



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2025 – 01:12 PM JST

PDB ID : 9IKF / pdb\_00009ikf  
Title : Bovine Heart Cytochrome c Oxidase in the Carbon Dioxide-bound Fully Oxidized State  
Authors : Muramoto, K.; Shinzawa-Itoh, K.  
Deposited on : 2024-06-27  
Resolution : 1.75 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

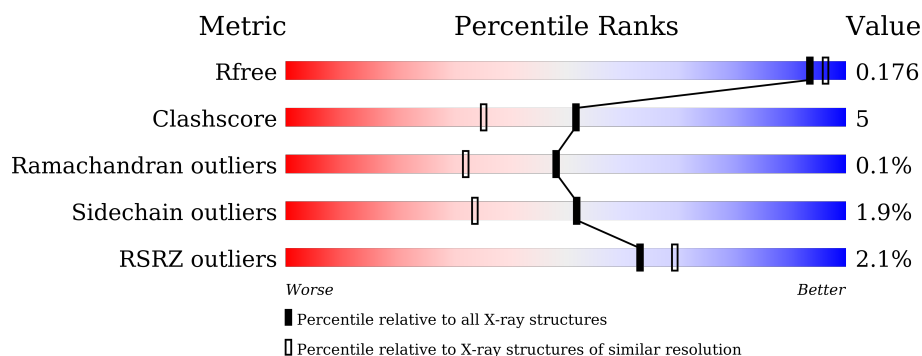
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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></div> <div>92% 7% .</div> </div>
1	N	514	<div> <div></div> <div>91% 9% .</div> </div>
2	B	227	<div> <div>5%</div> <div>81% 17% .</div> </div>
2	O	227	<div> <div>3%</div> <div>85% 13% .</div> </div>
3	C	261	<div> <div></div> <div>89% 10% .</div> </div>
3	P	261	<div> <div></div> <div>90% 9% .</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	LFA	C	308	-	-	-	X
21	LFA	P	311	-	-	-	X

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33055 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			

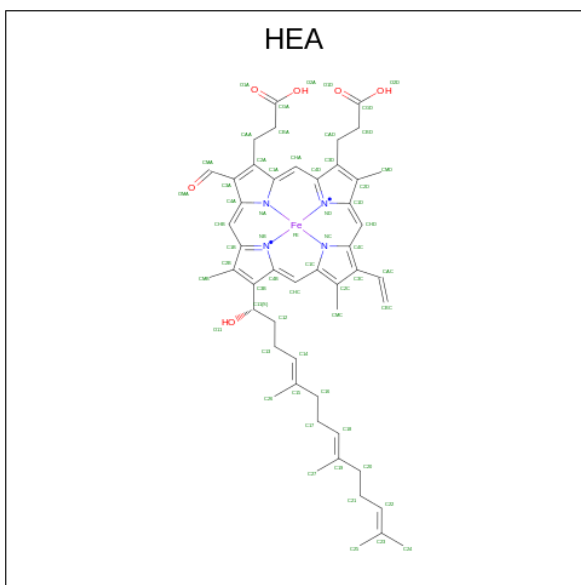
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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	C	Fe	N	O	
			69	58	1	4	6	1
14	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
14	N	1	Total	C	Fe	N	O	
			69	58	1	4	6	1
14	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	0

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

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

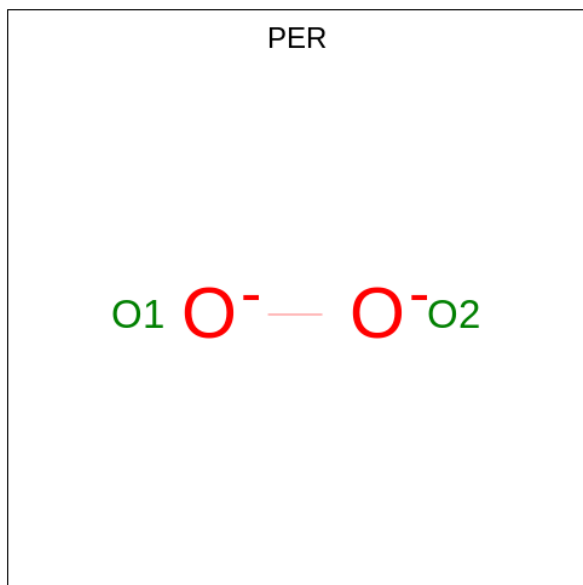
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

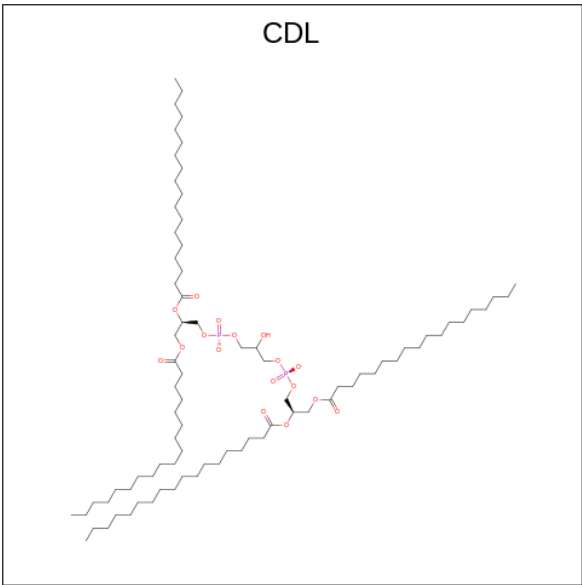
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total 1	Na 1	0	0
17	N	1	Total 1	Na 1	0	0

- Molecule 18 is PEROXIDE ION (CCD ID: PER) (formula: O<sub>2</sub>).



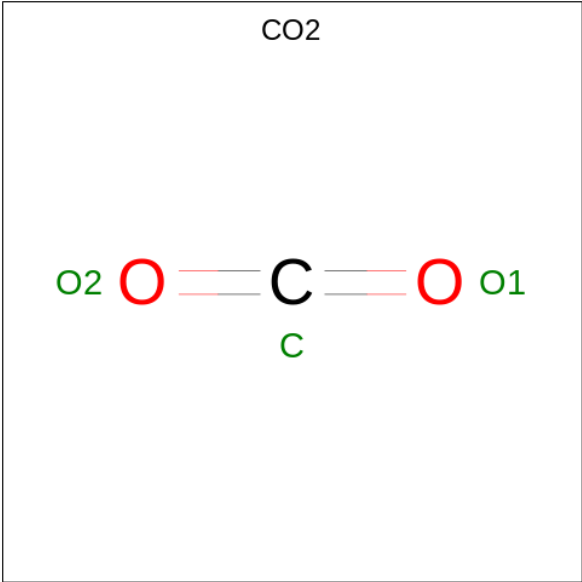
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total 2	O 2	0	0
18	N	1	Total 2	O 2	0	0

- Molecule 19 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



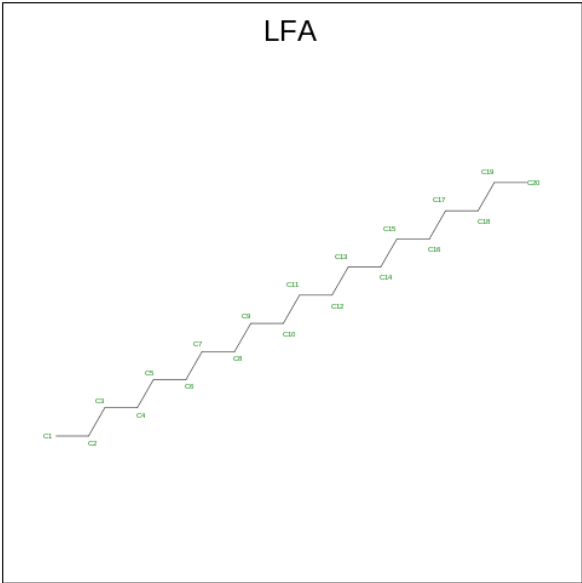
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			64	45	17	2		
19	C	1	Total	C	O	P	0	0
			87	68	17	2		
19	L	1	Total	C	O	P	0	0
			94	75	17	2		
19	P	1	Total	C	O	P	0	0
			87	68	17	2		
19	V	1	Total	C	O	P	0	0
			64	45	17	2		
19	Y	1	Total	C	O	P	0	0
			94	75	17	2		

- Molecule 20 is CARBON DIOXIDE (CCD ID: CO2) (formula: CO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			3	1	2		
20	N	1	Total	C	O	0	0
			3	1	2		

- Molecule 21 is EICOSANE (CCD ID: LFA) (formula: C<sub>20</sub>H<sub>42</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	C	0	0
			14	14		
21	A	1	Total	C	0	0
			14	14		

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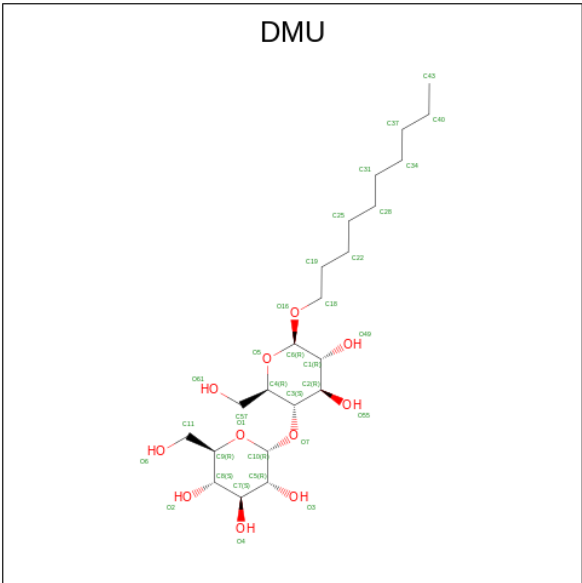
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total C 17 17	0	0
21	C	1	Total C 11 11	0	0
21	C	1	Total C 6 6	0	0
21	C	1	Total C 18 18	0	0
21	C	1	Total C 11 11	0	0
21	C	1	Total C 14 14	0	0
21	C	1	Total C 11 11	0	0
21	C	1	Total C 15 15	0	0
21	C	1	Total C 13 13	0	0
21	C	1	Total C 15 15	0	0
21	N	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	P	1	Total C 15 15	0	0
21	P	1	Total C 13 13	0	0
21	T	1	Total C 11 11	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 7 7	0	0
22	A	1	Total C O 33 22 11	0	0
22	A	1	Total C O 11 10 1	0	0
22	B	1	Total C O 11 10 1	0	0
22	B	1	Total C O 11 10 1	0	0
22	B	1	Total C O 22 16 6	0	0
22	B	1	Total C O 22 16 6	0	0
22	C	1	Total C O 11 10 1	0	0

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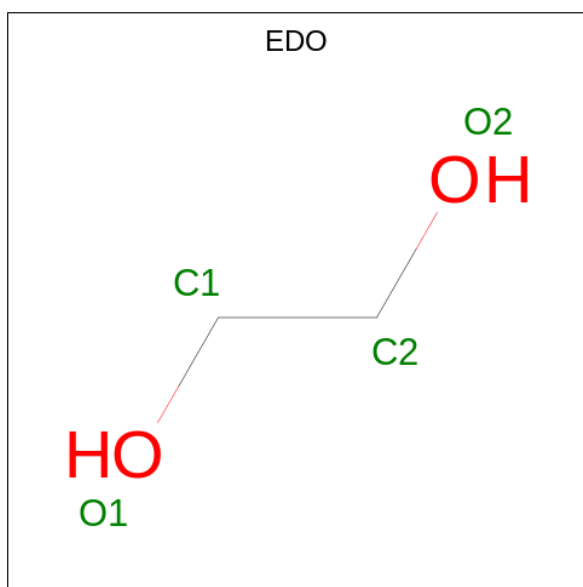
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O 33 22 11	0	0
22	C	1	Total C 7 7	0	0
22	C	1	Total C O 22 16 6	0	0
22	C	1	Total C O 33 22 11	0	0
22	C	1	Total C O 33 22 11	0	0
22	C	1	Total C O 22 16 6	0	0
22	C	1	Total C O 33 22 11	0	0
22	D	1	Total C O 33 22 11	0	0
22	G	1	Total C O 11 10 1	0	0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

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

- Molecule 23 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



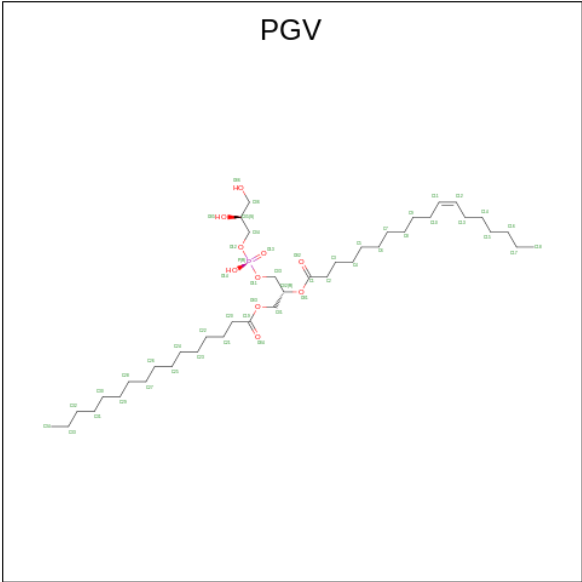
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			4	2	2		
23	A	1	Total	C	O	0	0
			4	2	2		
23	A	1	Total	C	O	0	0
			4	2	2		
23	A	1	Total	C	O	0	0
			4	2	2		
23	B	1	Total	C	O	0	0
			4	2	2		
23	C	1	Total	C	O	0	0
			4	2	2		
23	C	1	Total	C	O	0	0
			4	2	2		
23	C	1	Total	C	O	0	0
			4	2	2		
23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

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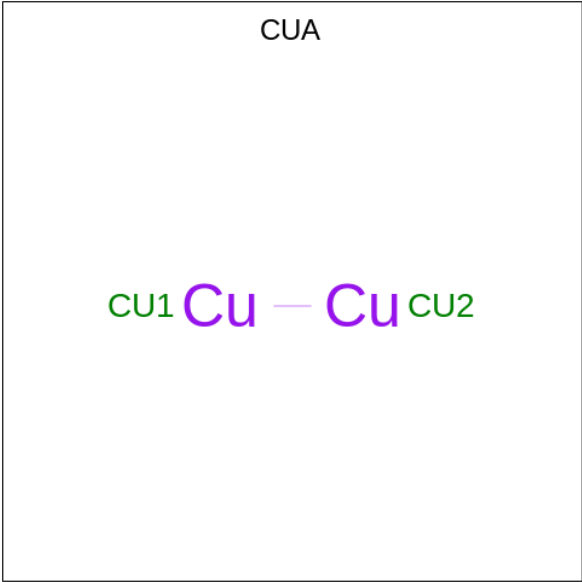
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	N	1	Total 4	C 2	O 2	0	0
23	N	1	Total 4	C 2	O 2	0	0
23	N	1	Total 4	C 2	O 2	0	0
23	N	1	Total 4	C 2	O 2	0	0
23	N	1	Total 4	C 2	O 2	0	0
23	O	1	Total 4	C 2	O 2	0	0
23	P	1	Total 4	C 2	O 2	0	0
23	P	1	Total 4	C 2	O 2	0	0
23	P	1	Total 4	C 2	O 2	0	0
23	R	1	Total 4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

- Molecule 24 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).



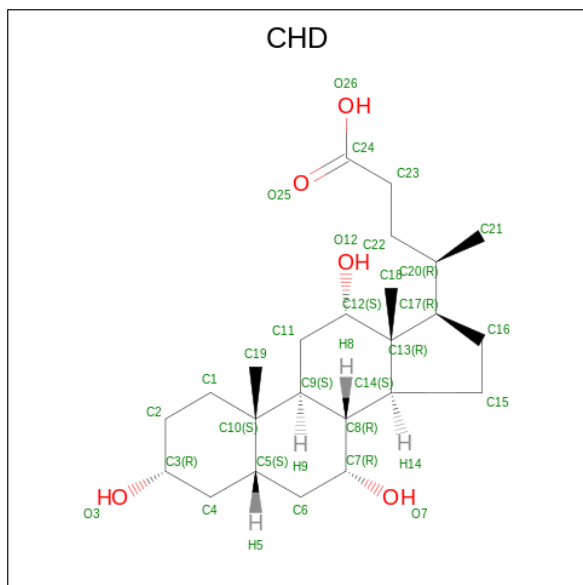
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	O	P	0	0
			51	40	10	1		
24	C	1	Total	C	O	P	0	0
			51	40	10	1		
24	N	1	Total	C	O	P	0	0
			51	40	10	1		
24	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 25 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 26 is CHOLIC ACID (CCD ID: CHD) (formula:  $C_{24}H_{40}O_5$ ).



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

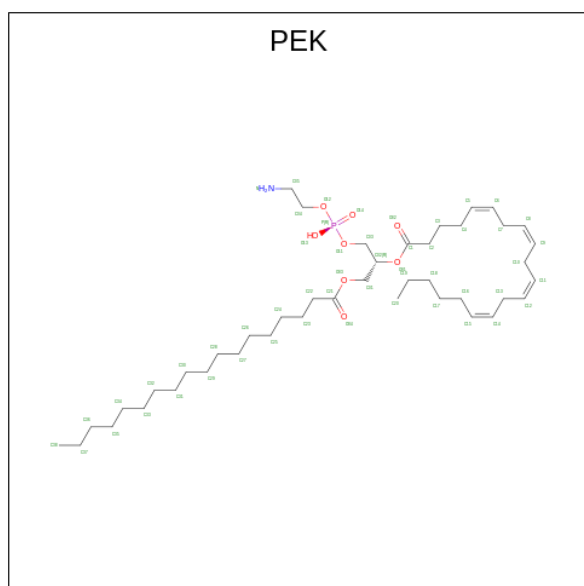
- Molecule 27 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

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

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 29 is (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
29	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
29	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	236	Total	O	0	11
			247	247		
30	B	177	Total	O	0	2
			179	179		
30	C	103	Total	O	0	1
			104	104		
30	D	138	Total	O	0	8
			146	146		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	E	109	Total 117	O 117	0	8
30	F	101	Total 108	O 108	0	7
30	G	43	Total 44	O 44	0	1
30	H	62	Total 62	O 62	0	0
30	I	39	Total 39	O 39	0	0
30	J	21	Total 21	O 21	0	0
30	K	21	Total 21	O 21	0	0
30	L	24	Total 26	O 26	0	2
30	M	22	Total 22	O 22	0	0
30	N	223	Total 233	O 233	0	10
30	O	149	Total 150	O 150	0	1
30	P	100	Total 101	O 101	0	1
30	Q	79	Total 84	O 84	0	5
30	R	88	Total 95	O 95	0	7
30	S	91	Total 97	O 97	0	6
30	T	35	Total 36	O 36	0	1
30	U	49	Total 49	O 49	0	0
30	V	23	Total 23	O 23	0	0
30	W	15	Total 15	O 15	0	0
30	X	19	Total 19	O 19	0	0
30	Y	23	Total 25	O 25	0	2

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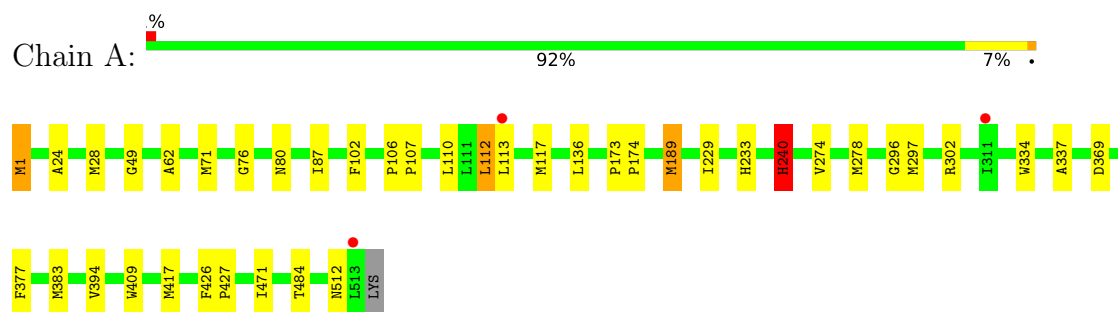
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	Z	17	Total	O	0	0
			17	17		

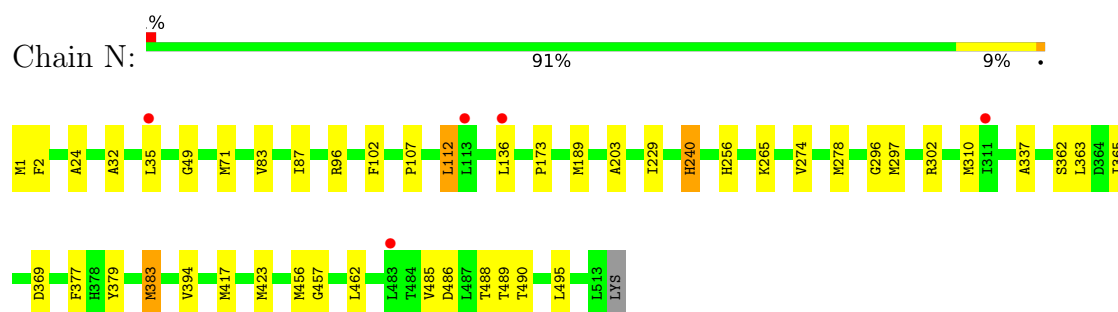
### 3 Residue-property plots

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

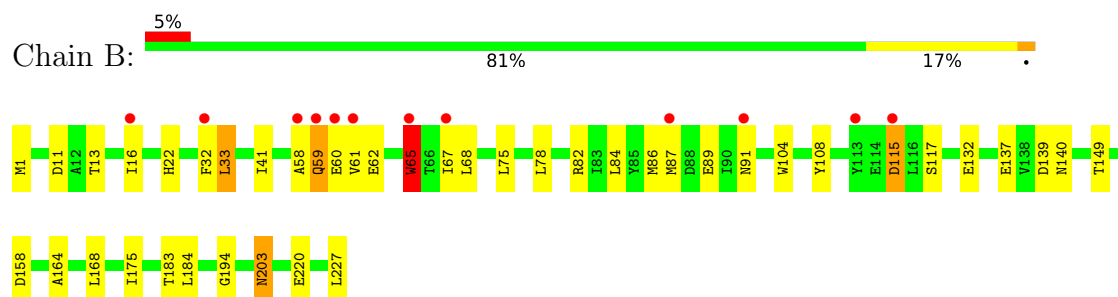
- Molecule 1: Cytochrome c oxidase subunit 1



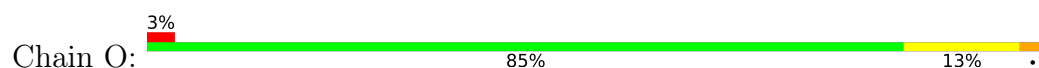
- Molecule 1: Cytochrome c oxidase subunit 1

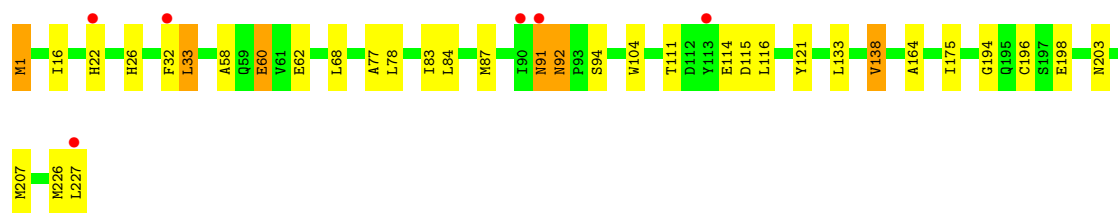


- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2





- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 89% 10%



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 90% 9%



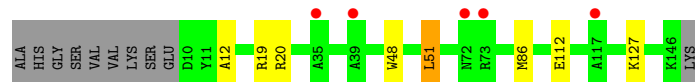
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 93% 2%



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

Chain Q: 88% 3% 5% 7%



- Molecule 5: Cytochrome c oxidase subunit 5A

Chain E: 89% 5% 6%

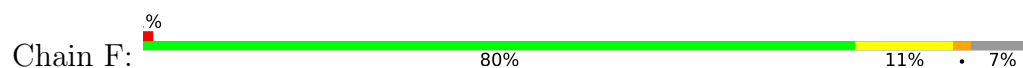


- Molecule 5: Cytochrome c oxidase subunit 5A

Chain R: 87% 2% 6% 6%



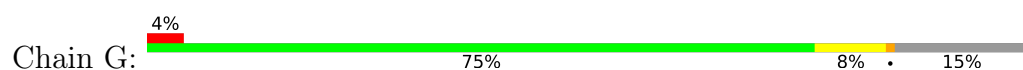
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



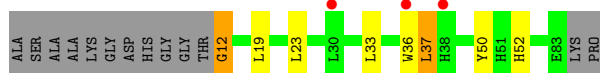
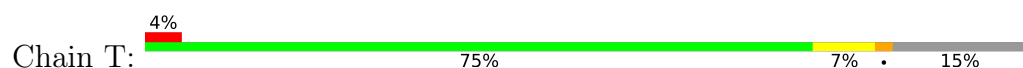
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



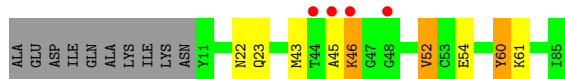
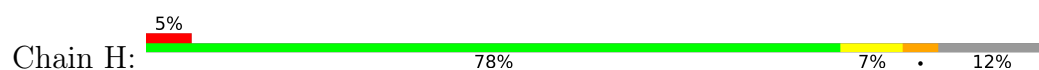
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



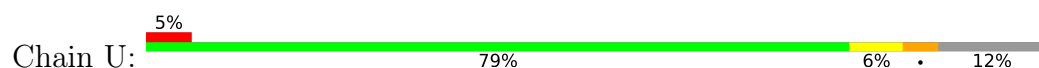
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



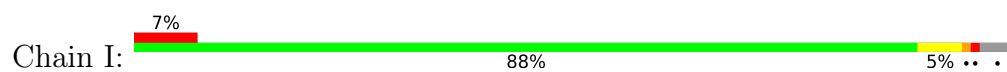
- Molecule 8: Cytochrome c oxidase subunit 6B1



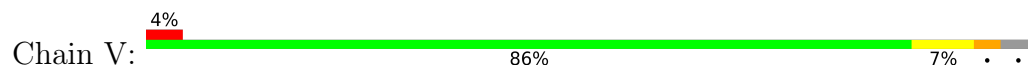
- Molecule 8: Cytochrome c oxidase subunit 6B1



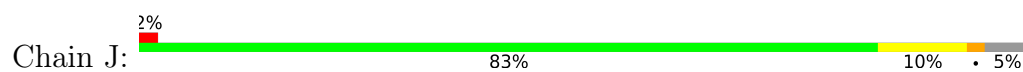
- Molecule 9: Cytochrome c oxidase subunit 6C



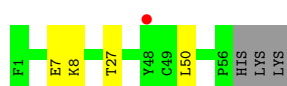
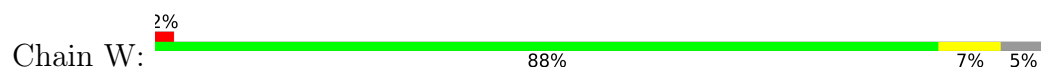
- Molecule 9: Cytochrome c oxidase subunit 6C



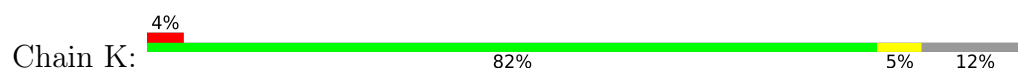
- Molecule 10: Cytochrome c oxidase subunit 7A1



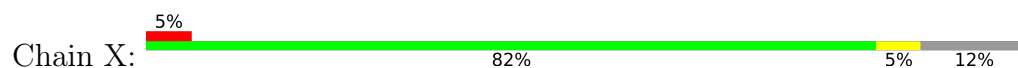
- Molecule 10: Cytochrome c oxidase subunit 7A1



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



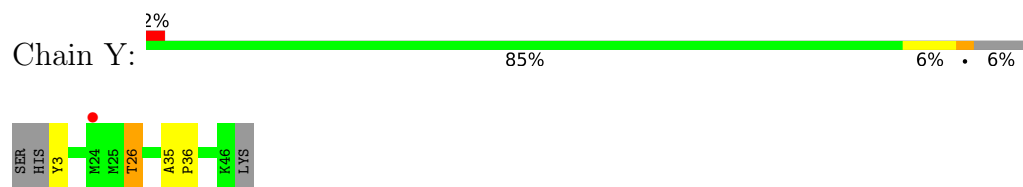
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



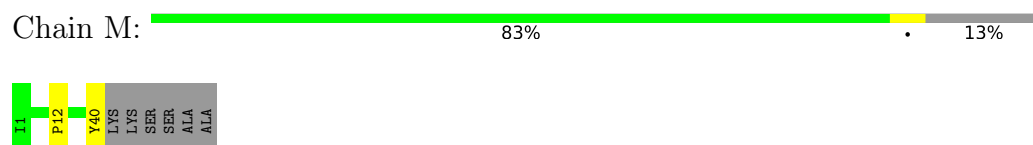
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



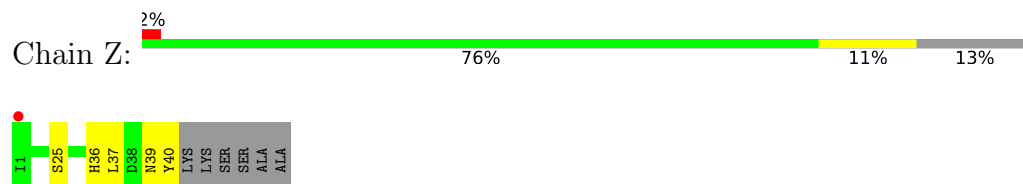
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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 204.40Å 177.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.75 40.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.75) 100.0 (40.00-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.130 , 0.167 0.145 , 0.176	Depositor DCC
$R_{free}$ test set	33113 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.667	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 59.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	33055	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: PGV, DMU, CHD, UNX, EDO, MG, ZN, CU, CUA, HEA, PEK, CO2, LFA, CDL, FME, PER, NA

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	1.08	4/4259 (0.1%)	1.18	5/5816 (0.1%)
1	N	1.07	4/4259 (0.1%)	1.20	6/5816 (0.1%)
2	B	1.12	1/1908 (0.1%)	1.33	18/2598 (0.7%)
2	O	1.09	2/1908 (0.1%)	1.25	1/2598 (0.0%)
3	C	1.04	1/2258 (0.0%)	1.16	3/3084 (0.1%)
3	P	1.05	1/2258 (0.0%)	1.19	4/3084 (0.1%)
4	D	1.11	1/1226 (0.1%)	1.21	2/1657 (0.1%)
4	Q	1.05	0/1182	1.31	0/1598
5	E	1.11	0/843	1.24	3/1145 (0.3%)
5	R	1.08	0/843	1.34	3/1145 (0.3%)
6	F	1.12	1/724 (0.1%)	1.21	0/983
6	S	1.19	0/724	1.21	0/983
7	G	1.10	2/633 (0.3%)	1.19	0/864
7	T	1.16	1/633 (0.2%)	1.28	0/864
8	H	1.04	0/648	1.33	0/877
8	U	1.07	0/648	1.32	0/877
9	I	1.15	2/588 (0.3%)	1.47	7/781 (0.9%)
9	V	1.10	0/588	1.44	1/781 (0.1%)
10	J	1.06	0/451	1.23	1/610 (0.2%)
10	W	1.08	0/451	1.27	0/610
11	K	1.14	1/398 (0.3%)	1.31	0/546
11	X	1.12	0/398	1.28	0/546
12	L	1.11	0/372	1.29	2/500 (0.4%)
12	Y	1.07	0/372	1.20	0/500
13	M	1.08	0/321	1.20	0/440
13	Z	1.00	0/321	1.34	0/440
All	All	1.09	21/29214 (0.1%)	1.24	56/39743 (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	2
6	S	0	1
All	All	0	3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	GLY	C-O	9.00	1.33	1.23
1	N	383	MET	C-O	-7.35	1.13	1.23
1	A	233	HIS	CE1-NE2	7.26	1.39	1.32
3	P	71	HIS	CE1-NE2	7.18	1.39	1.32
1	N	49	GLY	C-O	7.04	1.31	1.23
4	D	58	GLU	CD-OE1	6.92	1.38	1.25
9	I	72	ALA	C-O	6.54	1.36	1.23
1	N	203	ALA	C-O	6.41	1.31	1.24
7	T	12	GLY	N-CA	-6.34	1.35	1.45
7	G	12	GLY	N-CA	-6.06	1.35	1.45
2	O	198	GLU	C-O	6.06	1.30	1.23
9	I	31	PHE	C-O	5.82	1.31	1.24
1	A	174	PRO	C-O	-5.75	1.17	1.24
3	C	36	HIS	CE1-NE2	5.66	1.38	1.32
6	F	75	HIS	CE1-NE2	5.54	1.38	1.32
11	K	10	HIS	CE1-NE2	5.42	1.38	1.32
2	O	138	VAL	C-O	5.36	1.29	1.23
2	B	65	TRP	NE1-CE2	-5.20	1.31	1.37
1	A	189	MET	CB-CG	5.19	1.68	1.52
1	N	256	HIS	CE1-NE2	5.14	1.37	1.32
7	G	48	ILE	N-CA	5.10	1.49	1.45

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	65	TRP	CA-CB-CG	10.99	134.48	113.60
1	N	240	HIS	CA-CB-CG	-10.54	103.26	113.80
1	A	240	HIS	CA-CB-CG	-10.13	103.67	113.80
9	I	72	ALA	CA-C-O	-9.74	104.24	120.80
2	B	65	TRP	CB-CG-CD2	9.64	140.29	126.80
2	B	65	TRP	CB-CG-CD1	-8.23	114.56	126.90
5	E	108	LYS	CA-C-O	-7.93	107.31	120.80
3	P	122	HIS	CB-CA-C	7.35	118.29	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	58	GLU	CB-CG-CD	7.30	125.00	112.60
3	C	80	ARG	CG-CD-NE	-7.01	96.58	112.00
2	B	115	ASP	CB-CA-C	6.92	123.30	111.68
1	A	102	PHE	CA-CB-CG	-6.68	107.12	113.80
4	D	146	LYS	CA-C-O	-6.64	109.51	120.80
2	B	183	THR	CA-CB-OG1	-6.60	99.70	109.60
2	B	59	GLN	CB-CG-CD	6.56	123.76	112.60
3	P	233	PHE	CA-CB-CG	-6.43	107.37	113.80
12	L	25	MET	CA-C-N	6.35	129.11	120.54
12	L	25	MET	C-N-CA	6.35	129.11	120.54
1	N	102	PHE	CA-CB-CG	-6.29	107.50	113.80
5	R	78	HIS	CA-C-N	6.27	129.54	120.38
5	R	78	HIS	C-N-CA	6.27	129.54	120.38
1	N	71	MET	CG-SD-CE	-6.14	87.38	100.90
1	N	377	PHE	CA-CB-CG	6.10	119.90	113.80
3	P	80	ARG	CG-CD-NE	-5.92	98.97	112.00
2	B	82	ARG	CG-CD-NE	-5.88	99.07	112.00
2	B	89	GLU	CA-C-N	5.87	128.97	120.98
2	B	89	GLU	C-N-CA	5.87	128.97	120.98
2	B	149	THR	CA-CB-OG1	-5.77	100.95	109.60
3	P	76	GLN	CG-CD-NE2	-5.73	107.81	116.40
2	B	158	ASP	CA-CB-CG	5.62	118.22	112.60
2	B	139	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	512	ASN	CB-CA-C	5.41	119.80	110.45
2	B	184	LEU	N-CA-CB	-5.35	101.54	110.80
9	I	35	TYR	CA-C-N	5.32	127.67	120.38
9	I	35	TYR	C-N-CA	5.32	127.67	120.38
9	I	36	LYS	CA-C-N	5.32	129.59	120.71
9	I	36	LYS	C-N-CA	5.32	129.59	120.71
10	J	7	GLU	CB-CA-C	5.30	119.86	110.85
1	A	71	MET	CG-SD-CE	-5.26	89.32	100.90
2	O	92	ASN	CB-CA-C	5.26	115.69	110.33
9	V	8	GLN	N-CA-CB	5.25	117.73	109.69
3	C	76	GLN	CG-CD-NE2	-5.24	108.54	116.40
3	C	233	PHE	CA-CB-CG	-5.24	108.56	113.80
5	E	17	THR	CA-CB-OG1	-5.24	101.74	109.60
5	E	80	GLU	CB-CG-CD	5.19	121.42	112.60
2	B	11	ASP	CA-CB-CG	5.18	117.78	112.60
2	B	41	ILE	CA-C-O	-5.14	115.60	120.95
2	B	59	GLN	N-CA-CB	5.11	117.48	110.07
1	A	377	PHE	CA-CB-CG	5.09	118.89	113.80
2	B	203	ASN	CA-C-N	5.08	127.34	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	203	ASN	C-N-CA	5.08	127.34	120.38
1	N	83	VAL	N-CA-CB	5.04	114.38	110.45
9	I	22	VAL	CA-C-N	5.03	125.67	119.99
9	I	22	VAL	C-N-CA	5.03	125.67	119.99
5	R	80	GLU	CB-CG-CD	5.02	121.13	112.60
1	N	96	ARG	CB-CA-C	5.01	119.86	110.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	383	MET	Mainchain
6	S	92	VAL	Mainchain

## 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	42	0
1	N	4130	0	4102	45	0
2	B	1870	0	1870	24	0
2	O	1870	0	1870	32	0
3	C	2171	0	2080	32	0
3	P	2172	0	2081	19	0
4	D	1192	0	1178	5	0
4	Q	1148	0	1131	7	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	11	0
7	G	606	0	577	4	0
7	T	606	0	577	6	0
8	H	628	0	580	14	0
8	U	628	0	580	12	0
9	I	575	0	584	5	0
9	V	575	0	584	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	441	0	439	7	0
10	W	441	0	439	4	0
11	K	384	0	366	1	0
11	X	384	0	366	2	0
12	L	360	0	360	1	0
12	Y	360	0	360	7	0
13	M	311	0	321	2	0
13	Z	311	0	321	4	0
14	A	129	0	88	4	0
14	N	129	0	88	2	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	2	0	0	1	0
18	N	2	0	0	1	0
19	A	64	0	71	1	0
19	C	87	0	124	17	0
19	L	94	0	141	2	0
19	P	87	0	124	7	0
19	V	64	0	72	2	0
19	Y	94	0	141	4	0
20	A	3	0	0	0	0
20	N	3	0	0	0	0
21	A	28	0	54	11	0
21	B	17	0	33	3	0
21	C	114	0	203	5	0
21	N	28	0	54	10	0
21	O	28	0	54	0	0
21	P	114	0	202	7	0
21	T	11	0	21	0	0
22	A	51	0	76	1	0
22	B	66	0	104	0	0
22	C	194	0	262	8	0
22	D	33	0	41	2	0
22	G	11	0	21	0	0
22	H	33	0	30	1	0
22	J	11	0	21	0	0
22	L	22	0	31	0	0
22	M	41	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	N	40	0	55	0	0
22	O	66	0	104	2	0
22	P	194	0	262	2	0
22	Q	33	0	41	1	0
22	U	33	0	27	1	0
22	W	11	0	21	0	0
22	Z	63	0	87	2	0
23	A	16	0	24	1	0
23	B	4	0	6	0	0
23	C	12	0	17	0	0
23	E	12	0	18	0	0
23	F	8	0	12	0	0
23	G	4	0	6	0	0
23	N	20	0	30	0	0
23	O	4	0	6	0	0
23	P	12	0	17	0	0
23	R	12	0	18	0	0
23	S	8	0	12	0	0
23	T	4	0	6	0	0
24	A	51	0	76	0	0
24	C	51	0	76	1	0
24	N	51	0	76	1	0
24	P	51	0	76	0	0
25	B	2	0	0	0	0
25	O	2	0	0	0	0
26	B	29	0	39	1	0
26	C	58	0	78	2	0
26	O	29	0	39	1	0
26	P	58	0	78	4	0
27	C	1	0	0	1	0
27	P	1	0	0	0	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	G	53	0	77	0	0
29	T	53	0	77	5	0
30	A	247	0	0	8	0
30	B	179	0	0	4	0
30	C	104	0	0	5	0
30	D	146	0	0	3	0
30	E	117	0	0	0	0
30	F	108	0	0	1	0
30	G	44	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	H	62	0	0	0	0
30	I	39	0	0	1	0
30	J	21	0	0	0	0
30	K	21	0	0	0	0
30	L	26	0	0	0	0
30	M	22	0	0	1	0
30	N	233	0	0	6	0
30	O	150	0	0	2	0
30	P	101	0	0	5	0
30	Q	84	0	0	2	0
30	R	95	0	0	2	0
30	S	97	0	0	0	0
30	T	36	0	0	1	0
30	U	49	0	0	3	0
30	V	23	0	0	1	0
30	W	15	0	0	0	0
30	X	19	0	0	0	0
30	Y	25	0	0	1	0
30	Z	17	0	0	0	0
All	All	33055	0	31469	312	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 (312) 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)
1:A:112:LEU:HG	30:A:2025:HOH:O	1.45	1.16
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.25	1.12
18:N:606:PER:O2	18:N:606:PER:O1	1.68	1.09
18:A:606:PER:O2	18:A:606:PER:O1	1.70	1.09
1:N:112:LEU:HG	30:N:3014:HOH:O	1.60	1.00
3:P:4:GLN:N	30:P:403:HOH:O	1.93	0.99
7:G:19:LEU:HD23	21:N:609:LFA:H61	1.51	0.93
1:A:112:LEU:C	1:A:112:LEU:HD23	1.96	0.91
3:C:245:VAL:C	3:C:246[B]:ASP:CA	2.42	0.91
3:C:33[A]:MET:HE3	3:C:39:SER:OG	1.73	0.88
8:H:52:VAL:CG1	8:U:46:LYS:HG2	2.05	0.87
8:H:52:VAL:HG12	8:U:46:LYS:CG	2.06	0.85
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.16	0.85
1:A:136[B]:LEU:HD11	30:A:2031:HOH:O	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:43:MET:HE1	8:U:52:VAL:HG11	1.58	0.83
3:P:149:HIS:NE2	21:P:313:LFA:H11	1.95	0.81
19:P:305:CDL:H121	19:P:305:CDL:HA62	1.62	0.81
21:A:609:LFA:H12	21:A:610:LFA:H11	1.63	0.80
3:C:180[A]:GLU:OE2	30:C:402:HOH:O	2.01	0.78
1:N:112:LEU:HD23	1:N:112:LEU:C	2.08	0.78
8:H:52:VAL:HG21	8:U:43:MET:HE1	1.66	0.76
2:O:92:ASN:ND2	30:O:402:HOH:O	2.17	0.76
19:C:304:CDL:HB22	10:J:8:LYS:HE3	1.68	0.75
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:HG2	1.68	0.75
1:N:278[A]:MET:HE1	21:N:609:LFA:H51	1.69	0.75
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:HE3	1.67	0.75
1:A:297[B]:MET:SD	1:A:302:ARG:HG2	2.27	0.74
1:A:484:THR:HG22	30:A:2013:HOH:O	1.87	0.74
4:Q:112:GLU:OE2	30:Q:301:HOH:O	2.05	0.74
6:S:76:LYS:CE	6:S:93:PRO:HG2	2.18	0.72
1:N:2:PHE:CE2	19:Y:101:CDL:H712	2.24	0.72
3:C:51[B]:MET:HE2	19:C:304:CDL:H861	1.71	0.72
30:A:1865:HOH:O	3:C:77:LYS:HE3	1.89	0.71
19:C:304:CDL:HA62	19:C:304:CDL:H121	1.70	0.71
22:A:612:DMU:O6	30:A:1805:HOH:O	2.08	0.71
21:P:310:LFA:H32	30:U:223:HOH:O	1.89	0.71
3:C:33[A]:MET:CE	3:C:42:LEU:H	2.04	0.71
6:F:87[A]:THR:HG22	6:F:89:TYR:CE1	2.25	0.70
2:O:91:ASN:C	2:O:91:ASN:HD22	1.99	0.70
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.74	0.69
1:A:113[B]:LEU:HD11	1:A:117[B]:MET:SD	2.32	0.69
21:P:310:LFA:C3	30:U:223:HOH:O	2.41	0.69
19:Y:101:CDL:C41	19:Y:101:CDL:H801	2.22	0.69
19:C:304:CDL:HB22	10:J:8:LYS:CE	2.22	0.69
3:P:33[B]:MET:CE	3:P:42:LEU:HD12	2.22	0.69
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.29	0.68
1:A:112:LEU:CG	30:A:2025:HOH:O	2.19	0.67
1:A:278[A]:MET:CE	21:A:610:LFA:H51	2.23	0.67
27:C:302:UNX:UNK	30:C:497:HOH:O	1.76	0.67
19:C:304:CDL:CB6	19:C:304:CDL:HB21	2.24	0.67
2:B:220:GLU:OE1	30:B:402:HOH:O	2.13	0.66
8:H:46:LYS:HE2	8:H:46:LYS:O	1.96	0.66
3:C:33[B]:MET:HE1	22:C:324:DMU:H12	1.77	0.66
1:N:297[B]:MET:SD	1:N:302:ARG:CG	2.84	0.65
1:A:112:LEU:C	1:A:112:LEU:CD2	2.70	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:HD23	1:A:112:LEU:O	1.98	0.64
19:C:304:CDL:H531	19:C:304:CDL:HB4	1.79	0.64
22:C:324:DMU:H20	10:J:50:LEU:HB2	1.80	0.64
2:B:16[B]:ILE:HG23	30:B:542:HOH:O	1.97	0.64
6:F:37:LYS:HG2	30:F:293:HOH:O	1.98	0.64
1:A:28:MET:CE	14:A:601[A]:HEA:H271	2.28	0.64
21:N:608:LFA:H12	21:N:609:LFA:H11	1.80	0.64
3:P:258:TRP:CE2	21:P:308:LFA:H32	2.33	0.63
2:O:84:LEU:HA	2:O:87[A]:MET:HE2	1.80	0.63
3:P:156:ARG:HE	26:P:306:CHD:C24	2.12	0.63
1:A:1:FME:HE2	1:A:1:FME:HA	1.80	0.63
5:R:90:ARG:NH1	30:R:303:HOH:O	2.24	0.62
29:T:101:PEK:H32	29:T:101:PEK:H71	1.81	0.62
1:N:278[B]:MET:SD	21:N:608:LFA:H51	2.39	0.62
3:C:54[A]:MET:HE1	24:C:303:PGV:H141	1.82	0.62
19:C:304:CDL:HB21	19:C:304:CDL:HB61	1.81	0.62
2:O:114:GLU:HG3	2:O:227:LEU:HD21	1.81	0.62
26:C:305:CHD:H162	26:C:305:CHD:H231	1.81	0.62
1:A:189:MET:HE3	21:A:609:LFA:H31	1.80	0.61
1:N:274:VAL:HG12	1:N:278[A]:MET:HE2	1.81	0.61
1:A:274:VAL:HG12	1:A:278[A]:MET:HE2	1.81	0.61
3:C:180[B]:GLU:HG2	30:C:424:HOH:O	1.98	0.61
3:C:149:HIS:NE2	21:C:312:LFA:H11	2.15	0.60
3:C:33[B]:MET:CA	3:C:33[B]:MET:HE2	2.14	0.60
7:G:19:LEU:CD2	21:N:609:LFA:H61	2.30	0.60
3:C:33[B]:MET:CE	22:C:324:DMU:H12	2.30	0.60
1:N:486:ASP:OD2	4:Q:19:ARG:NE	2.35	0.60
3:C:258:TRP:NE1	21:C:307:LFA:H12	2.16	0.59
2:B:227:LEU:HD21	30:B:525:HOH:O	2.01	0.59
3:C:33[A]:MET:HE2	3:C:42:LEU:H	1.68	0.59
1:A:297[B]:MET:SD	1:A:302:ARG:CG	2.92	0.58
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.86	0.58
2:B:33:LEU:HD13	9:I:31:PHE:CD2	2.39	0.58
1:N:24:ALA:HB2	14:N:601[B]:HEA:H253	1.85	0.57
19:C:304:CDL:H121	19:C:304:CDL:CA6	2.33	0.57
6:S:76:LYS:HE2	6:S:93:PRO:HG2	1.87	0.57
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.87	0.56
22:P:325:DMU:O55	22:P:325:DMU:O3	2.21	0.56
1:A:278[A]:MET:SD	21:A:610:LFA:H51	2.46	0.56
2:B:22[B]:HIS:CE1	9:I:44:LYS:CE	2.88	0.56
1:N:310:MET:HE1	2:O:77:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:305:CDL:H752	10:W:27:THR:HG21	1.88	0.56
2:O:58:ALA:O	2:O:62:GLU:HG3	2.06	0.55
8:H:22:ASN:ND2	22:H:101:DMU:O3	2.40	0.55
1:N:136[B]:LEU:HD11	30:N:3021:HOH:O	2.07	0.55
12:Y:26:THR:HG21	22:Z:102:DMU:H26	1.89	0.55
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.38	0.54
19:P:305:CDL:O1	10:W:8:LYS:HD2	2.07	0.54
1:A:28:MET:CE	14:A:601[A]:HEA:C27	2.85	0.54
8:H:46:LYS:O	8:H:46:LYS:CE	2.55	0.54
22:Q:201:DMU:O55	22:Q:201:DMU:H36	2.08	0.54
2:B:13:THR:HB	2:B:168:LEU:HD23	1.90	0.54
1:N:112:LEU:CG	30:N:3014:HOH:O	2.35	0.54
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.36	0.54
7:G:12:GLY:HA3	30:G:236:HOH:O	2.08	0.53
1:N:2:PHE:CZ	19:Y:101:CDL:H712	2.42	0.53
1:A:278[A]:MET:HE1	21:A:610:LFA:H51	1.90	0.53
2:B:16[A]:ILE:HD12	2:B:87[A]:MET:HG2	1.91	0.53
3:C:258:TRP:CE2	21:C:307:LFA:H32	2.43	0.53
1:N:112:LEU:C	1:N:112:LEU:CD2	2.82	0.53
7:T:12:GLY:HA3	30:T:228:HOH:O	2.08	0.53
22:C:324:DMU:H11	10:J:49:CYS:HB3	1.90	0.52
2:O:33:LEU:HD13	9:V:31:PHE:CD2	2.44	0.52
6:S:54:ASN:HD22	6:S:54:ASN:C	2.17	0.52
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.90	0.52
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	2.97	0.52
9:I:36:LYS:HE3	9:I:36:LYS:HA	1.92	0.52
1:N:362[A]:SER:HA	2:O:87[A]:MET:HE1	1.93	0.51
3:C:33[A]:MET:HE1	3:C:42:LEU:H	1.74	0.51
1:N:278[B]:MET:HE1	21:N:608:LFA:H52	1.92	0.51
3:C:33[A]:MET:HE1	3:C:41:THR:HB	1.92	0.51
3:C:51[B]:MET:HE2	19:C:304:CDL:C86	2.40	0.51
1:N:297[B]:MET:HG2	1:N:302:ARG:HG3	1.93	0.51
1:N:365:ILE:HD11	30:N:2809:HOH:O	2.11	0.51
1:A:24:ALA:HB2	14:A:601[B]:HEA:H253	1.94	0.50
1:A:110:LEU:HD21	22:C:324:DMU:H24	1.93	0.50
1:A:278[B]:MET:HE1	21:A:609:LFA:H52	1.93	0.50
1:N:423[B]:MET:HE2	1:N:457:GLY:N	2.26	0.50
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.92	0.50
2:O:33:LEU:HB3	22:O:306:DMU:H23	1.94	0.50
12:Y:26:THR:CG2	22:Z:102:DMU:H26	2.40	0.50
1:A:28:MET:HE2	14:A:601[A]:HEA:C27	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:43:MET:CE	8:U:52:VAL:HG11	2.35	0.50
3:P:116:TRP:HA	3:P:117:PRO:C	2.36	0.50
2:B:84:LEU:O	2:B:87[B]:MET:HB2	2.12	0.50
1:N:362[B]:SER:O	2:O:87[B]:MET:HE1	2.12	0.50
3:C:59:ARG:HB2	19:C:304:CDL:OA9	2.12	0.50
4:D:42:GLU:OE2	30:D:301:HOH:O	2.20	0.50
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.47	0.50
1:N:488:THR:HB	1:N:495:LEU:HD13	1.94	0.49
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.94	0.49
6:S:19:GLU:OE1	6:S:31:TYR:OH	2.17	0.49
3:C:33[B]:MET:HE2	3:C:33[B]:MET:N	2.27	0.49
19:P:305:CDL:HB61	19:P:305:CDL:HB22	1.94	0.49
30:Q:305:HOH:O	5:R:108:LYS:HD3	2.12	0.49
2:B:61:VAL:HG22	2:B:65:TRP:CZ3	2.48	0.49
1:N:240:HIS:C	1:N:240:HIS:CD2	2.90	0.49
4:Q:86:MET:HE2	11:X:22:ALA:HA	1.94	0.49
8:H:52:VAL:CB	8:U:46:LYS:HG2	2.43	0.49
13:M:12:PRO:HG3	22:M:102:DMU:H16	1.95	0.49
19:L:101:CDL:OB9	19:L:101:CDL:H122	2.13	0.48
3:P:33[B]:MET:HE3	3:P:42:LEU:HD12	1.95	0.48
2:B:58:ALA:O	2:B:62:GLU:HG3	2.13	0.48
3:P:50:ASN:ND2	3:P:54[A]:MET:HE2	2.27	0.48
3:P:205:GLY:HA3	29:T:101:PEK:H182	1.94	0.48
8:U:22:ASN:ND2	22:U:101:DMU:O3	2.45	0.48
3:C:59:ARG:HG3	19:C:304:CDL:HA4	1.95	0.48
2:B:67:ILE:HD11	21:B:307:LFA:H42	1.96	0.48
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.95	0.48
29:T:101:PEK:H32	29:T:101:PEK:C7	2.44	0.48
21:A:610:LFA:C6	7:T:19:LEU:HD23	2.44	0.48
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:CG	2.41	0.48
1:A:297[B]:MET:HG2	1:A:302:ARG:HG3	1.96	0.47
6:F:92:VAL:HG23	6:F:92:VAL:O	2.13	0.47
2:B:67:ILE:CD1	21:B:307:LFA:H61	2.44	0.47
3:C:164:PHE:CD1	26:C:305:CHD:H192	2.49	0.47
1:N:417[B]:MET:CE	30:N:2986:HOH:O	2.62	0.47
1:N:278[A]:MET:CE	21:N:609:LFA:H51	2.43	0.47
19:C:304:CDL:CA3	19:C:304:CDL:OB9	2.63	0.47
30:N:2975:HOH:O	4:Q:20:ARG:HG2	2.14	0.47
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.97	0.47
22:P:325:DMU:H38	22:P:325:DMU:H28	1.57	0.47
22:D:201:DMU:H36	22:D:201:DMU:O55	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278[A]:MET:HE1	21:A:610:LFA:C5	2.45	0.47
4:D:86:MET:HE1	11:K:22:ALA:HB2	1.96	0.47
6:F:64:GLU:O	6:F:65:ASP:HB2	2.14	0.47
1:N:423[B]:MET:HE3	1:N:456:MET:HB2	1.96	0.47
24:N:617:PGV:H183	29:T:101:PEK:H331	1.97	0.47
3:P:258:TRP:CD2	21:P:308:LFA:H32	2.50	0.47
1:A:87:ILE:O	1:A:173:PRO:HD3	2.15	0.46
1:A:278[B]:MET:SD	21:A:609:LFA:H51	2.55	0.46
1:A:297[B]:MET:CG	1:A:302:ARG:HG3	2.45	0.46
1:N:297[B]:MET:CG	1:N:302:ARG:HG3	2.45	0.46
2:O:32[B]:PHE:CD2	9:V:31:PHE:CZ	3.03	0.46
6:F:53:THR:HG23	6:F:55:LYS:H	1.79	0.46
1:N:189:MET:HE3	21:N:608:LFA:H31	1.96	0.46
12:L:13:PHE:HB3	19:L:101:CDL:H512	1.98	0.46
2:O:121:TYR:O	2:O:138:VAL:HA	2.15	0.46
11:X:24:PHE:O	11:X:28:VAL:HG12	2.16	0.46
2:O:22[B]:HIS:CD2	9:V:44:LYS:HE2	2.51	0.46
3:C:226:HIS:HE1	19:C:304:CDL:H111	1.80	0.46
19:C:304:CDL:HB21	19:C:304:CDL:CB3	2.45	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.15	0.46
29:T:101:PEK:C11	29:T:101:PEK:C15	2.92	0.46
4:D:4:SER:HA	30:D:317:HOH:O	2.15	0.46
2:O:83:ILE:O	2:O:87[A]:MET:HG3	2.16	0.46
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.46	0.46
2:O:91:ASN:C	2:O:91:ASN:ND2	2.71	0.46
3:P:164:PHE:CD1	26:P:306:CHD:H192	2.51	0.46
1:N:423[B]:MET:HA	19:V:101:CDL:H782	1.98	0.45
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.98	0.45
26:O:301:CHD:H212	26:O:301:CHD:H12	1.98	0.45
3:P:258:TRP:NE1	21:P:308:LFA:H12	2.32	0.45
3:C:50:ASN:ND2	3:C:54[A]:MET:HE2	2.31	0.45
3:P:33[A]:MET:HG2	3:P:39:SER:O	2.16	0.45
26:P:306:CHD:H232	26:P:306:CHD:H162	1.98	0.45
1:A:240:HIS:C	1:A:240:HIS:CD2	2.95	0.45
21:A:610:LFA:H62	7:T:19:LEU:HD23	1.98	0.45
3:C:33[A]:MET:HG2	3:C:39:SER:O	2.17	0.45
3:P:4:GLN:CA	30:P:403:HOH:O	2.50	0.45
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.99	0.45
1:A:136[B]:LEU:CD1	30:A:2031:HOH:O	2.51	0.45
23:A:614:EDO:H12	2:B:58:ALA:HB3	1.98	0.45
2:B:16[A]:ILE:HD11	2:B:86:MET:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:33[B]:MET:HB2	3:P:33[B]:MET:HE2	1.53	0.45
21:N:608:LFA:H12	21:N:609:LFA:C1	2.46	0.45
2:O:164:ALA:O	2:O:194:GLY:HA3	2.16	0.45
6:S:64:GLU:O	6:S:65:ASP:HB2	2.16	0.45
7:T:50:TYR:HB3	7:T:52:HIS:CE1	2.52	0.45
3:C:133:ASN:ND2	30:C:406:HOH:O	2.49	0.45
30:C:459[B]:HOH:O	10:J:27:THR:HG22	2.17	0.45
1:A:334:TRP:HB2	22:D:201:DMU:C57	2.47	0.45
8:U:60:TYR:CD1	8:U:60:TYR:C	2.95	0.45
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.47	0.44
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.17	0.44
21:C:307:LFA:H31	26:P:302:CHD:H61	2.00	0.44
1:N:423[A]:MET:HA	19:V:101:CDL:H782	1.99	0.44
26:B:306:CHD:H212	26:B:306:CHD:H12	1.99	0.44
5:R:46:LYS:NZ	30:R:304:HOH:O	2.50	0.44
14:N:602:HEA:HBC1	14:N:602:HEA:HMC3	1.99	0.44
1:N:362[A]:SER:OG	2:O:87[A]:MET:HE2	2.18	0.44
2:O:16[B]:ILE:HG12	30:O:520:HOH:O	2.18	0.44
3:P:177:GLN:OE1	3:P:177:GLN:HA	2.17	0.44
12:Y:3:TYR:N	30:Y:202:HOH:O	2.50	0.44
1:N:423[B]:MET:HE3	1:N:456:MET:CB	2.48	0.44
2:O:60:GLU:CD	2:O:60:GLU:H	2.25	0.44
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.18	0.44
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.52	0.44
2:O:26:HIS:HE1	22:O:306:DMU:H9	1.82	0.44
19:P:305:CDL:C75	10:W:27:THR:HG21	2.48	0.43
4:D:127:LYS:HD2	30:I:137:HOH:O	2.18	0.43
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.19	0.43
1:A:409:TRP:HB3	1:A:471:ILE:HG12	1.99	0.43
3:C:116:TRP:HA	3:C:117:PRO:C	2.43	0.43
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.18	0.43
8:H:54:GLU:OE1	8:H:54:GLU:HA	2.19	0.43
3:P:149:HIS:NE2	21:P:313:LFA:C1	2.75	0.43
19:P:305:CDL:CA2	30:P:405:HOH:O	2.66	0.43
22:C:318:DMU:H22	10:J:41:GLY:HA3	2.01	0.43
2:O:1:FME:HE1	2:O:133:LEU:CD2	2.49	0.43
4:D:10:ASP:OD2	30:D:302:HOH:O	2.21	0.43
12:Y:26:THR:HG23	13:Z:25:SER:HB3	2.00	0.43
2:B:108:TYR:O	2:B:117:SER:HA	2.18	0.42
30:P:471[B]:HOH:O	10:W:27:THR:HG22	2.17	0.42
3:C:33[B]:MET:HE3	3:C:42:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:305:CDL:OB4	19:P:305:CDL:CA5	2.68	0.42
13:Z:37:LEU:HD23	13:Z:37:LEU:HA	1.91	0.42
13:M:40:TYR:C	30:M:201:HOH:O	2.62	0.42
1:N:278[B]:MET:SD	21:N:608:LFA:C5	3.07	0.42
7:T:37:LEU:HD12	7:T:37:LEU:HA	1.89	0.42
1:A:76:GLY:O	1:A:80:ASN:HB2	2.20	0.42
1:A:426:PHE:N	1:A:427:PRO:CD	2.82	0.42
19:C:304:CDL:CA5	19:C:304:CDL:OA8	2.68	0.42
8:H:60:TYR:CD1	8:H:60:TYR:C	2.97	0.42
1:A:106:PRO:HB2	1:A:107:PRO:HD3	2.01	0.42
4:Q:127:LYS:HD2	30:V:219:HOH:O	2.20	0.42
13:Z:36:HIS:HD2	13:Z:39:ASN:ND2	2.17	0.42
2:B:132:GLU:HB3	2:B:137:GLU:HG3	2.01	0.42
1:N:87:ILE:O	1:N:173:PRO:HD3	2.19	0.42
2:O:114:GLU:HG3	2:O:227:LEU:CD2	2.47	0.42
2:O:111:THR:HA	2:O:114:GLU:O	2.20	0.42
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.55	0.42
1:A:110:LEU:CD2	22:C:324:DMU:H24	2.50	0.41
2:O:22[B]:HIS:ND1	2:O:22[B]:HIS:O	2.52	0.41
19:C:304:CDL:H122	19:C:304:CDL:OB4	2.20	0.41
22:C:324:DMU:H10	10:J:53:ALA:HB2	2.01	0.41
1:A:229:ILE:HD11	2:B:175:ILE:HD13	2.02	0.41
21:A:610:LFA:C9	7:T:23:LEU:HB2	2.50	0.41
2:B:140:ASN:HB3	30:B:520:HOH:O	2.20	0.41
1:N:2:PHE:HE2	19:Y:101:CDL:H712	1.82	0.41
19:A:607:CDL:OA3	19:A:607:CDL:C1	2.68	0.41
30:A:1950:HOH:O	6:F:37:LYS:HE3	2.20	0.41
19:C:304:CDL:OA5	19:C:304:CDL:H1	2.17	0.41
8:H:46:LYS:HE2	8:H:46:LYS:C	2.46	0.41
6:S:10:GLU:OE2	6:S:25:ARG:NH1	2.42	0.41
8:U:43:MET:O	8:U:48:GLY:N	2.53	0.41
30:P:416:HOH:O	6:S:3:GLY:HA3	2.21	0.41
6:S:51:SER:O	6:S:93:PRO:HA	2.20	0.41
1:N:423[B]:MET:HE2	1:N:457:GLY:HA2	2.03	0.41
8:U:37:HIS:CE1	30:U:212:HOH:O	2.74	0.41
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.03	0.41
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	2.03	0.41
3:C:149:HIS:NE2	21:C:312:LFA:C1	2.83	0.40
6:F:85:CYS:SG	6:F:87[B]:THR:OG1	2.69	0.40
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	2.03	0.40
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:379:TYR:O	1:N:383:MET:HB2	2.22	0.40
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	2.03	0.40
3:C:51[A]:MET:SD	3:C:54[A]:MET:CE	3.10	0.40
6:F:21[B]:MET:HB3	6:F:21[B]:MET:HE3	1.86	0.40
1:N:489:THR:HA	6:S:71:TRP:O	2.22	0.40
2:B:67:ILE:HD11	21:B:307:LFA:H61	2.03	0.40
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.56	0.40
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.57	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%)	513 (98%)	13 (2%)	0	100	100
1	N	526/514 (102%)	513 (98%)	13 (2%)	0	100	100
2	B	230/227 (101%)	224 (97%)	6 (3%)	0	100	100
2	O	230/227 (101%)	225 (98%)	5 (2%)	0	100	100
3	C	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
3	P	265/261 (102%)	261 (98%)	4 (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%)	89 (98%)	2 (2%)	0	100	100
6	S	91/98 (93%)	89 (98%)	2 (2%)	0	100	100
7	G	71/85 (84%)	69 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	T	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
8	H	73/85 (86%)	69 (94%)	3 (4%)	1 (1%)	9	2
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%)	46 (98%)	1 (2%)	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%)	38 (100%)	0	0	100	100
13	Z	38/46 (83%)	37 (97%)	1 (3%)	0	100	100
All	All	3488/3614 (96%)	3415 (98%)	71 (2%)	2 (0%)	48	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	U	48	GLY
8	H	45	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/426 (103%)	438 (100%)	2 (0%)	86	82
1	N	440/426 (103%)	436 (99%)	4 (1%)	75	65
2	B	215/210 (102%)	206 (96%)	9 (4%)	25	8
2	O	215/210 (102%)	208 (97%)	7 (3%)	33	13
3	C	232/226 (103%)	230 (99%)	2 (1%)	75	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	232/226 (103%)	230 (99%)	2 (1%)	75	65
4	D	128/129 (99%)	127 (99%)	1 (1%)	79	71
4	Q	122/129 (95%)	121 (99%)	1 (1%)	79	71
5	E	89/95 (94%)	89 (100%)	0	100	100
5	R	89/95 (94%)	88 (99%)	1 (1%)	70	58
6	F	78/81 (96%)	74 (95%)	4 (5%)	20	5
6	S	78/81 (96%)	75 (96%)	3 (4%)	28	10
7	G	63/69 (91%)	60 (95%)	3 (5%)	21	6
7	T	63/69 (91%)	60 (95%)	3 (5%)	21	6
8	H	67/75 (89%)	63 (94%)	4 (6%)	16	3
8	U	67/75 (89%)	65 (97%)	2 (3%)	36	15
9	I	55/58 (95%)	54 (98%)	1 (2%)	54	37
9	V	55/58 (95%)	51 (93%)	4 (7%)	11	2
10	J	47/50 (94%)	46 (98%)	1 (2%)	48	29
10	W	47/50 (94%)	45 (96%)	2 (4%)	25	7
11	K	39/46 (85%)	38 (97%)	1 (3%)	41	21
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	19
13	M	34/38 (90%)	34 (100%)	0	100	100
13	Z	34/38 (90%)	33 (97%)	1 (3%)	37	17
All	All	3042/3086 (99%)	2983 (98%)	59 (2%)	52	34

