



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 08:02 PM JST

PDB ID : 7COH / pdb_00007coh
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

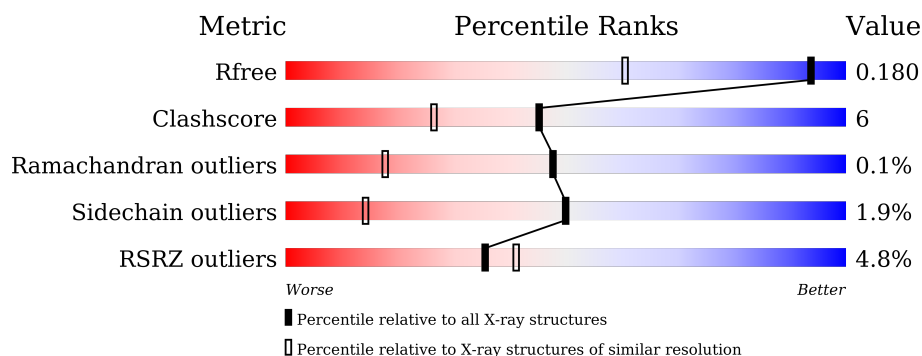
1 Overall quality at a glance

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.



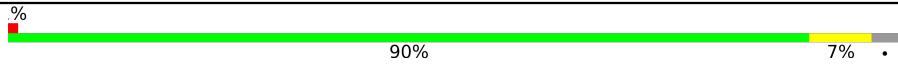
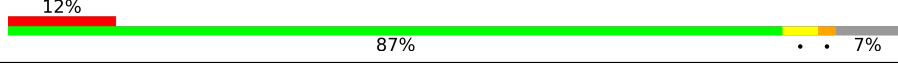
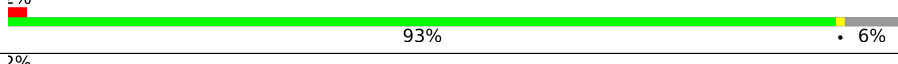
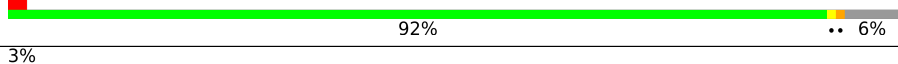
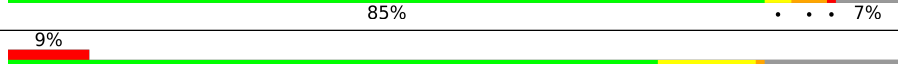
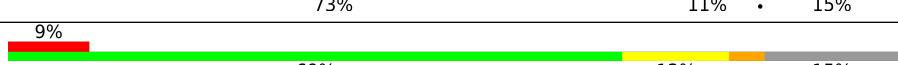
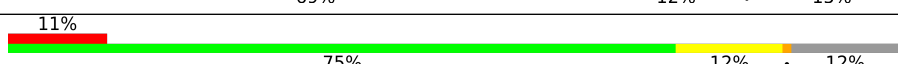
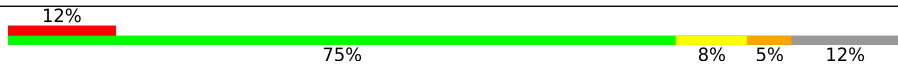
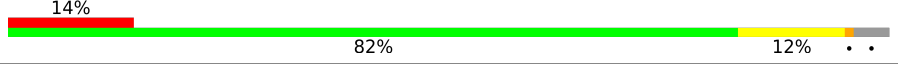
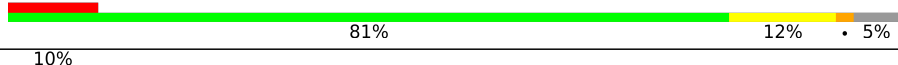
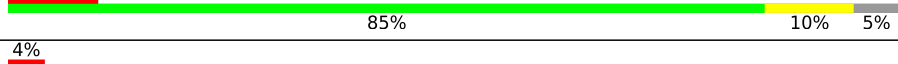
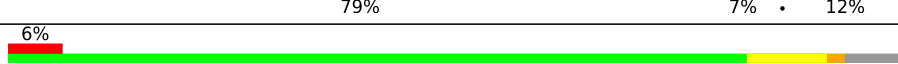
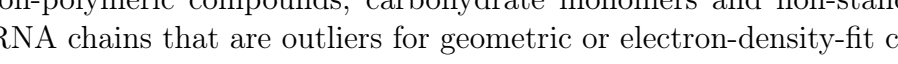
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	83% 15%
1	N	514	88% 11%
2	B	227	78% 17%
2	O	227	81% 16%
3	C	261	85% 14%
3	P	261	85% 13%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	PER	A	520	-	X	-	-
21	PER	N	520	-	X	-	-
22	LFA	C	612	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	LFA	C	615	-	-	-	X
22	LFA	P	614	-	-	-	X
22	LFA	P	615	-	-	-	X
22	LFA	P	623	-	-	-	X
22	LFA	P	624	-	-	-	X
23	EDO	C	807	-	-	-	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			

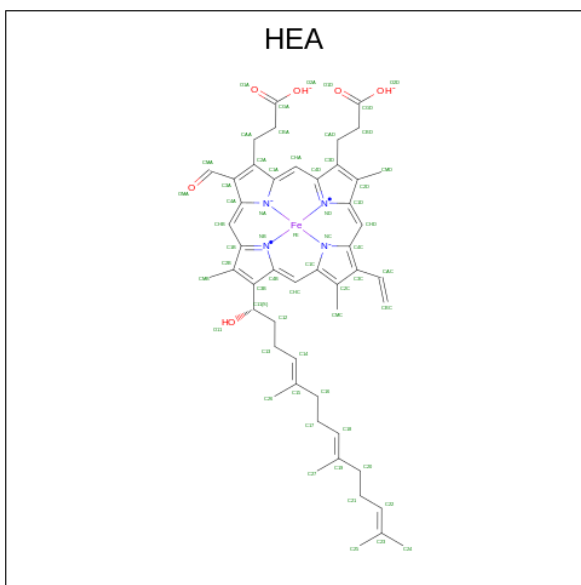
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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 (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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 (CCD ID: CU) (formula: Cu).

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

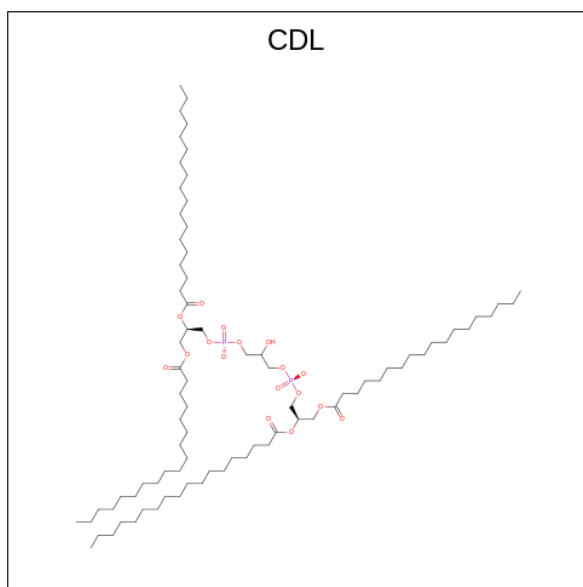
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

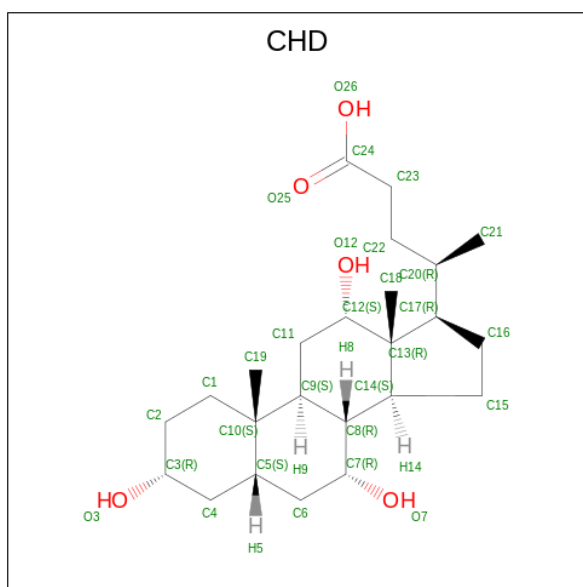
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

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



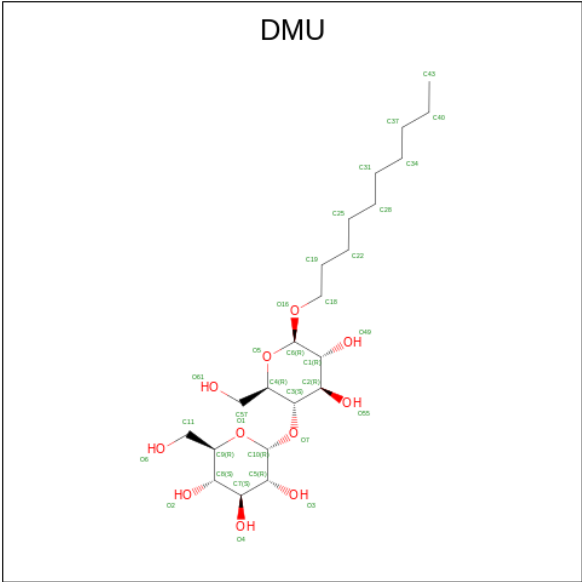
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			94	75	17	2		
18	A	1	Total	C	O	P	0	0
			64	45	17	2		
18	C	1	Total	C	O	P	0	0
			87	68	17	2		
18	N	1	Total	C	O	P	0	0
			94	75	17	2		
18	N	1	Total	C	O	P	0	0
			64	45	17	2		
18	P	1	Total	C	O	P	0	0
			87	68	17	2		

- Molecule 19 is CHOLIC ACID (CCD ID: 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 (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$) (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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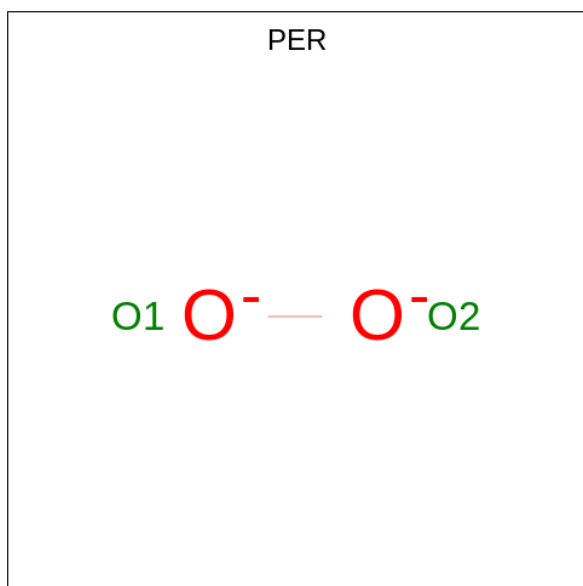
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			22	16	6		
20	G	1	Total	C	O	0	0
			11	10	1		
20	G	1	Total	C	O	0	0
			22	16	6		
20	J	1	Total	C	O	0	0
			11	10	1		
20	J	1	Total	C	O	0	0
			33	22	11		
20	L	1	Total	C	O	0	0
			22	16	6		
20	M	1	Total	C		0	0
			8	8			
20	N	1	Total	C	O	0	0
			33	22	11		
20	N	1	Total	C		0	0
			7	7			
20	N	1	Total	C	O	0	0
			33	22	11		
20	N	1	Total	C	O	0	0
			33	22	11		
20	O	1	Total	C	O	0	0
			11	10	1		
20	O	1	Total	C	O	0	0
			11	10	1		
20	O	1	Total	C	O	0	0
			22	16	6		
20	P	1	Total	C	O	0	0
			33	22	11		
20	P	1	Total	C	O	0	1
			33	22	11		
20	P	1	Total	C		0	0
			7	7			
20	P	1	Total	C	O	0	0
			22	16	6		
20	P	1	Total	C	O	0	0
			33	22	11		
20	P	1	Total	C	O	0	0
			33	22	11		
20	P	1	Total	C	O	0	0
			11	10	1		

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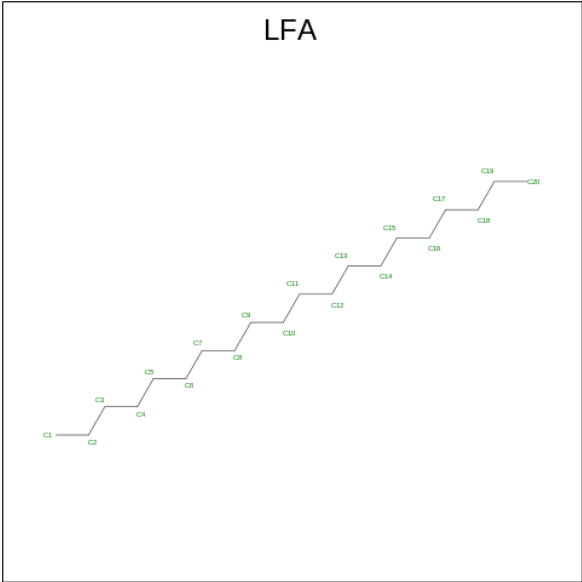
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	T	1	Total C O 22 16 6	0	0
20	T	1	Total C O 11 10 1	0	0
20	T	1	Total C O 22 16 6	0	0
20	W	1	Total C O 11 10 1	0	0
20	W	1	Total C O 33 22 11	0	0
20	Y	1	Total C O 22 16 6	0	0
20	Z	1	Total C 8 8	0	0

- Molecule 21 is PEROXIDE ION (CCD ID: 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 (CCD ID: LFA) (formula: C₂₀H₄₂) (labeled as "Ligand of Interest" by depositor).



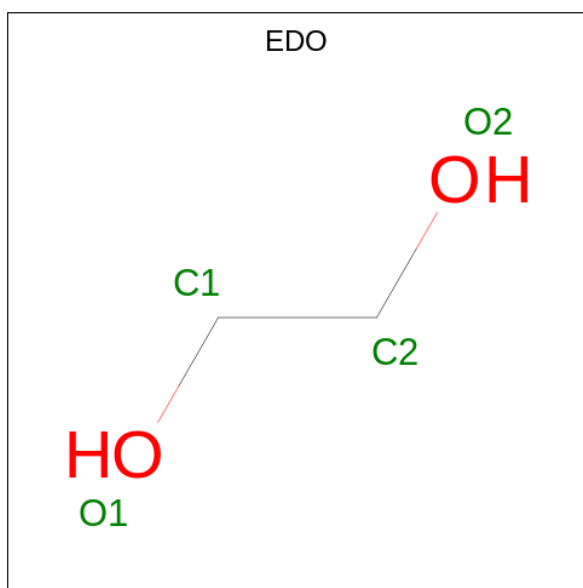
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	C	0	0
			14	14		
22	A	1	Total	C	0	0
			14	14		
22	C	1	Total	C	0	0
			11	11		
22	C	1	Total	C	0	0
			6	6		
22	C	1	Total	C	0	0
			15	15		
22	C	1	Total	C	0	0
			11	11		
22	C	1	Total	C	0	0
			14	14		
22	C	1	Total	C	0	0
			11	11		
22	C	1	Total	C	0	0
			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 (CCD ID: EDO) (formula: $C_2H_6O_2$).



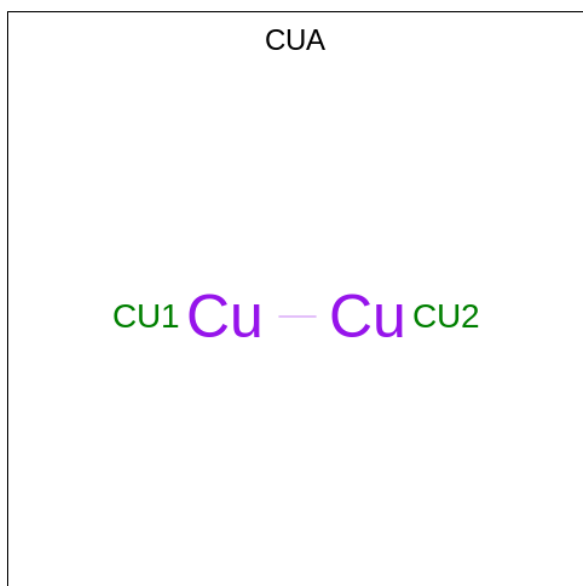
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total 4	C 2	O 2	0	0
23	A	1	Total 4	C 2	O 2	0	0
23	A	1	Total 4	C 2	O 2	0	0
23	A	1	Total 4	C 2	O 2	0	0
23	B	1	Total 4	C 2	O 2	0	0
23	C	1	Total 4	C 2	O 2	0	0
23	C	1	Total 4	C 2	O 2	0	0
23	C	1	Total 4	C 2	O 2	0	0
23	E	1	Total 4	C 2	O 2	0	0
23	E	1	Total 4	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 (CCD ID: CUA) (formula: Cu₂).

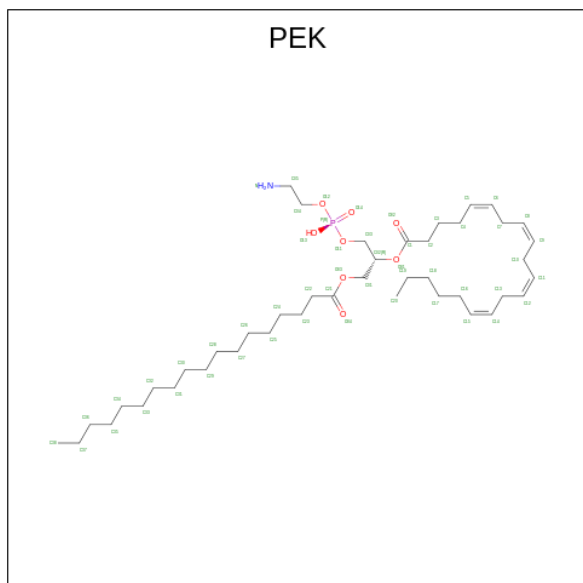


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total Cu 2 2	0	0
24	O	1	Total Cu 2 2	0	0

- Molecule 25 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

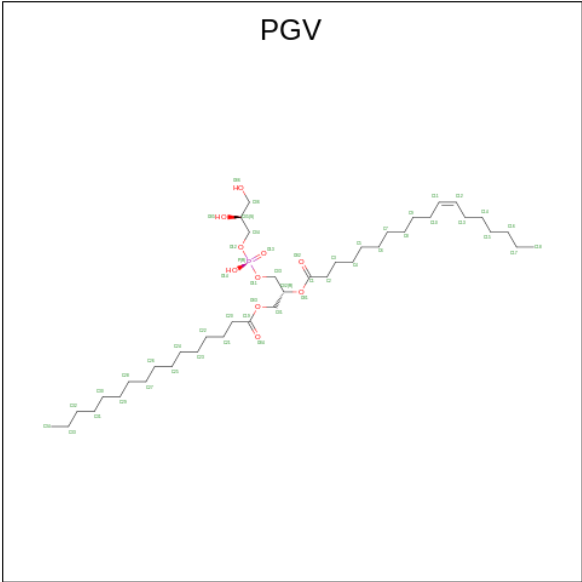
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total X 1 1	0	0
25	P	1	Total X 1 1	0	0

- Molecule 26 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: 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 (CCD ID: 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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 29 is 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
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	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	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

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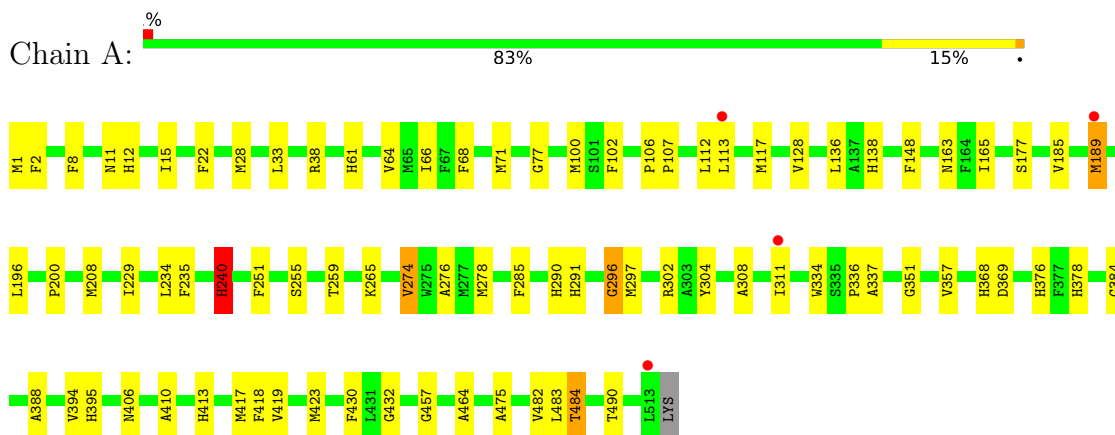
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1 1	0	0
29	Z	1	Total O 1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

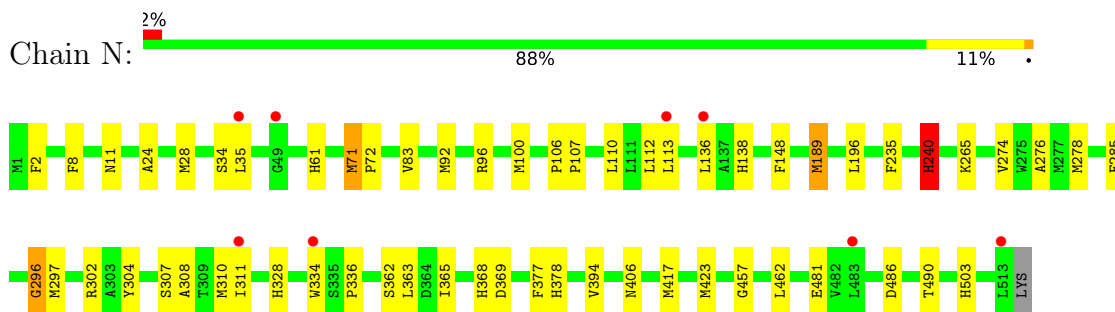
3 Residue-property plots [i](#)

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

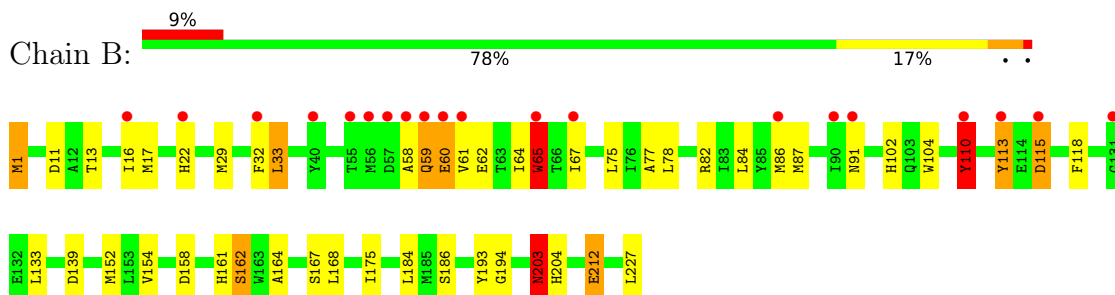
- Molecule 1: Cytochrome c oxidase subunit 1



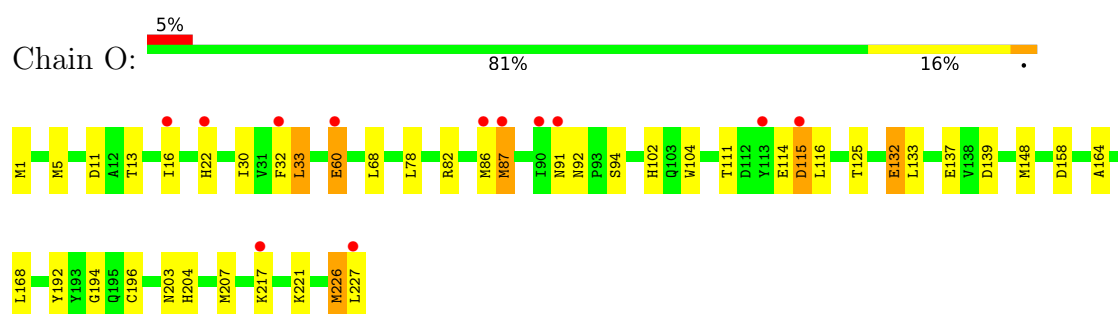
- Molecule 1: Cytochrome c oxidase subunit 1



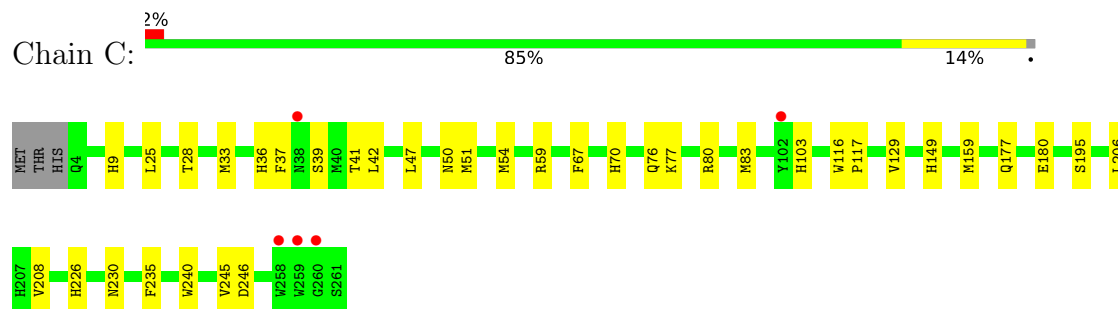
- Molecule 2: Cytochrome c oxidase subunit 2



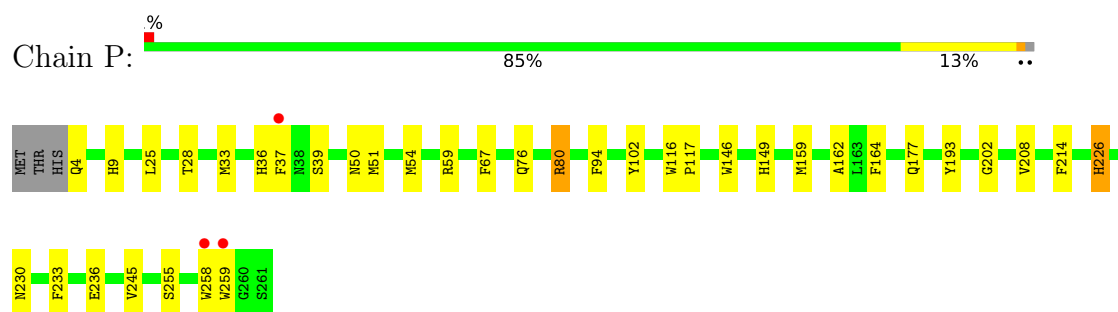
- Molecule 2: Cytochrome c oxidase subunit 2



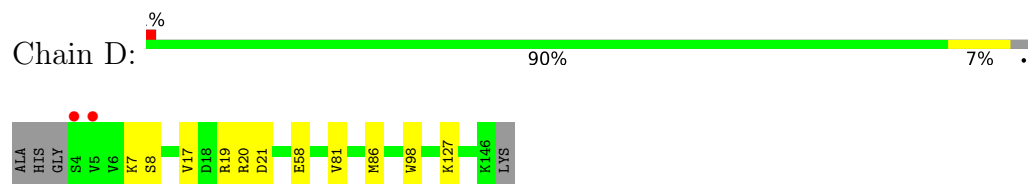
- Molecule 3: Cytochrome c oxidase subunit 3



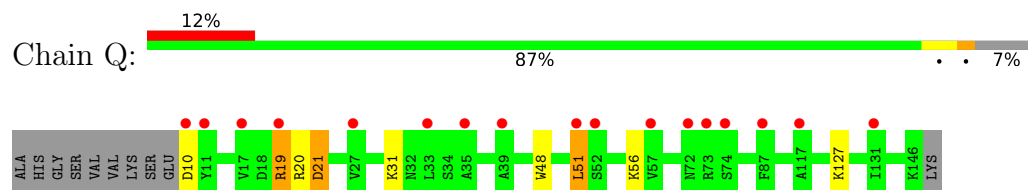
- Molecule 3: Cytochrome c oxidase subunit 3



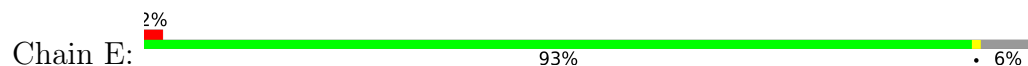
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

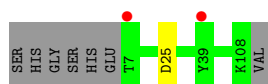


- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

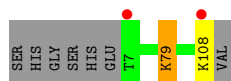


- Molecule 5: Cytochrome c oxidase subunit 5A

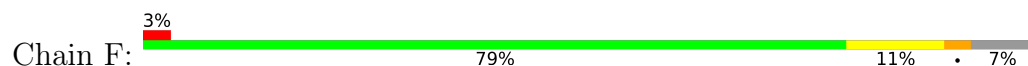




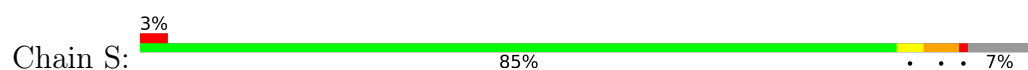
- Molecule 5: Cytochrome c oxidase subunit 5A



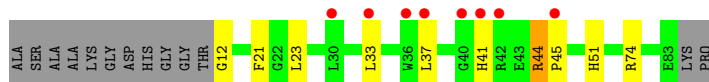
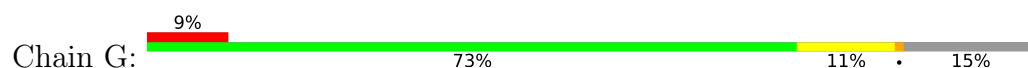
- Molecule 6: Cytochrome c oxidase subunit 5B



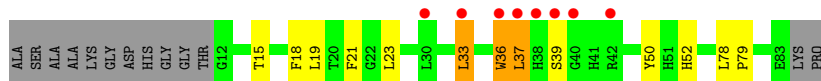
- Molecule 6: Cytochrome c oxidase subunit 5B



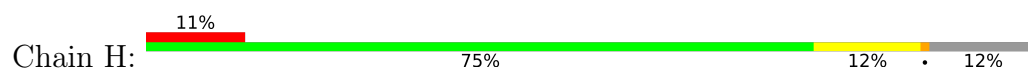
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



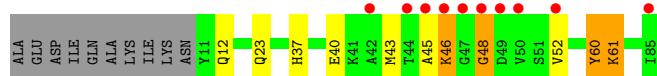
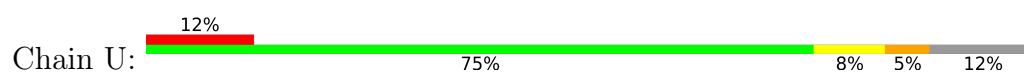
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



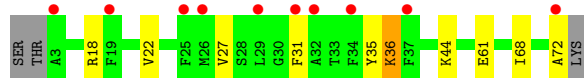
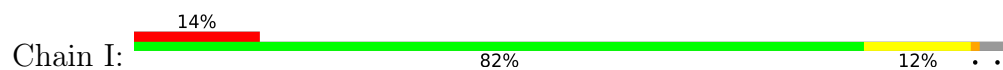
- Molecule 8: Cytochrome c oxidase subunit 6B1



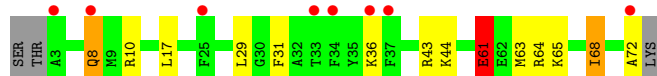
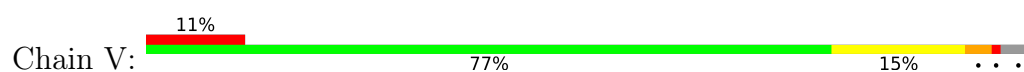
- Molecule 8: Cytochrome c oxidase subunit 6B1



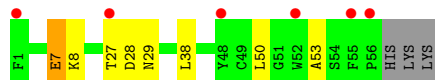
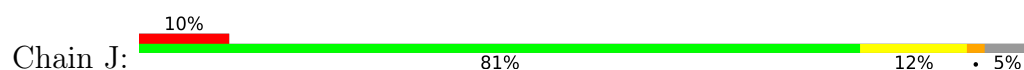
• Molecule 9: Cytochrome c oxidase subunit 6C



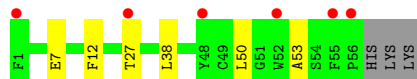
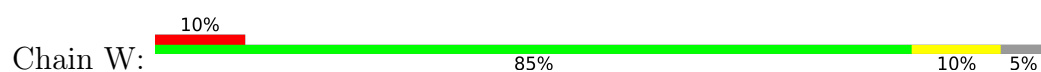
• Molecule 9: Cytochrome c oxidase subunit 6C



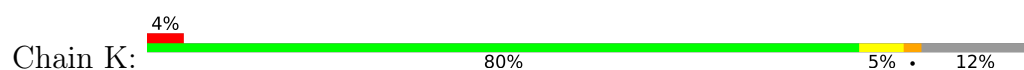
• Molecule 10: Cytochrome c oxidase subunit 7A1



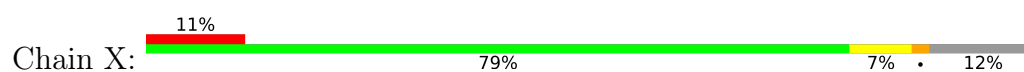
• Molecule 10: Cytochrome c oxidase subunit 7A1



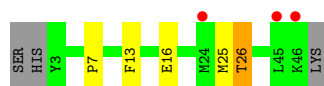
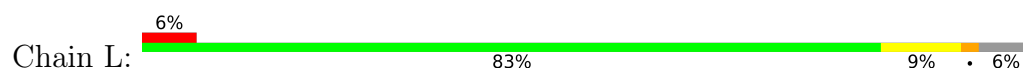
• Molecule 11: Cytochrome c oxidase subunit 7B



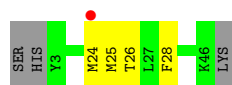
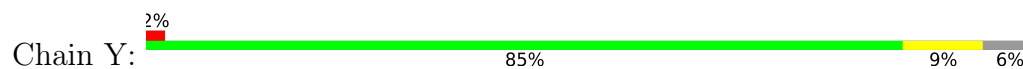
• Molecule 11: Cytochrome c oxidase subunit 7B



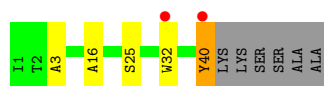
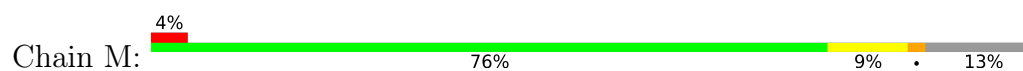
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



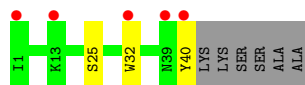
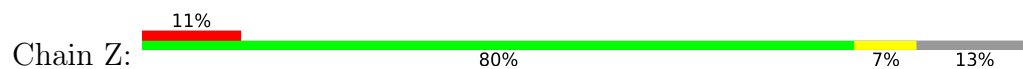
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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 40.00 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-1.30) 99.6 (40.00-1.30)	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 0.161 , 0.180	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)	0.33 , 51.0	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: ZN, CUA, CDL, EDO, CU, PER, MG, DMU, PGV, CHD, FME, LFA, HEA, NA, PEK, UNX

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	1.52	35/4259 (0.8%)	1.64	34/5816 (0.6%)
1	N	1.36	19/4259 (0.4%)	1.44	14/5816 (0.2%)
2	B	1.61	16/1908 (0.8%)	1.60	26/2598 (1.0%)
2	O	1.20	4/1908 (0.2%)	1.35	9/2598 (0.3%)
3	C	1.38	7/2258 (0.3%)	1.45	5/3084 (0.2%)
3	P	1.31	6/2258 (0.3%)	1.41	9/3084 (0.3%)
4	D	1.17	3/1226 (0.2%)	1.29	4/1657 (0.2%)
4	Q	1.05	0/1182	1.31	1/1598 (0.1%)
5	E	1.09	0/843	1.29	1/1145 (0.1%)
5	R	1.08	0/843	1.30	0/1145
6	F	1.28	2/724 (0.3%)	1.36	3/983 (0.3%)
6	S	1.26	2/724 (0.3%)	1.33	8/983 (0.8%)
7	G	1.12	1/633 (0.2%)	1.27	2/864 (0.2%)
7	T	1.15	0/633	1.33	2/864 (0.2%)
8	H	1.21	1/648 (0.2%)	1.35	1/877 (0.1%)
8	U	1.15	1/648 (0.2%)	1.36	3/877 (0.3%)
9	I	1.17	3/588 (0.5%)	1.49	4/781 (0.5%)
9	V	1.18	1/588 (0.2%)	1.45	1/781 (0.1%)
10	J	1.06	0/451	1.32	2/610 (0.3%)
10	W	1.05	0/451	1.28	1/610 (0.2%)
11	K	1.19	1/398 (0.3%)	1.51	1/546 (0.2%)
11	X	1.16	0/398	1.31	2/546 (0.4%)
12	L	1.27	0/372	1.44	4/500 (0.8%)
12	Y	1.14	0/372	1.24	2/500 (0.4%)
13	M	1.20	0/321	1.46	4/440 (0.9%)
13	Z	1.13	0/321	1.36	0/440
All	All	1.31	102/29214 (0.3%)	1.43	143/39743 (0.4%)

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 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	110	TYR	CE1-CZ	22.92	1.93	1.38
2	B	162	SER	C-O	-18.95	1.00	1.23
2	B	110	TYR	CG-CD1	17.21	1.75	1.39
2	B	212	GLU	C-N	11.88	1.50	1.33
2	B	110	TYR	CG-CD2	11.74	1.64	1.39

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	54	ARG	CA-C-O	-18.22	89.82	120.80
2	B	110	TYR	CB-CG-CD1	-12.43	102.16	120.80
2	B	64	ILE	CA-C-N	10.83	135.21	120.38
2	B	64	ILE	C-N-CA	10.83	135.21	120.38
1	N	71	MET	CG-SD-CE	-10.73	77.29	100.90

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	34	0
2	O	1870	0	1870	20	0
3	C	2171	0	2080	30	0
3	P	2172	0	2081	29	0
4	D	1192	0	1178	5	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	12	0
6	S	709	0	691	6	0
7	G	606	0	577	5	0
7	T	606	0	577	9	0
8	H	628	0	580	13	0
8	U	628	0	580	13	0
9	I	575	0	584	6	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	1	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	8	0
14	N	129	0	88	9	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	15	0
18	N	158	0	213	8	0
18	P	87	0	124	13	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	2	0
20	G	55	0	81	1	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	2	0
20	O	44	0	73	2	0
20	P	172	0	231	3	0
20	T	55	0	83	1	0
20	W	44	0	61	7	0
20	Y	22	0	31	0	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	17	0
22	C	114	0	219	7	0
22	G	28	0	54	1	0
22	N	28	0	54	9	0
22	P	114	0	219	4	0
22	T	28	0	54	4	0
23	A	16	0	24	0	0
23	B	4	0	6	0	0
23	C	12	0	18	0	0
23	E	12	0	18	0	0
23	F	8	0	12	0	0
23	G	4	0	6	0	0
23	N	20	0	30	0	0
23	O	4	0	6	0	0
23	P	12	0	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	3	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	11	0
29	B	179	0	0	2	0
29	C	101	0	0	1	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	7	0
29	O	147	0	0	0	0
29	P	102	0	0	5	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	0	0
All	All	33049	0	31527	366	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 366 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)
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.18	1.14
21:A:520:PER:O2	21:A:520:PER:O1	1.70	1.09

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	526/514 (102%)	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%)	9	1
8	U	73/85 (86%)	69 (94%)	2 (3%)	2 (3%)	4	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%)	48	18

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%)	437 (99%)	3 (1%)	76	50
1	N	440/426 (103%)	438 (100%)	2 (0%)	81	60
2	B	215/210 (102%)	207 (96%)	8 (4%)	30	3
2	O	215/210 (102%)	204 (95%)	11 (5%)	21	1
3	C	232/226 (103%)	230 (99%)	2 (1%)	70	42
3	P	232/226 (103%)	230 (99%)	2 (1%)	70	42
4	D	128/129 (99%)	128 (100%)	0	100	100
4	Q	122/129 (95%)	118 (97%)	4 (3%)	33	4
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%)	65	33
6	F	78/81 (96%)	76 (97%)	2 (3%)	40	7
6	S	78/81 (96%)	77 (99%)	1 (1%)	61	26
7	G	63/69 (91%)	61 (97%)	2 (3%)	34	4
7	T	63/69 (91%)	61 (97%)	2 (3%)	34	4
8	H	67/75 (89%)	65 (97%)	2 (3%)	36	5
8	U	67/75 (89%)	64 (96%)	3 (4%)	24	2
9	I	55/58 (95%)	54 (98%)	1 (2%)	51	16
9	V	55/58 (95%)	48 (87%)	7 (13%)	4	0
10	J	47/50 (94%)	46 (98%)	1 (2%)	47	11
10	W	47/50 (94%)	46 (98%)	1 (2%)	47	11
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	7
11	X	39/46 (85%)	38 (97%)	1 (3%)	40	7
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%)	2985 (98%)	57 (2%)	50	14

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	87[A]	MET
10	W	50	LEU
3	P	159	MET
9	V	68	ILE
9	V	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	35	GLN
1	N	422	ASN
8	U	37	HIS
1	N	170	ASN

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Mol	Chain	Res	Type
3	P	50	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	N	1	1	8,9,10	0.63	0	7,9,11	0.86	0
2	FME	O	1	2	8,9,10	0.85	0	7,9,11	0.92	0
1	FME	A	1	1	8,9,10	0.52	0	7,9,11	0.77	0
2	FME	B	1	2	8,9,10	3.32	3 (37%)	7,9,11	3.89	2 (28%)

