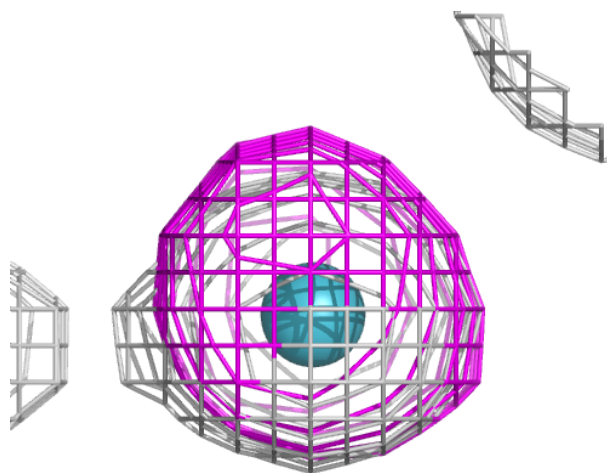
**Electron density around XE P 324:**

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



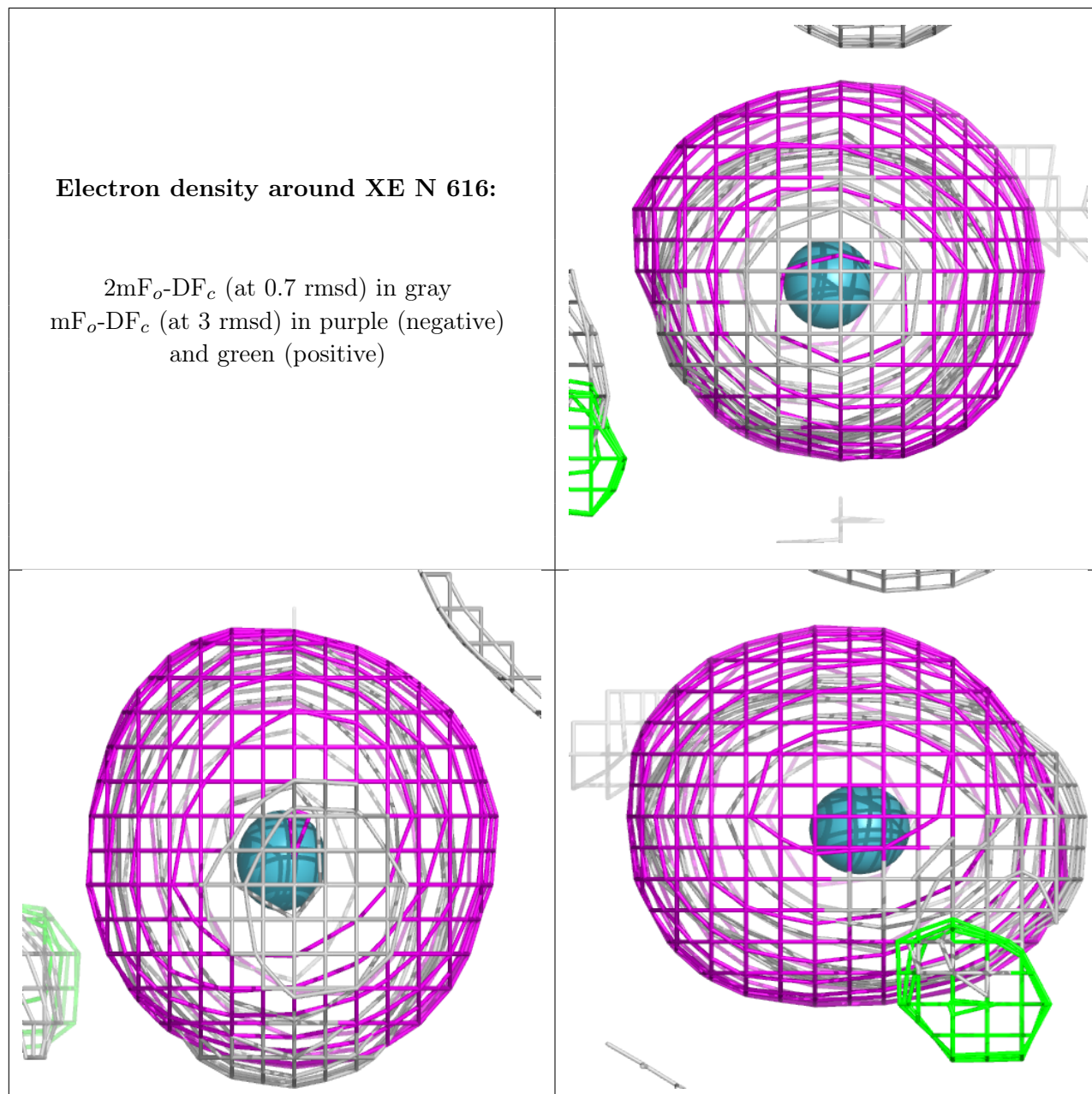
**Electron density around XE B 301:**

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