All (59) 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

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Mol	Chain	Res	Type
2	B	91	ASN
2	B	115	ASP
3	C	159	MET
3	C	230	ASN
4	D	4	SER
6	F	37	LYS
6	F	80	GLN
6	F	87[A]	THR
6	F	87[B]	THR
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
8	H	46	LYS
8	H	52	VAL
8	H	60	TYR
8	H	61	LYS
9	I	36	LYS
10	J	7	GLU
11	K	54	ARG
1	N	112	LEU
1	N	363	LEU
1	N	369	ASP
1	N	485	VAL
2	O	33	LEU
2	O	60	GLU
2	O	68	LEU
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	51	LEU
5	R	79	LYS
6	S	37	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

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Mol	Chain	Res	Type
9	V	8	GLN
9	V	29	LEU
9	V	61	GLU
9	V	65	LYS
10	W	7	GLU
10	W	50	LEU
12	Y	26	THR
13	Z	40	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	170	ASN
1	A	422	ASN
2	B	52	HIS
3	C	50	ASN
3	C	56	GLN
4	D	29	HIS
4	D	109	HIS
4	D	119	GLN
4	D	143	ASN
5	E	94	ASN
6	F	54	ASN
7	G	34	ASN
8	H	22	ASN
10	J	29	ASN
1	N	170	ASN
1	N	422	ASN
2	O	59	GLN
2	O	92	ASN
3	P	50	ASN
3	P	56	GLN
4	Q	32	ASN
4	Q	109	HIS
4	Q	119	GLN
5	R	94	ASN
6	S	54	ASN
7	T	34	ASN
8	U	22	ASN
8	U	28	ASN
8	U	32	ASN

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Mol	Chain	Res	Type
11	X	35	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	0.78	0	7,9,11	1.32	2 (28%)
2	FME	B	1	2	8,9,10	1.07	1 (12%)	7,9,11	1.30	1 (14%)
2	FME	O	1	2	8,9,10	0.78	0	7,9,11	1.16	1 (14%)
1	FME	A	1	1	8,9,10	0.48	0	7,9,11	1.13	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	-	2/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-2.55	1.67	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-2.68	105.50	112.95
1	N	1	FME	CA-N-CN	2.41	126.53	122.82
1	N	1	FME	O-C-CA	-2.29	118.77	124.78
1	A	1	FME	C-CA-N	2.18	113.66	109.73
2	O	1	FME	CA-N-CN	2.06	125.99	122.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 137 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 127 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	LFA	P	308	-	10,10,19	0.19	0	9,9,18	0.16	0
19	CDL	A	607	-	63,63,99	0.59	0	69,75,111	1.24	6 (8%)
22	DMU	N	610	-	6,6,34	0.41	0	5,5,45	0.33	0
22	DMU	O	308	-	22,22,34	0.70	0	27,27,45	1.21	4 (14%)
22	DMU	P	318	-	22,22,34	0.87	1 (4%)	27,27,45	1.29	3 (11%)
22	DMU	M	102	-	7,7,34	0.25	0	6,6,45	0.54	0
26	CHD	P	302	-	32,32,32	0.92	3 (9%)	51,51,51	0.86	0
22	DMU	B	304	-	22,22,34	0.77	1 (4%)	27,27,45	0.94	1 (3%)
23	EDO	A	613	-	3,3,3	0.26	0	2,2,2	0.21	0
22	DMU	C	306	-	10,10,34	0.40	0	9,9,45	0.52	0
21	LFA	C	311	-	13,13,19	0.23	0	12,12,18	0.16	0
18	PER	A	606	15,14	0,1,1	-	-	-	-	-
21	LFA	C	310	-	10,10,19	0.13	0	9,9,18	0.09	0
21	LFA	P	309	-	5,5,19	0.24	0	4,4,18	0.08	0
22	DMU	U	101	-	34,34,34	0.86	2 (5%)	45,45,45	1.27	5 (11%)
23	EDO	A	614	-	3,3,3	0.13	0	2,2,2	0.17	0
21	LFA	P	312	-	13,13,19	0.19	0	12,12,18	0.18	0
22	DMU	O	306	-	10,10,34	0.22	0	9,9,45	0.60	0
24	PGV	N	617	-	50,50,50	0.80	1 (2%)	53,56,56	1.29	4 (7%)
25	CUA	O	305	2	0,1,1	-	-	-	-	-
21	LFA	P	315	-	12,12,19	0.29	0	11,11,18	0.29	0
14	HEA	N	601[B]	-	57,67,67	1.83	16 (28%)	61,103,103	2.49	21 (34%)
18	PER	N	606	15,14	0,1,1	-	-	-	-	-
14	HEA	A	601[B]	-	57,67,67	1.88	15 (26%)	61,103,103	2.50	24 (39%)
22	DMU	P	307	-	10,10,34	0.28	0	9,9,45	0.66	0
23	EDO	P	321	-	3,3,3	0.14	0	2,2,2	0.10	0
22	DMU	W	101	-	10,10,34	0.24	0	9,9,45	0.57	0
21	LFA	C	307	-	10,10,19	0.22	0	9,9,18	0.23	0
21	LFA	N	609	-	13,13,19	0.65	0	12,12,18	0.39	0
21	LFA	O	302	-	16,16,19	0.27	0	15,15,18	0.19	0
19	CDL	P	305	-	86,86,99	0.57	1 (1%)	92,98,111	0.82	2 (2%)
14	HEA	A	601[A]	-	57,67,67	1.89	15 (26%)	61,103,103	2.42	22 (36%)
23	EDO	A	616	-	3,3,3	0.31	0	2,2,2	0.44	0
26	CHD	C	305	-	32,32,32	0.72	0	51,51,51	1.57	6 (11%)
19	CDL	C	304	-	86,86,99	0.59	0	92,98,111	1.13	11 (11%)
21	LFA	C	312	-	10,10,19	0.22	0	9,9,18	0.25	0
22	DMU	C	317	-	22,22,34	0.57	0	27,27,45	1.23	3 (11%)
23	EDO	E	202	-	3,3,3	0.26	0	2,2,2	0.09	0
26	CHD	C	301	-	32,32,32	0.95	3 (9%)	51,51,51	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	DMU	B	308	-	22,22,34	0.64	0	27,27,45	1.49	3 (11%)
22	DMU	Z	103	-	7,7,34	0.39	0	6,6,45	0.48	0
23	EDO	B	305	-	3,3,3	0.19	0	2,2,2	0.31	0
22	DMU	O	304	-	22,22,34	0.82	1 (4%)	27,27,45	1.23	3 (11%)
24	PGV	P	304	-	50,50,50	0.87	2 (4%)	53,56,56	0.92	3 (5%)
23	EDO	G	103	-	3,3,3	0.34	0	2,2,2	0.18	0
22	DMU	C	318	-	34,34,34	1.02	3 (8%)	45,45,45	1.25	4 (8%)
22	DMU	P	324	-	22,22,34	0.59	0	27,27,45	1.52	2 (7%)
22	DMU	C	316	-	6,6,34	0.24	0	5,5,45	0.56	0
23	EDO	N	614	-	3,3,3	0.27	0	2,2,2	0.15	0
22	DMU	M	101	-	34,34,34	0.98	2 (5%)	45,45,45	1.03	4 (8%)
14	HEA	N	602	1,18	57,67,67	1.84	12 (21%)	61,103,103	2.55	26 (42%)
23	EDO	N	615	-	3,3,3	0.32	0	2,2,2	0.15	0
29	PEK	G	101	-	52,52,52	0.59	1 (1%)	55,57,57	0.70	0
22	DMU	H	101	-	34,34,34	0.89	2 (5%)	45,45,45	1.17	4 (8%)
22	DMU	P	319	-	34,34,34	0.88	3 (8%)	45,45,45	1.14	2 (4%)
26	CHD	P	306	-	32,32,32	0.98	1 (3%)	51,51,51	0.88	1 (1%)
14	HEA	N	601[A]	-	57,67,67	1.82	16 (28%)	61,103,103	2.57	22 (36%)
23	EDO	R	203	-	3,3,3	0.39	0	2,2,2	0.57	0
23	EDO	N	616	-	3,3,3	0.39	0	2,2,2	0.33	0
22	DMU	N	611	-	34,34,34	1.43	5 (14%)	45,45,45	1.23	4 (8%)
21	LFA	C	314	-	12,12,19	0.28	0	11,11,18	0.18	0
21	LFA	P	311	-	10,10,19	0.17	0	9,9,18	0.08	0
22	DMU	Z	102	-	22,22,34	0.67	0	27,27,45	1.13	2 (7%)
19	CDL	L	101	-	93,93,99	0.39	0	99,105,111	0.69	2 (2%)
14	HEA	A	602	1,18	57,67,67	1.77	12 (21%)	61,103,103	2.34	24 (39%)
22	DMU	P	325	-	34,34,34	0.61	0	45,45,45	1.47	5 (11%)
22	DMU	O	307	-	10,10,34	0.35	0	9,9,45	0.56	0
20	CO2	A	608	-	2,2,2	0.22	0	1,1,1	0.31	0
24	PGV	C	303	-	50,50,50	0.73	1 (2%)	53,56,56	1.13	5 (9%)
21	LFA	C	325	-	14,14,19	0.17	0	13,13,18	0.08	0
21	LFA	B	307	-	16,16,19	0.38	0	15,15,18	0.20	0
21	LFA	P	301	-	14,14,19	0.16	0	13,13,18	0.10	0
23	EDO	A	615	-	3,3,3	0.55	0	2,2,2	0.30	0
22	DMU	B	302	-	10,10,34	0.24	0	9,9,45	0.62	0
23	EDO	T	103	-	3,3,3	0.27	0	2,2,2	0.18	0
21	LFA	T	102	-	10,10,19	0.21	0	9,9,18	0.17	0
22	DMU	D	201	-	34,34,34	1.43	5 (14%)	45,45,45	1.58	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	EDO	P	323	-	3,3,3	0.64	0	2,2,2	0.95	0
23	EDO	O	309	-	3,3,3	0.19	0	2,2,2	0.29	0
23	EDO	E	201	-	3,3,3	0.15	0	2,2,2	0.03	0
22	DMU	C	324	-	34,34,34	0.80	0	45,45,45	1.25	3 (6%)
21	LFA	N	608	-	13,13,19	0.35	0	12,12,18	0.36	0
29	PEK	T	101	-	52,52,52	0.65	2 (3%)	55,57,57	0.86	4 (7%)
22	DMU	P	317	-	6,6,34	0.30	0	5,5,45	0.40	0
22	DMU	P	316	-	34,34,34	0.75	0	45,45,45	1.44	5 (11%)
21	LFA	C	309	-	17,17,19	0.23	0	16,16,18	0.14	0
22	DMU	A	612	-	34,34,34	1.25	5 (14%)	45,45,45	1.20	4 (8%)
22	DMU	P	320	-	34,34,34	1.05	3 (8%)	45,45,45	1.31	2 (4%)
22	DMU	Z	101	-	34,34,34	0.97	2 (5%)	45,45,45	1.09	3 (6%)
21	LFA	C	313	-	14,14,19	0.30	0	13,13,18	0.43	0
20	CO2	N	607	-	2,2,2	0.08	0	1,1,1	0.29	0
22	DMU	C	319	-	34,34,34	0.72	0	45,45,45	1.27	7 (15%)
22	DMU	C	315	-	34,34,34	0.79	1 (2%)	45,45,45	1.39	7 (15%)
23	EDO	S	103	-	3,3,3	0.04	0	2,2,2	0.13	0
23	EDO	F	102	-	3,3,3	0.24	0	2,2,2	0.24	0
23	EDO	C	320	-	3,3,3	0.07	0	2,2,2	0.14	0
26	CHD	B	306	-	32,32,32	0.75	0	51,51,51	0.75	0
23	EDO	R	201	-	3,3,3	0.14	0	2,2,2	0.10	0
22	DMU	J	101	-	10,10,34	0.21	0	9,9,45	0.65	0
19	CDL	V	101	-	63,63,99	0.54	0	69,75,111	1.33	8 (11%)
21	LFA	P	313	-	10,10,19	0.18	0	9,9,18	0.27	0
23	EDO	E	203	-	3,3,3	0.18	0	2,2,2	0.19	0
21	LFA	P	314	-	14,14,19	0.27	0	13,13,18	0.17	0
24	PGV	A	617	-	50,50,50	0.78	2 (4%)	53,56,56	1.08	2 (3%)
21	LFA	P	310	-	17,17,19	0.20	0	16,16,18	0.18	0
21	LFA	O	303	-	10,10,19	0.18	0	9,9,18	0.09	0
19	CDL	Y	101	-	93,93,99	0.39	0	99,105,111	0.51	0
23	EDO	N	612	-	3,3,3	0.35	0	2,2,2	0.25	0
22	DMU	B	303	-	10,10,34	0.31	0	9,9,45	0.58	0
22	DMU	L	102	-	22,22,34	0.76	0	27,27,45	1.08	1 (3%)
21	LFA	A	610	-	13,13,19	0.58	0	12,12,18	0.40	0
22	DMU	A	618	-	10,10,34	0.30	0	9,9,45	0.55	0
23	EDO	C	322	-	3,3,3	0.87	0	2,2,2	0.71	0
22	DMU	A	611	-	6,6,34	0.59	0	5,5,45	0.27	0
23	EDO	F	103	-	3,3,3	0.18	0	2,2,2	0.35	0
25	CUA	B	301	2	0,1,1	-	-	-	-	-
22	DMU	G	102	-	10,10,34	0.29	0	9,9,45	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	EDO	R	202	-	3,3,3	0.16	0	2,2,2	0.27	0
22	DMU	Q	201	-	34,34,34	1.39	7 (20%)	45,45,45	1.69	8 (17%)
26	CHD	O	301	-	32,32,32	0.72	0	51,51,51	0.90	1 (1%)
23	EDO	P	322	-	3,3,3	0.14	0	2,2,2	0.29	0
22	DMU	C	323	-	22,22,34	0.75	0	27,27,45	1.02	1 (3%)
23	EDO	C	321	-	3,3,3	0.27	0	2,2,2	0.24	0
21	LFA	A	609	-	13,13,19	0.35	0	12,12,18	0.18	0
23	EDO	N	613	-	3,3,3	0.18	0	2,2,2	0.27	0
21	LFA	C	308	-	5,5,19	0.21	0	4,4,18	0.09	0
23	EDO	S	102	-	3,3,3	0.30	0	2,2,2	0.12	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LFA	P	308	-	-	7/8/8/17	-
19	CDL	A	607	-	-	38/74/74/110	-
22	DMU	N	610	-	-	2/4/4/59	-
22	DMU	O	308	-	-	4/13/33/59	0/1/1/2
22	DMU	P	318	-	-	6/13/33/59	0/1/1/2
22	DMU	M	102	-	-	4/5/5/59	-
26	CHD	P	302	-	-	2/9/74/74	0/4/4/4
22	DMU	B	304	-	-	6/13/33/59	0/1/1/2
23	EDO	A	613	-	-	0/1/1/1	-
22	DMU	C	306	-	-	2/8/8/59	-
21	LFA	C	311	-	-	7/11/11/17	-
21	LFA	C	310	-	-	7/8/8/17	-
21	LFA	P	309	-	-	0/3/3/17	-
22	DMU	U	101	-	-	5/19/59/59	0/2/2/2
23	EDO	A	614	-	-	1/1/1/1	-
21	LFA	P	312	-	-	5/11/11/17	-
22	DMU	O	306	-	-	3/8/8/59	-
24	PGV	N	617	-	-	6/55/55/55	-
21	LFA	P	315	-	-	6/10/10/17	-
14	HEA	N	601[B]	-	-	3/32/76/76	-
14	HEA	A	601[B]	-	-	4/32/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	DMU	P	307	-	-	2/8/8/59	-
23	EDO	P	321	-	-	0/1/1/1	-
22	DMU	W	101	-	-	5/8/8/59	-
21	LFA	C	307	-	-	6/8/8/17	-
21	LFA	N	609	-	-	4/11/11/17	-
21	LFA	O	302	-	-	12/14/14/17	-
19	CDL	P	305	-	-	53/97/97/110	-
14	HEA	A	601[A]	-	-	5/32/76/76	-
23	EDO	A	616	-	-	0/1/1/1	-
26	CHD	C	305	-	-	7/9/74/74	0/4/4/4
19	CDL	C	304	-	-	43/97/97/110	-
21	LFA	C	312	-	-	4/8/8/17	-
22	DMU	C	317	-	-	8/13/33/59	0/1/1/2
23	EDO	E	202	-	-	0/1/1/1	-
26	CHD	C	301	-	-	2/9/74/74	0/4/4/4
22	DMU	B	308	-	-	9/13/33/59	0/1/1/2
22	DMU	Z	103	-	-	2/5/5/59	-
23	EDO	B	305	-	-	0/1/1/1	-
22	DMU	O	304	-	-	7/13/33/59	0/1/1/2
24	PGV	P	304	-	-	10/55/55/55	-
23	EDO	G	103	-	-	0/1/1/1	-
22	DMU	C	318	-	-	12/19/59/59	0/2/2/2
22	DMU	P	324	-	-	7/13/33/59	0/1/1/2
22	DMU	C	316	-	-	3/4/4/59	-
23	EDO	N	614	-	-	0/1/1/1	-
22	DMU	M	101	-	-	4/19/59/59	0/2/2/2
14	HEA	N	602	1,18	-	4/32/76/76	-
23	EDO	N	615	-	-	0/1/1/1	-
29	PEK	G	101	-	-	15/56/56/56	-
22	DMU	H	101	-	-	7/19/59/59	0/2/2/2
22	DMU	P	319	-	-	15/19/59/59	0/2/2/2
26	CHD	P	306	-	-	5/9/74/74	0/4/4/4
14	HEA	N	601[A]	-	-	6/32/76/76	-
23	EDO	R	203	-	-	1/1/1/1	-
23	EDO	N	616	-	-	0/1/1/1	-
22	DMU	N	611	-	-	5/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LFA	C	314	-	-	3/10/10/17	-
21	LFA	P	311	-	-	6/8/8/17	-
22	DMU	Z	102	-	-	11/13/33/59	0/1/1/2
19	CDL	L	101	-	-	50/104/104/110	-
14	HEA	A	602	1,18	-	4/32/76/76	-
22	DMU	P	325	-	-	5/19/59/59	0/2/2/2
22	DMU	O	307	-	-	3/8/8/59	-
24	PGV	C	303	-	-	10/55/55/55	-
21	LFA	C	325	-	-	8/12/12/17	-
21	LFA	B	307	-	-	11/14/14/17	-
21	LFA	P	301	-	-	6/12/12/17	-
23	EDO	A	615	-	-	0/1/1/1	-
22	DMU	B	302	-	-	4/8/8/59	-
23	EDO	T	103	-	-	0/1/1/1	-
21	LFA	T	102	-	-	3/8/8/17	-
22	DMU	D	201	-	-	7/19/59/59	0/2/2/2
23	EDO	P	323	-	-	0/1/1/1	-
23	EDO	O	309	-	-	0/1/1/1	-
23	EDO	E	201	-	-	0/1/1/1	-
22	DMU	C	324	-	-	4/19/59/59	0/2/2/2
21	LFA	N	608	-	-	4/11/11/17	-
29	PEK	T	101	-	-	20/56/56/56	-
22	DMU	P	317	-	-	3/4/4/59	-
22	DMU	P	316	-	-	11/19/59/59	0/2/2/2
21	LFA	C	309	-	-	8/15/15/17	-
22	DMU	A	612	-	-	7/19/59/59	0/2/2/2
22	DMU	P	320	-	-	8/19/59/59	0/2/2/2
22	DMU	Z	101	-	-	7/19/59/59	0/2/2/2
21	LFA	C	313	-	-	2/12/12/17	-
22	DMU	C	319	-	-	10/19/59/59	0/2/2/2
22	DMU	C	315	-	-	11/19/59/59	0/2/2/2
23	EDO	S	103	-	-	0/1/1/1	-
23	EDO	F	102	-	-	0/1/1/1	-
23	EDO	C	320	-	-	1/1/1/1	-
26	CHD	B	306	-	-	2/9/74/74	0/4/4/4
23	EDO	R	201	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	DMU	J	101	-	-	3/8/8/59	-
19	CDL	V	101	-	-	41/74/74/110	-
21	LFA	P	313	-	-	5/8/8/17	-
23	EDO	E	203	-	-	0/1/1/1	-
21	LFA	P	314	-	-	6/12/12/17	-
24	PGV	A	617	-	-	8/55/55/55	-
21	LFA	P	310	-	-	9/15/15/17	-
21	LFA	O	303	-	-	2/8/8/17	-
19	CDL	Y	101	-	-	50/104/104/110	-
23	EDO	N	612	-	-	0/1/1/1	-
22	DMU	B	303	-	-	5/8/8/59	-
22	DMU	L	102	-	-	8/13/33/59	0/1/1/2
21	LFA	A	610	-	-	5/11/11/17	-
22	DMU	A	618	-	-	6/8/8/59	-
23	EDO	C	322	-	-	0/1/1/1	-
22	DMU	A	611	-	-	2/4/4/59	-
23	EDO	F	103	-	-	1/1/1/1	-
22	DMU	G	102	-	-	5/8/8/59	-
23	EDO	R	202	-	-	0/1/1/1	-
22	DMU	Q	201	-	-	9/19/59/59	0/2/2/2
26	CHD	O	301	-	-	2/9/74/74	0/4/4/4
23	EDO	P	322	-	-	0/1/1/1	-
22	DMU	C	323	-	-	9/13/33/59	0/1/1/2
23	EDO	C	321	-	-	0/1/1/1	-
21	LFA	A	609	-	-	4/11/11/17	-
23	EDO	N	613	-	-	0/1/1/1	-
21	LFA	C	308	-	-	1/3/3/17	-
23	EDO	S	102	-	-	0/1/1/1	-

All (146) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	611	DMU	O16-C6	-5.20	1.31	1.40
14	N	602	HEA	C1D-ND	-5.01	1.31	1.40
14	A	602	HEA	CHD-C1D	4.52	1.46	1.35
14	A	601[A]	HEA	C3A-C2A	4.51	1.46	1.40
14	A	601[B]	HEA	C3A-C2A	4.51	1.46	1.40
14	A	602	HEA	C1B-NB	-4.37	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	601[A]	HEA	C3C-C2C	4.33	1.46	1.40
14	N	601[B]	HEA	C3C-C2C	4.33	1.46	1.40
14	N	602	HEA	C1B-NB	-4.30	1.29	1.38
14	A	601[A]	HEA	C1D-ND	-4.22	1.33	1.40
14	A	601[B]	HEA	C1D-ND	-4.22	1.33	1.40
14	A	602	HEA	C3A-C2A	4.20	1.46	1.40
14	N	601[A]	HEA	CHC-C4B	4.09	1.45	1.35
14	N	601[B]	HEA	CHC-C4B	4.09	1.45	1.35
14	N	602	HEA	CHD-C1D	4.09	1.45	1.35
14	N	601[A]	HEA	C1D-ND	-3.96	1.33	1.40
14	N	601[B]	HEA	C1D-ND	-3.96	1.33	1.40
14	N	602	HEA	C3D-C2D	3.80	1.44	1.36
14	A	602	HEA	C1D-ND	-3.80	1.33	1.40
14	N	601[A]	HEA	C1B-NB	-3.73	1.31	1.38
14	N	601[B]	HEA	C1B-NB	-3.73	1.31	1.38
14	N	602	HEA	C3B-C2B	3.72	1.43	1.34
14	A	601[A]	HEA	C3C-C2C	3.65	1.45	1.40
14	A	601[B]	HEA	C3C-C2C	3.65	1.45	1.40
14	N	601[A]	HEA	C3B-C2B	3.64	1.42	1.34
14	N	601[B]	HEA	C3B-C2B	3.64	1.42	1.34
22	P	320	DMU	C7-C5	-3.63	1.43	1.52
14	A	601[A]	HEA	C3D-C2D	3.57	1.44	1.36
14	A	601[B]	HEA	C3D-C2D	3.57	1.44	1.36
14	A	601[A]	HEA	C16-C17	-3.56	1.41	1.53
14	A	601[B]	HEA	C16-C17	-3.56	1.41	1.53
14	N	601[A]	HEA	CHD-C1D	3.52	1.44	1.35
14	N	601[B]	HEA	CHD-C1D	3.52	1.44	1.35
22	D	201	DMU	O5-C6	-3.51	1.32	1.41
26	P	306	CHD	O25-C24	3.45	1.33	1.22
14	A	602	HEA	C4D-ND	-3.42	1.31	1.38
22	D	201	DMU	O16-C6	-3.42	1.34	1.40
14	A	601[A]	HEA	CHD-C1D	3.39	1.43	1.35
14	A	601[B]	HEA	CHD-C1D	3.39	1.43	1.35
14	A	601[A]	HEA	C4B-NB	-3.35	1.34	1.40
14	A	601[B]	HEA	C4B-NB	-3.35	1.34	1.40
22	P	318	DMU	O16-C6	3.35	1.45	1.40
14	N	602	HEA	CHC-C4B	3.34	1.43	1.35
14	A	602	HEA	C3B-C2B	3.32	1.42	1.34
22	C	318	DMU	C7-C5	-3.30	1.43	1.52
14	A	601[A]	HEA	C3B-C2B	3.29	1.42	1.34
14	A	601[B]	HEA	C3B-C2B	3.29	1.42	1.34
14	A	601[A]	HEA	CHC-C4B	3.26	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[B]	HEA	CHC-C4B	3.26	1.43	1.35
14	N	601[A]	HEA	C4B-C3B	3.25	1.50	1.44
14	N	601[B]	HEA	C4B-C3B	3.25	1.50	1.44
14	N	602	HEA	C4B-NB	-3.21	1.34	1.40
22	C	318	DMU	O5-C6	-3.14	1.33	1.41
24	N	617	PGV	O03-C19	3.13	1.42	1.33
22	A	612	DMU	C7-C5	-3.08	1.44	1.52
14	N	602	HEA	C3A-C2A	3.08	1.44	1.40
26	C	301	CHD	C22-C23	-3.05	1.43	1.52
24	A	617	PGV	O03-C19	3.04	1.42	1.33
14	A	601[A]	HEA	CMC-C2C	-3.03	1.45	1.51
14	A	601[B]	HEA	CMC-C2C	-3.03	1.45	1.51
14	N	602	HEA	C2A-C1A	2.97	1.49	1.42
24	P	304	PGV	O03-C19	2.92	1.41	1.33
22	Q	201	DMU	O5-C6	-2.90	1.34	1.41
14	A	601[A]	HEA	C1B-NB	-2.89	1.32	1.38
14	A	601[B]	HEA	C1B-NB	-2.89	1.32	1.38
14	A	601[A]	HEA	CAA-C2A	-2.88	1.47	1.52
14	A	601[B]	HEA	CAA-C2A	-2.88	1.47	1.52
22	P	320	DMU	C10-C5	-2.87	1.44	1.52
22	U	101	DMU	C7-C5	-2.87	1.45	1.52
14	N	601[A]	HEA	CAA-C2A	-2.86	1.47	1.52
14	N	601[B]	HEA	CAA-C2A	-2.86	1.47	1.52
22	Z	101	DMU	O3-C5	-2.84	1.36	1.43
22	M	101	DMU	O3-C5	-2.82	1.36	1.43
14	N	601[A]	HEA	C16-C17	-2.81	1.44	1.53
14	N	601[B]	HEA	C16-C17	-2.81	1.44	1.53
14	N	601[A]	HEA	C3D-C2D	2.78	1.42	1.36
14	N	601[B]	HEA	C3D-C2D	2.78	1.42	1.36
29	G	101	PEK	C23-C22	-2.77	1.42	1.52
29	T	101	PEK	C23-C22	-2.76	1.42	1.52
14	N	601[A]	HEA	C4D-ND	-2.76	1.33	1.38
14	N	601[B]	HEA	C4D-ND	-2.76	1.33	1.38
22	Q	201	DMU	C10-C5	-2.75	1.44	1.52
26	C	301	CHD	O26-C24	-2.74	1.21	1.30
26	P	302	CHD	C22-C23	-2.71	1.44	1.52
22	H	101	DMU	C7-C5	-2.71	1.45	1.52
14	A	602	HEA	C4B-NB	-2.70	1.35	1.40
14	A	602	HEA	C18-C19	2.69	1.39	1.33
26	P	302	CHD	O26-C24	-2.66	1.21	1.30
14	A	602	HEA	CHC-C4B	2.66	1.41	1.35
14	N	602	HEA	C1B-C2B	2.65	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Q	201	DMU	O3-C5	-2.64	1.36	1.43
14	A	601[A]	HEA	C4B-C3B	2.61	1.49	1.44
14	A	601[B]	HEA	C4B-C3B	2.61	1.49	1.44
14	N	601[A]	HEA	CBA-CGA	2.60	1.56	1.50
14	N	601[B]	HEA	CBA-CGA	2.60	1.56	1.50
14	N	601[A]	HEA	C3A-C2A	2.59	1.44	1.40
14	N	601[B]	HEA	C3A-C2A	2.59	1.44	1.40
22	A	612	DMU	O16-C6	-2.57	1.35	1.40
14	N	602	HEA	C4D-ND	-2.53	1.33	1.38
22	D	201	DMU	O3-C5	-2.53	1.37	1.43
22	A	612	DMU	O7-C10	2.51	1.48	1.41
22	D	201	DMU	O55-C2	2.49	1.48	1.43
14	A	602	HEA	C2A-C1A	2.46	1.48	1.42
22	N	611	DMU	C7-C5	-2.43	1.46	1.52
22	P	319	DMU	O3-C5	2.43	1.48	1.43
29	T	101	PEK	C2-C1	2.42	1.57	1.50
14	A	601[A]	HEA	O1D-CGD	2.40	1.30	1.22
14	A	601[B]	HEA	O1D-CGD	2.40	1.30	1.22
22	P	319	DMU	C7-C5	-2.37	1.46	1.52
14	N	601[A]	HEA	C1D-C2D	2.36	1.49	1.44
14	N	601[B]	HEA	C1D-C2D	2.36	1.49	1.44
22	N	611	DMU	O5-C6	-2.35	1.35	1.41
14	A	602	HEA	C4D-C3D	2.35	1.49	1.45
22	O	304	DMU	C3-C4	-2.31	1.48	1.53
22	U	101	DMU	C6-C1	-2.31	1.45	1.52
22	D	201	DMU	O61-C57	2.30	1.52	1.42
14	A	601[A]	HEA	C2A-C1A	2.29	1.47	1.42
14	A	601[B]	HEA	C2A-C1A	2.29	1.47	1.42
24	A	617	PGV	O01-C1	2.28	1.40	1.34
22	N	611	DMU	C10-C5	-2.28	1.45	1.52
14	N	601[A]	HEA	C2A-C1A	2.27	1.47	1.42
14	N	601[B]	HEA	C2A-C1A	2.27	1.47	1.42
22	P	320	DMU	O4-C7	2.27	1.48	1.43
22	M	101	DMU	C7-C5	-2.25	1.46	1.52
26	P	302	CHD	C8-C14	-2.24	1.49	1.53
22	Q	201	DMU	O16-C6	-2.22	1.36	1.40
22	C	318	DMU	O3-C5	2.22	1.48	1.43
26	C	301	CHD	O25-C24	2.19	1.29	1.22
22	Q	201	DMU	O55-C2	2.17	1.48	1.43
14	N	601[A]	HEA	C4B-NB	-2.17	1.36	1.40
14	N	601[B]	HEA	C4B-NB	-2.17	1.36	1.40
22	A	612	DMU	O3-C5	-2.17	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Q	201	DMU	O1-C10	2.16	1.47	1.41
22	H	101	DMU	C10-C5	-2.14	1.46	1.52
22	Z	101	DMU	O5-C6	-2.12	1.36	1.41
22	Q	201	DMU	C7-C5	-2.10	1.47	1.52
22	C	315	DMU	O3-C5	-2.10	1.38	1.43
24	P	304	PGV	O03-C01	-2.09	1.40	1.45
22	P	319	DMU	O5-C6	-2.09	1.36	1.41
24	C	303	PGV	O01-C1	2.08	1.40	1.34
14	A	602	HEA	CBD-CGD	2.08	1.55	1.50
22	N	611	DMU	C6-C1	-2.08	1.46	1.52
22	A	612	DMU	C10-C5	-2.07	1.46	1.52
19	P	305	CDL	C12-C11	-2.04	1.44	1.52
22	B	304	DMU	O16-C6	2.04	1.43	1.40
14	N	602	HEA	C4B-C3B	2.01	1.48	1.44

All (292) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601[A]	HEA	C3D-C4D-ND	7.88	117.99	110.36
14	N	601[B]	HEA	C3D-C4D-ND	7.88	117.99	110.36
14	N	602	HEA	C3D-C4D-ND	7.21	117.34	110.36
22	Q	201	DMU	O16-C6-C1	6.52	118.48	108.30
22	P	316	DMU	O16-C6-C1	6.14	117.89	108.30
14	A	601[A]	HEA	C3D-C4D-ND	6.06	116.22	110.36
14	A	601[B]	HEA	C3D-C4D-ND	6.06	116.22	110.36
14	N	601[A]	HEA	C2D-C1D-ND	5.80	116.71	109.84
14	N	601[B]	HEA	C2D-C1D-ND	5.80	116.71	109.84
22	P	324	DMU	O16-C6-C1	5.76	117.29	108.30
14	A	602	HEA	C3B-C4B-NB	5.68	116.57	109.84
22	C	324	DMU	O16-C6-C1	5.57	117.00	108.30
22	B	308	DMU	O16-C6-C1	5.51	116.91	108.30
14	A	601[A]	HEA	C2D-C1D-ND	5.44	116.29	109.84
14	A	601[B]	HEA	C2D-C1D-ND	5.44	116.29	109.84
14	A	602	HEA	C2B-C1B-NB	5.42	116.38	109.88
22	C	315	DMU	O16-C6-C1	5.41	116.75	108.30
19	V	101	CDL	OA6-CA4-CA3	5.39	127.92	108.40
14	N	601[A]	HEA	C2B-C1B-NB	5.39	116.34	109.88
14	N	601[B]	HEA	C2B-C1B-NB	5.39	116.34	109.88
26	C	305	CHD	C16-C17-C20	5.34	120.42	112.15
14	N	601[A]	HEA	C27-C19-C20	5.29	124.17	115.27
14	A	601[A]	HEA	C3C-C4C-NC	5.29	116.04	109.21
14	A	601[B]	HEA	C3C-C4C-NC	5.29	116.04	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	C3B-C4B-NB	5.25	116.06	109.84
14	N	602	HEA	C2B-C1B-NB	5.21	116.12	109.88
14	N	602	HEA	C2D-C1D-ND	5.19	115.99	109.84
14	A	601[A]	HEA	C2B-C1B-NB	5.12	116.01	109.88
14	A	601[B]	HEA	C2B-C1B-NB	5.12	116.01	109.88
22	P	325	DMU	C10-C5-C7	5.06	120.54	110.00
19	A	607	CDL	OA6-CA4-CA6	5.06	126.71	108.40
14	A	601[A]	HEA	C3B-C4B-NB	5.05	115.82	109.84
14	A	601[B]	HEA	C3B-C4B-NB	5.05	115.82	109.84
14	A	601[B]	HEA	C27-C19-C20	4.96	123.61	115.27
22	P	320	DMU	O16-C6-C1	4.84	115.86	108.30
14	A	602	HEA	C13-C12-C11	-4.80	107.14	114.35
22	D	201	DMU	O16-C6-C1	4.67	115.60	108.30
14	N	601[A]	HEA	C1D-C2D-C3D	-4.64	102.07	106.96
14	N	601[B]	HEA	C1D-C2D-C3D	-4.64	102.07	106.96
22	P	318	DMU	O5-C6-C1	4.61	120.11	110.35
26	C	305	CHD	C17-C13-C14	-4.52	95.53	100.09
14	N	602	HEA	C3C-C4C-NC	4.49	115.02	109.21
14	A	601[A]	HEA	C13-C12-C11	-4.47	107.64	114.35
14	A	601[B]	HEA	C13-C12-C11	-4.47	107.64	114.35
14	A	602	HEA	C2D-C1D-ND	4.39	115.04	109.84
14	N	602	HEA	CHB-C1B-C2B	-4.37	118.15	124.98
14	A	602	HEA	C3D-C4D-ND	4.36	114.58	110.36
14	A	601[A]	HEA	CHA-C4D-C3D	-4.34	118.46	124.84
14	A	601[B]	HEA	CHA-C4D-C3D	-4.34	118.46	124.84
19	V	101	CDL	OA6-CA5-C11	4.33	120.84	111.50
24	N	617	PGV	O03-C19-C20	4.33	125.49	111.91
24	N	617	PGV	O03-C19-O04	-4.31	112.72	123.59
14	N	602	HEA	C4D-C3D-C2D	-4.30	100.64	106.90
14	N	601[A]	HEA	CHB-C1B-C2B	-4.25	118.34	124.98
14	N	601[B]	HEA	CHB-C1B-C2B	-4.25	118.34	124.98
14	N	602	HEA	CHA-C4D-C3D	-4.23	118.63	124.84
14	N	601[A]	HEA	C1D-ND-C4D	-4.19	100.75	105.07
14	N	601[B]	HEA	C1D-ND-C4D	-4.19	100.75	105.07
14	A	601[A]	HEA	C27-C19-C20	4.19	122.32	115.27
24	A	617	PGV	O03-C19-O04	-4.18	113.05	123.59
22	P	325	DMU	O16-C6-C1	4.17	114.82	108.30
14	N	602	HEA	CAD-CBD-CGD	-4.16	104.66	113.60
19	V	101	CDL	OA6-CA4-CA6	-4.11	93.53	108.40
14	N	601[A]	HEA	C3B-C4B-NB	4.08	114.67	109.84
14	N	601[B]	HEA	C3B-C4B-NB	4.08	114.67	109.84
24	C	303	PGV	C27-C26-C25	-4.06	93.82	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	M	101	DMU	O16-C6-C1	4.06	114.64	108.30
19	C	304	CDL	OA6-CA5-C11	-4.04	102.79	111.50
26	C	305	CHD	C14-C13-C12	4.01	111.14	107.40
19	A	607	CDL	CA4-OA6-CA5	4.01	127.66	117.79
22	H	101	DMU	O16-C6-C1	4.01	114.56	108.30
14	A	601[A]	HEA	CHB-C1B-C2B	-4.00	118.73	124.98
14	A	601[B]	HEA	CHB-C1B-C2B	-4.00	118.73	124.98
14	N	601[A]	HEA	CMC-C2C-C3C	3.99	132.15	124.68
14	N	601[B]	HEA	CMC-C2C-C3C	3.99	132.15	124.68
19	A	607	CDL	OA5-PA1-OA3	3.97	124.57	109.07
14	N	601[A]	HEA	C3C-C4C-NC	3.92	114.28	109.21
14	N	601[B]	HEA	C3C-C4C-NC	3.92	114.28	109.21
22	O	304	DMU	O5-C6-C1	3.91	118.64	110.35
14	N	602	HEA	CAD-C3D-C4D	3.91	131.50	124.66
14	N	601[A]	HEA	C20-C19-C18	-3.83	113.36	121.12
22	D	201	DMU	O1-C9-C8	3.81	116.61	109.69
22	C	319	DMU	O16-C6-C1	3.80	114.24	108.30
14	A	602	HEA	CHA-C4D-C3D	-3.80	119.26	124.84
14	A	602	HEA	CAD-CBD-CGD	-3.80	105.43	113.60
14	A	601[B]	HEA	C20-C19-C18	-3.78	113.47	121.12
22	C	323	DMU	O16-C6-C1	3.74	114.14	108.30
22	L	102	DMU	O5-C6-O16	3.74	118.82	109.97
22	U	101	DMU	C10-C5-C7	3.69	117.69	110.00
22	D	201	DMU	C11-C9-C8	-3.66	104.43	113.00
14	A	602	HEA	CHB-C1B-C2B	-3.61	119.33	124.98
22	Z	101	DMU	O16-C6-C1	3.61	113.94	108.30
22	N	611	DMU	C10-O1-C9	3.59	120.73	113.69
14	N	601[A]	HEA	CHA-C4D-C3D	-3.57	119.58	124.84
14	N	601[B]	HEA	CHA-C4D-C3D	-3.57	119.58	124.84
14	A	602	HEA	C3C-C4C-NC	3.55	113.80	109.21
14	A	602	HEA	C4B-C3B-C2B	-3.55	101.35	107.41
22	C	317	DMU	O5-C6-C1	3.53	117.81	110.35
24	A	617	PGV	O03-C19-C20	3.52	122.96	111.91
22	P	320	DMU	C8-C7-C5	-3.51	104.69	110.82
22	U	101	DMU	O3-C5-C10	3.49	118.51	110.05
19	A	607	CDL	OA2-PA1-OA3	-3.46	95.56	109.07
22	P	319	DMU	C10-C5-C7	3.45	117.17	110.00
19	C	304	CDL	OB5-PB2-OB3	3.44	122.50	109.07
19	V	101	CDL	OA4-PA1-OA5	3.42	123.62	107.75
22	U	101	DMU	O16-C6-C1	3.41	113.63	108.30
14	A	602	HEA	C4B-NB-C1B	-3.38	101.58	105.07
24	N	617	PGV	O01-C1-O02	-3.38	115.53	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	319	DMU	O16-C6-C1	3.36	113.54	108.30
14	N	602	HEA	C1D-C2D-C3D	-3.35	103.43	106.96
22	Z	102	DMU	O5-C6-O16	3.35	117.90	109.97
19	L	101	CDL	OB4-PB2-OB2	3.35	123.28	107.75
14	A	601[A]	HEA	C4B-C3B-C2B	-3.33	101.72	107.41
14	A	601[B]	HEA	C4B-C3B-C2B	-3.33	101.72	107.41
14	A	601[A]	HEA	C4D-C3D-C2D	-3.33	102.05	106.90
14	A	601[B]	HEA	C4D-C3D-C2D	-3.33	102.05	106.90
14	A	602	HEA	C4D-C3D-C2D	-3.30	102.08	106.90
14	N	602	HEA	CBA-CAA-C2A	-3.30	107.04	112.60
14	N	602	HEA	C1B-C2B-C3B	-3.29	102.87	106.80
22	C	318	DMU	O16-C6-C1	3.26	113.40	108.30
22	Q	201	DMU	C6-O5-C4	-3.24	107.33	113.69
19	P	305	CDL	OA4-PA1-OA2	-3.22	92.77	107.75
14	N	602	HEA	C4B-C3B-C2B	-3.22	101.91	107.41
14	N	602	HEA	C4D-CHA-C1A	3.20	126.78	122.56
14	N	601[A]	HEA	C13-C12-C11	-3.19	109.55	114.35
14	N	601[B]	HEA	C13-C12-C11	-3.19	109.55	114.35
14	N	602	HEA	CMD-C2D-C1D	3.19	129.90	125.04
14	A	601[A]	HEA	C1D-C2D-C3D	-3.18	103.61	106.96
14	A	601[B]	HEA	C1D-C2D-C3D	-3.18	103.61	106.96
19	C	304	CDL	OA4-PA1-OA2	-3.17	93.01	107.75
14	N	601[A]	HEA	C4B-C3B-C2B	-3.16	102.01	107.41
14	N	601[B]	HEA	C4B-C3B-C2B	-3.16	102.01	107.41
14	A	601[A]	HEA	C1D-ND-C4D	-3.14	101.83	105.07
14	A	601[B]	HEA	C1D-ND-C4D	-3.14	101.83	105.07
19	A	607	CDL	OA6-CA5-C11	3.14	118.27	111.50
14	A	601[A]	HEA	CHC-C4B-NB	-3.12	120.52	124.38
14	A	601[B]	HEA	CHC-C4B-NB	-3.12	120.52	124.38
22	Q	201	DMU	C11-C9-C8	-3.12	105.70	113.00
22	D	201	DMU	C10-C5-C7	3.12	116.49	110.00
22	C	318	DMU	O3-C5-C10	3.11	117.60	110.05
14	N	602	HEA	C20-C19-C18	-3.10	114.83	121.12
14	N	601[A]	HEA	C4D-C3D-C2D	-3.09	102.39	106.90
14	N	601[B]	HEA	C4D-C3D-C2D	-3.09	102.39	106.90
14	A	602	HEA	CMB-C2B-C1B	3.08	129.74	125.04
22	C	315	DMU	C18-O16-C6	-3.08	108.74	113.84
19	C	304	CDL	OA7-CA5-C11	3.01	135.47	123.73
14	N	602	HEA	C13-C12-C11	-3.00	109.84	114.35
29	T	101	PEK	O01-C1-O02	-2.99	116.47	123.70
22	A	612	DMU	C10-O7-C3	-2.96	110.63	117.96
24	C	303	PGV	O03-C19-O04	-2.92	116.21	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	304	PGV	C27-C26-C25	-2.88	99.80	114.42
14	A	601[A]	HEA	CAD-C3D-C4D	2.87	129.68	124.66
14	A	601[B]	HEA	CAD-C3D-C4D	2.87	129.68	124.66
22	C	315	DMU	C10-C5-C7	2.87	115.97	110.00
22	U	101	DMU	C10-O7-C3	-2.83	110.97	117.96
22	C	319	DMU	O3-C5-C7	2.83	116.88	110.35
22	C	315	DMU	O5-C6-O16	-2.79	103.36	109.97
22	C	318	DMU	C8-C7-C5	-2.79	105.95	110.82
22	O	308	DMU	C57-C4-C3	-2.78	106.50	113.00
14	A	601[B]	HEA	C21-C22-C23	-2.77	118.27	127.75
26	C	305	CHD	C16-C17-C13	-2.77	100.84	103.55
19	P	305	CDL	OA4-PA1-OA3	2.75	125.82	112.24
14	A	602	HEA	C1B-C2B-C3B	-2.74	103.53	106.80
19	C	304	CDL	OB6-CB5-C51	2.73	117.39	111.50
19	V	101	CDL	OA7-CA5-C11	-2.73	113.08	123.73
29	T	101	PEK	C2-C3-C4	2.72	118.08	113.23
29	T	101	PEK	O02-C1-C2	2.72	134.33	123.73
26	C	305	CHD	C17-C13-C12	-2.71	115.20	117.67
22	C	317	DMU	C2-C3-C4	-2.69	105.43	110.24
26	C	305	CHD	C6-C7-C8	2.69	114.36	111.48
14	A	602	HEA	CMC-C2C-C3C	2.69	129.71	124.68
14	A	601[A]	HEA	C4B-NB-C1B	-2.69	102.30	105.07
14	A	601[B]	HEA	C4B-NB-C1B	-2.69	102.30	105.07
22	Q	201	DMU	O1-C9-C8	2.69	114.57	109.69
22	D	201	DMU	C7-C8-C9	2.68	115.01	110.24
14	A	601[A]	HEA	CMD-C2D-C1D	2.66	129.09	125.04
14	A	601[B]	HEA	CMD-C2D-C1D	2.66	129.09	125.04
14	A	602	HEA	CMD-C2D-C1D	2.65	129.08	125.04
22	Q	201	DMU	C10-O1-C9	2.65	118.88	113.69
19	C	304	CDL	OA4-PA1-OA3	2.63	125.26	112.24
22	C	319	DMU	O3-C5-C10	2.62	116.42	110.05
22	O	304	DMU	O16-C6-C1	2.61	112.38	108.30
19	C	304	CDL	OA4-PA1-OA5	-2.61	95.64	107.75
14	N	601[B]	HEA	C20-C19-C18	-2.60	115.85	121.12
22	Z	101	DMU	O3-C5-C7	2.60	116.35	110.35
14	N	602	HEA	C1D-ND-C4D	-2.59	102.40	105.07
19	V	101	CDL	OA4-PA1-OA2	-2.59	95.73	107.75
19	V	101	CDL	CA4-OA6-CA5	2.59	124.16	117.79
19	L	101	CDL	OB5-PB2-OB3	-2.58	98.97	109.07
22	C	324	DMU	C10-C5-C7	2.58	115.36	110.00
22	P	324	DMU	C18-O16-C6	-2.57	109.57	113.84
22	C	315	DMU	C6-O5-C4	2.56	118.72	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	CMB-C2B-C1B	2.55	128.93	125.04
22	H	101	DMU	C10-C5-C7	2.54	115.29	110.00
22	C	319	DMU	C10-C5-C7	2.51	115.23	110.00
14	N	601[A]	HEA	CMD-C2D-C1D	2.49	128.83	125.04
14	N	601[B]	HEA	CMD-C2D-C1D	2.49	128.83	125.04
22	O	304	DMU	C6-C1-C2	2.48	115.17	110.00
22	N	611	DMU	C7-C8-C9	2.48	114.67	110.24
22	B	304	DMU	O5-C6-C1	2.48	115.59	110.35
14	N	601[A]	HEA	C1B-C2B-C3B	-2.47	103.85	106.80
14	N	601[B]	HEA	C1B-C2B-C3B	-2.47	103.85	106.80
14	N	602	HEA	C27-C19-C20	2.47	119.42	115.27
22	C	317	DMU	C18-O16-C6	-2.45	109.77	113.84
14	A	601[A]	HEA	CMC-C2C-C3C	2.45	129.27	124.68
14	A	601[B]	HEA	CMC-C2C-C3C	2.45	129.27	124.68
22	P	318	DMU	C6-O5-C4	2.44	118.48	113.69
22	Q	201	DMU	C2-C3-C4	-2.44	105.33	110.93
22	H	101	DMU	O3-C5-C10	2.44	115.97	110.05
19	C	304	CDL	OA5-PA1-OA3	2.43	118.58	109.07
14	A	601[A]	HEA	CHD-C1D-C2D	-2.42	120.03	126.72
14	A	601[B]	HEA	CHD-C1D-C2D	-2.42	120.03	126.72
14	A	602	HEA	C4D-CHA-C1A	2.41	125.74	122.56
14	A	601[B]	HEA	C25-C23-C24	2.41	119.92	114.60
24	C	303	PGV	C22-C21-C20	-2.40	104.55	113.19
22	A	612	DMU	C10-C5-C7	2.40	114.99	110.00
22	D	201	DMU	C2-C3-C4	-2.39	105.44	110.93
22	P	325	DMU	O5-C6-O16	2.39	115.63	109.97
22	Z	102	DMU	C57-C4-C3	-2.38	107.42	113.00
22	C	319	DMU	C11-C9-C8	-2.38	107.43	113.00
22	O	308	DMU	O5-C6-O16	2.37	115.58	109.97
22	P	325	DMU	C10-O1-C9	-2.35	109.07	113.69
22	O	308	DMU	O5-C6-C1	2.35	115.32	110.35
14	A	602	HEA	C1D-C2D-C3D	-2.32	104.52	106.96
14	N	602	HEA	CMC-C2C-C3C	2.32	129.01	124.68
24	C	303	PGV	O01-C1-O02	-2.30	118.14	123.70
22	A	612	DMU	O5-C6-C1	2.29	115.20	110.35
22	C	315	DMU	O5-C6-C1	2.29	115.19	110.35
19	V	101	CDL	OA2-PA1-OA3	-2.27	100.19	109.07
14	A	601[A]	HEA	C26-C15-C16	2.27	119.09	115.27
14	A	601[B]	HEA	C26-C15-C16	2.27	119.09	115.27
14	A	601[A]	HEA	C1B-C2B-C3B	-2.26	104.09	106.80
14	A	601[B]	HEA	C1B-C2B-C3B	-2.26	104.09	106.80
22	D	201	DMU	O4-C7-C8	-2.26	105.13	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	611	DMU	C10-C5-C7	2.25	114.69	110.00
22	U	101	DMU	O5-C6-O16	2.25	115.30	109.97
19	C	304	CDL	CA6-CA4-CA3	2.24	117.08	111.79
22	D	201	DMU	C10-O1-C9	2.23	118.06	113.69
19	C	304	CDL	OB2-PB2-OB3	-2.21	100.42	109.07
22	M	101	DMU	O5-C6-C1	2.21	115.03	110.35
22	N	611	DMU	O5-C6-C1	2.21	115.03	110.35
22	P	316	DMU	C10-C5-C7	2.20	114.58	110.00
22	H	101	DMU	O5-C6-C1	2.20	115.00	110.35
14	A	602	HEA	O1A-CGA-CBA	-2.20	116.03	123.08
22	A	612	DMU	O3-C5-C7	2.19	115.42	110.35
14	N	602	HEA	CHD-C1D-C2D	-2.19	120.67	126.72
22	Q	201	DMU	C18-O16-C6	2.18	117.46	113.84
14	A	602	HEA	CAD-C3D-C4D	2.18	128.46	124.66
14	A	602	HEA	CMB-C2B-C3B	-2.17	126.20	130.34
22	B	308	DMU	O5-C6-C1	2.17	114.94	110.35
22	B	308	DMU	C6-O5-C4	2.16	117.92	113.69
22	P	316	DMU	O5-C6-C1	2.15	114.91	110.35
24	N	617	PGV	C01-O03-C19	-2.15	109.16	117.12
22	C	315	DMU	O3-C5-C10	2.15	115.26	110.05
22	C	319	DMU	O5-C6-C1	2.13	114.86	110.35
14	N	602	HEA	CHC-C4B-C3B	-2.13	120.31	125.80
14	N	601[A]	HEA	CAD-C3D-C4D	2.13	128.38	124.66
14	N	601[B]	HEA	CAD-C3D-C4D	2.13	128.38	124.66
22	P	318	DMU	C6-C1-C2	2.13	114.43	110.00
14	A	602	HEA	C4A-CHB-C1B	2.12	125.35	122.56
14	N	601[A]	HEA	CHD-C1D-C2D	-2.10	120.91	126.72
14	N	601[B]	HEA	CHD-C1D-C2D	-2.10	120.91	126.72
14	A	602	HEA	C20-C19-C18	-2.09	116.88	121.12
14	N	601[A]	HEA	C21-C22-C23	-2.08	120.65	127.75
22	C	324	DMU	O3-C5-C7	2.07	115.14	110.35
22	P	325	DMU	O5-C4-C57	2.07	111.58	106.44
24	C	303	PGV	C03-C02-C01	-2.06	106.92	111.79
22	M	101	DMU	O3-C5-C7	2.06	115.10	110.35
14	A	601[A]	HEA	C16-C17-C18	2.05	118.63	111.88
14	N	602	HEA	C4B-NB-C1B	-2.05	102.95	105.07
22	Z	101	DMU	C10-C5-C7	2.05	114.26	110.00
14	N	601[A]	HEA	C4A-CHB-C1B	2.05	125.26	122.56
14	N	601[B]	HEA	C4A-CHB-C1B	2.05	125.26	122.56
24	P	304	PGV	O03-C19-O04	-2.05	118.43	123.59
14	N	601[A]	HEA	O2A-CGA-CBA	2.04	120.58	114.03
14	N	601[B]	HEA	O2A-CGA-CBA	2.04	120.58	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	OMA-CMA-C3A	-2.04	120.47	124.91
19	A	607	CDL	OA7-CA5-C11	-2.03	115.81	123.73
22	Q	201	DMU	O3-C5-C7	2.03	115.04	110.35
22	O	308	DMU	C18-O16-C6	-2.02	110.48	113.84
19	C	304	CDL	OA2-PA1-OA3	2.02	116.97	109.07
29	T	101	PEK	O13-P-O14	2.02	122.24	112.24
22	P	316	DMU	O3-C5-C7	2.02	115.02	110.35
22	M	101	DMU	C10-C5-C7	2.02	114.20	110.00
22	P	316	DMU	C6-O5-C4	2.01	117.64	113.69
14	N	601[B]	HEA	C25-C23-C24	2.01	119.05	114.60
26	O	301	CHD	C13-C17-C20	-2.01	117.10	119.50
24	P	304	PGV	C22-C21-C20	-2.01	105.97	113.19
26	P	306	CHD	C15-C14-C13	2.01	105.52	103.55
22	C	318	DMU	C10-C5-C7	2.01	114.17	110.00
14	A	602	HEA	C16-C15-C14	-2.00	117.06	121.12
22	C	319	DMU	O1-C9-C11	2.00	111.41	106.44

There are no chirality outliers.

