



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2021 – 06:29 PM JST

PDB ID : 7COH
Title : Dimeric Form of Bovine Heart Cytochrome c Oxidase in the Fully Oxidized State
Authors : Shinzawa-Itoh, K.; Muramoto, K.
Deposited on : 2020-08-04
Resolution : 1.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

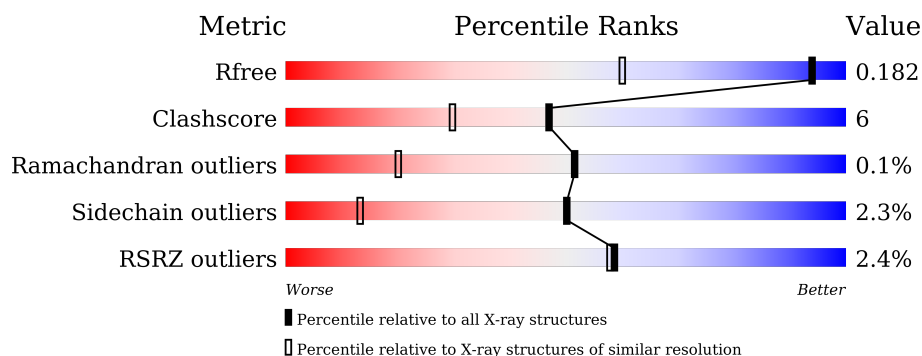
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



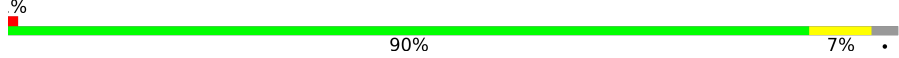

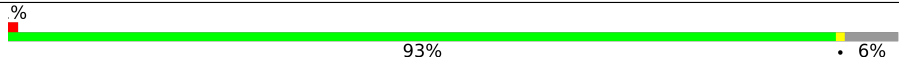
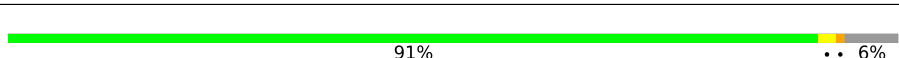
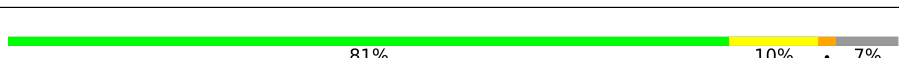
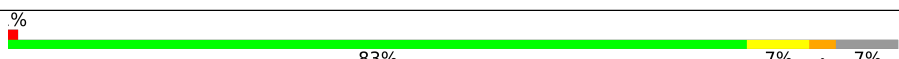
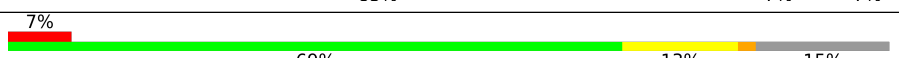
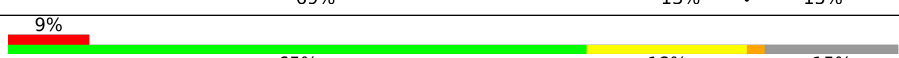
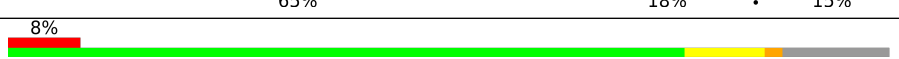

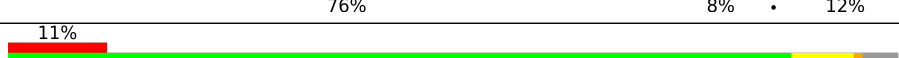







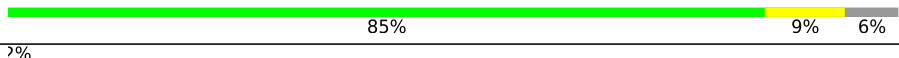
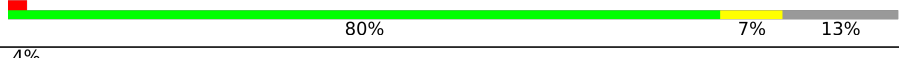
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>88%</div> <div>11%</div> </div>
1	N	514	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	B	227	<div> <div>5%</div> <div>80%</div> <div>15%</div> <div>.</div> <div>.</div> </div>
2	O	227	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
3	C	261	<div> <div>88%</div> <div>11%</div> <div>.</div> </div>
3	P	261	<div> <div>%</div> <div>87%</div> <div>11%</div> <div>.</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
14	HEA	A	516	X	-	-	-
14	HEA	N	516	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 33049 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.

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.

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.

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			

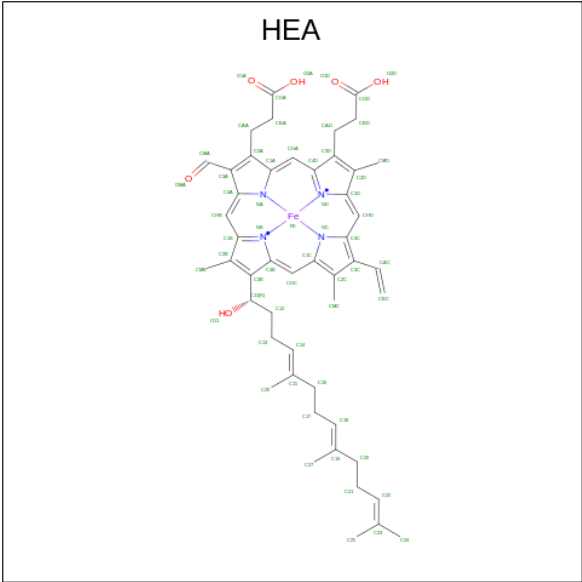
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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.

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 (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 69	C 58	Fe 1	N 4	O 6	0	1
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 69	C 58	Fe 1	N 4	O 6	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

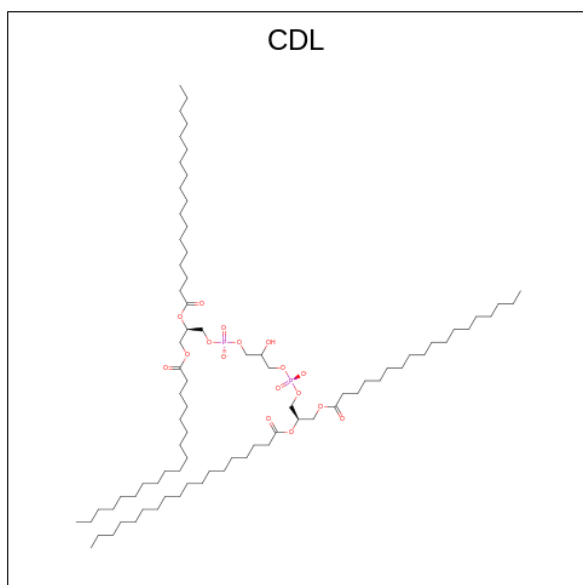
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

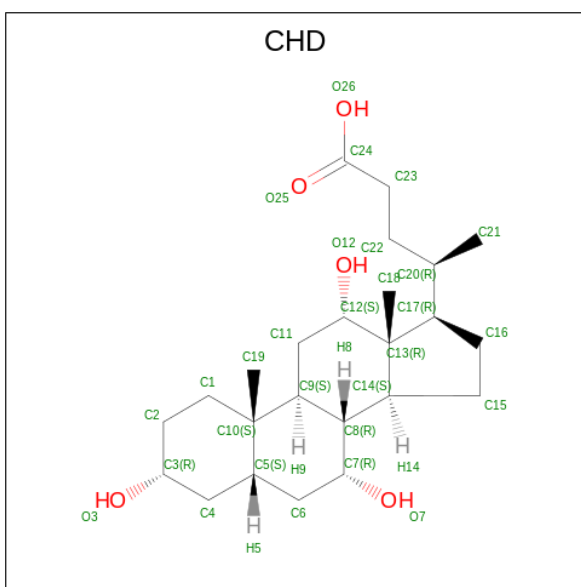
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



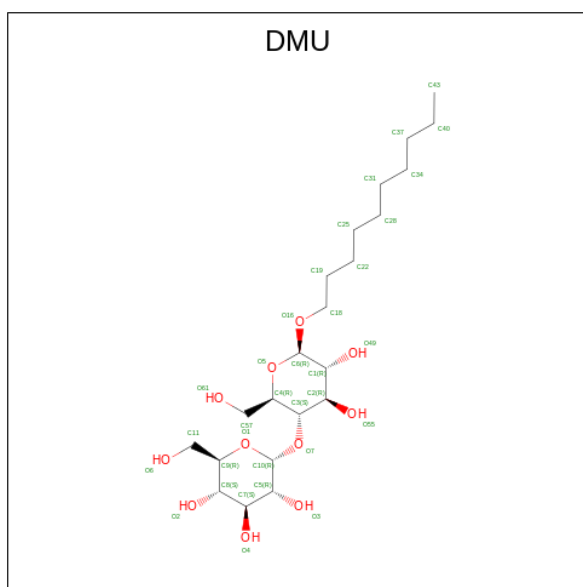
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			94	75	17	2		
18	A	1	Total	C	O	P	0	0
			64	45	17	2		
18	C	1	Total	C	O	P	0	0
			87	68	17	2		
18	N	1	Total	C	O	P	0	0
			94	75	17	2		
18	N	1	Total	C	O	P	0	0
			64	45	17	2		
18	P	1	Total	C	O	P	0	0
			87	68	17	2		

- Molecule 19 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			29	24	5		
19	C	1	Total	C	O	0	0
			29	24	5		
19	G	1	Total	C	O	0	0
			29	24	5		
19	N	1	Total	C	O	0	0
			29	24	5		
19	P	1	Total	C	O	0	0
			29	24	5		
19	T	1	Total	C	O	0	0
			29	24	5		

- Molecule 20 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁) (labeled as "Ligand of Interest" by depositor).



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

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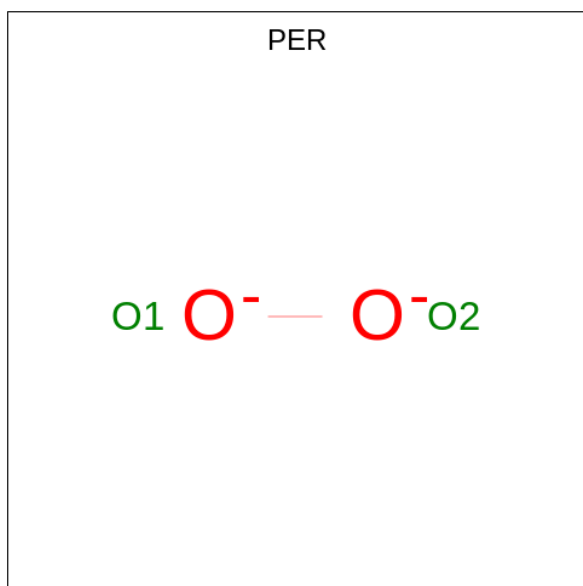
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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20	G	1	Total C O 11 10 1	0	0
20	G	1	Total C O 22 16 6	0	0
20	J	1	Total C O 11 10 1	0	0
20	J	1	Total C O 33 22 11	0	0
20	L	1	Total C O 22 16 6	0	0
20	M	1	Total C 8 8	0	0
20	N	1	Total C O 33 22 11	0	0
20	N	1	Total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

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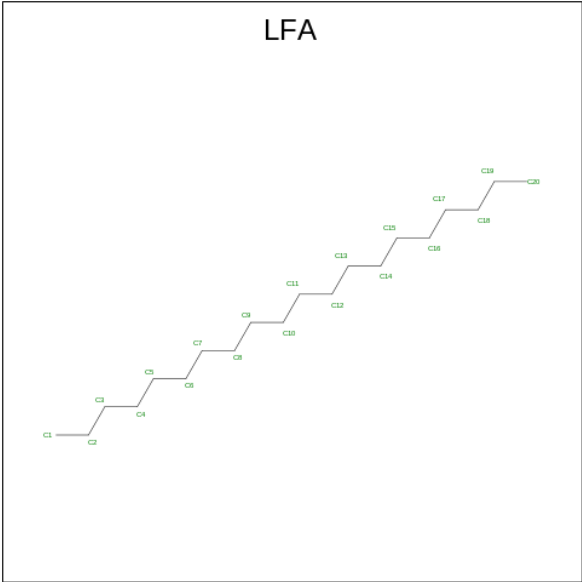
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	T	1	Total C O 22 16 6	0	0
20	T	1	Total C O 11 10 1	0	0
20	T	1	Total C O 22 16 6	0	0
20	W	1	Total C O 11 10 1	0	0
20	W	1	Total C O 33 22 11	0	0
20	Y	1	Total C O 22 16 6	0	0
20	Z	1	Total C 8 8	0	0

- Molecule 21 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



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

- Molecule 22 is EICOSANE (three-letter code: LFA) (formula: C₂₀H₄₂) (labeled as "Ligand of Interest" by depositor).



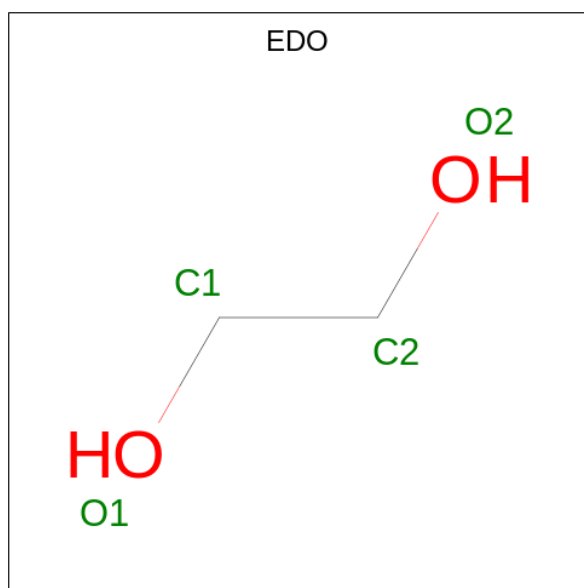
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	C	0	0
			14	14		
22	A	1	Total	C	0	0
			14	14		
22	C	1	Total	C	0	0
			11	11		
22	C	1	Total	C	0	0
			6	6		
22	C	1	Total	C	0	0
			15	15		
22	C	1	Total	C	0	0
			11	11		
22	C	1	Total	C	0	0
			14	14		
22	C	1	Total	C	0	0
			11	11		
22	C	1	Total	C	0	0
	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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	N	1	Total C 14 14	0	0
22	P	1	Total C 11 11	0	0
22	P	1	Total C 6 6	0	0
22	P	1	Total C 15 15	0	0
22	P	1	Total C 11 11	0	0
22	P	1	Total C 14 14	0	0
22	P	1	Total C 11 11	0	0
22	P	1	Total C 15 15	0	0
22	P	1	Total C 13 13	0	0
22	P	1	Total C 18 18	0	1
22	T	1	Total C 17 17	0	0
22	T	1	Total C 11 11	0	0

- Molecule 23 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



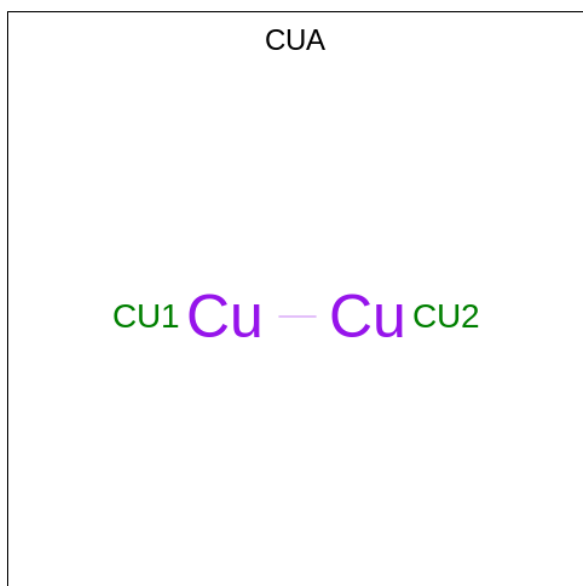
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total 4	C 2	O 2	0	0
23	A	1	Total 4	C 2	O 2	0	0
23	A	1	Total 4	C 2	O 2	0	0
23	A	1	Total 4	C 2	O 2	0	0
23	B	1	Total 4	C 2	O 2	0	0
23	C	1	Total 4	C 2	O 2	0	0
23	C	1	Total 4	C 2	O 2	0	0
23	C	1	Total 4	C 2	O 2	0	0
23	E	1	Total 4	C 2	O 2	0	0
23	E	1	Total 4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

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

- Molecule 24 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).

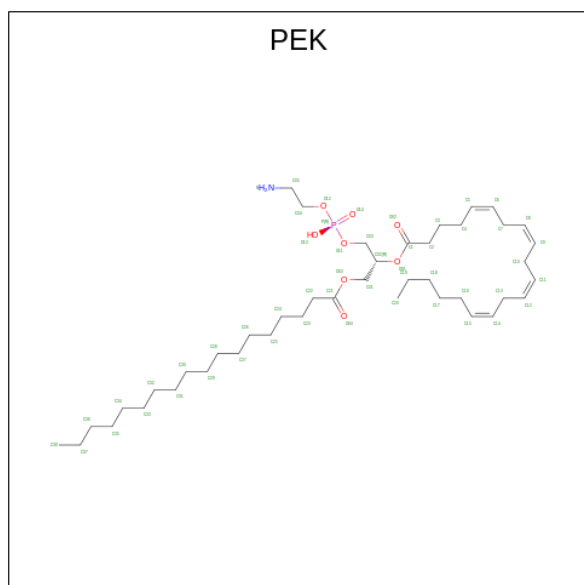


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total Cu 2 2	0	0
24	O	1	Total Cu 2 2	0	0

- Molecule 25 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

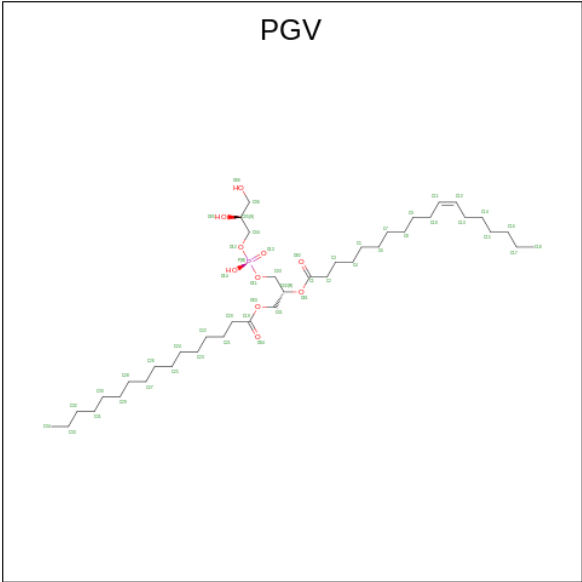
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total X 1 1	0	0
25	P	1	Total X 1 1	0	0

- Molecule 26 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 27 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P) (labeled as "Ligand of Interest" by depositor).



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

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

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

- Molecule 29 is water.

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	3	Total O 3 3	0	0
29	A	6	Total O 6 6	0	0
29	A	4	Total O 4 4	0	0
29	A	3	Total O 3 3	0	0
29	A	4	Total O 4 4	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	11	Total O 11 11	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	3	Total O 3 3	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	4	Total O 4 4	0	0
29	A	1	Total O 1 1	0	0
29	A	3	Total O 3 3	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	3	Total O 3 3	0	0
29	A	1	Total O 2 2	0	1
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	2	Total O 2 2	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	2	Total O 2 2	0	0
29	A	7	Total O 7 7	0	0
29	A	5	Total O 5 5	0	0
29	A	1	Total O 1 1	0	0
29	A	8	Total O 8 8	0	0
29	A	1	Total O 1 1	0	0
29	A	8	Total O 8 8	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 3 3	0	1
29	A	3	Total O 4 4	0	1
29	A	2	Total O 3 3	0	1
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 3 3	0	1
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 2 2	0	1
29	A	1	Total O 1 1	0	0
29	A	2	Total O 3 3	0	1
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 2 2	0	1

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	1	Total O 1 1	0	0
29	A	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	3	Total O 3 3	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	3	Total O 3 3	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	3	Total O 3 3	0	0
29	B	1	Total O 1 1	0	0
29	B	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0
29	B	3	Total O 3 3	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 2 2	0	1
29	B	2	Total O 2 2	0	0
29	B	4	Total O 4 4	0	0
29	B	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0
29	B	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	2	Total O 2 2	0	0
29	B	6	Total O 7 7	0	1
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	3	Total O 3 3	0	0
29	B	2	Total O 2 2	0	0
29	B	2	Total O 2 2	0	0
29	B	2	Total O 2 2	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0
29	B	1	Total O 1 1	0	0

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

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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 2 2	0	1
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 2 2	0	1
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 2 2	0	1
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 2 2	0	1
29	D	2	Total O 3 3	0	1
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 2 2	0	1
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 2 2	0	1
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 2 2	0	1
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 2 2	0	1
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	4	Total O 4 4	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	3	Total O 3 3	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	2	Total O 2 2	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0
29	D	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	2	Total O 2 2	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	2	Total O 2 2	0	0
29	E	2	Total O 2 2	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	2	Total O 2 2	0	0
29	E	2	Total O 2 2	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 2 2	0	1
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	2	Total O 2 2	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 2 2	0	1
29	E	1	Total O 1 1	0	0
29	E	1	Total O 2 2	0	1
29	E	1	Total O 2 2	0	1
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	E	2	Total O 2 2	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 2 2	0	1
29	E	1	Total O 1 1	0	0
29	E	1	Total O 2 2	0	1
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 2 2	0	1
29	E	1	Total O 1 1	0	0
29	E	2	Total O 2 2	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	2	Total O 2 2	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	3	Total O 3 3	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	1	Total O 1 1	0	0
29	E	3	Total O 3 3	0	0
29	E	1	Total O 1 1	0	0
29	E	6	Total O 6 6	0	0
29	E	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	2	Total O 2 2	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 2 2	0	1
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	2	Total O 2 2	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	2	Total O 4 4	0	2
29	F	2	Total O 2 2	0	0
29	F	1	Total O 1 1	0	0
29	F	2	Total O 2 2	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	F	1	Total O 1 1	0	0
29	F	1	Total O 2 2	0	1
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	2	Total O 3 3	0	1
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 2 2	0	1
29	F	1	Total O 1 1	0	0
29	F	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	1	Total O 1 1	0	0
29	F	2	Total O 2 2	0	0
29	F	4	Total O 4 4	0	0
29	F	7	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	F	1	Total O 1 1	0	0
29	F	2	Total O 2 2	0	0
29	F	1	Total O 1 1	0	0
29	F	2	Total O 3 3	0	1
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	G	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	2	Total O 2 2	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	2	Total O 2 2	0	0
29	H	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	H	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	I	1	Total O 1 1	0	0
29	I	2	Total O 2 2	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	I	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	J	1	Total O 1 1	0	0
29	J	2	Total O 2 2	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	J	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	K	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 2 2	0	1
29	L	1	Total O 1 1	0	0
29	L	1	Total O 2 2	0	1
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	L	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	M	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	2	Total O 2 2	0	0
29	N	3	Total O 3 3	0	0
29	N	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	N	4	Total O 4 4	0	0
29	N	3	Total O 3 3	0	0
29	N	4	Total O 4 4	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	11	Total O 11 11	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	3	Total O 3 3	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	3	Total O 3 3	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	4	Total O 4 4	0	0
29	N	1	Total O 1 1	0	0
29	N	3	Total O 3 3	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	3	Total O 3 3	0	0
29	N	1	Total O 2 2	0	1
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	2	Total O 2 2	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	3	Total O 3 3	0	0
29	N	7	Total O 7 7	0	0
29	N	5	Total O 5 5	0	0
29	N	1	Total O 1 1	0	0
29	N	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	N	1	Total O 1 1	0	0
29	N	8	Total O 8 8	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 3 3	0	1
29	N	2	Total O 3 3	0	1
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	3	Total O 3 3	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 2 2	0	1
29	N	1	Total O 2 2	0	1
29	N	1	Total O 2 2	0	1
29	N	1	Total O 2 2	0	1
29	N	1	Total O 2 2	0	1
29	N	2	Total O 4 4	0	2
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	N	2	Total O 2 2	0	0
29	N	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	2	Total O 2 2	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	3	Total O 3 3	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	3	Total O 3 3	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	3	Total O 3 3	0	0
29	O	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	O	2	Total O 2 2	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	2	Total O 2 2	0	0
29	O	2	Total O 2 2	0	0
29	O	3	Total O 3 3	0	0
29	O	1	Total O 1 1	0	0
29	O	3	Total O 3 3	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 2 2	0	1
29	O	2	Total O 2 2	0	0
29	O	4	Total O 4 4	0	0
29	O	2	Total O 2 2	0	0
29	O	1	Total O 1 1	0	0

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	2	Total O 2 2	0	0
29	O	5	Total O 5 5	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	2	Total O 2 2	0	0
29	O	3	Total O 3 3	0	0
29	O	2	Total O 2 2	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	O	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0
29	P	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	4	Total O 4 4	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 2 2	0	1
29	P	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0
29	P	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	2	Total O 2 2	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	3	Total O 3 3	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	P	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	Q	2	Total O 2 2	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	2	Total O 2 2	0	0
29	Q	1	Total O 1 1	0	0
29	Q	2	Total O 2 2	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 2 2	0	1
29	Q	1	Total O 2 2	0	1
29	Q	1	Total O 2 2	0	1
29	Q	1	Total O 2 2	0	1
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	4	Total O 4 4	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	3	Total O 3 3	0	0
29	Q	2	Total O 2 2	0	0
29	Q	3	Total O 3 3	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0
29	Q	2	Total O 2 2	0	0
29	Q	1	Total O 1 1	0	0
29	Q	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	Q	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	2	Total O 2 2	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	3	Total O 3 3	0	0
29	R	1	Total O 1 1	0	0
29	R	2	Total O 2 2	0	0
29	R	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 2 2	0	1
29	R	1	Total O 2 2	0	1
29	R	2	Total O 4 4	0	2
29	R	1	Total O 2 2	0	1
29	R	1	Total O 2 2	0	1
29	R	1	Total O 2 2	0	1
29	R	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	3	Total O 3 3	0	0
29	R	2	Total O 2 2	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	1	Total O 1 1	0	0
29	R	3	Total O 3 3	0	0
29	R	1	Total O 1 1	0	0
29	R	6	Total O 6 6	0	0
29	R	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	2	Total O 2 2	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 2 2	0	1
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	2	Total O 2 2	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	2	Total O 4 4	0	2

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	2	Total O 2 2	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 2 2	0	1
29	S	1	Total O 2 2	0	1
29	S	2	Total O 4 4	0	2
29	S	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	S	8	Total O 8 8	0	0
29	S	1	Total O 1 1	0	0
29	S	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 2 2	0	1
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	T	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	2	Total O 2 2	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	2	Total O 2 2	0	0
29	U	1	Total O 1 1	0	0
29	U	2	Total O 2 2	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	2	Total O 2 2	0	0
29	U	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	U	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	V	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	W	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	2	Total O 4 4	0	2
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	1	Total O 1 1	0	0
29	Y	3	Total O 3 3	0	0
29	Y	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0

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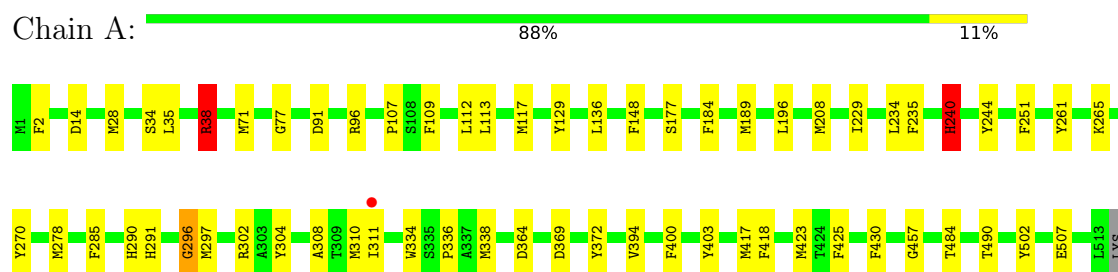
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0

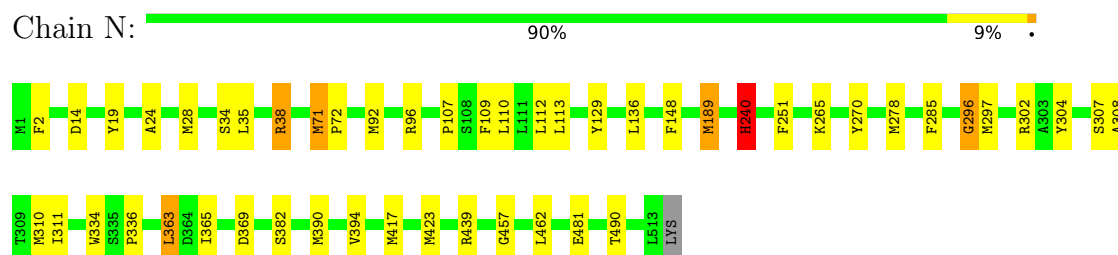
3 Residue-property plots

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

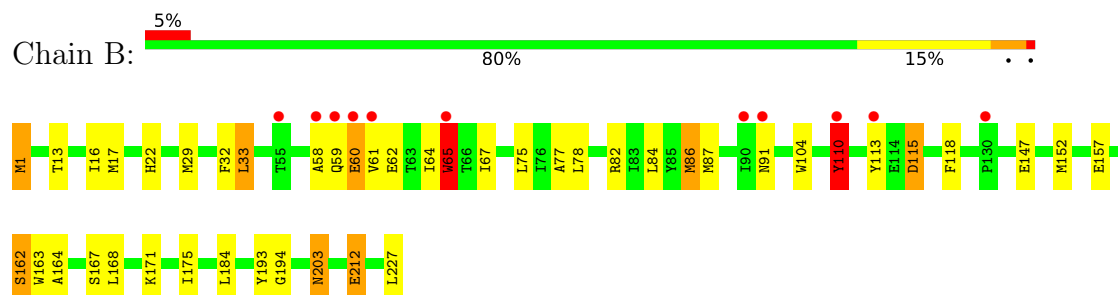
• Molecule 1: Cytochrome c oxidase subunit 1



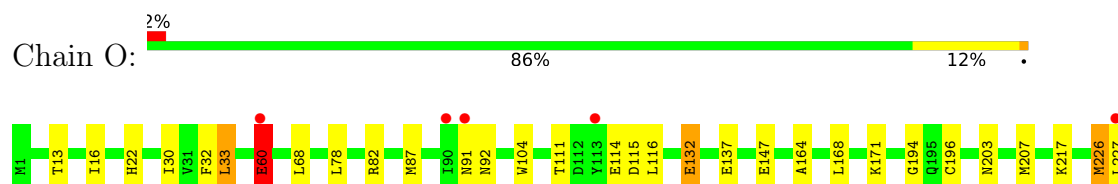
• Molecule 1: Cytochrome c oxidase subunit 1



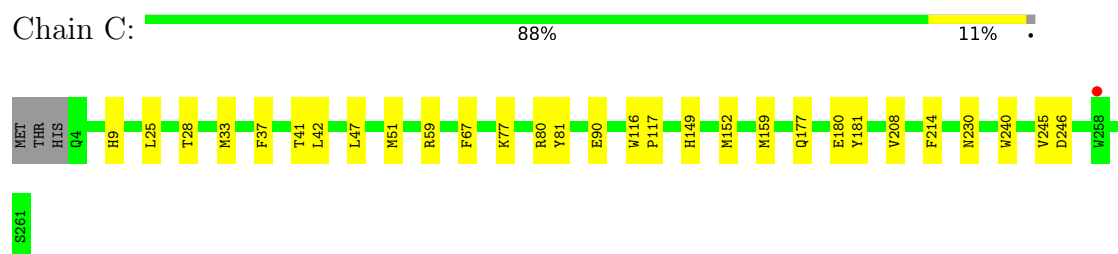
• Molecule 2: Cytochrome c oxidase subunit 2



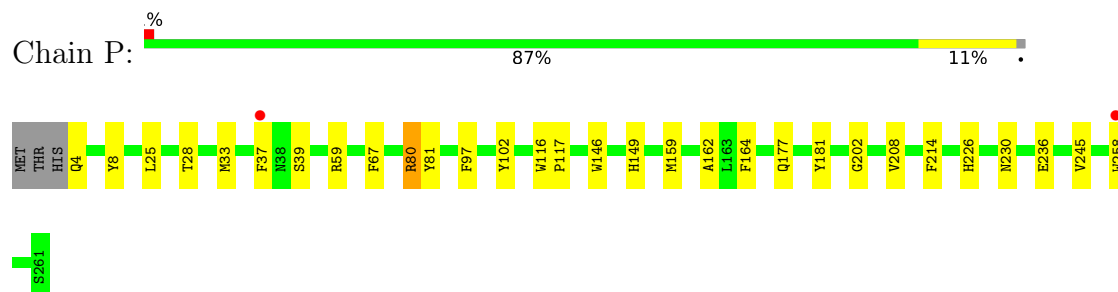
• Molecule 2: Cytochrome c oxidase subunit 2



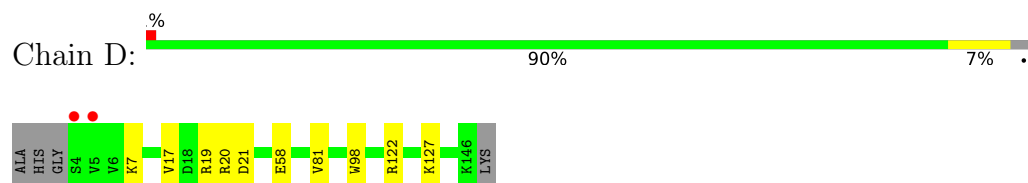
• Molecule 3: Cytochrome c oxidase subunit 3



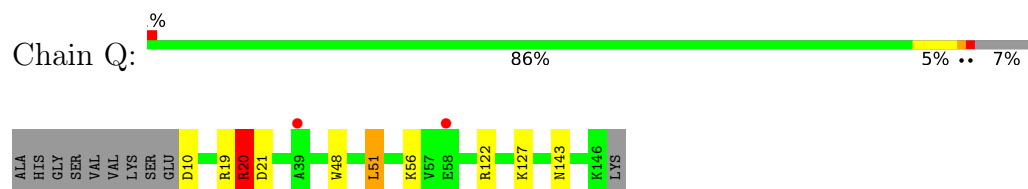
• Molecule 3: Cytochrome c oxidase subunit 3



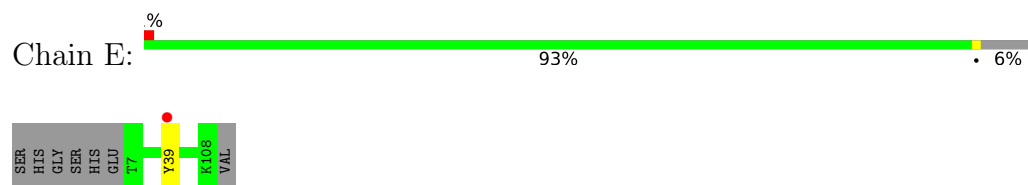
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



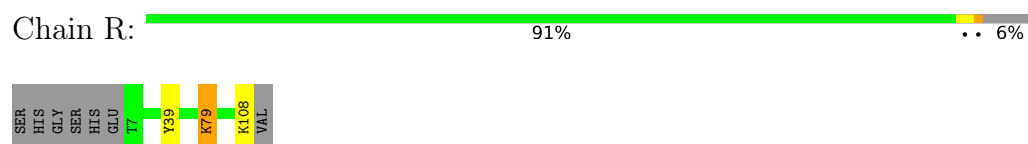
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1




• Molecule 5: Cytochrome c oxidase subunit 5A

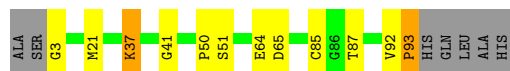


• Molecule 5: Cytochrome c oxidase subunit 5A




- Molecule 6: Cytochrome c oxidase subunit 5B

Chain F:  81% 10% 7%



- Molecule 6: Cytochrome c oxidase subunit 5B

Chain S:  83% 7% 7%



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

Chain G:  69% 13% 15%




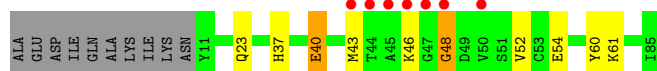
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:  65% 18% 15%




- Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:  76% 9% 12%




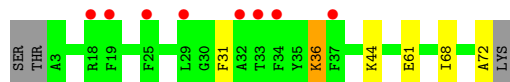
- Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:  76% 8% 12%

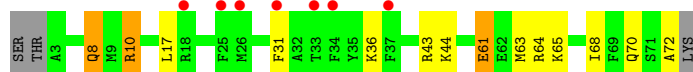
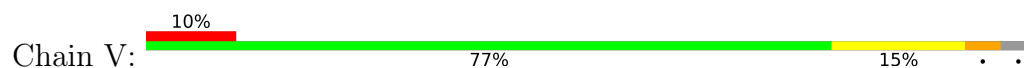


- Molecule 9: Cytochrome c oxidase subunit 6C

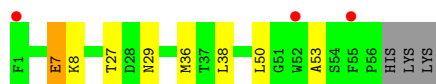
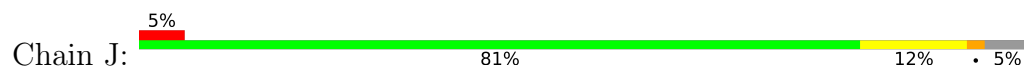
Chain I:  88% 7% 7%



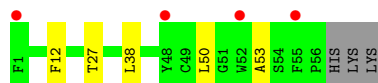
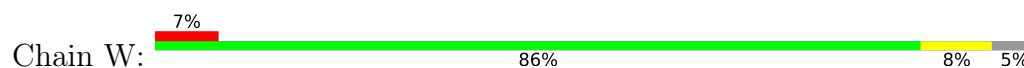
- Molecule 9: Cytochrome c oxidase subunit 6C



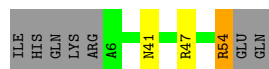
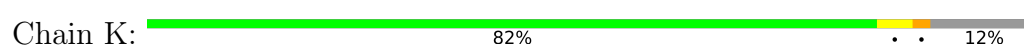
- Molecule 10: Cytochrome c oxidase subunit 7A1



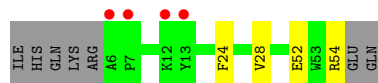
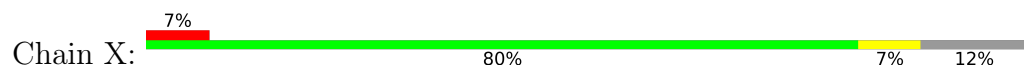
- Molecule 10: Cytochrome c oxidase subunit 7A1



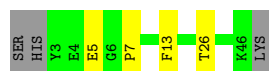
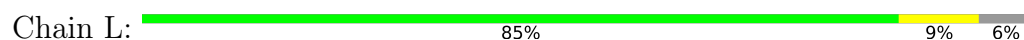
- Molecule 11: Cytochrome c oxidase subunit 7B



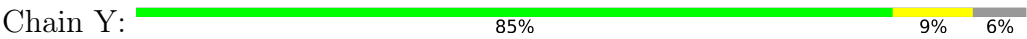
- Molecule 11: Cytochrome c oxidase subunit 7B



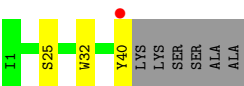
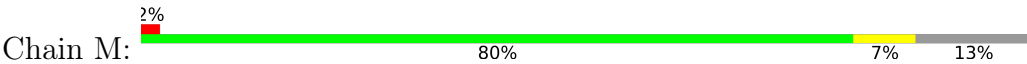
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



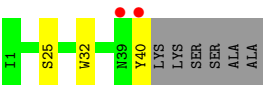
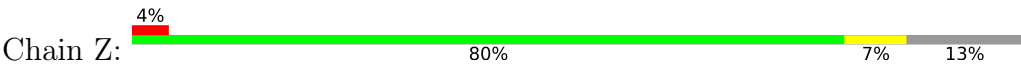
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



● Molecule 13: Cytochrome c oxidase subunit 8B



● Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.00Å 204.19Å 177.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.30 135.86 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-1.30) 99.6 (135.86-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.148 , 0.170 0.163 , 0.182	Depositor DCC
R_{free} test set	79184 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33049	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.13	6/4259 (0.1%)	1.29	30/5816 (0.5%)
1	N	1.05	8/4259 (0.2%)	1.13	19/5816 (0.3%)
2	B	1.67	11/1908 (0.6%)	1.50	21/2598 (0.8%)
2	O	0.92	4/1908 (0.2%)	1.10	4/2598 (0.2%)
3	C	1.02	2/2258 (0.1%)	1.06	6/3084 (0.2%)
3	P	0.96	0/2258	1.00	7/3084 (0.2%)
4	D	0.95	2/1226 (0.2%)	1.09	4/1657 (0.2%)
4	Q	0.74	0/1182	0.93	3/1598 (0.2%)
5	E	0.82	0/843	0.96	2/1145 (0.2%)
5	R	0.77	0/843	0.88	2/1145 (0.2%)
6	F	0.96	1/724 (0.1%)	1.07	1/983 (0.1%)
6	S	0.94	1/724 (0.1%)	1.07	1/983 (0.1%)
7	G	0.83	2/633 (0.3%)	0.94	1/864 (0.1%)
7	T	0.84	1/633 (0.2%)	0.97	2/864 (0.2%)
8	H	0.98	2/648 (0.3%)	0.99	0/877
8	U	0.88	2/648 (0.3%)	0.98	1/877 (0.1%)
9	I	0.96	2/588 (0.3%)	1.07	1/781 (0.1%)
9	V	0.83	0/588	1.04	3/781 (0.4%)
10	J	0.72	0/451	0.89	2/610 (0.3%)
10	W	0.74	0/451	0.84	0/610
11	K	0.84	0/398	1.14	2/546 (0.4%)
11	X	0.83	0/398	0.84	0/546
12	L	1.02	1/372 (0.3%)	1.06	0/500
12	Y	0.88	1/372 (0.3%)	0.83	0/500
13	M	0.92	0/321	1.05	0/440
13	Z	0.79	0/321	0.88	0/440
All	All	1.03	46/29214 (0.2%)	1.11	112/39743 (0.3%)

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	4
1	N	0	3
2	B	0	5
6	S	0	1
11	K	0	1
All	All	0	14

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	110	TYR	CE1-CZ	42.08	1.93	1.38
2	B	110	TYR	CG-CD1	27.95	1.75	1.39
2	B	110	TYR	CG-CD2	19.12	1.64	1.39
1	N	481	GLU	CD-OE2	18.10	1.45	1.25
2	B	110	TYR	CE2-CZ	12.35	1.54	1.38

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	110	TYR	CB-CG-CD1	-31.40	102.16	121.00
2	O	82	ARG	NE-CZ-NH2	-19.74	110.43	120.30
2	B	82	ARG	NE-CZ-NH2	-17.76	111.42	120.30
2	B	110	TYR	CD1-CE1-CZ	-17.49	104.06	119.80
11	K	54	ARG	CA-C-O	-14.42	89.82	120.10

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
1	A	304	TYR	Sidechain
1	A	38	ARG	Sidechain
2	B	110	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	56	0
1	N	4130	0	4102	60	0
2	B	1870	0	1870	31	0
2	O	1870	0	1870	15	0
3	C	2171	0	2080	26	0
3	P	2172	0	2081	24	0
4	D	1192	0	1178	4	0
4	Q	1148	0	1131	6	0
5	E	825	0	823	0	0
5	R	825	0	823	2	0
6	F	709	0	691	11	0
6	S	709	0	691	7	0
7	G	606	0	577	5	0
7	T	606	0	577	9	0
8	H	628	0	580	11	0
8	U	628	0	580	10	0
9	I	575	0	584	5	0
9	V	575	0	584	9	0
10	J	441	0	439	8	0
10	W	441	0	439	6	0
11	K	384	0	366	0	0
11	X	384	0	366	2	0
12	L	360	0	360	4	0
12	Y	360	0	360	4	0
13	M	311	0	321	3	0
13	Z	311	0	321	3	0
14	A	129	0	88	7	0
14	N	129	0	88	8	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	158	0	213	10	0
18	C	87	0	124	14	0
18	N	158	0	213	8	0
18	P	87	0	124	12	0
19	A	29	0	39	0	0
19	C	29	0	39	0	0
19	G	29	0	39	1	0
19	N	29	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	P	29	0	39	1	0
19	T	29	0	39	1	0
20	A	106	0	138	6	0
20	B	44	0	73	0	0
20	C	172	0	230	7	0
20	G	55	0	81	9	0
20	J	44	0	61	6	0
20	L	22	0	31	0	0
20	M	8	0	15	0	0
20	N	106	0	138	4	0
20	O	44	0	73	2	0
20	P	172	0	231	7	0
20	T	55	0	83	18	0
20	W	44	0	61	7	0
20	Y	22	0	31	1	0
20	Z	8	0	15	0	0
21	A	2	0	0	1	0
21	N	2	0	0	1	0
22	A	28	0	54	16	0
22	C	114	0	219	12	0
22	G	28	0	54	1	0
22	N	28	0	54	7	0
22	P	114	0	219	7	0
22	T	28	0	54	4	0
23	A	16	0	24	1	0
23	B	4	0	6	0	0
23	C	12	0	18	2	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	1	0
23	O	4	0	6	0	0
23	P	12	0	18	0	0
23	R	12	0	18	0	0
23	S	8	0	12	0	0
23	T	4	0	6	0	0
24	B	2	0	0	0	0
24	O	2	0	0	0	0
25	C	1	0	0	0	0
25	P	1	0	0	1	0
26	C	53	0	77	5	0
26	P	53	0	77	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	C	102	0	152	2	0
27	P	102	0	152	1	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	254	0	0	15	0
29	B	179	0	0	2	0
29	C	101	0	0	5	0
29	D	147	0	0	0	0
29	E	117	0	0	0	0
29	F	107	0	0	1	0
29	G	43	0	0	1	0
29	H	59	0	0	2	0
29	I	39	0	0	1	0
29	J	21	0	0	0	0
29	K	20	0	0	0	0
29	L	27	0	0	1	0
29	M	21	0	0	0	0
29	N	236	0	0	11	0
29	O	147	0	0	0	0
29	P	102	0	0	6	0
29	Q	78	0	0	1	0
29	R	96	0	0	0	0
29	S	97	0	0	0	0
29	T	37	0	0	0	0
29	U	50	0	0	3	0
29	V	21	0	0	1	0
29	W	16	0	0	0	0
29	X	20	0	0	0	0
29	Y	27	0	0	1	0
29	Z	18	0	0	2	0
All	All	33049	0	31527	387	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 387 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)
2:B:110:TYR:CG	2:B:110:TYR:CD1	1.75	1.69
1:N:189:MET:CG	1:N:189:MET:CB	1.76	1.62
2:B:110:TYR:CZ	2:B:110:TYR:CE1	1.93	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297[B]:MET:CB	29:A:4142:HOH:O	1.86	1.20
1:A:297[B]:MET:HB2	29:A:4142:HOH:O	1.38	1.15

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	510 (97%)	16 (3%)	0	100	100
1	N	526/514 (102%)	510 (97%)	16 (3%)	0	100	100
2	B	230/227 (101%)	225 (98%)	5 (2%)	0	100	100
2	O	230/227 (101%)	226 (98%)	4 (2%)	0	100	100
3	C	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
3	P	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	136/147 (92%)	133 (98%)	3 (2%)	0	100	100
5	E	100/109 (92%)	100 (100%)	0	0	100	100
5	R	100/109 (92%)	100 (100%)	0	0	100	100
6	F	91/98 (93%)	91 (100%)	0	0	100	100
6	S	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
7	G	71/85 (84%)	68 (96%)	3 (4%)	0	100	100
7	T	71/85 (84%)	68 (96%)	3 (4%)	0	100	100
8	H	73/85 (86%)	70 (96%)	2 (3%)	1 (1%)	11	1
8	U	73/85 (86%)	69 (94%)	2 (3%)	2 (3%)	5	0
9	I	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
9	V	68/73 (93%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	40 (95%)	2 (5%)	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%)	38 (100%)	0	0	100	100
All	All	3488/3614 (96%)	3411 (98%)	74 (2%)	3 (0%)	51	20

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/426 (103%)	436 (99%)	4 (1%)	78	53
1	N	440/426 (103%)	436 (99%)	4 (1%)	78	53
2	B	215/210 (102%)	205 (95%)	10 (5%)	26	2
2	O	215/210 (102%)	205 (95%)	10 (5%)	26	2
3	C	232/226 (103%)	229 (99%)	3 (1%)	69	35
3	P	232/226 (103%)	229 (99%)	3 (1%)	69	35
4	D	128/129 (99%)	128 (100%)	0	100	100
4	Q	122/129 (95%)	118 (97%)	4 (3%)	38	5
5	E	89/95 (94%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	R	89/95 (94%)	88 (99%)	1 (1%)	73	45
6	F	78/81 (96%)	77 (99%)	1 (1%)	69	35
6	S	78/81 (96%)	77 (99%)	1 (1%)	69	35
7	G	63/69 (91%)	58 (92%)	5 (8%)	12	0
7	T	63/69 (91%)	59 (94%)	4 (6%)	18	0
8	H	67/75 (89%)	65 (97%)	2 (3%)	41	7
8	U	67/75 (89%)	64 (96%)	3 (4%)	27	2
9	I	55/58 (95%)	54 (98%)	1 (2%)	59	24
9	V	55/58 (95%)	49 (89%)	6 (11%)	6	0
10	J	47/50 (94%)	46 (98%)	1 (2%)	53	16
10	W	47/50 (94%)	46 (98%)	1 (2%)	53	16
11	K	39/46 (85%)	37 (95%)	2 (5%)	24	2
11	X	39/46 (85%)	38 (97%)	1 (3%)	46	10
12	L	37/40 (92%)	37 (100%)	0	100	100
12	Y	37/40 (92%)	37 (100%)	0	100	100
13	M	34/38 (90%)	34 (100%)	0	100	100
13	Z	34/38 (90%)	34 (100%)	0	100	100
All	All	3042/3086 (99%)	2975 (98%)	67 (2%)	50	15

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	U	60	TYR
9	V	8	GLN
10	W	50	LEU
8	H	61	LYS
8	H	60	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
4	Q	109	HIS
8	U	31	GLN
6	S	54	ASN
8	U	37	HIS

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Mol	Chain	Res	Type
5	E	94	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	A	1	1	8,9,10	0.52	0	7,9,11	0.77	0
2	FME	O	1	2	8,9,10	0.85	0	7,9,11	0.92	0
2	FME	B	1	2	8,9,10	3.32	3 (37%)	7,9,11	3.89	2 (28%)
1	FME	N	1	1	8,9,10	0.63	0	7,9,11	0.86	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
1	FME	A	1	1	-	2/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
2	FME	B	1	2	-	2/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CA-N	8.61	1.58	1.46
2	B	1	FME	CG-SD	-2.53	1.68	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CB-CG	2.42	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-7.41	111.43	122.82
2	B	1	FME	C-CA-N	6.34	121.17	109.73

