



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2021 – 06:29 PM JST

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

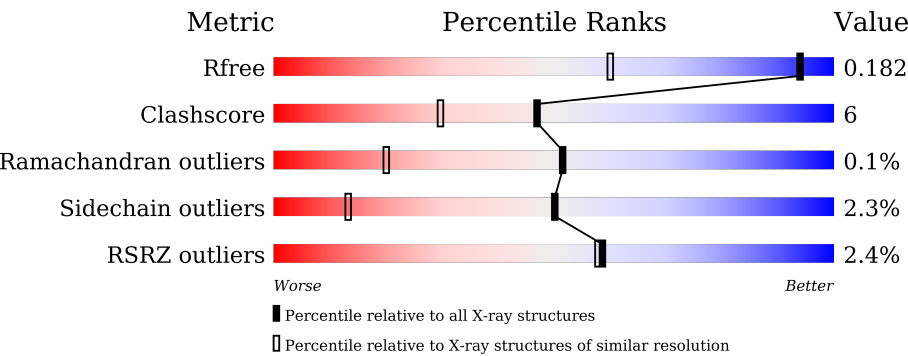
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.30 Å.

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



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

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

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	516	X	-	-	-
14	HEA	N	516	X	-	-	-

## 2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 33049 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

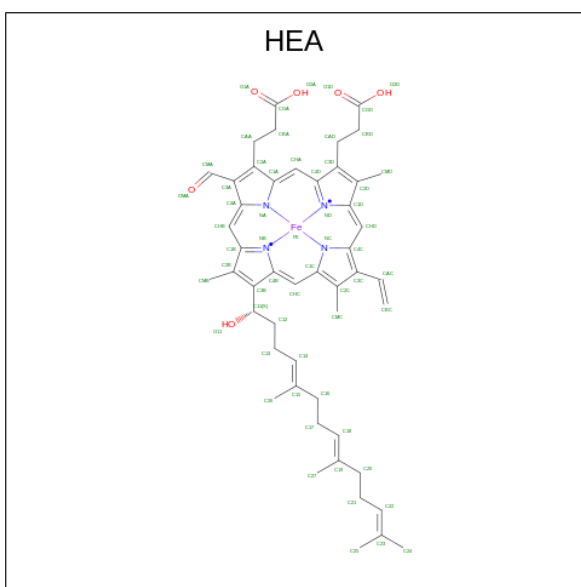
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



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

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

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

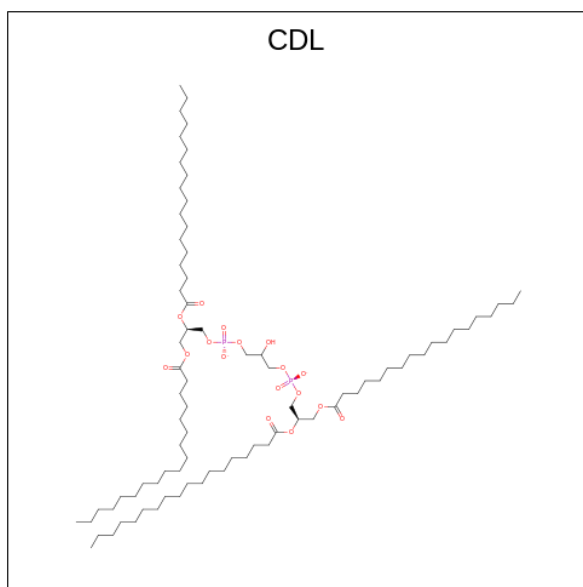
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

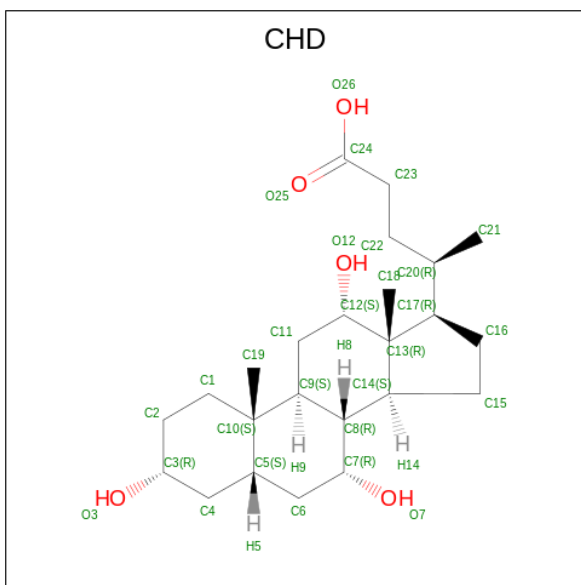
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

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



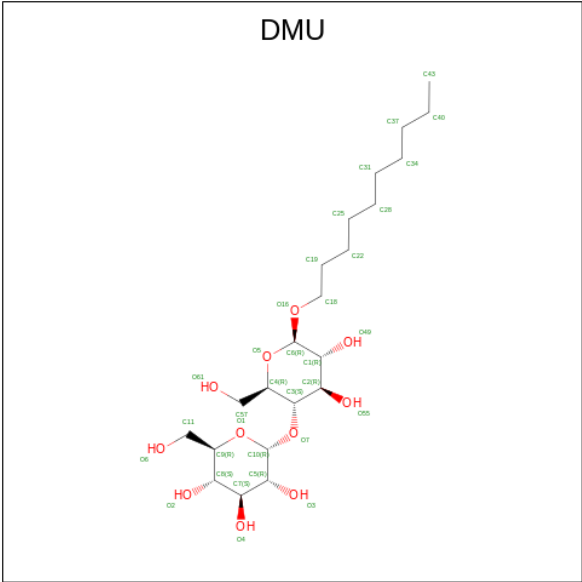
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			94	75	17	2		
18	A	1	Total	C	O	P	0	0
			64	45	17	2		
18	C	1	Total	C	O	P	0	0
			87	68	17	2		
18	N	1	Total	C	O	P	0	0
			94	75	17	2		
18	N	1	Total	C	O	P	0	0
			64	45	17	2		
18	P	1	Total	C	O	P	0	0
			87	68	17	2		

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



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

- Molecule 20 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: 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	0	0
			33	22	11		
20	A	1	Total	C		0	0
			7	7			
20	A	1	Total	C	O	0	0
			33	22	11		
20	A	1	Total	C	O	0	0
			33	22	11		
20	B	1	Total	C	O	0	0
			11	10	1		
20	B	1	Total	C	O	0	0
			11	10	1		
20	B	1	Total	C	O	0	0
			22	16	6		
20	C	1	Total	C	O	0	0
			33	22	11		
20	C	1	Total	C	O	0	1
			33	22	11		
20	C	1	Total	C		0	0
			7	7			
20	C	1	Total	C	O	0	0
			22	16	6		
20	C	1	Total	C	O	0	0
			33	22	11		
20	C	1	Total	C	O	0	0
			33	22	11		
20	C	1	Total	C	O	0	0
			11	10	1		

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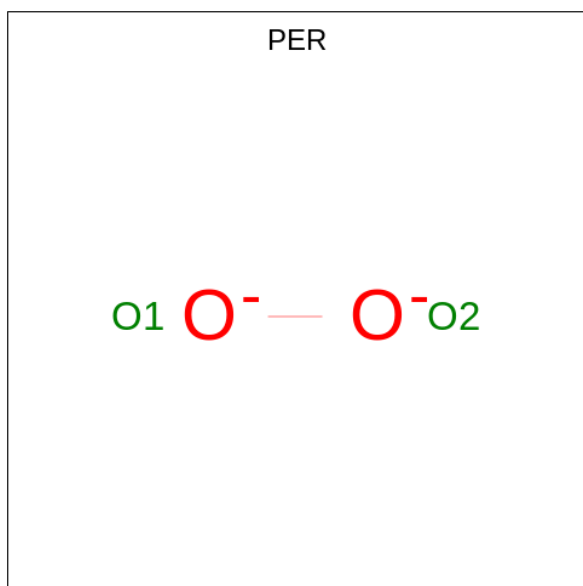
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	G	1	Total C O 22 16 6	0	0
20	G	1	Total C O 11 10 1	0	0
20	G	1	Total C O 22 16 6	0	0
20	J	1	Total C O 11 10 1	0	0
20	J	1	Total C O 33 22 11	0	0
20	L	1	Total C O 22 16 6	0	0
20	M	1	Total C 8 8	0	0
20	N	1	Total C O 33 22 11	0	0
20	N	1	Total C 7 7	0	0
20	N	1	Total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

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

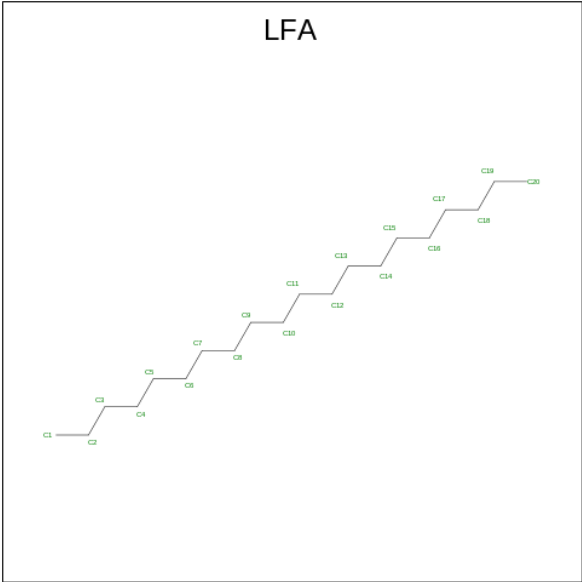
- Molecule 21 is PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



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

- Molecule 22 is EICOSANE (three-letter code: LFA) (formula: C<sub>20</sub>H<sub>42</sub>) (labeled as "Ligand of Interest" by depositor).





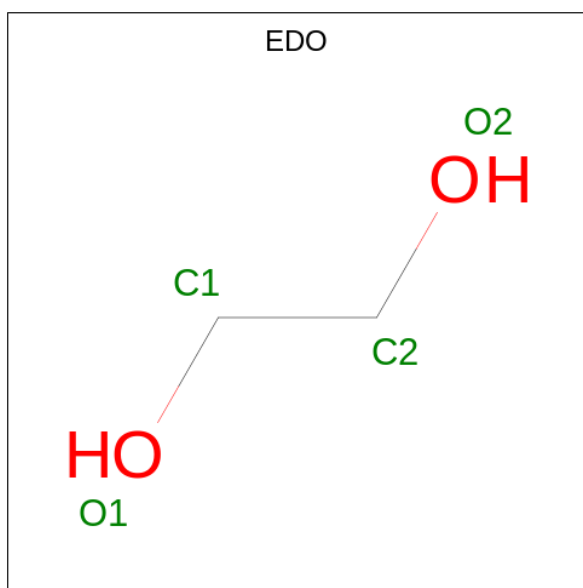
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	C	0	0
			14	14		
22	A	1	Total	C	0	0
			14	14		
22	C	1	Total	C	0	0
			11	11		
22	C	1	Total	C	0	0
			6	6		
22	C	1	Total	C	0	0
			15	15		
22	C	1	Total	C	0	0
			11	11		
22	C	1	Total	C	0	0
			14	14		
22	C	1	Total	C	0	0
			11	11		
22	C	1	Total	C	0	0
	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

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

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



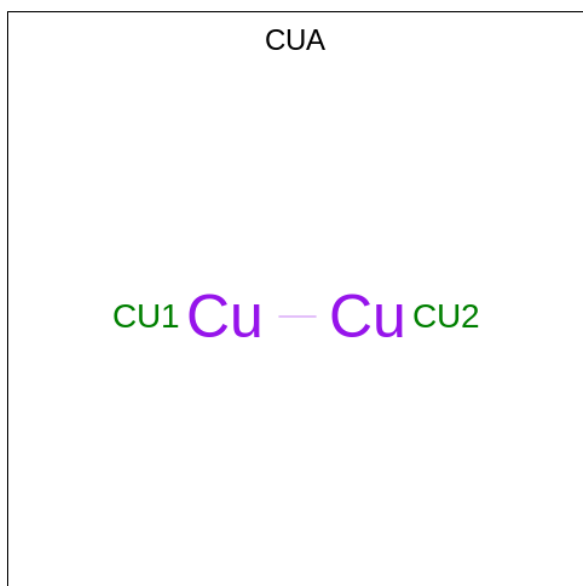
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 4 2 2	0	0
23	A	1	Total C O 4 2 2	0	0
23	A	1	Total C O 4 2 2	0	0
23	A	1	Total C O 4 2 2	0	0
23	B	1	Total C O 4 2 2	0	0
23	C	1	Total C O 4 2 2	0	0
23	C	1	Total C O 4 2 2	0	0
23	C	1	Total C O 4 2 2	0	0
23	E	1	Total C O 4 2 2	0	0
23	E	1	Total C O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

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

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

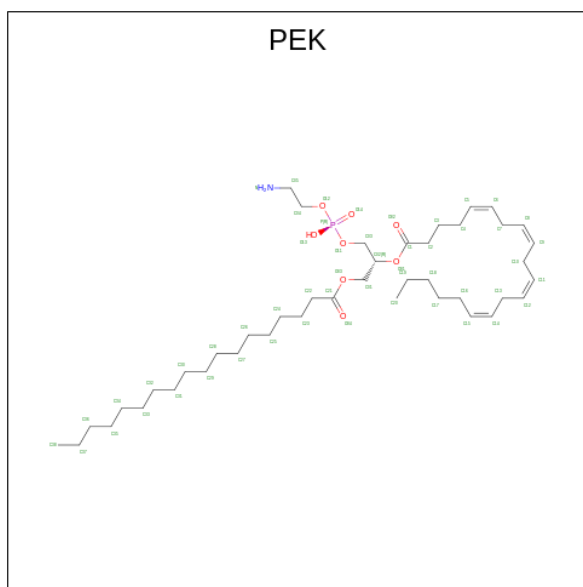


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total Cu 2 2	0	0
24	O	1	Total Cu 2 2	0	0

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

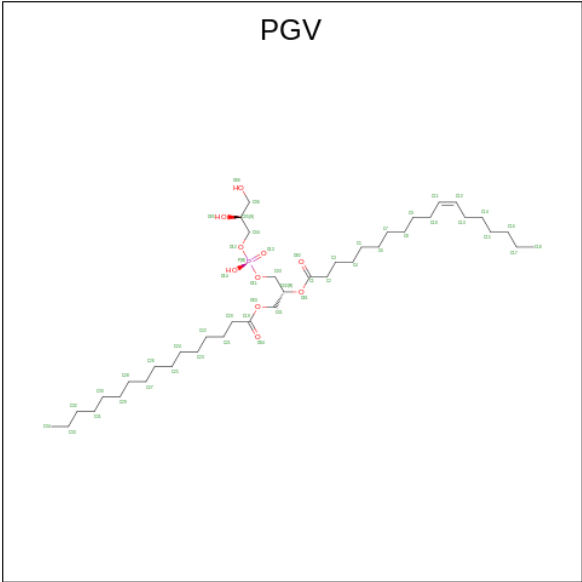
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	C	1	Total	X	0	0
			1	1		
25	P	1	Total	X	0	0
			1	1		

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



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

- Molecule 27 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



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

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

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

- Molecule 29 is water.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	X	1	Total O 1 1	0	0
29	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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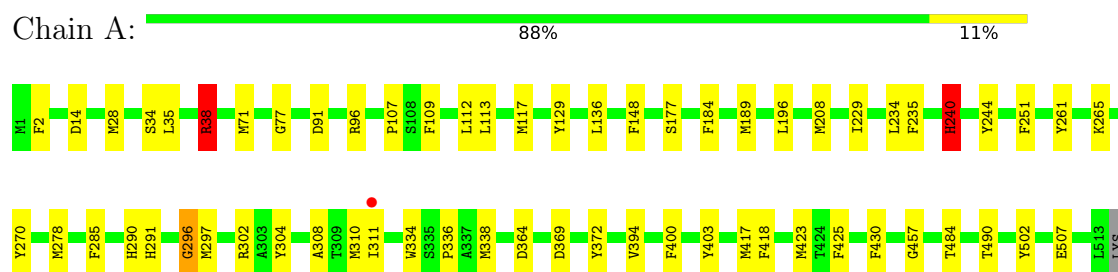
*Continued from previous page...*

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

### 3 Residue-property plots

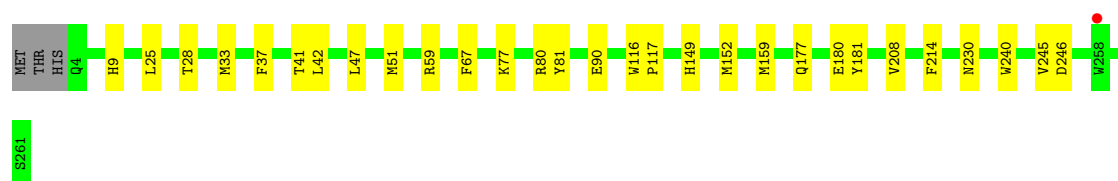
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Cytochrome c oxidase subunit 1

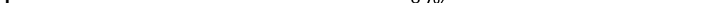


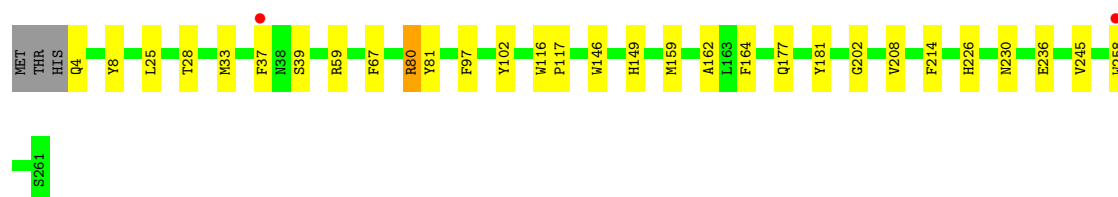
- Molecule 3: Cytochrome c oxidase subunit 3

Chain C:  88% 11%



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P:  87% 11%

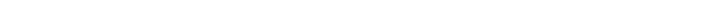


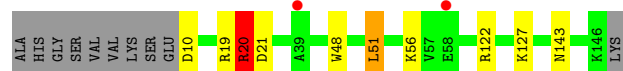
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:  90% 7% .



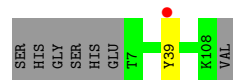
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:  86% 5% .. 7%



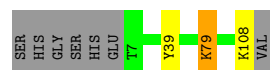
- Molecule 5: Cytochrome c oxidase subunit 5A

Chain E:  93% • 6%




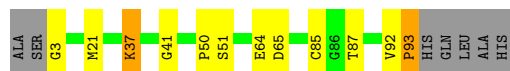
- Molecule 5: Cytochrome c oxidase subunit 5A

Chain R:  91% .. 6%




- Molecule 6: Cytochrome c oxidase subunit 5B

Chain F: 



- Molecule 6: Cytochrome c oxidase subunit 5B

Chain S: 



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

Chain G: 




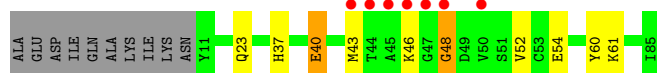
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T: 




- Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H: 




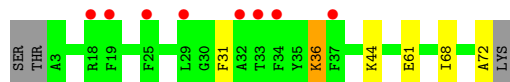
- Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U: 

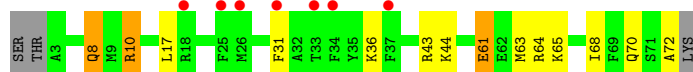
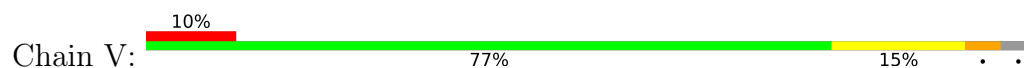


- Molecule 9: Cytochrome c oxidase subunit 6C

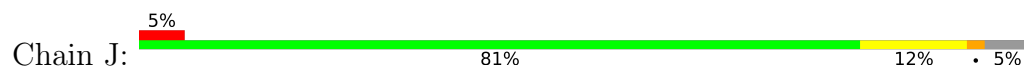
Chain I: 



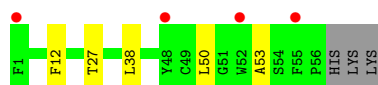
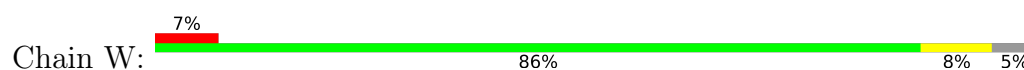
- Molecule 9: Cytochrome c oxidase subunit 6C



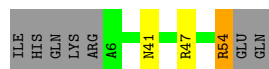
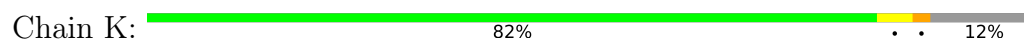
- Molecule 10: Cytochrome c oxidase subunit 7A1



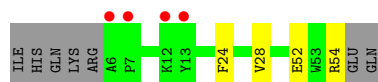
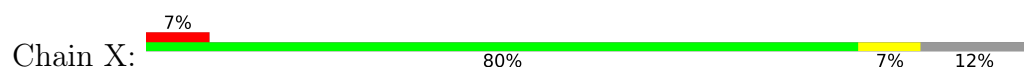
- Molecule 10: Cytochrome c oxidase subunit 7A1



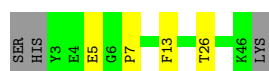
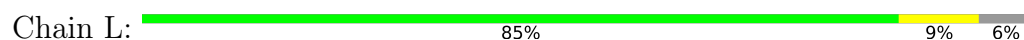
- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 11: Cytochrome c oxidase subunit 7B

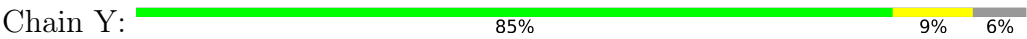


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

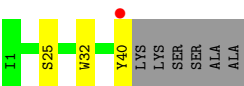
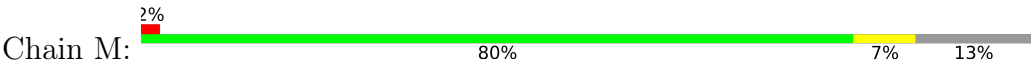


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

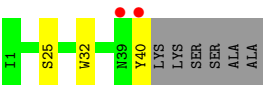
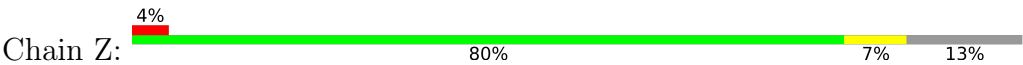




● Molecule 13: Cytochrome c oxidase subunit 8B



● 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, $\alpha$ , $\beta$ , $\gamma$	182.00Å 204.19Å 177.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.30 135.86 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-1.30) 99.6 (135.86-1.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.148 , 0.170 0.163 , 0.182	Depositor DCC
$R_{free}$ test set	79184 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	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 <sup>2</sup> )	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.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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

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

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	N	0	3
2	B	0	5
6	S	0	1
11	K	0	1
All	All	0	14

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	110	TYR	CE1-CZ	42.08	1.93	1.38
2	B	110	TYR	CG-CD1	27.95	1.75	1.39
2	B	110	TYR	CG-CD2	19.12	1.64	1.39
1	N	481	GLU	CD-OE2	18.10	1.45	1.25
2	B	110	TYR	CE2-CZ	12.35	1.54	1.38
2	B	162	SER	C-O	-12.17	1.00	1.23
4	D	58	GLU	CD-OE1	11.05	1.37	1.25
9	I	61	GLU	CD-OE2	-10.69	1.13	1.25
2	O	132	GLU	CD-OE2	9.83	1.36	1.25
1	N	481	GLU	CD-OE1	8.02	1.34	1.25
1	N	189	MET	CB-CG	7.99	1.76	1.51
2	B	167	SER	CB-OG	7.40	1.51	1.42
2	B	212	GLU	C-N	7.05	1.50	1.34
9	I	72	ALA	C-O	6.83	1.36	1.23
6	F	3	GLY	C-O	6.64	1.34	1.23
3	C	90	GLU	CD-OE1	6.59	1.32	1.25
8	U	61	LYS	C-O	6.29	1.35	1.23
1	N	481	GLU	CG-CD	6.23	1.61	1.51
1	A	507	GLU	CD-OE1	-6.22	1.18	1.25
7	G	12	GLY	C-O	6.19	1.33	1.23
2	O	60	GLU	CD-OE1	6.12	1.32	1.25
1	A	77	GLY	C-O	6.10	1.33	1.23
2	O	60	GLU	CD-OE2	6.02	1.32	1.25
2	B	152	MET	CB-CG	-6.02	1.32	1.51
1	N	189	MET	CG-SD	-5.98	1.65	1.81
6	S	3	GLY	C-O	5.97	1.33	1.23
7	T	12	GLY	C-O	5.83	1.32	1.23
8	H	54	GLU	CD-OE2	5.80	1.32	1.25
12	L	5	GLU	CD-OE2	-5.73	1.19	1.25
1	N	92	MET	CB-CG	5.68	1.69	1.51
2	B	147	GLU	CD-OE1	-5.63	1.19	1.25
1	N	382	SER	CB-OG	-5.57	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	115	ASP	CG-OD2	5.48	1.38	1.25
7	G	83	GLU	CD-OE1	5.40	1.31	1.25
2	B	157	GLU	CD-OE2	-5.40	1.19	1.25
8	U	78	GLU	CD-OE2	5.35	1.31	1.25
1	A	34	SER	CB-OG	-5.27	1.35	1.42
8	H	40	GLU	CD-OE2	5.25	1.31	1.25
2	O	147	GLU	CD-OE1	-5.20	1.20	1.25
1	A	177	SER	CA-CB	-5.17	1.45	1.52
12	Y	5	GLU	CD-OE1	-5.15	1.20	1.25
1	A	235	PHE	C-O	5.15	1.33	1.23
1	A	189	MET	CG-SD	-5.07	1.68	1.81
1	N	71	MET	CG-SD	5.07	1.94	1.81
4	D	7	LYS	C-O	5.03	1.32	1.23
3	C	9	HIS	CE1-NE2	5.02	1.44	1.32

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	110	TYR	CB-CG-CD1	-31.40	102.16	121.00
2	O	82	ARG	NE-CZ-NH2	-19.74	110.43	120.30
2	B	82	ARG	NE-CZ-NH2	-17.76	111.42	120.30
2	B	110	TYR	CD1-CE1-CZ	-17.49	104.06	119.80
11	K	54	ARG	CA-C-O	-14.42	89.82	120.10
1	N	71	MET	CG-SD-CE	-14.32	77.29	100.20
4	D	20	ARG	NE-CZ-NH2	13.45	127.03	120.30
4	D	20	ARG	NE-CZ-NH1	-12.94	113.83	120.30
2	B	110	TYR	CD1-CG-CD2	12.12	131.23	117.90
2	B	110	TYR	OH-CZ-CE2	-11.76	88.34	120.10
1	A	71	MET	CG-SD-CE	-11.33	82.06	100.20
4	Q	20	ARG	NE-CZ-NH2	-10.48	115.06	120.30
1	A	184	PHE	CB-CG-CD2	10.15	127.90	120.80
1	N	481	GLU	OE1-CD-OE2	9.26	134.41	123.30
2	B	110	TYR	CZ-CE2-CD2	-9.13	111.58	119.80
5	E	39	TYR	CB-CG-CD1	9.02	126.41	121.00
4	Q	20	ARG	NE-CZ-NH1	8.97	124.79	120.30
1	A	129	TYR	CD1-CE1-CZ	8.88	127.79	119.80
2	B	212	GLU	CA-C-N	-8.42	98.67	117.20
1	N	19	TYR	CB-CG-CD2	8.41	126.05	121.00
1	N	310	MET	CG-SD-CE	-8.40	86.76	100.20
2	B	82	ARG	CG-CD-NE	-8.27	94.44	111.80
1	N	38	ARG	NE-CZ-NH1	8.22	124.41	120.30
2	B	65	TRP	CA-CB-CG	8.20	129.27	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	10	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	N	481	GLU	CG-CD-OE2	-7.97	102.37	118.30
2	B	115	ASP	CB-CA-C	7.89	126.19	110.40
9	I	72	ALA	CA-C-O	-7.87	103.58	120.10
1	A	38	ARG	NE-CZ-NH1	7.54	124.07	120.30
2	B	110	TYR	CE1-CZ-CE2	7.42	131.67	119.80
1	N	38	ARG	NE-CZ-NH2	-7.41	116.60	120.30
6	S	93	PRO	CA-C-O	-7.37	102.52	120.20
1	A	129	TYR	CG-CD2-CE2	7.27	127.12	121.30
2	O	82	ARG	NE-CZ-NH1	7.27	123.93	120.30
9	V	10	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	N	96	ARG	NE-CZ-NH2	-7.03	116.78	120.30
5	R	39	TYR	CB-CG-CD1	6.93	125.16	121.00
3	P	81	TYR	CB-CG-CD1	6.92	125.15	121.00
9	V	72	ALA	CA-C-O	-6.85	105.72	120.10
1	A	129	TYR	CG-CD1-CE1	-6.82	115.85	121.30
1	N	14	ASP	CB-CG-OD2	-6.78	112.20	118.30
2	B	65	TRP	CB-CA-C	-6.77	96.86	110.40
1	A	96	ARG	NE-CZ-NH2	-6.71	116.94	120.30
3	P	181	TYR	CB-CG-CD2	-6.71	116.97	121.00
2	B	110	TYR	CG-CD2-CE2	-6.71	115.94	121.30
1	A	261	TYR	CB-CG-CD2	6.64	124.98	121.00
5	R	39	TYR	CB-CG-CD2	-6.61	117.04	121.00
4	D	21	ASP	CB-CG-OD2	6.58	124.22	118.30
2	B	110	TYR	CG-CD1-CE1	-6.55	116.06	121.30
1	A	38	ARG	NE-CZ-NH2	-6.53	117.03	120.30
2	B	184	LEU	N-CA-CB	-6.51	97.38	110.40
3	P	80	ARG	CG-CD-NE	-6.48	98.18	111.80
2	B	82	ARG	NH1-CZ-NH2	6.41	126.45	119.40
2	O	82	ARG	CG-CD-NE	-6.39	98.39	111.80
1	N	439	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	N	19	TYR	CB-CG-CD1	-6.18	117.29	121.00
1	A	403	TYR	CD1-CE1-CZ	6.18	125.36	119.80
11	K	54	ARG	NE-CZ-NH1	-6.18	117.21	120.30
3	C	181	TYR	CB-CG-CD1	6.13	124.68	121.00
1	A	310	MET	CG-SD-CE	-6.09	90.45	100.20
2	B	162	SER	CA-C-N	-6.09	103.79	117.20
3	C	81	TYR	CB-CG-CD1	5.96	124.58	121.00
8	U	61	LYS	O-C-N	5.91	132.15	122.70
1	A	184	PHE	CB-CG-CD1	-5.88	116.69	120.80
1	A	251	PHE	CB-CG-CD1	5.87	124.91	120.80
1	N	129	TYR	CG-CD2-CE2	5.86	125.99	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	167	SER	N-CA-CB	5.82	119.23	110.50
1	A	35	LEU	CB-CG-CD2	5.81	120.88	111.00
7	T	44	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	372	TYR	CB-CG-CD1	5.72	124.43	121.00
1	A	14	ASP	CB-CG-OD2	-5.72	113.16	118.30
3	C	181	TYR	CB-CG-CD2	-5.71	117.58	121.00
3	C	80	ARG	CG-CD-NE	-5.71	99.82	111.80
1	A	400	PHE	CB-CG-CD1	5.70	124.79	120.80
1	A	196	LEU	O-C-N	5.63	131.71	122.70
6	F	93	PRO	CA-C-O	-5.63	106.69	120.20
1	A	502	TYR	CB-CG-CD1	-5.63	117.62	121.00
2	O	82	ARG	NH1-CZ-NH2	5.51	125.46	119.40
10	J	36	MET	CG-SD-CE	-5.51	91.39	100.20
5	E	39	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	A	244	TYR	CZ-CE2-CD2	5.48	124.73	119.80
1	N	270	TYR	CD1-CE1-CZ	5.46	124.72	119.80
1	A	364	ASP	CB-CG-OD2	5.45	123.20	118.30
3	P	97	PHE	CB-CG-CD1	5.43	124.61	120.80
1	N	129	TYR	CD1-CE1-CZ	5.42	124.68	119.80
2	B	64	ILE	C-N-CA	5.41	135.21	121.70
1	N	285	PHE	CB-CG-CD1	5.41	124.58	120.80
2	B	163	TRP	CD1-CG-CD2	5.38	110.61	106.30
1	A	403	TYR	CG-CD2-CE2	5.35	125.58	121.30
3	C	80	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	N	390	MET	CG-SD-CE	5.33	108.72	100.20
1	A	430	PHE	CB-CG-CD2	-5.28	117.11	120.80
7	G	44	ARG	NE-CZ-NH1	5.27	122.94	120.30
10	J	7	GLU	CB-CA-C	5.24	120.88	110.40
4	Q	122	ARG	NE-CZ-NH2	-5.24	117.68	120.30
3	P	81	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	A	364	ASP	CB-CG-OD1	-5.20	113.62	118.30
3	P	8	TYR	CB-CG-CD2	5.18	124.11	121.00
1	A	372	TYR	CG-CD1-CE1	5.18	125.44	121.30
7	T	14	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	270	TYR	CB-CG-CD2	5.16	124.09	121.00
1	N	363	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	502	TYR	CB-CG-CD2	5.14	124.09	121.00
4	D	122	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	N	251	PHE	CB-CG-CD1	5.13	124.39	120.80
3	C	152	MET	CG-SD-CE	-5.09	92.05	100.20
3	P	80	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	B	212	GLU	C-N-CA	-5.07	109.03	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ASP	CB-CG-OD2	5.05	122.84	118.30
1	N	240	HIS	CA-CB-CG	-5.05	105.02	113.60
1	A	425	PHE	CB-CG-CD1	5.04	124.33	120.80
1	A	240	HIS	CA-CB-CG	-5.01	105.08	113.60

There are no chirality outliers.

All (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
2	B	113	TYR	Mainchain
2	B	162	SER	Mainchain
2	B	203	ASN	Sidechain
2	B	212	GLU	Mainchain
11	K	41	ASN	Sidechain
1	N	240	HIS	Sidechain
1	N	296	GLY	Mainchain
1	N	304	TYR	Sidechain
6	S	92	VAL	Mainchain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4102	56	0
1	N	4130	0	4102	60	0
2	B	1870	0	1870	31	0
2	O	1870	0	1870	15	0
3	C	2171	0	2080	26	0
3	P	2172	0	2081	24	0
4	D	1192	0	1178	4	0
4	Q	1148	0	1131	6	0
5	E	825	0	823	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	825	0	823	2	0
6	F	709	0	691	11	0
6	S	709	0	691	7	0
7	G	606	0	577	5	0
7	T	606	0	577	9	0
8	H	628	0	580	11	0
8	U	628	0	580	10	0
9	I	575	0	584	5	0
9	V	575	0	584	9	0
10	J	441	0	439	8	0
10	W	441	0	439	6	0
11	K	384	0	366	0	0
11	X	384	0	366	2	0
12	L	360	0	360	4	0
12	Y	360	0	360	4	0
13	M	311	0	321	3	0
13	Z	311	0	321	3	0
14	A	129	0	88	7	0
14	N	129	0	88	8	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	158	0	213	10	0
18	C	87	0	124	14	0
18	N	158	0	213	8	0
18	P	87	0	124	12	0
19	A	29	0	39	0	0
19	C	29	0	39	0	0
19	G	29	0	39	1	0
19	N	29	0	39	0	0
19	P	29	0	39	1	0
19	T	29	0	39	1	0
20	A	106	0	138	6	0
20	B	44	0	73	0	0
20	C	172	0	230	7	0
20	G	55	0	81	9	0
20	J	44	0	61	6	0
20	L	22	0	31	0	0
20	M	8	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	N	106	0	138	4	0
20	O	44	0	73	2	0
20	P	172	0	231	7	0
20	T	55	0	83	18	0
20	W	44	0	61	7	0
20	Y	22	0	31	1	0
20	Z	8	0	15	0	0
21	A	2	0	0	1	0
21	N	2	0	0	1	0
22	A	28	0	54	16	0
22	C	114	0	219	12	0
22	G	28	0	54	1	0
22	N	28	0	54	7	0
22	P	114	0	219	7	0
22	T	28	0	54	4	0
23	A	16	0	24	1	0
23	B	4	0	6	0	0
23	C	12	0	18	2	0
23	E	12	0	18	0	0
23	F	8	0	12	0	0
23	G	4	0	6	0	0
23	N	20	0	30	1	0
23	O	4	0	6	0	0
23	P	12	0	18	0	0
23	R	12	0	18	0	0
23	S	8	0	12	0	0
23	T	4	0	6	0	0
24	B	2	0	0	0	0
24	O	2	0	0	0	0
25	C	1	0	0	0	0
25	P	1	0	0	1	0
26	C	53	0	77	5	0
26	P	53	0	77	3	0
27	C	102	0	152	2	0
27	P	102	0	152	1	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	254	0	0	15	0
29	B	179	0	0	2	0
29	C	101	0	0	5	0
29	D	147	0	0	0	0
29	E	117	0	0	0	0