All (792) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C18-C19-C20-C21
14	A	601[A]	HEA	C27-C19-C20-C21
14	A	601[B]	HEA	C18-C19-C20-C21
14	A	601[B]	HEA	C27-C19-C20-C21
14	N	601[A]	HEA	C27-C19-C20-C21
19	A	607	CDL	C1-CA2-OA2-PA1
19	A	607	CDL	CA3-OA5-PA1-OA3
19	A	607	CDL	C11-CA5-OA6-CA4
19	A	607	CDL	CB2-OB2-PB2-OB3
19	A	607	CDL	CB2-OB2-PB2-OB4
19	A	607	CDL	CB3-OB5-PB2-OB4
19	A	607	CDL	C51-CB5-OB6-CB4
19	C	304	CDL	CB2-C1-CA2-OA2
19	C	304	CDL	C1-CA2-OA2-PA1
19	C	304	CDL	CA3-OA5-PA1-OA2
19	C	304	CDL	C11-CA5-OA6-CA4
19	C	304	CDL	CB2-OB2-PB2-OB4
19	C	304	CDL	CB3-OB5-PB2-OB4
19	C	304	CDL	OB7-CB5-OB6-CB4
19	C	304	CDL	C51-CB5-OB6-CB4
19	L	101	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
19	L	101	CDL	C11-CA5-OA6-CA4
19	P	305	CDL	O1-C1-CB2-OB2
19	P	305	CDL	C1-CA2-OA2-PA1
19	P	305	CDL	CA2-OA2-PA1-OA3
19	P	305	CDL	C11-CA5-OA6-CA4
19	P	305	CDL	CB3-OB5-PB2-OB4
19	P	305	CDL	OB7-CB5-OB6-CB4
19	V	101	CDL	CA3-OA5-PA1-OA2
19	V	101	CDL	CA3-OA5-PA1-OA3
19	V	101	CDL	CB2-OB2-PB2-OB3
19	V	101	CDL	CB2-OB2-PB2-OB4
19	V	101	CDL	CB3-OB5-PB2-OB2
19	V	101	CDL	CB3-OB5-PB2-OB3
19	V	101	CDL	CB3-OB5-PB2-OB4
19	V	101	CDL	C51-CB5-OB6-CB4
19	Y	101	CDL	CA2-C1-CB2-OB2
19	Y	101	CDL	CA3-OA5-PA1-OA3
19	Y	101	CDL	CA3-OA5-PA1-OA4
19	Y	101	CDL	C11-CA5-OA6-CA4
19	Y	101	CDL	C51-CB5-OB6-CB4
22	B	304	DMU	C1-C6-O16-C18
22	B	304	DMU	O5-C6-O16-C18
22	B	308	DMU	C19-C18-O16-C6
22	C	318	DMU	C1-C6-O16-C18
22	C	318	DMU	C19-C18-O16-C6
22	D	201	DMU	C19-C18-O16-C6
22	O	304	DMU	C19-C18-O16-C6
22	O	308	DMU	C19-C18-O16-C6
22	P	324	DMU	C1-C6-O16-C18
22	P	324	DMU	O5-C6-O16-C18
22	Q	201	DMU	O5-C6-O16-C18
22	Q	201	DMU	C19-C18-O16-C6
22	U	101	DMU	C1-C6-O16-C18
22	Z	102	DMU	C1-C6-O16-C18
22	Z	102	DMU	O5-C6-O16-C18
22	Z	102	DMU	C19-C18-O16-C6
26	C	305	CHD	C13-C17-C20-C21
26	C	305	CHD	C16-C17-C20-C22
29	T	101	PEK	C11-C12-C13-C14
29	T	101	PEK	C12-C13-C14-C15
19	L	101	CDL	OA9-CA7-OA8-CA6
26	C	305	CHD	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
26	C	305	CHD	C13-C17-C20-C22
19	A	607	CDL	OA7-CA5-OA6-CA4
19	C	304	CDL	OA7-CA5-OA6-CA4
19	V	101	CDL	OA7-CA5-OA6-CA4
22	B	308	DMU	C3-C4-C57-O61
22	C	323	DMU	O5-C4-C57-O61
19	P	305	CDL	C51-CB5-OB6-CB4
22	P	325	DMU	O6-C11-C9-O1
21	N	609	LFA	C9-C10-C11-C12
21	P	310	LFA	C11-C10-C9-C8
19	L	101	CDL	C31-CA7-OA8-CA6
19	A	607	CDL	OB7-CB5-OB6-CB4
19	L	101	CDL	OA7-CA5-OA6-CA4
19	V	101	CDL	OB7-CB5-OB6-CB4
19	Y	101	CDL	OA7-CA5-OA6-CA4
19	Y	101	CDL	OB7-CB5-OB6-CB4
22	C	315	DMU	O6-C11-C9-C8
22	P	316	DMU	O5-C4-C57-O61
22	U	101	DMU	O5-C4-C57-O61
22	Z	102	DMU	O5-C4-C57-O61
19	L	101	CDL	C72-C73-C74-C75
21	P	301	LFA	C2-C3-C4-C5
19	A	607	CDL	O1-C1-CA2-OA2
19	C	304	CDL	O1-C1-CA2-OA2
19	Y	101	CDL	O1-C1-CB2-OB2
19	Y	101	CDL	C31-CA7-OA8-CA6
22	O	304	DMU	O5-C4-C57-O61
22	P	319	DMU	O5-C4-C57-O61
22	H	101	DMU	C3-C4-C57-O61
22	A	612	DMU	O6-C11-C9-O1
22	C	323	DMU	C3-C4-C57-O61
24	A	617	PGV	C26-C27-C28-C29
24	C	303	PGV	C28-C29-C30-C31
22	H	101	DMU	O5-C4-C57-O61
22	P	320	DMU	O6-C11-C9-O1
22	A	612	DMU	O6-C11-C9-C8
19	P	305	CDL	OA7-CA5-OA6-CA4
22	O	304	DMU	C3-C4-C57-O61
22	P	316	DMU	C31-C34-C37-C40
22	B	308	DMU	O5-C4-C57-O61
22	P	325	DMU	O6-C11-C9-C8
22	Z	102	DMU	C3-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
14	N	601[A]	HEA	C18-C19-C20-C21
22	L	102	DMU	O5-C4-C57-O61
19	Y	101	CDL	OA9-CA7-OA8-CA6
22	P	319	DMU	C3-C4-C57-O61
22	B	308	DMU	O5-C6-O16-C18
22	N	611	DMU	O5-C6-O16-C18
14	A	601[A]	HEA	C15-C16-C17-C18
21	P	310	LFA	C12-C13-C14-C15
19	P	305	CDL	C31-CA7-OA8-CA6
26	P	306	CHD	C17-C20-C22-C23
21	C	325	LFA	C9-C10-C11-C12
19	Y	101	CDL	CB2-C1-CA2-OA2
22	N	611	DMU	O6-C11-C9-C8
19	C	304	CDL	C31-CA7-OA8-CA6
19	V	101	CDL	C31-CA7-OA8-CA6
22	P	316	DMU	C3-C4-C57-O61
21	C	309	LFA	C12-C13-C14-C15
19	Y	101	CDL	O1-C1-CA2-OA2
19	C	304	CDL	CA7-C31-C32-C33
19	Y	101	CDL	C31-C32-C33-C34
22	C	315	DMU	O6-C11-C9-O1
19	A	607	CDL	C78-C79-C80-C81
22	P	320	DMU	C2-C3-O7-C10
22	C	317	DMU	C3-C4-C57-O61
19	P	305	CDL	CB5-C51-C52-C53
19	V	101	CDL	OA9-CA7-OA8-CA6
22	P	319	DMU	O6-C11-C9-O1
26	P	306	CHD	C21-C20-C22-C23
21	C	309	LFA	C11-C10-C9-C8
22	A	612	DMU	O5-C4-C57-O61
22	P	320	DMU	O6-C11-C9-C8
19	A	607	CDL	CA5-C11-C12-C13
19	C	304	CDL	CB7-C71-C72-C73
19	L	101	CDL	CB7-C71-C72-C73
19	C	304	CDL	C71-CB7-OB8-CB6
22	Z	102	DMU	O16-C18-C19-C22
22	C	319	DMU	O16-C18-C19-C22
19	C	304	CDL	CB5-C51-C52-C53
19	L	101	CDL	C31-C32-C33-C34
22	A	612	DMU	C3-C4-C57-O61
22	C	317	DMU	O16-C18-C19-C22
22	C	318	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
22	L	102	DMU	O16-C18-C19-C22
22	C	318	DMU	O5-C6-O16-C18
22	P	320	DMU	C4-C3-O7-C10
19	V	101	CDL	CA7-C31-C32-C33
19	C	304	CDL	OA9-CA7-OA8-CA6
22	U	101	DMU	C3-C4-C57-O61
29	T	101	PEK	C7-C8-C9-C10
22	B	304	DMU	O16-C18-C19-C22
19	P	305	CDL	OA9-CA7-OA8-CA6
19	A	607	CDL	CB2-OB2-PB2-OB5
19	C	304	CDL	CB2-OB2-PB2-OB5
19	L	101	CDL	CA3-OA5-PA1-OA2
19	L	101	CDL	CB2-OB2-PB2-OB5
19	P	305	CDL	CA2-OA2-PA1-OA5
19	P	305	CDL	CA3-OA5-PA1-OA2
19	V	101	CDL	CB2-OB2-PB2-OB5
19	Y	101	CDL	CA3-OA5-PA1-OA2
21	C	307	LFA	C7-C8-C9-C10
22	D	201	DMU	O16-C18-C19-C22
22	O	308	DMU	O16-C18-C19-C22
22	C	319	DMU	O5-C4-C57-O61
21	A	610	LFA	C9-C10-C11-C12
22	B	308	DMU	O16-C18-C19-C22
29	T	101	PEK	C1-C2-C3-C4
22	A	618	DMU	C19-C22-C25-C28
19	C	304	CDL	C22-C23-C24-C25
19	P	305	CDL	C53-C54-C55-C56
19	V	101	CDL	C76-C77-C78-C79
21	O	302	LFA	C11-C12-C13-C14
21	O	302	LFA	C13-C14-C15-C16
21	P	312	LFA	C3-C4-C5-C6
21	T	102	LFA	C4-C5-C6-C7
22	C	315	DMU	C19-C22-C25-C28
22	P	317	DMU	C28-C31-C34-C37
24	C	303	PGV	C7-C8-C9-C10
24	P	304	PGV	C7-C8-C9-C10
29	T	101	PEK	C22-C23-C24-C25
19	V	101	CDL	C72-C73-C74-C75
21	P	311	LFA	C6-C7-C8-C9
22	Z	101	DMU	C22-C25-C28-C31
24	C	303	PGV	C14-C15-C16-C17
19	V	101	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
19	Y	101	CDL	C63-C64-C65-C66
24	P	304	PGV	C14-C15-C16-C17
21	N	608	LFA	C6-C7-C8-C9
19	P	305	CDL	O1-C1-CA2-OA2
21	C	307	LFA	C4-C5-C6-C7
22	C	317	DMU	C19-C22-C25-C28
22	L	102	DMU	C31-C34-C37-C40
22	Z	101	DMU	O16-C18-C19-C22
24	A	617	PGV	C29-C30-C31-C32
22	C	319	DMU	C1-C6-O16-C18
22	O	304	DMU	C1-C6-O16-C18
21	B	307	LFA	C13-C14-C15-C16
19	C	304	CDL	OB9-CB7-OB8-CB6
22	C	317	DMU	O5-C4-C57-O61
22	W	101	DMU	C25-C28-C31-C34
19	P	305	CDL	C74-C75-C76-C77
21	C	325	LFA	C7-C8-C9-C10
21	T	102	LFA	C3-C4-C5-C6
22	C	315	DMU	C28-C31-C34-C37
22	Z	102	DMU	C25-C28-C31-C34
22	Z	102	DMU	C31-C34-C37-C40
19	L	101	CDL	C58-C59-C60-C61
21	B	307	LFA	C10-C11-C12-C13
19	L	101	CDL	C51-CB5-OB6-CB4
19	V	101	CDL	C31-C32-C33-C34
19	Y	101	CDL	C76-C77-C78-C79
21	C	310	LFA	C7-C8-C9-C10
21	O	303	LFA	C2-C3-C4-C5
22	A	611	DMU	C28-C31-C34-C37
22	C	317	DMU	C31-C34-C37-C40
22	P	319	DMU	C28-C31-C34-C37
19	A	607	CDL	C73-C74-C75-C76
19	L	101	CDL	C74-C75-C76-C77
19	P	305	CDL	C35-C36-C37-C38
19	V	101	CDL	C73-C74-C75-C76
21	A	609	LFA	C6-C7-C8-C9
21	C	309	LFA	C5-C6-C7-C8
21	O	302	LFA	C4-C5-C6-C7
21	P	301	LFA	C9-C10-C11-C12
21	P	308	LFA	C4-C5-C6-C7
21	P	310	LFA	C4-C5-C6-C7
22	M	102	DMU	C25-C28-C31-C34

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Mol	Chain	Res	Type	Atoms
29	T	101	PEK	C26-C27-C28-C29
22	U	101	DMU	O5-C6-O16-C18
14	N	601[A]	HEA	C15-C16-C17-C18
19	L	101	CDL	C59-C60-C61-C62
19	Y	101	CDL	C37-C38-C39-C40
19	C	304	CDL	C75-C76-C77-C78
19	L	101	CDL	C17-C18-C19-C20
21	C	309	LFA	C3-C4-C5-C6
21	C	311	LFA	C4-C5-C6-C7
22	C	318	DMU	C31-C34-C37-C40
19	P	305	CDL	CB7-C71-C72-C73
19	Y	101	CDL	C13-C14-C15-C16
21	C	310	LFA	C3-C4-C5-C6
21	N	609	LFA	C5-C6-C7-C8
21	P	311	LFA	C2-C3-C4-C5
22	B	303	DMU	C25-C28-C31-C34
22	C	316	DMU	C28-C31-C34-C37
22	C	319	DMU	C3-C4-C57-O61
19	Y	101	CDL	C73-C74-C75-C76
22	N	611	DMU	O16-C18-C19-C22
22	C	306	DMU	C18-C19-C22-C25
22	C	317	DMU	C19-C18-O16-C6
22	C	323	DMU	C19-C18-O16-C6
22	L	102	DMU	C19-C18-O16-C6
24	C	303	PGV	C30-C31-C32-C33
24	P	304	PGV	C24-C25-C26-C27
19	A	607	CDL	C17-C18-C19-C20
21	C	307	LFA	C5-C6-C7-C8
21	B	307	LFA	C4-C5-C6-C7
21	B	307	LFA	C11-C12-C13-C14
22	P	320	DMU	C31-C34-C37-C40
22	Z	101	DMU	C25-C28-C31-C34
19	L	101	CDL	CA5-C11-C12-C13
22	P	324	DMU	C18-C19-C22-C25
29	G	101	PEK	C16-C17-C18-C19
21	C	312	LFA	C1-C2-C3-C4
22	P	320	DMU	C22-C25-C28-C31
21	C	309	LFA	C2-C3-C4-C5
22	C	318	DMU	C19-C22-C25-C28
22	M	101	DMU	C22-C25-C28-C31
24	A	617	PGV	C11-C10-C9-C8
29	G	101	PEK	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	L	102	DMU	C25-C28-C31-C34
22	Z	101	DMU	O6-C11-C9-C8
19	P	305	CDL	C75-C76-C77-C78
19	Y	101	CDL	C79-C80-C81-C82
21	P	315	LFA	C2-C3-C4-C5
19	L	101	CDL	OB7-CB5-OB6-CB4
19	L	101	CDL	C34-C35-C36-C37
21	P	313	LFA	C1-C2-C3-C4
22	A	612	DMU	C31-C34-C37-C40
22	B	303	DMU	C28-C31-C34-C37
19	Y	101	CDL	OB9-CB7-OB8-CB6
21	P	312	LFA	C11-C10-C9-C8
23	R	201	EDO	O1-C1-C2-O2
21	B	307	LFA	C12-C13-C14-C15
21	O	302	LFA	C6-C7-C8-C9
22	O	308	DMU	C34-C37-C40-C43
19	Y	101	CDL	C71-CB7-OB8-CB6
19	L	101	CDL	C12-C13-C14-C15
21	C	311	LFA	C11-C10-C9-C8
22	B	308	DMU	C31-C34-C37-C40
19	A	607	CDL	C19-C20-C21-C22
22	C	323	DMU	O16-C18-C19-C22
22	B	308	DMU	C18-C19-C22-C25
22	O	306	DMU	C18-C19-C22-C25
21	P	311	LFA	C5-C6-C7-C8
19	P	305	CDL	C57-C58-C59-C60
22	M	101	DMU	C19-C22-C25-C28
24	N	617	PGV	C11-C10-C9-C8
24	P	304	PGV	C12-C13-C14-C15
21	P	308	LFA	C6-C7-C8-C9
21	P	308	LFA	C7-C8-C9-C10
22	P	325	DMU	O16-C18-C19-C22
22	P	324	DMU	C22-C25-C28-C31
19	A	607	CDL	C76-C77-C78-C79
19	V	101	CDL	C17-C18-C19-C20
22	N	611	DMU	C31-C34-C37-C40
19	V	101	CDL	C78-C79-C80-C81
22	O	306	DMU	C19-C22-C25-C28
22	Q	201	DMU	C4-C3-O7-C10
22	Z	102	DMU	C22-C25-C28-C31
22	D	201	DMU	C19-C22-C25-C28
22	L	102	DMU	C3-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
19	Y	101	CDL	C22-C23-C24-C25
21	P	301	LFA	C6-C7-C8-C9
21	P	313	LFA	C3-C4-C5-C6
22	C	324	DMU	O16-C18-C19-C22
19	P	305	CDL	CA7-C31-C32-C33
19	Y	101	CDL	CA5-C11-C12-C13
19	V	101	CDL	C11-CA5-OA6-CA4
22	N	611	DMU	O6-C11-C9-O1
19	P	305	CDL	C56-C57-C58-C59
22	P	319	DMU	C25-C28-C31-C34
22	B	302	DMU	C18-C19-C22-C25
21	P	314	LFA	C5-C6-C7-C8
19	L	101	CDL	OB6-CB4-CB6-OB8
19	V	101	CDL	OA6-CA4-CA6-OA8
19	P	305	CDL	C71-C72-C73-C74
21	O	302	LFA	C5-C6-C7-C8
24	C	303	PGV	C13-C14-C15-C16
29	T	101	PEK	C15-C16-C17-C18
21	P	301	LFA	C7-C8-C9-C10
22	P	318	DMU	C18-C19-C22-C25
19	A	607	CDL	C18-C19-C20-C21
22	B	303	DMU	C18-C19-C22-C25
26	C	305	CHD	C21-C20-C22-C23
22	B	302	DMU	C19-C22-C25-C28
22	C	316	DMU	C31-C34-C37-C40
22	C	323	DMU	C19-C22-C25-C28
22	P	316	DMU	O6-C11-C9-O1
19	L	101	CDL	C51-C52-C53-C54
21	P	310	LFA	C3-C4-C5-C6
22	P	307	DMU	C31-C34-C37-C40
29	G	101	PEK	C26-C27-C28-C29
29	G	101	PEK	C28-C29-C30-C31
22	C	323	DMU	C18-C19-C22-C25
21	C	313	LFA	C4-C5-C6-C7
21	P	310	LFA	C5-C6-C7-C8
22	O	307	DMU	C19-C22-C25-C28
29	G	101	PEK	C29-C30-C31-C32
19	P	305	CDL	C13-C14-C15-C16
21	C	325	LFA	C10-C11-C12-C13
22	H	101	DMU	C19-C22-C25-C28
21	N	609	LFA	C11-C10-C9-C8
22	J	101	DMU	C18-C19-C22-C25

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Mol	Chain	Res	Type	Atoms
22	O	307	DMU	C18-C19-C22-C25
21	C	307	LFA	C6-C7-C8-C9
21	P	312	LFA	C5-C6-C7-C8
22	M	101	DMU	C25-C28-C31-C34
22	P	318	DMU	C22-C25-C28-C31
19	L	101	CDL	C76-C77-C78-C79
21	C	311	LFA	C5-C6-C7-C8
19	C	304	CDL	C71-C72-C73-C74
19	L	101	CDL	CB2-C1-CA2-OA2
21	C	310	LFA	C4-C5-C6-C7
22	C	323	DMU	C22-C25-C28-C31
22	P	318	DMU	C19-C22-C25-C28
24	N	617	PGV	C23-C24-C25-C26
29	G	101	PEK	C34-C35-C36-C37
19	P	305	CDL	C54-C55-C56-C57
22	P	319	DMU	C31-C34-C37-C40
24	A	617	PGV	C14-C15-C16-C17
19	C	304	CDL	CB3-CB4-CB6-OB8
19	L	101	CDL	CA3-CA4-CA6-OA8
19	P	305	CDL	CA3-CA4-CA6-OA8
19	P	305	CDL	CB3-CB4-CB6-OB8
19	V	101	CDL	CA3-CA4-CA6-OA8
19	Y	101	CDL	C80-C81-C82-C83
19	P	305	CDL	C20-C21-C22-C23
19	Y	101	CDL	C64-C65-C66-C67
22	B	304	DMU	C34-C37-C40-C43
22	C	319	DMU	C34-C37-C40-C43
22	J	101	DMU	C34-C37-C40-C43
21	O	302	LFA	C2-C3-C4-C5
22	B	308	DMU	C34-C37-C40-C43
22	C	316	DMU	C34-C37-C40-C43
19	C	304	CDL	C59-C60-C61-C62
19	V	101	CDL	C74-C75-C76-C77
19	Y	101	CDL	C61-C62-C63-C64
21	P	311	LFA	C7-C8-C9-C10
21	C	310	LFA	C6-C7-C8-C9
29	T	101	PEK	C17-C18-C19-C20
19	A	607	CDL	C16-C17-C18-C19
22	B	304	DMU	C31-C34-C37-C40
29	T	101	PEK	C2-C3-C4-C5
21	B	307	LFA	C14-C15-C16-C17
21	P	313	LFA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
22	Z	101	DMU	C34-C37-C40-C43
22	C	318	DMU	O6-C11-C9-O1
22	Z	101	DMU	O6-C11-C9-O1
19	A	607	CDL	C12-C13-C14-C15
21	N	608	LFA	C7-C8-C9-C10
19	V	101	CDL	C71-CB7-OB8-CB6
19	L	101	CDL	C38-C39-C40-C41
21	C	325	LFA	C12-C13-C14-C15
19	A	607	CDL	CA6-CA4-OA6-CA5
22	B	302	DMU	O16-C18-C19-C22
22	B	303	DMU	O16-C18-C19-C22
22	O	306	DMU	O16-C18-C19-C22
22	O	307	DMU	O16-C18-C19-C22
22	W	101	DMU	O16-C18-C19-C22
21	C	307	LFA	C11-C10-C9-C8
21	C	312	LFA	C11-C10-C9-C8
22	G	102	DMU	C34-C37-C40-C43
21	P	310	LFA	C13-C14-C15-C16
22	W	101	DMU	C34-C37-C40-C43
21	B	307	LFA	C1-C2-C3-C4
22	P	316	DMU	C19-C22-C25-C28
19	Y	101	CDL	C19-C20-C21-C22
19	Y	101	CDL	C84-C85-C86-C87
21	C	314	LFA	C1-C2-C3-C4
22	P	318	DMU	C31-C34-C37-C40
19	L	101	CDL	C75-C76-C77-C78
21	C	310	LFA	C11-C10-C9-C8
22	Z	103	DMU	C22-C25-C28-C31
22	Z	103	DMU	C31-C34-C37-C40
21	O	302	LFA	C7-C8-C9-C10
24	P	304	PGV	C15-C16-C17-C18
22	D	201	DMU	C4-C3-O7-C10
22	C	306	DMU	O16-C18-C19-C22
22	P	307	DMU	O16-C18-C19-C22
19	C	304	CDL	C12-C11-CA5-OA6
19	V	101	CDL	C75-C76-C77-C78
22	B	303	DMU	C19-C22-C25-C28
22	P	317	DMU	C25-C28-C31-C34
19	L	101	CDL	C84-C85-C86-C87
22	C	319	DMU	C25-C28-C31-C34
19	L	101	CDL	C22-C23-C24-C25
21	N	608	LFA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	P	313	LFA	C4-C5-C6-C7
19	V	101	CDL	C32-C33-C34-C35
19	Y	101	CDL	C51-C52-C53-C54
21	O	302	LFA	C14-C15-C16-C17
29	T	101	PEK	C4-C5-C6-C7
19	L	101	CDL	C18-C19-C20-C21
24	P	304	PGV	C11-C12-C13-C14
29	T	101	PEK	C14-C15-C16-C17
22	Q	201	DMU	C2-C3-O7-C10
21	P	314	LFA	C9-C10-C11-C12
22	C	317	DMU	C25-C28-C31-C34
19	C	304	CDL	C23-C24-C25-C26
19	C	304	CDL	C57-C58-C59-C60
22	P	319	DMU	C34-C37-C40-C43
19	P	305	CDL	C71-CB7-OB8-CB6
24	C	303	PGV	C02-C03-O11-P
19	A	607	CDL	C71-C72-C73-C74
21	P	312	LFA	C10-C11-C12-C13
22	C	315	DMU	C34-C37-C40-C43
22	B	304	DMU	C19-C18-O16-C6
22	P	318	DMU	C19-C18-O16-C6
22	P	320	DMU	C19-C18-O16-C6
19	L	101	CDL	C80-C81-C82-C83
21	C	312	LFA	C6-C7-C8-C9
21	P	311	LFA	C11-C10-C9-C8
22	A	618	DMU	O16-C18-C19-C22
22	M	102	DMU	C22-C25-C28-C31
19	L	101	CDL	CB3-CB4-CB6-OB8
22	L	102	DMU	C22-C25-C28-C31
19	C	304	CDL	C52-C53-C54-C55
22	A	618	DMU	C25-C28-C31-C34
19	P	305	CDL	C12-C11-CA5-OA6
19	Y	101	CDL	C77-C78-C79-C80
19	L	101	CDL	CA2-OA2-PA1-OA5
29	G	101	PEK	C9-C10-C11-C12
29	G	101	PEK	C11-C12-C13-C14
29	G	101	PEK	C12-C13-C14-C15
29	T	101	PEK	C11-C10-C9-C8
19	L	101	CDL	C36-C37-C38-C39
24	N	617	PGV	C31-C32-C33-C34
19	L	101	CDL	C21-C22-C23-C24
19	Y	101	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
21	N	608	LFA	C2-C3-C4-C5
22	C	315	DMU	C25-C28-C31-C34
22	M	102	DMU	C31-C34-C37-C40
22	G	102	DMU	O16-C18-C19-C22
21	B	307	LFA	C6-C7-C8-C9
21	C	325	LFA	C1-C2-C3-C4
21	T	102	LFA	C7-C8-C9-C10
24	C	303	PGV	C25-C26-C27-C28
19	C	304	CDL	O1-C1-CB2-OB2
21	C	325	LFA	C6-C7-C8-C9
22	A	611	DMU	C25-C28-C31-C34
22	P	319	DMU	C4-C3-O7-C10
19	A	607	CDL	OA6-CA4-CA6-OA8
19	L	101	CDL	OA6-CA4-CA6-OA8
22	H	101	DMU	C25-C28-C31-C34
22	C	319	DMU	O5-C6-O16-C18
19	A	607	CDL	CB2-C1-CA2-OA2
19	C	304	CDL	C73-C74-C75-C76
22	Z	102	DMU	C34-C37-C40-C43
19	Y	101	CDL	C57-C58-C59-C60
21	C	309	LFA	C14-C15-C16-C17
22	G	102	DMU	C28-C31-C34-C37
24	P	304	PGV	C02-C03-O11-P
19	Y	101	CDL	C16-C17-C18-C19
21	P	315	LFA	C6-C7-C8-C9
24	P	304	PGV	C30-C31-C32-C33
19	Y	101	CDL	C59-C60-C61-C62
21	C	310	LFA	C1-C2-C3-C4
22	P	319	DMU	C19-C22-C25-C28
19	Y	101	CDL	C21-C22-C23-C24
21	C	308	LFA	C3-C4-C5-C6
22	P	318	DMU	C28-C31-C34-C37
22	W	101	DMU	C22-C25-C28-C31
21	A	609	LFA	C7-C8-C9-C10
21	A	610	LFA	C2-C3-C4-C5
21	C	307	LFA	C3-C4-C5-C6
22	A	618	DMU	C18-C19-C22-C25
22	C	318	DMU	C3-C4-C57-O61
22	B	308	DMU	C25-C28-C31-C34
19	P	305	CDL	C33-C34-C35-C36
22	P	319	DMU	O6-C11-C9-C8
22	H	101	DMU	O6-C11-C9-O1

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Mol	Chain	Res	Type	Atoms
19	V	101	CDL	C18-C19-C20-C21
22	Z	101	DMU	C28-C31-C34-C37
24	A	617	PGV	C31-C32-C33-C34
19	V	101	CDL	OA5-CA3-CA4-OA6
29	G	101	PEK	C27-C28-C29-C30
19	V	101	CDL	C77-C78-C79-C80
22	D	201	DMU	C2-C3-O7-C10
22	P	319	DMU	C2-C3-O7-C10
19	P	305	CDL	OB9-CB7-OB8-CB6
19	V	101	CDL	OB9-CB7-OB8-CB6
21	P	315	LFA	C3-C4-C5-C6
29	G	101	PEK	C17-C18-C19-C20
21	P	301	LFA	C1-C2-C3-C4
21	P	315	LFA	C10-C11-C12-C13
22	P	324	DMU	O16-C18-C19-C22
29	G	101	PEK	C25-C26-C27-C28
22	C	324	DMU	C28-C31-C34-C37
19	V	101	CDL	C19-C20-C21-C22
21	P	308	LFA	C3-C4-C5-C6
21	A	610	LFA	C11-C12-C13-C14
21	A	610	LFA	C5-C6-C7-C8
21	O	302	LFA	C12-C13-C14-C15
22	C	315	DMU	C4-C3-O7-C10
22	Q	201	DMU	O5-C4-C57-O61
21	P	308	LFA	C1-C2-C3-C4
21	C	325	LFA	C11-C10-C9-C8
22	O	304	DMU	C22-C25-C28-C31
22	D	201	DMU	O6-C11-C9-C8
21	A	610	LFA	C6-C7-C8-C9
19	C	304	CDL	CA4-CA3-OA5-PA1
19	C	304	CDL	CA3-OA5-PA1-OA3
19	C	304	CDL	CB2-OB2-PB2-OB3
19	L	101	CDL	CA2-OA2-PA1-OA4
19	L	101	CDL	CA3-OA5-PA1-OA3
19	L	101	CDL	CA3-OA5-PA1-OA4
19	L	101	CDL	CB2-OB2-PB2-OB3
19	P	305	CDL	CA3-OA5-PA1-OA3
19	V	101	CDL	OA5-CA3-CA4-CA6
19	Y	101	CDL	OA5-CA3-CA4-CA6
21	C	311	LFA	C6-C7-C8-C9
23	R	203	EDO	O1-C1-C2-O2
19	P	305	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
19	L	101	CDL	C72-C71-CB7-OB8
19	P	305	CDL	C52-C53-C54-C55
22	P	316	DMU	C4-C3-O7-C10
19	Y	101	CDL	OA5-CA3-CA4-OA6
24	C	303	PGV	C1-C2-C3-C4
21	P	310	LFA	C11-C12-C13-C14
22	N	610	DMU	C34-C37-C40-C43
19	L	101	CDL	O1-C1-CA2-OA2
21	P	310	LFA	C2-C3-C4-C5
22	C	318	DMU	C2-C3-O7-C10
19	L	101	CDL	C56-C57-C58-C59
24	C	303	PGV	C29-C30-C31-C32
19	P	305	CDL	OB6-CB4-CB6-OB8
19	L	101	CDL	C60-C61-C62-C63
21	P	312	LFA	C4-C5-C6-C7
22	A	618	DMU	C28-C31-C34-C37
29	G	101	PEK	C32-C33-C34-C35
21	A	609	LFA	C9-C10-C11-C12
19	P	305	CDL	CA4-CA3-OA5-PA1
19	V	101	CDL	C1-CA2-OA2-PA1
21	C	313	LFA	C5-C6-C7-C8
22	C	318	DMU	O1-C10-O7-C3
19	L	101	CDL	C15-C16-C17-C18
22	C	315	DMU	C2-C3-O7-C10
21	N	609	LFA	C3-C4-C5-C6
19	C	304	CDL	C12-C13-C14-C15
22	C	319	DMU	C28-C31-C34-C37
22	C	323	DMU	C34-C37-C40-C43
19	Y	101	CDL	C32-C33-C34-C35
21	P	314	LFA	C6-C7-C8-C9
19	P	305	CDL	C78-C79-C80-C81
22	C	315	DMU	C18-C19-C22-C25
21	C	325	LFA	C4-C5-C6-C7
24	A	617	PGV	C30-C31-C32-C33
21	A	609	LFA	C2-C3-C4-C5
19	Y	101	CDL	C1-CA2-OA2-PA1
21	P	313	LFA	C6-C7-C8-C9
22	C	319	DMU	C19-C22-C25-C28
22	Z	102	DMU	C19-C22-C25-C28
29	T	101	PEK	C10-C11-C12-C13
21	B	307	LFA	C9-C10-C11-C12
22	P	316	DMU	C2-C3-O7-C10

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Mol	Chain	Res	Type	Atoms
19	A	607	CDL	C32-C33-C34-C35
22	P	319	DMU	C5-C10-O7-C3
19	A	607	CDL	C15-C16-C17-C18
29	T	101	PEK	C23-C24-C25-C26
29	T	101	PEK	C2-C1-O01-C02
22	Q	201	DMU	O6-C11-C9-C8
22	Q	201	DMU	C25-C28-C31-C34
19	A	607	CDL	C71-CB7-OB8-CB6
19	A	607	CDL	CA3-OA5-PA1-OA2
21	C	309	LFA	C11-C12-C13-C14
22	P	317	DMU	C31-C34-C37-C40
24	N	617	PGV	C15-C16-C17-C18
22	C	318	DMU	C4-C3-O7-C10
19	L	101	CDL	C78-C79-C80-C81
19	V	101	CDL	C52-C51-CB5-OB6
24	P	304	PGV	C22-C23-C24-C25
21	C	314	LFA	C6-C7-C8-C9
22	P	319	DMU	C22-C25-C28-C31
21	C	309	LFA	C13-C14-C15-C16
19	C	304	CDL	C79-C80-C81-C82
19	A	607	CDL	C13-C14-C15-C16
22	N	610	DMU	C31-C34-C37-C40
21	P	315	LFA	C9-C10-C11-C12
19	C	304	CDL	C55-C56-C57-C58
21	P	308	LFA	C2-C3-C4-C5
19	Y	101	CDL	C60-C61-C62-C63
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
14	A	601[B]	HEA	CAD-CBD-CGD-O1D
14	A	602	HEA	CAA-CBA-CGA-O1A
24	N	617	PGV	C29-C30-C31-C32
21	P	314	LFA	C11-C10-C9-C8
22	C	318	DMU	C5-C10-O7-C3
19	P	305	CDL	C23-C24-C25-C26
21	O	302	LFA	C3-C4-C5-C6
19	P	305	CDL	C22-C23-C24-C25
26	B	306	CHD	C22-C23-C24-O25
22	H	101	DMU	C1-C6-O16-C18
22	C	323	DMU	C28-C31-C34-C37
26	P	306	CHD	C20-C22-C23-C24
22	C	317	DMU	C28-C31-C34-C37
21	P	310	LFA	C6-C7-C8-C9
19	L	101	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
21	C	311	LFA	C9-C10-C11-C12
26	O	301	CHD	C22-C23-C24-O26
19	P	305	CDL	C21-C22-C23-C24
19	P	305	CDL	C73-C74-C75-C76
19	P	305	CDL	C18-C19-C20-C21
14	N	602	HEA	CAA-CBA-CGA-O1A
22	P	316	DMU	C28-C31-C34-C37
19	C	304	CDL	C11-C12-C13-C14
14	N	601[A]	HEA	CAD-CBD-CGD-O1D
14	N	601[B]	HEA	CAD-CBD-CGD-O1D
26	B	306	CHD	C22-C23-C24-O26
19	C	304	CDL	C12-C11-CA5-OA7
19	Y	101	CDL	C14-C15-C16-C17
21	O	302	LFA	C1-C2-C3-C4
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
14	A	601[B]	HEA	CAD-CBD-CGD-O2D
26	C	305	CHD	C22-C23-C24-O26
26	O	301	CHD	C22-C23-C24-O25
21	C	314	LFA	C11-C10-C9-C8
21	P	314	LFA	C4-C5-C6-C7
19	A	607	CDL	C52-C51-CB5-OB6
21	O	302	LFA	C11-C10-C9-C8
26	C	305	CHD	C22-C23-C24-O25
19	P	305	CDL	OB5-CB3-CB4-OB6
22	P	316	DMU	C5-C10-O7-C3
14	N	602	HEA	CAD-CBD-CGD-O1D
21	O	303	LFA	C5-C6-C7-C8
22	O	304	DMU	C18-C19-C22-C25
29	G	101	PEK	C23-C24-C25-C26
22	P	316	DMU	O1-C10-O7-C3
21	B	307	LFA	C11-C10-C9-C8
14	N	602	HEA	CAA-CBA-CGA-O2A
19	P	305	CDL	C76-C77-C78-C79
19	C	304	CDL	OB6-CB4-CB6-OB8
22	C	324	DMU	C18-C19-C22-C25
22	D	201	DMU	C28-C31-C34-C37
24	P	304	PGV	C27-C28-C29-C30
19	Y	101	CDL	C38-C39-C40-C41
21	B	307	LFA	C5-C6-C7-C8
19	A	607	CDL	OB9-CB7-OB8-CB6
24	N	617	PGV	O03-C19-C20-C21
19	Y	101	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
22	C	315	DMU	C5-C10-O7-C3
14	A	602	HEA	CAD-CBD-CGD-O1D
21	C	311	LFA	C10-C11-C12-C13
21	C	311	LFA	C11-C12-C13-C14
22	G	102	DMU	C19-C22-C25-C28
19	P	305	CDL	C17-C18-C19-C20
19	P	305	CDL	C12-C11-CA5-OA7
24	A	617	PGV	O03-C19-C20-C21
19	V	101	CDL	C52-C51-CB5-OB7
29	T	101	PEK	C13-C14-C15-C16
14	A	602	HEA	CAA-CBA-CGA-O2A
26	C	301	CHD	C22-C23-C24-O26
19	C	304	CDL	C72-C73-C74-C75
19	L	101	CDL	C23-C24-C25-C26
21	P	301	LFA	C11-C12-C13-C14
14	N	602	HEA	CAD-CBD-CGD-O2D
26	P	306	CHD	C22-C23-C24-O26
22	O	304	DMU	O16-C18-C19-C22
19	V	101	CDL	C20-C21-C22-C23
14	A	602	HEA	CAD-CBD-CGD-O2D
22	C	315	DMU	O1-C10-O7-C3
22	P	319	DMU	O1-C10-O7-C3
22	O	308	DMU	C1-C6-O16-C18
26	P	302	CHD	C22-C23-C24-O26
29	T	101	PEK	C30-C31-C32-C33
22	B	302	DMU	C34-C37-C40-C43
22	G	102	DMU	C25-C28-C31-C34
22	M	102	DMU	C34-C37-C40-C43
22	Q	201	DMU	C31-C34-C37-C40
19	V	101	CDL	C72-C71-CB7-OB8
19	A	607	CDL	C72-C71-CB7-OB8
22	P	320	DMU	O5-C4-C57-O61
29	T	101	PEK	C32-C33-C34-C35
29	T	101	PEK	O02-C1-O01-C02
22	U	101	DMU	C25-C28-C31-C34
19	L	101	CDL	C52-C53-C54-C55
29	G	101	PEK	C24-C25-C26-C27
19	P	305	CDL	C52-C51-CB5-OB6
19	Y	101	CDL	C17-C18-C19-C20
21	P	308	LFA	C11-C10-C9-C8
22	A	612	DMU	C19-C22-C25-C28
19	Y	101	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
23	A	614	EDO	O1-C1-C2-O2
23	C	320	EDO	O1-C1-C2-O2
26	C	301	CHD	C22-C23-C24-O25
26	P	302	CHD	C22-C23-C24-O25
26	P	306	CHD	C22-C23-C24-O25
19	P	305	CDL	CB4-CB6-OB8-CB7
19	C	304	CDL	C52-C51-CB5-OB6
19	A	607	CDL	C52-C51-CB5-OB7
21	P	314	LFA	C2-C3-C4-C5
22	P	325	DMU	C25-C28-C31-C34
19	P	305	CDL	C72-C71-CB7-OB8
19	V	101	CDL	C32-C31-CA7-OA8
19	Y	101	CDL	C12-C13-C14-C15
14	N	601[A]	HEA	CAD-CBD-CGD-O2D
14	N	601[B]	HEA	CAD-CBD-CGD-O2D
22	C	324	DMU	O1-C10-O7-C3
21	P	311	LFA	C3-C4-C5-C6
22	J	101	DMU	O16-C18-C19-C22
22	L	102	DMU	C19-C22-C25-C28
22	P	324	DMU	C31-C34-C37-C40
19	A	607	CDL	CA2-C1-CB2-OB2
22	A	618	DMU	C34-C37-C40-C43
19	C	304	CDL	C52-C51-CB5-OB7
19	V	101	CDL	C72-C71-CB7-OB9
19	L	101	CDL	C19-C20-C21-C22
19	A	607	CDL	C72-C71-CB7-OB9
19	P	305	CDL	C72-C71-CB7-OB9
19	C	304	CDL	C19-C20-C21-C22
21	P	315	LFA	C5-C6-C7-C8
19	C	304	CDL	C72-C71-CB7-OB8
19	Y	101	CDL	C72-C71-CB7-OB8
24	C	303	PGV	C05-C04-O12-P
19	A	607	CDL	CA2-OA2-PA1-OA3
19	A	607	CDL	CB3-OB5-PB2-OB3
19	Y	101	CDL	CB3-OB5-PB2-OB3
19	Y	101	CDL	C58-C59-C60-C61
22	C	319	DMU	C18-C19-C22-C25
22	W	101	DMU	C31-C34-C37-C40
23	F	103	EDO	O1-C1-C2-O2
22	H	101	DMU	C28-C31-C34-C37
19	P	305	CDL	C52-C51-CB5-OB7
21	C	312	LFA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
21	C	310	LFA	C5-C6-C7-C8
19	L	101	CDL	C53-C54-C55-C56
29	T	101	PEK	O01-C1-C2-C3
22	P	316	DMU	C18-C19-C22-C25
19	A	607	CDL	C74-C75-C76-C77
19	P	305	CDL	CA2-C1-CB2-OB2
22	M	101	DMU	C34-C37-C40-C43
22	Q	201	DMU	C28-C31-C34-C37
22	P	319	DMU	O16-C18-C19-C22
22	P	324	DMU	O5-C4-C57-O61
22	A	612	DMU	C4-C3-O7-C10
24	A	617	PGV	C15-C16-C17-C18
22	P	325	DMU	C19-C18-O16-C6
14	N	601[A]	HEA	CAA-CBA-CGA-O2A
14	N	601[B]	HEA	CAA-CBA-CGA-O2A

There are no ring outliers.

42 monomers are involved in 112 short contacts:

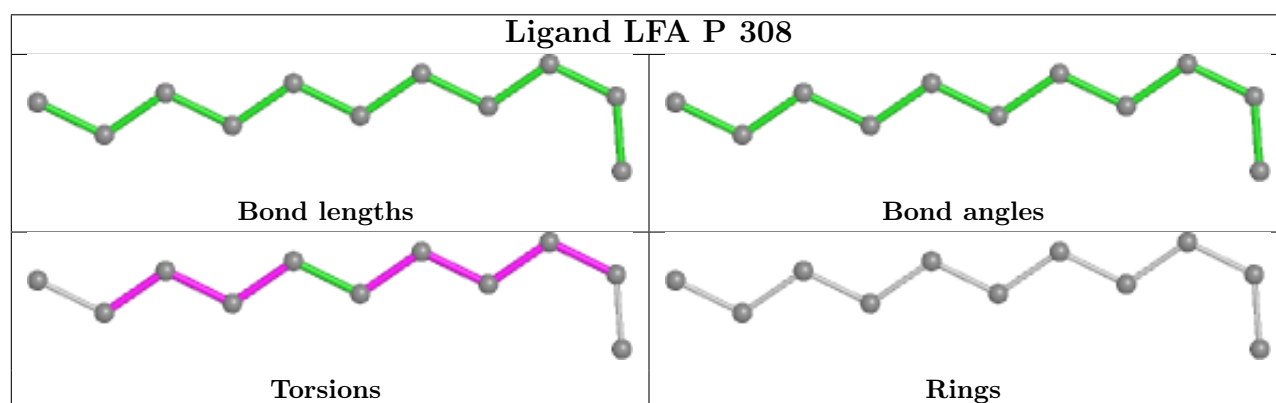
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	P	308	LFA	3	0
19	A	607	CDL	1	0
22	M	102	DMU	1	0
26	P	302	CHD	1	0
18	A	606	PER	1	0
22	U	101	DMU	1	0
23	A	614	EDO	1	0
22	O	306	DMU	2	0
24	N	617	PGV	1	0
14	N	601[B]	HEA	1	0
18	N	606	PER	1	0
14	A	601[B]	HEA	1	0
21	C	307	LFA	3	0
21	N	609	LFA	6	0
19	P	305	CDL	7	0
14	A	601[A]	HEA	3	0
26	C	305	CHD	2	0
19	C	304	CDL	17	0
21	C	312	LFA	2	0
22	C	318	DMU	1	0
14	N	602	HEA	1	0
22	H	101	DMU	1	0

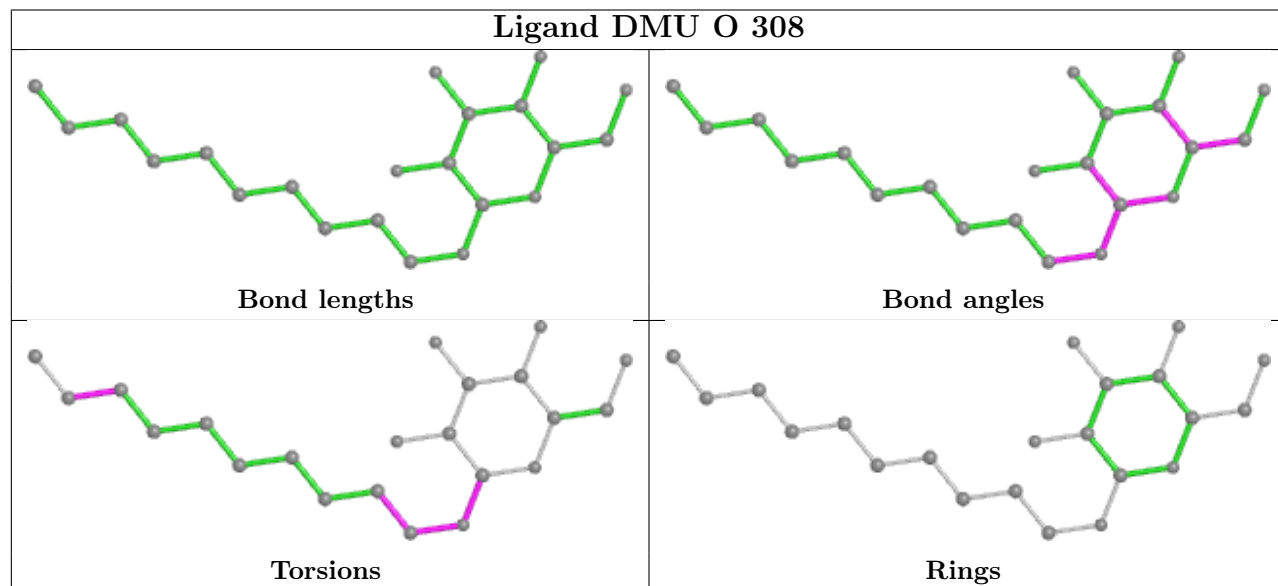
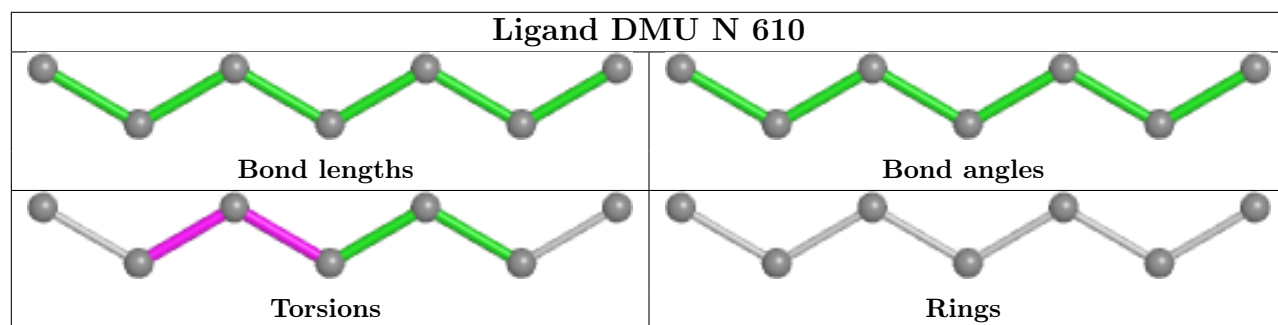
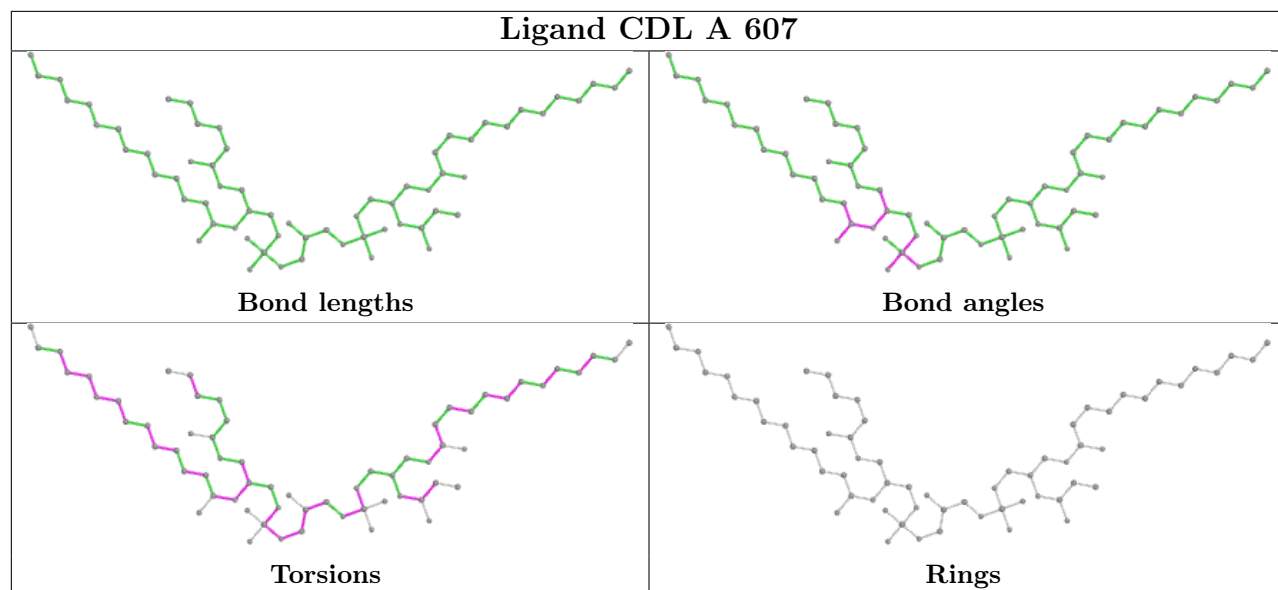
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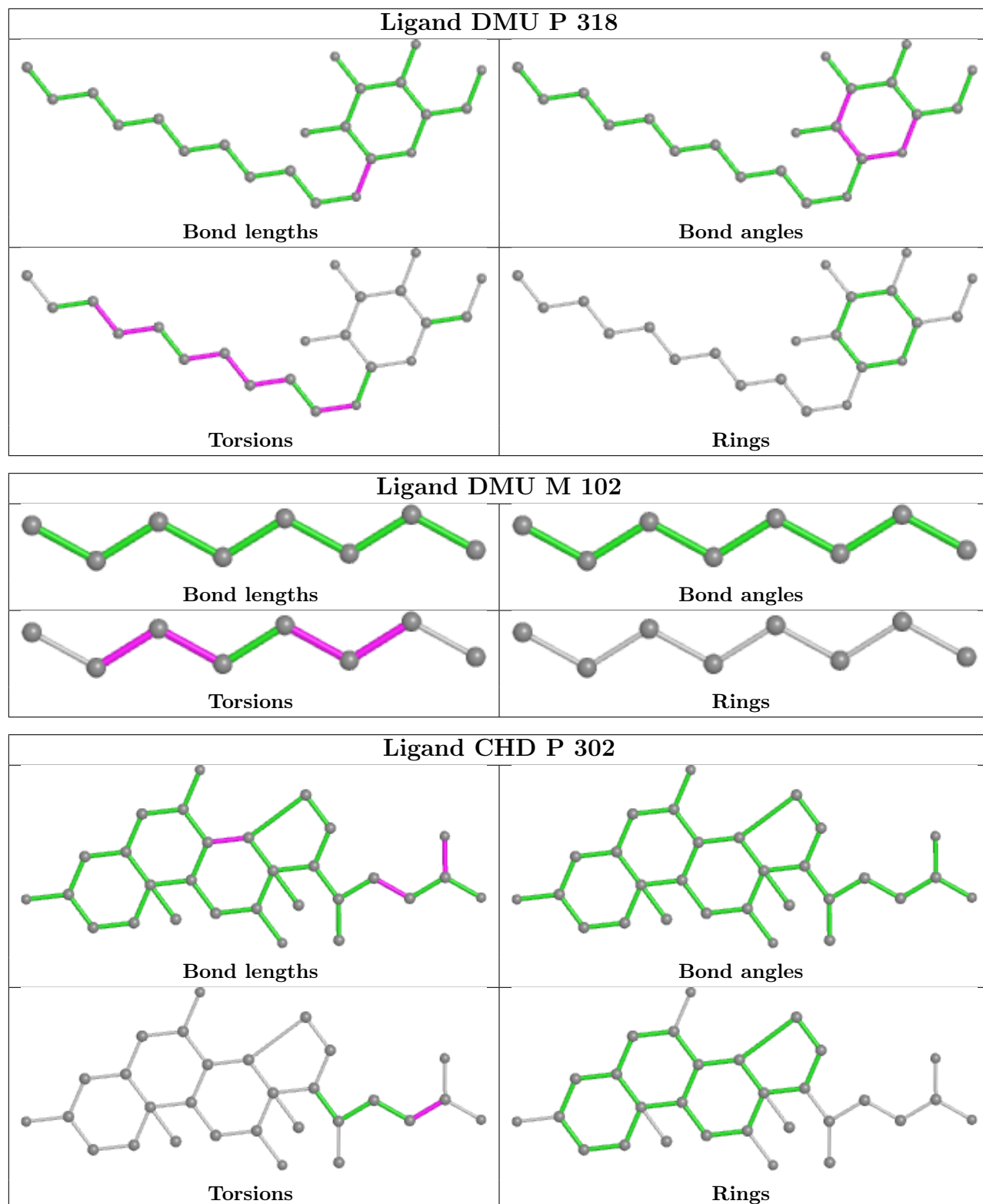
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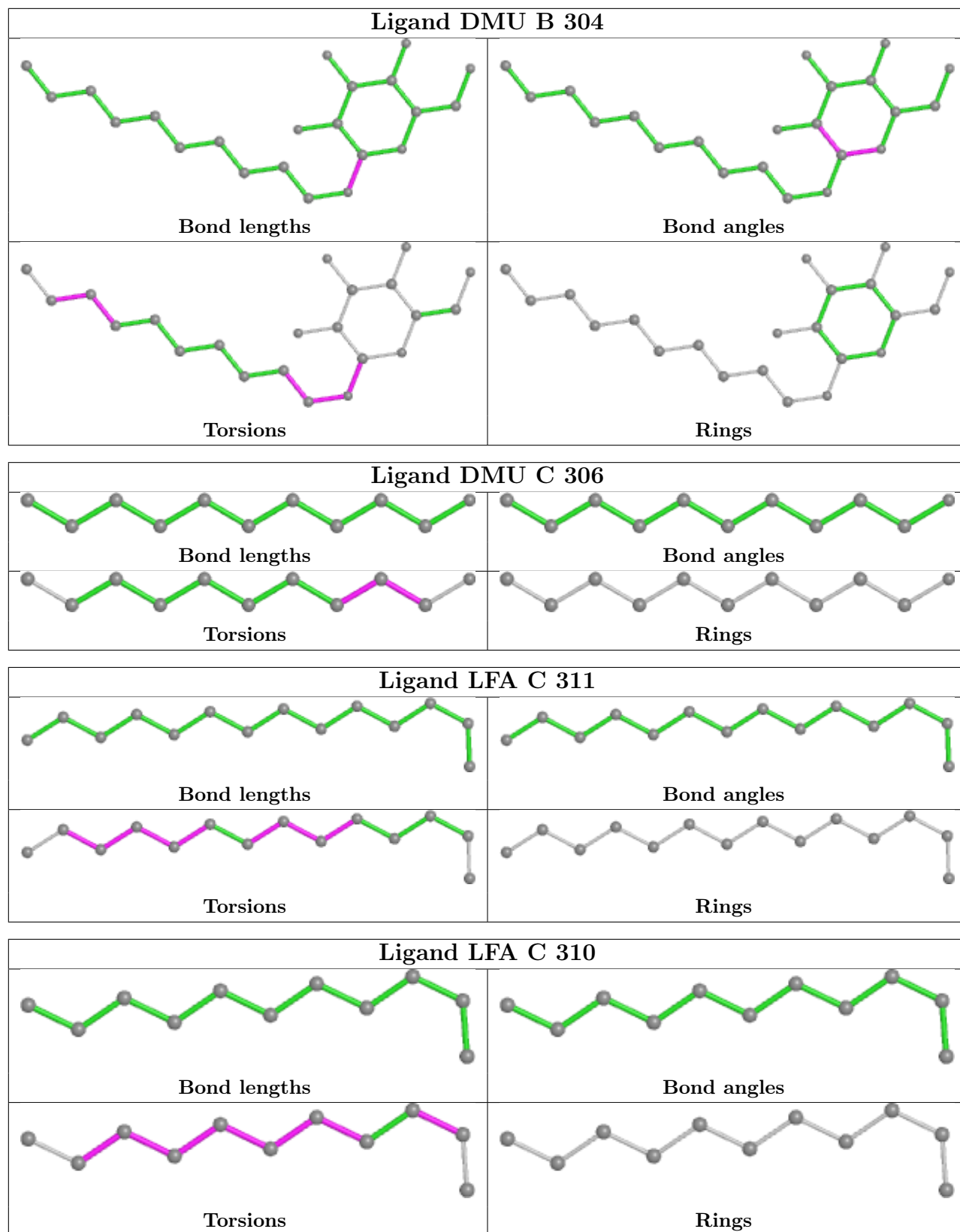
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	P	306	CHD	3	0
22	Z	102	DMU	2	0
19	L	101	CDL	2	0
22	P	325	DMU	2	0
24	C	303	PGV	1	0
21	B	307	LFA	3	0
22	D	201	DMU	2	0
22	C	324	DMU	7	0
21	N	608	LFA	6	0
29	T	101	PEK	5	0
22	A	612	DMU	1	0
26	B	306	CHD	1	0
19	V	101	CDL	2	0
21	P	313	LFA	2	0
21	P	310	LFA	2	0
19	Y	101	CDL	4	0
21	A	610	LFA	8	0
22	Q	201	DMU	1	0
26	O	301	CHD	1	0
21	A	609	LFA	4	0