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
2	B	1	FME	CB-CA-N-CN
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 135 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 125 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
20	DMU	B	731	-	10,10,34	0.29	0	9,9,45	0.54	0
22	LFA	T	622	-	10,10,19	0.21	0	9,9,18	0.12	0
22	LFA	P	625	-	14,14,19	0.30	0	13,13,18	0.54	0
26	PEK	P	264	-	52,52,52	0.73	2 (3%)	55,57,57	1.03	4 (7%)
19	CHD	C	271	-	29,32,32	0.63	0	48,51,51	1.63	9 (18%)
20	DMU	N	745	-	34,34,34	1.43	4 (11%)	45,45,45	1.33	6 (13%)
20	DMU	P	733	-	34,34,34	0.81	2 (5%)	45,45,45	1.46	4 (8%)
23	EDO	N	829	-	3,3,3	0.16	0	2,2,2	0.18	0
23	EDO	T	821	-	3,3,3	0.44	0	2,2,2	0.24	0
23	EDO	A	803	-	3,3,3	0.09	0	2,2,2	0.12	0
20	DMU	G	711	-	22,22,34	0.74	1 (4%)	27,27,45	1.37	3 (11%)
20	DMU	T	712	-	10,10,34	0.45	0	9,9,45	0.58	0
22	LFA	C	615	-	10,10,19	0.16	0	9,9,18	0.15	0
20	DMU	N	743	-	6,6,34	0.34	0	5,5,45	0.35	0
20	DMU	C	715[A]	-	34,34,34	1.31	6 (17%)	45,45,45	1.36	3 (6%)
23	EDO	C	809	-	3,3,3	0.20	0	2,2,2	0.54	0
22	LFA	C	625	-	14,14,19	0.26	0	13,13,18	0.44	0
20	DMU	O	741	-	10,10,34	0.53	0	9,9,45	0.55	0
27	PGV	P	266	-	50,50,50	0.91	3 (6%)	53,56,56	1.20	2 (3%)
14	HEA	N	516	21,1	44,67,67	1.24	6 (13%)	37,103,103	2.39	7 (18%)
22	LFA	C	611	-	10,10,19	0.26	0	9,9,18	0.30	0
23	EDO	R	811	-	3,3,3	0.12	0	2,2,2	0.08	0
18	CDL	C	270	-	86,86,99	0.56	1 (1%)	92,98,111	1.07	9 (9%)
20	DMU	P	734	-	34,34,34	0.94	1 (2%)	45,45,45	1.19	2 (4%)
22	LFA	T	621	-	16,16,19	0.40	0	15,15,18	0.31	0
20	DMU	A	745	-	34,34,34	1.18	3 (8%)	45,45,45	1.03	2 (4%)
22	LFA	C	626	-	12,12,19	0.21	0	11,11,18	0.24	0
27	PGV	C	266	-	50,50,50	1.08	4 (8%)	53,56,56	1.08	3 (5%)
18	CDL	N	521	-	93,93,99	0.36	0	99,105,111	0.46	0
22	LFA	N	627	-	13,13,19	0.32	0	12,12,18	0.53	0
20	DMU	B	742	-	22,22,34	0.69	0	27,27,45	1.16	2 (7%)
20	DMU	P	715[A]	-	34,34,34	1.22	4 (11%)	45,45,45	1.25	3 (6%)
23	EDO	P	827	-	3,3,3	0.54	0	2,2,2	1.16	0
20	DMU	G	713	-	22,22,34	0.54	0	27,27,45	1.18	2 (7%)
23	EDO	C	827	-	3,3,3	0.49	0	2,2,2	0.75	0
20	DMU	J	732	-	10,10,34	0.15	0	9,9,45	0.64	0
20	DMU	O	742	-	22,22,34	1.00	2 (9%)	27,27,45	1.09	3 (11%)
23	EDO	S	819	-	3,3,3	0.33	0	2,2,2	0.24	0
20	DMU	P	272	-	10,10,34	0.25	0	9,9,45	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LFA	N	628	-	13,13,19	0.49	0	12,12,18	0.52	0
24	CUA	O	228	2	0,1,1	0.00	-	-		
22	LFA	P	611	-	10,10,19	0.25	0	9,9,18	0.19	0
23	EDO	A	823	-	3,3,3	0.53	0	2,2,2	0.57	0
14	HEA	N	515[A]	-	44,67,67	1.27	6 (13%)	37,103,103	1.98	9 (24%)
21	PER	N	520	15,14	0,1,1	0.00	-	-		
22	LFA	A	628	-	13,13,19	0.45	0	12,12,18	0.69	0
22	LFA	P	624	-	10,10,19	0.19	0	9,9,18	0.14	0
20	DMU	C	272	-	10,10,34	0.33	0	9,9,45	0.59	0
19	CHD	A	525	-	29,32,32	0.72	0	48,51,51	1.15	6 (12%)
23	EDO	E	813	-	3,3,3	0.36	0	2,2,2	0.20	0
23	EDO	F	817	-	3,3,3	0.64	0	2,2,2	0.34	0
22	LFA	C	612	-	5,5,19	0.20	0	4,4,18	0.16	0
20	DMU	P	722	-	22,22,34	0.46	0	27,27,45	1.06	2 (7%)
23	EDO	G	821	-	3,3,3	0.22	0	2,2,2	0.27	0
23	EDO	N	803	-	3,3,3	0.20	0	2,2,2	0.41	0
22	LFA	G	621	-	16,16,19	0.30	0	15,15,18	0.60	0
20	DMU	T	711	-	22,22,34	0.79	0	27,27,45	1.45	4 (14%)
20	DMU	A	743	-	6,6,34	0.30	0	5,5,45	0.38	0
22	LFA	P	716[B]	-	17,17,19	0.13	0	16,16,18	0.12	0
24	CUA	B	228	2	0,1,1	0.00	-	-		
14	HEA	A	515[A]	-	44,67,67	1.38	6 (13%)	37,103,103	2.37	11 (29%)
23	EDO	B	805	-	3,3,3	1.04	0	2,2,2	0.97	0
20	DMU	P	721	-	6,6,34	0.18	0	5,5,45	0.62	0
20	DMU	C	721	-	6,6,34	0.21	0	5,5,45	0.58	0
20	DMU	C	733	-	34,34,34	1.17	5 (14%)	45,45,45	1.20	5 (11%)
19	CHD	T	86	-	29,32,32	0.74	0	48,51,51	1.10	2 (4%)
20	DMU	Y	747	-	22,22,34	0.56	0	27,27,45	1.18	2 (7%)
20	DMU	Z	746	-	7,7,34	0.16	0	6,6,45	0.48	0
21	PER	A	520	15,14	0,1,1	0.00	-	-		
23	EDO	P	807	-	3,3,3	0.07	0	2,2,2	0.13	0
23	EDO	O	805	-	3,3,3	0.55	0	2,2,2	0.13	0
20	DMU	N	526	-	34,34,34	0.96	2 (5%)	45,45,45	1.14	2 (4%)
20	DMU	B	741	-	10,10,34	0.34	0	9,9,45	0.56	0
23	EDO	E	811	-	3,3,3	0.19	0	2,2,2	0.44	0
22	LFA	C	716[B]	-	17,17,19	0.17	0	16,16,18	0.16	0
22	LFA	A	627	-	13,13,19	0.72	0	12,12,18	0.30	0
22	LFA	P	615	-	10,10,19	0.19	0	9,9,18	0.17	0
27	PGV	P	267	-	50,50,50	0.75	1 (2%)	53,56,56	0.92	1 (1%)
19	CHD	G	86	-	29,32,32	0.73	0	48,51,51	1.08	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PGV	C	267	-	50,50,50	0.87	3 (6%)	53,56,56	1.09	3 (5%)
20	DMU	L	747	-	22,22,34	0.72	0	27,27,45	1.27	3 (11%)
23	EDO	P	809	-	3,3,3	0.40	0	2,2,2	0.38	0
23	EDO	F	819	-	3,3,3	0.44	0	2,2,2	0.39	0
22	LFA	G	622	-	10,10,19	0.18	0	9,9,18	0.16	0
20	DMU	W	732	-	10,10,34	0.16	0	9,9,45	0.57	0
23	EDO	N	801	-	3,3,3	0.53	0	2,2,2	0.12	0
23	EDO	N	825	-	3,3,3	0.51	0	2,2,2	0.23	0
20	DMU	C	734	-	34,34,34	0.99	1 (2%)	45,45,45	1.06	3 (6%)
20	DMU	P	714	-	34,34,34	0.73	0	45,45,45	1.06	3 (6%)
22	LFA	P	623	-	13,13,19	0.25	0	12,12,18	0.26	0
19	CHD	P	271	-	29,32,32	0.51	0	48,51,51	1.60	7 (14%)
18	CDL	P	270	-	86,86,99	0.47	0	92,98,111	0.95	6 (6%)
14	HEA	A	516	21,1	44,67,67	1.46	8 (18%)	37,103,103	2.63	6 (16%)
22	LFA	P	626	-	12,12,19	0.31	0	11,11,18	0.30	0
20	DMU	C	714	-	34,34,34	0.85	1 (2%)	45,45,45	1.25	6 (13%)
14	HEA	A	515[B]	-	44,67,67	1.35	6 (13%)	37,103,103	2.33	11 (29%)
23	EDO	E	815	-	3,3,3	0.40	0	2,2,2	0.60	0
23	EDO	N	823	-	3,3,3	0.61	0	2,2,2	0.41	0
20	DMU	G	712	-	10,10,34	0.23	0	9,9,45	0.59	0
23	EDO	A	825	-	3,3,3	0.41	0	2,2,2	0.51	0
19	CHD	N	525	-	29,32,32	0.82	0	48,51,51	0.91	2 (4%)
23	EDO	R	815	-	3,3,3	0.15	0	2,2,2	0.04	0
20	DMU	T	713	-	22,22,34	0.68	1 (4%)	27,27,45	1.39	5 (18%)
20	DMU	N	744	-	34,34,34	1.42	7 (20%)	45,45,45	1.54	5 (11%)
26	PEK	C	264	-	52,52,52	0.59	2 (3%)	55,57,57	0.81	2 (3%)
23	EDO	R	813	-	3,3,3	0.18	0	2,2,2	0.03	0
23	EDO	S	817	-	3,3,3	0.93	0	2,2,2	0.06	0
22	LFA	C	623	-	13,13,19	0.28	0	12,12,18	0.18	0
20	DMU	J	61	-	34,34,34	0.84	1 (2%)	45,45,45	1.05	2 (4%)
18	CDL	A	521	-	93,93,99	0.46	0	99,105,111	0.60	2 (2%)
22	LFA	C	624	-	10,10,19	0.28	0	9,9,18	0.20	0
18	CDL	A	522	-	63,63,99	0.53	0	69,75,111	1.18	6 (8%)
14	HEA	N	515[B]	-	44,67,67	1.30	6 (13%)	37,103,103	1.84	10 (27%)
20	DMU	M	746	-	7,7,34	0.19	0	6,6,45	0.79	0
20	DMU	C	722	-	22,22,34	0.52	0	27,27,45	0.94	2 (7%)
22	LFA	P	612	-	5,5,19	0.09	0	4,4,18	0.20	0
20	DMU	W	61	-	34,34,34	0.72	0	45,45,45	1.49	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LFA	P	614	-	14,14,19	0.17	0	13,13,18	0.16	0
20	DMU	A	526	-	34,34,34	1.05	2 (5%)	45,45,45	1.12	2 (4%)
20	DMU	A	744	-	34,34,34	1.47	6 (17%)	45,45,45	1.19	3 (6%)
20	DMU	O	731	-	10,10,34	0.21	0	9,9,45	0.46	0
22	LFA	C	614	-	14,14,19	0.21	0	13,13,18	0.21	0
18	CDL	N	522	-	63,63,99	0.50	1 (1%)	69,75,111	1.04	5 (7%)
23	EDO	C	807	-	3,3,3	0.17	0	2,2,2	0.20	0
23	EDO	A	801	-	3,3,3	0.66	0	2,2,2	0.87	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
20	DMU	B	731	-	-	6/8/8/59	-
22	LFA	T	622	-	-	4/8/8/17	-
22	LFA	P	625	-	-	4/12/12/17	-
26	PEK	P	264	-	-	18/56/56/56	-
19	CHD	C	271	-	-	6/7/74/74	0/4/4/4
20	DMU	N	745	-	-	7/19/59/59	0/2/2/2
20	DMU	P	733	-	-	6/19/59/59	0/2/2/2
23	EDO	N	829	-	-	0/1/1/1	-
23	EDO	T	821	-	-	0/1/1/1	-
23	EDO	A	803	-	-	0/1/1/1	-
20	DMU	G	711	-	-	3/13/33/59	0/1/1/2
20	DMU	T	712	-	-	4/8/8/59	-
22	LFA	C	615	-	-	2/8/8/17	-
20	DMU	N	743	-	-	3/4/4/59	-
20	DMU	C	715[A]	-	-	3/19/59/59	0/2/2/2
23	EDO	C	809	-	-	0/1/1/1	-
22	LFA	C	625	-	-	3/12/12/17	-
20	DMU	O	741	-	-	4/8/8/59	-
27	PGV	P	266	-	-	8/55/55/55	-
14	HEA	N	516	21,1	3/3/7/16	0/24/76/76	-
22	LFA	C	611	-	-	5/8/8/17	-
23	EDO	R	811	-	-	1/1/1/1	-
18	CDL	C	270	-	-	49/97/97/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	P	734	-	-	10/19/59/59	0/2/2/2
22	LFA	T	621	-	-	9/14/14/17	-
20	DMU	A	745	-	-	5/19/59/59	0/2/2/2
22	LFA	C	626	-	-	4/10/10/17	-
27	PGV	C	266	-	-	7/55/55/55	-
18	CDL	N	521	-	-	53/104/104/110	-
22	LFA	N	627	-	-	5/11/11/17	-
20	DMU	B	742	-	-	8/13/33/59	0/1/1/2
20	DMU	P	715[A]	-	-	6/19/59/59	0/2/2/2
23	EDO	P	827	-	-	0/1/1/1	-
20	DMU	G	713	-	-	8/13/33/59	0/1/1/2
23	EDO	C	827	-	-	1/1/1/1	-
20	DMU	J	732	-	-	5/8/8/59	-
20	DMU	O	742	-	-	7/13/33/59	0/1/1/2
23	EDO	S	819	-	-	0/1/1/1	-
20	DMU	P	272	-	-	0/8/8/59	-
22	LFA	N	628	-	-	6/11/11/17	-
22	LFA	P	611	-	-	5/8/8/17	-
23	EDO	A	823	-	-	0/1/1/1	-
14	HEA	N	515[A]	-	-	4/24/76/76	-
22	LFA	A	628	-	-	5/11/11/17	-
22	LFA	P	624	-	-	6/8/8/17	-
20	DMU	C	272	-	-	4/8/8/59	-
19	CHD	A	525	-	-	0/7/74/74	0/4/4/4
23	EDO	E	813	-	-	0/1/1/1	-
23	EDO	F	817	-	-	0/1/1/1	-
22	LFA	C	612	-	-	1/3/3/17	-
20	DMU	P	722	-	-	8/13/33/59	0/1/1/2
23	EDO	G	821	-	-	0/1/1/1	-
23	EDO	N	803	-	-	1/1/1/1	-
22	LFA	G	621	-	-	9/14/14/17	-
20	DMU	T	711	-	-	7/13/33/59	0/1/1/2
20	DMU	A	743	-	-	2/4/4/59	-
22	LFA	P	716[B]	-	-	6/15/15/17	-
14	HEA	A	515[A]	-	-	3/24/76/76	-
23	EDO	B	805	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	P	721	-	-	3/4/4/59	-
20	DMU	C	721	-	-	2/4/4/59	-
20	DMU	C	733	-	-	9/19/59/59	0/2/2/2
19	CHD	T	86	-	-	0/7/74/74	0/4/4/4
20	DMU	Y	747	-	-	9/13/33/59	0/1/1/2
20	DMU	Z	746	-	-	2/5/5/59	-
23	EDO	P	807	-	-	1/1/1/1	-
23	EDO	O	805	-	-	0/1/1/1	-
20	DMU	N	526	-	-	6/19/59/59	0/2/2/2
20	DMU	B	741	-	-	4/8/8/59	-
23	EDO	E	811	-	-	0/1/1/1	-
22	LFA	C	716[B]	-	-	5/15/15/17	-
22	LFA	A	627	-	-	5/11/11/17	-
22	LFA	P	615	-	-	5/8/8/17	-
27	PGV	P	267	-	-	12/55/55/55	-
19	CHD	G	86	-	-	0/7/74/74	0/4/4/4
27	PGV	C	267	-	-	13/55/55/55	-
23	EDO	P	809	-	-	0/1/1/1	-
23	EDO	F	819	-	-	0/1/1/1	-
22	LFA	G	622	-	-	3/8/8/17	-
20	DMU	W	732	-	-	7/8/8/59	-
23	EDO	N	801	-	-	0/1/1/1	-
23	EDO	N	825	-	-	0/1/1/1	-
20	DMU	C	734	-	-	8/19/59/59	0/2/2/2
20	DMU	P	714	-	-	5/19/59/59	0/2/2/2
22	LFA	P	623	-	-	5/11/11/17	-
19	CHD	P	271	-	-	6/7/74/74	0/4/4/4
18	CDL	P	270	-	-	49/97/97/110	-
14	HEA	A	516	21,1	3/3/7/16	0/24/76/76	-
22	LFA	P	626	-	-	5/10/10/17	-
20	DMU	C	714	-	-	8/19/59/59	0/2/2/2
14	HEA	A	515[B]	-	-	0/24/76/76	-
23	EDO	E	815	-	-	1/1/1/1	-
23	EDO	N	823	-	-	0/1/1/1	-
20	DMU	G	712	-	-	4/8/8/59	-
23	EDO	A	825	-	-	1/1/1/1	-
19	CHD	N	525	-	-	0/7/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	EDO	R	815	-	-	1/1/1/1	-
20	DMU	T	713	-	-	5/13/33/59	0/1/1/2
20	DMU	N	744	-	-	5/19/59/59	0/2/2/2
26	PEK	C	264	-	-	15/56/56/56	-
23	EDO	R	813	-	-	0/1/1/1	-
23	EDO	S	817	-	-	0/1/1/1	-
22	LFA	C	623	-	-	5/11/11/17	-
20	DMU	J	61	-	-	5/19/59/59	0/2/2/2
18	CDL	A	521	-	-	51/104/104/110	-
22	LFA	C	624	-	-	4/8/8/17	-
18	CDL	A	522	-	-	31/74/74/110	-
14	HEA	N	515[B]	-	-	0/24/76/76	-
20	DMU	M	746	-	-	5/5/5/59	-
20	DMU	C	722	-	-	10/13/33/59	0/1/1/2
22	LFA	P	612	-	-	1/3/3/17	-
20	DMU	W	61	-	-	3/19/59/59	0/2/2/2
22	LFA	P	614	-	-	6/12/12/17	-
20	DMU	A	526	-	-	4/19/59/59	0/2/2/2
20	DMU	A	744	-	-	7/19/59/59	0/2/2/2
20	DMU	O	731	-	-	4/8/8/59	-
22	LFA	C	614	-	-	7/12/12/17	-
18	CDL	N	522	-	-	34/74/74/110	-
23	EDO	C	807	-	-	0/1/1/1	-
23	EDO	A	801	-	-	0/1/1/1	-

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	745	DMU	O16-C6	-4.51	1.32	1.40
14	A	516	HEA	CMB-C2B	-4.43	1.42	1.51
20	A	744	DMU	O49-C1	-4.38	1.32	1.43
20	P	715[A]	DMU	O3-C5	-4.35	1.32	1.43
14	A	515[A]	HEA	C16-C17	-4.29	1.39	1.53

The worst 5 of 208 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	516	HEA	C1B-C2B-C3B	-12.95	97.99	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	516	HEA	C1B-C2B-C3B	-10.94	99.39	107.00
14	A	515[A]	HEA	C1B-C2B-C3B	-7.14	102.03	107.00
14	A	515[B]	HEA	C1B-C2B-C3B	-7.14	102.03	107.00
20	N	744	DMU	O16-C6-C1	6.36	118.23	108.30

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	516	HEA	NB
14	A	516	HEA	ND
14	A	516	HEA	NA
14	N	516	HEA	NB
14	N	516	HEA	ND

5 of 712 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	515[A]	HEA	C18-C19-C20-C21
14	A	515[A]	HEA	C27-C19-C20-C21
18	A	521	CDL	CA2-OA2-PA1-OA3
18	A	521	CDL	C11-CA5-OA6-CA4
18	A	521	CDL	CB2-OB2-PB2-OB3

There are no ring outliers.

64 monomers are involved in 188 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	T	622	LFA	1	0
26	P	264	PEK	3	0
20	N	745	DMU	2	0
20	P	733	DMU	4	0
23	N	829	EDO	1	0
20	G	711	DMU	3	0
20	T	712	DMU	8	0
23	C	809	EDO	2	0
22	C	625	LFA	1	0
27	P	266	PGV	1	0
14	N	516	HEA	1	0
18	C	270	CDL	14	0
20	P	734	DMU	3	0
22	T	621	LFA	3	0
22	C	626	LFA	4	0

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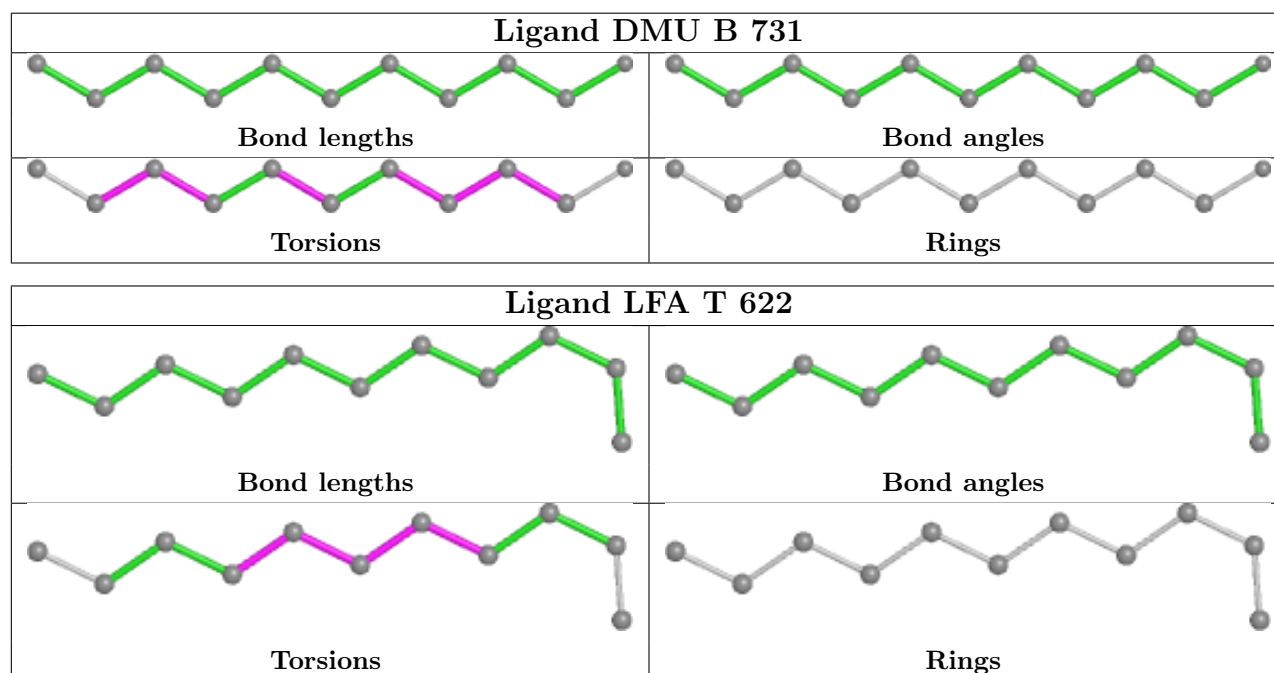
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	C	266	PGV	2	0
18	N	521	CDL	7	0
22	N	627	LFA	1	0
20	P	715[A]	DMU	1	0
20	G	713	DMU	4	0
20	O	742	DMU	1	0
22	N	628	LFA	6	0
22	P	611	LFA	1	0
14	N	515[A]	HEA	6	0
21	N	520	PER	1	0
22	A	628	LFA	11	0
22	P	624	LFA	2	0
20	T	711	DMU	12	0
20	A	743	DMU	1	0
22	P	716[B]	LFA	1	0
14	A	515[A]	HEA	6	0
20	C	721	DMU	2	0
20	C	733	DMU	2	0
19	T	86	CHD	1	0
20	Y	747	DMU	1	0
21	A	520	PER	1	0
22	C	716[B]	LFA	3	0
22	A	627	LFA	6	0
22	P	615	LFA	2	0
19	G	86	CHD	1	0
22	G	622	LFA	1	0
20	P	714	DMU	2	0
22	P	623	LFA	1	0
19	P	271	CHD	1	0
18	P	270	CDL	12	0
14	A	516	HEA	1	0
22	P	626	LFA	1	0
20	C	714	DMU	3	0
20	G	712	DMU	8	0
20	T	713	DMU	13	0
20	N	744	DMU	2	0
26	C	264	PEK	5	0
20	J	61	DMU	6	0
18	A	521	CDL	9	0
22	C	624	LFA	4	0
18	A	522	CDL	1	0
14	N	515[B]	HEA	1	0

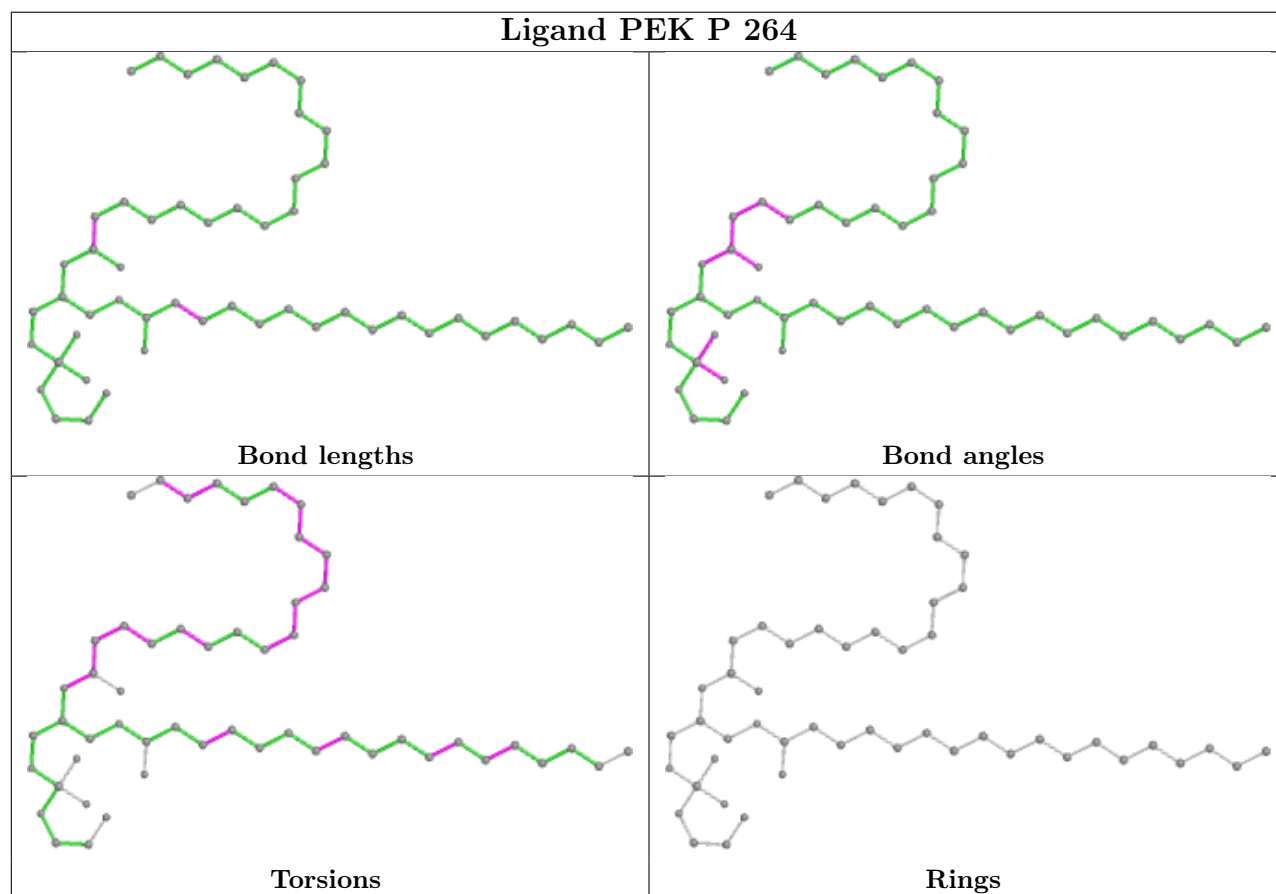
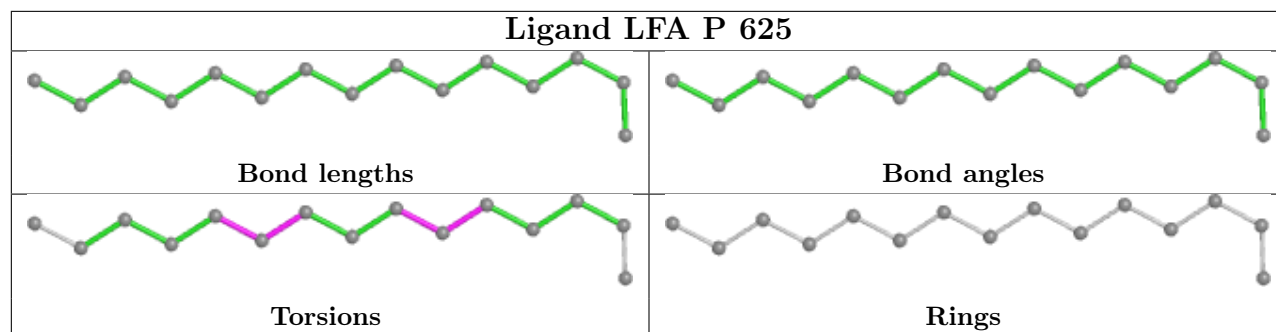
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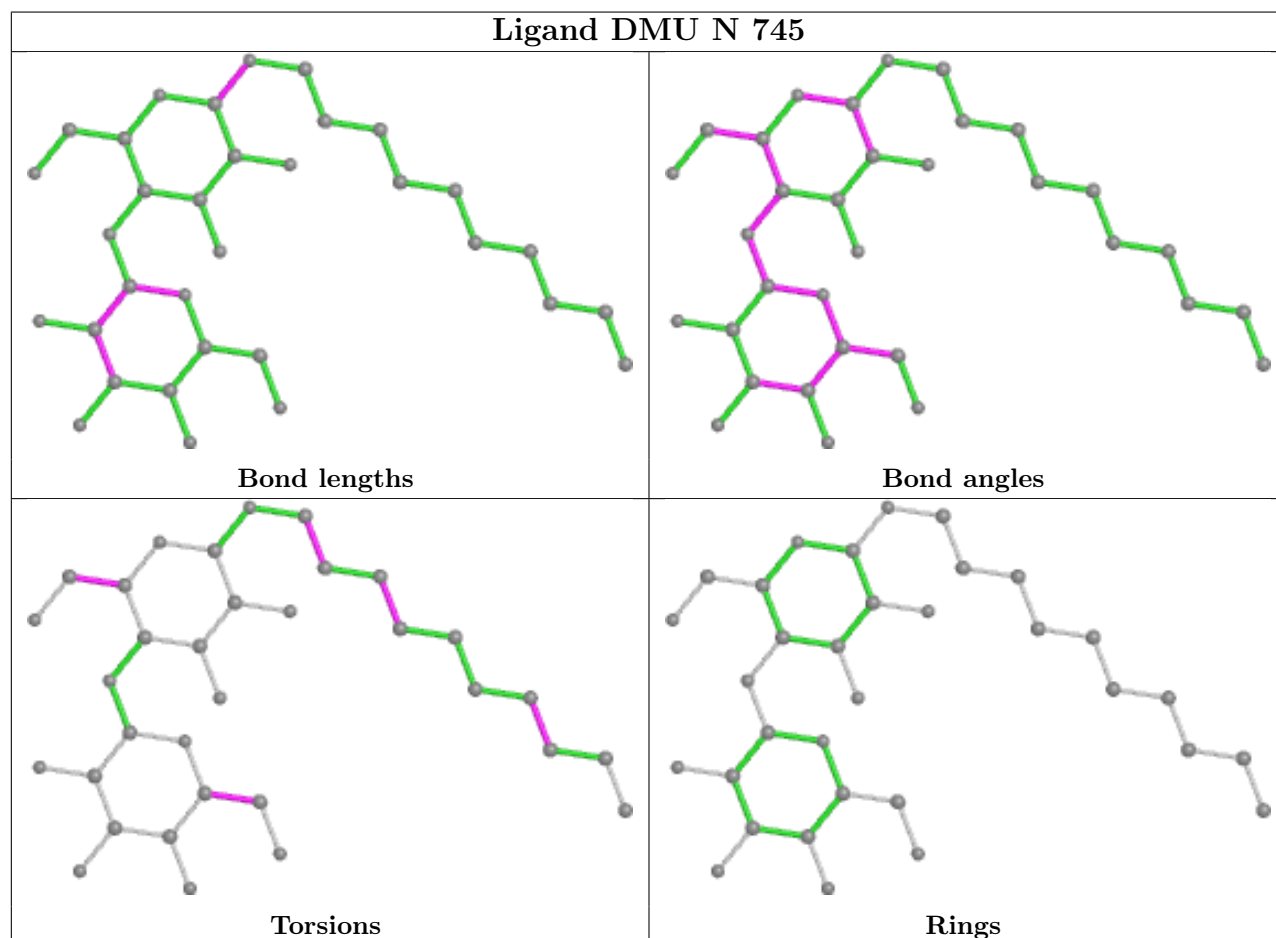
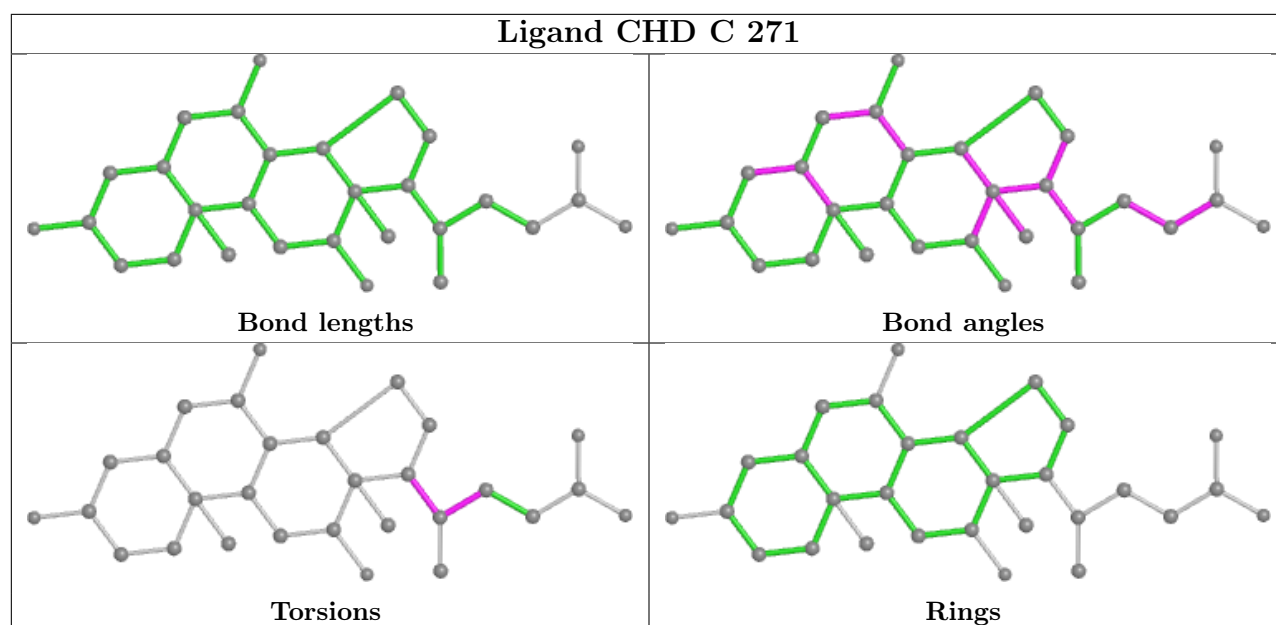
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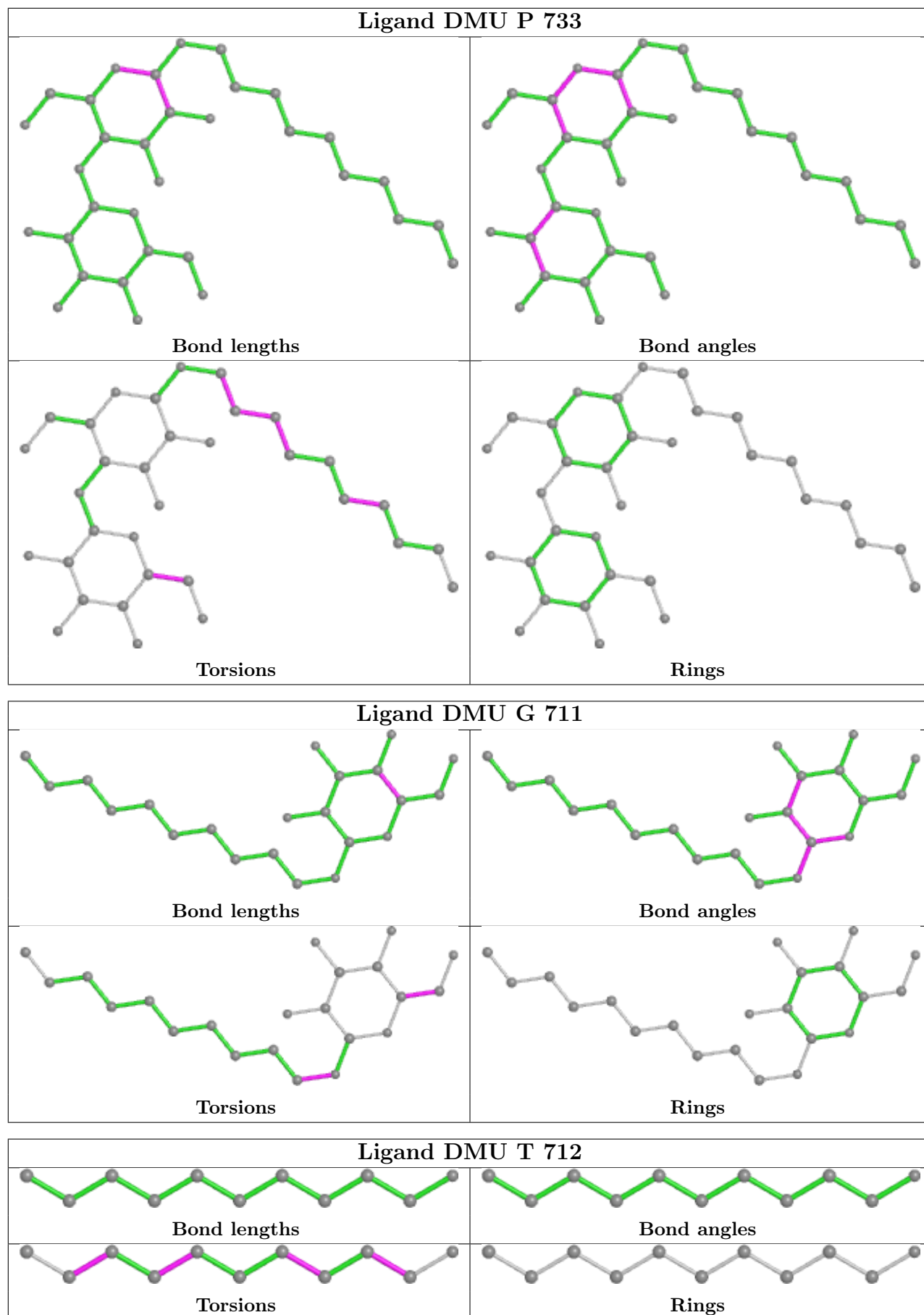
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	W	61	DMU	7	0
20	A	526	DMU	1	0
20	A	744	DMU	4	0
20	O	731	DMU	1	0
22	C	614	LFA	1	0
18	N	522	CDL	1	0
23	A	801	EDO	1	0

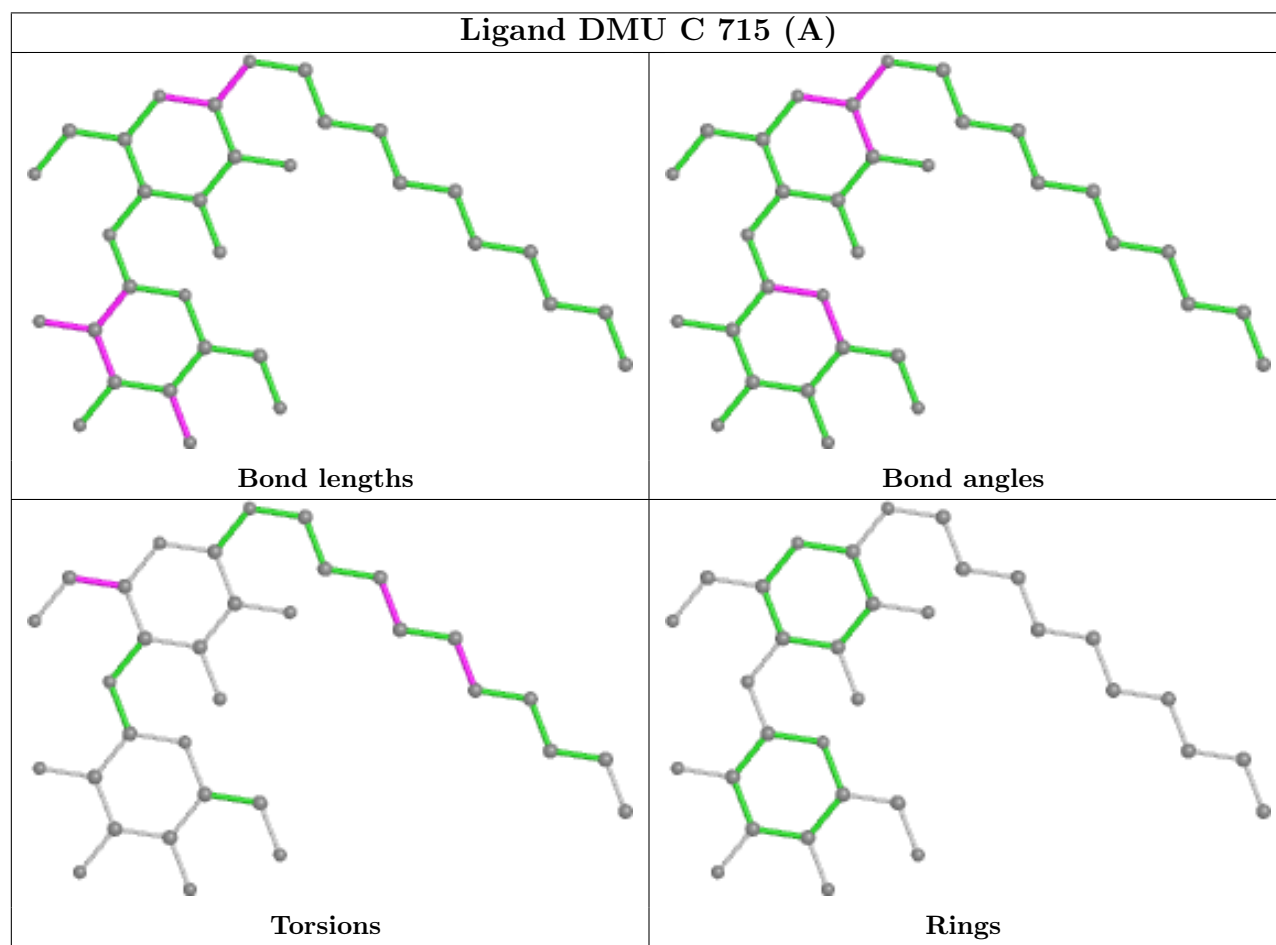
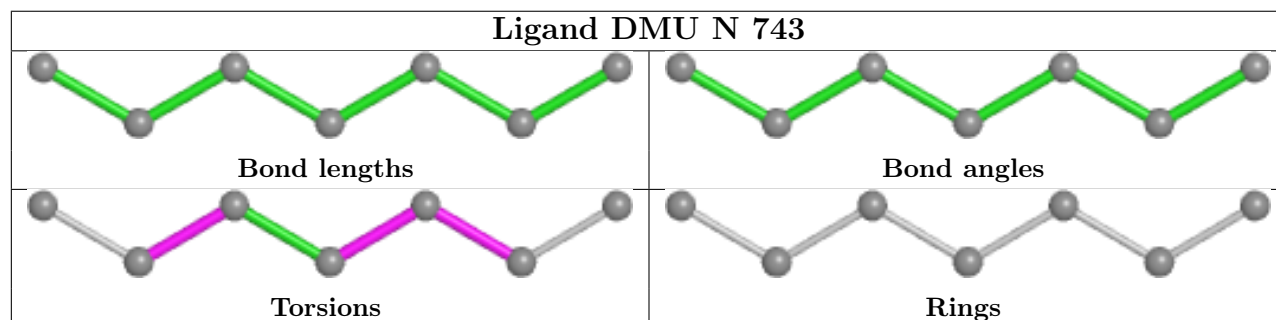
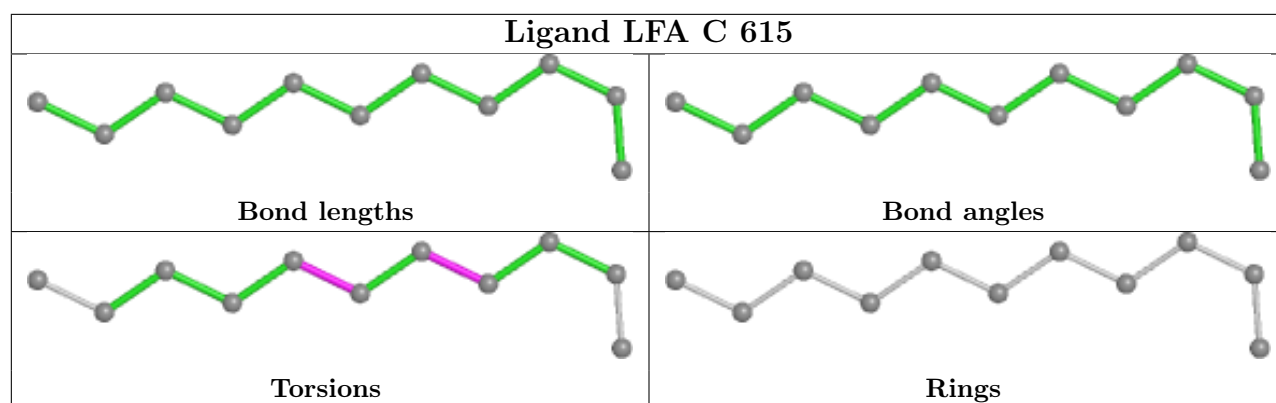
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