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

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

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	FME	2	0
1	A	1	FME	1	0
2	B	1	FME	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	C	722	-	22,22,34	0.52	0	27,27,45	0.94	2 (7%)
20	DMU	G	713	-	22,22,34	0.54	0	27,27,45	1.18	2 (7%)
20	DMU	N	745	-	34,34,34	1.43	4 (11%)	45,45,45	1.33	6 (13%)
20	DMU	C	715[A]	-	34,34,34	1.31	6 (17%)	45,45,45	1.36	3 (6%)
22	LFA	A	627	-	13,13,19	0.72	0	12,12,18	0.30	0
23	EDO	A	803	-	3,3,3	0.09	0	2,2,2	0.12	0
20	DMU	C	272	-	10,10,34	0.33	0	9,9,45	0.59	0
22	LFA	P	611	-	10,10,19	0.25	0	9,9,18	0.19	0
20	DMU	Z	746	-	7,7,34	0.16	0	6,6,45	0.48	0
22	LFA	P	626	-	12,12,19	0.31	0	11,11,18	0.30	0
22	LFA	T	621	-	16,16,19	0.40	0	15,15,18	0.31	0
18	CDL	P	270	-	86,86,99	0.47	0	92,98,111	0.95	6 (6%)
22	LFA	N	627	-	13,13,19	0.32	0	12,12,18	0.53	0
20	DMU	J	61	-	34,34,34	0.84	1 (2%)	45,45,45	1.05	2 (4%)
23	EDO	P	827	-	3,3,3	0.54	0	2,2,2	1.16	0
20	DMU	B	742	-	22,22,34	0.69	0	27,27,45	1.16	2 (7%)
20	DMU	O	741	-	10,10,34	0.53	0	9,9,45	0.55	0
20	DMU	T	713	-	22,22,34	0.68	1 (4%)	27,27,45	1.39	5 (18%)
23	EDO	C	827	-	3,3,3	0.49	0	2,2,2	0.75	0
27	PGV	C	267	-	50,50,50	0.87	3 (6%)	53,56,56	1.09	3 (5%)
18	CDL	A	522	-	63,63,99	0.53	0	69,75,111	1.18	6 (8%)
23	EDO	A	825	-	3,3,3	0.41	0	2,2,2	0.51	0
21	PER	N	520	15,14	1,1,1	2.41	1 (100%)	-		
21	PER	A	520	15,14	1,1,1	2.71	1 (100%)	-		
20	DMU	A	744	-	34,34,34	1.47	6 (17%)	45,45,45	1.19	3 (6%)
14	HEA	A	516	1,21	66,67,67	2.01	17 (25%)	78,103,103	2.66	31 (39%)
23	EDO	O	805	-	3,3,3	0.55	0	2,2,2	0.13	0
23	EDO	N	823	-	3,3,3	0.61	0	2,2,2	0.41	0
20	DMU	P	734	-	34,34,34	0.94	1 (2%)	45,45,45	1.19	2 (4%)
20	DMU	M	746	-	7,7,34	0.19	0	6,6,45	0.79	0
23	EDO	S	817	-	3,3,3	0.93	0	2,2,2	0.06	0
18	CDL	N	521	-	93,93,99	0.36	0	99,105,111	0.46	0
26	PEK	P	264	-	52,52,52	0.73	2 (3%)	55,57,57	1.03	4 (7%)
20	DMU	C	733	-	34,34,34	1.17	5 (14%)	45,45,45	1.20	5 (11%)
19	CHD	A	525	-	32,32,32	0.98	2 (6%)	51,51,51	1.13	5 (9%)
22	LFA	A	628	-	13,13,19	0.45	0	12,12,18	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	DMU	N	744	-	34,34,34	1.42	7 (20%)	45,45,45	1.54	5 (11%)
23	EDO	N	801	-	3,3,3	0.53	0	2,2,2	0.12	0
22	LFA	C	624	-	10,10,19	0.28	0	9,9,18	0.20	0
23	EDO	F	817	-	3,3,3	0.64	0	2,2,2	0.34	0
20	DMU	W	732	-	10,10,34	0.16	0	9,9,45	0.57	0
20	DMU	A	745	-	34,34,34	1.18	3 (8%)	45,45,45	1.03	2 (4%)
23	EDO	C	807	-	3,3,3	0.17	0	2,2,2	0.20	0
22	LFA	P	612	-	5,5,19	0.09	0	4,4,18	0.20	0
20	DMU	T	712	-	10,10,34	0.45	0	9,9,45	0.58	0
20	DMU	P	272	-	10,10,34	0.25	0	9,9,45	0.70	0
22	LFA	P	624	-	10,10,19	0.19	0	9,9,18	0.14	0
22	LFA	N	628	-	13,13,19	0.49	0	12,12,18	0.52	0
19	CHD	T	86	-	32,32,32	0.85	1 (3%)	51,51,51	1.08	2 (3%)
14	HEA	A	515[B]	-	66,67,67	1.68	15 (22%)	78,103,103	2.47	26 (33%)
20	DMU	J	732	-	10,10,34	0.15	0	9,9,45	0.64	0
20	DMU	C	714	-	34,34,34	0.85	1 (2%)	45,45,45	1.25	6 (13%)
20	DMU	P	722	-	22,22,34	0.46	0	27,27,45	1.06	2 (7%)
23	EDO	E	815	-	3,3,3	0.40	0	2,2,2	0.60	0
18	CDL	C	270	-	86,86,99	0.56	1 (1%)	92,98,111	1.07	9 (9%)
19	CHD	C	271	-	32,32,32	0.69	0	51,51,51	1.56	9 (17%)
22	LFA	C	625	-	14,14,19	0.26	0	13,13,18	0.44	0
24	CUA	O	228	2	0,1,1	-	-	-	-	-
27	PGV	P	266	-	50,50,50	0.91	3 (6%)	53,56,56	1.20	2 (3%)
20	DMU	L	747	-	22,22,34	0.72	0	27,27,45	1.27	3 (11%)
23	EDO	F	819	-	3,3,3	0.44	0	2,2,2	0.39	0
22	LFA	C	612	-	5,5,19	0.20	0	4,4,18	0.16	0
20	DMU	N	526	-	34,34,34	0.96	2 (5%)	45,45,45	1.14	2 (4%)
23	EDO	A	823	-	3,3,3	0.53	0	2,2,2	0.57	0
23	EDO	P	809	-	3,3,3	0.40	0	2,2,2	0.38	0
18	CDL	A	521	-	93,93,99	0.46	0	99,105,111	0.60	2 (2%)
20	DMU	O	742	-	22,22,34	1.00	2 (9%)	27,27,45	1.09	3 (11%)
26	PEK	C	264	-	52,52,52	0.59	2 (3%)	55,57,57	0.81	2 (3%)
27	PGV	C	266	-	50,50,50	1.08	4 (8%)	53,56,56	1.08	3 (5%)
14	HEA	N	516	1,21	66,67,67	1.98	16 (24%)	78,103,103	2.97	26 (33%)
20	DMU	G	711	-	22,22,34	0.74	1 (4%)	27,27,45	1.37	3 (11%)
19	CHD	N	525	-	32,32,32	1.01	2 (6%)	51,51,51	0.94	2 (3%)
22	LFA	C	611	-	10,10,19	0.26	0	9,9,18	0.30	0
22	LFA	C	716[B]	-	17,17,19	0.17	0	16,16,18	0.16	0
23	EDO	E	813	-	3,3,3	0.36	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	EDO	B	805	-	3,3,3	1.04	0	2,2,2	0.97	0
20	DMU	P	715[A]	-	34,34,34	1.22	4 (11%)	45,45,45	1.25	3 (6%)
20	DMU	N	743	-	6,6,34	0.34	0	5,5,45	0.35	0
14	HEA	N	515[B]	-	66,67,67	1.61	12 (18%)	78,103,103	2.12	22 (28%)
22	LFA	P	623	-	13,13,19	0.25	0	12,12,18	0.26	0
20	DMU	B	731	-	10,10,34	0.29	0	9,9,45	0.54	0
23	EDO	T	821	-	3,3,3	0.44	0	2,2,2	0.24	0
23	EDO	A	801	-	3,3,3	0.66	0	2,2,2	0.87	0
22	LFA	G	622	-	10,10,19	0.18	0	9,9,18	0.16	0
20	DMU	Y	747	-	22,22,34	0.56	0	27,27,45	1.18	2 (7%)
20	DMU	P	714	-	34,34,34	0.73	0	45,45,45	1.06	3 (6%)
19	CHD	G	86	-	32,32,32	0.76	0	51,51,51	1.10	3 (5%)
22	LFA	C	615	-	10,10,19	0.16	0	9,9,18	0.15	0
22	LFA	P	625	-	14,14,19	0.30	0	13,13,18	0.54	0
20	DMU	G	712	-	10,10,34	0.23	0	9,9,45	0.59	0
23	EDO	E	811	-	3,3,3	0.19	0	2,2,2	0.44	0
23	EDO	N	803	-	3,3,3	0.20	0	2,2,2	0.41	0
20	DMU	T	711	-	22,22,34	0.79	0	27,27,45	1.45	4 (14%)
24	CUA	B	228	2	0,1,1	-	-	-	-	-
22	LFA	C	626	-	12,12,19	0.21	0	11,11,18	0.24	0
20	DMU	C	721	-	6,6,34	0.21	0	5,5,45	0.58	0
20	DMU	O	731	-	10,10,34	0.21	0	9,9,45	0.46	0
27	PGV	P	267	-	50,50,50	0.75	1 (2%)	53,56,56	0.92	1 (1%)
20	DMU	A	526	-	34,34,34	1.05	2 (5%)	45,45,45	1.12	2 (4%)
20	DMU	P	721	-	6,6,34	0.18	0	5,5,45	0.62	0
23	EDO	R	811	-	3,3,3	0.12	0	2,2,2	0.08	0
22	LFA	P	716[B]	-	17,17,19	0.13	0	16,16,18	0.12	0
23	EDO	R	813	-	3,3,3	0.18	0	2,2,2	0.03	0
23	EDO	N	829	-	3,3,3	0.16	0	2,2,2	0.18	0
20	DMU	P	733	-	34,34,34	0.81	2 (5%)	45,45,45	1.46	4 (8%)
19	CHD	P	271	-	32,32,32	0.58	0	51,51,51	1.59	8 (15%)
22	LFA	P	614	-	14,14,19	0.17	0	13,13,18	0.16	0
18	CDL	N	522	-	63,63,99	0.50	1 (1%)	69,75,111	1.04	5 (7%)
20	DMU	C	734	-	34,34,34	0.99	1 (2%)	45,45,45	1.06	3 (6%)
23	EDO	N	825	-	3,3,3	0.51	0	2,2,2	0.23	0
23	EDO	C	809	-	3,3,3	0.20	0	2,2,2	0.54	0
23	EDO	P	807	-	3,3,3	0.07	0	2,2,2	0.13	0
20	DMU	A	743	-	6,6,34	0.30	0	5,5,45	0.38	0
23	EDO	G	821	-	3,3,3	0.22	0	2,2,2	0.27	0
23	EDO	R	815	-	3,3,3	0.15	0	2,2,2	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LFA	C	623	-	13,13,19	0.28	0	12,12,18	0.18	0
22	LFA	T	622	-	10,10,19	0.21	0	9,9,18	0.12	0
23	EDO	S	819	-	3,3,3	0.33	0	2,2,2	0.24	0
22	LFA	G	621	-	16,16,19	0.30	0	15,15,18	0.60	0
20	DMU	B	741	-	10,10,34	0.34	0	9,9,45	0.56	0
14	HEA	N	515[A]	-	66,67,67	1.59	12 (18%)	78,103,103	2.18	21 (26%)
22	LFA	C	614	-	14,14,19	0.21	0	13,13,18	0.21	0
20	DMU	W	61	-	34,34,34	0.72	0	45,45,45	1.49	4 (8%)
14	HEA	A	515[A]	-	66,67,67	1.69	15 (22%)	78,103,103	2.49	26 (33%)
22	LFA	P	615	-	10,10,19	0.19	0	9,9,18	0.17	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	C	722	-	-	10/13/33/59	0/1/1/2
20	DMU	G	713	-	-	8/13/33/59	0/1/1/2
20	DMU	N	745	-	-	7/19/59/59	0/2/2/2
20	DMU	C	715[A]	-	-	3/19/59/59	0/2/2/2
22	LFA	A	627	-	-	5/11/11/17	-
23	EDO	A	803	-	-	0/1/1/1	-
20	DMU	C	272	-	-	4/8/8/59	-
22	LFA	P	611	-	-	5/8/8/17	-
20	DMU	Z	746	-	-	2/5/5/59	-
22	LFA	P	626	-	-	5/10/10/17	-
22	LFA	T	621	-	-	9/14/14/17	-
18	CDL	P	270	-	-	49/97/97/110	-
22	LFA	N	627	-	-	5/11/11/17	-
20	DMU	J	61	-	-	5/19/59/59	0/2/2/2
23	EDO	P	827	-	-	0/1/1/1	-
20	DMU	B	742	-	-	8/13/33/59	0/1/1/2
20	DMU	O	741	-	-	4/8/8/59	-
20	DMU	T	713	-	-	5/13/33/59	0/1/1/2
23	EDO	C	827	-	-	1/1/1/1	-
27	PGV	C	267	-	-	13/55/55/55	-
18	CDL	A	522	-	-	31/74/74/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	EDO	A	825	-	-	1/1/1/1	-
20	DMU	A	744	-	-	7/19/59/59	0/2/2/2
14	HEA	A	516	1,21	-	4/36/76/76	-
23	EDO	O	805	-	-	0/1/1/1	-
23	EDO	N	823	-	-	0/1/1/1	-
20	DMU	P	734	-	-	10/19/59/59	0/2/2/2
20	DMU	M	746	-	-	5/5/5/59	-
23	EDO	S	817	-	-	0/1/1/1	-
18	CDL	N	521	-	-	53/104/104/110	-
26	PEK	P	264	-	-	18/56/56/56	-
20	DMU	C	733	-	-	9/19/59/59	0/2/2/2
19	CHD	A	525	-	-	2/9/74/74	0/4/4/4
22	LFA	A	628	-	-	5/11/11/17	-
20	DMU	N	744	-	-	5/19/59/59	0/2/2/2
23	EDO	N	801	-	-	0/1/1/1	-
22	LFA	C	624	-	-	4/8/8/17	-
23	EDO	F	817	-	-	0/1/1/1	-
20	DMU	W	732	-	-	7/8/8/59	-
20	DMU	A	745	-	-	5/19/59/59	0/2/2/2
23	EDO	C	807	-	-	0/1/1/1	-
22	LFA	P	612	-	-	1/3/3/17	-
20	DMU	T	712	-	-	4/8/8/59	-
20	DMU	P	272	-	-	0/8/8/59	-
22	LFA	P	624	-	-	6/8/8/17	-
22	LFA	N	628	-	-	6/11/11/17	-
19	CHD	T	86	-	-	2/9/74/74	0/4/4/4
14	HEA	A	515[B]	-	-	4/36/76/76	-
20	DMU	J	732	-	-	5/8/8/59	-
20	DMU	C	714	-	-	8/19/59/59	0/2/2/2
20	DMU	P	722	-	-	8/13/33/59	0/1/1/2
23	EDO	E	815	-	-	1/1/1/1	-
18	CDL	C	270	-	-	49/97/97/110	-
19	CHD	C	271	-	-	8/9/74/74	0/4/4/4
22	LFA	C	625	-	-	3/12/12/17	-
27	PGV	P	266	-	-	8/55/55/55	-
20	DMU	L	747	-	-	10/13/33/59	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	EDO	F	819	-	-	0/1/1/1	-
22	LFA	C	612	-	-	1/3/3/17	-
20	DMU	N	526	-	-	6/19/59/59	0/2/2/2
23	EDO	A	823	-	-	0/1/1/1	-
23	EDO	P	809	-	-	0/1/1/1	-
18	CDL	A	521	-	-	51/104/104/110	-
20	DMU	O	742	-	-	7/13/33/59	0/1/1/2
26	PEK	C	264	-	-	15/56/56/56	-
27	PGV	C	266	-	-	7/55/55/55	-
14	HEA	N	516	1,21	-	4/36/76/76	-
20	DMU	G	711	-	-	3/13/33/59	0/1/1/2
19	CHD	N	525	-	-	2/9/74/74	0/4/4/4
22	LFA	C	611	-	-	5/8/8/17	-
22	LFA	C	716[B]	-	-	5/15/15/17	-
23	EDO	E	813	-	-	0/1/1/1	-
23	EDO	B	805	-	-	0/1/1/1	-
20	DMU	P	715[A]	-	-	6/19/59/59	0/2/2/2
20	DMU	N	743	-	-	3/4/4/59	-
14	HEA	N	515[B]	-	-	3/36/76/76	-
22	LFA	P	623	-	-	5/11/11/17	-
20	DMU	B	731	-	-	6/8/8/59	-
23	EDO	T	821	-	-	0/1/1/1	-
23	EDO	A	801	-	-	0/1/1/1	-
22	LFA	G	622	-	-	3/8/8/17	-
20	DMU	Y	747	-	-	9/13/33/59	0/1/1/2
20	DMU	P	714	-	-	5/19/59/59	0/2/2/2
19	CHD	G	86	-	-	2/9/74/74	0/4/4/4
22	LFA	C	615	-	-	2/8/8/17	-
22	LFA	P	625	-	-	4/12/12/17	-
20	DMU	G	712	-	-	4/8/8/59	-
23	EDO	E	811	-	-	0/1/1/1	-
23	EDO	N	803	-	-	1/1/1/1	-
20	DMU	T	711	-	-	7/13/33/59	0/1/1/2
22	LFA	C	626	-	-	4/10/10/17	-
20	DMU	C	721	-	-	2/4/4/59	-
20	DMU	O	731	-	-	4/8/8/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PGV	P	267	-	-	12/55/55/55	-
20	DMU	A	526	-	-	4/19/59/59	0/2/2/2
20	DMU	P	721	-	-	3/4/4/59	-
23	EDO	R	811	-	-	1/1/1/1	-
22	LFA	P	716[B]	-	-	6/15/15/17	-
23	EDO	R	813	-	-	0/1/1/1	-
23	EDO	N	829	-	-	0/1/1/1	-
20	DMU	P	733	-	-	6/19/59/59	0/2/2/2
19	CHD	P	271	-	-	8/9/74/74	0/4/4/4
22	LFA	P	614	-	-	6/12/12/17	-
18	CDL	N	522	-	-	34/74/74/110	-
20	DMU	C	734	-	-	8/19/59/59	0/2/2/2
23	EDO	N	825	-	-	0/1/1/1	-
23	EDO	C	809	-	-	0/1/1/1	-
23	EDO	P	807	-	-	1/1/1/1	-
20	DMU	A	743	-	-	2/4/4/59	-
23	EDO	G	821	-	-	0/1/1/1	-
23	EDO	R	815	-	-	1/1/1/1	-
22	LFA	C	623	-	-	5/11/11/17	-
22	LFA	T	622	-	-	4/8/8/17	-
23	EDO	S	819	-	-	0/1/1/1	-
22	LFA	G	621	-	-	9/14/14/17	-
20	DMU	B	741	-	-	4/8/8/59	-
14	HEA	N	515[A]	-	-	7/36/76/76	-
22	LFA	C	614	-	-	7/12/12/17	-
20	DMU	W	61	-	-	3/19/59/59	0/2/2/2
14	HEA	A	515[A]	-	-	7/36/76/76	-
22	LFA	P	615	-	-	5/8/8/17	-

The worst 5 of 160 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	516	HEA	C1D-ND	-6.76	1.28	1.40
14	A	516	HEA	CHD-C1D	6.63	1.52	1.38
14	N	516	HEA	C3C-C4C	5.61	1.55	1.42
14	A	516	HEA	C3B-C2B	5.46	1.47	1.34
14	N	515[A]	HEA	CHB-C4A	4.84	1.47	1.38

The worst 5 of 307 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	516	HEA	C2D-C1D-ND	10.08	121.78	109.84
14	A	515[A]	HEA	C3C-C4C-NC	10.06	116.44	110.25
14	A	515[B]	HEA	C3C-C4C-NC	10.06	116.44	110.25
14	N	516	HEA	C1D-C2D-C3D	-8.08	98.46	106.96
14	N	516	HEA	CMD-C2D-C1D	7.93	137.11	125.04

There are no chirality outliers.

5 of 756 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.

50 monomers are involved in 150 short contacts:

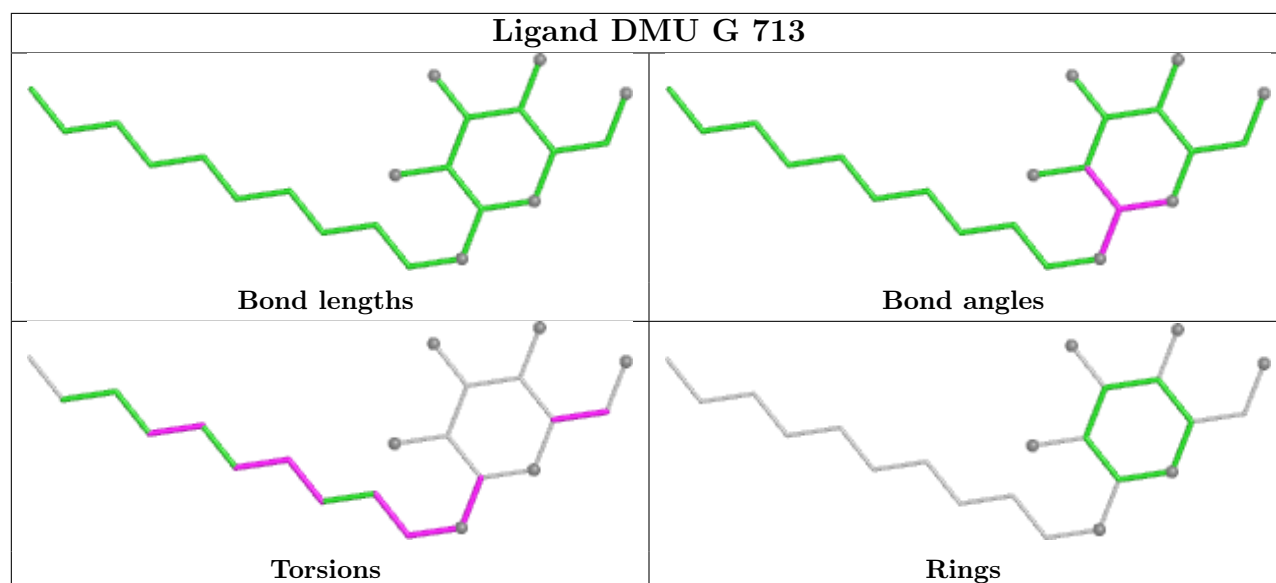
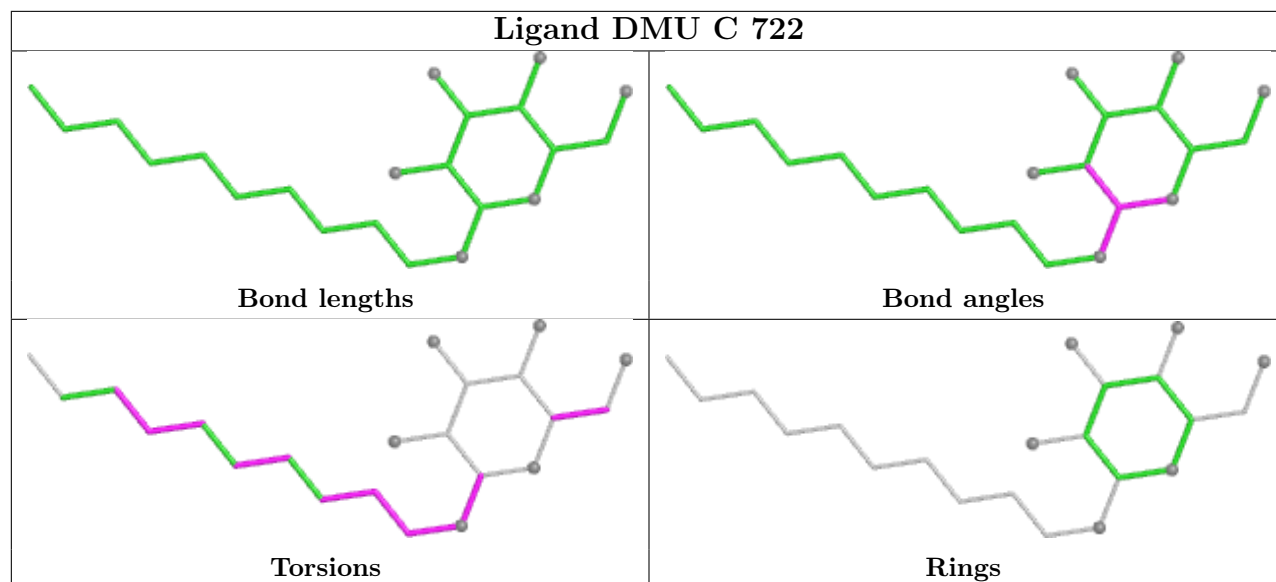
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	627	LFA	7	0
22	P	611	LFA	1	0
22	T	621	LFA	3	0
18	P	270	CDL	13	0
22	N	627	LFA	3	0
20	J	61	DMU	6	0
27	C	267	PGV	1	0
18	A	522	CDL	1	0
21	N	520	PER	1	0
21	A	520	PER	1	0
20	A	744	DMU	4	0
14	A	516	HEA	1	0
18	N	521	CDL	7	0
26	P	264	PEK	3	0
20	C	733	DMU	2	0
22	A	628	LFA	11	0
20	N	744	DMU	2	0
22	C	624	LFA	2	0
22	P	624	LFA	1	0
22	N	628	LFA	6	0
19	T	86	CHD	1	0

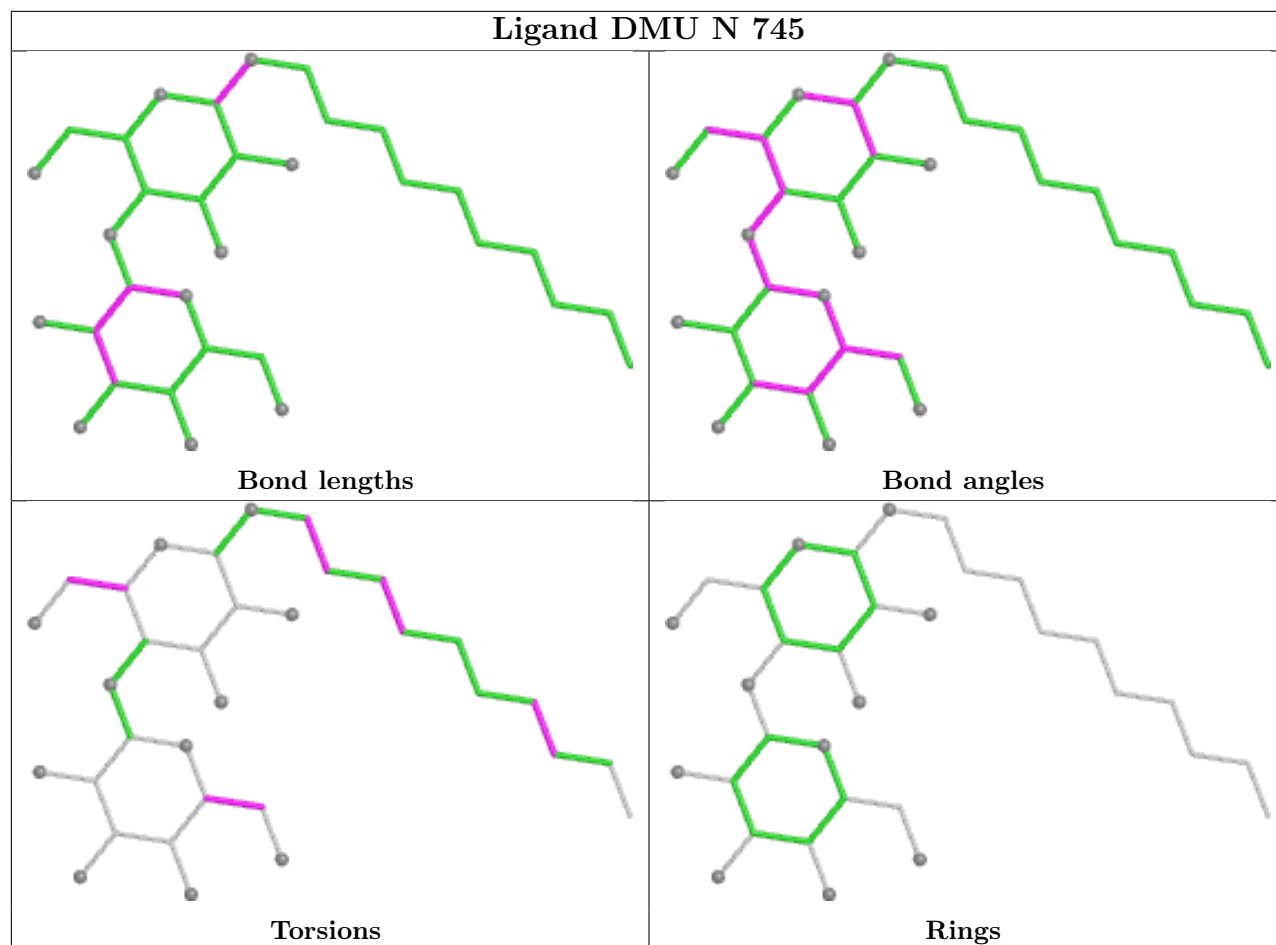
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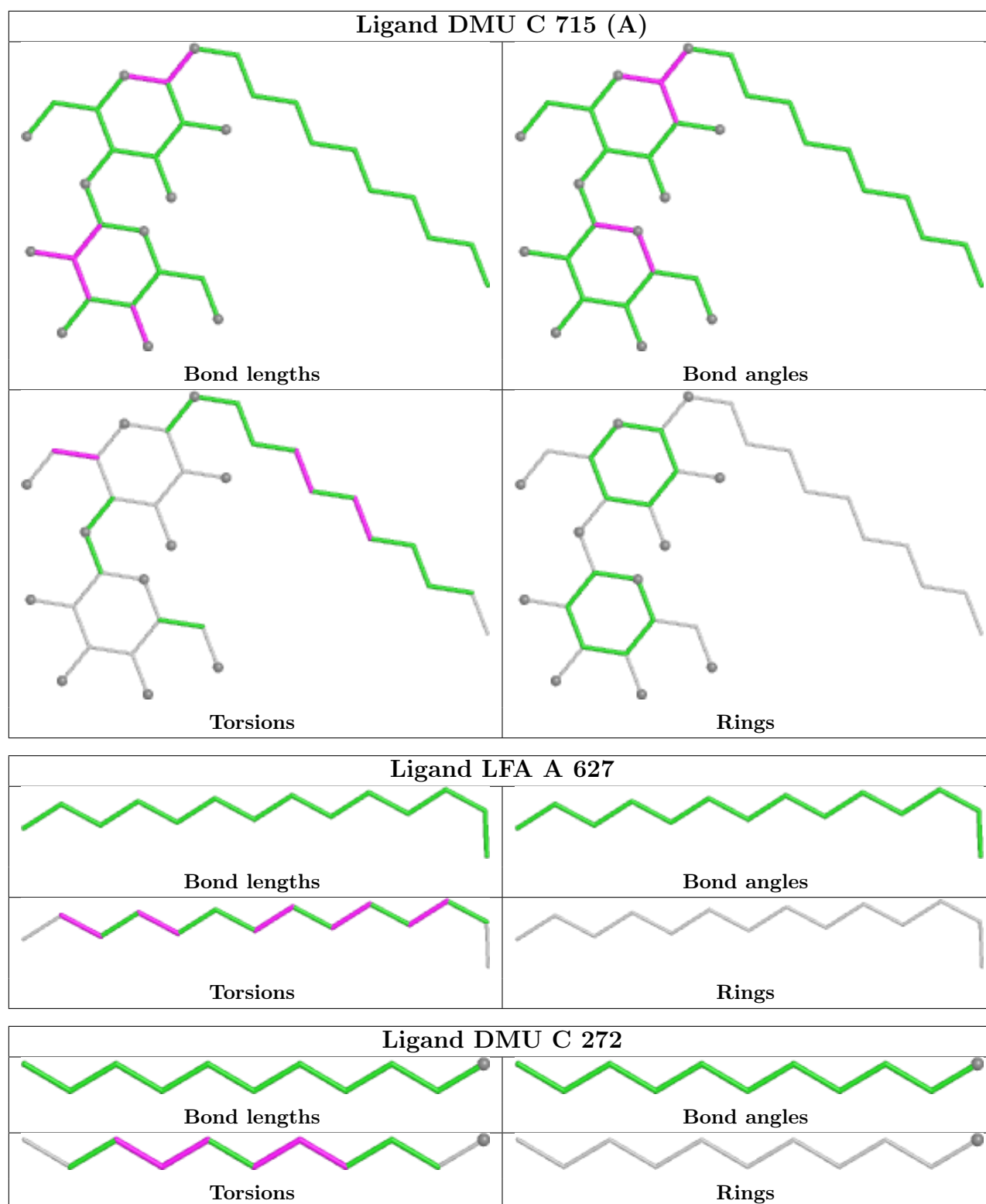
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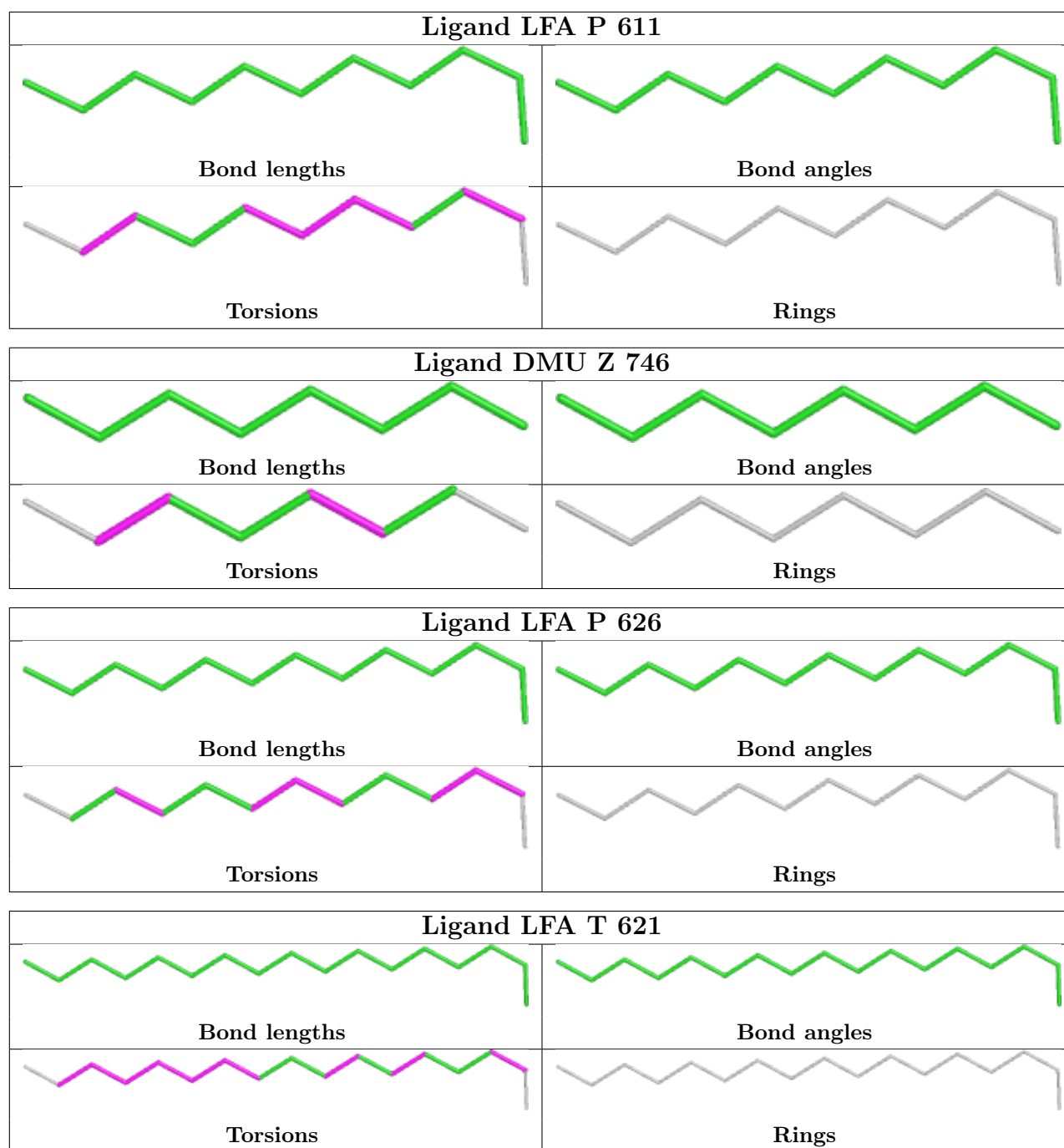
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	270	CDL	15	0
22	C	625	LFA	1	0
27	P	266	PGV	1	0
18	A	521	CDL	9	0
20	O	742	DMU	1	0
26	C	264	PEK	5	0
27	C	266	PGV	2	0
14	N	516	HEA	2	0
22	C	716[B]	LFA	3	0
20	P	715[A]	DMU	1	0
14	N	515[B]	HEA	1	0
22	G	622	LFA	1	0
20	P	714	DMU	1	0
19	G	86	CHD	1	0
20	G	712	DMU	1	0
20	T	711	DMU	1	0
22	C	626	LFA	2	0
20	O	731	DMU	1	0
20	A	526	DMU	1	0
22	P	716[B]	LFA	1	0
20	P	733	DMU	1	0
19	P	271	CHD	1	0
18	N	522	CDL	1	0
20	A	743	DMU	1	0
22	T	622	LFA	1	0
14	N	515[A]	HEA	6	0
20	W	61	DMU	7	0
14	A	515[A]	HEA	7	0
22	P	615	LFA	1	0

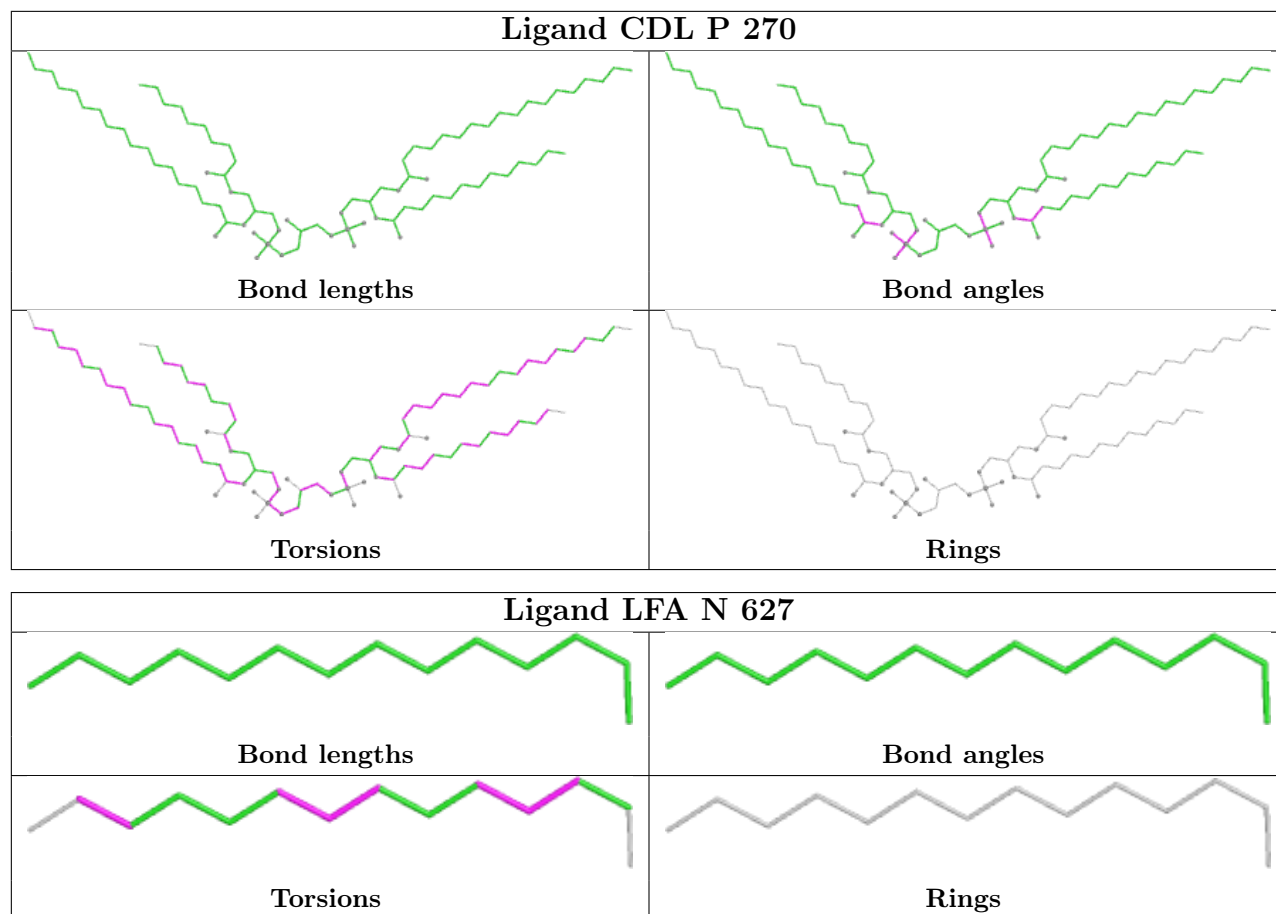
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

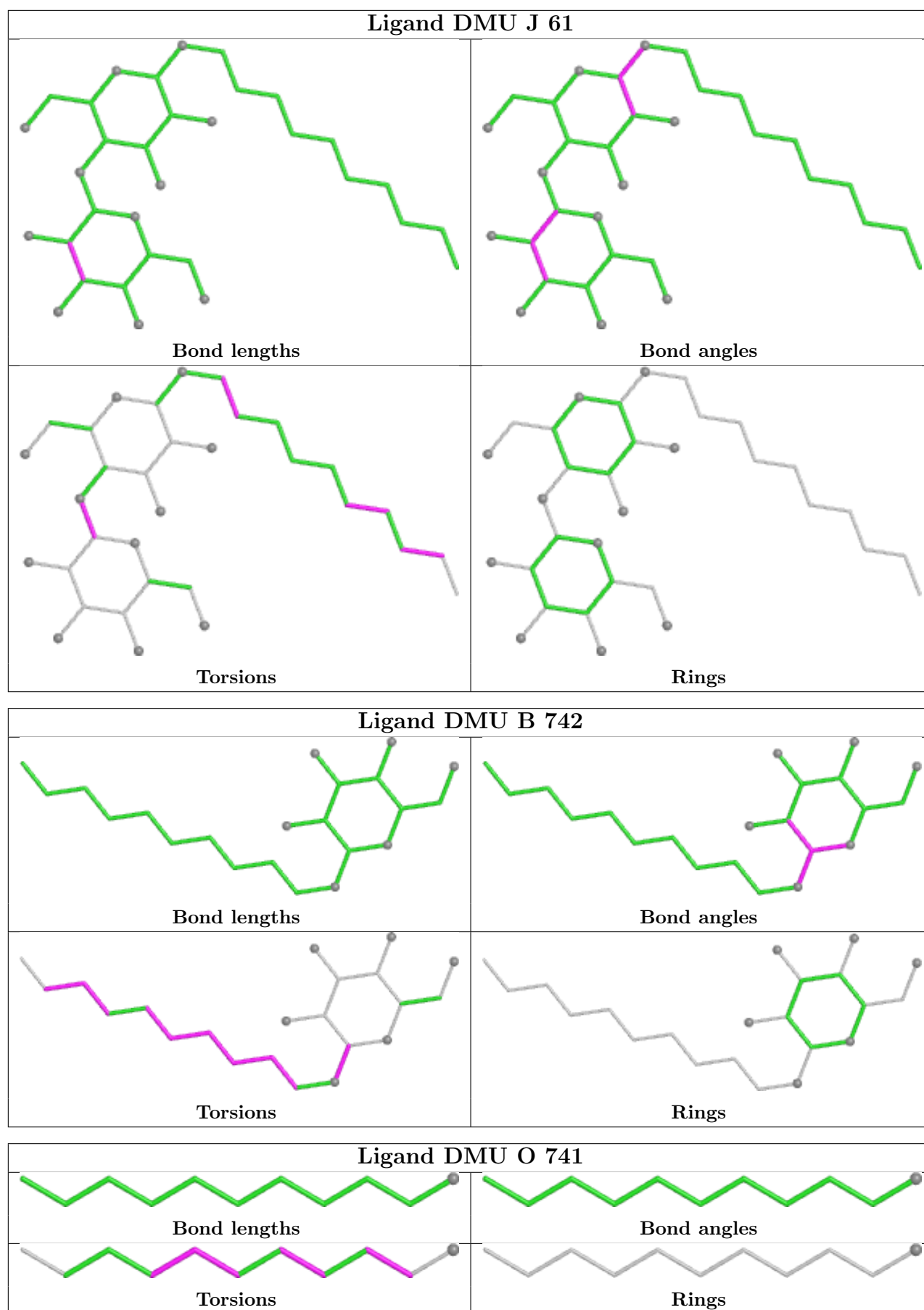


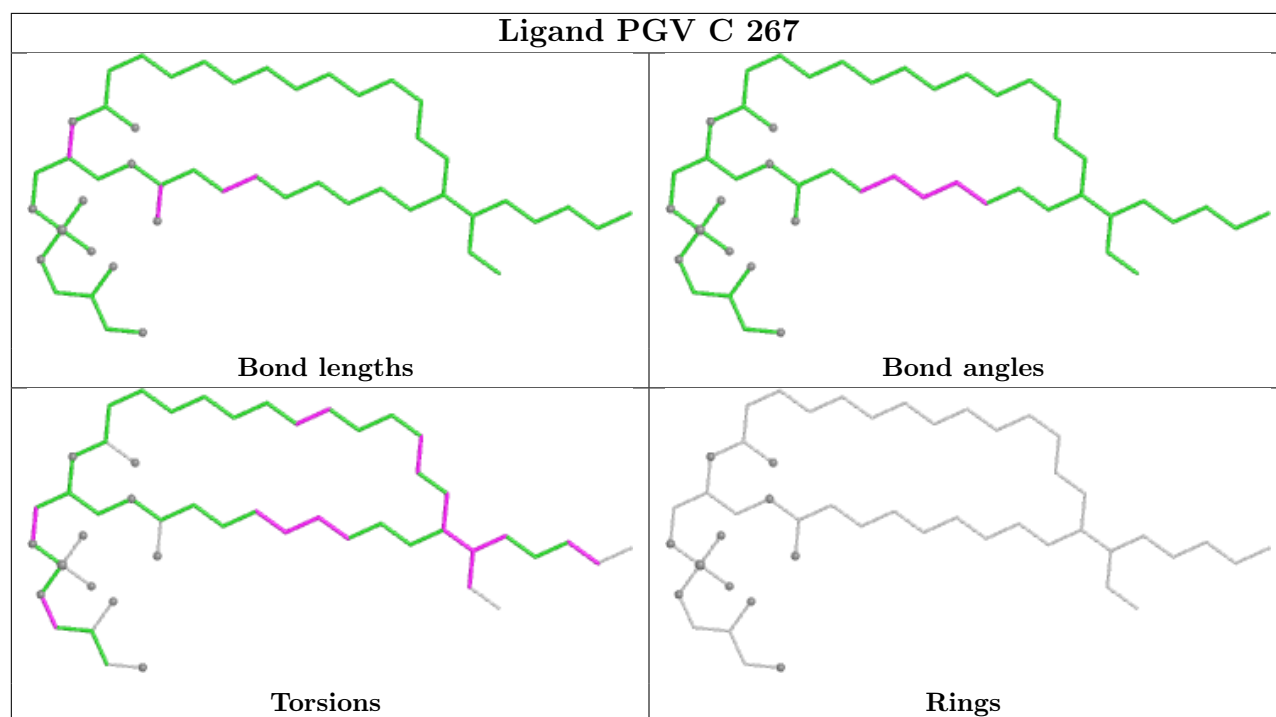
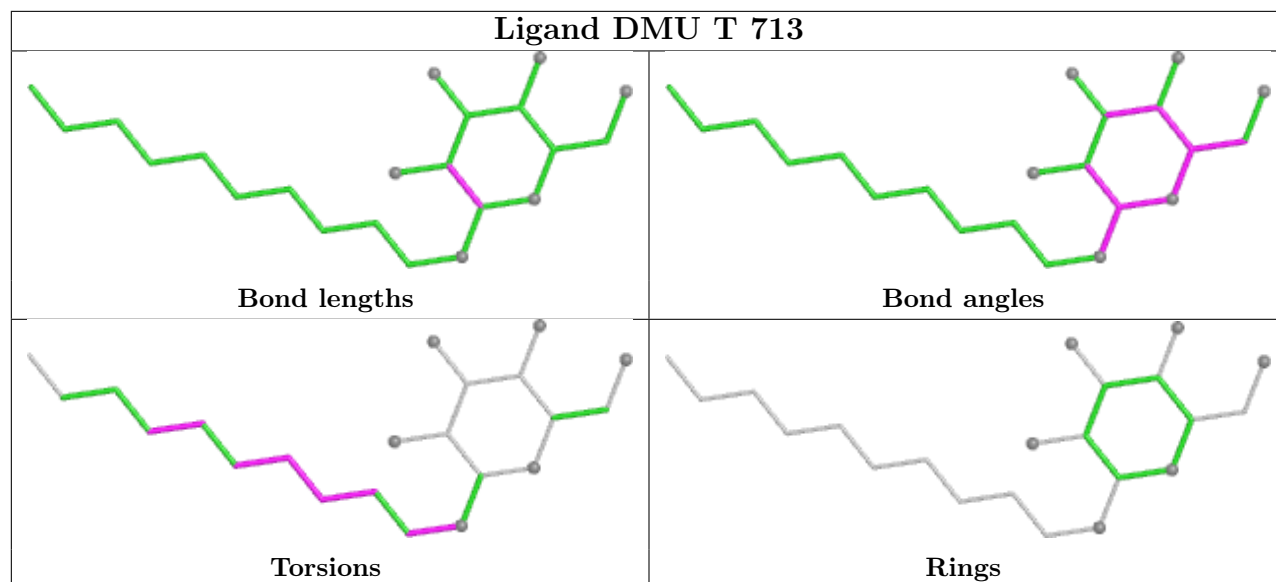