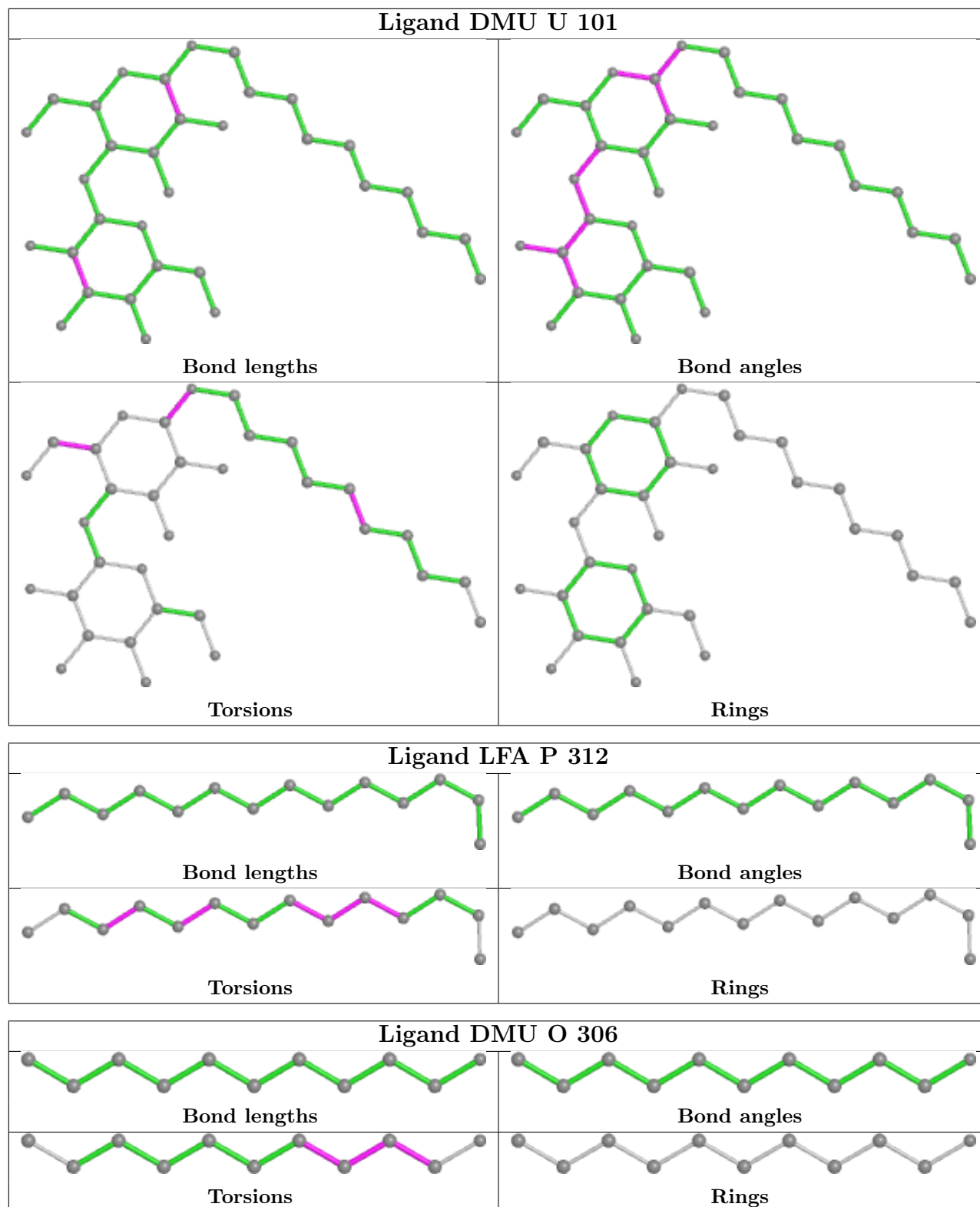
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

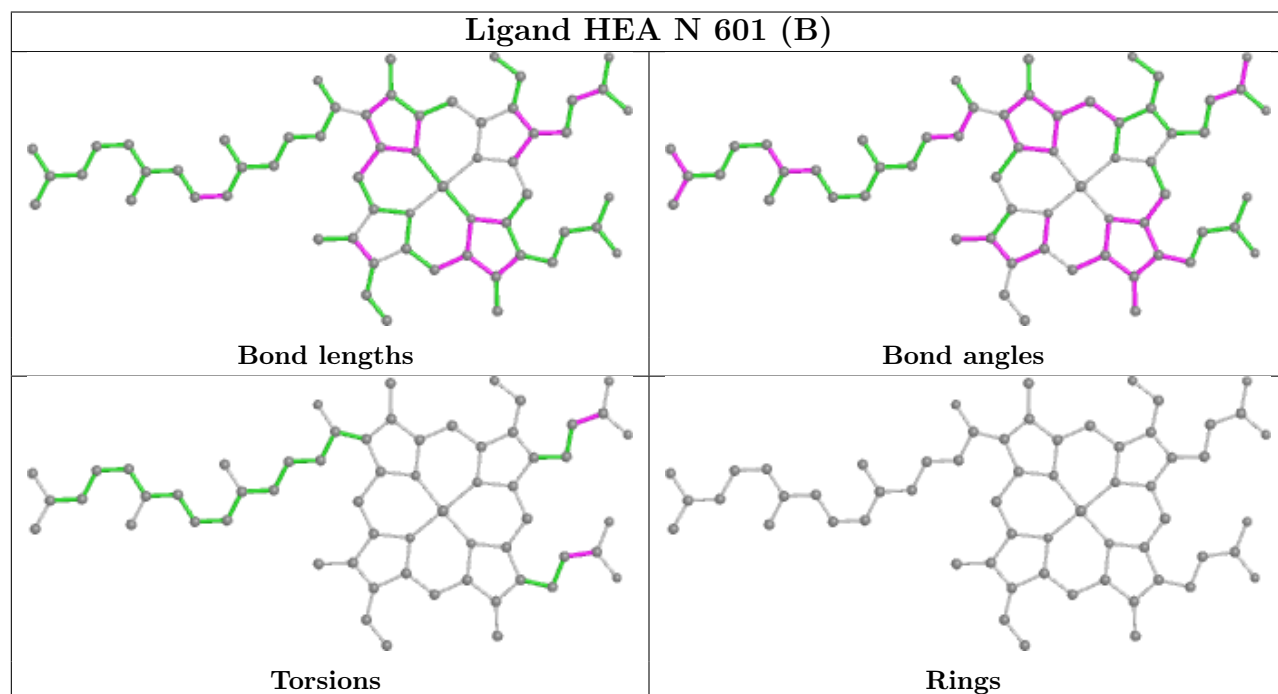
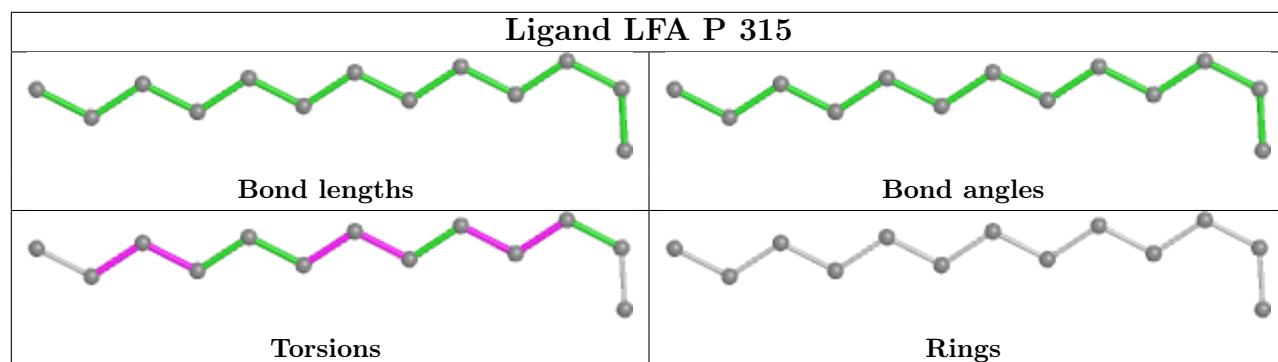
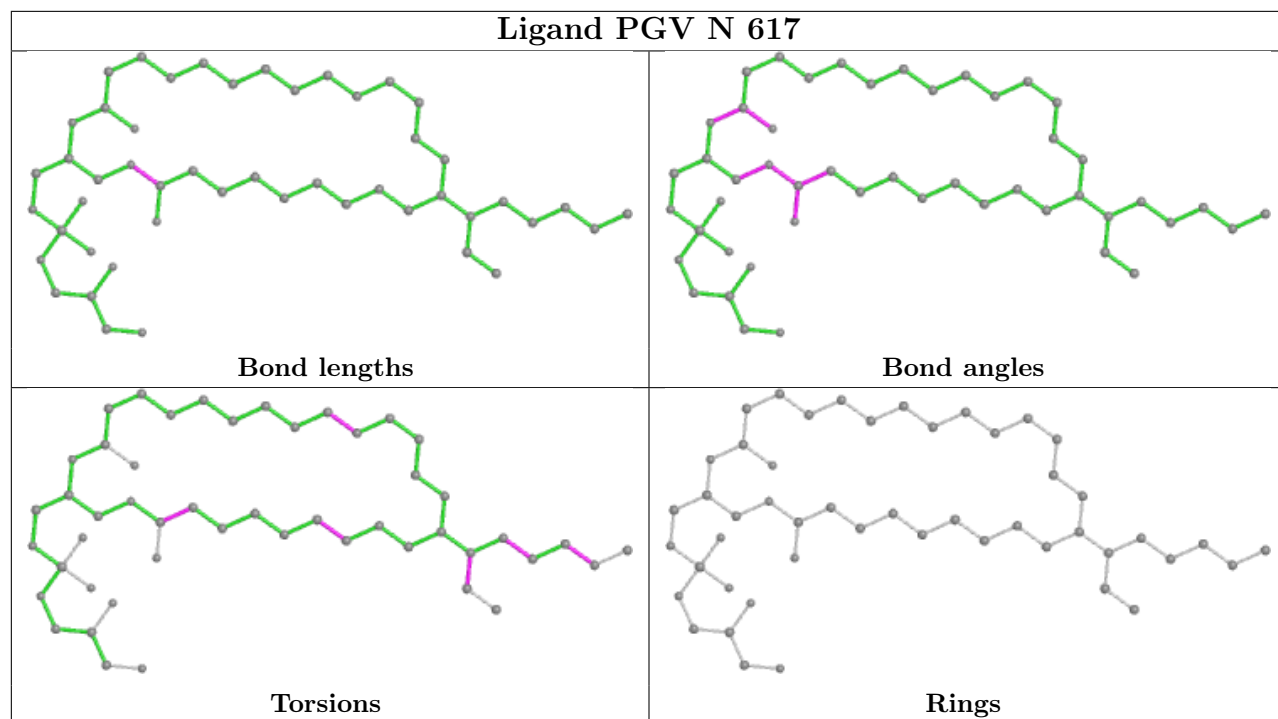


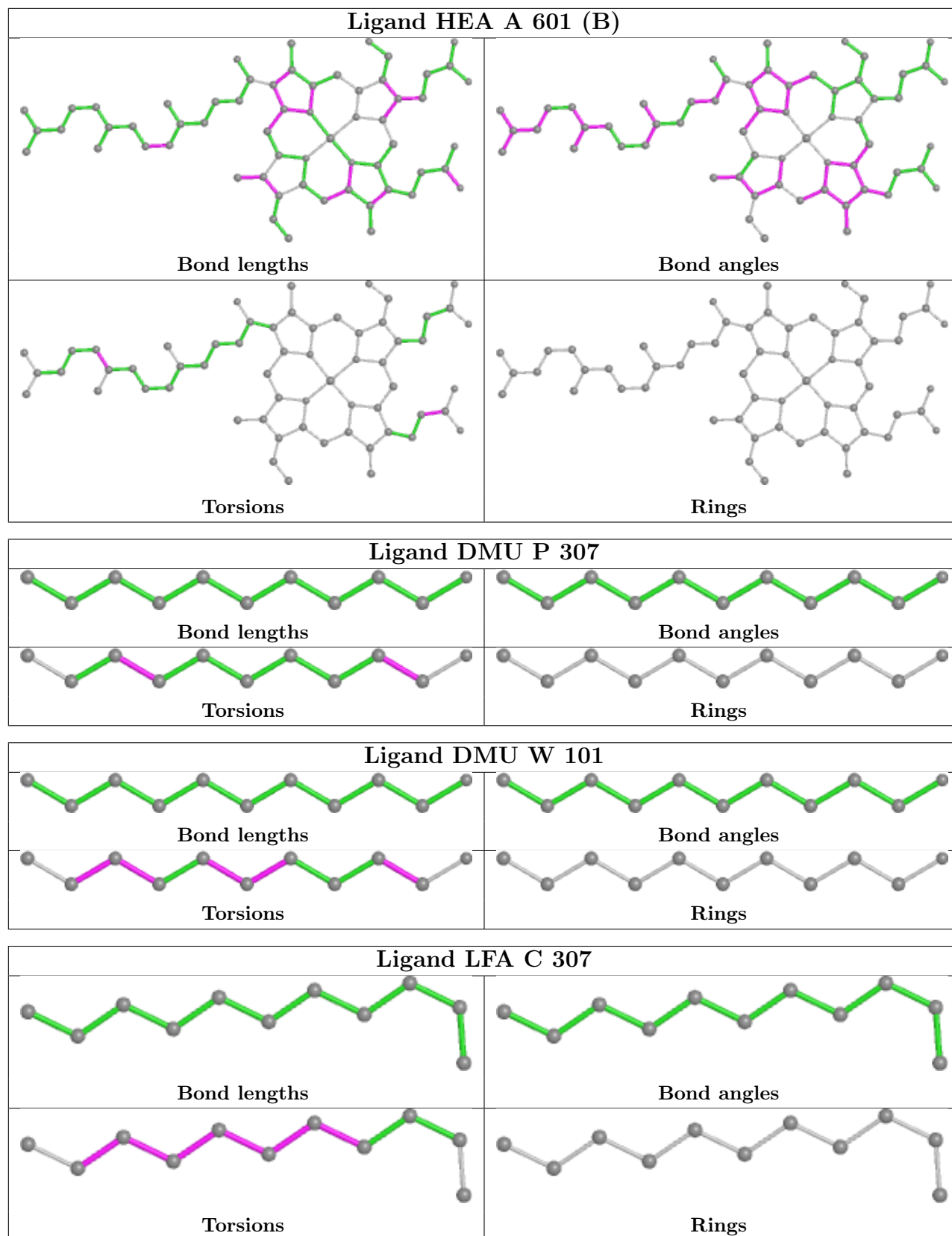




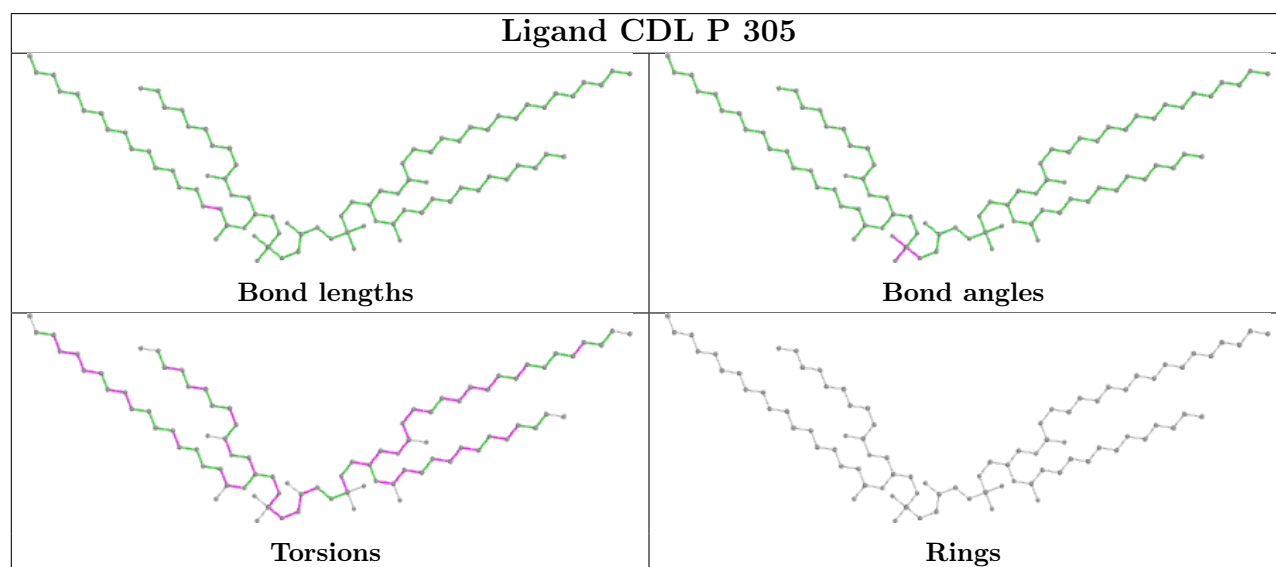
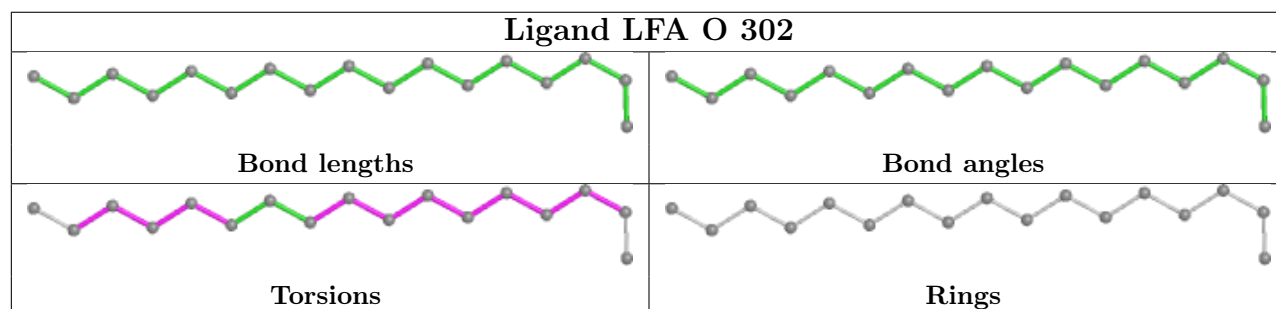
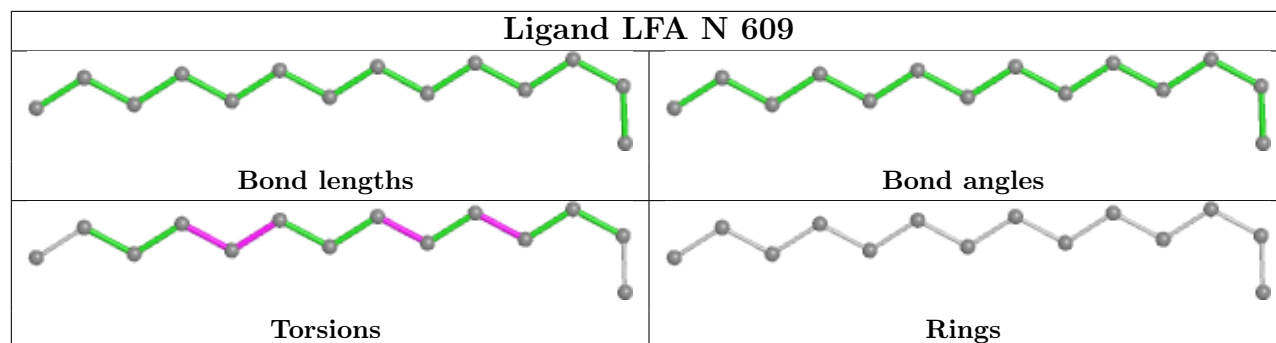




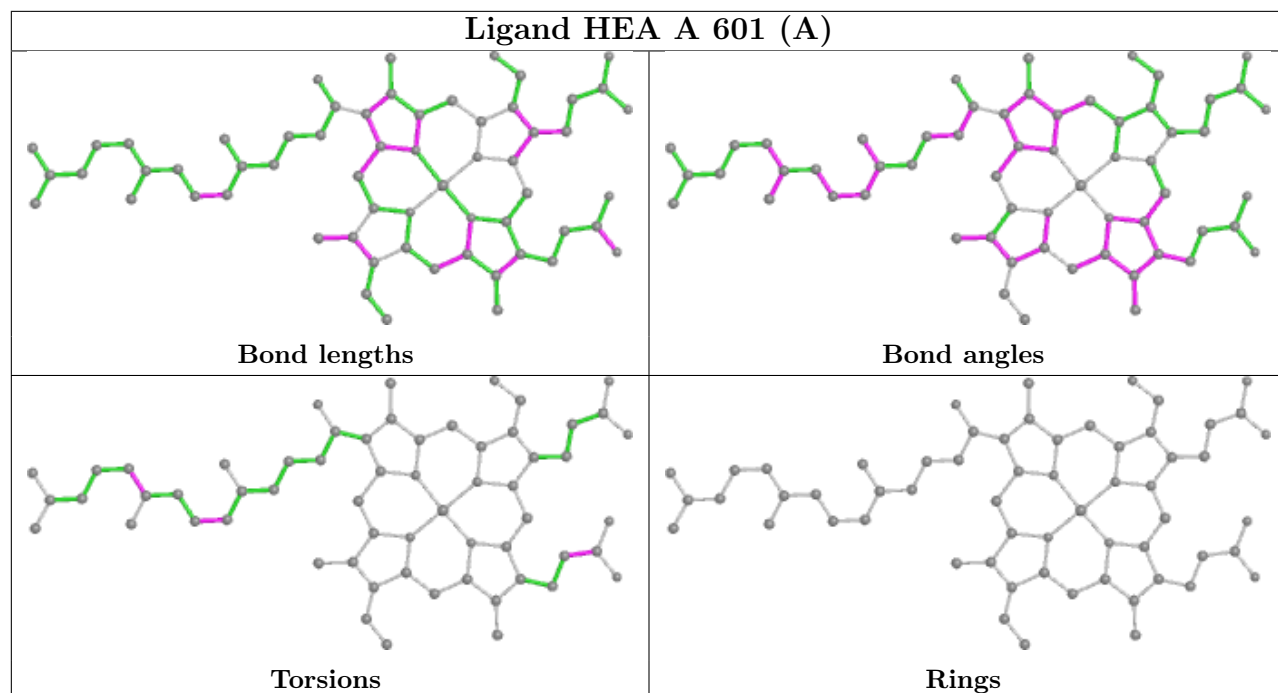




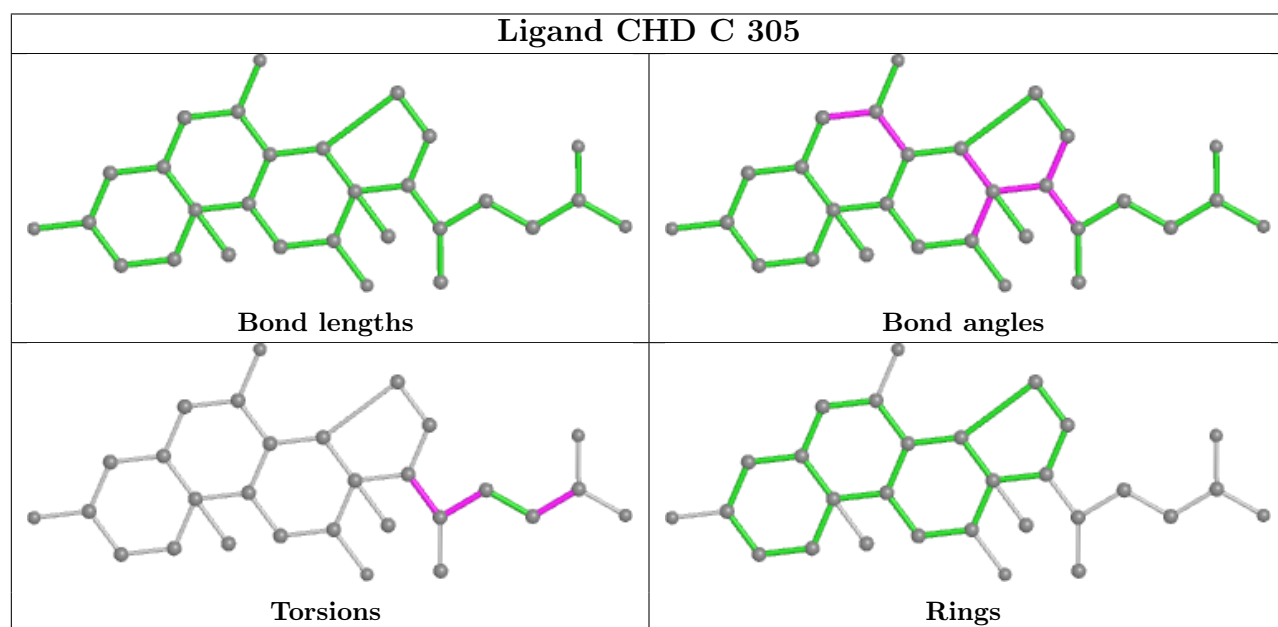


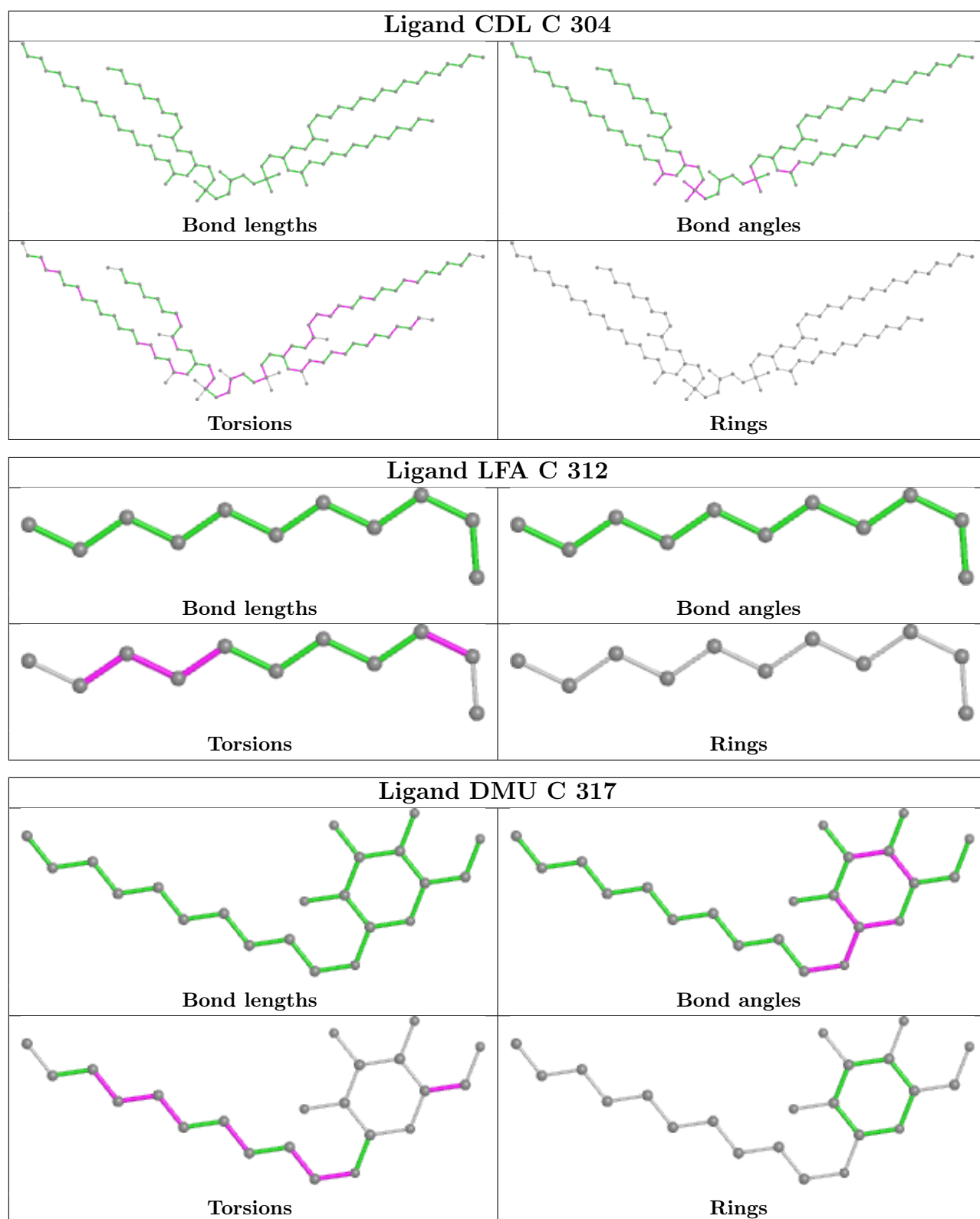


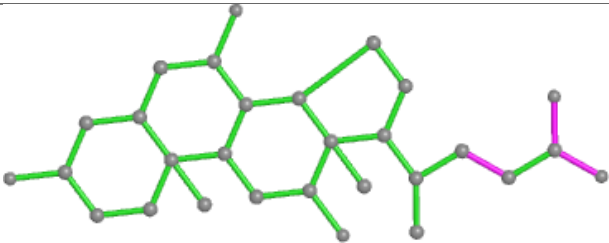
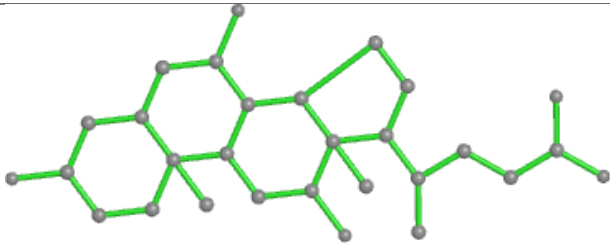
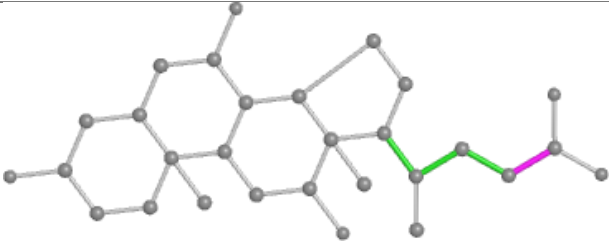
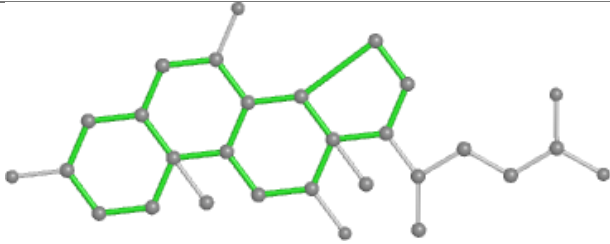
## Ligand HEA A 601 (A)

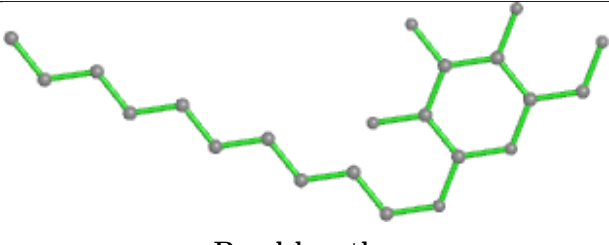
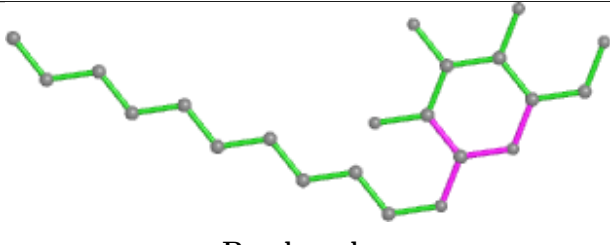
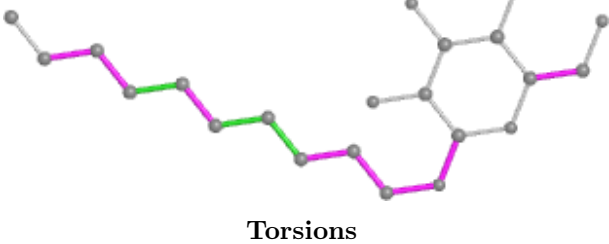



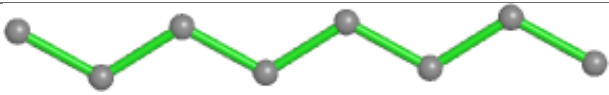
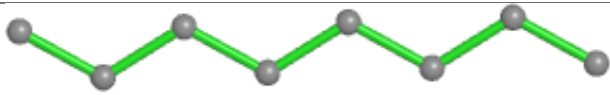


## Ligand CHD C 305

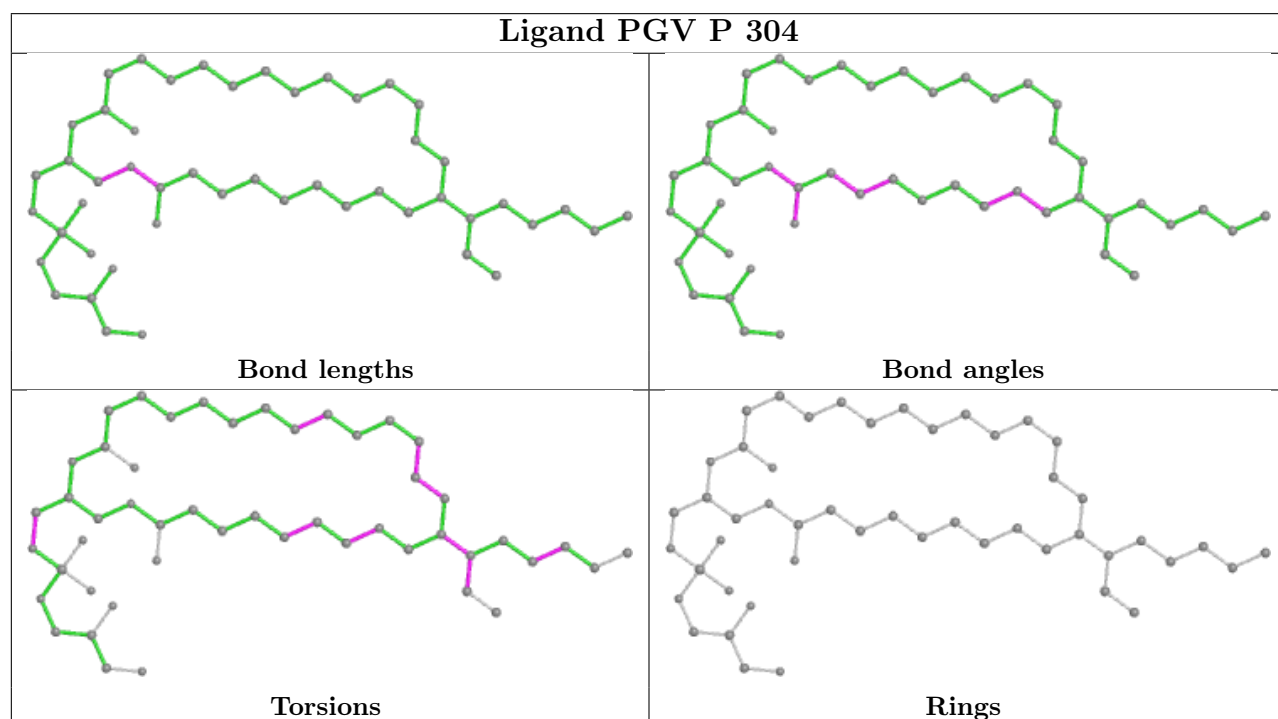
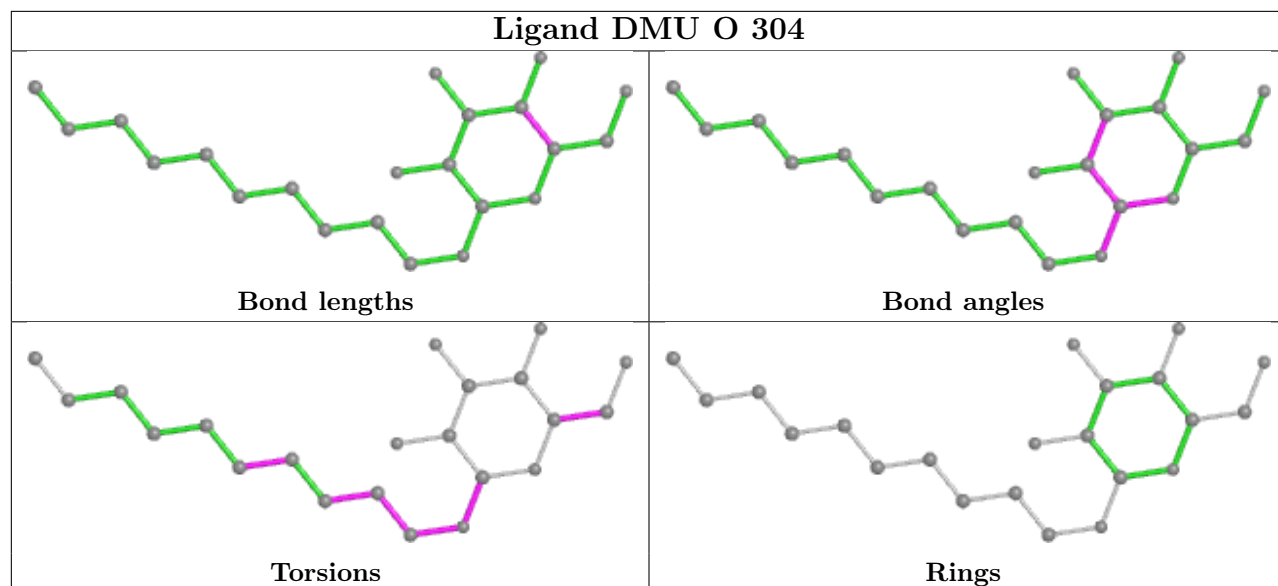


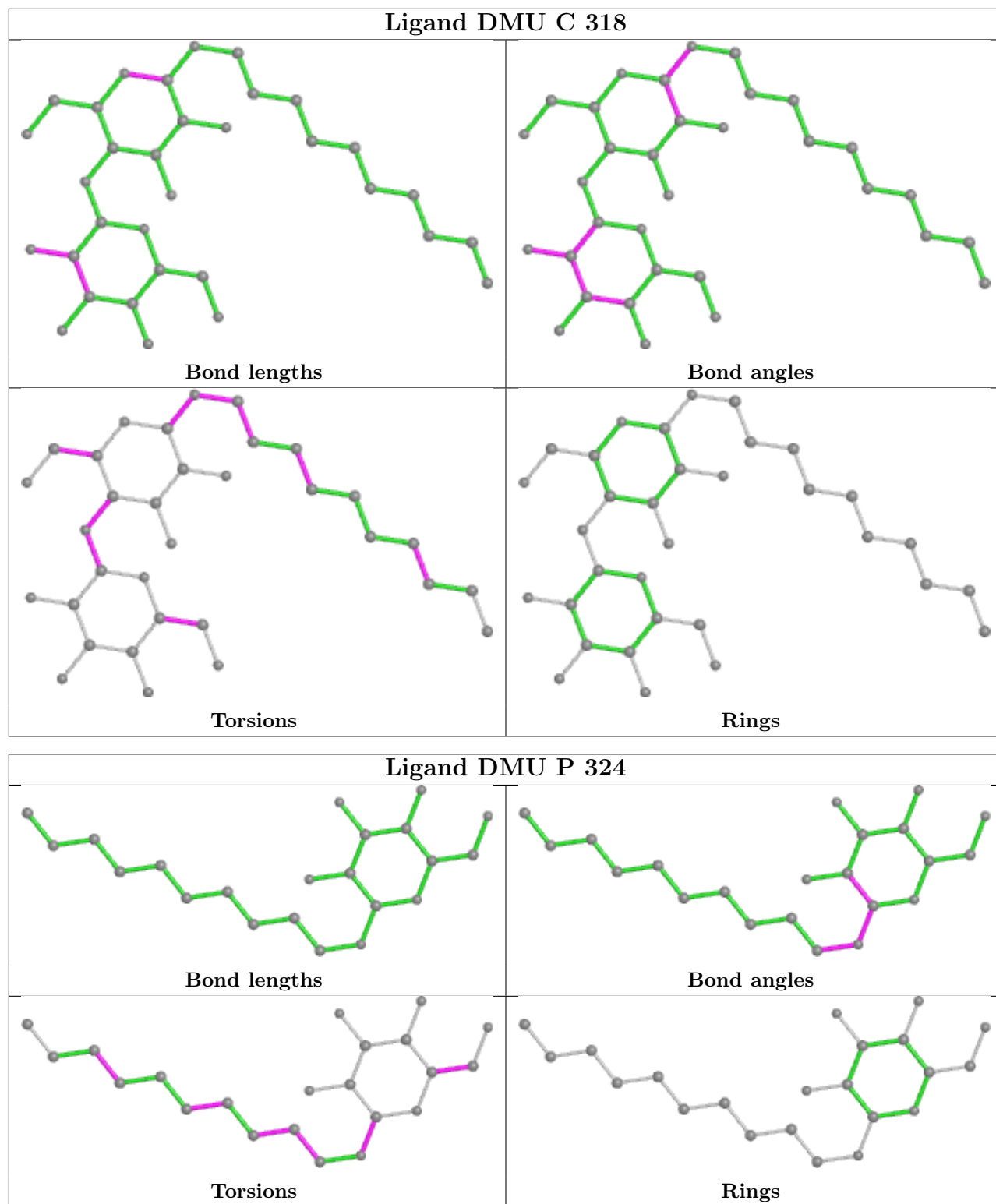


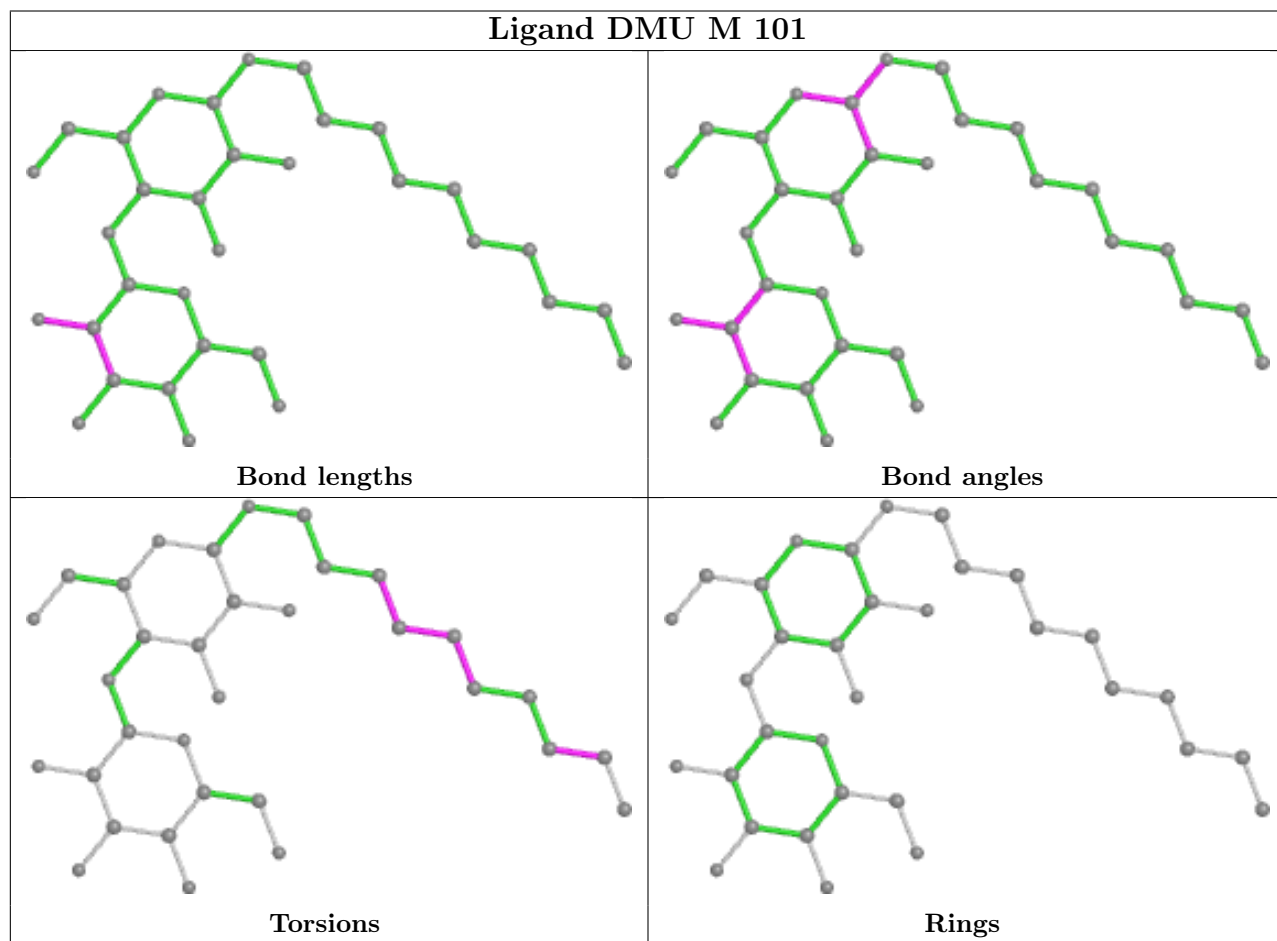
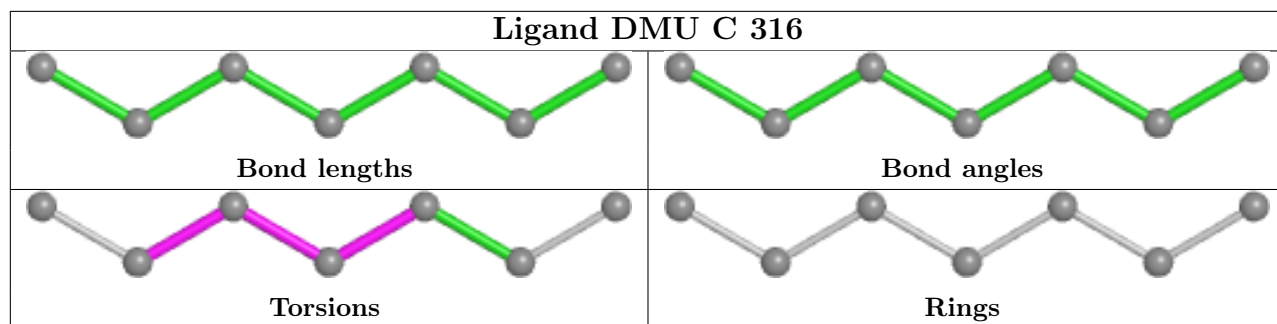
Ligand CHD C 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

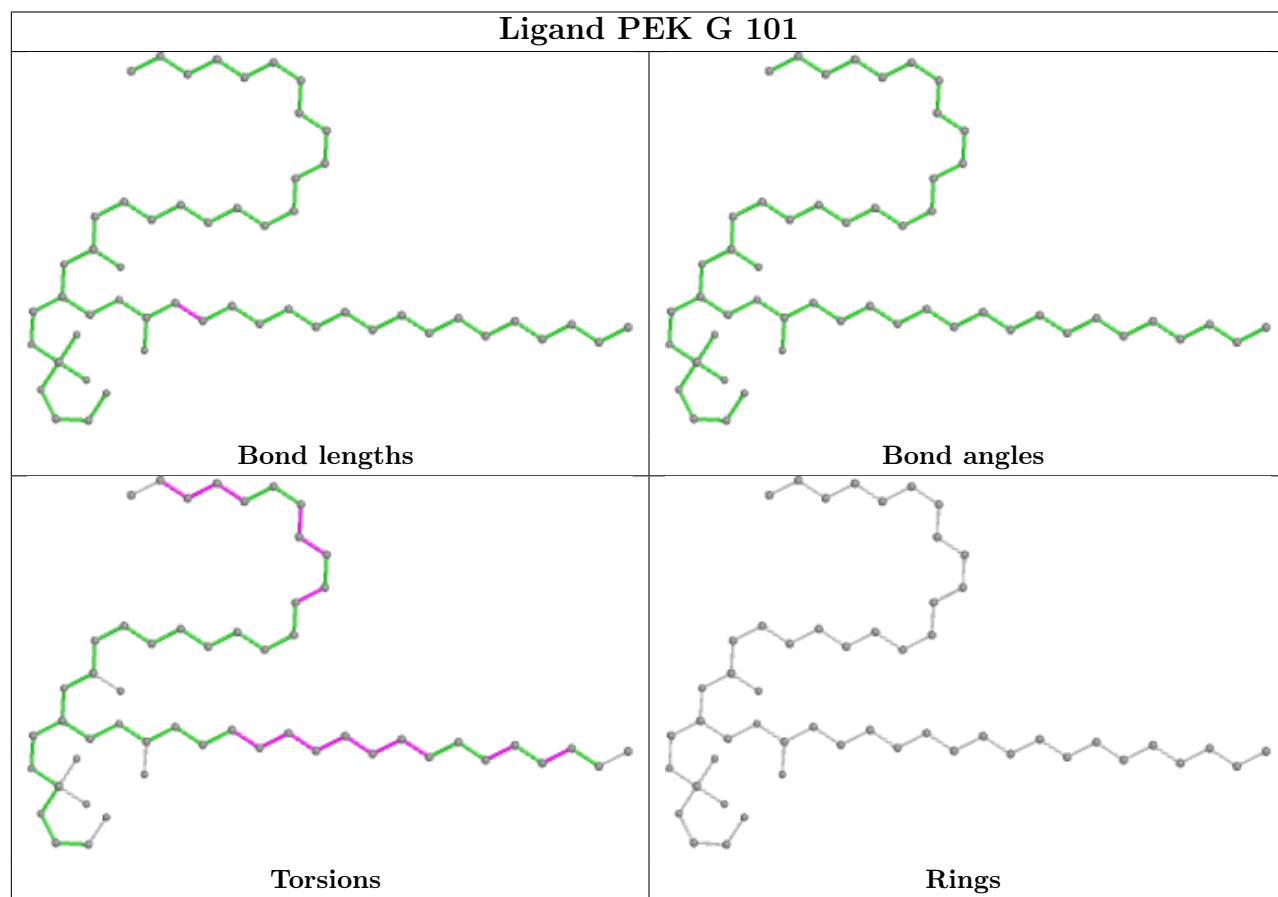
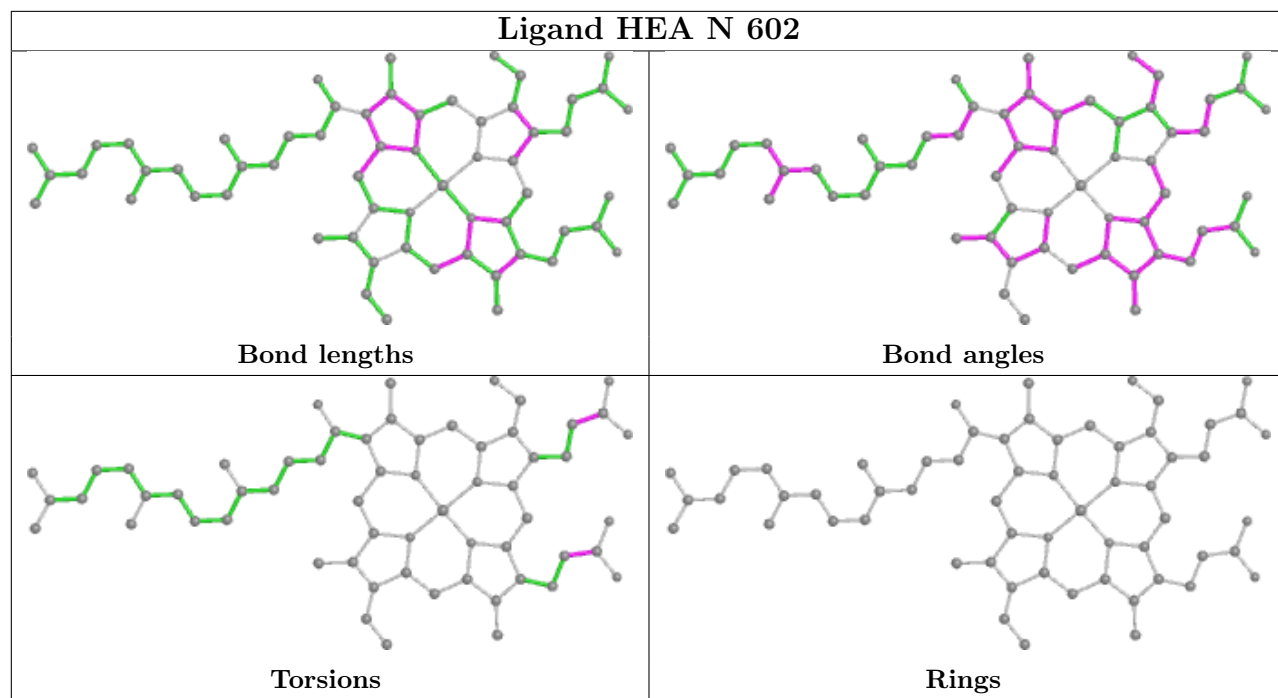
Ligand DMU B 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DMU Z 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