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

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

All (387) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:TYR:CG	2:B:110:TYR:CD1	1.75	1.69
1:N:189:MET:CG	1:N:189:MET:CB	1.76	1.62
2:B:110:TYR:CZ	2:B:110:TYR:CE1	1.93	1.57
1:A:297[B]:MET:CB	29:A:4142:HOH:O	1.86	1.20
1:A:297[B]:MET:HB2	29:A:4142:HOH:O	1.38	1.15
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
21:N:520:PER:O1	21:N:520:PER:O2	1.67	1.09
20:T:711:DMU:O49	20:T:713:DMU:C57	1.99	1.09
20:T:711:DMU:O49	20:T:713:DMU:O61	1.75	1.04
1:N:297[B]:MET:CB	29:N:3098:HOH:O	2.02	1.03
1:N:297[B]:MET:HB2	29:N:3098:HOH:O	1.57	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:711:DMU:O49	20:T:713:DMU:H29	1.59	1.02
1:N:136[B]:LEU:HD11	29:N:3268:HOH:O	1.64	0.98
1:A:136[B]:LEU:HD11	29:A:3514:HOH:O	1.63	0.97
3:C:245:VAL:C	3:C:246[B]:ASP:CA	2.32	0.96
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.08	0.93
20:T:712:DMU:H8	20:T:713:DMU:H6	1.50	0.93
8:H:52:VAL:HG12	8:U:46:LYS:CG	1.99	0.92
2:B:110:TYR:CD1	2:B:110:TYR:CB	2.55	0.88
8:H:52:VAL:CG1	8:U:46:LYS:HG2	2.03	0.88
3:C:33[B]:MET:CE	20:J:61:DMU:H12	2.03	0.88
3:P:149:HIS:NE2	22:P:624:LFA:H11	1.89	0.88
20:T:711:DMU:O49	20:T:712:DMU:O16	1.92	0.87
1:N:417[B]:MET:HE2	29:N:2011:HOH:O	1.75	0.87
25:P:262:UNX:UNK	29:P:2021:HOH:O	1.52	0.86
18:C:270:CDL:HB61	18:C:270:CDL:HB21	1.58	0.86
1:N:423[B]:MET:HE2	1:N:457:GLY:HA2	1.55	0.86
1:A:297[B]:MET:HB3	29:A:4142:HOH:O	1.63	0.86
3:C:33[A]:MET:HE1	3:C:42:LEU:H	1.41	0.85
22:C:624:LFA:H102	20:C:721:DMU:H25	1.61	0.83
1:A:28:MET:CE	14:A:515[A]:HEA:C27	2.57	0.82
22:C:626:LFA:H13	29:C:3800:HOH:O	1.80	0.82
1:N:278[B]:MET:SD	22:N:627:LFA:H51	2.20	0.82
1:A:297[B]:MET:SD	1:A:302:ARG:HG2	2.20	0.82
1:A:423[B]:MET:HE2	1:A:457:GLY:HA2	1.59	0.82
10:J:50:LEU:HB2	20:J:61:DMU:H20	1.62	0.81
1:A:113[A]:LEU:HD12	18:A:521:CDL:C87	2.10	0.81
1:A:297[B]:MET:HG2	1:A:302:ARG:HG3	1.62	0.81
3:C:33[B]:MET:HE2	20:J:61:DMU:H12	1.64	0.80
1:N:189:MET:CB	1:N:189:MET:SD	2.70	0.79
20:T:711:DMU:H2	20:T:713:DMU:O61	1.83	0.79
18:A:521:CDL:O1	29:L:3766[B]:HOH:O	2.00	0.77
1:A:297[B]:MET:SD	1:A:302:ARG:CG	2.74	0.76
2:O:22[B]:HIS:CE1	9:V:44:LYS:HE2	2.20	0.76
1:N:297[B]:MET:HB3	29:N:3098:HOH:O	1.72	0.76
1:N:297[B]:MET:SD	1:N:302:ARG:CG	2.73	0.76
7:T:33:LEU:HD22	7:T:37:LEU:HD22	1.66	0.75
1:A:28:MET:CE	14:A:515[A]:HEA:H271	2.16	0.75
20:T:712:DMU:H21	20:T:713:DMU:H20	1.69	0.75
1:A:484:THR:HG22	29:A:3347:HOH:O	1.86	0.75
1:A:113[A]:LEU:HD12	18:A:521:CDL:H873	1.68	0.74
1:A:28:MET:HE2	14:A:515[A]:HEA:H273	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:28:MET:CE	14:N:515[A]:HEA:C27	2.65	0.74
1:A:297[B]:MET:CG	1:A:302:ARG:HG3	2.17	0.74
2:B:110:TYR:CD1	2:B:110:TYR:CZ	2.59	0.74
18:P:270:CDL:HB61	18:P:270:CDL:HB21	1.70	0.73
14:N:516:HEA:HMC1	14:N:516:HEA:HBC1	1.68	0.73
14:A:516:HEA:HBC1	14:A:516:HEA:HMC1	1.70	0.73
2:B:110:TYR:CG	2:B:110:TYR:CE1	2.62	0.73
20:P:733:DMU:O3	20:P:734:DMU:C57	2.38	0.72
22:P:626:LFA:H12	29:P:3527:HOH:O	1.88	0.72
3:P:4:GLN:N	29:P:3471:HOH:O	2.23	0.71
18:C:270:CDL:HA62	18:C:270:CDL:H121	1.72	0.71
1:A:278[B]:MET:SD	22:A:627:LFA:H52	2.30	0.71
23:C:809:EDO:O2	29:C:1810:HOH:O	0.72	0.71
20:G:712:DMU:H22	1:N:311[A]:ILE:HD11	1.73	0.70
2:B:13:THR:HB	2:B:168:LEU:HD23	1.73	0.70
1:A:278[A]:MET:CE	22:A:628:LFA:H51	2.21	0.70
1:A:28:MET:HE2	14:A:515[A]:HEA:C27	2.21	0.70
1:N:28:MET:CE	14:N:515[A]:HEA:H271	2.22	0.70
1:N:28:MET:HE2	14:N:515[A]:HEA:H273	1.73	0.69
1:N:28:MET:HE2	14:N:515[A]:HEA:C27	2.23	0.69
20:P:733:DMU:O3	20:P:734:DMU:O61	2.09	0.69
3:C:180[B]:GLU:HG2	29:C:3893:HOH:O	1.91	0.69
1:N:113[A]:LEU:HD12	18:N:521:CDL:H871	1.74	0.68
1:A:423[B]:MET:HE3	1:A:457:GLY:N	2.08	0.67
3:C:149:HIS:NE2	22:C:624:LFA:H11	2.09	0.67
18:P:270:CDL:HA62	18:P:270:CDL:H121	1.77	0.67
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.77	0.67
1:N:189:MET:CG	1:N:189:MET:CA	2.72	0.66
29:A:3305:HOH:O	3:C:77:LYS:HE3	1.96	0.66
20:P:733:DMU:O3	20:P:734:DMU:H29	1.96	0.66
2:B:16[A]:ILE:HD11	2:B:86:MET:HG2	1.76	0.65
1:N:297[B]:MET:HG2	1:N:302:ARG:HG3	1.78	0.65
1:N:278[A]:MET:CE	22:N:628:LFA:H51	2.26	0.65
1:A:423[B]:MET:HE2	1:A:457:GLY:CA	2.26	0.65
29:A:3684:HOH:O	22:C:716[B]:LFA:H52	1.95	0.65
2:B:61:VAL:HG22	2:B:65:TRP:CZ3	2.32	0.65
18:P:270:CDL:HB61	18:P:270:CDL:CB2	2.26	0.64
1:A:311[A]:ILE:HD11	20:T:712:DMU:H22	1.77	0.64
3:P:33[B]:MET:CA	3:P:33[B]:MET:HE2	2.28	0.64
2:B:110:TYR:HE1	2:B:118:PHE:CE2	2.17	0.63
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:37:HIS:HE1	29:U:3552:HOH:O	1.80	0.63
23:A:801:EDO:O1	29:A:1801[B]:HOH:O	0.63	0.62
1:N:423[B]:MET:HE3	1:N:457:GLY:N	2.13	0.62
29:A:3684:HOH:O	22:C:716[B]:LFA:C5	2.46	0.62
1:A:297[B]:MET:SD	1:A:302:ARG:HG3	2.40	0.62
1:A:113[B]:LEU:HD11	1:A:117[B]:MET:SD	2.39	0.62
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:HG3	1.80	0.62
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.35	0.62
20:T:711:DMU:C1	20:T:713:DMU:O61	2.47	0.61
1:A:278[A]:MET:HE3	22:A:628:LFA:H51	1.81	0.61
1:N:417[B]:MET:CE	29:N:2011:HOH:O	2.41	0.61
3:P:226:HIS:HE1	18:P:270:CDL:H111	1.64	0.61
1:A:423[B]:MET:CE	1:A:457:GLY:N	2.63	0.61
1:N:278[A]:MET:SD	22:N:628:LFA:H51	2.41	0.61
1:A:297[B]:MET:O	1:A:302:ARG:NE	2.29	0.61
3:C:33[A]:MET:CE	3:C:42:LEU:H	2.11	0.60
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.01	0.60
6:F:64:GLU:O	6:F:65:ASP:HB2	2.02	0.60
1:A:28:MET:HE1	14:A:515[A]:HEA:H271	1.83	0.59
20:N:745:DMU:H40	29:Z:2097:HOH:O	2.01	0.59
3:C:33[B]:MET:HE1	20:J:61:DMU:H12	1.82	0.59
6:F:37:LYS:HG2	29:F:3928:HOH:O	2.01	0.59
29:N:3540:HOH:O	4:Q:20:ARG:HG2	2.03	0.59
20:T:711:DMU:H2	20:T:713:DMU:C57	2.32	0.59
20:T:711:DMU:C2	20:T:713:DMU:O61	2.51	0.59
1:N:297[B]:MET:CG	1:N:302:ARG:HG3	2.32	0.59
3:P:33[B]:MET:CE	20:W:61:DMU:H12	2.32	0.59
20:A:744:DMU:H11	4:D:81:VAL:HG11	1.84	0.58
1:A:28:MET:HE1	14:A:515[A]:HEA:C27	2.33	0.58
29:A:3932:HOH:O	6:F:37:LYS:HE3	2.03	0.58
3:C:33[B]:MET:CE	20:J:61:DMU:C25	2.81	0.58
29:N:3838[B]:HOH:O	4:Q:19:ARG:HD3	2.02	0.58
1:N:2:PHE:HE2	18:N:521:CDL:H712	1.69	0.58
3:P:59:ARG:HB2	18:P:270:CDL:OA9	2.04	0.57
18:A:521:CDL:H842	18:A:521:CDL:C41	2.34	0.57
20:N:745:DMU:C11	29:Z:2097:HOH:O	2.53	0.57
3:P:33[B]:MET:HE2	20:W:61:DMU:H12	1.85	0.57
3:C:33[B]:MET:HE2	3:C:33[B]:MET:CA	2.31	0.57
2:B:110:TYR:CD1	2:B:110:TYR:N	2.73	0.57
20:T:711:DMU:C1	20:T:713:DMU:H31	2.14	0.57
18:P:270:CDL:HA21	10:W:12:PHE:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:2:PHE:CE2	18:N:521:CDL:H712	2.40	0.56
9:V:61:GLU:OE1	9:V:64:ARG:NE	2.39	0.56
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.88	0.56
6:S:64:GLU:O	6:S:65:ASP:HB2	2.04	0.56
8:U:37:HIS:CE1	29:U:3552:HOH:O	2.58	0.56
23:N:829:EDO:O2	29:N:2829:HOH:O	0.57	0.56
20:P:714:DMU:H35	20:P:714:DMU:H30	1.88	0.56
3:C:149:HIS:NE2	22:C:624:LFA:C1	2.69	0.55
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.07	0.55
8:H:46:LYS:CE	8:H:46:LYS:O	2.55	0.55
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	2.95	0.55
22:C:625:LFA:H22	22:C:626:LFA:H71	1.88	0.55
2:B:16[B]:ILE:HG23	29:B:1078:HOH:O	2.05	0.55
2:B:29:MET:SD	9:I:36:LYS:NZ	2.76	0.55
1:N:28:MET:HE1	14:N:515[A]:HEA:H271	1.87	0.55
18:A:521:CDL:H512	12:L:13:PHE:HB3	1.89	0.55
20:G:712:DMU:H20	20:G:713:DMU:H20	1.89	0.55
1:A:113[A]:LEU:CD1	18:A:521:CDL:C87	2.83	0.54
26:P:264:PEK:H71	26:P:264:PEK:H32	1.89	0.54
1:N:308:ALA:HA	1:N:311[A]:ILE:HD12	1.88	0.54
1:N:423[B]:MET:HE2	1:N:457:GLY:CA	2.32	0.54
3:C:33[A]:MET:HE1	3:C:42:LEU:N	2.17	0.54
1:N:365:ILE:HD11	29:N:3309:HOH:O	2.08	0.53
18:C:270:CDL:HB21	18:C:270:CDL:CB6	2.35	0.53
8:H:46:LYS:O	8:H:46:LYS:HE2	2.09	0.53
3:C:59:ARG:HG3	18:C:270:CDL:HA4	1.91	0.53
3:P:4:GLN:CA	29:P:3471:HOH:O	2.57	0.53
26:C:264:PEK:C11	26:C:264:PEK:H161	2.39	0.53
9:V:8:GLN:OE1	9:V:10:ARG:O	2.27	0.53
2:O:13:THR:HB	2:O:168:LEU:HD23	1.90	0.52
1:N:28:MET:CE	14:N:515[A]:HEA:H273	2.36	0.52
20:G:712:DMU:H22	1:N:311[A]:ILE:CD1	2.39	0.52
1:A:2:PHE:CE1	18:A:521:CDL:H712	2.44	0.52
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.39	0.52
2:B:67:ILE:HD11	22:T:621:LFA:H61	1.92	0.52
22:C:624:LFA:C10	20:C:721:DMU:H25	2.38	0.51
2:O:22[B]:HIS:CE1	9:V:44:LYS:CE	2.91	0.51
3:P:164:PHE:CD1	19:P:271:CHD:H192	2.45	0.51
3:P:226:HIS:CE1	18:P:270:CDL:H111	2.45	0.51
1:A:112:LEU:HG	29:A:1053:HOH:O	2.10	0.51
1:N:278[A]:MET:HE3	22:N:628:LFA:H51	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:53:ALA:HB2	20:W:61:DMU:H10	1.93	0.51
3:P:67:PHE:CE2	18:P:270:CDL:O1	2.55	0.50
1:N:113[A]:LEU:CD1	18:N:521:CDL:H871	2.40	0.50
2:B:1:FME:HCN	2:B:193:TYR:HD1	1.76	0.50
26:C:264:PEK:H161	26:C:264:PEK:C12	2.42	0.50
1:A:112:LEU:C	1:A:112:LEU:HD23	2.32	0.50
20:G:712:DMU:H19	1:N:307:SER:HB3	1.93	0.50
18:P:270:CDL:HA21	10:W:12:PHE:CE2	2.47	0.50
29:Q:4067:HOH:O	5:R:108:LYS:HD3	2.10	0.50
1:A:278[A]:MET:SD	22:A:628:LFA:H51	2.51	0.50
2:B:67:ILE:CD1	22:T:621:LFA:H61	2.41	0.50
7:G:12:GLY:HA3	29:G:1207:HOH:O	2.11	0.50
2:O:32[B]:PHE:CD2	9:V:31:PHE:CZ	2.99	0.50
18:P:270:CDL:H751	10:W:27:THR:HG21	1.94	0.50
18:C:270:CDL:CA5	18:C:270:CDL:OA8	2.60	0.50
1:N:278[A]:MET:CE	22:N:628:LFA:C5	2.90	0.50
20:T:711:DMU:C2	20:T:713:DMU:C57	2.90	0.50
26:C:264:PEK:C38	27:C:266:PGV:H343	2.42	0.49
1:N:113[A]:LEU:HD12	18:N:521:CDL:C87	2.42	0.49
18:P:270:CDL:H121	18:P:270:CDL:CA6	2.40	0.49
12:Y:24:MET:HG3	29:Y:4051:HOH:O	2.11	0.49
1:N:110:LEU:HD21	20:W:61:DMU:H24	1.94	0.49
22:P:623:LFA:H101	22:P:624:LFA:C11	2.42	0.49
1:N:110:LEU:CD2	20:W:61:DMU:H24	2.42	0.49
22:A:628:LFA:C6	7:T:19:LEU:HD23	2.43	0.49
3:C:33[B]:MET:HG3	3:C:37:PHE:HB2	1.94	0.49
18:C:270:CDL:CA5	18:C:270:CDL:OB4	2.61	0.49
18:N:522:CDL:H1	18:N:522:CDL:OA3	2.13	0.49
1:A:418:PHE:CD1	20:A:744:DMU:H24	2.48	0.49
2:B:33:LEU:HD13	9:I:31:PHE:CD2	2.48	0.48
3:P:258:TRP:CE2	22:P:611:LFA:H32	2.48	0.48
1:A:285:PHE:CD2	22:A:627:LFA:H121	2.49	0.48
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.95	0.48
20:P:715[A]:DMU:O61	20:P:715[A]:DMU:H35	2.13	0.48
6:F:51:SER:O	6:F:93:PRO:HA	2.14	0.48
1:N:278[A]:MET:HE3	22:N:628:LFA:C5	2.43	0.48
1:N:423[B]:MET:CE	1:N:457:GLY:HA2	2.35	0.48
3:P:33[B]:MET:HG3	3:P:37:PHE:HB2	1.95	0.48
18:C:270:CDL:HB22	10:J:8:LYS:HE3	1.94	0.48
3:P:102:TYR:CE1	22:P:615:LFA:H91	2.49	0.48
1:A:278[B]:MET:CE	22:A:627:LFA:H52	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:336:PRO:HB2	1:N:394[B]:VAL:HG11	1.96	0.48
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.95	0.48
6:F:64:GLU:O	6:F:65:ASP:CB	2.59	0.48
1:A:423[B]:MET:CE	1:A:457:GLY:CA	2.90	0.48
2:O:30:ILE:HG12	20:O:731:DMU:H16	1.94	0.48
6:F:85:CYS:SG	6:F:87[B]:THR:OG1	2.70	0.48
20:Y:747:DMU:C18	20:Y:747:DMU:O49	2.62	0.48
1:N:423[B]:MET:CE	1:N:457:GLY:CA	2.92	0.47
8:H:37:HIS:HD2	8:H:40:GLU:OE2	1.97	0.47
1:N:297[B]:MET:SD	1:N:302:ARG:HG3	2.53	0.47
2:B:110:TYR:N	2:B:110:TYR:HD1	2.13	0.47
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.02	0.47
18:C:270:CDL:HB61	18:C:270:CDL:CB2	2.36	0.47
20:G:712:DMU:H13	20:G:713:DMU:H10	1.96	0.47
10:J:53:ALA:HB2	20:J:61:DMU:H10	1.97	0.47
1:N:297[B]:MET:O	1:N:302:ARG:NE	2.41	0.47
1:A:417[B]:MET:CE	29:A:1011:HOH:O	2.63	0.47
3:C:33[A]:MET:CE	3:C:41:THR:HB	2.45	0.47
8:H:43:MET:O	8:H:48:GLY:N	2.48	0.47
29:P:2107[B]:HOH:O	10:W:27:THR:HG22	2.14	0.47
20:G:711:DMU:H2	20:G:713:DMU:C57	2.45	0.47
2:O:116:LEU:HD13	2:O:226:MET:HG3	1.96	0.47
8:U:37:HIS:HD2	8:U:40:GLU:OE2	1.98	0.47
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.50	0.46
18:C:270:CDL:H121	18:C:270:CDL:CA6	2.44	0.46
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.15	0.46
6:F:21[B]:MET:HB2	6:F:21[B]:MET:HE2	1.46	0.46
2:B:86:MET:HE2	2:B:86:MET:HB2	1.71	0.46
3:P:33[A]:MET:HG2	3:P:39:SER:O	2.16	0.46
3:P:116:TRP:HA	3:P:117:PRO:C	2.35	0.46
1:A:208[B]:MET:HE1	1:A:234:LEU:CD1	2.46	0.46
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.44	0.46
18:A:522:CDL:OA3	18:A:522:CDL:H1	2.15	0.46
11:X:54:ARG:HD2	11:X:54:ARG:C	2.36	0.46
1:A:148:PHE:HB3	3:C:28:THR:HB	1.97	0.46
20:G:711:DMU:H5	20:G:712:DMU:H6	1.97	0.46
1:A:308:ALA:O	1:A:311[B]:ILE:HG12	2.16	0.45
18:A:521:CDL:H722	18:A:521:CDL:H752	1.51	0.45
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.97	0.45
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.97	0.45
1:A:417[B]:MET:HE2	29:A:1011:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:628:LFA:H121	22:A:628:LFA:H81	1.99	0.45
26:P:264:PEK:H32	26:P:264:PEK:C7	2.46	0.45
6:S:21[B]:MET:HE2	6:S:21[B]:MET:HB2	1.60	0.45
7:T:36:TRP:HE3	7:T:39:SER:HB3	1.81	0.45
22:A:628:LFA:H61	7:T:19:LEU:HD23	1.98	0.45
2:O:33:LEU:HD13	9:V:31:PHE:CD2	2.51	0.45
13:M:32:TRP:CZ3	13:M:40:TYR:OH	2.68	0.45
22:C:626:LFA:C1	29:C:3800:HOH:O	2.50	0.45
2:B:16[B]:ILE:HG13	2:B:17:MET:N	2.31	0.45
2:B:84:LEU:O	2:B:87[B]:MET:HB2	2.17	0.45
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.98	0.45
20:N:744:DMU:H36	20:N:744:DMU:O55	2.17	0.45
1:A:336:PRO:HB2	1:A:394[B]:VAL:HG11	1.98	0.44
22:A:627:LFA:H12	22:A:628:LFA:C1	2.47	0.44
2:B:60:GLU:H	2:B:60:GLU:CD	2.19	0.44
2:O:60:GLU:CD	2:O:60:GLU:H	2.20	0.44
8:U:43:MET:O	8:U:48:GLY:N	2.50	0.44
1:A:278[A]:MET:CE	22:A:628:LFA:C5	2.95	0.44
1:N:136[B]:LEU:CD1	29:N:3268:HOH:O	2.42	0.44
2:O:164:ALA:O	2:O:194:GLY:HA3	2.18	0.44
1:A:278[B]:MET:SD	22:A:627:LFA:C5	3.04	0.44
3:C:51[B]:MET:HE1	18:C:270:CDL:H861	2.00	0.44
20:A:526:DMU:H11	4:D:98:TRP:CE2	2.53	0.44
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.99	0.44
2:O:196:CYS:HB2	2:O:207:MET:HG3	2.00	0.44
5:R:79:LYS:HD2	5:R:79:LYS:N	2.32	0.44
1:A:334:TRP:CE3	20:A:743:DMU:H19	2.53	0.44
11:X:24:PHE:O	11:X:28:VAL:HG12	2.18	0.44
1:N:334:TRP:HB2	20:N:744:DMU:C57	2.48	0.44
18:P:270:CDL:CA5	18:P:270:CDL:OB4	2.65	0.44
3:P:202:GLY:HA3	26:P:264:PEK:H21	1.99	0.44
6:S:64:GLU:O	6:S:65:ASP:CB	2.65	0.44
1:A:278[B]:MET:HE1	22:A:627:LFA:H52	2.00	0.43
3:C:208:VAL:HG22	3:C:245:VAL:CG1	2.47	0.43
20:O:742:DMU:H16	9:V:17:LEU:HD21	2.00	0.43
9:V:63:MET:HB3	9:V:68:ILE:HD11	2.00	0.43
1:N:148:PHE:HB3	3:P:28:THR:HB	1.98	0.43
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.70	0.43
22:A:628:LFA:H92	7:T:23:LEU:HB2	1.99	0.43
2:B:67:ILE:HD11	22:T:621:LFA:C6	2.48	0.43
20:C:733:DMU:H25	10:J:38:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:127:LYS:HD2	29:I:1320:HOH:O	2.18	0.43
12:L:26:THR:HG23	13:M:25:SER:CB	2.47	0.43
20:T:712:DMU:H26	20:T:713:DMU:H25	2.00	0.43
4:D:17[B]:VAL:HG22	4:D:19:ARG:HG3	1.99	0.43
6:S:51:SER:O	6:S:93:PRO:HA	2.18	0.43
2:B:110:TYR:CE1	2:B:118:PHE:CE2	3.02	0.43
23:C:809:EDO:C2	29:C:1810:HOH:O	1.76	0.43
1:N:112:LEU:HD23	1:N:112:LEU:C	2.39	0.43
20:P:714:DMU:H36	20:P:714:DMU:O55	2.19	0.43
1:A:240:HIS:C	1:A:240:HIS:CD2	2.92	0.43
2:B:164:ALA:O	2:B:194:GLY:HA3	2.19	0.43
26:C:264:PEK:H382	27:C:266:PGV:H343	2.00	0.43
20:G:711:DMU:H12	20:G:712:DMU:H10	2.00	0.43
1:N:423[B]:MET:CE	1:N:457:GLY:N	2.79	0.43
4:Q:127:LYS:HD2	29:V:2320:HOH:O	2.18	0.43
20:C:714:DMU:H29	22:P:615:LFA:H31	2.00	0.43
7:T:21:PHE:CD1	22:T:622:LFA:H62	2.54	0.43
22:C:614:LFA:H102	22:C:614:LFA:H131	1.51	0.42
1:N:24:ALA:HB2	14:N:515[B]:HEA:H253	1.99	0.42
20:C:714:DMU:O55	20:C:714:DMU:H36	2.19	0.42
18:C:270:CDL:OA3	18:C:270:CDL:H1	2.19	0.42
18:C:270:CDL:H751	10:J:27:THR:HG21	2.00	0.42
6:F:92:VAL:HG23	6:F:92:VAL:O	2.18	0.42
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.54	0.42
20:W:61:DMU:O55	20:W:61:DMU:O3	2.32	0.42
29:A:1275:HOH:O	12:L:7:PRO:HG3	2.18	0.42
3:P:208:VAL:HG22	3:P:245:VAL:CG1	2.50	0.42
1:A:334:TRP:HB2	20:A:744:DMU:C57	2.50	0.42
18:C:270:CDL:CB2	10:J:8:LYS:HE3	2.49	0.42
7:G:21:PHE:CD1	22:G:622:LFA:H62	2.54	0.42
20:A:744:DMU:H36	20:A:744:DMU:O55	2.19	0.42
8:H:37:HIS:HE1	29:H:3679:HOH:O	2.01	0.42
3:P:177:GLN:OE1	3:P:177:GLN:HA	2.19	0.42
3:C:240:TRP:CE2	22:C:626:LFA:H51	2.55	0.42
12:L:26:THR:HG23	13:M:25:SER:HB3	2.01	0.42
7:G:41:HIS:HB3	7:G:74:ARG:NH1	2.34	0.42
2:O:111:THR:HA	2:O:114:GLU:O	2.20	0.42
2:O:114:GLU:HG3	2:O:227:LEU:HD21	2.01	0.42
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.55	0.42
9:I:68:ILE:HD13	9:I:68:ILE:HG21	1.85	0.42
3:P:28:THR:HG22	27:P:266:PGV:H182	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:23:LEU:HB2	22:N:628:LFA:H92	2.01	0.41
29:P:2093:HOH:O	6:S:3:GLY:HA3	2.18	0.41
1:N:189:MET:CB	1:N:189:MET:CE	2.98	0.41
18:N:521:CDL:H532	12:Y:28:PHE:CD1	2.55	0.41
20:C:714:DMU:H30	20:C:714:DMU:H35	2.02	0.41
1:A:107:PRO:HB3	3:C:25:LEU:HB2	2.02	0.41
1:A:278[A]:MET:HE3	22:A:628:LFA:C5	2.49	0.41
1:A:311[A]:ILE:CD1	20:T:712:DMU:H22	2.49	0.41
1:N:240:HIS:CD2	1:N:240:HIS:C	2.93	0.41
19:T:86:CHD:H212	19:T:86:CHD:H12	2.01	0.41
2:B:58:ALA:O	2:B:62:GLU:HG3	2.20	0.41
3:C:33[B]:MET:HB2	3:C:33[B]:MET:HE3	0.72	0.41
7:G:44:ARG:HA	7:G:45:PRO:HD3	1.88	0.41
20:T:712:DMU:H13	20:T:713:DMU:H10	2.03	0.41
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.20	0.41
2:B:227:LEU:HD21	29:B:3750:HOH:O	2.18	0.41
18:A:521:CDL:H362	18:A:521:CDL:H711	2.02	0.41
20:G:712:DMU:C37	20:G:713:DMU:H20	2.51	0.41
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.21	0.41
29:A:3684:HOH:O	22:C:716[B]:LFA:H51	2.16	0.41
3:C:116:TRP:HA	3:C:117:PRO:C	2.40	0.41
26:C:264:PEK:H11	26:C:264:PEK:H42	2.03	0.41
20:P:733:DMU:H25	10:W:38:LEU:HD23	2.03	0.41
4:Q:51:LEU:HB3	4:Q:56:LYS:HG3	2.02	0.41
6:S:19:GLU:OE1	6:S:31:TYR:OH	2.24	0.41
6:F:50:PRO:HA	6:F:92:VAL:CG2	2.51	0.41
8:U:46:LYS:CD	8:U:46:LYS:O	2.69	0.41
2:B:77:ALA:CB	20:T:711:DMU:H19	2.51	0.40
3:P:80:ARG:NH2	3:P:236:GLU:OE1	2.48	0.40
6:S:54:ASN:C	6:S:54:ASN:HD22	2.25	0.40
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.21	0.40
22:A:628:LFA:H21	7:T:15:THR:HG23	2.03	0.40
19:G:86:CHD:H212	19:G:86:CHD:H12	2.02	0.40
8:H:37:HIS:CE1	29:H:3679:HOH:O	2.74	0.40
18:N:521:CDL:H801	18:N:521:CDL:C41	2.51	0.40
22:P:716[B]:LFA:C5	29:U:3543:HOH:O	2.69	0.40
20:C:733:DMU:C43	10:J:38:LEU:HD23	2.51	0.40
10:J:29:ASN:HD22	10:J:29:ASN:H	1.69	0.40
7:T:78:LEU:HB3	7:T:79:PRO:HD2	2.03	0.40
20:T:711:DMU:H5	20:T:712:DMU:O16	2.21	0.40
3:C:67:PHE:CE2	18:C:270:CDL:O1	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:50:TYR:HB3	7:T:52:HIS:CE1	2.56	0.40
1:A:229:ILE:HD11	2:B:175:ILE:HD13	2.03	0.40
8:H:52:VAL:CB	8:U:46:LYS:HG2	2.50	0.40
20:W:61:DMU:O3	20:W:61:DMU:C2	2.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
9	V	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
10	J	54/59 (92%)	54 (100%)	0	0	100	100
10	W	54/59 (92%)	54 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	42/47 (89%)	40 (95%)	2 (5%)	0	100	100
12	Y	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
13	M	38/46 (83%)	38 (100%)	0	0	100	100
13	Z	38/46 (83%)	38 (100%)	0	0	100	100
All	All	3488/3614 (96%)	3411 (98%)	74 (2%)	3 (0%)	51	20

All (3) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Q	122/129 (95%)	118 (97%)	4 (3%)	38	5
5	E	89/95 (94%)	89 (100%)	0	100	100
5	R	89/95 (94%)	88 (99%)	1 (1%)	73	45
6	F	78/81 (96%)	77 (99%)	1 (1%)	69	35
6	S	78/81 (96%)	77 (99%)	1 (1%)	69	35
7	G	63/69 (91%)	58 (92%)	5 (8%)	12	0
7	T	63/69 (91%)	59 (94%)	4 (6%)	18	0
8	H	67/75 (89%)	65 (97%)	2 (3%)	41	7
8	U	67/75 (89%)	64 (96%)	3 (4%)	27	2
9	I	55/58 (95%)	54 (98%)	1 (2%)	59	24
9	V	55/58 (95%)	49 (89%)	6 (11%)	6	0
10	J	47/50 (94%)	46 (98%)	1 (2%)	53	16
10	W	47/50 (94%)	46 (98%)	1 (2%)	53	16
11	K	39/46 (85%)	37 (95%)	2 (5%)	24	2
11	X	39/46 (85%)	38 (97%)	1 (3%)	46	10
12	L	37/40 (92%)	37 (100%)	0	100	100
12	Y	37/40 (92%)	37 (100%)	0	100	100
13	M	34/38 (90%)	34 (100%)	0	100	100
13	Z	34/38 (90%)	34 (100%)	0	100	100
All	All	3042/3086 (99%)	2975 (98%)	67 (2%)	50	15

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	338	MET
1	A	369	ASP
2	B	33	LEU
2	B	59	GLN
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	86	MET

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Mol	Chain	Res	Type
2	B	91	ASN
2	B	115	ASP
2	B	171	LYS
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
6	F	37	LYS
7	G	18	PHE
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
7	G	54	ARG
8	H	60	TYR
8	H	61	LYS
9	I	36	LYS
10	J	7	GLU
11	K	47	ARG
11	K	54	ARG
1	N	38	ARG
1	N	109	PHE
1	N	363	LEU
1	N	369	ASP
2	O	33	LEU
2	O	60	GLU
2	O	68	LEU
2	O	78	LEU
2	O	91	ASN
2	O	92	ASN
2	O	115	ASP
2	O	171	LYS
2	O	217	LYS
2	O	226	MET
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	10	ASP
4	Q	20	ARG
4	Q	51	LEU
4	Q	143	ASN
5	R	79	LYS
6	S	54	ASN
7	T	18	PHE

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Mol	Chain	Res	Type
7	T	33	LEU
7	T	37	LEU
7	T	54	ARG
8	U	46	LYS
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	36	LYS
9	V	43	ARG
9	V	61	GLU
9	V	65	LYS
9	V	70	GLN
10	W	50	LEU
11	X	52	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	10	GLN
2	B	59	GLN
2	B	195	GLN
3	C	50	ASN
4	D	109	HIS
4	D	143	ASN
5	E	94	ASN
6	F	54	ASN
8	H	37	HIS
10	J	29	ASN
2	O	10	GLN
2	O	195	GLN
3	P	50	ASN
4	Q	101	HIS
4	Q	109	HIS
5	R	94	ASN
6	S	54	ASN
8	U	31	GLN
8	U	37	HIS
9	V	8	GLN
10	W	29	ASN
11	X	35	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	FME	A	1	1	8,9,10	0.52	0	7,9,11	0.77	0
2	FME	O	1	2	8,9,10	0.85	0	7,9,11	0.92	0
2	FME	B	1	2	8,9,10	3.32	3 (37%)	7,9,11	3.89	2 (28%)
1	FME	N	1	1	8,9,10	0.63	0	7,9,11	0.86	0

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

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

All (3) bond length outliers are listed below:

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

All (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
1	A	1	FME	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 135 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 125 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
20	DMU	B	731	-	10,10,34	0.29	0	9,9,45	0.54	0
22	LFA	T	622	-	10,10,19	0.21	0	9,9,18	0.12	0
22	LFA	P	625	-	14,14,19	0.30	0	13,13,18	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	PEK	P	264	-	52,52,52	0.73	2 (3%)	55,57,57	1.03	4 (7%)
19	CHD	C	271	-	29,32,32	0.63	0	48,51,51	1.63	9 (18%)
20	DMU	N	745	-	34,34,34	1.43	4 (11%)	45,45,45	1.33	6 (13%)
20	DMU	P	733	-	34,34,34	0.81	2 (5%)	45,45,45	1.46	4 (8%)
23	EDO	N	829	-	3,3,3	0.16	0	2,2,2	0.18	0
23	EDO	T	821	-	3,3,3	0.44	0	2,2,2	0.24	0
23	EDO	A	803	-	3,3,3	0.09	0	2,2,2	0.12	0
20	DMU	G	711	-	22,22,34	0.74	1 (4%)	27,27,45	1.37	3 (11%)
20	DMU	T	712	-	10,10,34	0.45	0	9,9,45	0.58	0
22	LFA	C	615	-	10,10,19	0.16	0	9,9,18	0.15	0
20	DMU	N	743	-	6,6,34	0.34	0	5,5,45	0.35	0
20	DMU	C	715[A]	-	34,34,34	1.31	6 (17%)	45,45,45	1.36	3 (6%)
23	EDO	C	809	-	3,3,3	0.20	0	2,2,2	0.54	0
22	LFA	C	625	-	14,14,19	0.26	0	13,13,18	0.44	0
20	DMU	O	741	-	10,10,34	0.53	0	9,9,45	0.55	0
27	PGV	P	266	-	50,50,50	0.91	3 (6%)	53,56,56	1.20	2 (3%)
14	HEA	N	516	21,1	44,67,67	1.24	6 (13%)	37,103,103	2.39	7 (18%)
22	LFA	C	611	-	10,10,19	0.26	0	9,9,18	0.30	0
23	EDO	R	811	-	3,3,3	0.12	0	2,2,2	0.08	0
18	CDL	C	270	-	86,86,99	0.56	1 (1%)	92,98,111	1.07	9 (9%)
20	DMU	P	734	-	34,34,34	0.94	1 (2%)	45,45,45	1.19	2 (4%)
22	LFA	T	621	-	16,16,19	0.40	0	15,15,18	0.31	0
20	DMU	A	745	-	34,34,34	1.18	3 (8%)	45,45,45	1.03	2 (4%)
22	LFA	C	626	-	12,12,19	0.21	0	11,11,18	0.24	0
27	PGV	C	266	-	50,50,50	1.08	4 (8%)	53,56,56	1.08	3 (5%)
18	CDL	N	521	-	93,93,99	0.36	0	99,105,111	0.46	0
22	LFA	N	627	-	13,13,19	0.32	0	12,12,18	0.53	0
20	DMU	B	742	-	22,22,34	0.69	0	27,27,45	1.16	2 (7%)
20	DMU	P	715[A]	-	34,34,34	1.22	4 (11%)	45,45,45	1.25	3 (6%)
23	EDO	P	827	-	3,3,3	0.54	0	2,2,2	1.16	0
20	DMU	G	713	-	22,22,34	0.54	0	27,27,45	1.18	2 (7%)
23	EDO	C	827	-	3,3,3	0.49	0	2,2,2	0.75	0
20	DMU	J	732	-	10,10,34	0.15	0	9,9,45	0.64	0
20	DMU	O	742	-	22,22,34	1.00	2 (9%)	27,27,45	1.09	3 (11%)
23	EDO	S	819	-	3,3,3	0.33	0	2,2,2	0.24	0
20	DMU	P	272	-	10,10,34	0.25	0	9,9,45	0.70	0
22	LFA	N	628	-	13,13,19	0.49	0	12,12,18	0.52	0
24	CUA	O	228	2	0,1,1	0.00	-	-	-	-
22	LFA	P	611	-	10,10,19	0.25	0	9,9,18	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	EDO	A	823	-	3,3,3	0.53	0	2,2,2	0.57	0
14	HEA	N	515[A]	-	44,67,67	1.27	6 (13%)	37,103,103	1.98	9 (24%)
21	PER	N	520	15,14	0,1,1	0.00	-	-	-	-
22	LFA	A	628	-	13,13,19	0.45	0	12,12,18	0.69	0
22	LFA	P	624	-	10,10,19	0.19	0	9,9,18	0.14	0
20	DMU	C	272	-	10,10,34	0.33	0	9,9,45	0.59	0
19	CHD	A	525	-	29,32,32	0.72	0	48,51,51	1.15	6 (12%)
23	EDO	E	813	-	3,3,3	0.36	0	2,2,2	0.20	0
23	EDO	F	817	-	3,3,3	0.64	0	2,2,2	0.34	0
22	LFA	C	612	-	5,5,19	0.20	0	4,4,18	0.16	0
20	DMU	P	722	-	22,22,34	0.46	0	27,27,45	1.06	2 (7%)
23	EDO	G	821	-	3,3,3	0.22	0	2,2,2	0.27	0
23	EDO	N	803	-	3,3,3	0.20	0	2,2,2	0.41	0
22	LFA	G	621	-	16,16,19	0.30	0	15,15,18	0.60	0
20	DMU	T	711	-	22,22,34	0.79	0	27,27,45	1.45	4 (14%)
20	DMU	A	743	-	6,6,34	0.30	0	5,5,45	0.38	0
22	LFA	P	716[B]	-	17,17,19	0.13	0	16,16,18	0.12	0
24	CUA	B	228	2	0,1,1	0.00	-	-	-	-
14	HEA	A	515[A]	-	44,67,67	1.38	6 (13%)	37,103,103	2.37	11 (29%)
23	EDO	B	805	-	3,3,3	1.04	0	2,2,2	0.97	0
20	DMU	P	721	-	6,6,34	0.18	0	5,5,45	0.62	0
20	DMU	C	721	-	6,6,34	0.21	0	5,5,45	0.58	0
20	DMU	C	733	-	34,34,34	1.17	5 (14%)	45,45,45	1.20	5 (11%)
19	CHD	T	86	-	29,32,32	0.74	0	48,51,51	1.10	2 (4%)
20	DMU	Y	747	-	22,22,34	0.56	0	27,27,45	1.18	2 (7%)
20	DMU	Z	746	-	7,7,34	0.16	0	6,6,45	0.48	0
21	PER	A	520	15,14	0,1,1	0.00	-	-	-	-
23	EDO	P	807	-	3,3,3	0.07	0	2,2,2	0.13	0
23	EDO	O	805	-	3,3,3	0.55	0	2,2,2	0.13	0
20	DMU	N	526	-	34,34,34	0.96	2 (5%)	45,45,45	1.14	2 (4%)
20	DMU	B	741	-	10,10,34	0.34	0	9,9,45	0.56	0
23	EDO	E	811	-	3,3,3	0.19	0	2,2,2	0.44	0
22	LFA	C	716[B]	-	17,17,19	0.17	0	16,16,18	0.16	0
22	LFA	A	627	-	13,13,19	0.72	0	12,12,18	0.30	0
22	LFA	P	615	-	10,10,19	0.19	0	9,9,18	0.17	0
27	PGV	P	267	-	50,50,50	0.75	1 (2%)	53,56,56	0.92	1 (1%)
19	CHD	G	86	-	29,32,32	0.73	0	48,51,51	1.08	2 (4%)
27	PGV	C	267	-	50,50,50	0.87	3 (6%)	53,56,56	1.09	3 (5%)
20	DMU	L	747	-	22,22,34	0.72	0	27,27,45	1.27	3 (11%)
23	EDO	P	809	-	3,3,3	0.40	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	EDO	F	819	-	3,3,3	0.44	0	2,2,2	0.39	0
22	LFA	G	622	-	10,10,19	0.18	0	9,9,18	0.16	0
20	DMU	W	732	-	10,10,34	0.16	0	9,9,45	0.57	0
23	EDO	N	801	-	3,3,3	0.53	0	2,2,2	0.12	0
23	EDO	N	825	-	3,3,3	0.51	0	2,2,2	0.23	0
20	DMU	C	734	-	34,34,34	0.99	1 (2%)	45,45,45	1.06	3 (6%)
20	DMU	P	714	-	34,34,34	0.73	0	45,45,45	1.06	3 (6%)
22	LFA	P	623	-	13,13,19	0.25	0	12,12,18	0.26	0
19	CHD	P	271	-	29,32,32	0.51	0	48,51,51	1.60	7 (14%)
18	CDL	P	270	-	86,86,99	0.47	0	92,98,111	0.95	6 (6%)
14	HEA	A	516	21,1	44,67,67	1.46	8 (18%)	37,103,103	2.63	6 (16%)
22	LFA	P	626	-	12,12,19	0.31	0	11,11,18	0.30	0
20	DMU	C	714	-	34,34,34	0.85	1 (2%)	45,45,45	1.25	6 (13%)
14	HEA	A	515[B]	-	44,67,67	1.35	6 (13%)	37,103,103	2.33	11 (29%)
23	EDO	E	815	-	3,3,3	0.40	0	2,2,2	0.60	0
23	EDO	N	823	-	3,3,3	0.61	0	2,2,2	0.41	0
20	DMU	G	712	-	10,10,34	0.23	0	9,9,45	0.59	0
23	EDO	A	825	-	3,3,3	0.41	0	2,2,2	0.51	0
19	CHD	N	525	-	29,32,32	0.82	0	48,51,51	0.91	2 (4%)
23	EDO	R	815	-	3,3,3	0.15	0	2,2,2	0.04	0
20	DMU	T	713	-	22,22,34	0.68	1 (4%)	27,27,45	1.39	5 (18%)
20	DMU	N	744	-	34,34,34	1.42	7 (20%)	45,45,45	1.54	5 (11%)
26	PEK	C	264	-	52,52,52	0.59	2 (3%)	55,57,57	0.81	2 (3%)
23	EDO	R	813	-	3,3,3	0.18	0	2,2,2	0.03	0
23	EDO	S	817	-	3,3,3	0.93	0	2,2,2	0.06	0
22	LFA	C	623	-	13,13,19	0.28	0	12,12,18	0.18	0
20	DMU	J	61	-	34,34,34	0.84	1 (2%)	45,45,45	1.05	2 (4%)
18	CDL	A	521	-	93,93,99	0.46	0	99,105,111	0.60	2 (2%)
22	LFA	C	624	-	10,10,19	0.28	0	9,9,18	0.20	0
18	CDL	A	522	-	63,63,99	0.53	0	69,75,111	1.18	6 (8%)
14	HEA	N	515[B]	-	44,67,67	1.30	6 (13%)	37,103,103	1.84	10 (27%)
20	DMU	M	746	-	7,7,34	0.19	0	6,6,45	0.79	0
20	DMU	C	722	-	22,22,34	0.52	0	27,27,45	0.94	2 (7%)
22	LFA	P	612	-	5,5,19	0.09	0	4,4,18	0.20	0
20	DMU	W	61	-	34,34,34	0.72	0	45,45,45	1.49	4 (8%)
22	LFA	P	614	-	14,14,19	0.17	0	13,13,18	0.16	0
20	DMU	A	526	-	34,34,34	1.05	2 (5%)	45,45,45	1.12	2 (4%)
20	DMU	A	744	-	34,34,34	1.47	6 (17%)	45,45,45	1.19	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	DMU	O	731	-	10,10,34	0.21	0	9,9,45	0.46	0
22	LFA	C	614	-	14,14,19	0.21	0	13,13,18	0.21	0
18	CDL	N	522	-	63,63,99	0.50	1 (1%)	69,75,111	1.04	5 (7%)
23	EDO	C	807	-	3,3,3	0.17	0	2,2,2	0.20	0
23	EDO	A	801	-	3,3,3	0.66	0	2,2,2	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	B	731	-	-	6/8/8/59	-
22	LFA	T	622	-	-	4/8/8/17	-
22	LFA	P	625	-	-	4/12/12/17	-
26	PEK	P	264	-	-	18/56/56/56	-
19	CHD	C	271	-	-	6/7/74/74	0/4/4/4
20	DMU	N	745	-	-	7/19/59/59	0/2/2/2
20	DMU	P	733	-	-	6/19/59/59	0/2/2/2
23	EDO	N	829	-	-	0/1/1/1	-
23	EDO	T	821	-	-	0/1/1/1	-
23	EDO	A	803	-	-	0/1/1/1	-
20	DMU	G	711	-	-	3/13/33/59	0/1/1/2
20	DMU	T	712	-	-	4/8/8/59	-
22	LFA	C	615	-	-	2/8/8/17	-
20	DMU	N	743	-	-	3/4/4/59	-
20	DMU	C	715[A]	-	-	3/19/59/59	0/2/2/2
23	EDO	C	809	-	-	0/1/1/1	-
22	LFA	C	625	-	-	3/12/12/17	-
20	DMU	O	741	-	-	4/8/8/59	-
27	PGV	P	266	-	-	8/55/55/55	-
14	HEA	N	516	21,1	3/3/7/16	0/24/76/76	-
22	LFA	C	611	-	-	5/8/8/17	-
23	EDO	R	811	-	-	1/1/1/1	-
18	CDL	C	270	-	-	49/97/97/110	-
20	DMU	P	734	-	-	10/19/59/59	0/2/2/2
22	LFA	T	621	-	-	9/14/14/17	-
20	DMU	A	745	-	-	5/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LFA	C	626	-	-	4/10/10/17	-
27	PGV	C	266	-	-	7/55/55/55	-
18	CDL	N	521	-	-	53/104/104/110	-
22	LFA	N	627	-	-	5/11/11/17	-
20	DMU	B	742	-	-	8/13/33/59	0/1/1/2
20	DMU	P	715[A]	-	-	6/19/59/59	0/2/2/2
23	EDO	P	827	-	-	0/1/1/1	-
20	DMU	G	713	-	-	8/13/33/59	0/1/1/2
23	EDO	C	827	-	-	1/1/1/1	-
20	DMU	J	732	-	-	5/8/8/59	-
20	DMU	O	742	-	-	7/13/33/59	0/1/1/2
23	EDO	S	819	-	-	0/1/1/1	-
20	DMU	P	272	-	-	0/8/8/59	-
22	LFA	N	628	-	-	6/11/11/17	-
22	LFA	P	611	-	-	5/8/8/17	-
23	EDO	A	823	-	-	0/1/1/1	-
14	HEA	N	515[A]	-	-	4/24/76/76	-
22	LFA	A	628	-	-	5/11/11/17	-
22	LFA	P	624	-	-	6/8/8/17	-
20	DMU	C	272	-	-	4/8/8/59	-
19	CHD	A	525	-	-	0/7/74/74	0/4/4/4
23	EDO	E	813	-	-	0/1/1/1	-
23	EDO	F	817	-	-	0/1/1/1	-
22	LFA	C	612	-	-	1/3/3/17	-
20	DMU	P	722	-	-	8/13/33/59	0/1/1/2
23	EDO	G	821	-	-	0/1/1/1	-
23	EDO	N	803	-	-	1/1/1/1	-
22	LFA	G	621	-	-	9/14/14/17	-
20	DMU	T	711	-	-	7/13/33/59	0/1/1/2
20	DMU	A	743	-	-	2/4/4/59	-
22	LFA	P	716[B]	-	-	6/15/15/17	-
14	HEA	A	515[A]	-	-	3/24/76/76	-
23	EDO	B	805	-	-	0/1/1/1	-
20	DMU	P	721	-	-	3/4/4/59	-
20	DMU	C	721	-	-	2/4/4/59	-
20	DMU	C	733	-	-	9/19/59/59	0/2/2/2
19	CHD	T	86	-	-	0/7/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	Y	747	-	-	9/13/33/59	0/1/1/2
20	DMU	Z	746	-	-	2/5/5/59	-
23	EDO	P	807	-	-	1/1/1/1	-
23	EDO	O	805	-	-	0/1/1/1	-
20	DMU	N	526	-	-	6/19/59/59	0/2/2/2
20	DMU	B	741	-	-	4/8/8/59	-
23	EDO	E	811	-	-	0/1/1/1	-
22	LFA	C	716[B]	-	-	5/15/15/17	-
22	LFA	A	627	-	-	5/11/11/17	-
22	LFA	P	615	-	-	5/8/8/17	-
27	PGV	P	267	-	-	12/55/55/55	-
19	CHD	G	86	-	-	0/7/74/74	0/4/4/4
27	PGV	C	267	-	-	13/55/55/55	-
23	EDO	P	809	-	-	0/1/1/1	-
23	EDO	F	819	-	-	0/1/1/1	-
22	LFA	G	622	-	-	3/8/8/17	-
20	DMU	W	732	-	-	7/8/8/59	-
23	EDO	N	801	-	-	0/1/1/1	-
23	EDO	N	825	-	-	0/1/1/1	-
20	DMU	C	734	-	-	8/19/59/59	0/2/2/2
20	DMU	P	714	-	-	5/19/59/59	0/2/2/2
22	LFA	P	623	-	-	5/11/11/17	-
19	CHD	P	271	-	-	6/7/74/74	0/4/4/4
18	CDL	P	270	-	-	49/97/97/110	-
14	HEA	A	516	21,1	3/3/7/16	0/24/76/76	-
22	LFA	P	626	-	-	5/10/10/17	-
20	DMU	C	714	-	-	8/19/59/59	0/2/2/2
14	HEA	A	515[B]	-	-	0/24/76/76	-
23	EDO	E	815	-	-	1/1/1/1	-
23	EDO	N	823	-	-	0/1/1/1	-
20	DMU	G	712	-	-	4/8/8/59	-
23	EDO	A	825	-	-	1/1/1/1	-
19	CHD	N	525	-	-	0/7/74/74	0/4/4/4
23	EDO	R	815	-	-	1/1/1/1	-
20	DMU	T	713	-	-	5/13/33/59	0/1/1/2
20	DMU	N	744	-	-	5/19/59/59	0/2/2/2
26	PEK	C	264	-	-	15/56/56/56	-

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

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	745	DMU	O16-C6	-4.51	1.32	1.40
14	A	516	HEA	CMB-C2B	-4.43	1.42	1.51
20	A	744	DMU	O49-C1	-4.38	1.32	1.43
20	P	715[A]	DMU	O3-C5	-4.35	1.32	1.43
14	A	515[A]	HEA	C16-C17	-4.29	1.39	1.53
14	A	515[B]	HEA	C16-C17	-4.29	1.39	1.53
14	A	516	HEA	C3C-C2C	-4.07	1.34	1.40
20	C	733	DMU	O16-C6	-3.68	1.33	1.40
20	P	734	DMU	O3-C5	-3.65	1.34	1.43
14	N	516	HEA	CMD-C2D	-3.63	1.42	1.51
14	N	515[A]	HEA	C16-C17	-3.62	1.41	1.53
14	N	515[B]	HEA	C16-C17	-3.62	1.41	1.53
27	C	266	PGV	C21-C20	3.62	1.65	1.52
20	N	744	DMU	O49-C1	-3.42	1.34	1.43
26	P	264	PEK	C2-C1	3.32	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	734	DMU	O3-C5	-3.28	1.35	1.43
20	N	745	DMU	C10-C5	-3.23	1.43	1.52
20	C	715[A]	DMU	O5-C6	-3.22	1.33	1.41
20	N	744	DMU	O5-C6	-3.18	1.33	1.41
14	A	516	HEA	CAD-C3D	-3.00	1.47	1.52
14	N	516	HEA	CMB-C2B	-2.97	1.45	1.51
20	C	715[A]	DMU	O3-C5	-2.96	1.36	1.43
20	A	745	DMU	C10-C5	-2.93	1.44	1.52
14	N	515[A]	HEA	C3C-C2C	-2.92	1.36	1.40
14	N	515[B]	HEA	C3C-C2C	-2.92	1.36	1.40
20	N	526	DMU	O16-C6	-2.90	1.35	1.40
14	A	515[A]	HEA	C14-C15	-2.83	1.26	1.33
14	A	515[B]	HEA	C14-C15	-2.83	1.26	1.33
14	A	516	HEA	CMD-C2D	-2.82	1.44	1.51
20	A	744	DMU	O55-C2	2.78	1.49	1.43
20	C	733	DMU	O3-C5	-2.71	1.36	1.43
20	O	742	DMU	O16-C6	-2.67	1.35	1.40
26	P	264	PEK	C23-C22	-2.67	1.42	1.52
20	N	744	DMU	O1-C10	2.63	1.48	1.41
14	N	515[A]	HEA	C1B-NB	2.63	1.41	1.36
14	N	515[B]	HEA	C1B-NB	2.63	1.41	1.36
20	O	742	DMU	O16-C18	2.62	1.50	1.43
20	N	744	DMU	C10-C5	-2.61	1.45	1.52
27	C	267	PGV	O01-C02	-2.58	1.40	1.46
20	N	745	DMU	C7-C5	-2.55	1.45	1.52
18	C	270	CDL	C11-CA5	2.54	1.58	1.50
20	C	715[A]	DMU	C10-C5	-2.54	1.45	1.52
14	A	516	HEA	C1C-CHC	-2.48	1.34	1.41
27	P	267	PGV	P-O14	-2.48	1.43	1.55
20	C	715[A]	DMU	O2-C8	2.47	1.48	1.43
20	A	744	DMU	O3-C5	-2.47	1.37	1.43
20	N	744	DMU	O3-C5	-2.47	1.37	1.43
14	N	516	HEA	C4D-ND	2.44	1.41	1.36
20	C	733	DMU	O5-C6	-2.41	1.35	1.41
14	A	516	HEA	C3D-C2D	2.38	1.44	1.37
26	C	264	PEK	C22-C21	2.38	1.57	1.50
27	C	266	PGV	P-O13	-2.37	1.42	1.50
20	C	714	DMU	C7-C5	-2.36	1.46	1.52
27	C	266	PGV	P-O14	-2.36	1.44	1.55
20	G	711	DMU	C3-C4	-2.34	1.48	1.53
14	N	516	HEA	C3D-C2D	2.34	1.44	1.37
20	P	715[A]	DMU	C7-C5	-2.34	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	P	715[A]	DMU	C10-C5	-2.31	1.45	1.52
14	A	515[A]	HEA	C1C-NC	2.30	1.40	1.36
14	A	515[B]	HEA	C1C-NC	2.30	1.40	1.36
27	C	267	PGV	O04-C19	-2.30	1.15	1.22
20	C	715[A]	DMU	C7-C5	-2.29	1.46	1.52
18	N	522	CDL	OA7-CA5	-2.27	1.15	1.22
20	N	744	DMU	O16-C6	-2.27	1.36	1.40
20	A	744	DMU	O16-C6	-2.27	1.36	1.40
14	N	516	HEA	C1B-CHB	2.26	1.47	1.41
20	N	526	DMU	O1-C10	2.25	1.47	1.41
20	A	526	DMU	C10-C5	-2.24	1.46	1.52
20	C	715[A]	DMU	O16-C6	-2.23	1.36	1.40
20	P	733	DMU	O5-C6	-2.22	1.36	1.41
14	N	515[A]	HEA	C1C-NC	2.21	1.40	1.36
14	N	515[B]	HEA	C1C-NC	2.21	1.40	1.36
20	N	745	DMU	O1-C10	2.20	1.47	1.41
20	N	744	DMU	C7-C5	-2.20	1.46	1.52
20	C	733	DMU	C7-C5	-2.19	1.46	1.52
20	A	526	DMU	C7-C5	-2.17	1.46	1.52
20	A	744	DMU	O5-C6	-2.17	1.36	1.41
20	J	61	DMU	C7-C5	-2.15	1.46	1.52
27	C	266	PGV	C03-C02	2.14	1.57	1.50
20	A	745	DMU	C3-C4	2.13	1.58	1.52
27	P	266	PGV	O03-C01	2.13	1.50	1.45
26	C	264	PEK	C23-C22	-2.12	1.44	1.52
20	P	715[A]	DMU	O5-C6	-2.11	1.36	1.41
20	C	733	DMU	C10-C5	-2.10	1.46	1.52
14	N	515[A]	HEA	CMC-C2C	-2.10	1.47	1.51
14	N	515[B]	HEA	CMC-C2C	-2.10	1.47	1.51
20	A	745	DMU	O7-C10	2.08	1.47	1.41
14	A	515[A]	HEA	CMB-C2B	-2.08	1.47	1.51
14	A	515[B]	HEA	CMB-C2B	-2.08	1.47	1.51
14	A	515[A]	HEA	C27-C19	-2.08	1.45	1.50
20	P	733	DMU	C6-C1	-2.08	1.46	1.52
20	A	744	DMU	O1-C10	2.07	1.47	1.41
14	A	516	HEA	C1B-CHB	2.07	1.46	1.41
27	P	266	PGV	P-O14	-2.06	1.45	1.55
14	A	515[A]	HEA	C12-C13	2.05	1.60	1.53
14	A	515[B]	HEA	C12-C13	2.05	1.60	1.53
27	C	267	PGV	C22-C21	2.05	1.63	1.51
27	P	266	PGV	C01-C02	2.05	1.57	1.50
14	A	515[B]	HEA	C22-C23	2.04	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	516	HEA	C3B-C11	-2.04	1.51	1.52
14	A	516	HEA	C18-C19	2.04	1.37	1.33
14	N	515[A]	HEA	O11-C11	2.01	1.47	1.42
14	N	515[B]	HEA	O11-C11	2.01	1.47	1.42
20	T	713	DMU	C6-C1	-2.01	1.46	1.52