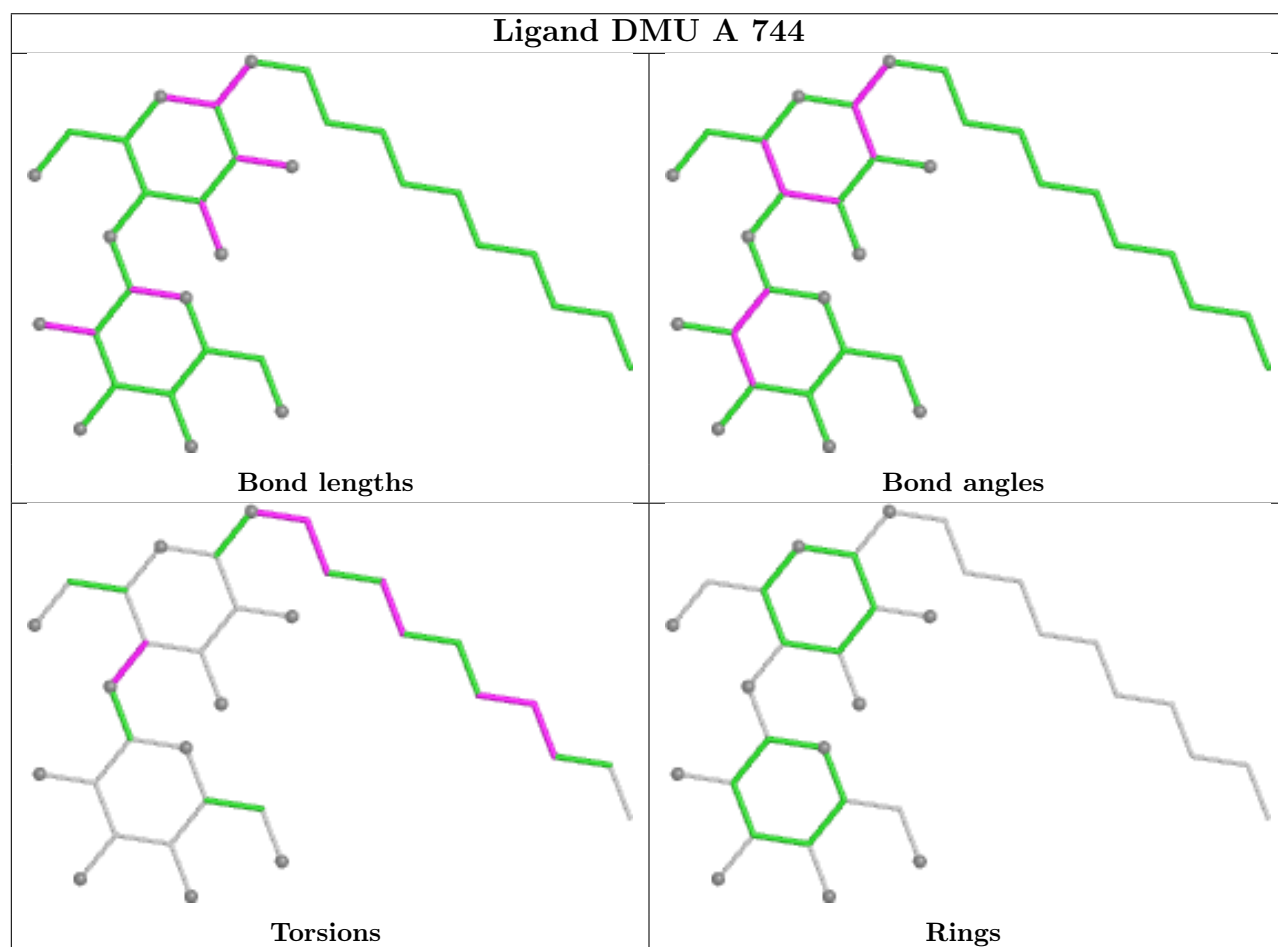
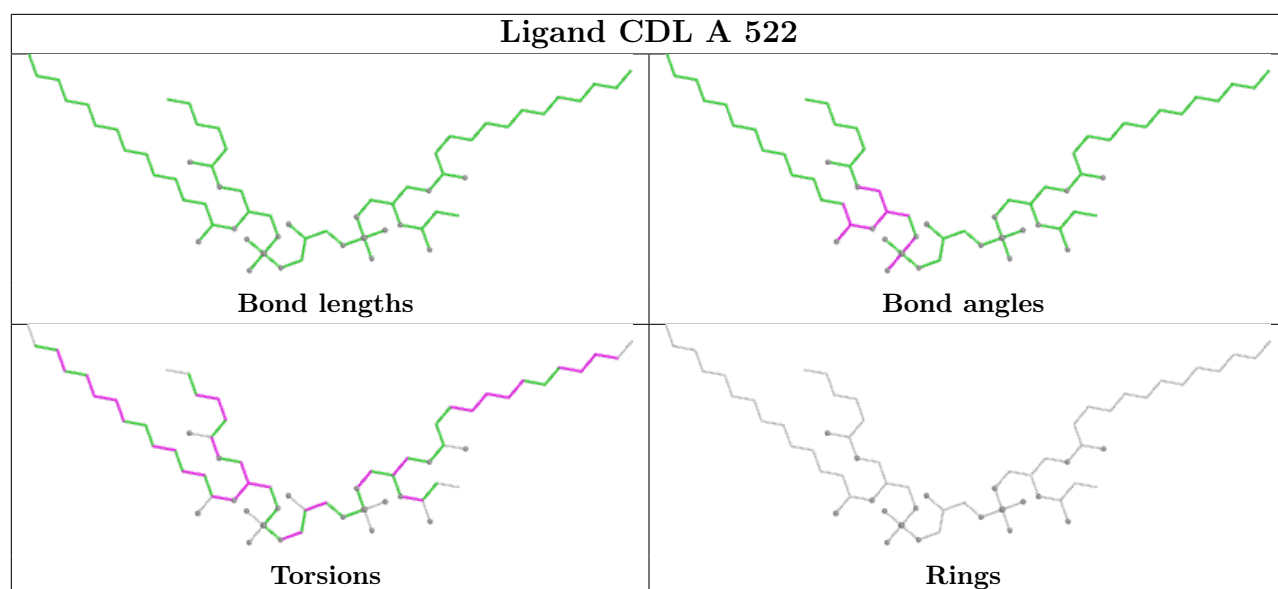


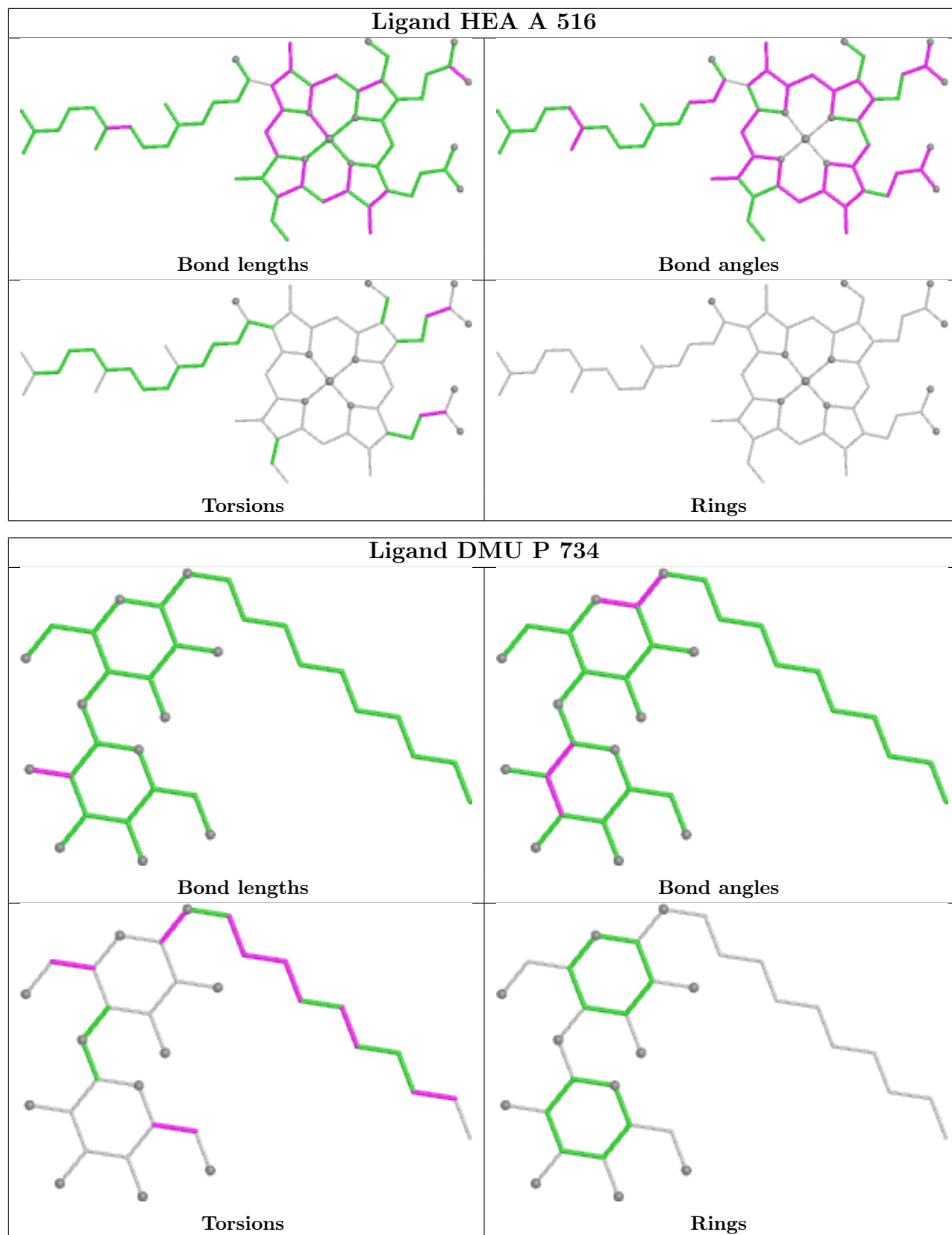


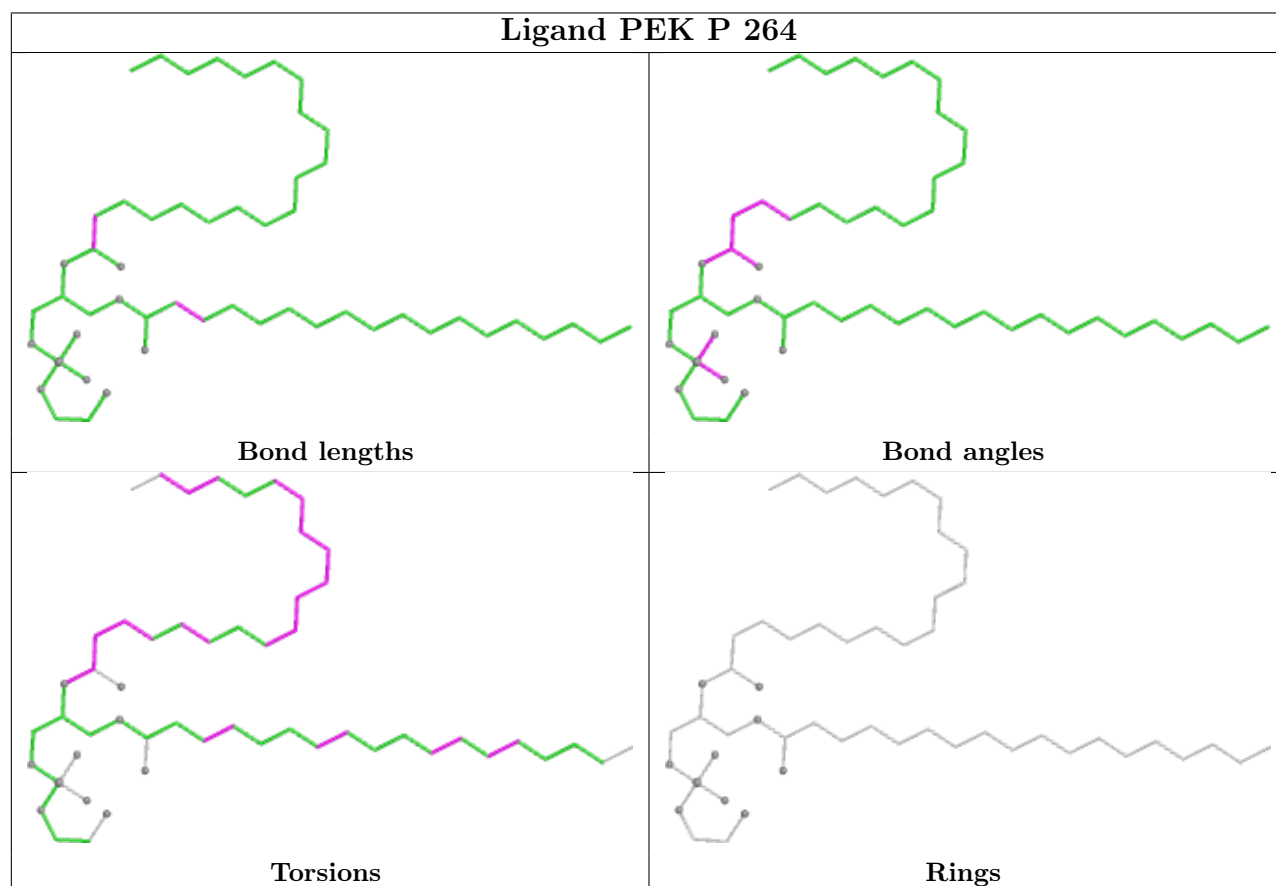
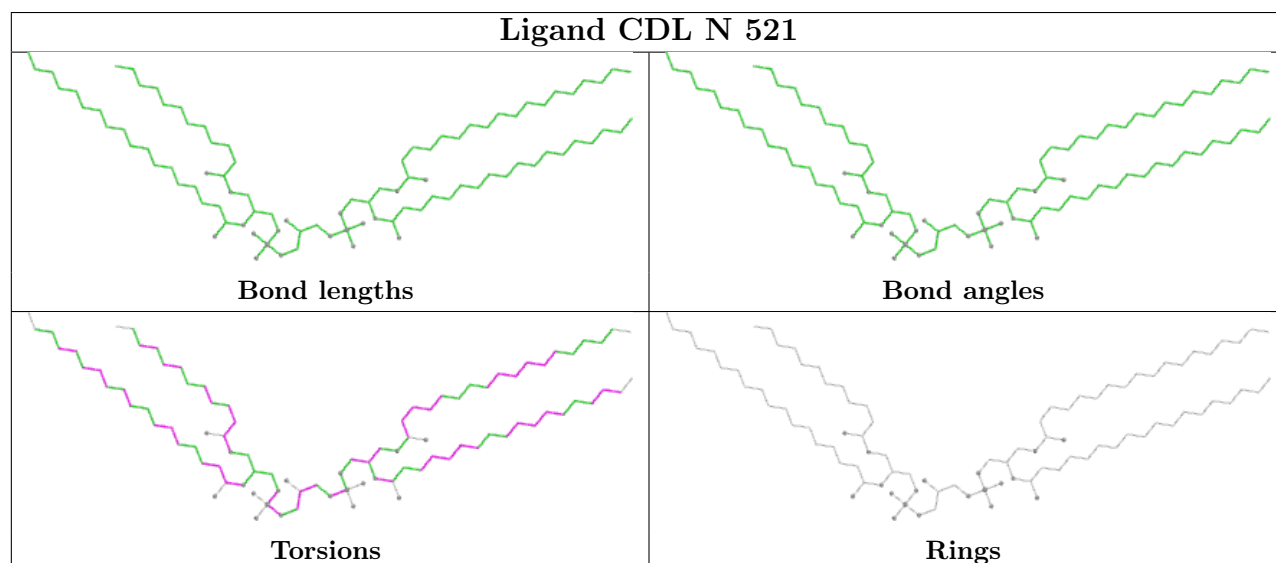
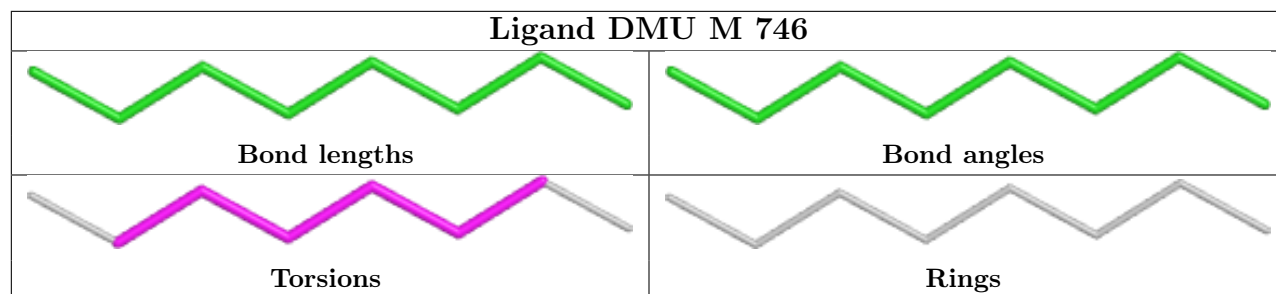


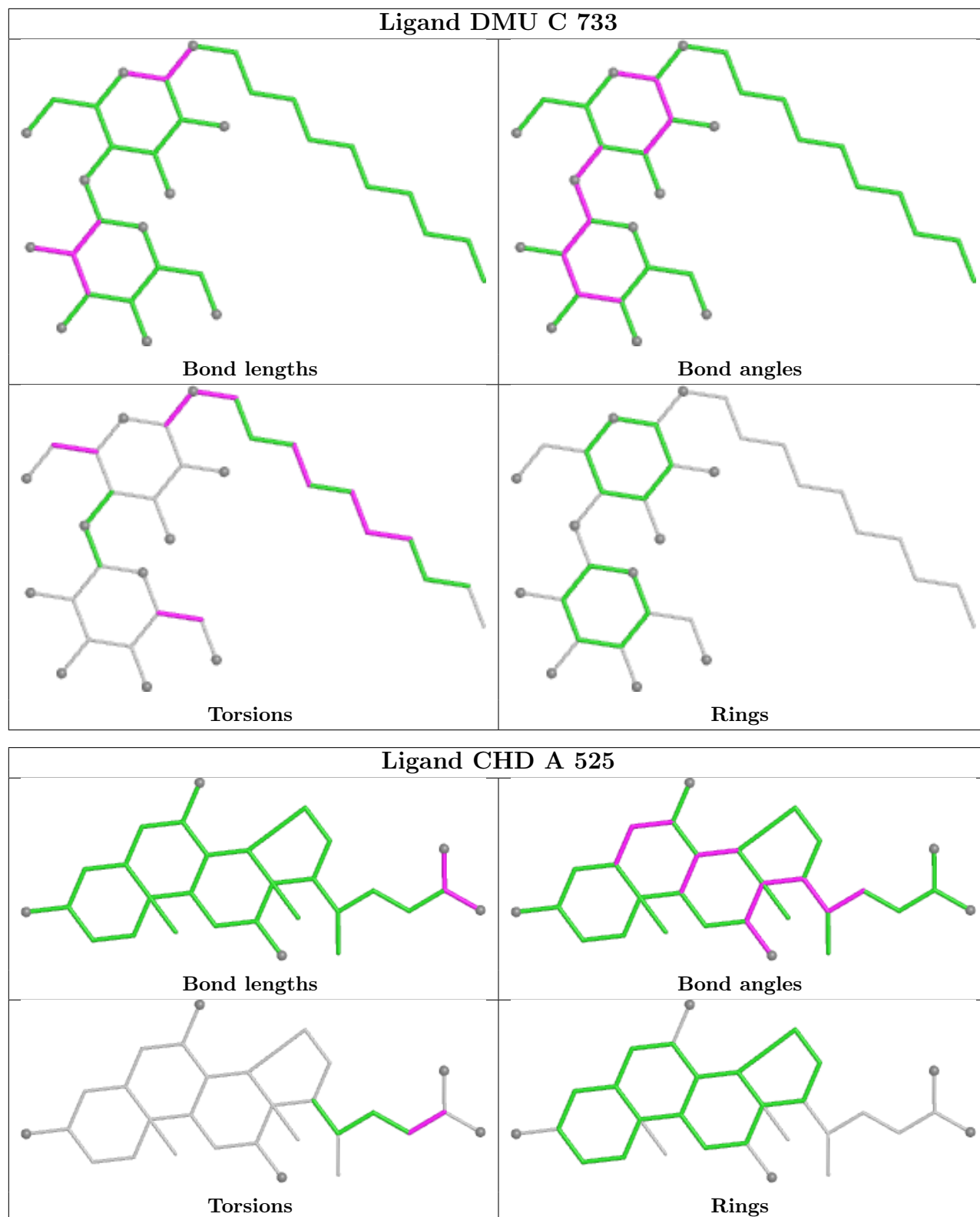


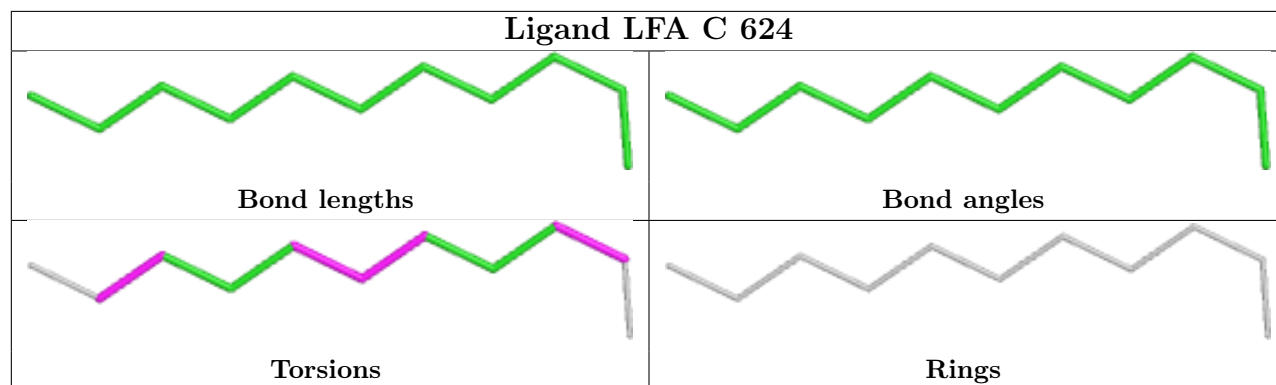
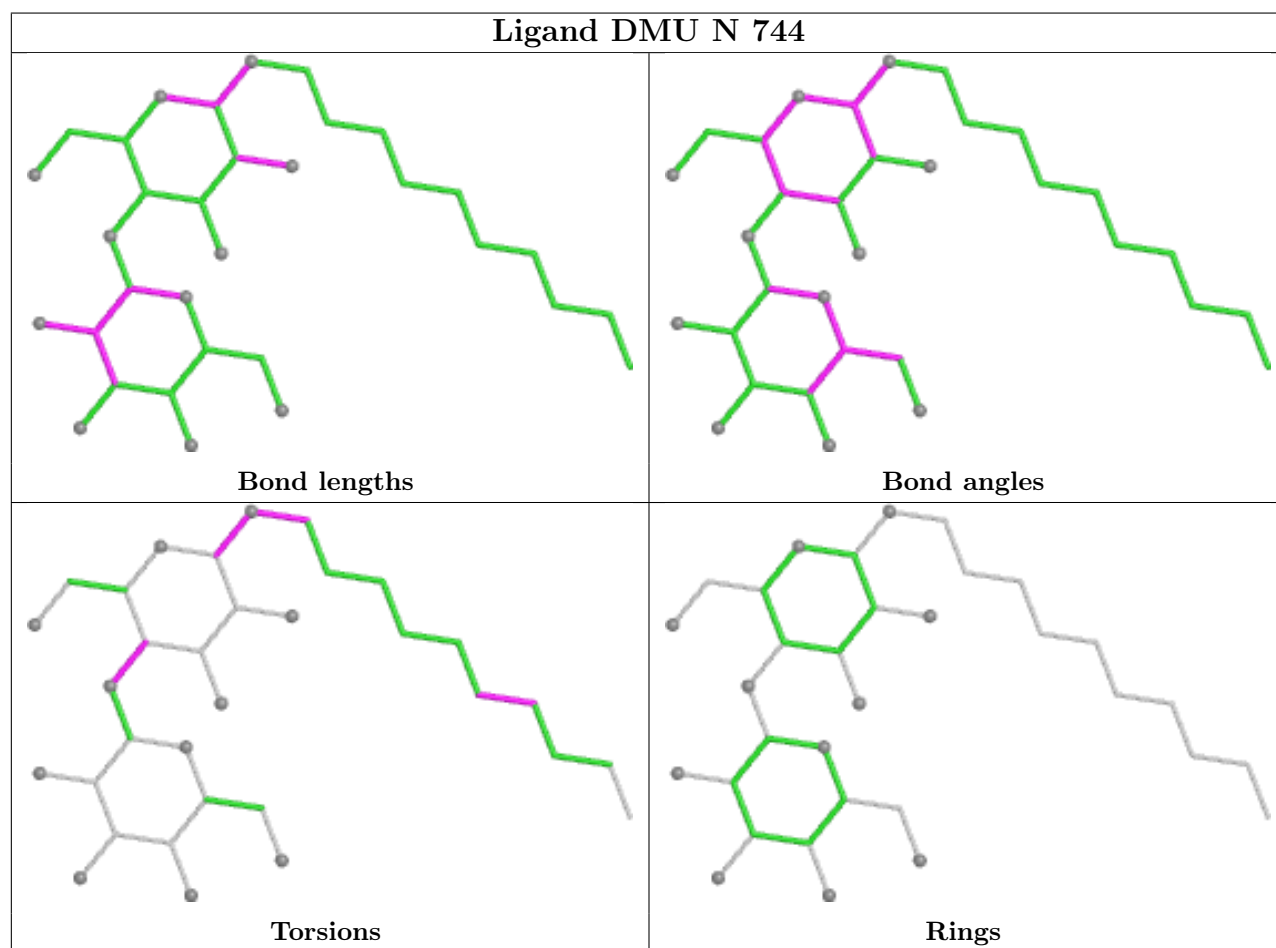
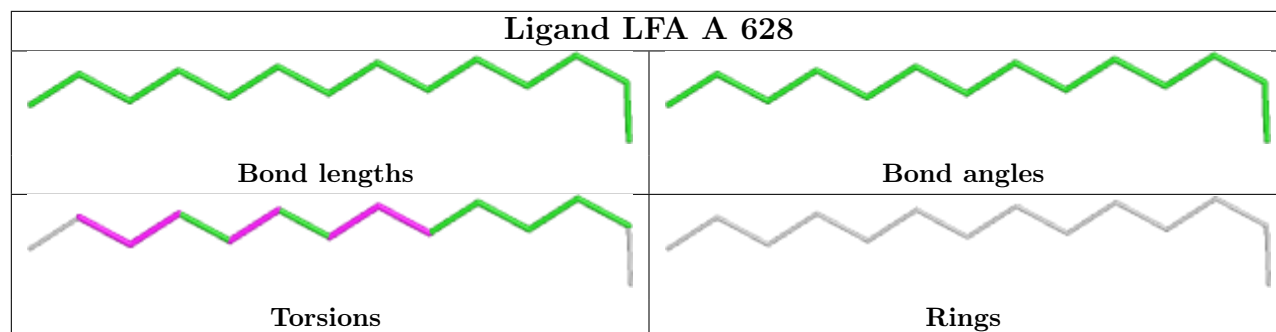


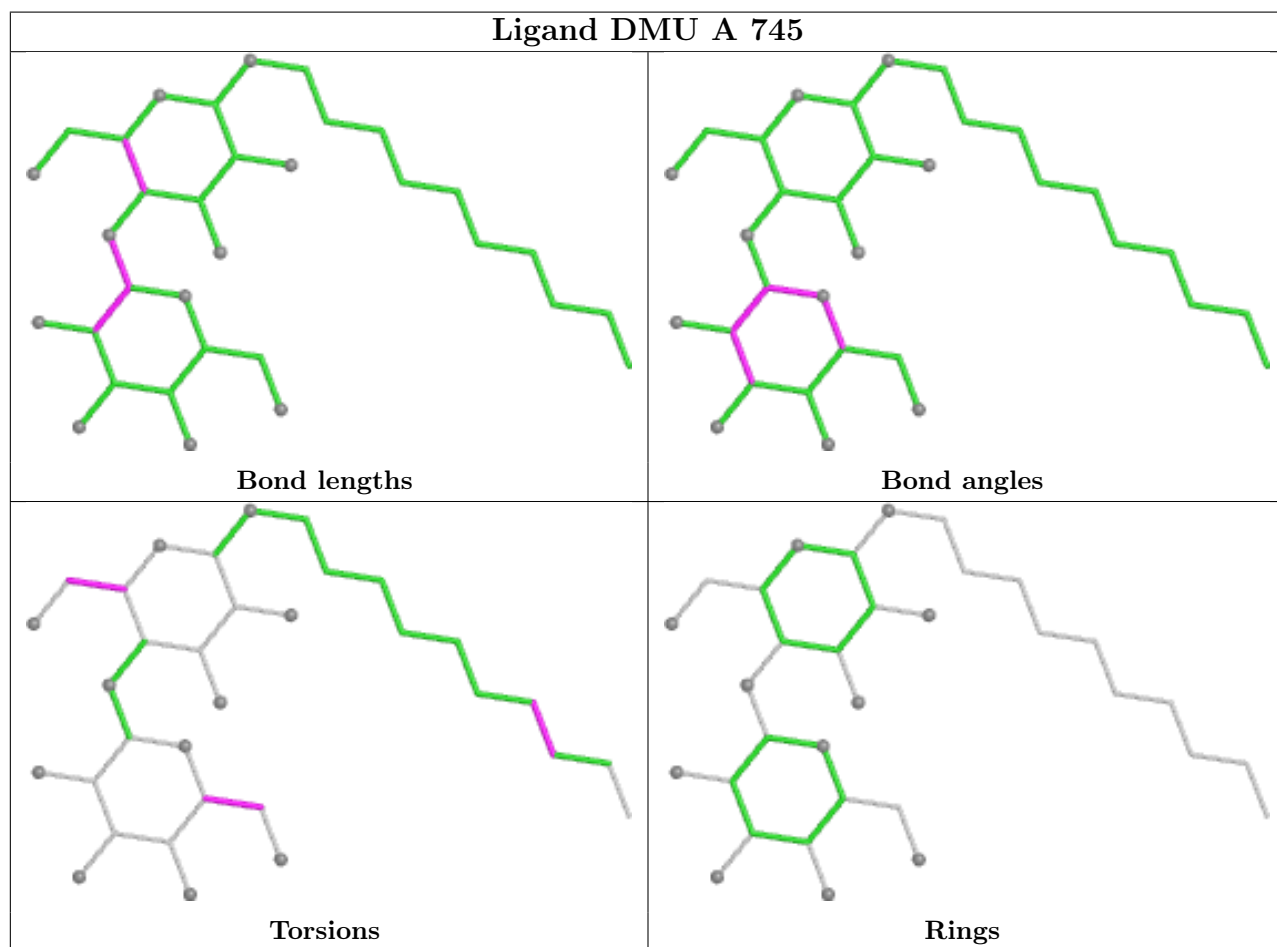
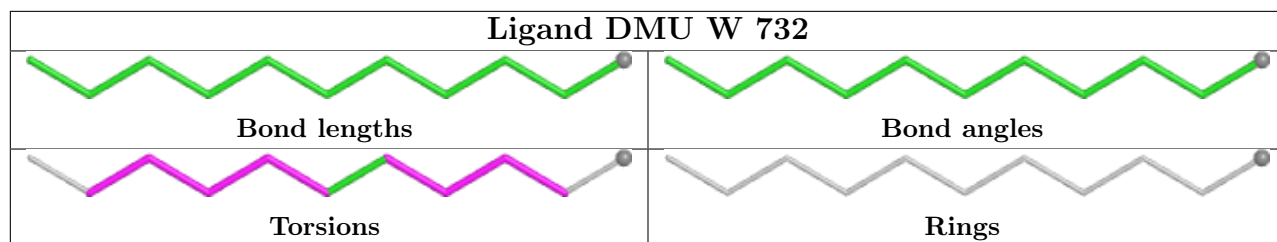


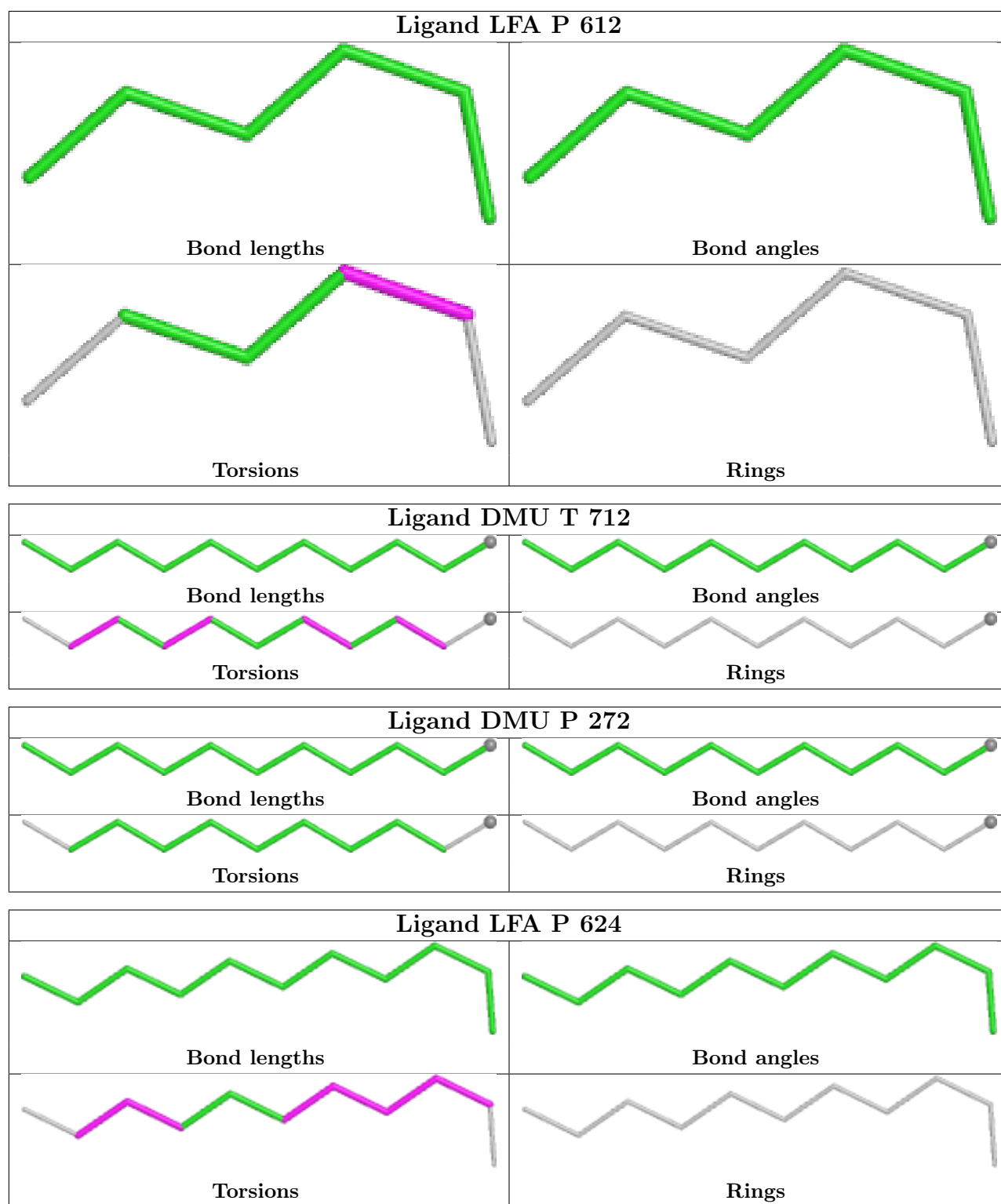


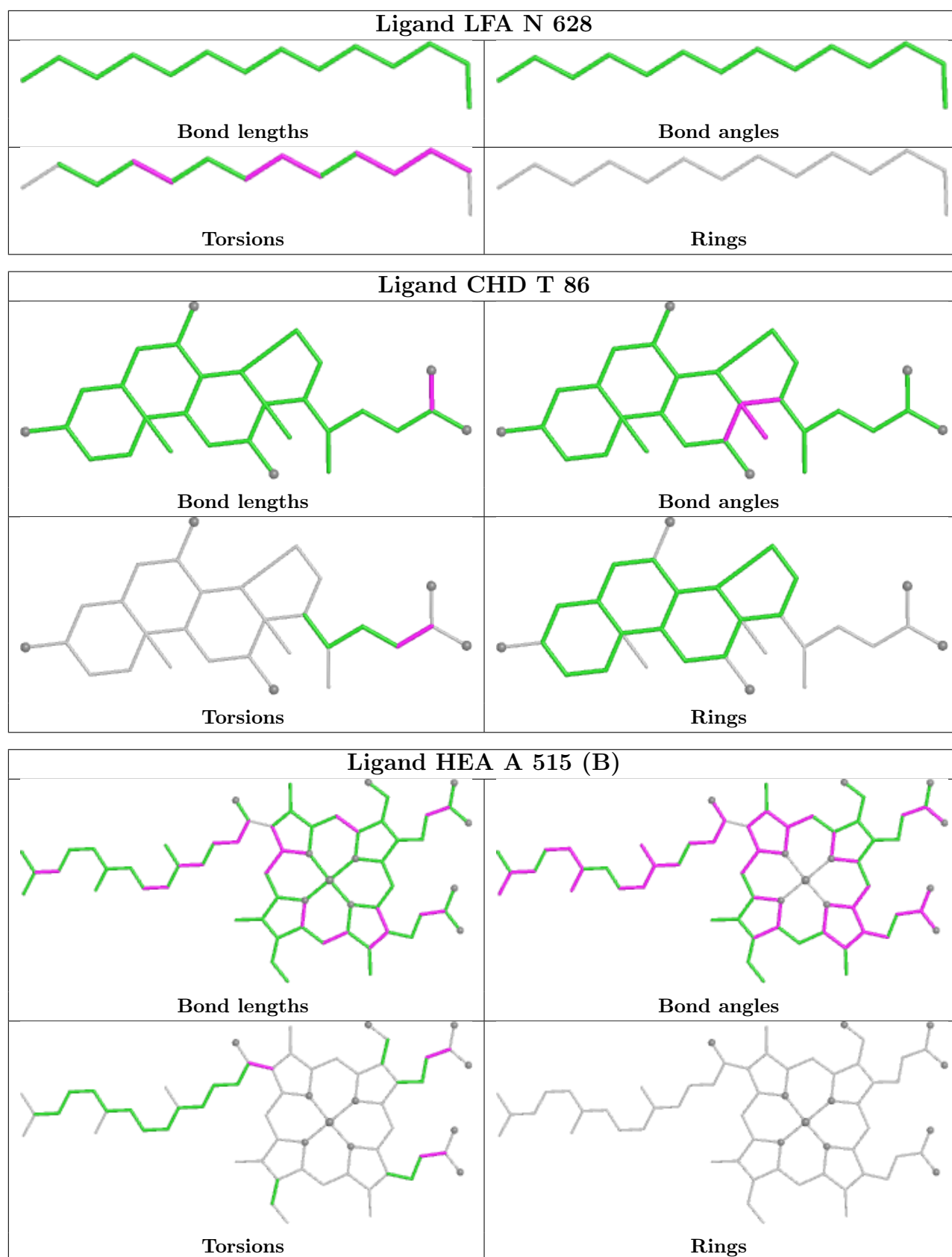


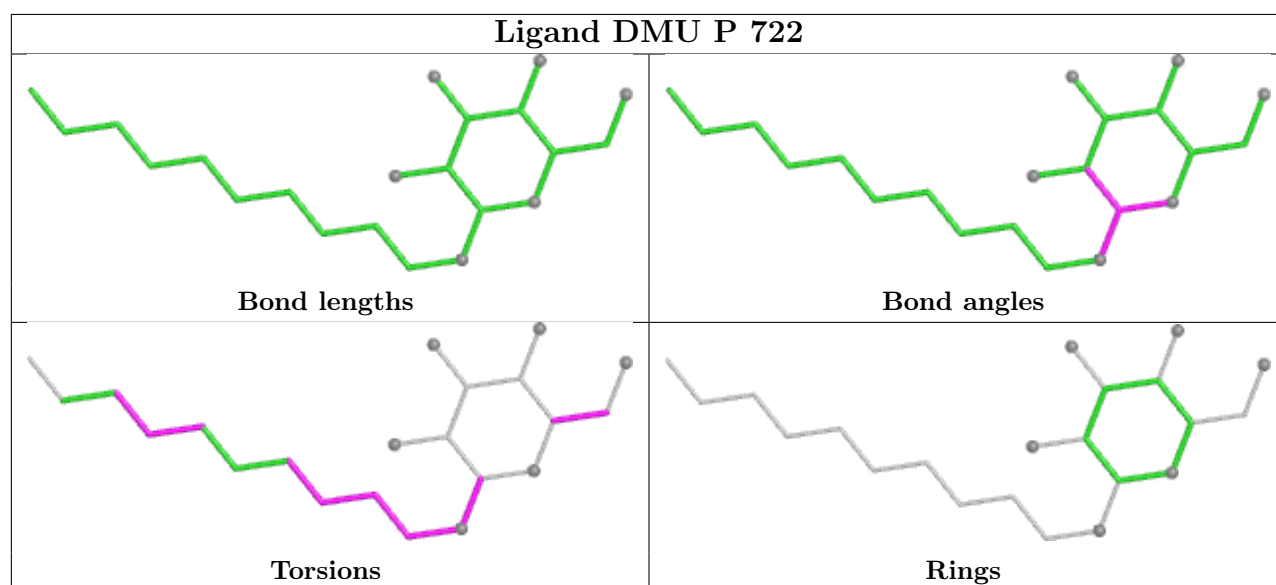
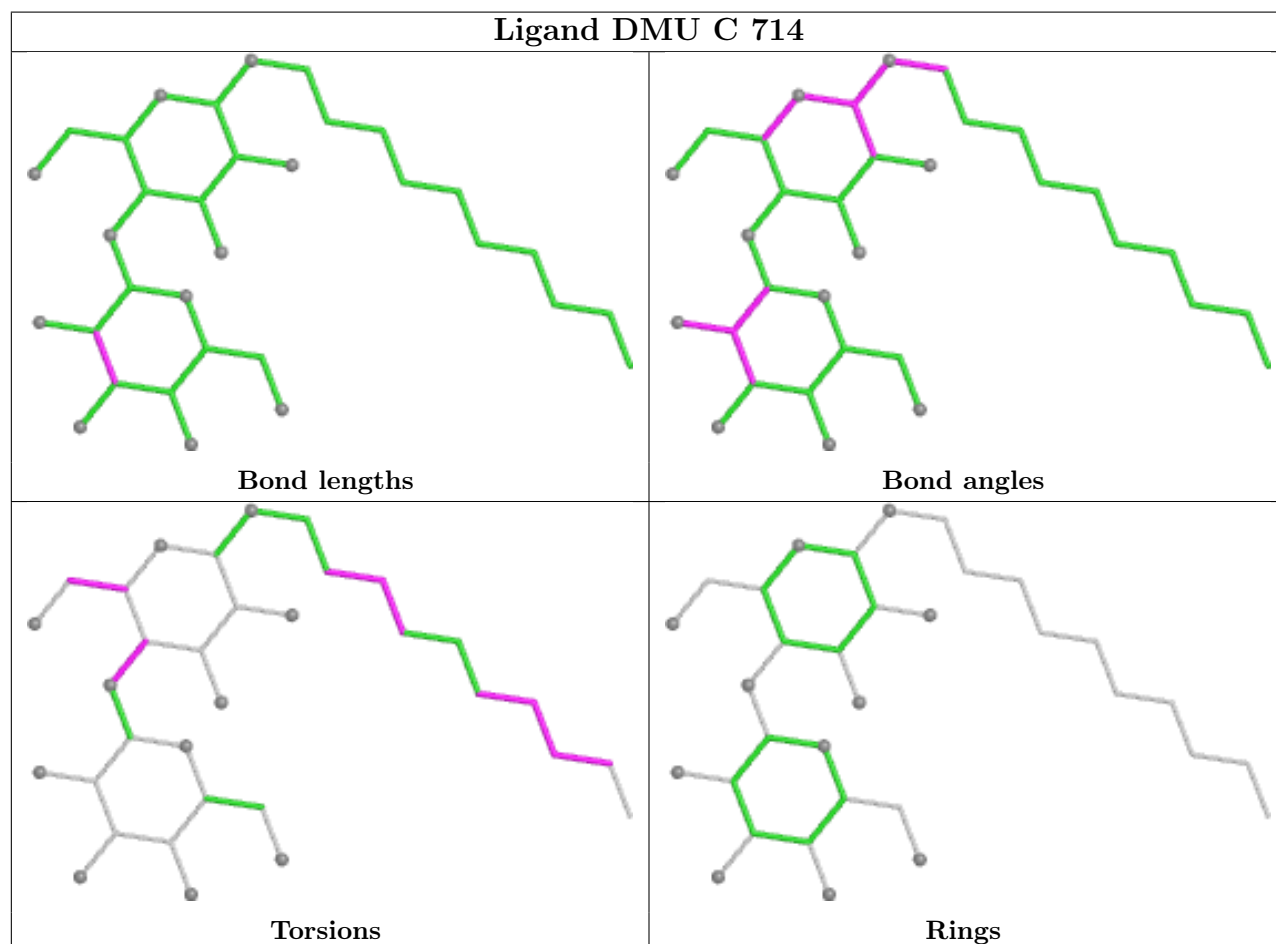
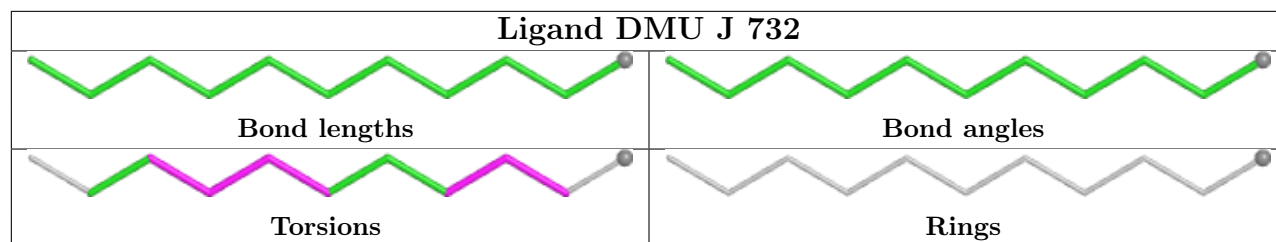