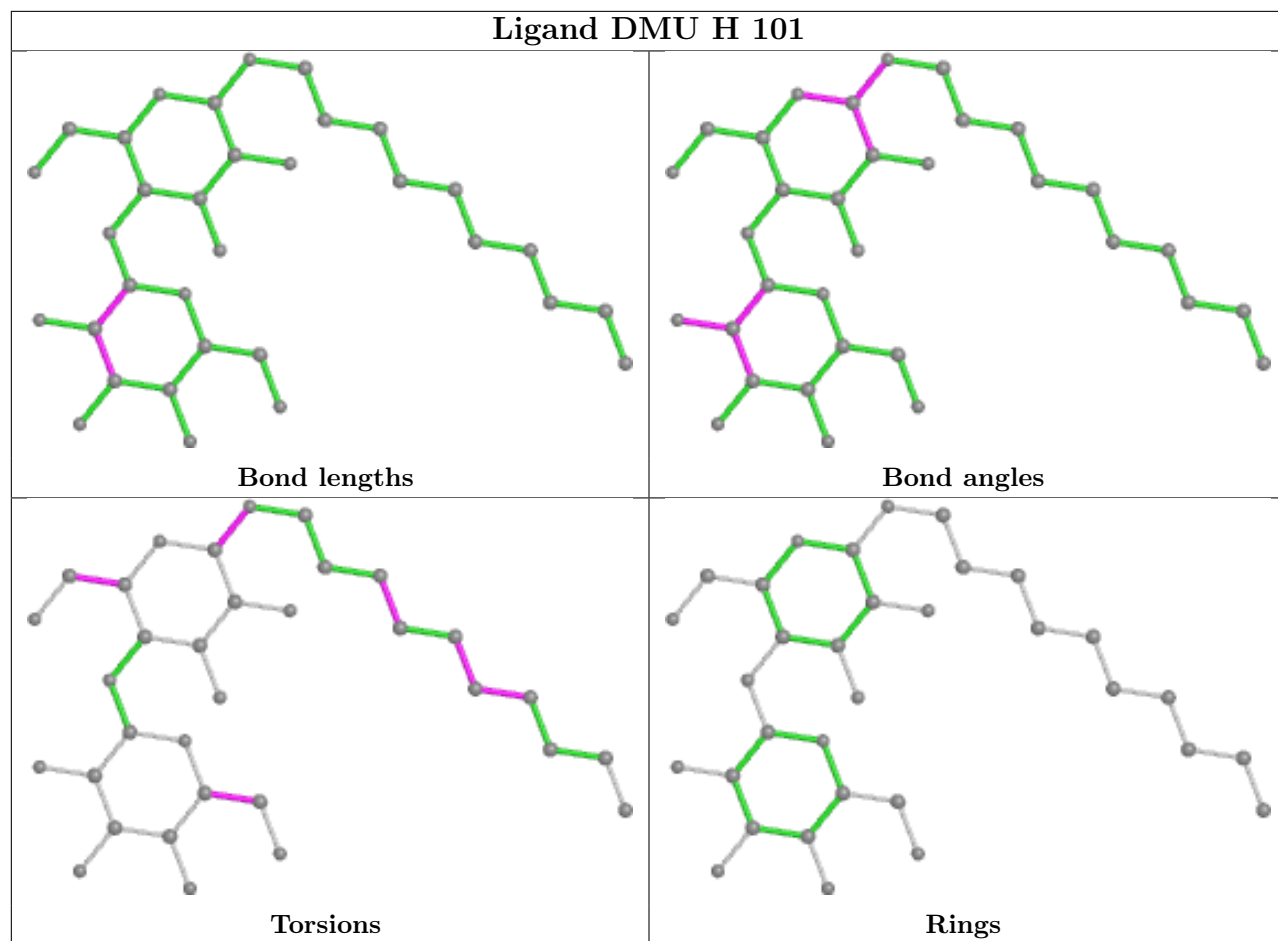


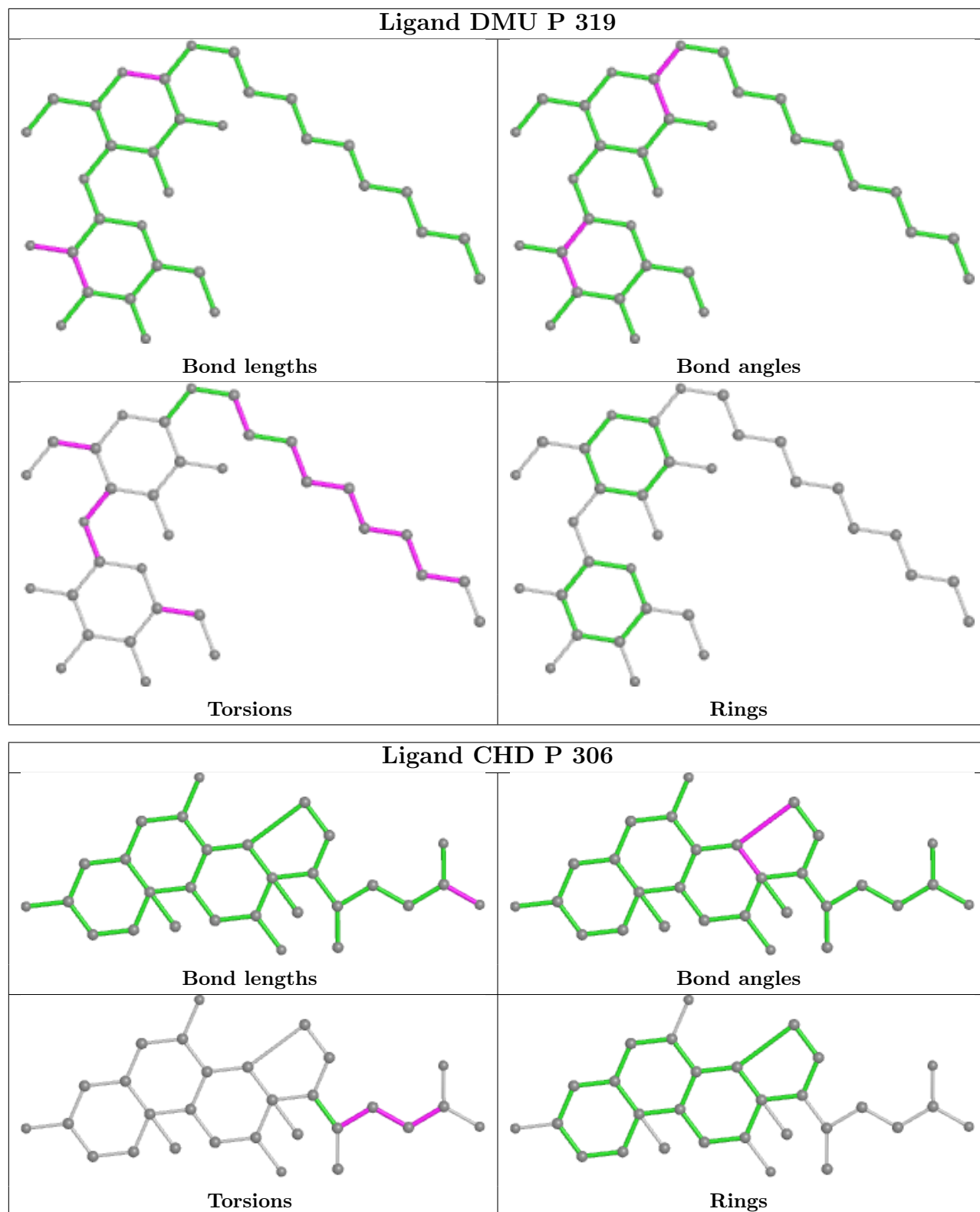




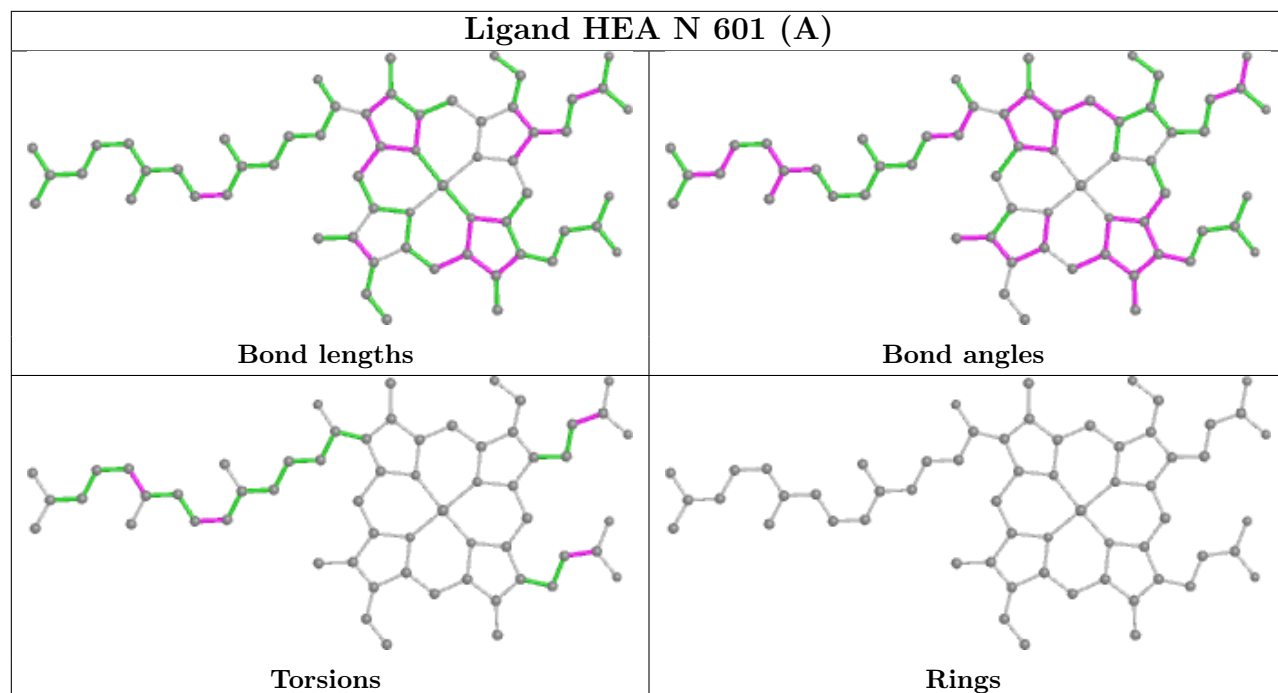




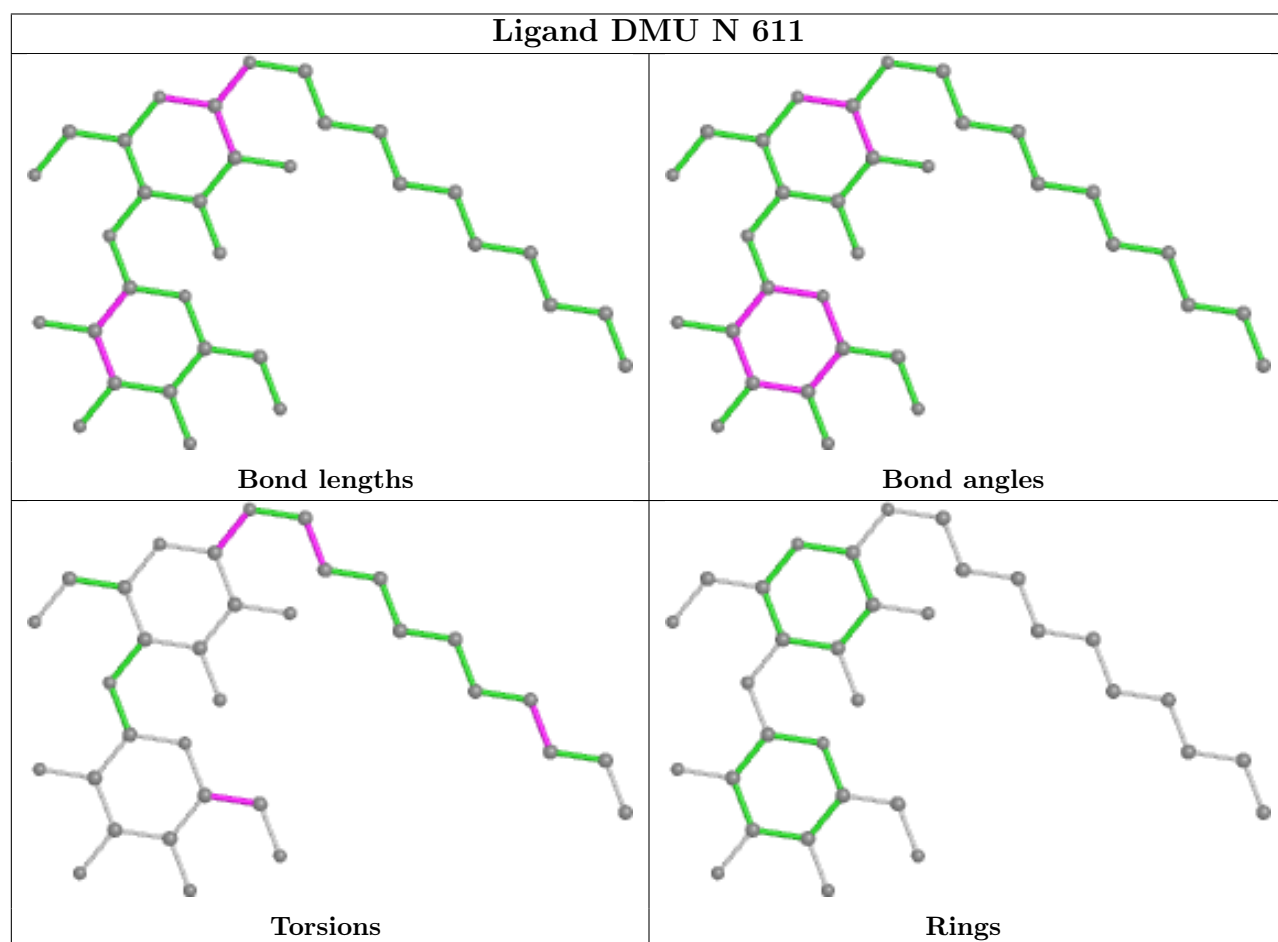


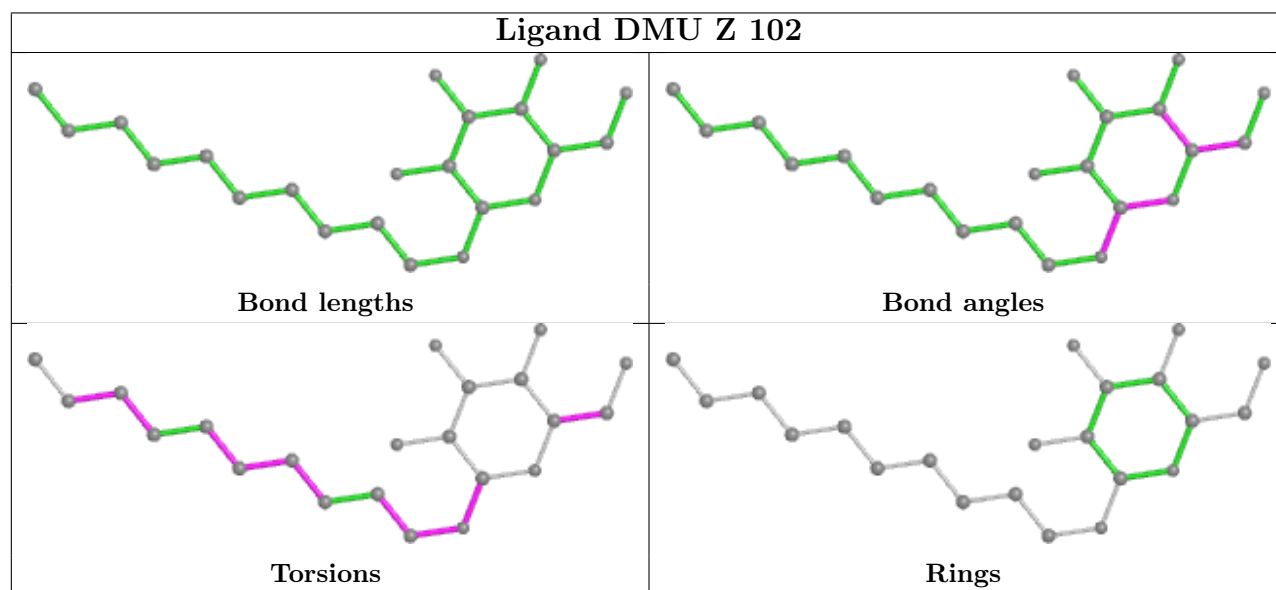
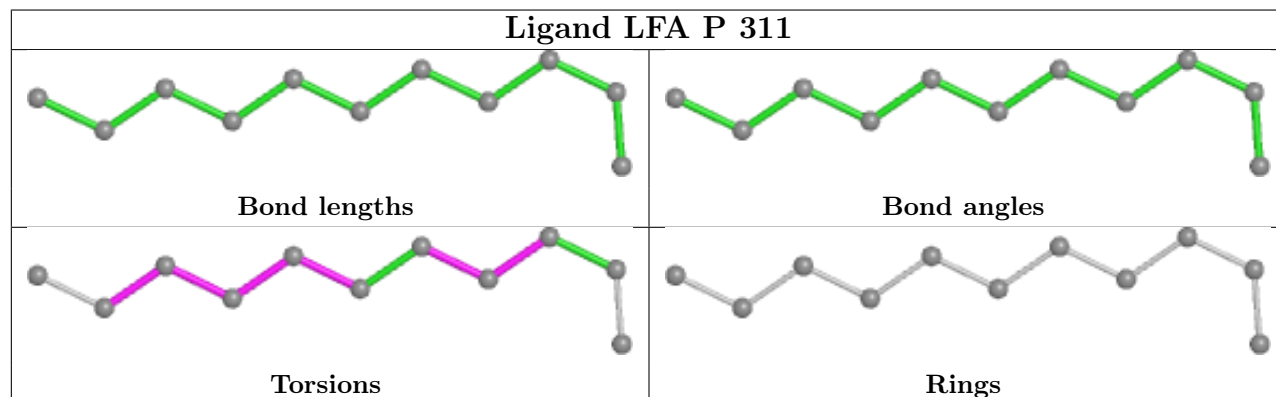
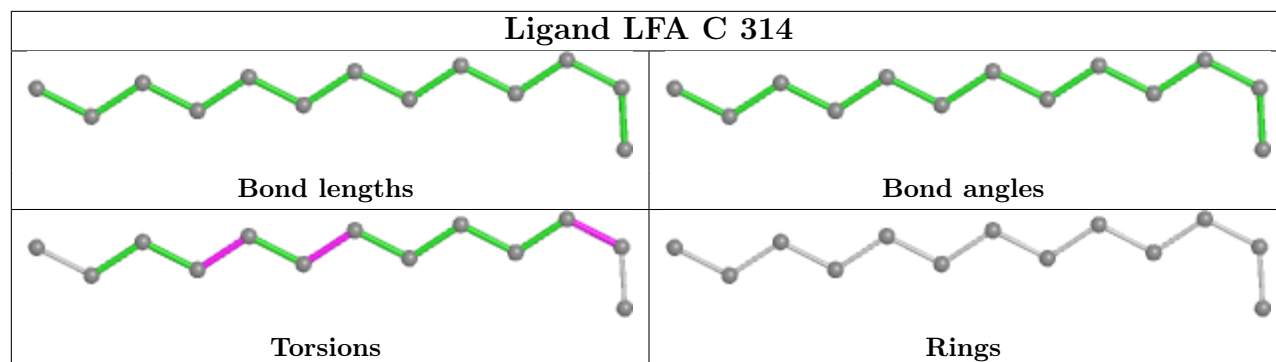


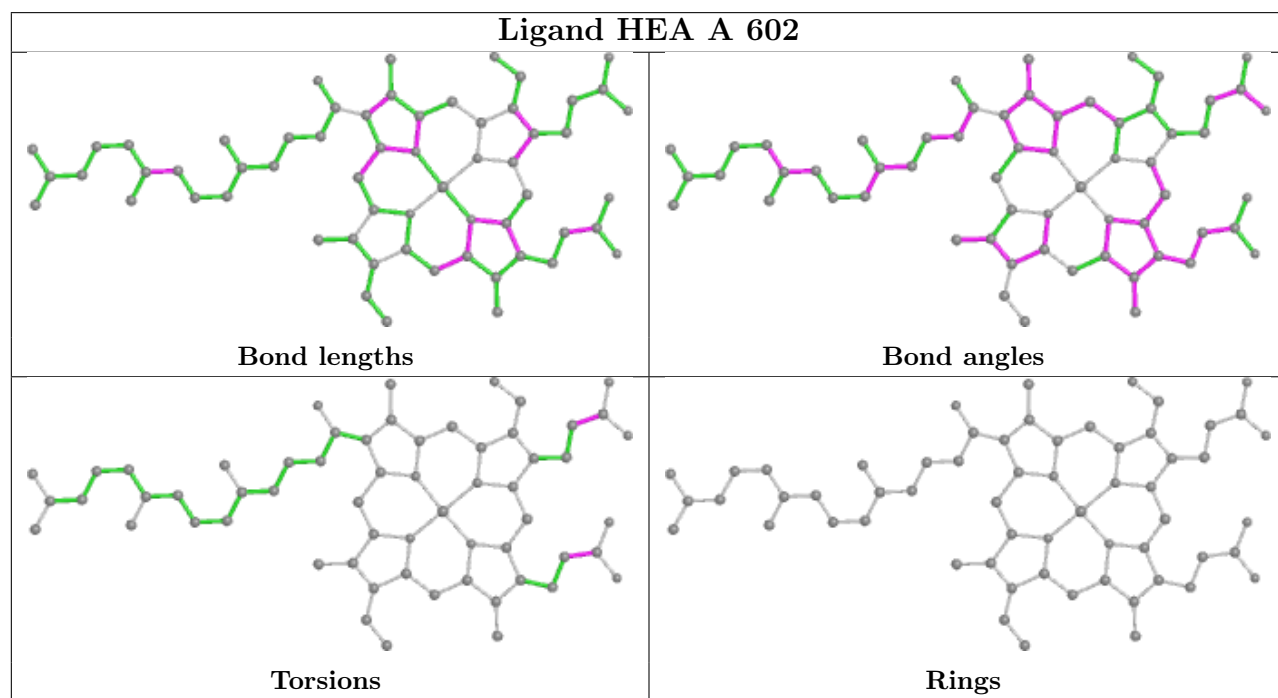
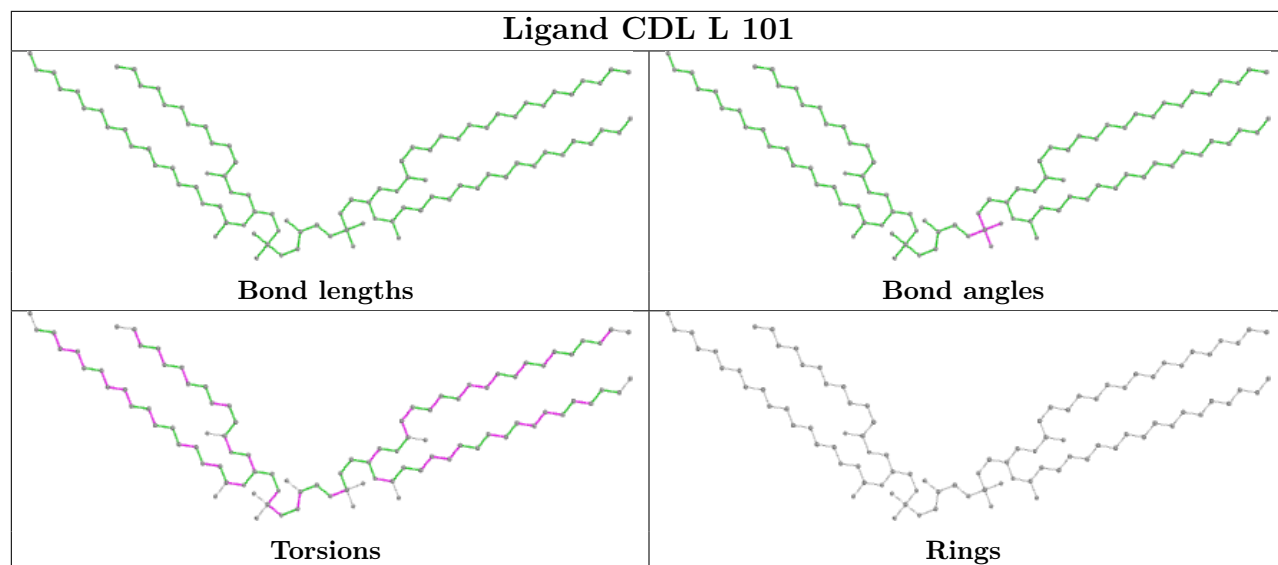
## Ligand HEA N 601 (A)

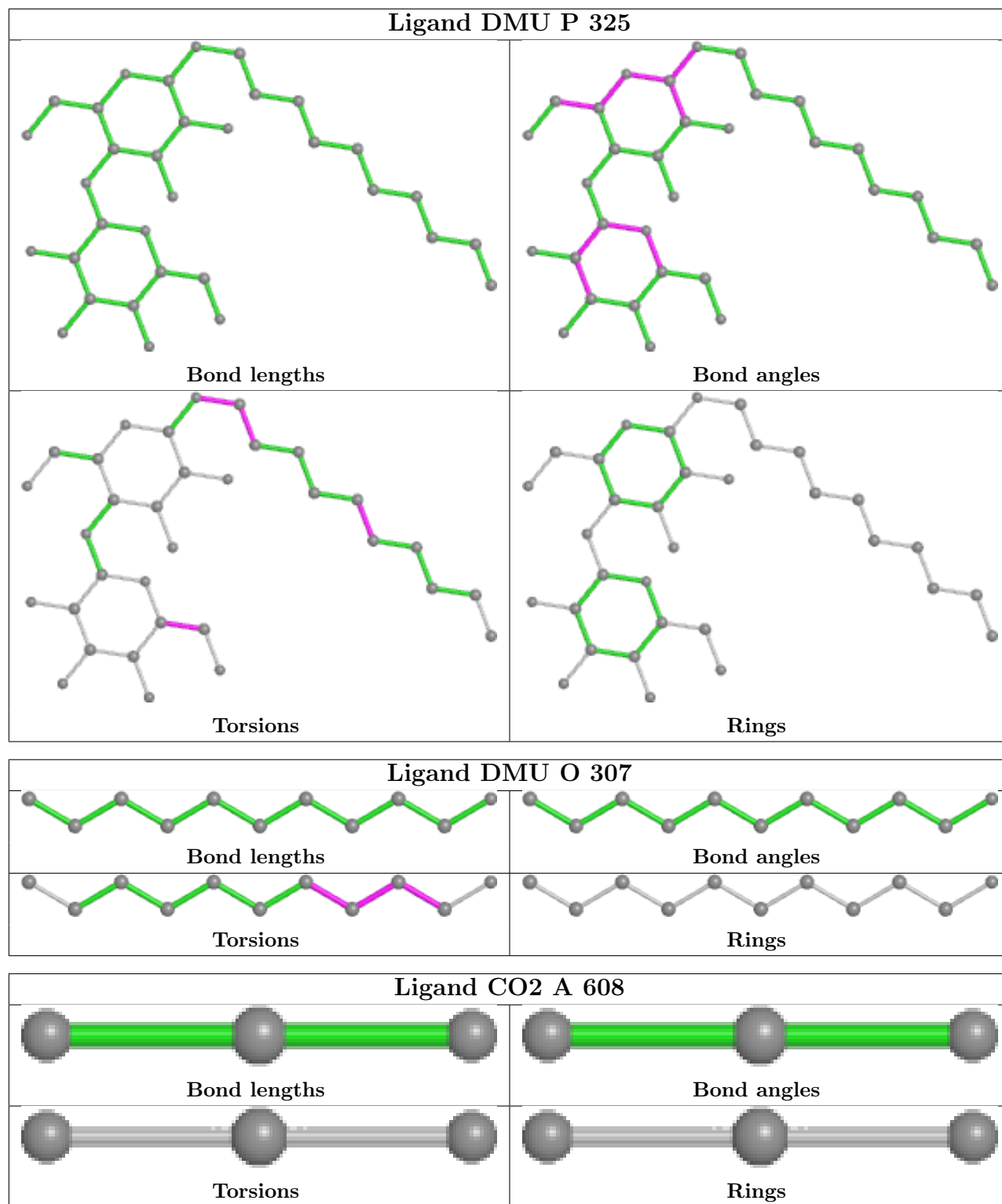


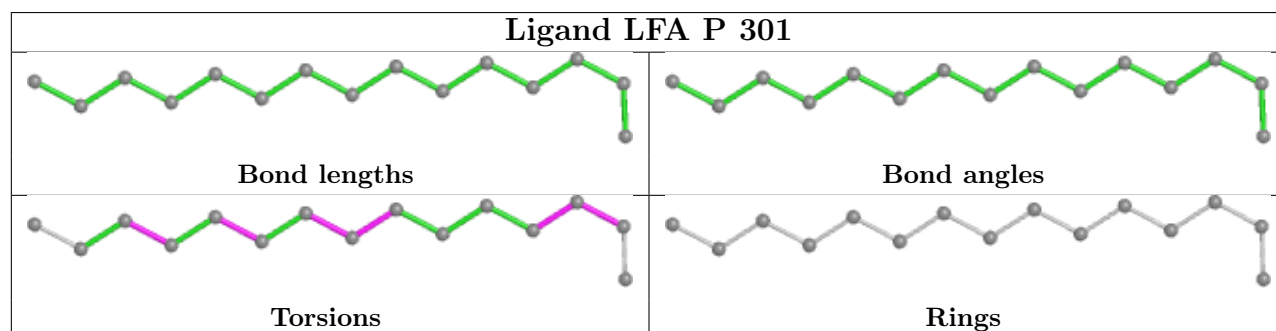
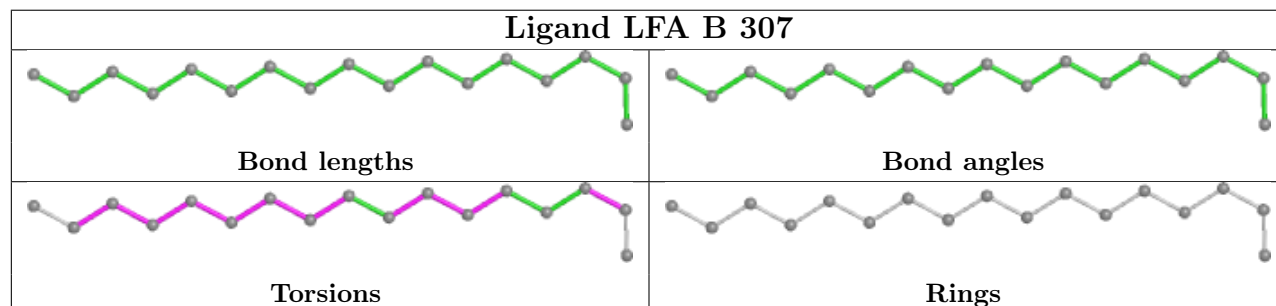
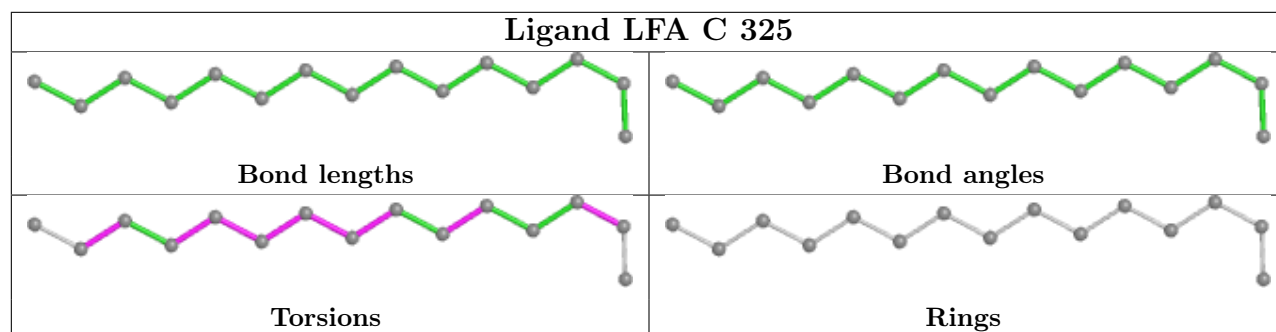
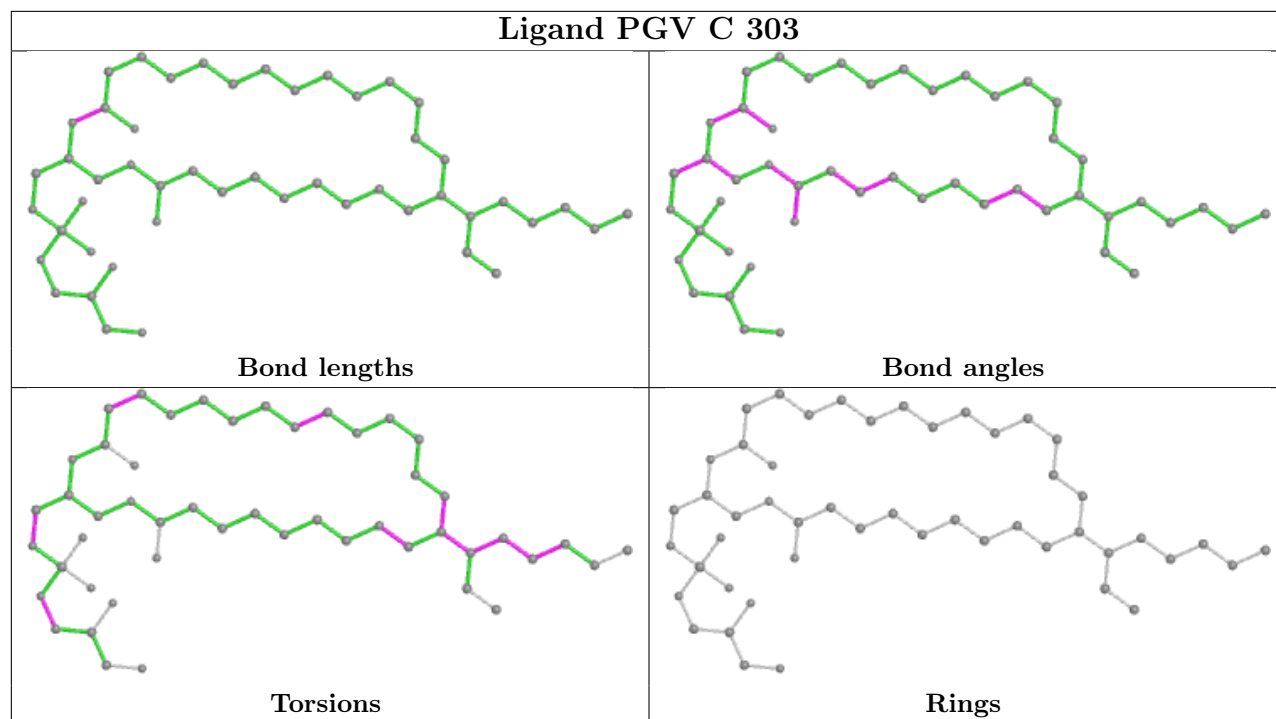
## Ligand DMU N 611