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	516	HEA	C1B-C2B-C3B	-12.95	97.99	107.00
14	N	516	HEA	C1B-C2B-C3B	-10.94	99.39	107.00
14	A	515[A]	HEA	C1B-C2B-C3B	-7.14	102.03	107.00
14	A	515[B]	HEA	C1B-C2B-C3B	-7.14	102.03	107.00
20	N	744	DMU	O16-C6-C1	6.36	118.23	108.30
19	P	271	CHD	C17-C13-C14	-6.31	93.73	100.09
18	A	522	CDL	OA6-CA4-CA3	5.79	129.36	108.40
14	A	515[A]	HEA	C3C-C4C-NC	5.59	116.44	109.21
14	A	515[B]	HEA	C3C-C4C-NC	5.59	116.44	109.21
14	N	515[A]	HEA	C27-C19-C20	5.51	124.54	115.27
20	P	715[A]	DMU	O16-C6-C1	5.44	116.80	108.30
20	W	61	DMU	C10-C5-C7	5.42	121.29	110.00
20	C	715[A]	DMU	O16-C6-C1	5.28	116.55	108.30
19	C	271	CHD	C17-C13-C14	-5.17	94.88	100.09
20	P	734	DMU	C10-C5-C7	5.08	120.58	110.00
27	P	266	PGV	O03-C19-O04	-5.04	110.86	123.59
14	A	516	HEA	C4B-C3B-C2B	5.03	110.38	106.87
20	P	733	DMU	C10-C5-C7	4.95	120.31	110.00
14	N	516	HEA	CMB-C2B-C1B	4.92	136.03	128.46
14	A	516	HEA	CMB-C2B-C1B	4.84	135.90	128.46
14	A	515[A]	HEA	C26-C15-C16	-4.79	107.21	115.27
14	A	515[B]	HEA	C26-C15-C16	-4.79	107.21	115.27
20	W	61	DMU	O16-C6-C1	4.79	115.78	108.30
14	N	515[A]	HEA	C1B-C2B-C3B	-4.76	103.68	107.00
14	N	515[B]	HEA	C1B-C2B-C3B	-4.76	103.68	107.00
20	T	711	DMU	O5-C6-C1	4.74	120.38	110.35
20	G	711	DMU	O5-C6-C1	4.72	120.34	110.35
20	T	713	DMU	O16-C6-C1	4.69	115.63	108.30
18	N	522	CDL	OA6-CA5-C11	4.69	121.60	111.50
19	C	271	CHD	C16-C17-C20	4.66	119.35	112.15
27	C	267	PGV	C23-C22-C21	4.64	137.97	114.42
20	Y	747	DMU	O16-C6-C1	4.49	115.32	108.30
19	C	271	CHD	C14-C13-C12	4.49	111.58	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	61	DMU	O16-C6-C1	4.31	115.04	108.30
14	N	516	HEA	CAD-CBD-CGD	-4.29	105.48	112.67
26	P	264	PEK	O01-C1-O02	-4.27	113.37	123.70
20	L	747	DMU	O16-C6-C1	4.25	114.94	108.30
14	A	515[A]	HEA	C27-C19-C20	4.24	122.40	115.27
19	P	271	CHD	C14-C13-C12	4.16	111.28	107.40
20	B	742	DMU	O16-C6-C1	4.09	114.69	108.30
20	A	744	DMU	O16-C6-C1	4.08	114.67	108.30
20	A	745	DMU	C10-O1-C9	4.06	121.65	113.69
18	A	522	CDL	CA4-OA6-CA5	4.06	127.78	117.79
20	N	526	DMU	O16-C6-C1	4.00	114.54	108.30
20	P	733	DMU	C6-O5-C4	3.98	121.50	113.69
20	A	526	DMU	O16-C6-C1	3.95	114.47	108.30
19	P	271	CHD	C16-C17-C20	3.95	118.25	112.15
14	N	515[A]	HEA	C13-C12-C11	-3.90	108.48	114.35
14	N	515[B]	HEA	C13-C12-C11	-3.90	108.48	114.35
20	P	714	DMU	O16-C6-C1	3.90	114.39	108.30
14	A	515[A]	HEA	CMB-C2B-C3B	3.88	132.29	124.69
14	A	515[B]	HEA	CMB-C2B-C3B	3.88	132.29	124.69
18	C	270	CDL	OB6-CB5-C51	3.87	119.84	111.50
18	P	270	CDL	OB6-CB5-C51	3.80	119.70	111.50
19	C	271	CHD	C22-C23-C24	-3.80	105.42	113.59
20	G	713	DMU	O16-C6-C1	3.79	114.22	108.30
20	C	714	DMU	O16-C6-C1	3.76	114.17	108.30
20	C	734	DMU	C10-C5-C7	3.68	117.66	110.00
14	N	515[A]	HEA	C3C-C4C-NC	3.63	113.91	109.21
14	N	515[B]	HEA	C3C-C4C-NC	3.63	113.91	109.21
20	P	733	DMU	O5-C6-C1	3.62	118.02	110.35
18	C	270	CDL	OA6-CA5-OA7	-3.56	115.09	123.70
20	N	745	DMU	C10-O1-C9	3.56	120.67	113.69
20	C	715[A]	DMU	C10-O1-C9	3.55	120.66	113.69
20	P	733	DMU	O5-C4-C3	3.47	117.07	109.75
14	N	515[B]	HEA	C27-C19-C20	3.45	121.08	115.27
14	A	515[A]	HEA	C13-C12-C11	-3.43	109.19	114.35
14	A	515[B]	HEA	C13-C12-C11	-3.43	109.19	114.35
18	C	270	CDL	OA7-CA5-C11	3.41	137.02	123.73
27	P	266	PGV	O03-C19-C20	3.40	122.57	111.91
18	P	270	CDL	OB5-PB2-OB3	3.29	121.93	109.07
18	C	270	CDL	OB5-PB2-OB3	3.27	121.86	109.07
19	G	86	CHD	C18-C13-C12	3.26	112.38	109.07
20	A	744	DMU	C10-C5-C7	3.21	116.68	110.00
14	A	515[A]	HEA	C20-C19-C18	-3.18	114.68	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	264	PEK	C2-C3-C4	3.11	118.77	113.23
14	A	516	HEA	CAD-CBD-CGD	-3.11	107.46	112.67
14	N	515[A]	HEA	CMB-C2B-C3B	3.08	130.71	124.69
14	N	515[B]	HEA	CMB-C2B-C3B	3.08	130.71	124.69
20	N	526	DMU	O3-C5-C10	3.07	117.51	110.05
18	N	522	CDL	OA6-CA4-CA3	3.07	119.50	108.40
20	T	711	DMU	O16-C6-C1	3.02	113.02	108.30
20	C	714	DMU	C6-O5-C4	3.02	119.61	113.69
27	C	267	PGV	C24-C23-C22	2.99	129.61	114.42
19	T	86	CHD	C18-C13-C12	2.97	112.09	109.07
20	C	733	DMU	C10-C5-C7	2.95	116.13	110.00
20	G	711	DMU	C6-C1-C2	2.92	116.07	110.00
26	P	264	PEK	O02-C1-C2	2.86	134.89	123.73
14	A	515[B]	HEA	C27-C19-C20	2.84	120.05	115.27
18	N	522	CDL	OA8-CA6-CA4	2.82	116.64	108.43
20	O	742	DMU	O16-C6-C1	2.75	112.60	108.30
20	O	742	DMU	C57-C4-C3	-2.75	106.56	113.00
18	A	521	CDL	OB5-PB2-OB3	-2.75	98.34	109.07
20	N	744	DMU	C11-C9-C8	-2.74	106.58	113.00
19	C	271	CHD	C16-C17-C13	-2.73	100.87	103.55
18	A	522	CDL	OA8-CA6-CA4	2.71	116.31	108.43
20	N	744	DMU	C6-O5-C4	-2.70	108.40	113.69
27	C	266	PGV	O03-C19-O04	-2.67	116.85	123.59
20	C	714	DMU	O5-C6-C1	2.65	115.96	110.35
19	A	525	CHD	C22-C20-C17	-2.65	104.81	110.28
14	N	515[A]	HEA	CMC-C2C-C1C	-2.63	124.42	128.46
14	N	515[B]	HEA	CMC-C2C-C1C	-2.63	124.42	128.46
20	P	722	DMU	O5-C6-C1	2.62	115.90	110.35
19	A	525	CHD	C5-C6-C7	2.62	117.35	114.46
20	T	711	DMU	C6-C1-C2	2.61	115.43	110.00
20	N	745	DMU	C57-C4-C3	-2.61	105.74	113.33
18	N	522	CDL	OA6-CA4-CA6	-2.61	98.97	108.40
20	C	714	DMU	O3-C5-C10	2.60	116.37	110.05
14	A	515[A]	HEA	C16-C15-C14	2.60	126.37	121.12
14	A	515[B]	HEA	C16-C15-C14	2.60	126.37	121.12
18	P	270	CDL	OA5-PA1-OA3	2.59	119.18	109.07
20	C	733	DMU	O5-C6-C1	2.58	115.82	110.35
18	A	522	CDL	OA6-CA5-C11	2.58	117.06	111.50
14	A	515[A]	HEA	CMD-C2D-C3D	2.57	129.79	124.94
14	A	515[B]	HEA	CMD-C2D-C3D	2.57	129.79	124.94
27	C	266	PGV	C15-C14-C13	-2.56	102.63	113.79
19	T	86	CHD	C17-C13-C12	-2.55	115.34	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	270	CDL	OA5-PA1-OA3	2.53	118.97	109.07
18	N	522	CDL	OA6-CA5-OA7	-2.51	117.63	123.70
20	N	745	DMU	C10-O7-C3	-2.50	111.77	117.96
26	P	264	PEK	O13-P-O14	2.50	124.60	112.24
18	P	270	CDL	OA4-PA1-OA3	2.49	124.57	112.24
20	C	734	DMU	O5-C6-O16	2.48	115.84	109.97
20	N	745	DMU	C7-C8-C9	2.46	114.64	110.24
14	A	515[A]	HEA	C17-C16-C15	2.46	121.08	112.98
14	A	515[B]	HEA	C17-C16-C15	2.46	121.08	112.98
19	P	271	CHD	C16-C17-C13	-2.46	101.14	103.55
20	L	747	DMU	C6-O5-C4	2.46	118.51	113.69
14	N	516	HEA	C13-C12-C11	-2.45	110.67	114.35
18	A	522	CDL	OA7-CA5-C11	-2.45	114.17	123.73
19	P	271	CHD	C18-C13-C17	2.45	115.04	111.21
19	A	525	CHD	O12-C12-C13	-2.44	106.90	111.03
20	T	713	DMU	O5-C4-C3	2.43	114.11	109.69
20	T	713	DMU	C2-C3-C4	2.42	114.56	110.24
20	A	526	DMU	C10-C5-C7	2.41	115.02	110.00
18	C	270	CDL	OB2-PB2-OB3	-2.40	99.69	109.07
20	C	722	DMU	O5-C6-C1	2.38	115.39	110.35
20	P	734	DMU	O5-C6-O16	2.38	115.60	109.97
20	L	747	DMU	O5-C6-C1	2.38	115.38	110.35
20	A	744	DMU	C2-C3-C4	-2.36	105.52	110.93
20	J	61	DMU	C10-C5-C7	2.35	114.88	110.00
20	C	733	DMU	C8-C7-C5	2.33	114.88	110.82
20	C	733	DMU	C6-C1-C2	2.32	114.83	110.00
20	C	715[A]	DMU	O5-C6-C1	2.32	115.26	110.35
14	N	516	HEA	C3C-C4C-NC	2.31	112.19	109.21
20	W	61	DMU	O1-C10-C5	2.30	115.23	110.35
18	A	522	CDL	OA5-PA1-OA3	-2.30	100.08	109.07
20	B	742	DMU	O5-C6-C1	2.29	115.21	110.35
20	G	711	DMU	O16-C6-C1	2.29	111.89	108.30
20	P	714	DMU	O3-C5-C10	2.29	115.61	110.05
20	O	742	DMU	O5-C4-C57	2.29	112.13	106.44
20	G	713	DMU	O5-C6-O16	2.29	115.40	109.97
14	N	515[A]	HEA	C20-C19-C18	-2.29	116.48	121.12
20	Y	747	DMU	O5-C6-C1	2.28	115.17	110.35
20	P	714	DMU	C10-C5-C7	2.28	114.74	110.00
14	A	516	HEA	C27-C19-C20	2.27	119.09	115.27
20	P	715[A]	DMU	C10-O7-C3	-2.26	112.38	117.96
20	T	713	DMU	O5-C6-O16	2.25	115.31	109.97
14	N	516	HEA	C25-C23-C22	-2.25	116.13	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	744	DMU	C2-C3-C4	-2.25	105.77	110.93
18	P	270	CDL	OA6-CA5-C11	-2.25	106.66	111.50
19	A	525	CHD	C13-C17-C20	2.24	122.17	119.50
19	G	86	CHD	C14-C13-C12	-2.23	105.32	107.40
18	P	270	CDL	OA4-PA1-OA5	-2.23	97.38	107.75
19	A	525	CHD	C23-C22-C20	-2.23	111.72	114.72
19	N	525	CHD	C22-C20-C17	-2.22	105.69	110.28
14	A	515[B]	HEA	C21-C20-C19	-2.21	105.70	112.98
18	C	270	CDL	O1-C1-CB2	2.20	117.27	109.56
27	C	266	PGV	O14-P-O12	-2.18	97.60	107.75
20	C	714	DMU	C18-O16-C6	-2.18	110.23	113.84
20	C	733	DMU	C10-O7-C3	-2.18	112.58	117.96
19	C	271	CHD	C6-C7-C8	2.17	113.80	111.48
20	N	745	DMU	O5-C6-C1	2.17	114.94	110.35
20	C	714	DMU	C10-C5-C7	2.17	114.51	110.00
14	N	516	HEA	C27-C19-C20	2.16	118.90	115.27
20	T	711	DMU	C57-C4-C3	-2.15	107.96	113.00
20	N	744	DMU	C10-O1-C9	2.15	117.91	113.69
20	C	734	DMU	O3-C5-C7	2.15	115.31	110.35
20	W	61	DMU	O1-C9-C8	-2.15	105.79	109.69
19	P	271	CHD	C17-C13-C12	-2.14	115.71	117.67
27	P	267	PGV	O04-C19-C20	2.13	132.06	123.73
14	N	515[A]	HEA	C3A-C4A-NA	2.13	114.97	110.94
14	N	515[B]	HEA	C3A-C4A-NA	2.13	114.97	110.94
26	C	264	PEK	O13-P-O14	2.12	122.74	112.24
26	C	264	PEK	C03-C02-C01	2.12	116.80	111.79
14	N	515[A]	HEA	C16-C17-C18	2.12	118.83	111.88
14	N	515[B]	HEA	C25-C23-C22	-2.12	116.53	122.65
18	A	521	CDL	OB4-PB2-OB2	2.11	117.56	107.75
20	T	713	DMU	C57-C4-C3	-2.11	108.07	113.00
19	C	271	CHD	C4-C5-C10	2.09	114.88	112.66
27	C	267	PGV	C25-C24-C23	2.08	124.98	114.42
20	P	722	DMU	O16-C6-C1	2.07	111.54	108.30
19	A	525	CHD	C14-C8-C9	2.06	112.54	109.71
20	P	715[A]	DMU	O5-C4-C57	2.05	111.54	106.44
20	A	745	DMU	C10-C5-C7	2.05	114.27	110.00
19	N	525	CHD	O7-C7-C8	2.05	114.01	109.43
19	C	271	CHD	C18-C13-C17	2.05	114.42	111.21
14	A	515[B]	HEA	C25-C23-C22	-2.05	116.73	122.65
20	N	745	DMU	C11-C9-C8	-2.04	108.23	113.00
19	C	271	CHD	C17-C13-C12	-2.04	115.81	117.67
14	N	515[B]	HEA	C17-C18-C19	2.03	132.56	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	516	HEA	C13-C12-C11	-2.03	111.30	114.35
14	N	515[B]	HEA	C21-C20-C19	-2.03	106.30	112.98
18	C	270	CDL	OA6-CA4-CA6	-2.03	101.05	108.40
18	C	270	CDL	CA6-CA4-CA3	2.03	116.58	111.79
19	P	271	CHD	C15-C14-C8	2.02	121.15	118.33
14	A	515[A]	HEA	C20-C21-C22	-2.01	105.26	111.88
20	C	722	DMU	O16-C6-C1	2.01	111.44	108.30

All (6) chirality outliers are listed below:

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

All (712) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	515[A]	HEA	C18-C19-C20-C21
14	A	515[A]	HEA	C27-C19-C20-C21
18	A	521	CDL	CA2-OA2-PA1-OA3
18	A	521	CDL	C11-CA5-OA6-CA4
18	A	521	CDL	CB2-OB2-PB2-OB3
18	A	521	CDL	C51-CB5-OB6-CB4
18	A	522	CDL	C1-CA2-OA2-PA1
18	A	522	CDL	C51-CB5-OB6-CB4
18	C	270	CDL	C1-CA2-OA2-PA1
18	C	270	CDL	CA2-OA2-PA1-OA3
18	C	270	CDL	C11-CA5-OA6-CA4
18	C	270	CDL	CB3-OB5-PB2-OB4
18	C	270	CDL	OB7-CB5-OB6-CB4
18	C	270	CDL	C51-CB5-OB6-CB4
18	N	521	CDL	CA2-OA2-PA1-OA3
18	N	521	CDL	CA3-OA5-PA1-OA3
18	N	521	CDL	C11-CA5-OA6-CA4
18	N	521	CDL	CB2-OB2-PB2-OB5
18	N	521	CDL	C51-CB5-OB6-CB4
18	N	522	CDL	CA2-C1-CB2-OB2
18	N	522	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
18	N	522	CDL	C11-CA5-OA6-CA4
18	N	522	CDL	CB3-OB5-PB2-OB3
18	N	522	CDL	CB3-OB5-PB2-OB4
18	N	522	CDL	C51-CB5-OB6-CB4
18	P	270	CDL	C1-CA2-OA2-PA1
18	P	270	CDL	CA2-OA2-PA1-OA3
18	P	270	CDL	CB3-OB5-PB2-OB4
18	P	270	CDL	OB7-CB5-OB6-CB4
18	P	270	CDL	C51-CB5-OB6-CB4
19	P	271	CHD	C13-C17-C20-C21
20	A	744	DMU	C19-C18-O16-C6
20	C	722	DMU	C1-C6-O16-C18
20	C	722	DMU	O5-C6-O16-C18
20	C	733	DMU	C1-C6-O16-C18
20	G	711	DMU	C19-C18-O16-C6
20	N	744	DMU	O5-C6-O16-C18
20	O	742	DMU	C19-C18-O16-C6
20	P	722	DMU	C19-C18-O16-C6
20	T	711	DMU	C19-C18-O16-C6
20	Y	747	DMU	O5-C6-O16-C18
26	C	264	PEK	C12-C13-C14-C15
26	P	264	PEK	C9-C10-C11-C12
26	P	264	PEK	C11-C12-C13-C14
26	P	264	PEK	C12-C13-C14-C15
18	C	270	CDL	OB9-CB7-OB8-CB6
19	P	271	CHD	C16-C17-C20-C21
19	C	271	CHD	C13-C17-C20-C21
19	C	271	CHD	C13-C17-C20-C22
19	P	271	CHD	C13-C17-C20-C22
18	A	521	CDL	OA7-CA5-OA6-CA4
18	A	521	CDL	OB7-CB5-OB6-CB4
18	A	522	CDL	OB7-CB5-OB6-CB4
18	C	270	CDL	OA7-CA5-OA6-CA4
18	N	521	CDL	OA7-CA5-OA6-CA4
18	N	521	CDL	OB7-CB5-OB6-CB4
18	N	522	CDL	OA7-CA5-OA6-CA4
18	N	522	CDL	OB7-CB5-OB6-CB4
20	C	734	DMU	O5-C4-C57-O61
19	C	271	CHD	C16-C17-C20-C21
19	P	271	CHD	C16-C17-C20-C22
18	A	521	CDL	C31-CA7-OA8-CA6
18	C	270	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
18	N	521	CDL	C31-CA7-OA8-CA6
18	A	521	CDL	OA9-CA7-OA8-CA6
18	N	521	CDL	OA9-CA7-OA8-CA6
19	C	271	CHD	C16-C17-C20-C22
20	P	734	DMU	O5-C4-C57-O61
18	C	270	CDL	O1-C1-CB2-OB2
18	N	522	CDL	O1-C1-CB2-OB2
18	P	270	CDL	O1-C1-CB2-OB2
18	N	522	CDL	C31-CA7-OA8-CA6
20	A	745	DMU	O5-C4-C57-O61
18	P	270	CDL	C11-CA5-OA6-CA4
20	G	711	DMU	O5-C4-C57-O61
20	C	714	DMU	C3-C4-C57-O61
22	P	716[B]	LFA	C12-C13-C14-C15
18	A	521	CDL	C72-C73-C74-C75
18	C	270	CDL	C51-C52-C53-C54
22	C	614	LFA	C10-C11-C12-C13
22	P	614	LFA	C9-C10-C11-C12
20	C	714	DMU	O5-C4-C57-O61
20	P	734	DMU	O6-C11-C9-O1
20	W	61	DMU	O6-C11-C9-O1
20	P	733	DMU	O6-C11-C9-C8
20	T	711	DMU	O5-C4-C57-O61
20	P	734	DMU	C3-C4-C57-O61
20	P	733	DMU	O6-C11-C9-O1
20	A	745	DMU	O6-C11-C9-C8
22	N	628	LFA	C9-C10-C11-C12
20	C	733	DMU	O6-C11-C9-C8
20	C	734	DMU	C3-C4-C57-O61
14	N	515[A]	HEA	C15-C16-C17-C18
27	P	267	PGV	C28-C29-C30-C31
20	N	745	DMU	O6-C11-C9-C8
20	W	61	DMU	O6-C11-C9-C8
27	C	266	PGV	C26-C27-C28-C29
27	P	266	PGV	C23-C24-C25-C26
20	A	745	DMU	O6-C11-C9-O1
18	A	522	CDL	OA7-CA5-OA6-CA4
18	N	522	CDL	OA9-CA7-OA8-CA6
18	P	270	CDL	C31-CA7-OA8-CA6
18	P	270	CDL	C71-CB7-OB8-CB6
20	T	711	DMU	C3-C4-C57-O61
20	A	745	DMU	C3-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
20	G	711	DMU	C3-C4-C57-O61
20	P	734	DMU	O6-C11-C9-C8
19	P	271	CHD	C21-C20-C22-C23
18	N	521	CDL	CA5-C11-C12-C13
18	N	521	CDL	OB6-CB4-CB6-OB8
14	N	515[A]	HEA	C27-C19-C20-C21
20	G	713	DMU	O5-C4-C57-O61
18	P	270	CDL	C51-C52-C53-C54
19	P	271	CHD	C17-C20-C22-C23
20	C	733	DMU	O6-C11-C9-O1
27	P	266	PGV	C26-C27-C28-C29
18	A	521	CDL	CA5-C11-C12-C13
18	A	521	CDL	CA7-C31-C32-C33
18	A	522	CDL	CA5-C11-C12-C13
18	A	522	CDL	CA7-C31-C32-C33
18	C	270	CDL	CB5-C51-C52-C53
18	N	522	CDL	CA7-C31-C32-C33
18	P	270	CDL	CA7-C31-C32-C33
18	P	270	CDL	CB5-C51-C52-C53
18	P	270	CDL	OA7-CA5-OA6-CA4
22	C	716[B]	LFA	C12-C13-C14-C15
22	P	716[B]	LFA	C11-C10-C9-C8
20	N	745	DMU	O5-C4-C57-O61
18	P	270	CDL	OB9-CB7-OB8-CB6
20	G	713	DMU	C3-C4-C57-O61
20	C	733	DMU	O5-C6-O16-C18
20	C	722	DMU	O16-C18-C19-C22
20	G	713	DMU	O16-C18-C19-C22
18	A	521	CDL	O1-C1-CB2-OB2
18	N	521	CDL	O1-C1-CB2-OB2
18	N	522	CDL	CA5-C11-C12-C13
18	A	521	CDL	CB3-OB5-PB2-OB2
18	C	270	CDL	CA2-OA2-PA1-OA5
18	C	270	CDL	CA3-OA5-PA1-OA2
18	N	522	CDL	CB3-OB5-PB2-OB2
18	P	270	CDL	CA2-OA2-PA1-OA5
18	P	270	CDL	CA3-OA5-PA1-OA2
20	P	733	DMU	O16-C18-C19-C22
18	A	521	CDL	CA2-C1-CB2-OB2
18	N	521	CDL	CA2-C1-CB2-OB2
14	N	515[A]	HEA	C18-C19-C20-C21
20	P	715[A]	DMU	O5-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
18	C	270	CDL	C31-CA7-OA8-CA6
20	C	722	DMU	C31-C34-C37-C40
18	A	521	CDL	C22-C23-C24-C25
18	A	521	CDL	C77-C78-C79-C80
18	C	270	CDL	C73-C74-C75-C76
18	P	270	CDL	C54-C55-C56-C57
20	B	741	DMU	C19-C22-C25-C28
20	C	721	DMU	C31-C34-C37-C40
20	C	722	DMU	C22-C25-C28-C31
22	G	621	LFA	C11-C12-C13-C14
22	P	614	LFA	C2-C3-C4-C5
20	B	742	DMU	C19-C22-C25-C28
20	N	526	DMU	O16-C18-C19-C22
20	W	732	DMU	C31-C34-C37-C40
22	C	614	LFA	C7-C8-C9-C10
27	C	267	PGV	C7-C8-C9-C10
18	N	521	CDL	C14-C15-C16-C17
22	P	623	LFA	C4-C5-C6-C7
26	C	264	PEK	C26-C27-C28-C29
20	N	526	DMU	O6-C11-C9-O1
26	P	264	PEK	C7-C8-C9-C10
18	A	522	CDL	C73-C74-C75-C76
18	C	270	CDL	C35-C36-C37-C38
20	C	714	DMU	C19-C22-C25-C28
22	T	621	LFA	C4-C5-C6-C7
27	C	266	PGV	C29-C30-C31-C32
27	C	266	PGV	C30-C31-C32-C33
20	C	733	DMU	C25-C28-C31-C34
20	G	712	DMU	C19-C22-C25-C28
20	Y	747	DMU	O16-C18-C19-C22
22	C	615	LFA	C5-C6-C7-C8
20	B	742	DMU	C1-C6-O16-C18
20	G	713	DMU	C1-C6-O16-C18
20	P	715[A]	DMU	C1-C6-O16-C18
18	A	521	CDL	C76-C77-C78-C79
18	P	270	CDL	C71-C72-C73-C74
22	C	614	LFA	C6-C7-C8-C9
26	C	264	PEK	C28-C29-C30-C31
27	C	267	PGV	C22-C23-C24-C25
27	P	267	PGV	C30-C31-C32-C33
20	N	745	DMU	O6-C11-C9-O1
22	C	624	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	P	611	LFA	C5-C6-C7-C8
22	P	615	LFA	C3-C4-C5-C6
27	C	267	PGV	C28-C29-C30-C31
26	P	264	PEK	C1-C2-C3-C4
18	A	522	CDL	C31-C32-C33-C34
20	C	714	DMU	C28-C31-C34-C37
20	C	733	DMU	C19-C22-C25-C28
20	C	733	DMU	C28-C31-C34-C37
20	N	526	DMU	C22-C25-C28-C31
20	O	741	DMU	C19-C22-C25-C28
20	P	733	DMU	C28-C31-C34-C37
20	Y	747	DMU	C22-C25-C28-C31
22	C	611	LFA	C5-C6-C7-C8
22	P	623	LFA	C3-C4-C5-C6
20	N	526	DMU	O6-C11-C9-C8
18	P	270	CDL	OA9-CA7-OA8-CA6
18	C	270	CDL	C56-C57-C58-C59
18	N	521	CDL	C13-C14-C15-C16
20	B	731	DMU	C19-C22-C25-C28
20	Z	746	DMU	C25-C28-C31-C34
22	P	611	LFA	C4-C5-C6-C7
18	A	522	CDL	C11-CA5-OA6-CA4
20	B	731	DMU	C31-C34-C37-C40
22	N	627	LFA	C6-C7-C8-C9
26	C	264	PEK	C34-C35-C36-C37
27	P	266	PGV	C12-C13-C14-C15
18	A	521	CDL	C14-C15-C16-C17
18	N	521	CDL	C80-C81-C82-C83
18	N	522	CDL	C73-C74-C75-C76
20	J	732	DMU	C31-C34-C37-C40
20	M	746	DMU	C25-C28-C31-C34
22	C	625	LFA	C4-C5-C6-C7
22	P	614	LFA	C7-C8-C9-C10
22	P	615	LFA	C7-C8-C9-C10
18	P	270	CDL	C75-C76-C77-C78
20	N	745	DMU	C31-C34-C37-C40
22	P	614	LFA	C11-C12-C13-C14
22	P	623	LFA	C6-C7-C8-C9
27	P	266	PGV	C29-C30-C31-C32
27	P	267	PGV	C7-C8-C9-C10
22	C	611	LFA	C4-C5-C6-C7
22	C	615	LFA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
22	C	625	LFA	C9-C10-C11-C12
26	C	264	PEK	C25-C26-C27-C28
27	C	267	PGV	C14-C15-C16-C17
20	C	734	DMU	O6-C11-C9-C8
18	C	270	CDL	CA7-C31-C32-C33
18	N	521	CDL	C77-C78-C79-C80
20	P	721	DMU	C28-C31-C34-C37
22	C	611	LFA	C3-C4-C5-C6
22	T	621	LFA	C11-C12-C13-C14
18	C	270	CDL	C54-C55-C56-C57
22	P	716[B]	LFA	C2-C3-C4-C5
20	C	722	DMU	C19-C18-O16-C6
20	C	733	DMU	C19-C18-O16-C6
20	G	713	DMU	C19-C18-O16-C6
20	N	744	DMU	C19-C18-O16-C6
18	C	270	CDL	C78-C79-C80-C81
22	C	626	LFA	C2-C3-C4-C5
22	C	716[B]	LFA	C2-C3-C4-C5
18	N	522	CDL	C15-C16-C17-C18
18	N	522	CDL	C71-C72-C73-C74
20	A	526	DMU	C22-C25-C28-C31
27	C	267	PGV	C13-C14-C15-C16
27	C	267	PGV	C27-C28-C29-C30
18	P	270	CDL	C73-C74-C75-C76
18	A	521	CDL	C74-C75-C76-C77
20	B	742	DMU	O16-C18-C19-C22
18	C	270	CDL	C33-C34-C35-C36
18	N	521	CDL	C63-C64-C65-C66
18	N	521	CDL	C76-C77-C78-C79
18	A	521	CDL	C13-C14-C15-C16
18	A	521	CDL	C17-C18-C19-C20
18	N	522	CDL	C74-C75-C76-C77
18	P	270	CDL	C11-C12-C13-C14
22	P	615	LFA	C4-C5-C6-C7
27	C	267	PGV	C21-C22-C23-C24
27	P	266	PGV	C30-C31-C32-C33
26	C	264	PEK	C15-C16-C17-C18
18	C	270	CDL	OA9-CA7-OA8-CA6
18	A	521	CDL	C71-C72-C73-C74
18	C	270	CDL	C71-C72-C73-C74
22	N	628	LFA	C6-C7-C8-C9
18	A	522	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
18	A	522	CDL	C77-C78-C79-C80
20	A	526	DMU	C19-C22-C25-C28
20	G	712	DMU	C31-C34-C37-C40
20	W	61	DMU	O16-C18-C19-C22
22	C	623	LFA	C4-C5-C6-C7
22	P	615	LFA	C6-C7-C8-C9
18	C	270	CDL	C79-C80-C81-C82
22	A	628	LFA	C6-C7-C8-C9
22	P	716[B]	LFA	C6-C7-C8-C9
23	P	807	EDO	O1-C1-C2-O2
18	A	522	CDL	C78-C79-C80-C81
18	P	270	CDL	C56-C57-C58-C59
22	G	621	LFA	C6-C7-C8-C9
27	P	267	PGV	C24-C25-C26-C27
22	T	621	LFA	C13-C14-C15-C16
20	P	733	DMU	C18-C19-C22-C25
18	A	522	CDL	C74-C75-C76-C77
20	B	741	DMU	C25-C28-C31-C34
22	C	624	LFA	C1-C2-C3-C4
26	P	264	PEK	C17-C18-C19-C20
18	N	521	CDL	C22-C23-C24-C25
20	C	722	DMU	O5-C4-C57-O61
20	A	745	DMU	C31-C34-C37-C40
20	N	526	DMU	C25-C28-C31-C34
22	T	622	LFA	C4-C5-C6-C7
20	Y	747	DMU	C18-C19-C22-C25
20	P	715[A]	DMU	C25-C28-C31-C34
18	C	270	CDL	C22-C23-C24-C25
22	C	626	LFA	C4-C5-C6-C7
20	B	731	DMU	C18-C19-C22-C25
18	A	521	CDL	C51-C52-C53-C54
18	A	522	CDL	C16-C17-C18-C19
22	C	614	LFA	C11-C10-C9-C8
22	P	624	LFA	C7-C8-C9-C10
18	N	521	CDL	C57-C58-C59-C60
18	P	270	CDL	C22-C23-C24-C25
22	C	626	LFA	C5-C6-C7-C8
22	G	621	LFA	C4-C5-C6-C7
20	B	742	DMU	C18-C19-C22-C25
20	B	742	DMU	C31-C34-C37-C40
20	P	734	DMU	O16-C18-C19-C22
26	C	264	PEK	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
20	Y	747	DMU	C1-C6-O16-C18
18	N	522	CDL	OA6-CA4-CA6-OA8
18	N	521	CDL	C19-C20-C21-C22
18	N	521	CDL	C71-C72-C73-C74
20	P	714	DMU	C19-C22-C25-C28
18	A	522	CDL	C17-C18-C19-C20
19	C	271	CHD	C21-C20-C22-C23
18	A	521	CDL	C80-C81-C82-C83
20	P	722	DMU	C28-C31-C34-C37
18	A	521	CDL	C36-C37-C38-C39
18	A	522	CDL	C12-C13-C14-C15
18	P	270	CDL	CB3-OB5-PB2-OB2
18	A	521	CDL	C58-C59-C60-C61
18	N	522	CDL	C16-C17-C18-C19
18	P	270	CDL	C13-C14-C15-C16
20	C	721	DMU	C28-C31-C34-C37
18	P	270	CDL	C33-C34-C35-C36
20	P	733	DMU	C19-C22-C25-C28
22	N	627	LFA	C2-C3-C4-C5
20	A	744	DMU	C4-C3-O7-C10
20	C	722	DMU	C28-C31-C34-C37
20	P	722	DMU	O16-C18-C19-C22
22	C	624	LFA	C4-C5-C6-C7
27	P	267	PGV	C12-C13-C14-C15
18	A	521	CDL	C59-C60-C61-C62
18	P	270	CDL	C82-C83-C84-C85
20	O	742	DMU	O16-C18-C19-C22
20	P	734	DMU	C25-C28-C31-C34
20	G	713	DMU	C19-C22-C25-C28
20	T	713	DMU	C22-C25-C28-C31
20	W	732	DMU	C25-C28-C31-C34
18	N	521	CDL	O1-C1-CA2-OA2
22	T	622	LFA	C3-C4-C5-C6
20	C	734	DMU	O6-C11-C9-O1
18	A	522	CDL	CB3-CB4-CB6-OB8
18	N	521	CDL	CB3-CB4-CB6-OB8
20	J	61	DMU	C34-C37-C40-C43
22	C	623	LFA	C11-C10-C9-C8
18	A	521	CDL	C12-C13-C14-C15
20	C	714	DMU	C34-C37-C40-C43
20	C	272	DMU	C28-C31-C34-C37
22	T	621	LFA	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	O	731	DMU	O16-C18-C19-C22
18	A	521	CDL	C84-C85-C86-C87
22	P	626	LFA	C1-C2-C3-C4
20	W	732	DMU	C19-C22-C25-C28
22	G	621	LFA	C5-C6-C7-C8
22	G	621	LFA	C7-C8-C9-C10
20	C	272	DMU	C22-C25-C28-C31
20	P	714	DMU	C18-C19-C22-C25
22	P	624	LFA	C11-C10-C9-C8
18	N	522	CDL	C78-C79-C80-C81
18	P	270	CDL	C35-C36-C37-C38
26	P	264	PEK	C2-C3-C4-C5
18	N	522	CDL	C17-C18-C19-C20
20	G	712	DMU	C18-C19-C22-C25
22	A	627	LFA	C9-C10-C11-C12
22	C	624	LFA	C11-C10-C9-C8
20	A	743	DMU	C34-C37-C40-C43
20	B	742	DMU	C25-C28-C31-C34
20	T	711	DMU	C34-C37-C40-C43
26	C	264	PEK	C17-C18-C19-C20
26	P	264	PEK	C26-C27-C28-C29
22	C	611	LFA	C11-C10-C9-C8
22	N	628	LFA	C1-C2-C3-C4
20	B	731	DMU	O16-C18-C19-C22
20	G	712	DMU	O16-C18-C19-C22
20	O	741	DMU	O16-C18-C19-C22
20	T	712	DMU	O16-C18-C19-C22
18	N	521	CDL	C78-C79-C80-C81
22	N	628	LFA	C2-C3-C4-C5
20	Y	747	DMU	O5-C4-C57-O61
18	A	522	CDL	C15-C16-C17-C18
20	O	742	DMU	C19-C22-C25-C28
22	P	626	LFA	C6-C7-C8-C9
26	P	264	PEK	C4-C5-C6-C7
20	T	713	DMU	C18-C19-C22-C25
18	P	270	CDL	C57-C58-C59-C60
18	A	521	CDL	C34-C35-C36-C37
22	T	621	LFA	C6-C7-C8-C9
18	C	270	CDL	C13-C14-C15-C16
26	C	264	PEK	C35-C36-C37-C38
18	N	521	CDL	C52-C53-C54-C55
18	P	270	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	P	626	LFA	C9-C10-C11-C12
27	C	267	PGV	C23-C24-C25-C26
26	C	264	PEK	C29-C30-C31-C32
20	J	732	DMU	O16-C18-C19-C22
18	A	522	CDL	C79-C80-C81-C82
18	N	521	CDL	C79-C80-C81-C82
22	N	628	LFA	C5-C6-C7-C8
20	P	722	DMU	C31-C34-C37-C40
22	N	627	LFA	C7-C8-C9-C10
27	P	267	PGV	C22-C23-C24-C25
20	B	741	DMU	C18-C19-C22-C25
20	N	526	DMU	C34-C37-C40-C43
22	C	612	LFA	C2-C3-C4-C5
20	B	742	DMU	C34-C37-C40-C43
20	J	61	DMU	O16-C18-C19-C22
18	A	521	CDL	C57-C58-C59-C60
18	N	521	CDL	C53-C54-C55-C56
22	P	611	LFA	C11-C10-C9-C8
20	A	743	DMU	C25-C28-C31-C34
22	C	611	LFA	C7-C8-C9-C10
22	P	625	LFA	C5-C6-C7-C8
20	W	732	DMU	C18-C19-C22-C25
20	Y	747	DMU	C19-C18-O16-C6
20	P	734	DMU	C34-C37-C40-C43
20	P	714	DMU	C28-C31-C34-C37
20	B	741	DMU	O16-C18-C19-C22
18	A	522	CDL	CA3-CA4-CA6-OA8
18	C	270	CDL	CB3-CB4-CB6-OB8
18	P	270	CDL	C59-C60-C61-C62
26	P	264	PEK	C13-C14-C15-C16
22	A	627	LFA	C2-C3-C4-C5
20	T	713	DMU	C19-C22-C25-C28
18	N	521	CDL	C37-C38-C39-C40
22	P	716[B]	LFA	C7-C8-C9-C10
22	G	621	LFA	C14-C15-C16-C17
26	C	264	PEK	C9-C10-C11-C12
26	P	264	PEK	C11-C10-C9-C8
18	N	521	CDL	CA7-C31-C32-C33
18	N	521	CDL	OB5-CB3-CB4-OB6
18	A	522	CDL	C31-CA7-OA8-CA6
18	P	270	CDL	C24-C25-C26-C27
22	P	624	LFA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	P	266	PGV	C14-C15-C16-C17
20	O	742	DMU	C18-C19-C22-C25
20	O	731	DMU	C18-C19-C22-C25
18	N	522	CDL	C77-C78-C79-C80
22	C	614	LFA	C9-C10-C11-C12
14	A	515[A]	HEA	C15-C16-C17-C18
18	A	522	CDL	CA2-C1-CB2-OB2
20	T	712	DMU	C28-C31-C34-C37
18	P	270	CDL	C79-C80-C81-C82
20	T	712	DMU	C19-C22-C25-C28
22	G	622	LFA	C5-C6-C7-C8
27	P	267	PGV	C02-C03-O11-P
20	C	715[A]	DMU	C19-C22-C25-C28
20	C	734	DMU	C25-C28-C31-C34
20	N	743	DMU	C34-C37-C40-C43
20	W	732	DMU	C28-C31-C34-C37
22	C	614	LFA	C2-C3-C4-C5
20	A	744	DMU	C2-C3-O7-C10
27	P	267	PGV	C11-C12-C13-C14
20	P	721	DMU	C31-C34-C37-C40
20	Y	747	DMU	C31-C34-C37-C40
22	C	625	LFA	C5-C6-C7-C8
18	A	521	CDL	C20-C21-C22-C23
22	P	625	LFA	C4-C5-C6-C7
18	C	270	CDL	C74-C75-C76-C77
18	C	270	CDL	C75-C76-C77-C78
18	P	270	CDL	C72-C73-C74-C75
20	P	721	DMU	C25-C28-C31-C34
22	T	621	LFA	C10-C11-C12-C13
22	T	622	LFA	C6-C7-C8-C9
18	N	521	CDL	C60-C61-C62-C63
26	P	264	PEK	C22-C23-C24-C25
22	A	628	LFA	C11-C12-C13-C14
18	P	270	CDL	C78-C79-C80-C81
22	P	624	LFA	C1-C2-C3-C4
18	N	521	CDL	C54-C55-C56-C57
18	N	521	CDL	C51-C52-C53-C54
22	A	628	LFA	C11-C10-C9-C8
20	P	734	DMU	C19-C22-C25-C28
22	C	623	LFA	C5-C6-C7-C8
22	G	622	LFA	C2-C3-C4-C5
26	C	264	PEK	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
18	A	521	CDL	C53-C54-C55-C56
18	P	270	CDL	C19-C20-C21-C22
20	O	742	DMU	O5-C4-C57-O61
20	T	711	DMU	C18-C19-C22-C25
20	O	742	DMU	C31-C34-C37-C40
22	P	623	LFA	C10-C11-C12-C13
18	C	270	CDL	CA4-CA3-OA5-PA1
18	N	522	CDL	CA3-CA4-CA6-OA8
18	P	270	CDL	CB3-CB4-CB6-OB8
27	C	267	PGV	C02-C03-O11-P
20	N	745	DMU	C3-C4-C57-O61
20	W	732	DMU	C34-C37-C40-C43
20	O	731	DMU	C19-C22-C25-C28
18	C	270	CDL	O1-C1-CA2-OA2
20	P	722	DMU	C18-C19-C22-C25
22	P	626	LFA	C5-C6-C7-C8
20	M	746	DMU	C34-C37-C40-C43
18	C	270	CDL	C18-C19-C20-C21
20	O	741	DMU	C28-C31-C34-C37
22	P	626	LFA	C2-C3-C4-C5
27	C	266	PGV	C11-C10-C9-C8
20	O	741	DMU	C25-C28-C31-C34
22	T	621	LFA	C1-C2-C3-C4
18	N	522	CDL	C75-C76-C77-C78
20	N	744	DMU	C4-C3-O7-C10
22	P	611	LFA	C1-C2-C3-C4
18	A	521	CDL	C78-C79-C80-C81
22	P	625	LFA	C9-C10-C11-C12
18	A	521	CDL	OB9-CB7-OB8-CB6
18	C	270	CDL	C36-C37-C38-C39
18	N	521	CDL	C32-C33-C34-C35
18	N	522	CDL	C79-C80-C81-C82
20	C	714	DMU	C18-C19-C22-C25
20	C	722	DMU	C18-C19-C22-C25
18	N	521	CDL	C35-C36-C37-C38
18	A	521	CDL	CA2-OA2-PA1-OA5
20	Z	746	DMU	C34-C37-C40-C43
18	P	270	CDL	CA4-CA3-OA5-PA1
20	C	715[A]	DMU	C3-C4-C57-O61
18	P	270	CDL	C80-C81-C82-C83
22	A	627	LFA	C11-C12-C13-C14
18	A	521	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
18	A	521	CDL	CB3-OB5-PB2-OB4
18	C	270	CDL	CA2-OA2-PA1-OA4
18	C	270	CDL	CA3-OA5-PA1-OA3
18	N	521	CDL	CA3-OA5-PA1-OA4
18	P	270	CDL	CA3-OA5-PA1-OA3
18	A	521	CDL	C71-CB7-OB8-CB6
18	A	521	CDL	OA5-CA3-CA4-CA6
18	N	521	CDL	OB5-CB3-CB4-CB6
20	T	711	DMU	C31-C34-C37-C40
26	P	264	PEK	C30-C31-C32-C33
20	C	733	DMU	C3-C4-C57-O61
18	N	521	CDL	C64-C65-C66-C67
18	N	522	CDL	C72-C73-C74-C75
22	G	622	LFA	C1-C2-C3-C4
27	P	266	PGV	C11-C10-C9-C8
18	P	270	CDL	CB7-C71-C72-C73
18	C	270	CDL	C12-C11-CA5-OA6
18	N	521	CDL	CB2-C1-CA2-OA2
18	C	270	CDL	C14-C15-C16-C17
20	B	731	DMU	C25-C28-C31-C34
18	A	521	CDL	OA5-CA3-CA4-OA6
18	A	522	CDL	OA5-CA3-CA4-OA6
20	B	731	DMU	C34-C37-C40-C43
20	P	722	DMU	C19-C22-C25-C28
22	A	628	LFA	C10-C11-C12-C13
20	A	526	DMU	C25-C28-C31-C34
22	G	621	LFA	C2-C3-C4-C5
18	C	270	CDL	CB7-C71-C72-C73
18	C	270	CDL	OB6-CB4-CB6-OB8
22	P	614	LFA	C1-C2-C3-C4
18	P	270	CDL	C14-C15-C16-C17
20	A	526	DMU	C34-C37-C40-C43
22	A	628	LFA	C5-C6-C7-C8
18	P	270	CDL	C12-C11-CA5-OA6
20	J	732	DMU	C25-C28-C31-C34
20	T	712	DMU	C34-C37-C40-C43
20	A	744	DMU	C28-C31-C34-C37
20	N	745	DMU	C19-C22-C25-C28
22	P	612	LFA	C1-C2-C3-C4
18	A	521	CDL	C38-C39-C40-C41
22	C	626	LFA	C10-C11-C12-C13
20	C	734	DMU	C31-C34-C37-C40

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Mol	Chain	Res	Type	Atoms
27	P	267	PGV	C15-C16-C17-C18
20	C	734	DMU	C34-C37-C40-C43
22	N	628	LFA	C3-C4-C5-C6
20	M	746	DMU	C22-C25-C28-C31
18	N	522	CDL	CB2-C1-CA2-OA2
20	N	743	DMU	C28-C31-C34-C37
22	C	614	LFA	C11-C12-C13-C14
18	A	522	CDL	C72-C73-C74-C75
27	C	267	PGV	C31-C32-C33-C34
18	N	522	CDL	C31-C32-C33-C34
18	N	521	CDL	C72-C73-C74-C75
20	C	715[A]	DMU	C25-C28-C31-C34
22	A	627	LFA	C4-C5-C6-C7
22	T	622	LFA	C5-C6-C7-C8
23	N	803	EDO	O1-C1-C2-O2
23	R	811	EDO	O1-C1-C2-O2
22	P	615	LFA	C5-C6-C7-C8
18	A	522	CDL	OB6-CB4-CB6-OB8
18	C	270	CDL	C82-C83-C84-C85
18	A	521	CDL	CB2-OB2-PB2-OB5
18	N	521	CDL	CA2-OA2-PA1-OA5
18	C	270	CDL	C11-C12-C13-C14
18	A	522	CDL	OA9-CA7-OA8-CA6
20	W	732	DMU	O16-C18-C19-C22
22	N	627	LFA	C11-C12-C13-C14
18	N	522	CDL	C52-C51-CB5-OB6
20	N	744	DMU	C2-C3-O7-C10
22	N	627	LFA	C3-C4-C5-C6
20	P	734	DMU	C18-C19-C22-C25
18	A	522	CDL	CB4-CB3-OB5-PB2
18	C	270	CDL	C20-C21-C22-C23
26	P	264	PEK	C10-C11-C12-C13
22	C	623	LFA	C6-C7-C8-C9
20	O	742	DMU	C25-C28-C31-C34
22	C	716[B]	LFA	C5-C6-C7-C8
22	P	624	LFA	C2-C3-C4-C5
22	A	627	LFA	C6-C7-C8-C9
22	C	716[B]	LFA	C14-C15-C16-C17
18	N	521	CDL	C17-C18-C19-C20
18	P	270	CDL	C18-C19-C20-C21
20	M	746	DMU	C28-C31-C34-C37
22	P	624	LFA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
18	N	522	CDL	C52-C51-CB5-OB7
20	A	744	DMU	O16-C18-C19-C22
20	P	715[A]	DMU	C19-C22-C25-C28
27	C	267	PGV	C05-C04-O12-P
27	P	267	PGV	C29-C30-C31-C32
27	C	266	PGV	C11-C12-C13-C14
18	N	521	CDL	C20-C21-C22-C23
18	P	270	CDL	C74-C75-C76-C77
20	Y	747	DMU	C34-C37-C40-C43
18	C	270	CDL	C84-C85-C86-C87
20	P	722	DMU	C3-C4-C57-O61
18	C	270	CDL	C21-C22-C23-C24
18	A	521	CDL	C19-C20-C21-C22
18	A	522	CDL	CA3-CA4-OA6-CA5
20	P	714	DMU	C4-C3-O7-C10
18	C	270	CDL	CB3-OB5-PB2-OB2
18	A	521	CDL	C52-C53-C54-C55
20	A	744	DMU	C31-C34-C37-C40
26	P	264	PEK	C16-C17-C18-C19
20	P	714	DMU	C2-C3-O7-C10
26	P	264	PEK	C32-C33-C34-C35
27	P	267	PGV	C1-C2-C3-C4
27	C	266	PGV	O03-C19-C20-C21
20	B	742	DMU	C22-C25-C28-C31
20	C	272	DMU	C31-C34-C37-C40
27	P	266	PGV	O03-C19-C20-C21
20	G	713	DMU	C28-C31-C34-C37
22	C	623	LFA	C10-C11-C12-C13
22	G	621	LFA	C3-C4-C5-C6
22	P	625	LFA	C11-C10-C9-C8
23	A	825	EDO	O1-C1-C2-O2
23	E	815	EDO	O1-C1-C2-O2
23	R	815	EDO	O1-C1-C2-O2
18	P	270	CDL	C17-C18-C19-C20
20	N	743	DMU	C25-C28-C31-C34
20	T	713	DMU	C28-C31-C34-C37
18	A	522	CDL	OA5-CA3-CA4-CA6
18	N	522	CDL	C20-C21-C22-C23
20	J	61	DMU	C28-C31-C34-C37
20	P	722	DMU	C1-C6-O16-C18
20	P	734	DMU	C1-C6-O16-C18
18	A	521	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
22	C	716[B]	LFA	C1-C2-C3-C4
20	N	744	DMU	C28-C31-C34-C37
22	P	716[B]	LFA	C3-C4-C5-C6
18	C	270	CDL	C57-C58-C59-C60
18	N	521	CDL	C59-C60-C61-C62
18	A	521	CDL	C54-C55-C56-C57
18	N	522	CDL	C32-C31-CA7-OA8
18	A	521	CDL	C73-C74-C75-C76
22	P	611	LFA	C3-C4-C5-C6
20	T	711	DMU	C25-C28-C31-C34
18	A	521	CDL	C60-C61-C62-C63
20	N	745	DMU	O16-C18-C19-C22
26	C	264	PEK	C23-C24-C25-C26
20	P	715[A]	DMU	C3-C4-C57-O61
27	C	266	PGV	C31-C32-C33-C34
20	A	744	DMU	C19-C22-C25-C28
18	A	521	CDL	C72-C71-CB7-OB8
20	M	746	DMU	C31-C34-C37-C40
20	J	61	DMU	C5-C10-O7-C3
20	O	731	DMU	C22-C25-C28-C31
20	C	722	DMU	C3-C4-C57-O61
18	N	521	CDL	C12-C11-CA5-OA6
18	N	521	CDL	C58-C59-C60-C61
20	C	714	DMU	C4-C3-O7-C10
22	T	621	LFA	C12-C13-C14-C15
18	N	522	CDL	C32-C31-CA7-OA9
18	A	522	CDL	C19-C20-C21-C22
20	C	714	DMU	C31-C34-C37-C40
18	N	521	CDL	CB7-C71-C72-C73
26	P	264	PEK	O01-C1-C2-C3
20	J	61	DMU	O1-C10-O7-C3
20	J	732	DMU	C18-C19-C22-C25
22	T	621	LFA	C9-C10-C11-C12
18	P	270	CDL	C1-CB2-OB2-PB2
27	P	267	PGV	C05-C04-O12-P
18	P	270	CDL	CB3-OB5-PB2-OB3
20	P	715[A]	DMU	O5-C6-O16-C18
19	C	271	CHD	C17-C20-C22-C23
26	C	264	PEK	C31-C32-C33-C34
23	C	827	EDO	O1-C1-C2-O2
18	C	270	CDL	C80-C81-C82-C83
20	C	734	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
18	N	521	CDL	C12-C11-CA5-OA7
26	P	264	PEK	C2-C1-O01-C02
18	A	522	CDL	O1-C1-CB2-OB2
18	N	521	CDL	C32-C31-CA7-OA8
18	N	521	CDL	C32-C31-CA7-OA9
14	N	515[A]	HEA	C16-C17-C18-C19
22	G	621	LFA	C11-C10-C9-C8
22	P	614	LFA	C4-C5-C6-C7
20	J	732	DMU	C28-C31-C34-C37
22	P	623	LFA	C1-C2-C3-C4
27	C	267	PGV	C15-C16-C17-C18
18	A	521	CDL	C72-C71-CB7-OB9
20	T	713	DMU	C19-C18-O16-C6
18	N	521	CDL	C72-C71-CB7-OB8
26	C	264	PEK	O03-C21-C22-C23
20	G	713	DMU	C22-C25-C28-C31
27	C	267	PGV	C11-C12-C13-C14
20	C	272	DMU	C19-C22-C25-C28
18	C	270	CDL	C12-C11-CA5-OA7

There are no ring outliers.