**Electron density around XE N 616:**

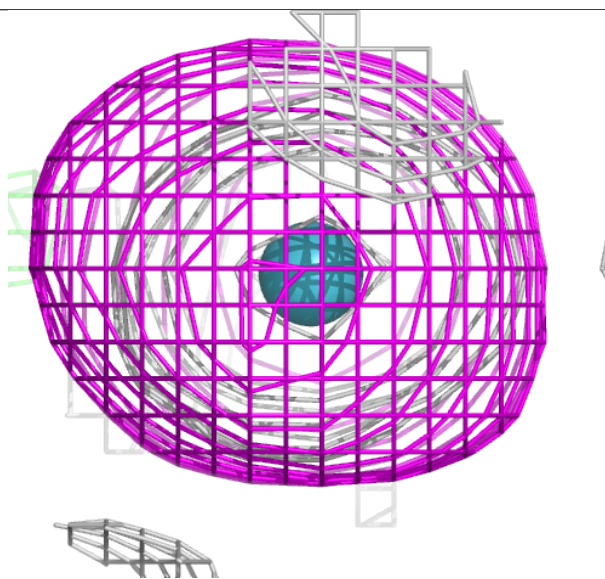
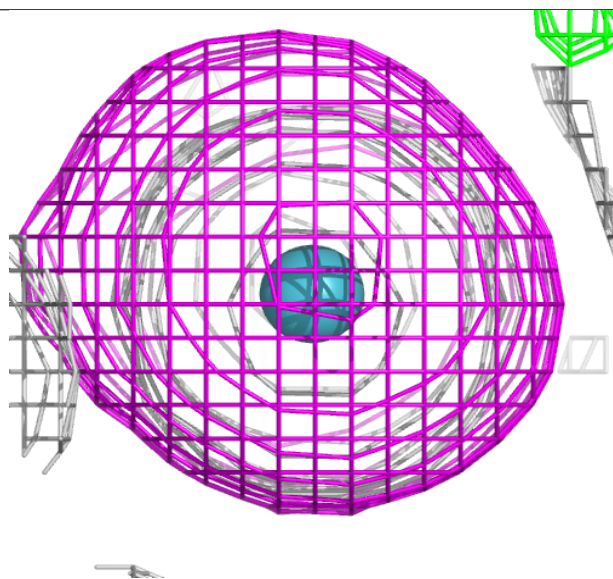
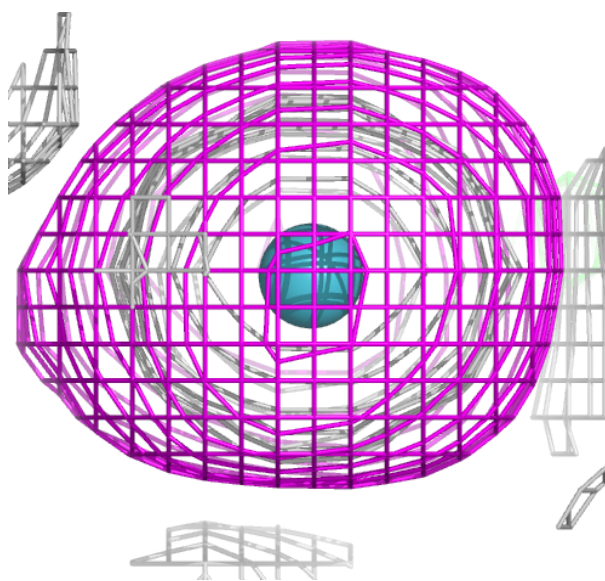
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