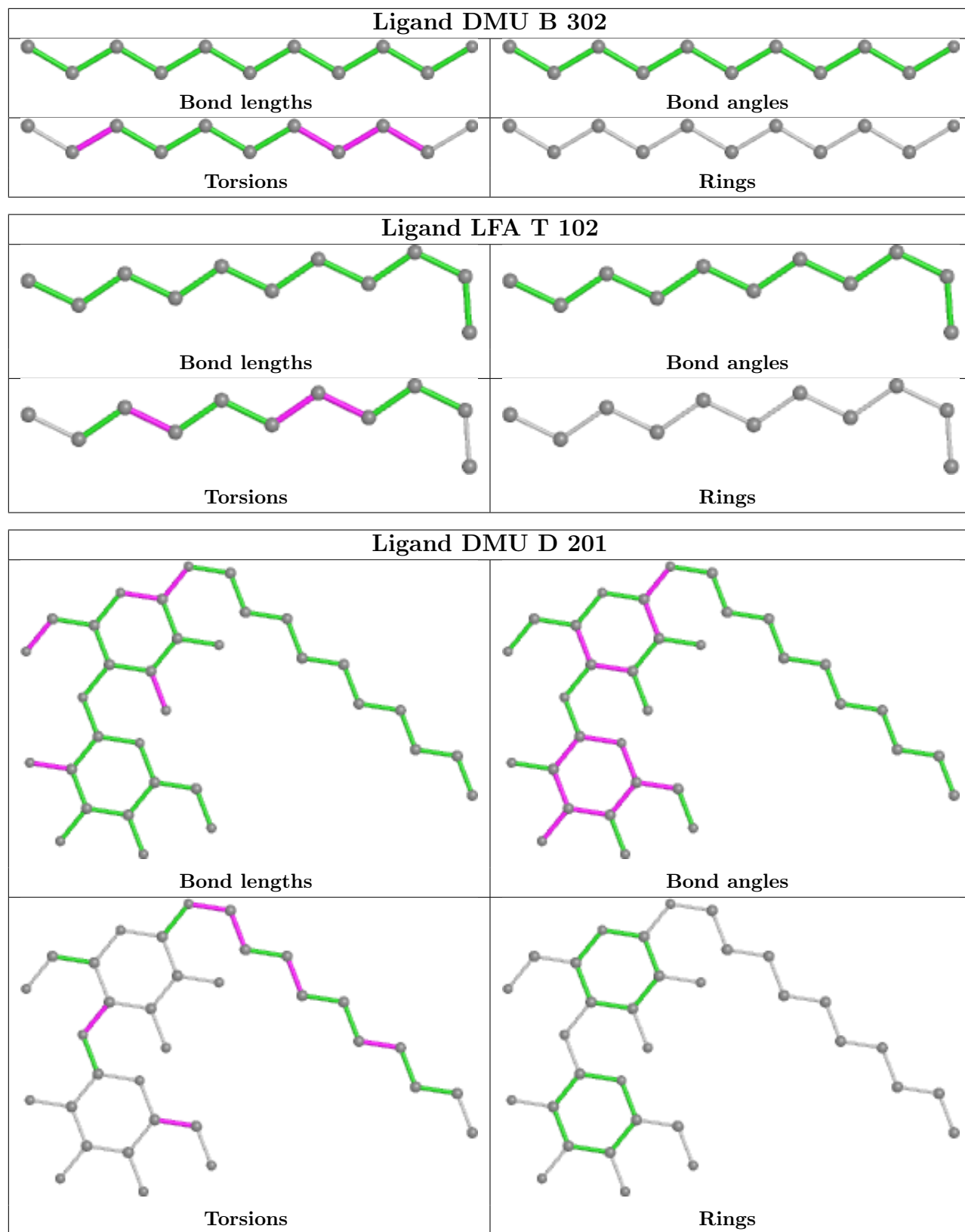




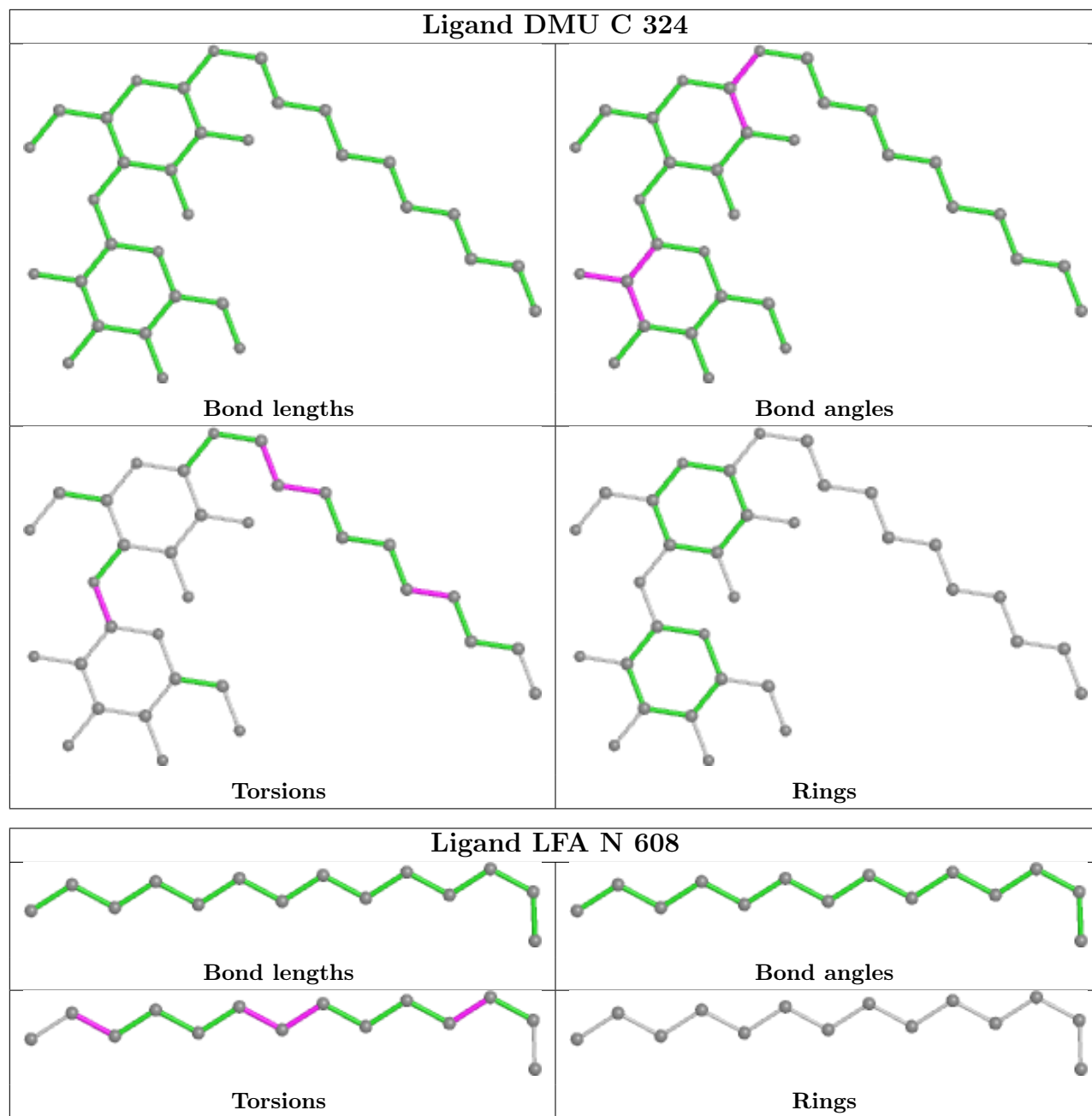


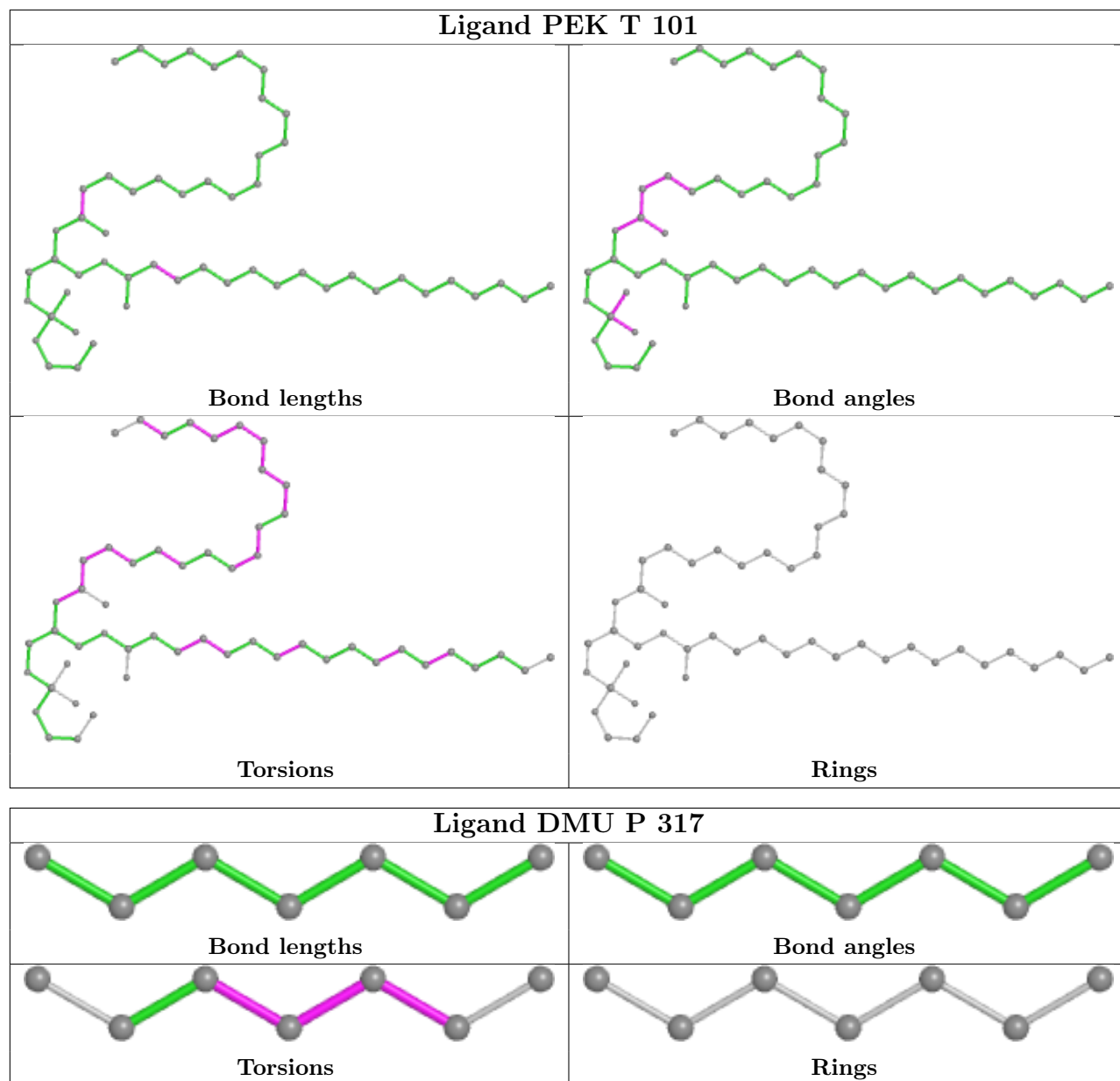


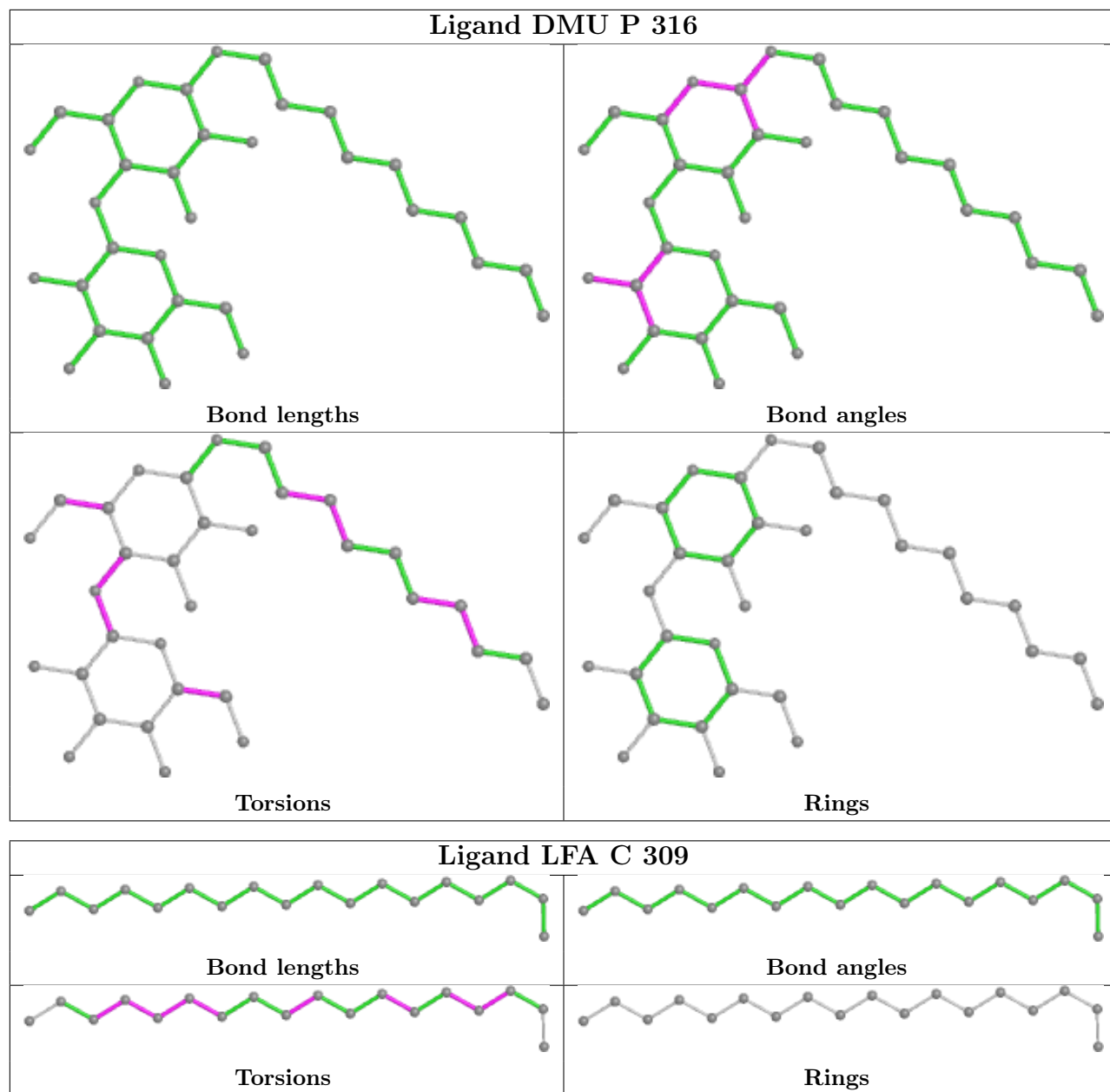


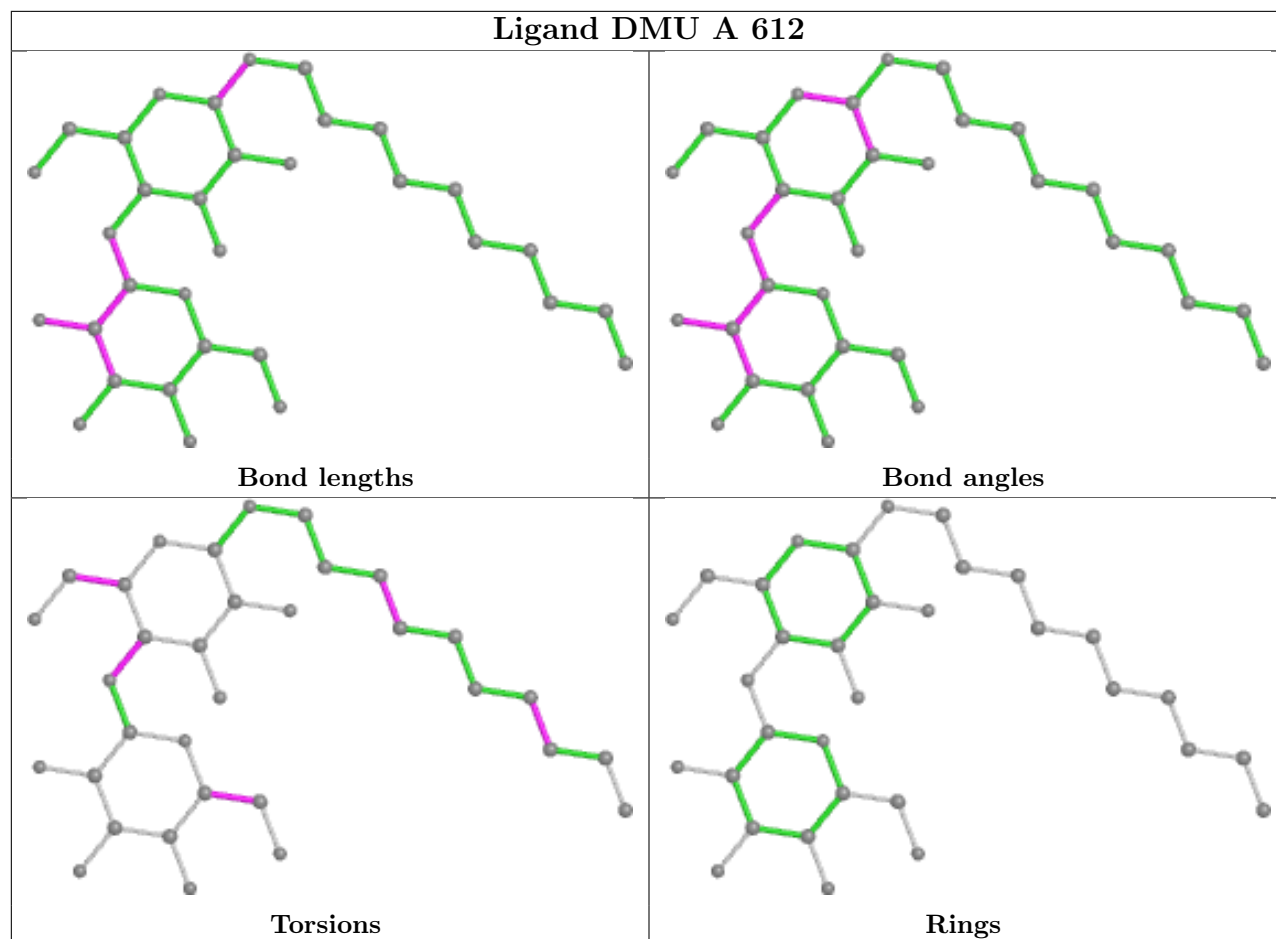


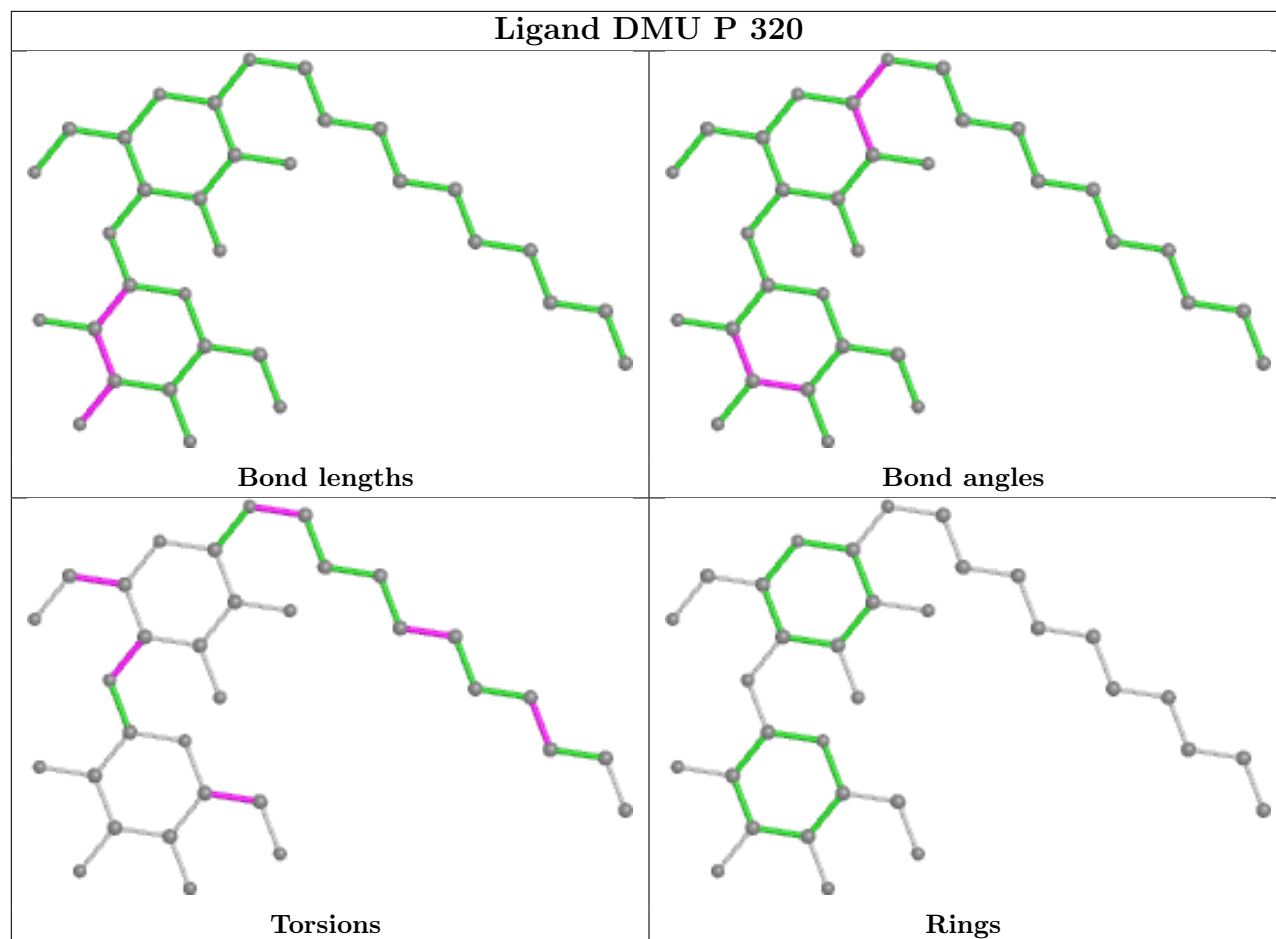


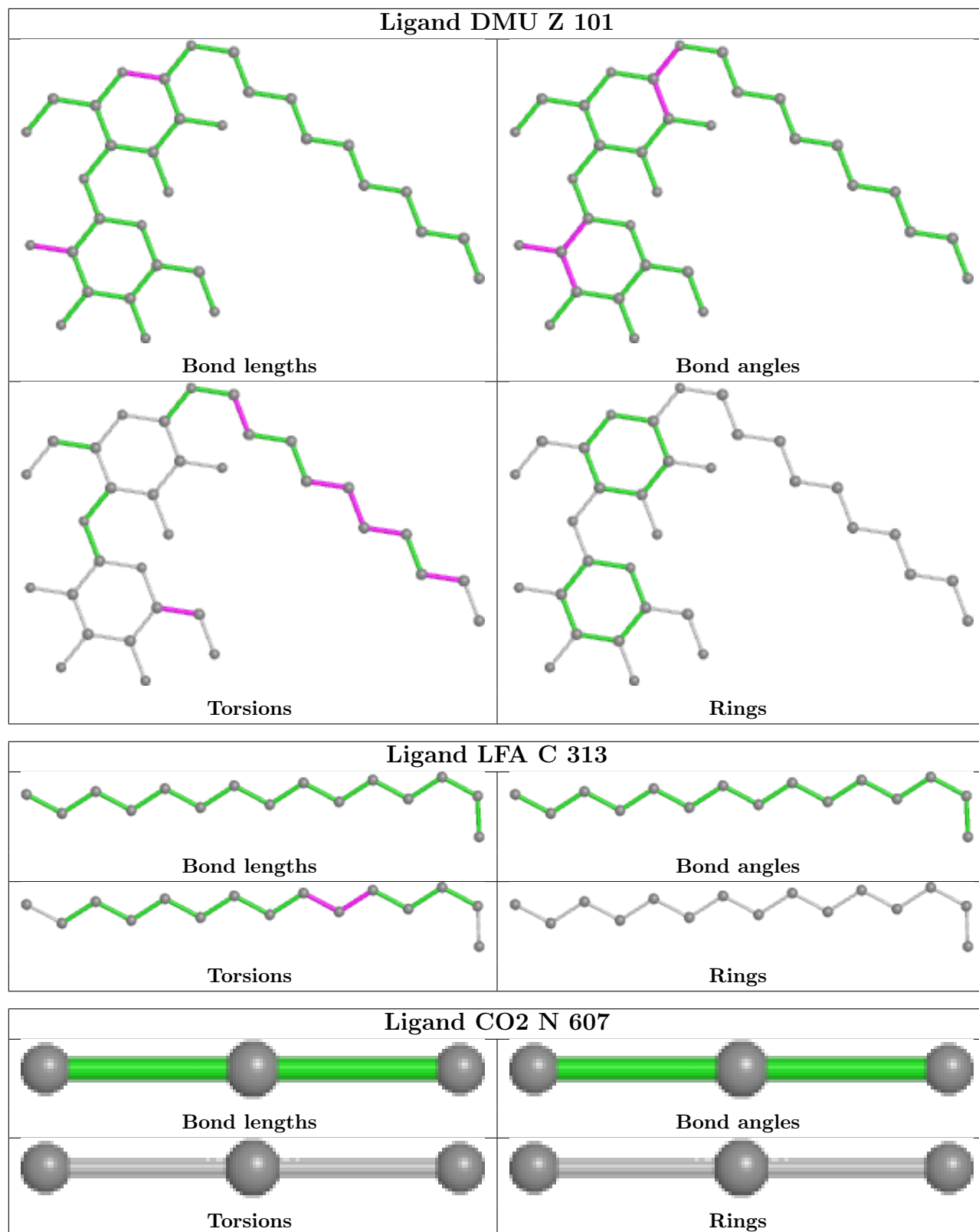


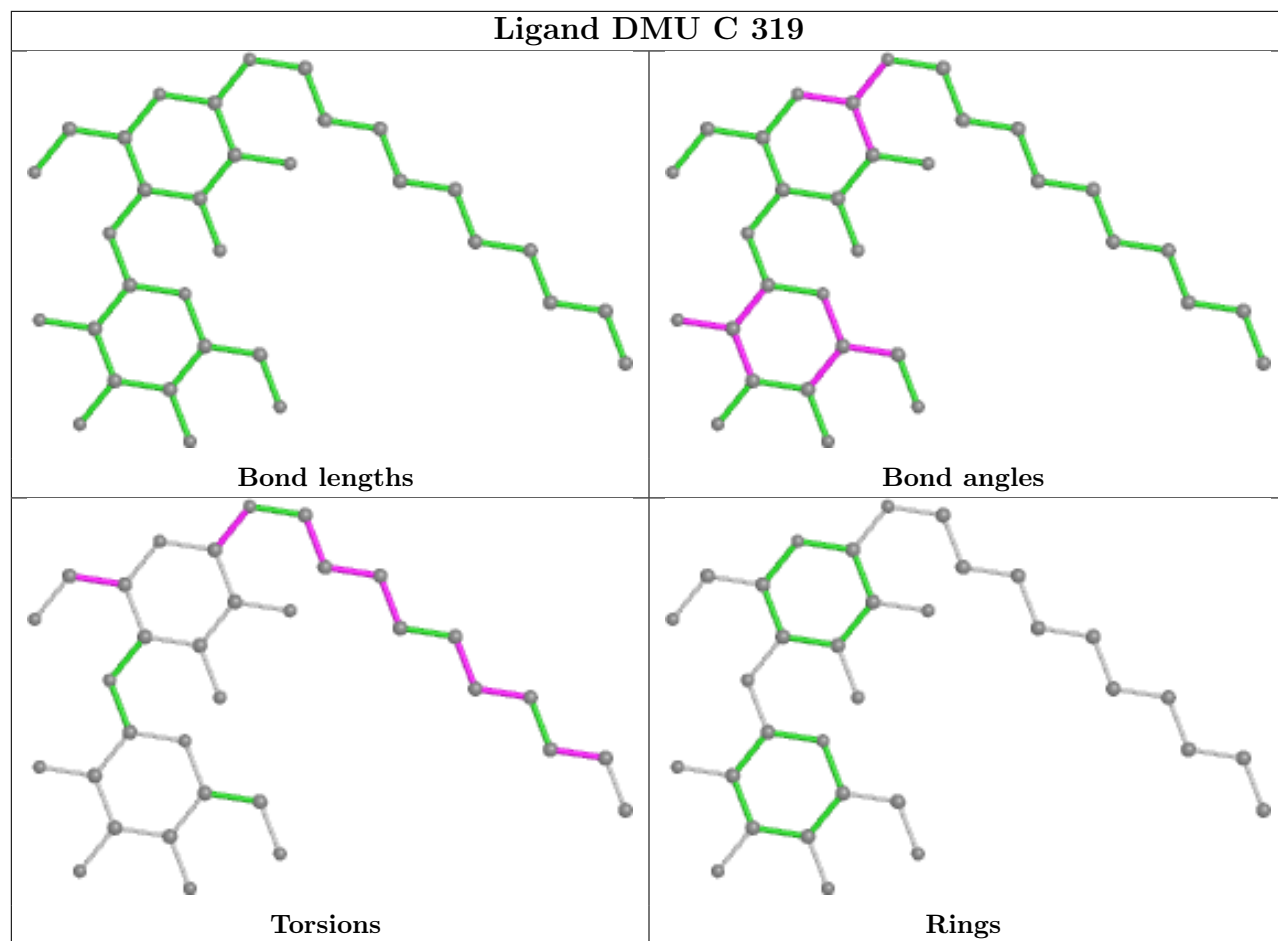


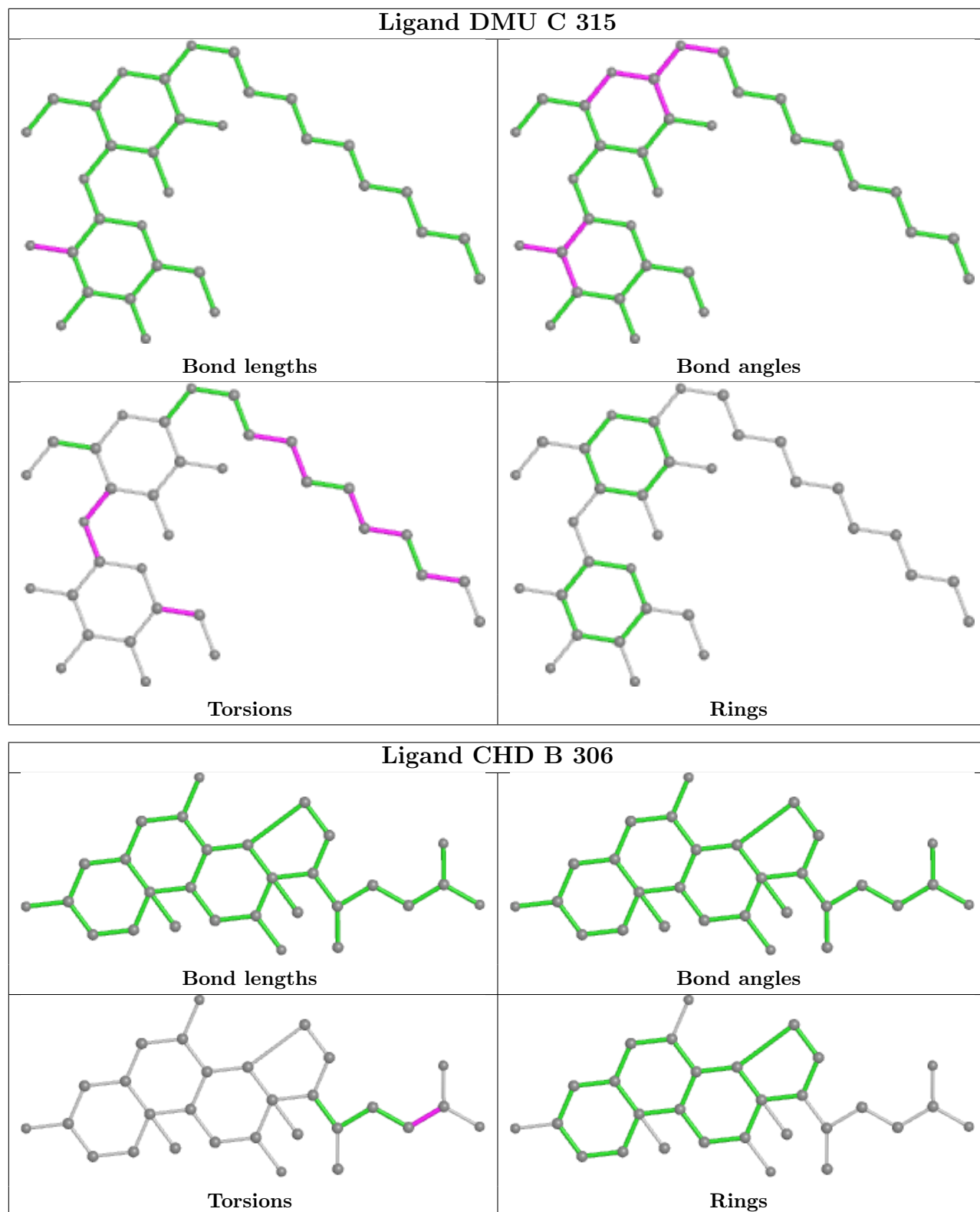




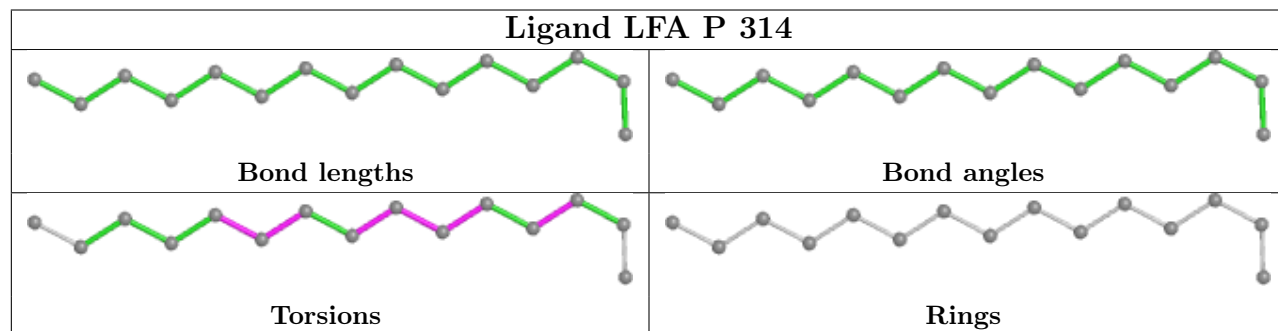
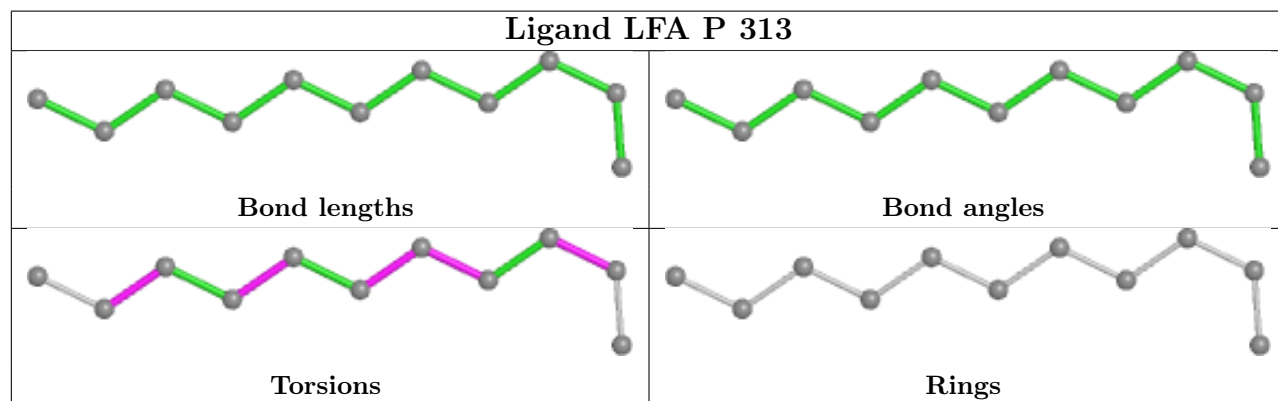
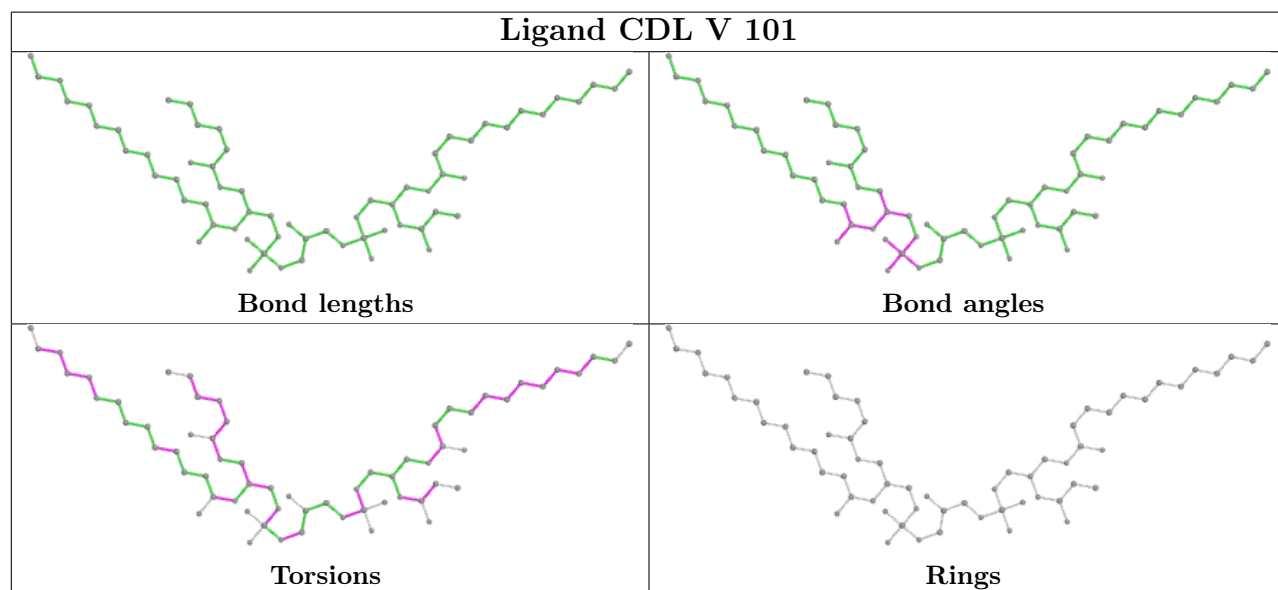
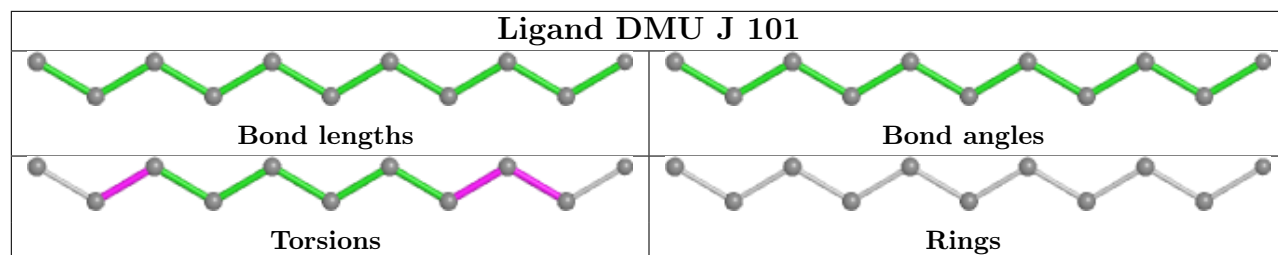


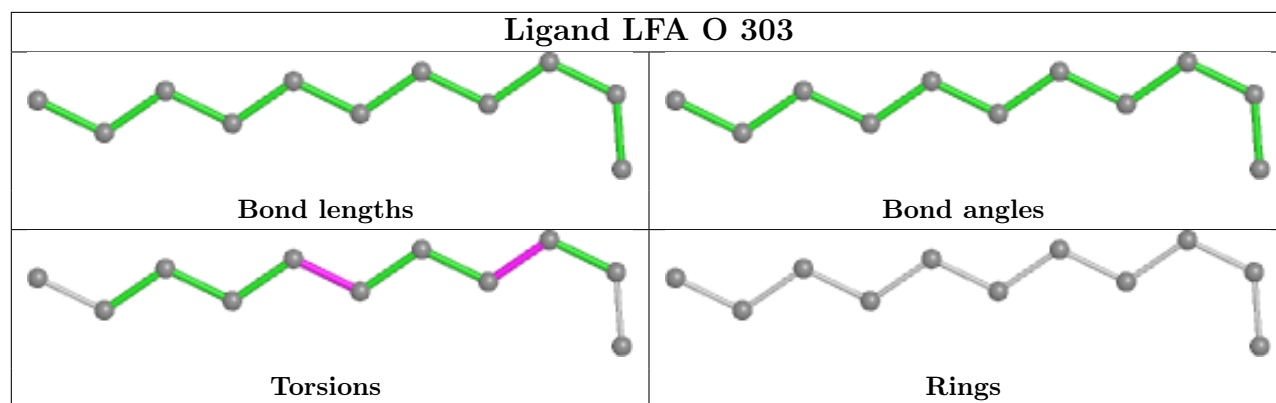
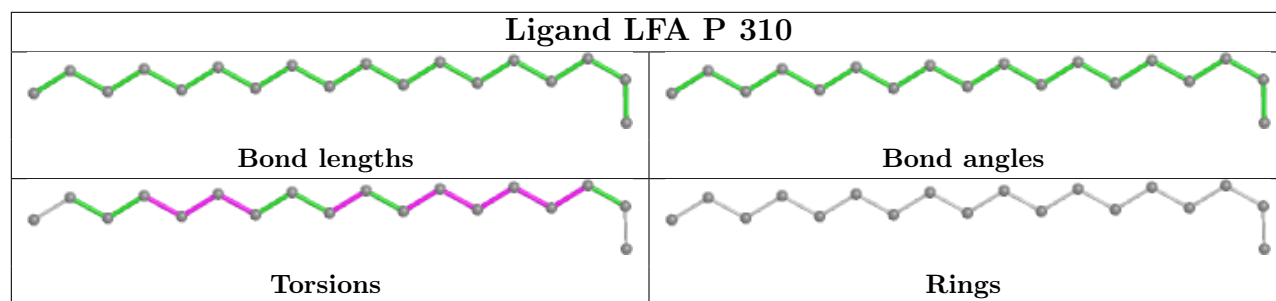
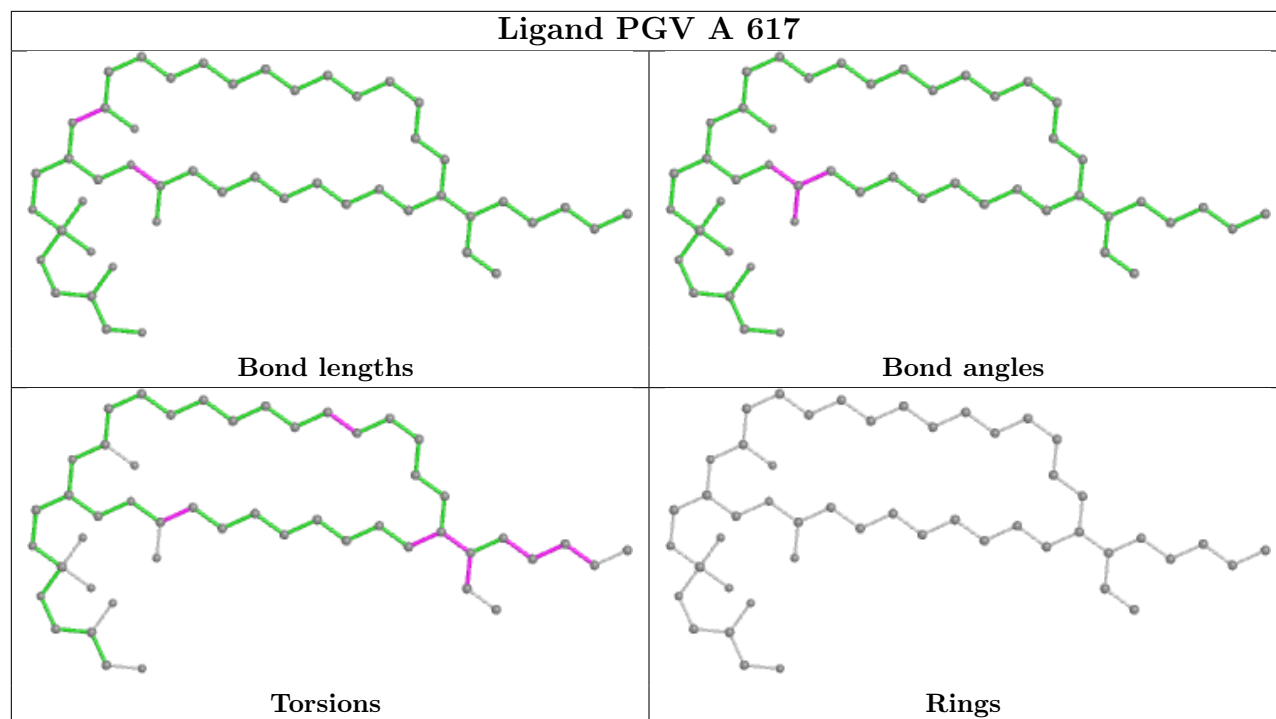


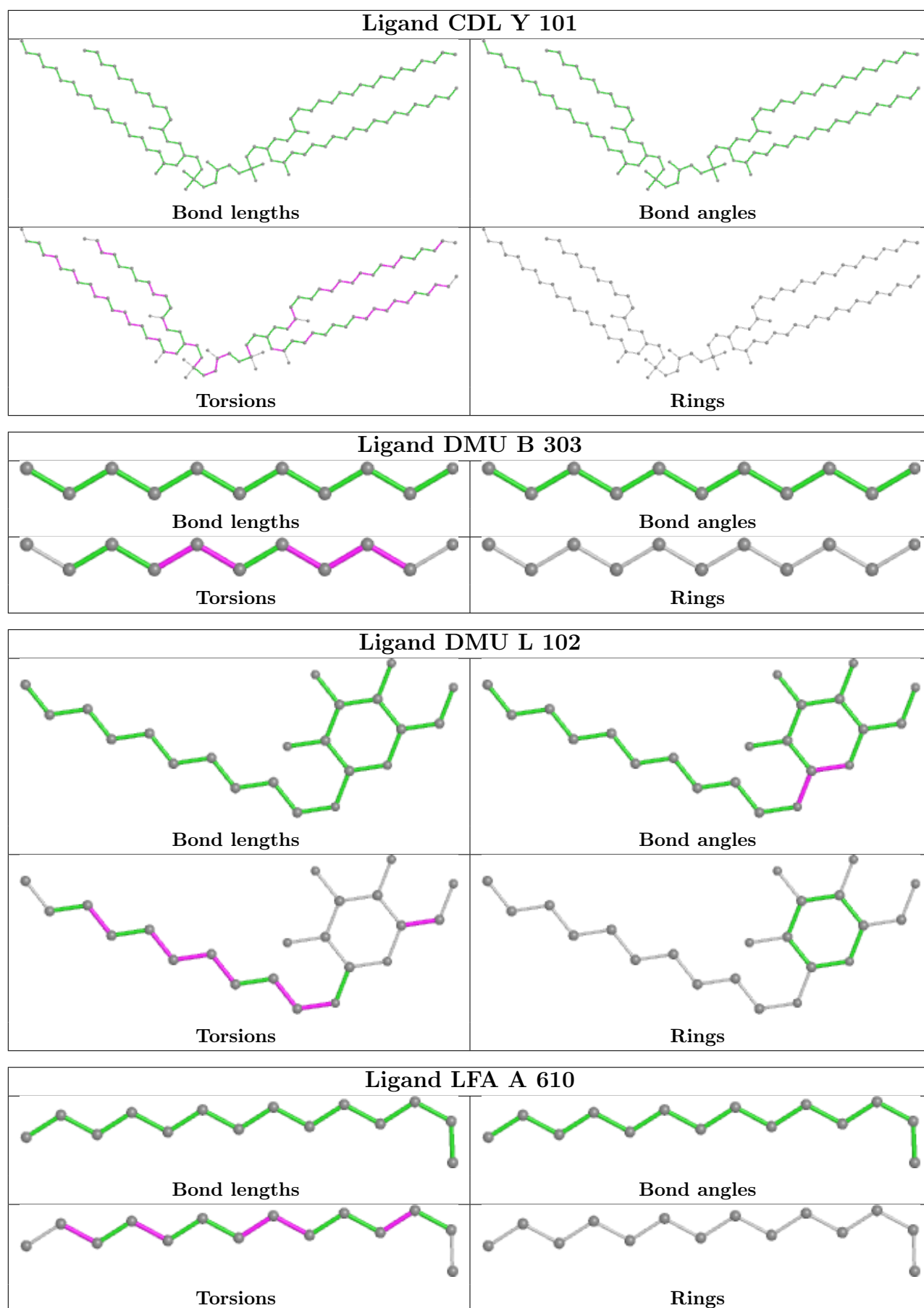


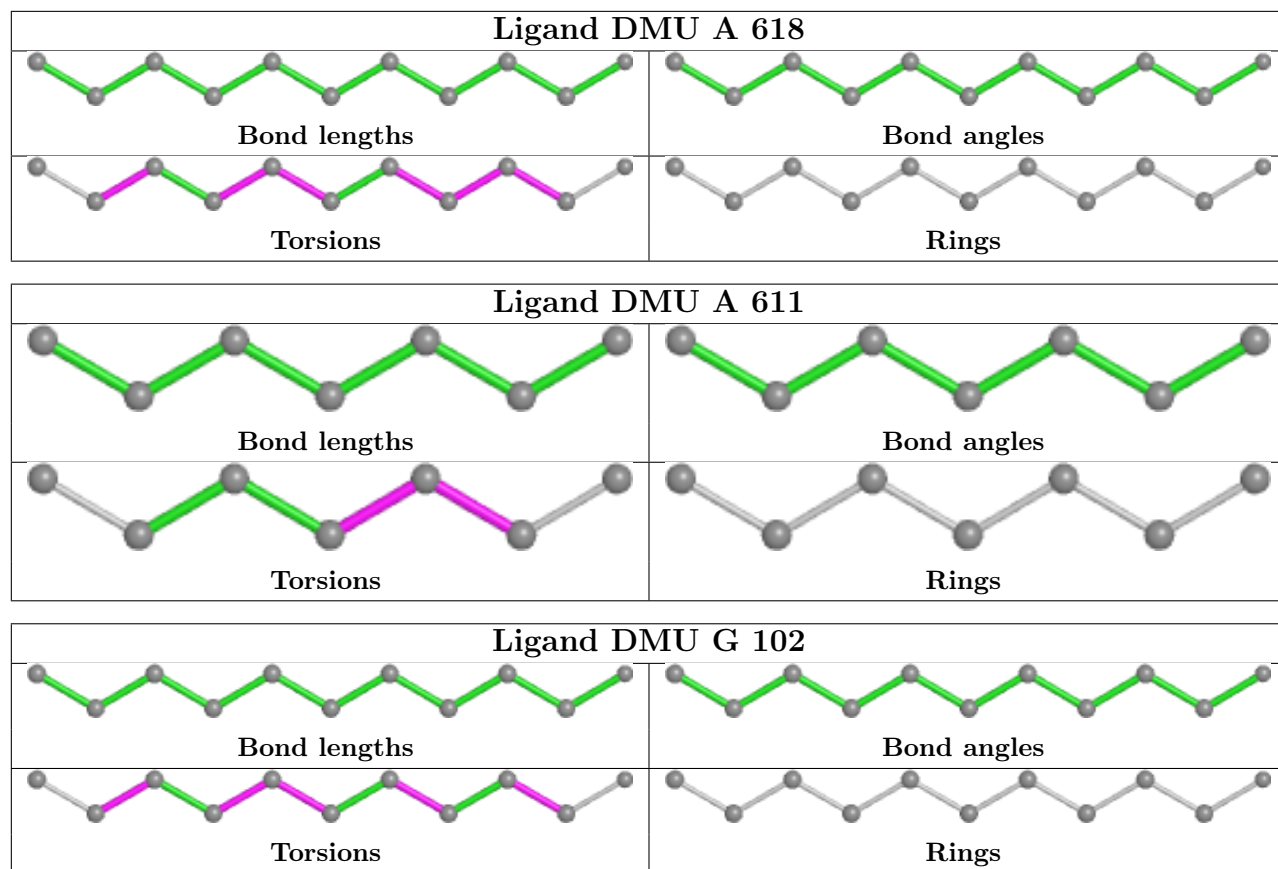


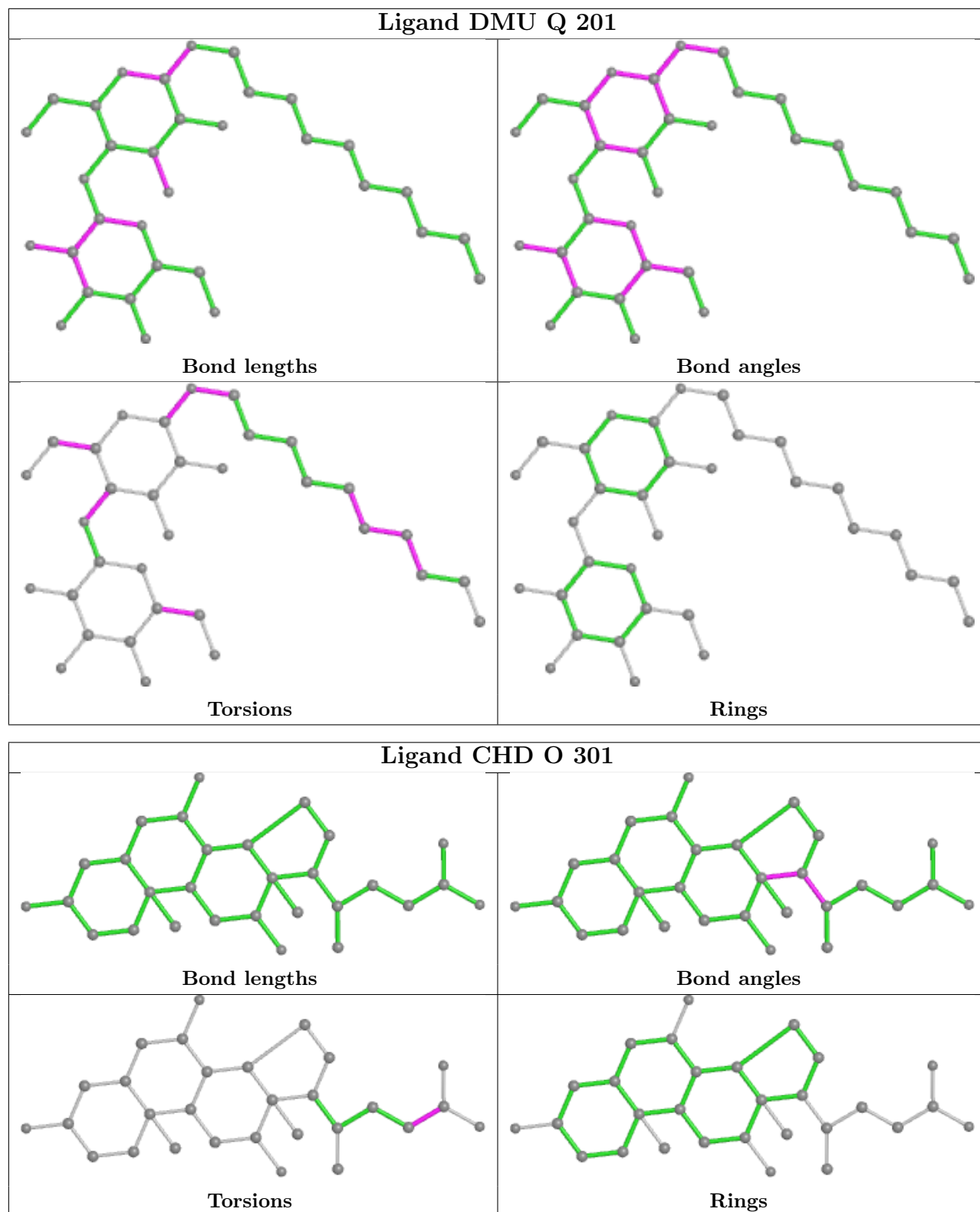


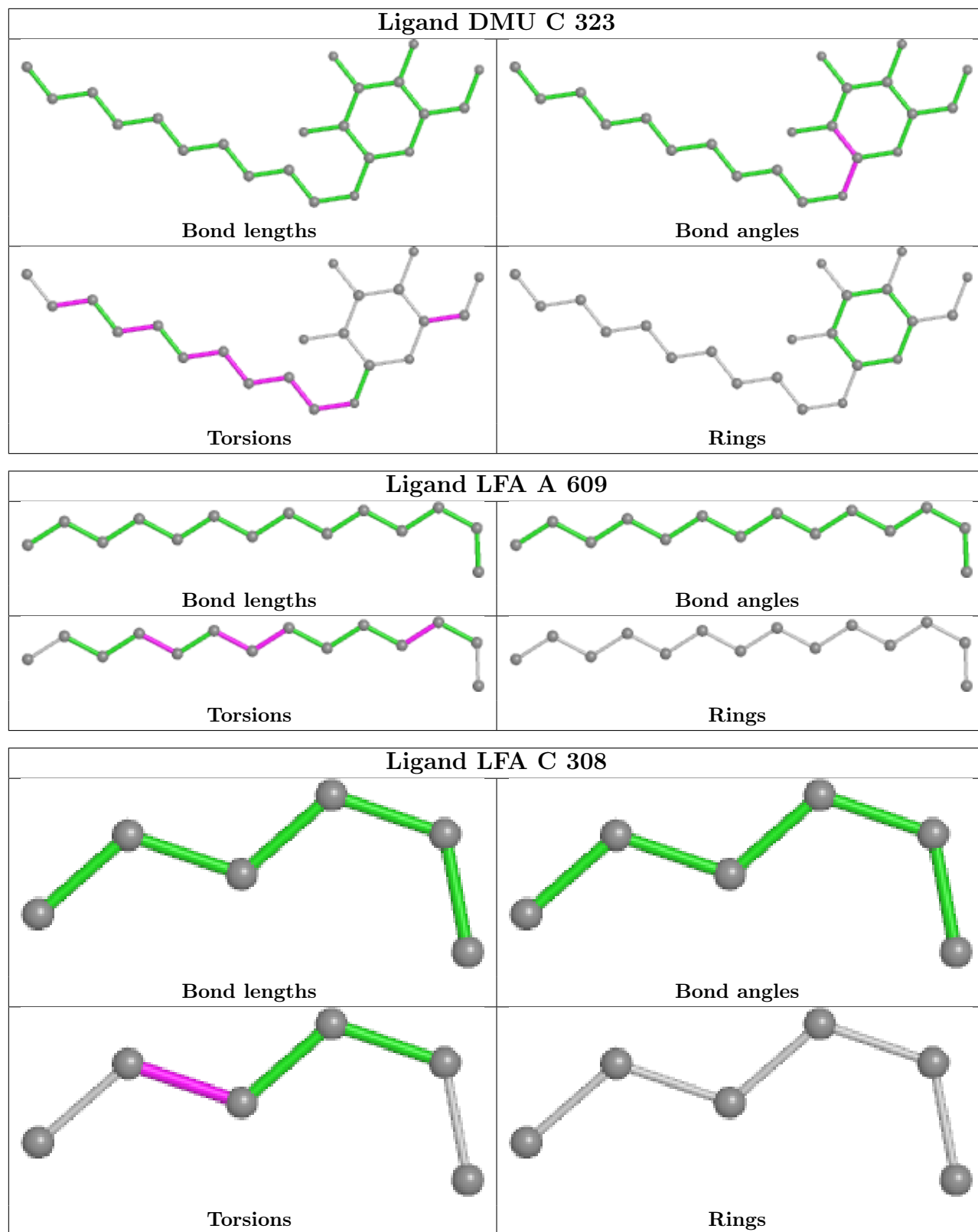












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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%)	-0.32	3 (0%) 85 89	16, 33, 40, 58	15 (2%)
1	N	512/514 (99%)	-0.21	5 (0%) 79 84	17, 36, 44, 63	15 (2%)
2	B	226/227 (99%)	0.04	12 (5%) 33 36	20, 40, 58, 77	5 (2%)
2	O	226/227 (99%)	0.10	6 (2%) 56 62	22, 44, 69, 94	5 (2%)
3	C	258/261 (98%)	-0.16	1 (0%) 89 92	16, 36, 47, 61	9 (3%)
3	P	258/261 (98%)	-0.22	1 (0%) 89 92	16, 37, 48, 68	9 (3%)
4	D	143/147 (97%)	-0.01	3 (2%) 63 69	19, 43, 59, 74	1 (0%)
4	Q	137/147 (93%)	0.37	5 (3%) 46 53	24, 53, 76, 90	1 (0%)
5	E	102/109 (93%)	-0.20	1 (0%) 79 84	35, 41, 55, 73	0
5	R	102/109 (93%)	-0.08	2 (1%) 64 71	39, 49, 66, 80	0
6	F	91/98 (92%)	-0.06	1 (1%) 77 83	20, 42, 61, 72	2 (2%)
6	S	91/98 (92%)	0.07	2 (2%) 62 68	20, 41, 62, 70	2 (2%)
7	G	72/85 (84%)	0.24	3 (4%) 41 47	21, 44, 87, 104	1 (1%)
7	T	72/85 (84%)	0.29	3 (4%) 41 47	23, 46, 87, 102	1 (1%)
8	H	75/85 (88%)	0.23	4 (5%) 33 36	38, 46, 85, 109	0
8	U	75/85 (88%)	0.23	4 (5%) 33 36	41, 50, 89, 113	0
9	I	70/73 (95%)	0.36	5 (7%) 23 26	38, 51, 76, 96	0
9	V	70/73 (95%)	0.39	3 (4%) 40 45	38, 58, 76, 106	0
10	J	56/59 (94%)	0.12	1 (1%) 67 73	37, 47, 68, 76	0
10	W	56/59 (94%)	0.14	1 (1%) 67 73	39, 49, 69, 80	0
11	K	49/56 (87%)	0.27	2 (4%) 42 48	41, 47, 63, 74	0
11	X	49/56 (87%)	0.69	3 (6%) 28 32	46, 56, 74, 90	0
12	L	44/47 (93%)	-0.09	0 100 100	35, 39, 50, 65	0
12	Y	44/47 (93%)	0.06	1 (2%) 61 67	38, 45, 60, 68	0

*Continued on next page...*



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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	40/46 (86%)	0.05	0 100 100	37, 40, 58, 68	0
13	Z	40/46 (86%)	0.46	1 (2%) 58 65	44, 50, 73, 82	0
All	All	3470/3614 (96%)	-0.03	73 (2%) 63 69	16, 40, 66, 113	66 (1%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	36	TRP	5.9
6	S	3	GLY	5.0
6	S	93	PRO	4.9
9	V	72	ALA	4.8
1	N	136[A]	LEU	4.7
7	G	36	TRP	4.5
4	D	5	VAL	4.4
11	X	6	ALA	4.3
2	B	59	GLN	4.2
1	N	113[A]	LEU	4.2
4	D	4	SER	3.9
2	O	113	TYR	3.8
6	F	3	GLY	3.6
9	I	3	ALA	3.6
2	O	32[A]	PHE	3.6
11	K	6	ALA	3.5
8	H	45	ALA	3.4
9	V	37	PHE	3.4
2	O	91	ASN	3.2
10	J	1	PHE	3.2
7	G	30	LEU	3.2
4	Q	39	ALA	3.2
8	U	48	GLY	3.1
8	H	46	LYS	3.0
1	N	311[A]	ILE	2.9
1	A	311[A]	ILE	2.9
2	O	90	ILE	2.9
8	U	49	ASP	2.9
7	T	38	HIS	2.9
10	W	48	TYR	2.9
1	A	113[A]	LEU	2.8
9	V	3	ALA	2.8
2	B	65	TRP	2.8
4	Q	35	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	61	VAL	2.7
2	B	32[A]	PHE	2.7
8	U	45	ALA	2.6
9	I	72	ALA	2.6
1	A	513	LEU	2.6
5	R	7	THR	2.6
11	X	13	TYR	2.5
2	B	87[A]	MET	2.5
3	P	37	PHE	2.5
2	B	60	GLU	2.4
8	H	48	GLY	2.4
9	I	37	PHE	2.4
11	X	7	PRO	2.4
2	B	67	ILE	2.3
2	B	115	ASP	2.3
12	Y	24	MET	2.3
2	O	22[A]	HIS	2.3
7	G	41	HIS	2.3
2	O	227	LEU	2.3
4	Q	72	ASN	2.2
7	T	30	LEU	2.2
4	Q	117	ALA	2.2
5	E	7	THR	2.2
2	B	91	ASN	2.2
2	B	113	TYR	2.2
9	I	25	PHE	2.1
1	N	35	LEU	2.1
1	N	483	LEU	2.1
3	C	258	TRP	2.1
4	D	102	TYR	2.1
8	U	50	VAL	2.1
2	B	58	ALA	2.1
9	I	21	ILE	2.1
2	B	16[A]	ILE	2.0
5	R	108	LYS	2.0
4	Q	73	ARG	2.0
11	K	26	VAL	2.0
8	H	44	THR	2.0
13	Z	1	ILE	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	0.13	43,52,80,92	0
1	FME	N	1	10/11	0.95	0.14	46,54,85,98	0
2	FME	B	1	10/11	0.97	0.09	37,39,50,88	0
2	FME	O	1	10/11	0.98	0.09	43,46,55,80	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
22	DMU	C	317	22/33	0.71	0.32	42,61,70,87	22
22	DMU	P	318	22/33	0.76	0.31	38,64,77,84	22
21	LFA	P	311	11/20	0.78	0.42	46,58,68,75	11
21	LFA	C	308	6/20	0.79	0.43	41,46,52,52	6
23	EDO	C	322	4/4	0.79	0.35	36,38,40,41	4
23	EDO	E	201	4/4	0.81	0.42	38,42,45,49	4
23	EDO	P	323	4/4	0.81	0.28	33,33,38,40	4
22	DMU	C	318	33/33	0.82	0.36	42,56,75,87	33
22	DMU	N	610	7/33	0.83	0.40	54,61,67,68	7
22	DMU	A	611	7/33	0.83	0.34	53,59,64,69	7
22	DMU	C	315	33/33	0.83	0.35	43,57,63,68	33
21	LFA	C	325	15/20	0.83	0.41	49,55,70,73	15
21	LFA	C	311	14/20	0.83	0.37	43,60,66,66	14
21	LFA	C	313	15/20	0.84	0.28	47,53,74,75	15
21	LFA	N	609	14/20	0.84	0.29	41,49,59,60	14
22	DMU	C	319	33/33	0.84	0.25	41,63,75,77	33
23	EDO	N	613	4/4	0.84	0.28	40,44,47,47	4
21	LFA	O	302	17/20	0.84	0.32	39,58,72,73	17

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	EDO	R	203	4/4	0.84	0.31	39,42,51,53	4
21	LFA	O	303	11/20	0.85	0.32	45,58,67,71	11
21	LFA	C	314	13/20	0.85	0.30	50,59,70,73	13
26	CHD	P	306	29/29	0.85	0.17	62,71,94,103	0
21	LFA	P	301	15/20	0.86	0.33	45,53,61,63	15
22	DMU	P	320	33/33	0.86	0.25	49,73,82,86	33
21	LFA	P	309	6/20	0.86	0.36	46,50,52,55	6
21	LFA	C	310	11/20	0.86	0.34	56,65,78,80	11
21	LFA	A	610	14/20	0.86	0.27	40,48,60,62	14
22	DMU	C	324	33/33	0.86	0.19	40,57,74,87	33
22	DMU	M	102	8/33	0.86	0.23	42,45,50,58	8
22	DMU	A	618	11/33	0.86	0.37	50,58,66,69	11
21	LFA	T	102	11/20	0.87	0.28	49,56,66,69	11
22	DMU	N	611	33/33	0.87	0.22	41,53,77,79	33
21	LFA	B	307	17/20	0.87	0.31	41,56,72,73	17
22	DMU	P	319	33/33	0.87	0.31	49,58,71,86	33
21	LFA	A	609	14/20	0.87	0.26	38,46,72,75	14
22	DMU	P	325	33/33	0.87	0.18	43,61,86,89	33
22	DMU	Q	201	33/33	0.87	0.22	40,55,65,76	33
21	LFA	P	308	11/20	0.87	0.33	50,54,59,63	11
21	LFA	C	312	11/20	0.87	0.29	43,53,63,63	11
21	LFA	C	309	18/20	0.87	0.24	39,48,62,64	18
21	LFA	P	312	14/20	0.87	0.33	39,64,68,70	14
21	LFA	P	313	11/20	0.87	0.29	41,52,66,70	11
21	LFA	P	315	13/20	0.87	0.28	43,56,67,68	13
23	EDO	C	320	4/4	0.88	0.27	48,51,53,65	4
22	DMU	C	323	22/33	0.88	0.29	51,60,68,72	22
19	CDL	P	305	87/100	0.88	0.19	46,83,134,163	0
22	DMU	H	101	33/33	0.88	0.24	34,48,58,76	33
22	DMU	O	304	22/33	0.88	0.29	56,66,78,99	22
22	DMU	P	316	33/33	0.88	0.28	46,56,69,77	33
26	CHD	C	305	29/29	0.88	0.14	59,69,87,106	0
23	EDO	A	613	4/4	0.88	0.20	30,33,33,35	4
22	DMU	W	101	11/33	0.89	0.33	63,68,73,76	11
19	CDL	C	304	87/100	0.89	0.18	47,83,117,131	0
23	EDO	A	614	4/4	0.89	0.23	36,45,49,52	4
21	LFA	P	314	15/20	0.89	0.21	43,48,55,62	15
19	CDL	A	607	64/100	0.89	0.16	46,78,105,127	0
19	CDL	V	101	64/100	0.89	0.16	56,81,114,138	0
21	LFA	P	310	18/20	0.89	0.26	41,54,64,64	18
21	LFA	C	307	11/20	0.89	0.30	45,49,62,66	11
22	DMU	P	324	22/33	0.89	0.24	50,60,66,75	22

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	DMU	B	308	22/33	0.89	0.28	55,74,80,84	22
19	CDL	Y	101	94/100	0.89	0.17	51,84,134,164	0
22	DMU	U	101	33/33	0.90	0.24	36,48,60,64	33
22	DMU	C	316	7/33	0.91	0.29	50,53,58,69	7
22	DMU	B	302	11/33	0.91	0.29	45,51,57,64	11
22	DMU	G	102	11/33	0.91	0.28	44,54,65,66	11
22	DMU	O	306	11/33	0.91	0.27	41,45,52,65	11
22	DMU	O	308	22/33	0.91	0.19	34,48,55,56	22
22	DMU	A	612	33/33	0.91	0.18	32,45,58,61	33
22	DMU	P	317	7/33	0.91	0.26	55,57,63,67	7
22	DMU	Z	102	22/33	0.91	0.31	53,62,67,74	22
21	LFA	N	608	14/20	0.91	0.23	40,49,65,66	14
22	DMU	B	303	11/33	0.92	0.23	46,54,64,65	11
22	DMU	J	101	11/33	0.92	0.30	56,62,68,74	11
22	DMU	L	102	22/33	0.92	0.27	47,57,66,73	22
19	CDL	L	101	94/100	0.92	0.15	44,80,120,132	0
22	DMU	Z	103	8/33	0.92	0.21	47,49,51,54	8
23	EDO	C	321	4/4	0.93	0.21	36,37,38,43	4
22	DMU	Z	101	33/33	0.93	0.10	55,62,75,84	0
22	DMU	D	201	33/33	0.93	0.14	27,44,58,63	33
23	EDO	E	202	4/4	0.93	0.24	33,34,35,35	4
23	EDO	F	102	4/4	0.93	0.16	25,25,30,32	4
22	DMU	C	306	11/33	0.94	0.22	53,56,60,67	11
23	EDO	R	202	4/4	0.94	0.21	35,37,42,42	4
23	EDO	E	203	4/4	0.94	0.25	35,37,40,45	4
26	CHD	C	301	29/29	0.94	0.08	35,39,41,44	0
22	DMU	P	307	11/33	0.94	0.24	48,50,57,64	11
22	DMU	B	304	22/33	0.94	0.17	44,60,67,81	22
27	UNX	P	303	1/1	0.94	0.29	46,46,46,46	0
23	EDO	P	321	4/4	0.95	0.18	49,56,64,72	4
23	EDO	P	322	4/4	0.95	0.22	36,39,40,42	4
22	DMU	M	101	33/33	0.95	0.08	47,54,69,76	0
23	EDO	N	612	4/4	0.95	0.12	32,32,35,36	4
23	EDO	A	615	4/4	0.95	0.19	27,27,28,31	4
23	EDO	N	614	4/4	0.95	0.20	31,32,33,34	4
23	EDO	N	615	4/4	0.95	0.17	35,39,44,44	4
23	EDO	N	616	4/4	0.95	0.15	32,34,34,40	4
23	EDO	O	309	4/4	0.95	0.14	34,38,40,41	4
20	CO2	N	607	3/3	0.96	0.25	41,41,46,49	0
23	EDO	T	103	4/4	0.96	0.12	37,39,39,40	4
23	EDO	G	103	4/4	0.96	0.14	33,34,34,36	4
22	DMU	O	307	11/33	0.96	0.21	46,50,58,59	11

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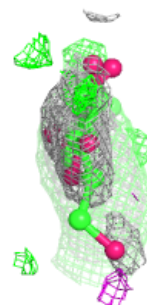
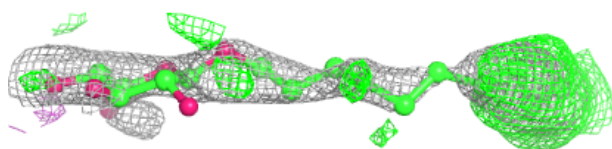
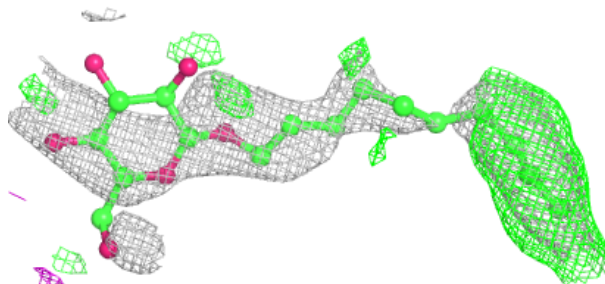
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	CHD	P	302	29/29	0.96	0.07	34,39,44,45	0
23	EDO	R	201	4/4	0.96	0.25	56,59,66,67	4
23	EDO	A	616	4/4	0.96	0.13	44,44,46,48	4
29	PEK	G	101	53/53	0.96	0.11	36,52,93,120	0
29	PEK	T	101	53/53	0.96	0.11	38,55,100,111	0
24	PGV	N	617	51/51	0.97	0.09	34,46,75,80	0
26	CHD	B	306	29/29	0.97	0.06	33,36,40,49	0
27	UNX	C	302	1/1	0.97	0.18	44,44,44,44	0
23	EDO	S	102	4/4	0.97	0.07	24,28,28,31	4
23	EDO	B	305	4/4	0.97	0.09	26,29,30,33	4
26	CHD	O	301	29/29	0.97	0.06	33,36,39,46	0
18	PER	N	606	2/2	0.98	0.09	35,35,35,35	0
24	PGV	A	617	51/51	0.98	0.09	32,43,77,83	0
24	PGV	C	303	51/51	0.98	0.08	33,40,92,100	0
23	EDO	F	103	4/4	0.98	0.09	33,33,36,37	4
24	PGV	P	304	51/51	0.98	0.08	32,41,88,111	0
17	NA	A	605	1/1	0.99	0.05	35,35,35,35	0
18	PER	A	606	2/2	0.99	0.04	32,32,32,33	0
14	HEA	A	601[A]	60/60	0.99	0.05	26,30,41,45	9
14	HEA	A	601[B]	60/60	0.99	0.05	26,30,46,49	9
14	HEA	A	602	60/60	0.99	0.05	28,30,37,42	0
14	HEA	N	601[A]	60/60	0.99	0.05	30,34,45,52	9
23	EDO	S	103	4/4	0.99	0.08	29,38,38,38	4
14	HEA	N	601[B]	60/60	0.99	0.05	30,34,44,48	9
14	HEA	N	602	60/60	0.99	0.06	29,33,37,42	0
16	MG	N	604	1/1	0.99	0.03	35,35,35,35	0
20	CO2	A	608	3/3	0.99	0.16	37,37,39,46	0
25	CUA	B	301	2/2	1.00	0.02	32,32,32,33	0
25	CUA	O	305	2/2	1.00	0.02	37,37,37,37	0
17	NA	N	605	1/1	1.00	0.05	41,41,41,41	0
16	MG	A	604	1/1	1.00	0.02	32,32,32,32	0
28	ZN	F	101	1/1	1.00	0.01	36,36,36,36	0
28	ZN	S	101	1/1	1.00	0.01	37,37,37,37	0
15	CU	A	603	1/1	1.00	0.01	31,31,31,31	0
15	CU	N	603	1/1	1.00	0.01	33,33,33,33	0

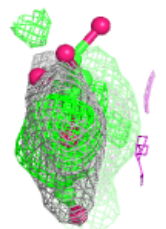
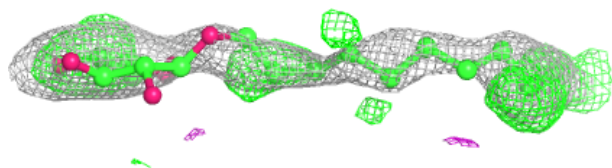
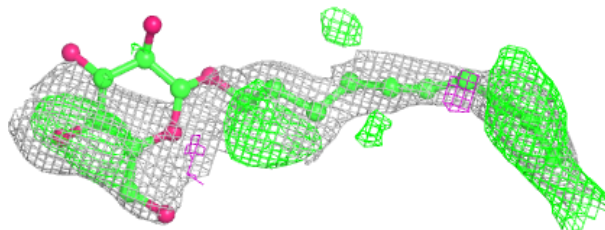
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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 318:**

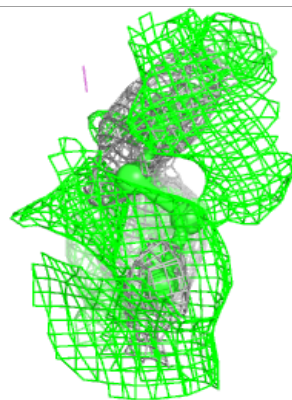
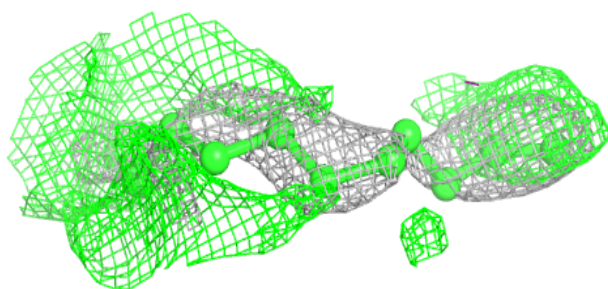
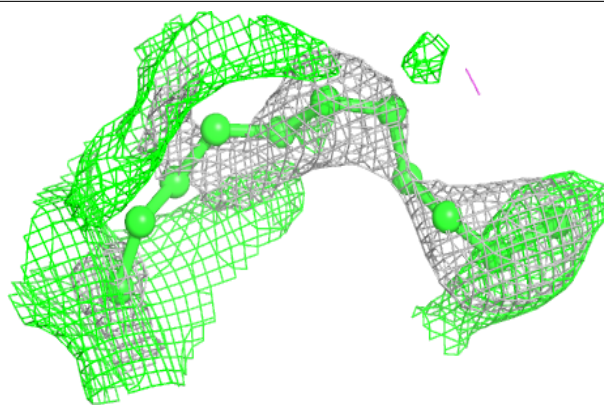
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