64 monomers are involved in 188 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	T	622	LFA	1	0
26	P	264	PEK	3	0
20	N	745	DMU	2	0
20	P	733	DMU	4	0
23	N	829	EDO	1	0
20	G	711	DMU	3	0
20	T	712	DMU	8	0
23	C	809	EDO	2	0
22	C	625	LFA	1	0
27	P	266	PGV	1	0
14	N	516	HEA	1	0
18	C	270	CDL	14	0
20	P	734	DMU	3	0
22	T	621	LFA	3	0
22	C	626	LFA	4	0
27	C	266	PGV	2	0
18	N	521	CDL	7	0
22	N	627	LFA	1	0

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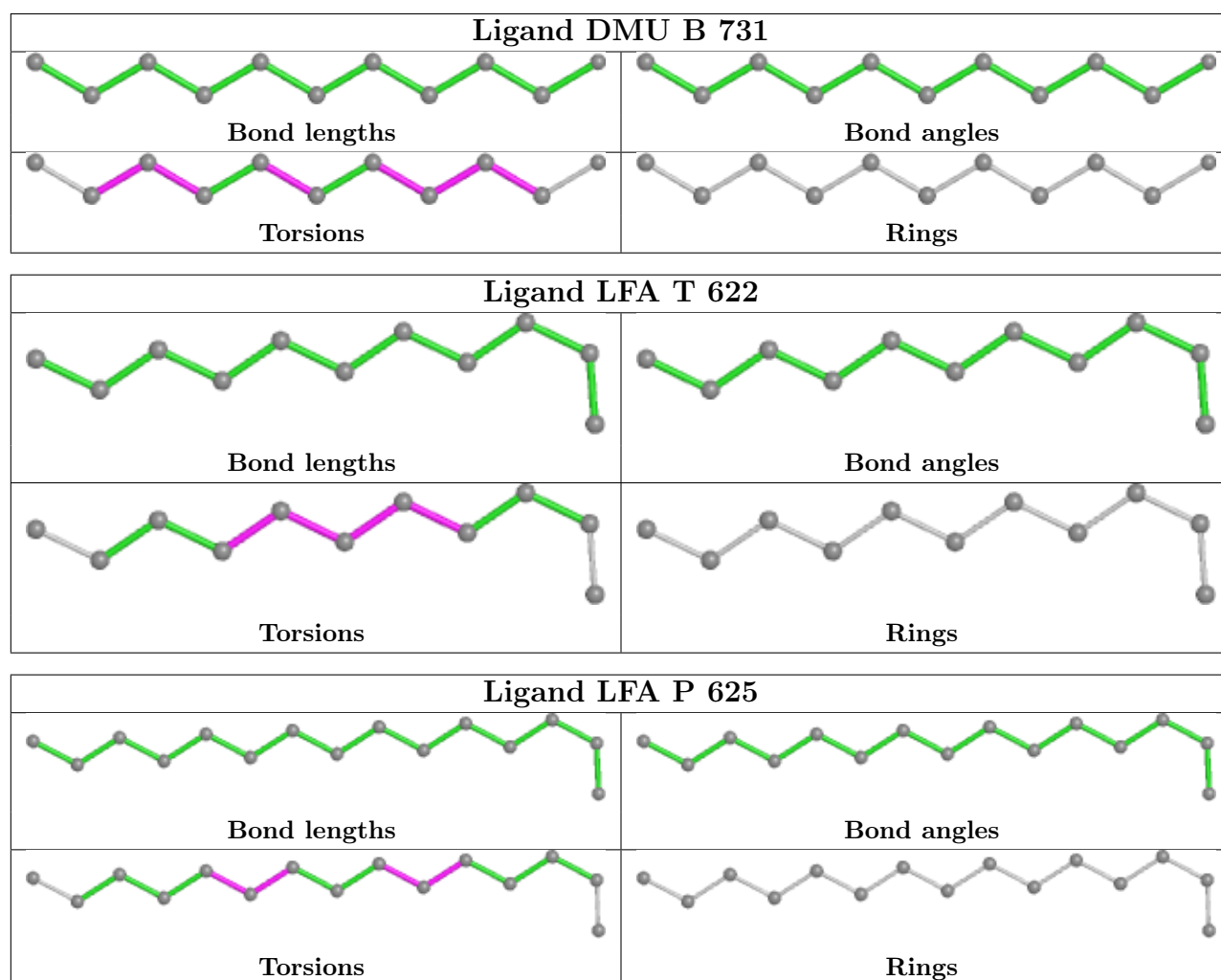
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	P	715[A]	DMU	1	0
20	G	713	DMU	4	0
20	O	742	DMU	1	0
22	N	628	LFA	6	0
22	P	611	LFA	1	0
14	N	515[A]	HEA	6	0
21	N	520	PER	1	0
22	A	628	LFA	11	0
22	P	624	LFA	2	0
20	T	711	DMU	12	0
20	A	743	DMU	1	0
22	P	716[B]	LFA	1	0
14	A	515[A]	HEA	6	0
20	C	721	DMU	2	0
20	C	733	DMU	2	0
19	T	86	CHD	1	0
20	Y	747	DMU	1	0
21	A	520	PER	1	0
22	C	716[B]	LFA	3	0
22	A	627	LFA	6	0
22	P	615	LFA	2	0
19	G	86	CHD	1	0
22	G	622	LFA	1	0
20	P	714	DMU	2	0
22	P	623	LFA	1	0
19	P	271	CHD	1	0
18	P	270	CDL	12	0
14	A	516	HEA	1	0
22	P	626	LFA	1	0
20	C	714	DMU	3	0
20	G	712	DMU	8	0
20	T	713	DMU	13	0
20	N	744	DMU	2	0
26	C	264	PEK	5	0
20	J	61	DMU	6	0
18	A	521	CDL	9	0
22	C	624	LFA	4	0
18	A	522	CDL	1	0
14	N	515[B]	HEA	1	0
20	W	61	DMU	7	0
20	A	526	DMU	1	0
20	A	744	DMU	4	0

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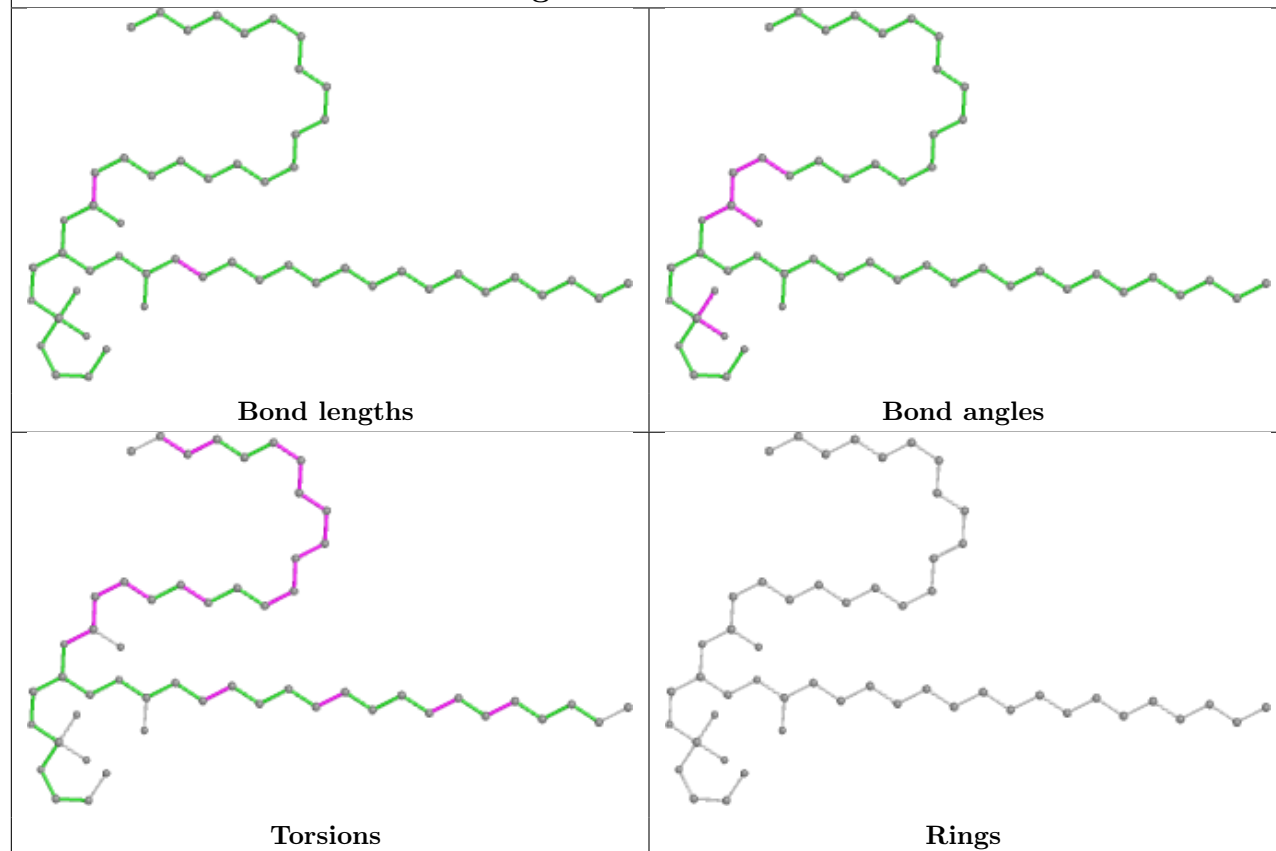
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	O	731	DMU	1	0
22	C	614	LFA	1	0
18	N	522	CDL	1	0
23	A	801	EDO	1	0

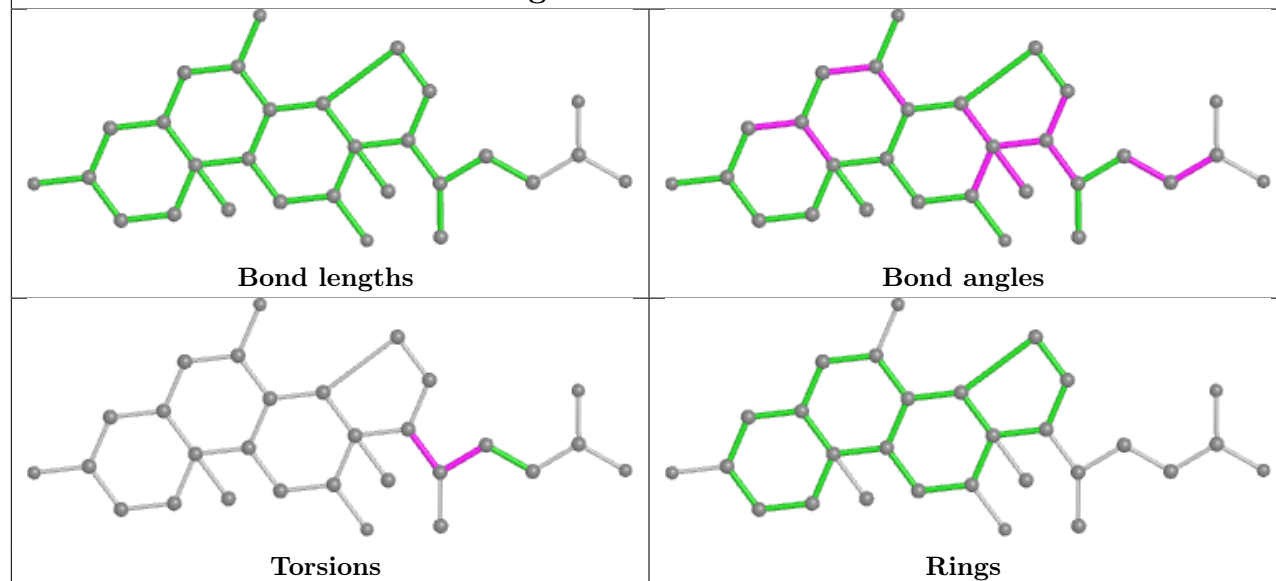
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

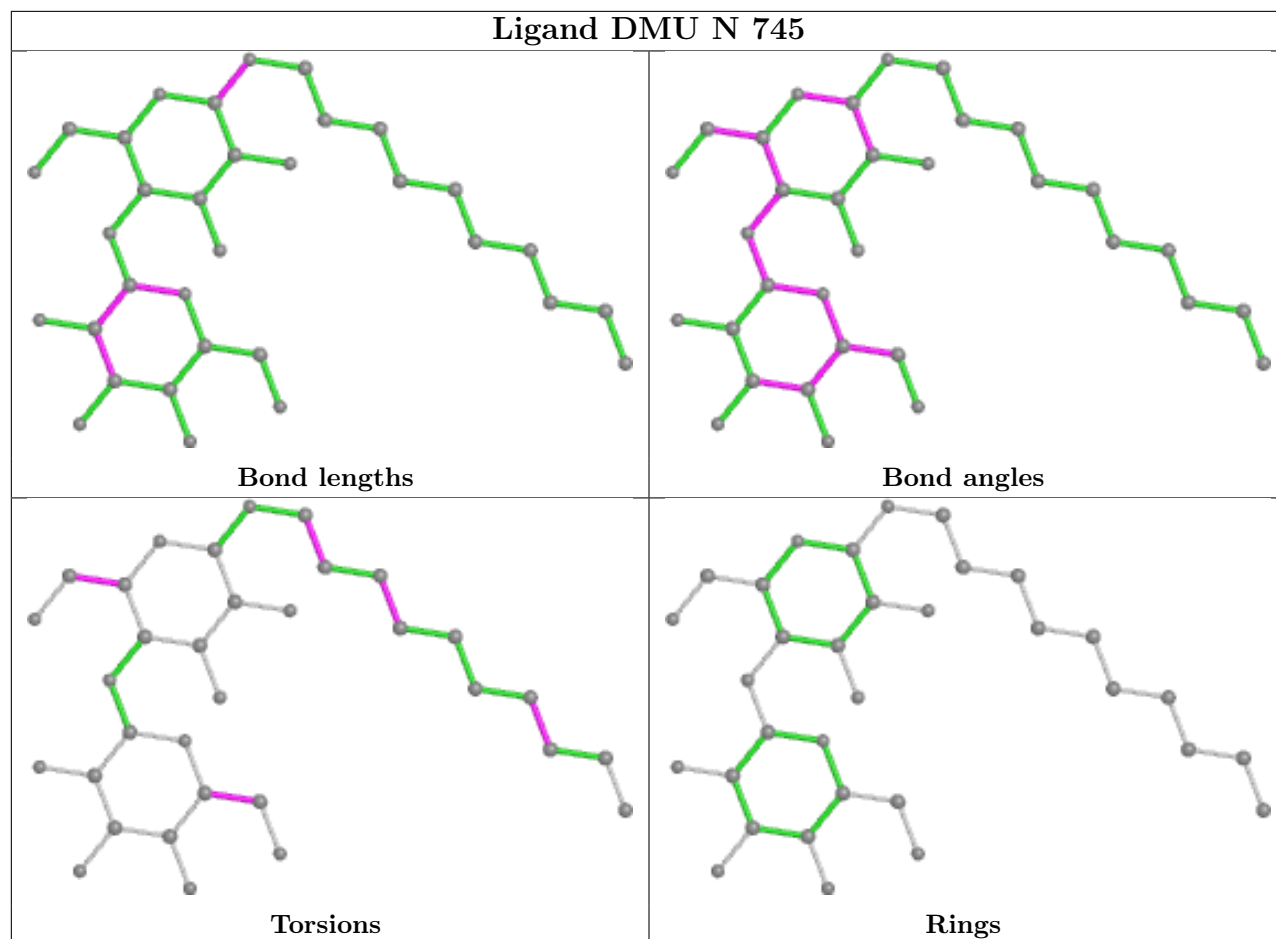


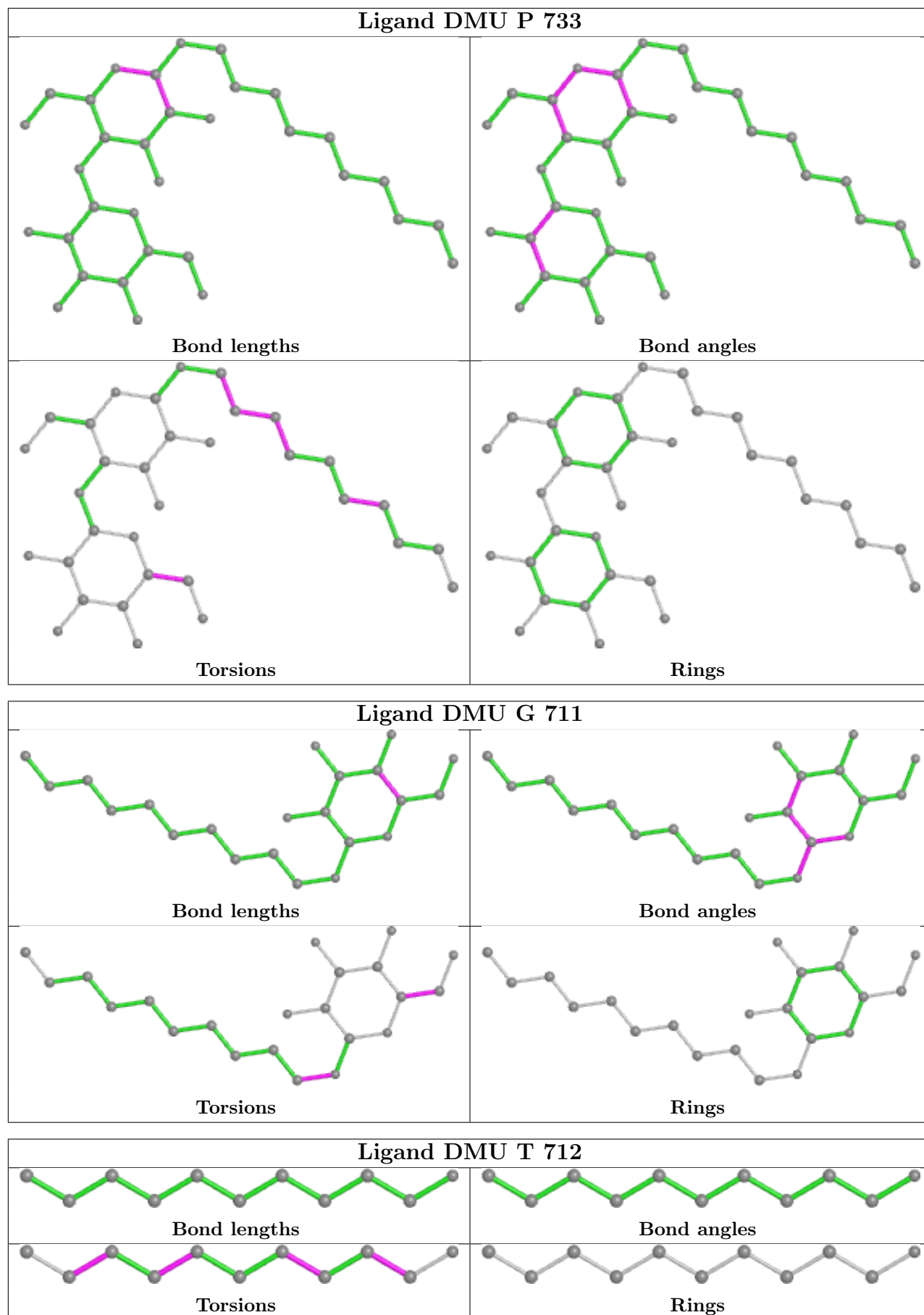
## Ligand PEK P 264



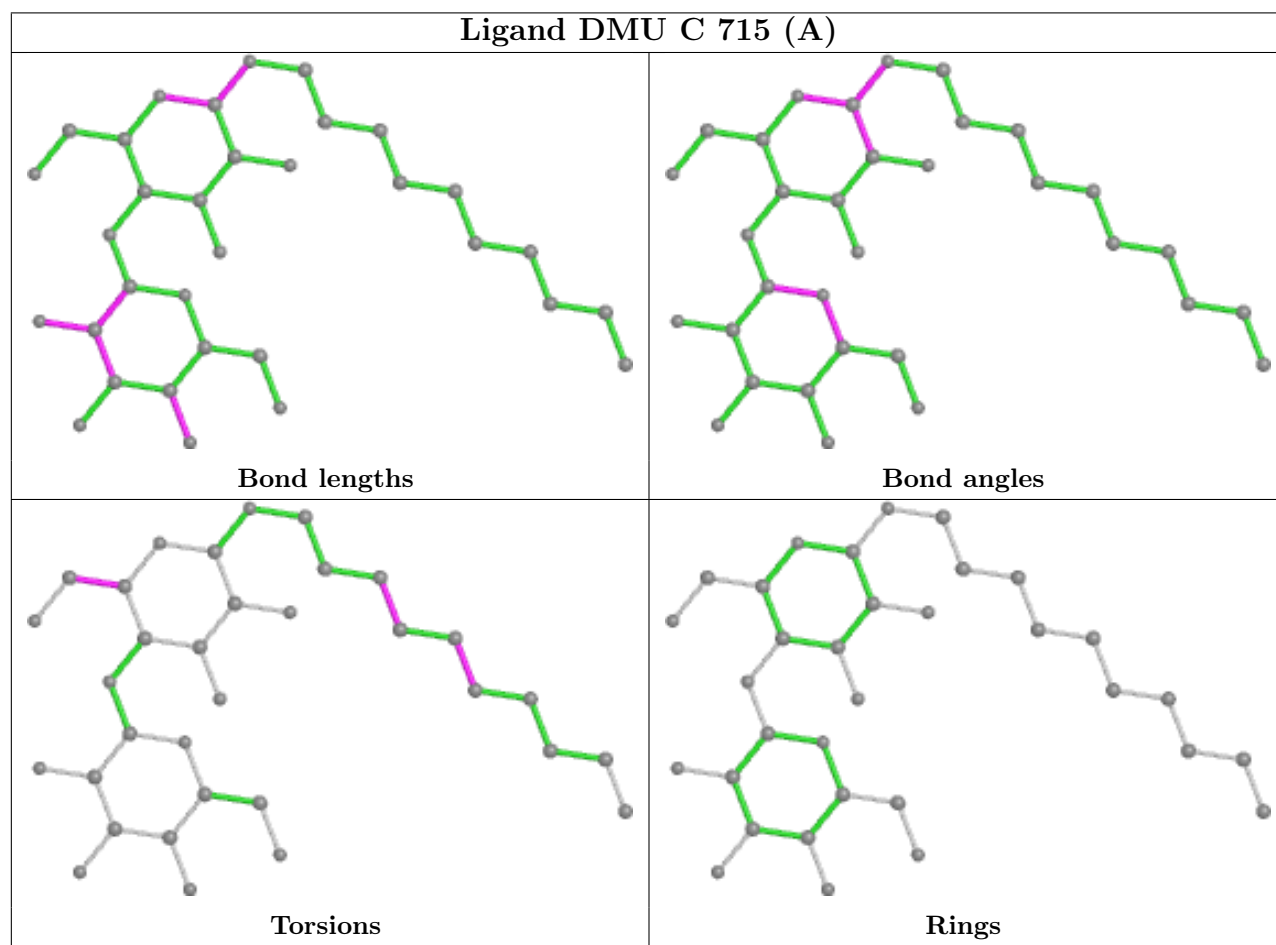
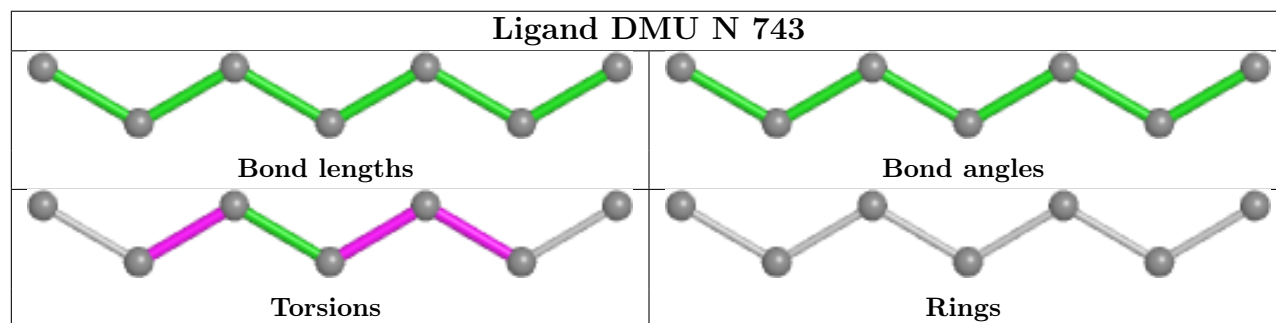
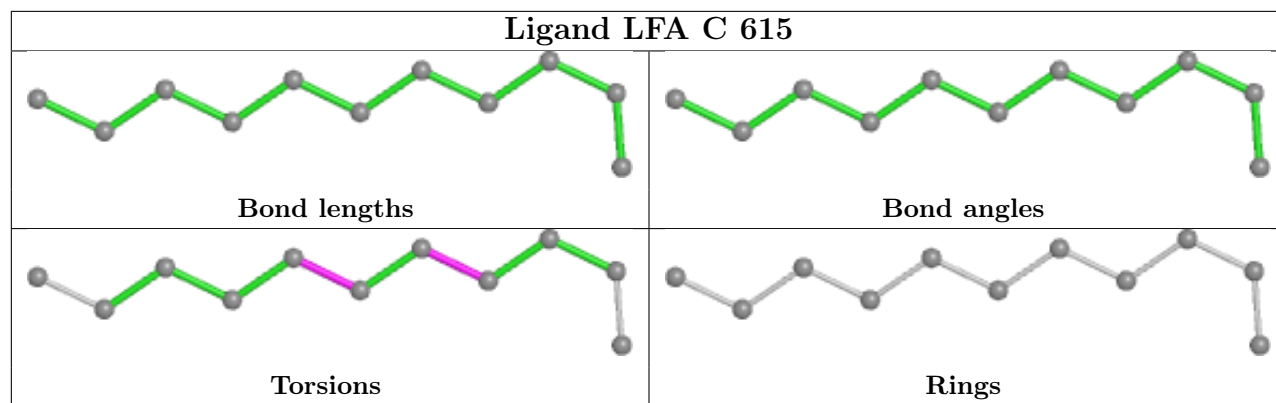
## Ligand CHD C 271

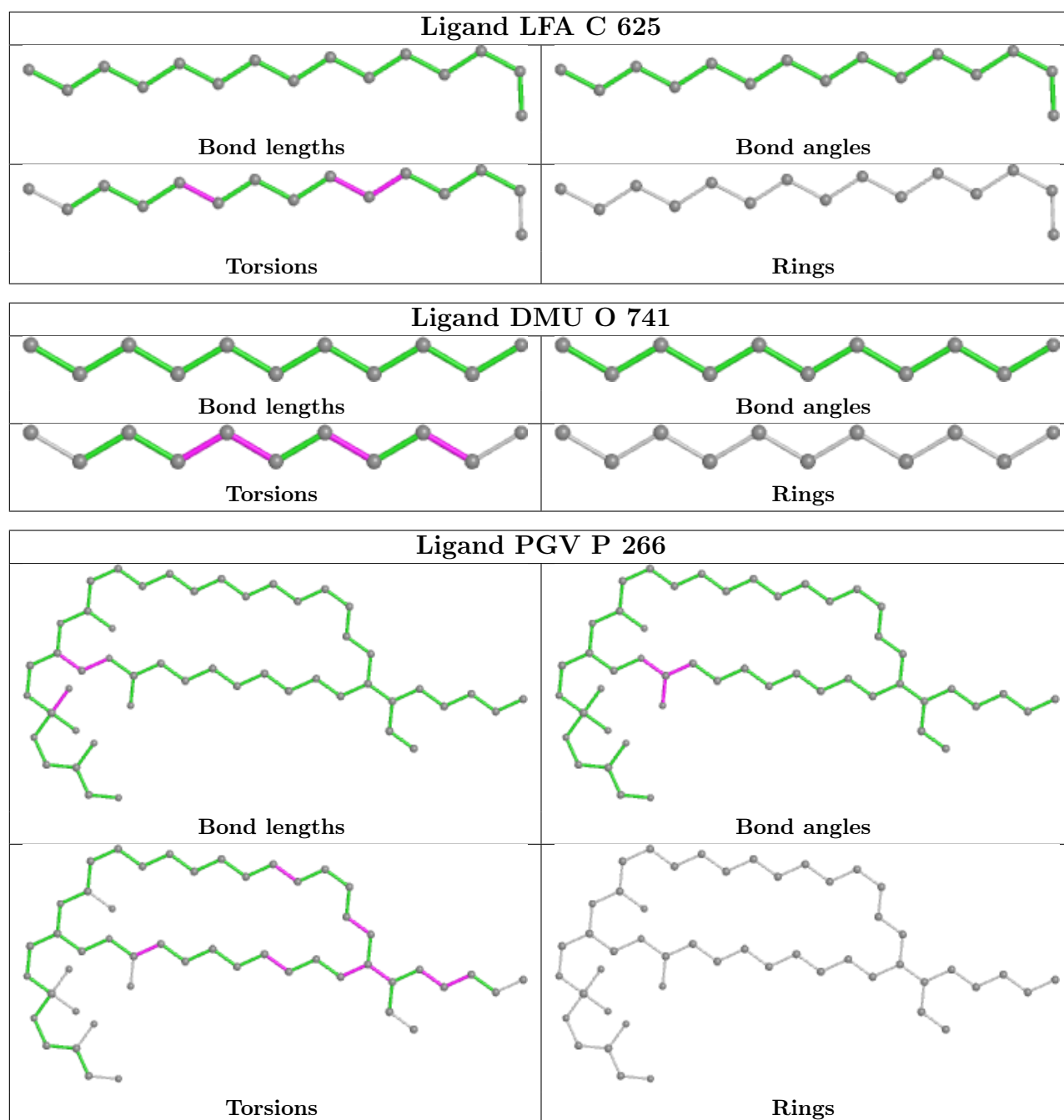


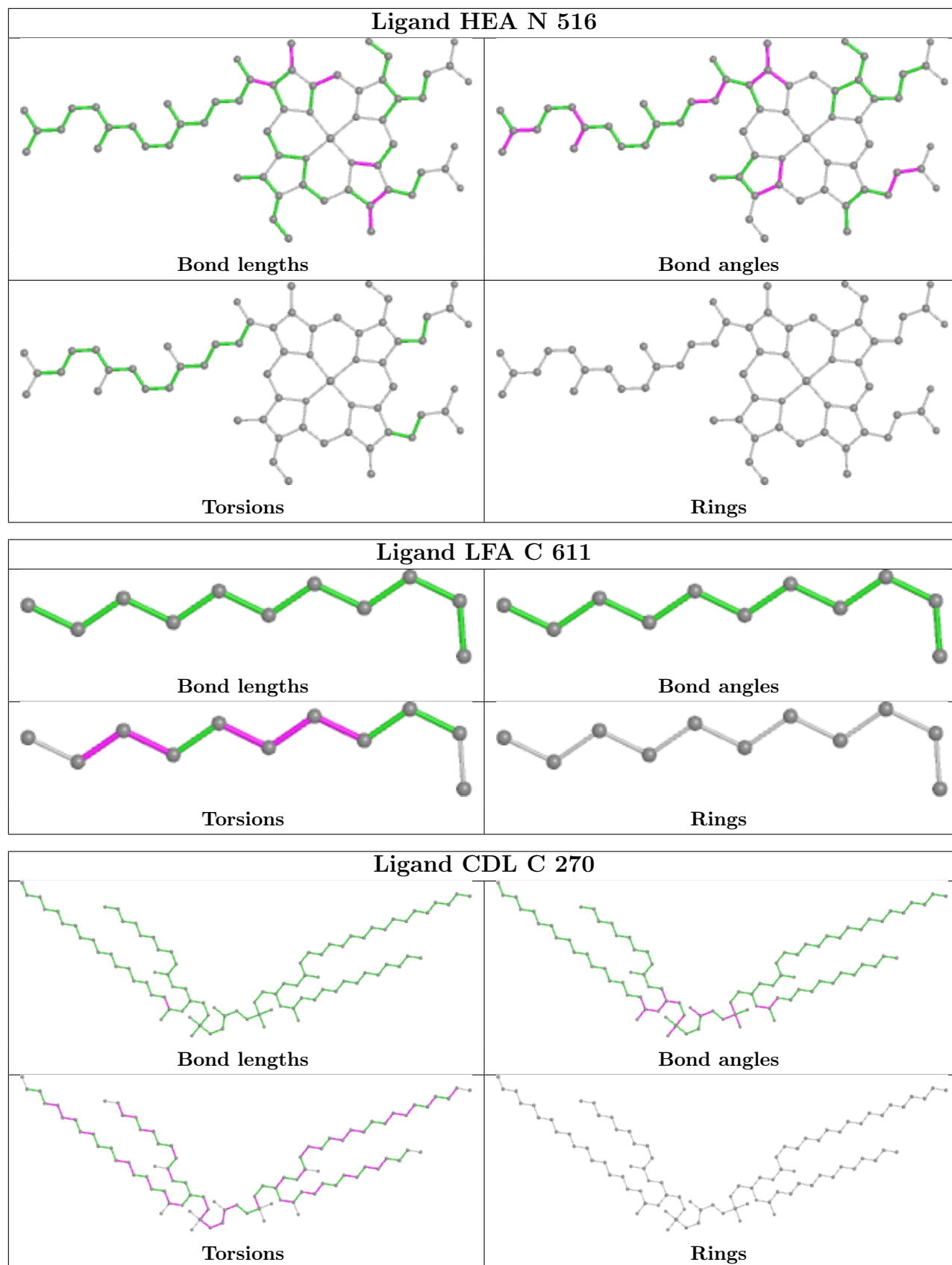


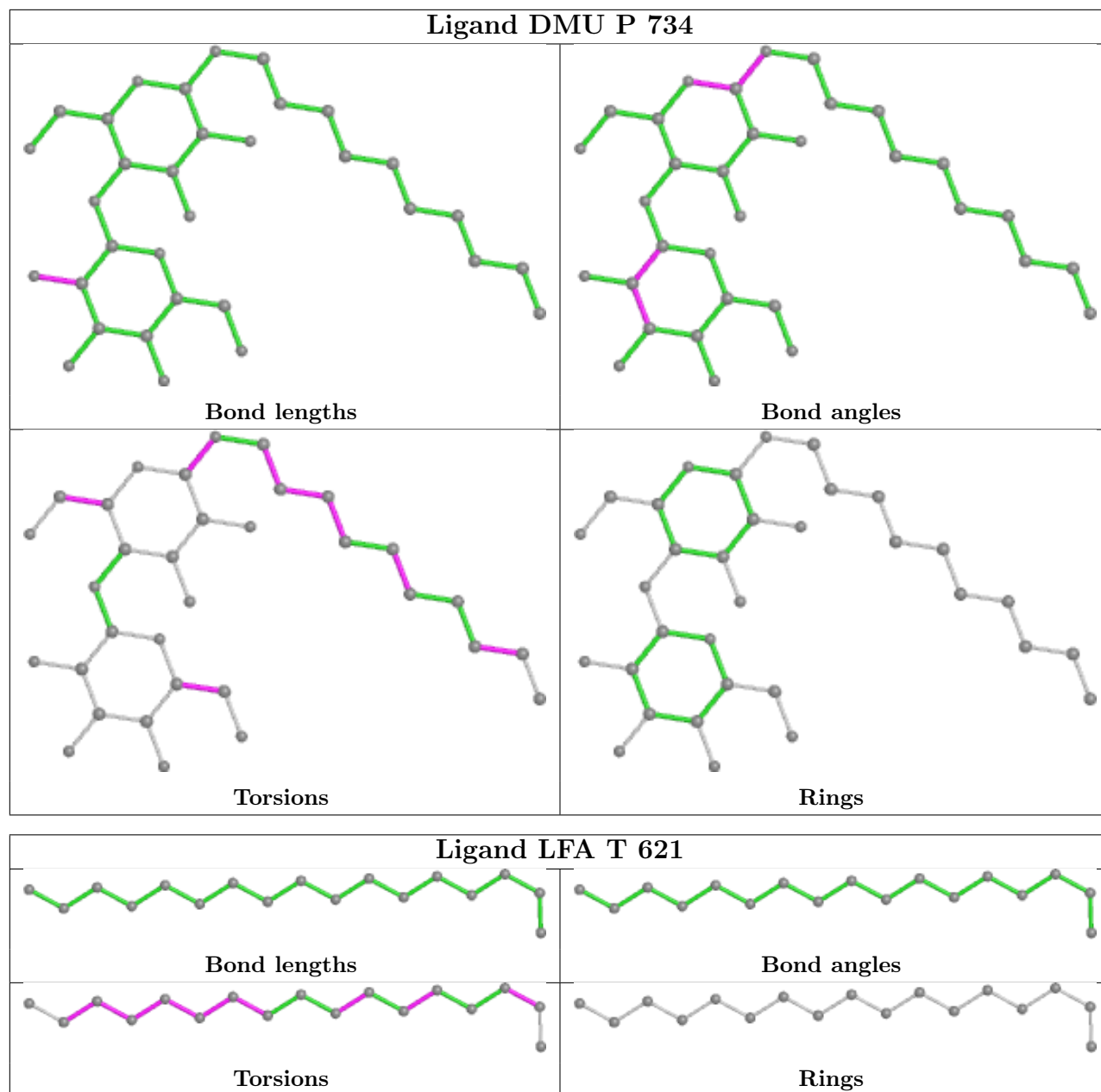


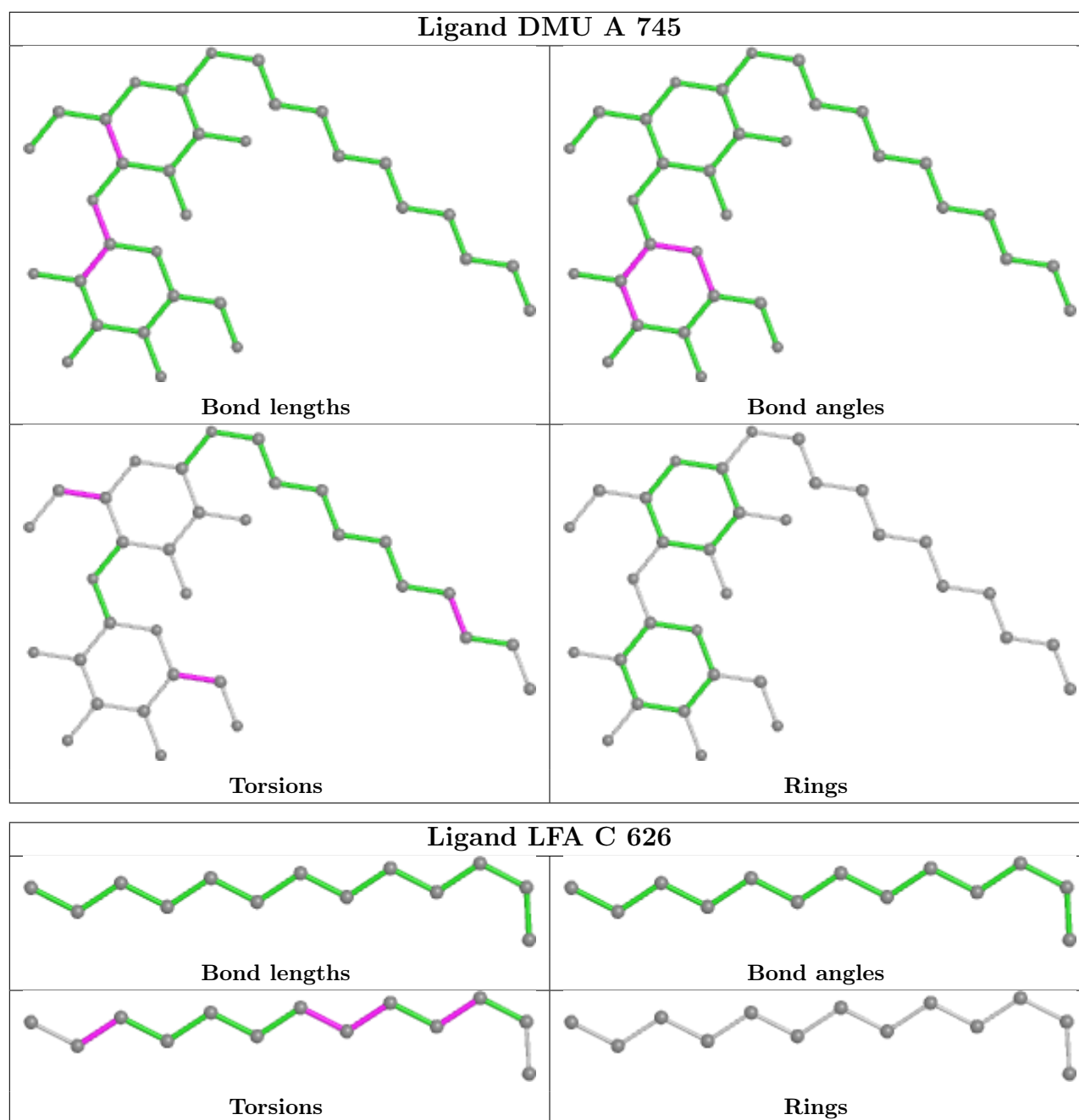


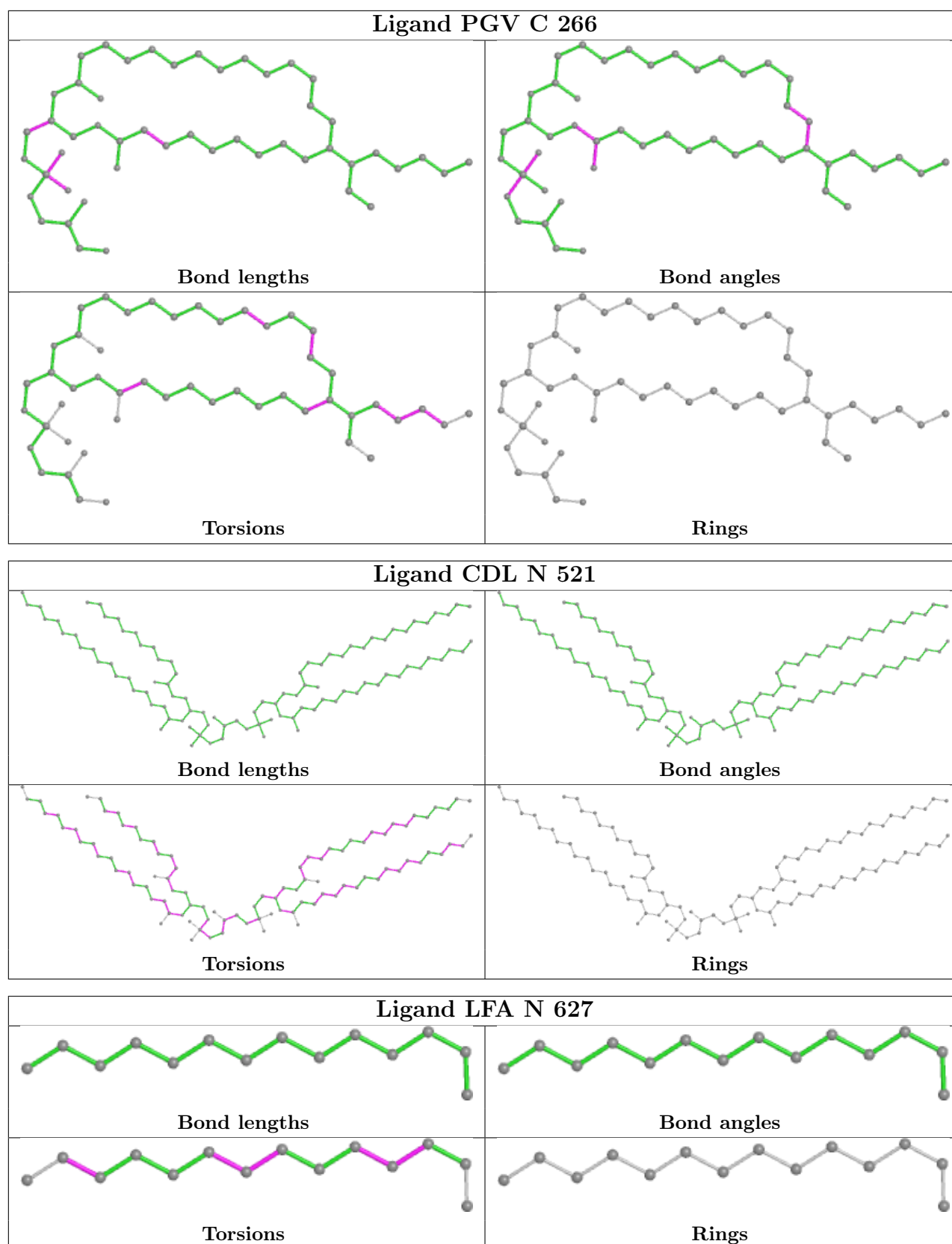


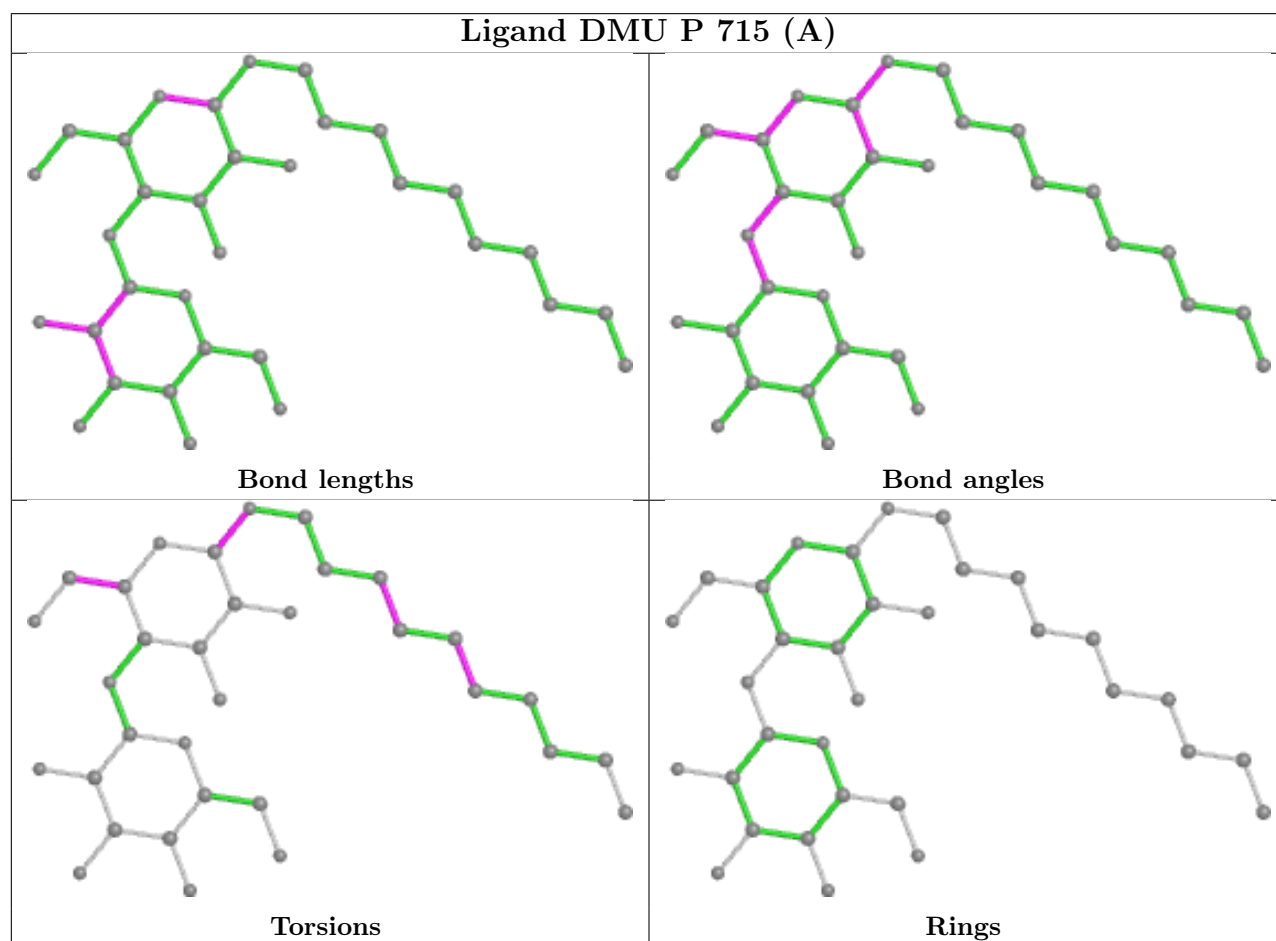
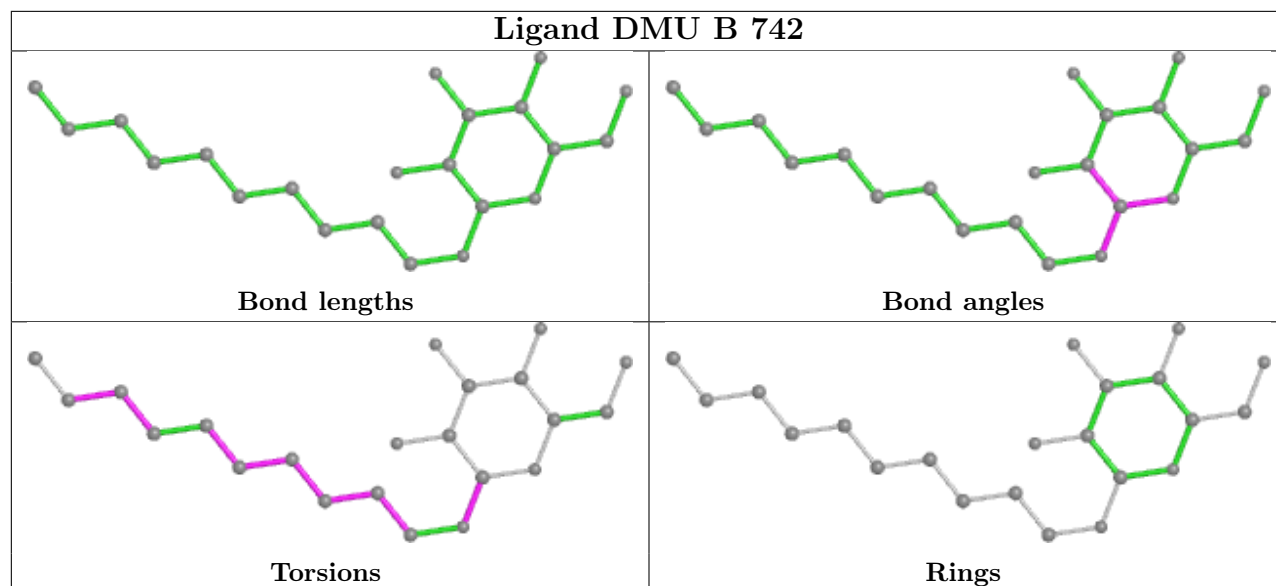


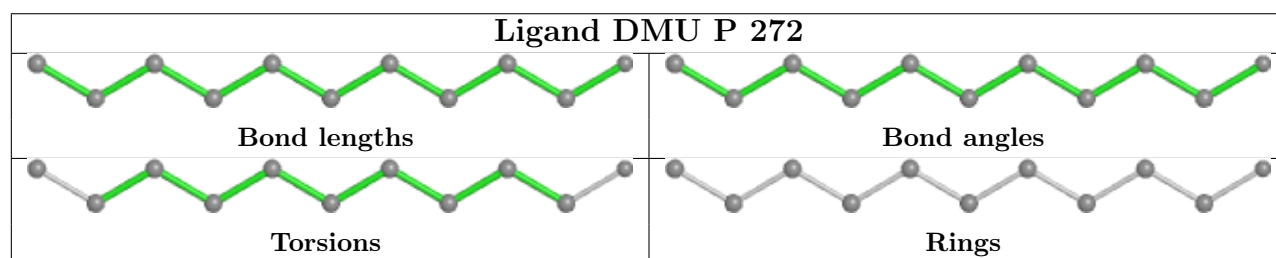
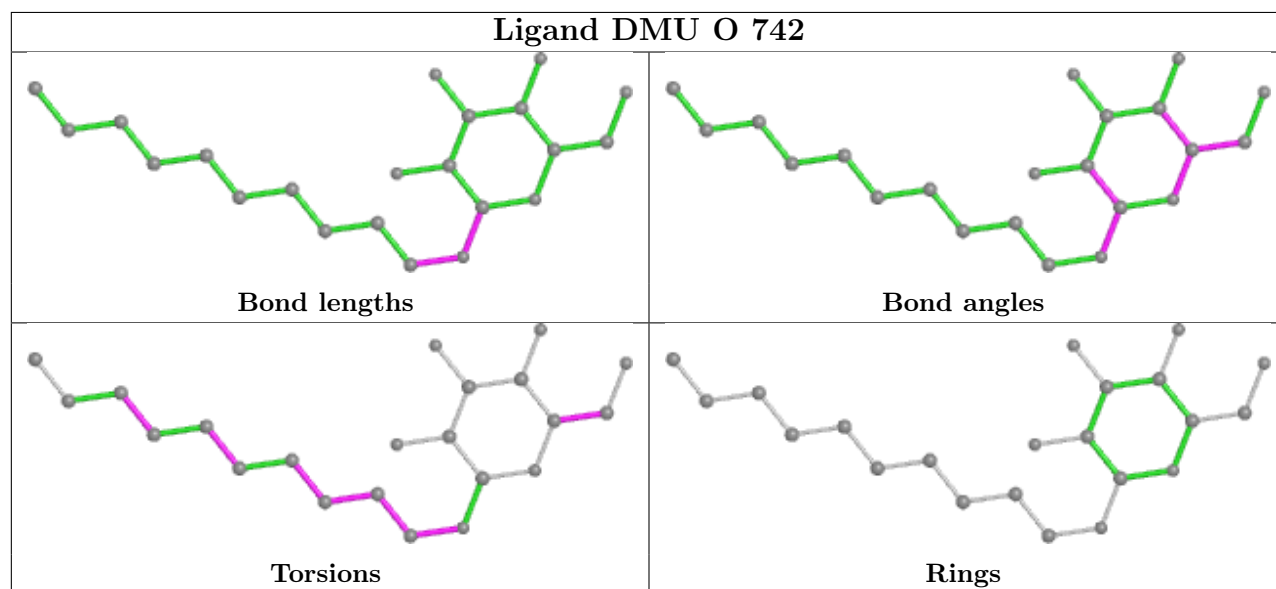
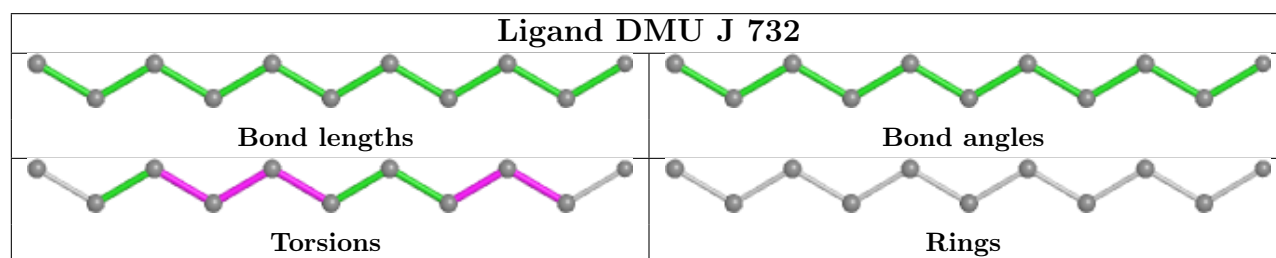
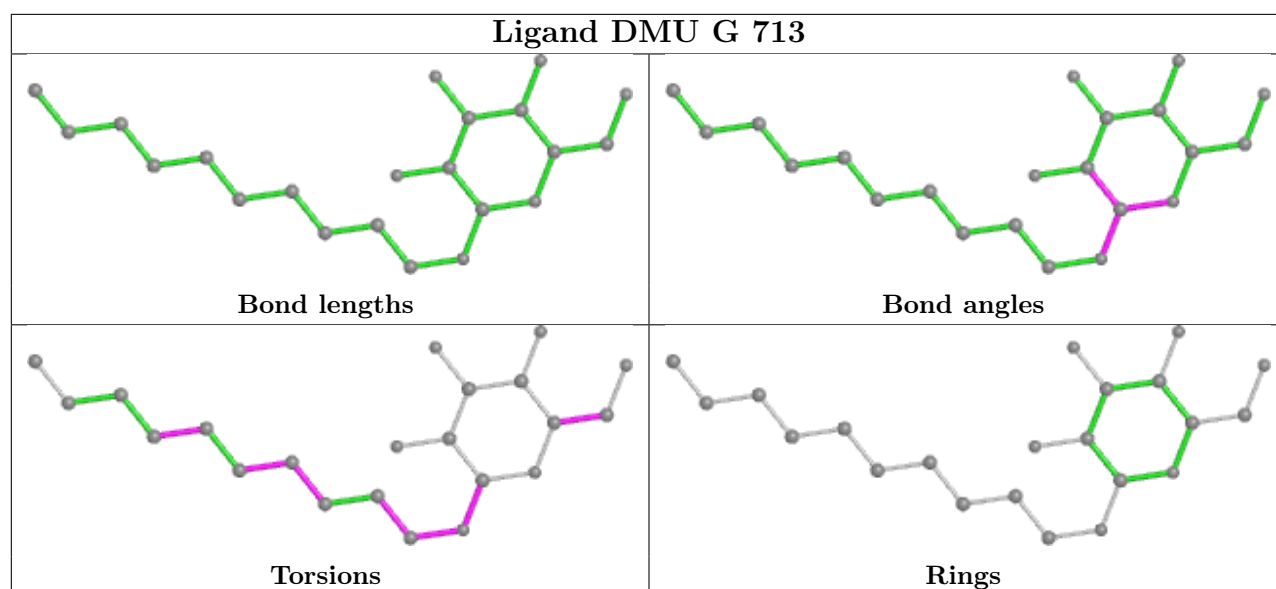