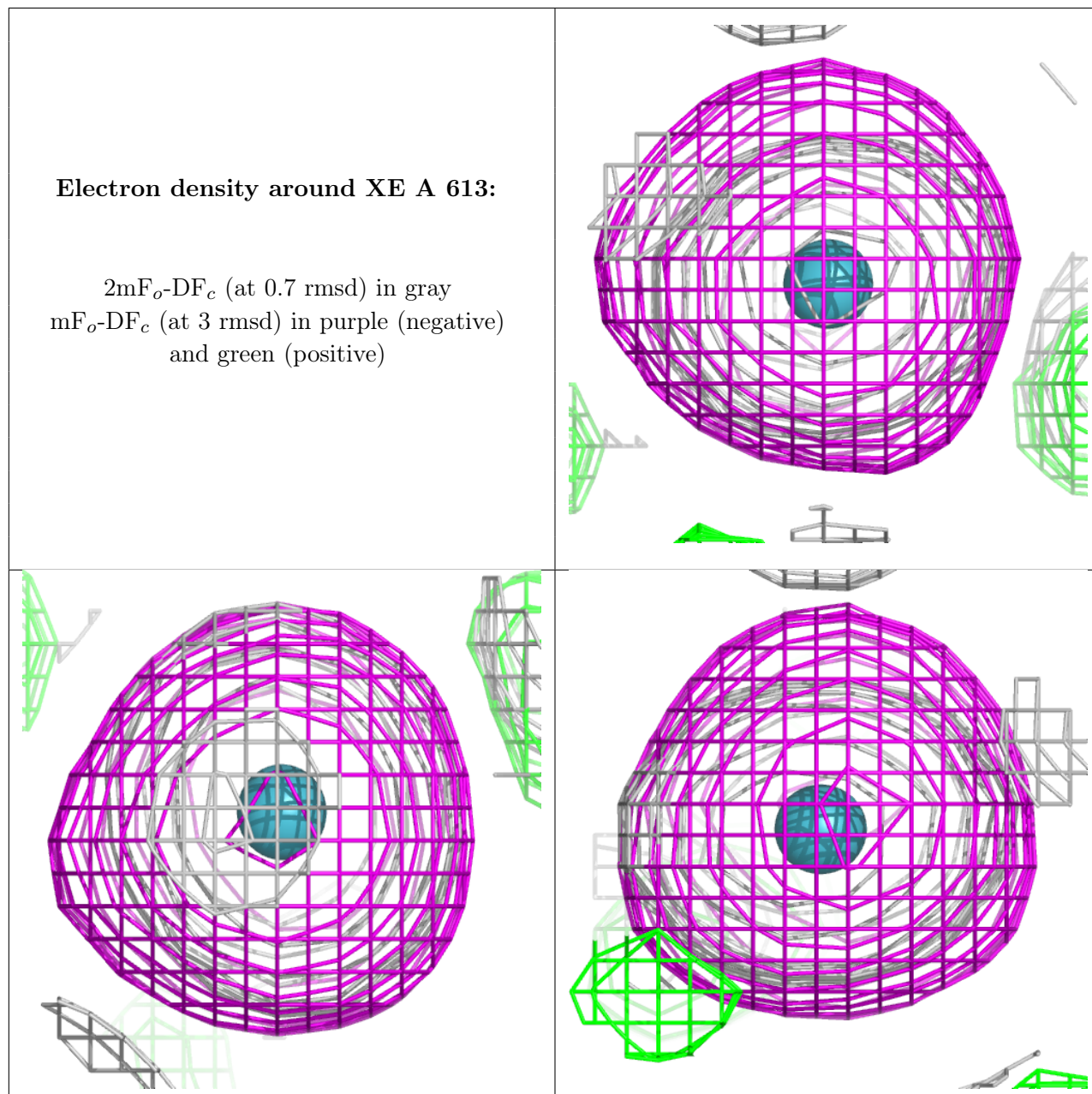
**Electron density around XE N 617:**

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



**Electron density around XE A 613:**