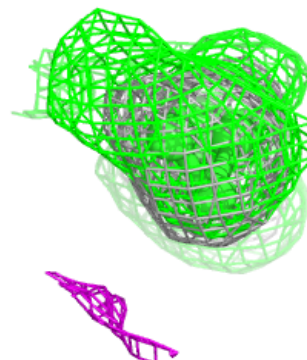
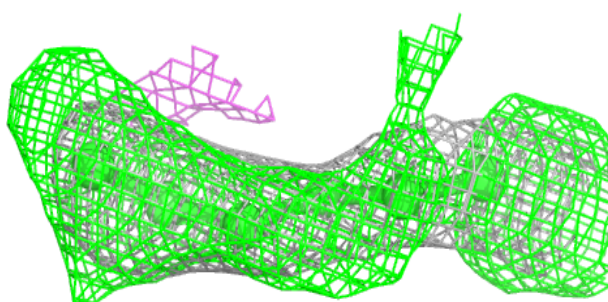
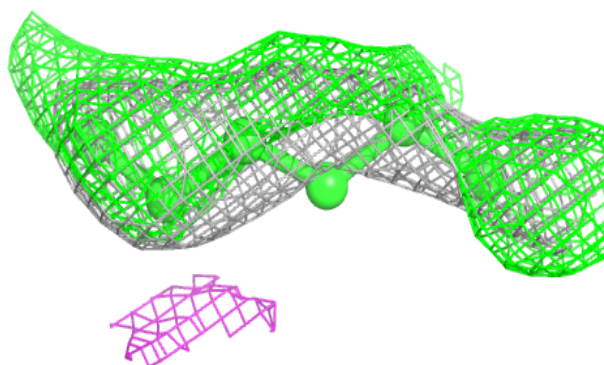


**Electron density around LFA P 311:**

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

**Electron density around LFA C 308:**

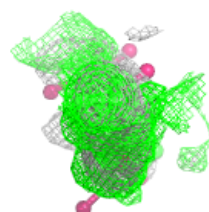
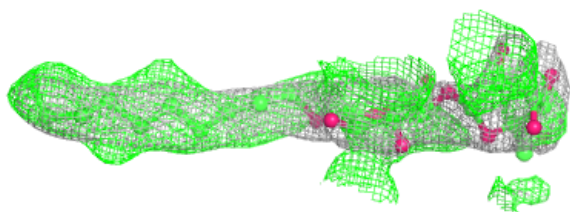
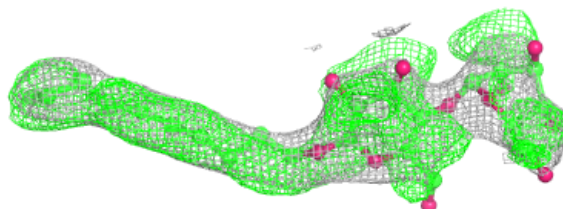
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



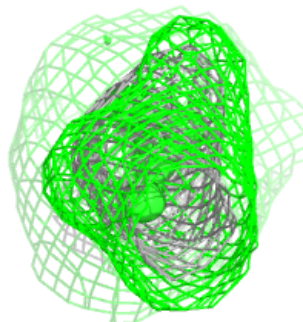
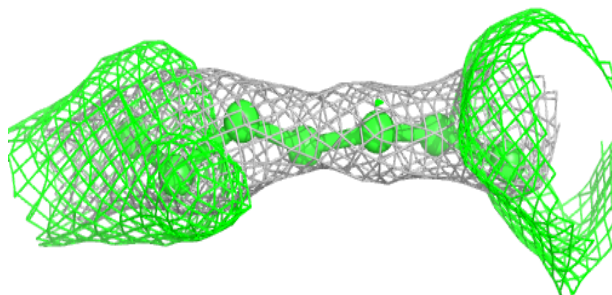
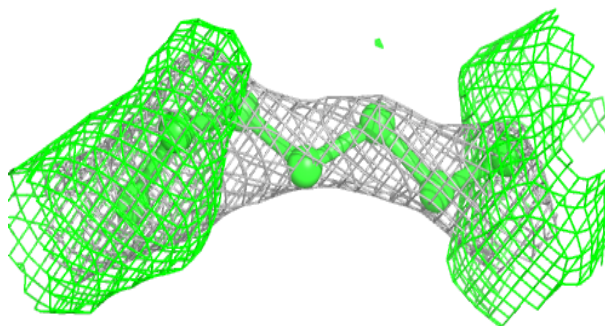


**Electron density around DMU C 318:**

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

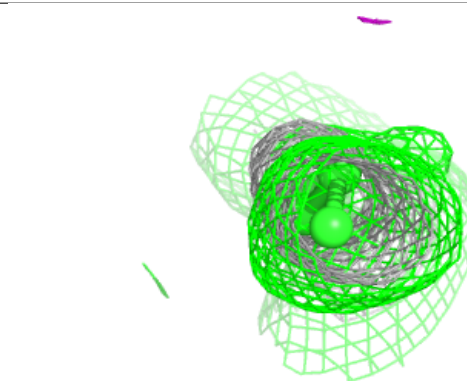
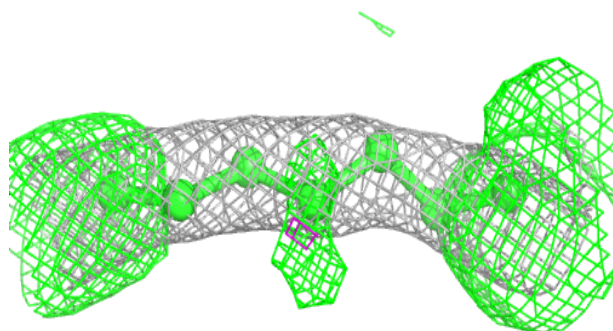
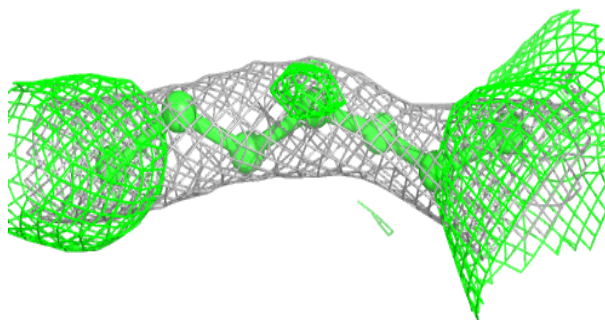
**Electron density around DMU N 610:**

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

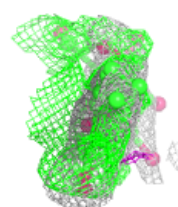
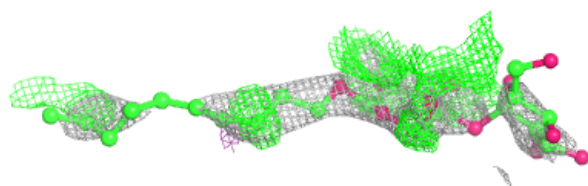
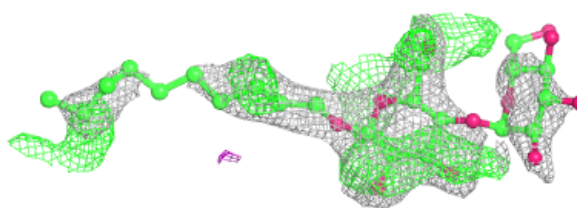


**Electron density around DMU A 611:**

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

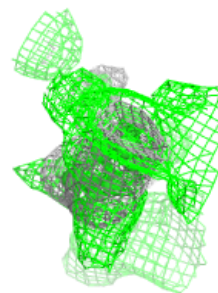
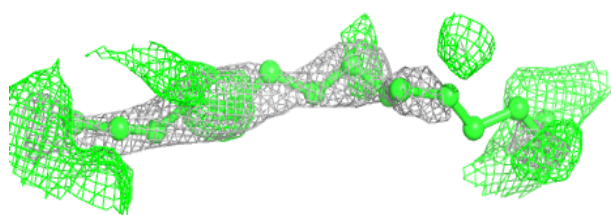
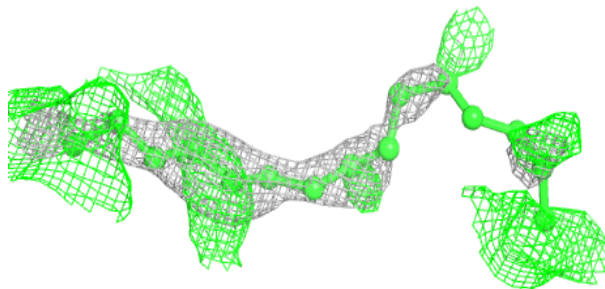
**Electron density around DMU C 315:**

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

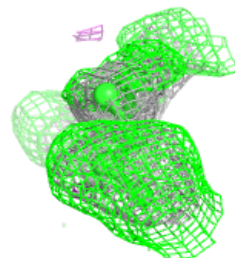
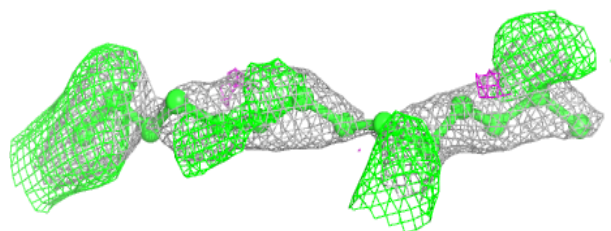
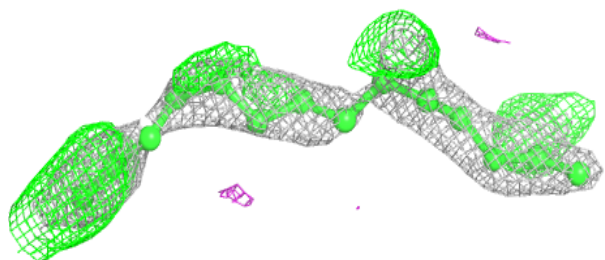


**Electron density around LFA C 325:**

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

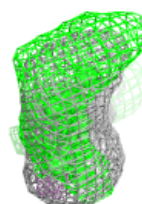
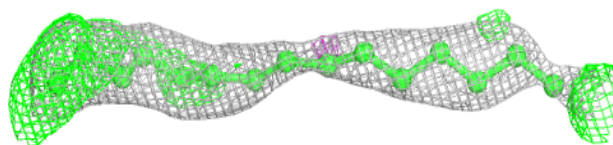
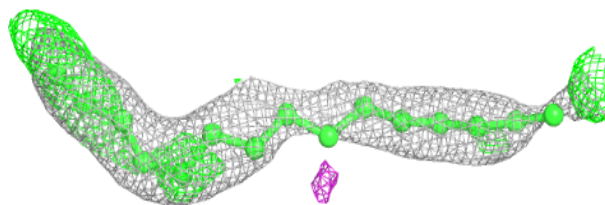
**Electron density around LFA C 311:**

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

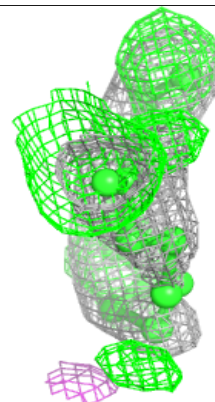
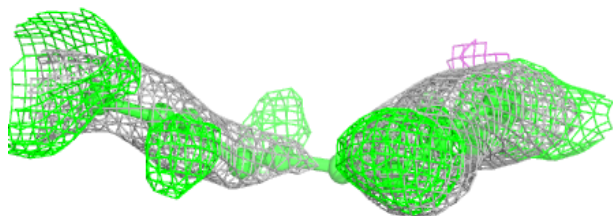
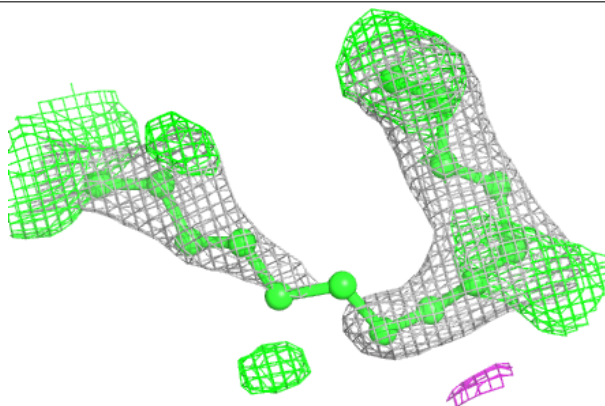


**Electron density around LFA C 313:**

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

**Electron density around LFA N 609:**

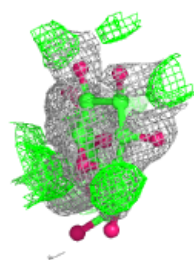
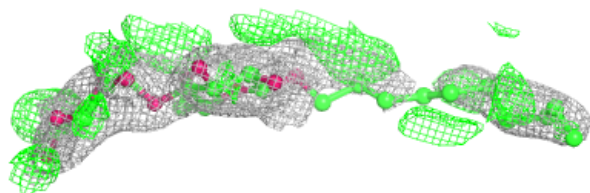
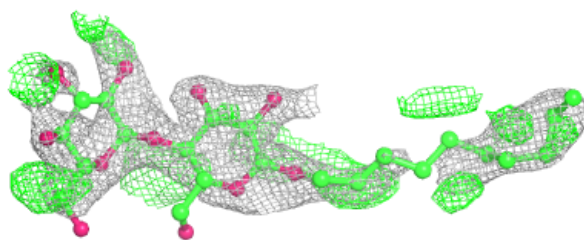
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



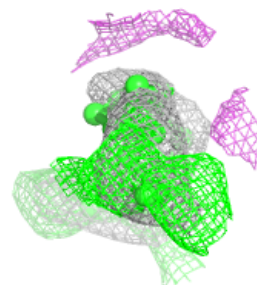
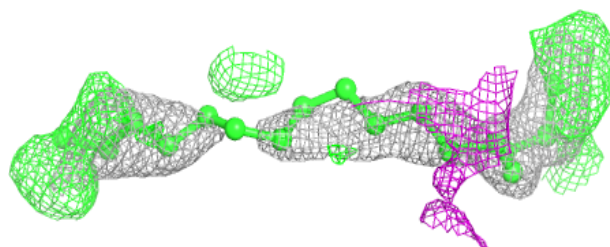
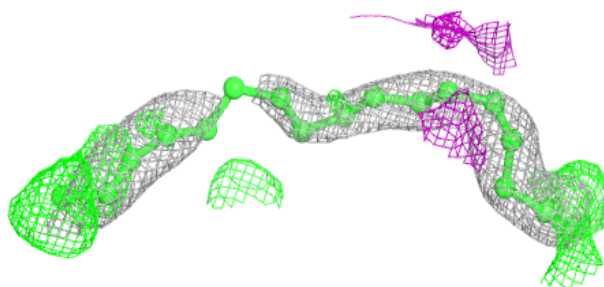


**Electron density around DMU C 319:**

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

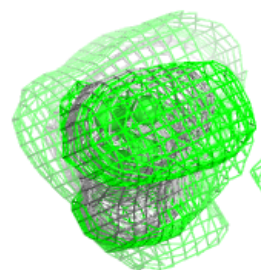
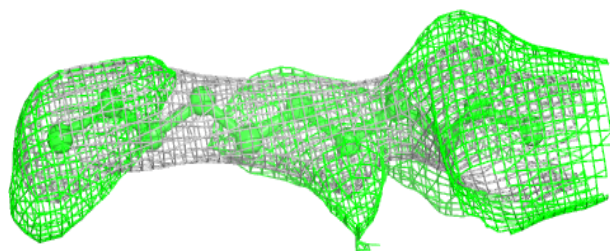
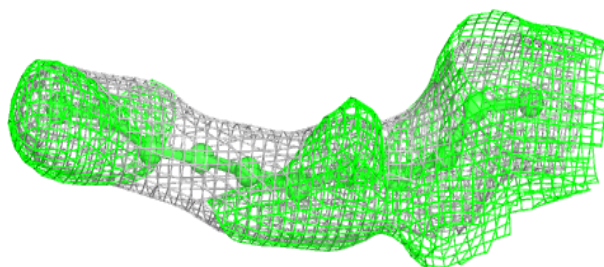
**Electron density around LFA O 302:**

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

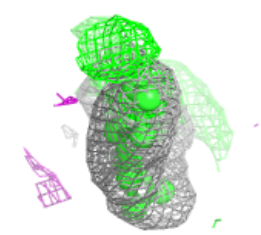
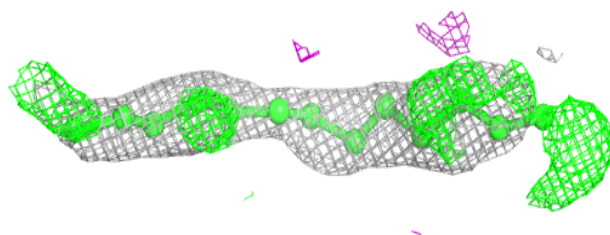
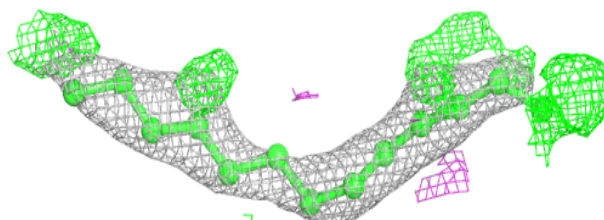


**Electron density around LFA O 303:**

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

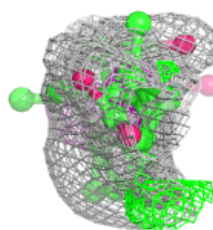
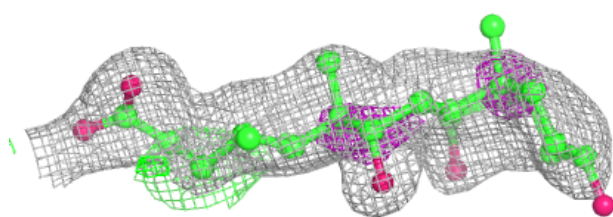
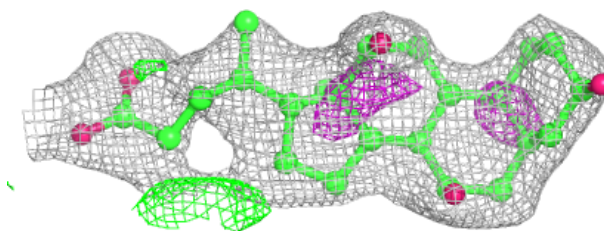
**Electron density around LFA C 314:**

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

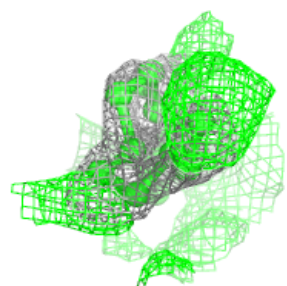
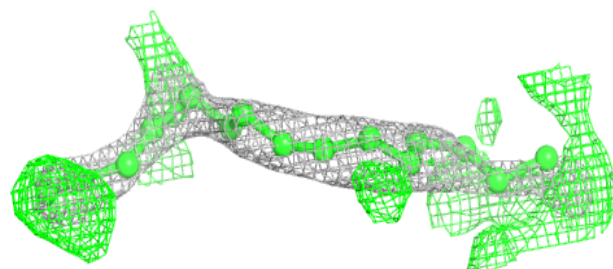
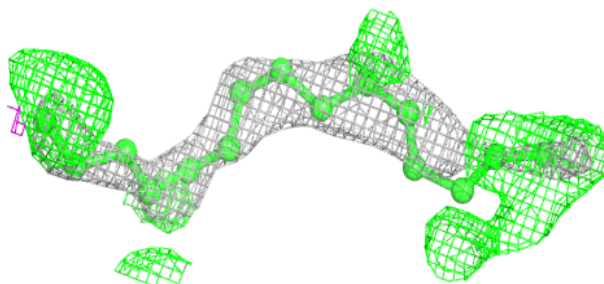


**Electron density around CHD P 306:**

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

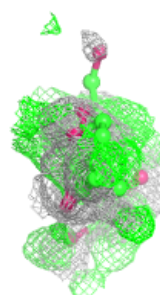
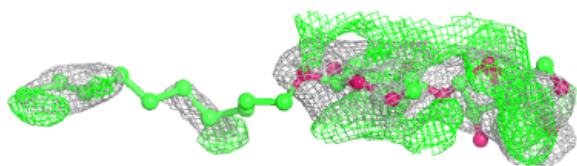
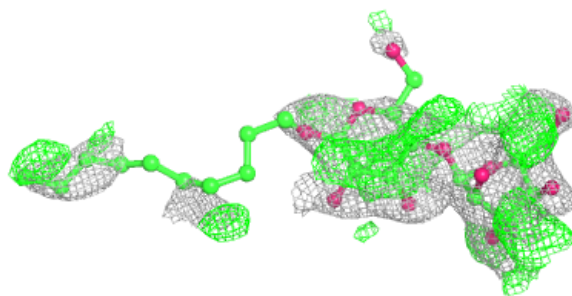
**Electron density around LFA P 301:**

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

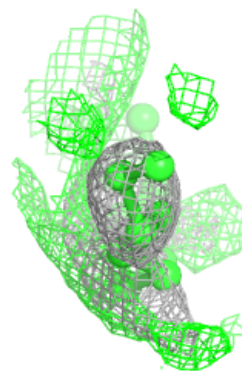
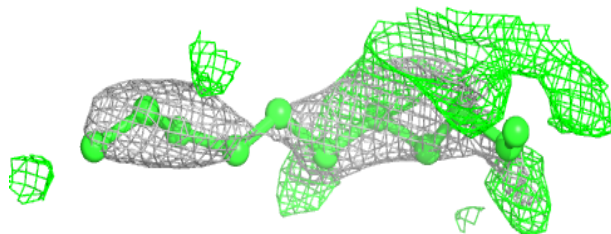
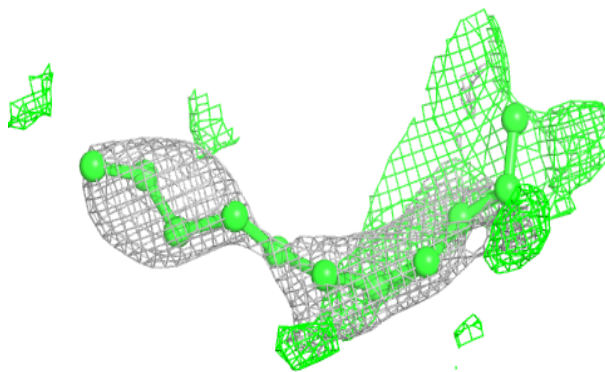


**Electron density around DMU P 320:**

$2mF_o-DF_c$  (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:**

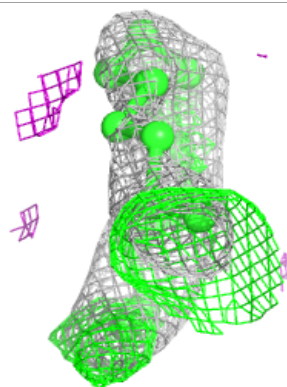
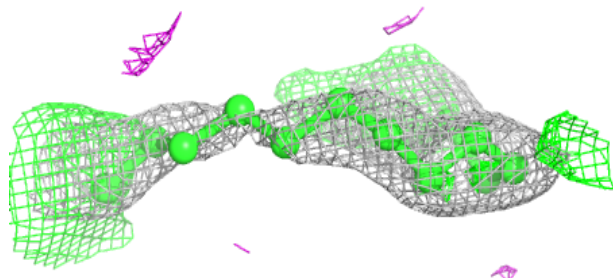
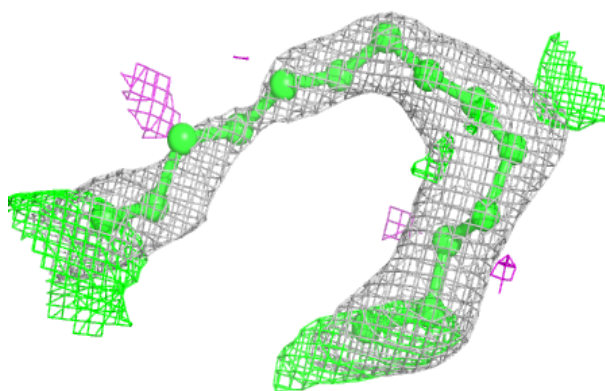
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



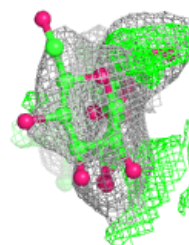
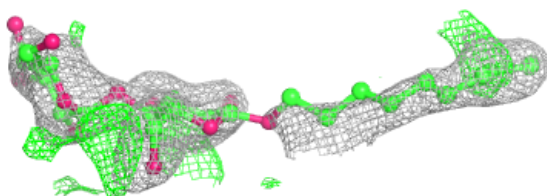
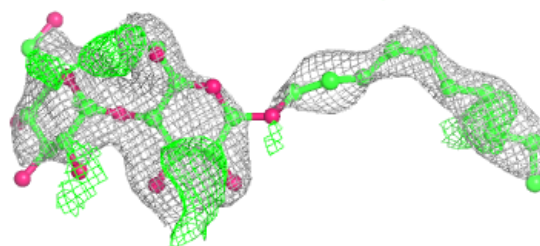


**Electron density around LFA A 610:**

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

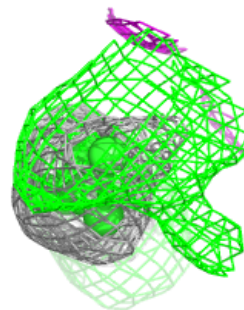
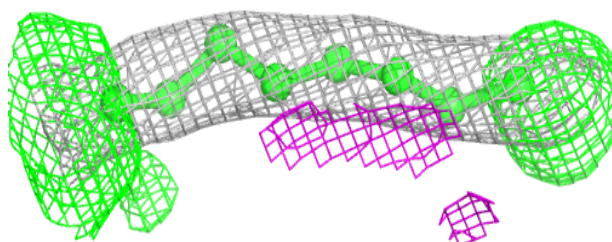
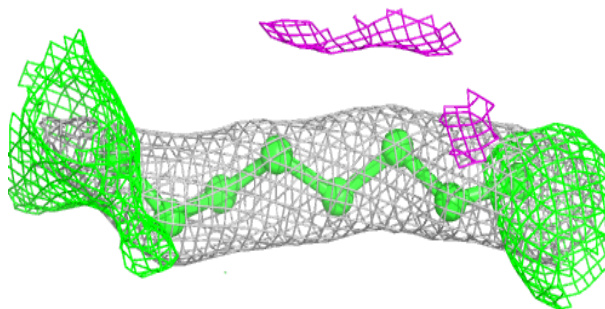
**Electron density around DMU C 324:**

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

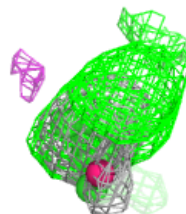
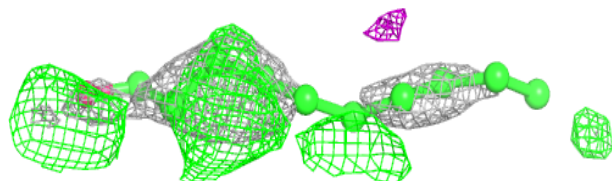
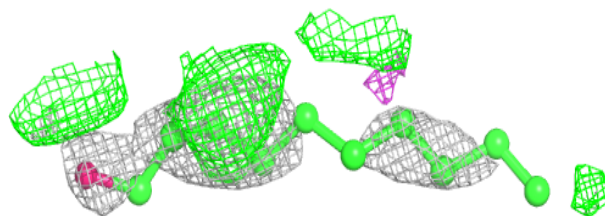


**Electron density around DMU M 102:**

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

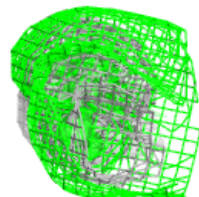
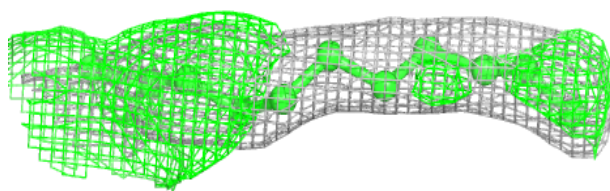
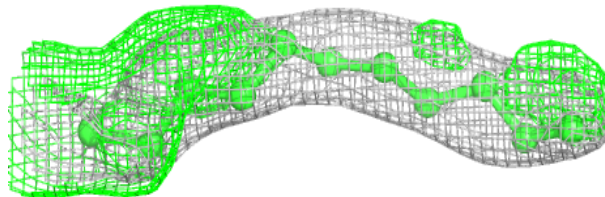
**Electron density around DMU A 618:**

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

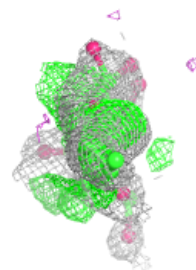
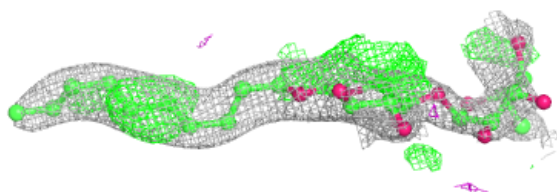
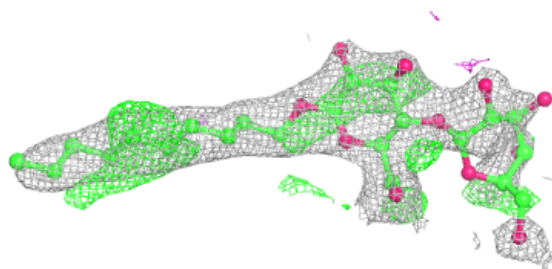


**Electron density around LFA T 102:**

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

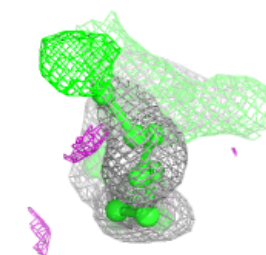
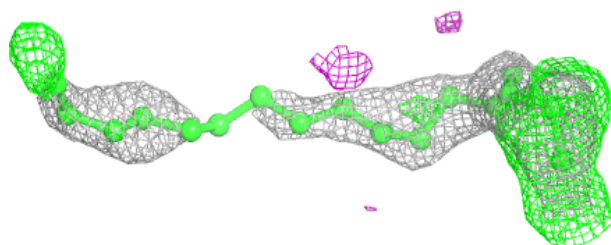
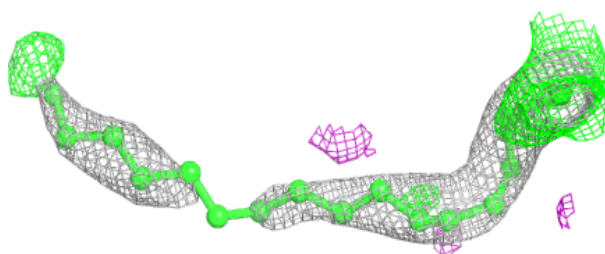
**Electron density around DMU N 611:**

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

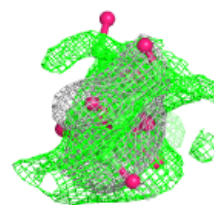
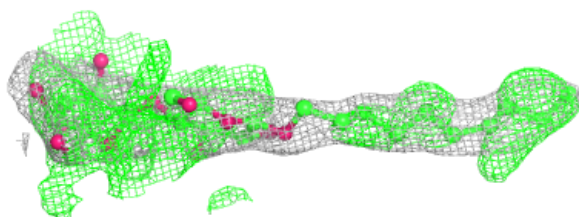
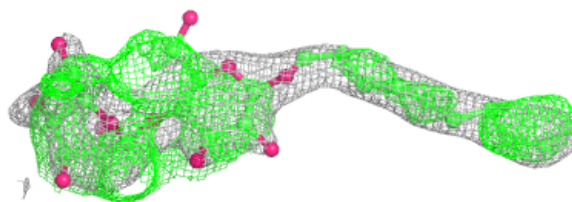


**Electron density around LFA B 307:**

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

**Electron density around DMU P 319:**

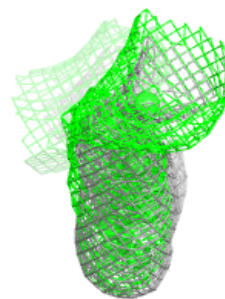
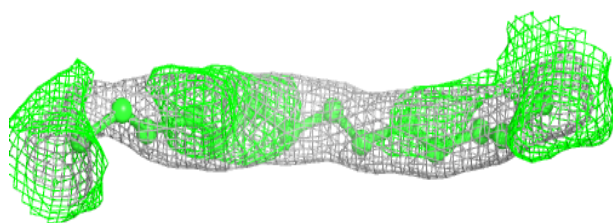
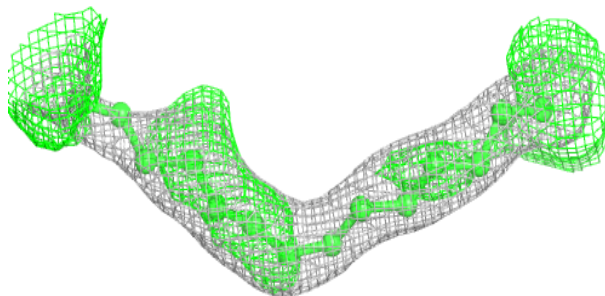
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



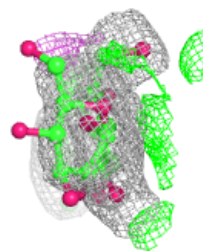
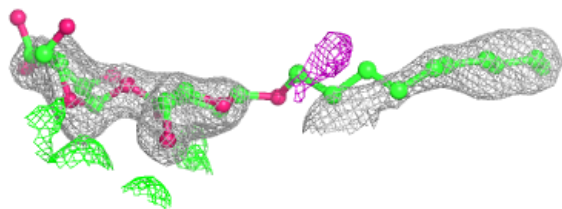
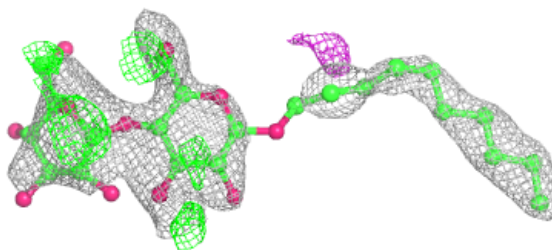


**Electron density around LFA A 609:**

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

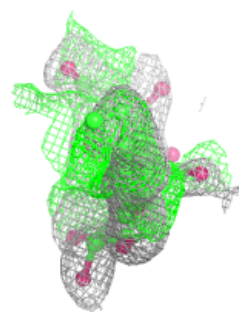
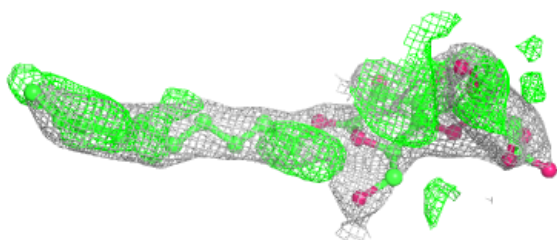
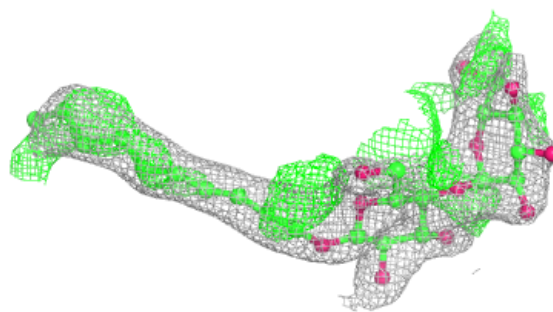
**Electron density around DMU P 325:**

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

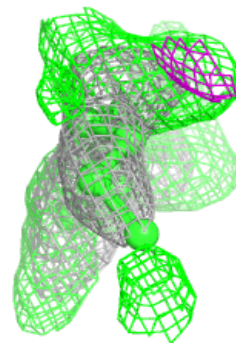
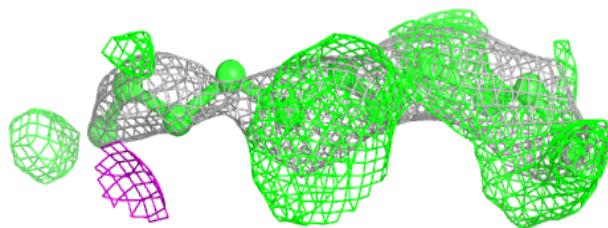
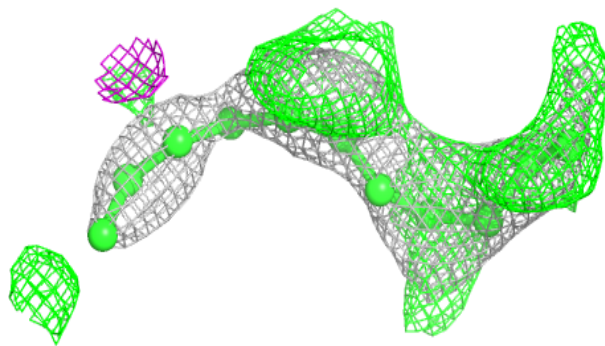


**Electron density around DMU Q 201:**

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

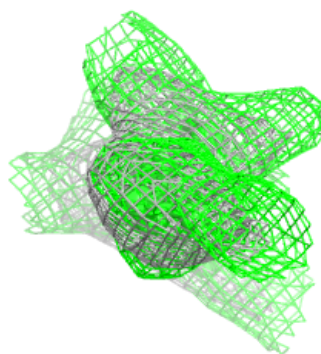
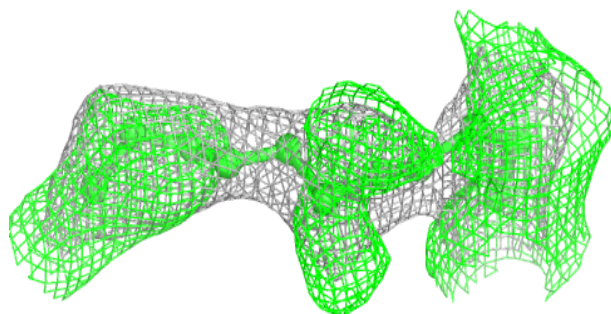
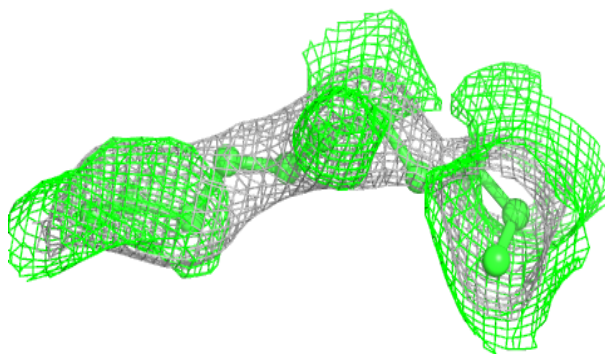
**Electron density around LFA P 308:**

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

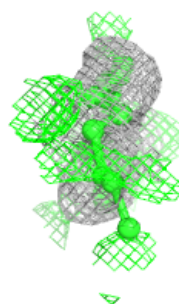
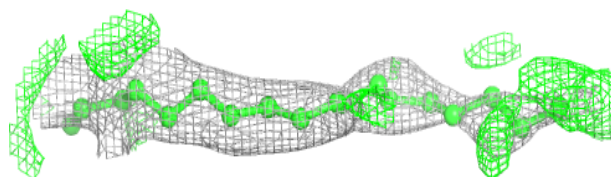
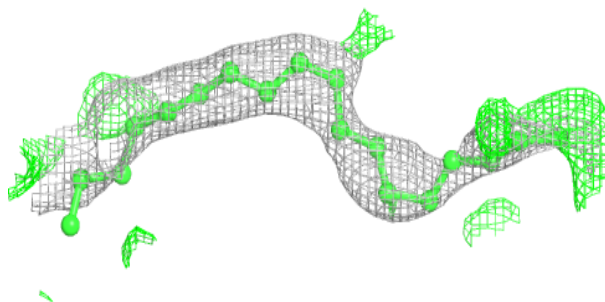


**Electron density around LFA C 312:**

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

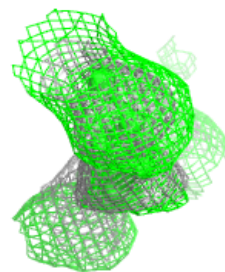
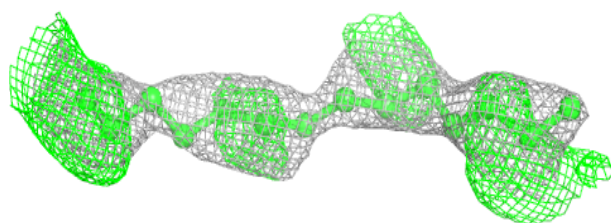
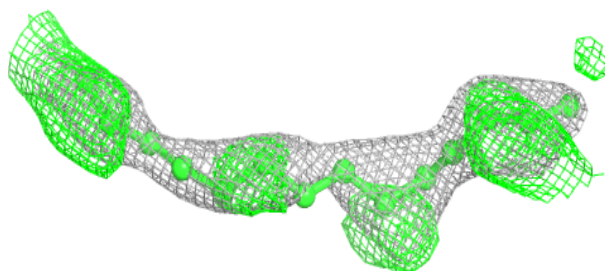
**Electron density around LFA C 309:**

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

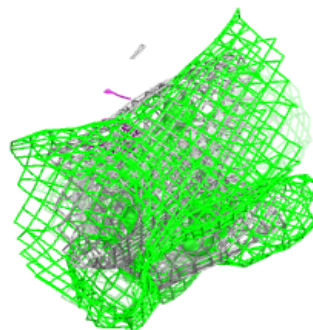
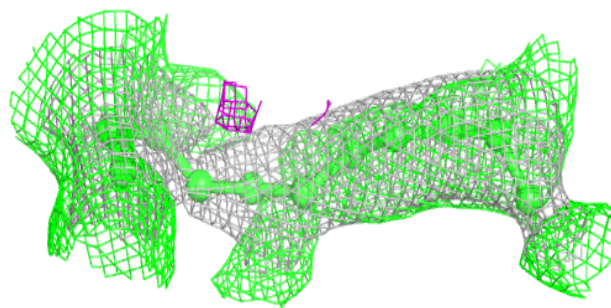
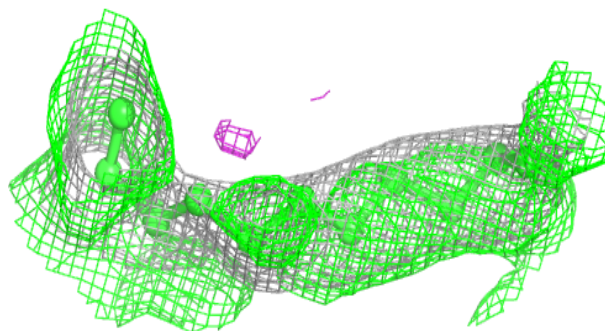


**Electron density around LFA P 312:**

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

**Electron density around LFA P 313:**

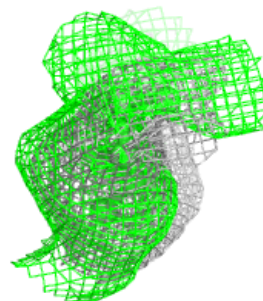
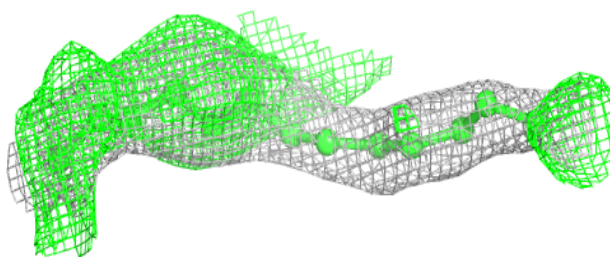
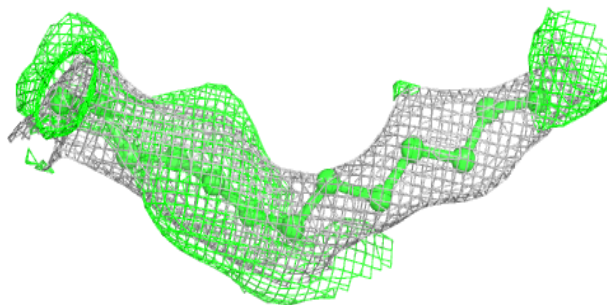
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



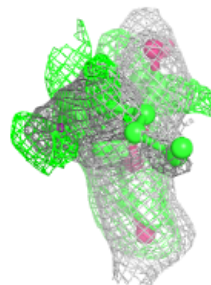
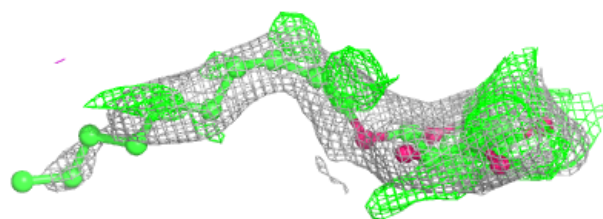
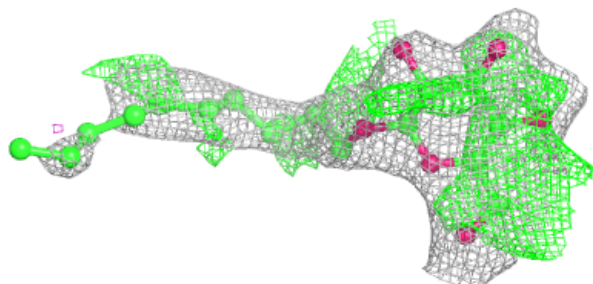


**Electron density around LFA P 315:**

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

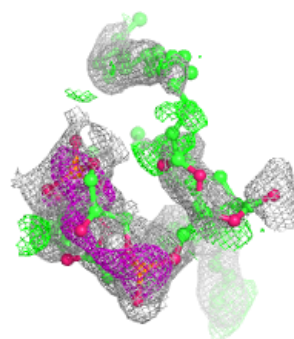
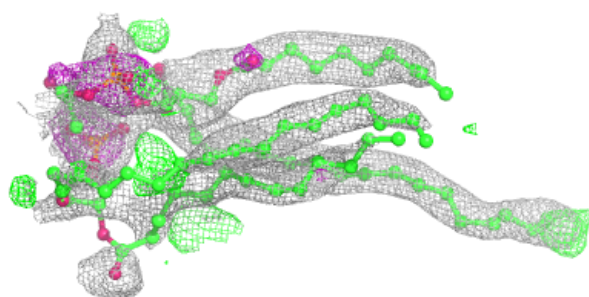
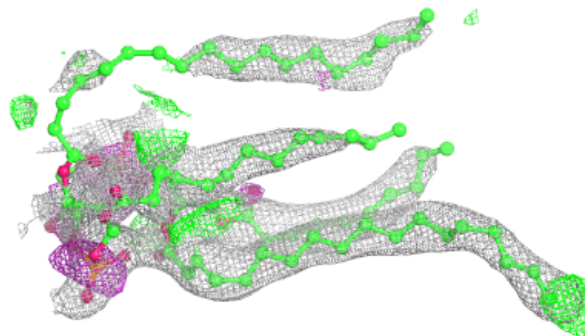
**Electron density around DMU C 323:**

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

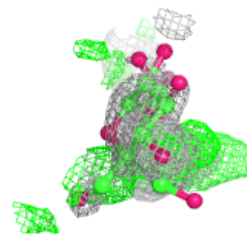
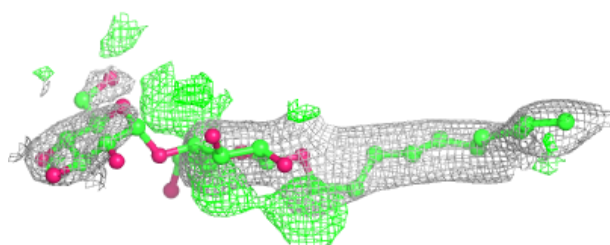
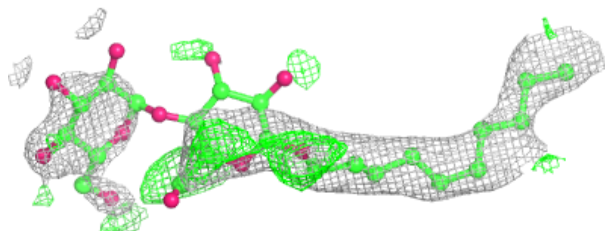


**Electron density around CDL P 305:**

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

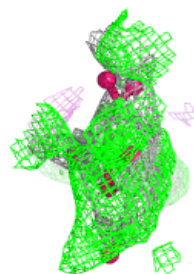
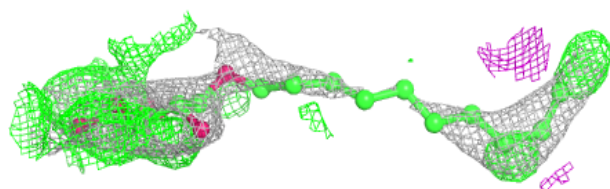
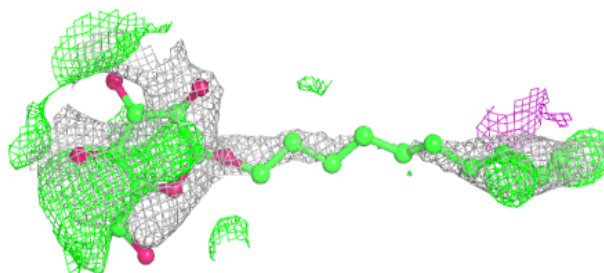
**Electron density around DMU H 101:**

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

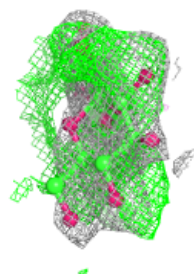
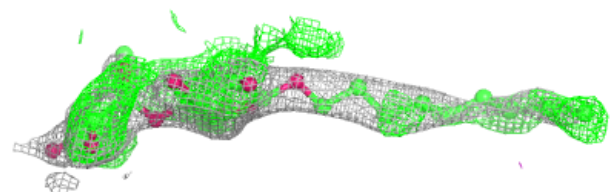
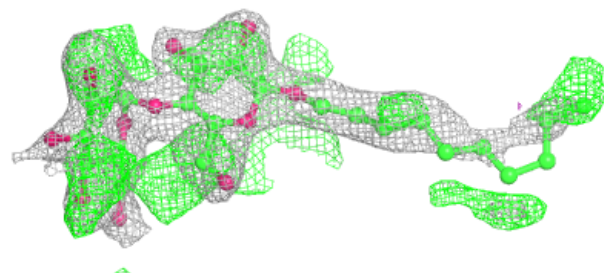


**Electron density around DMU O 304:**

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

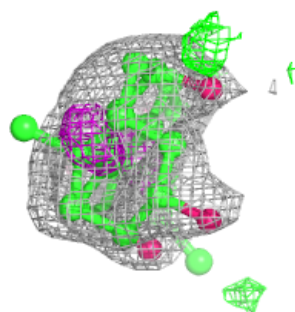
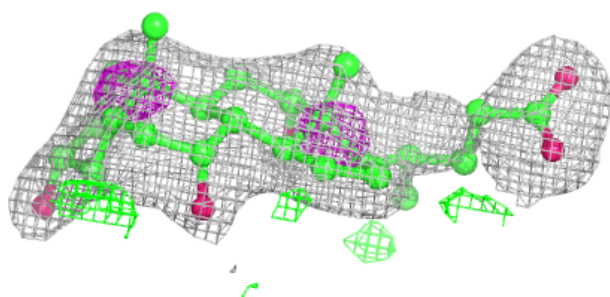
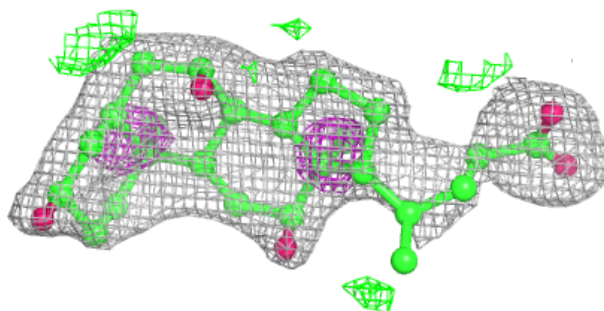
**Electron density around DMU P 316:**

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

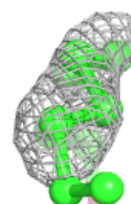
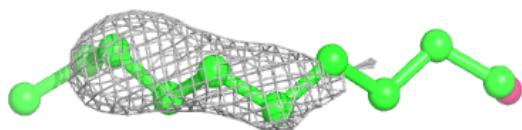
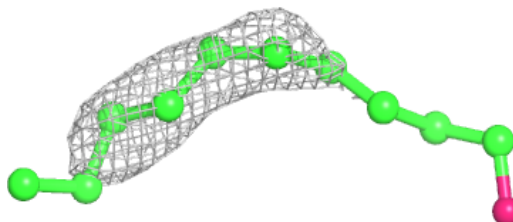


**Electron density around CHD C 305:**

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

**Electron density around DMU W 101:**

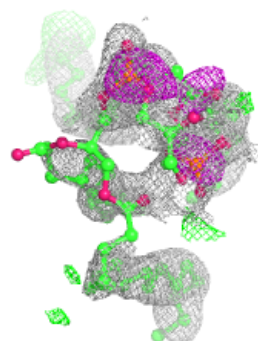
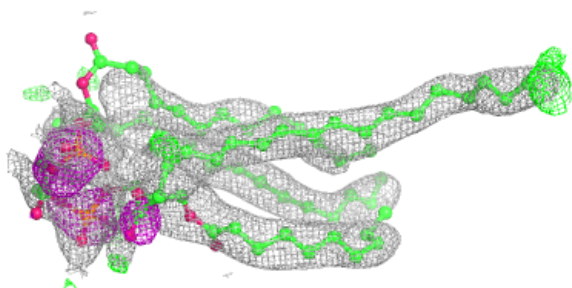
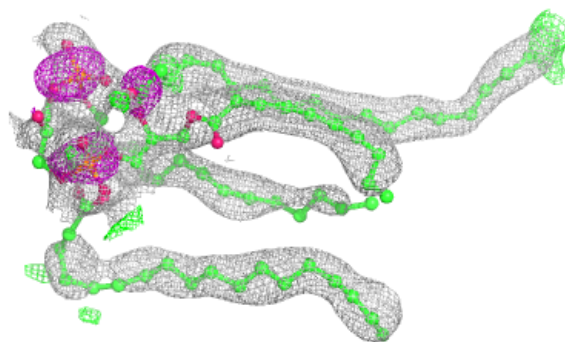
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



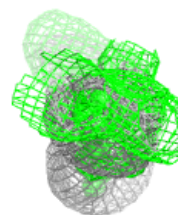
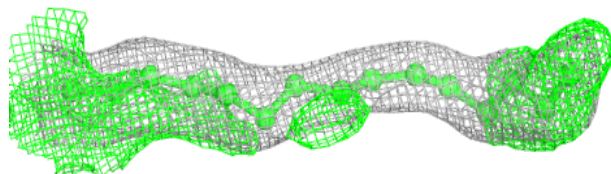
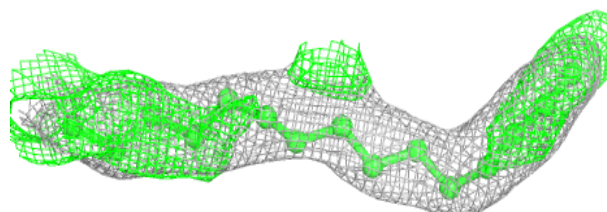


**Electron density around CDL C 304:**

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

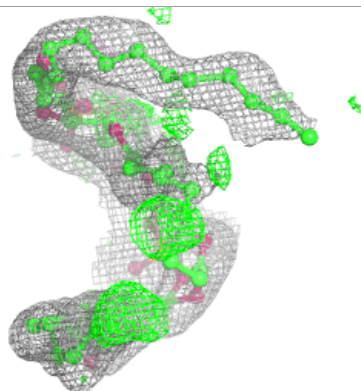
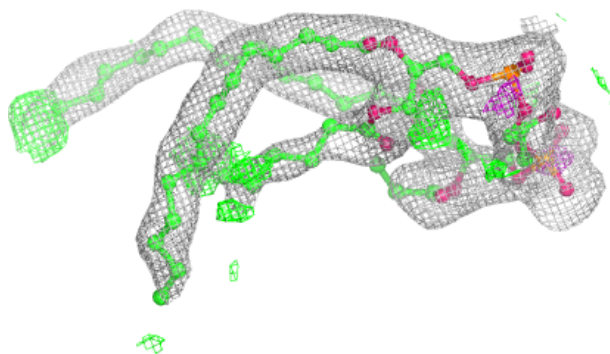
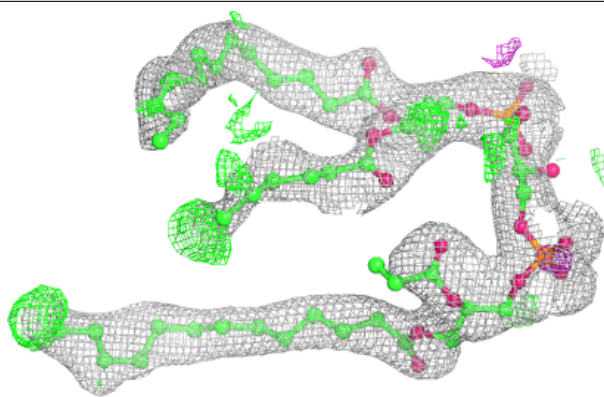
**Electron density around LFA P 314:**

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

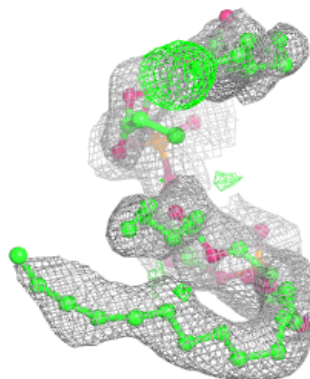
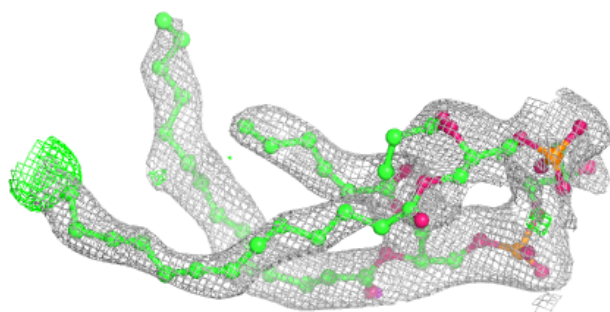
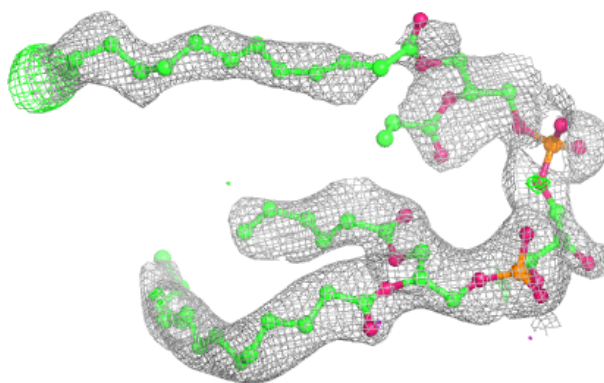