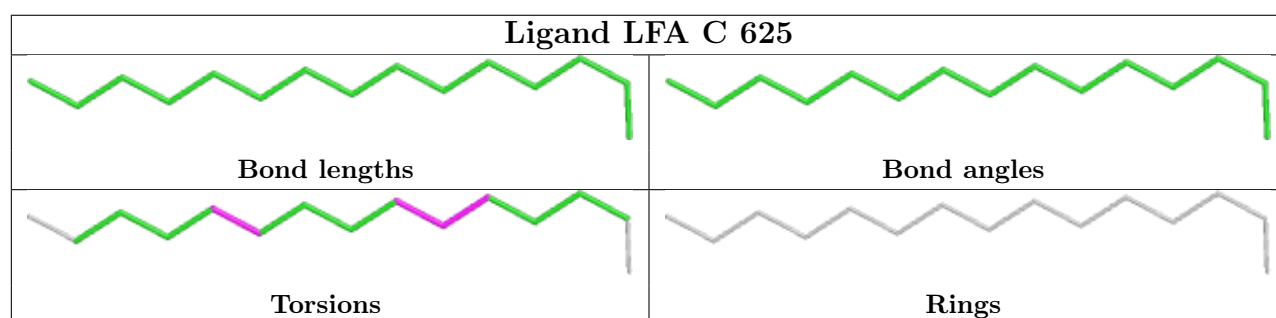
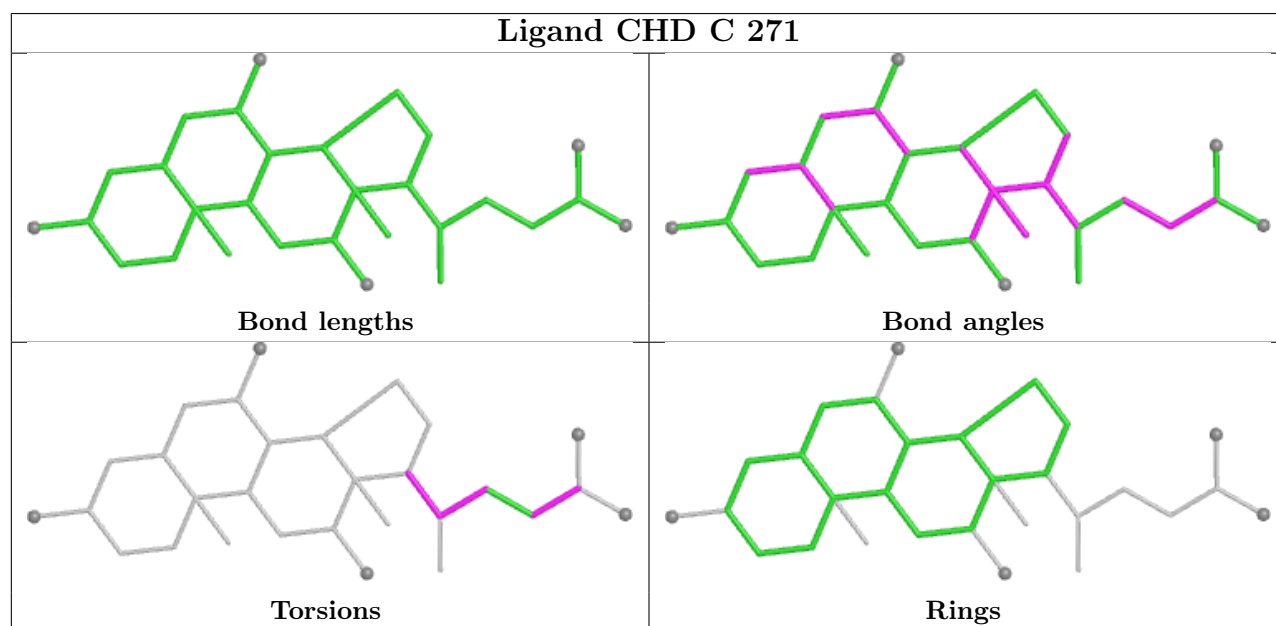
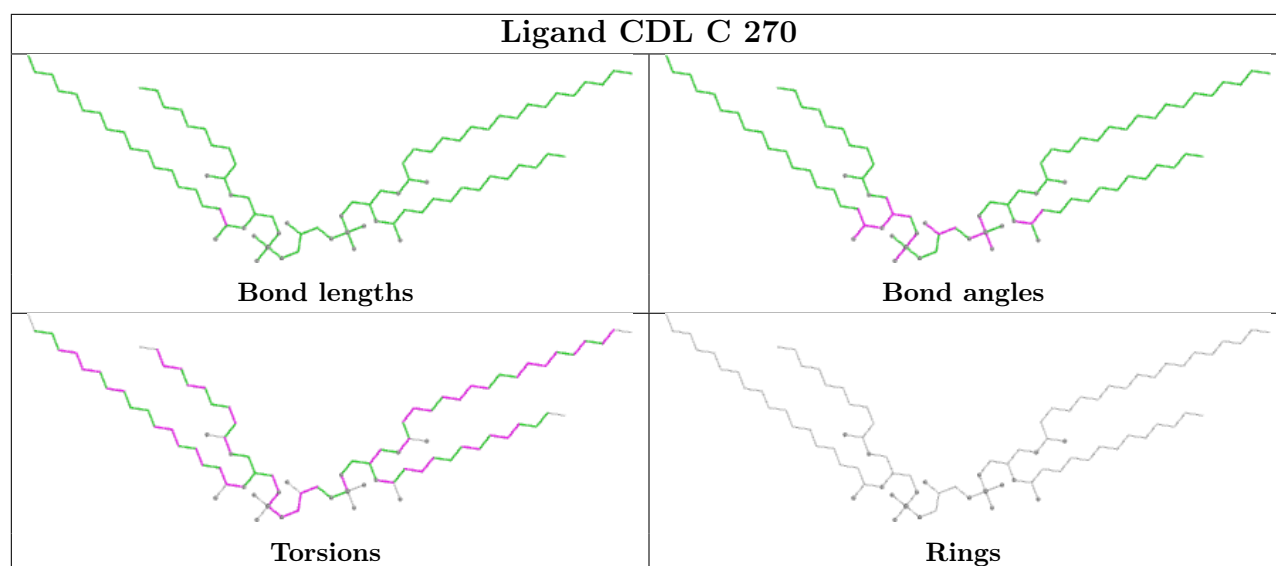


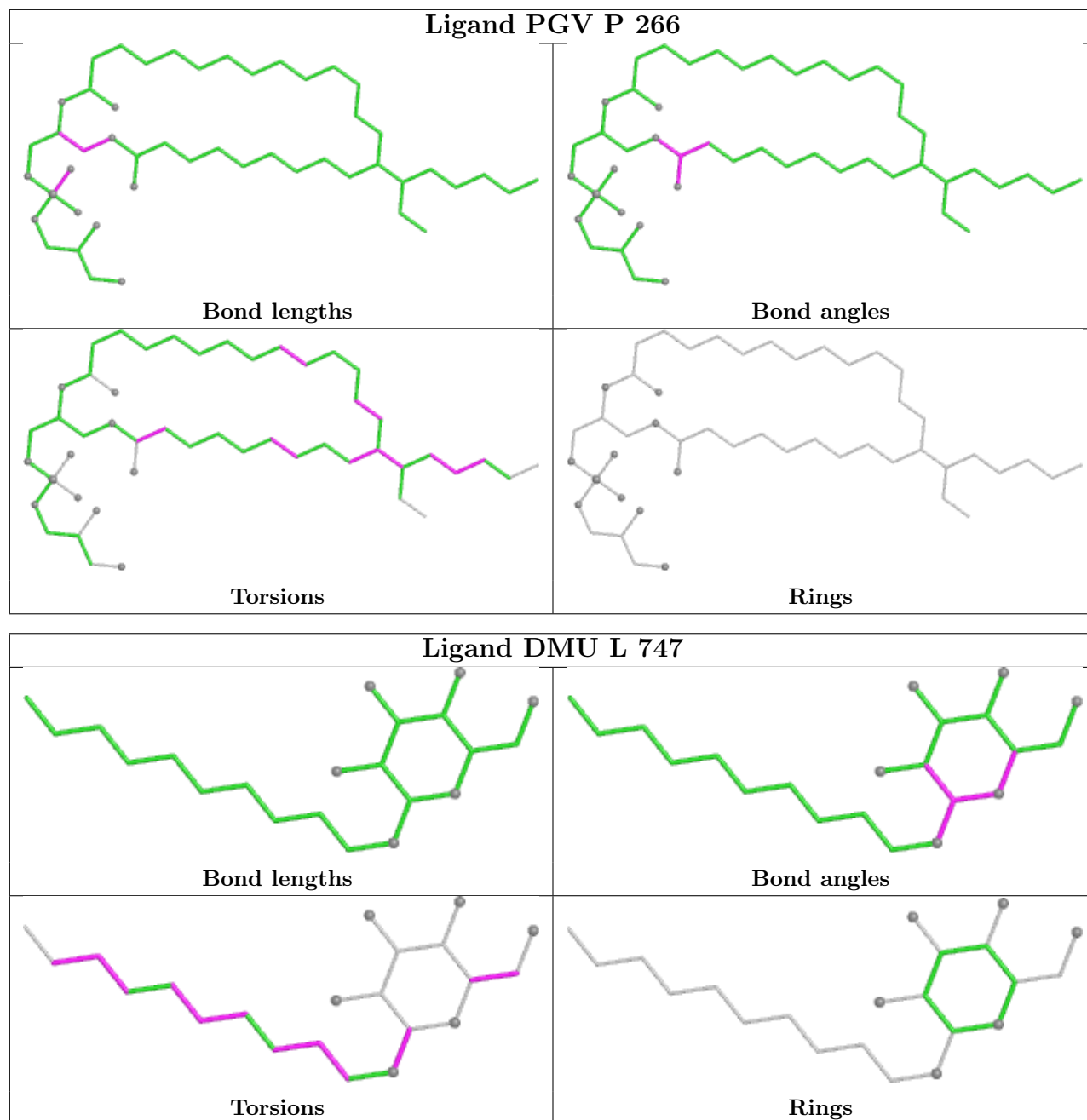


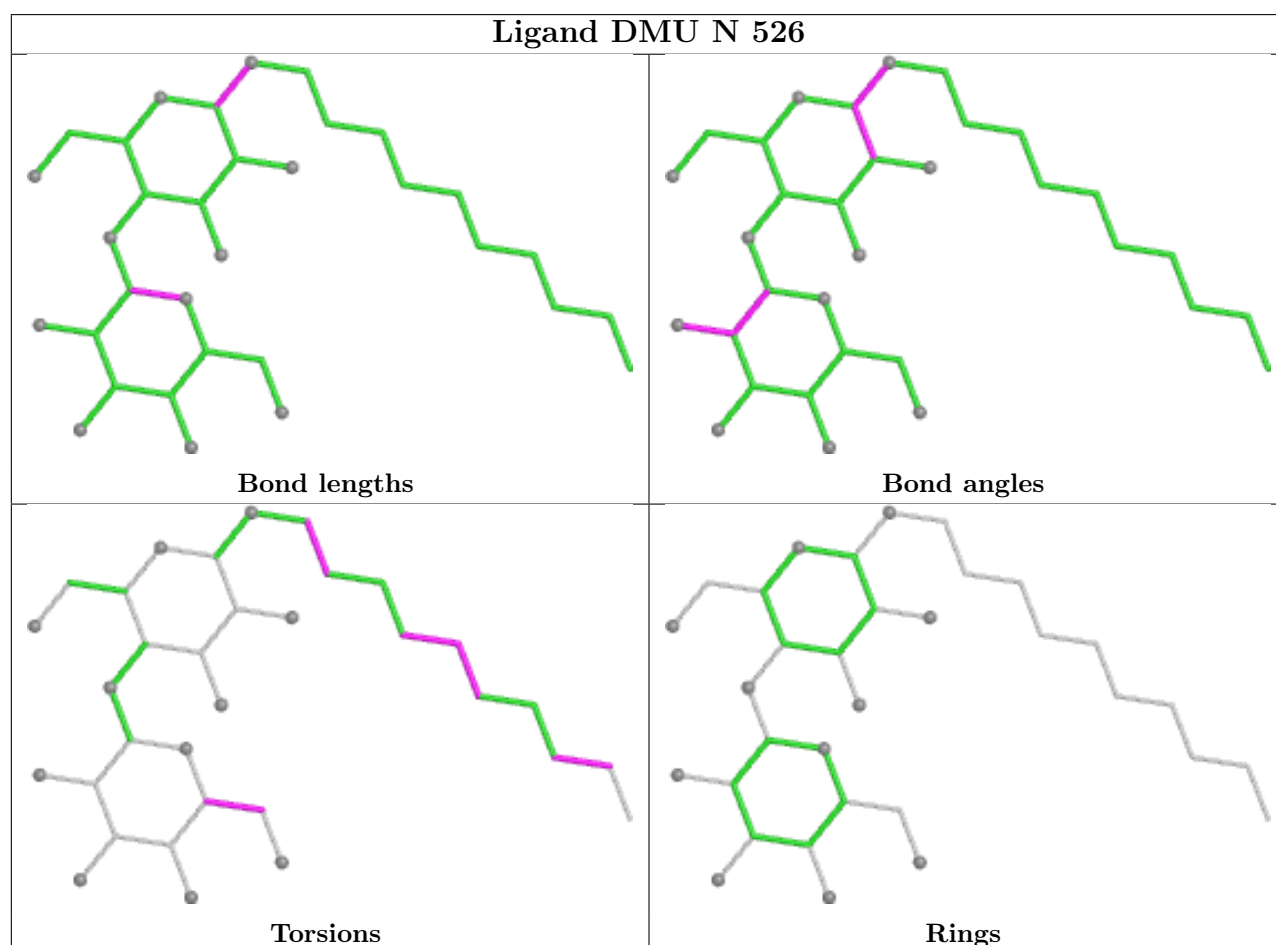
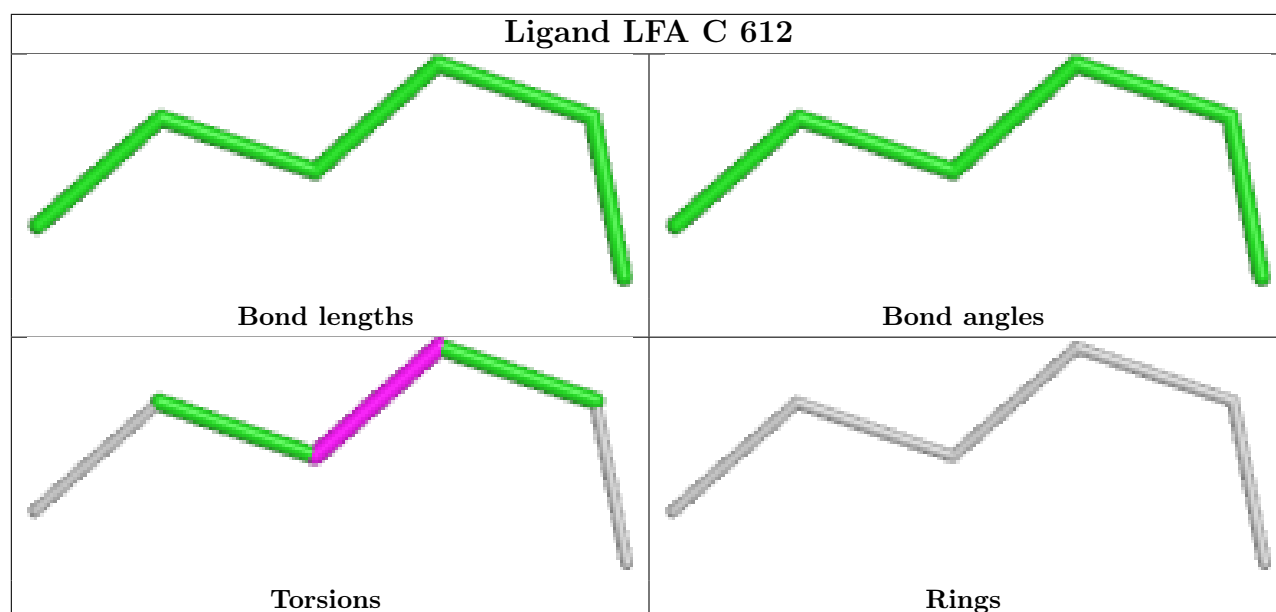


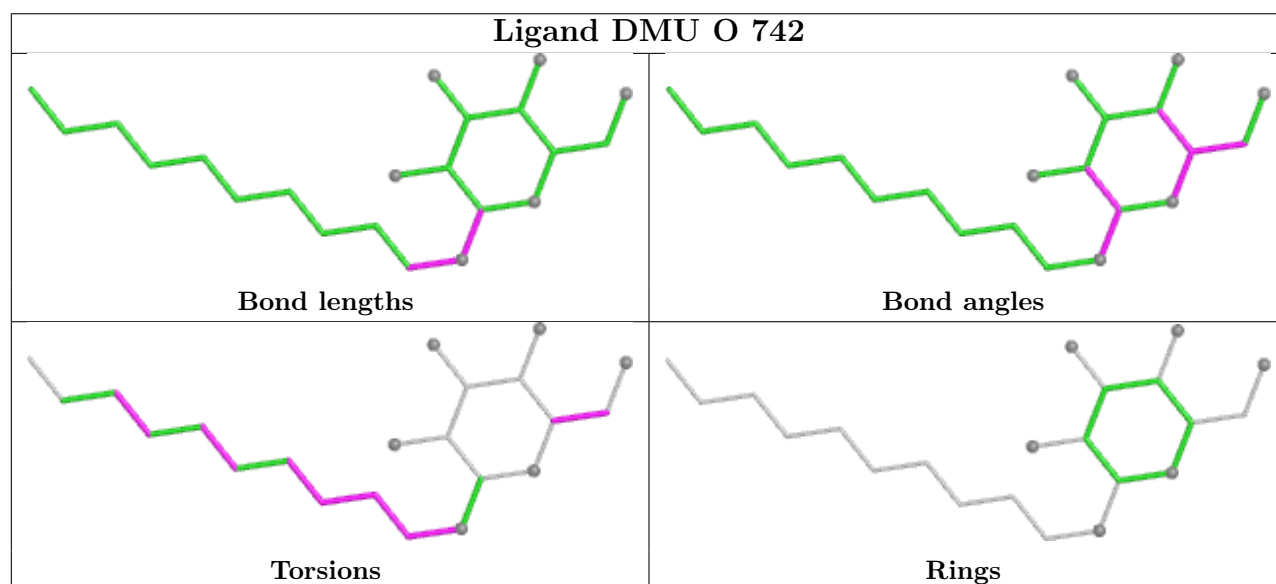
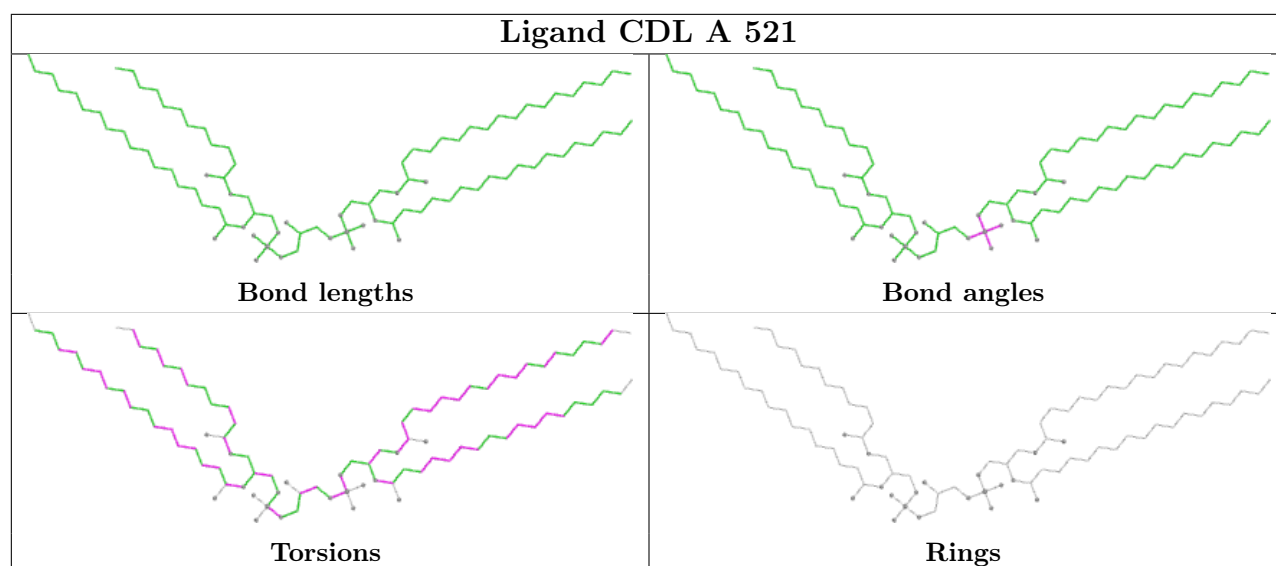




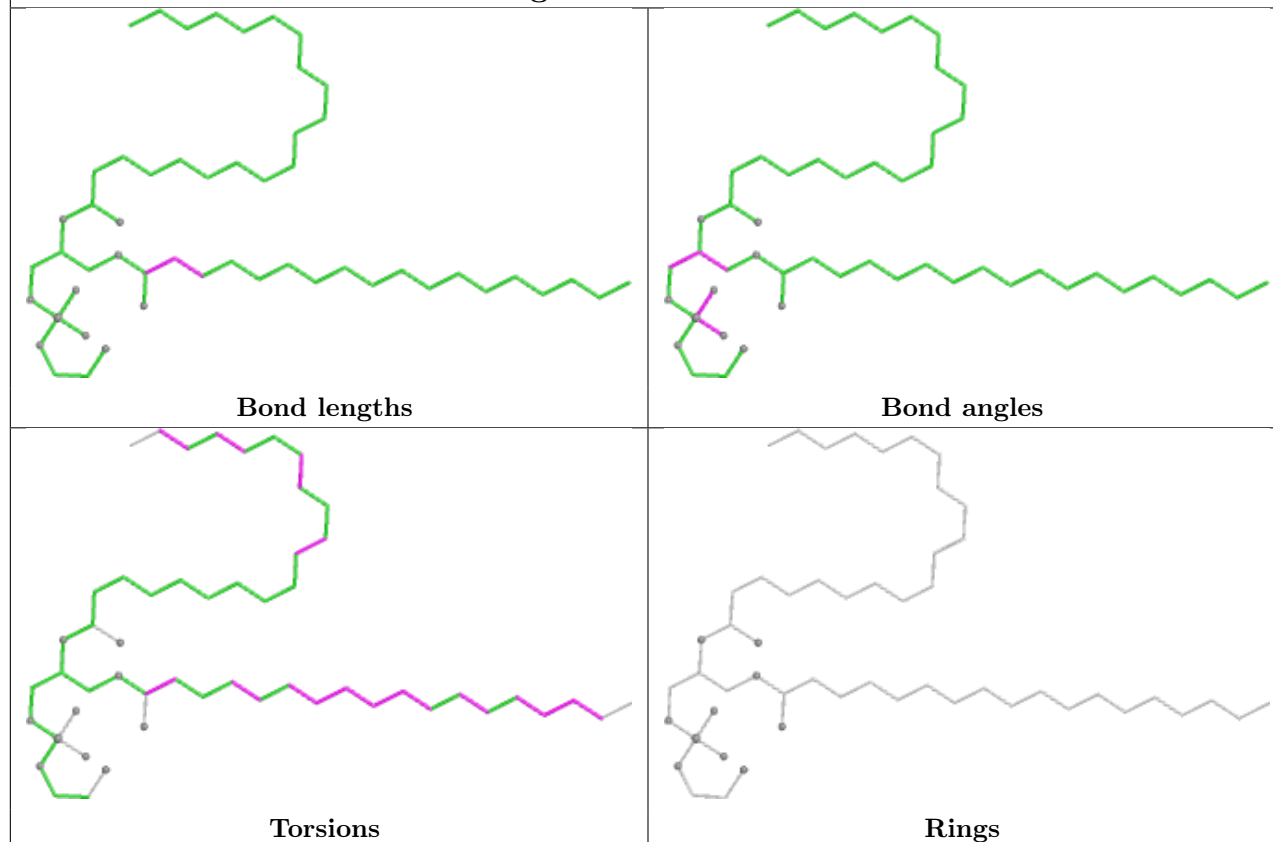




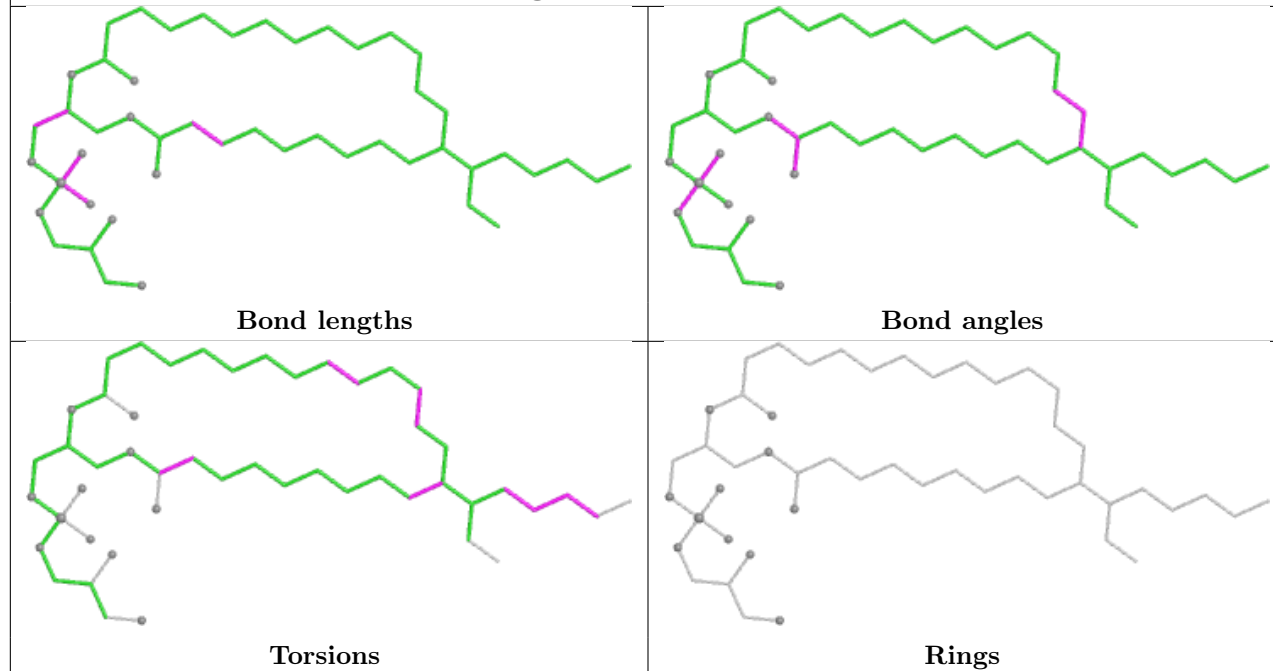


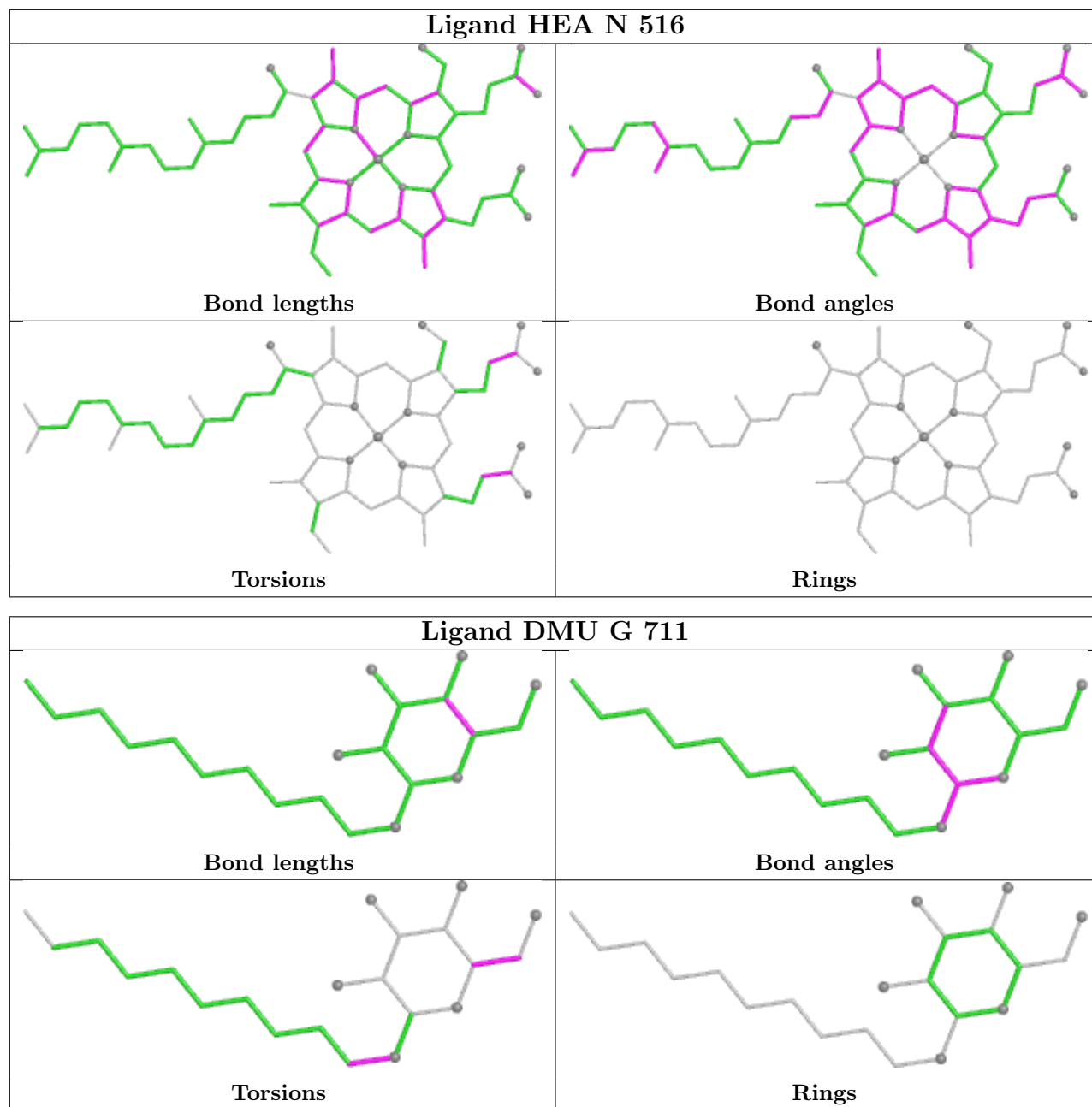


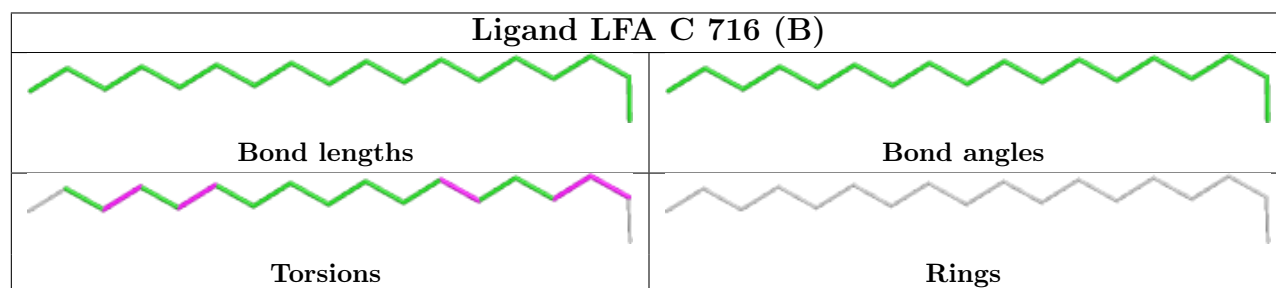
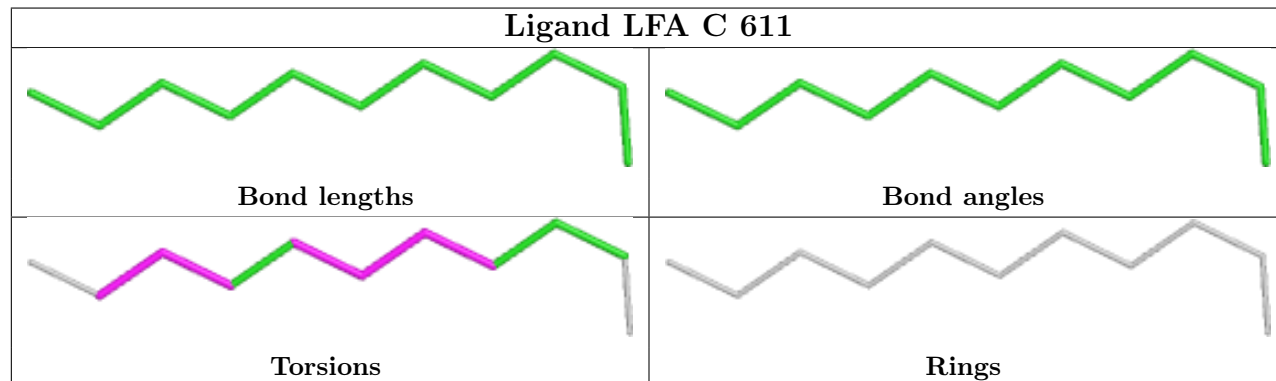
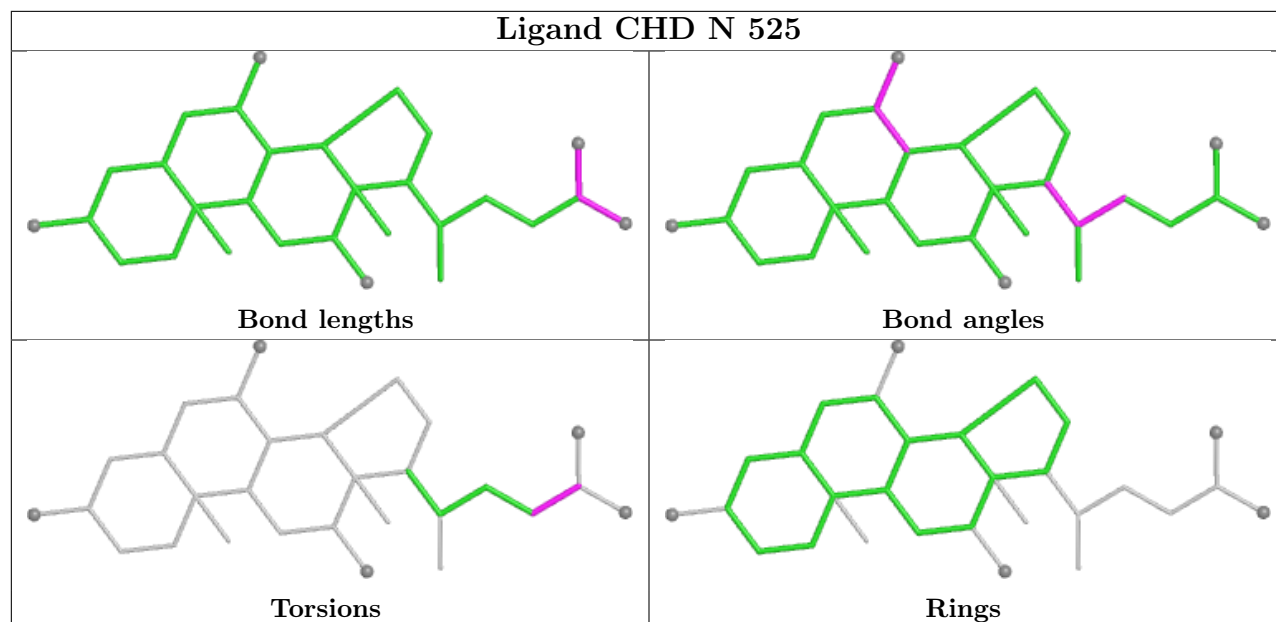
Ligand PEK C 264

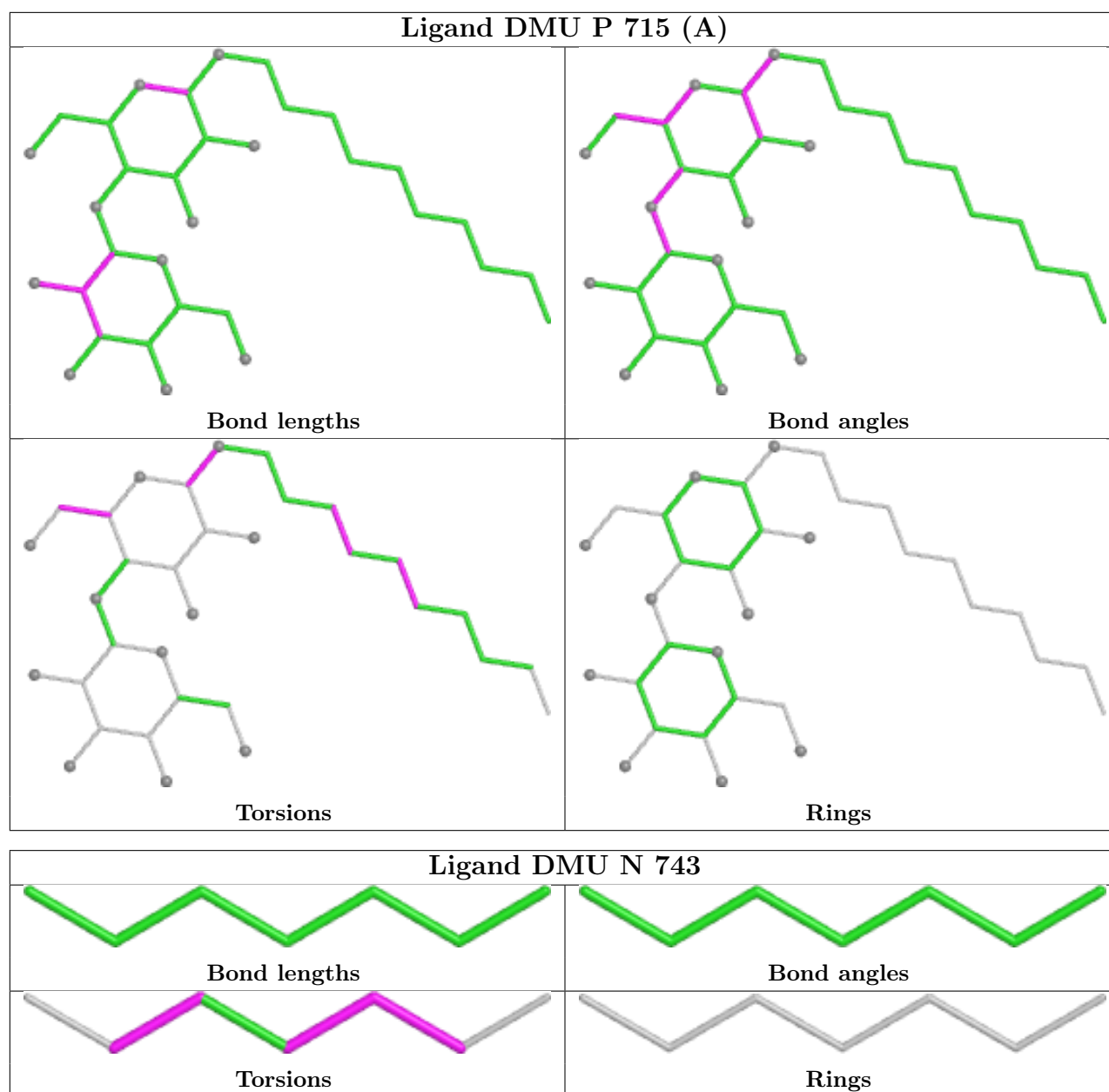


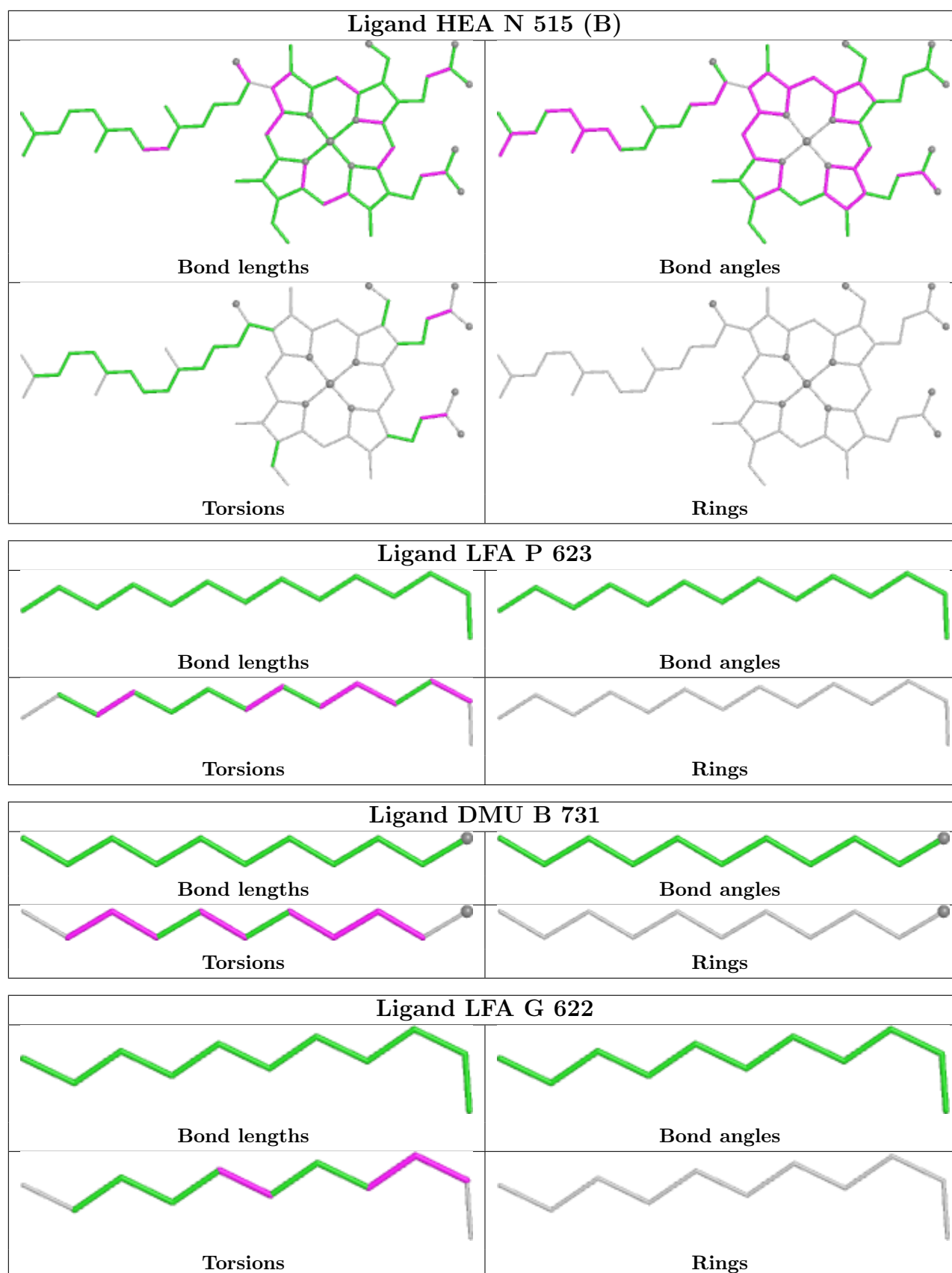
Ligand PGV C 266

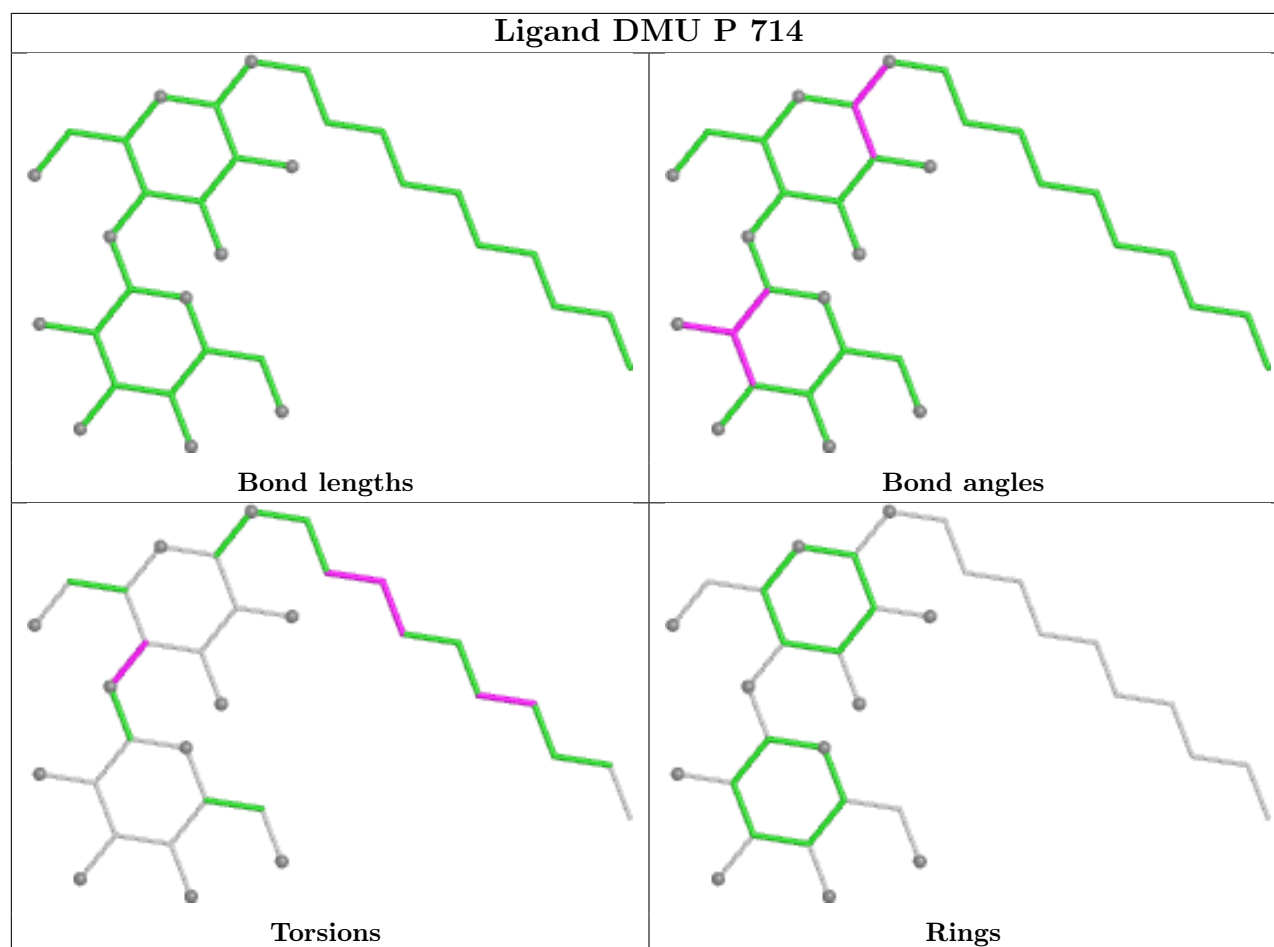
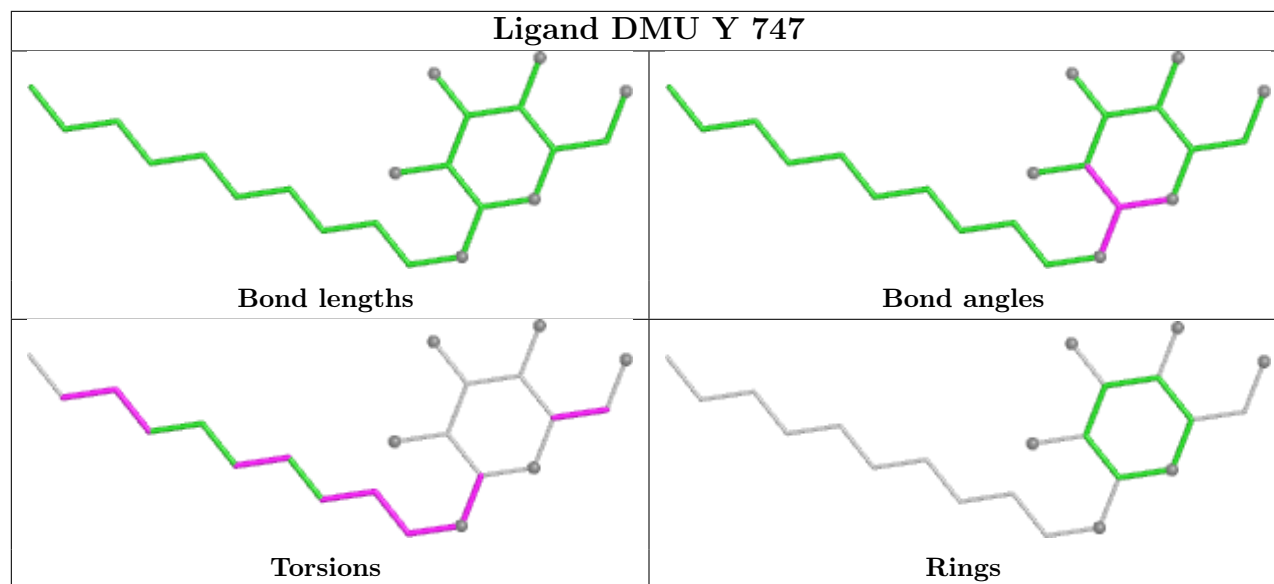