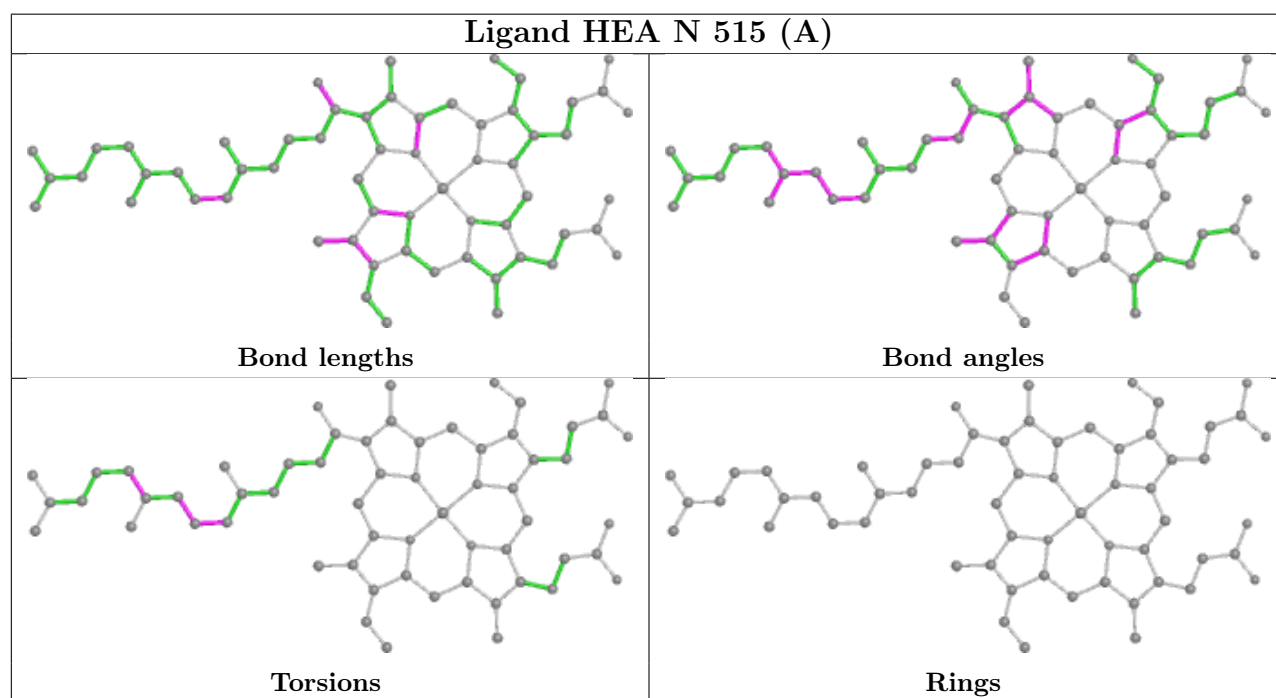
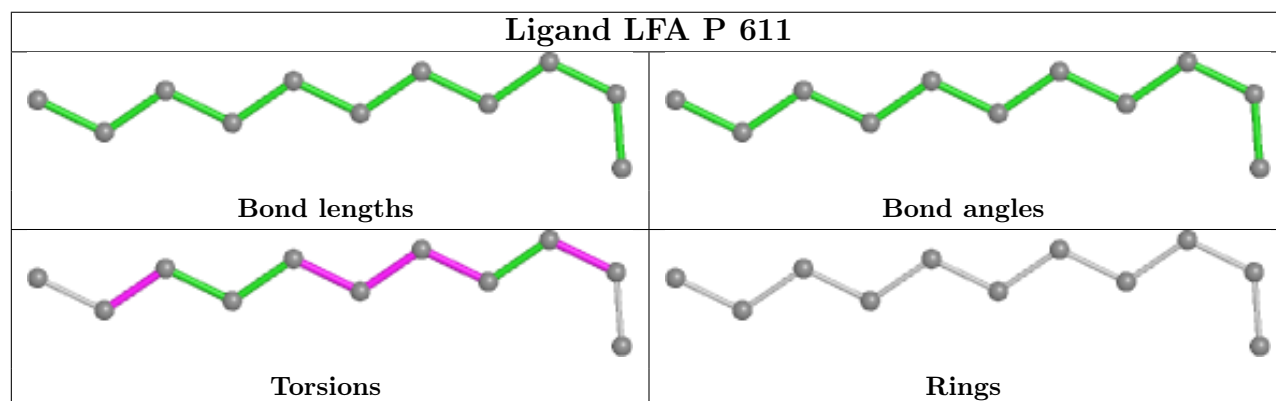
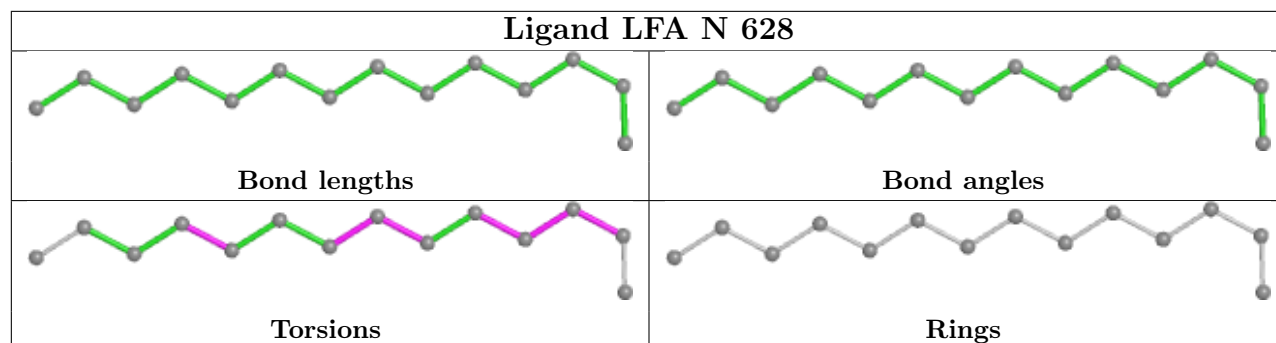


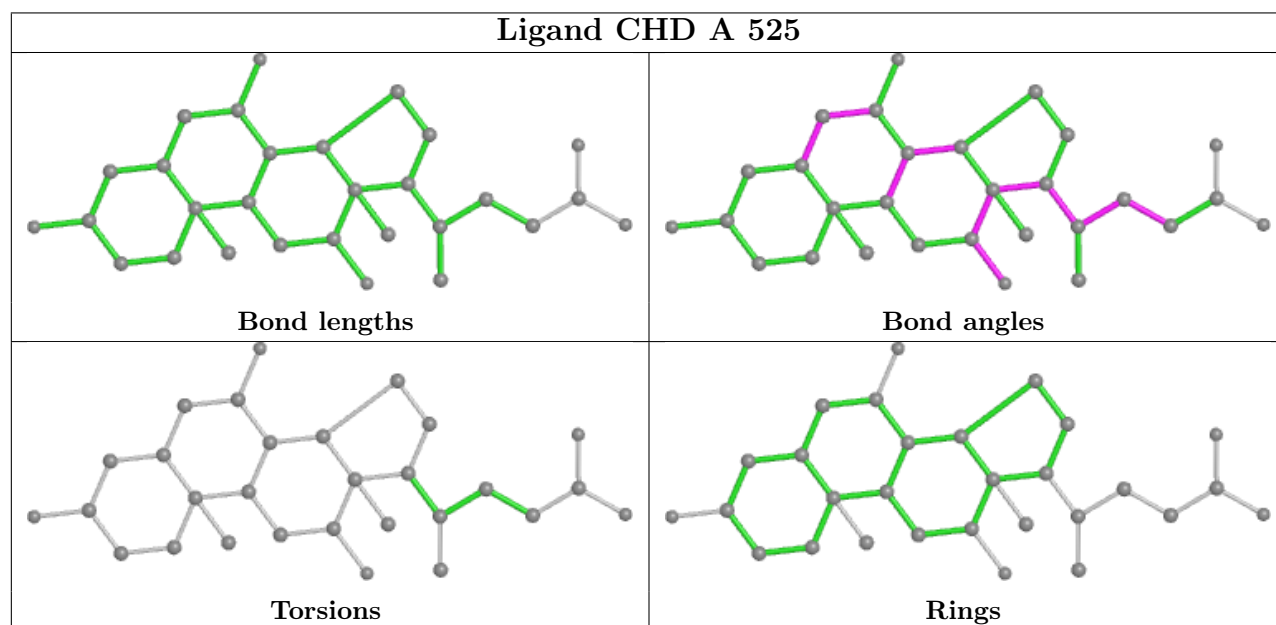
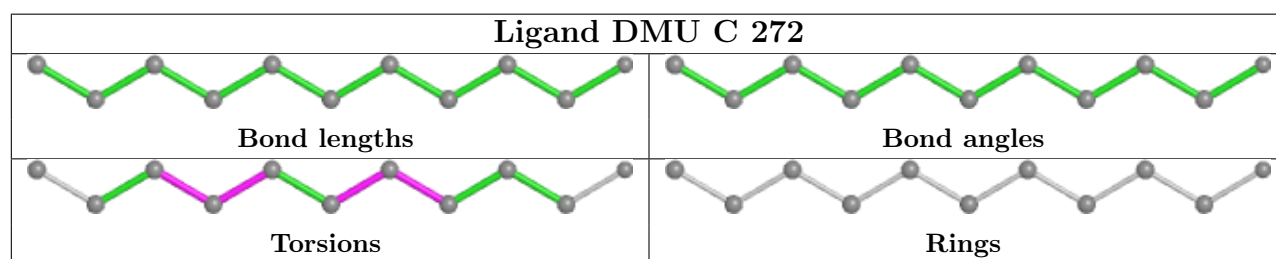
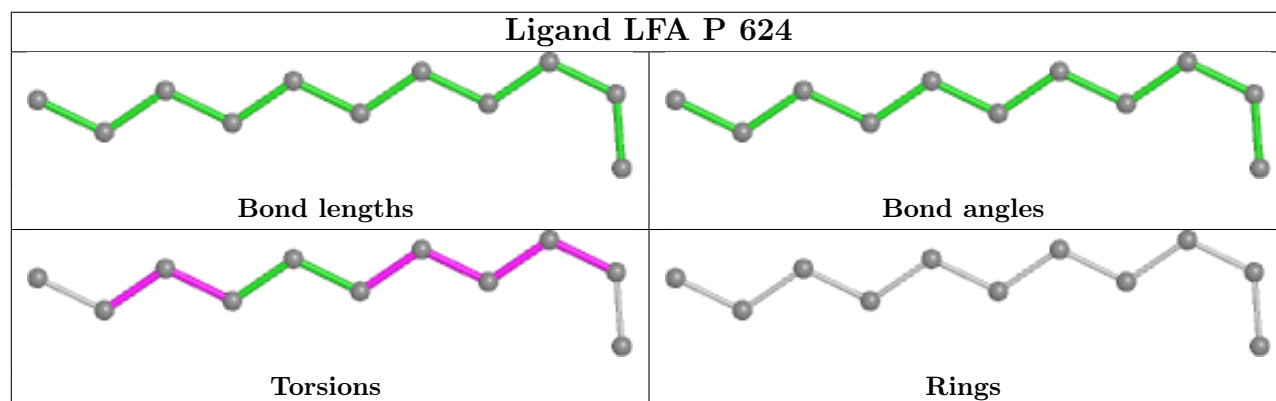
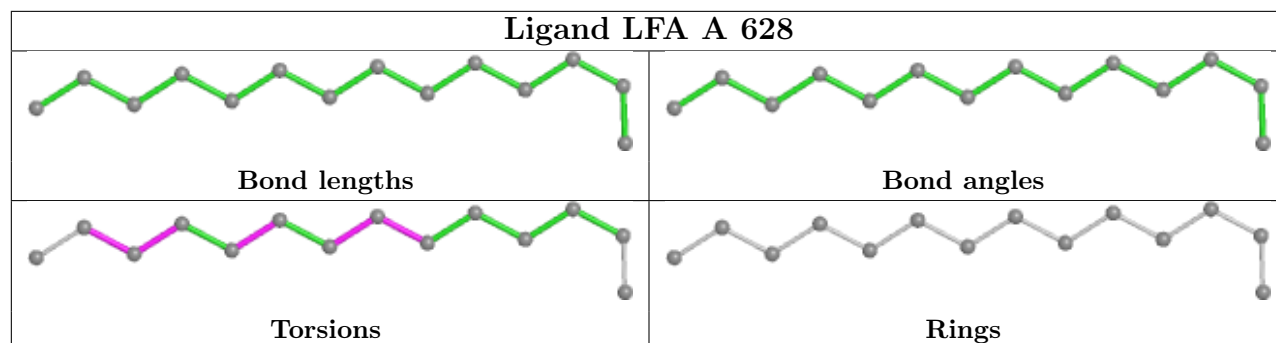


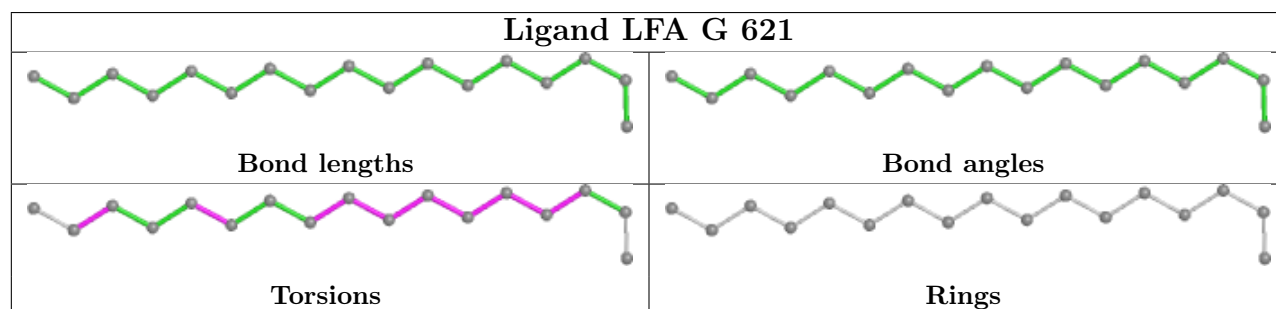
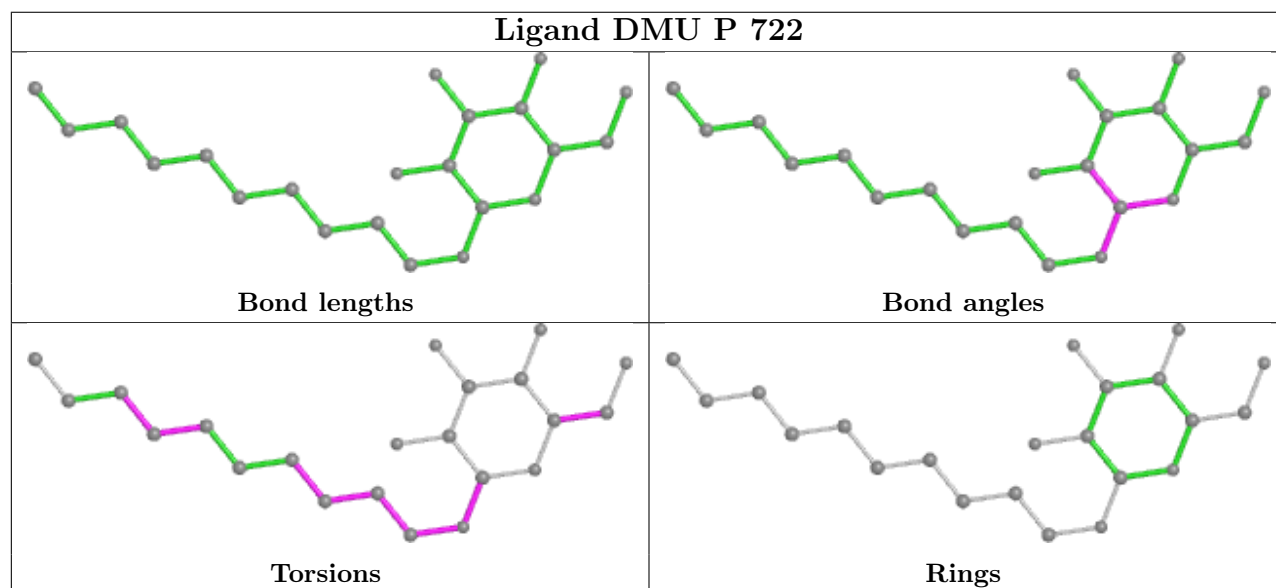
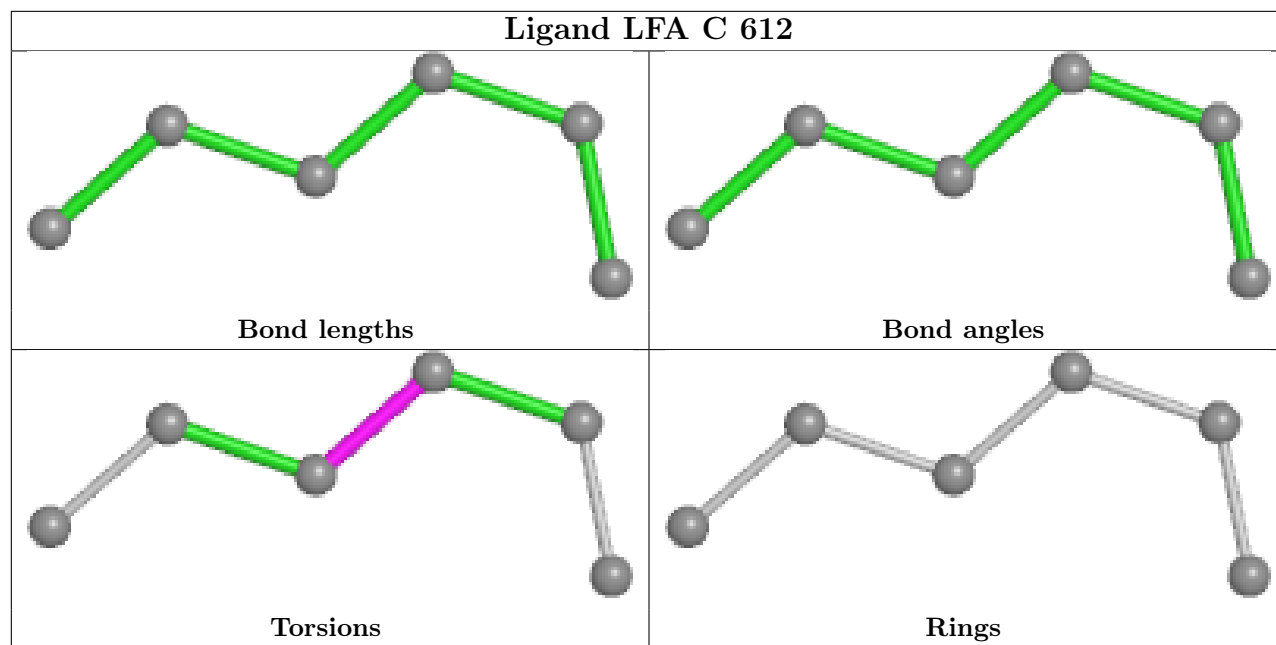


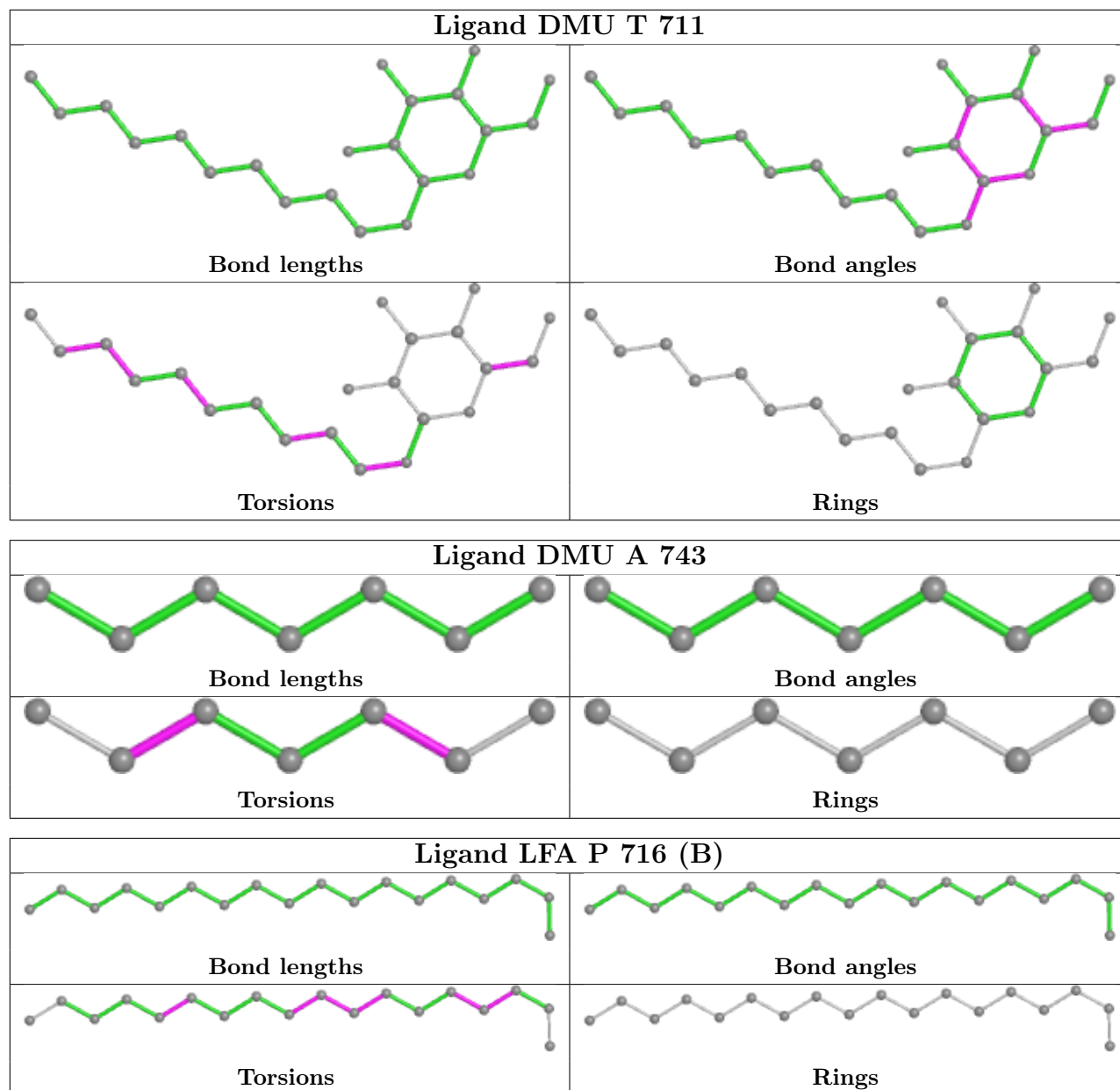


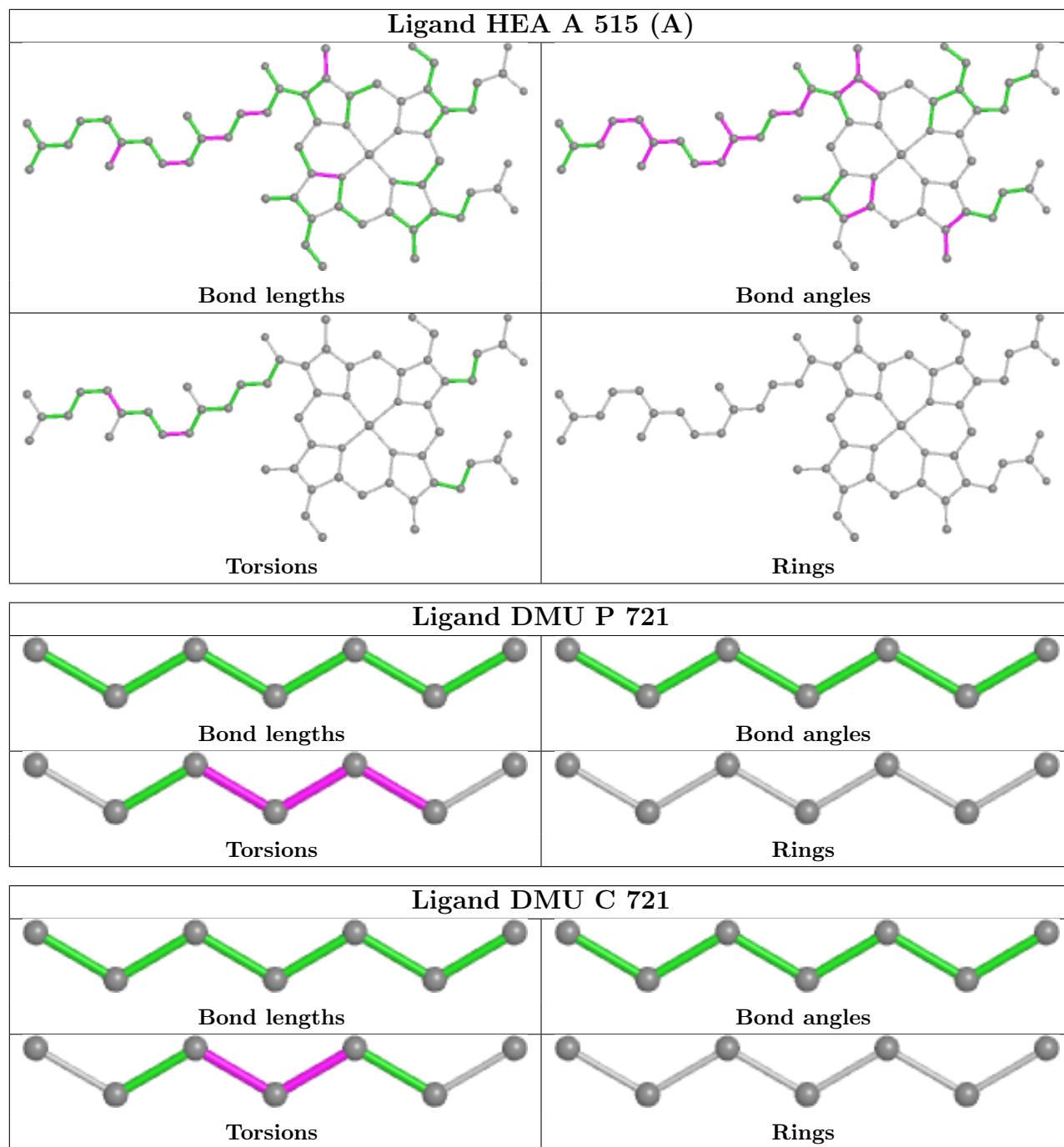


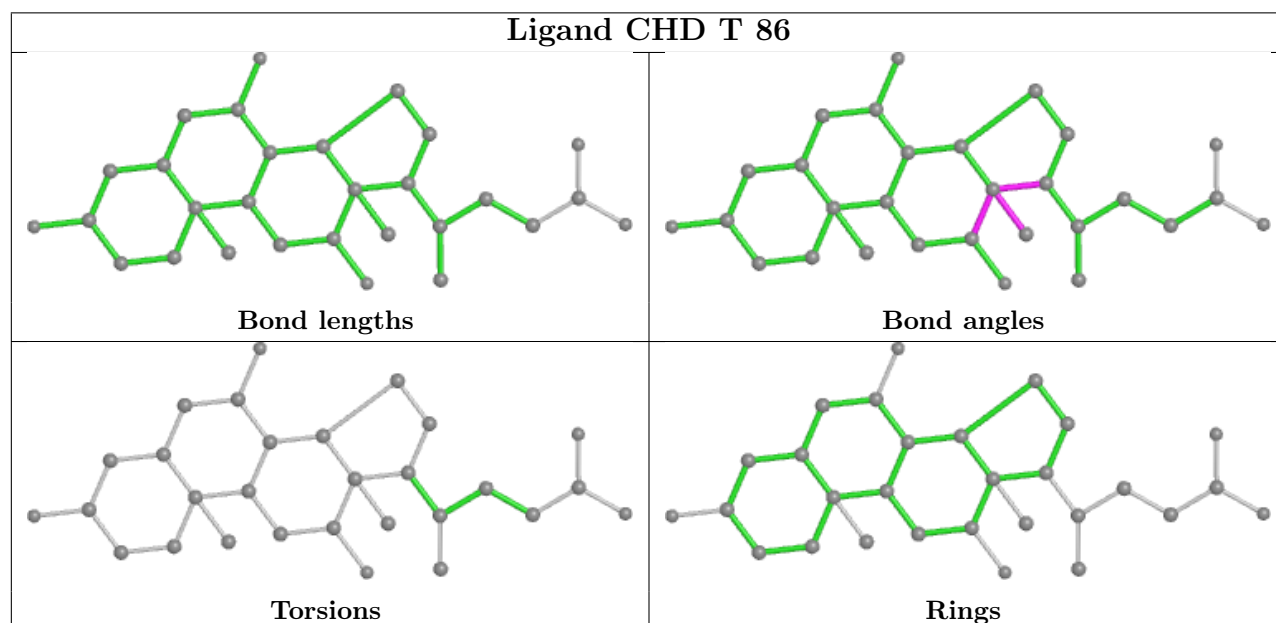
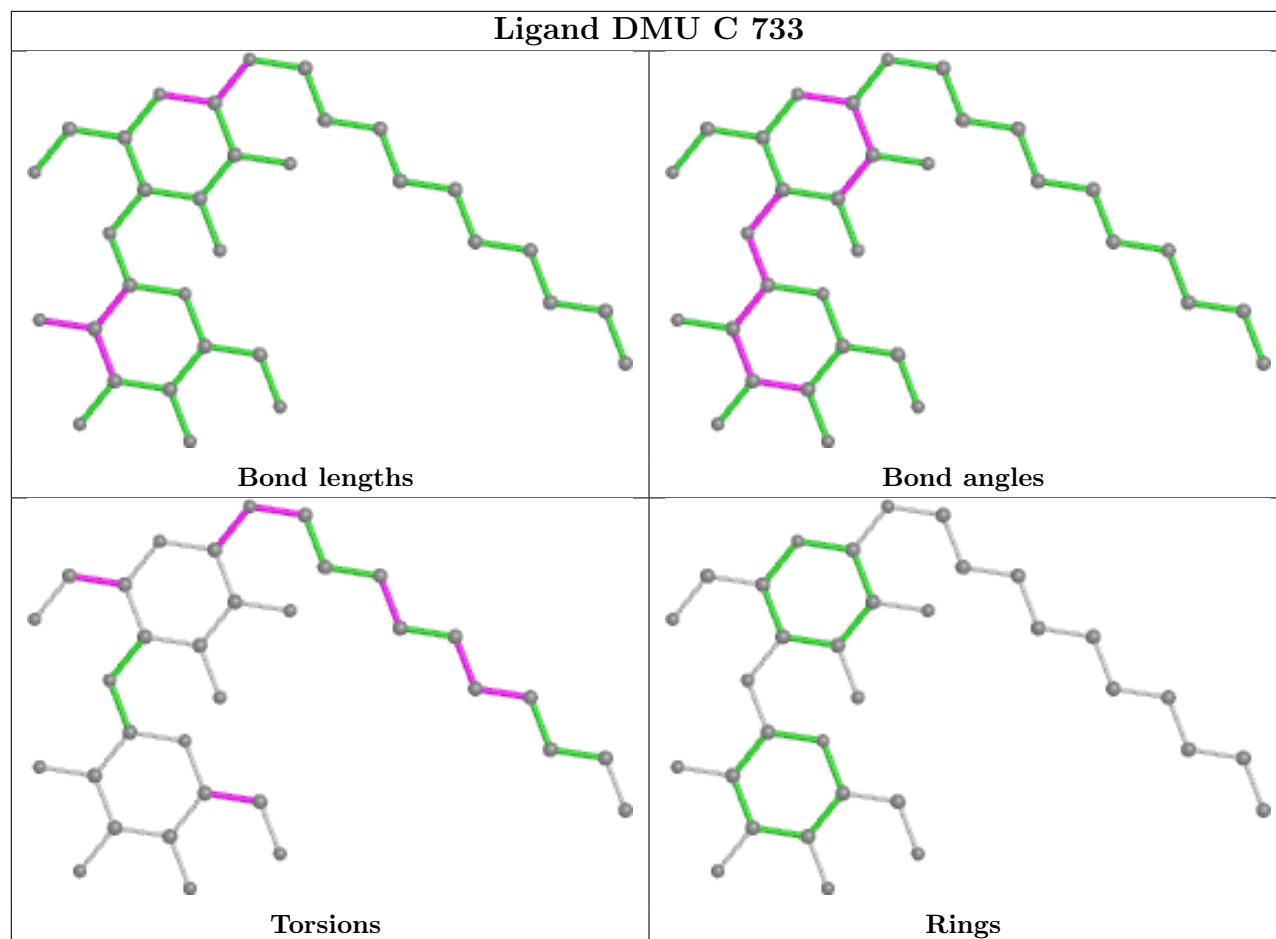


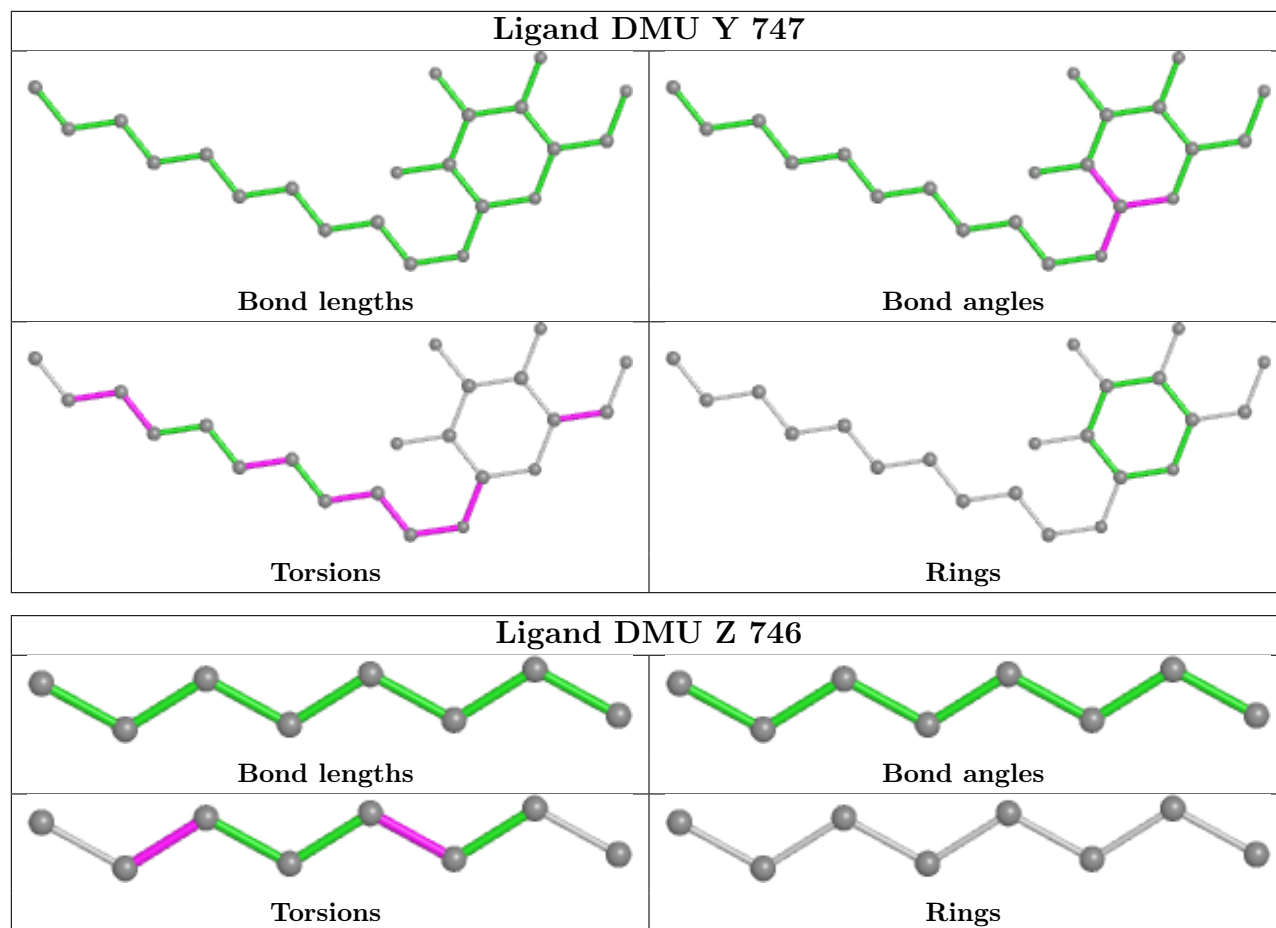


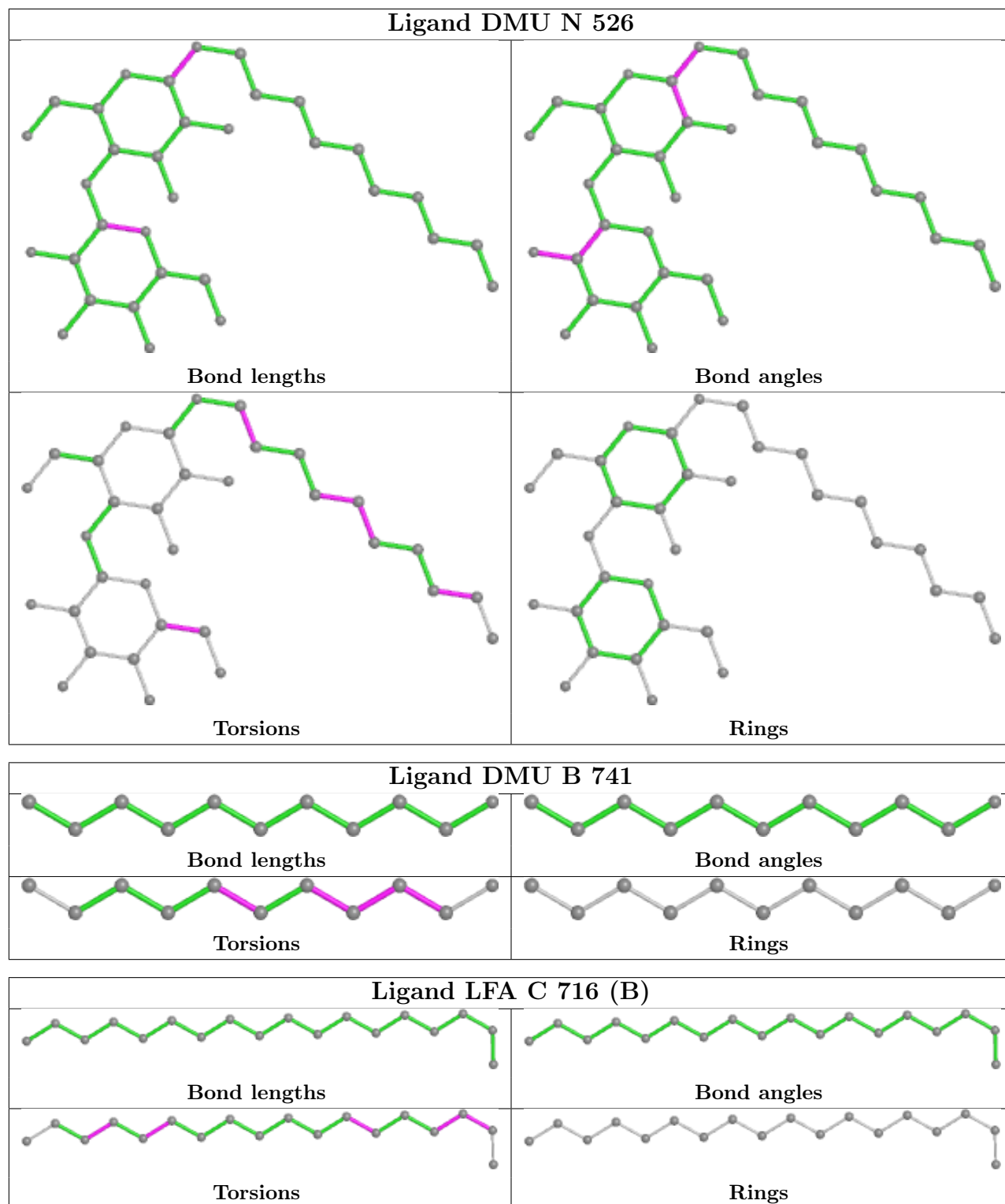




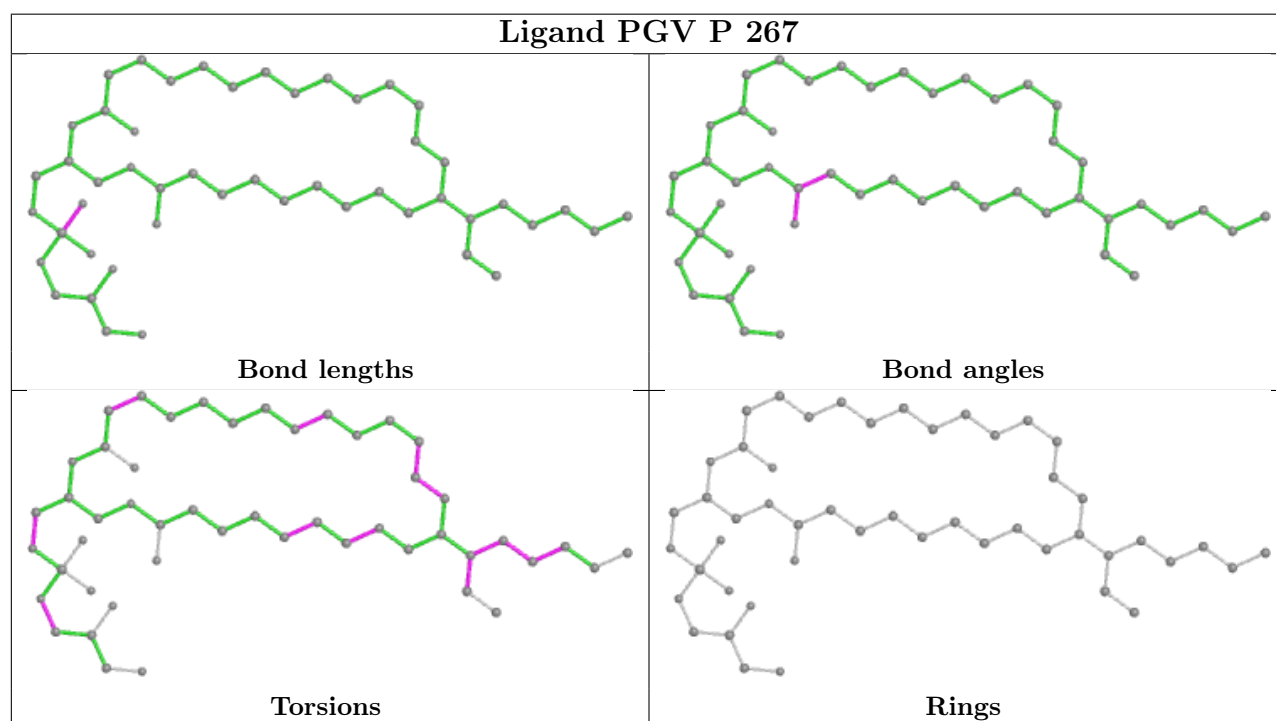
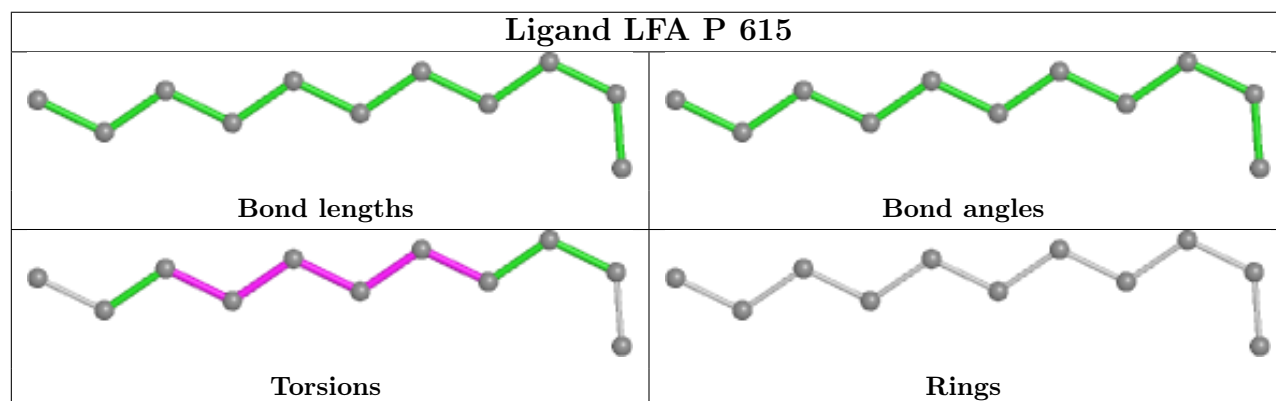
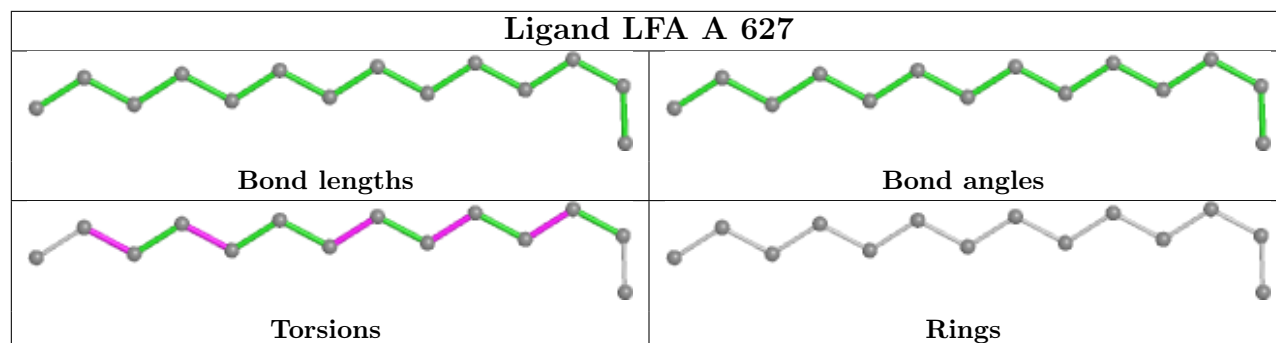