**Electron density around CDL A 607:**

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

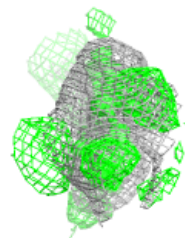
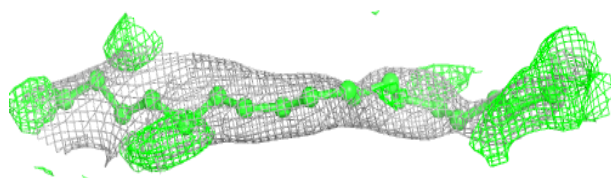
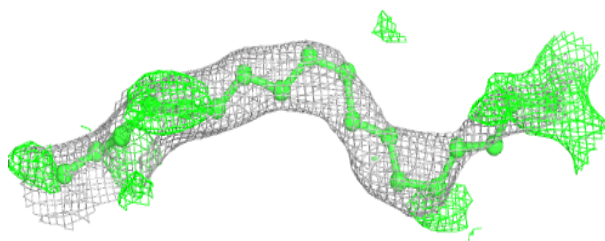
**Electron density around CDL V 101:**

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

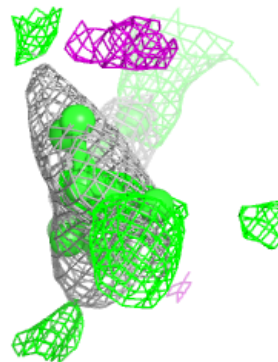
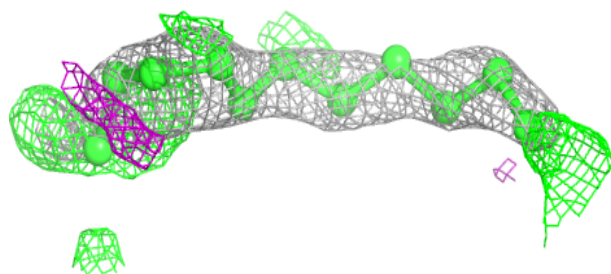
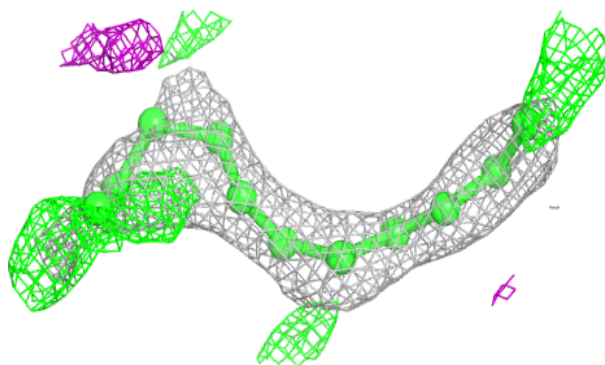


**Electron density around LFA P 310:**

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

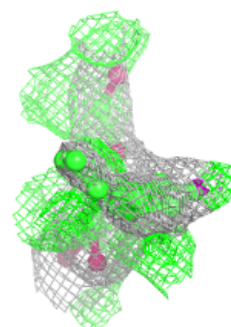
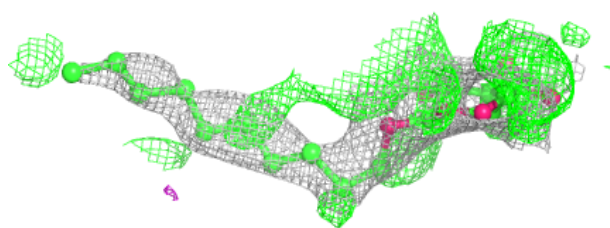
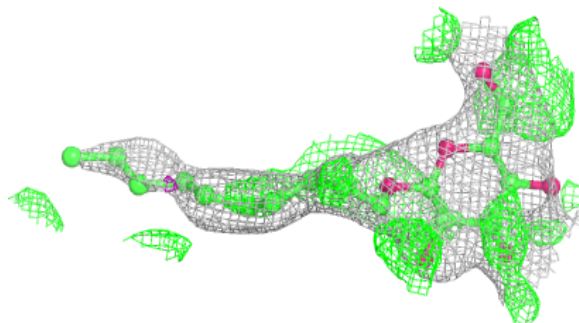
**Electron density around LFA C 307:**

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

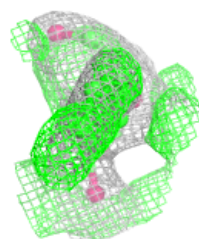
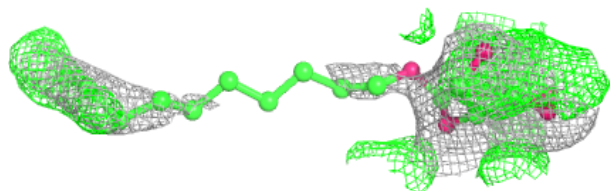
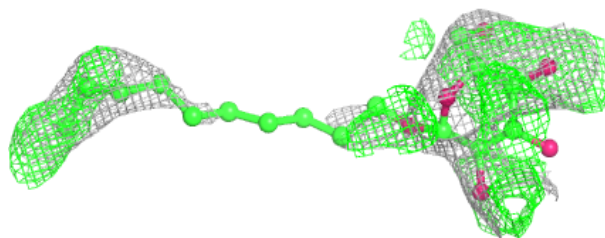


**Electron density around DMU P 324:**

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

**Electron density around DMU B 308:**

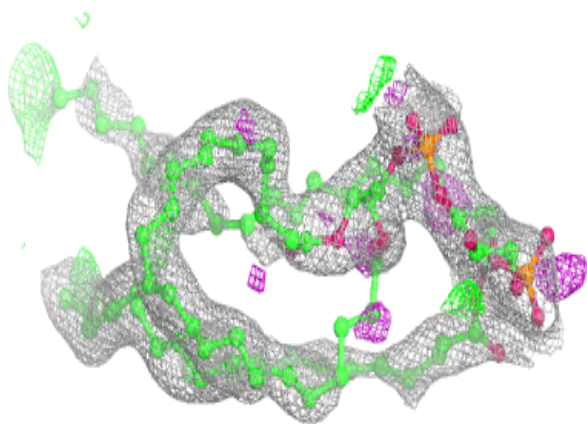
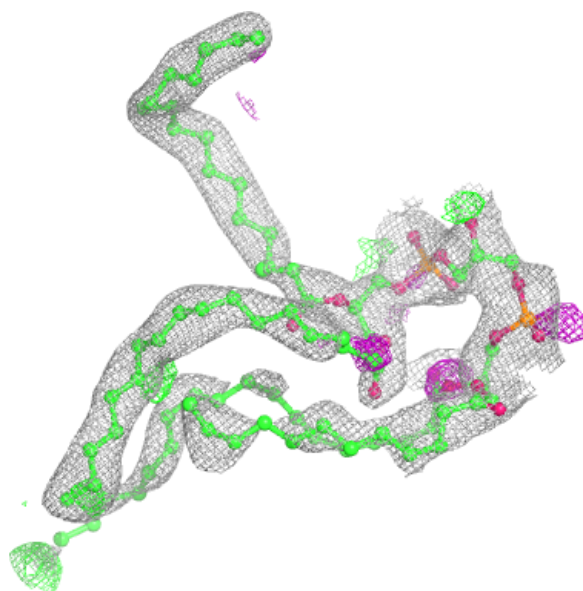
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





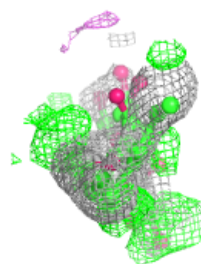
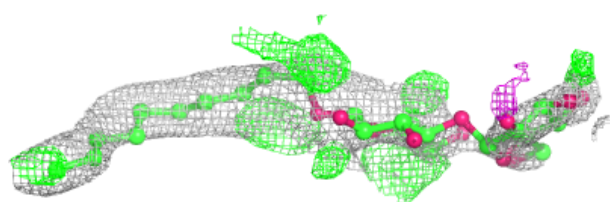
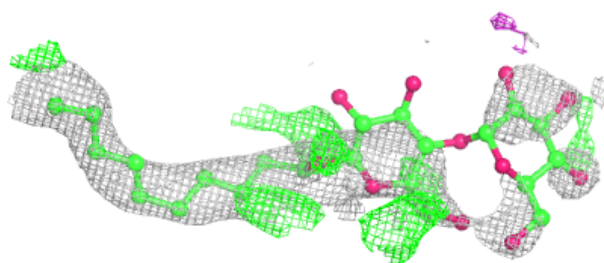
**Electron density around CDL Y 101:**

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

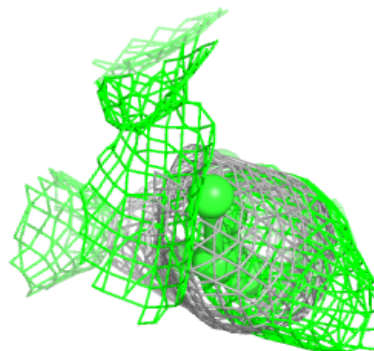
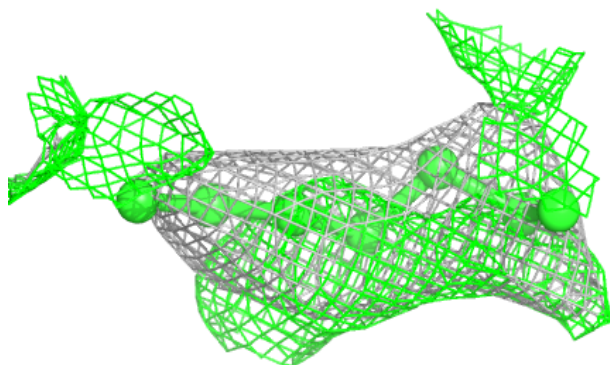
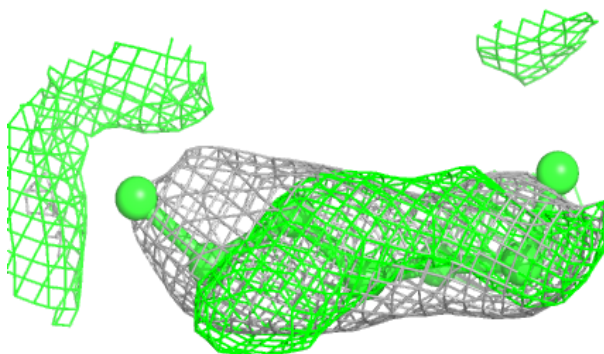


**Electron density around DMU U 101:**

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

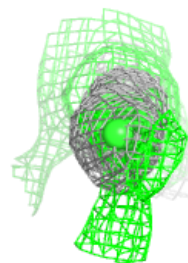
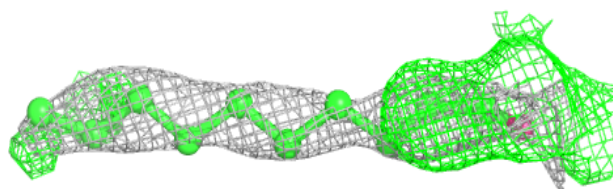
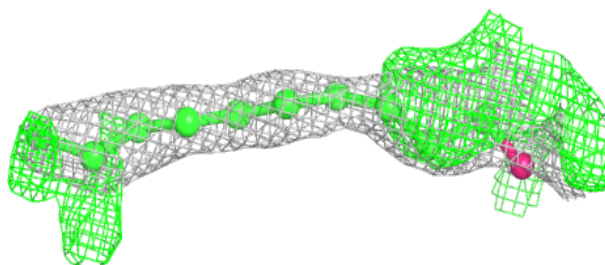
**Electron density around DMU C 316:**

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

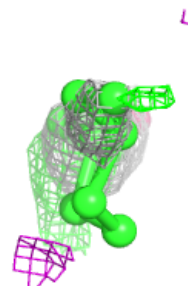
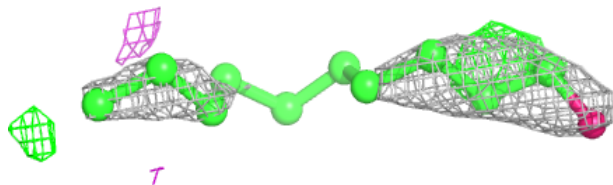
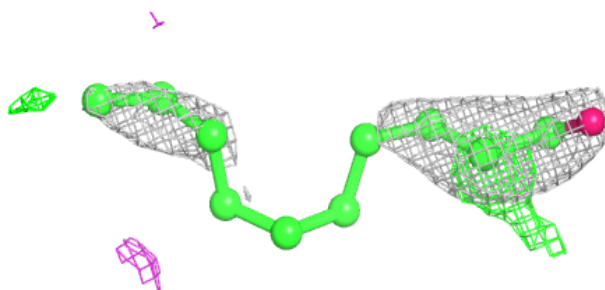


**Electron density around DMU B 302:**

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

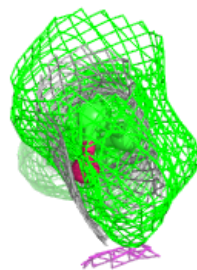
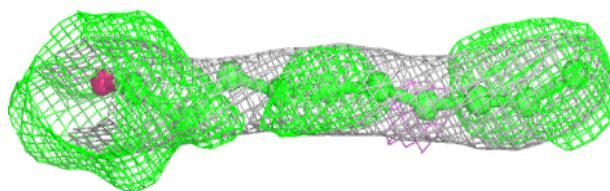
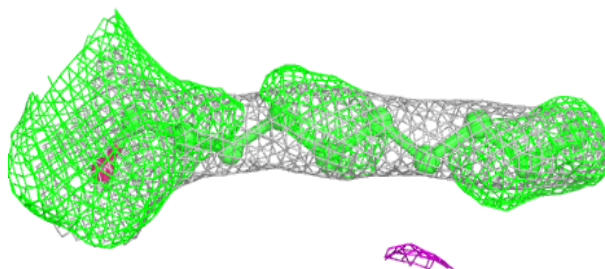
**Electron density around DMU G 102:**

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

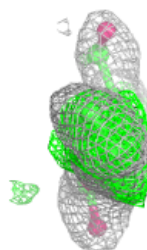
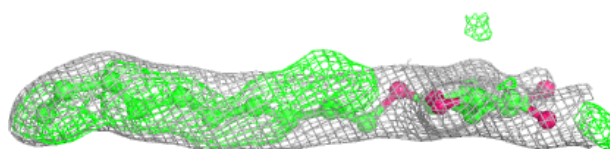
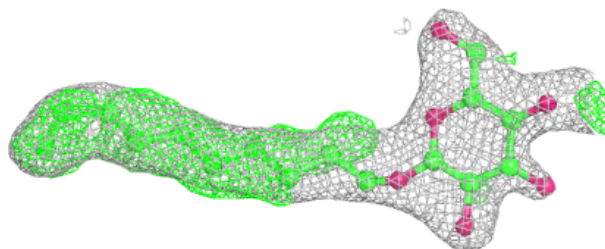


**Electron density around DMU O 306:**

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

**Electron density around DMU O 308:**

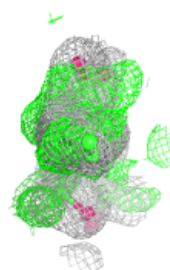
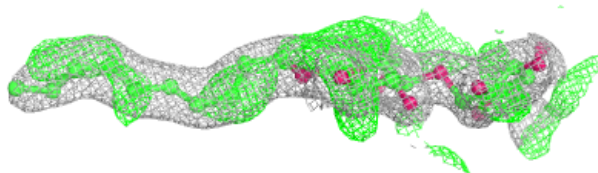
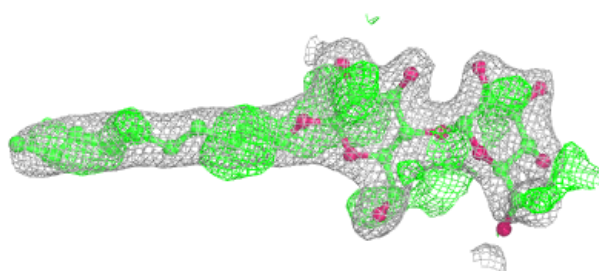
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



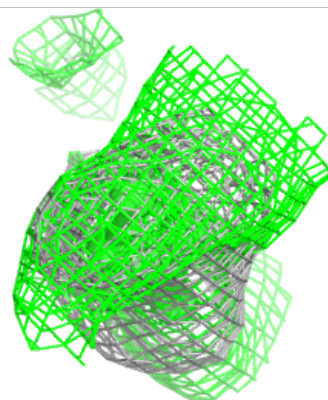
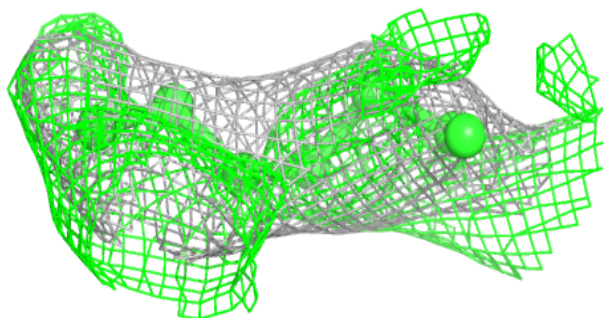
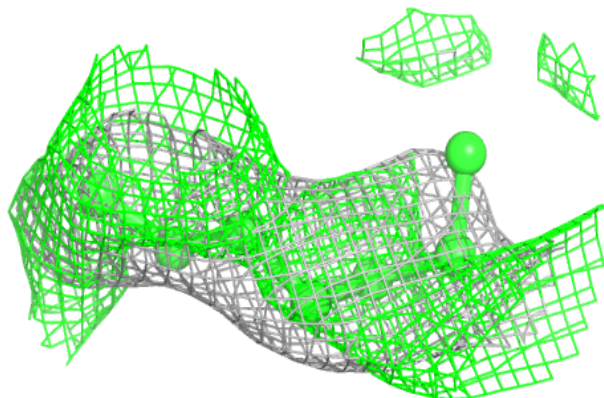


**Electron density around DMU A 612:**

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

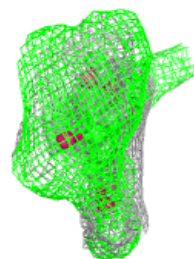
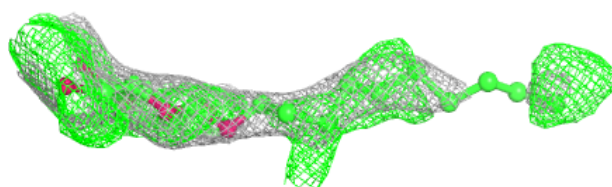
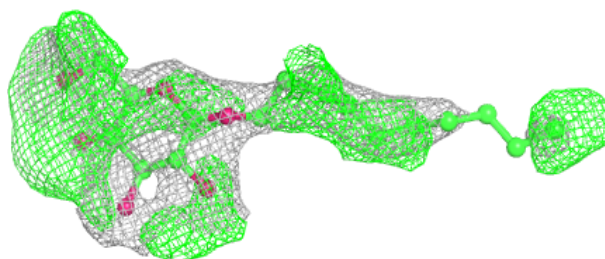
**Electron density around DMU P 317:**

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

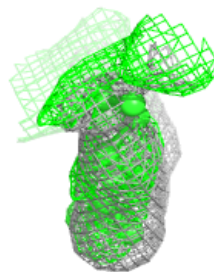
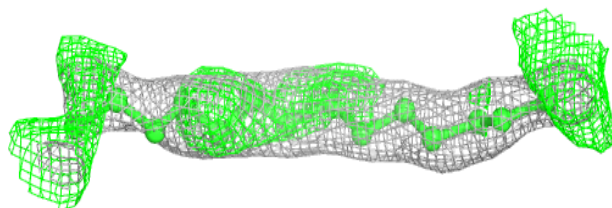
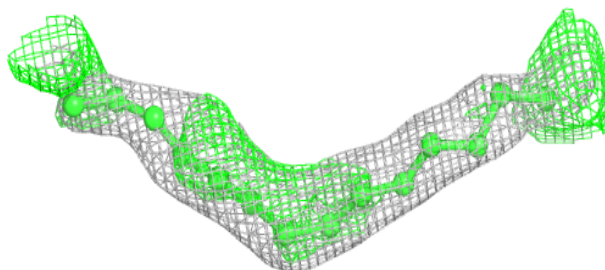


**Electron density around DMU Z 102:**

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

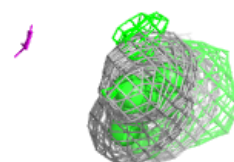
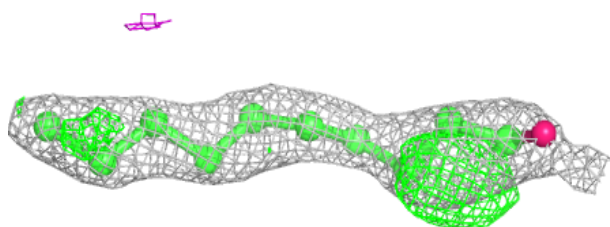
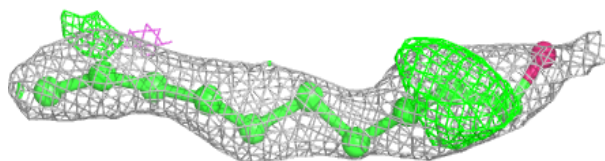
**Electron density around LFA N 608:**

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

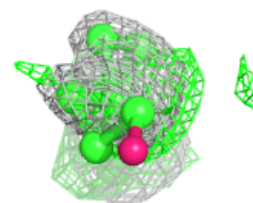
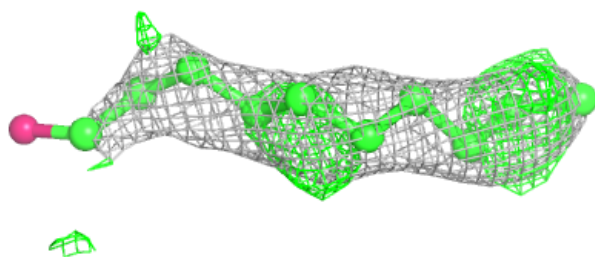
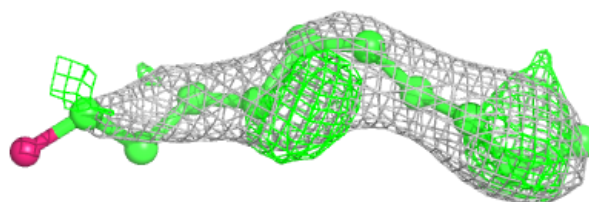


**Electron density around DMU B 303:**

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

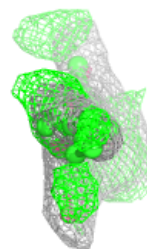
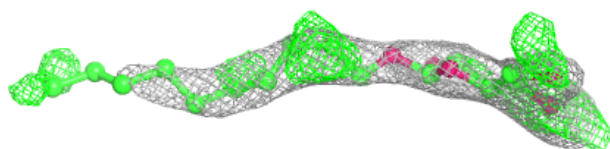
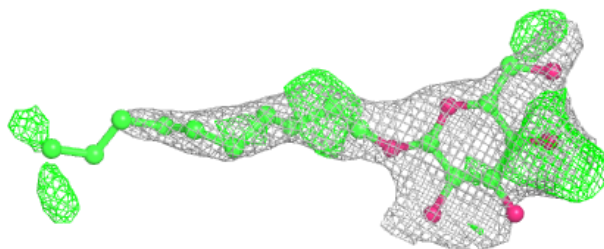
**Electron density around DMU J 101:**

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



**Electron density around DMU L 102:**

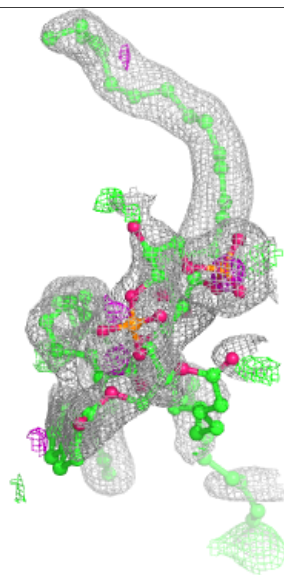
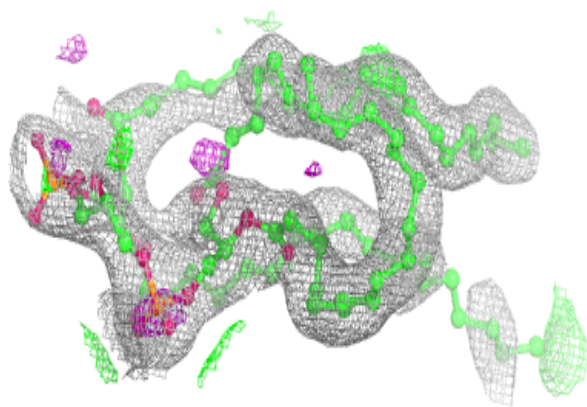
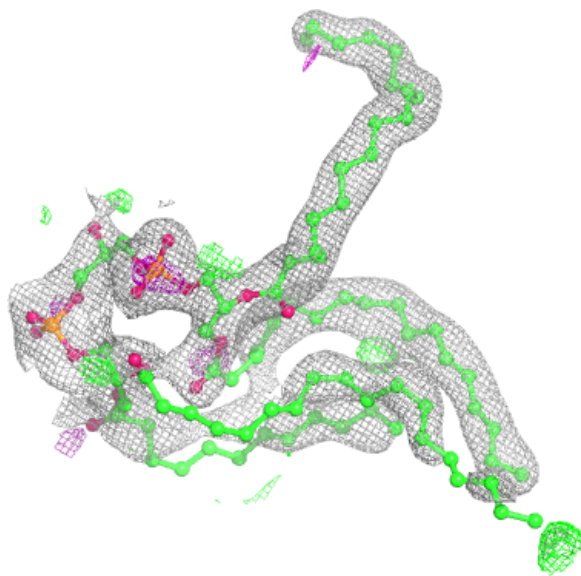
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





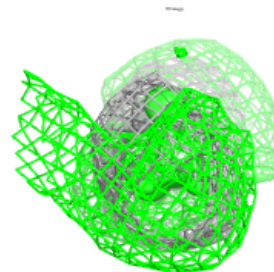
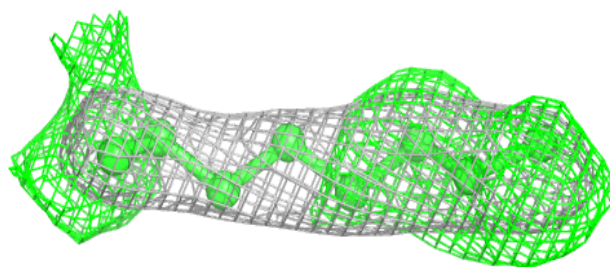
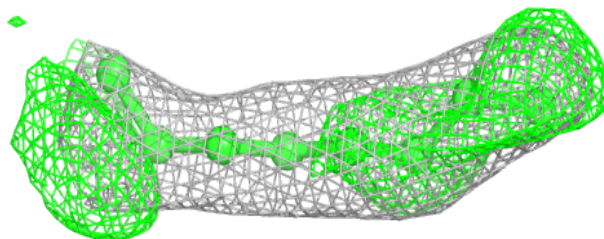
**Electron density around CDL L 101:**

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

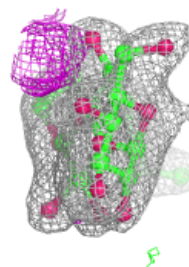
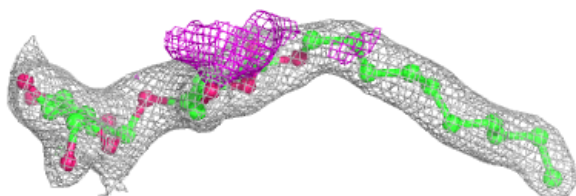
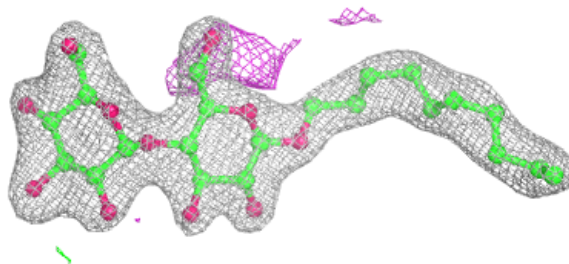


**Electron density around DMU Z 103:**

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

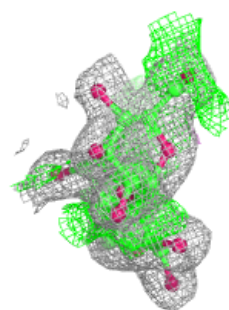
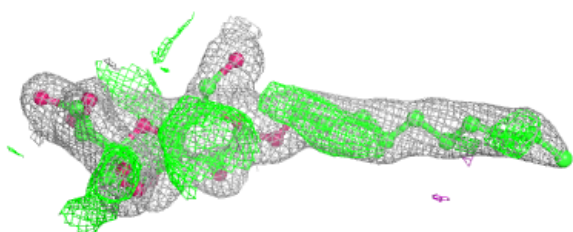
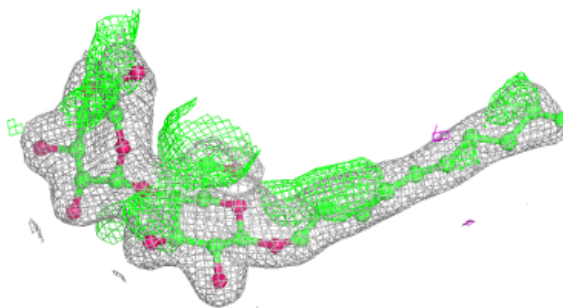
**Electron density around DMU Z 101:**

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

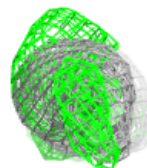
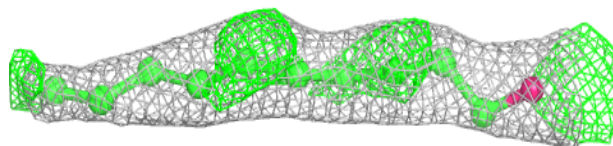
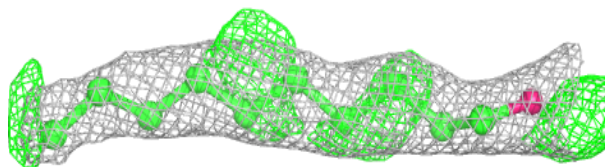


**Electron density around DMU D 201:**

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

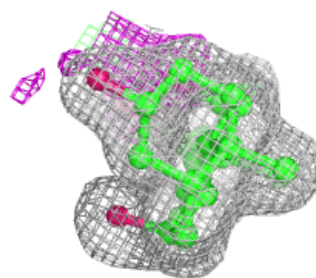
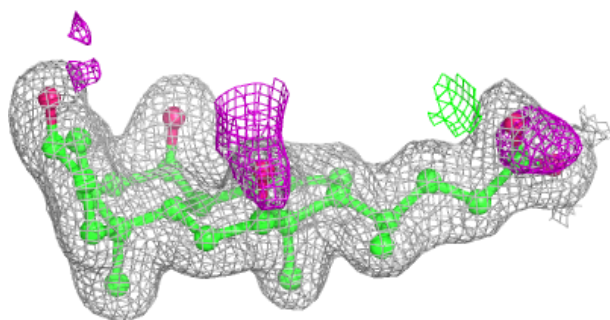
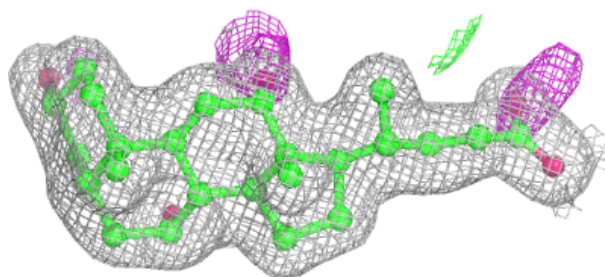
**Electron density around DMU C 306:**

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

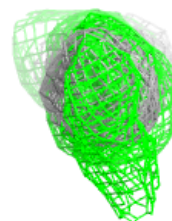
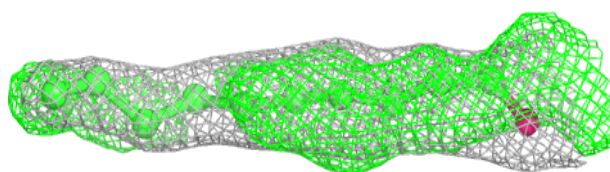
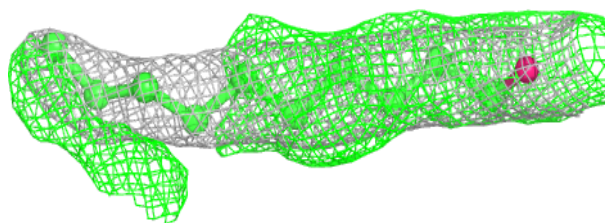


**Electron density around CHD C 301:**

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

**Electron density around DMU P 307:**

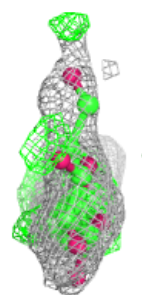
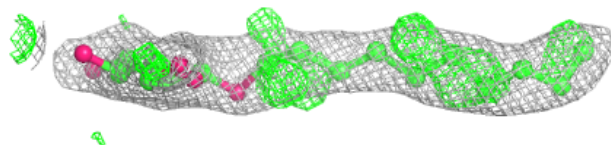
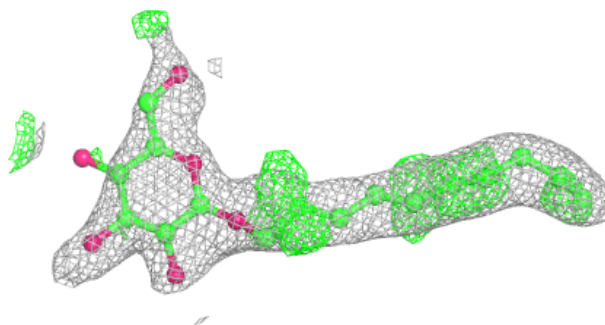
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



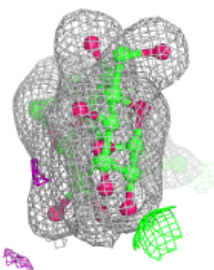
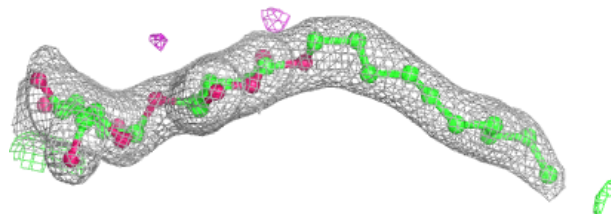
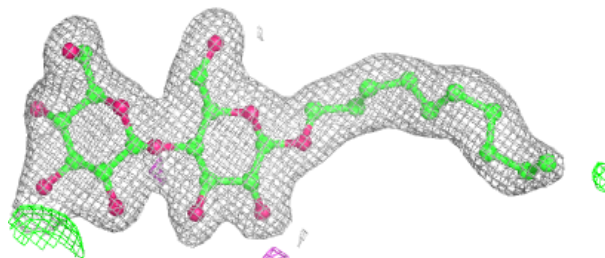


**Electron density around DMU B 304:**

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

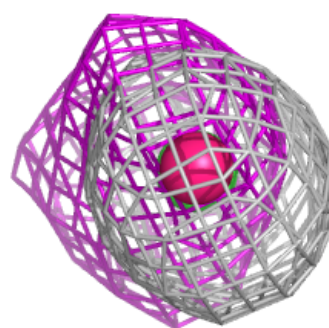
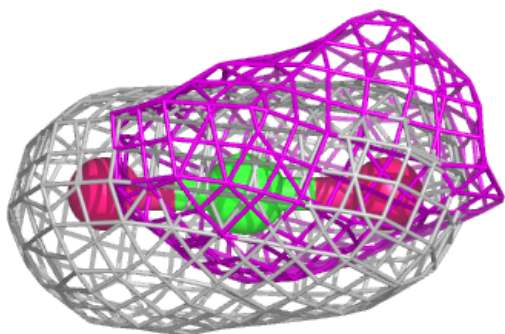
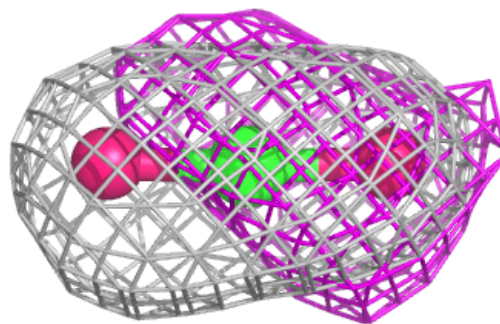
**Electron density around DMU M 101:**

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

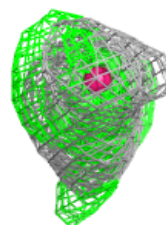
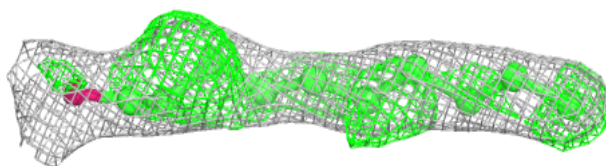
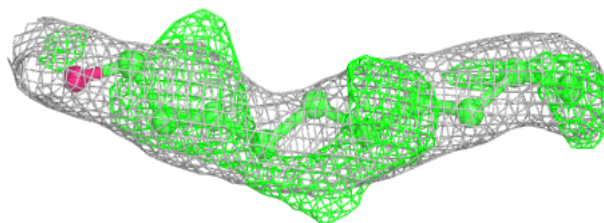


**Electron density around CO2 N 607:**

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

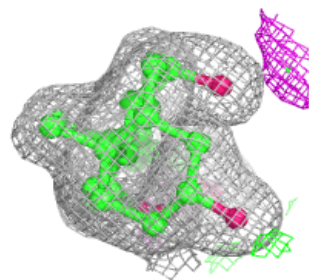
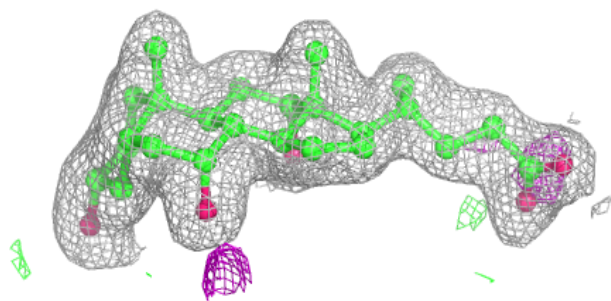
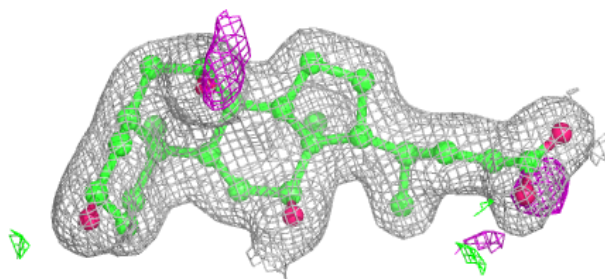
**Electron density around DMU O 307:**

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

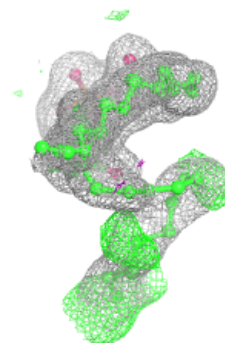
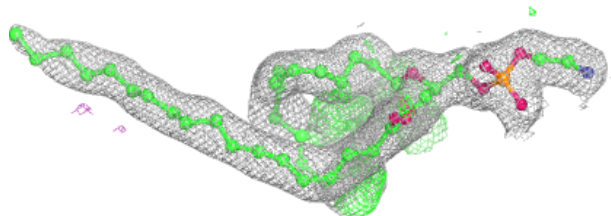
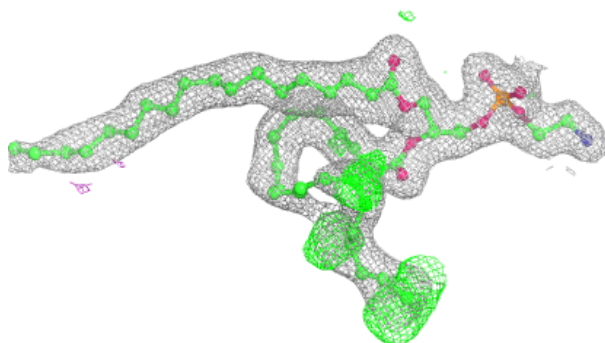


**Electron density around CHD P 302:**

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

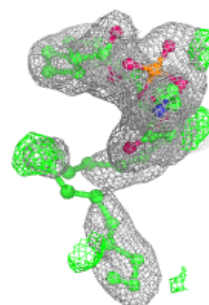
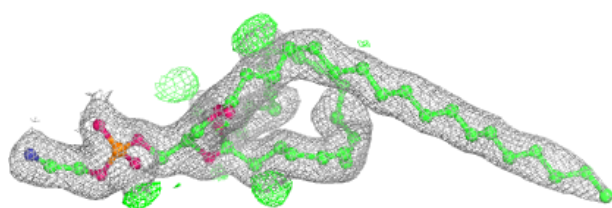
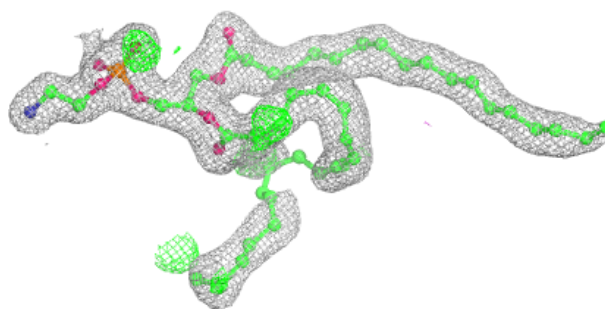
**Electron density around PEK G 101:**

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

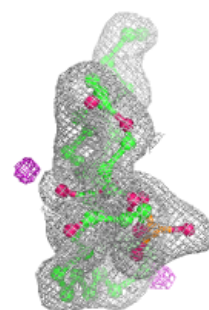
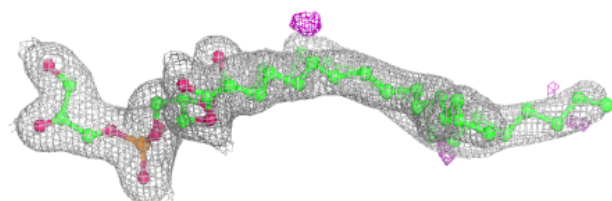
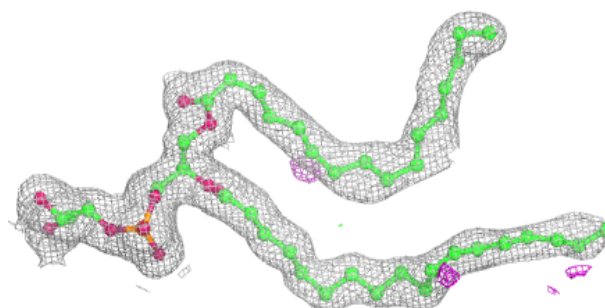


**Electron density around PEK T 101:**

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

**Electron density around PGV N 617:**

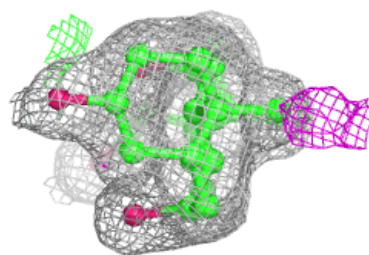
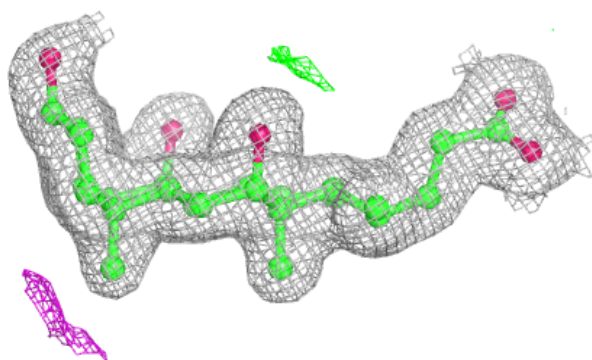
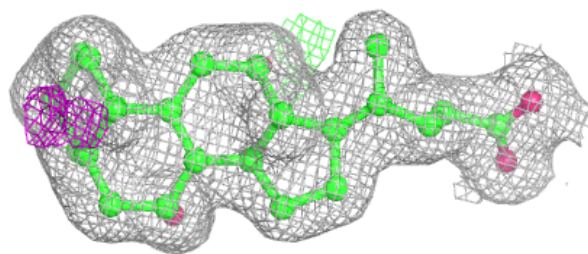
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



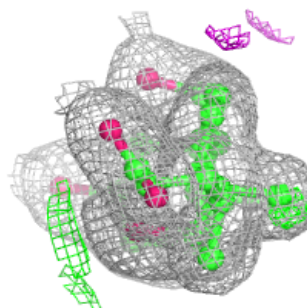
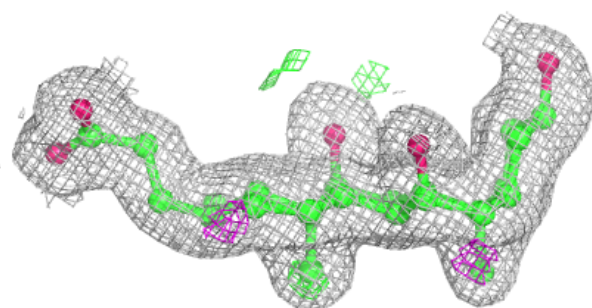
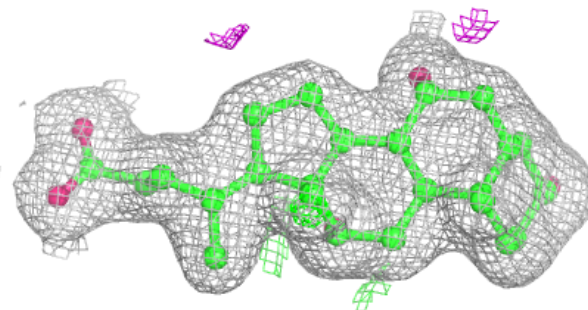


**Electron density around CHD B 306:**

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

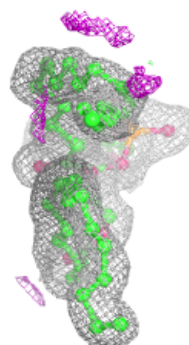
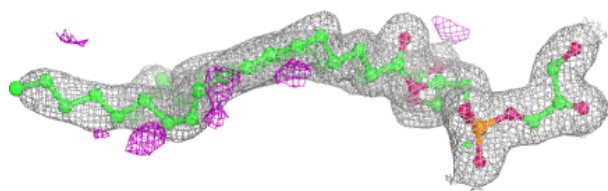
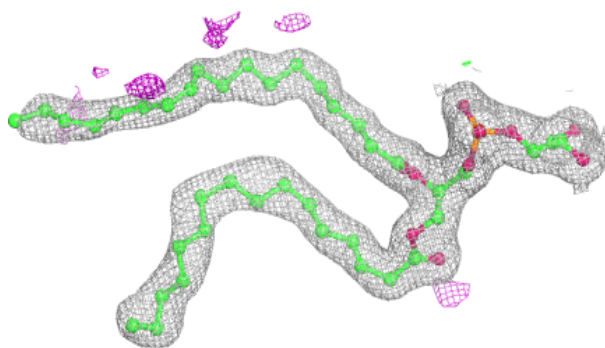
**Electron density around CHD O 301:**

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

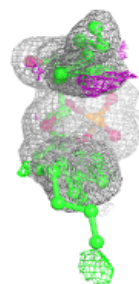
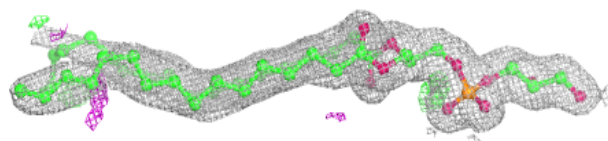
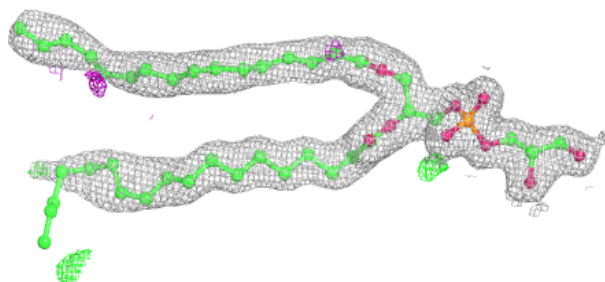


**Electron density around PGV A 617:**

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

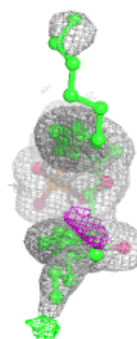
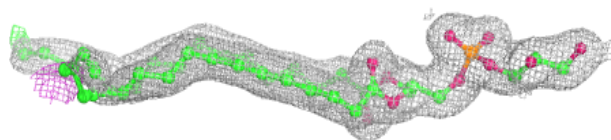
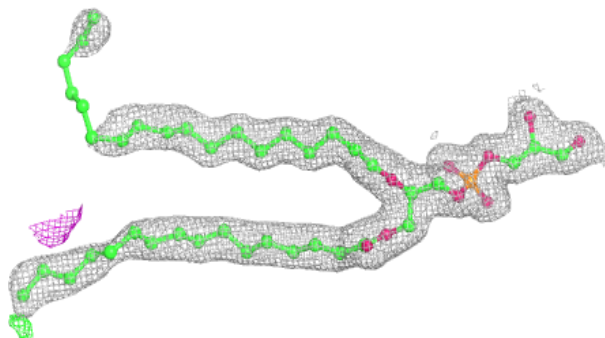
**Electron density around PGV C 303:**

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

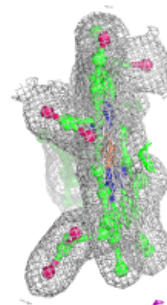
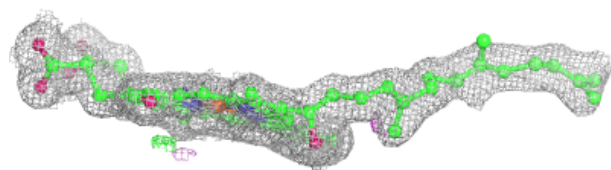
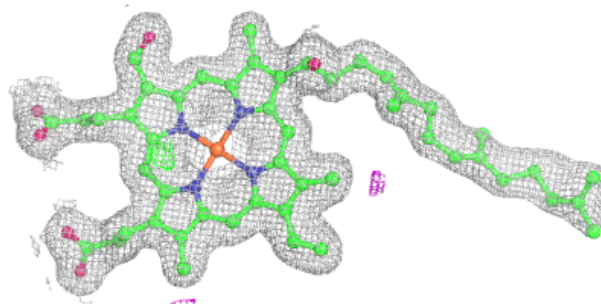


**Electron density around PGV P 304:**

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

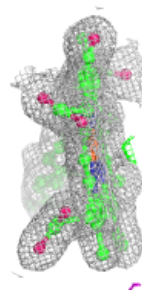
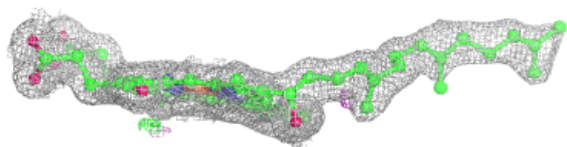
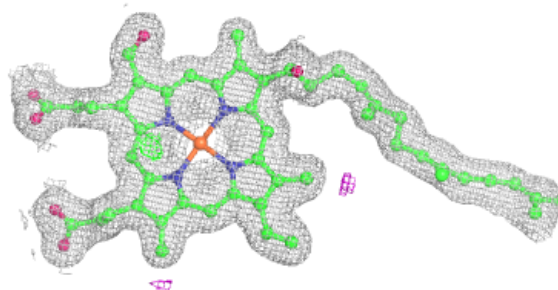
**Electron density around HEA A 601 (A):**

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

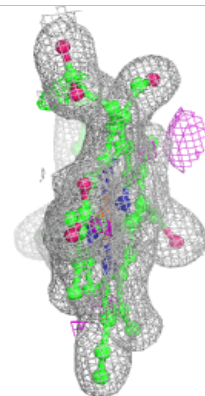
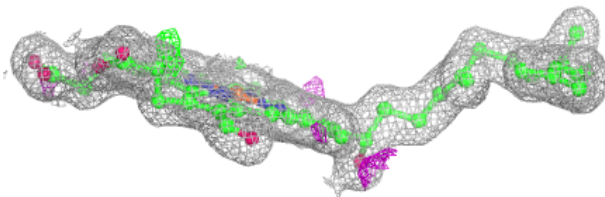
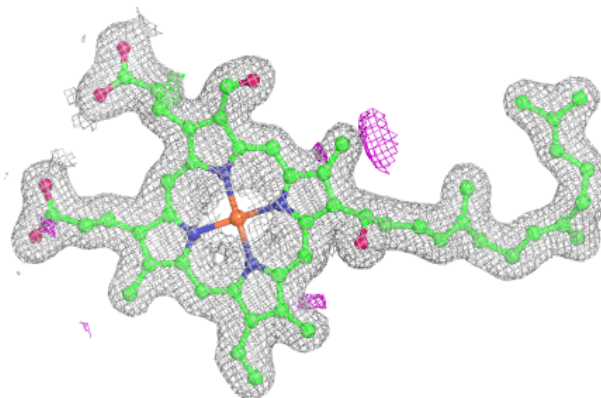


**Electron density around HEA A 601 (B):**

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

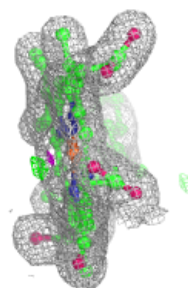
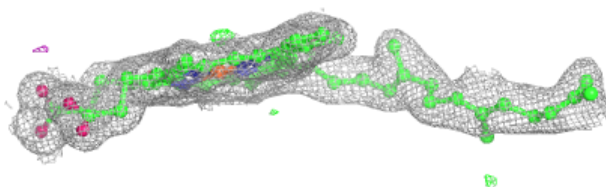
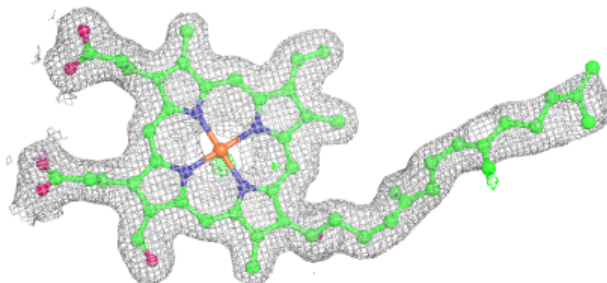
**Electron density around HEA A 602:**

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

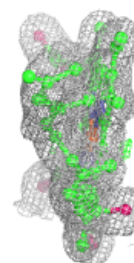
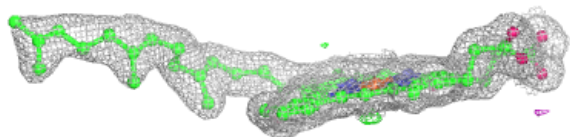
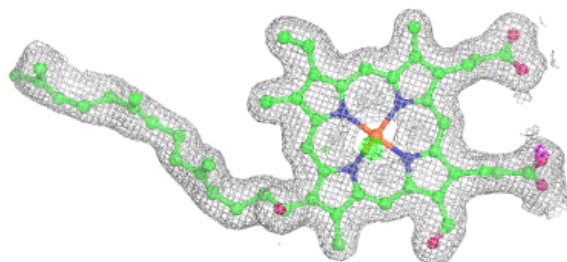


**Electron density around HEA N 601 (A):**

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

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

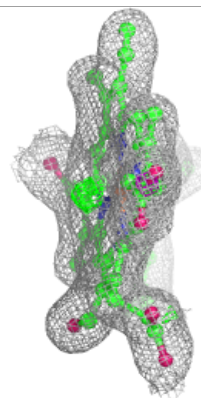
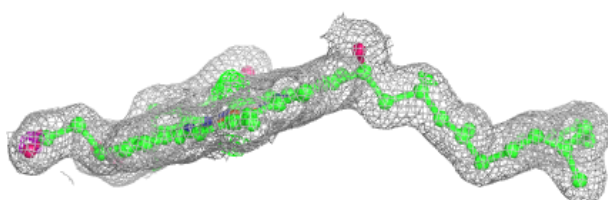
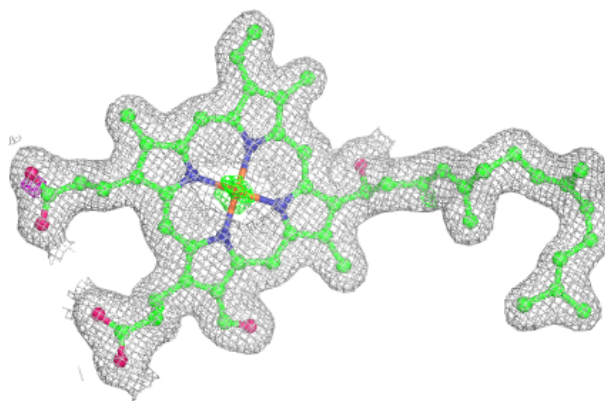
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



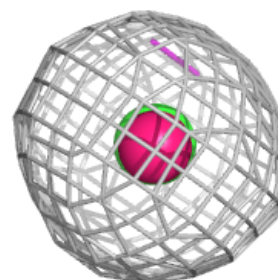
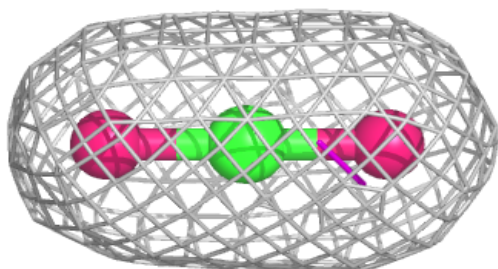
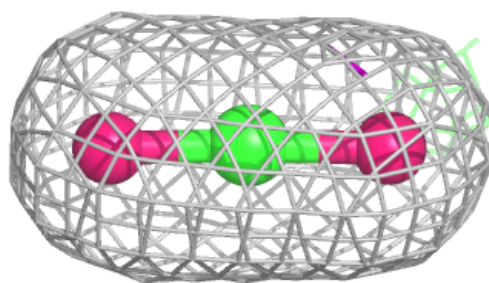


**Electron density around HEA N 602:**

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

**Electron density around CO2 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.