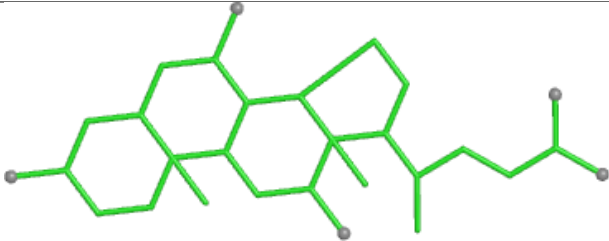
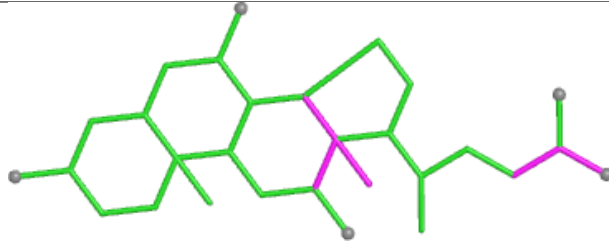
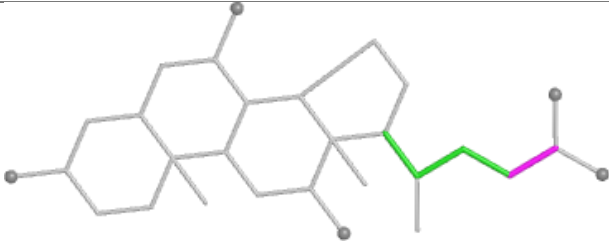
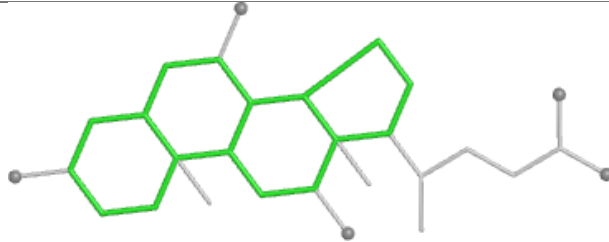


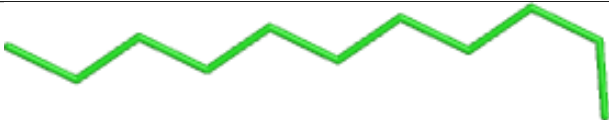
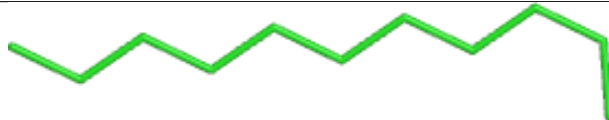
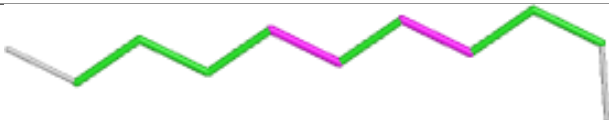
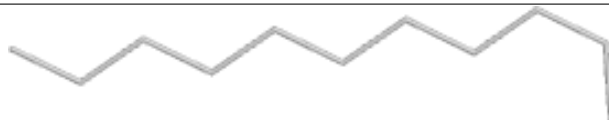


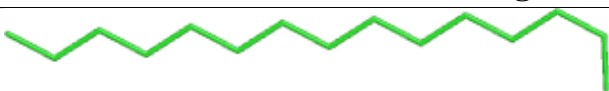
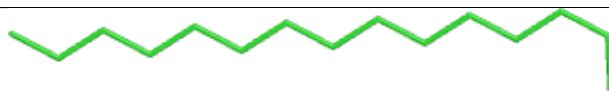
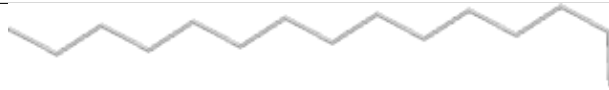




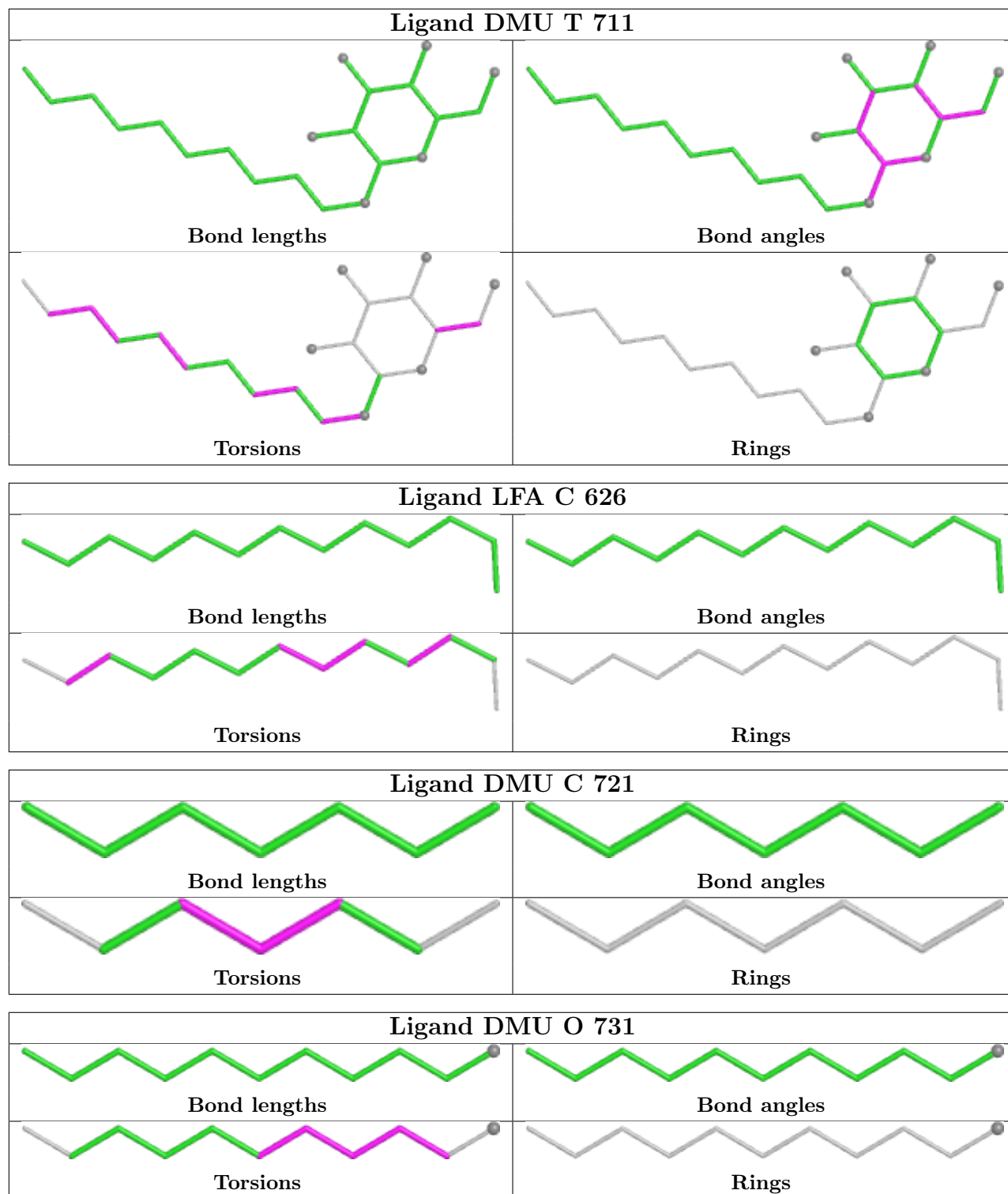


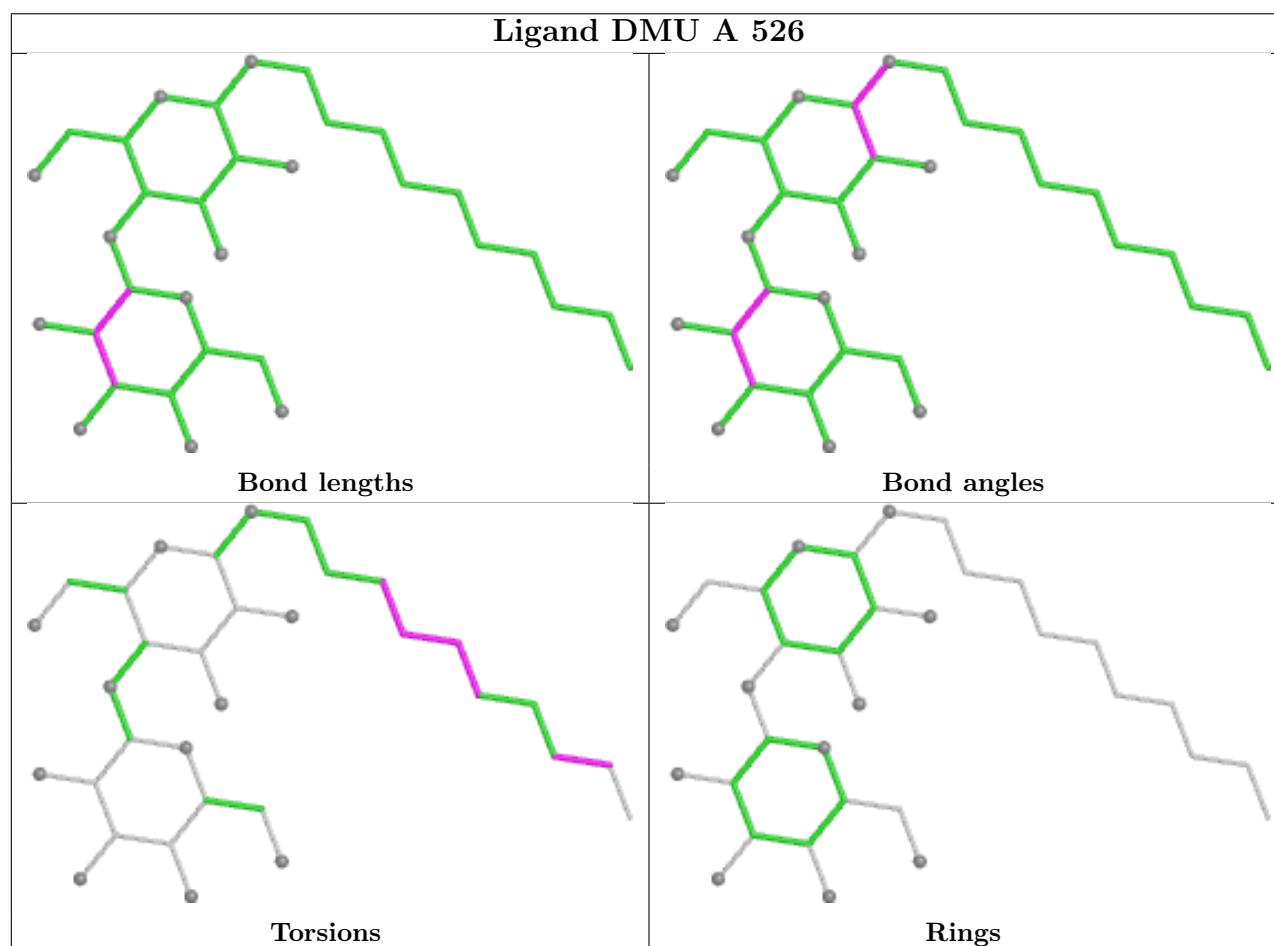
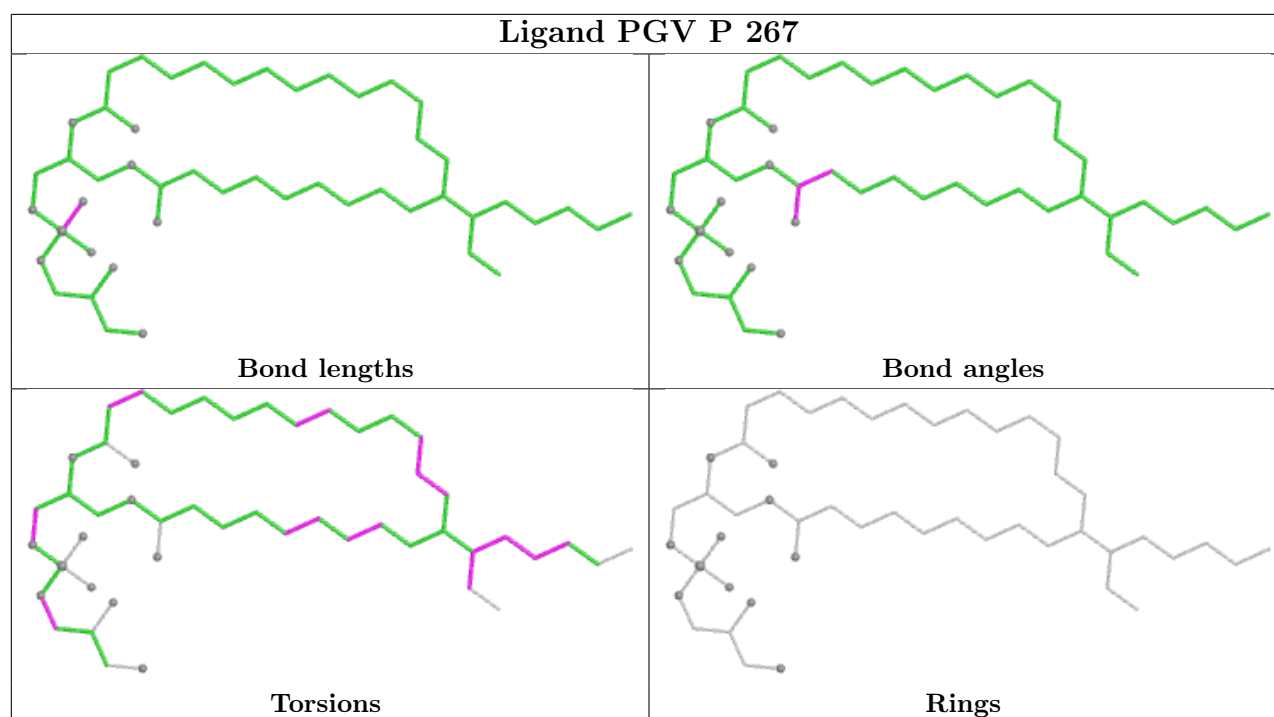
Ligand CHD G 86	
	
Bond lengths	Bond angles
	
Torsions	Rings

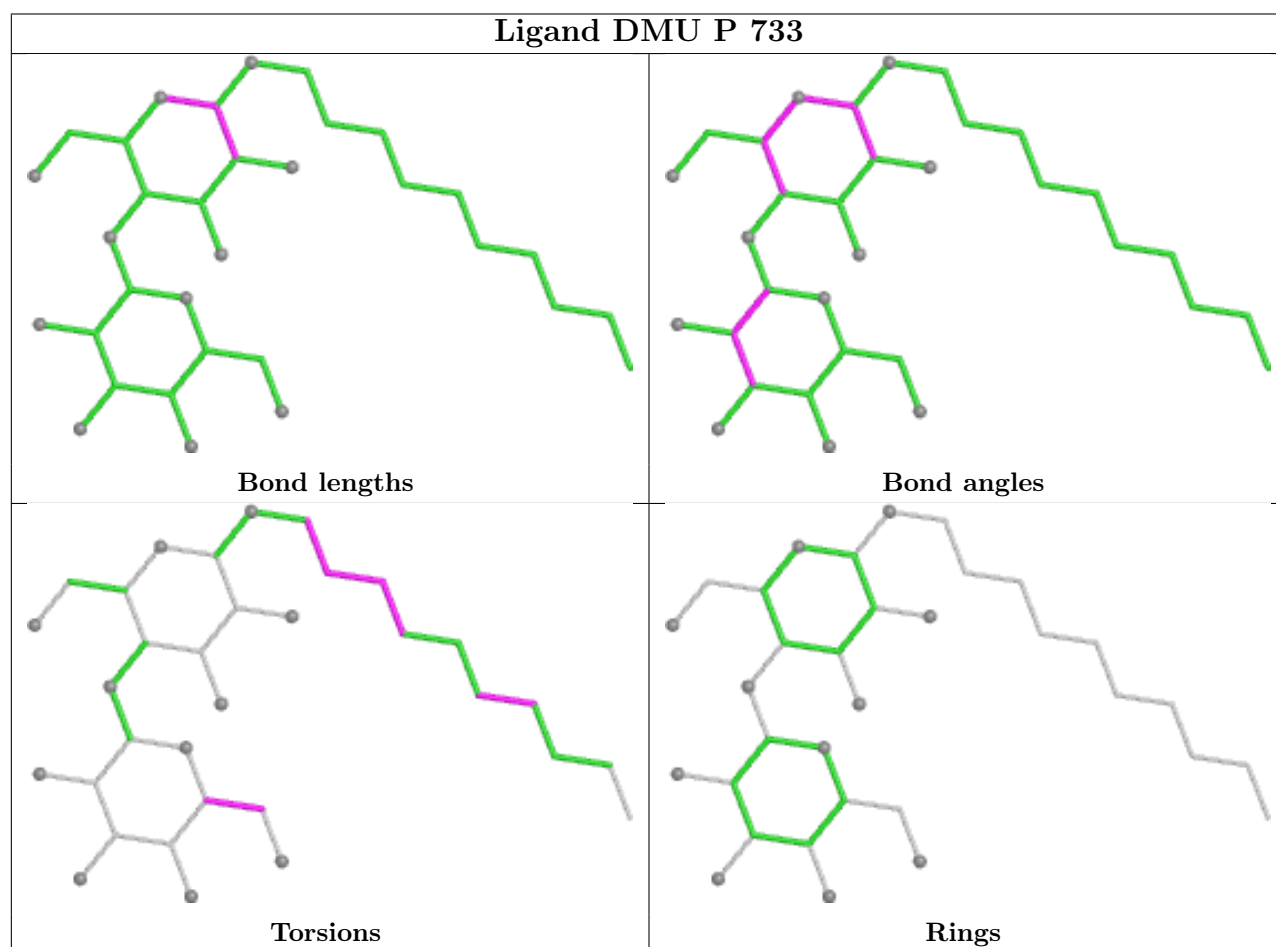
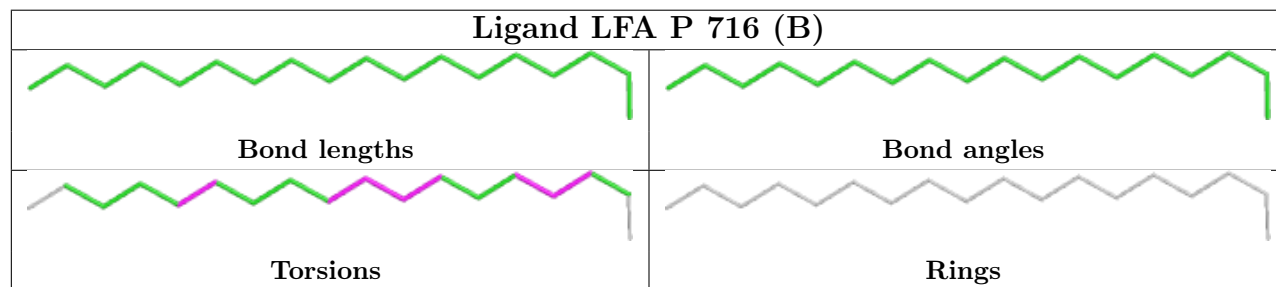
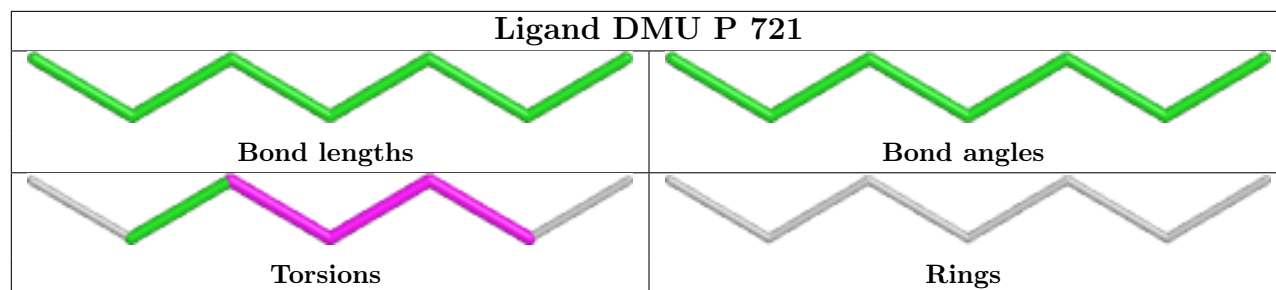
Ligand LFA C 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

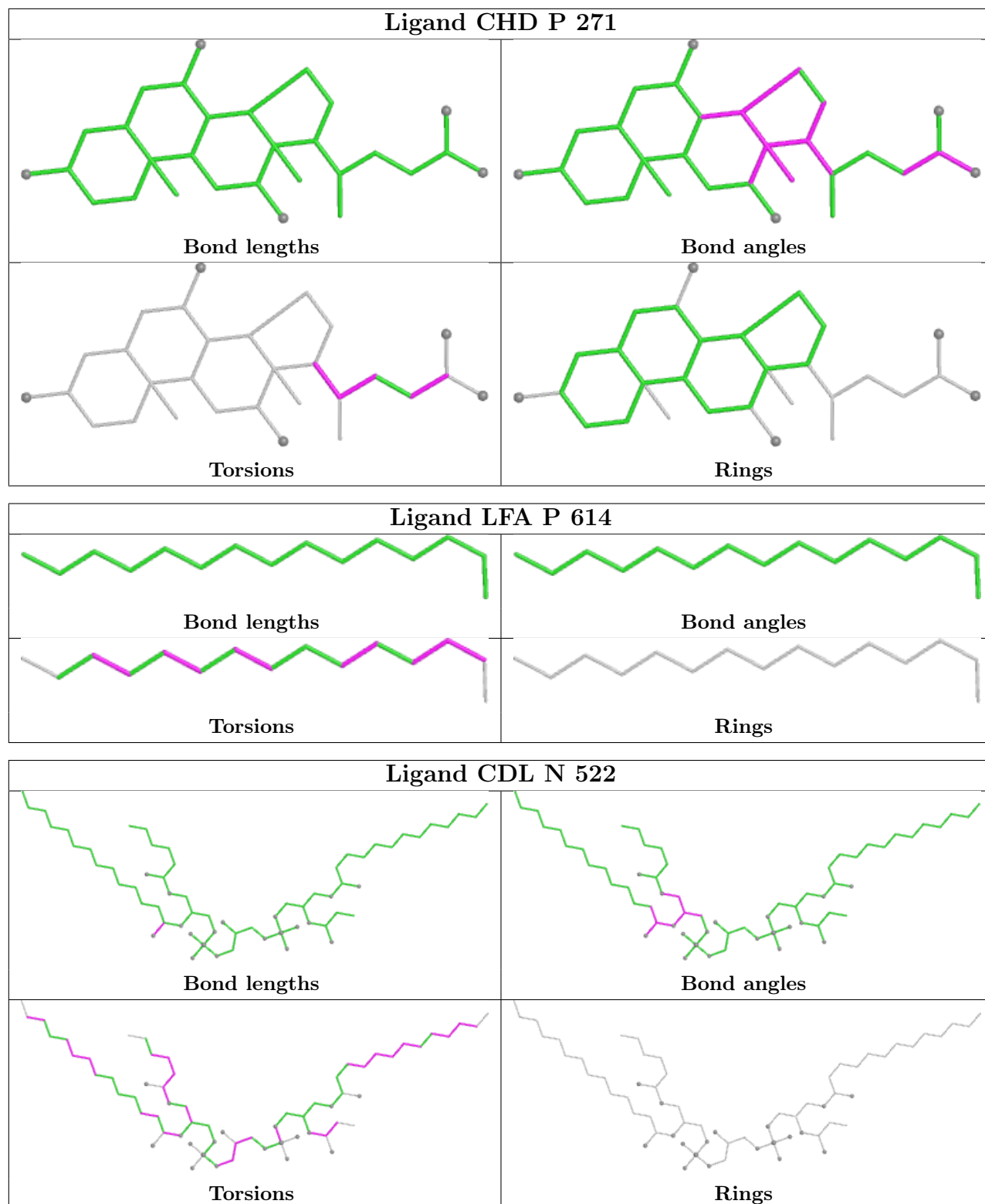
Ligand LFA P 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

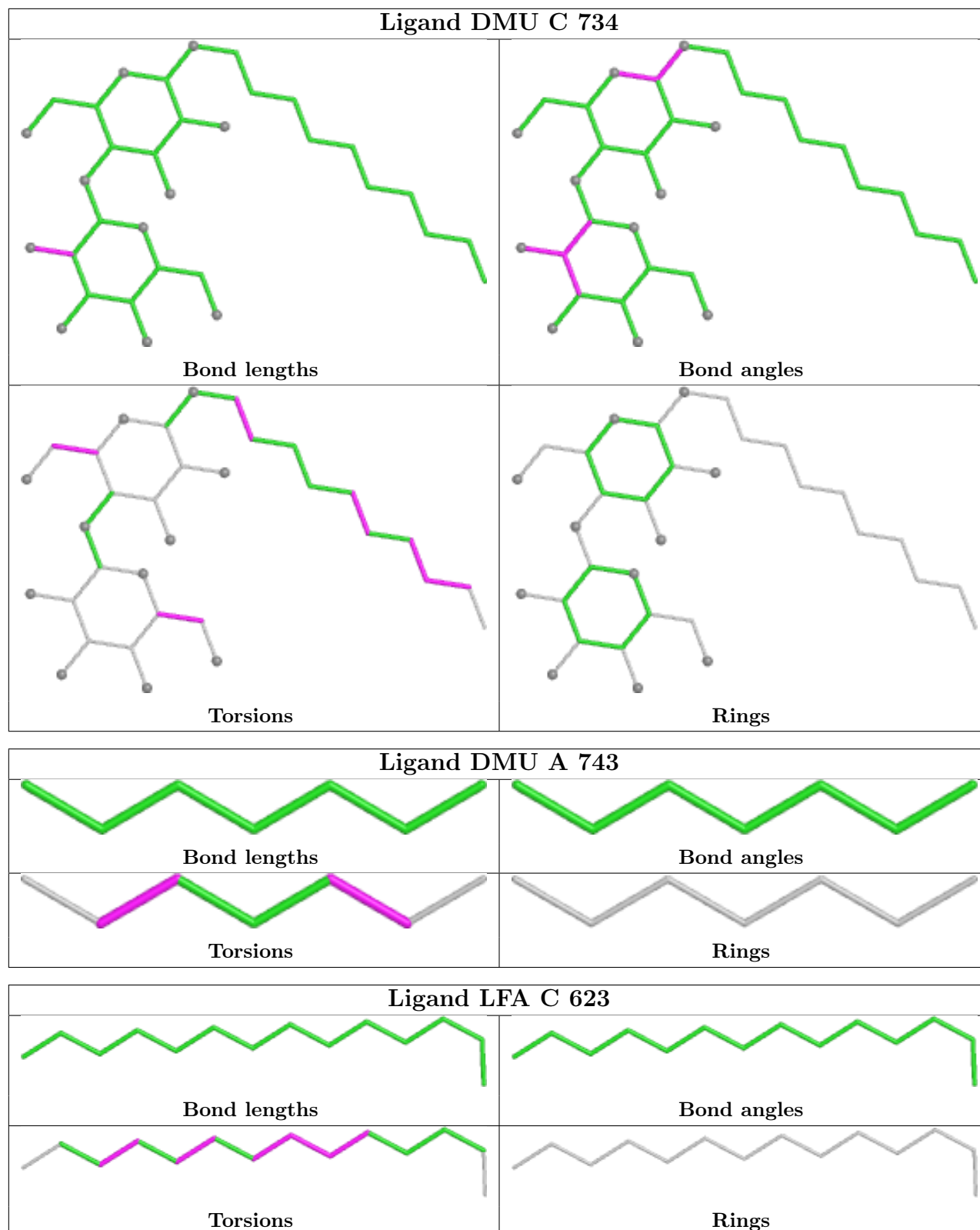
Ligand DMU G 712	
	
Bond lengths	Bond angles
	
Torsions	Rings

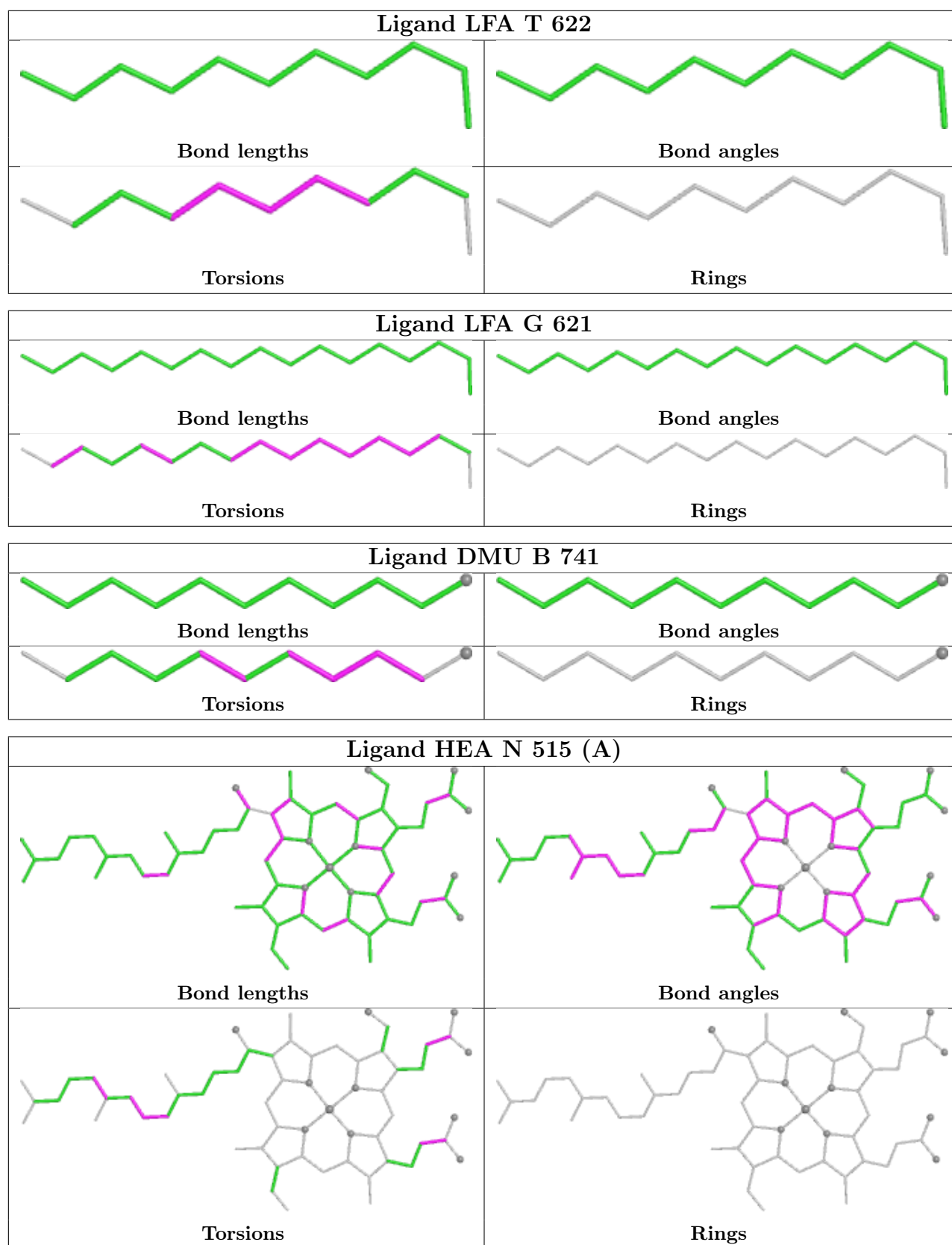


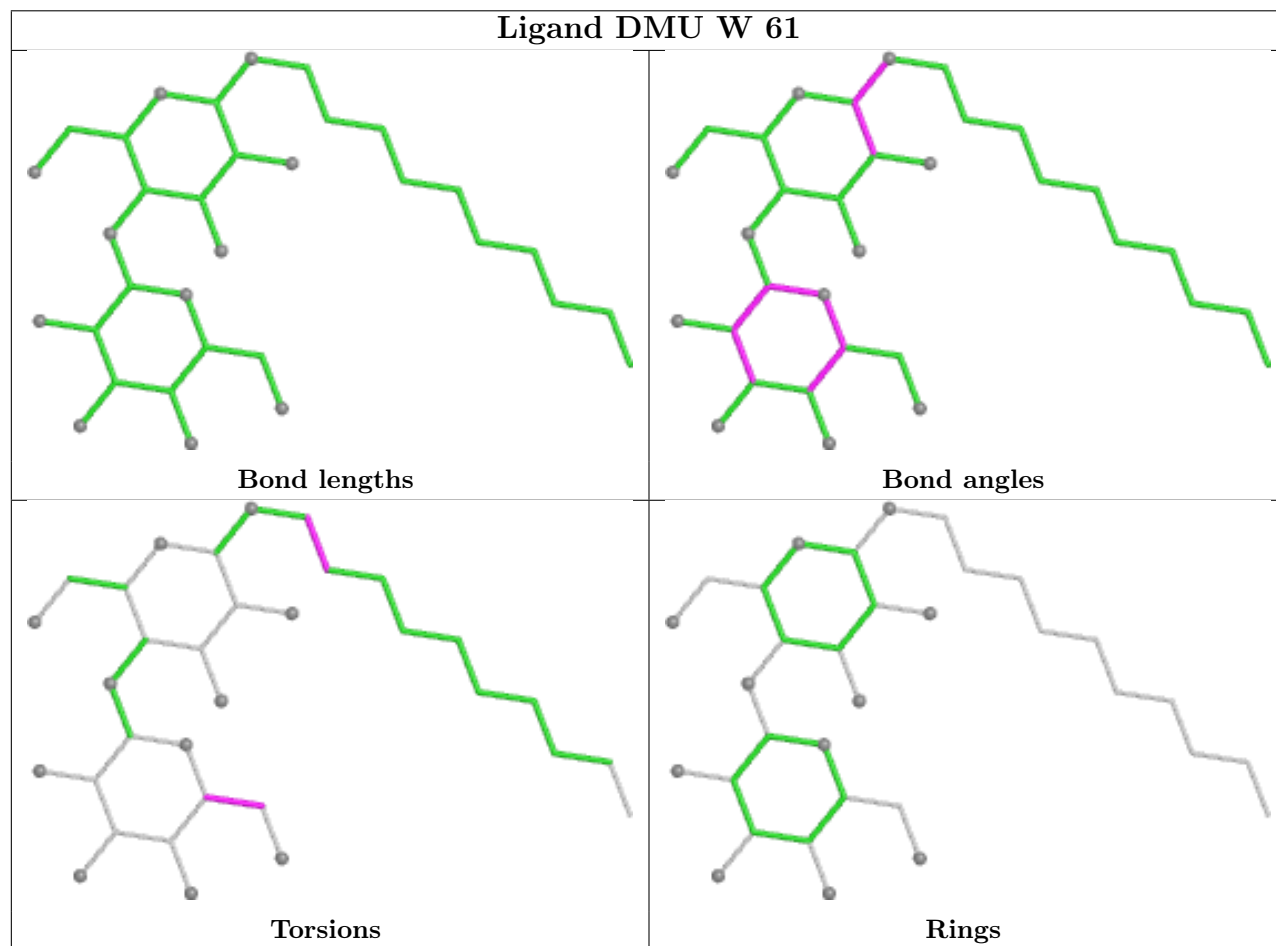
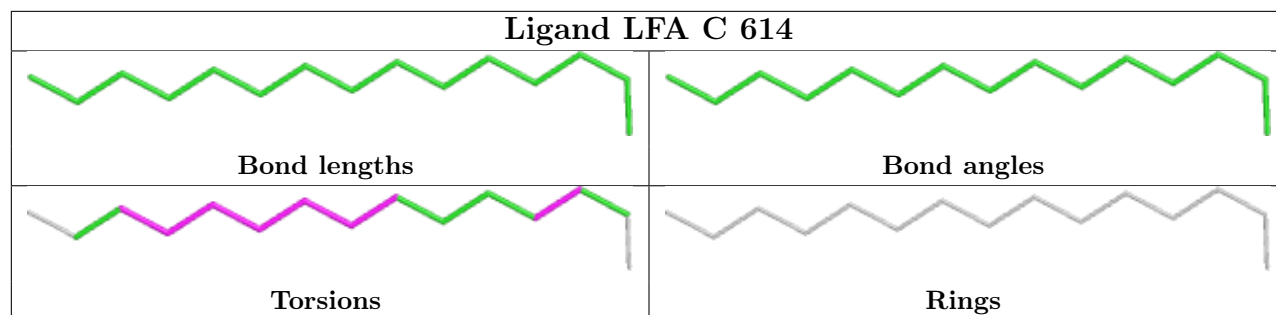


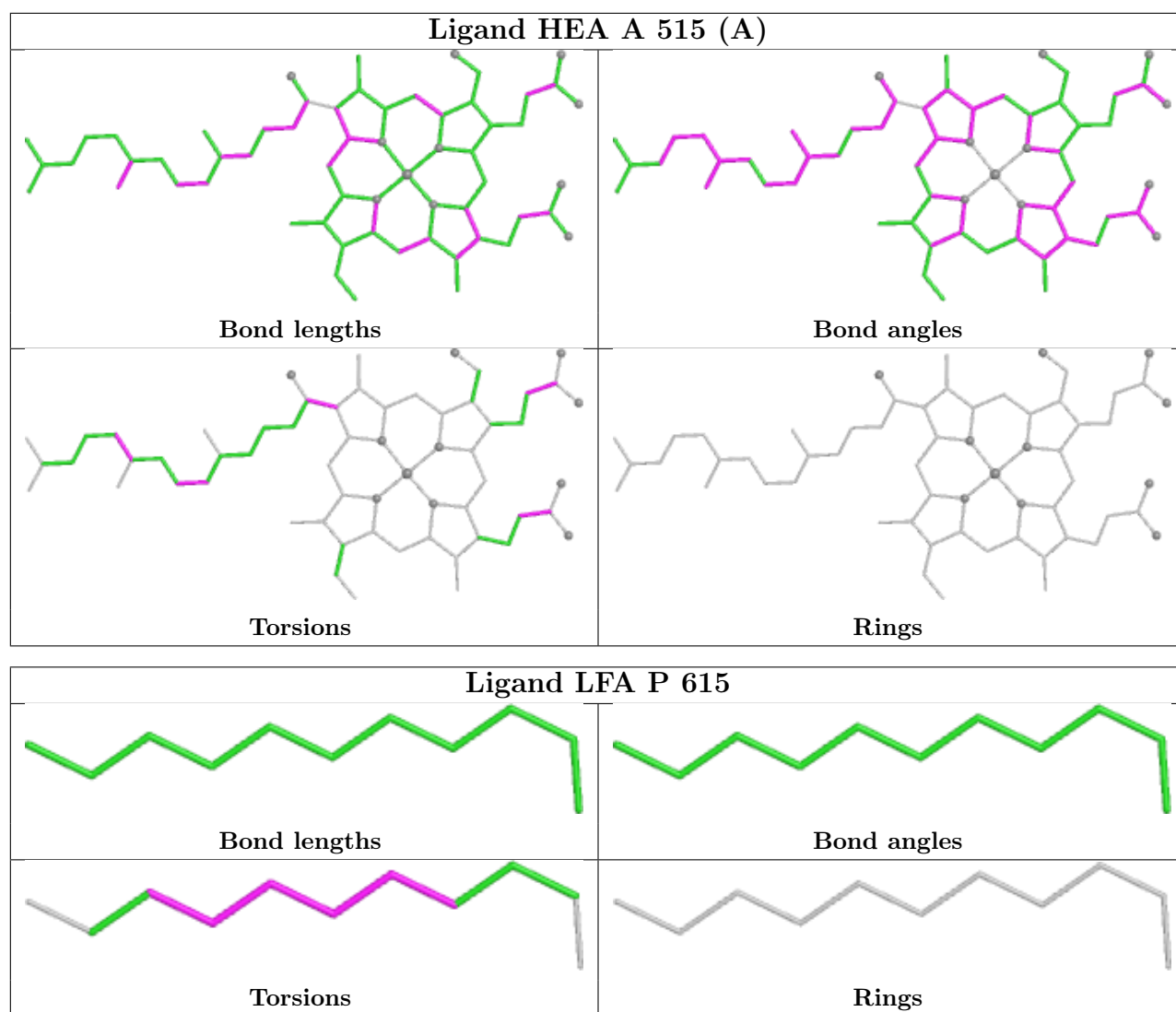












5.7 Other polymers [i](#)

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%)	-0.11	4 (0%) 82 86	9, 20, 27, 45	15 (2%)
1	N	512/514 (99%)	0.12	8 (1%) 70 74	10, 23, 32, 48	15 (2%)
2	B	226/227 (99%)	0.37	20 (8%) 15 17	14, 25, 47, 74	5 (2%)
2	O	226/227 (99%)	0.49	12 (5%) 32 37	16, 31, 57, 113	5 (2%)
3	C	258/261 (98%)	0.17	5 (1%) 66 70	10, 23, 34, 49	9 (3%)
3	P	258/261 (98%)	0.23	3 (1%) 76 80	10, 25, 37, 58	9 (3%)
4	D	143/147 (97%)	0.27	2 (1%) 73 77	13, 28, 42, 61	1 (0%)
4	Q	137/147 (93%)	0.90	17 (12%) 8 9	19, 41, 72, 88	1 (0%)
5	E	102/109 (93%)	0.15	2 (1%) 65 69	22, 28, 44, 60	0
5	R	102/109 (93%)	0.41	2 (1%) 65 69	26, 38, 54, 68	0
6	F	91/98 (92%)	0.29	3 (3%) 49 55	14, 29, 50, 59	2 (2%)
6	S	91/98 (92%)	0.49	3 (3%) 49 55	14, 28, 51, 57	2 (2%)
7	G	72/85 (84%)	0.71	8 (11%) 10 11	15, 30, 76, 94	1 (1%)
7	T	72/85 (84%)	0.81	8 (11%) 10 11	16, 34, 77, 99	1 (1%)
8	H	75/85 (88%)	0.71	9 (12%) 9 10	23, 32, 79, 107	0
8	U	75/85 (88%)	0.77	10 (13%) 7 8	28, 36, 79, 101	0
9	I	70/73 (95%)	0.88	10 (14%) 6 6	26, 38, 63, 85	0
9	V	70/73 (95%)	1.00	8 (11%) 10 11	25, 46, 64, 94	0
10	J	56/59 (94%)	0.66	6 (10%) 11 12	25, 34, 61, 67	0
10	W	56/59 (94%)	0.99	6 (10%) 11 12	27, 38, 58, 81	0
11	K	49/56 (87%)	0.66	2 (4%) 41 47	26, 33, 49, 59	0
11	X	49/56 (87%)	1.15	6 (12%) 8 9	33, 43, 69, 81	0
12	L	44/47 (93%)	0.27	3 (6%) 23 27	21, 25, 38, 57	0
12	Y	44/47 (93%)	0.63	1 (2%) 61 66	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%)	0.42	2 (5%) 34 39	21, 25, 46, 63	0
13	Z	40/46 (86%)	0.86	5 (12%) 8 9	30, 37, 69, 71	0
All	All	3470/3614 (96%)	0.35	165 (4%) 35 41	9, 27, 54, 113	66 (1%)

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	36	TRP	9.1
7	G	36	TRP	6.8
2	O	227	LEU	6.6
6	S	93	PRO	6.6
10	W	1	PHE	6.2

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	0.15	21,34,59,119	0
1	FME	A	1	10/11	0.95	0.12	32,41,68,95	0
1	FME	N	1	10/11	0.95	0.12	35,41,72,79	0
2	FME	O	1	10/11	0.96	0.09	28,32,40,54	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	C	722	22/33	0.66	0.40	32,56,76,90	22