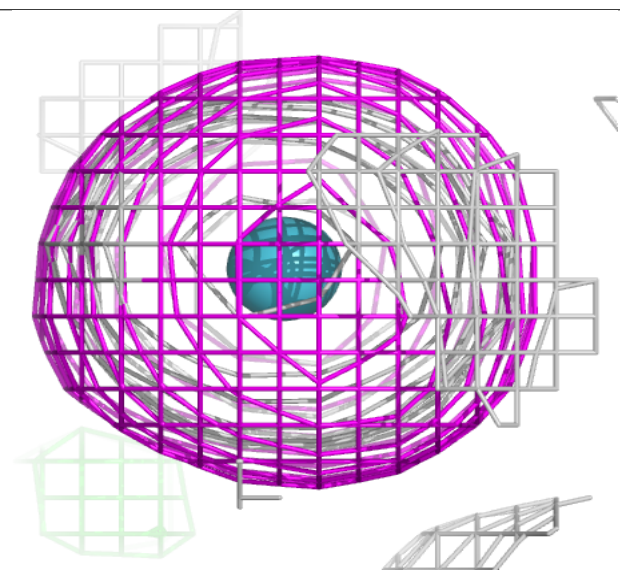
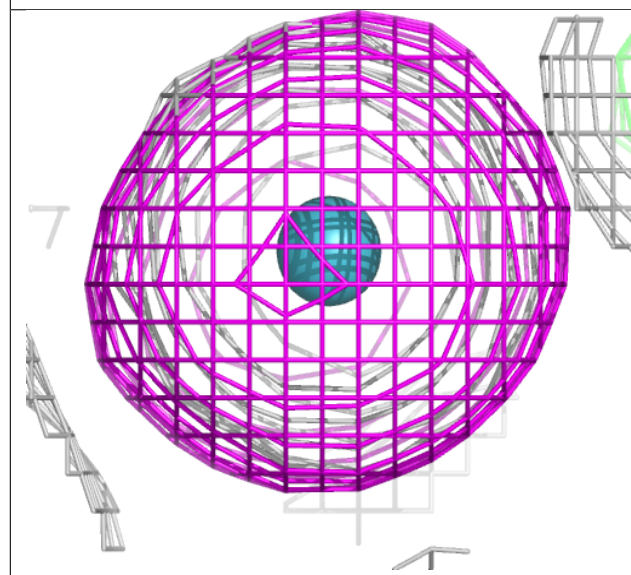
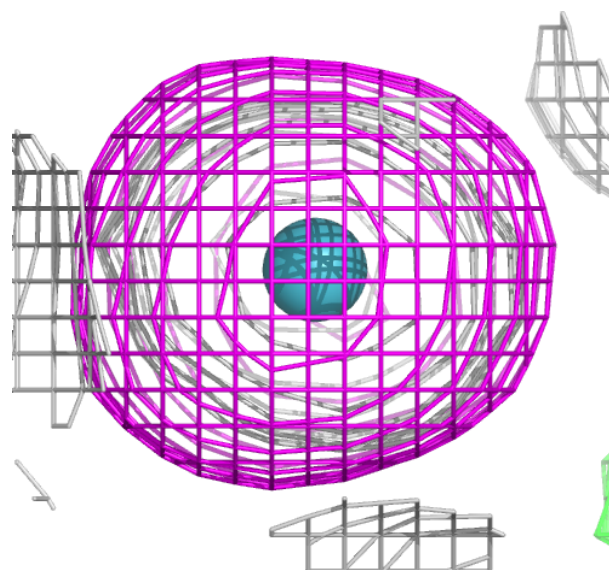
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