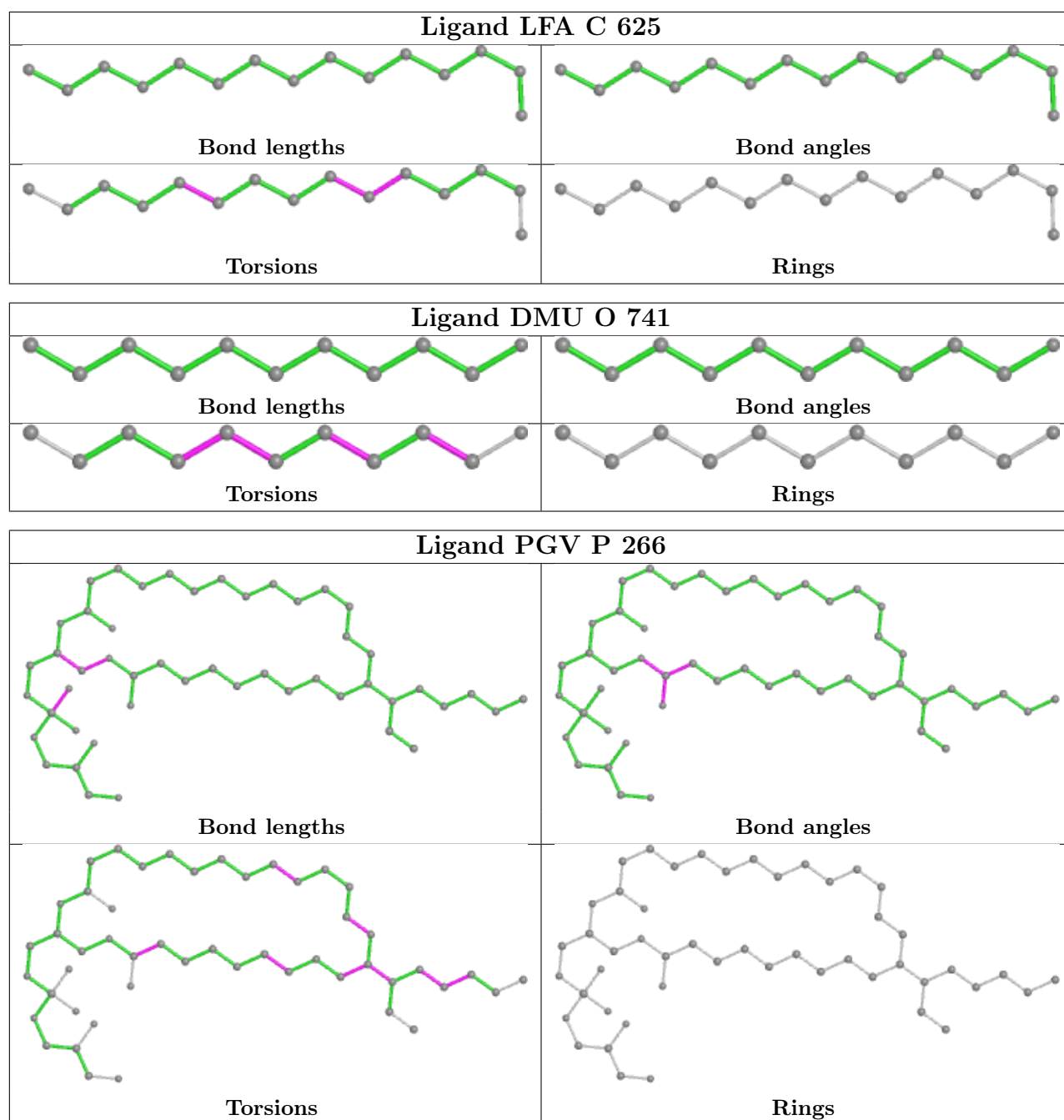


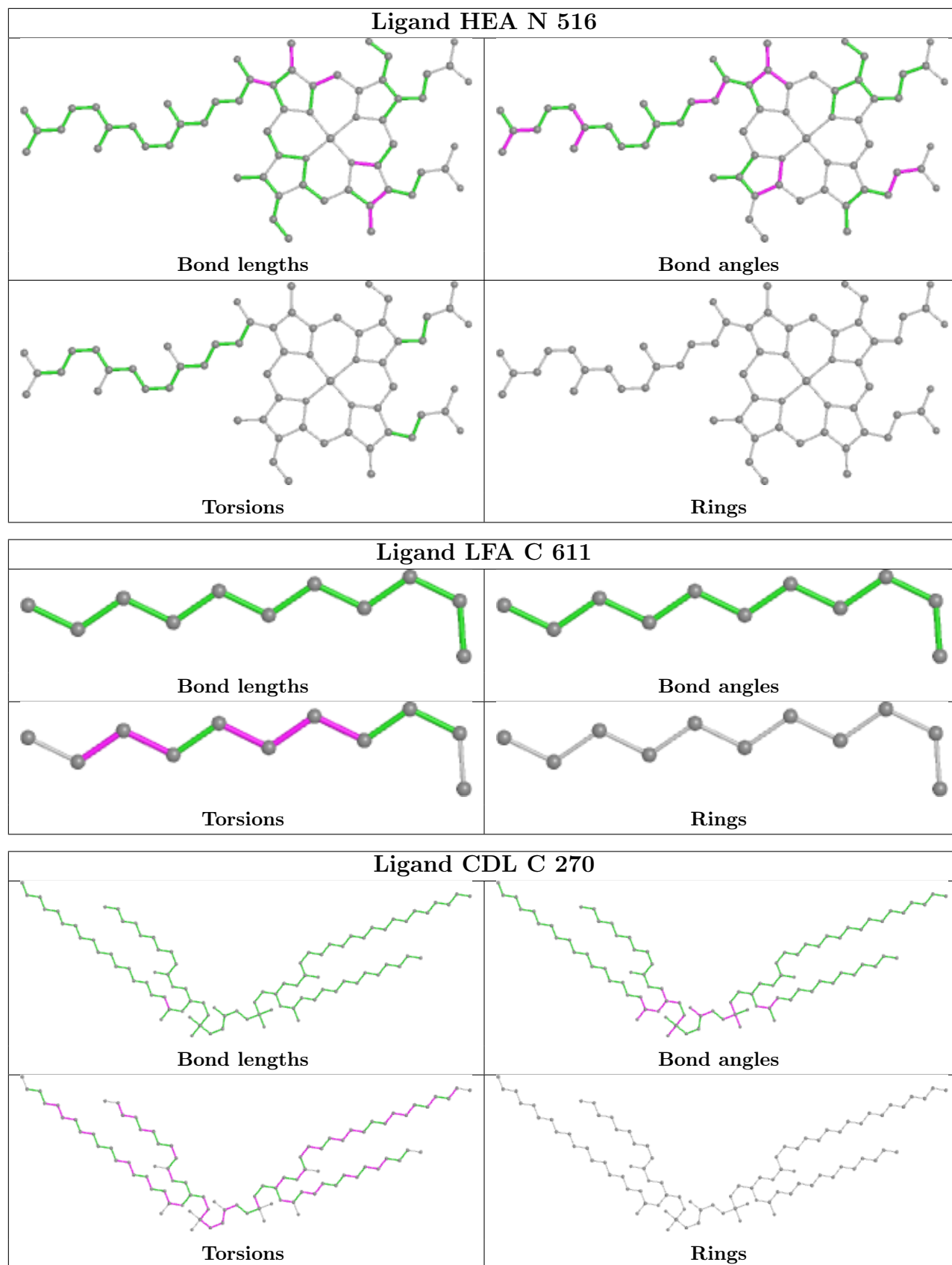


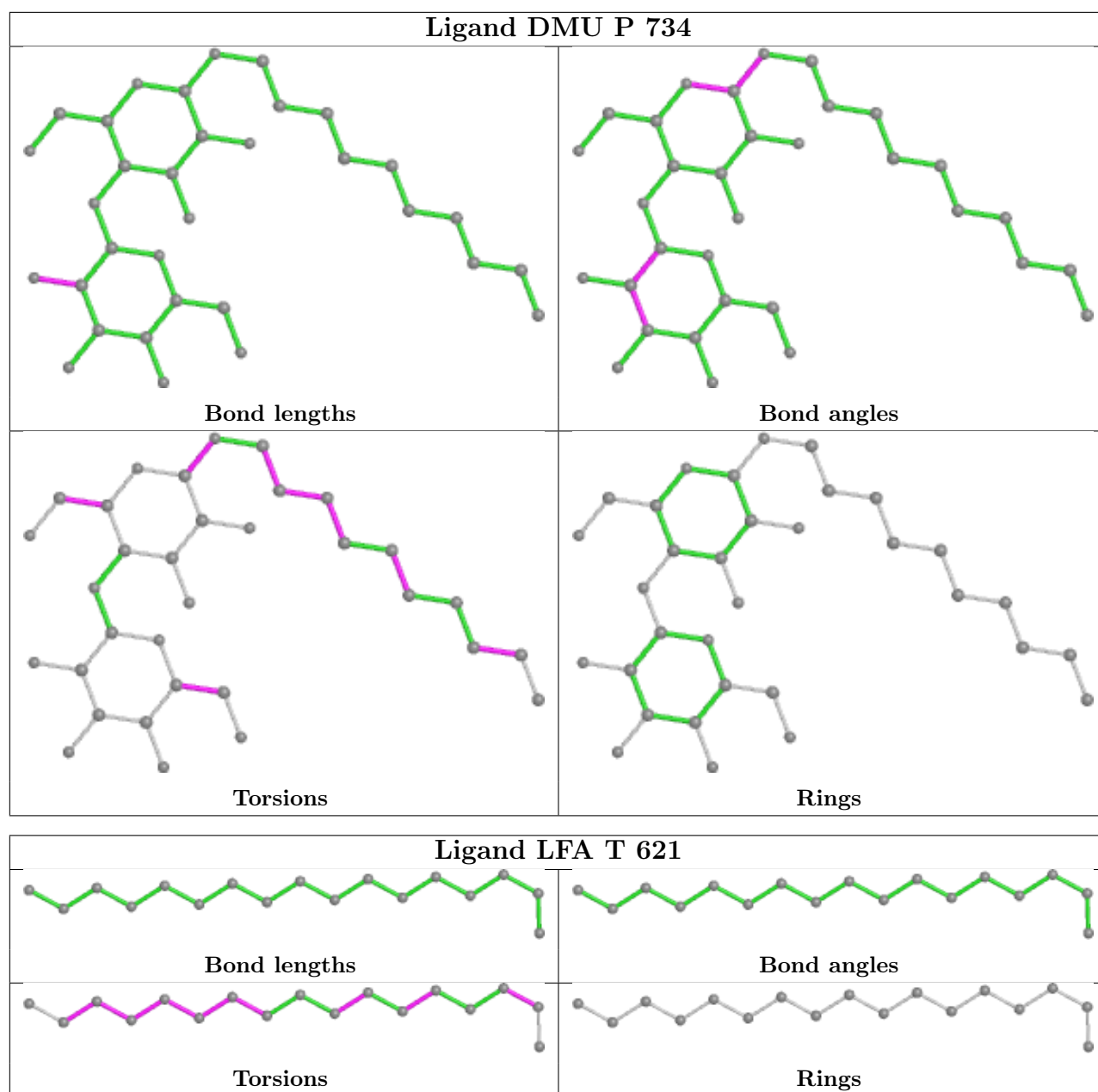


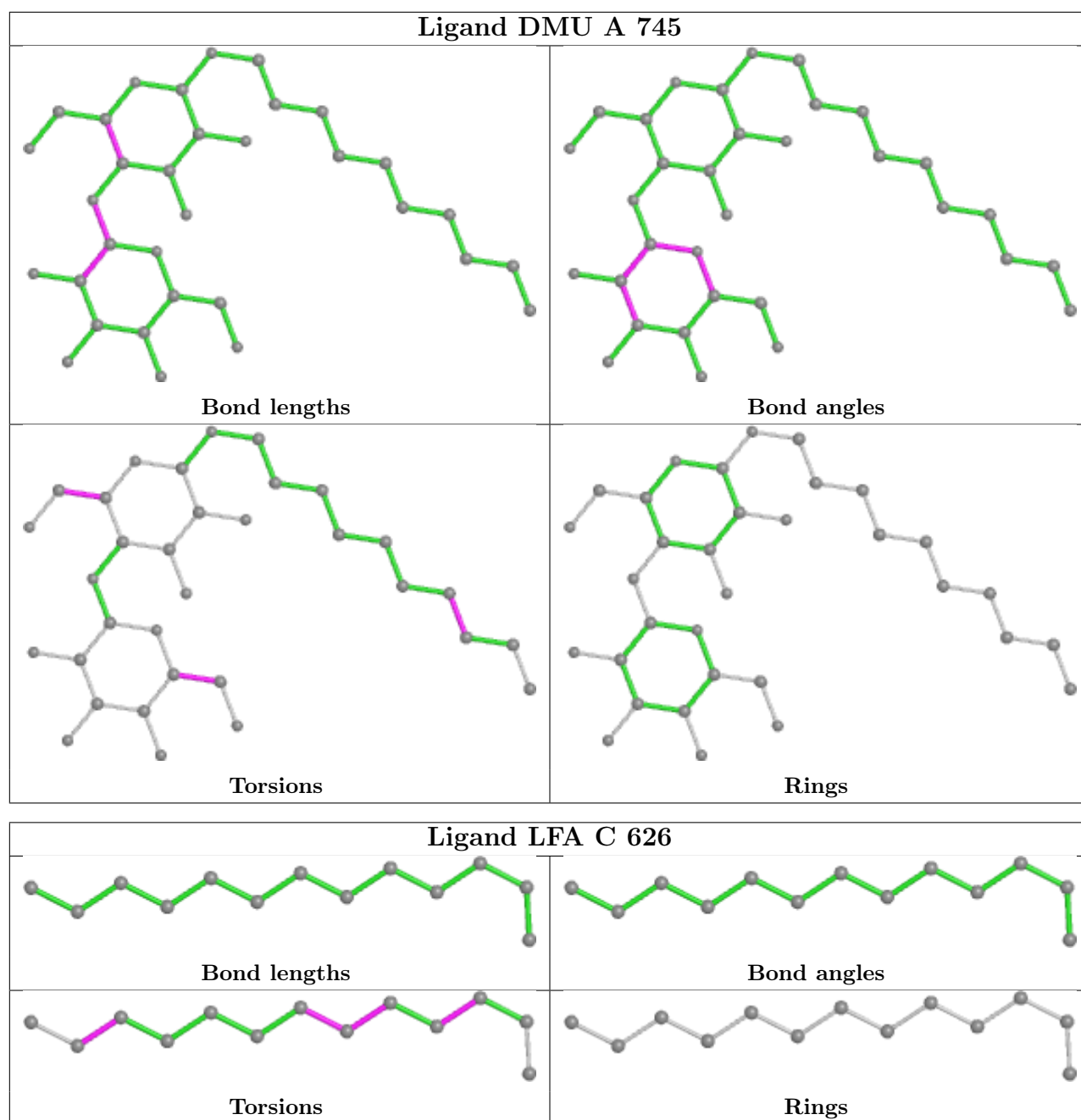


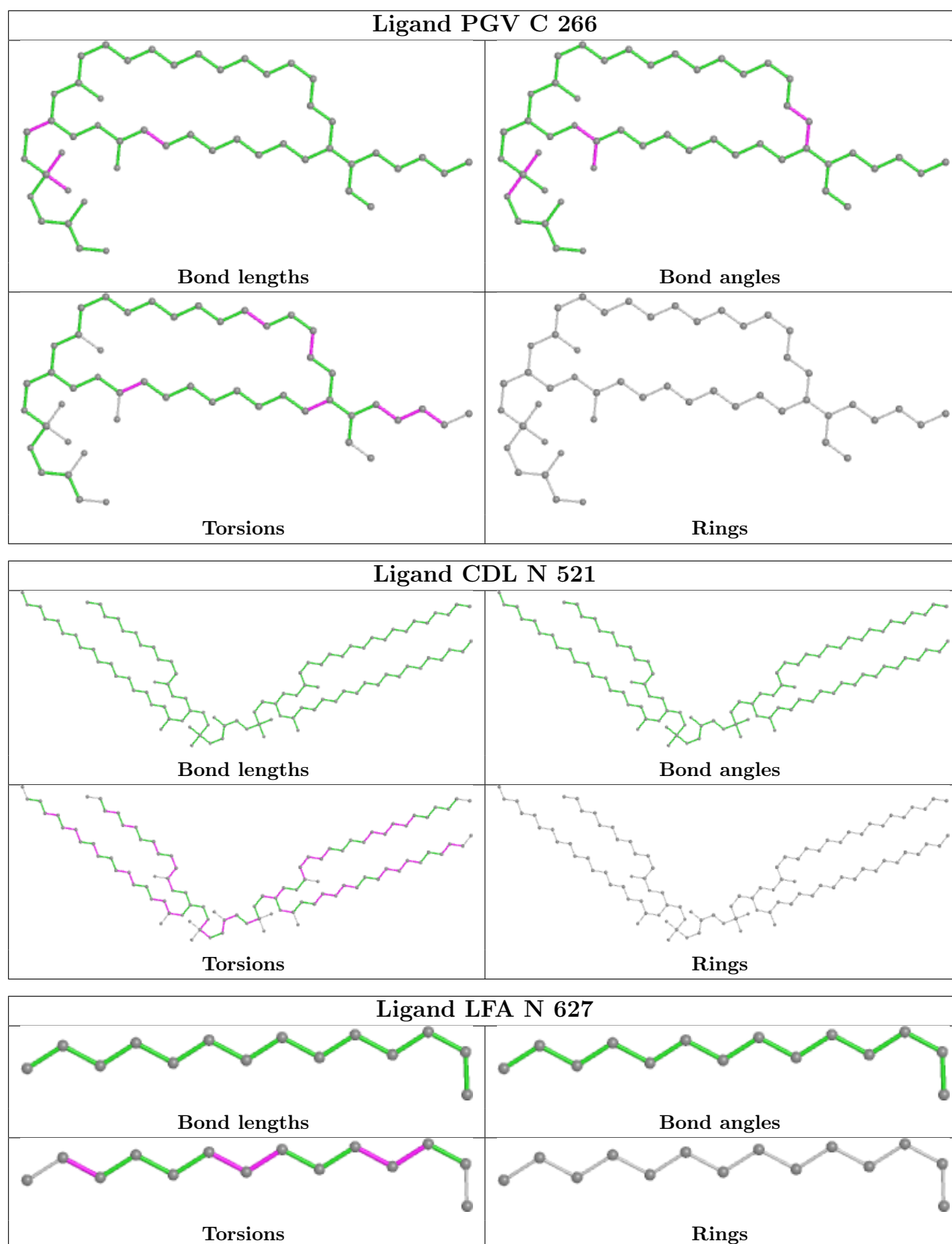


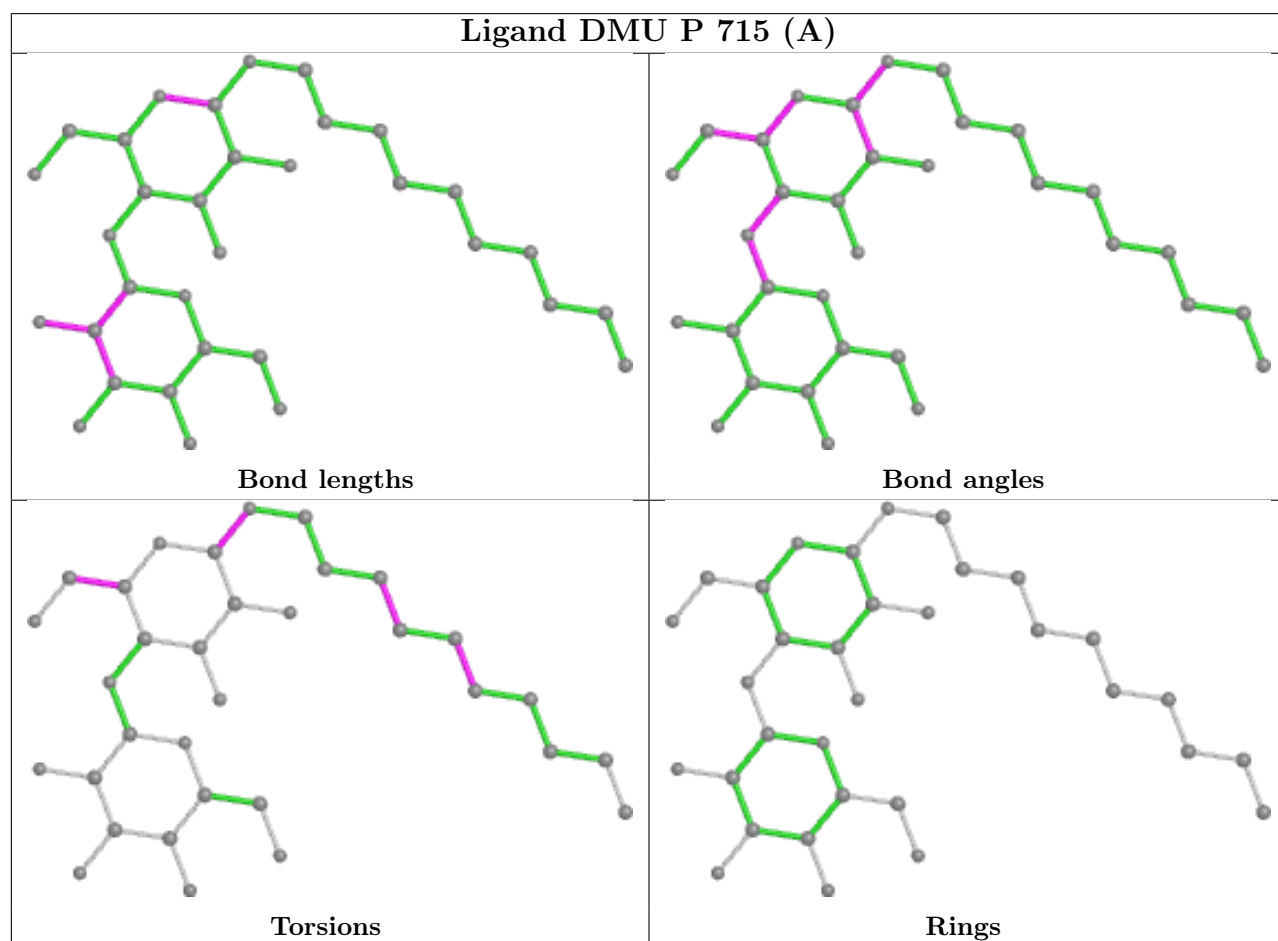
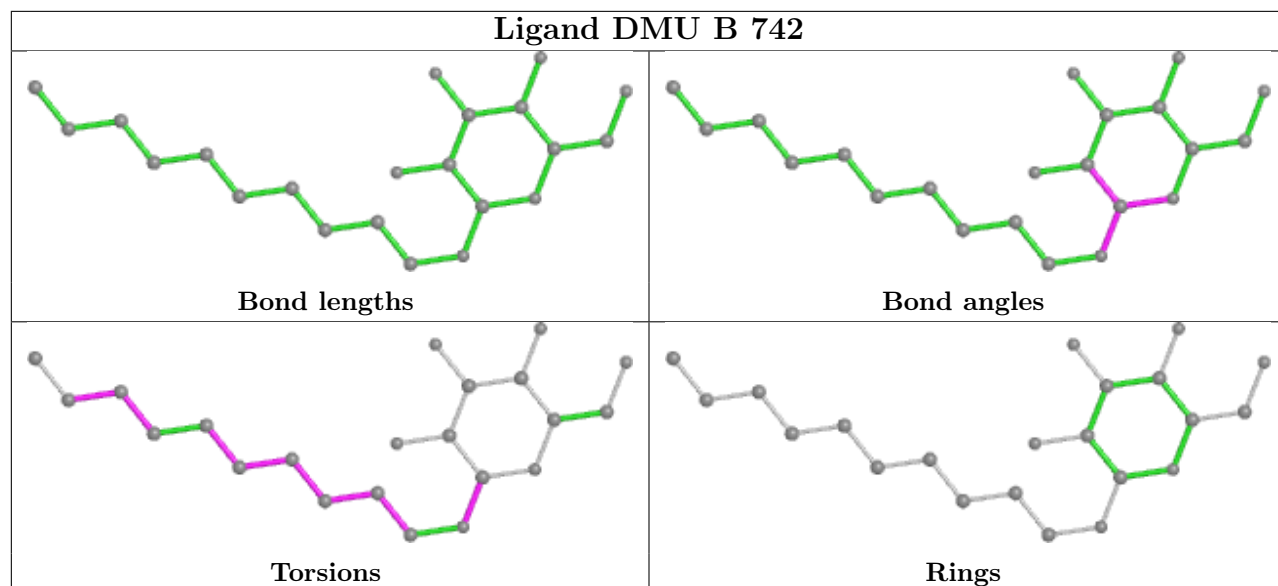


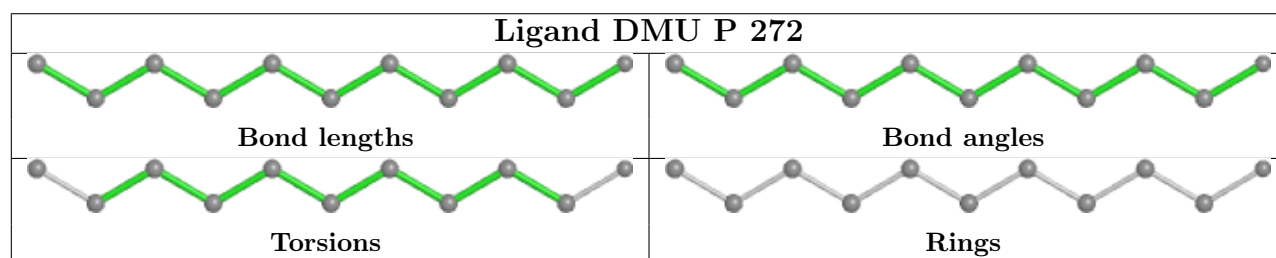
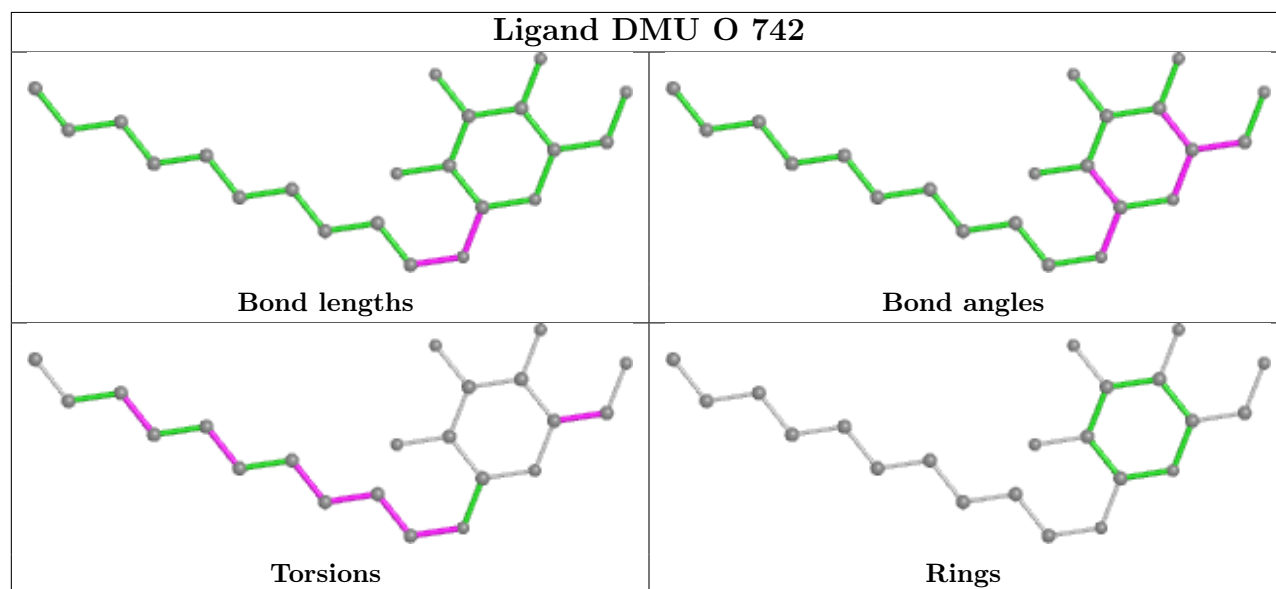
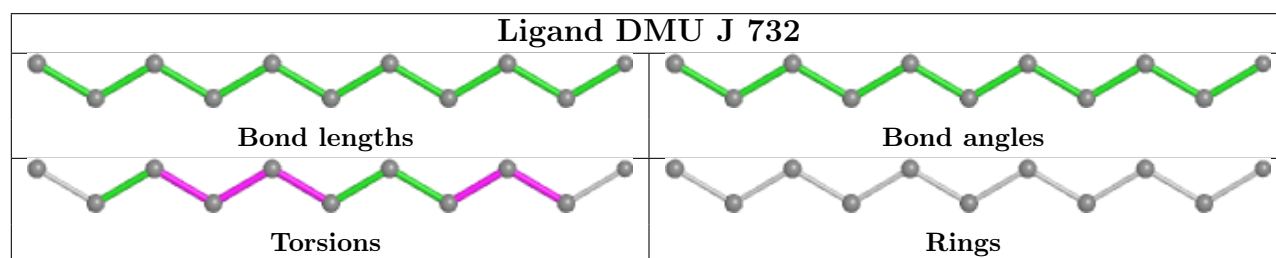
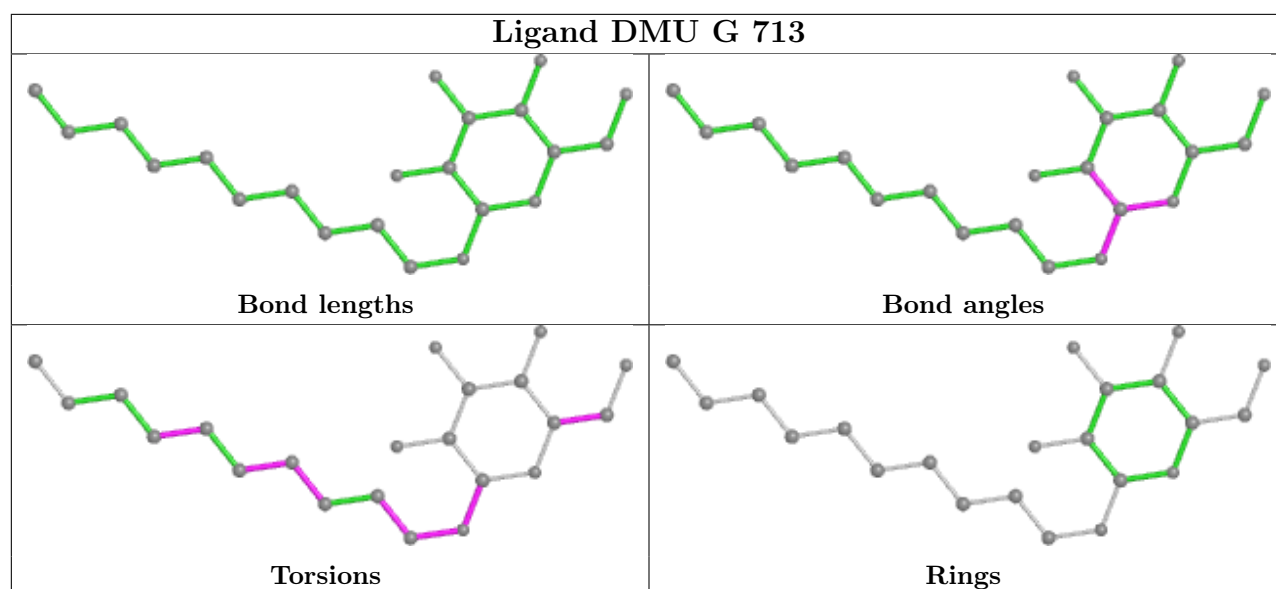


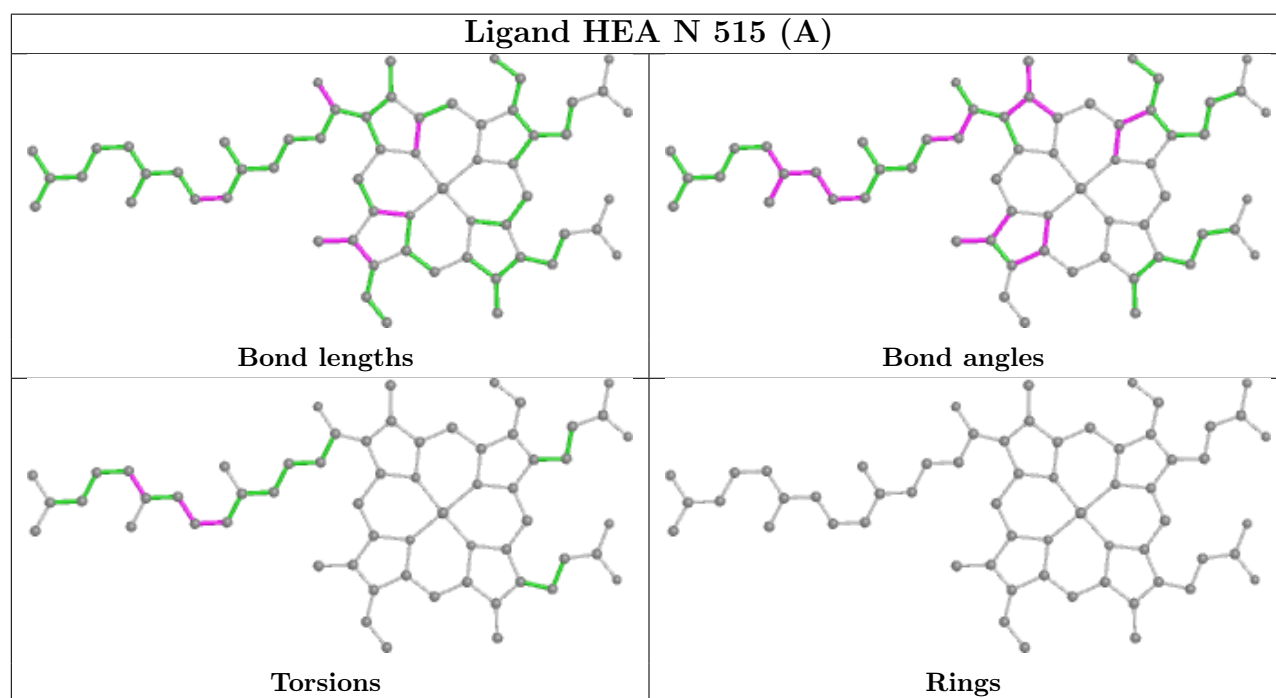
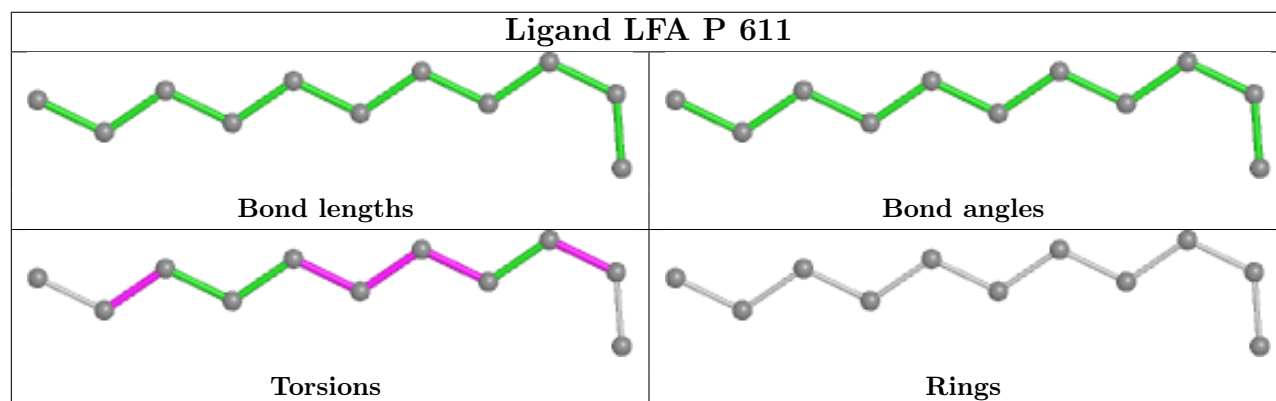
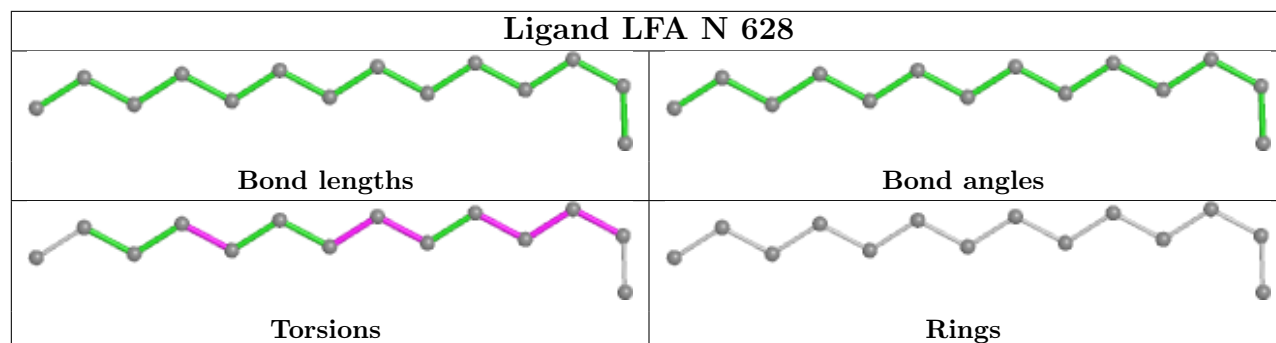


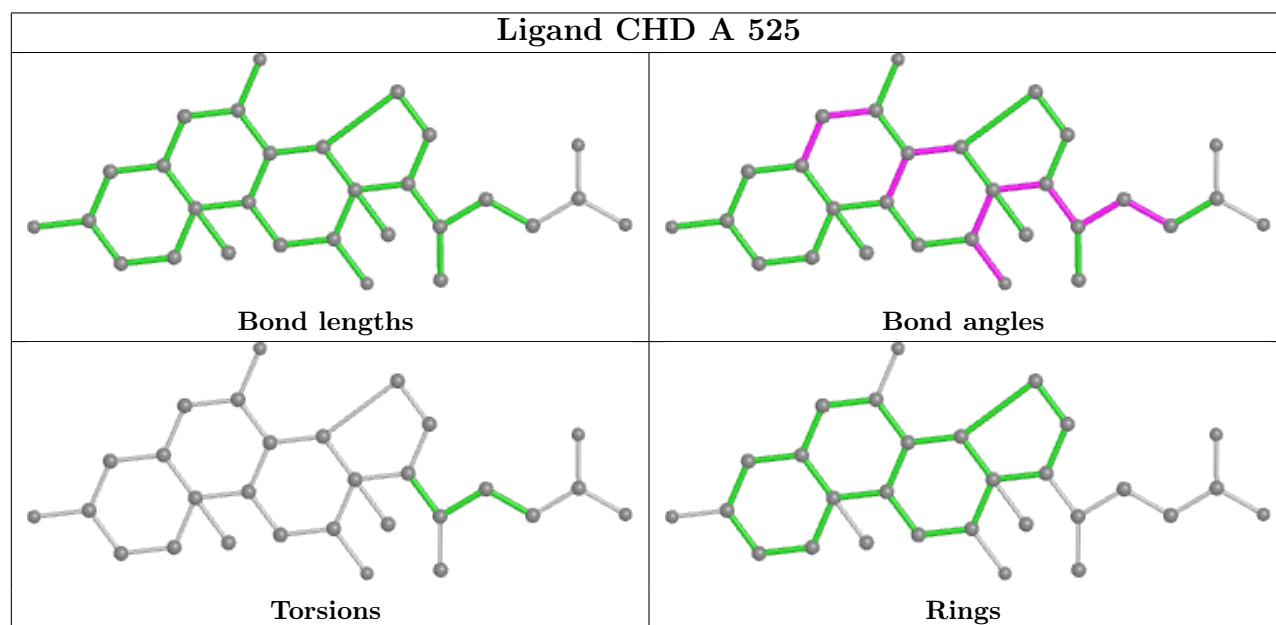
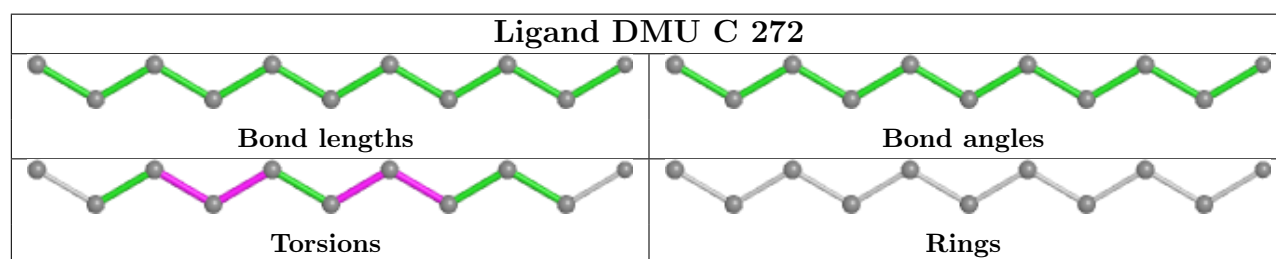
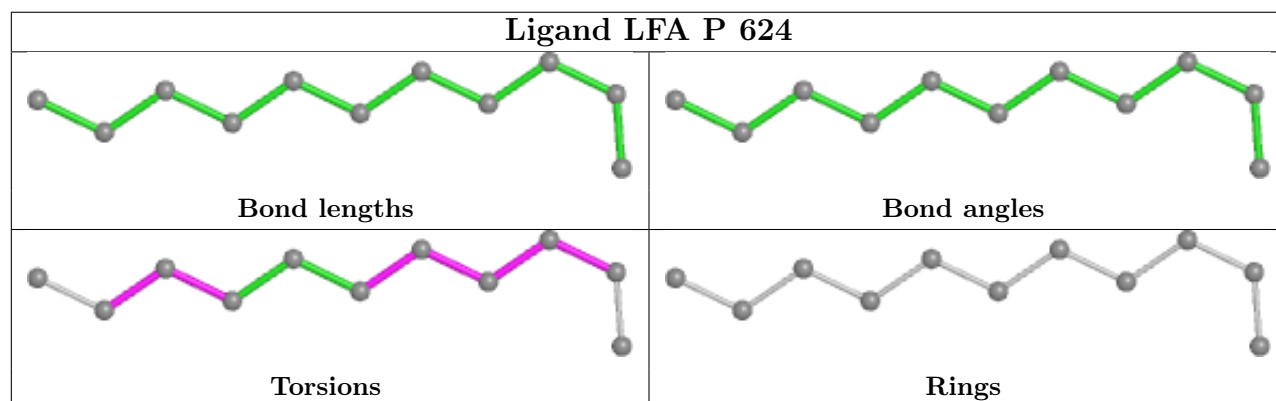
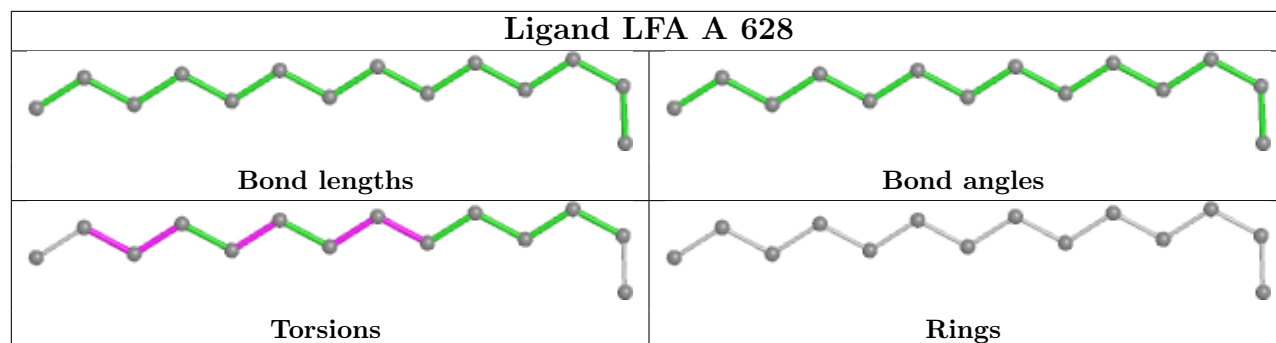


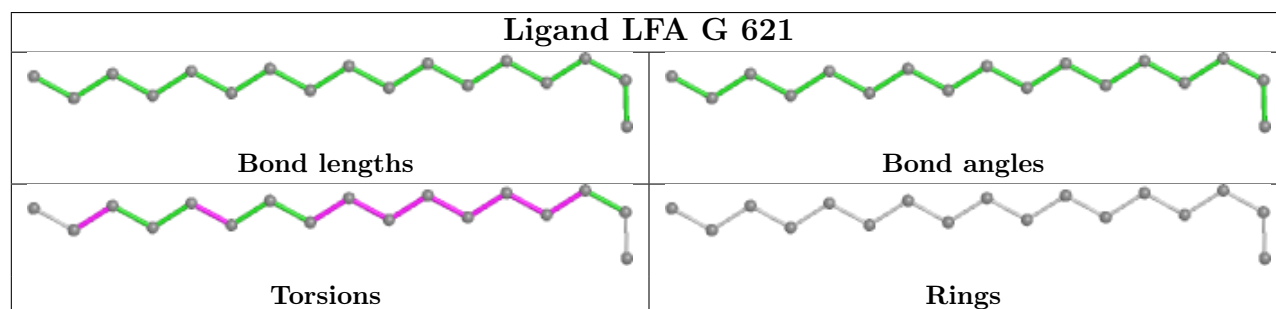
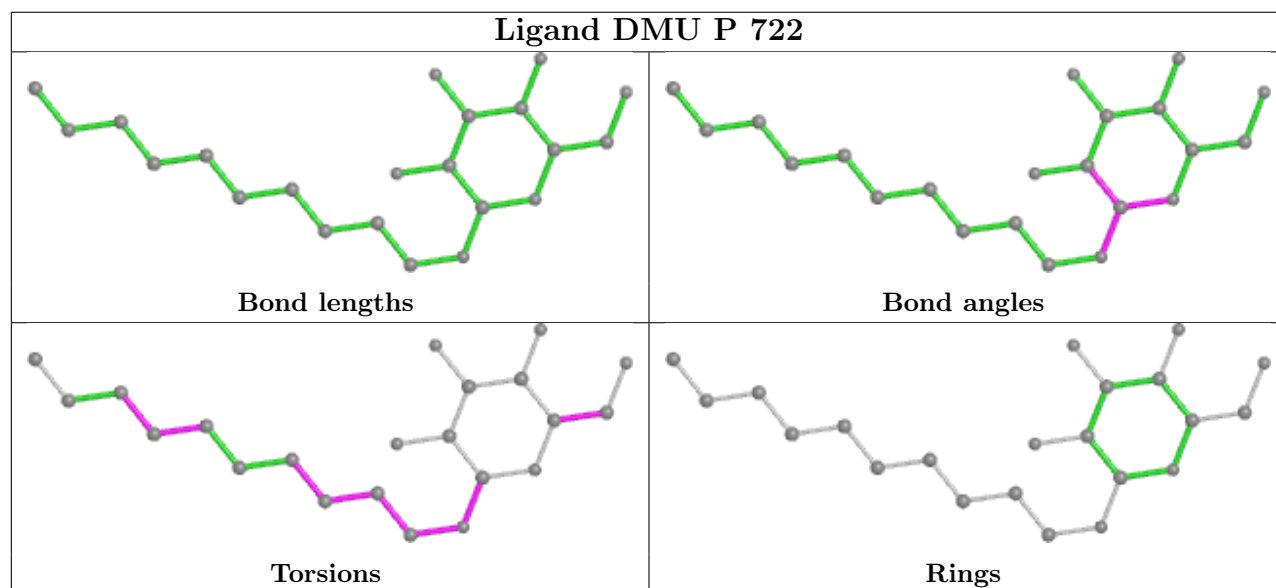
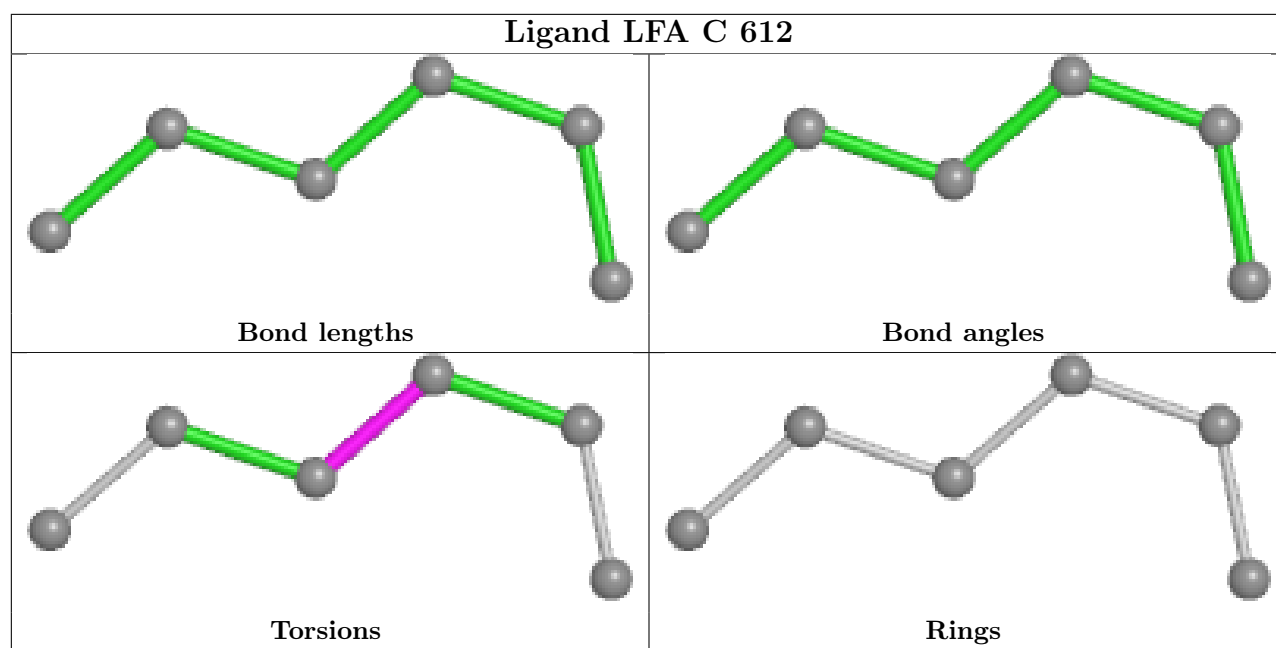


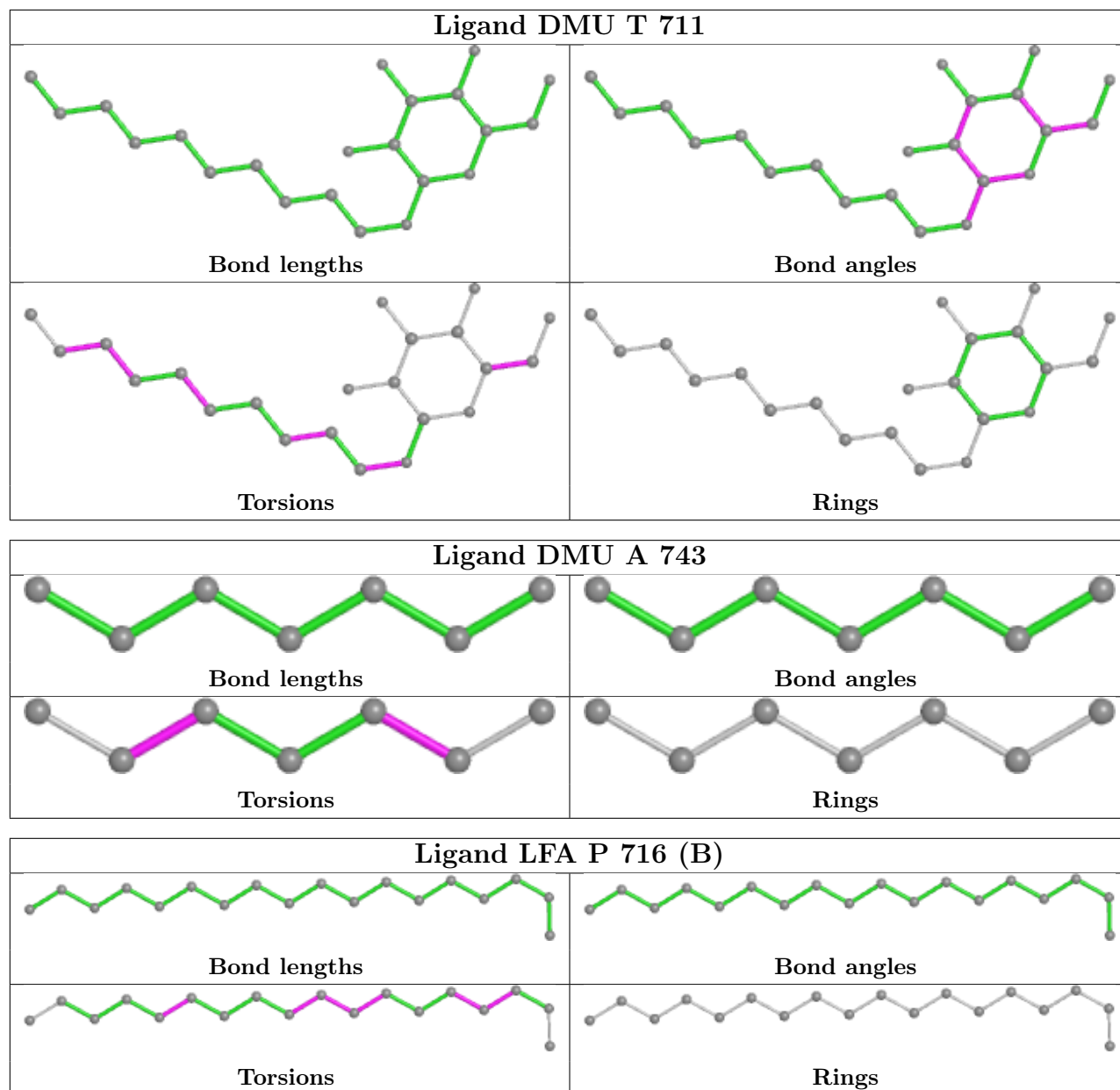


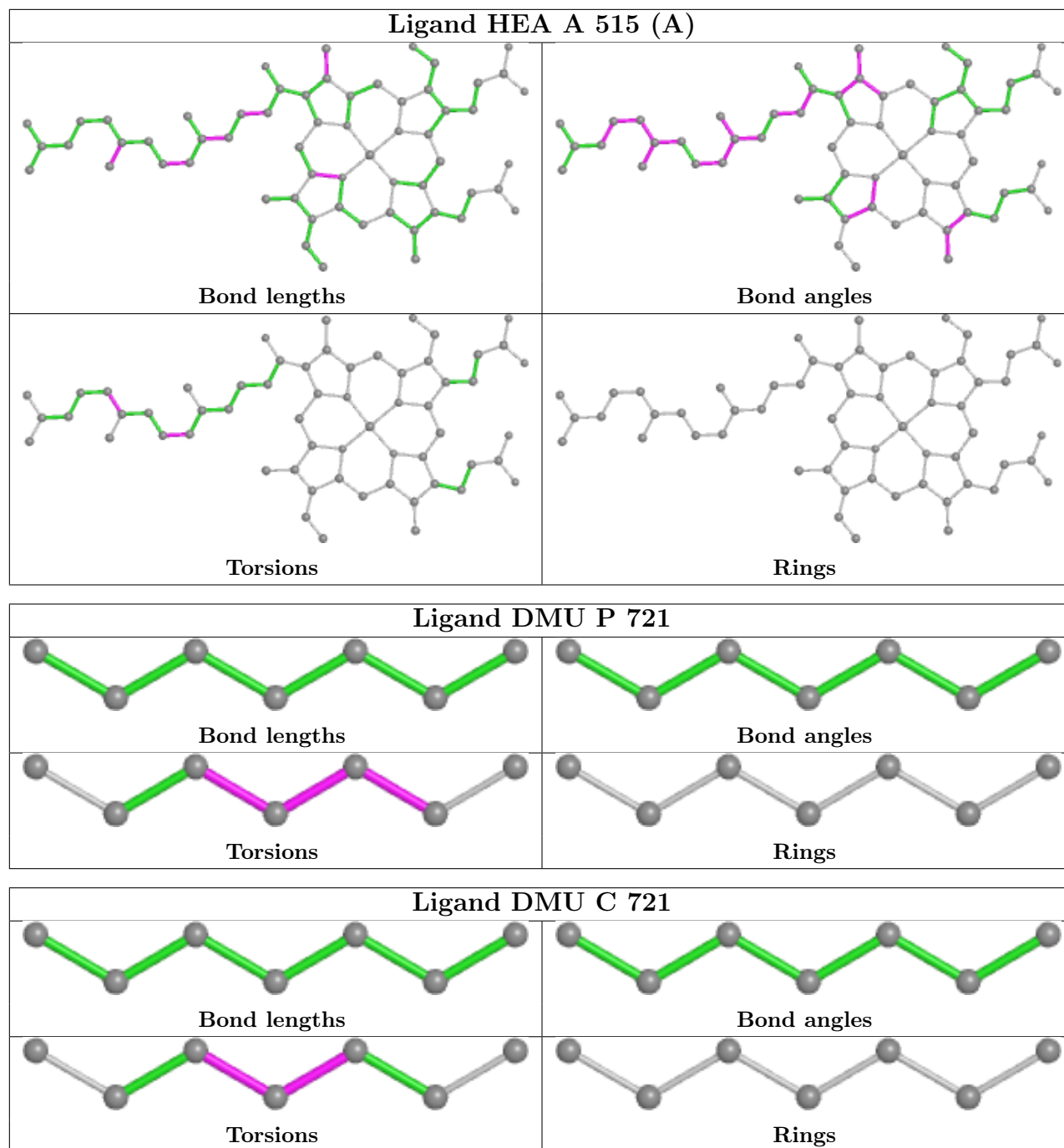


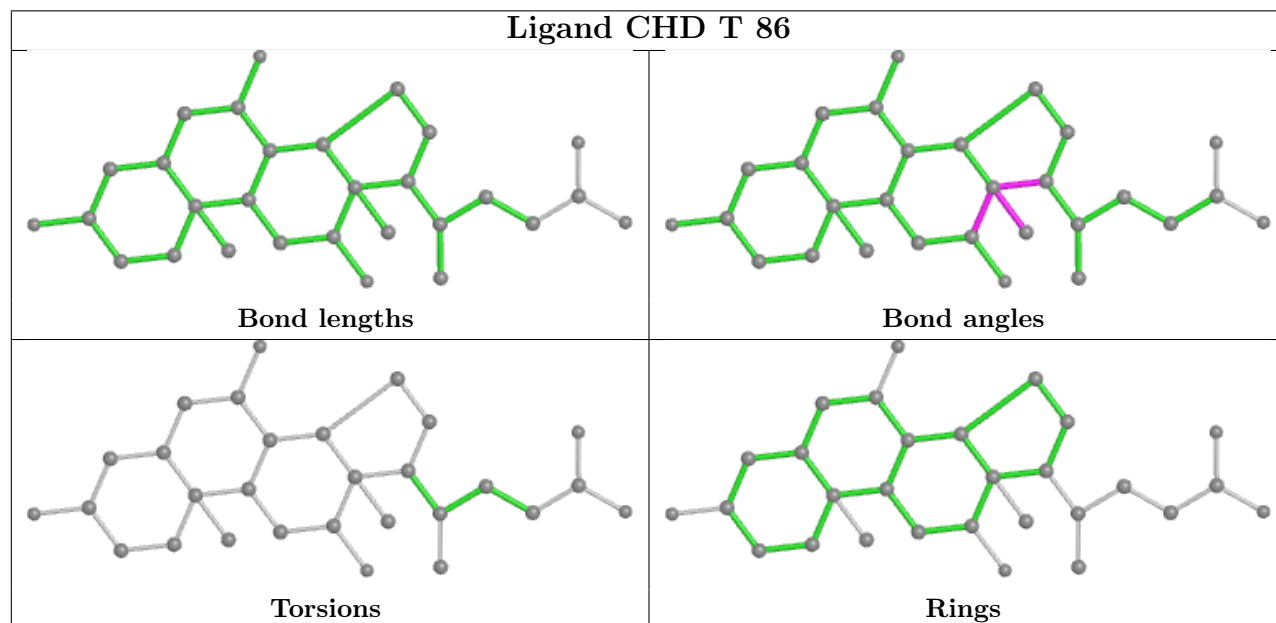
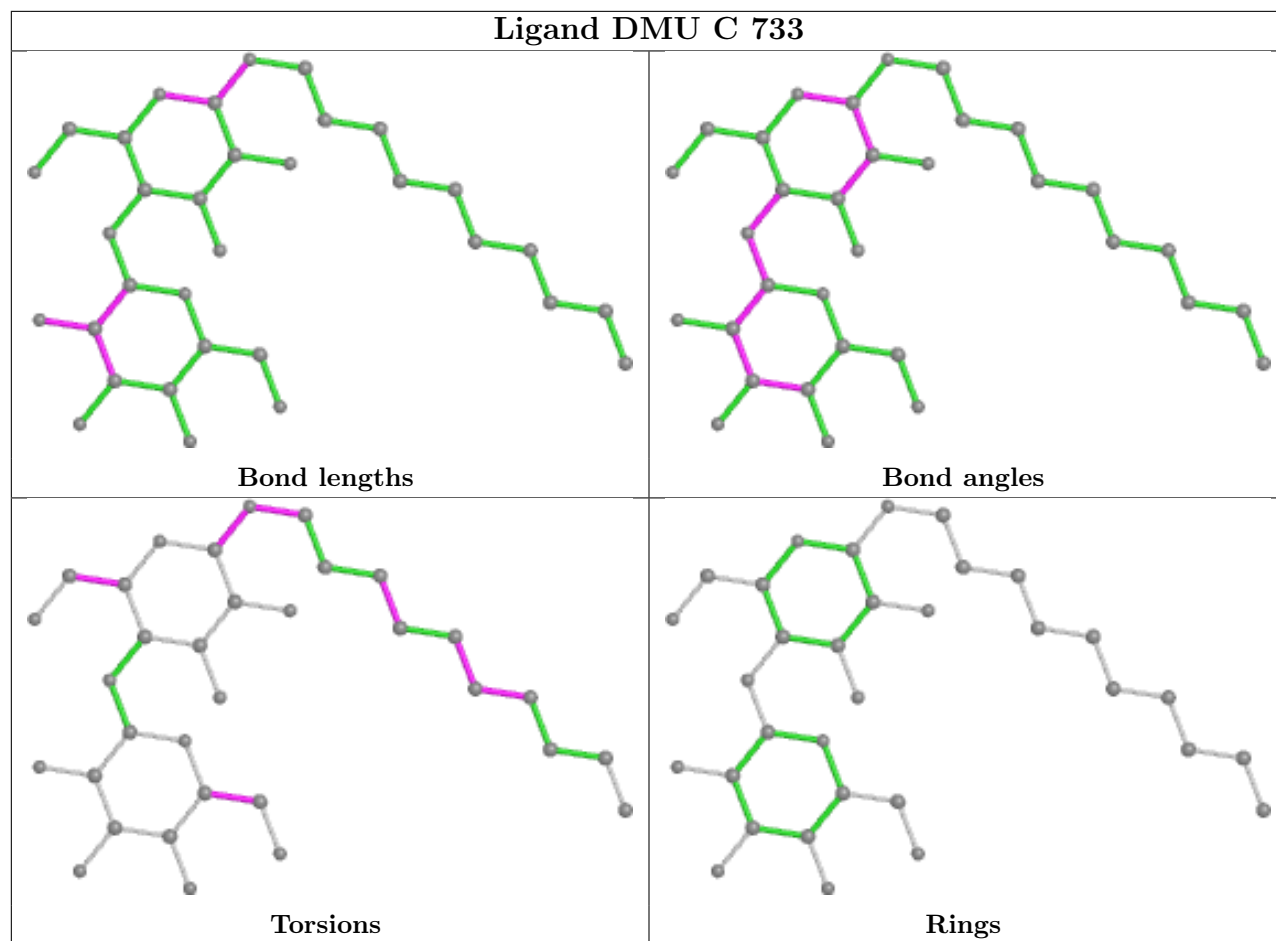