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	DMU	P	722	22/33	0.68	0.38	31,63,73,87	22
22	LFA	P	615	11/20	0.68	0.49	52,57,67,74	11
22	LFA	C	626	13/20	0.73	0.31	41,45,51,54	13
23	EDO	C	807	4/4	0.74	0.41	42,45,46,60	4
19	CHD	P	271	29/29	0.76	0.20	48,66,110,128	0
22	LFA	P	716[B]	18/20	0.77	0.28	37,49,60,62	18
22	LFA	P	624	11/20	0.77	0.41	42,47,54,60	11
22	LFA	P	623	14/20	0.78	0.41	32,53,60,63	14
22	LFA	C	615	11/20	0.78	0.45	45,55,74,75	11
20	DMU	G	711	22/33	0.78	0.33	42,56,77,88	22
20	DMU	P	733	33/33	0.78	0.38	40,50,59,68	33
22	LFA	P	614	15/20	0.79	0.41	40,46,58,59	15
20	DMU	T	711	22/33	0.79	0.33	43,53,69,80	22
22	LFA	C	612	6/20	0.79	0.44	39,43,45,49	6
20	DMU	B	741	11/33	0.79	0.33	49,56,63,66	11
22	LFA	C	623	14/20	0.79	0.38	34,48,54,55	14
20	DMU	P	714	33/33	0.79	0.33	34,42,59,78	33
22	LFA	C	614	15/20	0.80	0.38	38,46,57,58	15
20	DMU	C	733	33/33	0.80	0.38	38,48,60,65	33
20	DMU	W	732	11/33	0.80	0.40	49,54,59,70	11
22	LFA	C	625	15/20	0.80	0.28	33,41,54,57	15
20	DMU	P	734	33/33	0.80	0.31	48,60,72,80	33
22	LFA	T	622	11/20	0.80	0.36	41,54,62,65	11
22	LFA	G	622	11/20	0.80	0.34	39,51,56,60	11
23	EDO	E	811	4/4	0.80	0.31	29,31,33,35	4
20	DMU	C	714	33/33	0.81	0.33	33,39,57,61	33
20	DMU	N	744	33/33	0.81	0.24	28,43,59,67	33
22	LFA	C	624	11/20	0.81	0.37	37,48,53,54	11
23	EDO	C	827	4/4	0.81	0.28	23,26,27,29	4
22	LFA	P	611	11/20	0.81	0.33	28,39,44,46	11
22	LFA	C	716[B]	18/20	0.82	0.29	34,49,89,90	18
22	LFA	P	626	13/20	0.82	0.32	38,50,62,64	13
20	DMU	C	734	33/33	0.82	0.27	38,54,63,66	33
20	DMU	W	61	33/33	0.82	0.22	36,48,77,81	33
22	LFA	A	628	14/20	0.82	0.29	33,41,48,51	14
19	CHD	C	271	29/29	0.82	0.17	44,58,76,95	0
20	DMU	J	732	11/33	0.82	0.41	47,50,57,68	11
20	DMU	T	712	11/33	0.83	0.36	45,52,60,60	11
20	DMU	J	61	33/33	0.83	0.20	33,43,65,71	33
20	DMU	N	743	7/33	0.83	0.34	45,49,56,57	7
20	DMU	A	743	7/33	0.83	0.34	42,46,50,53	7
20	DMU	N	745	33/33	0.83	0.28	33,46,72,87	33

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	DMU	O	742	22/33	0.83	0.26	33,38,44,48	22
22	LFA	A	627	14/20	0.84	0.28	28,38,66,70	14
22	LFA	G	621	17/20	0.84	0.29	29,53,64,64	17
23	EDO	N	801	4/4	0.84	0.17	17,17,19,23	4
23	EDO	P	827	4/4	0.84	0.25	23,24,30,32	4
23	EDO	A	801	4/4	0.85	0.14	17,18,20,22	4
22	LFA	P	625	15/20	0.85	0.22	35,41,61,63	15
23	EDO	C	809	4/4	0.85	0.17	22,23,29,32	4
20	DMU	Y	747	22/33	0.85	0.38	35,55,76,79	22
20	DMU	O	731	11/33	0.85	0.38	46,48,52,67	11
22	LFA	T	621	17/20	0.85	0.31	34,49,66,69	17
18	CDL	P	270	87/100	0.85	0.21	34,78,126,150	0
20	DMU	C	715[A]	33/33	0.86	0.23	26,35,43,61	33
20	DMU	G	713	22/33	0.86	0.30	41,52,58,61	22
18	CDL	C	270	87/100	0.86	0.20	34,82,121,135	0
20	DMU	B	742	22/33	0.86	0.25	34,48,57,69	22
18	CDL	N	522	64/100	0.86	0.18	46,82,132,158	0
20	DMU	P	715[A]	33/33	0.86	0.23	27,37,49,61	33
20	DMU	P	721	7/33	0.86	0.37	43,53,63,70	7
22	LFA	P	612	6/20	0.86	0.33	39,40,41,44	6
20	DMU	T	713	22/33	0.87	0.27	37,48,54,59	22
20	DMU	G	712	11/33	0.87	0.33	35,46,52,65	11
20	DMU	A	745	33/33	0.87	0.21	24,32,44,57	33
23	EDO	A	803	4/4	0.87	0.23	23,29,37,39	4
20	DMU	C	721	7/33	0.87	0.32	45,49,53,64	7
18	CDL	N	521	94/100	0.87	0.19	37,83,124,140	0
20	DMU	O	741	11/33	0.87	0.30	40,45,52,66	11
20	DMU	L	747	22/33	0.87	0.33	37,47,57,64	22
23	EDO	F	817	4/4	0.87	0.15	13,13,16,20	4
20	DMU	M	746	8/33	0.87	0.26	35,44,48,49	8
23	EDO	N	803	4/4	0.87	0.21	26,26,37,42	4
22	LFA	N	628	14/20	0.87	0.28	35,42,66,68	14
22	LFA	C	611	11/20	0.88	0.32	36,43,48,49	11
22	LFA	N	627	14/20	0.88	0.26	28,38,54,55	14
18	CDL	A	522	64/100	0.88	0.17	38,71,110,133	0
23	EDO	A	825	4/4	0.89	0.19	33,33,34,42	4
20	DMU	B	731	11/33	0.89	0.31	36,51,59,63	11
20	DMU	P	272	11/33	0.89	0.27	42,47,55,60	11
20	DMU	A	744	33/33	0.90	0.17	21,32,44,65	33
20	DMU	Z	746	8/33	0.90	0.26	44,47,52,56	8
23	EDO	P	807	4/4	0.90	0.23	47,48,50,59	4
18	CDL	A	521	94/100	0.90	0.17	28,71,121,139	0

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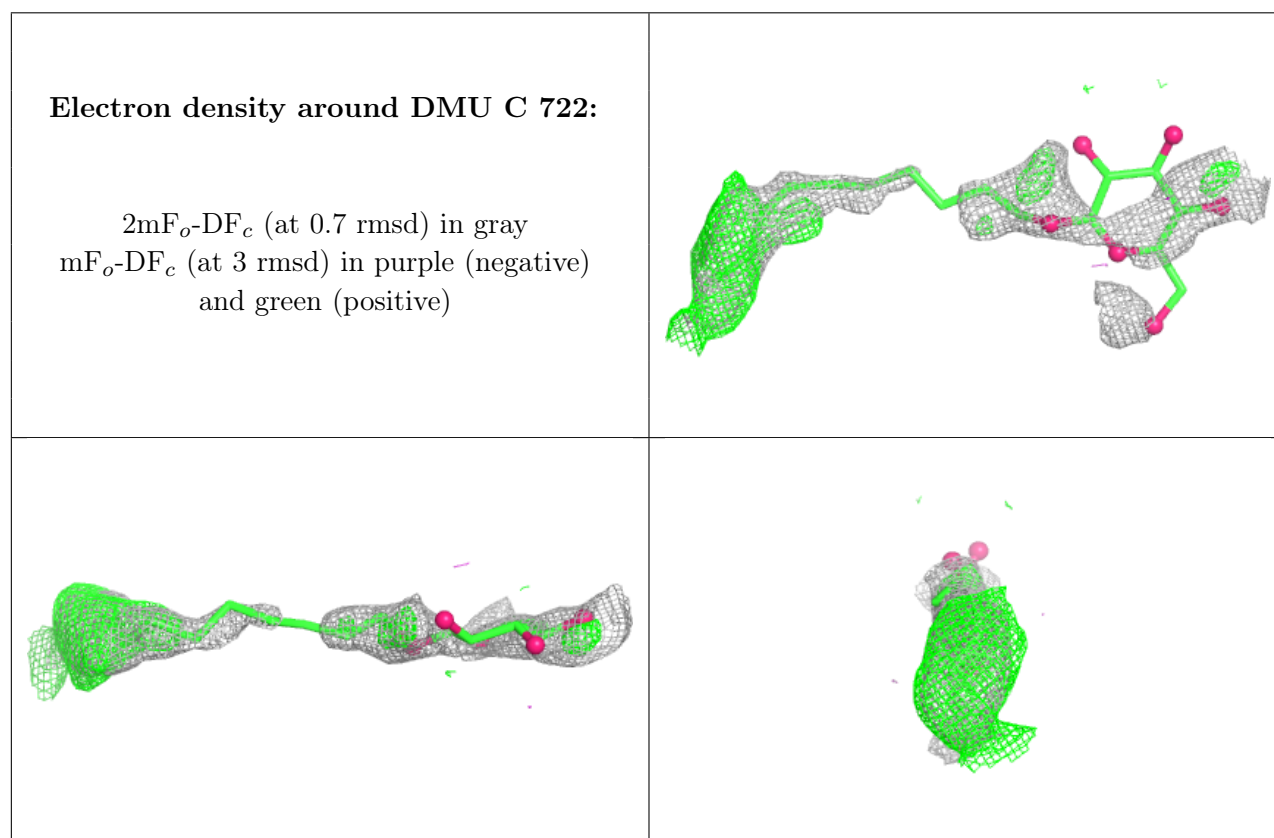
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	DMU	C	272	11/33	0.91	0.23	45,51,57,68	11
23	EDO	F	819	4/4	0.91	0.14	22,22,27,29	4
23	EDO	S	817	4/4	0.91	0.11	13,14,16,19	4
23	EDO	N	829	4/4	0.92	0.14	27,30,31,33	4
20	DMU	N	526	33/33	0.92	0.11	41,49,61,72	0
23	EDO	R	815	4/4	0.93	0.17	38,39,42,43	4
23	EDO	P	809	4/4	0.93	0.15	27,28,28,36	4
23	EDO	G	821	4/4	0.94	0.12	23,24,29,30	4
23	EDO	A	823	4/4	0.94	0.15	17,17,19,24	4
23	EDO	B	805	4/4	0.94	0.13	17,21,21,25	4
23	EDO	S	819	4/4	0.94	0.12	20,21,21,30	4
23	EDO	N	825	4/4	0.95	0.13	27,28,29,30	4
23	EDO	E	815	4/4	0.95	0.13	25,28,29,32	4
19	CHD	A	525	29/29	0.95	0.08	22,26,29,33	0
20	DMU	A	526	33/33	0.95	0.09	32,39,54,58	0
23	EDO	R	811	4/4	0.96	0.26	45,46,50,53	4
23	EDO	N	823	4/4	0.96	0.15	19,21,22,22	4
19	CHD	N	525	29/29	0.96	0.07	23,26,29,34	0
23	EDO	E	813	4/4	0.96	0.12	22,24,25,25	4
26	PEK	P	264	53/53	0.96	0.13	26,46,102,108	0
19	CHD	G	86	29/29	0.97	0.06	20,23,28,36	0
23	EDO	R	813	4/4	0.97	0.11	27,28,29,29	4
23	EDO	T	821	4/4	0.97	0.07	25,27,29,32	4
26	PEK	C	264	53/53	0.97	0.12	24,42,96,129	0
19	CHD	T	86	29/29	0.97	0.07	21,24,28,35	0
27	PGV	P	266	51/51	0.97	0.10	22,31,61,65	0
23	EDO	O	805	4/4	0.98	0.10	23,24,27,29	4
25	UNX	C	262	1/1	0.98	0.25	36,36,36,36	0
27	PGV	C	266	51/51	0.98	0.10	19,28,65,76	0
27	PGV	C	267	51/51	0.98	0.10	20,28,75,94	0
25	UNX	P	262	1/1	0.98	0.21	34,34,34,34	0
27	PGV	P	267	51/51	0.98	0.10	20,30,91,105	0
21	PER	N	520	2/2	0.99	0.12	19,19,19,26	0
14	HEA	A	515[A]	60/60	0.99	0.05	15,18,29,35	9
14	HEA	A	515[B]	60/60	0.99	0.05	15,18,29,34	9
14	HEA	A	516	60/60	0.99	0.05	15,17,23,26	0
14	HEA	N	515[A]	60/60	0.99	0.05	19,21,32,39	9
14	HEA	N	515[B]	60/60	0.99	0.05	19,21,29,33	9
14	HEA	N	516	60/60	0.99	0.05	18,19,25,28	0
21	PER	A	520	2/2	0.99	0.10	20,20,20,26	0
16	MG	N	518	1/1	1.00	0.02	23,23,23,23	0
17	NA	A	519	1/1	1.00	0.03	21,21,21,21	0

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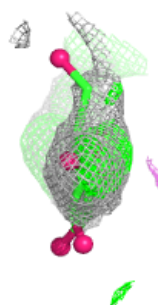
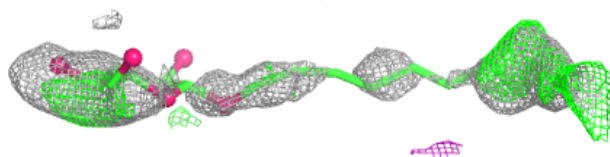
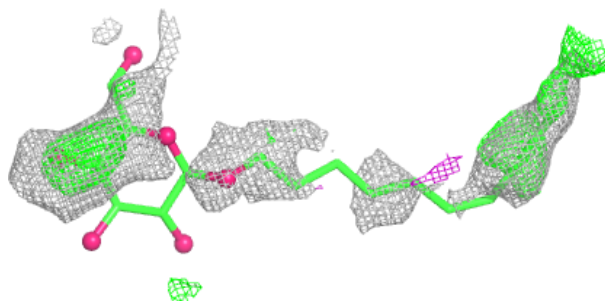
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	NA	N	519	1/1	1.00	0.02	28,28,28,28	0
15	CU	A	517	1/1	1.00	0.02	17,17,17,17	0
15	CU	N	517	1/1	1.00	0.02	20,20,20,20	0
16	MG	A	518	1/1	1.00	0.03	19,19,19,19	0
24	CUA	B	228	2/2	1.00	0.01	19,19,19,19	0
24	CUA	O	228	2/2	1.00	0.01	24,24,24,25	0
28	ZN	F	99	1/1	1.00	0.02	24,24,24,24	0
28	ZN	S	99	1/1	1.00	0.02	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.

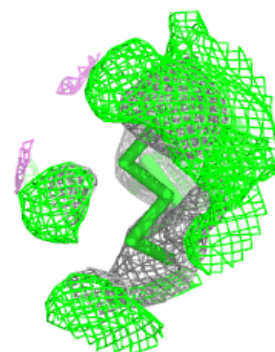
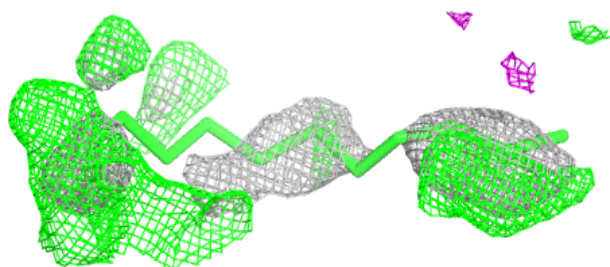
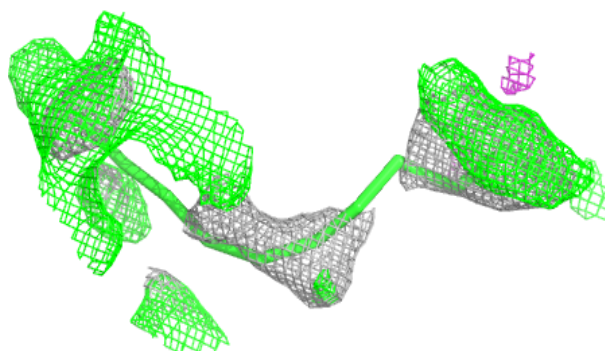


Electron density around DMU P 722:

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

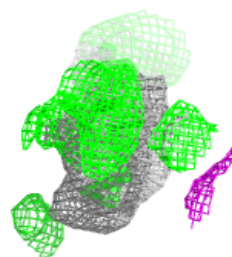
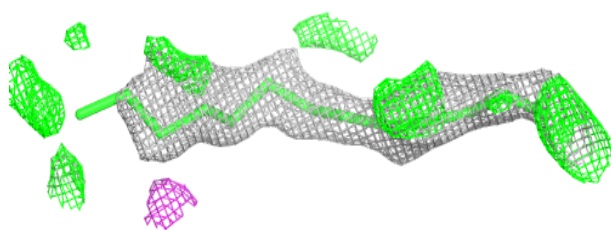
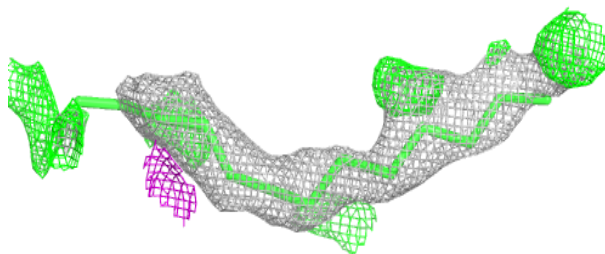
**Electron density around LFA P 615:**

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

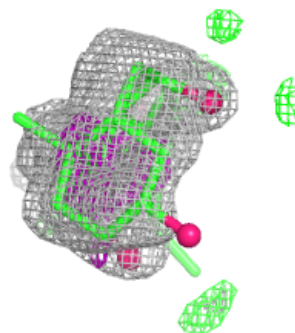
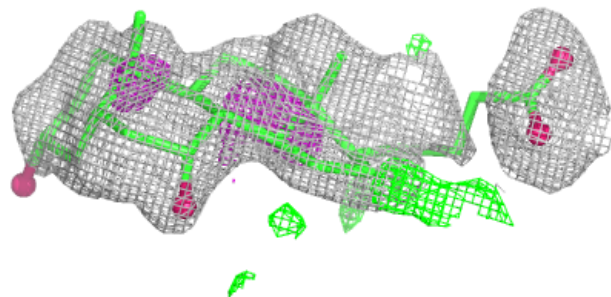
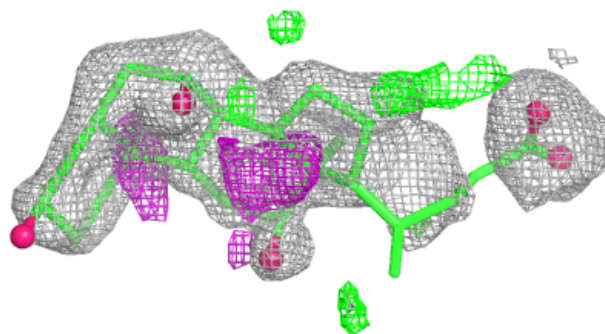


Electron density around LFA C 626:

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

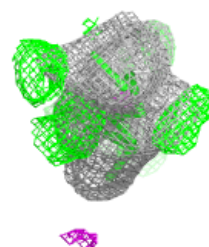
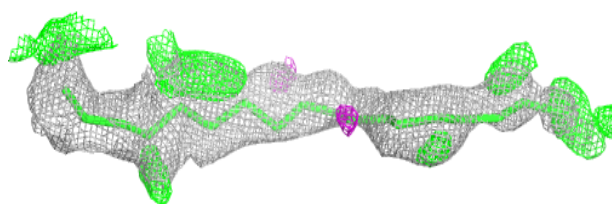
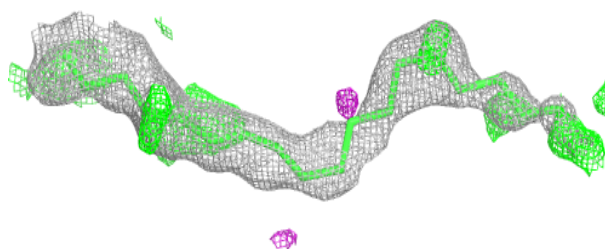
**Electron density around CHD P 271:**

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

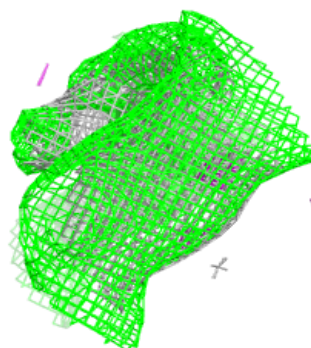
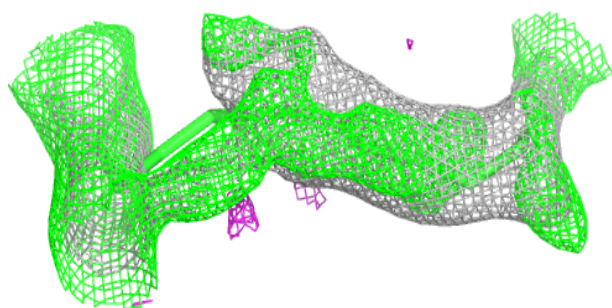
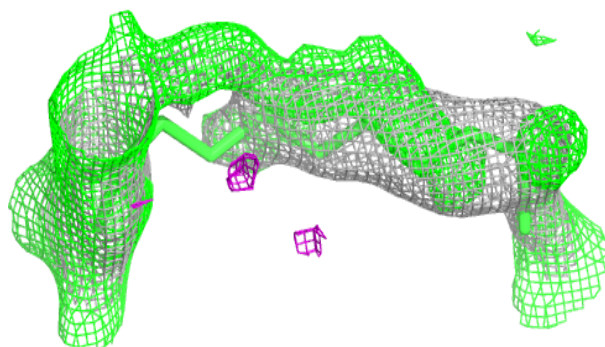


Electron density around LFA P 716 (B):

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

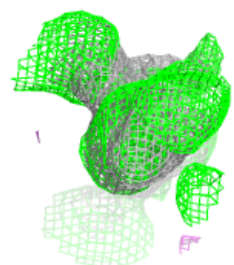
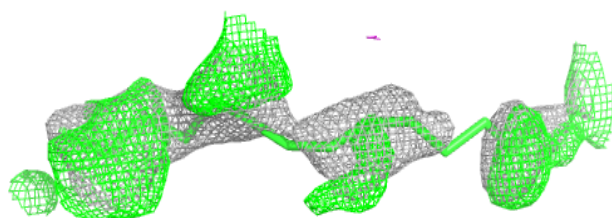
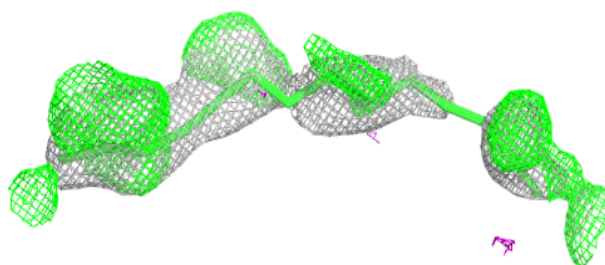
**Electron density around LFA P 624:**

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

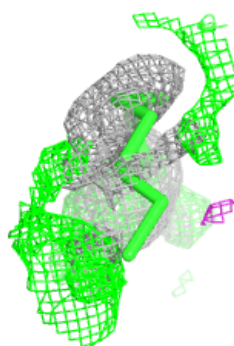
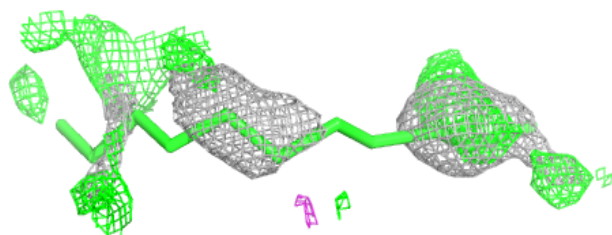
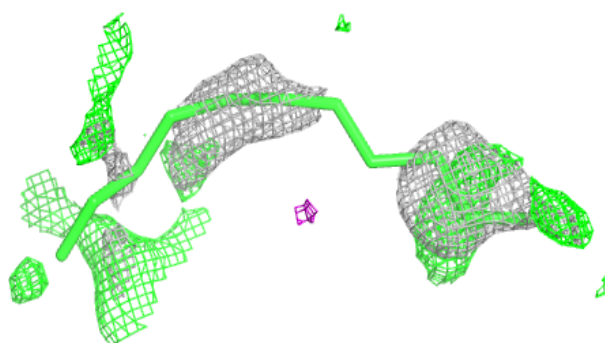


Electron density around LFA P 623:

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

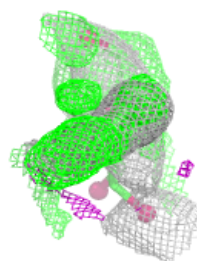
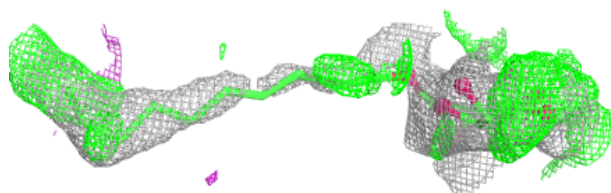
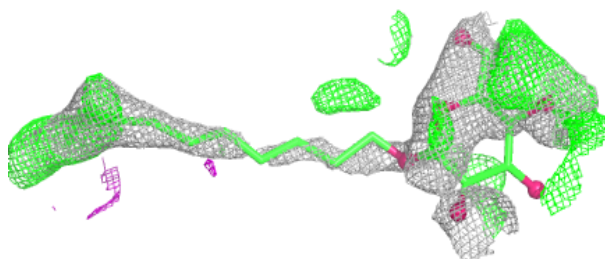
**Electron density around LFA C 615:**

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

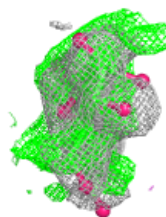
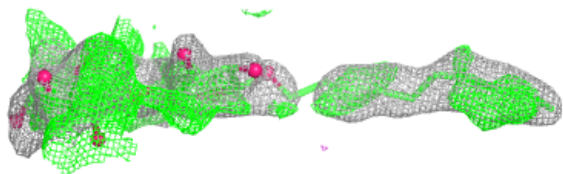
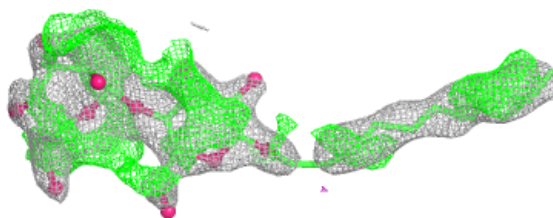


Electron density around DMU G 711:

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

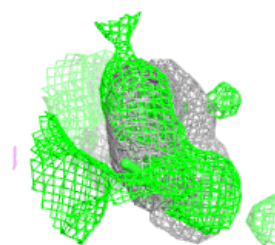
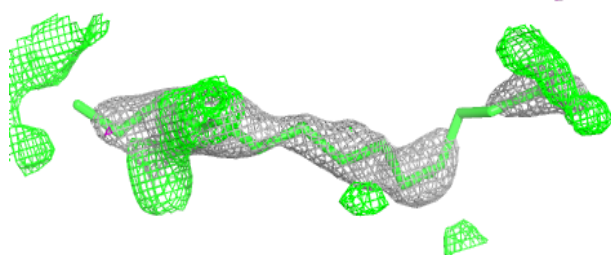
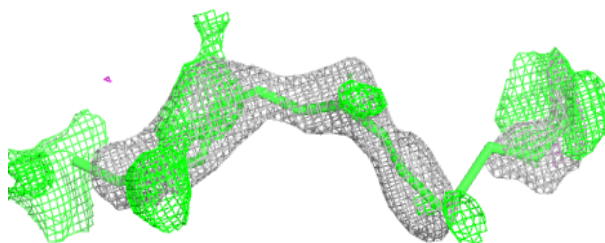
**Electron density around DMU P 733:**

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

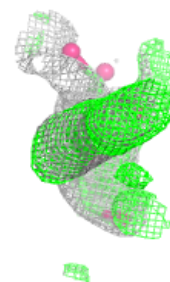
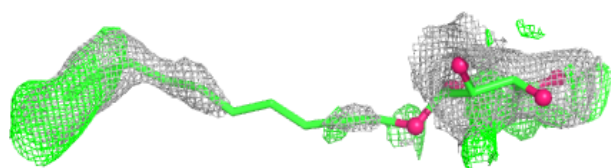
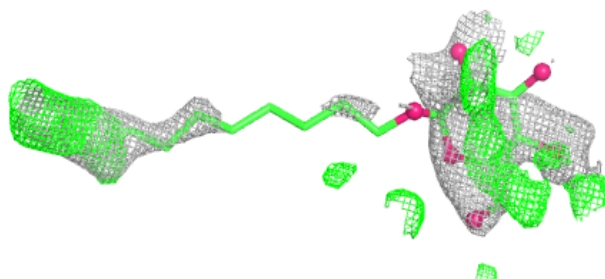


Electron density around LFA P 614:

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

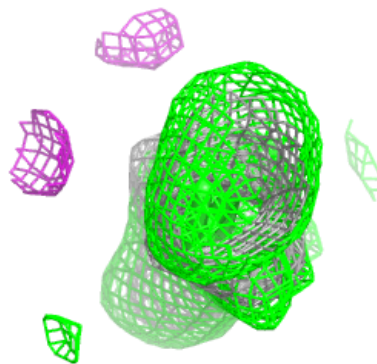
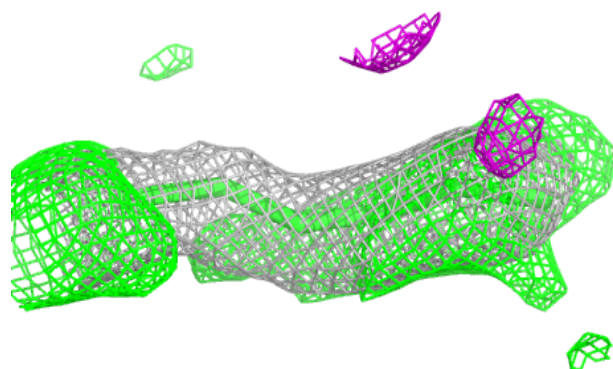
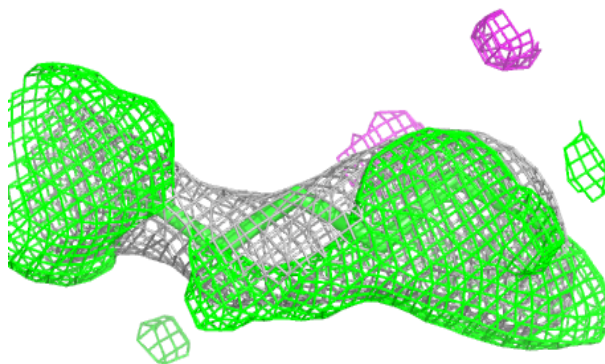
**Electron density around DMU T 711:**

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

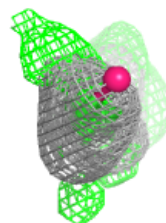
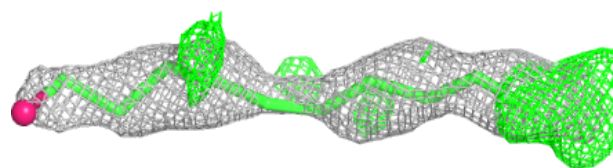
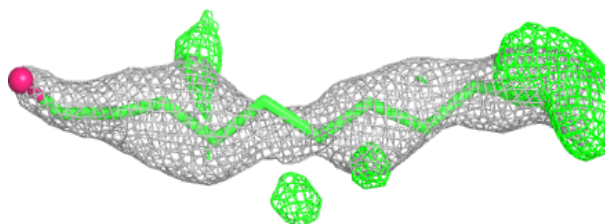


Electron density around LFA C 612:

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

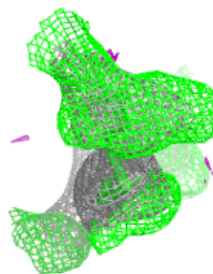
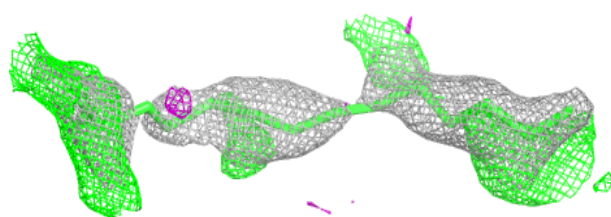
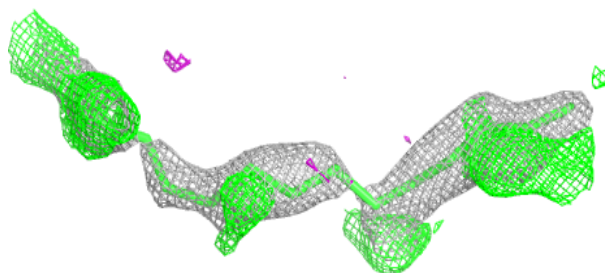
**Electron density around DMU B 741:**

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

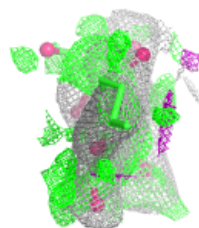
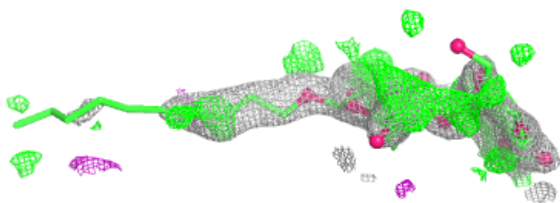
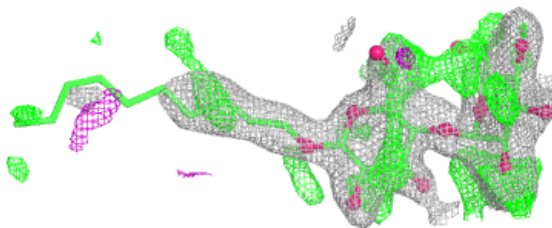


Electron density around LFA C 623:

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

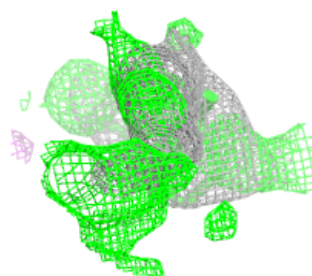
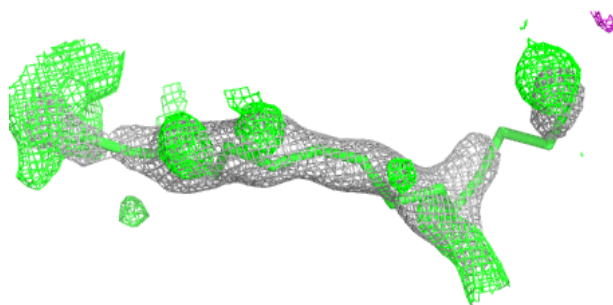
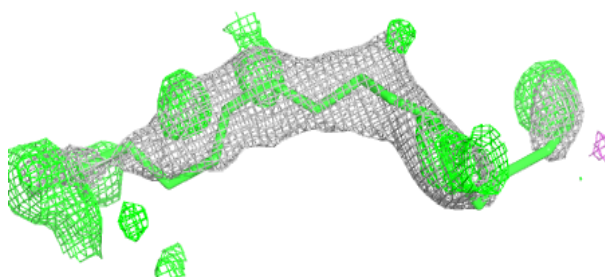
**Electron density around DMU P 714:**

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

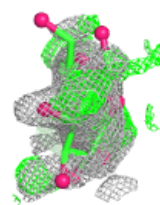
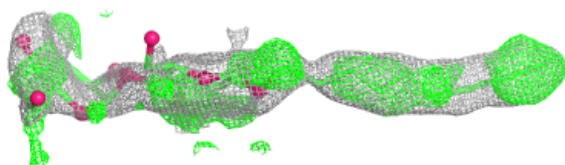
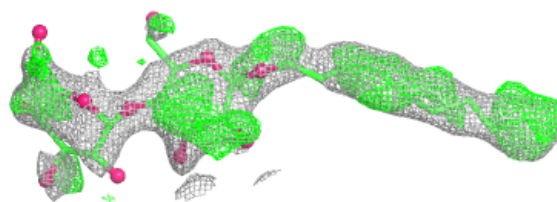


Electron density around LFA C 614:

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

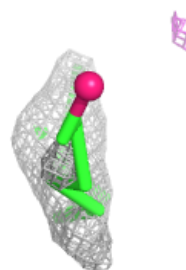
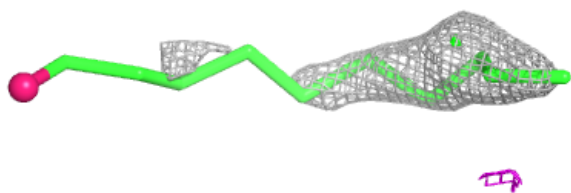
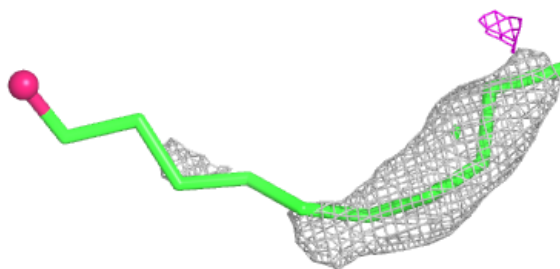
**Electron density around DMU C 733:**

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

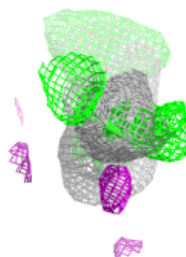
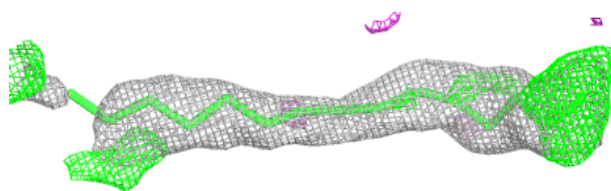
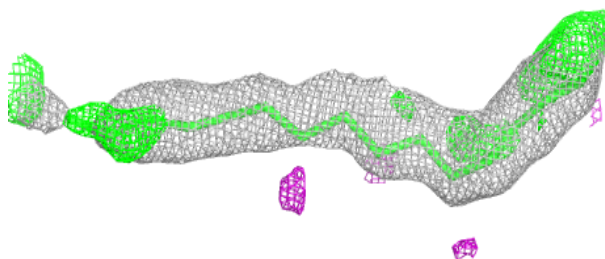


Electron density around DMU W 732:

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

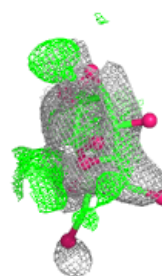
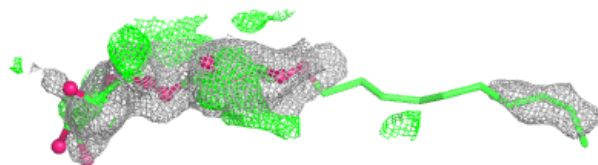
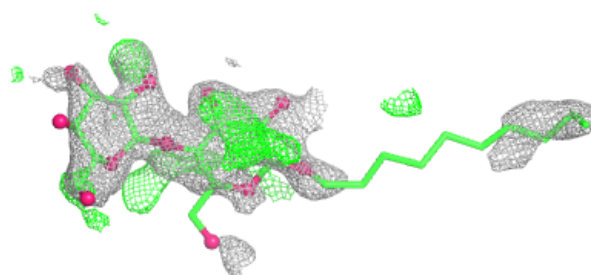
**Electron density around LFA C 625:**

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

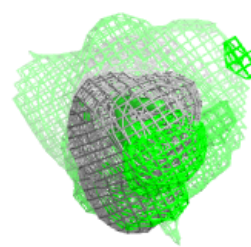
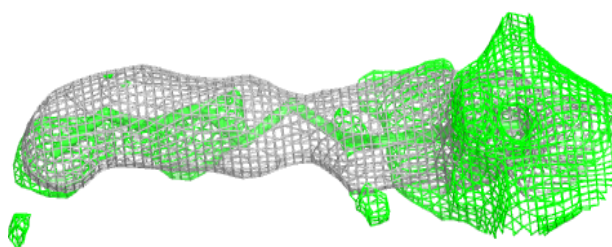
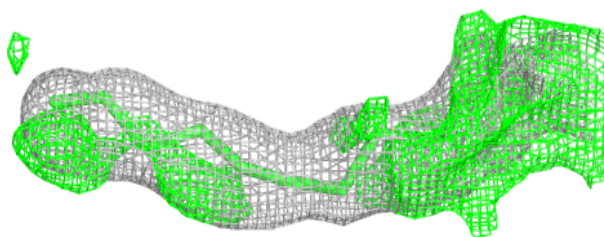


Electron density around DMU P 734:

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

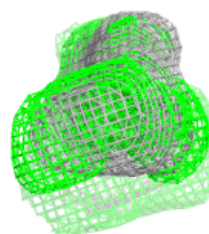
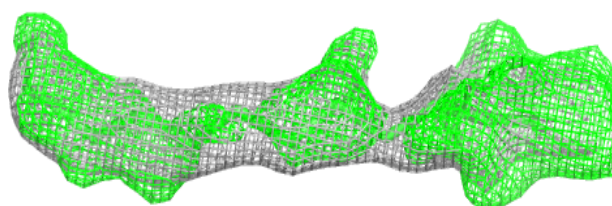
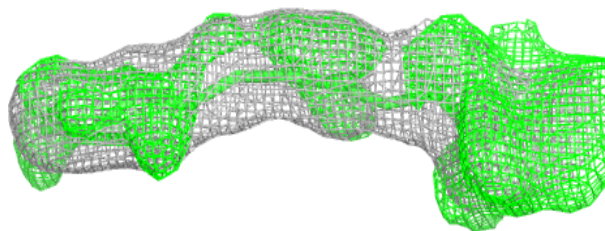
**Electron density around LFA T 622:**

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

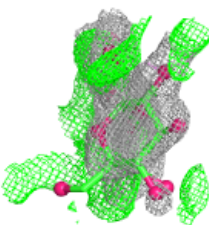
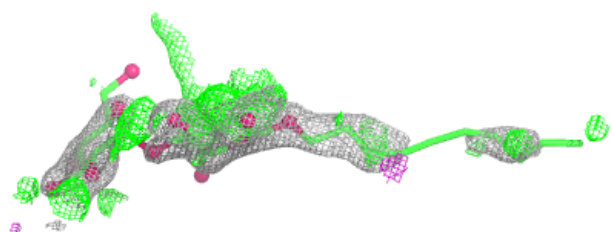
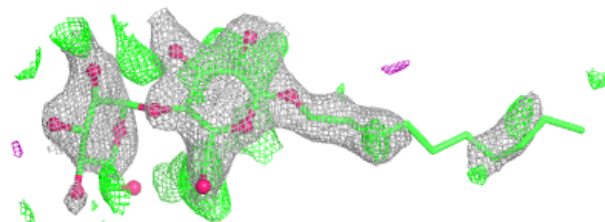


Electron density around LFA G 622:

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

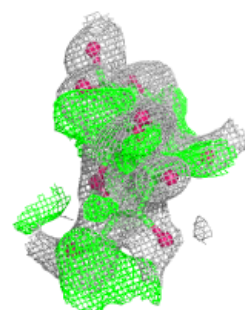
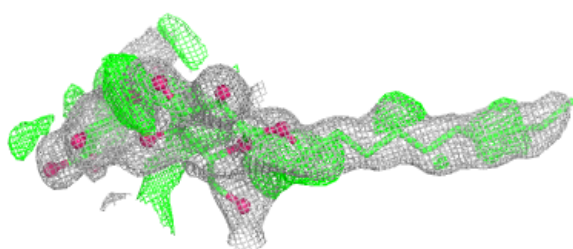
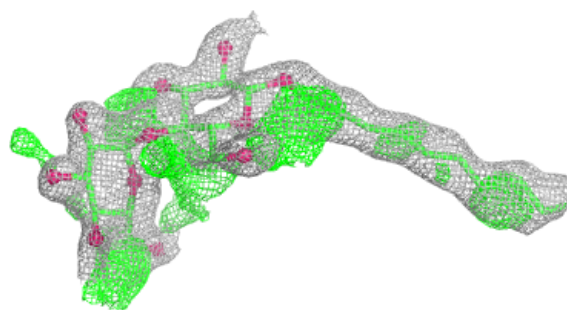
**Electron density around DMU C 714:**

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

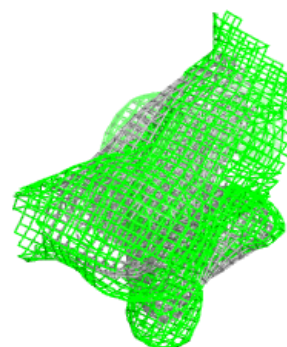
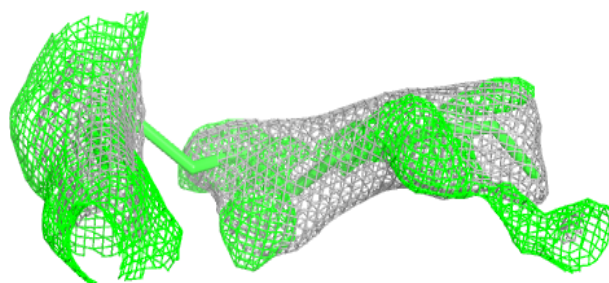
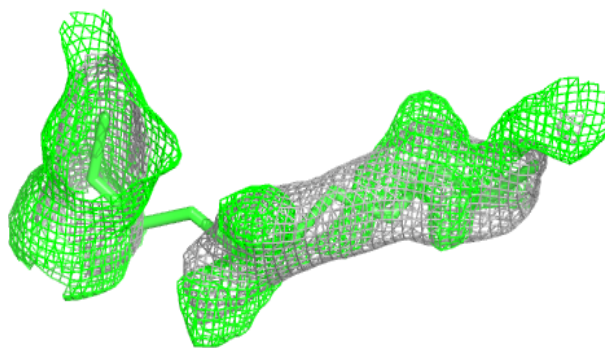


Electron density around DMU N 744:

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

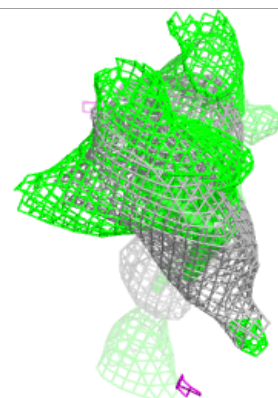
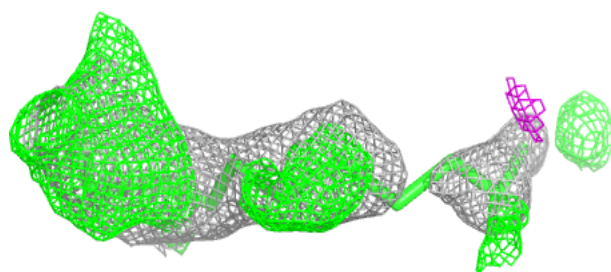
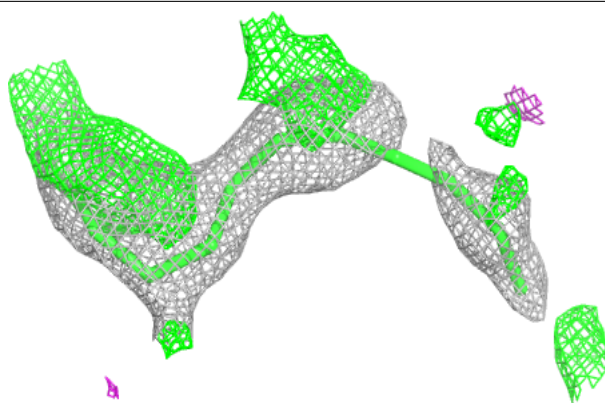
**Electron density around LFA C 624:**

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

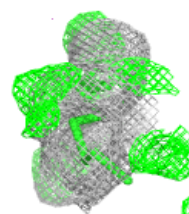
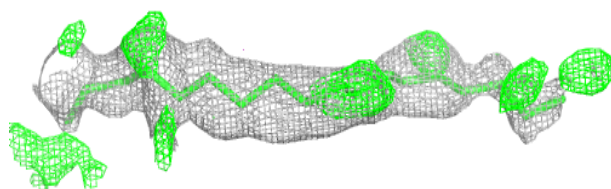
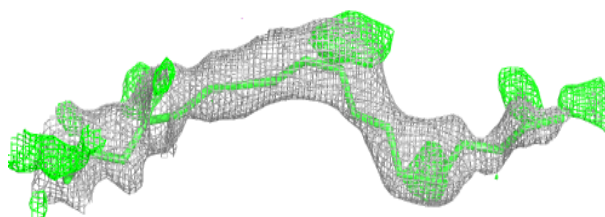


Electron density around LFA P 611:

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

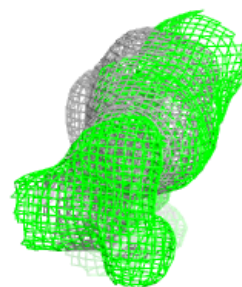
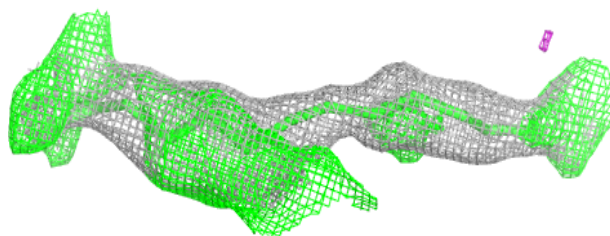
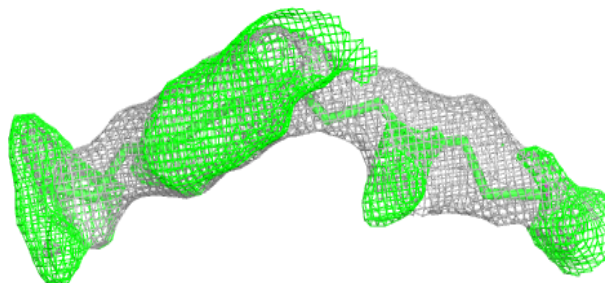
**Electron density around LFA C 716 (B):**

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

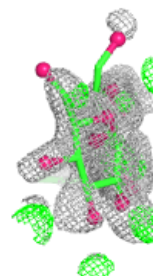
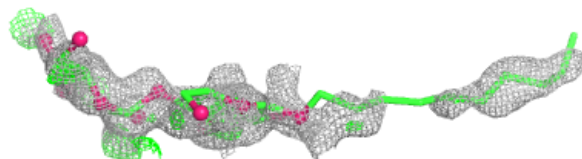
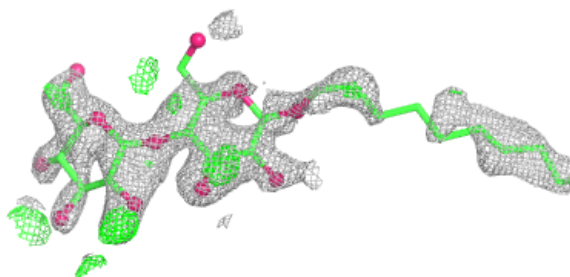


Electron density around LFA P 626:

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

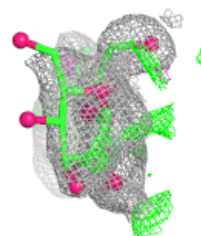
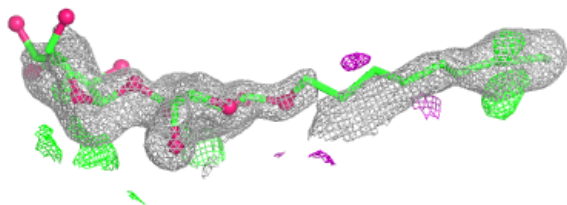
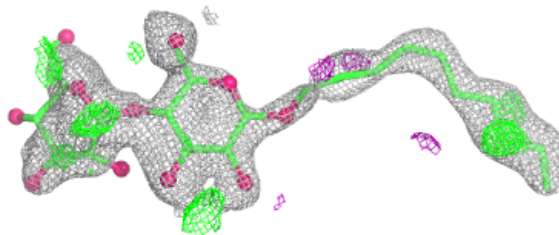
**Electron density around DMU C 734:**

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

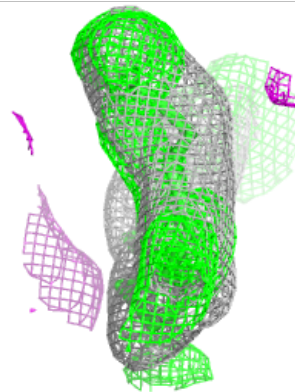
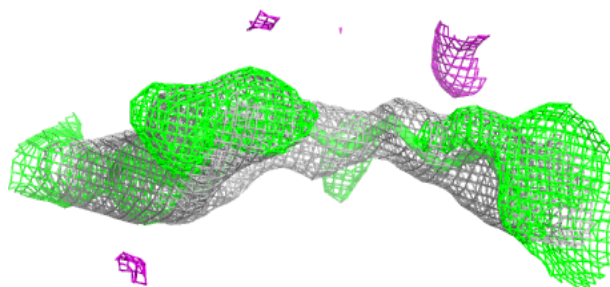
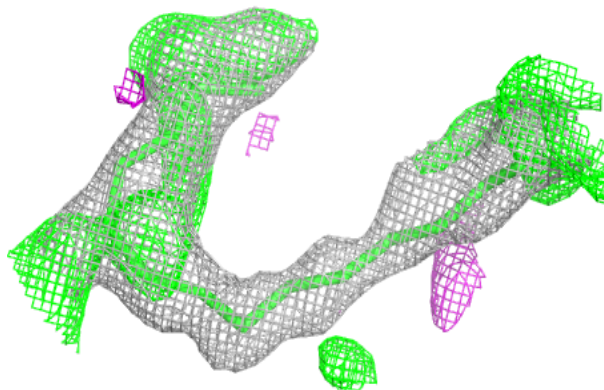


Electron density around DMU W 61:

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

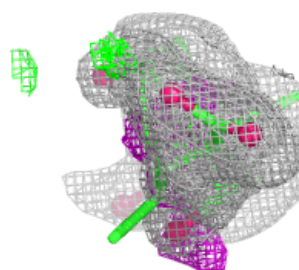
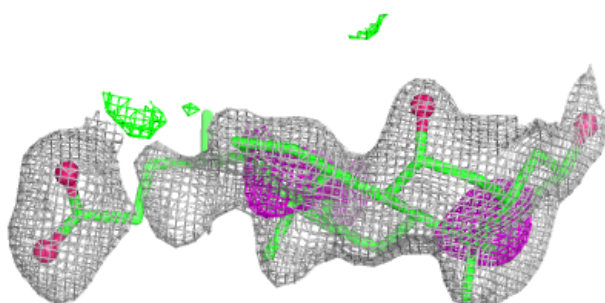
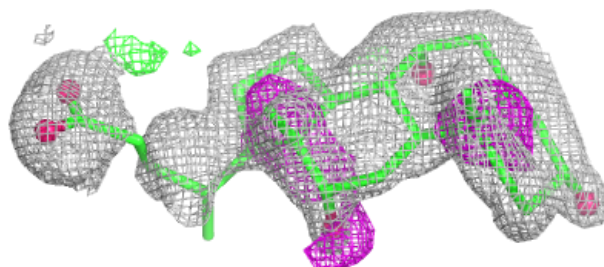
**Electron density around LFA A 628:**

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

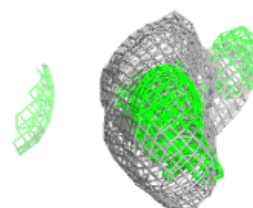
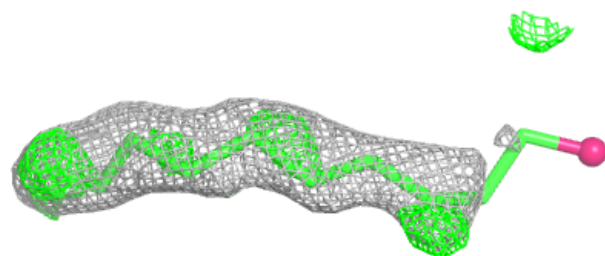
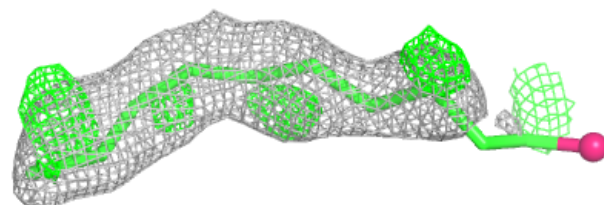


Electron density around CHD C 271:

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

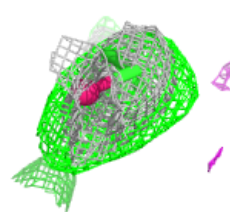
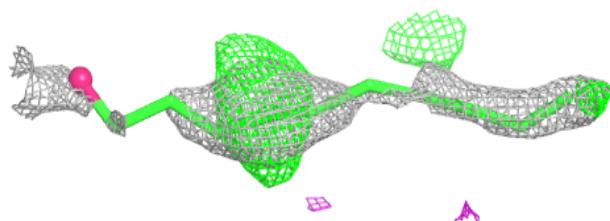
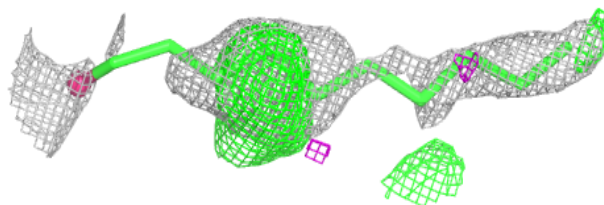
**Electron density around DMU J 732:**

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

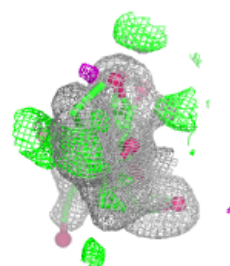
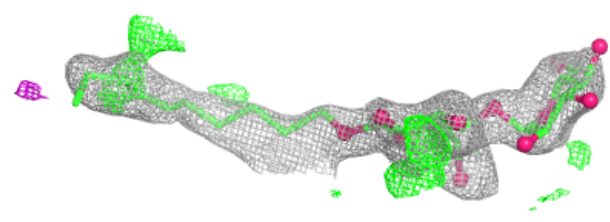
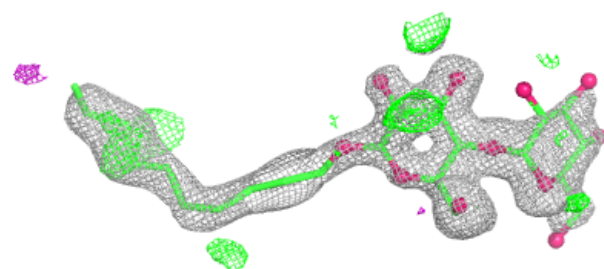


Electron density around DMU T 712:

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

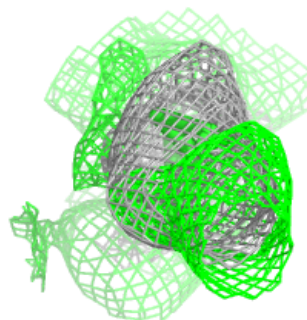
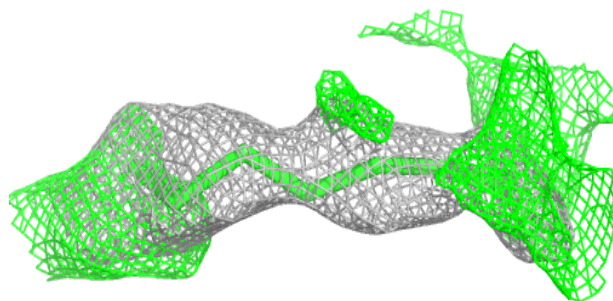
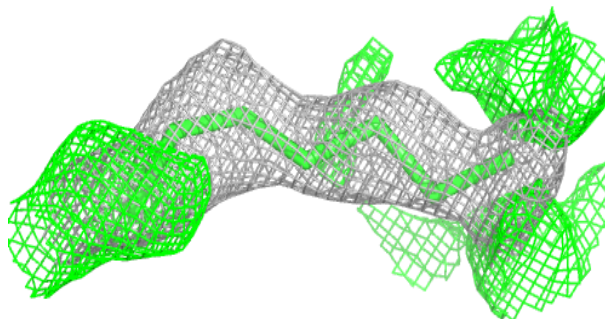
**Electron density around DMU J 61:**

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

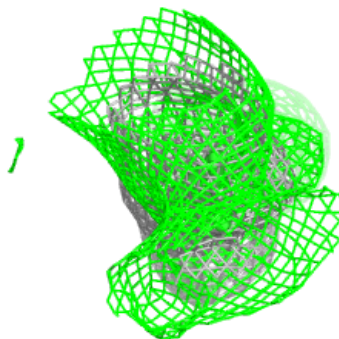
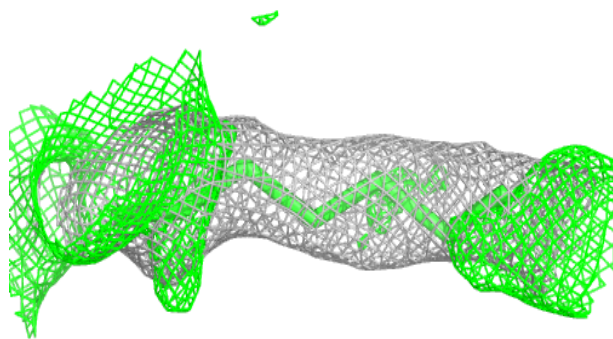
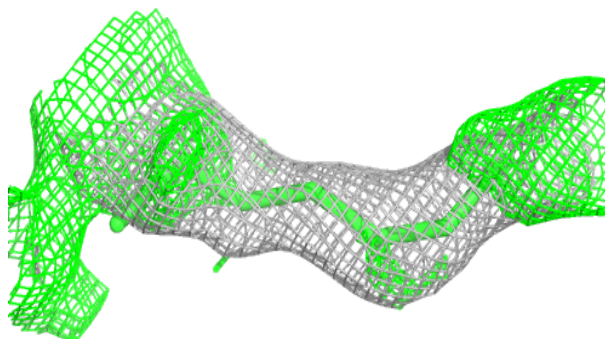


Electron density around DMU N 743:

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

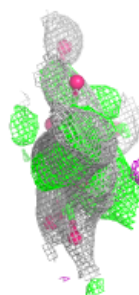
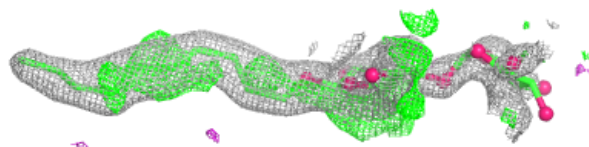
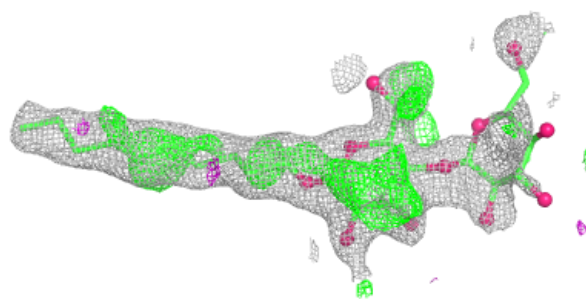
**Electron density around DMU A 743:**

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

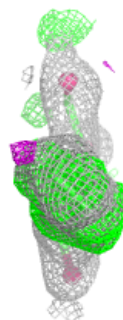
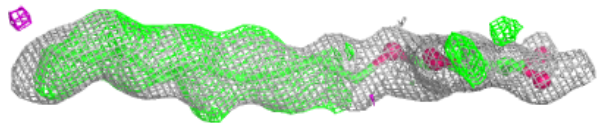
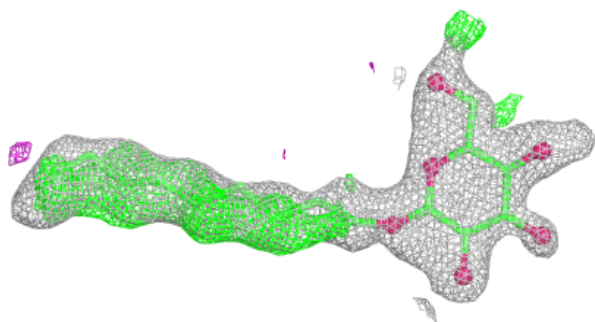


Electron density around DMU N 745:

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

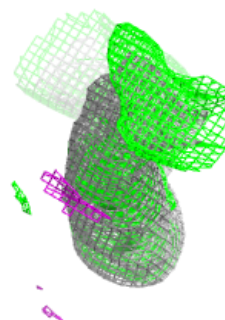
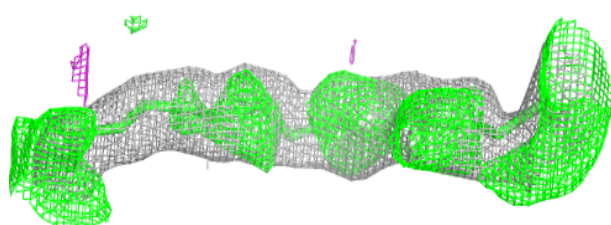
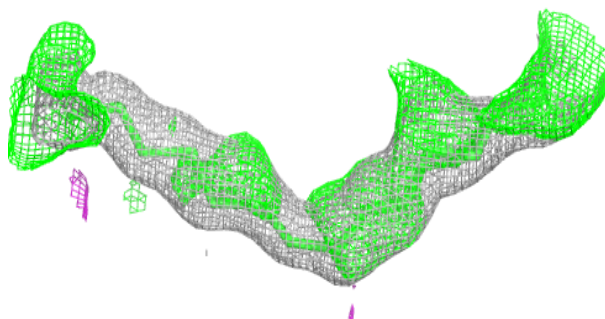
**Electron density around DMU O 742:**

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

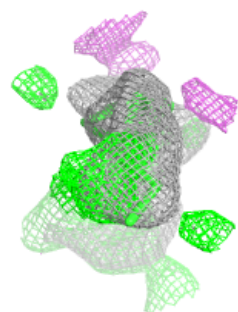
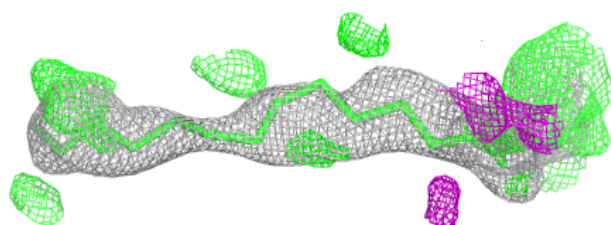
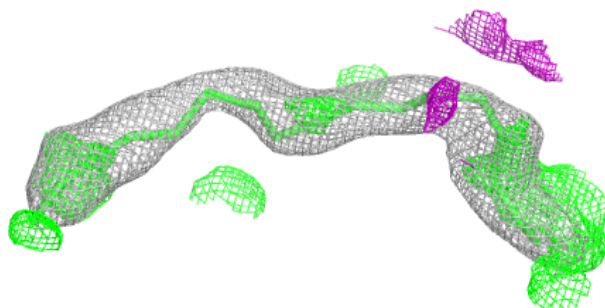


Electron density around LFA A 627:

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

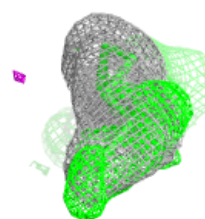
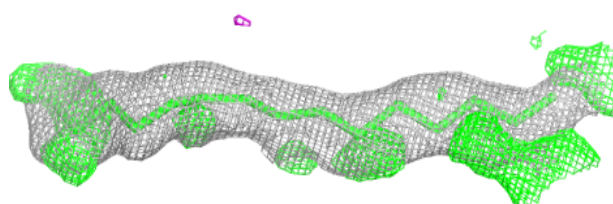
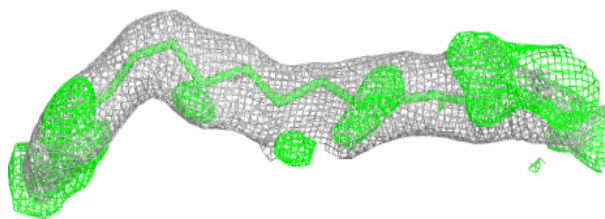
**Electron density around LFA G 621:**

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

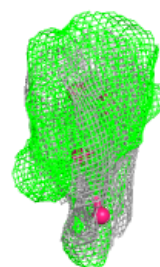
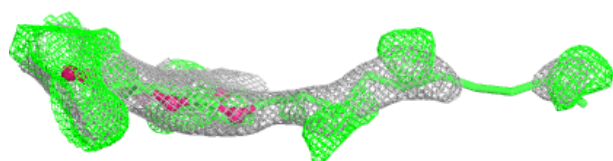
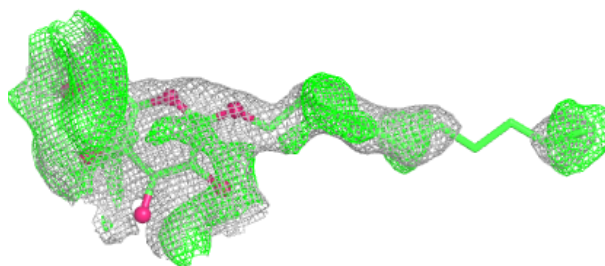


Electron density around LFA P 625:

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

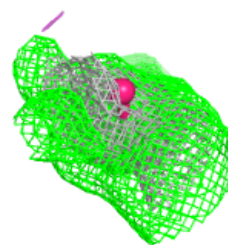
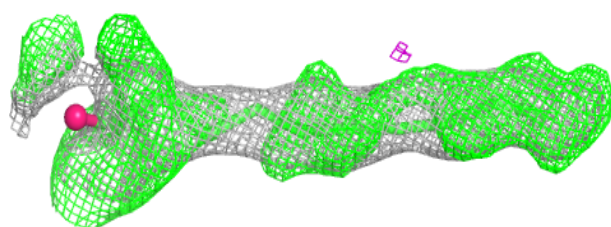
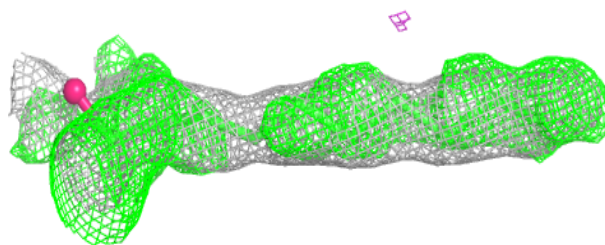
**Electron density around DMU Y 747:**

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

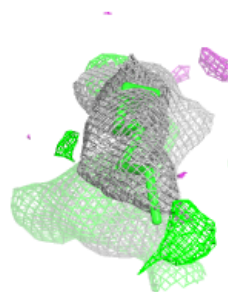
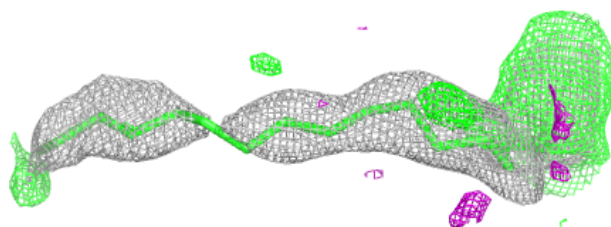
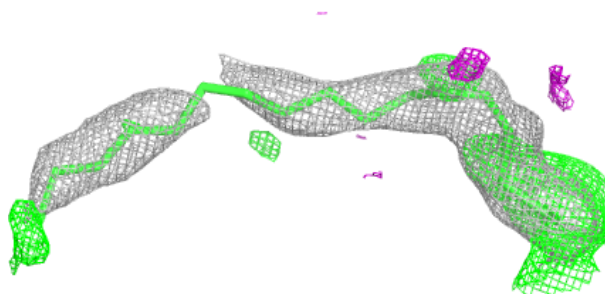


Electron density around DMU O 731:

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

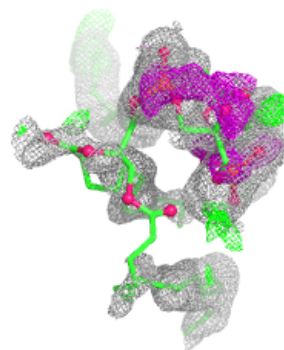
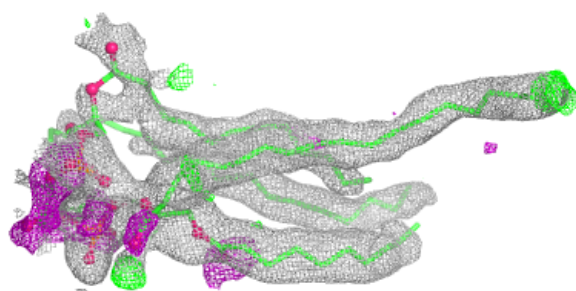
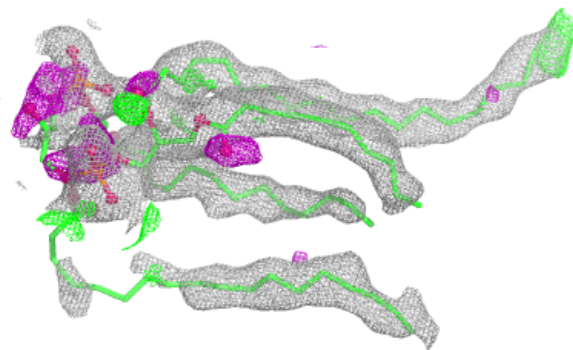
**Electron density around LFA T 621:**

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

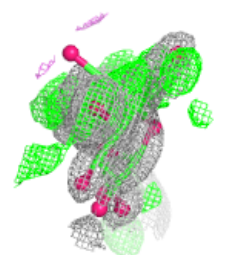
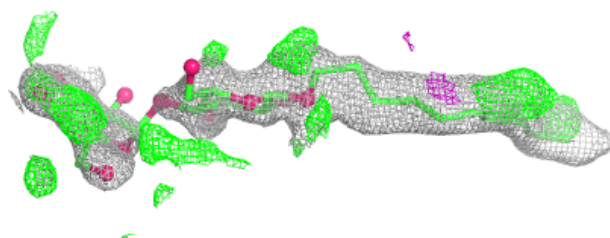
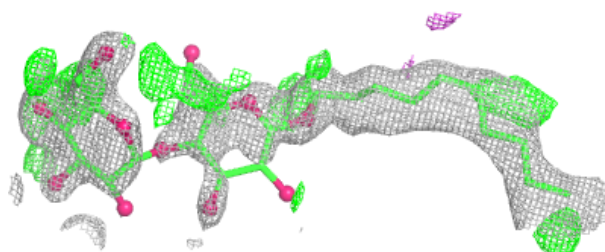


Electron density around CDL P 270:

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

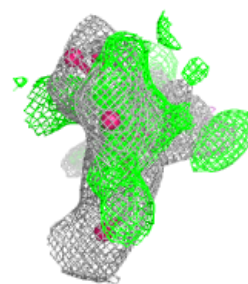
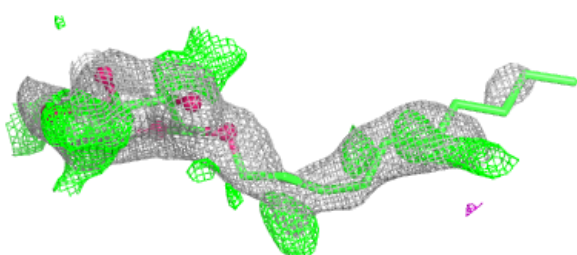
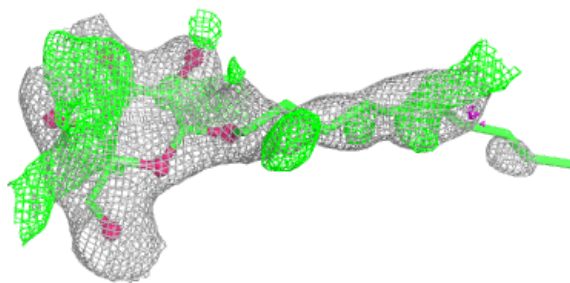
**Electron density around DMU C 715 (A):**

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

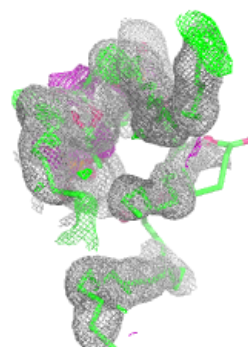
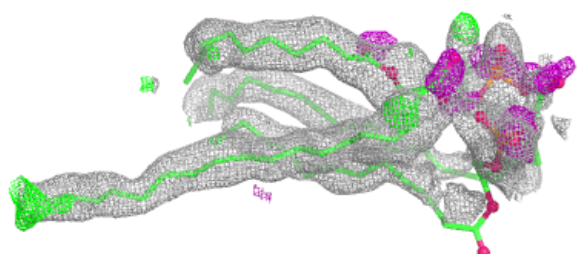
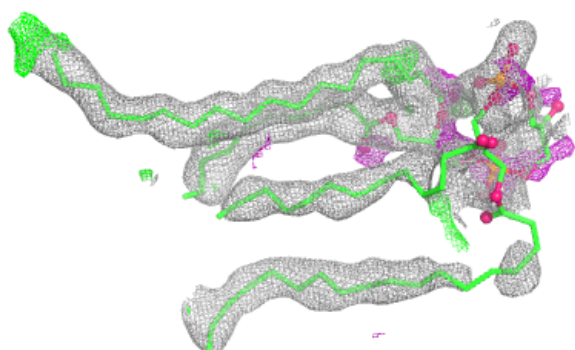


Electron density around DMU G 713:

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

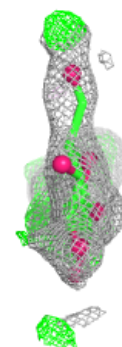
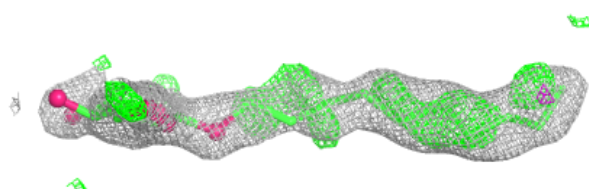
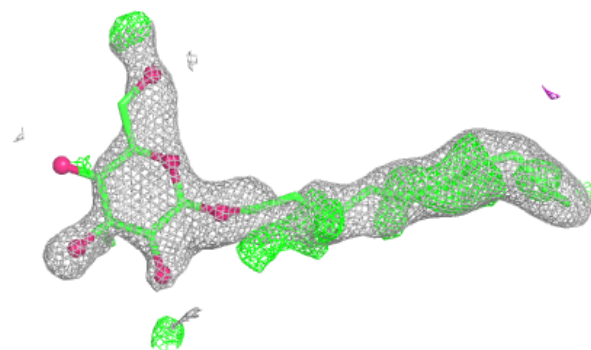
**Electron density around CDL C 270:**

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

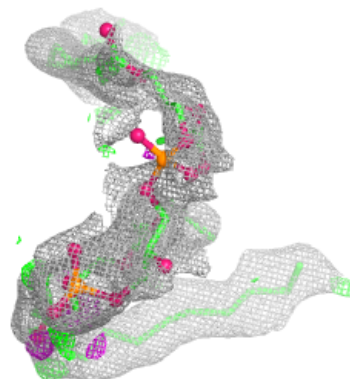
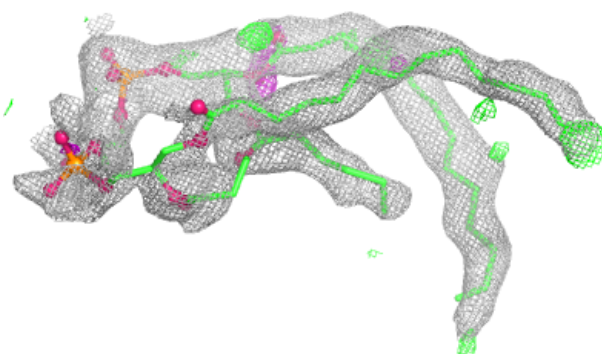
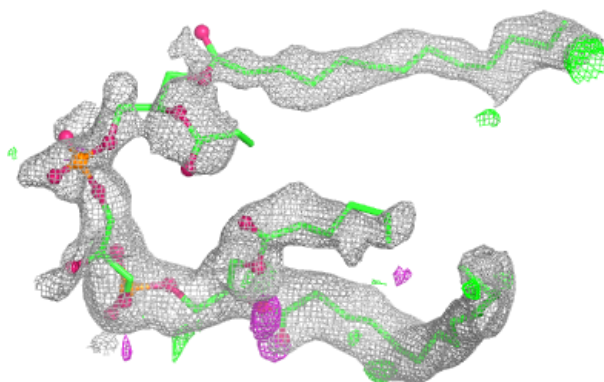


Electron density around DMU B 742:

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

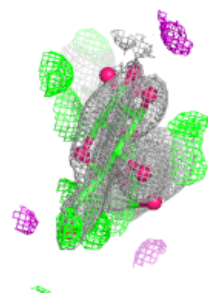
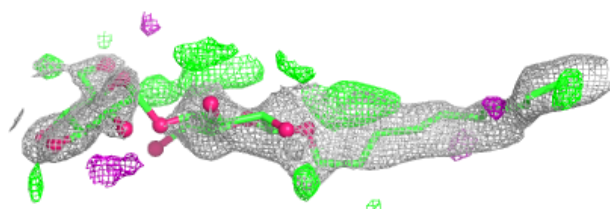
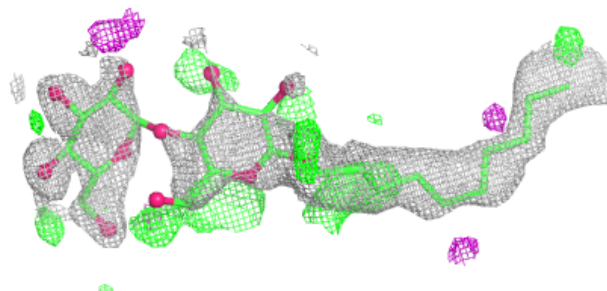
**Electron density around CDL N 522:**

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

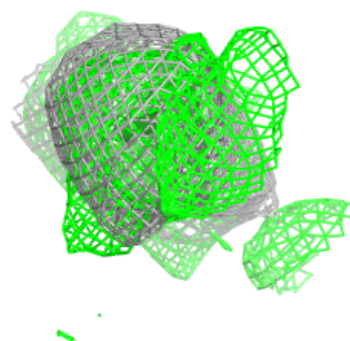
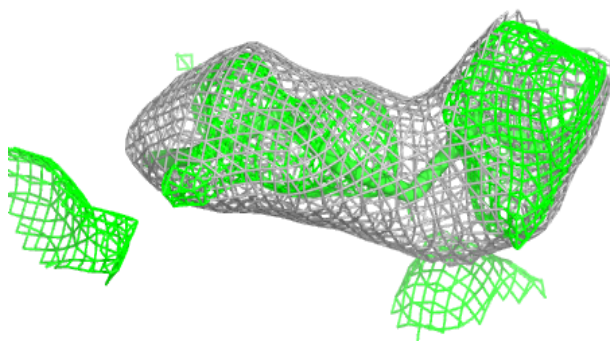
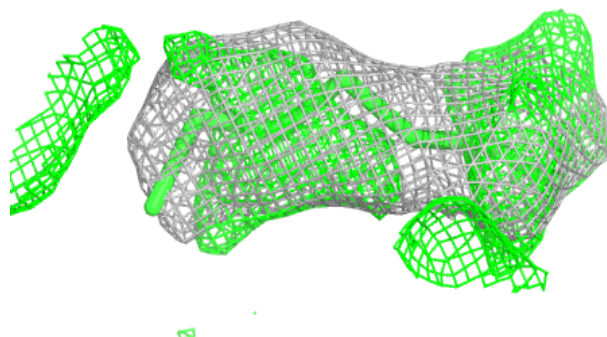


Electron density around DMU P 715 (A):

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

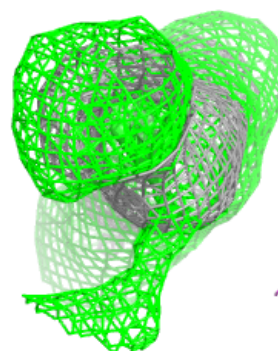
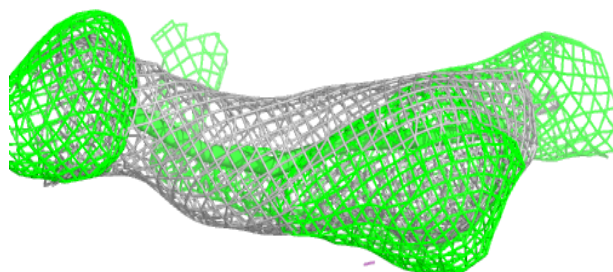
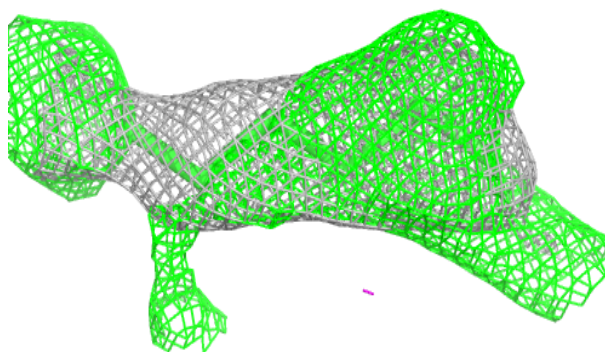
**Electron density around DMU P 721:**

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

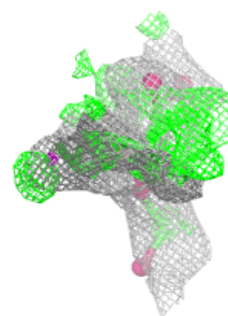
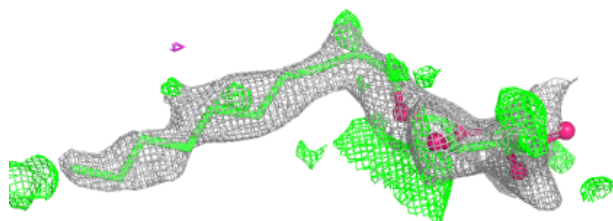
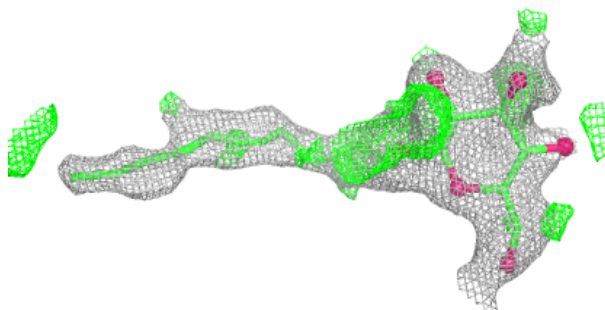


Electron density around LFA P 612:

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

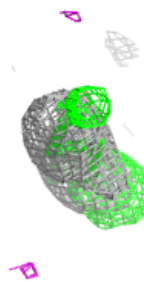
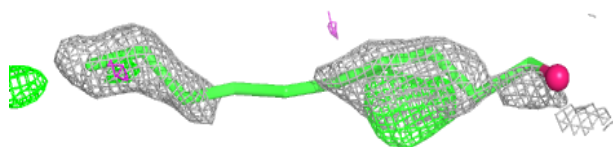
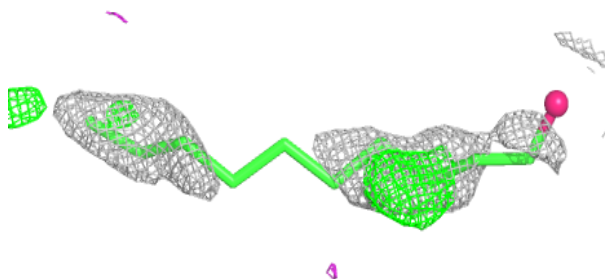
**Electron density around DMU T 713:**

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

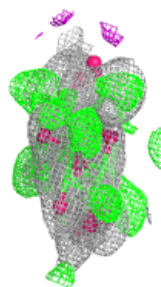
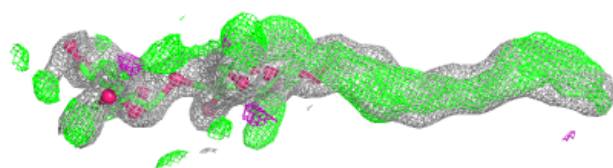
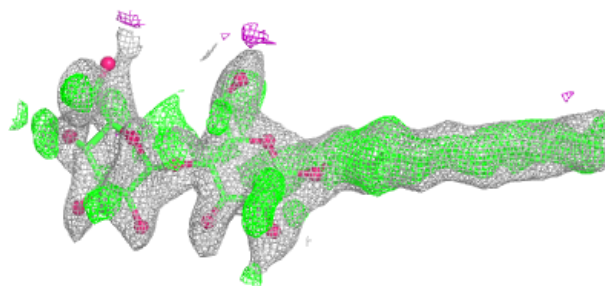


Electron density around DMU G 712:

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

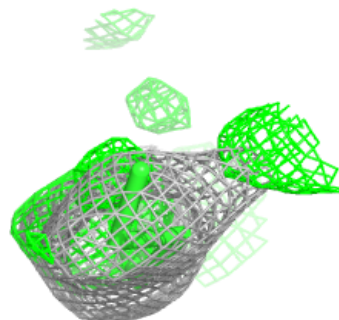
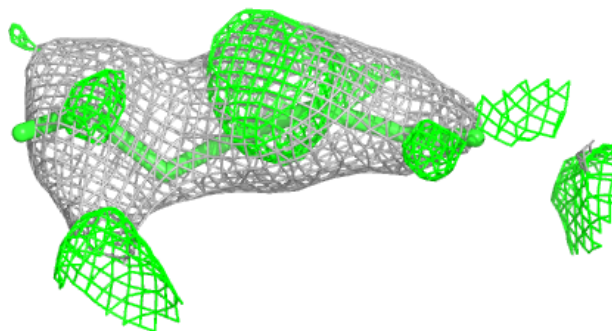
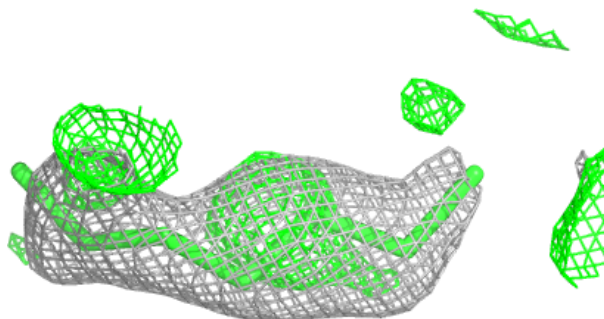
**Electron density around DMU A 745:**

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



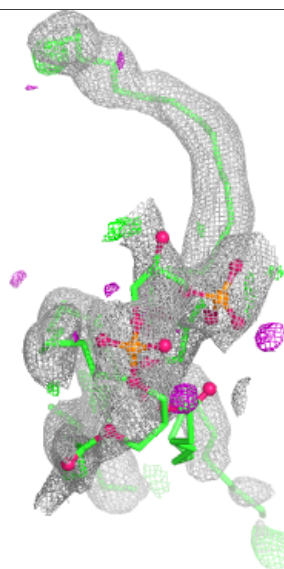
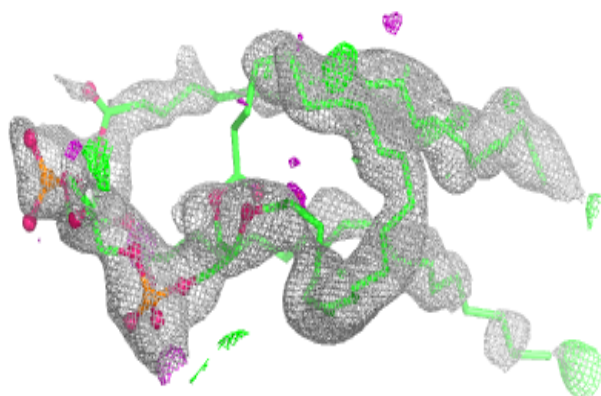
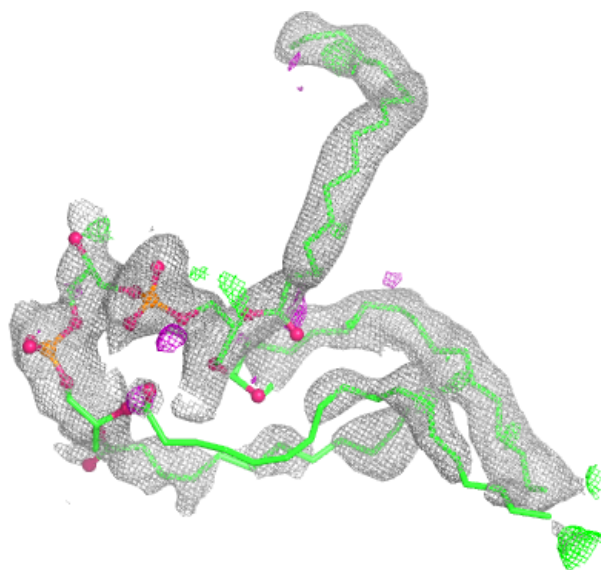
Electron density around DMU C 721:

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



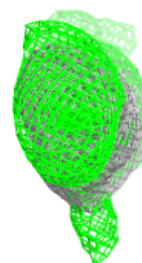
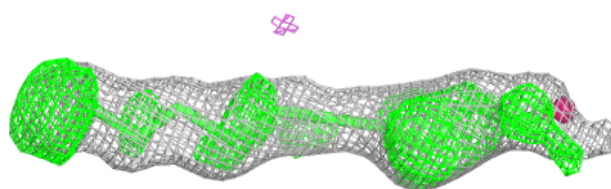
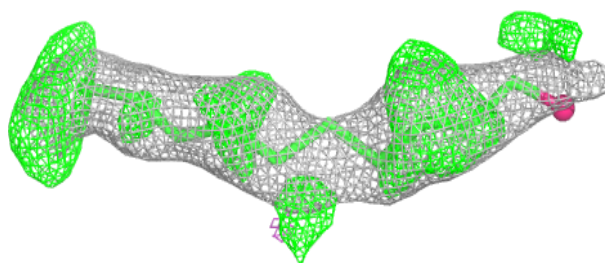
Electron density around CDL N 521:

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

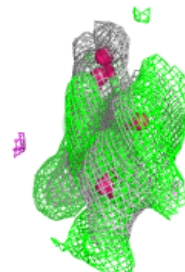
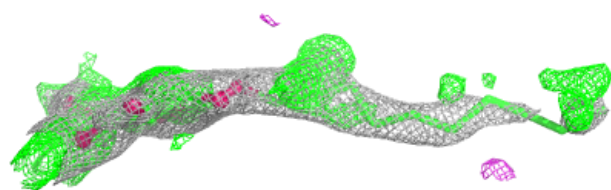
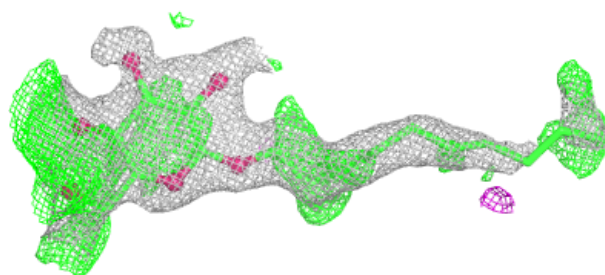


Electron density around DMU O 741:

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

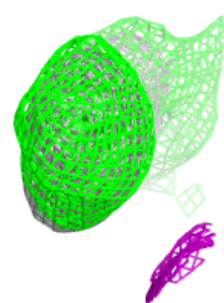
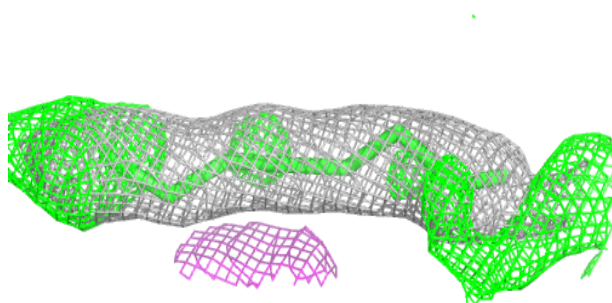
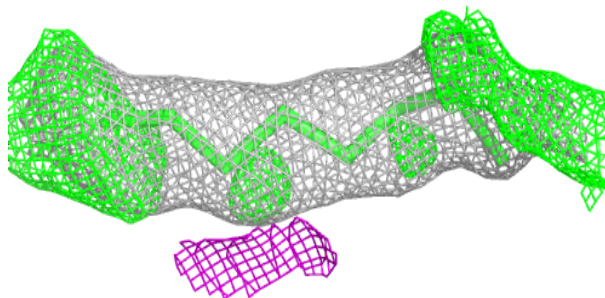
**Electron density around DMU L 747:**

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

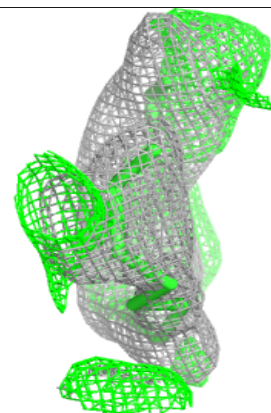
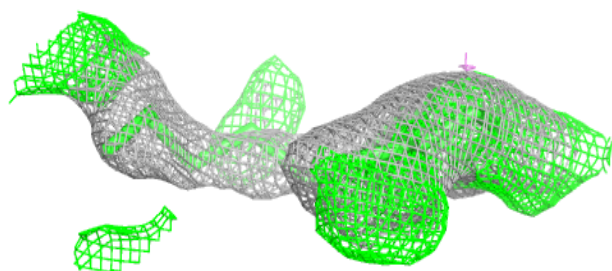
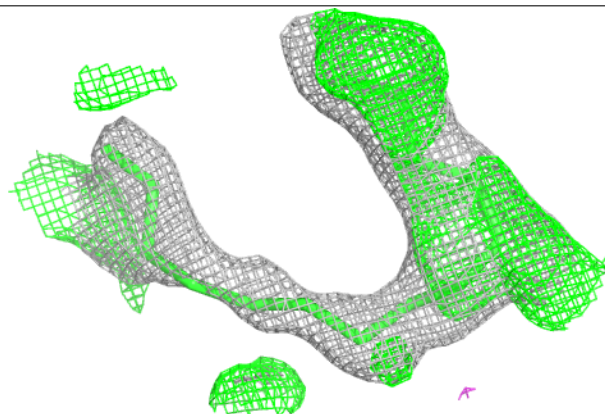


Electron density around DMU M 746:

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

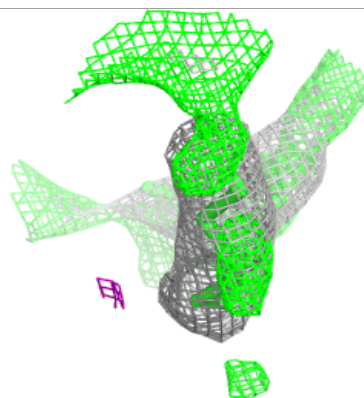
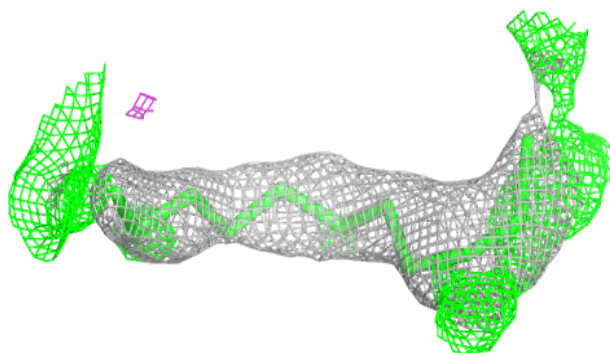
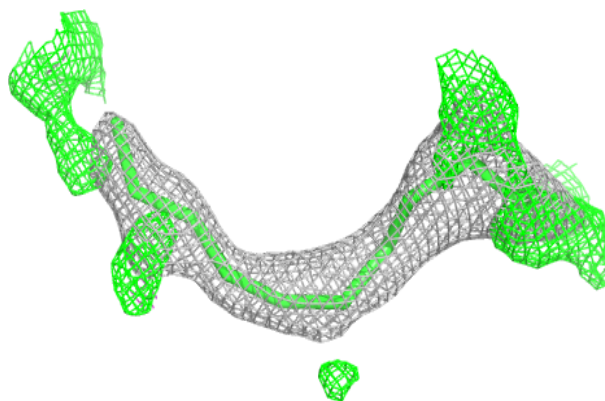
**Electron density around LFA N 628:**

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

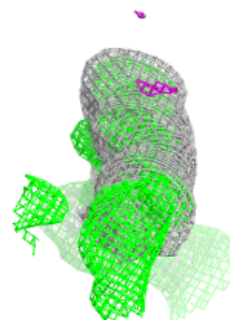
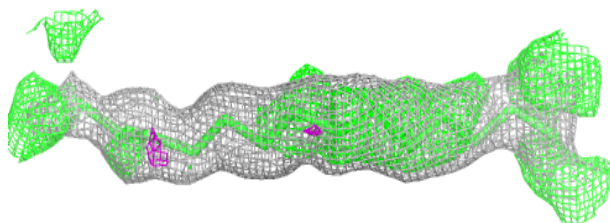
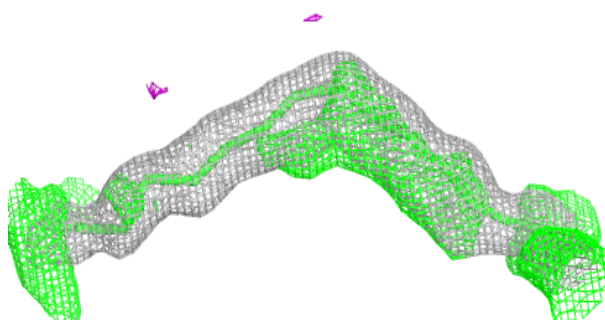


Electron density around LFA C 611:

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

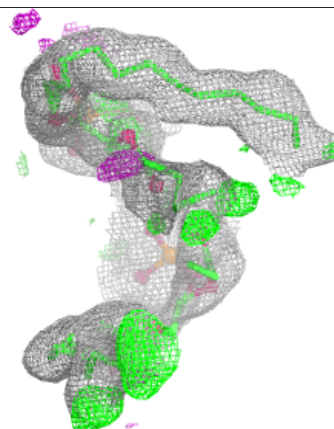
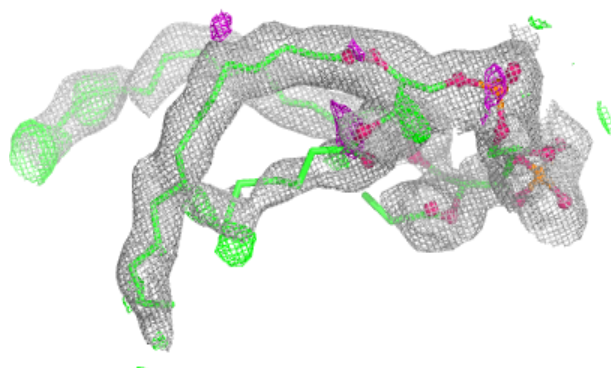
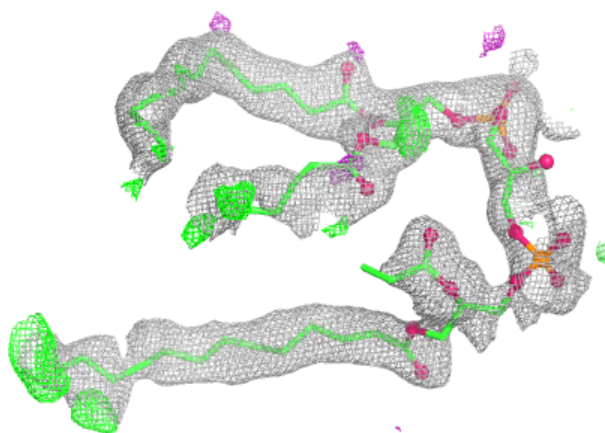
**Electron density around LFA N 627:**

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

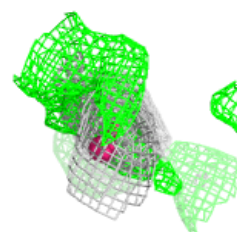
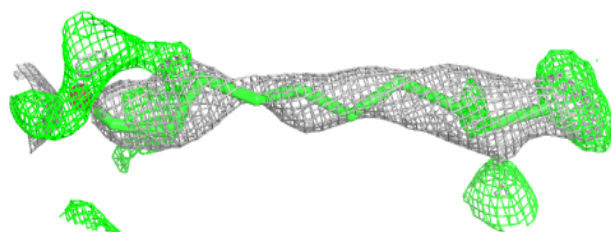
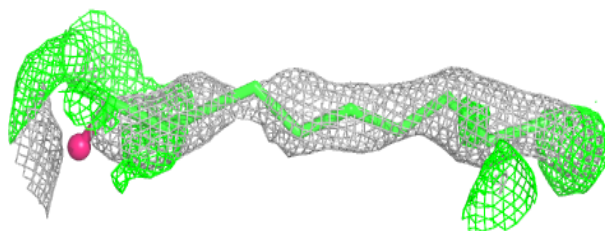


Electron density around CDL A 522:

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

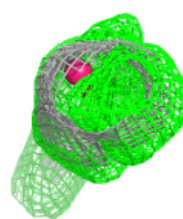
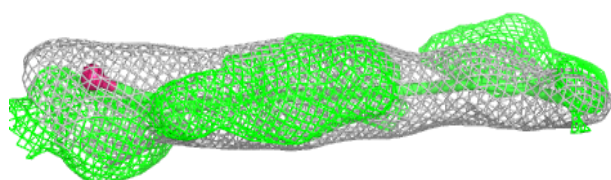
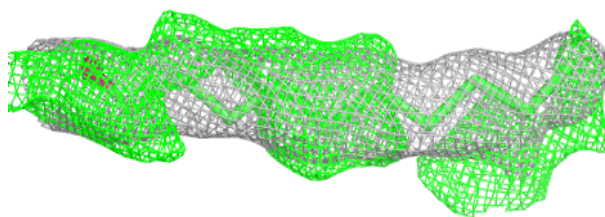
**Electron density around DMU B 731:**

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

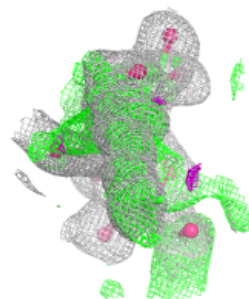
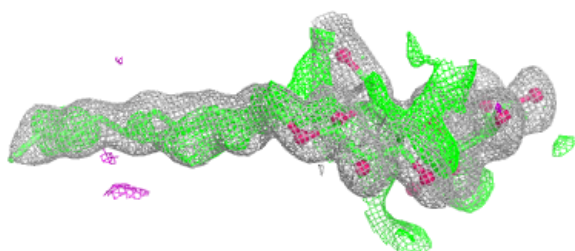
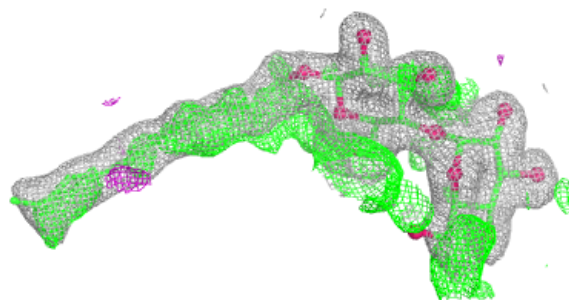


Electron density around DMU P 272:

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

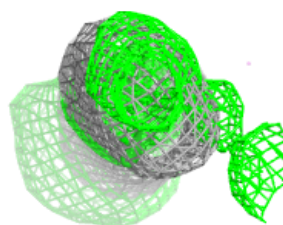
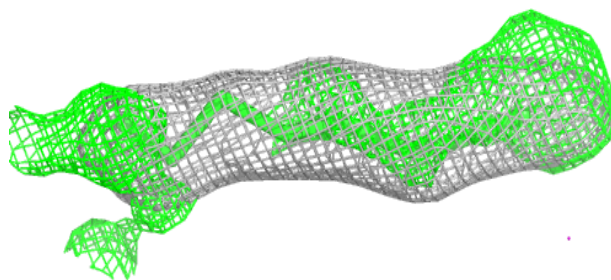
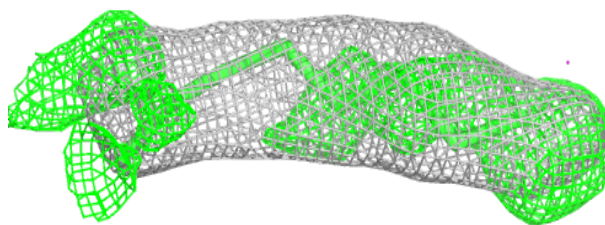
**Electron density around DMU A 744:**

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



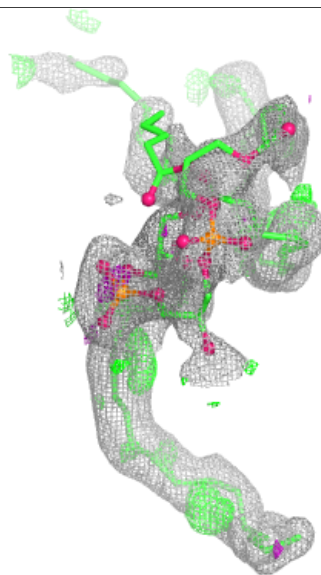
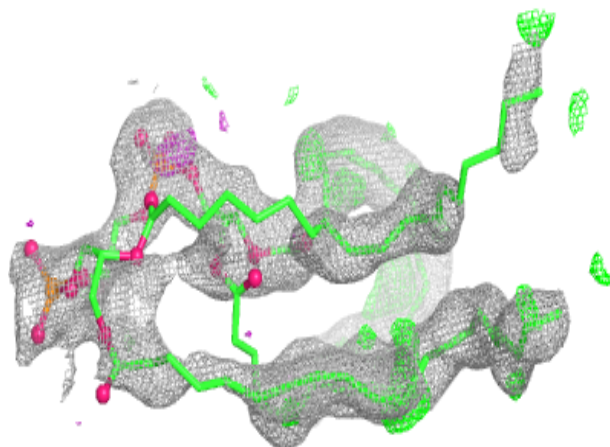
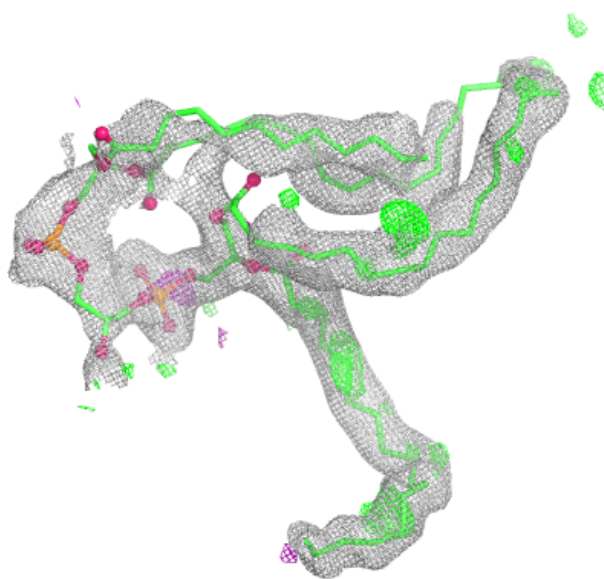
Electron density around DMU Z 746:

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



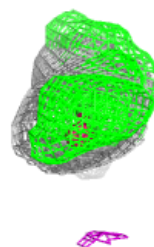
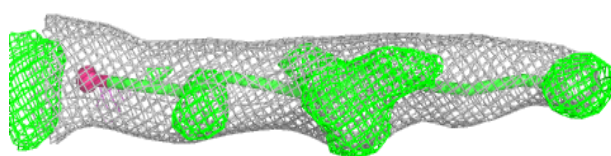
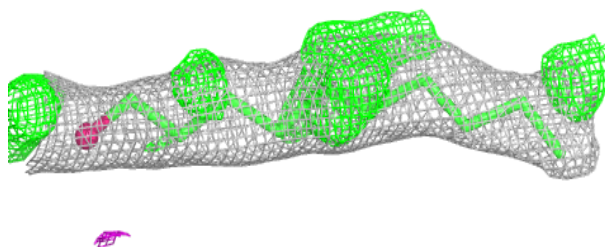
Electron density around CDL A 521:

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

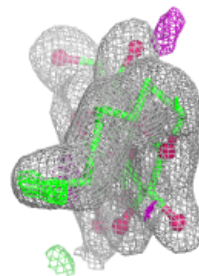
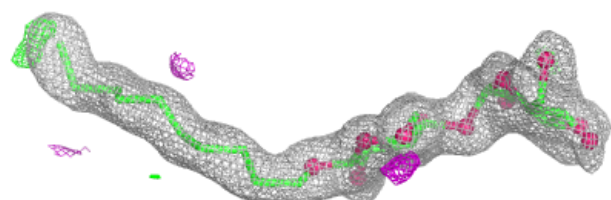
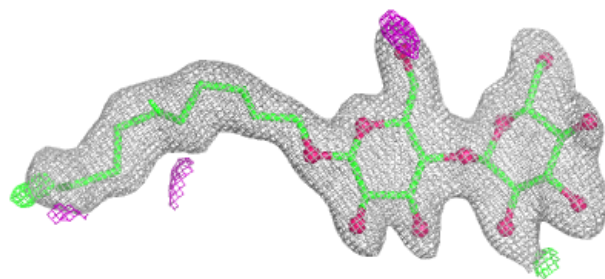


Electron density around DMU C 272:

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

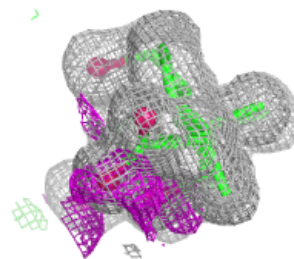
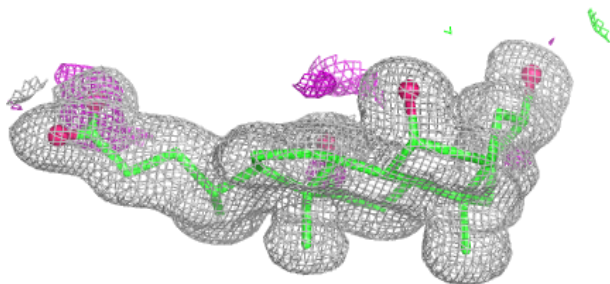
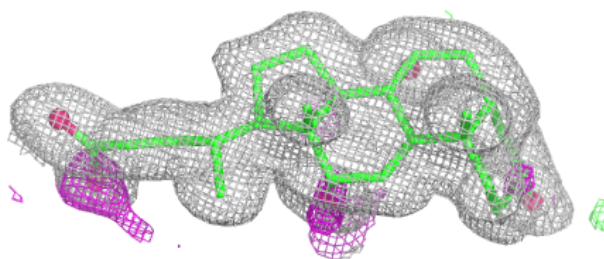
**Electron density around DMU N 526:**

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

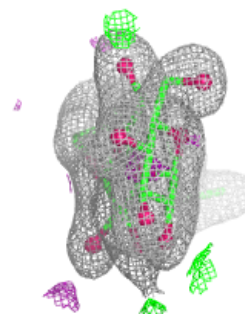
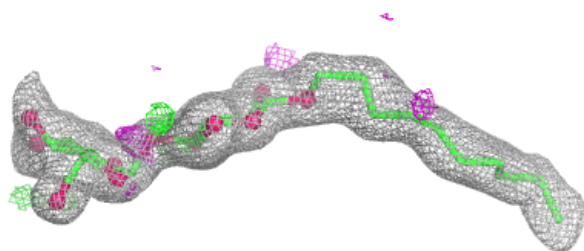
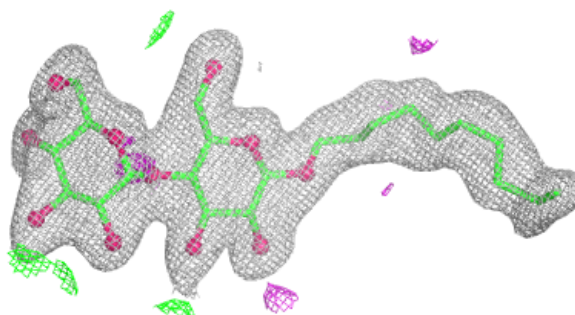


Electron density around CHD A 525:

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

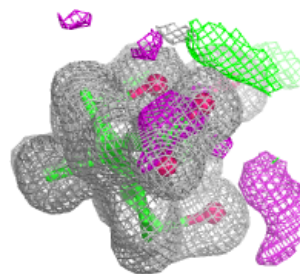
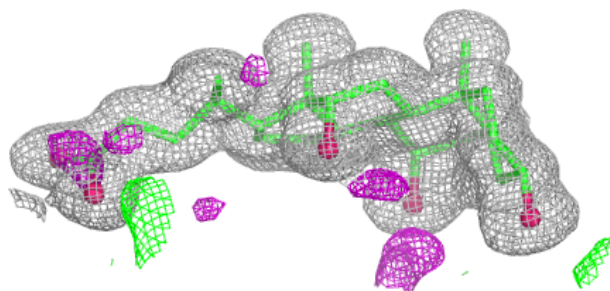
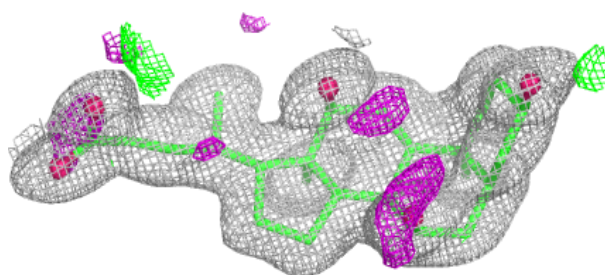
**Electron density around DMU A 526:**

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

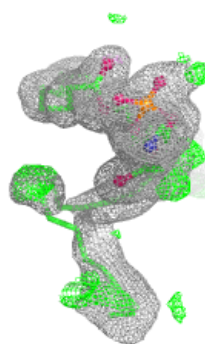
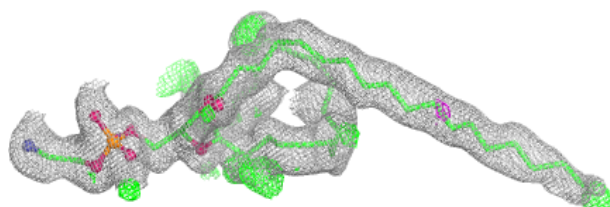
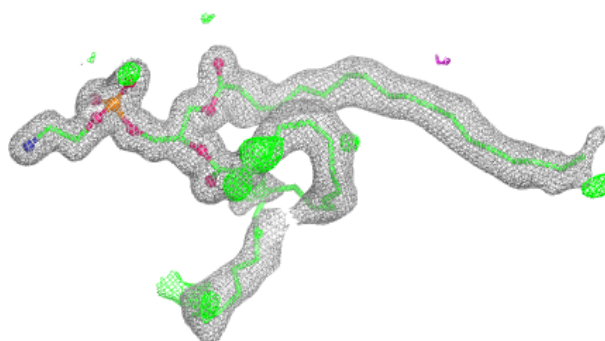


Electron density around CHD N 525:

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

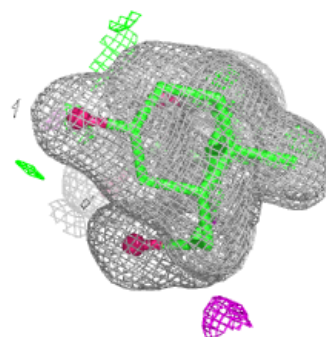
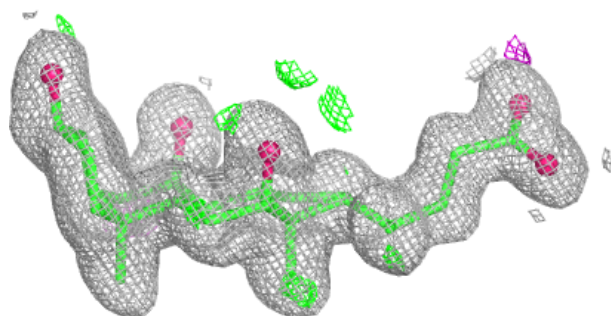
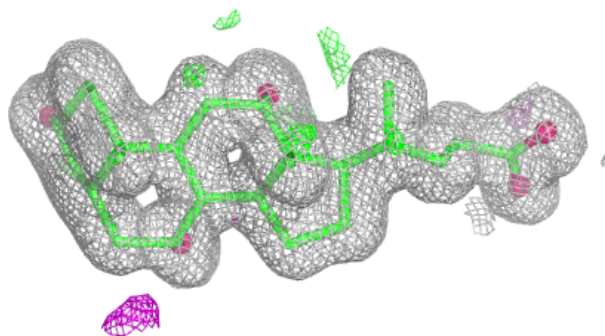
**Electron density around PEK P 264:**

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

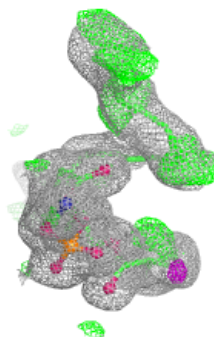
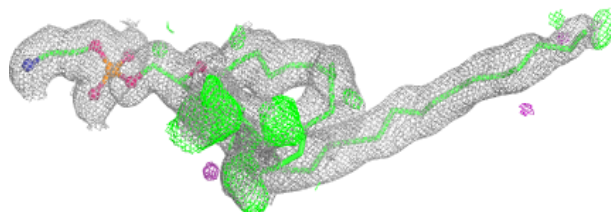
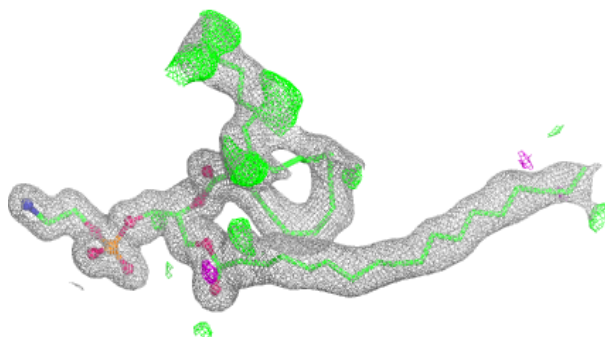


Electron density around CHD G 86:

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

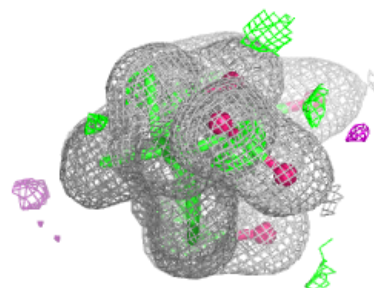
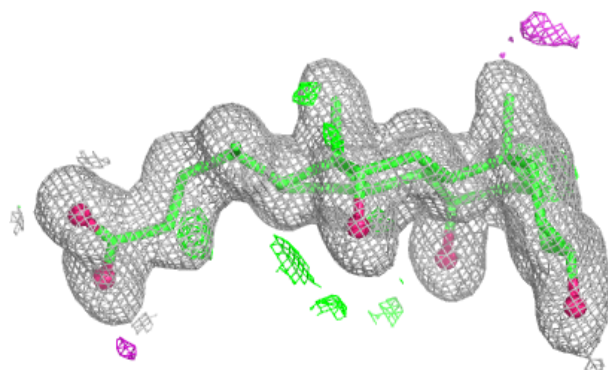
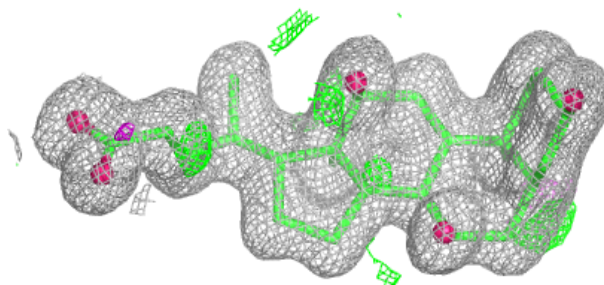
**Electron density around PEK C 264:**

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

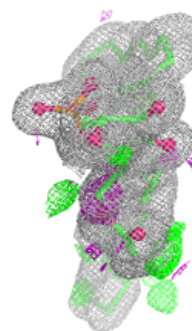
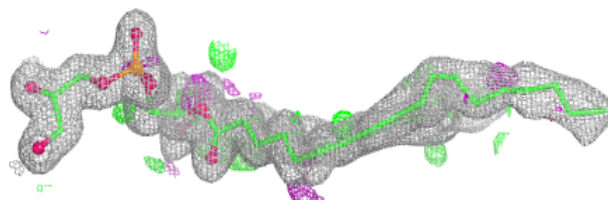
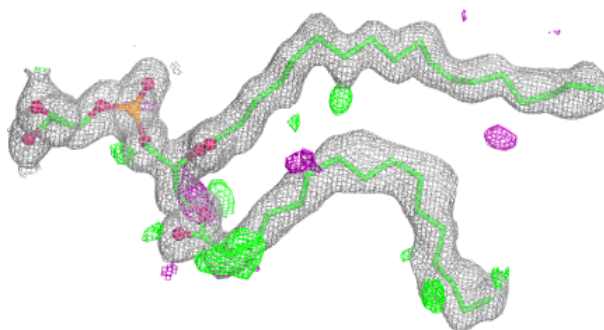


Electron density around CHD T 86:

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

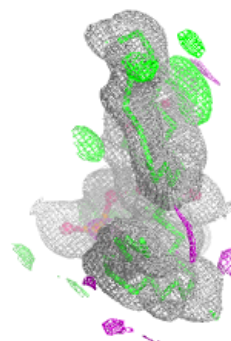
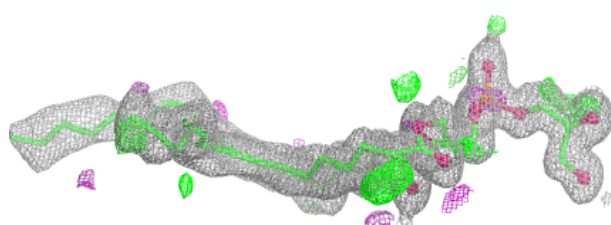
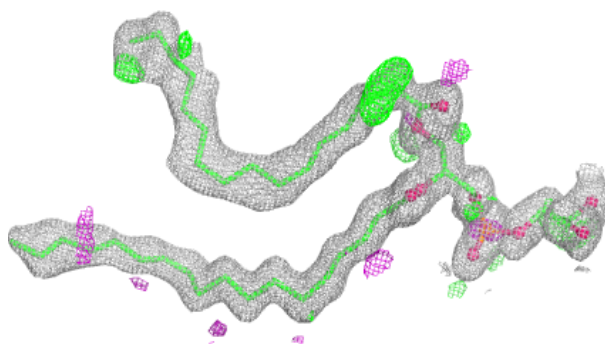
**Electron density around PGV P 266:**

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

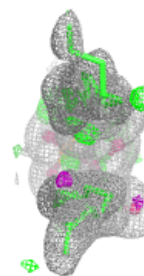
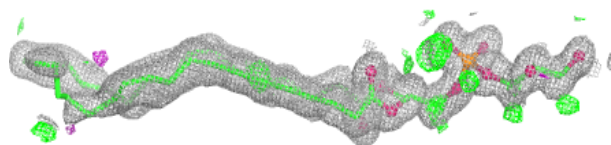
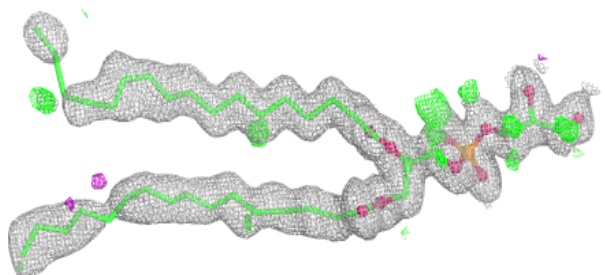


Electron density around PGV C 266:

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

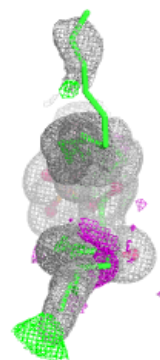
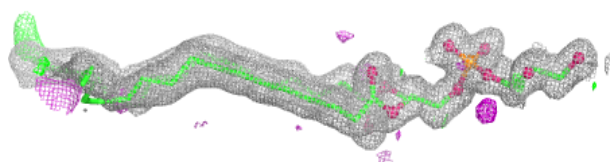
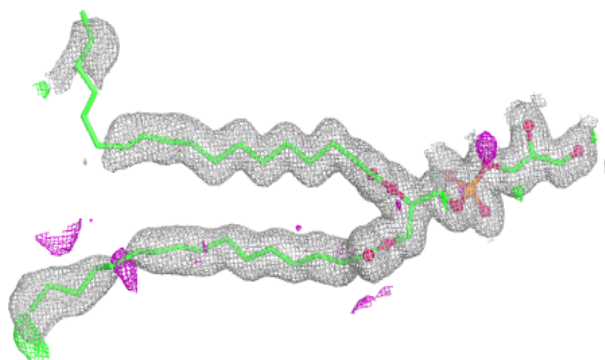
**Electron density around PGV C 267:**

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

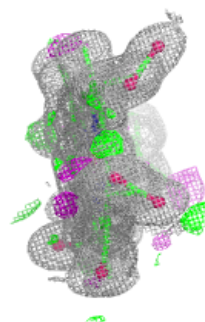
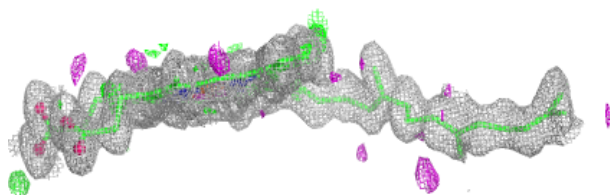
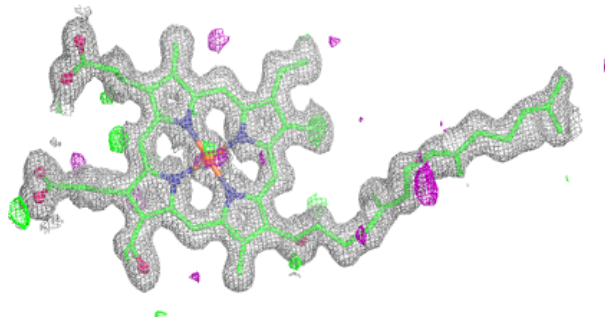


Electron density around PGV P 267:

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

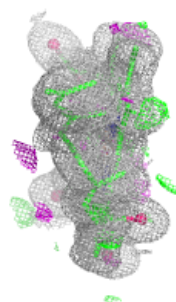
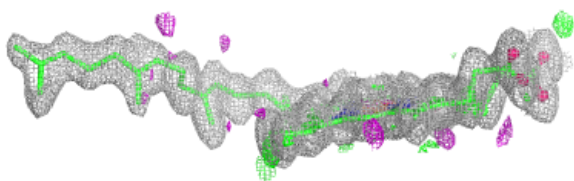
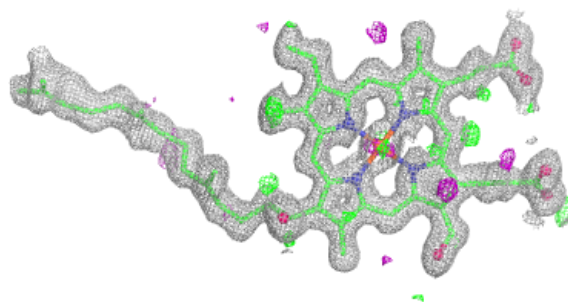
**Electron density around HEA A 515 (A):**

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

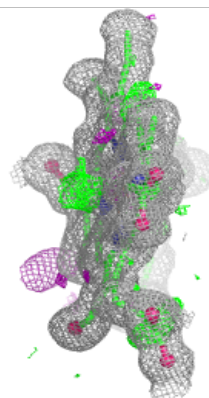
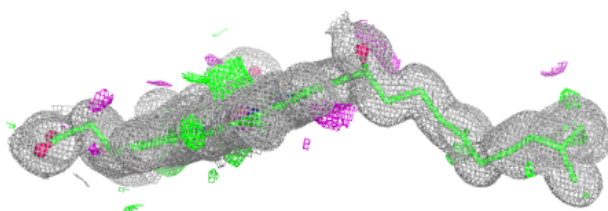
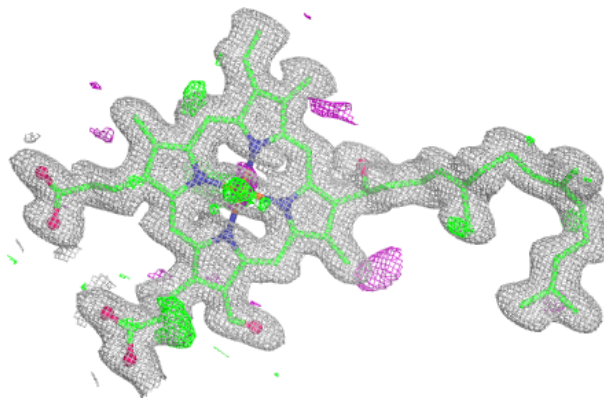


Electron density around HEA A 515 (B):

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

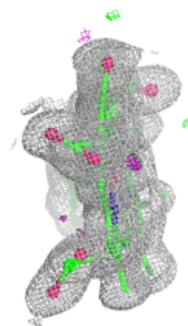
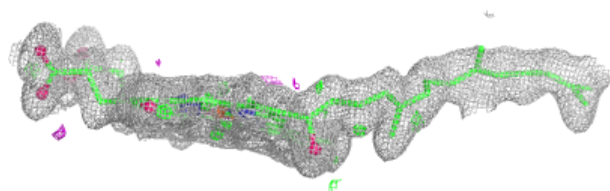
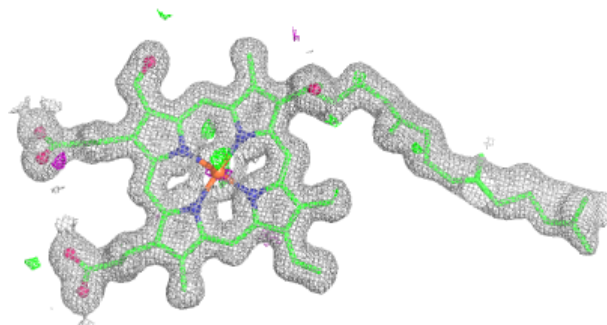
**Electron density around HEA A 516:**

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

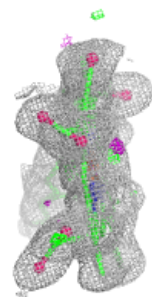
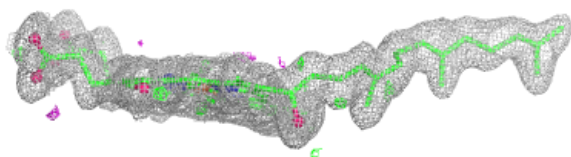
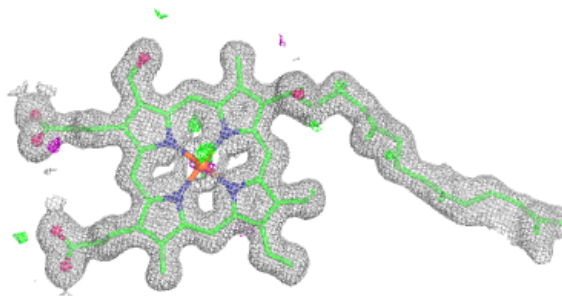


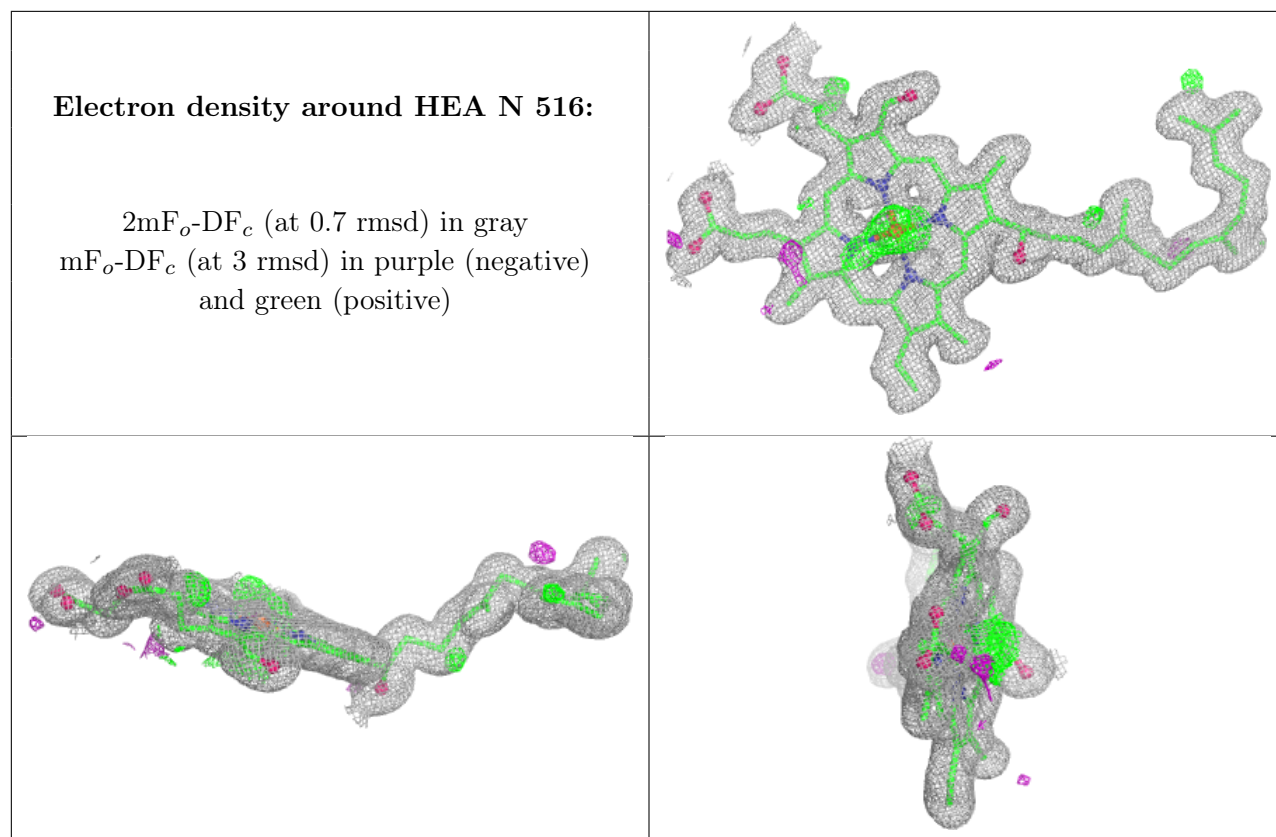
Electron density around HEA N 515 (A):

$2mF_o-DF_c$ (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.