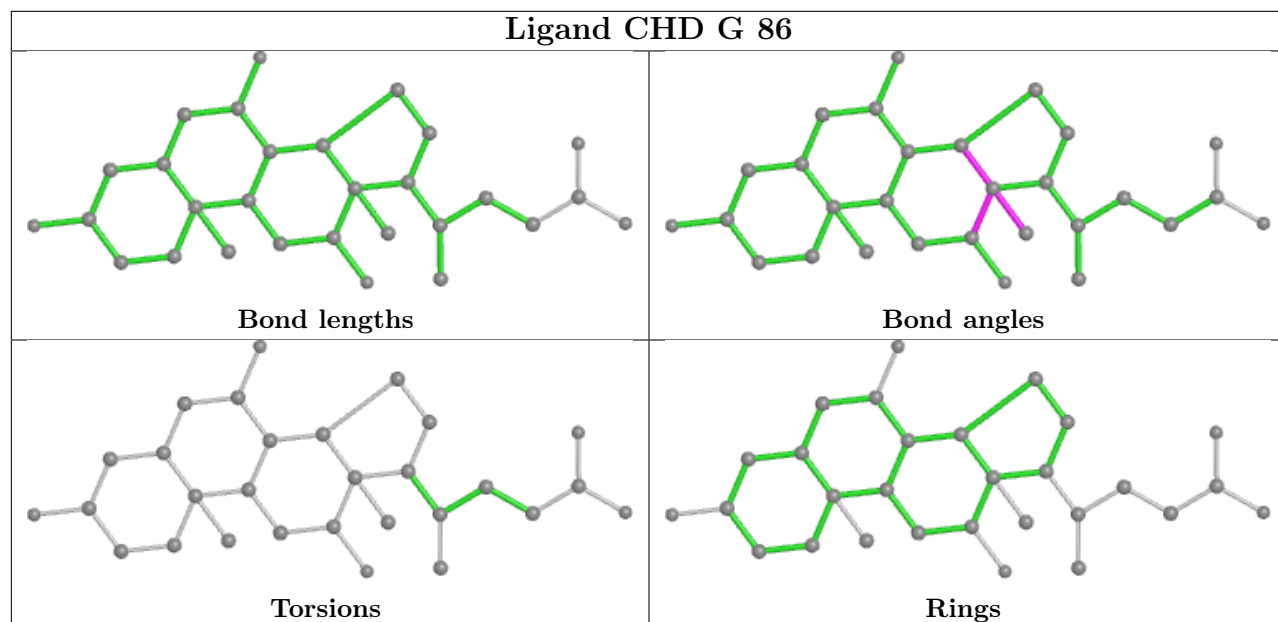




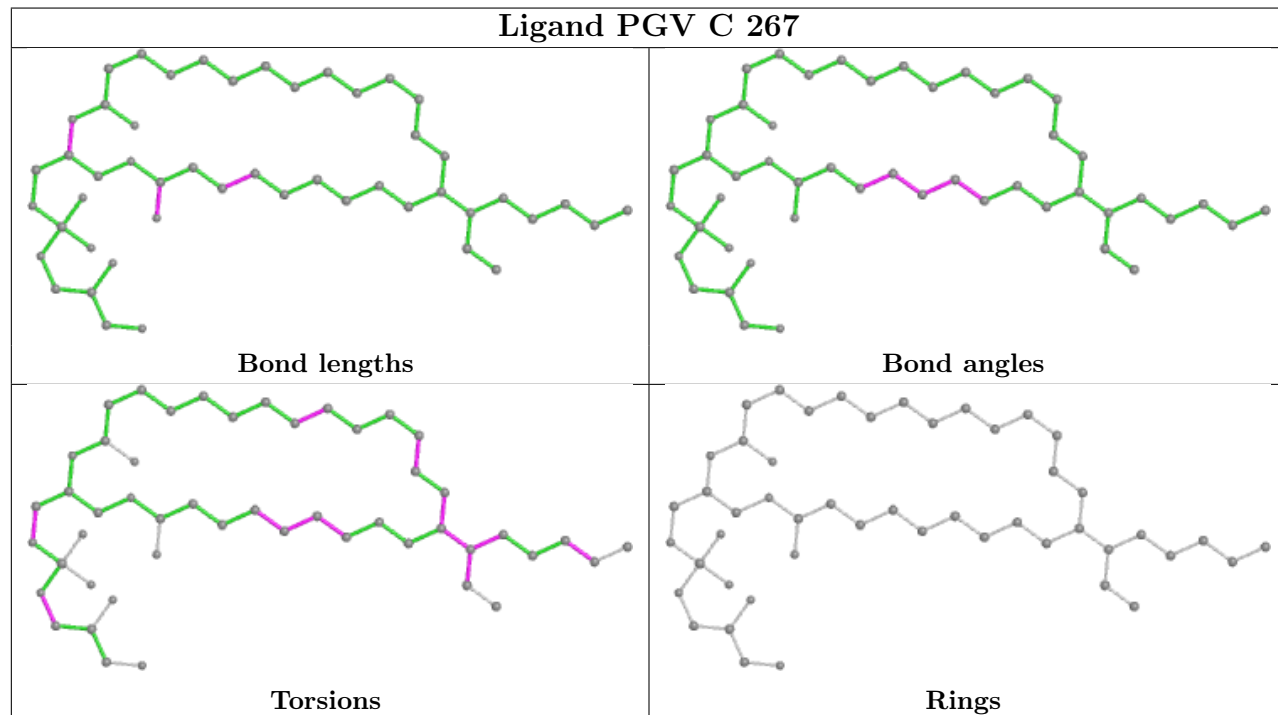


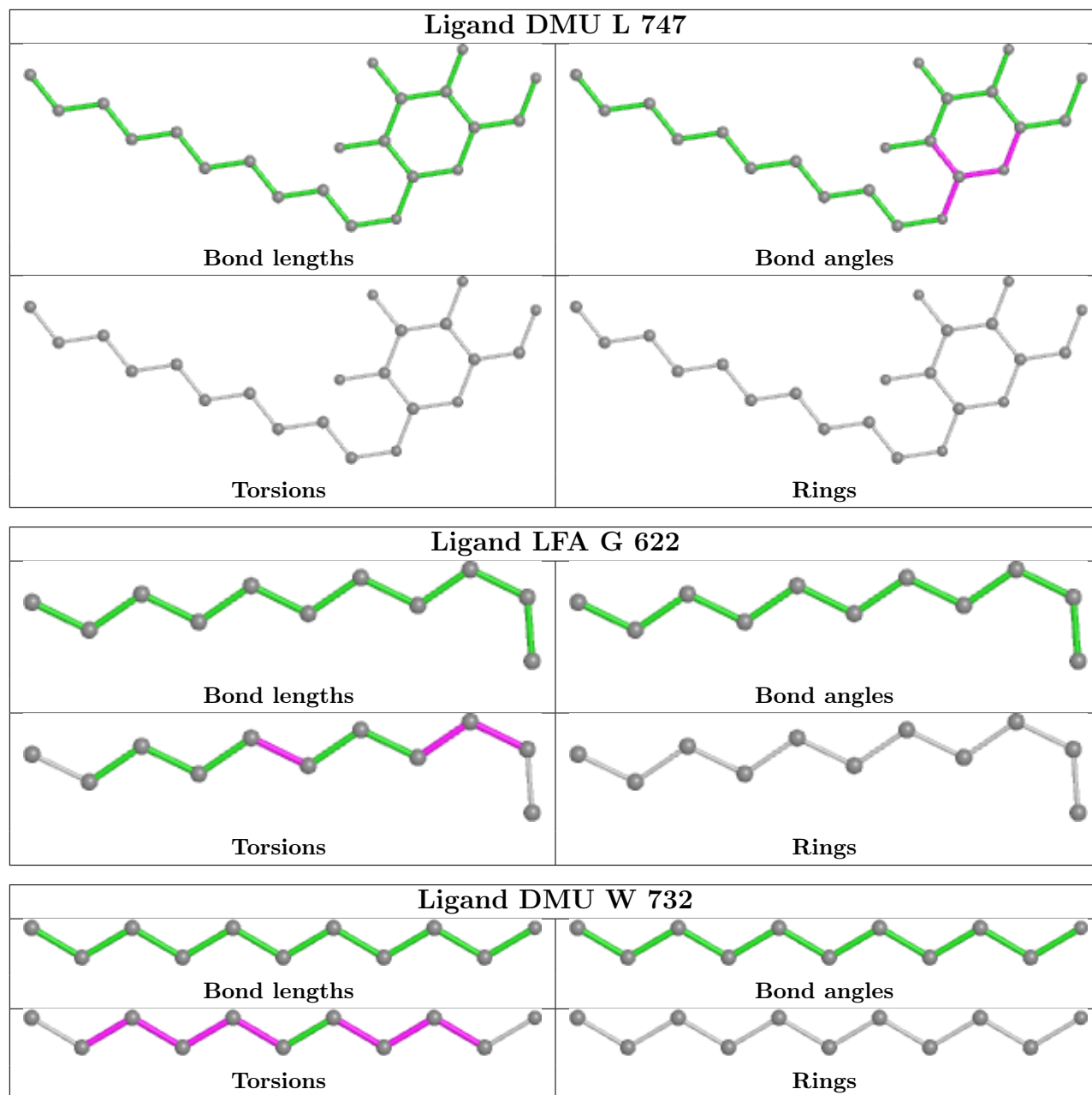


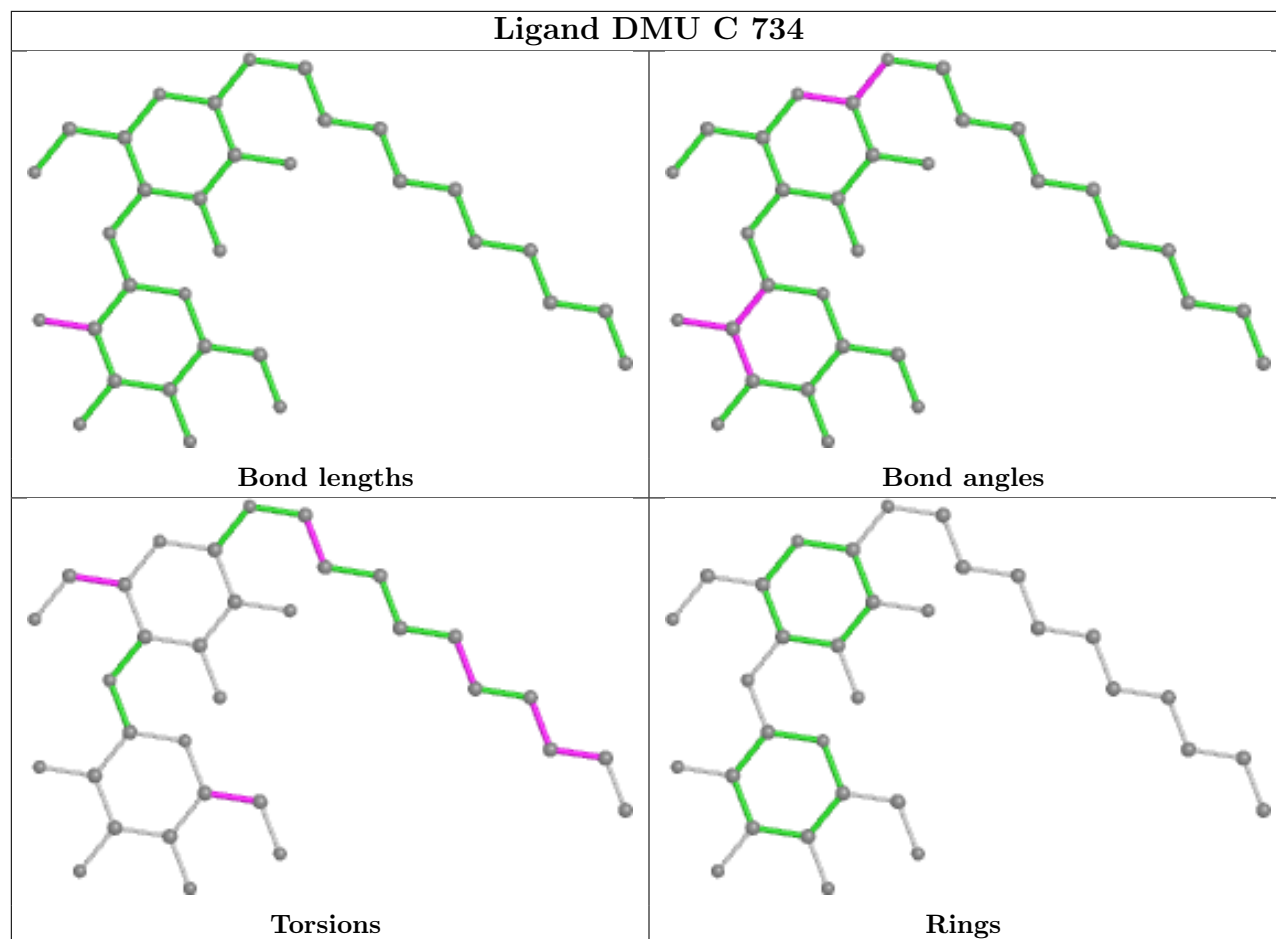
## Ligand CHD G 86

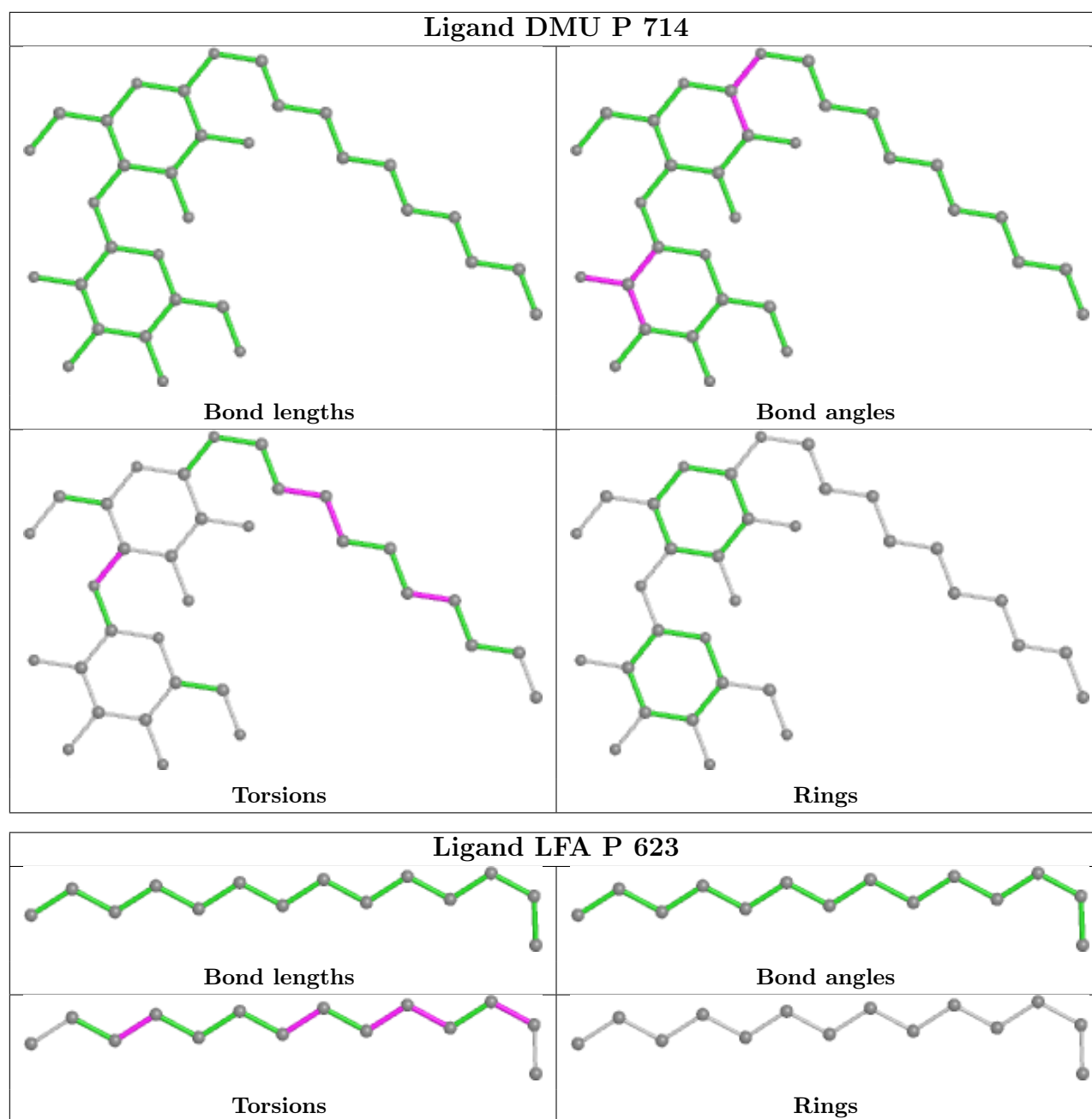


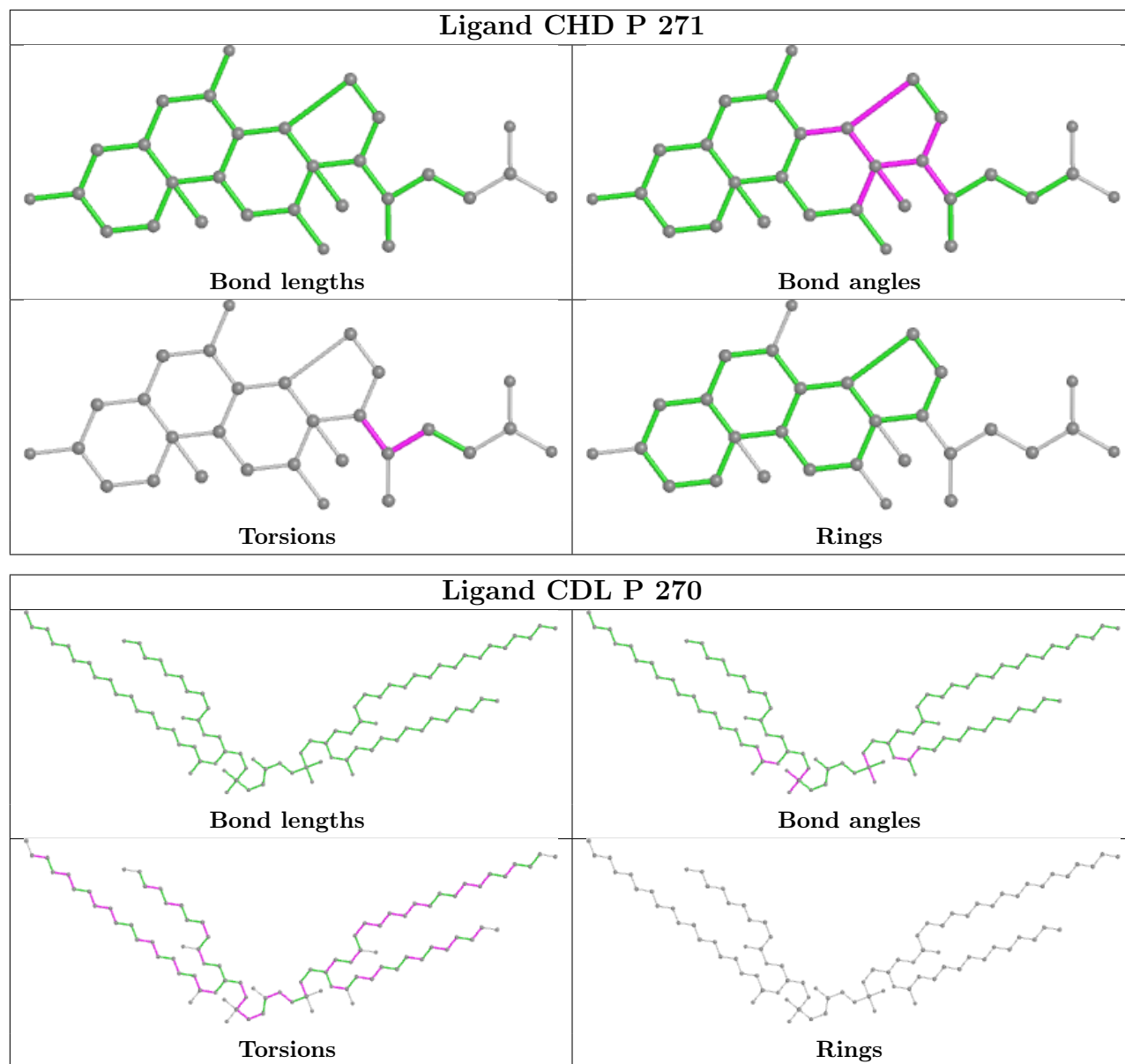
## Ligand PGV C 267

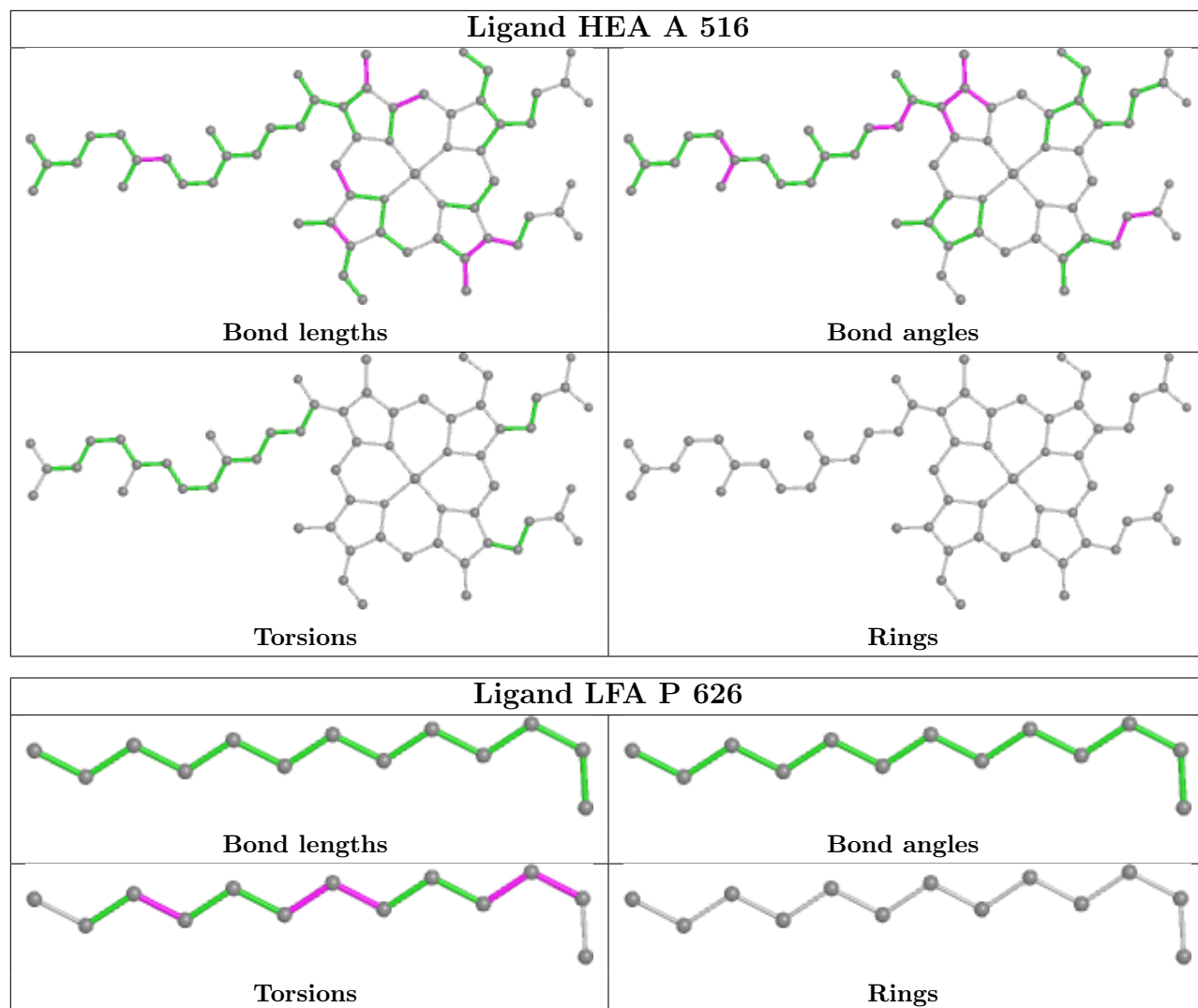


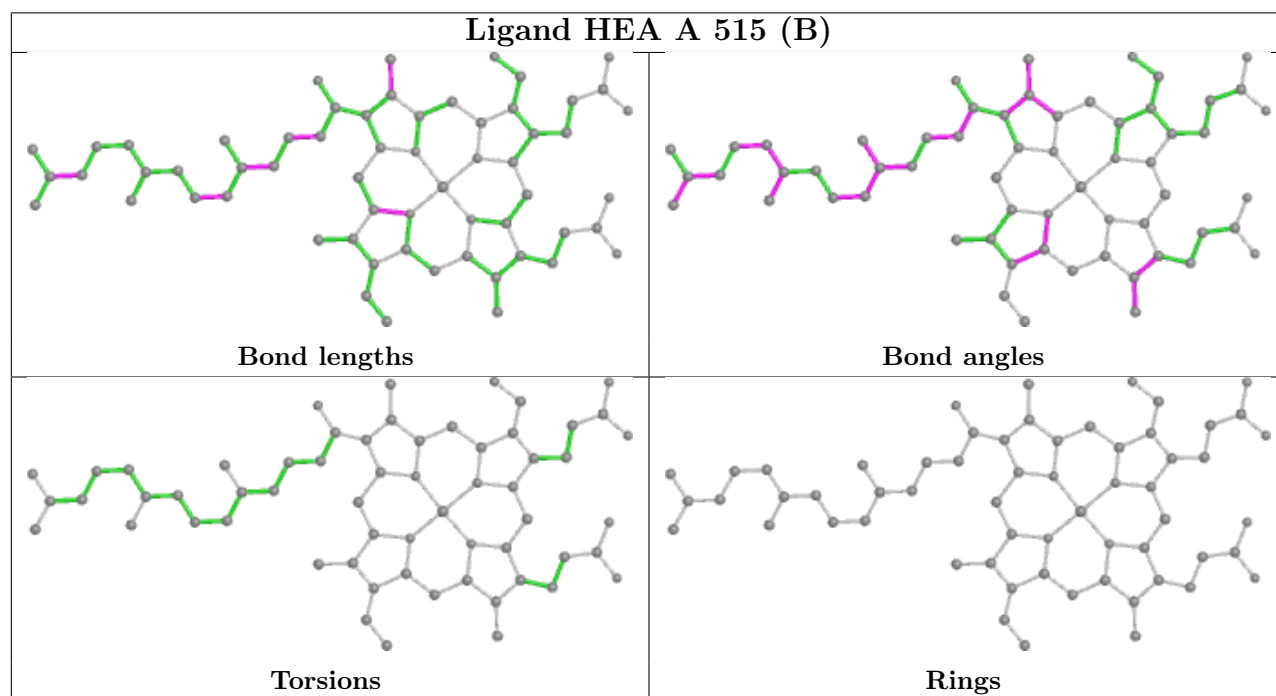
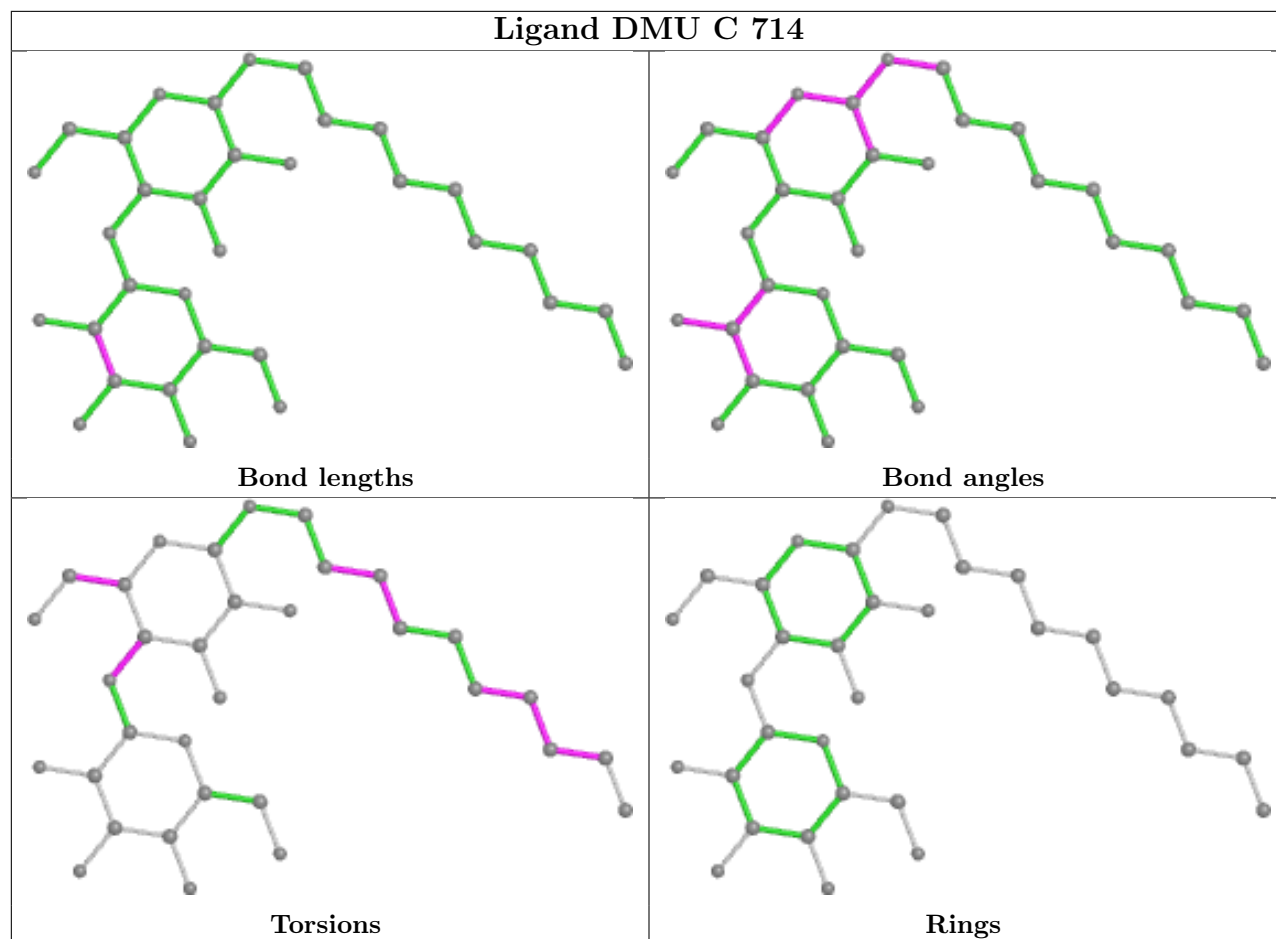




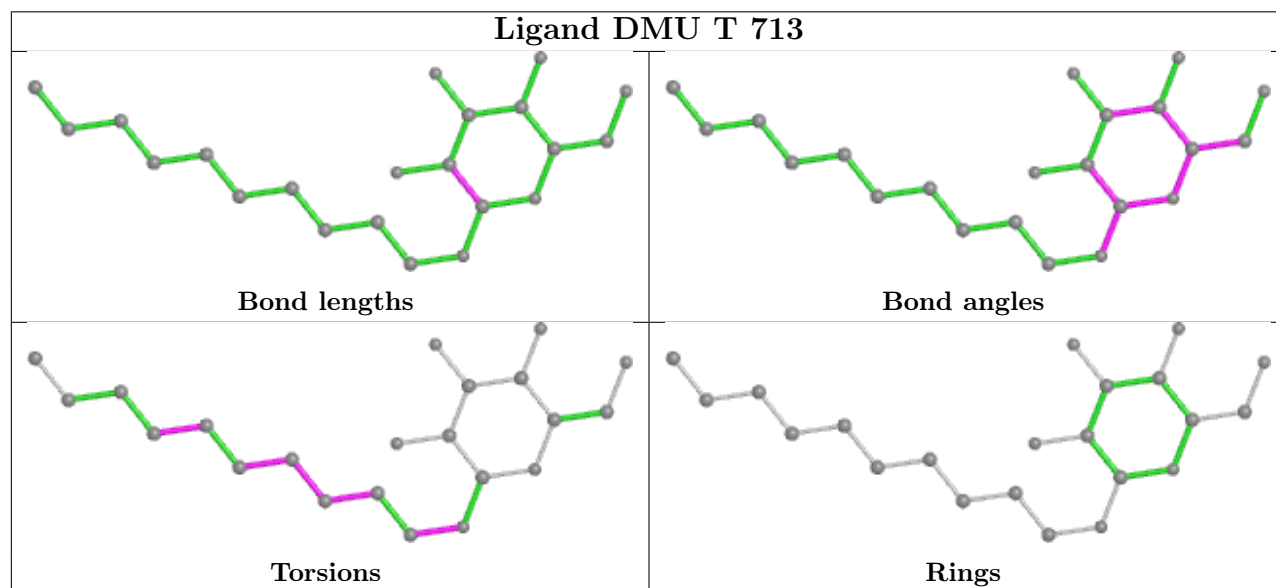
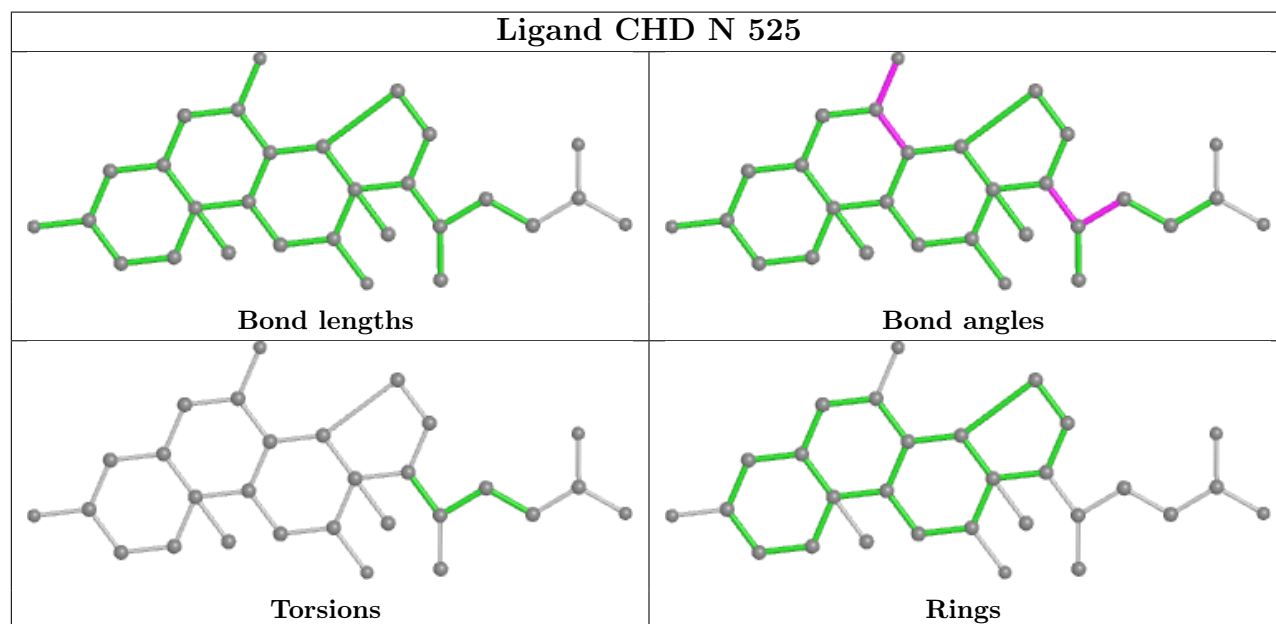
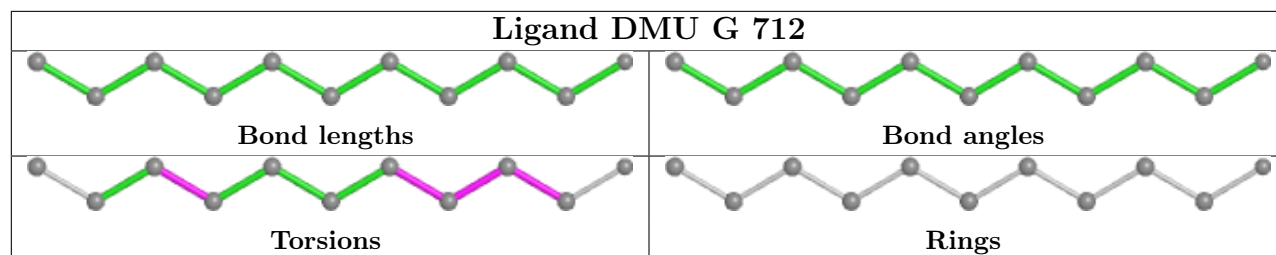


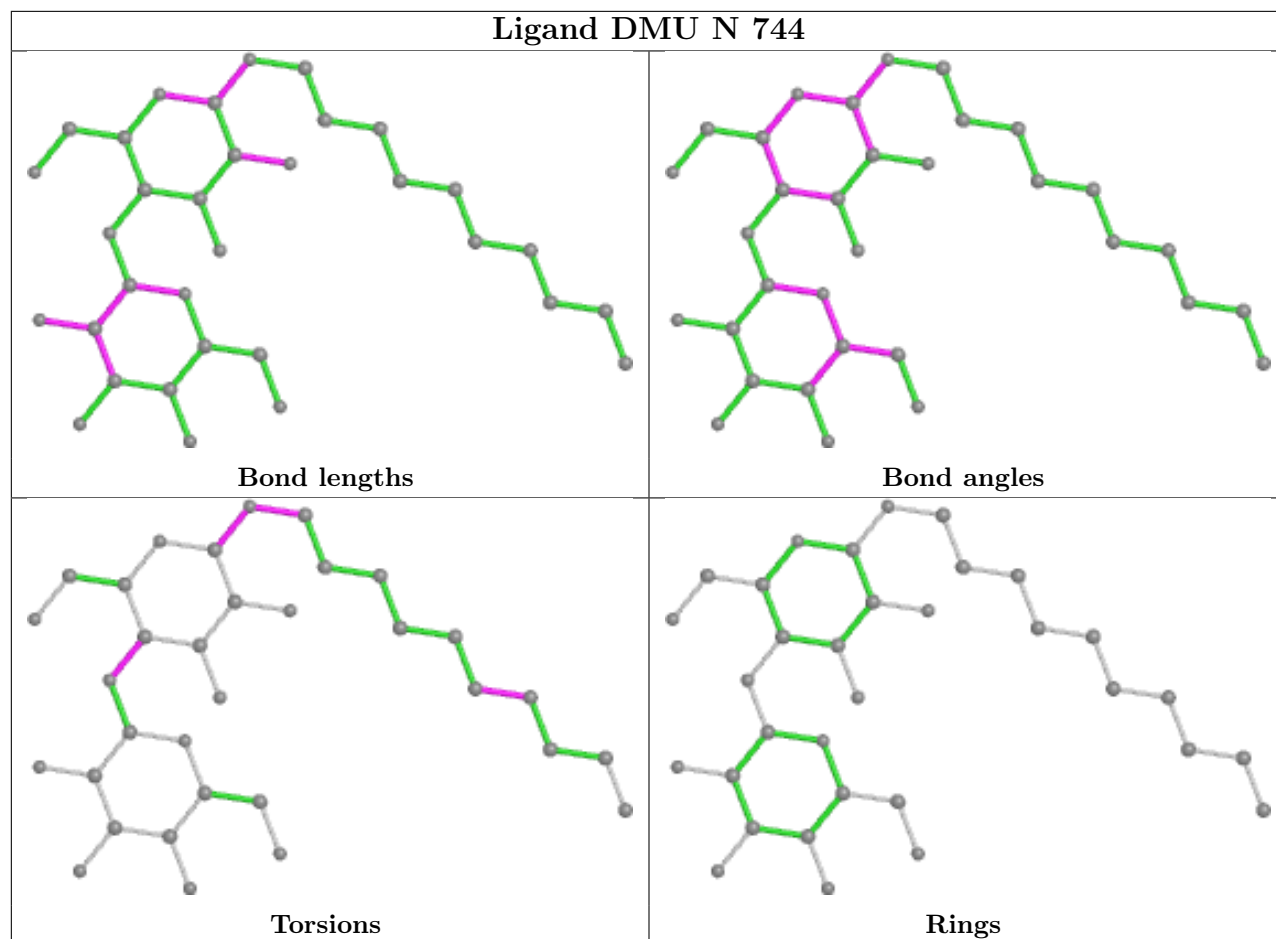


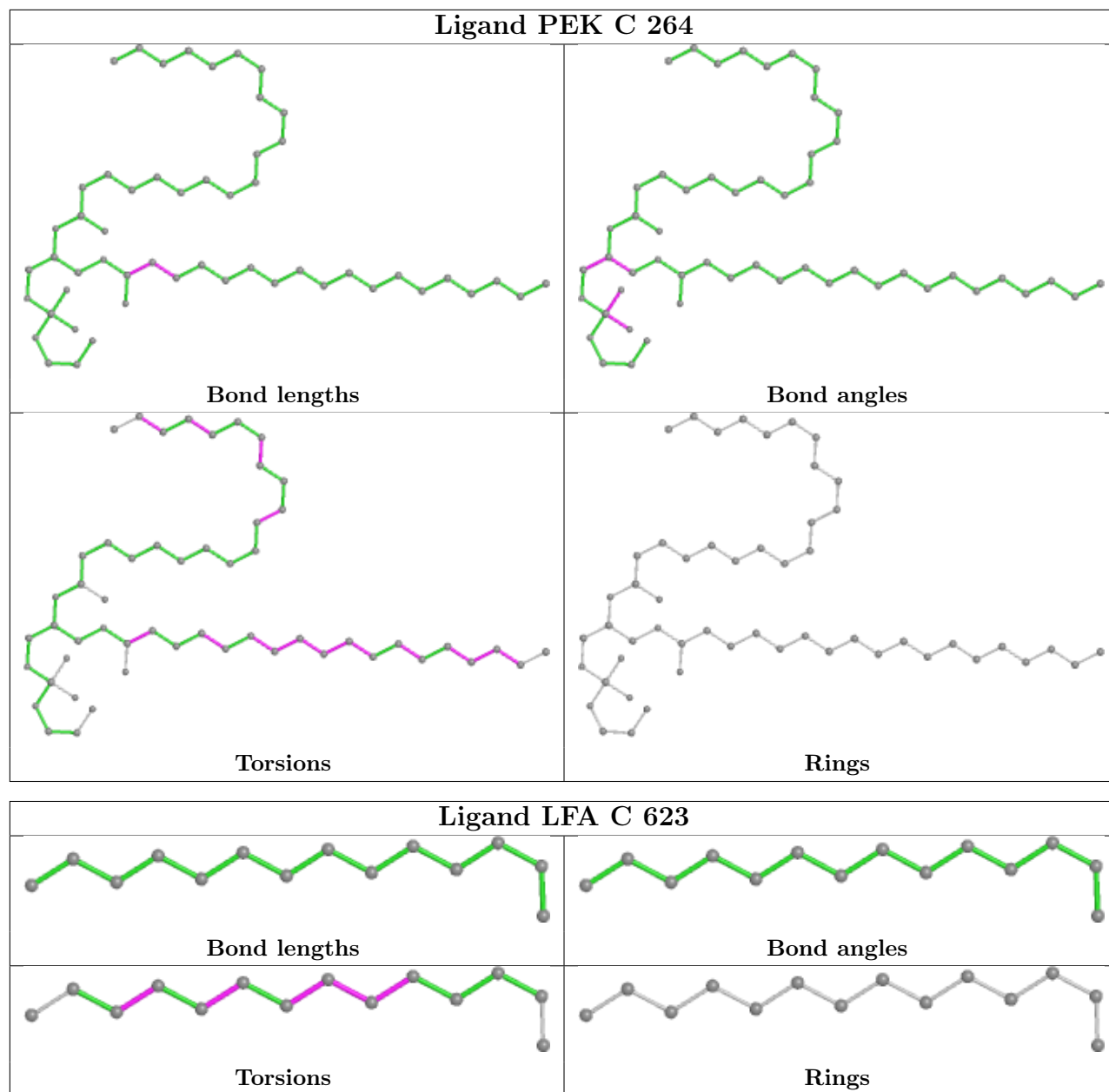


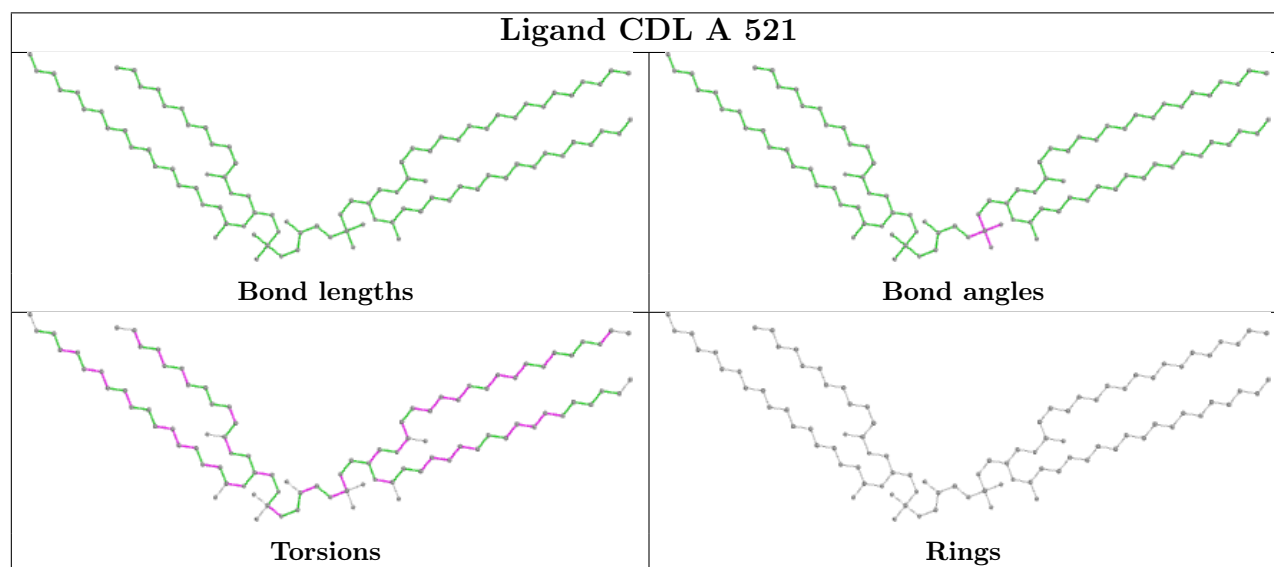
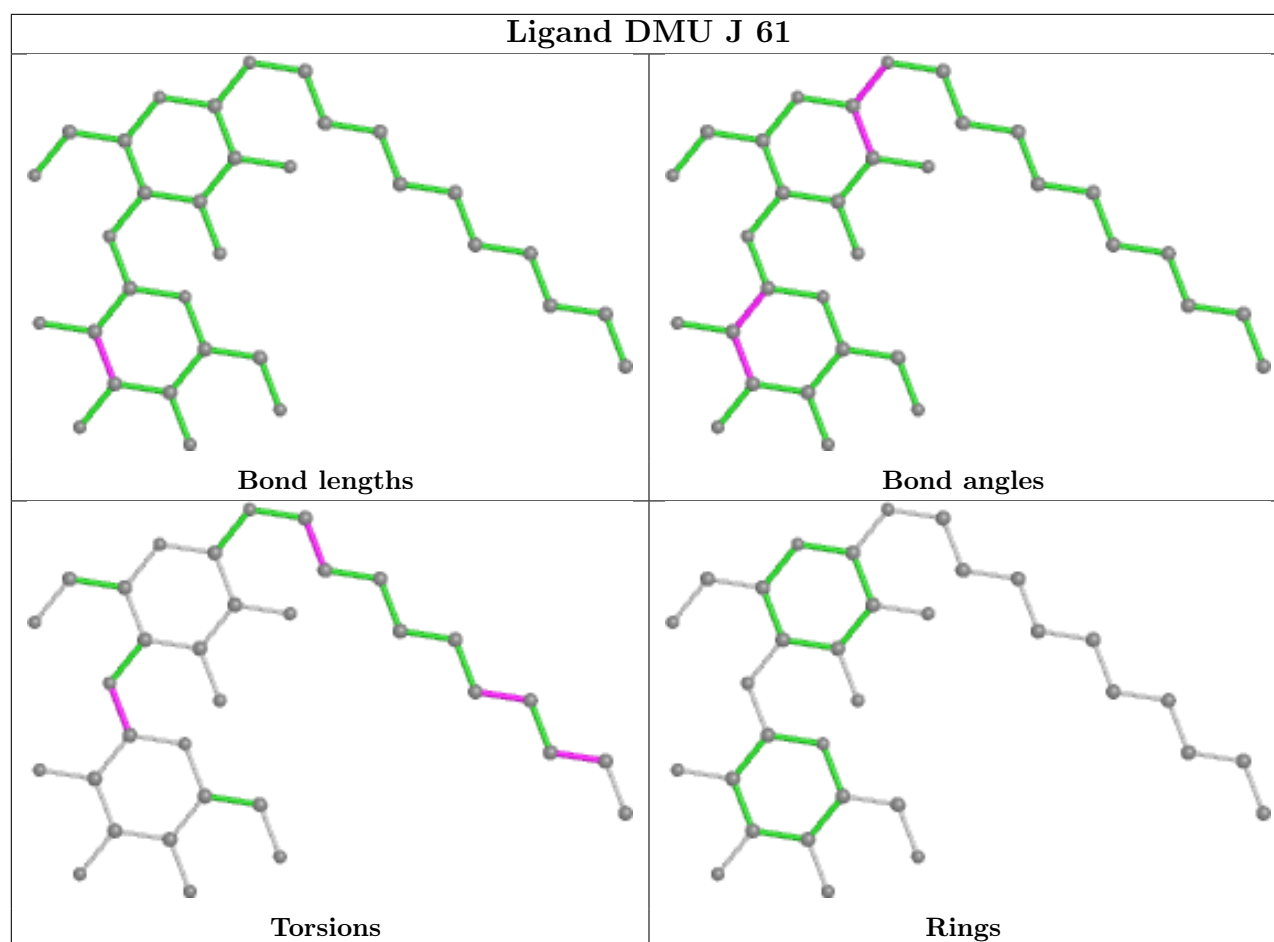


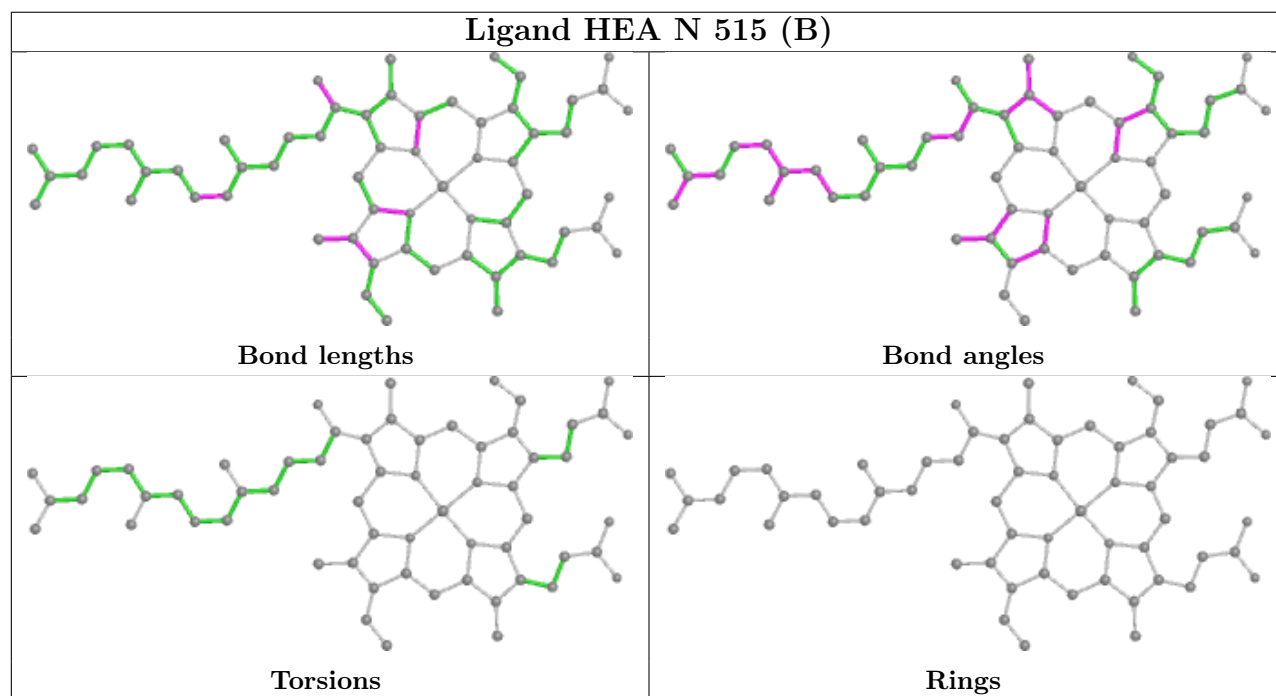
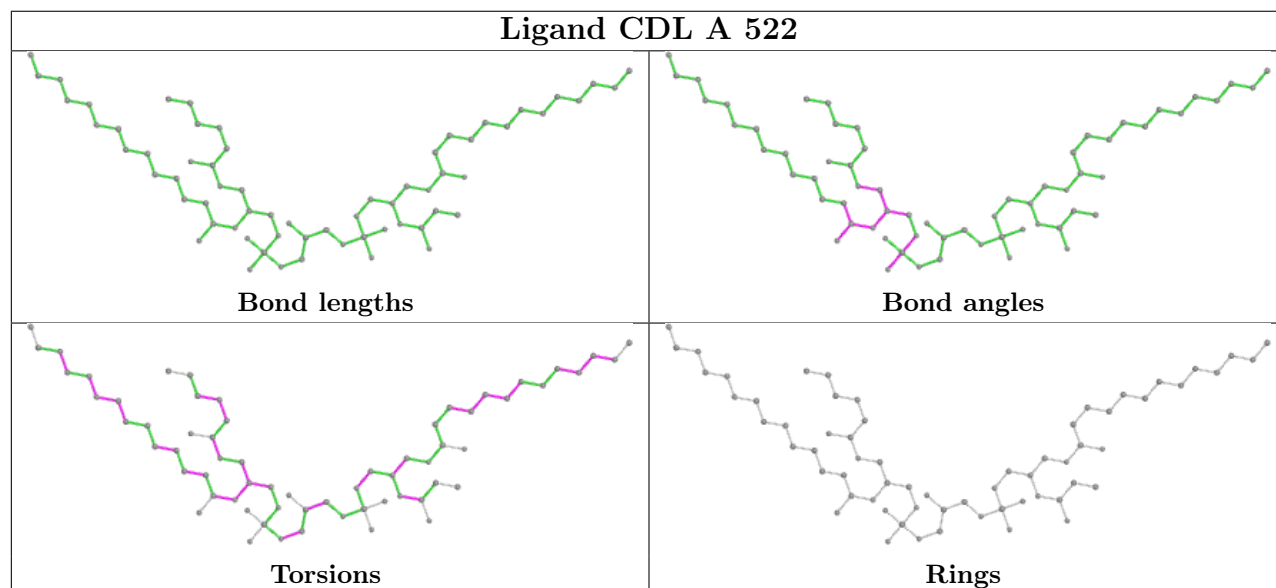
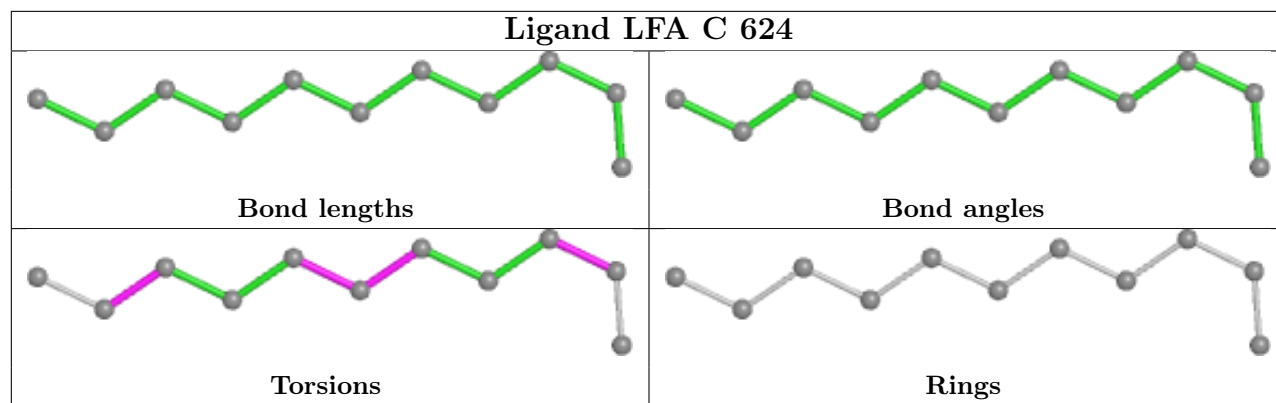