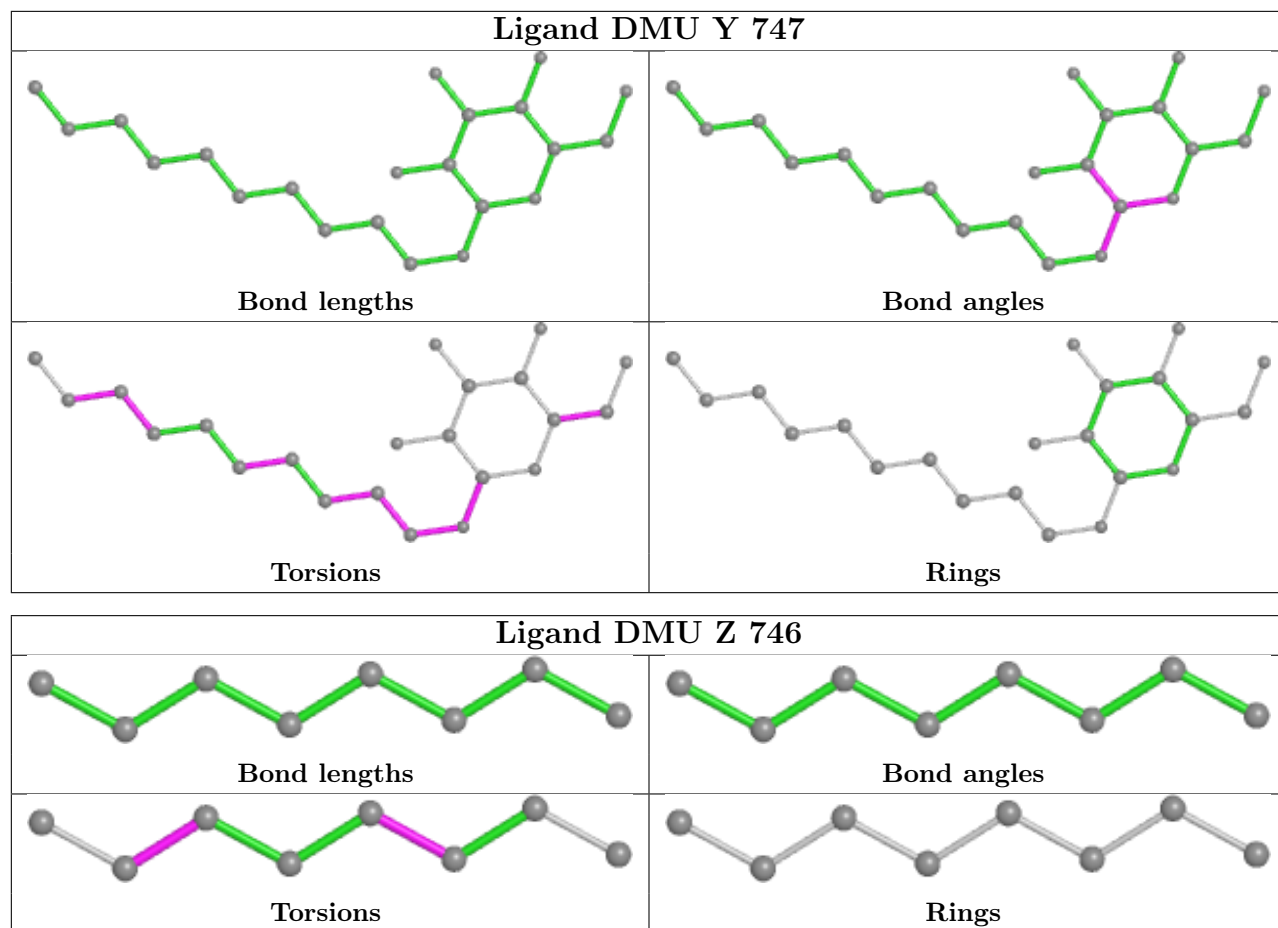


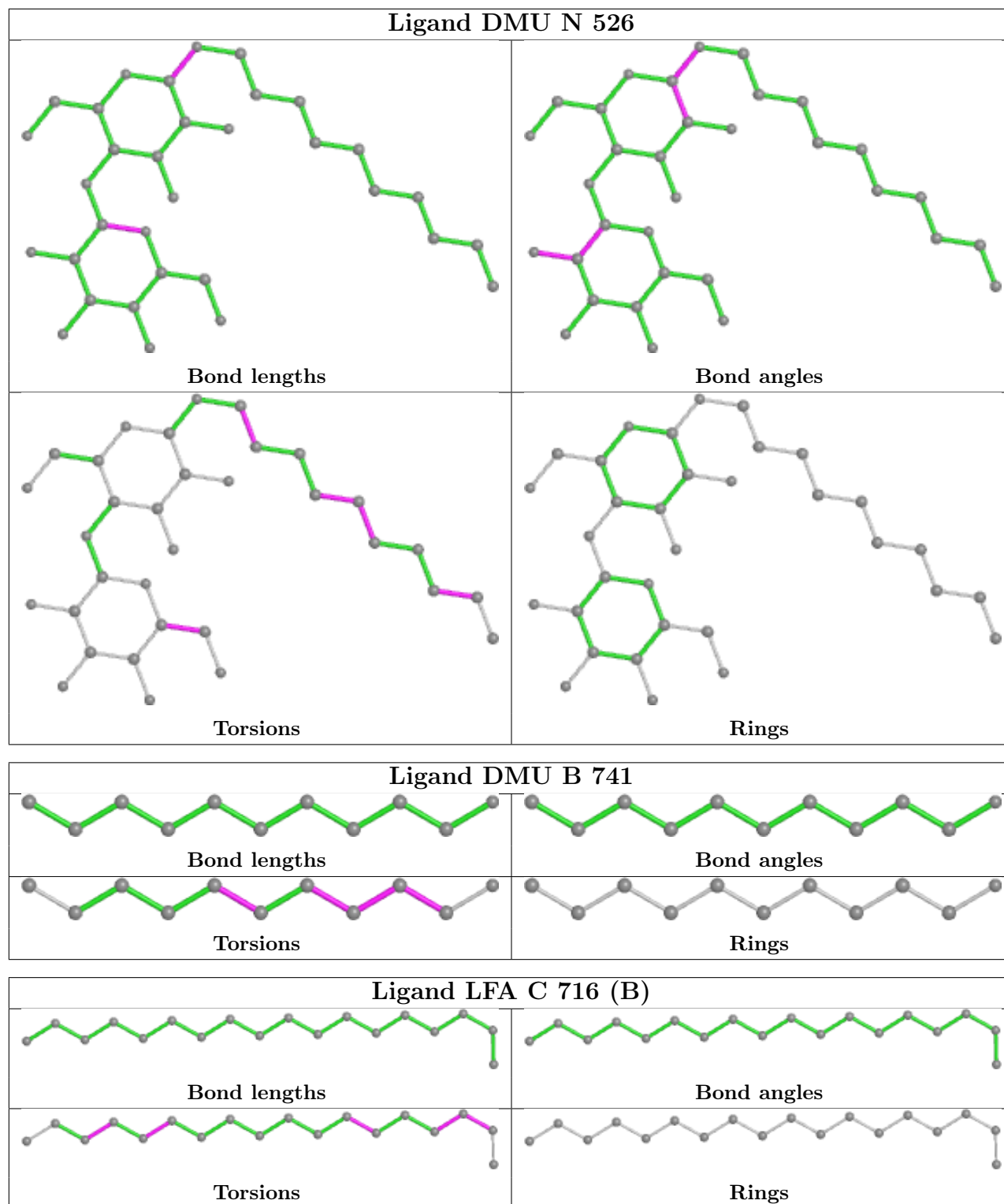


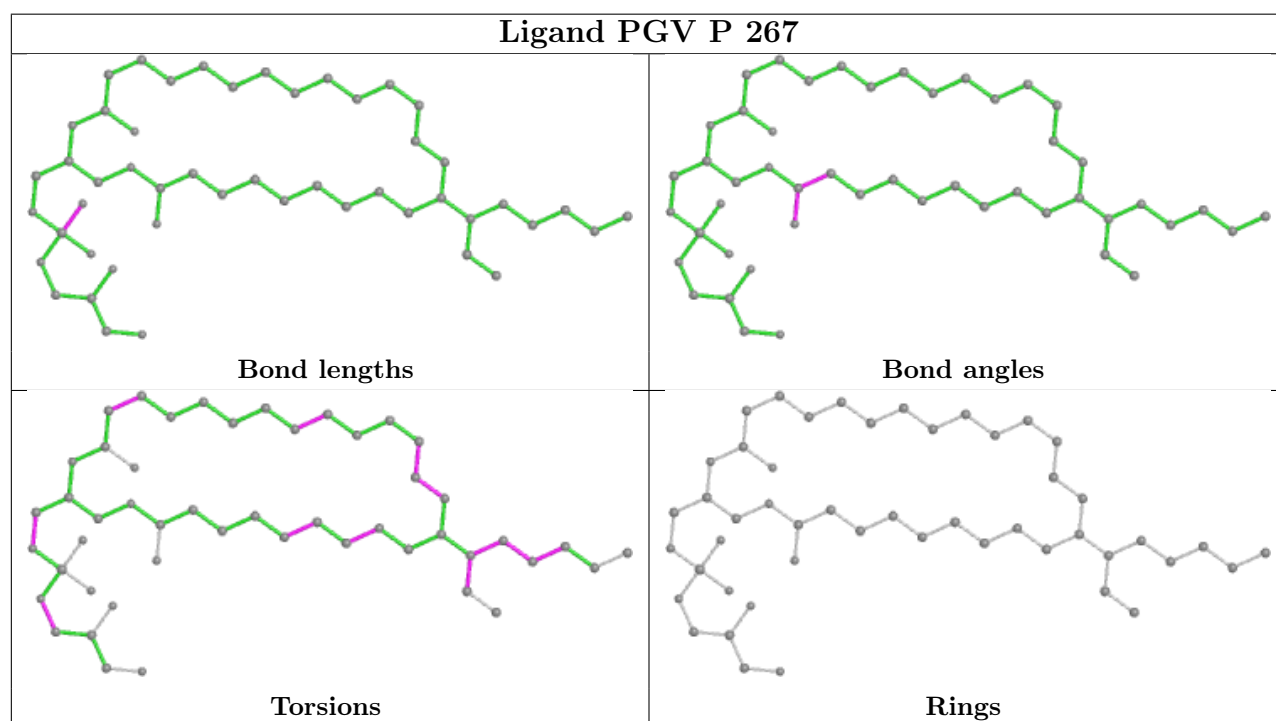
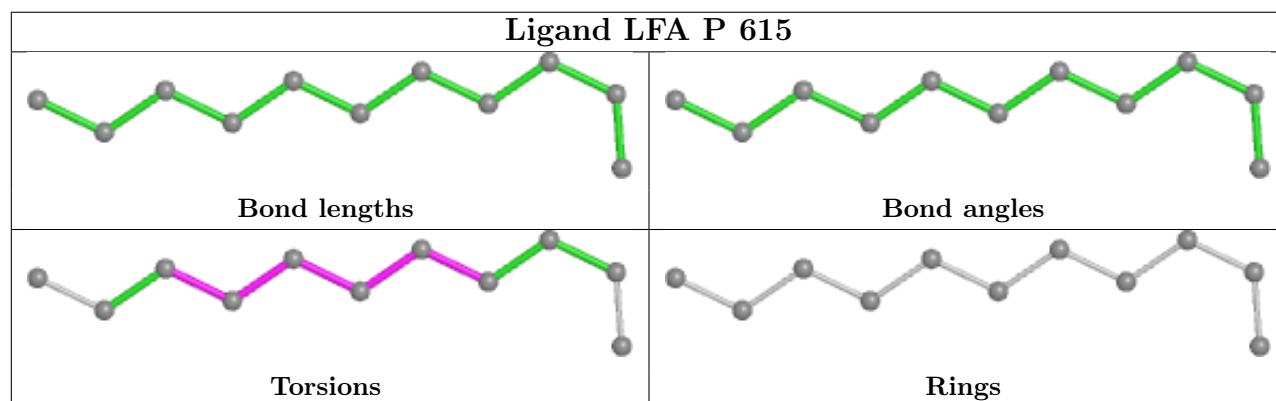
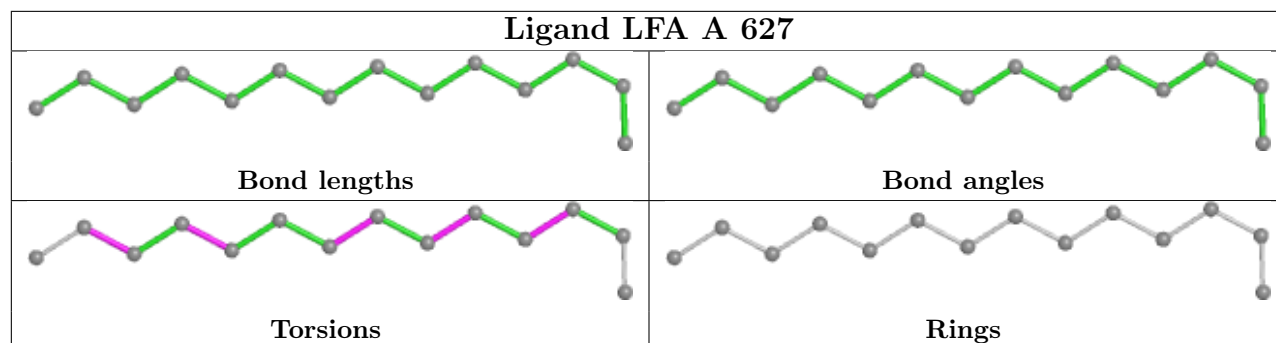


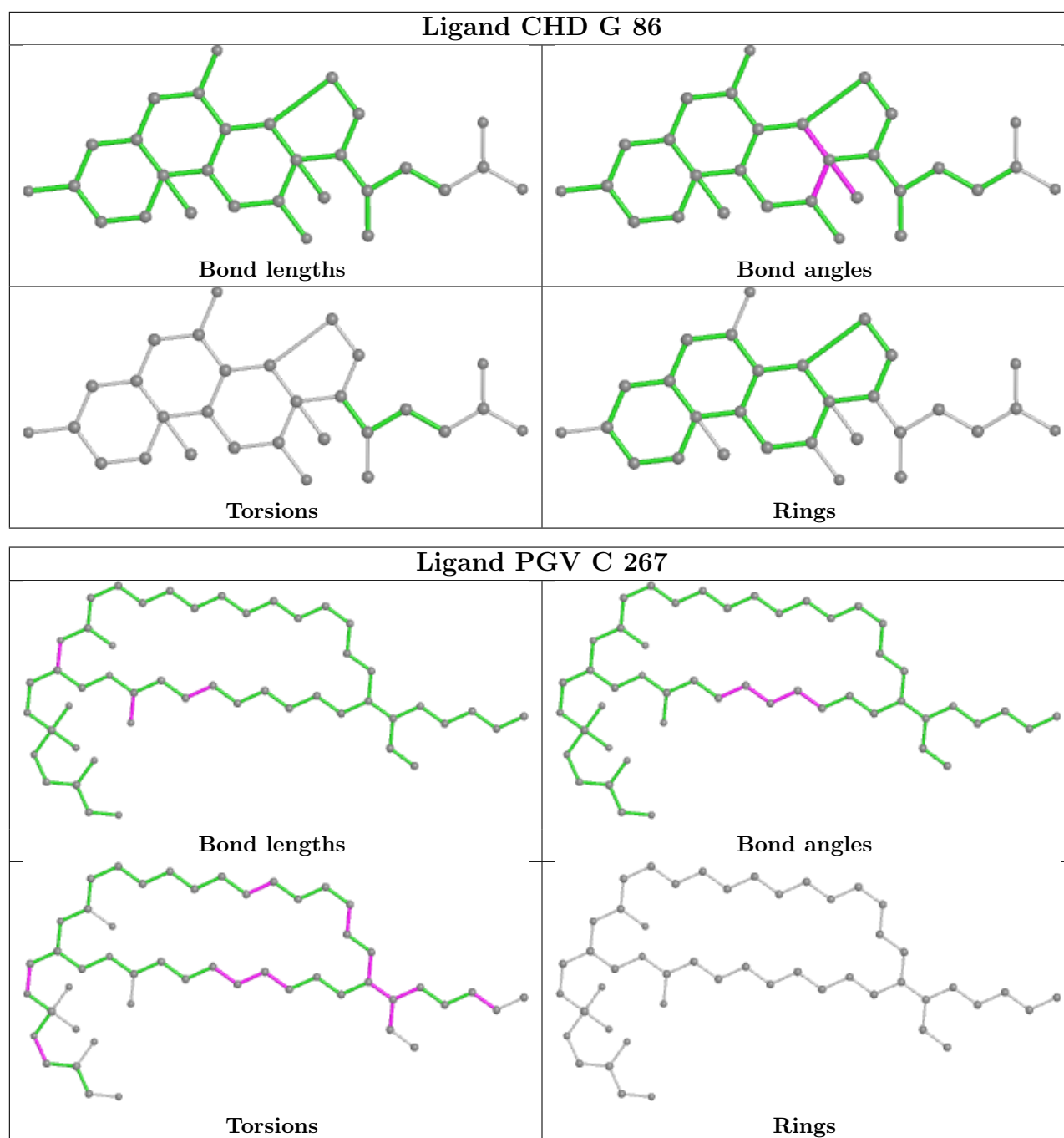


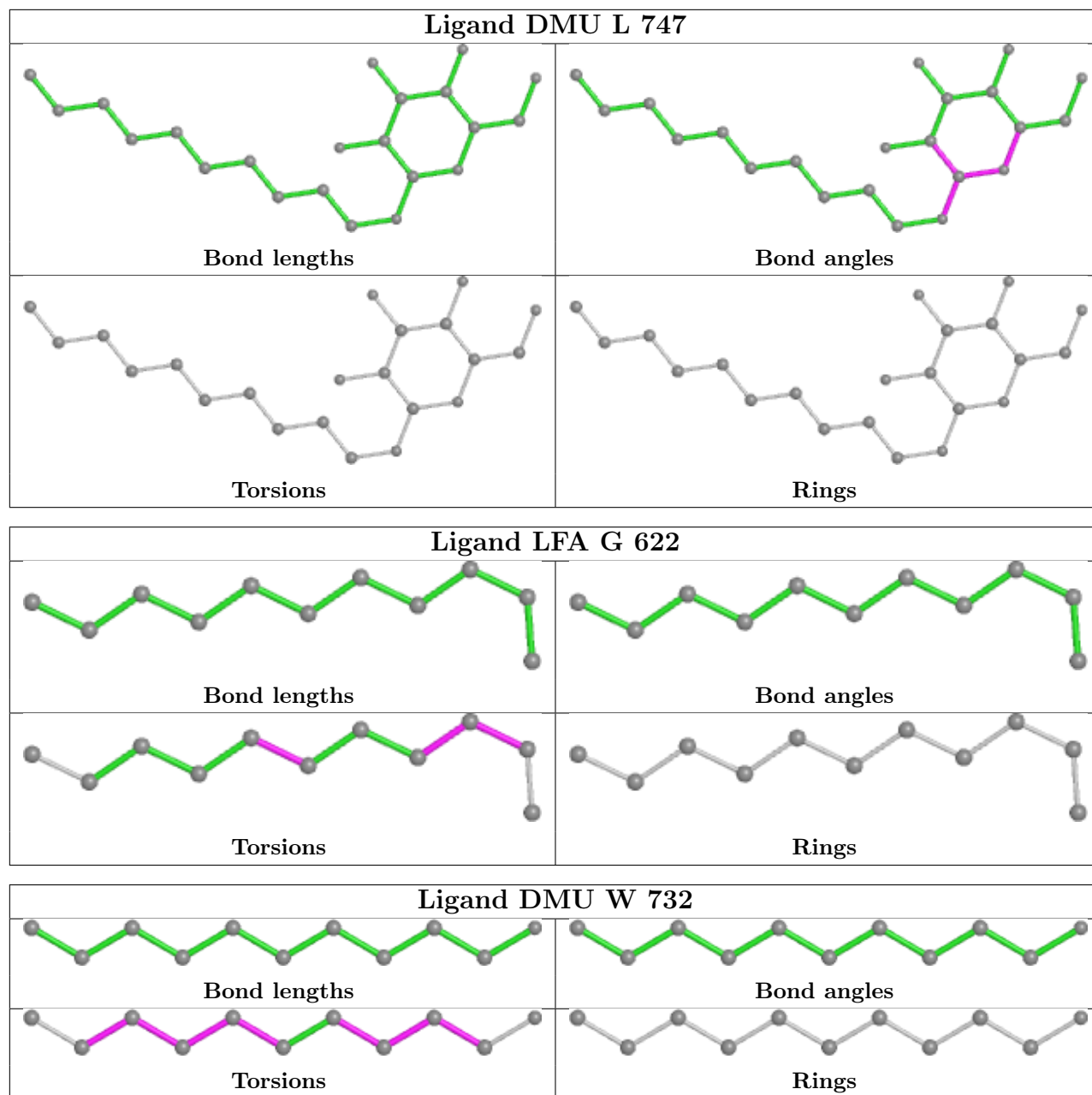


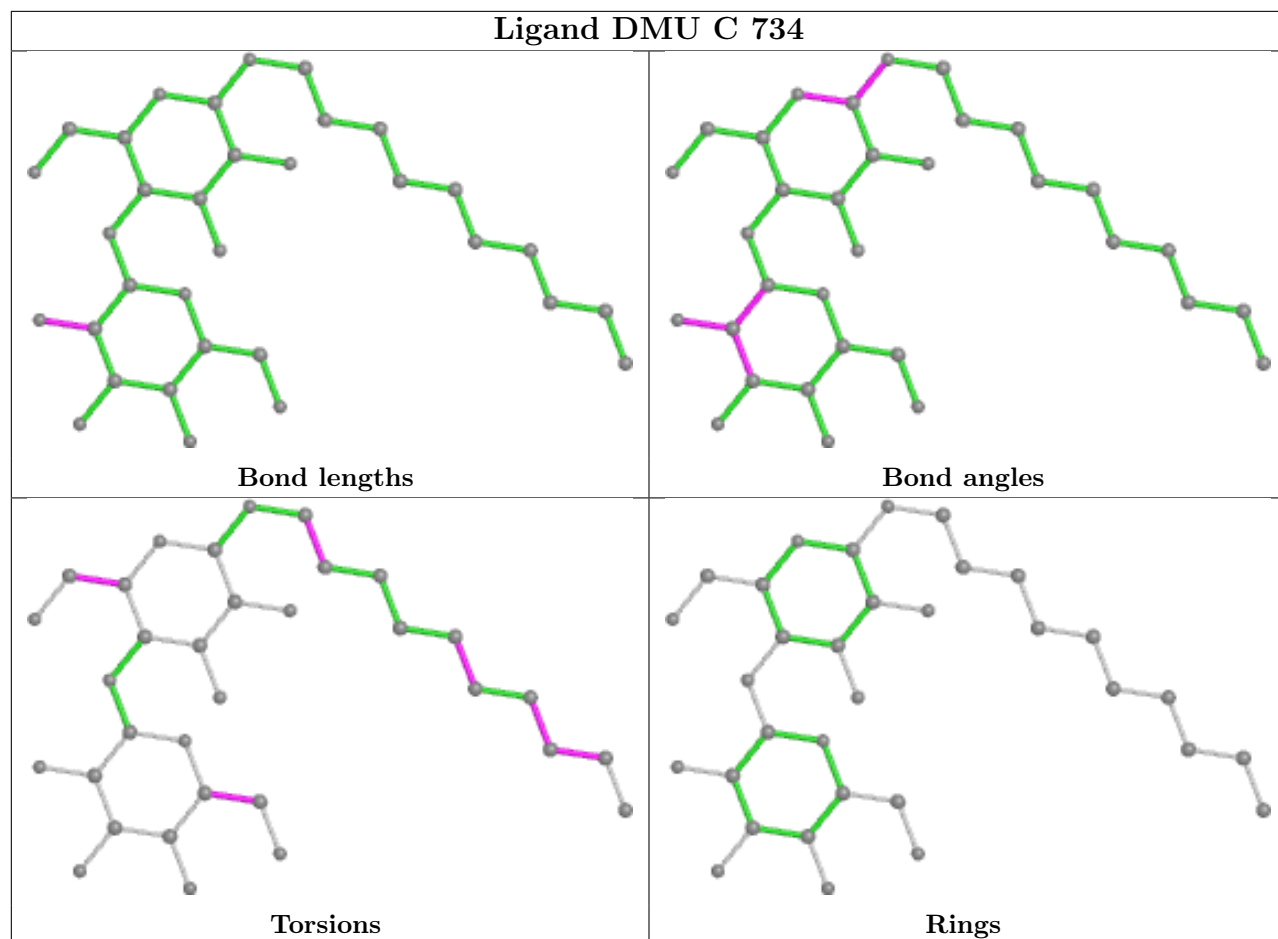


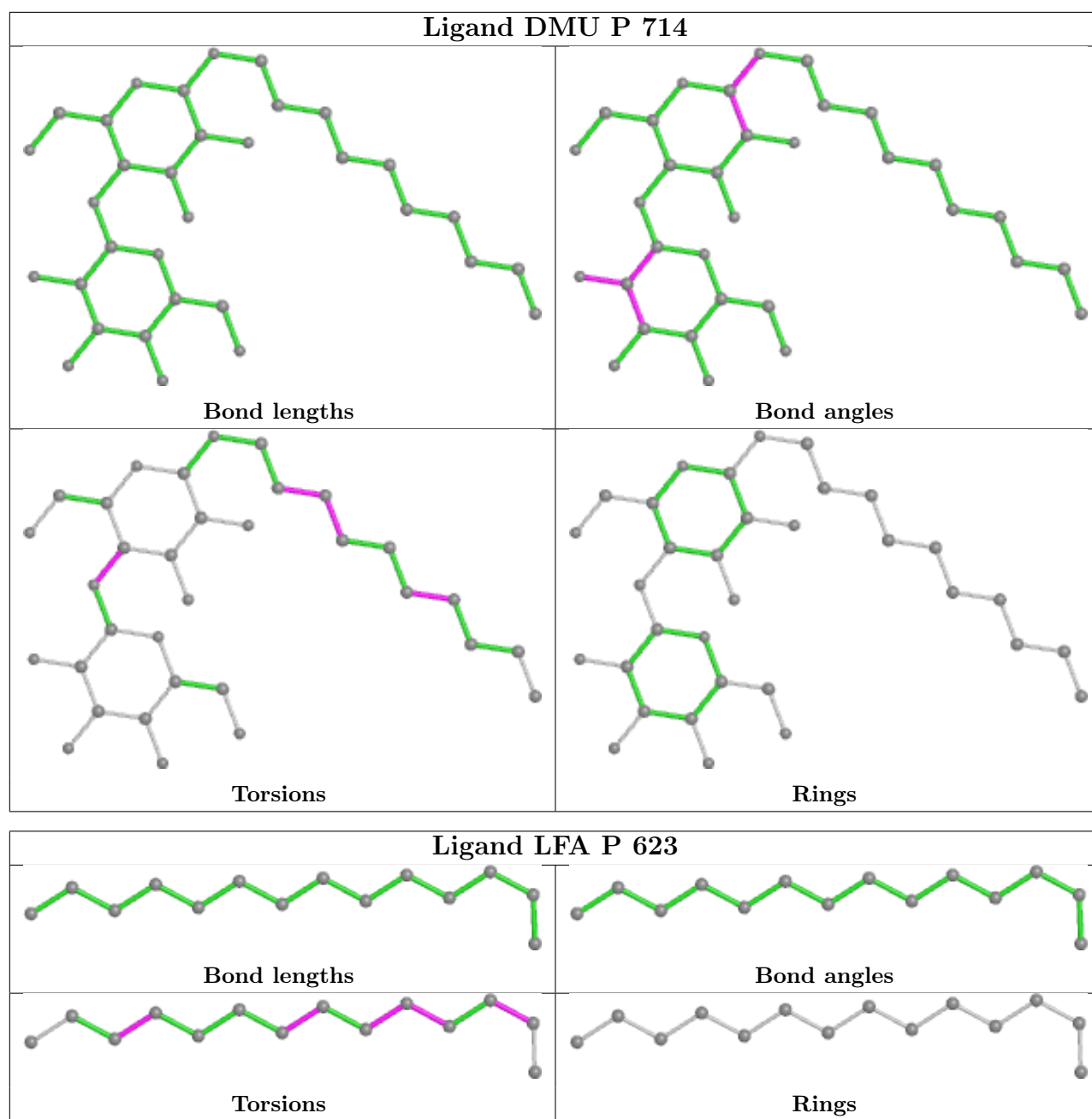


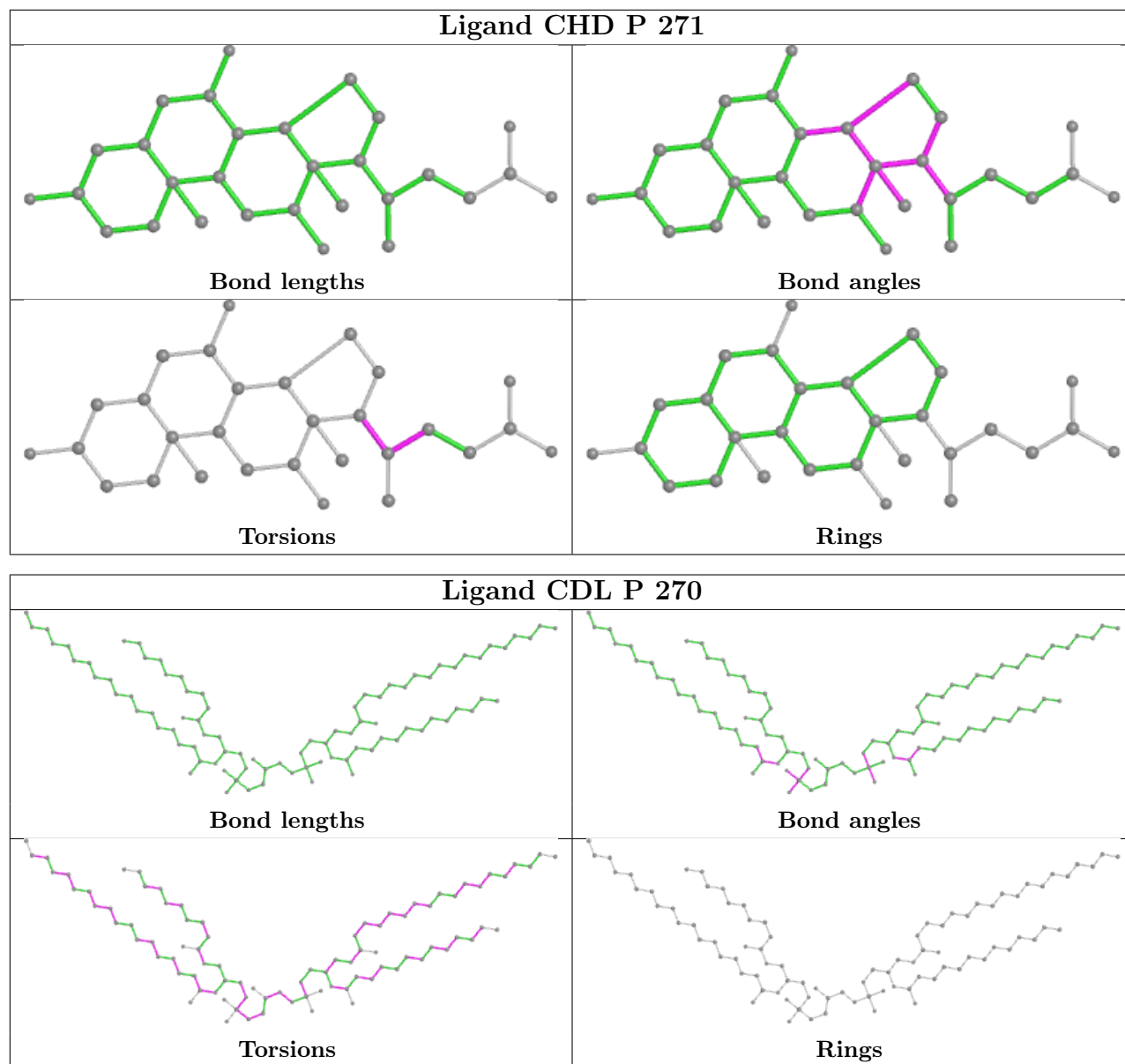


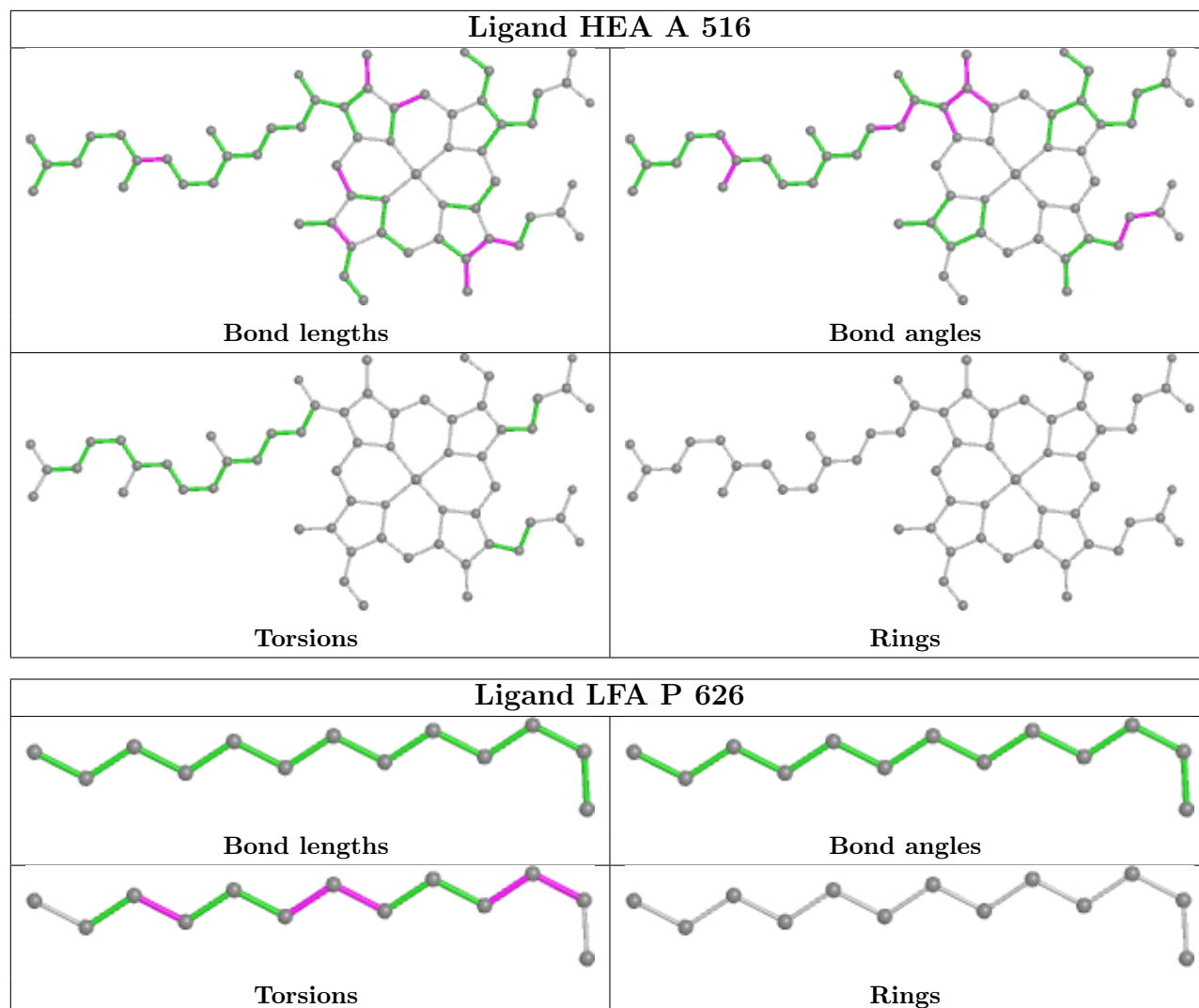


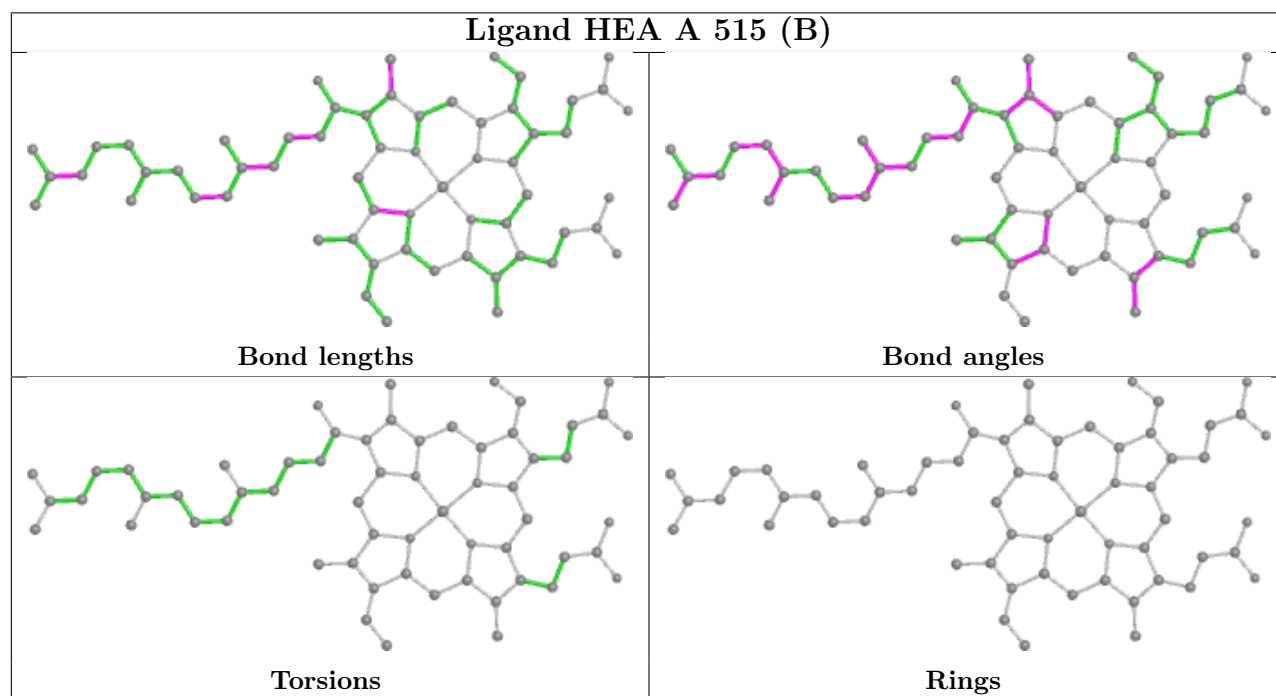
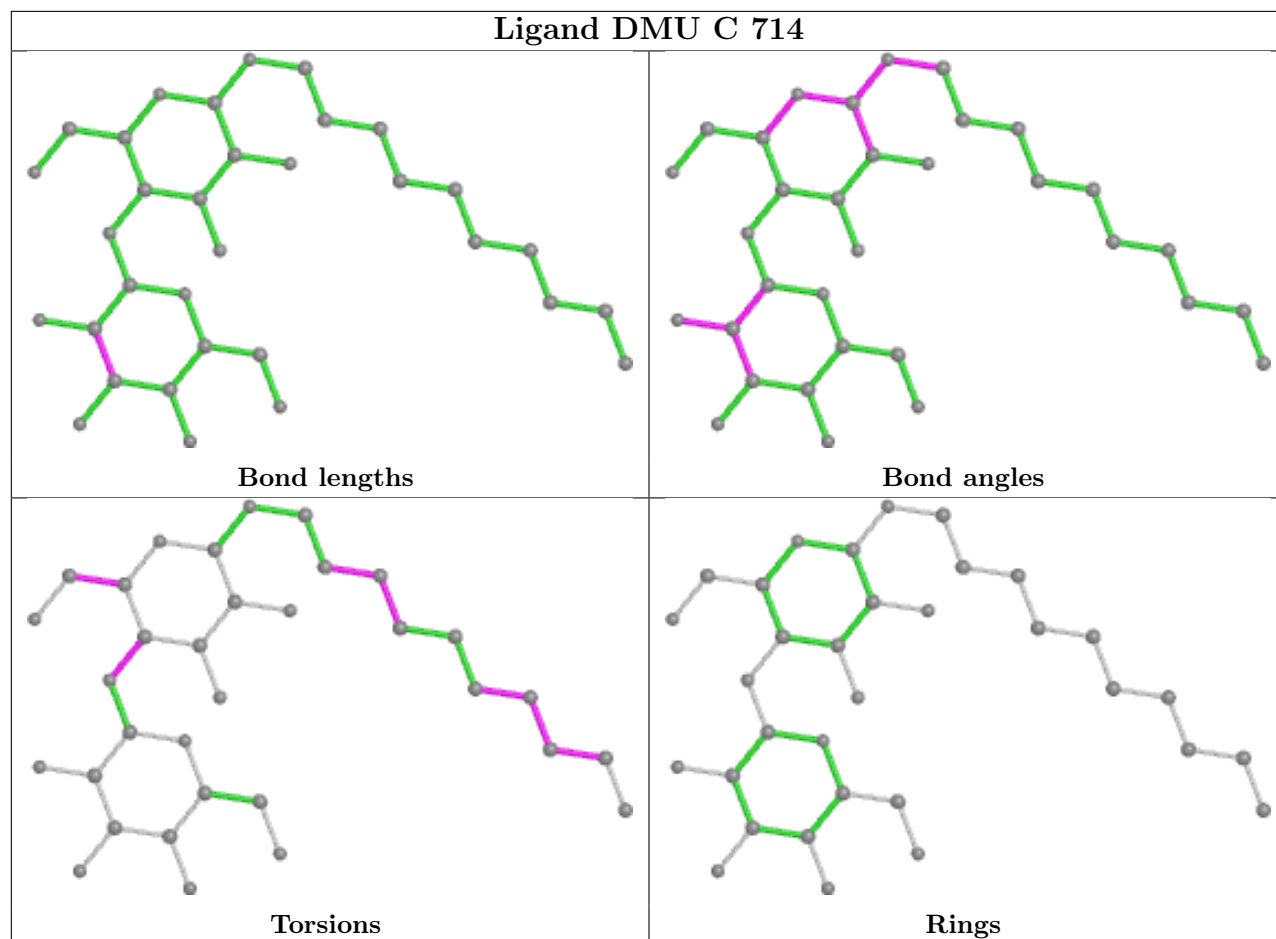


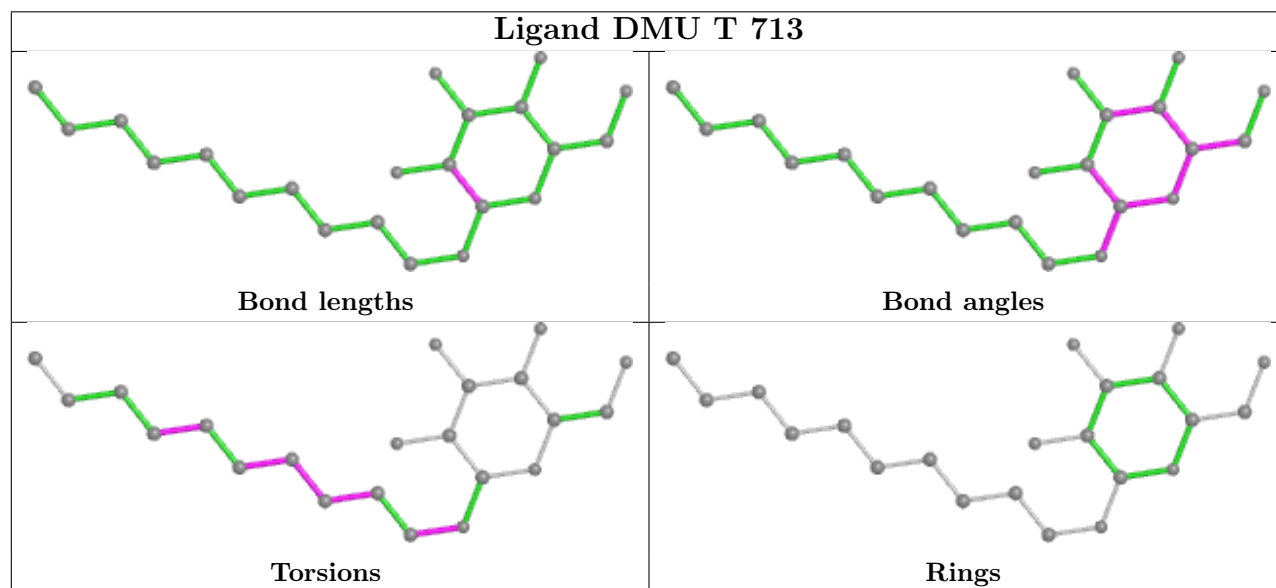
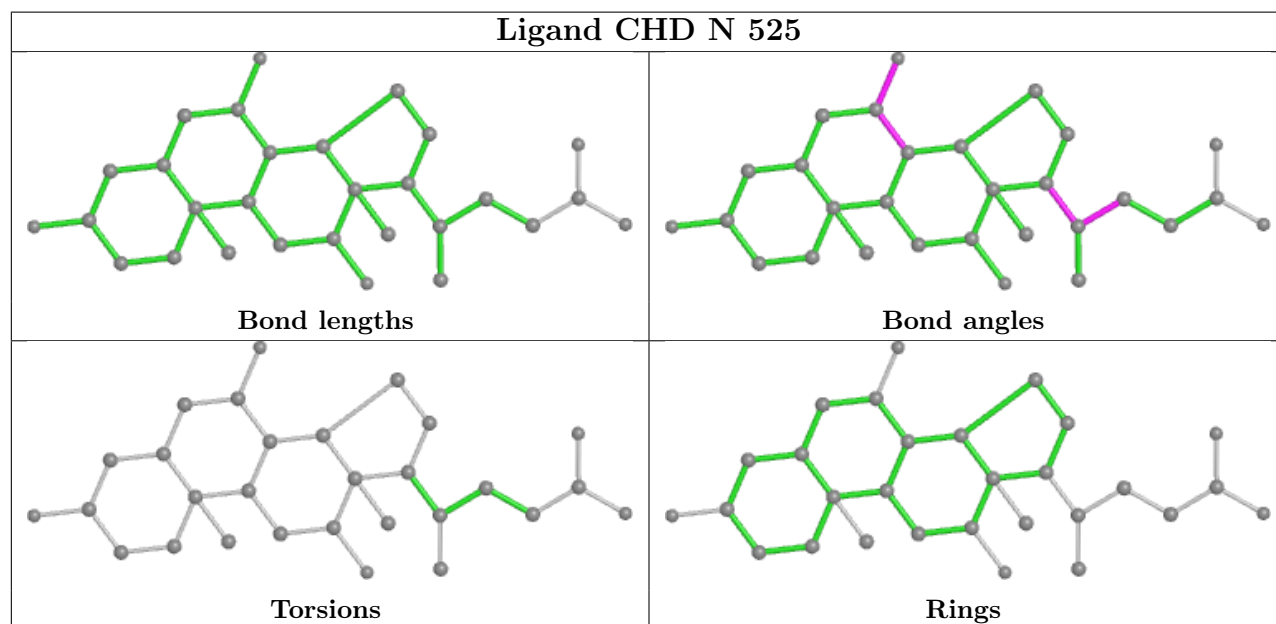
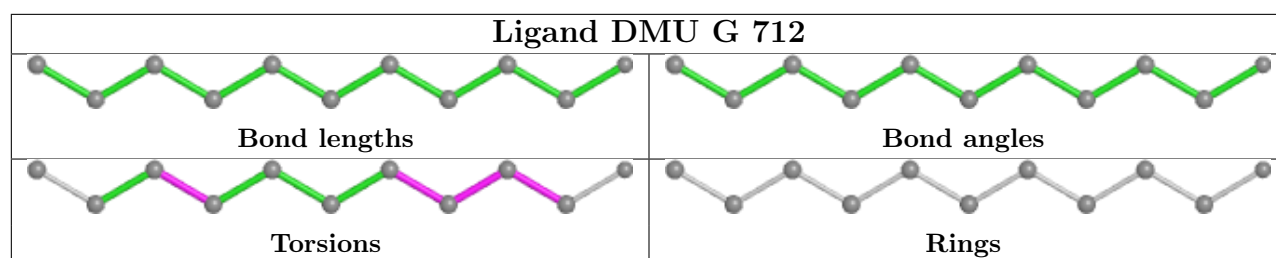