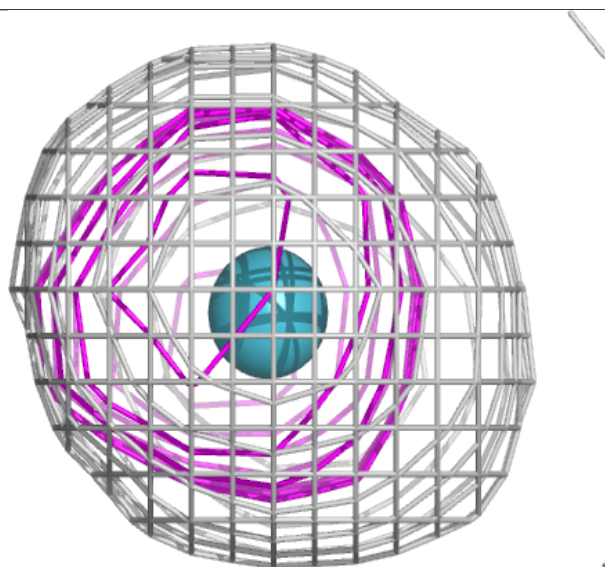
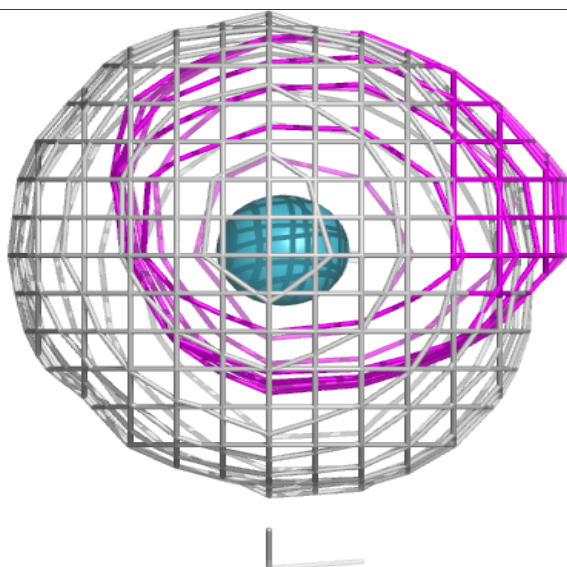
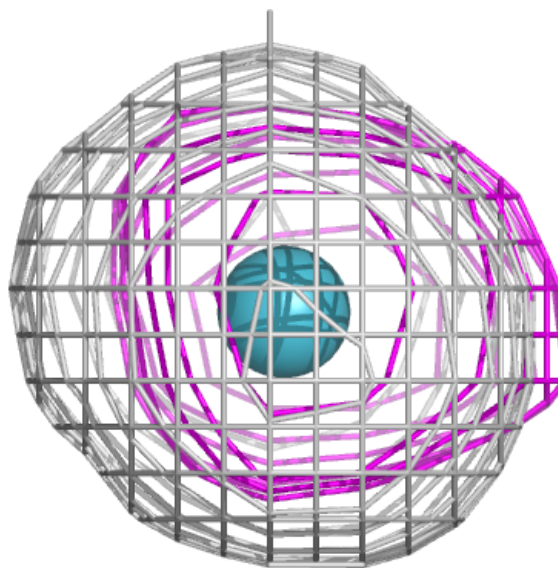
**Electron density around XE A 614:**

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



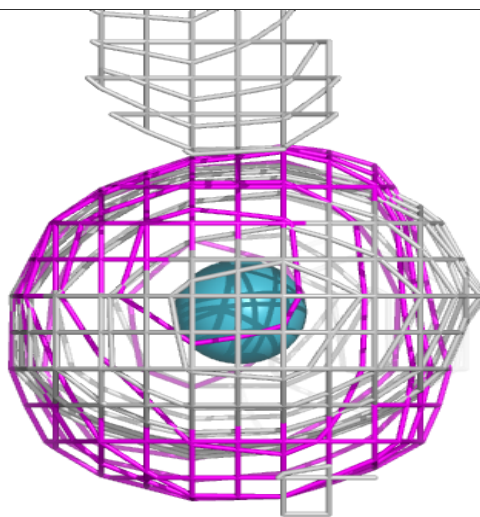
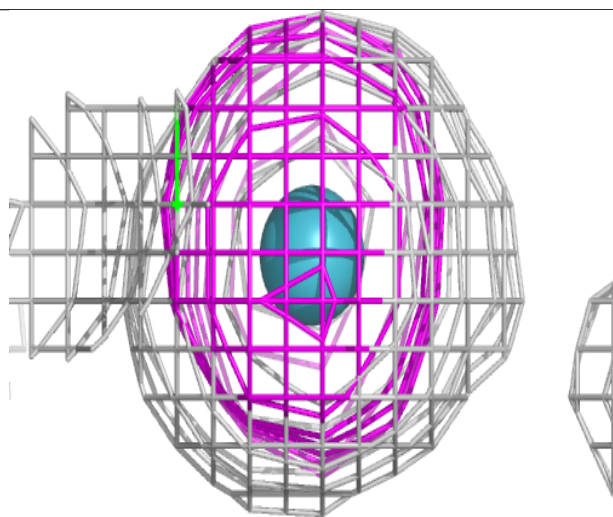
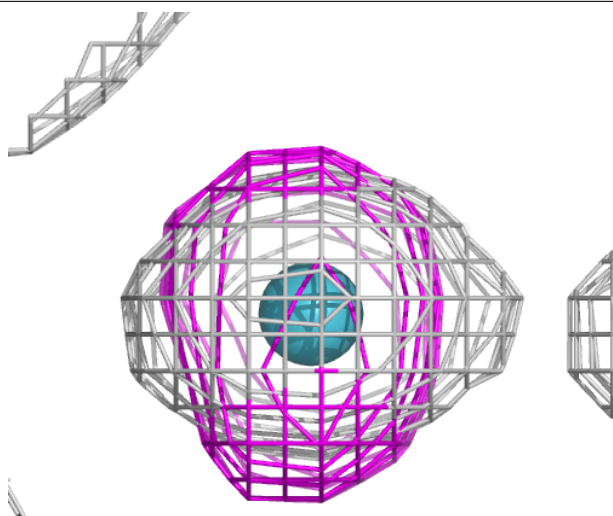
**Electron density around XE N 620:**