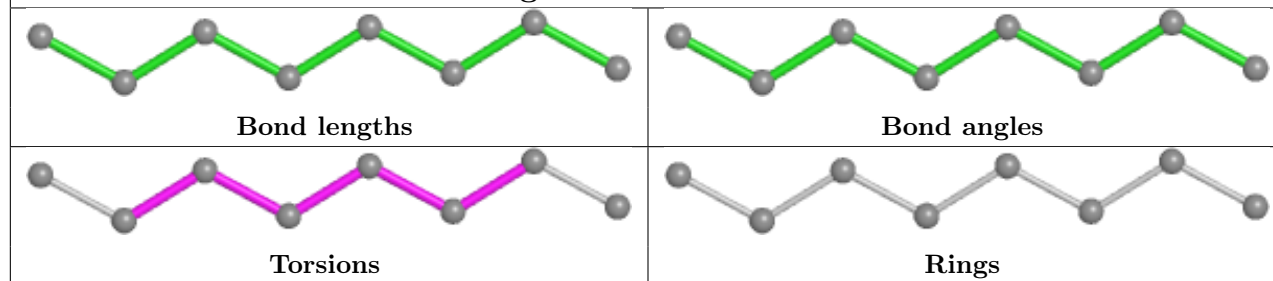




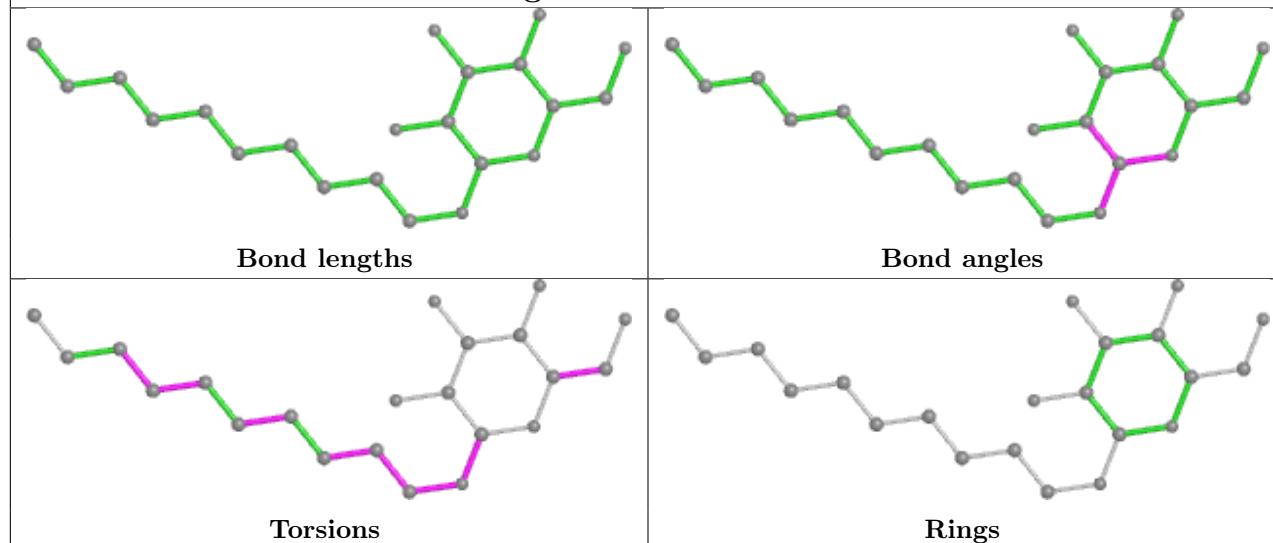




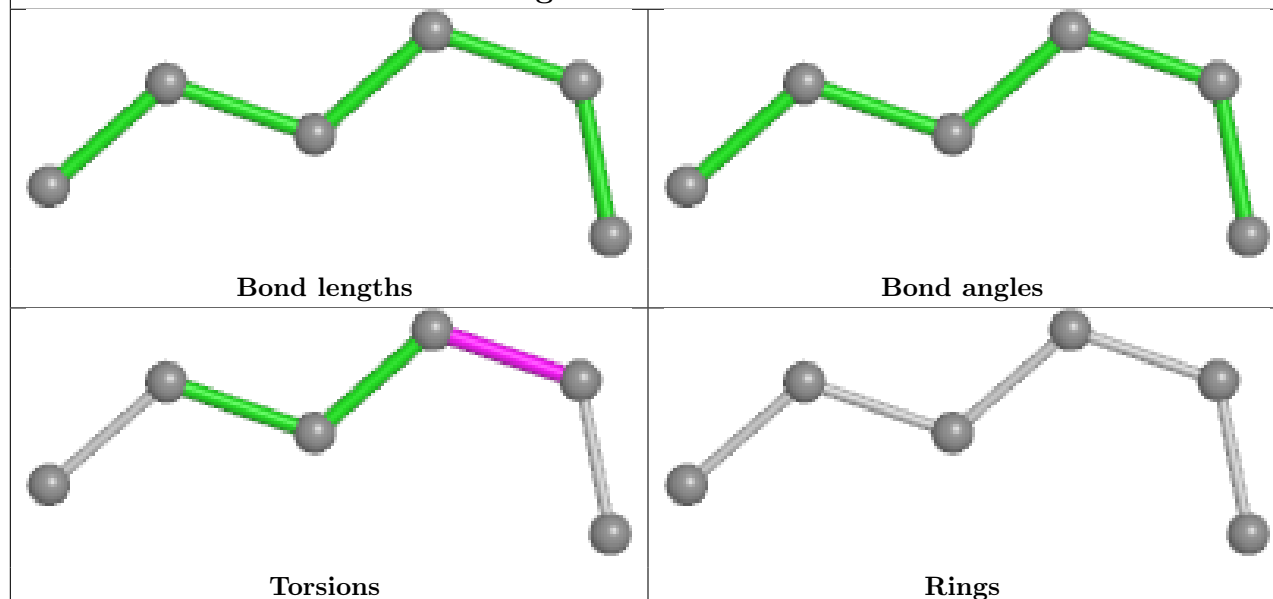
## Ligand DMU M 746

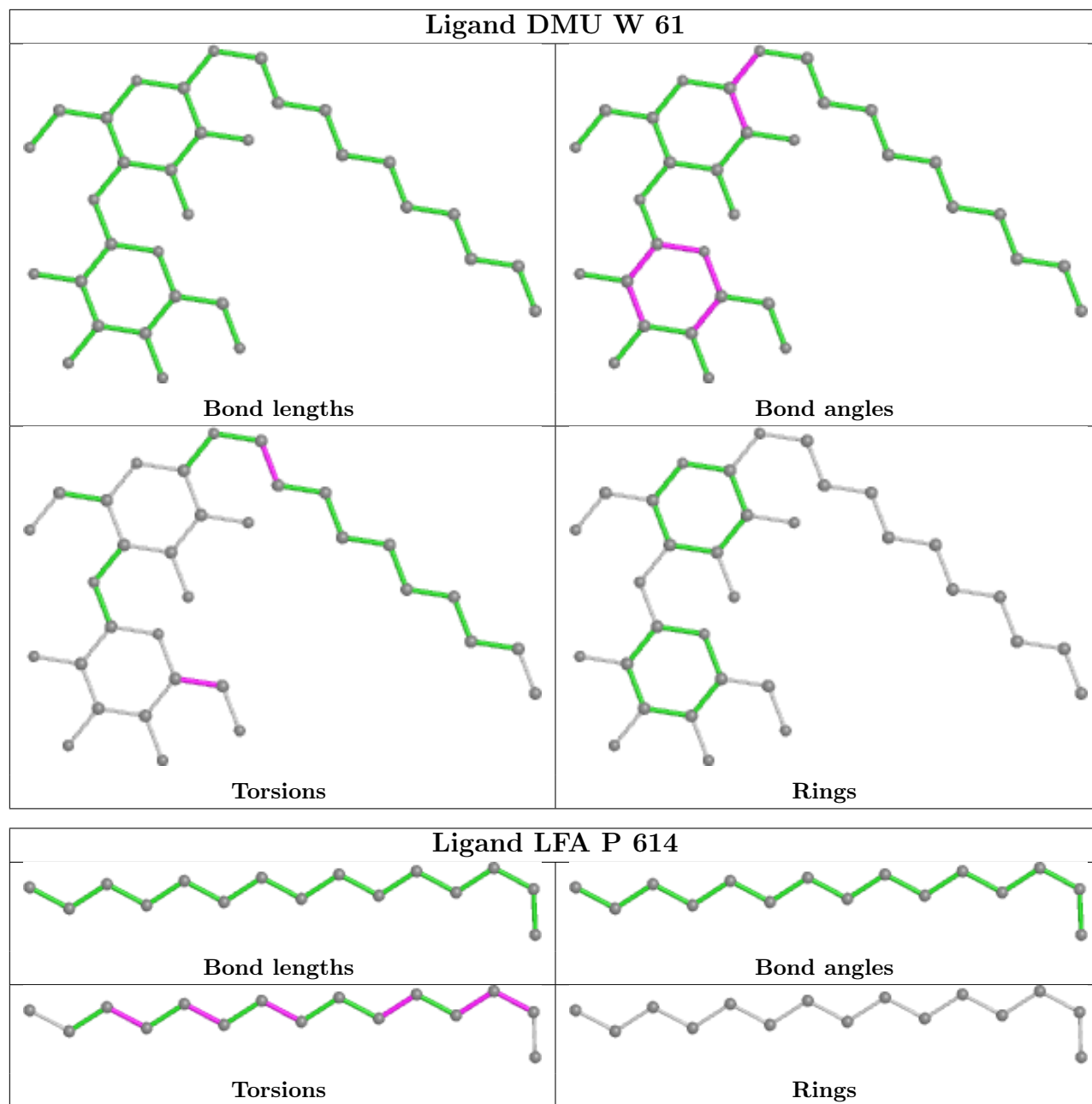


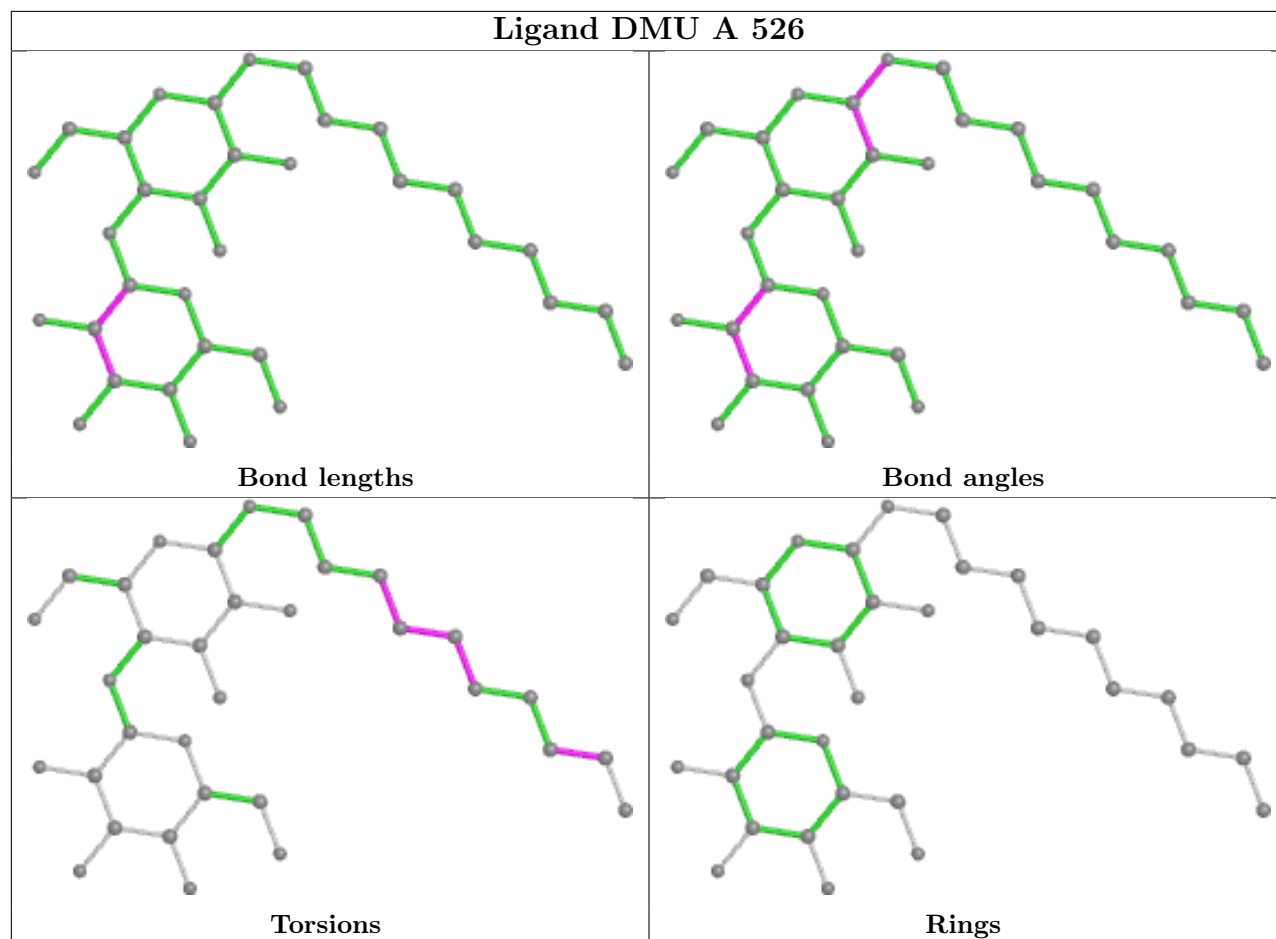
## Ligand DMU C 722



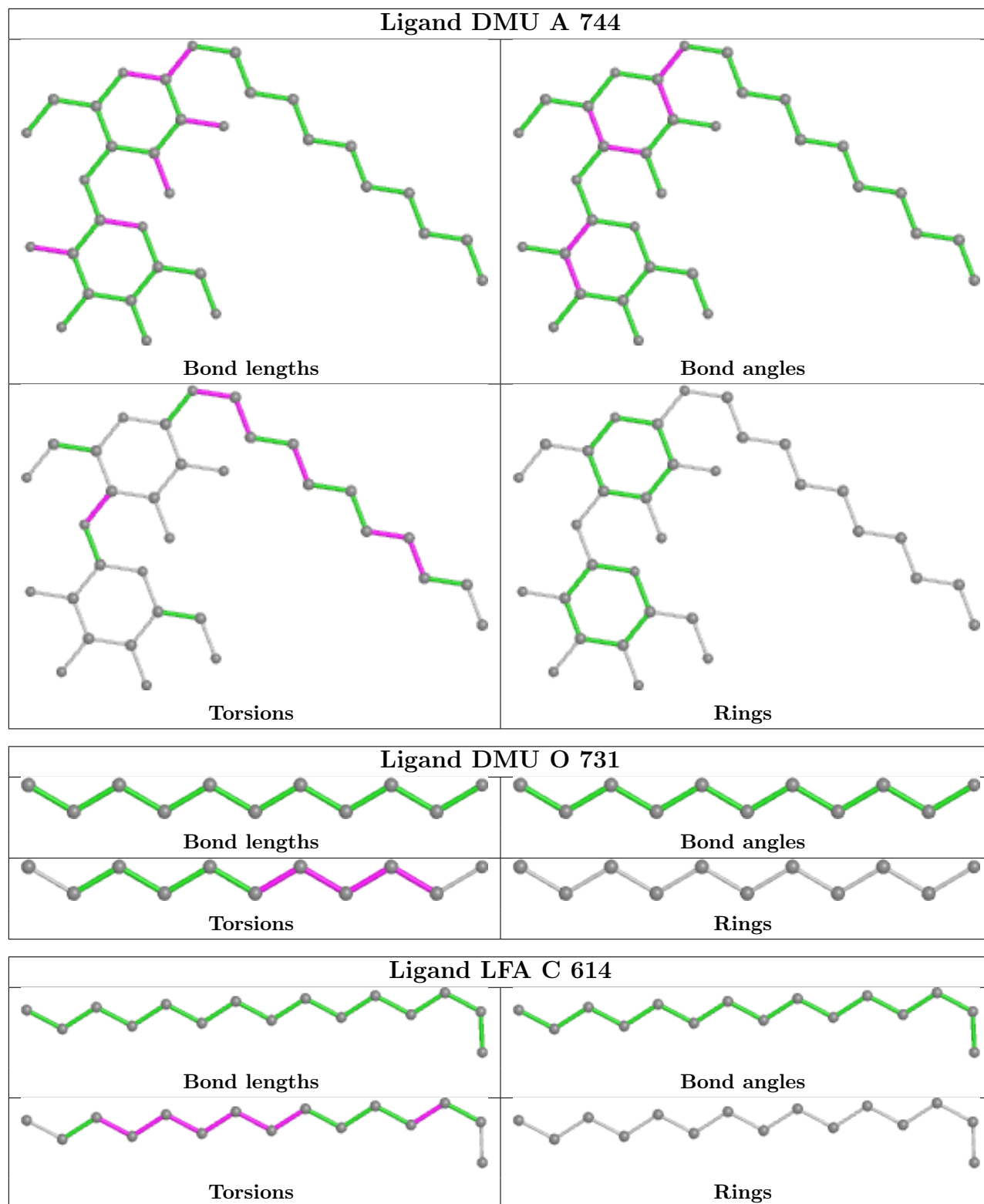
## Ligand LFA P 612

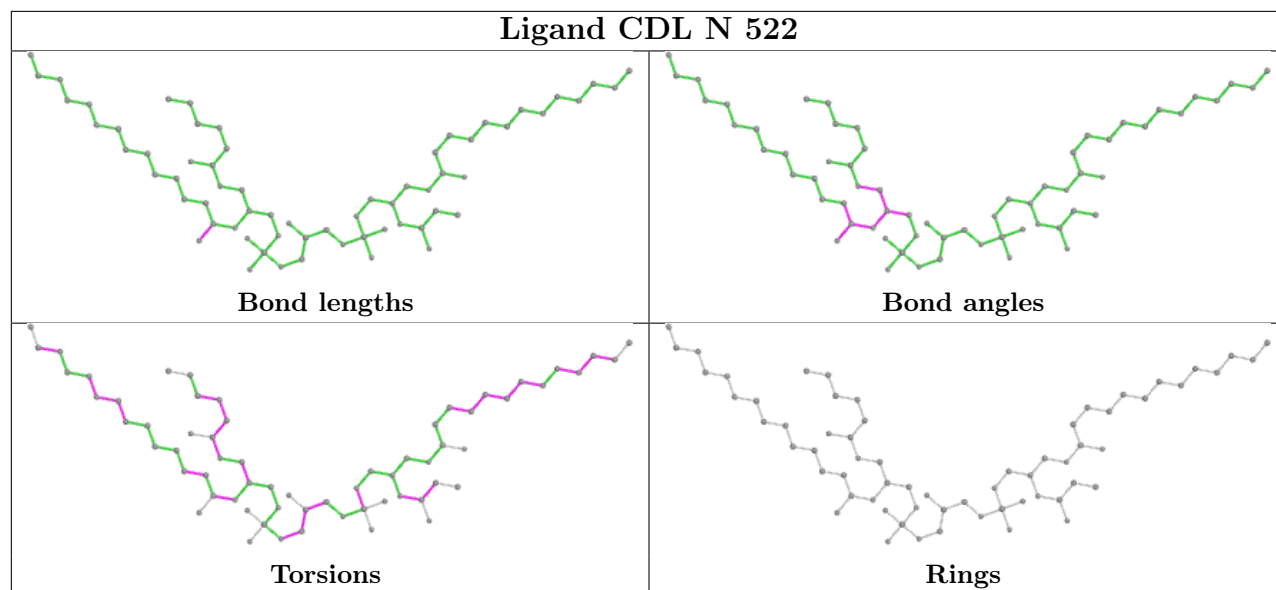












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	36	TRP	8.2
10	W	1	PHE	8.0
8	H	45	ALA	7.9
10	J	1	PHE	7.5
11	X	6	ALA	7.3
9	V	37	PHE	7.1
8	H	47	GLY	6.7
7	G	36	TRP	6.2
8	U	47	GLY	6.1
7	G	42	ARG	6.0
11	X	7	PRO	5.9
9	I	37	PHE	5.7
10	W	52	TRP	5.5
2	B	59	GLN	5.1
2	B	61	VAL	5.1
9	I	25	PHE	5.0
11	X	13	TYR	4.8
2	B	60	GLU	4.7
2	B	65	TRP	4.6
8	U	48	GLY	4.5
2	O	113	TYR	4.3
9	V	25	PHE	4.3
8	H	44	THR	4.2
10	W	55	PHE	4.2
2	O	90	ILE	4.1
9	V	34	PHE	4.0
10	W	48	TYR	4.0
7	T	42	ARG	4.0
10	J	52	TRP	3.9
6	S	93	PRO	3.8
9	I	29	LEU	3.7
4	Q	39	ALA	3.7
8	U	45	ALA	3.7
8	H	48	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	O	91	ASN	3.6
2	B	58	ALA	3.5
13	M	40	TYR	3.5
7	G	40	GLY	3.5
8	U	44	THR	3.4
8	H	46	LYS	3.4
7	T	38	HIS	3.3
3	P	37	PHE	3.3
7	G	37	LEU	3.2
8	U	46	LYS	3.2
8	U	49	ASP	3.2
7	T	40	GLY	3.1
4	D	4	SER	2.9
3	P	258	TRP	2.9
9	V	18	ARG	2.8
3	C	258	TRP	2.7
7	G	41	HIS	2.7
13	Z	40	TYR	2.7
9	V	33	THR	2.7
13	Z	39	ASN	2.6
7	T	39	SER	2.6
8	H	43	MET	2.6
9	I	19	PHE	2.6
2	B	55	THR	2.6
2	B	91	ASN	2.6
9	I	18	ARG	2.5
4	D	5	VAL	2.5
9	I	34	PHE	2.5
2	O	227	LEU	2.5
7	T	37	LEU	2.4
7	T	43	GLU	2.4
9	I	32	ALA	2.4
7	T	41	HIS	2.4
5	E	39	TYR	2.4
2	B	90	ILE	2.3
9	V	26	MET	2.3
9	I	33	THR	2.3
2	B	110	TYR	2.3
2	B	113	TYR	2.3
2	B	130	PRO	2.2
9	V	31	PHE	2.2
8	U	52	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
10	J	55	PHE	2.2
7	G	38	HIS	2.2
8	H	50	VAL	2.1
1	A	311[A]	ILE	2.1
2	O	60	GLU	2.1
4	Q	58	GLU	2.1
11	X	12	LYS	2.0

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

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
20	DMU	B	741	11/33	0.56	0.20	49,56,63,66	11
20	DMU	T	712	11/33	0.58	0.32	45,52,60,60	11
20	DMU	G	711	22/33	0.61	0.23	42,56,77,88	22
20	DMU	P	722	22/33	0.61	0.37	31,63,73,87	22
20	DMU	C	722	22/33	0.61	0.33	32,56,76,90	22
20	DMU	T	711	22/33	0.64	0.23	43,53,69,80	22
22	LFA	P	615	11/20	0.64	0.38	52,57,67,74	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	DMU	J	732	11/33	0.65	0.24	47,50,57,68	11
20	DMU	W	61	33/33	0.68	0.22	36,48,77,81	33
20	DMU	B	742	22/33	0.68	0.20	34,48,57,69	22
20	DMU	P	721	7/33	0.69	0.32	43,53,63,70	7
20	DMU	N	743	7/33	0.69	0.18	45,49,56,57	7
22	LFA	C	615	11/20	0.69	0.38	45,55,74,75	11
20	DMU	O	742	22/33	0.69	0.17	33,38,44,48	22
22	LFA	C	625	15/20	0.71	0.19	33,41,54,57	15
22	LFA	C	614	15/20	0.72	0.27	38,46,57,58	15
20	DMU	W	732	11/33	0.72	0.34	49,54,59,70	11
20	DMU	C	733	33/33	0.72	0.24	38,48,60,65	33
20	DMU	Y	747	22/33	0.72	0.24	35,55,76,79	22
22	LFA	P	623	14/20	0.73	0.24	32,53,60,63	14
20	DMU	O	741	11/33	0.74	0.23	40,45,52,66	11
20	DMU	A	743	7/33	0.74	0.19	42,46,50,53	7
23	EDO	E	811	4/4	0.74	0.19	29,31,33,35	4
22	LFA	P	614	15/20	0.75	0.25	40,46,58,59	15
22	LFA	P	626	13/20	0.76	0.23	38,50,62,64	13
22	LFA	A	628	14/20	0.76	0.21	33,41,48,51	14
22	LFA	C	612	6/20	0.77	0.29	39,43,45,49	6
20	DMU	G	712	11/33	0.77	0.26	35,46,52,65	11
20	DMU	N	744	33/33	0.77	0.14	28,43,59,67	33
22	LFA	P	611	11/20	0.78	0.25	28,39,44,46	11
20	DMU	C	734	33/33	0.78	0.20	38,54,63,66	33
22	LFA	P	716[B]	18/20	0.78	0.14	37,49,60,62	18
20	DMU	P	733	33/33	0.78	0.21	40,50,59,68	33
22	LFA	P	624	11/20	0.79	0.30	42,47,54,60	11
22	LFA	C	623	14/20	0.79	0.18	34,48,54,55	14
20	DMU	J	61	33/33	0.79	0.23	33,43,65,71	33
20	DMU	N	745	33/33	0.79	0.22	33,46,72,87	33
22	LFA	N	628	14/20	0.80	0.22	35,42,66,68	14
22	LFA	C	624	11/20	0.80	0.27	37,48,53,54	11
20	DMU	C	714	33/33	0.80	0.22	33,39,57,61	33
20	DMU	G	713	22/33	0.81	0.19	41,52,58,61	22
20	DMU	C	721	7/33	0.81	0.23	45,49,53,64	7
22	LFA	G	622	11/20	0.81	0.21	39,51,56,60	11
22	LFA	P	625	15/20	0.81	0.17	35,41,61,63	15
20	DMU	A	745	33/33	0.81	0.15	24,32,44,57	33
20	DMU	L	747	22/33	0.81	0.20	37,47,57,64	22
20	DMU	P	734	33/33	0.81	0.20	48,60,72,80	33
22	LFA	G	621	17/20	0.82	0.17	29,53,64,64	17
20	DMU	C	715[A]	33/33	0.82	0.19	26,35,43,61	33

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
19	CHD	P	271	29/29	0.82	0.29	48,66,110,128	0
22	LFA	C	716[B]	18/20	0.82	0.15	34,49,89,90	18
20	DMU	P	714	33/33	0.83	0.18	34,42,59,78	33
20	DMU	B	731	11/33	0.83	0.17	36,51,59,63	11
22	LFA	C	626	13/20	0.83	0.17	41,45,51,54	13
18	CDL	C	270	87/100	0.83	0.24	34,82,121,135	0
20	DMU	O	731	11/33	0.85	0.26	46,48,52,67	11
20	DMU	P	272	11/33	0.85	0.20	42,47,55,60	11
18	CDL	P	270	87/100	0.85	0.24	34,78,126,150	0
20	DMU	Z	746	8/33	0.85	0.17	44,47,52,56	8
22	LFA	T	621	17/20	0.85	0.18	34,49,66,69	17
20	DMU	P	715[A]	33/33	0.85	0.20	27,37,49,61	33
19	CHD	C	271	29/29	0.86	0.29	44,58,76,95	0
22	LFA	T	622	11/20	0.86	0.17	41,54,62,65	11
23	EDO	C	807	4/4	0.86	0.20	42,45,46,60	4
20	DMU	T	713	22/33	0.86	0.15	37,48,54,59	22
22	LFA	P	612	6/20	0.87	0.28	39,40,41,44	6
22	LFA	N	627	14/20	0.87	0.18	28,38,54,55	14
20	DMU	C	272	11/33	0.87	0.14	45,51,57,68	11
18	CDL	N	522	64/100	0.87	0.20	46,82,132,158	0
18	CDL	N	521	94/100	0.88	0.27	37,83,124,140	0
22	LFA	C	611	11/20	0.88	0.21	36,43,48,49	11
20	DMU	M	746	8/33	0.88	0.16	35,44,48,49	8
20	DMU	N	526	33/33	0.89	0.16	41,49,61,72	0
18	CDL	A	522	64/100	0.89	0.17	38,71,110,133	0
23	EDO	N	801	4/4	0.89	0.09	17,17,19,23	4
18	CDL	A	521	94/100	0.90	0.21	28,71,121,139	0
22	LFA	A	627	14/20	0.90	0.20	28,38,66,70	14
23	EDO	P	807	4/4	0.90	0.13	47,48,50,59	4
23	EDO	N	829	4/4	0.91	0.09	27,30,31,33	4
20	DMU	A	744	33/33	0.91	0.11	21,32,44,65	33
23	EDO	P	827	4/4	0.91	0.17	23,24,30,32	4
19	CHD	A	525	29/29	0.92	0.08	22,26,29,33	0
23	EDO	A	801	4/4	0.92	0.10	17,18,20,22	4
23	EDO	R	811	4/4	0.92	0.12	45,46,50,53	4
23	EDO	A	825	4/4	0.93	0.08	33,33,34,42	4
19	CHD	G	86	29/29	0.94	0.07	20,23,28,36	0
23	EDO	C	809	4/4	0.94	0.08	22,23,29,32	4
23	EDO	C	827	4/4	0.94	0.16	23,26,27,29	4
19	CHD	N	525	29/29	0.94	0.06	23,26,29,34	0
23	EDO	G	821	4/4	0.94	0.13	23,24,29,30	4
23	EDO	S	817	4/4	0.94	0.10	13,14,16,19	4

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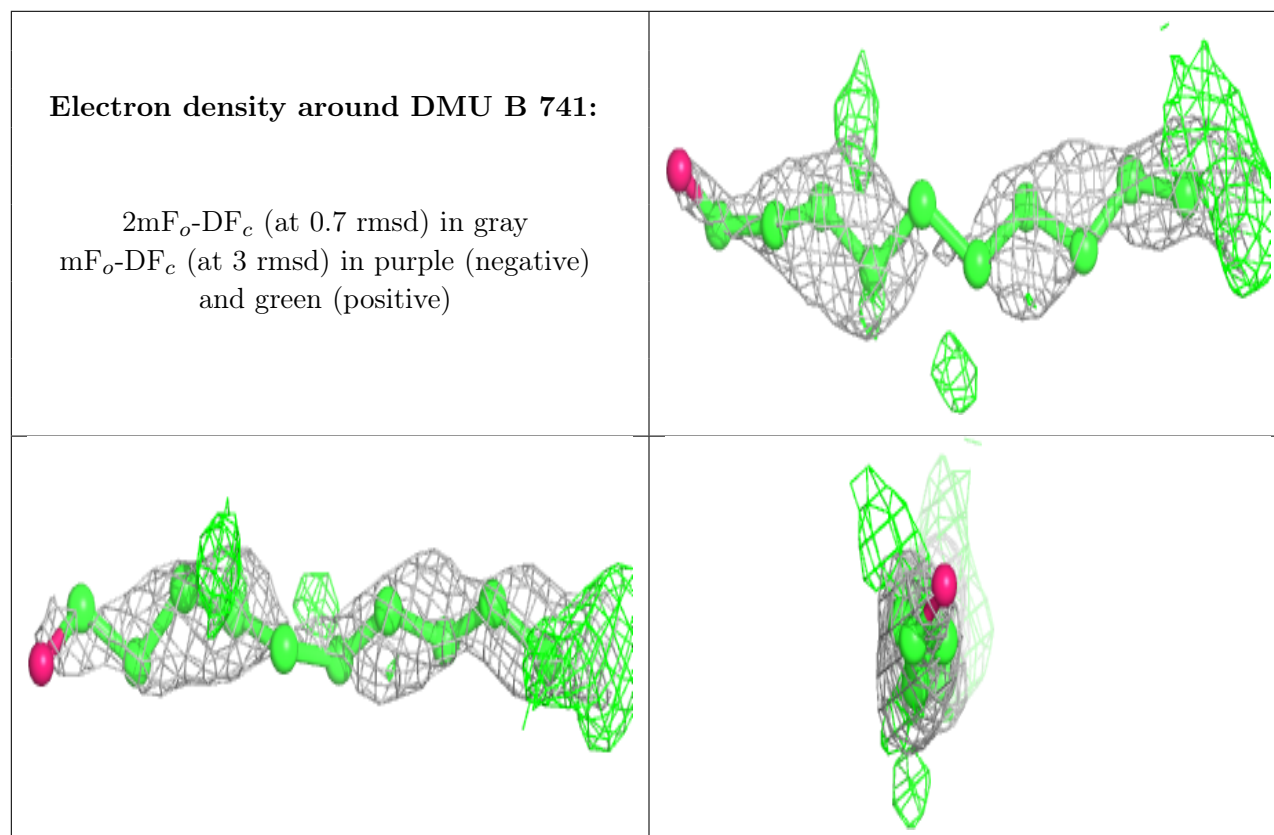
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	EDO	B	805	4/4	0.95	0.13	17,21,21,25	4
20	DMU	A	526	33/33	0.95	0.09	32,39,54,58	0
19	CHD	T	86	29/29	0.95	0.07	21,24,28,35	0
23	EDO	E	813	4/4	0.96	0.14	22,24,25,25	4
23	EDO	F	817	4/4	0.96	0.13	13,13,16,20	4
23	EDO	R	813	4/4	0.96	0.13	27,28,29,29	4
23	EDO	P	809	4/4	0.96	0.07	27,28,28,36	4
23	EDO	S	819	4/4	0.96	0.08	20,21,21,30	4
23	EDO	F	819	4/4	0.97	0.07	22,22,27,29	4
23	EDO	E	815	4/4	0.97	0.16	25,28,29,32	4
23	EDO	R	815	4/4	0.97	0.11	38,39,42,43	4
23	EDO	A	803	4/4	0.97	0.10	23,29,37,39	4
23	EDO	N	803	4/4	0.97	0.11	26,26,37,42	4
23	EDO	T	821	4/4	0.97	0.09	25,27,29,32	4
25	UNX	P	262	1/1	0.97	0.21	34,34,34,34	0
26	PEK	P	264	53/53	0.97	0.09	26,46,102,108	0
23	EDO	O	805	4/4	0.98	0.08	23,24,27,29	4
23	EDO	N	823	4/4	0.98	0.13	19,21,22,22	4
23	EDO	N	825	4/4	0.98	0.08	27,28,29,30	4
26	PEK	C	264	53/53	0.98	0.09	24,42,96,129	0
23	EDO	A	823	4/4	0.98	0.15	17,17,19,24	4
27	PGV	C	266	51/51	0.98	0.09	19,28,65,76	0
27	PGV	C	267	51/51	0.98	0.09	20,28,75,94	0
27	PGV	P	266	51/51	0.98	0.09	22,31,61,65	0
27	PGV	P	267	51/51	0.98	0.09	20,30,91,105	0
14	HEA	A	515[A]	60/60	0.99	0.09	15,18,29,35	9
14	HEA	A	515[B]	60/60	0.99	0.09	15,18,29,34	9
14	HEA	A	516	60/60	0.99	0.07	15,17,23,26	0
25	UNX	C	262	1/1	0.99	0.24	36,36,36,36	0
14	HEA	N	515[A]	60/60	0.99	0.07	19,21,32,39	9
14	HEA	N	515[B]	60/60	0.99	0.07	19,21,29,33	9
14	HEA	N	516	60/60	0.99	0.07	18,19,25,28	0
21	PER	A	520	2/2	0.99	0.17	20,20,20,26	0
21	PER	N	520	2/2	0.99	0.17	19,19,19,26	0
15	CU	N	517	1/1	0.99	0.12	20,20,20,20	0
16	MG	A	518	1/1	0.99	0.08	19,19,19,19	0
28	ZN	F	99	1/1	0.99	0.11	24,24,24,24	0
17	NA	A	519	1/1	1.00	0.09	21,21,21,21	0
24	CUA	B	228	2/2	1.00	0.13	19,19,19,19	0
24	CUA	O	228	2/2	1.00	0.12	24,24,24,25	0
17	NA	N	519	1/1	1.00	0.07	28,28,28,28	0
15	CU	A	517	1/1	1.00	0.12	17,17,17,17	0

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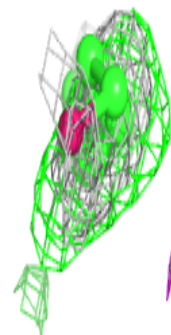
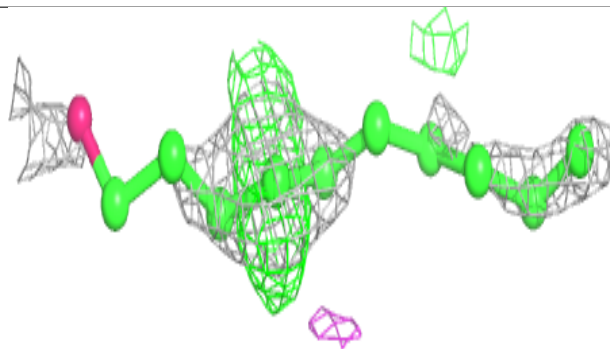
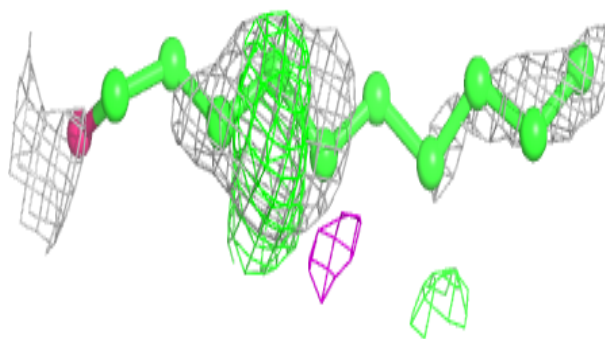
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
16	MG	N	518	1/1	1.00	0.08	23,23,23,23	0
28	ZN	S	99	1/1	1.00	0.11	25,25,25,25	0

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

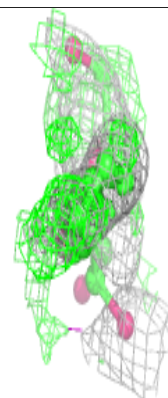
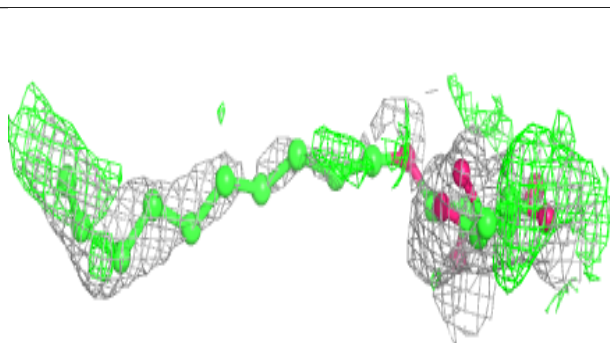
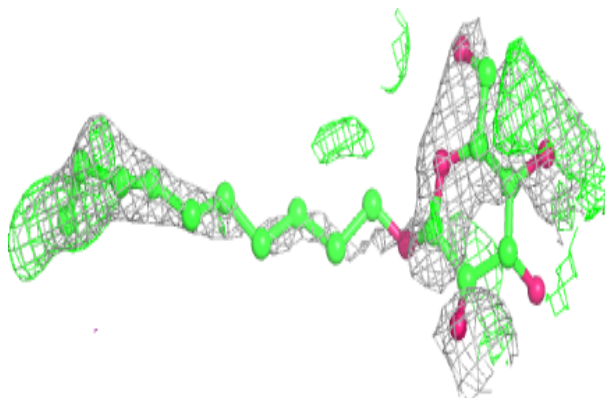


**Electron density around DMU T 712:**

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

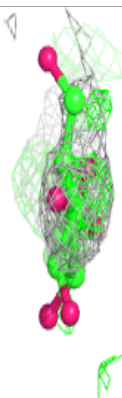
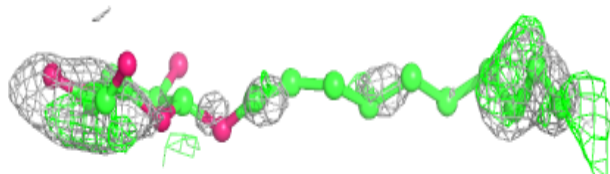
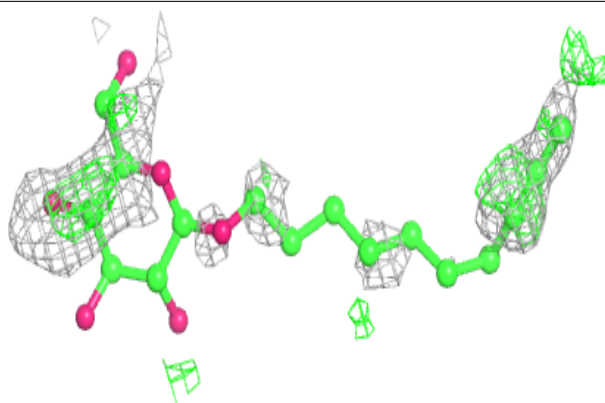
**Electron density around DMU G 711:**

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

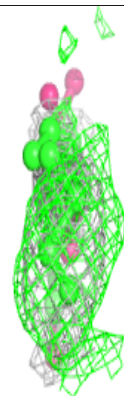
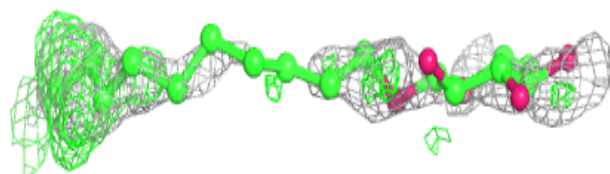
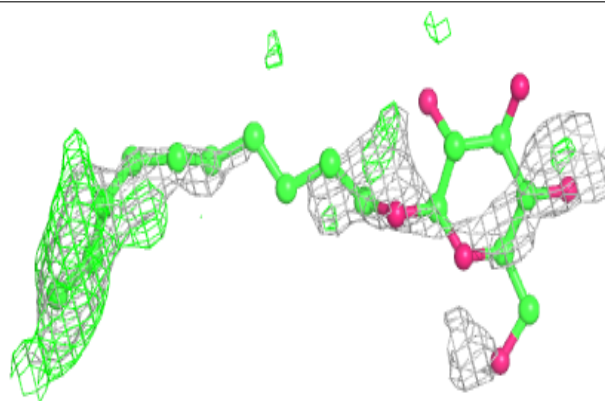


**Electron density around DMU P 722:**

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

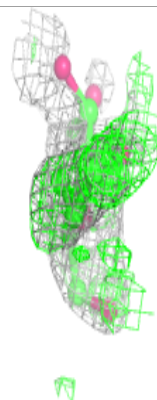
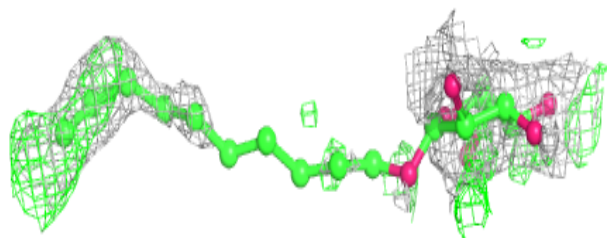
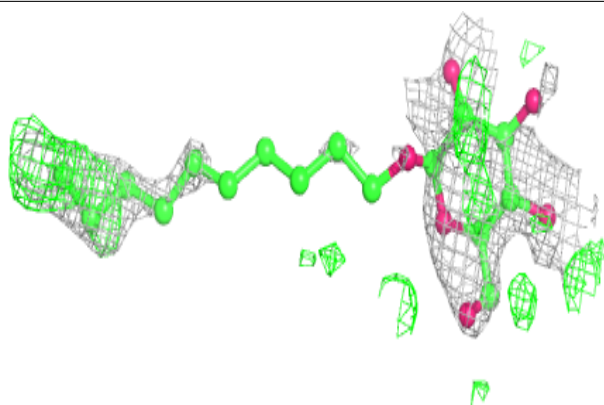
**Electron density around DMU C 722:**

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

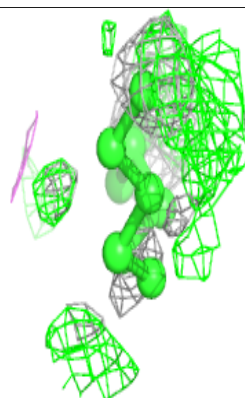
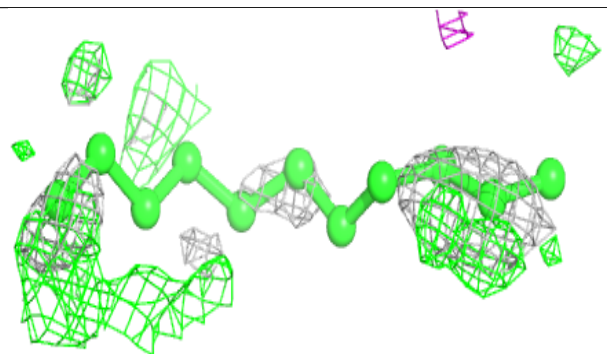
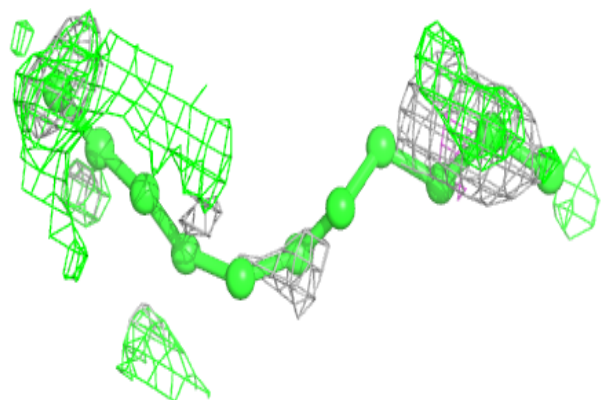


**Electron density around DMU T 711:**

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

**Electron density around LFA P 615:**

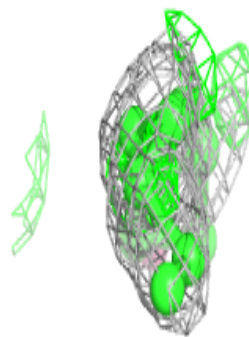
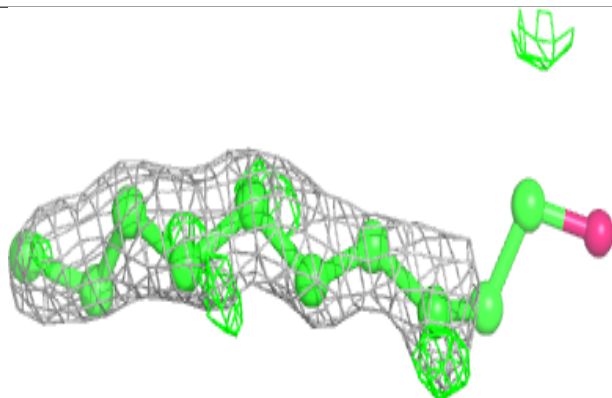
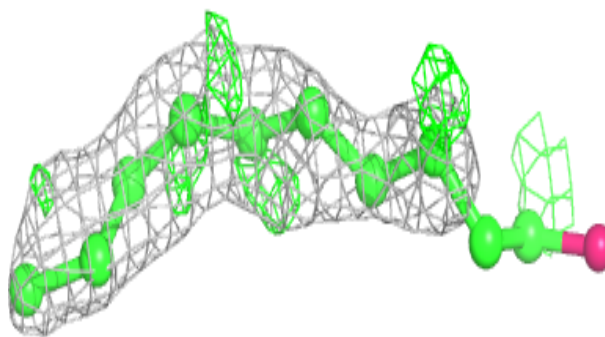
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