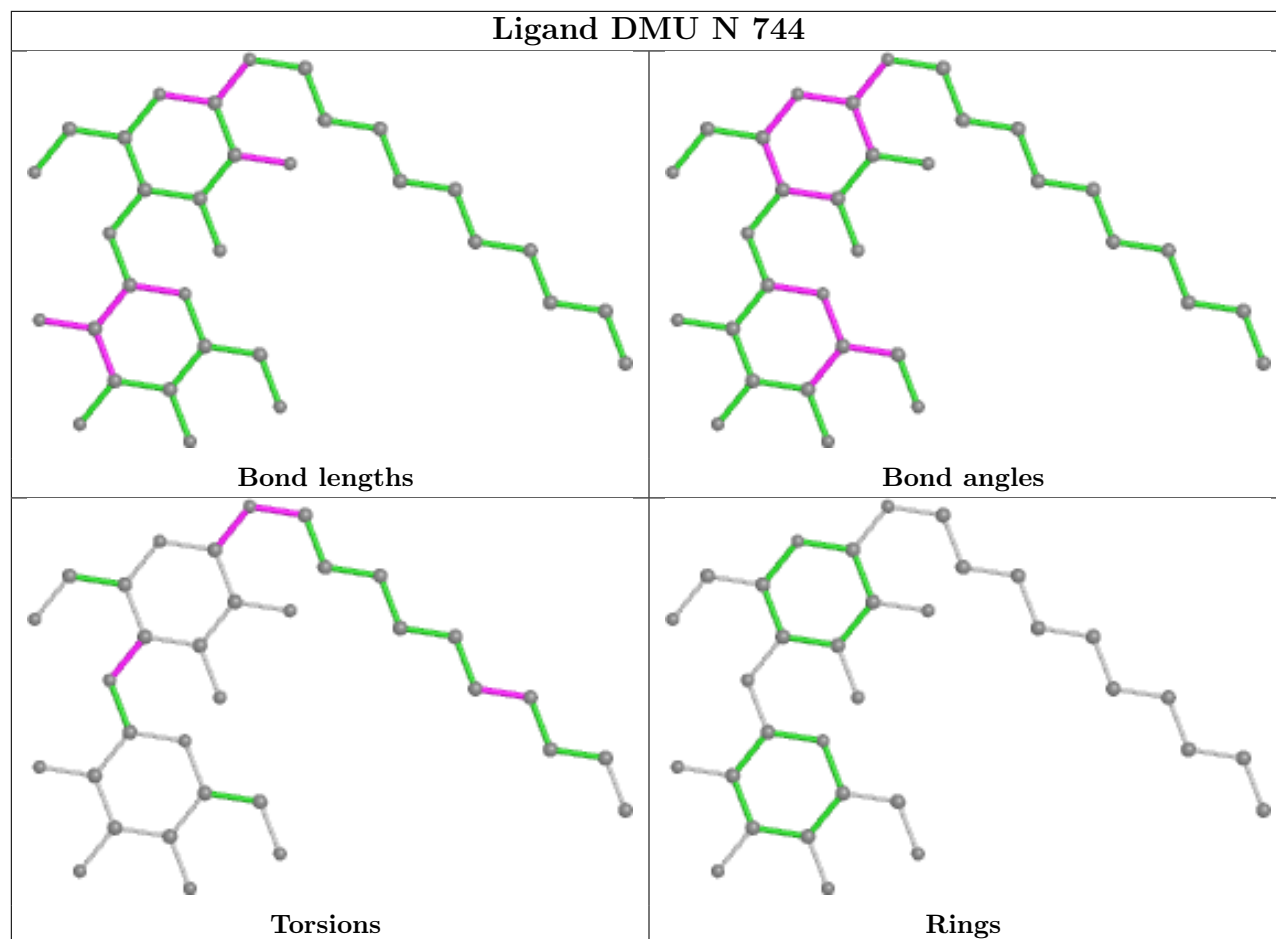


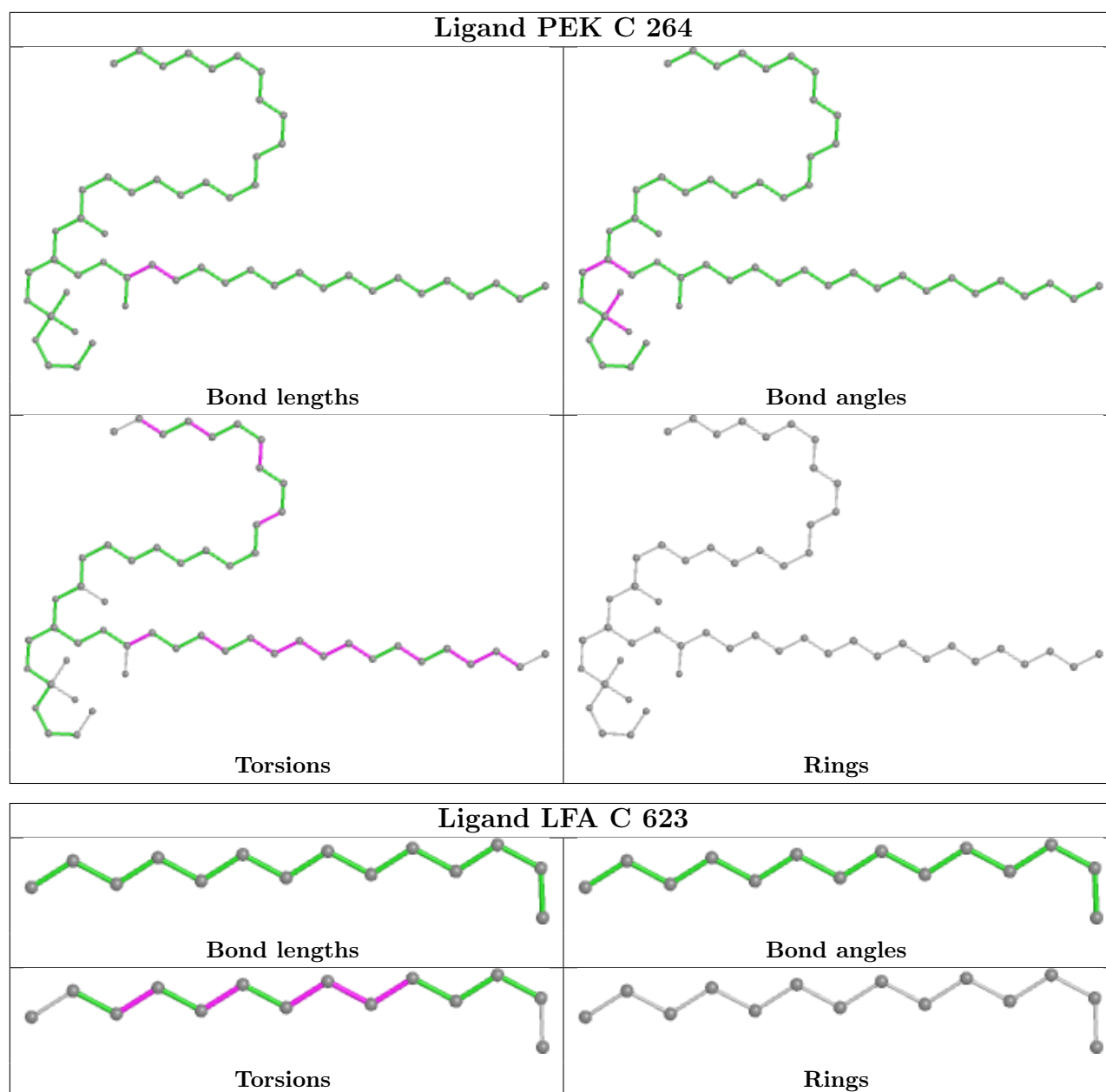


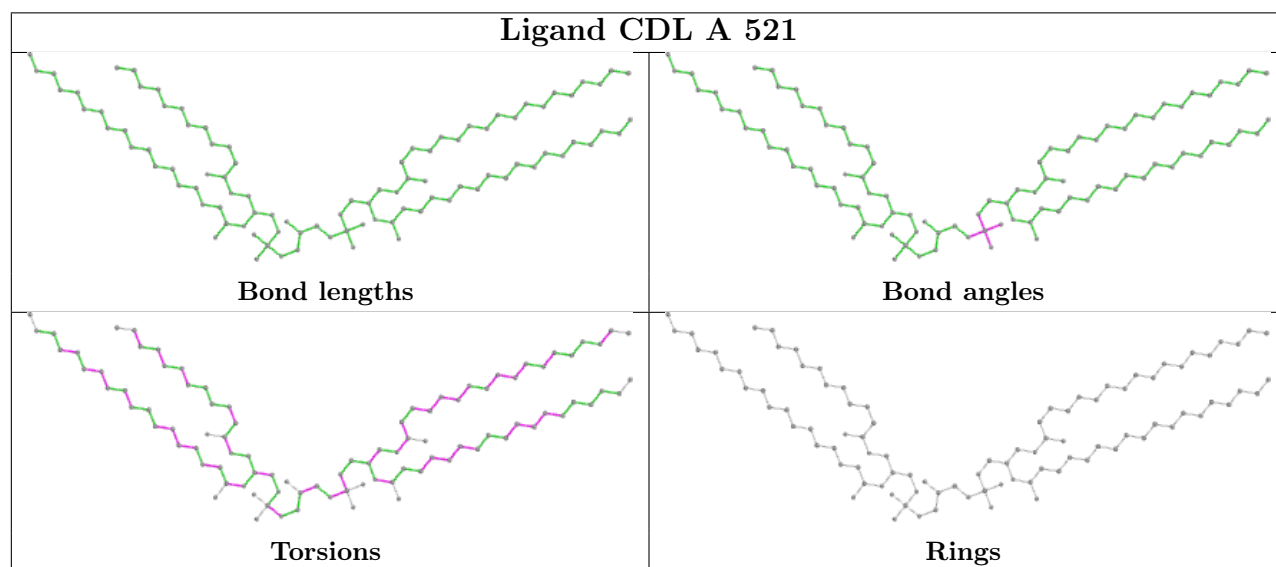
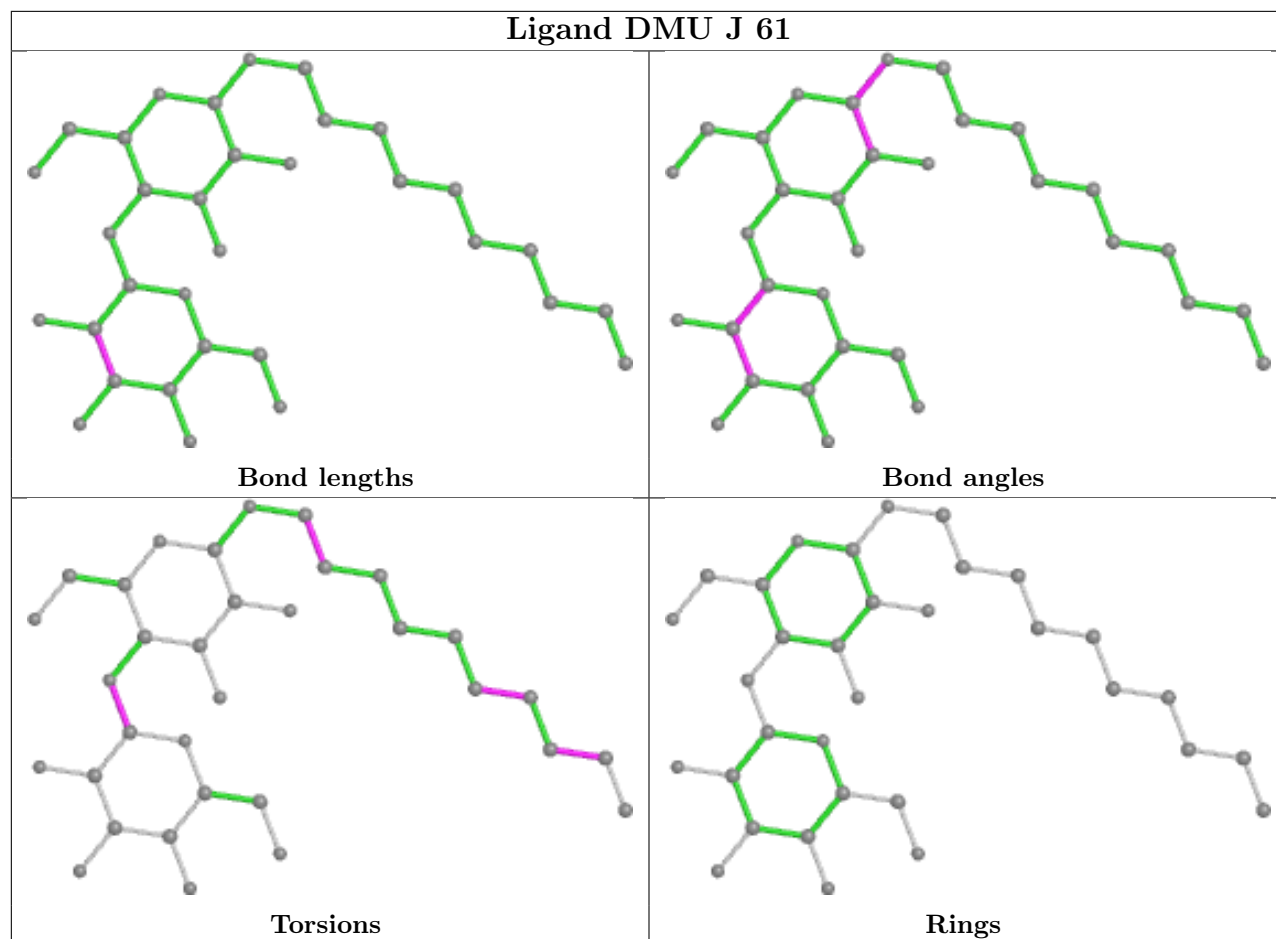


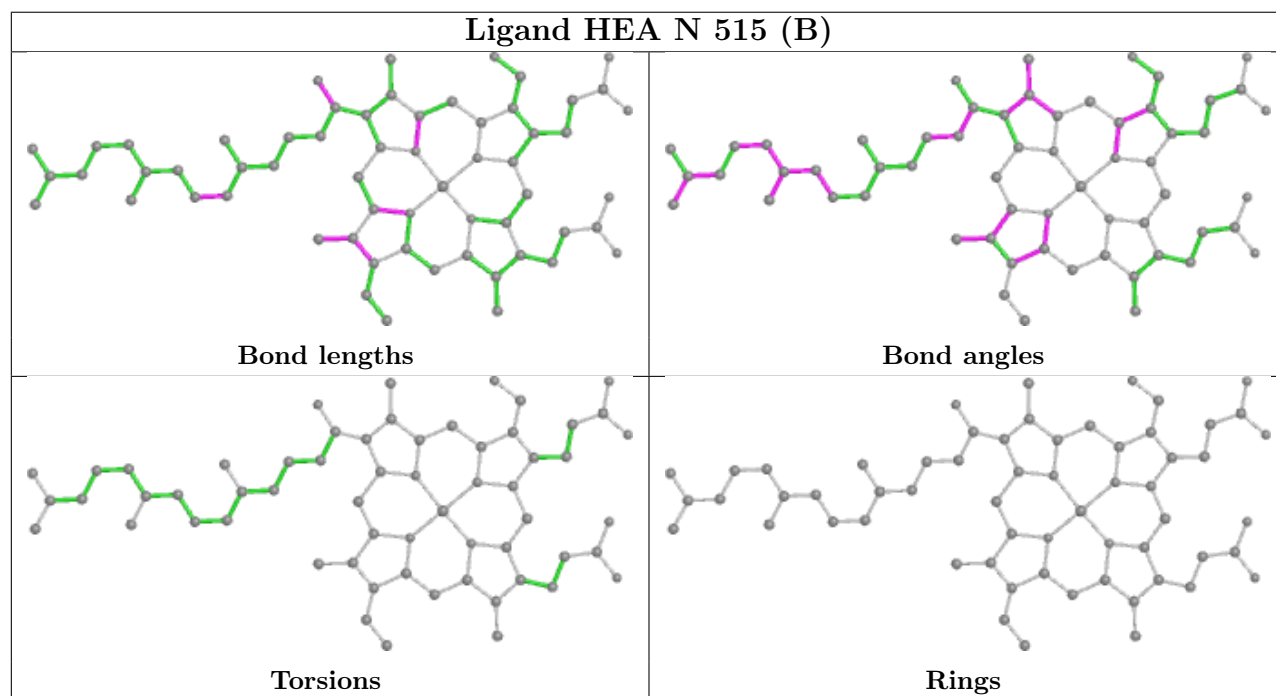
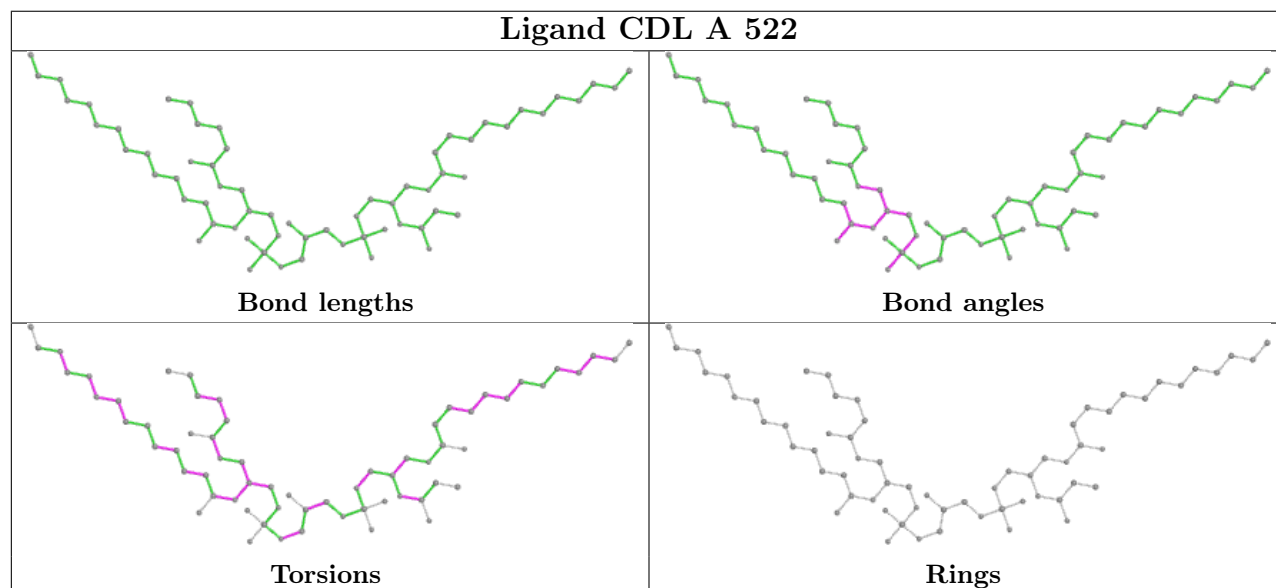
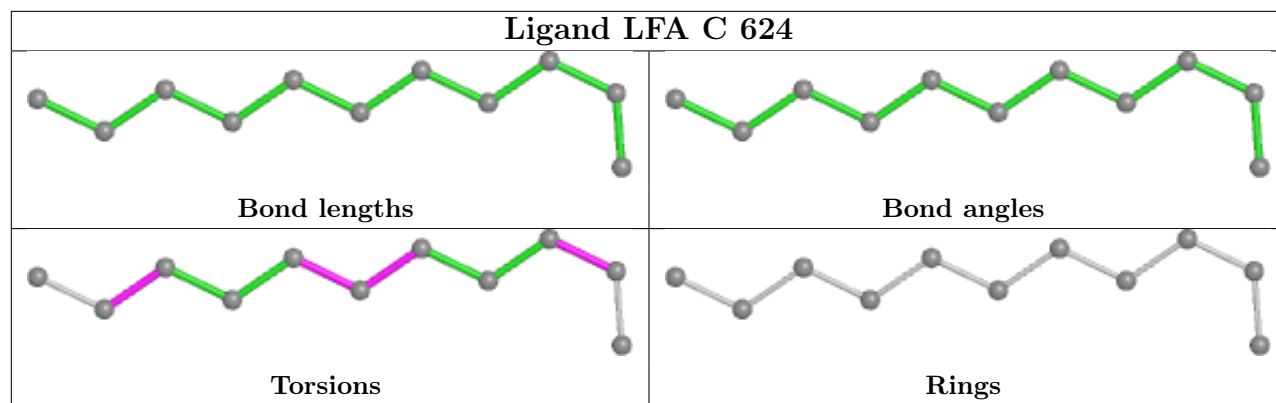


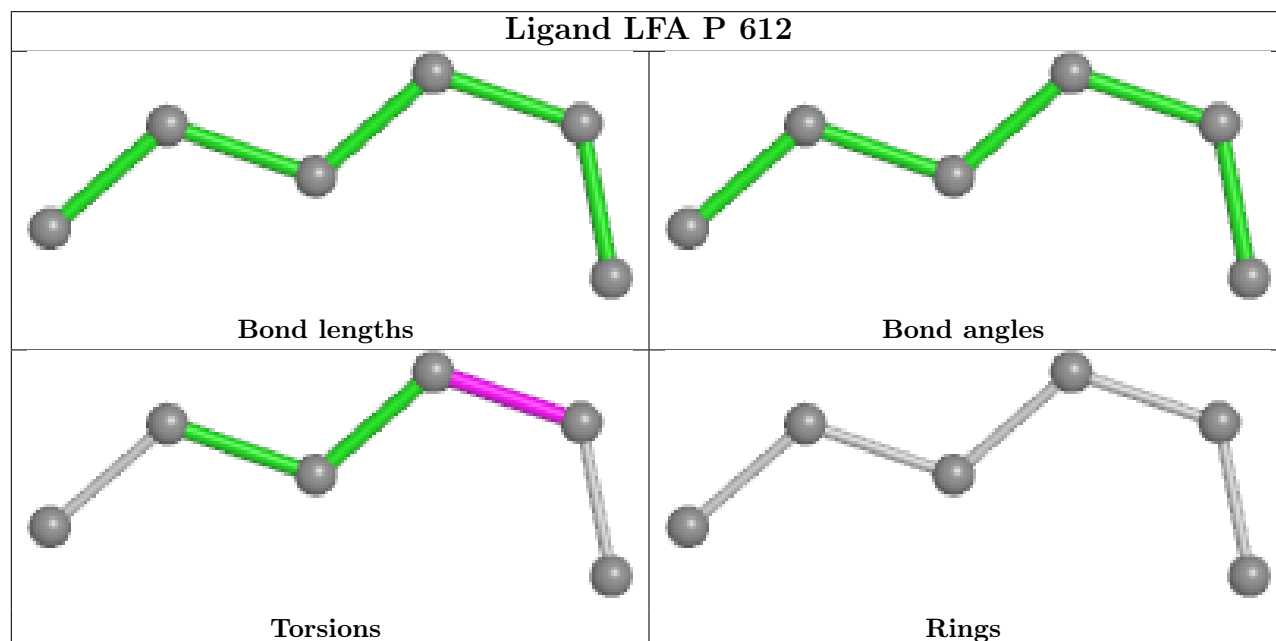
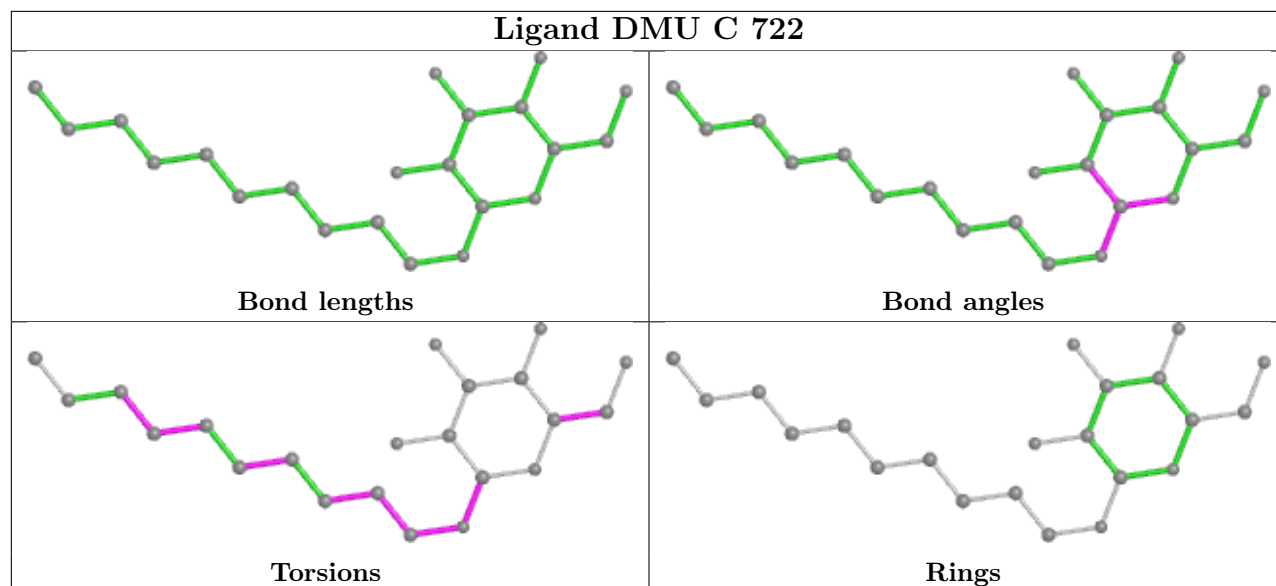
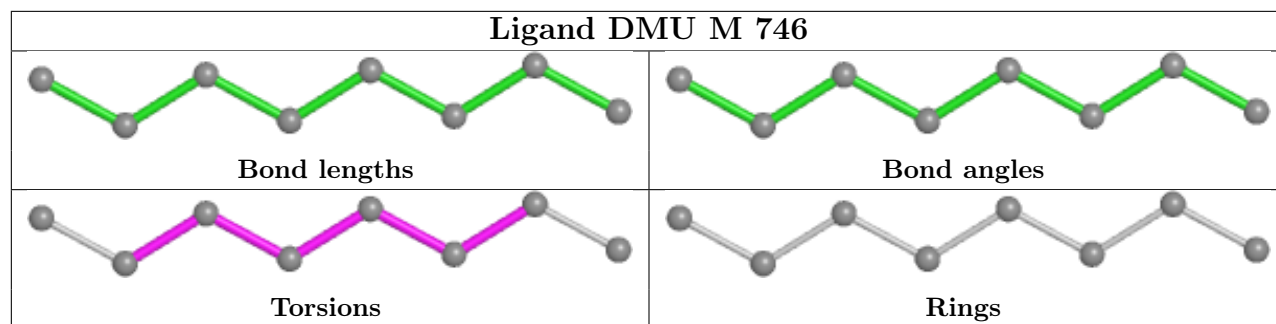


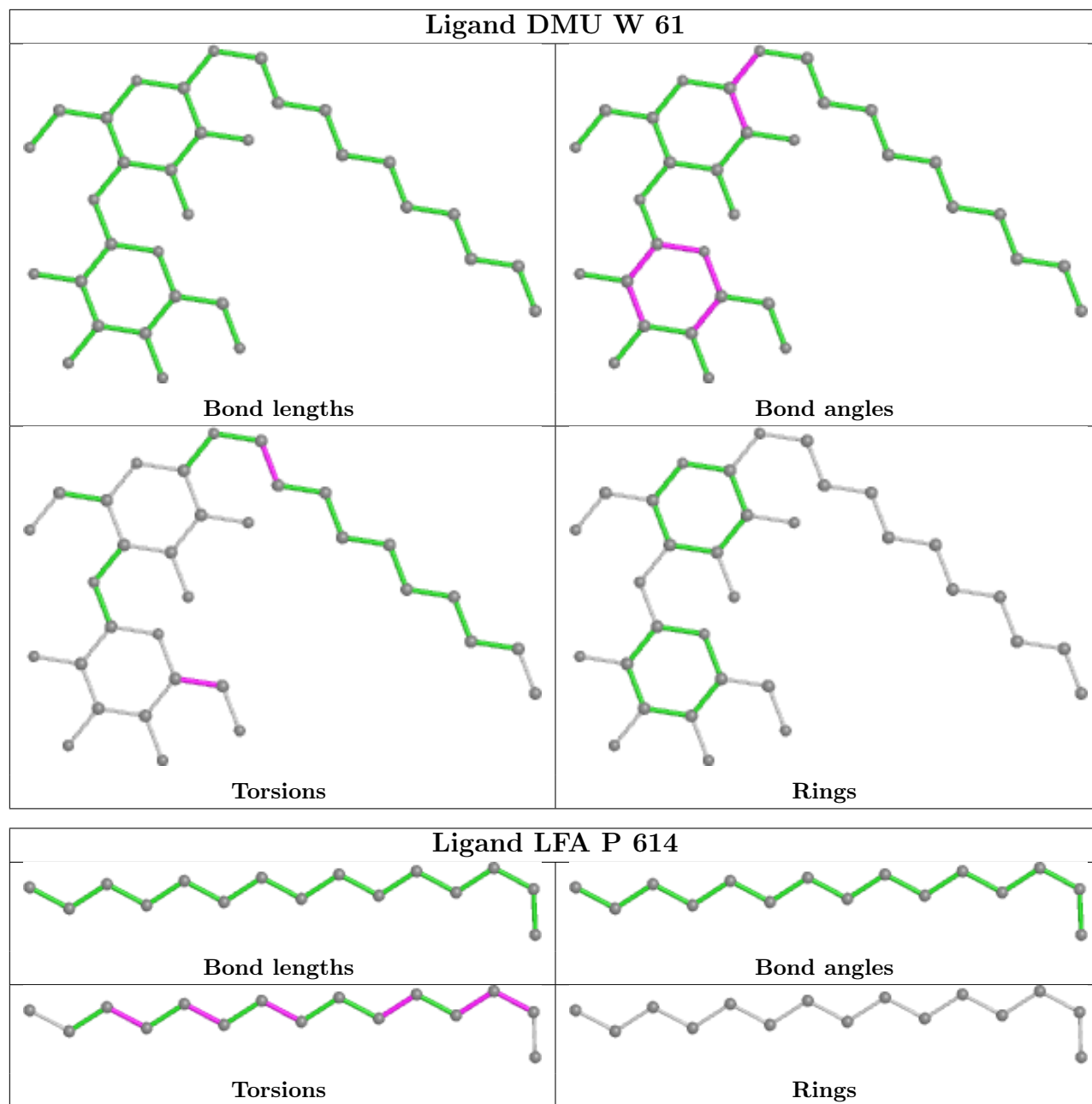


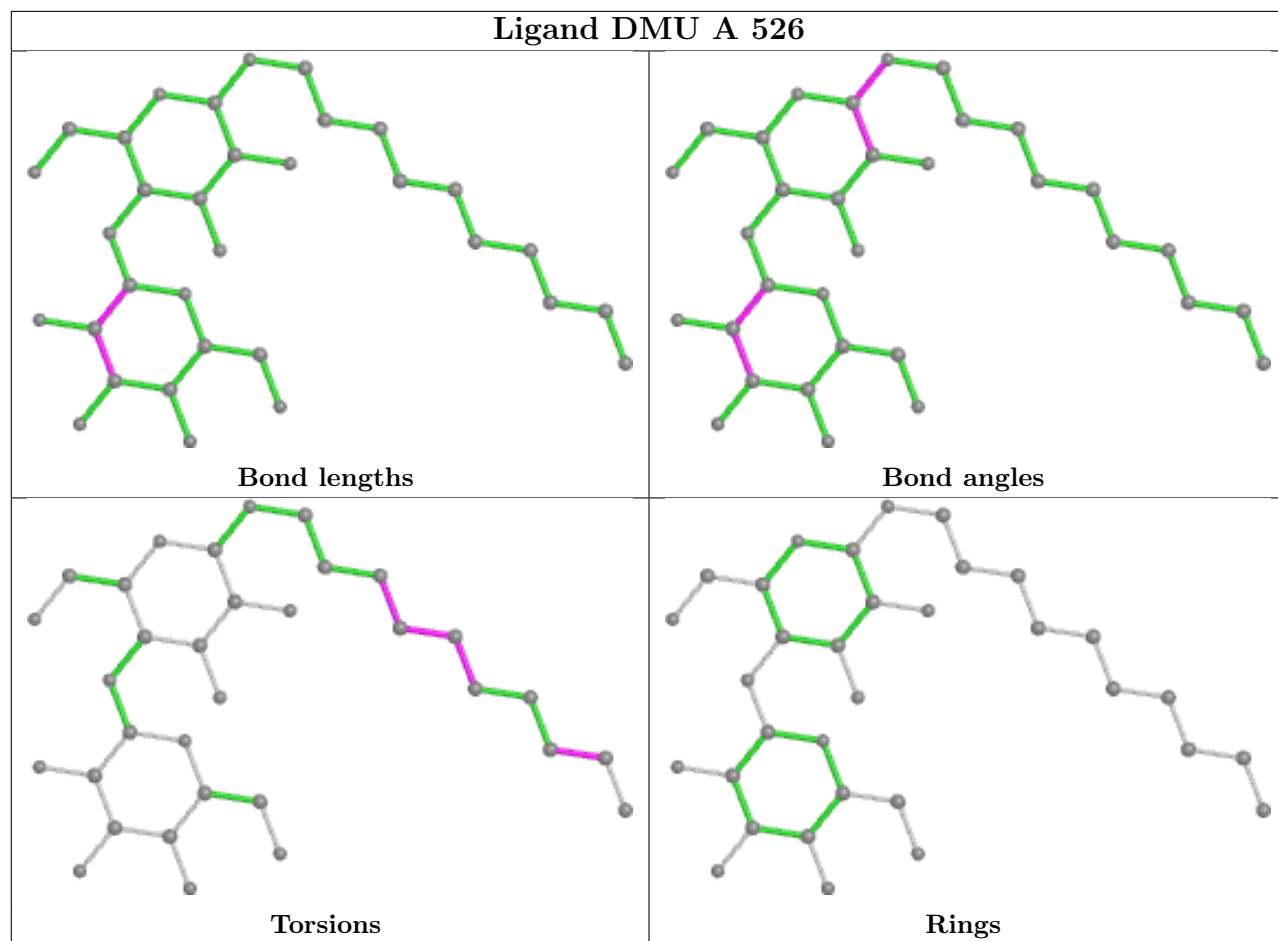


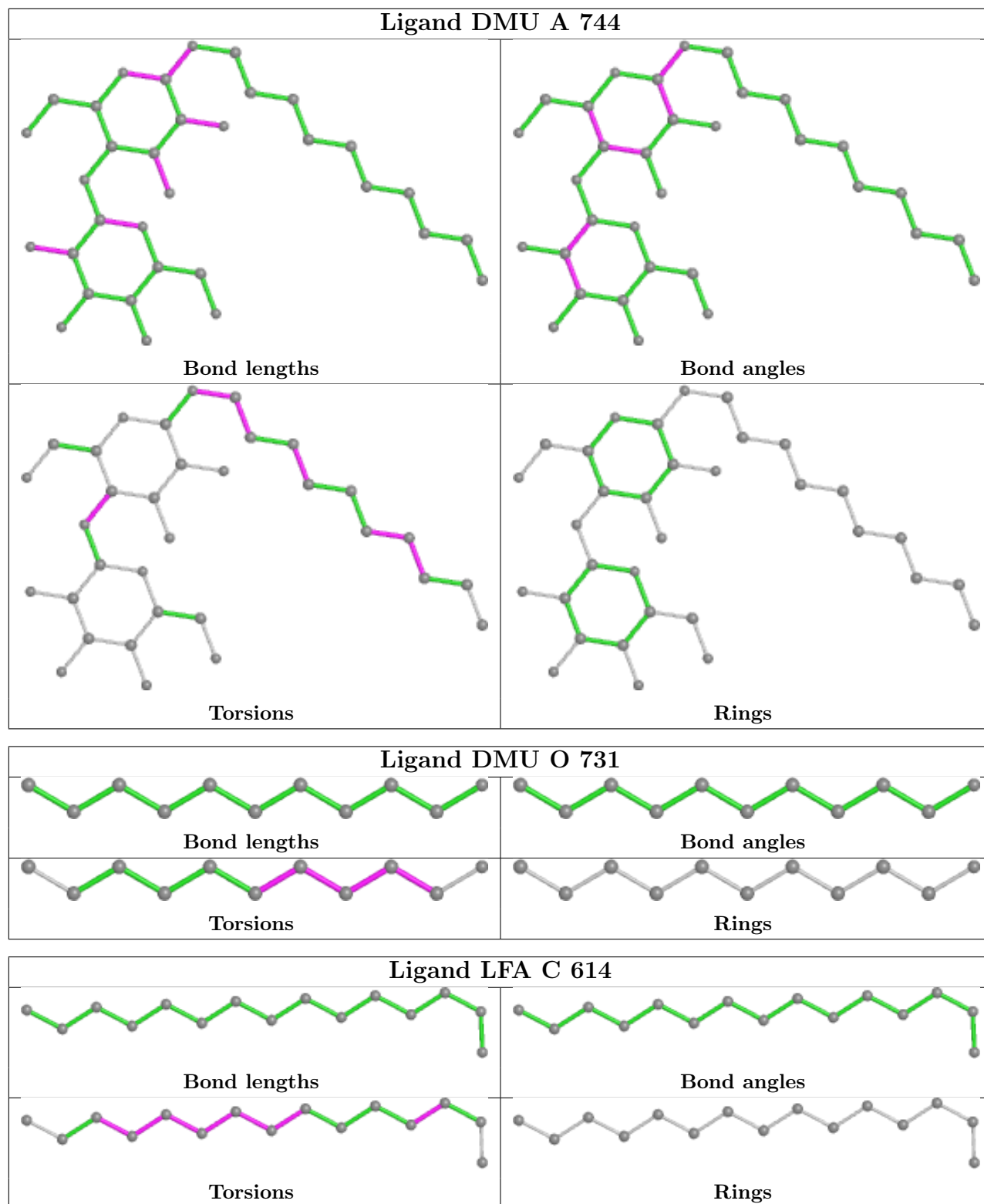


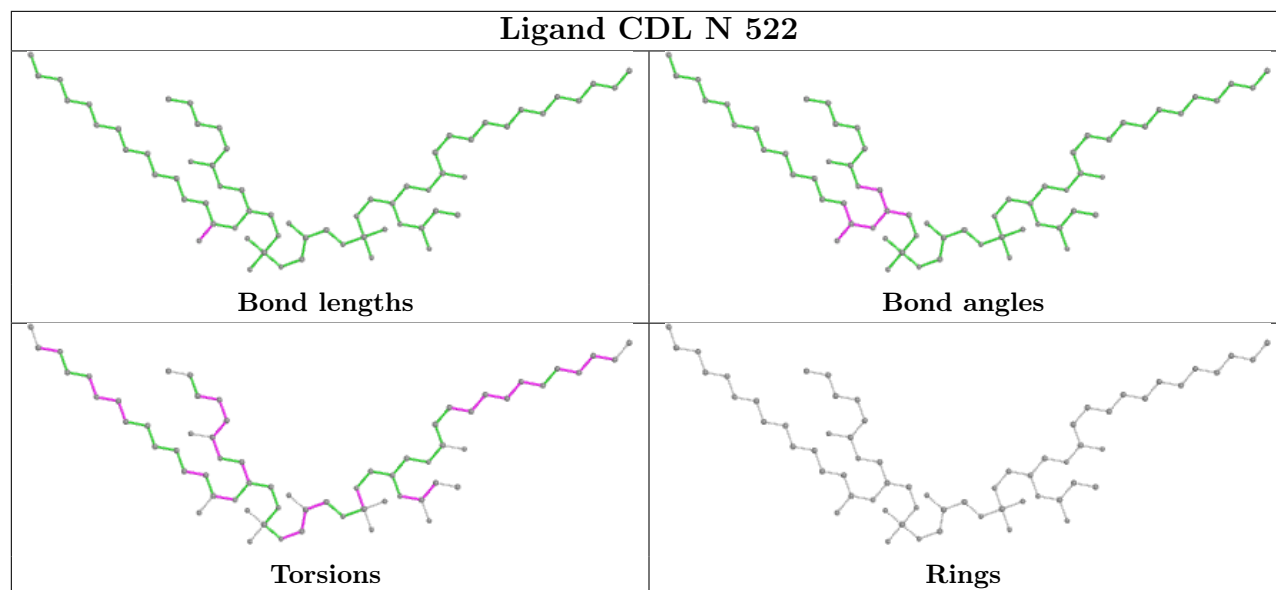












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	512/514 (99%)	-0.13	1 (0%) 95 94	16, 20, 28, 45	0
1	N	512/514 (99%)	-0.28	0 100 100	18, 23, 32, 48	0
2	B	226/227 (99%)	0.04	11 (4%) 29 27	18, 26, 48, 74	0
2	O	226/227 (99%)	-0.13	5 (2%) 62 61	23, 32, 57, 113	0
3	C	258/261 (98%)	-0.28	1 (0%) 92 91	18, 23, 34, 49	0
3	P	258/261 (98%)	-0.30	2 (0%) 86 86	19, 25, 37, 58	0
4	D	143/147 (97%)	-0.27	2 (1%) 75 77	22, 28, 42, 61	0
4	Q	137/147 (93%)	-0.04	2 (1%) 73 75	29, 41, 72, 88	0
5	E	102/109 (93%)	-0.43	1 (0%) 82 83	22, 28, 44, 60	0
5	R	102/109 (93%)	-0.49	0 100 100	26, 38, 54, 68	0
6	F	91/98 (92%)	-0.22	0 100 100	20, 29, 50, 59	0
6	S	91/98 (92%)	-0.21	1 (1%) 80 82	20, 28, 51, 57	0
7	G	72/85 (84%)	0.07	6 (8%) 11 8	22, 30, 76, 94	0
7	T	72/85 (84%)	0.11	8 (11%) 5 4	21, 34, 77, 99	0
8	H	75/85 (88%)	0.21	7 (9%) 8 6	23, 32, 79, 107	0
8	U	75/85 (88%)	0.14	7 (9%) 8 6	28, 36, 79, 101	0
9	I	70/73 (95%)	0.40	8 (11%) 5 4	26, 38, 63, 85	0
9	V	70/73 (95%)	0.52	7 (10%) 7 5	25, 46, 64, 94	0
10	J	56/59 (94%)	-0.02	3 (5%) 25 23	25, 34, 61, 67	0
10	W	56/59 (94%)	0.18	4 (7%) 16 13	27, 38, 58, 81	0
11	K	49/56 (87%)	-0.24	0 100 100	26, 33, 49, 59	0
11	X	49/56 (87%)	0.33	4 (8%) 11 8	33, 43, 69, 81	0
12	L	44/47 (93%)	-0.23	0 100 100	21, 25, 38, 57	0
12	Y	44/47 (93%)	-0.27	0 100 100	27, 33, 50, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	40/46 (86%)	-0.06	1 (2%) 57 56	21, 25, 46, 63	0
13	Z	40/46 (86%)	-0.06	2 (5%) 28 26	30, 37, 69, 71	0
All	All	3470/3614 (96%)	-0.13	83 (2%) 59 58	16, 27, 54, 113	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	36	TRP	8.2
10	W	1	PHE	8.0
8	H	45	ALA	7.9
10	J	1	PHE	7.5
11	X	6	ALA	7.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FME	B	1	10/11	0.94	0.13	21,34,59,119	0
2	FME	O	1	10/11	0.96	0.09	28,32,40,54	0
1	FME	N	1	10/11	0.97	0.10	35,41,72,79	0
1	FME	A	1	10/11	0.97	0.11	32,41,68,95	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	DMU	B	741	11/33	0.56	0.20	49,56,63,66	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	DMU	T	712	11/33	0.58	0.32	45,52,60,60	11
20	DMU	G	711	22/33	0.61	0.23	42,56,77,88	22
20	DMU	P	722	22/33	0.61	0.37	31,63,73,87	22
20	DMU	C	722	22/33	0.61	0.33	32,56,76,90	22
20	DMU	T	711	22/33	0.64	0.23	43,53,69,80	22
22	LFA	P	615	11/20	0.64	0.38	52,57,67,74	11
20	DMU	J	732	11/33	0.65	0.24	47,50,57,68	11
20	DMU	W	61	33/33	0.68	0.22	36,48,77,81	33
20	DMU	B	742	22/33	0.68	0.20	34,48,57,69	22
20	DMU	P	721	7/33	0.69	0.32	43,53,63,70	7
20	DMU	N	743	7/33	0.69	0.18	45,49,56,57	7
22	LFA	C	615	11/20	0.69	0.38	45,55,74,75	11
20	DMU	O	742	22/33	0.69	0.17	33,38,44,48	22
22	LFA	C	625	15/20	0.71	0.19	33,41,54,57	15
22	LFA	C	614	15/20	0.72	0.27	38,46,57,58	15
20	DMU	W	732	11/33	0.72	0.34	49,54,59,70	11
20	DMU	C	733	33/33	0.72	0.24	38,48,60,65	33
20	DMU	Y	747	22/33	0.72	0.24	35,55,76,79	22
22	LFA	P	623	14/20	0.73	0.24	32,53,60,63	14
20	DMU	O	741	11/33	0.74	0.23	40,45,52,66	11
20	DMU	A	743	7/33	0.74	0.19	42,46,50,53	7
23	EDO	E	811	4/4	0.74	0.19	29,31,33,35	4
22	LFA	P	614	15/20	0.75	0.25	40,46,58,59	15
22	LFA	P	626	13/20	0.76	0.23	38,50,62,64	13
22	LFA	A	628	14/20	0.76	0.21	33,41,48,51	14
22	LFA	C	612	6/20	0.77	0.29	39,43,45,49	6
20	DMU	G	712	11/33	0.77	0.26	35,46,52,65	11
20	DMU	N	744	33/33	0.77	0.14	28,43,59,67	33
22	LFA	P	611	11/20	0.78	0.25	28,39,44,46	11
20	DMU	C	734	33/33	0.78	0.20	38,54,63,66	33
22	LFA	P	716[B]	18/20	0.78	0.14	37,49,60,62	18
20	DMU	P	733	33/33	0.78	0.21	40,50,59,68	33
22	LFA	P	624	11/20	0.79	0.30	42,47,54,60	11
22	LFA	C	623	14/20	0.79	0.18	34,48,54,55	14
20	DMU	J	61	33/33	0.79	0.23	33,43,65,71	33
20	DMU	N	745	33/33	0.79	0.22	33,46,72,87	33
22	LFA	N	628	14/20	0.80	0.22	35,42,66,68	14
22	LFA	C	624	11/20	0.80	0.27	37,48,53,54	11
20	DMU	C	714	33/33	0.80	0.22	33,39,57,61	33
20	DMU	G	713	22/33	0.81	0.19	41,52,58,61	22
20	DMU	C	721	7/33	0.81	0.23	45,49,53,64	7
22	LFA	G	622	11/20	0.81	0.21	39,51,56,60	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	LFA	P	625	15/20	0.81	0.17	35,41,61,63	15
20	DMU	A	745	33/33	0.81	0.15	24,32,44,57	33
20	DMU	L	747	22/33	0.81	0.20	37,47,57,64	22
20	DMU	P	734	33/33	0.81	0.20	48,60,72,80	33
22	LFA	G	621	17/20	0.82	0.17	29,53,64,64	17
20	DMU	C	715[A]	33/33	0.82	0.19	26,35,43,61	33
19	CHD	P	271	29/29	0.82	0.29	48,66,110,128	0
22	LFA	C	716[B]	18/20	0.82	0.15	34,49,89,90	18
20	DMU	P	714	33/33	0.83	0.18	34,42,59,78	33
20	DMU	B	731	11/33	0.83	0.17	36,51,59,63	11
22	LFA	C	626	13/20	0.83	0.17	41,45,51,54	13
18	CDL	C	270	87/100	0.83	0.24	34,82,121,135	0
20	DMU	O	731	11/33	0.85	0.26	46,48,52,67	11
20	DMU	P	272	11/33	0.85	0.20	42,47,55,60	11
18	CDL	P	270	87/100	0.85	0.24	34,78,126,150	0
20	DMU	Z	746	8/33	0.85	0.17	44,47,52,56	8
22	LFA	T	621	17/20	0.85	0.18	34,49,66,69	17
20	DMU	P	715[A]	33/33	0.85	0.20	27,37,49,61	33
19	CHD	C	271	29/29	0.86	0.29	44,58,76,95	0
22	LFA	T	622	11/20	0.86	0.17	41,54,62,65	11
23	EDO	C	807	4/4	0.86	0.20	42,45,46,60	4
20	DMU	T	713	22/33	0.86	0.15	37,48,54,59	22
22	LFA	P	612	6/20	0.87	0.28	39,40,41,44	6
22	LFA	N	627	14/20	0.87	0.18	28,38,54,55	14
20	DMU	C	272	11/33	0.87	0.14	45,51,57,68	11
18	CDL	N	522	64/100	0.87	0.20	46,82,132,158	0
18	CDL	N	521	94/100	0.88	0.27	37,83,124,140	0
22	LFA	C	611	11/20	0.88	0.21	36,43,48,49	11
20	DMU	M	746	8/33	0.88	0.16	35,44,48,49	8
20	DMU	N	526	33/33	0.89	0.16	41,49,61,72	0
18	CDL	A	522	64/100	0.89	0.17	38,71,110,133	0
23	EDO	N	801	4/4	0.89	0.09	17,17,19,23	4
18	CDL	A	521	94/100	0.90	0.21	28,71,121,139	0
22	LFA	A	627	14/20	0.90	0.20	28,38,66,70	14
23	EDO	P	807	4/4	0.90	0.13	47,48,50,59	4
23	EDO	N	829	4/4	0.91	0.09	27,30,31,33	4
20	DMU	A	744	33/33	0.91	0.11	21,32,44,65	33
23	EDO	P	827	4/4	0.91	0.17	23,24,30,32	4
19	CHD	A	525	29/29	0.92	0.08	22,26,29,33	0
23	EDO	A	801	4/4	0.92	0.10	17,18,20,22	4
23	EDO	R	811	4/4	0.92	0.12	45,46,50,53	4
23	EDO	A	825	4/4	0.93	0.08	33,33,34,42	4

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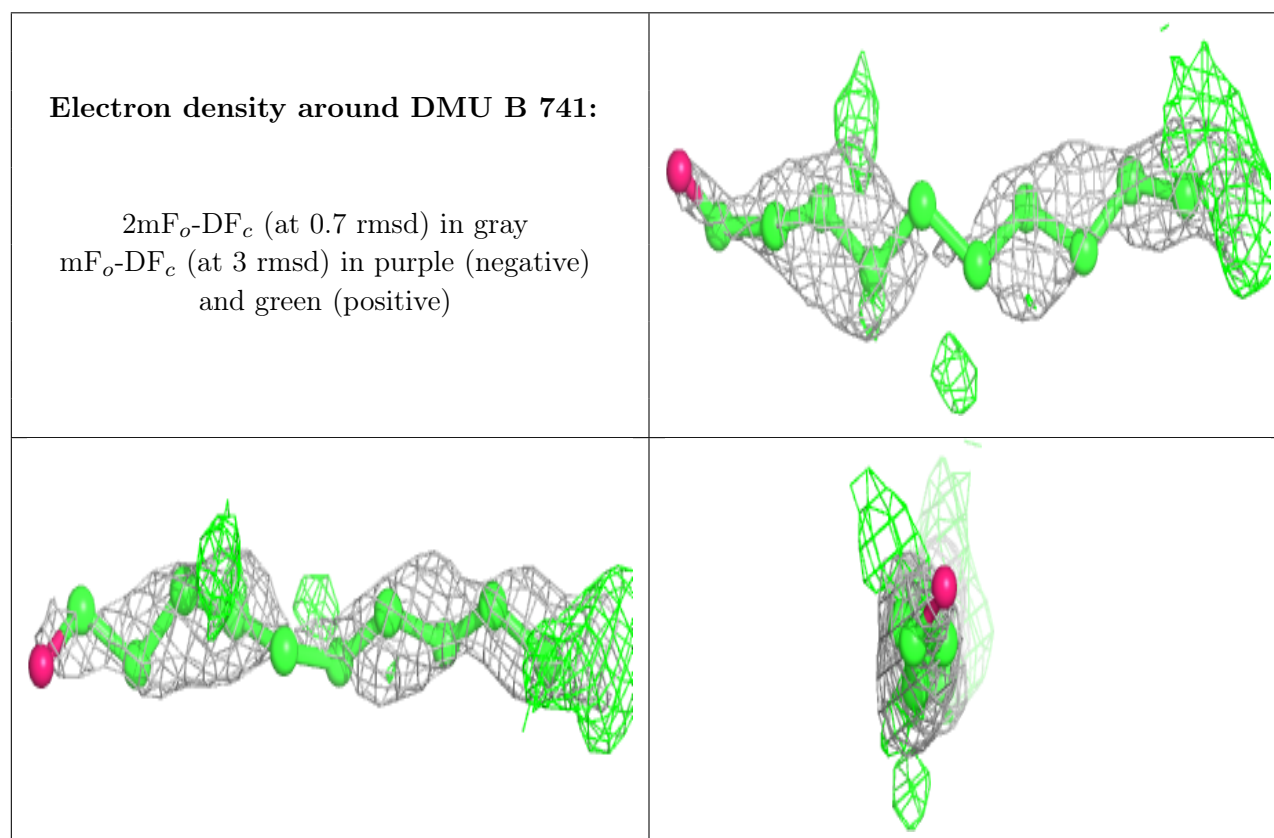
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	CHD	G	86	29/29	0.94	0.07	20,23,28,36	0
23	EDO	C	809	4/4	0.94	0.08	22,23,29,32	4
23	EDO	C	827	4/4	0.94	0.16	23,26,27,29	4
19	CHD	N	525	29/29	0.94	0.06	23,26,29,34	0
23	EDO	G	821	4/4	0.94	0.13	23,24,29,30	4
23	EDO	S	817	4/4	0.94	0.10	13,14,16,19	4
23	EDO	B	805	4/4	0.95	0.13	17,21,21,25	4
20	DMU	A	526	33/33	0.95	0.09	32,39,54,58	0
19	CHD	T	86	29/29	0.95	0.07	21,24,28,35	0
23	EDO	E	813	4/4	0.96	0.14	22,24,25,25	4
23	EDO	F	817	4/4	0.96	0.13	13,13,16,20	4
23	EDO	R	813	4/4	0.96	0.13	27,28,29,29	4
23	EDO	P	809	4/4	0.96	0.07	27,28,28,36	4
23	EDO	S	819	4/4	0.96	0.08	20,21,21,30	4
23	EDO	F	819	4/4	0.97	0.07	22,22,27,29	4
23	EDO	E	815	4/4	0.97	0.16	25,28,29,32	4
23	EDO	R	815	4/4	0.97	0.11	38,39,42,43	4
23	EDO	A	803	4/4	0.97	0.10	23,29,37,39	4
23	EDO	N	803	4/4	0.97	0.11	26,26,37,42	4
23	EDO	T	821	4/4	0.97	0.09	25,27,29,32	4
25	UNX	P	262	1/1	0.97	0.21	34,34,34,34	0
26	PEK	P	264	53/53	0.97	0.09	26,46,102,108	0
23	EDO	O	805	4/4	0.98	0.08	23,24,27,29	4
23	EDO	N	823	4/4	0.98	0.13	19,21,22,22	4
23	EDO	N	825	4/4	0.98	0.08	27,28,29,30	4
26	PEK	C	264	53/53	0.98	0.09	24,42,96,129	0
23	EDO	A	823	4/4	0.98	0.15	17,17,19,24	4
27	PGV	C	266	51/51	0.98	0.09	19,28,65,76	0
27	PGV	C	267	51/51	0.98	0.09	20,28,75,94	0
27	PGV	P	266	51/51	0.98	0.09	22,31,61,65	0
27	PGV	P	267	51/51	0.98	0.09	20,30,91,105	0
14	HEA	A	515[A]	60/60	0.99	0.09	15,18,29,35	9
14	HEA	A	515[B]	60/60	0.99	0.09	15,18,29,34	9
14	HEA	A	516	60/60	0.99	0.07	15,17,23,26	0
25	UNX	C	262	1/1	0.99	0.24	36,36,36,36	0
14	HEA	N	515[A]	60/60	0.99	0.07	19,21,32,39	9
14	HEA	N	515[B]	60/60	0.99	0.07	19,21,29,33	9
14	HEA	N	516	60/60	0.99	0.07	18,19,25,28	0
21	PER	A	520	2/2	0.99	0.17	20,20,20,26	0
21	PER	N	520	2/2	0.99	0.17	19,19,19,26	0
15	CU	N	517	1/1	0.99	0.12	20,20,20,20	0
16	MG	A	518	1/1	0.99	0.08	19,19,19,19	0

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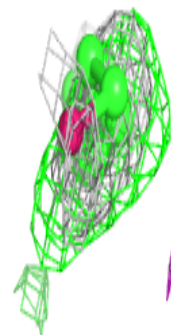
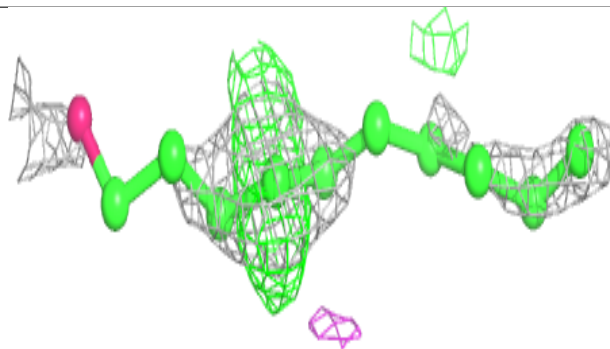
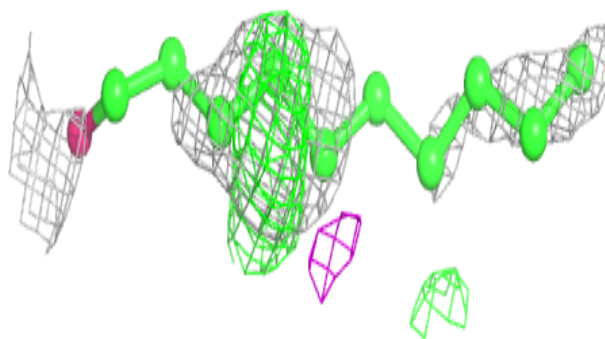
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	ZN	F	99	1/1	0.99	0.11	24,24,24,24	0
17	NA	A	519	1/1	1.00	0.09	21,21,21,21	0
24	CUA	B	228	2/2	1.00	0.13	19,19,19,19	0
24	CUA	O	228	2/2	1.00	0.12	24,24,24,25	0
17	NA	N	519	1/1	1.00	0.07	28,28,28,28	0
15	CU	A	517	1/1	1.00	0.12	17,17,17,17	0
16	MG	N	518	1/1	1.00	0.08	23,23,23,23	0
28	ZN	S	99	1/1	1.00	0.11	25,25,25,25	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.