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



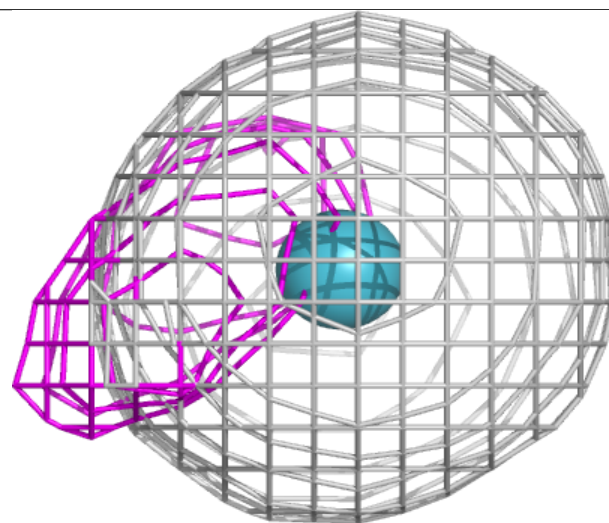
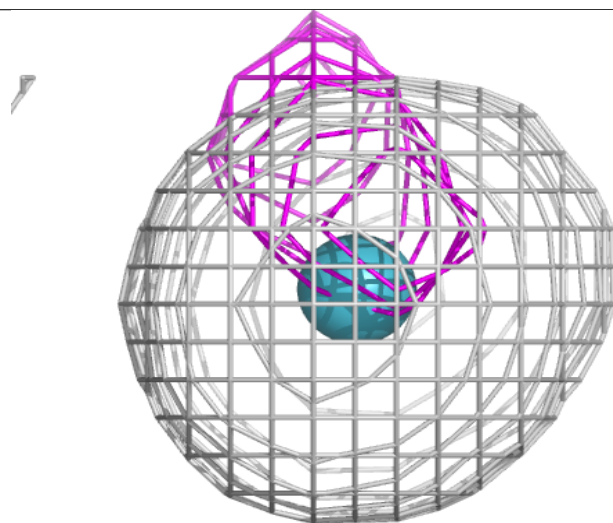
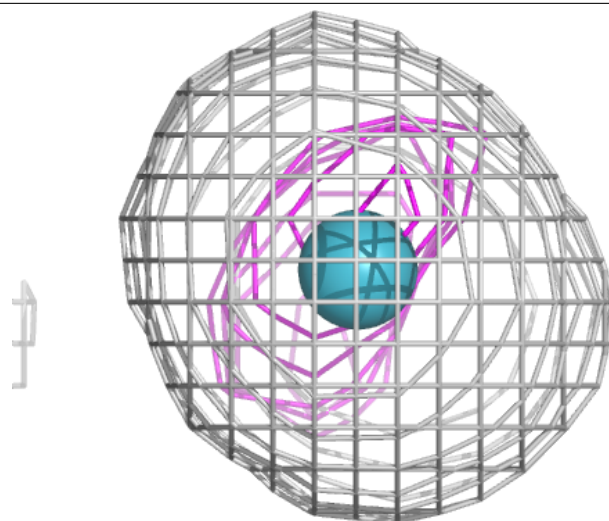
**Electron density around XE O 305:**

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



**Electron density around XE A 617:**

$2mF_o-DF_c$  (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.