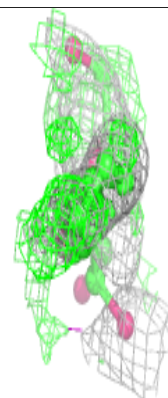
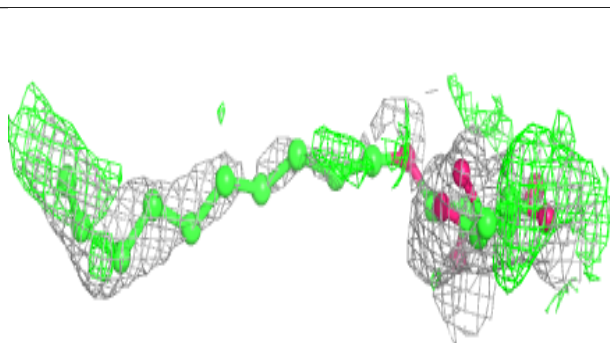
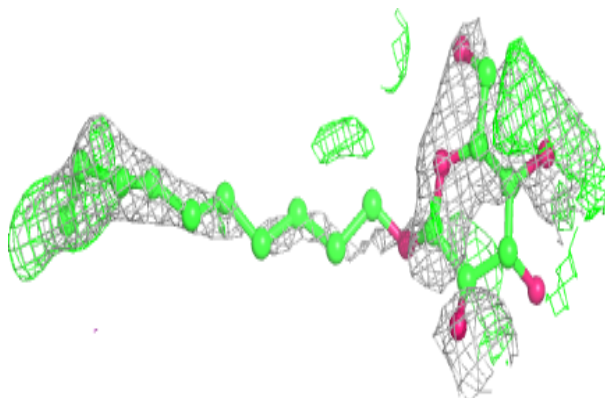


Electron density around DMU T 712:

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

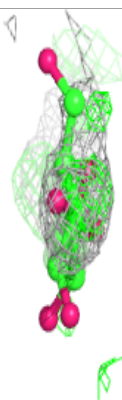
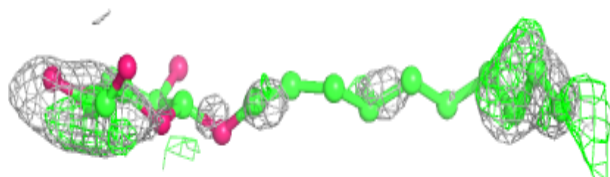
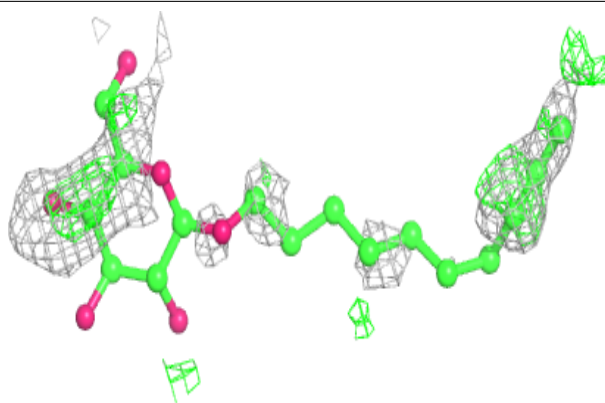
**Electron density around DMU G 711:**

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

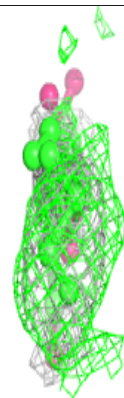
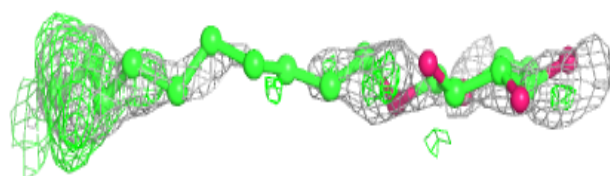
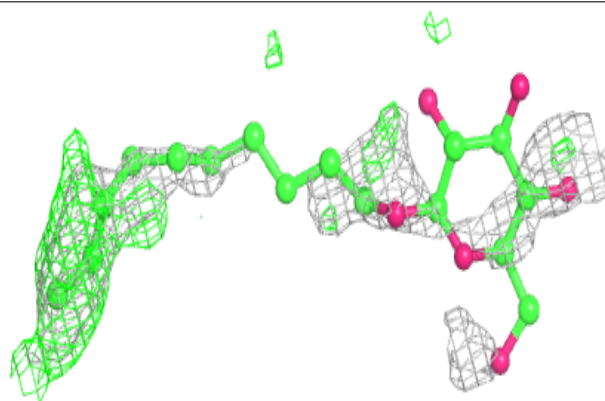


Electron density around DMU P 722:

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

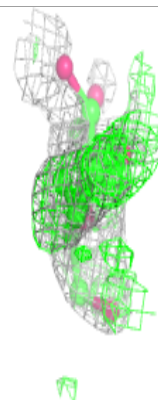
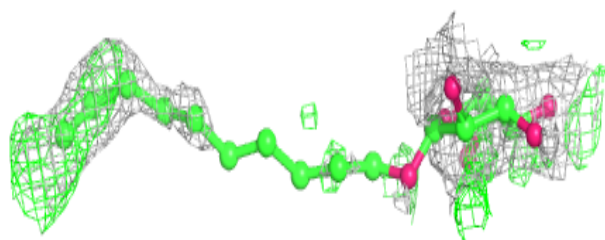
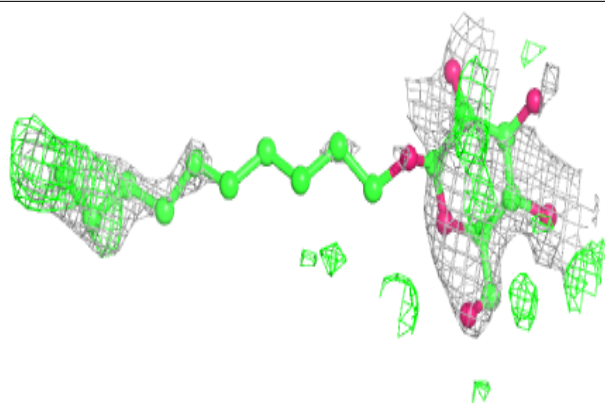
**Electron density around DMU C 722:**

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

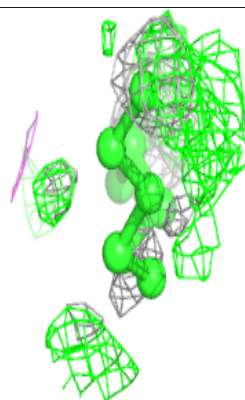
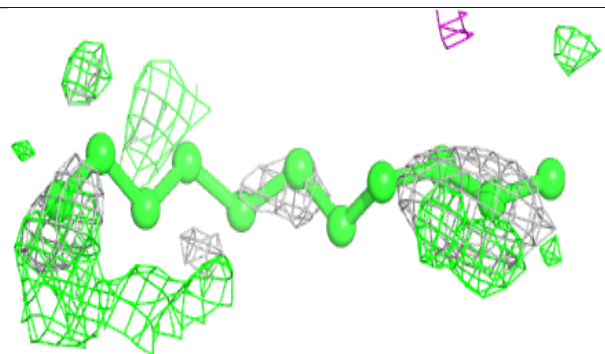
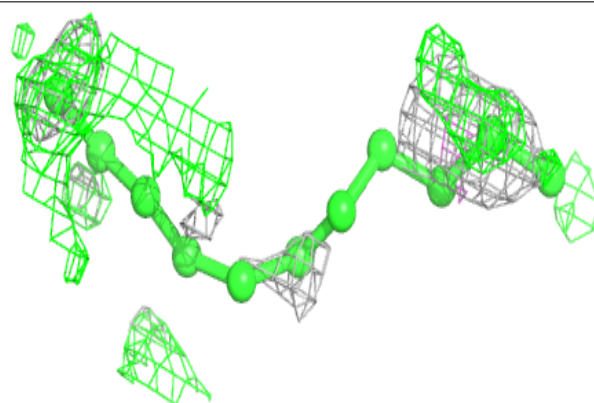


Electron density around DMU T 711:

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

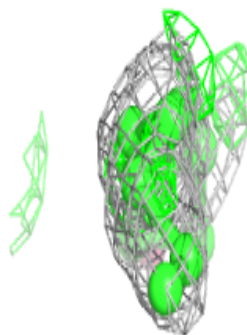
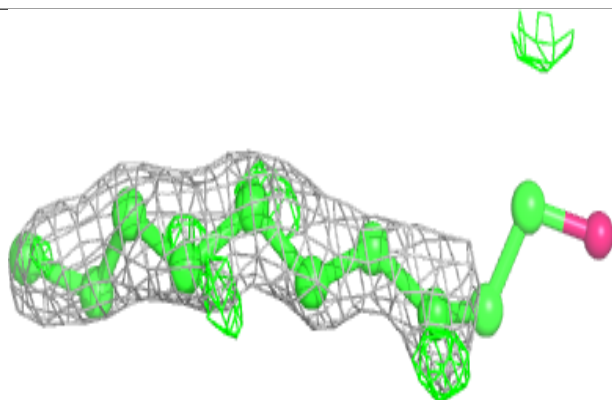
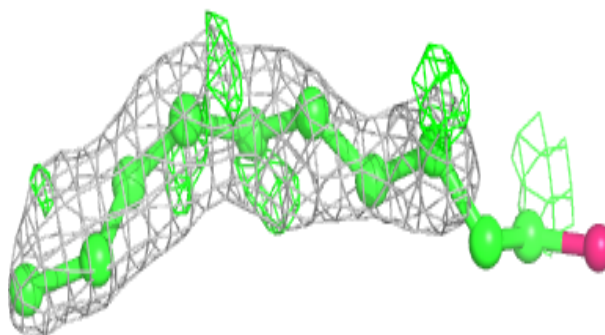
**Electron density around LFA P 615:**

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

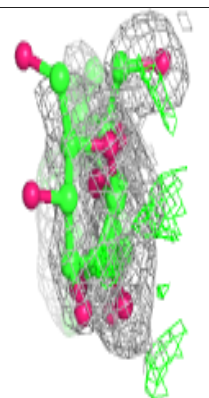
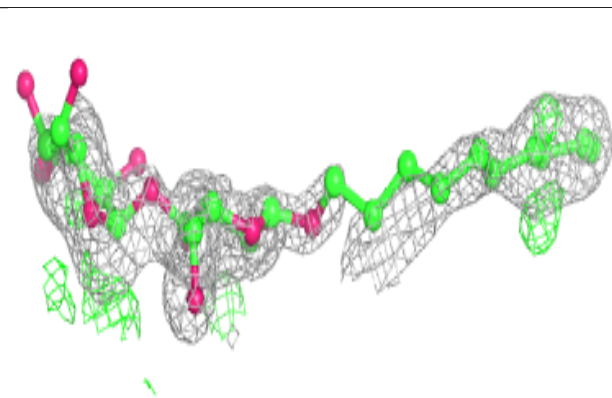
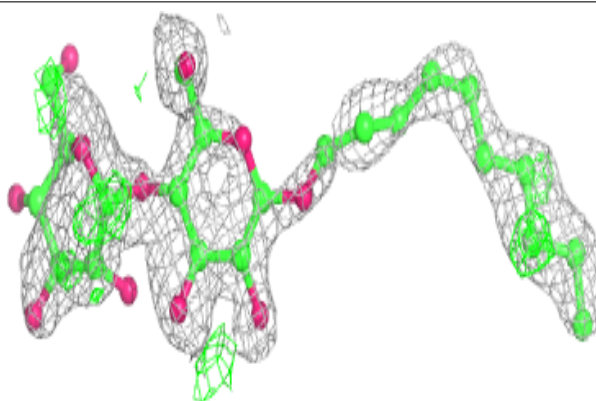


Electron density around DMU J 732:

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

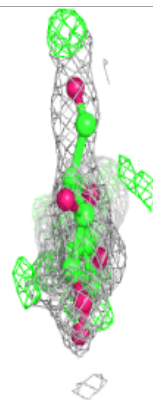
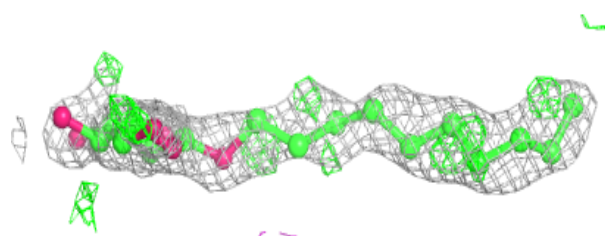
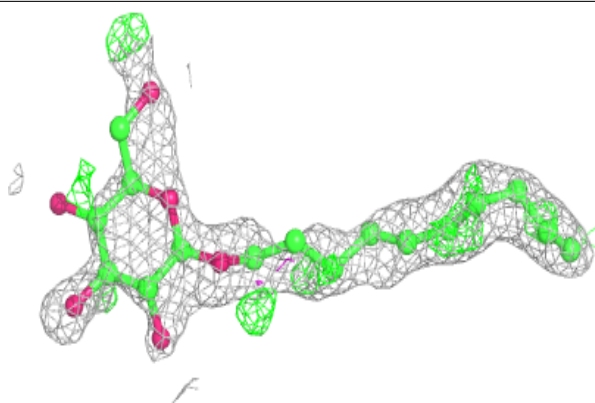
**Electron density around DMU W 61:**

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

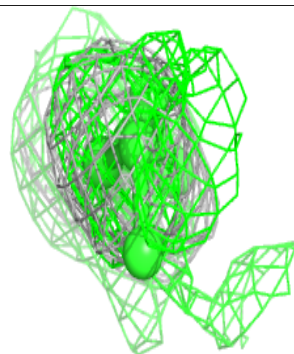
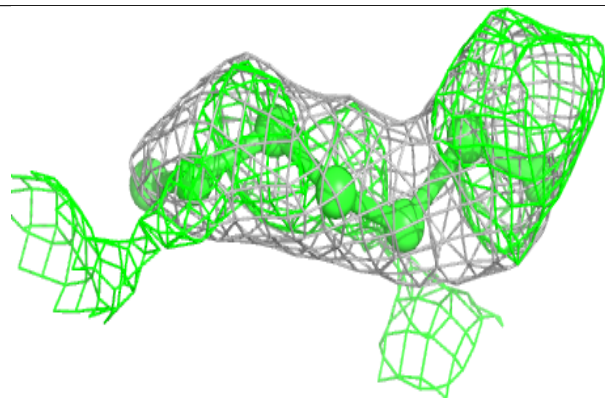
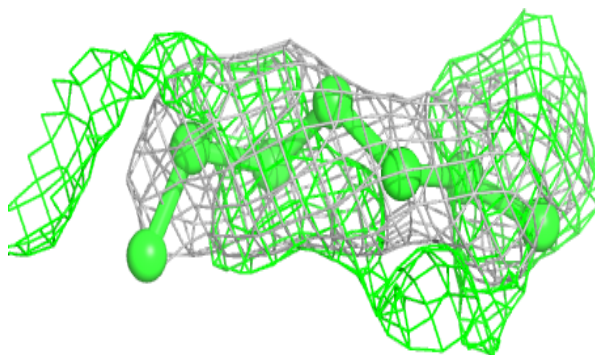


Electron density around DMU B 742:

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

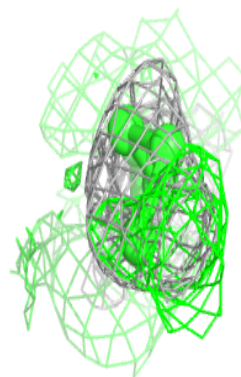
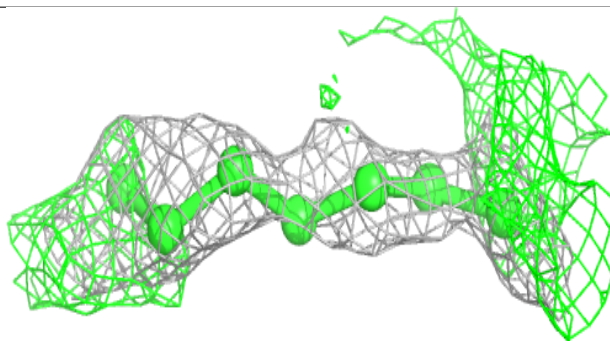
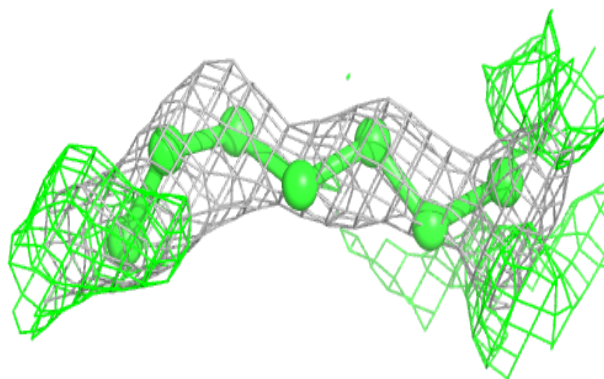
**Electron density around DMU P 721:**

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

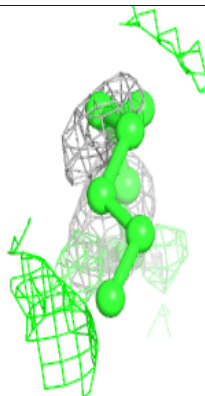
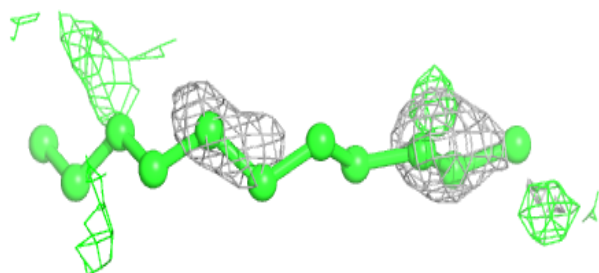
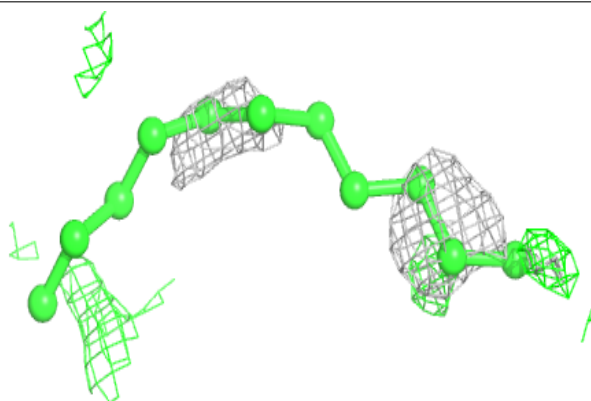


Electron density around DMU N 743:

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

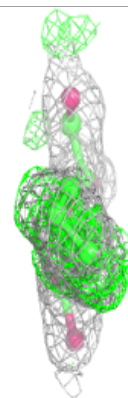
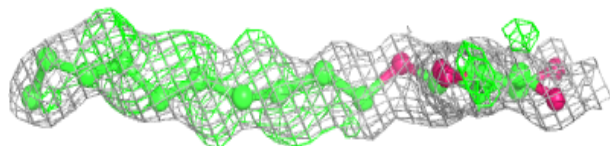
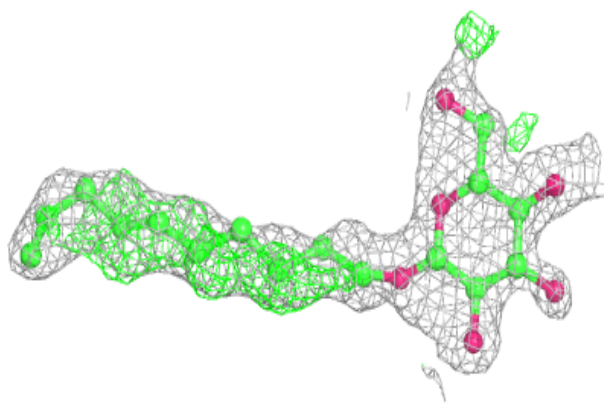
**Electron density around LFA C 615:**

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

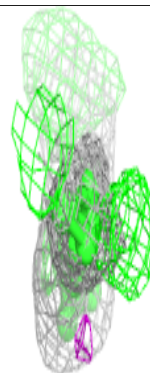
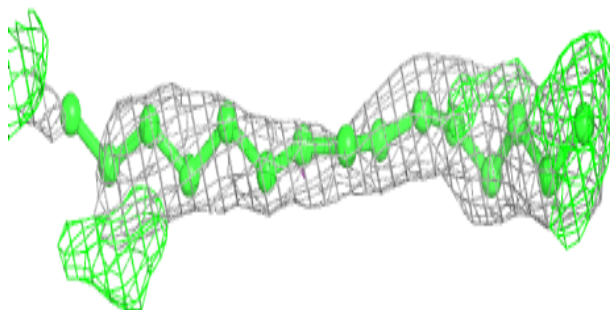
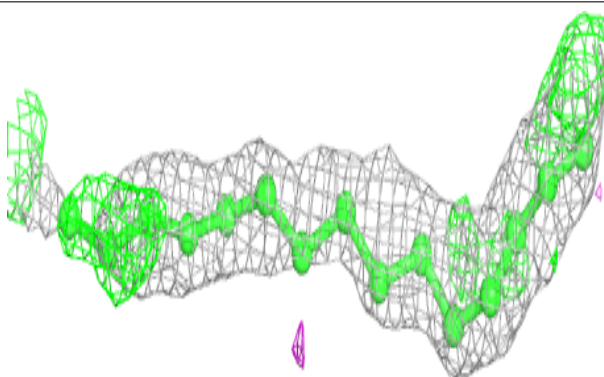


Electron density around DMU O 742:

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

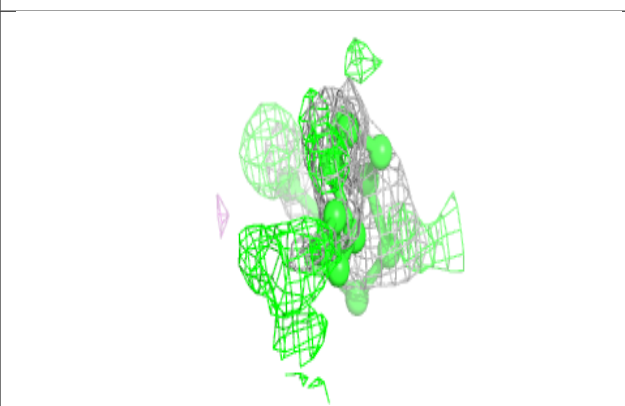
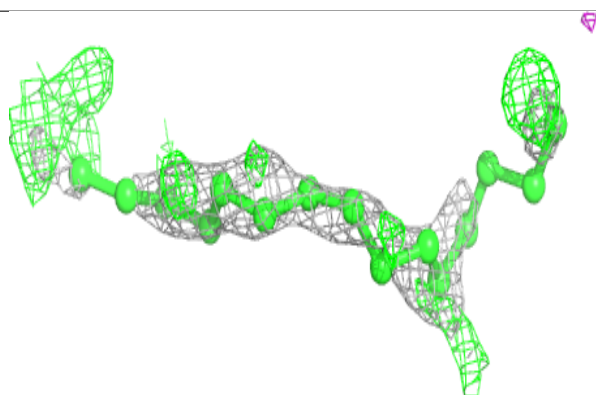
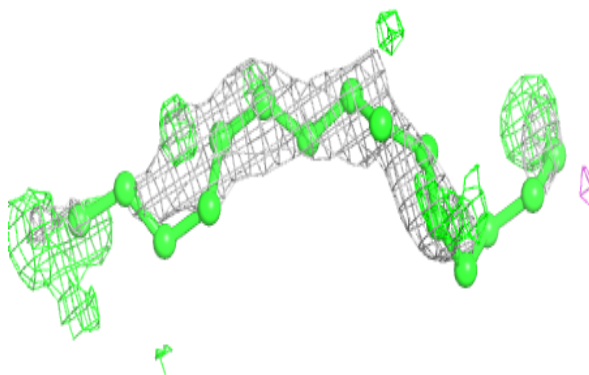
**Electron density around LFA C 625:**

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

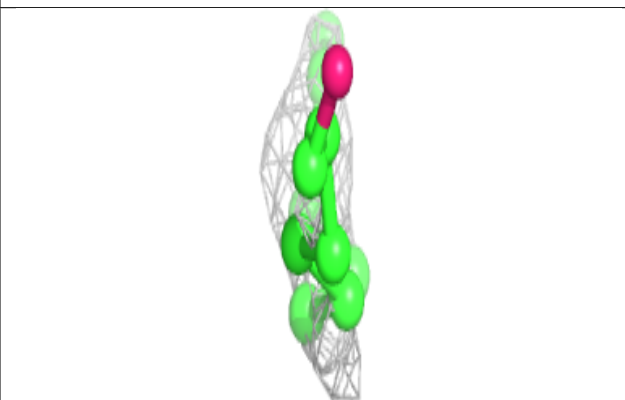
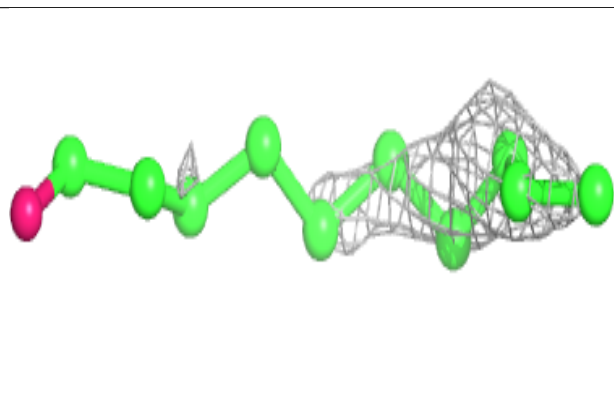
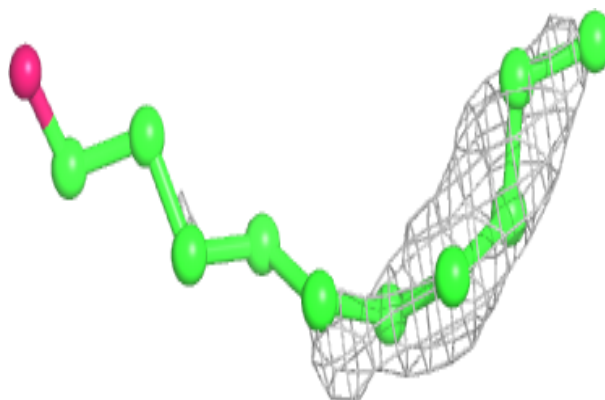


Electron density around LFA C 614:

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

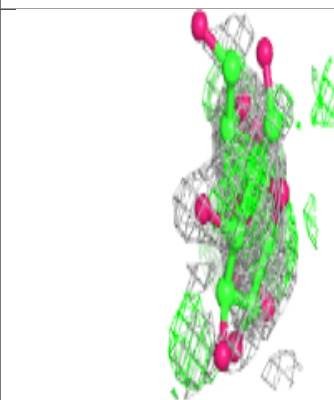
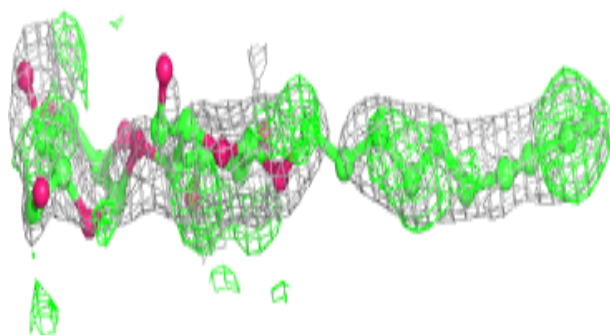
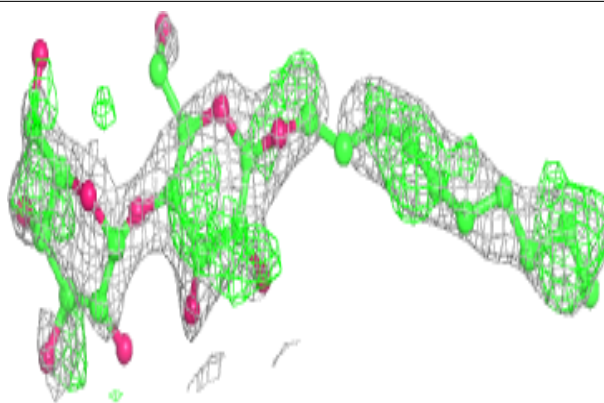
**Electron density around DMU W 732:**

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

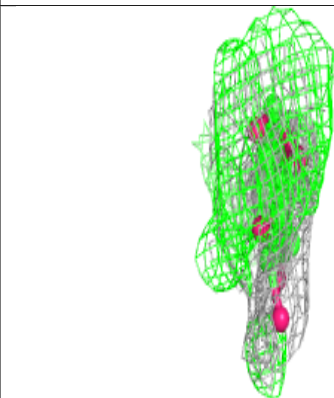
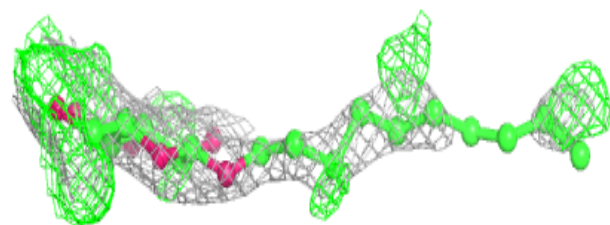
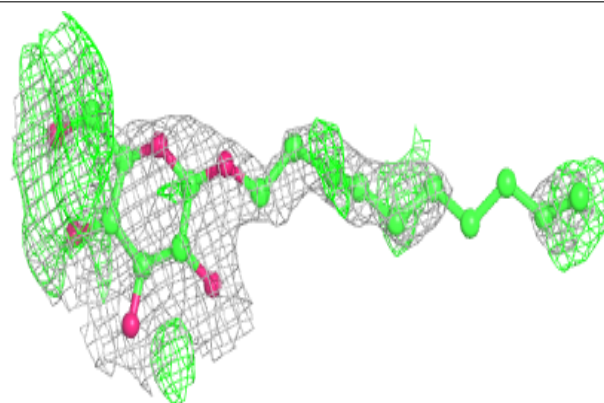


Electron density around DMU C 733:

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

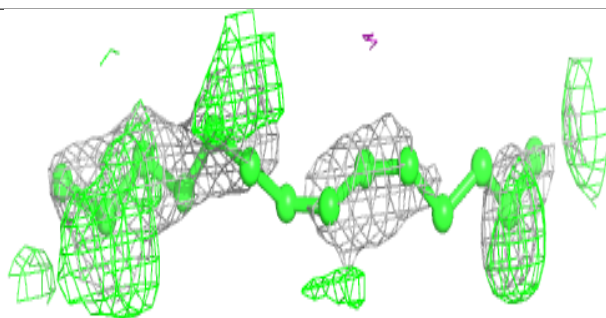
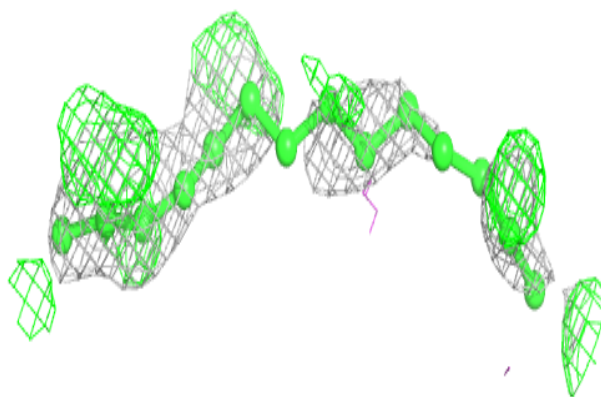
**Electron density around DMU Y 747:**

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

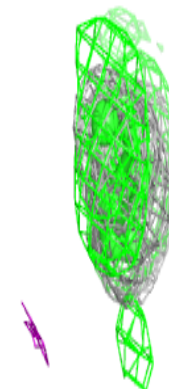
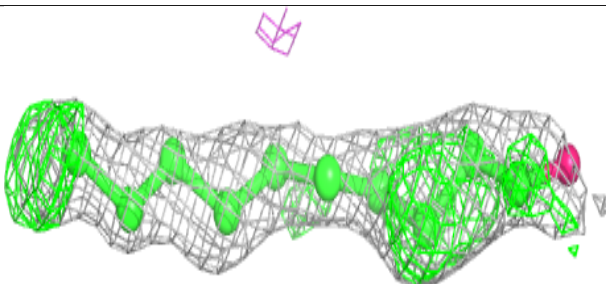
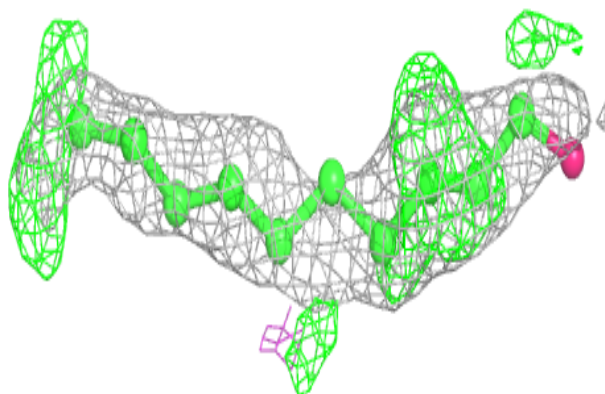


Electron density around LFA P 623:

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

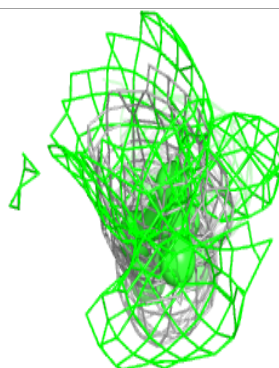
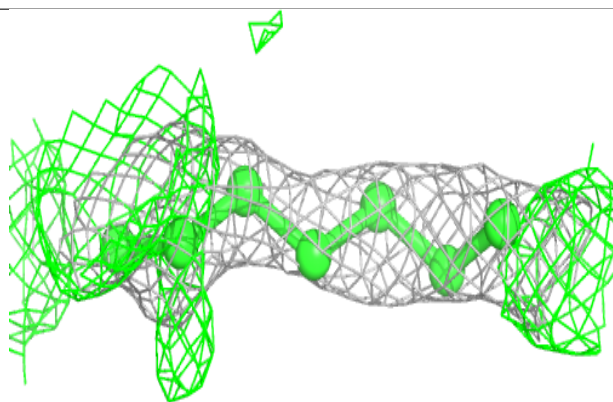
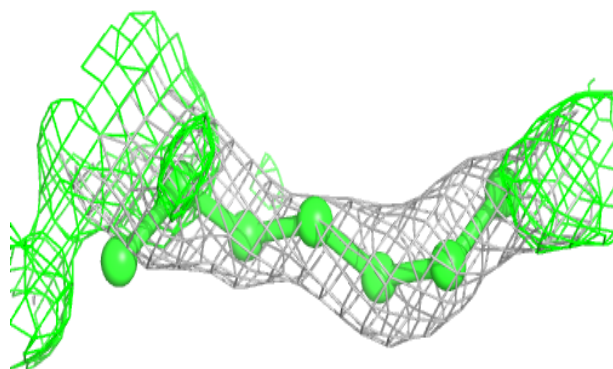
**Electron density around DMU O 741:**

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

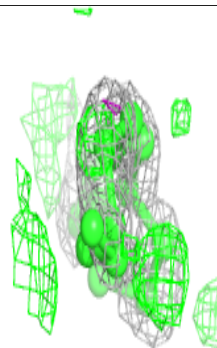
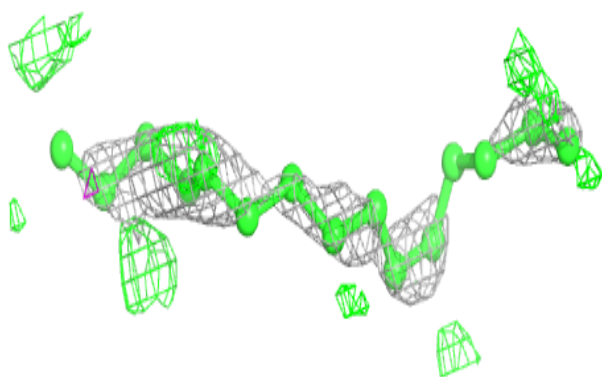
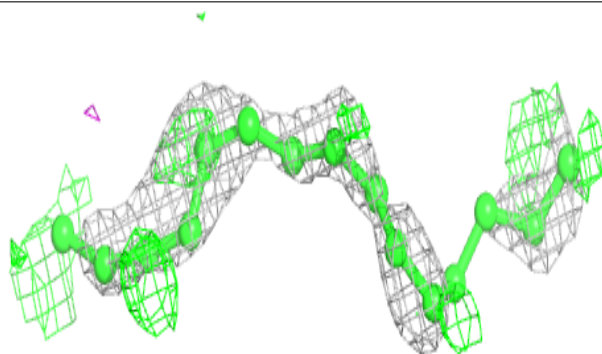


Electron density around DMU A 743:

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

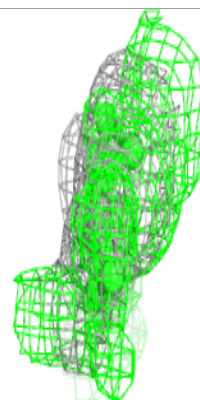
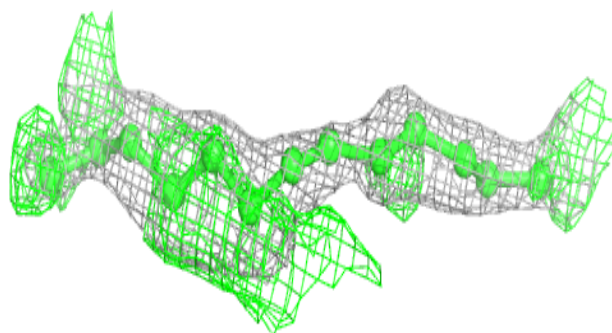
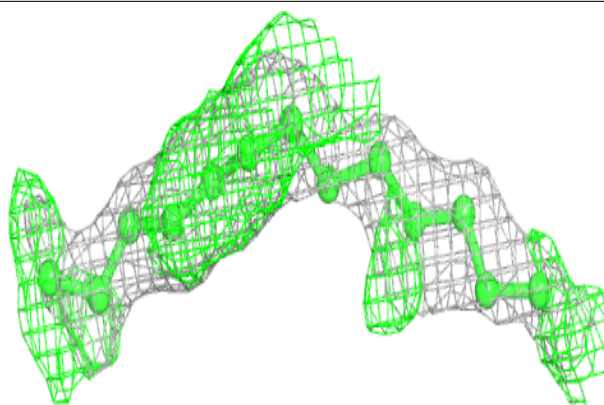
**Electron density around LFA P 614:**

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

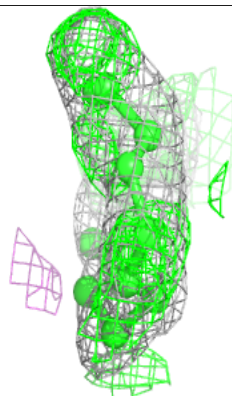
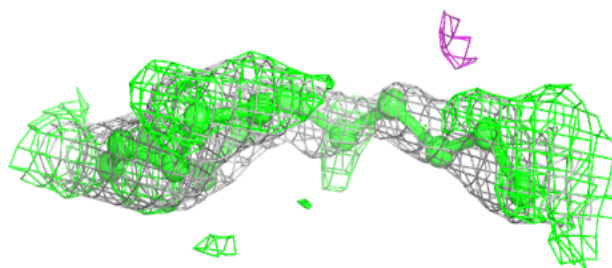
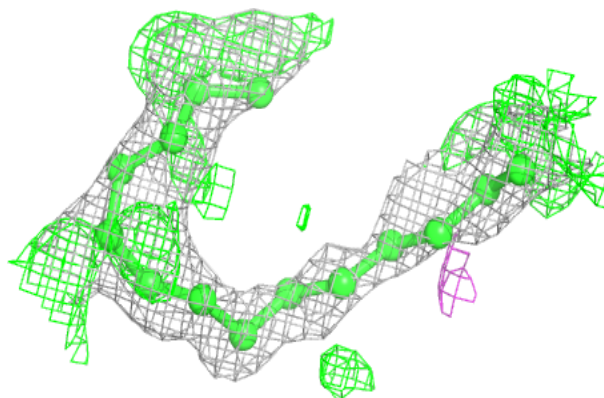


Electron density around LFA P 626:

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

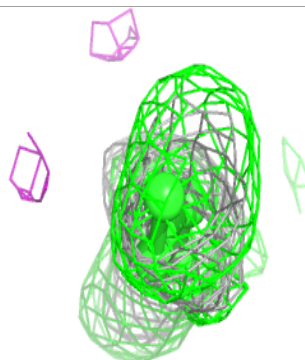
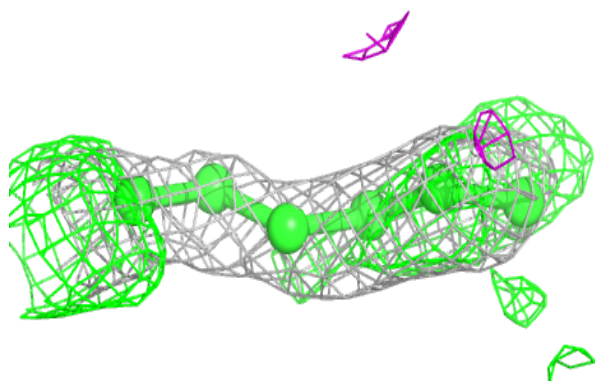
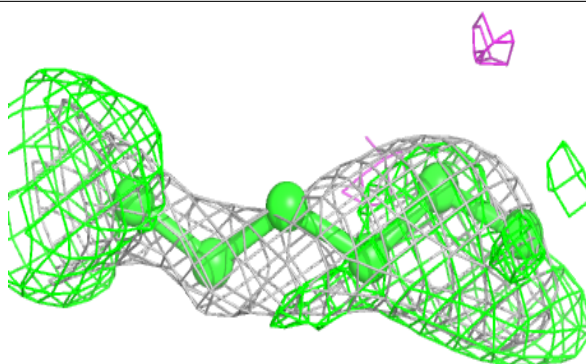
**Electron density around LFA A 628:**

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

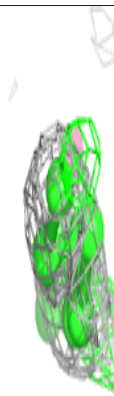
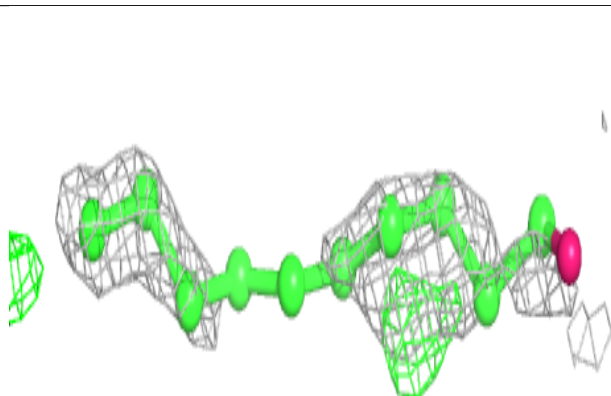
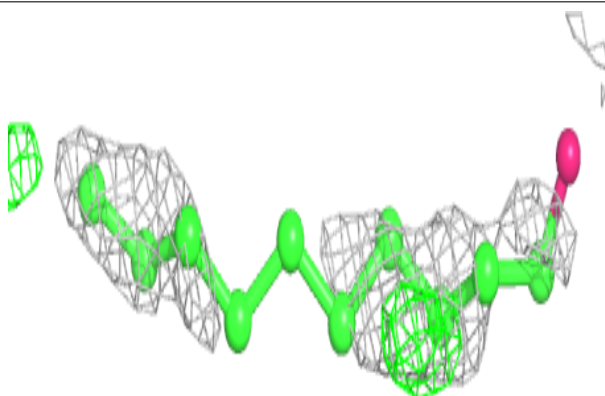


Electron density around LFA C 612:

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

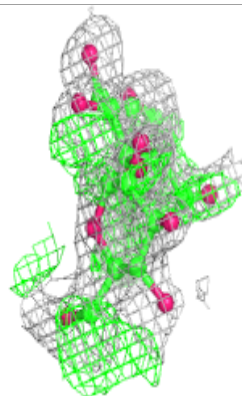
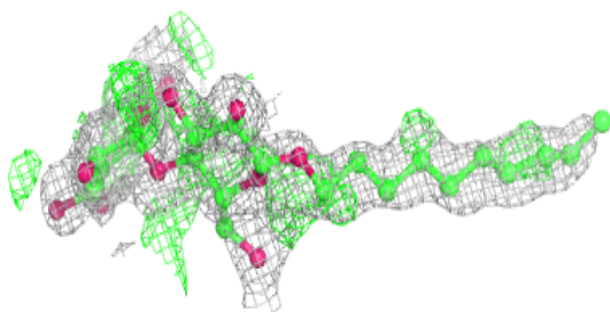
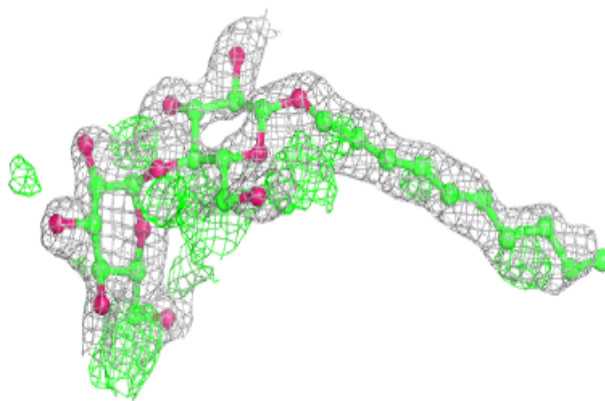
**Electron density around DMU G 712:**

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

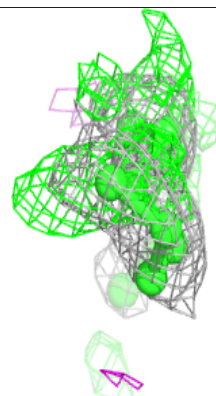
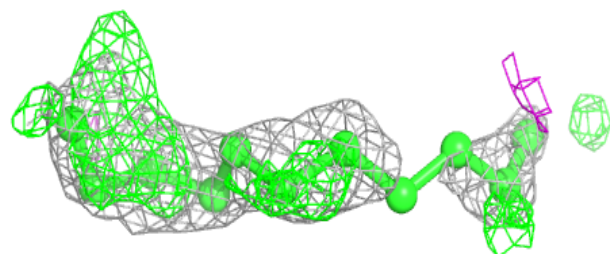
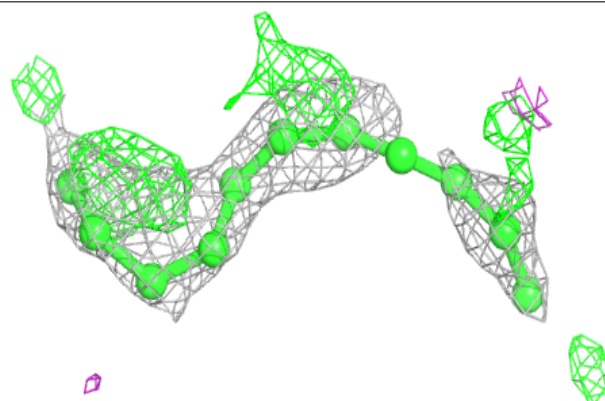


Electron density around DMU N 744:

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

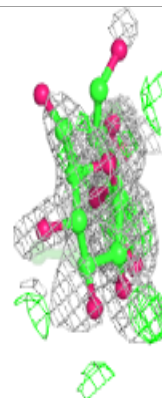
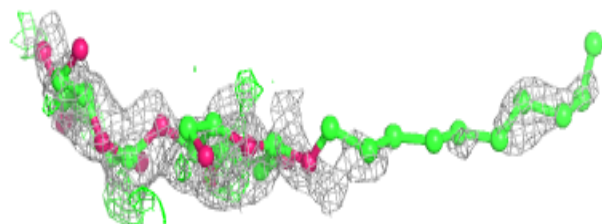
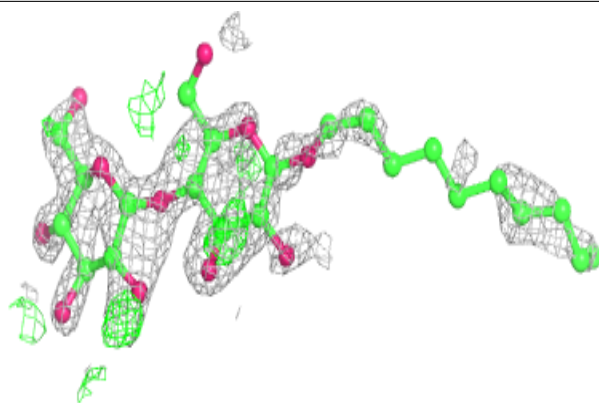
**Electron density around LFA P 611:**

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

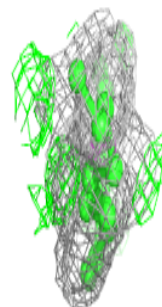
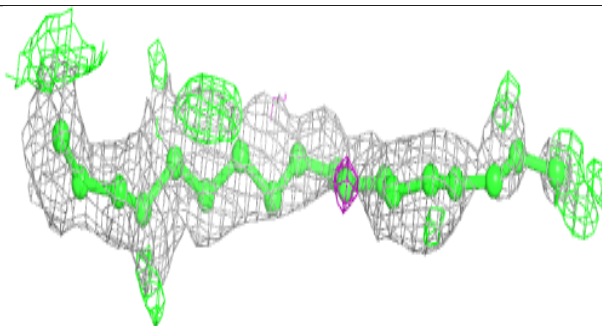
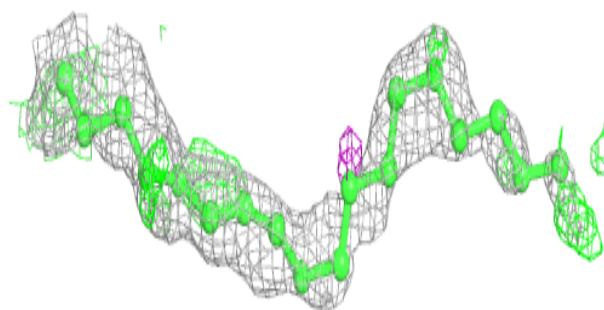


Electron density around DMU C 734:

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

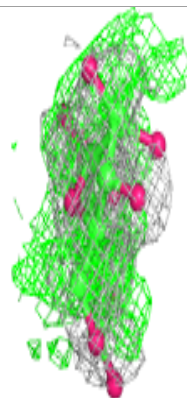
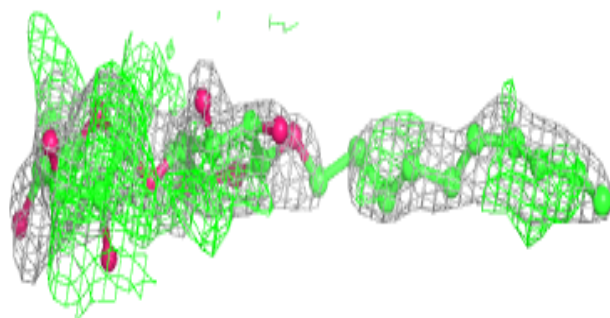
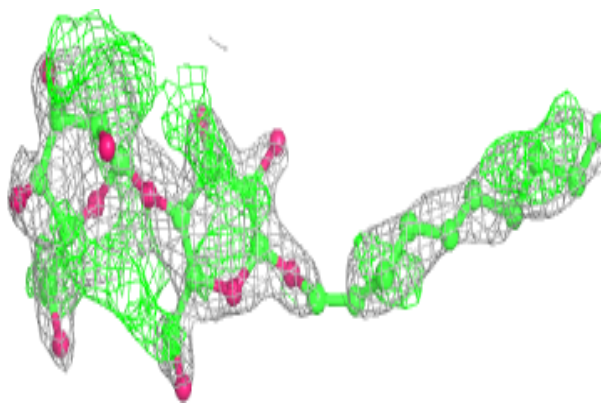
**Electron density around LFA P 716 (B):**

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

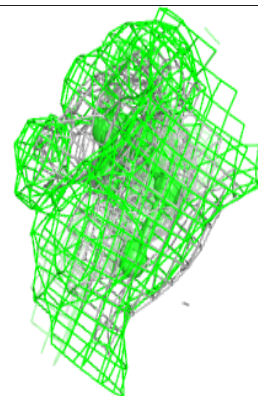
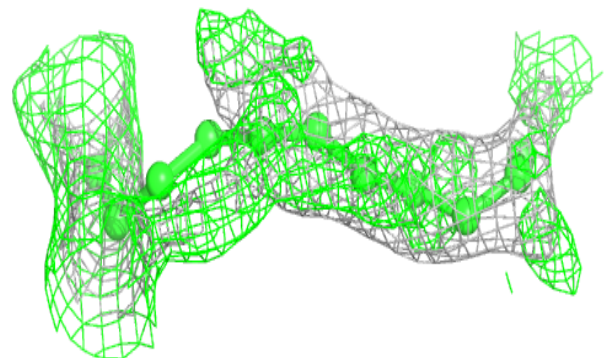
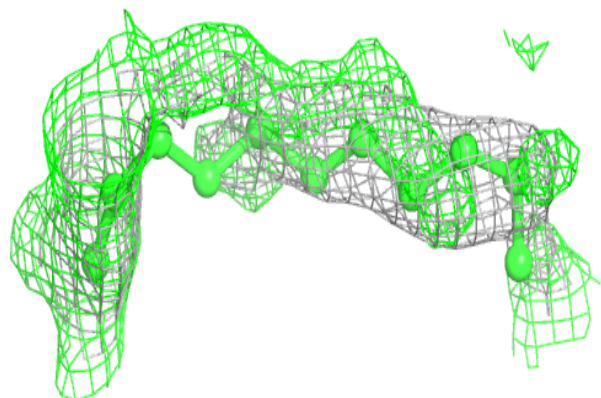


Electron density around DMU P 733:

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

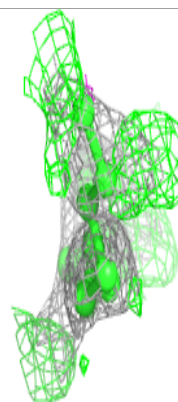
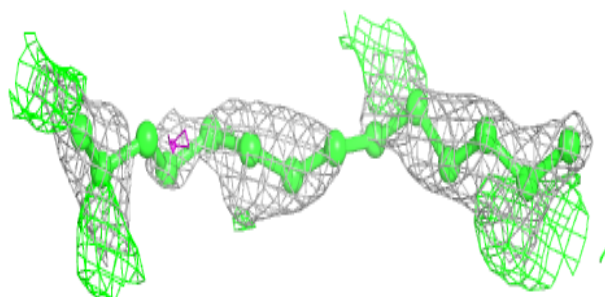
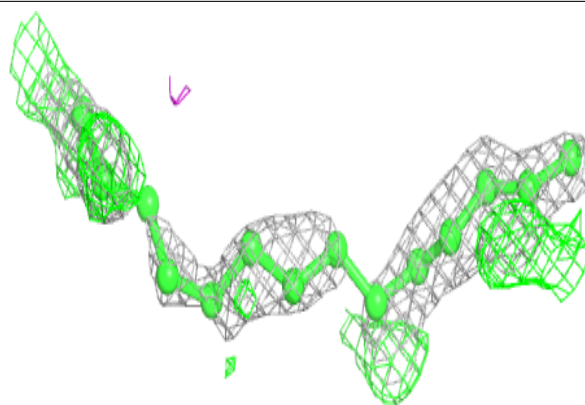
**Electron density around LFA P 624:**

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

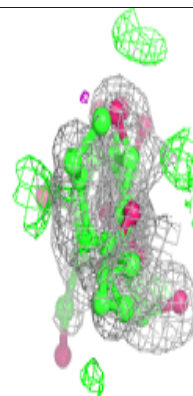
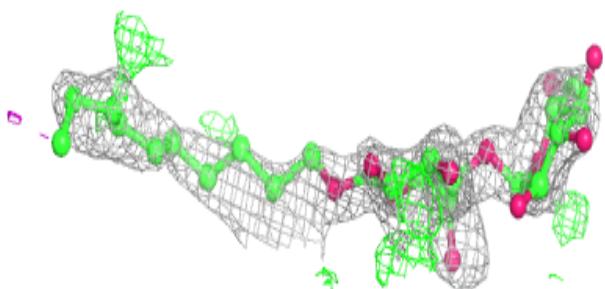
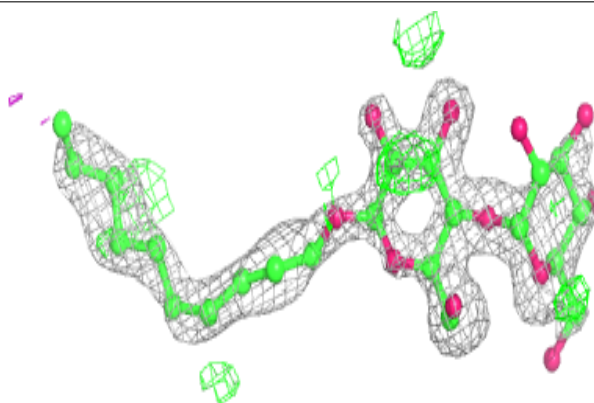


Electron density around LFA C 623:

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

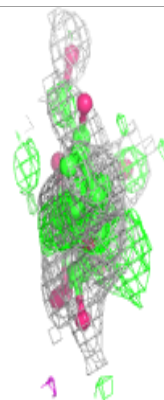
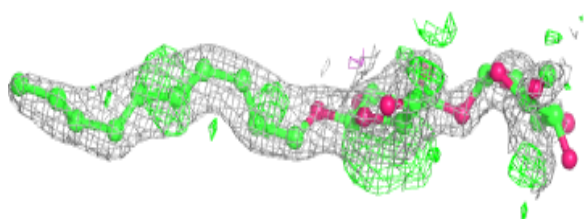
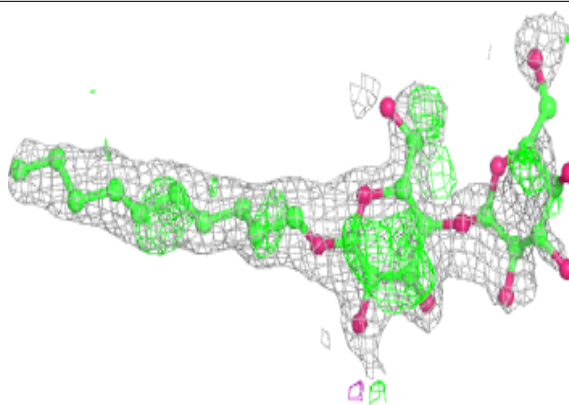
**Electron density around DMU J 61:**

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

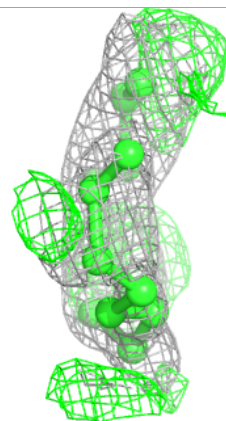
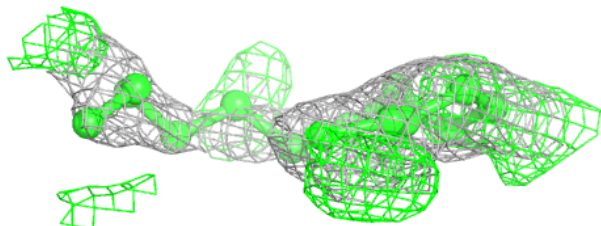
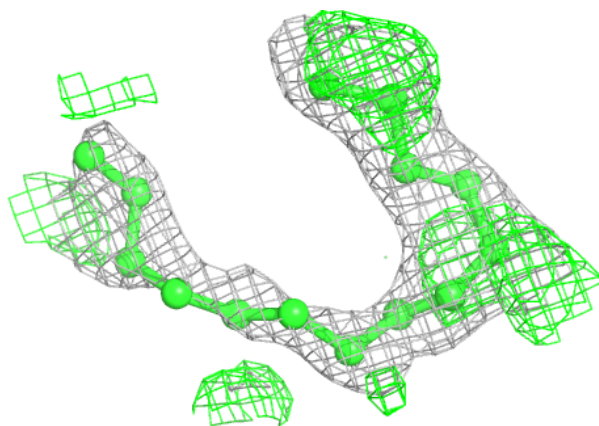


Electron density around DMU N 745:

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

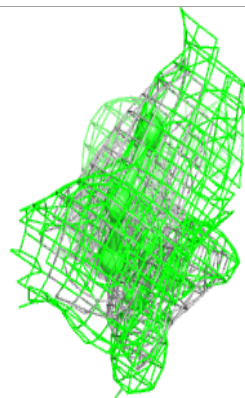
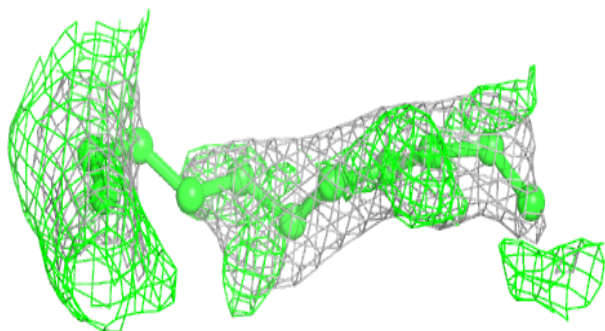
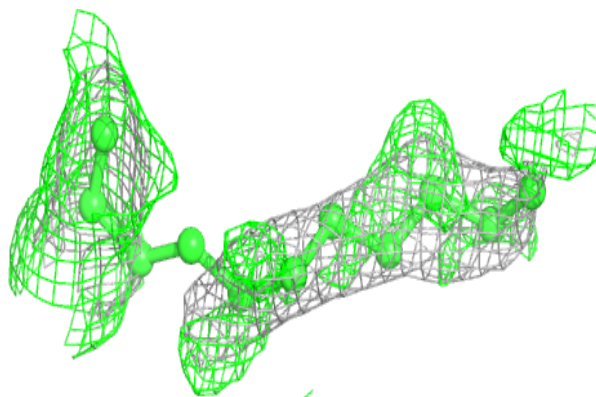
**Electron density around LFA N 628:**

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

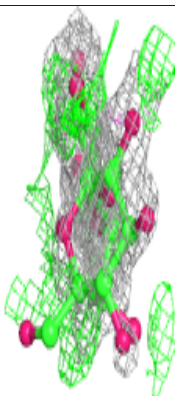
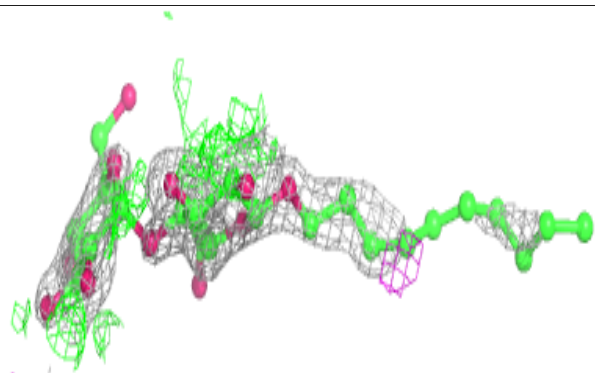
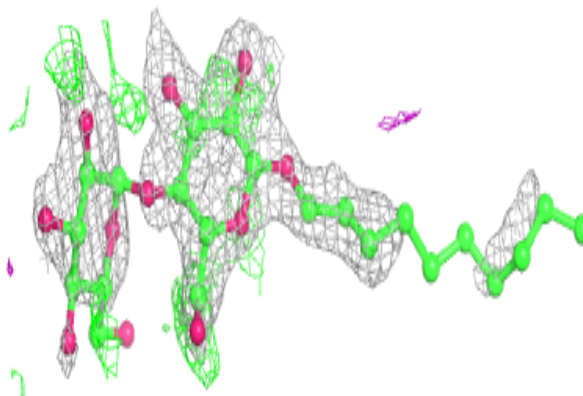


Electron density around LFA C 624:

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

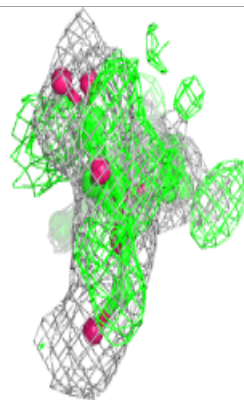
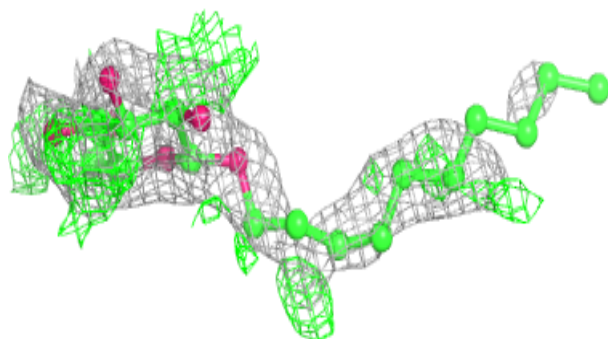
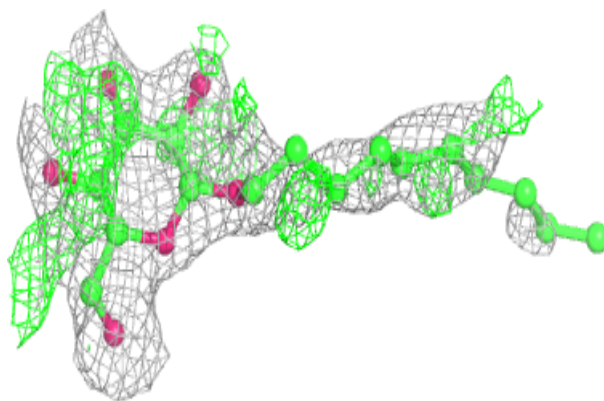
**Electron density around DMU C 714:**

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

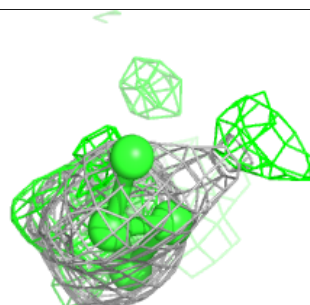
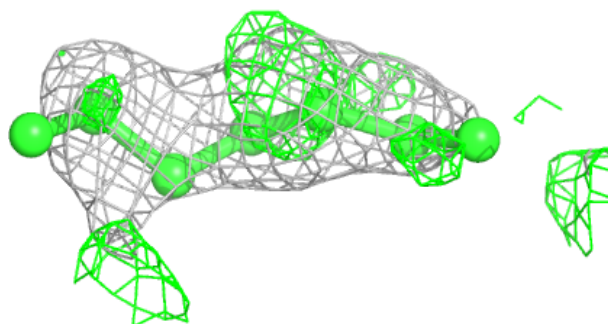
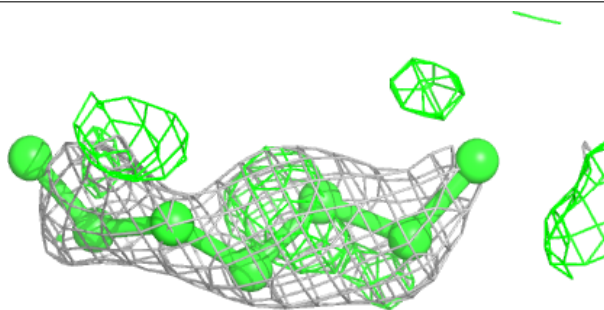


Electron density around DMU G 713:

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

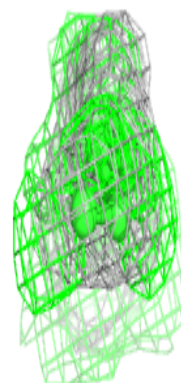
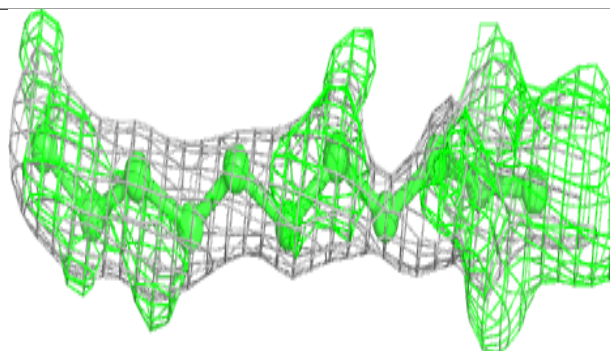
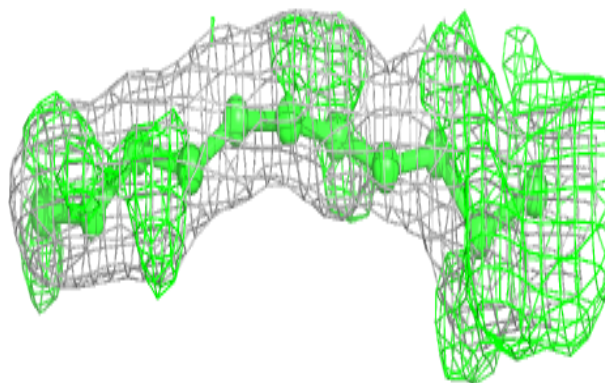
**Electron density around DMU C 721:**

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

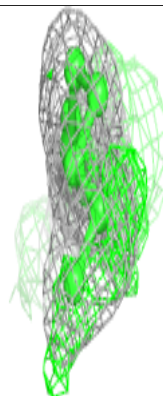
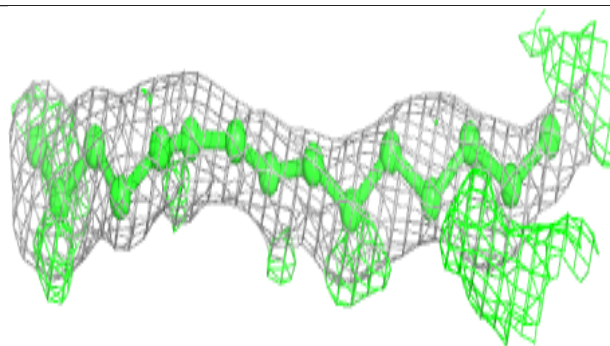
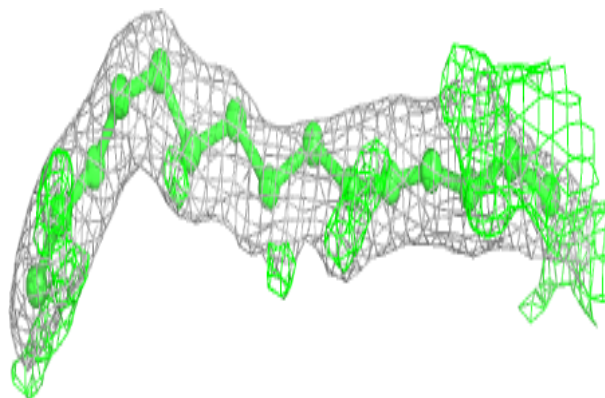


Electron density around LFA G 622:

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

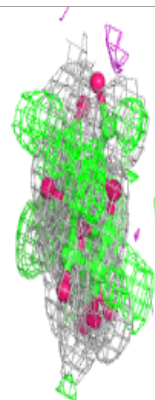
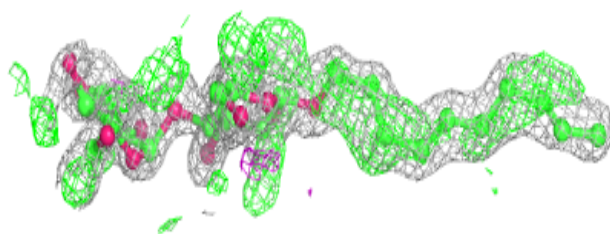
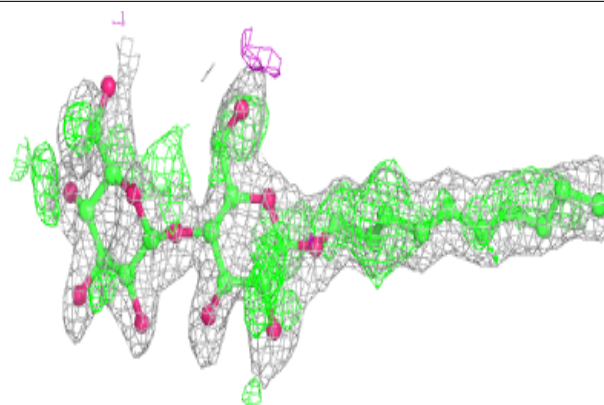
**Electron density around LFA P 625:**

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

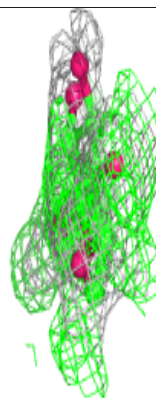
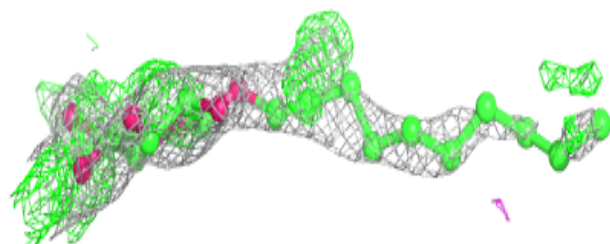
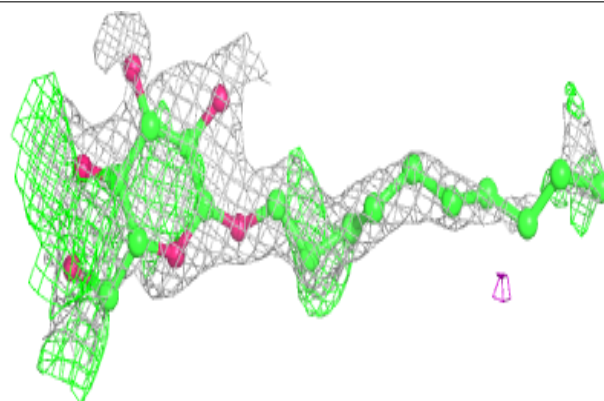


Electron density around DMU A 745:

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

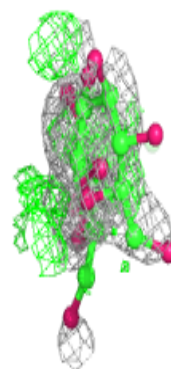
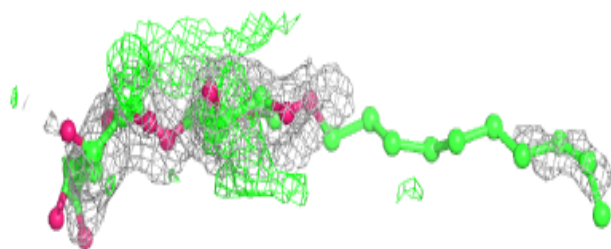
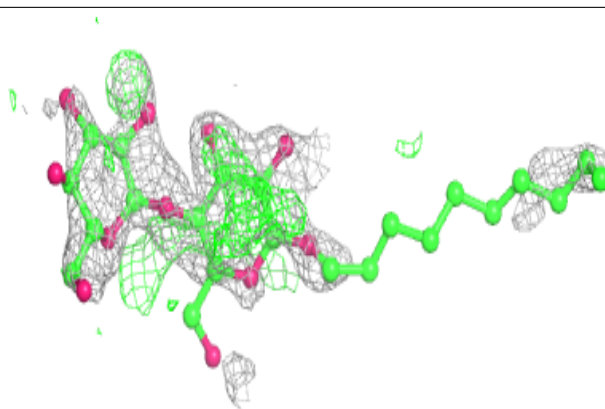
**Electron density around DMU L 747:**

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

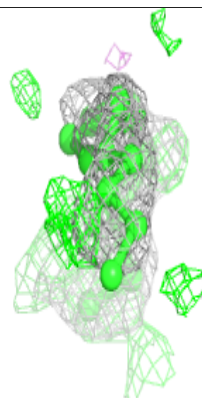
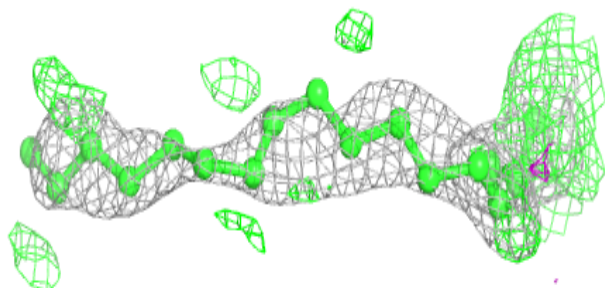
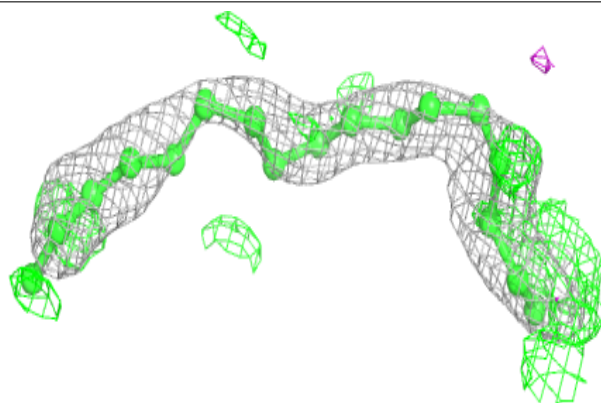


Electron density around DMU P 734:

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

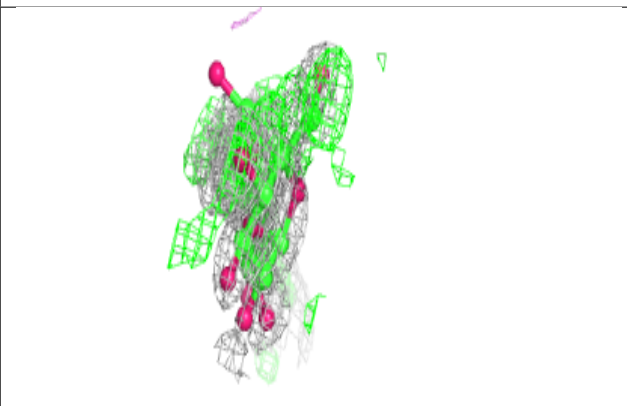
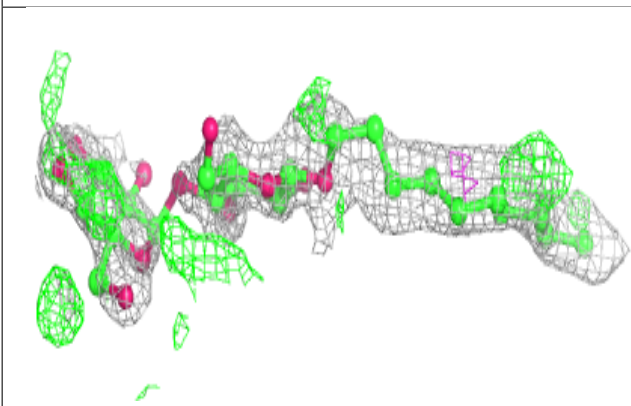
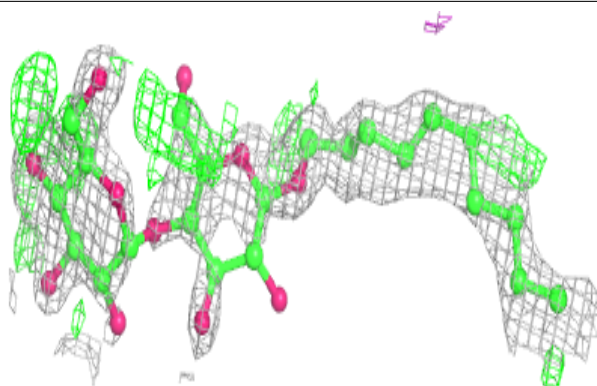
**Electron density around LFA G 621:**

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

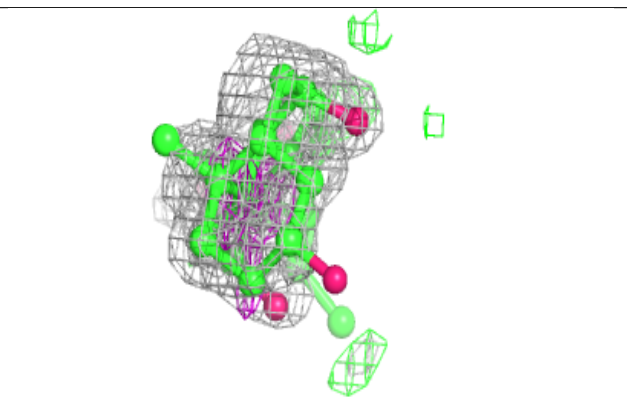
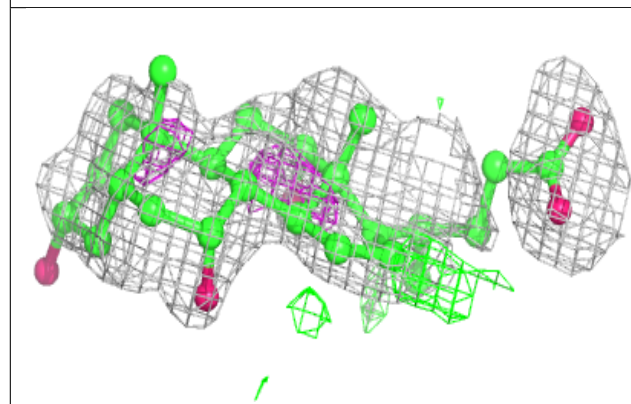
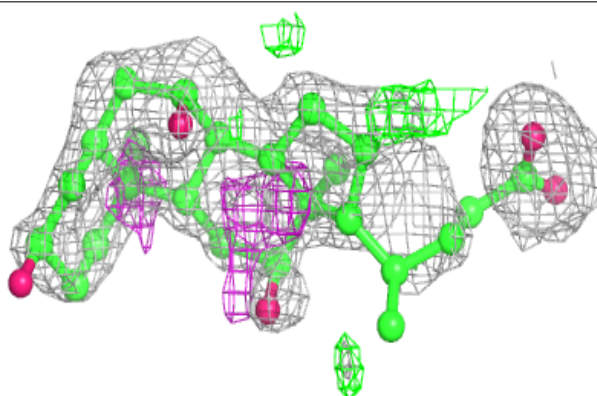


Electron density around DMU C 715 (A):

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

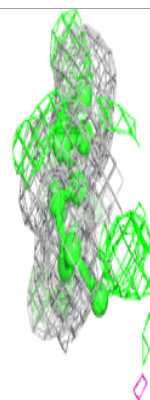
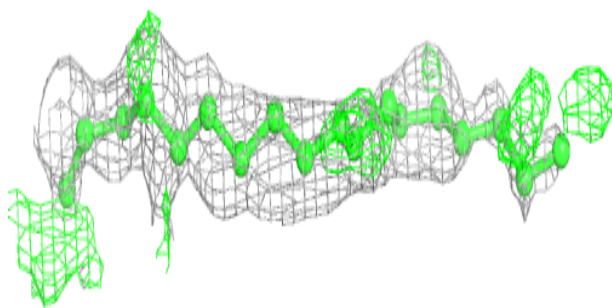
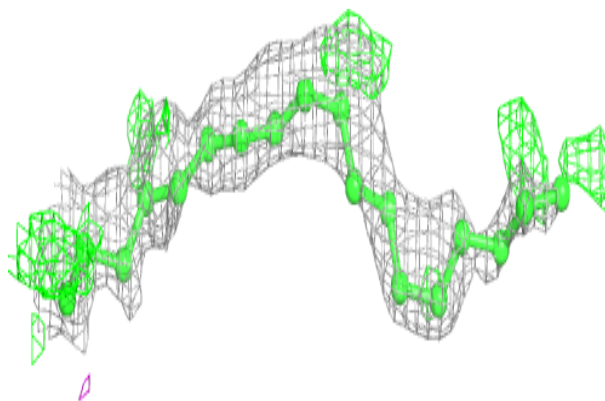
**Electron density around CHD P 271:**

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

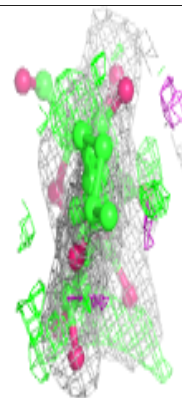
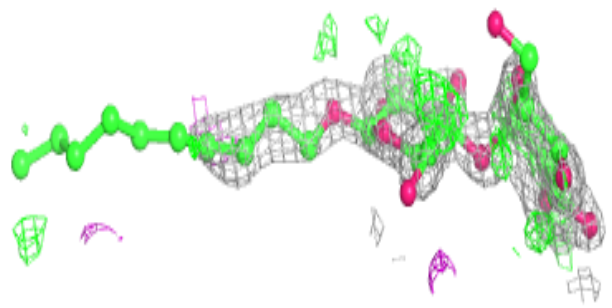
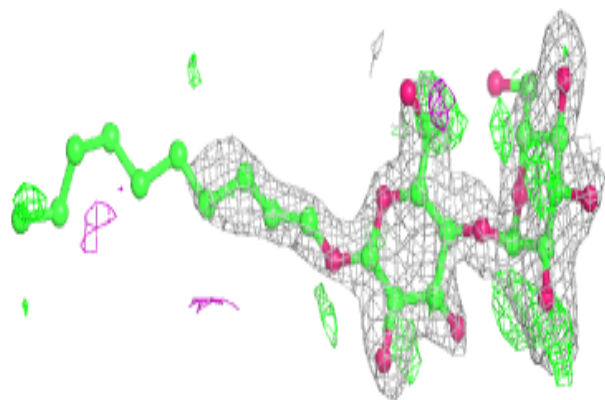


Electron density around LFA C 716 (B):

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

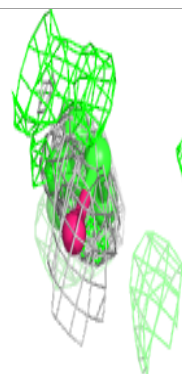
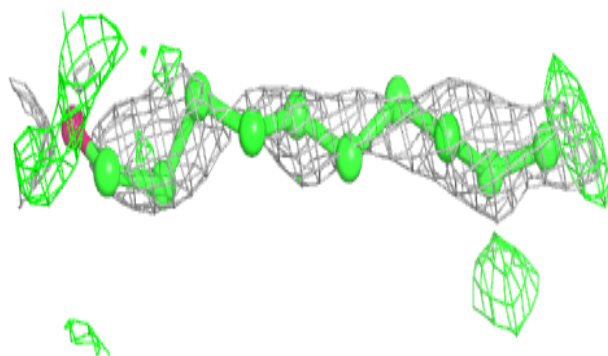
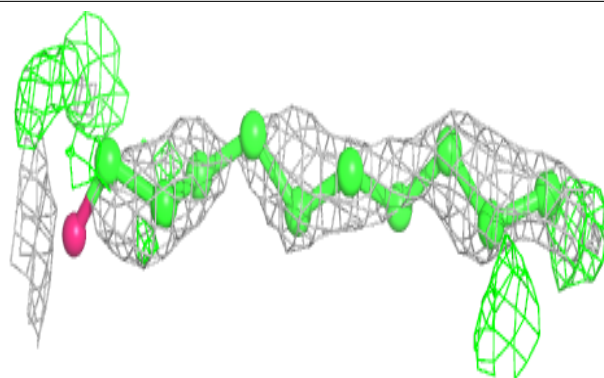
**Electron density around DMU P 714:**

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

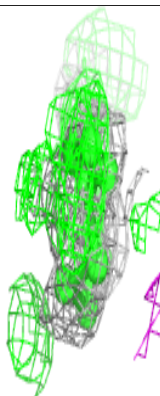
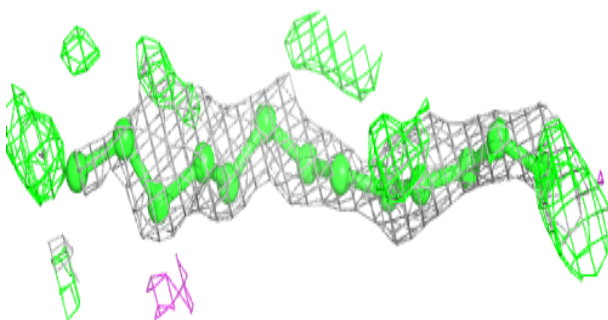
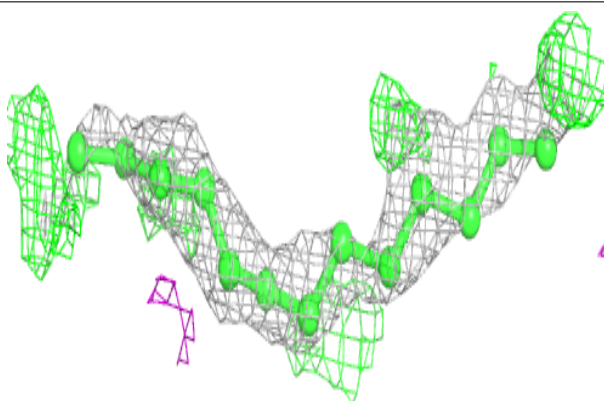


Electron density around DMU B 731:

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

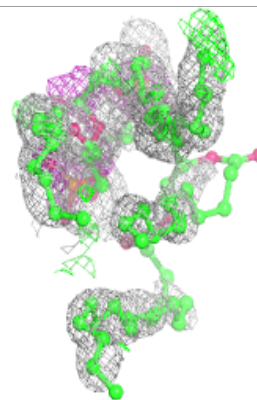
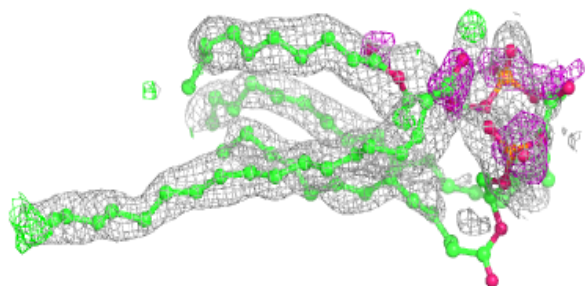
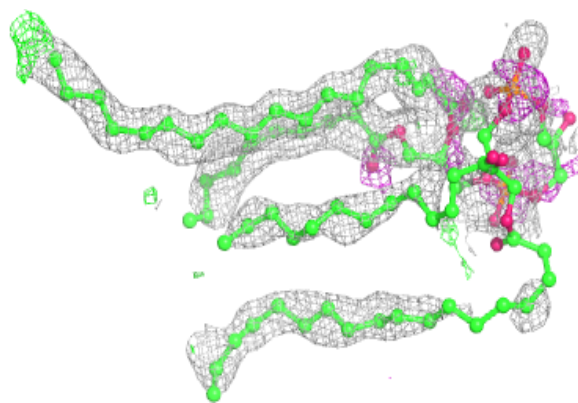
**Electron density around LFA C 626:**

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

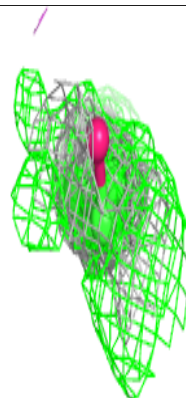
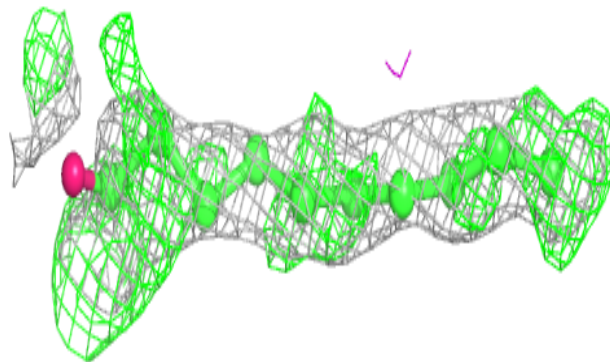
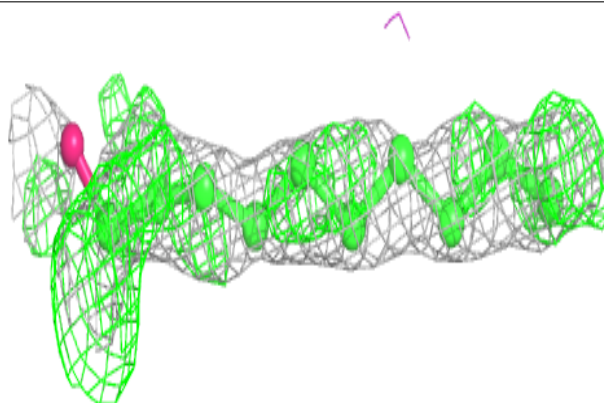


Electron density around CDL C 270:

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

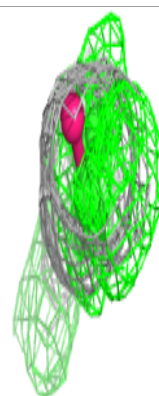
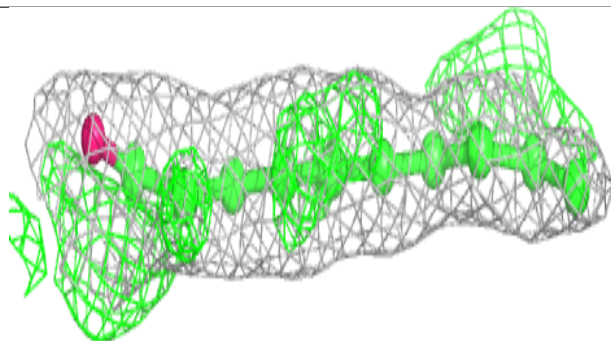
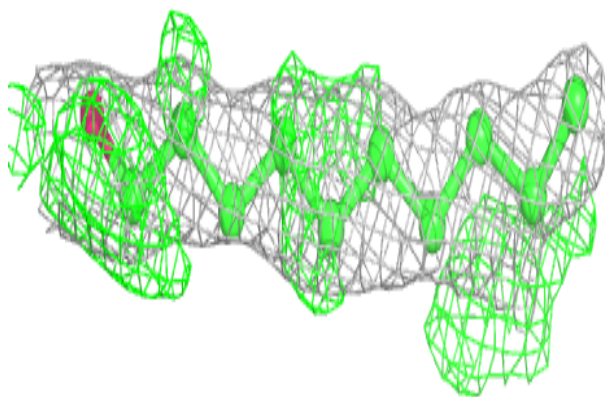
**Electron density around DMU O 731:**

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

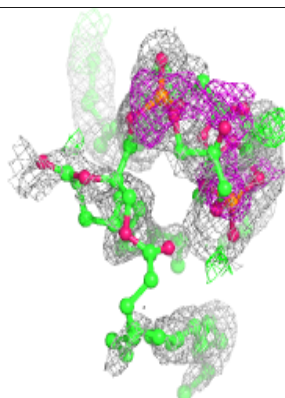
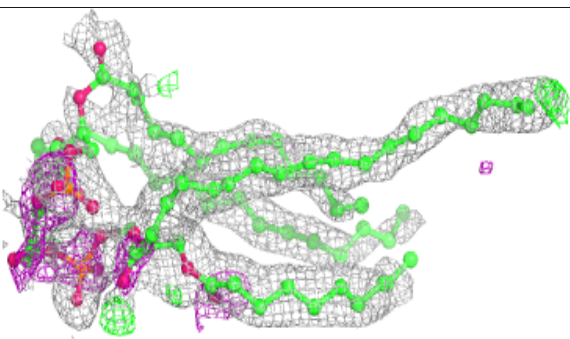
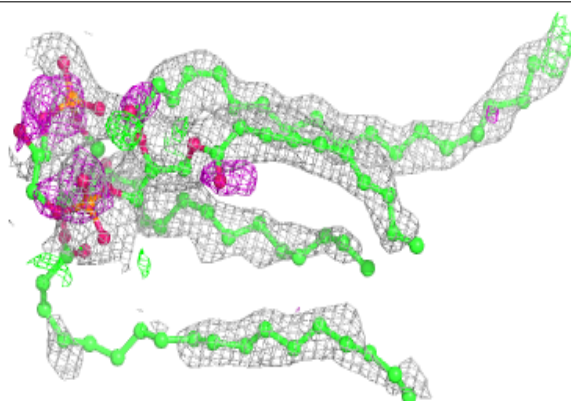


Electron density around DMU P 272:

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

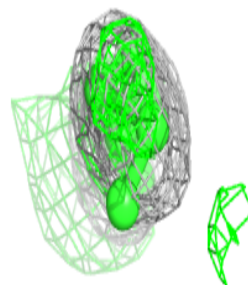
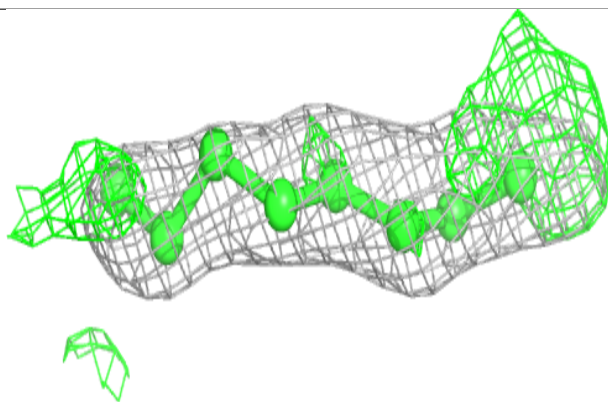
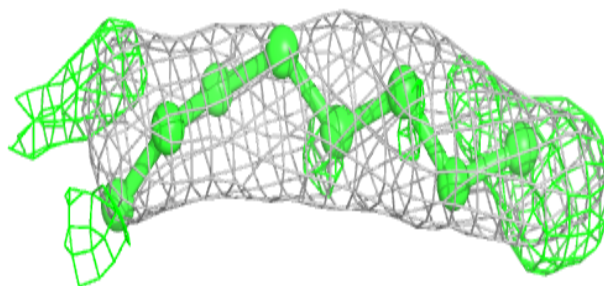
**Electron density around CDL P 270:**

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

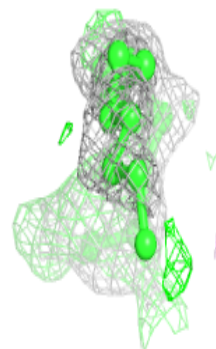
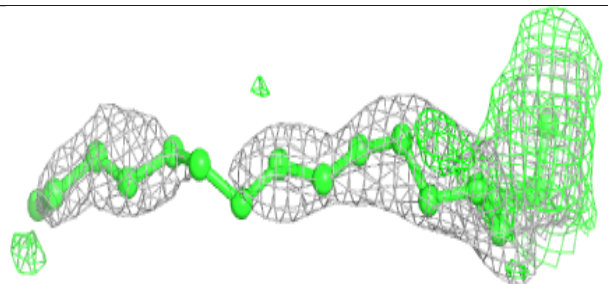
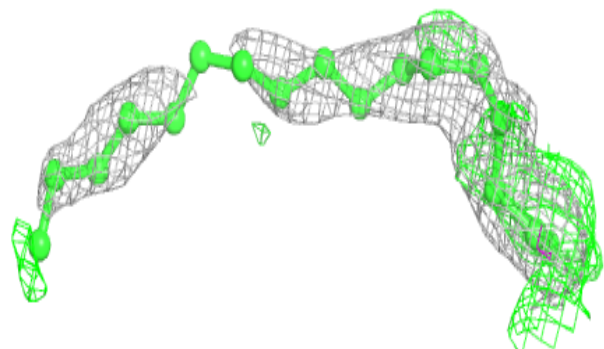


Electron density around DMU Z 746:

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

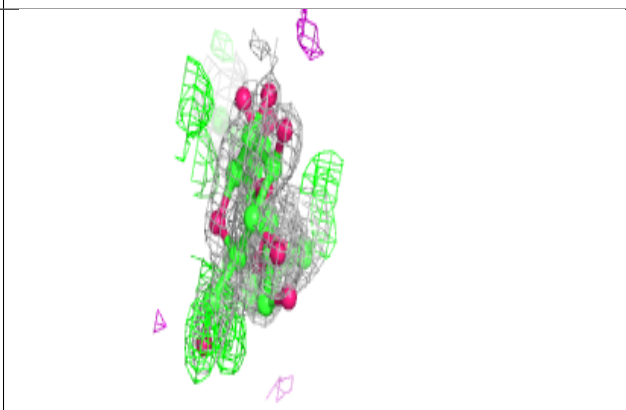
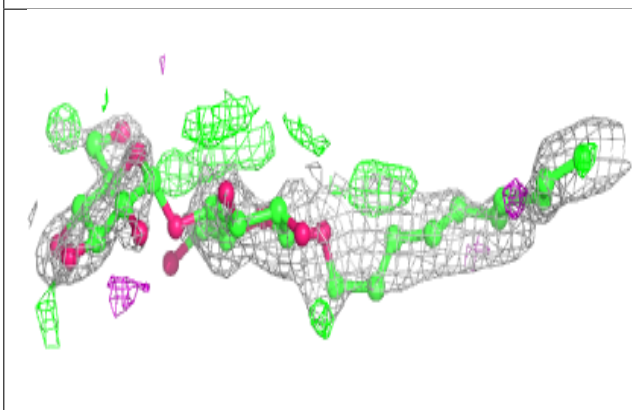
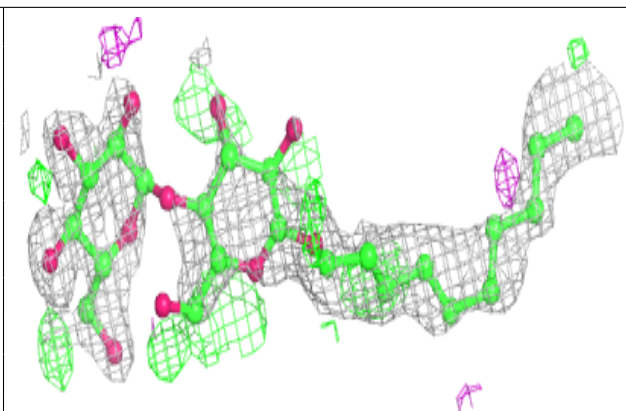
**Electron density around LFA T 621:**

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

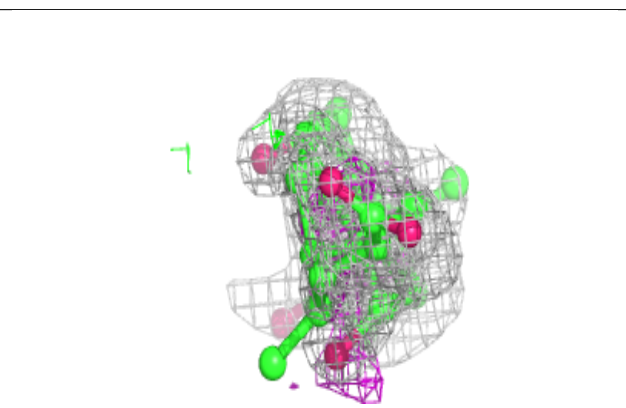
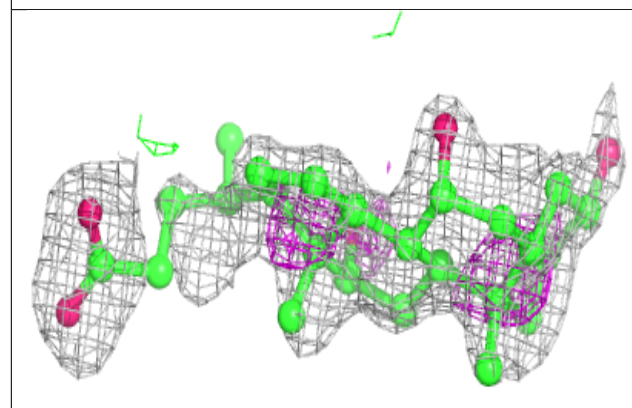
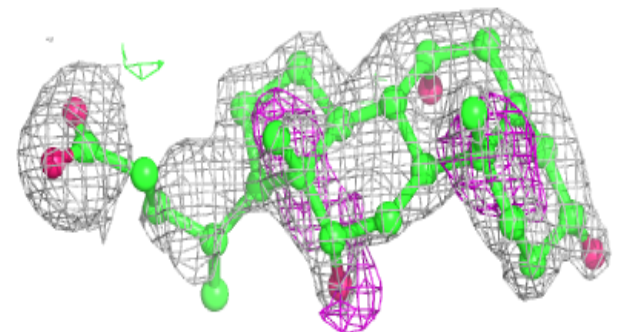


Electron density around DMU P 715 (A):

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

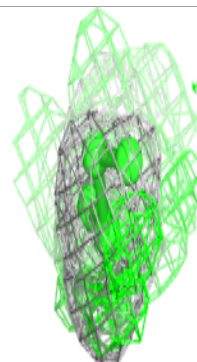
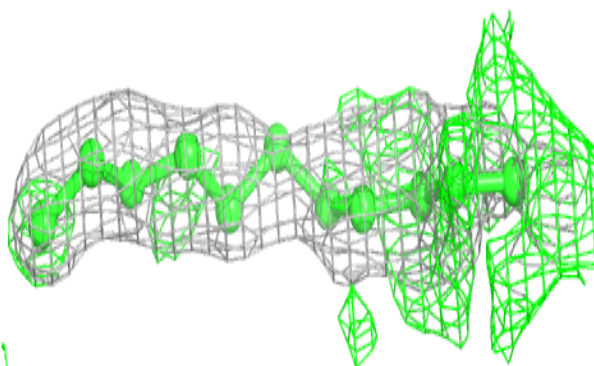
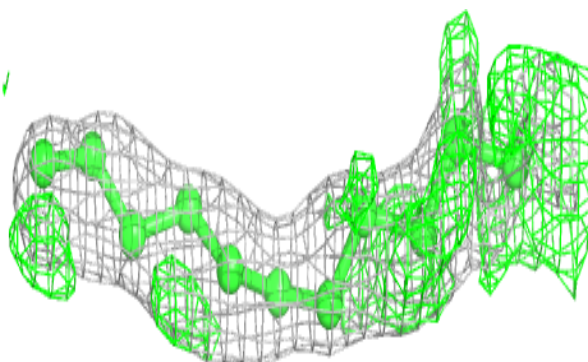
**Electron density around CHD C 271:**

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

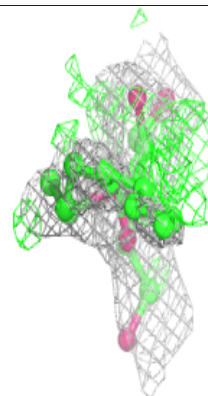
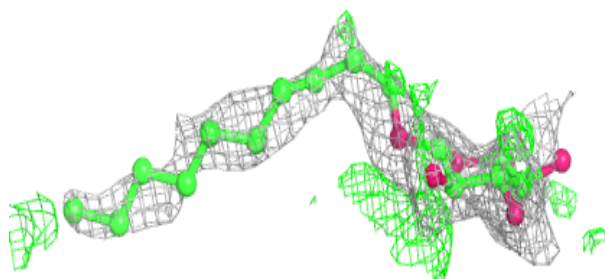
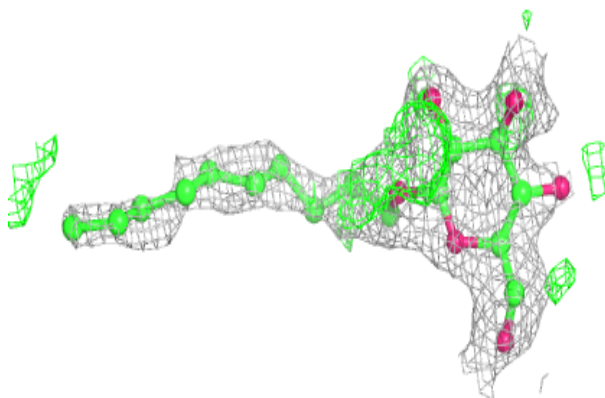


Electron density around LFA T 622:

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

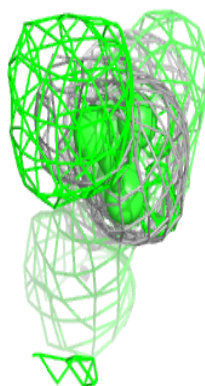
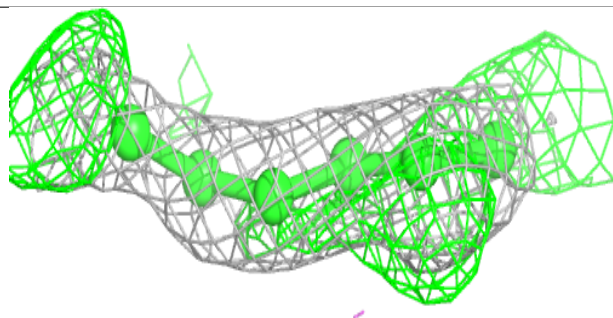
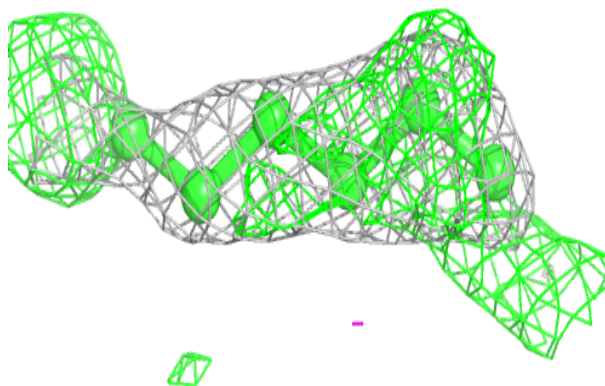
**Electron density around DMU T 713:**

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

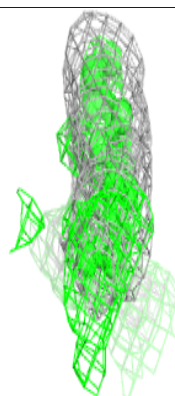
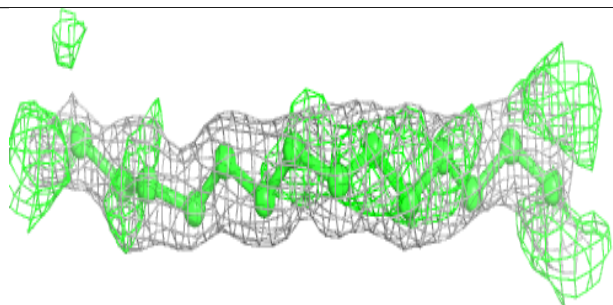
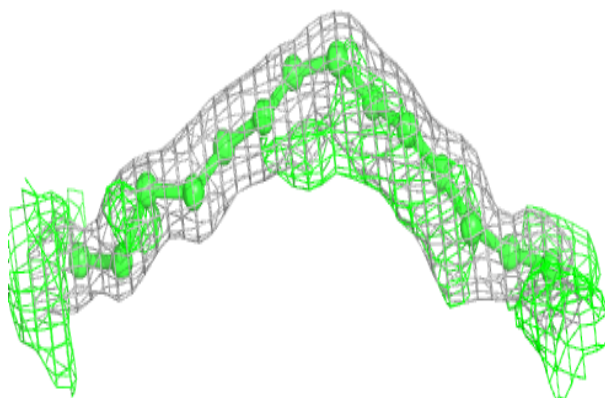


Electron density around LFA P 612:

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

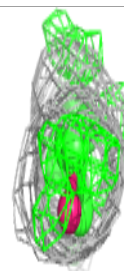
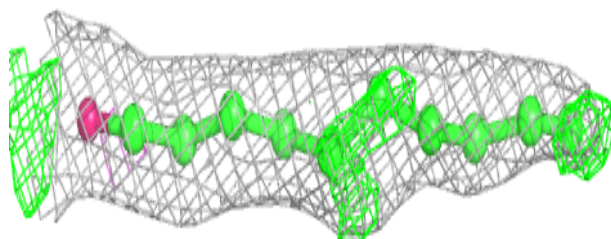
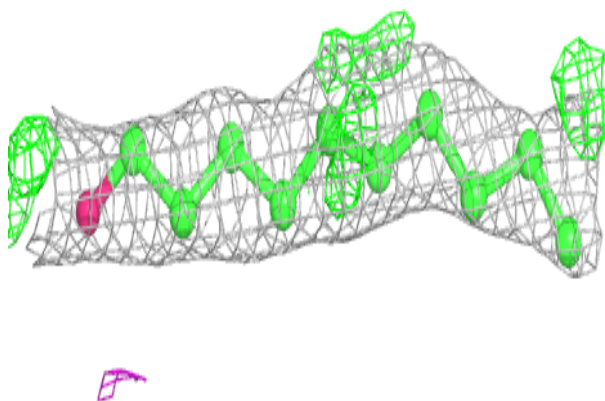
**Electron density around LFA N 627:**

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

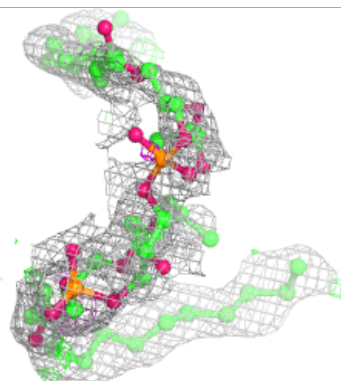
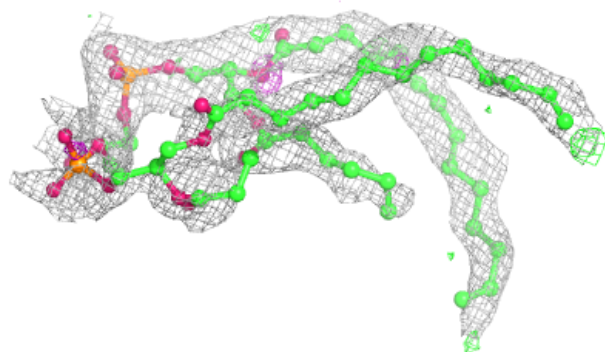
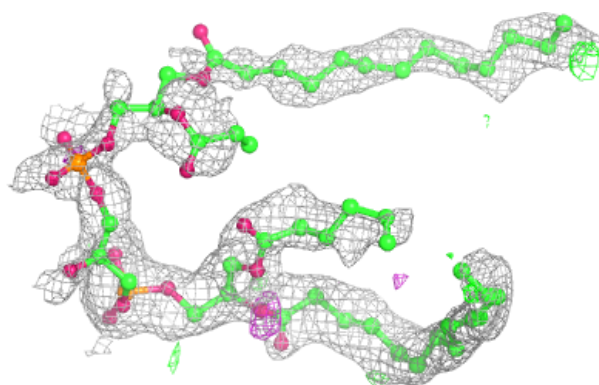


Electron density around DMU C 272:

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

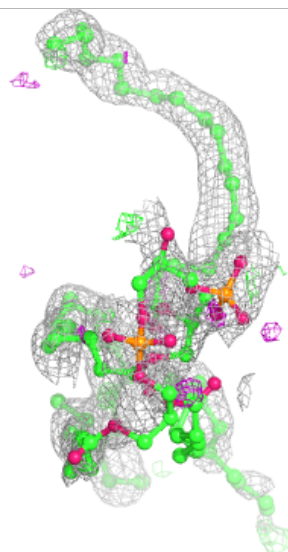
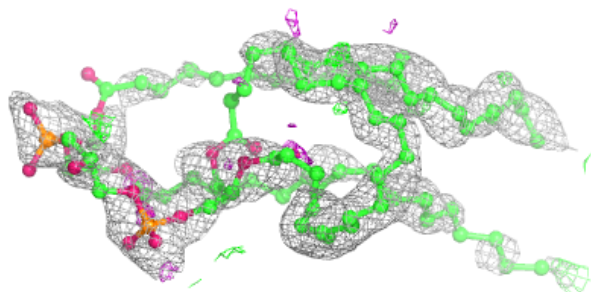
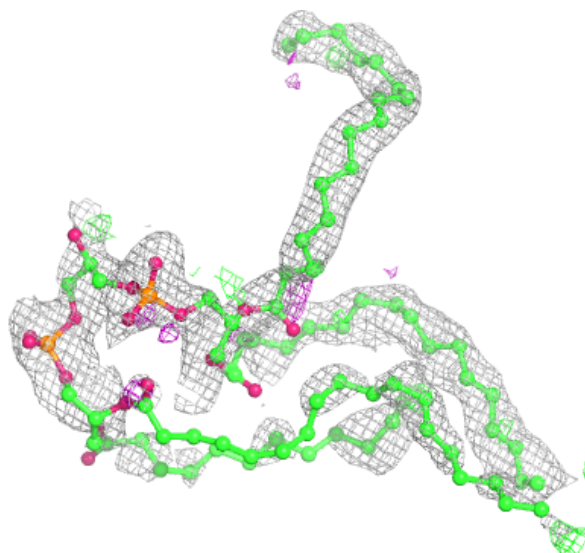
**Electron density around CDL N 522:**

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



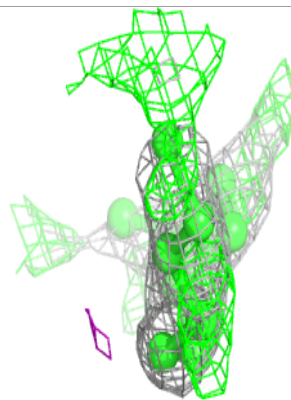
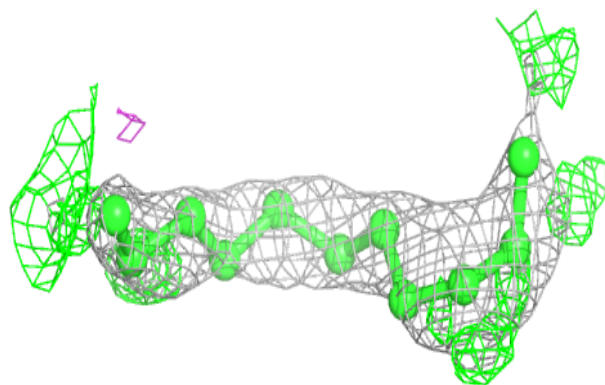
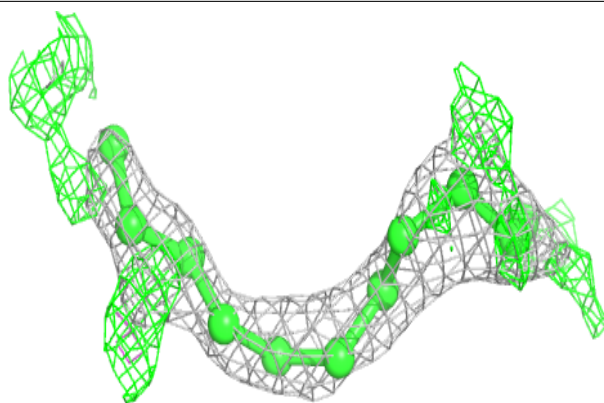
Electron density around CDL N 521:

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

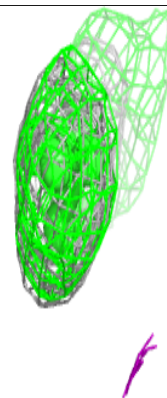
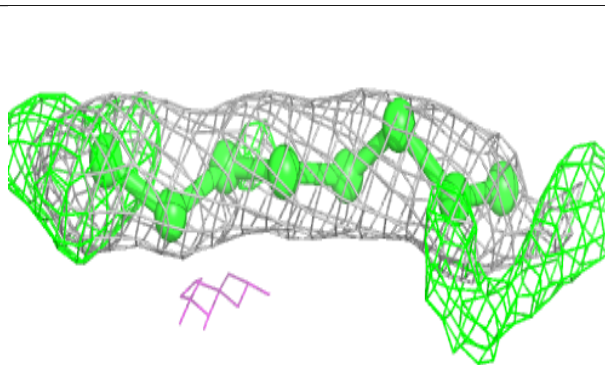
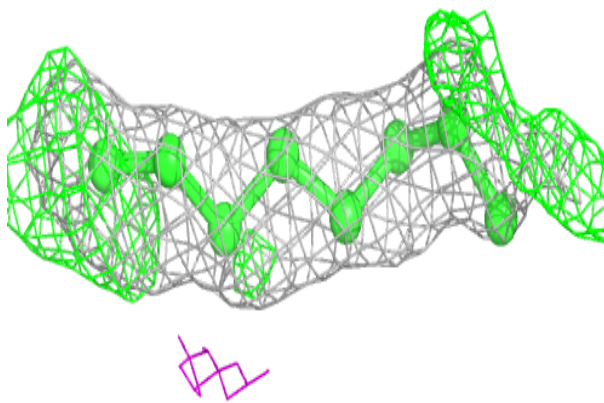


Electron density around LFA C 611:

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

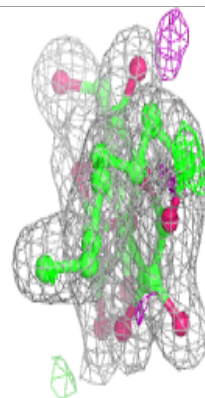
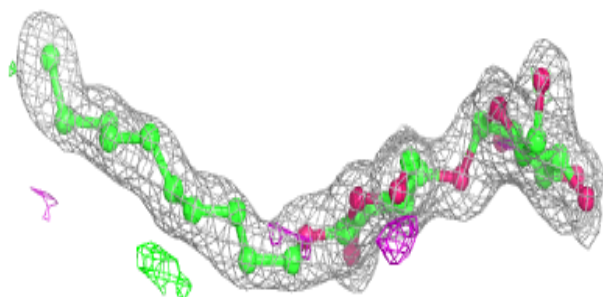
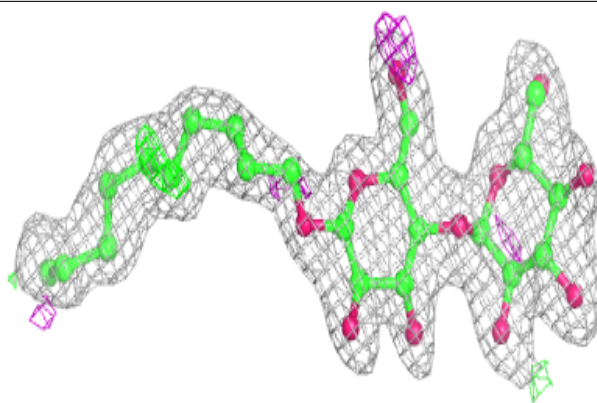
**Electron density around DMU M 746:**

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

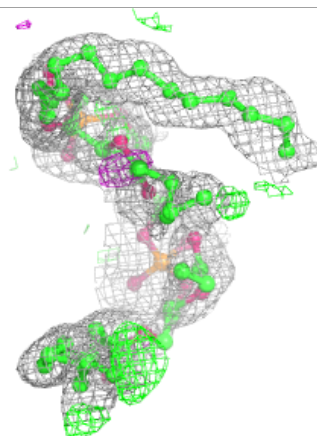
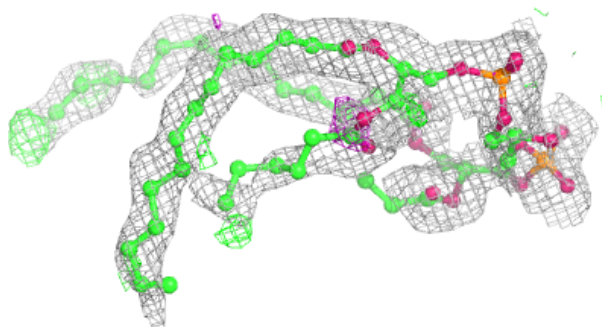
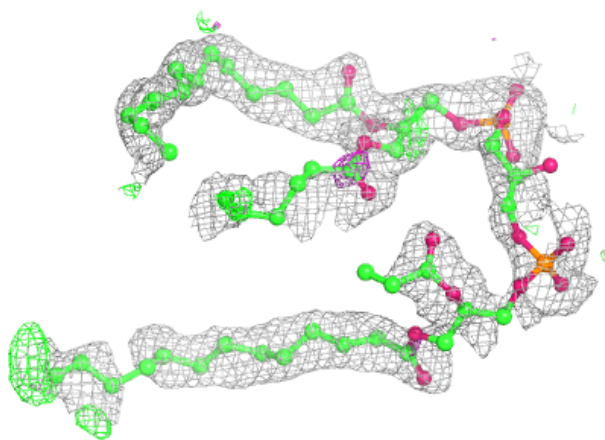


Electron density around DMU N 526:

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

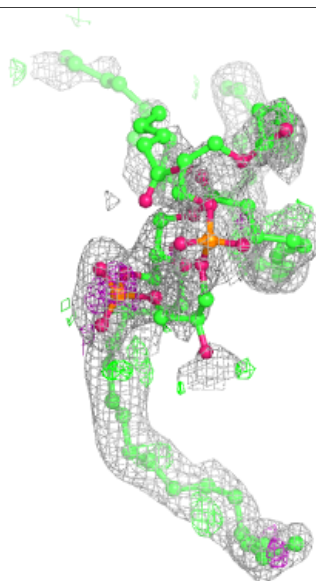
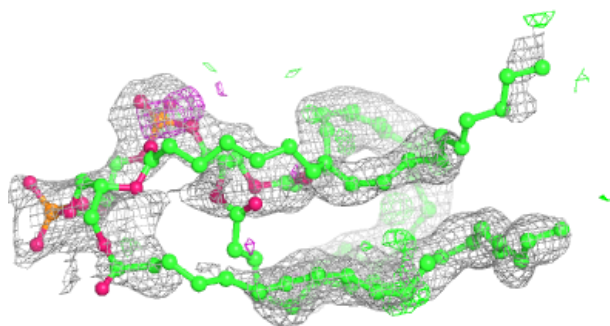
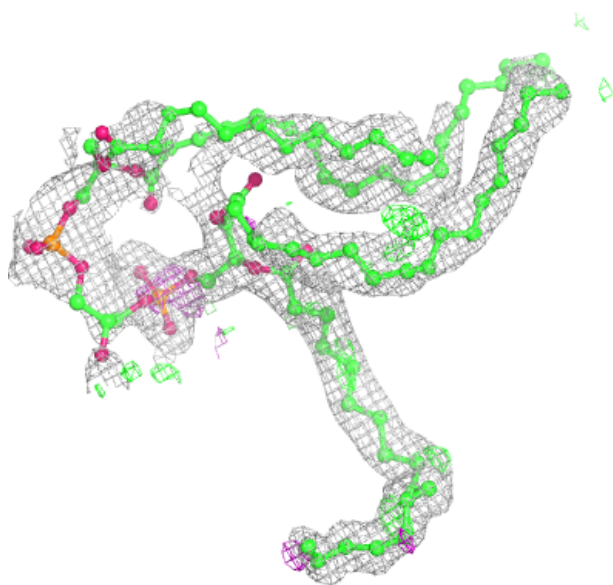
**Electron density around CDL A 522:**

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



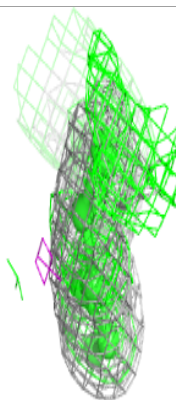
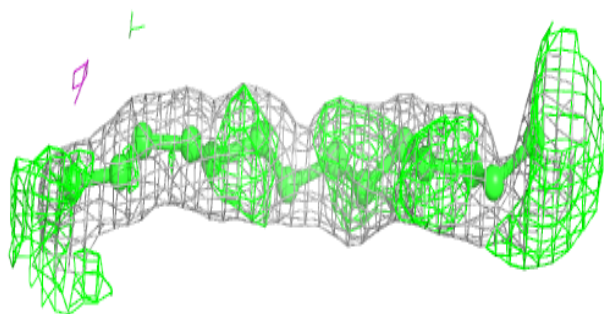
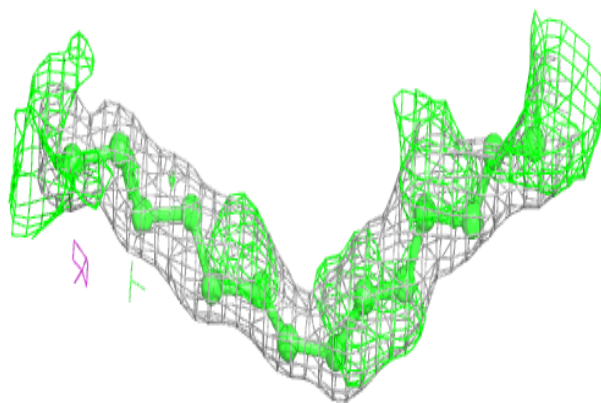
Electron density around CDL A 521:

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

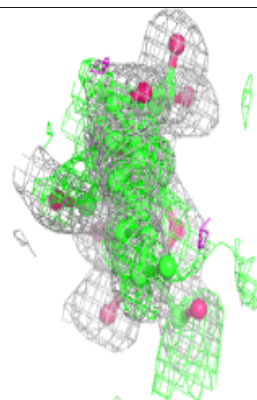
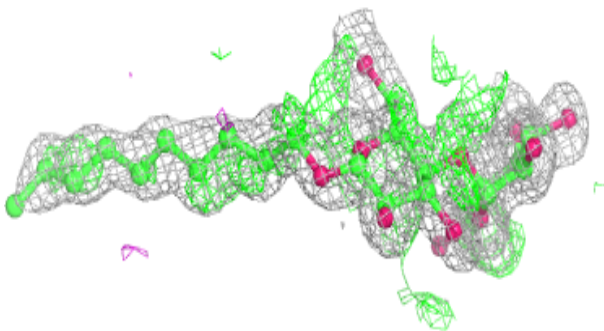
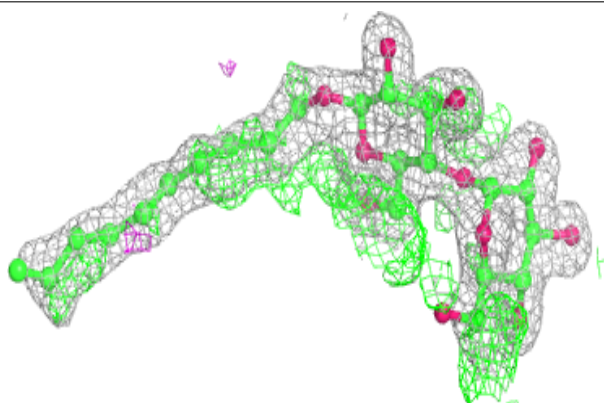


Electron density around LFA A 627:

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

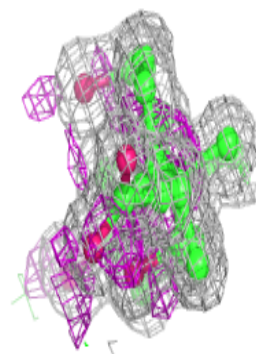
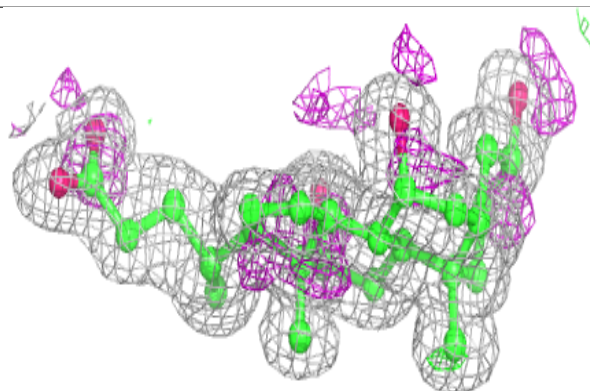
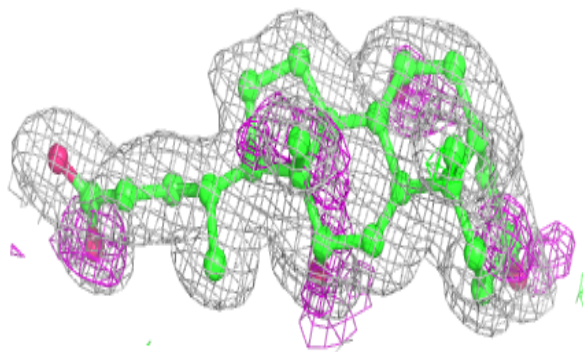
**Electron density around DMU A 744:**

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

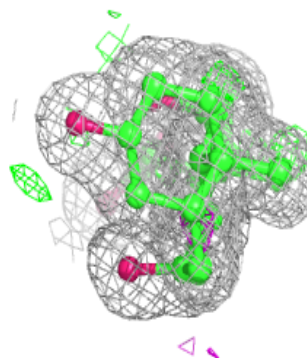
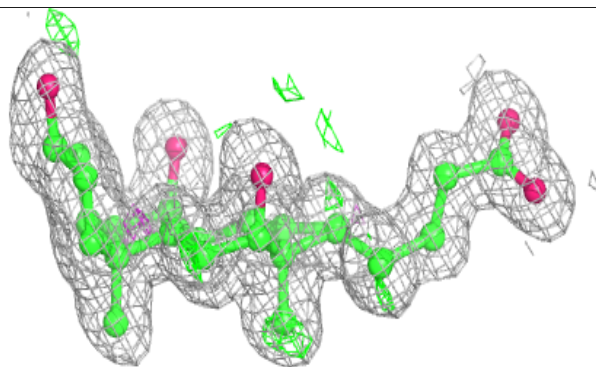
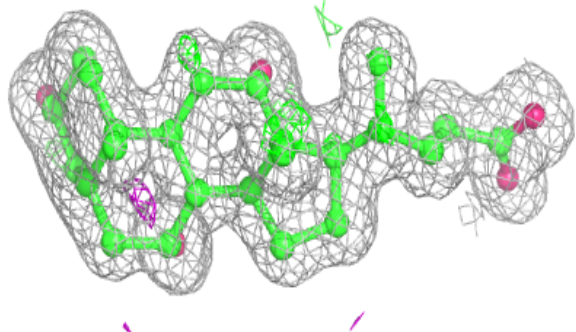


Electron density around CHD A 525:

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

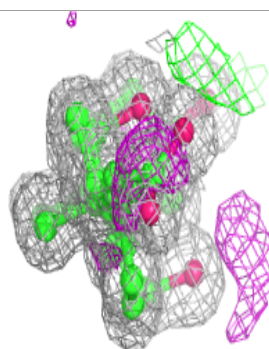
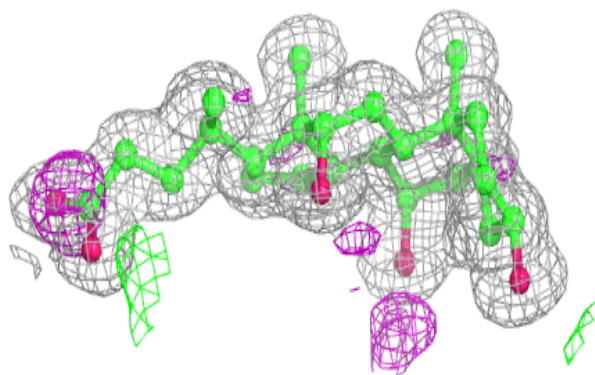
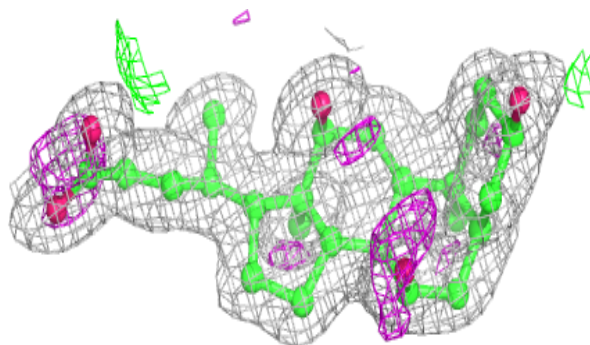
**Electron density around CHD G 86:**

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

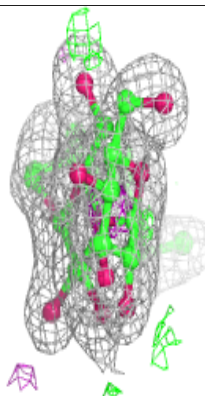
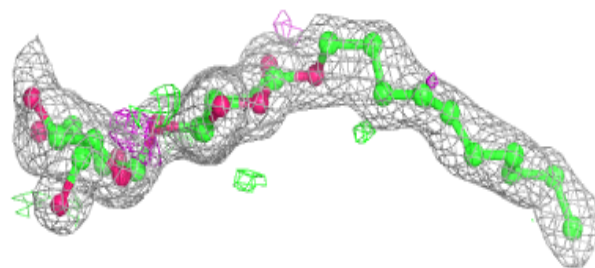
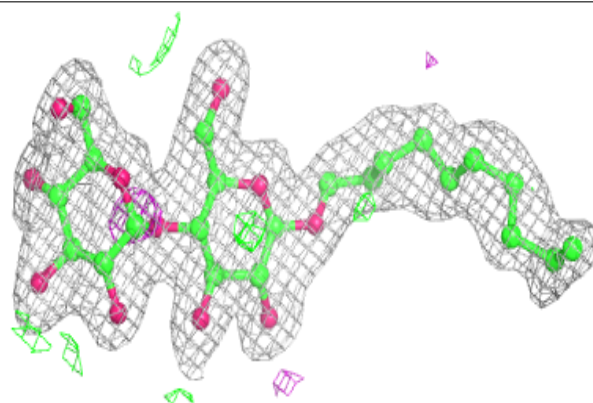


Electron density around CHD N 525:

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

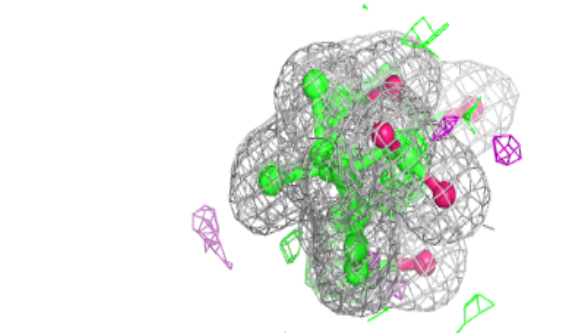
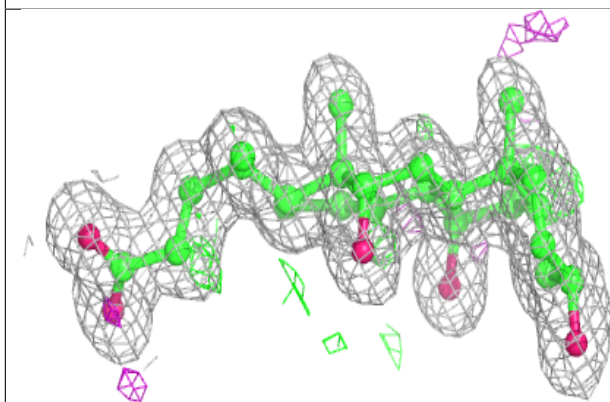
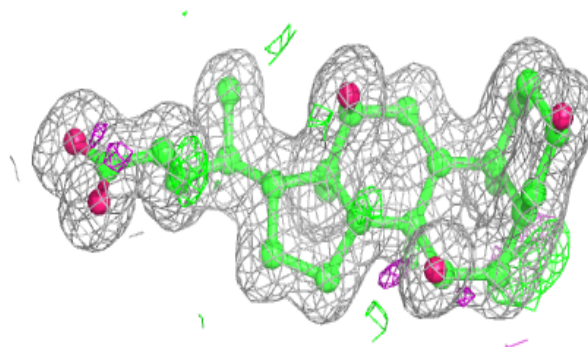
**Electron density around DMU A 526:**

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

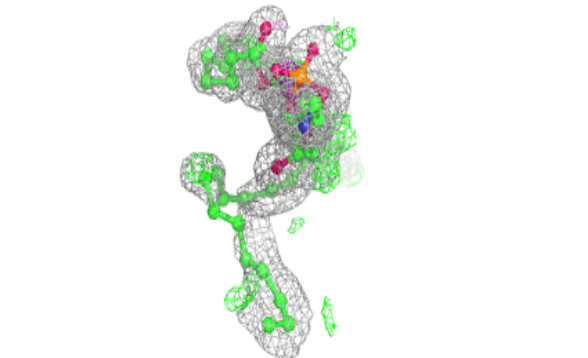
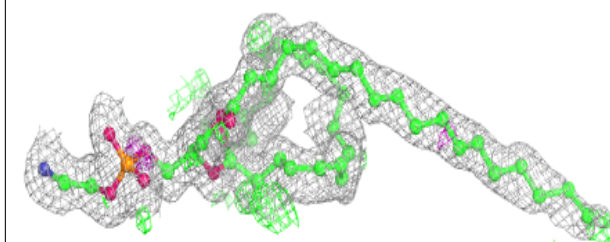
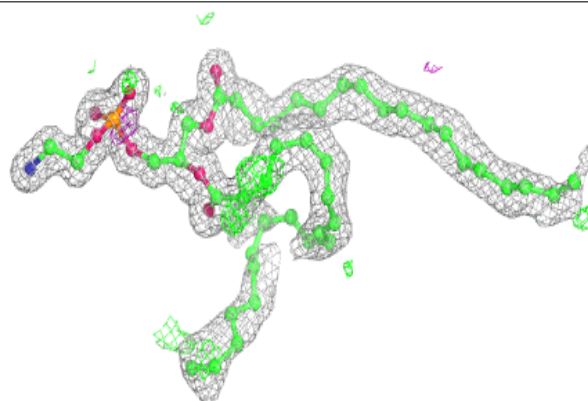


Electron density around CHD T 86:

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

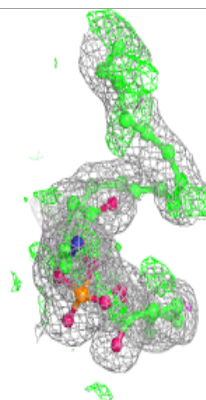
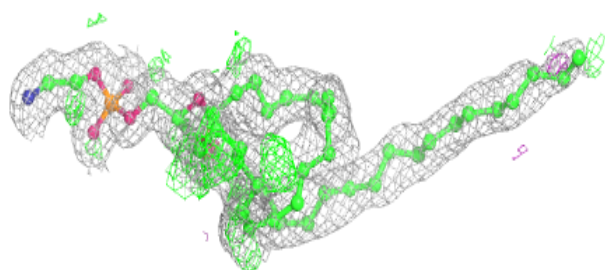
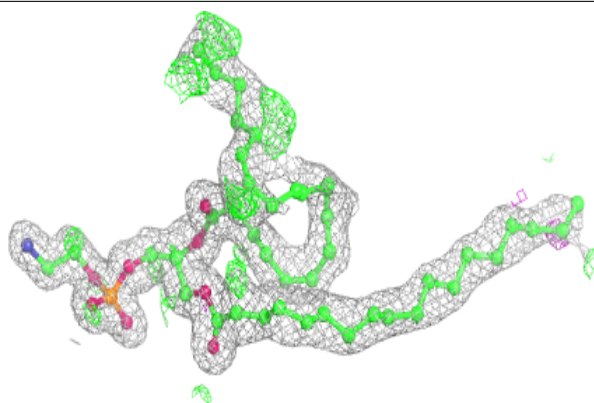
**Electron density around PEK P 264:**

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

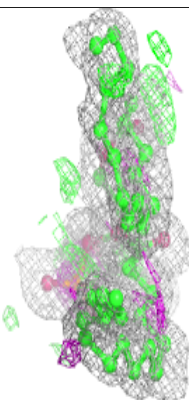
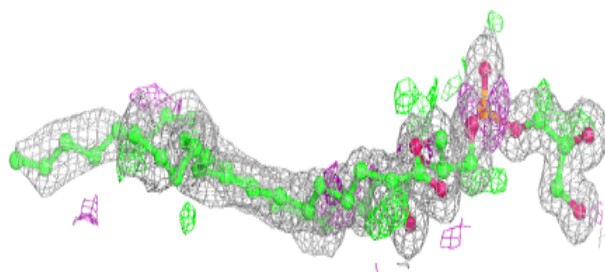
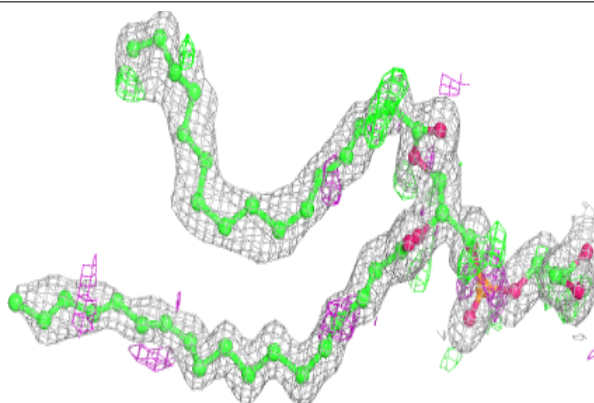


Electron density around PEK C 264:

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

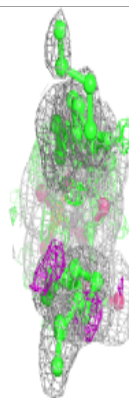
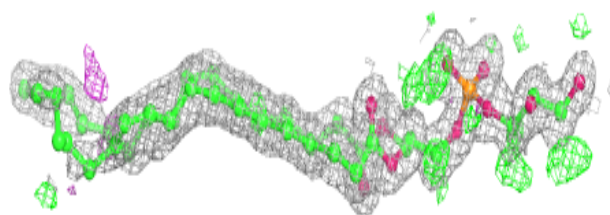
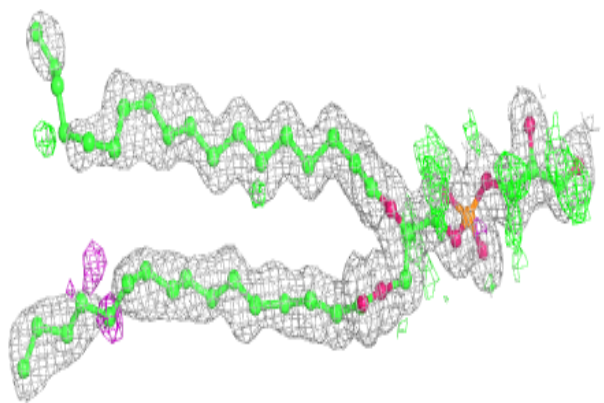
**Electron density around PGV C 266:**

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

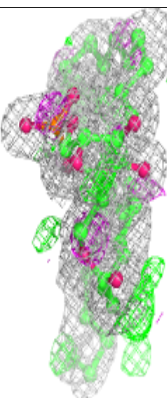
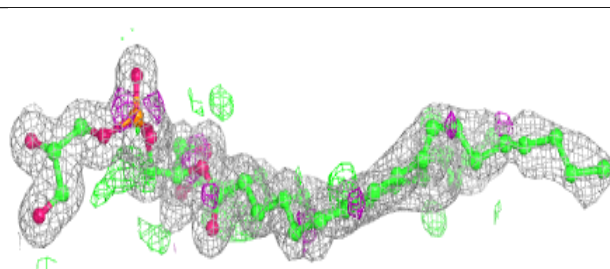
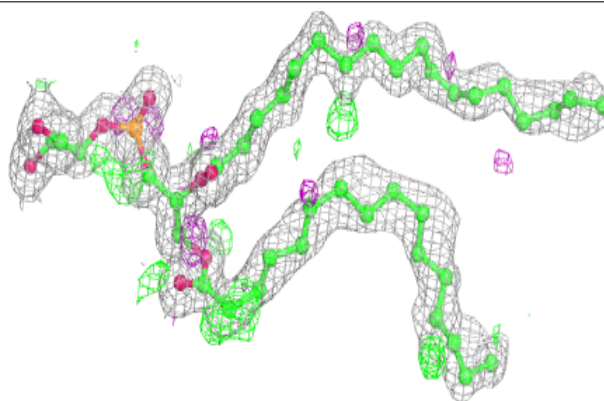


Electron density around PGV C 267:

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

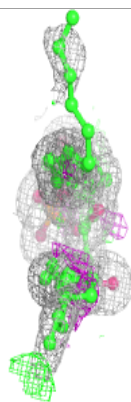
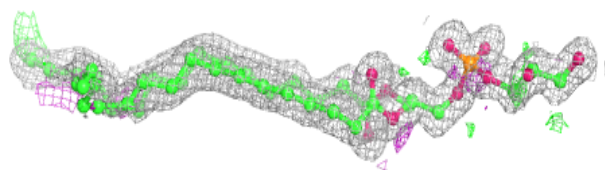
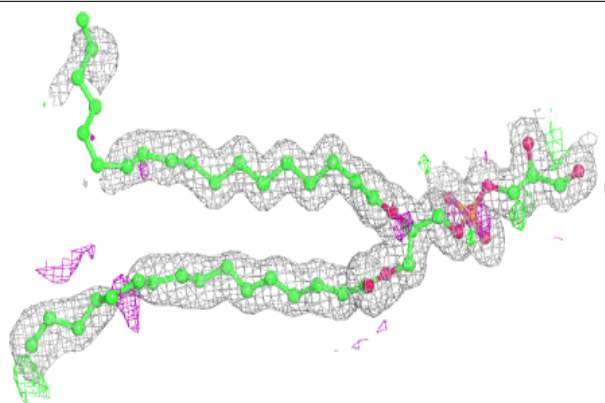
**Electron density around PGV P 266:**

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

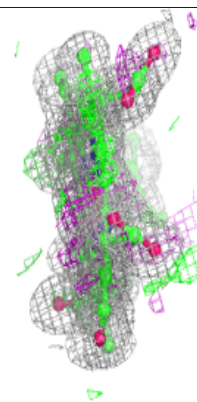
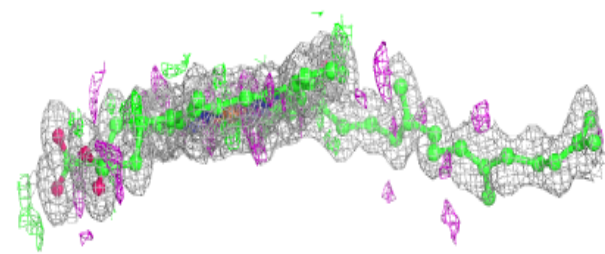
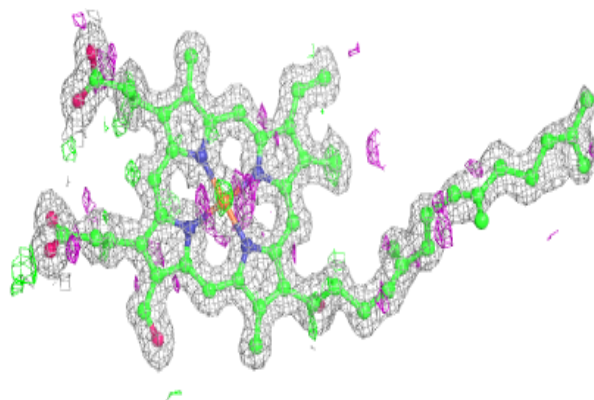


Electron density around PGV P 267:

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

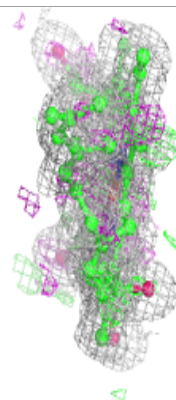
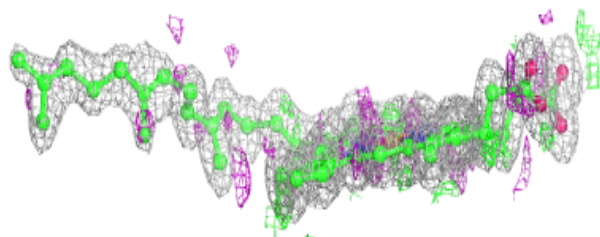
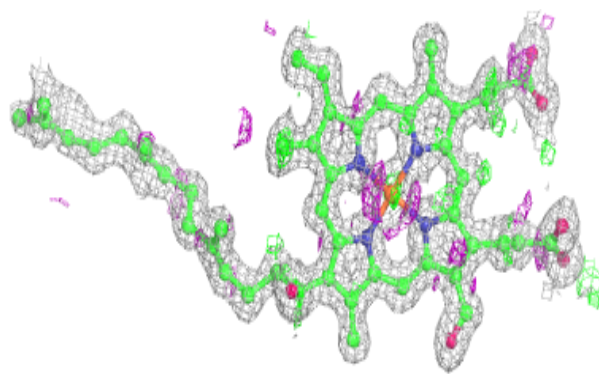
**Electron density around HEA A 515 (A):**

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

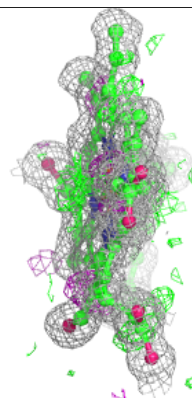
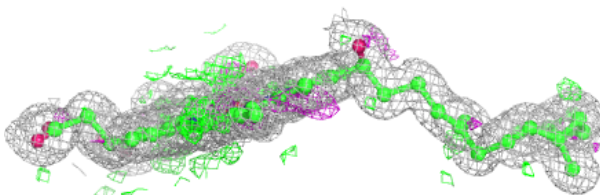
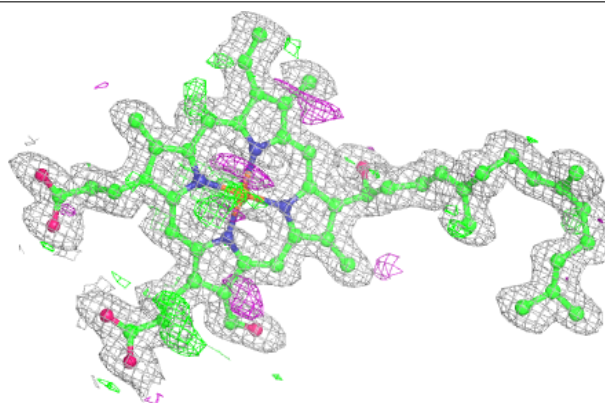


Electron density around HEA A 515 (B):

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

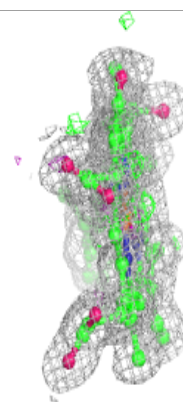
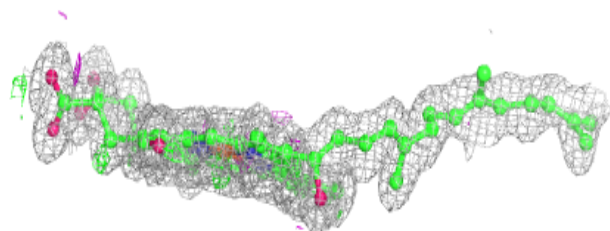
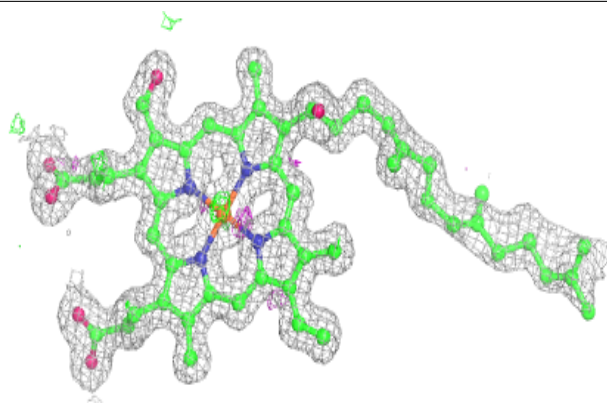
**Electron density around HEA A 516:**

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

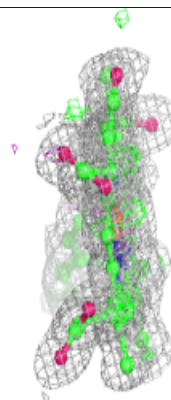
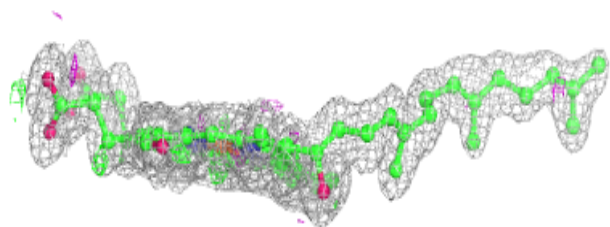
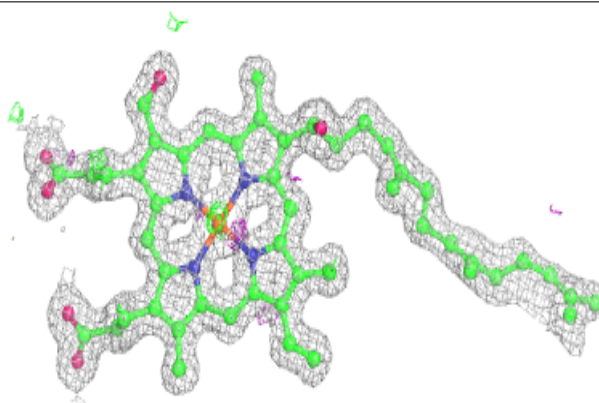


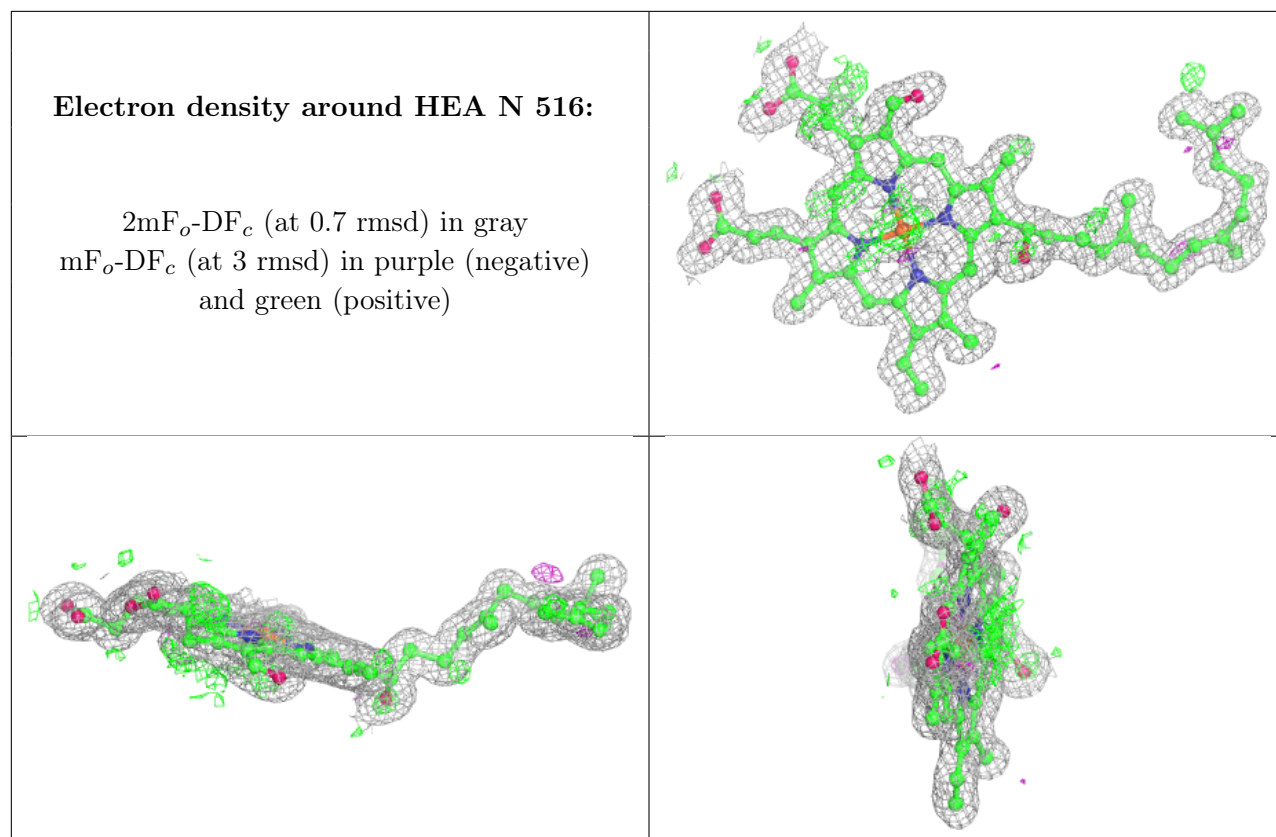
Electron density around HEA N 515 (A):

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

**Electron density around HEA N 515 (B):**

$2mF_o-DF_c$ (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.