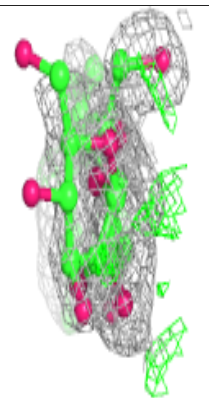
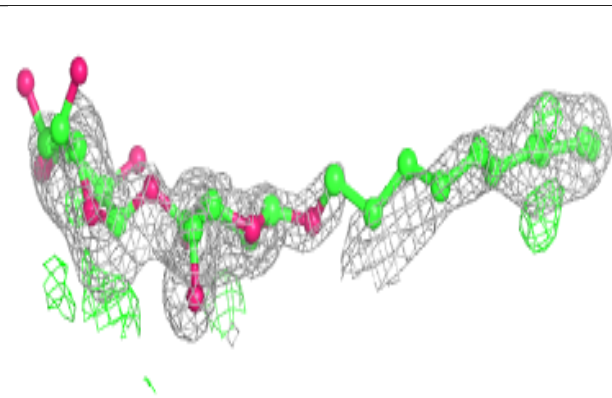
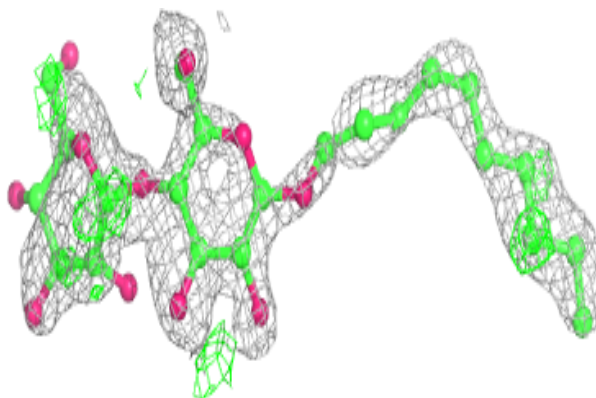


**Electron density around DMU J 732:**

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

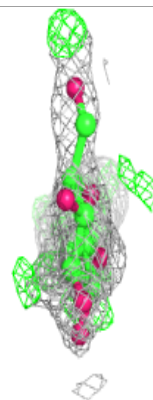
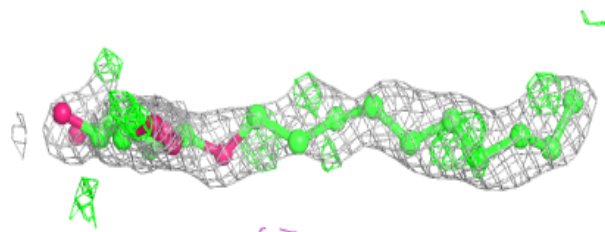
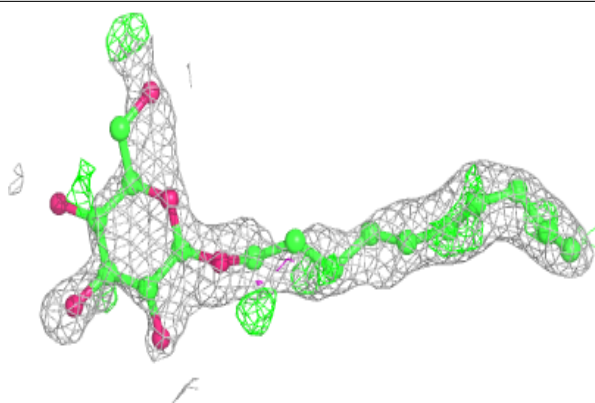
**Electron density around DMU W 61:**

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

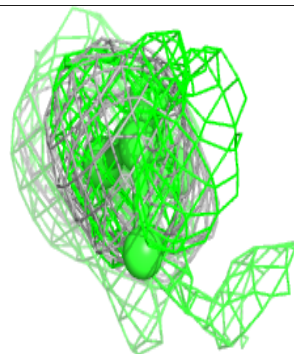
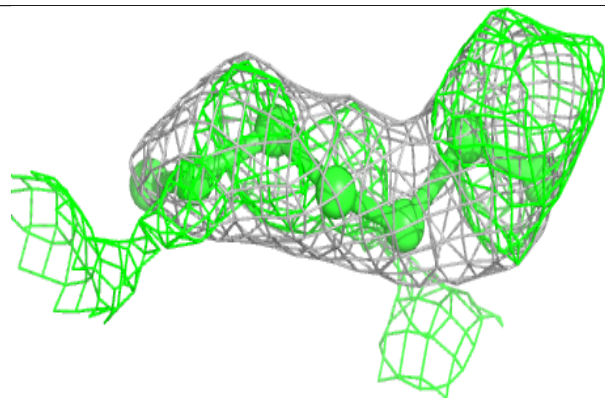
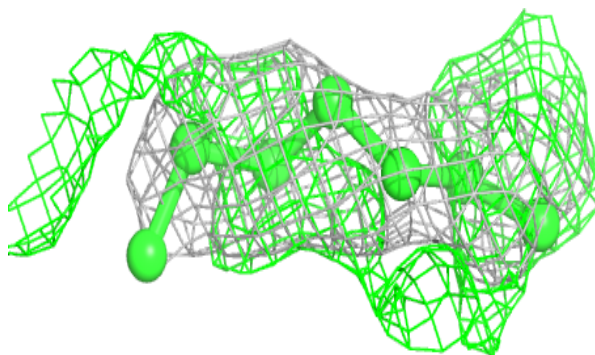


**Electron density around DMU B 742:**

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

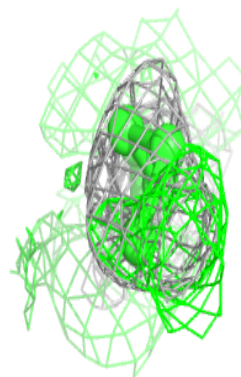
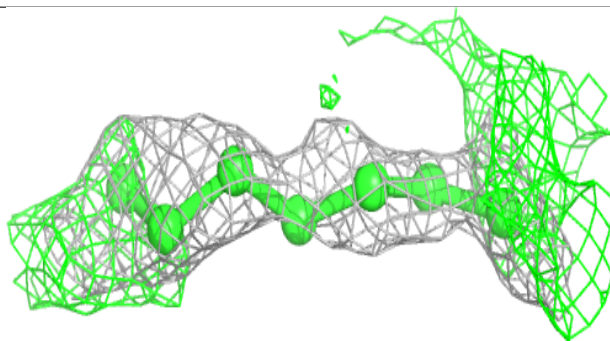
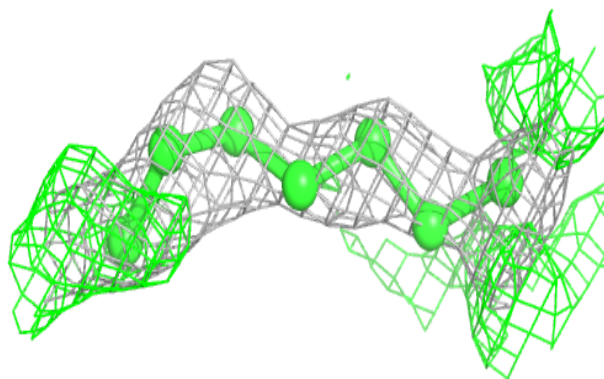
**Electron density around DMU P 721:**

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

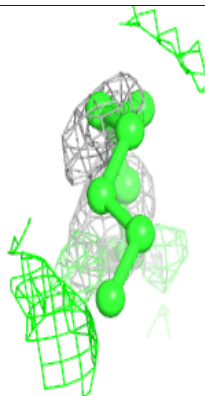
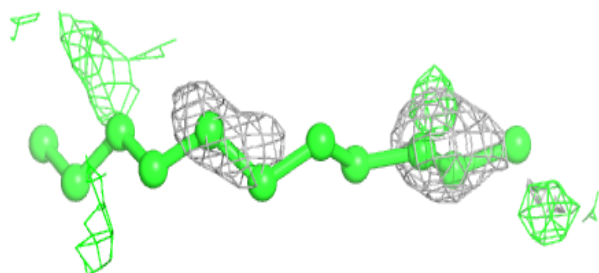
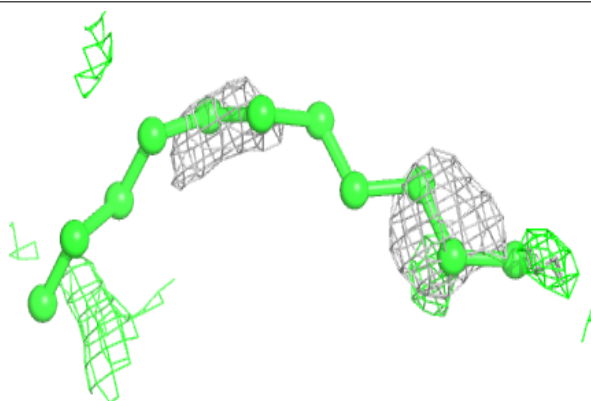


**Electron density around DMU N 743:**

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

**Electron density around LFA C 615:**

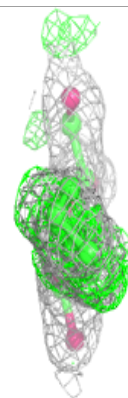
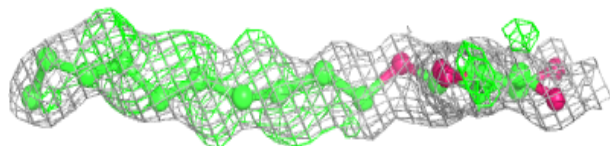
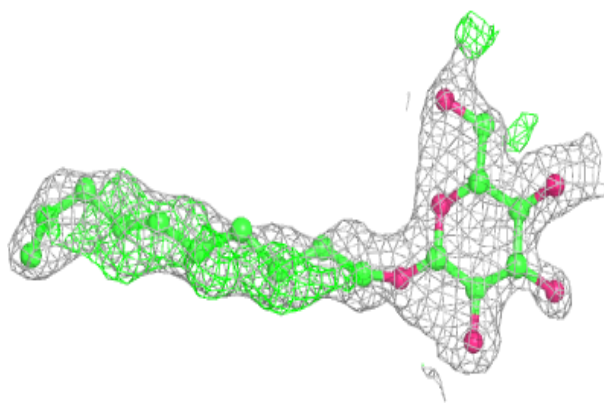
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



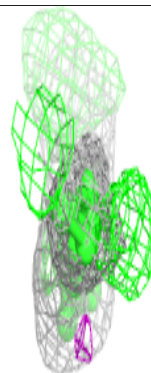
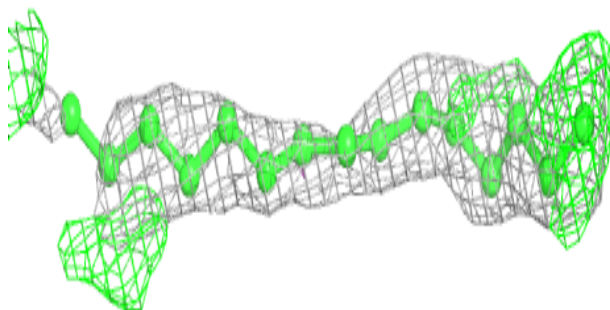
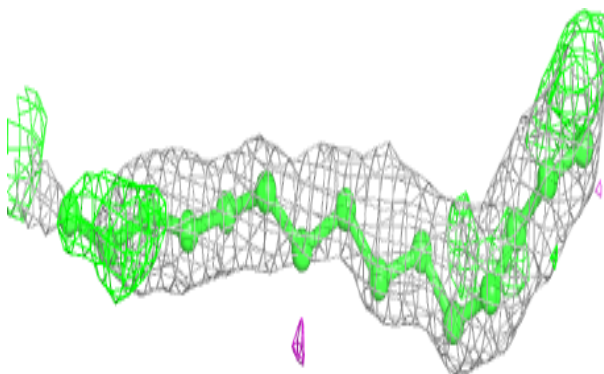


**Electron density around DMU O 742:**

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

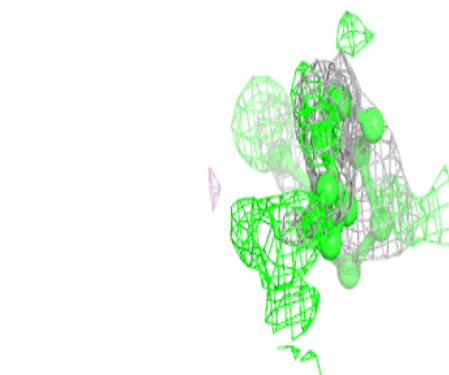
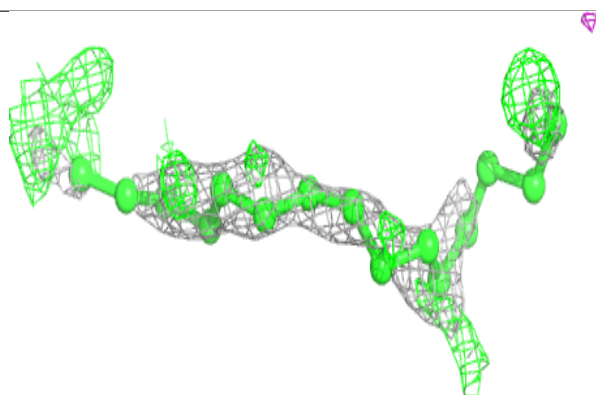
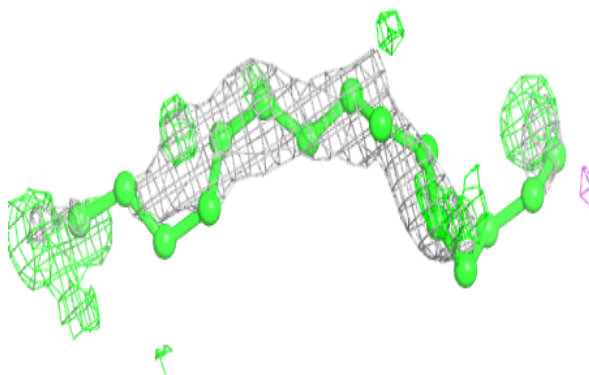
**Electron density around LFA C 625:**

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

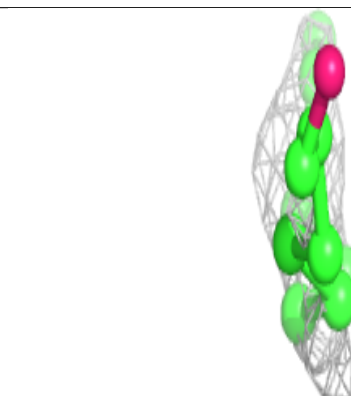
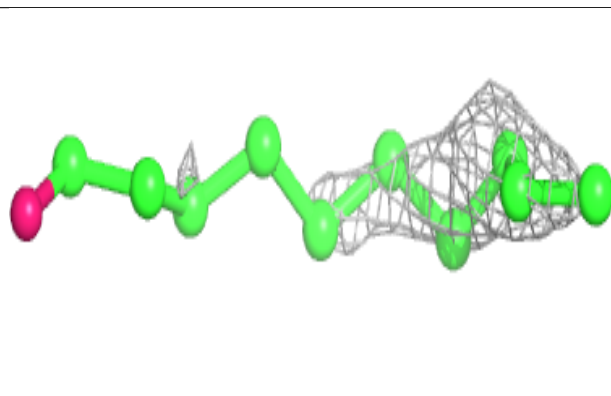
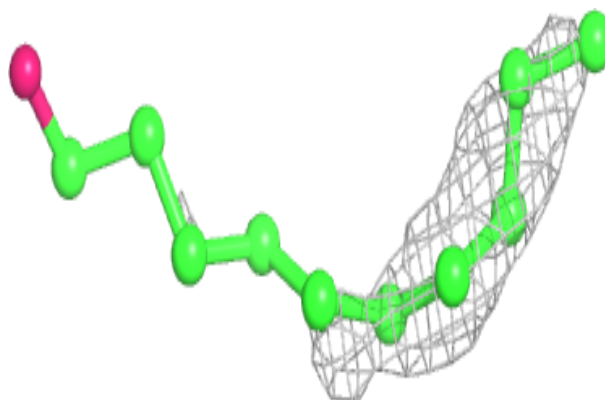


**Electron density around LFA C 614:**

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

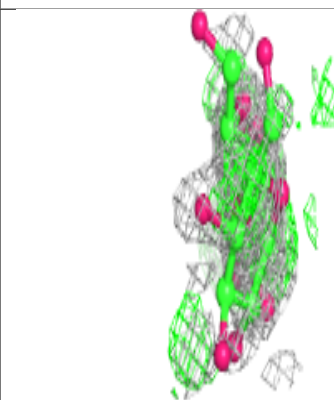
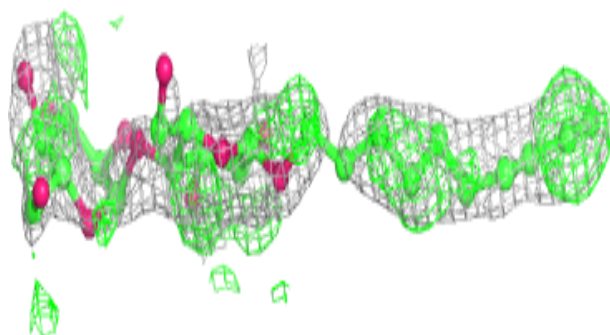
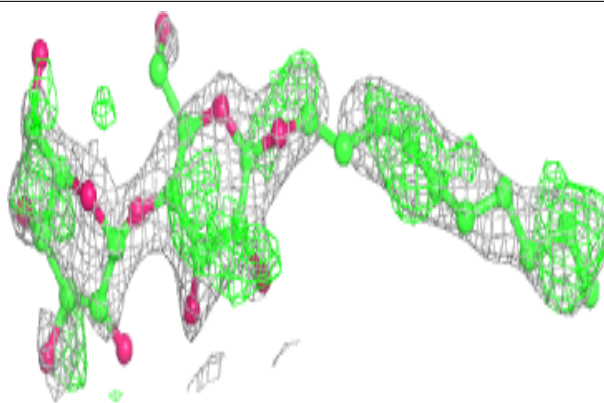
**Electron density around DMU W 732:**

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

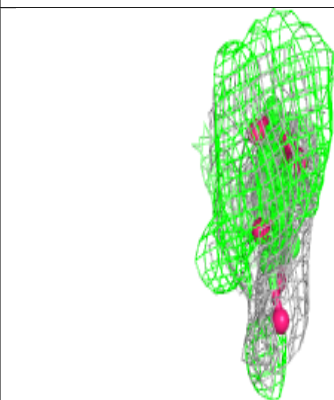
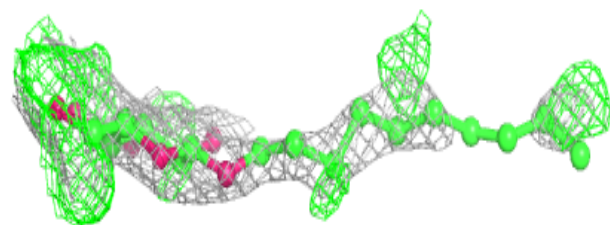
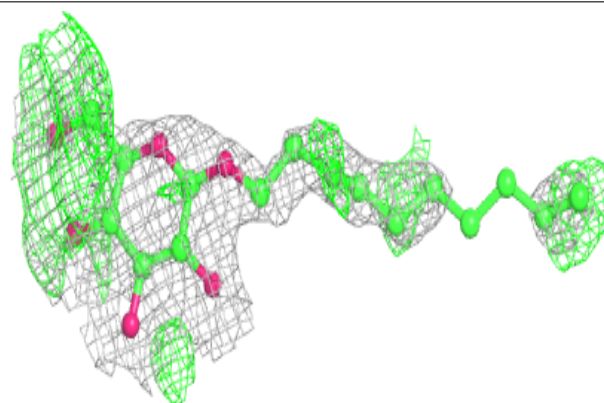


**Electron density around DMU C 733:**

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

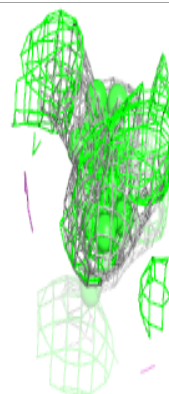
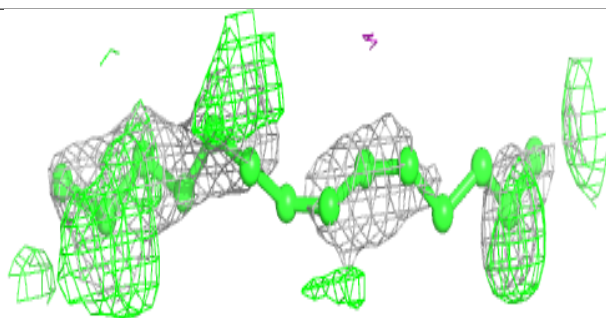
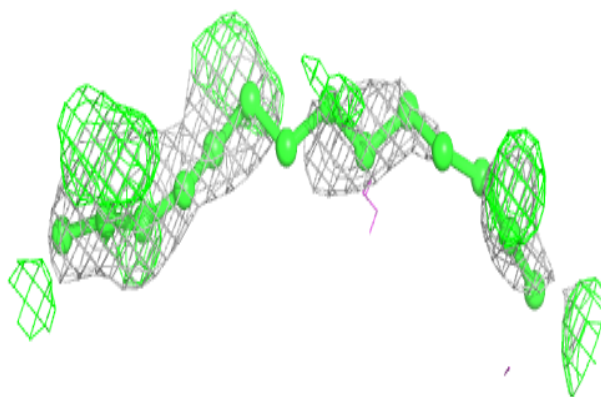
**Electron density around DMU Y 747:**

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

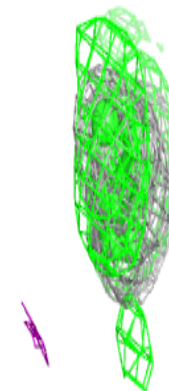
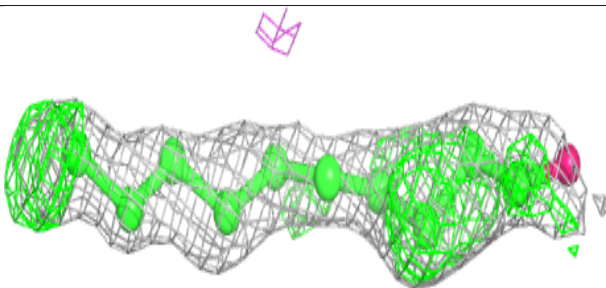
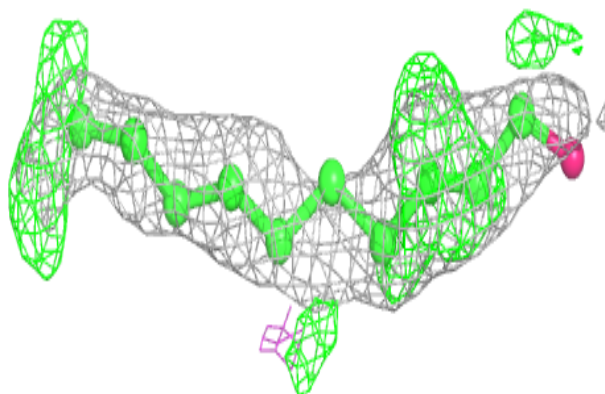


**Electron density around LFA P 623:**

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

**Electron density around DMU O 741:**

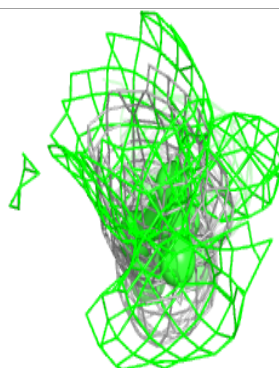
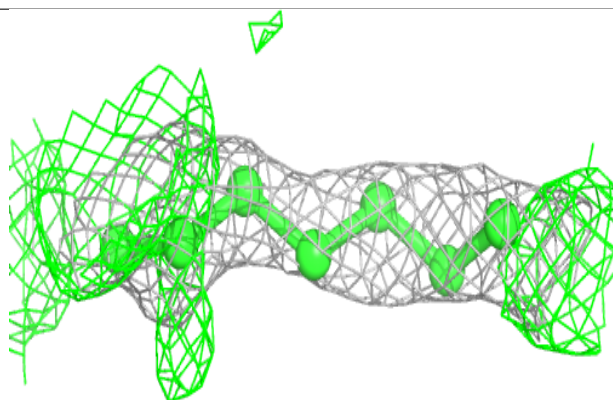
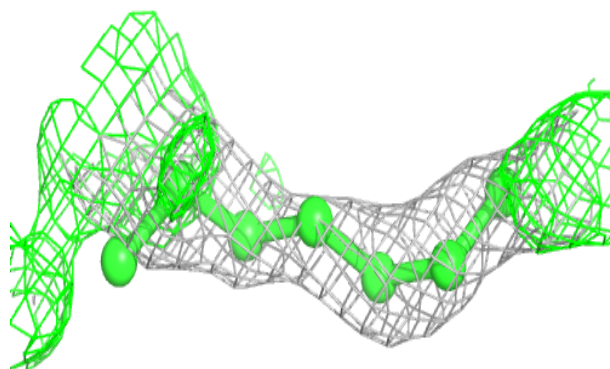
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



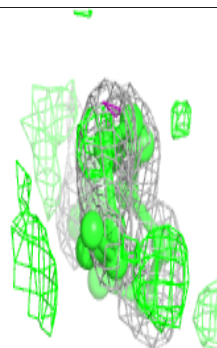
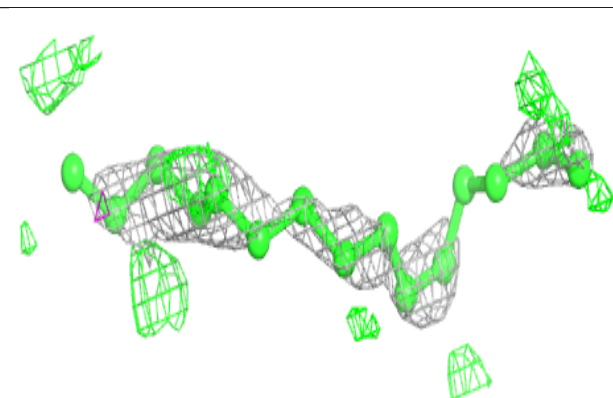
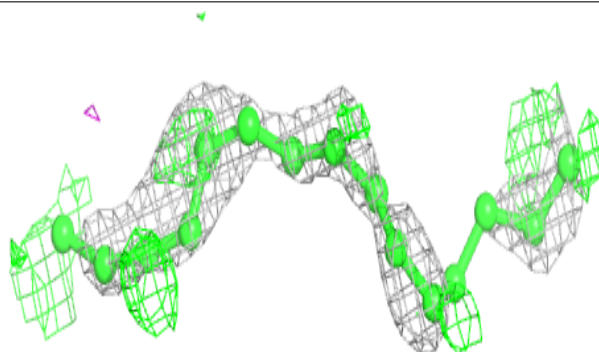


**Electron density around DMU A 743:**

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

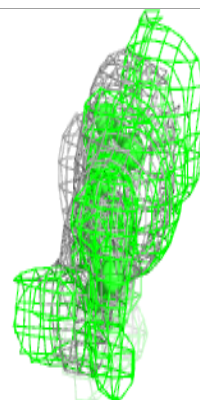
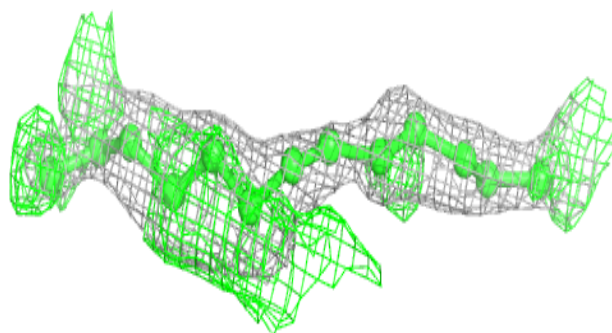
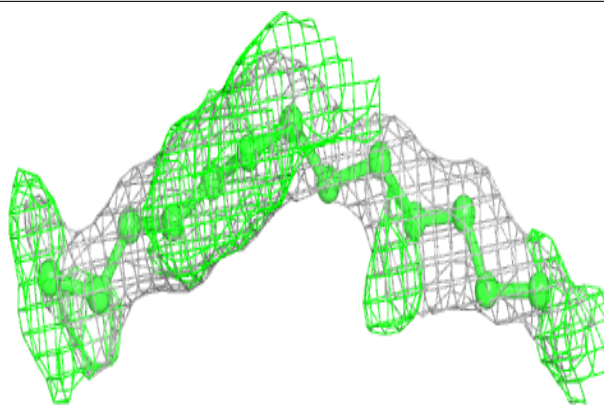
**Electron density around LFA P 614:**

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

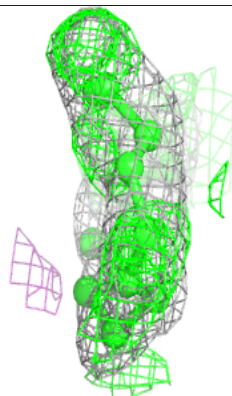
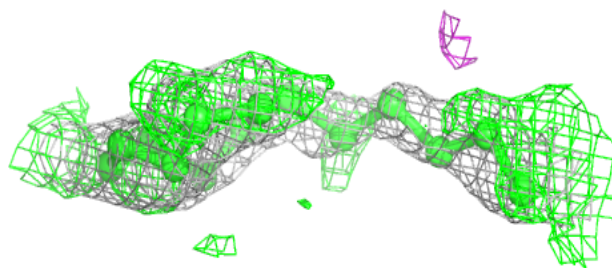
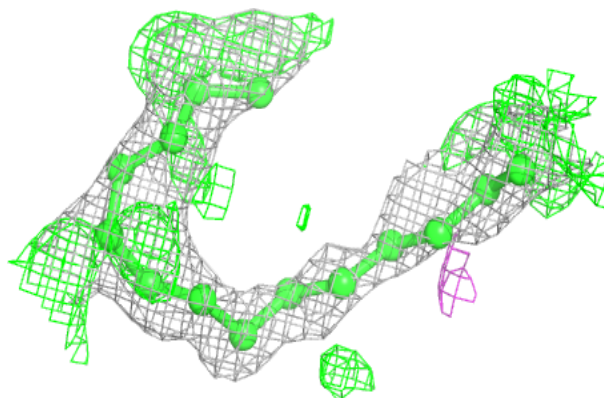


**Electron density around LFA P 626:**

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

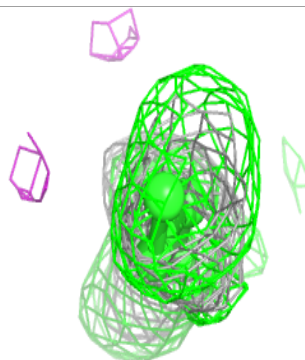
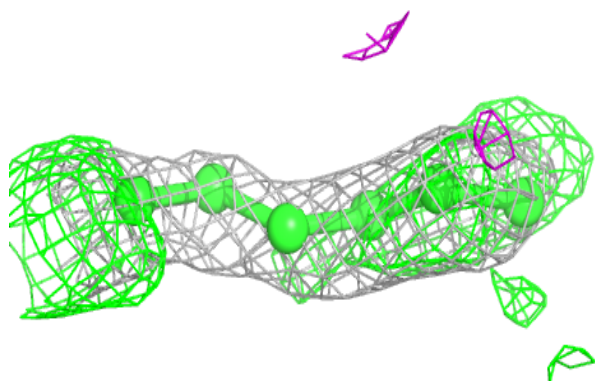
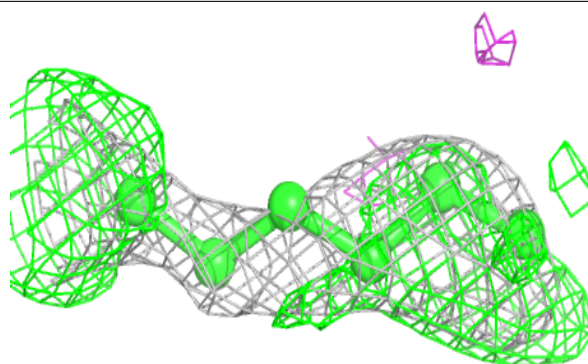
**Electron density around LFA A 628:**

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

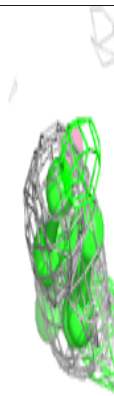
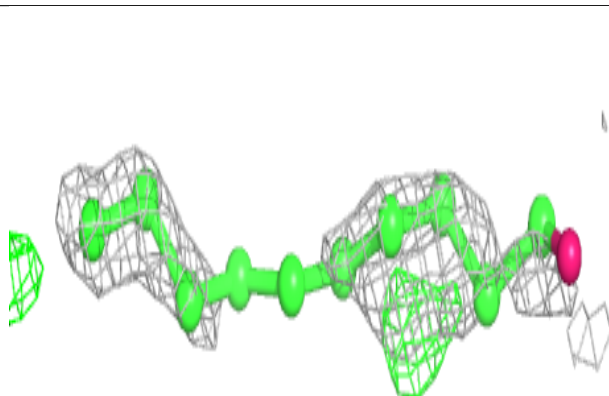
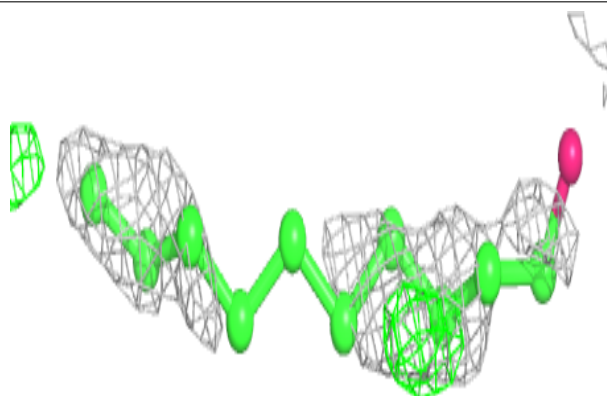


**Electron density around LFA C 612:**

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

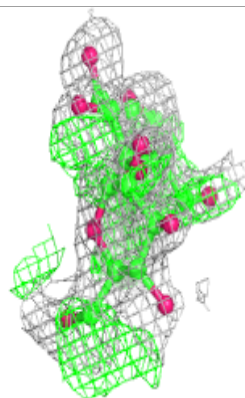
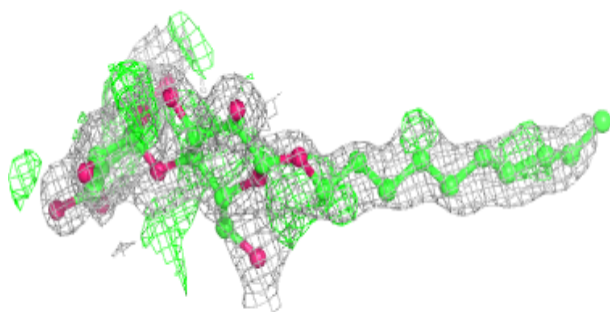
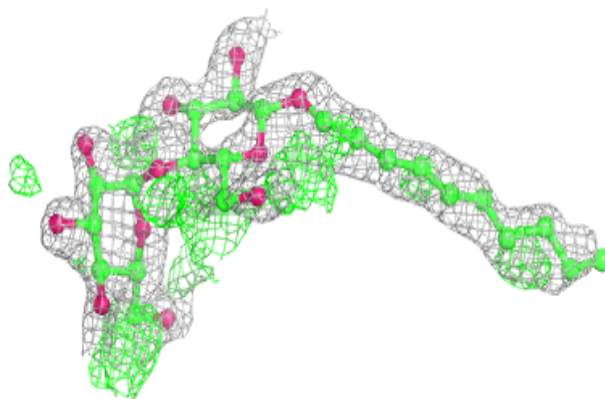
**Electron density around DMU G 712:**

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

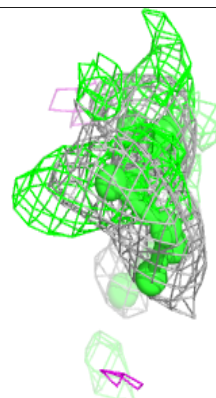
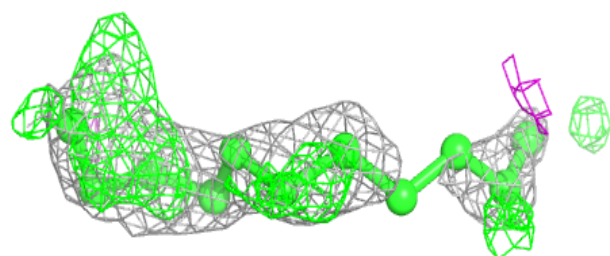
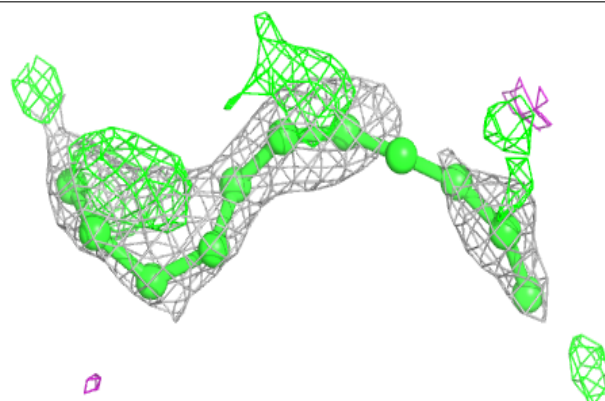


**Electron density around DMU N 744:**

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

**Electron density around LFA P 611:**

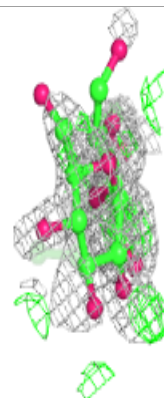
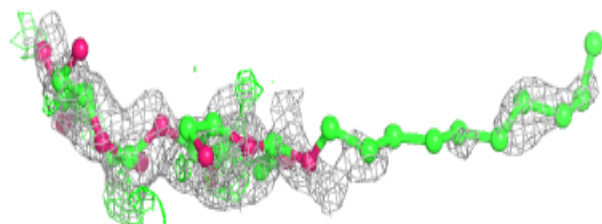
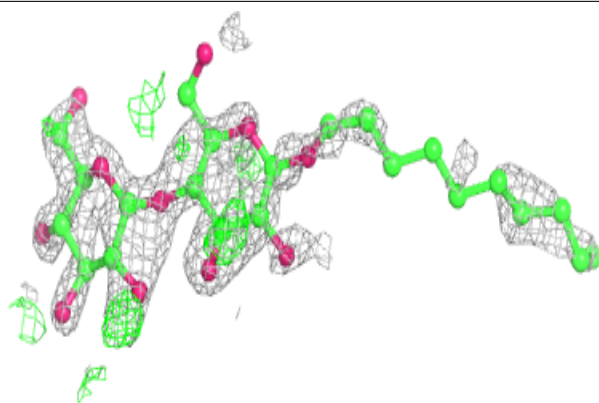
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



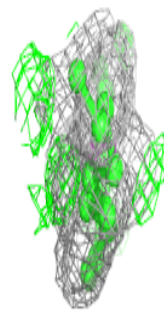
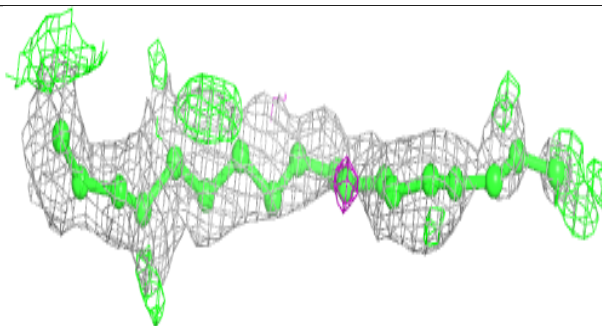
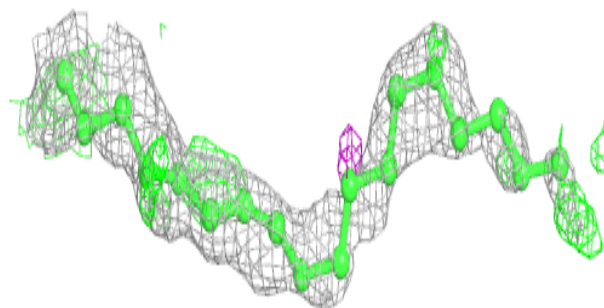


**Electron density around DMU C 734:**

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

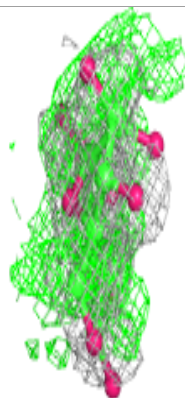
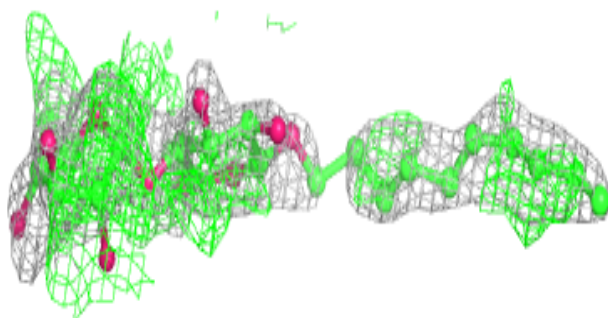
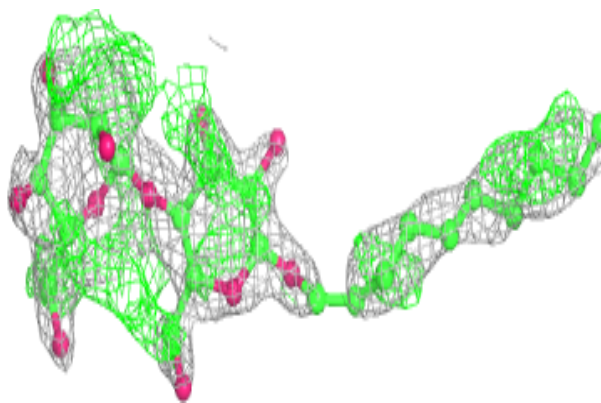
**Electron density around LFA P 716 (B):**

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

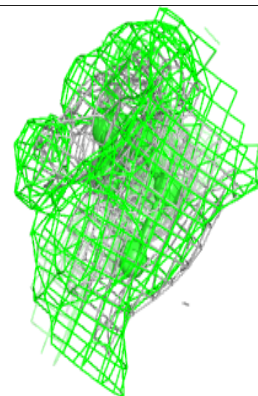
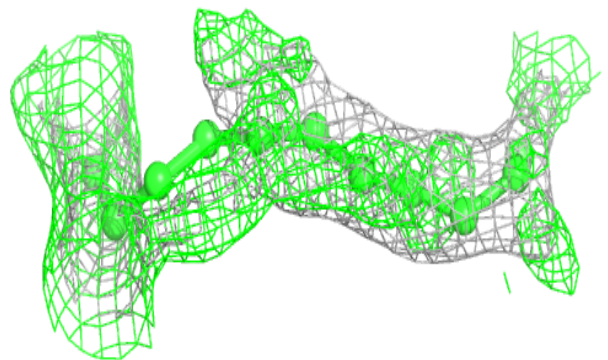
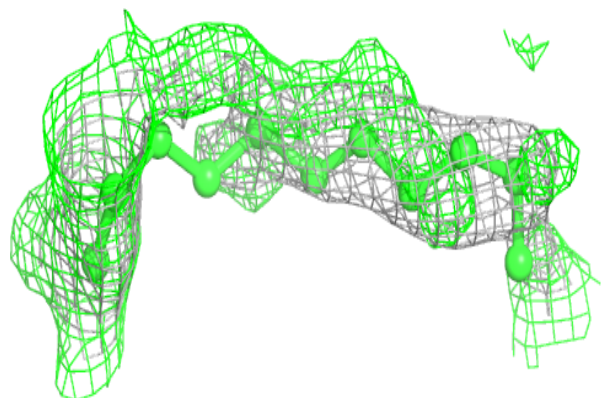


**Electron density around DMU P 733:**

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

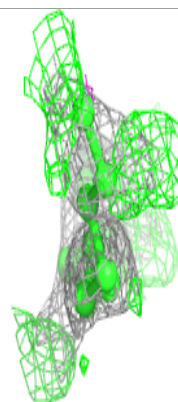
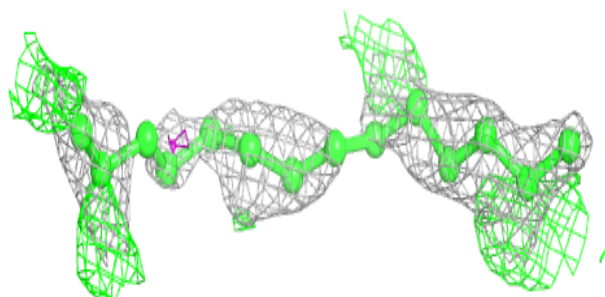
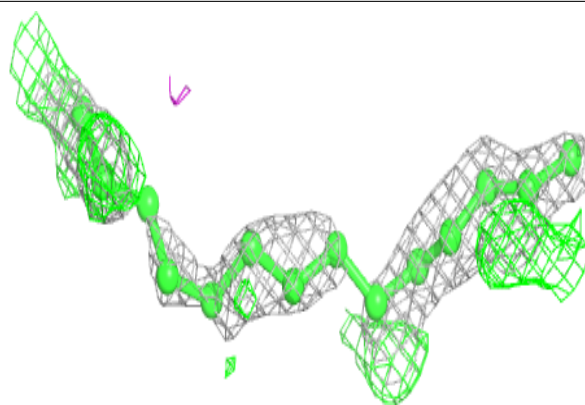
**Electron density around LFA P 624:**

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

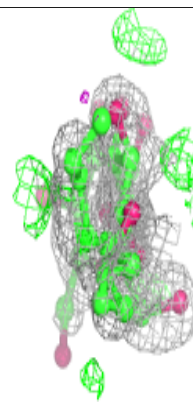
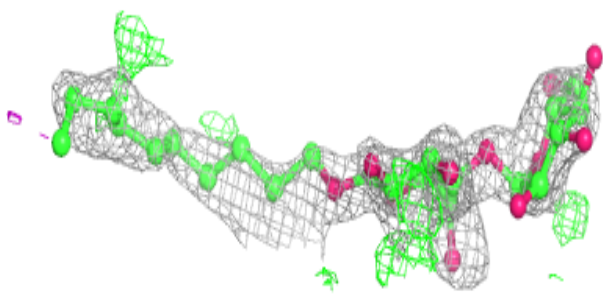
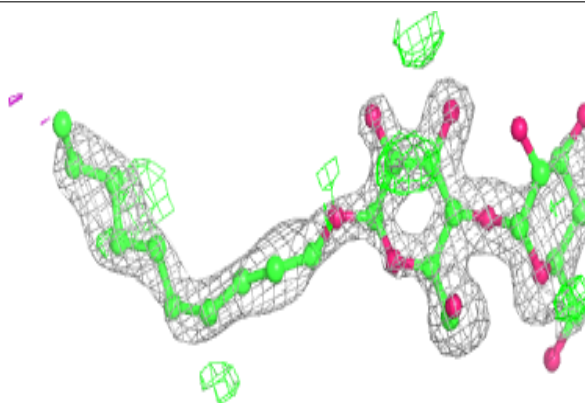


**Electron density around LFA C 623:**

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

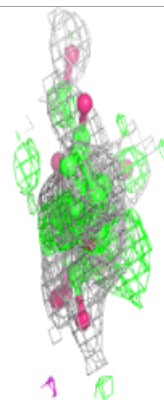
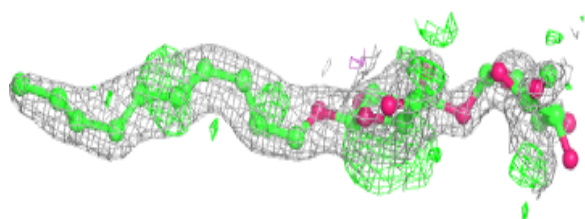
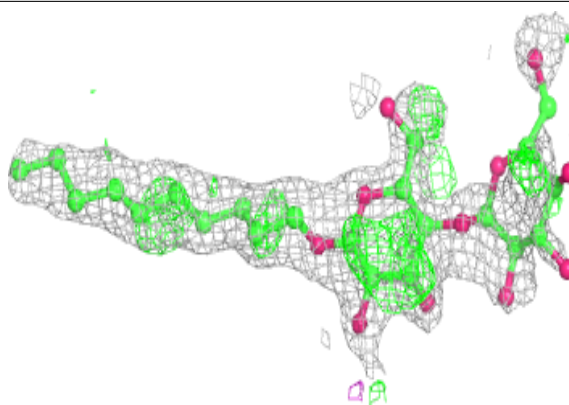
**Electron density around DMU J 61:**

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

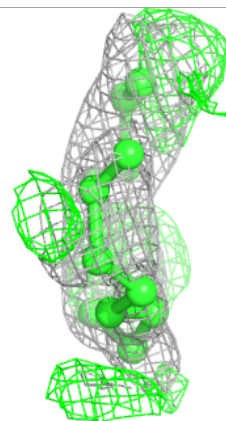
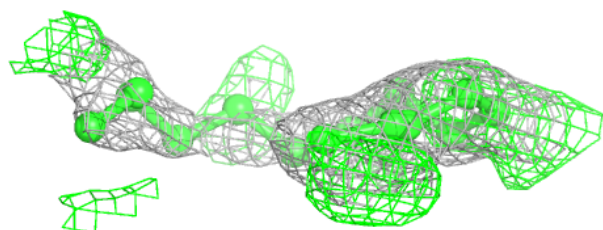
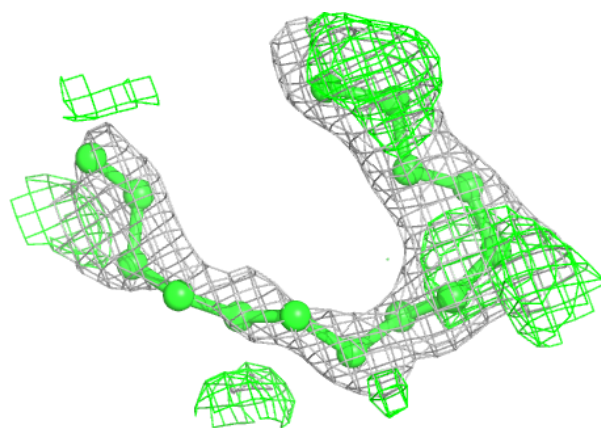


**Electron density around DMU N 745:**

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

**Electron density around LFA N 628:**

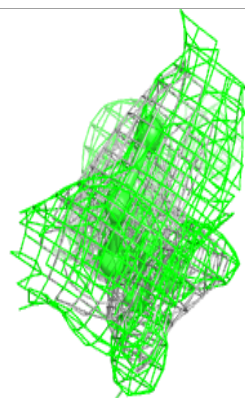
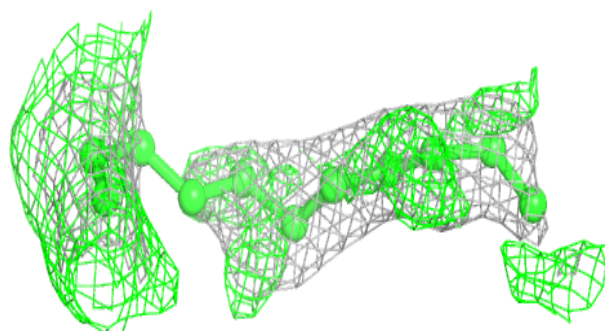
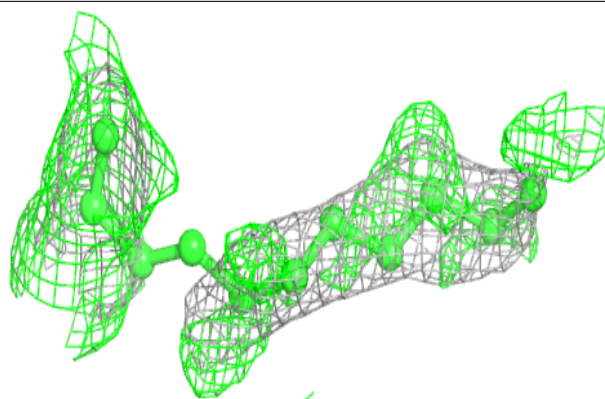
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



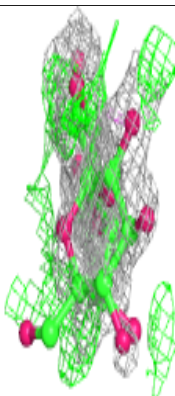
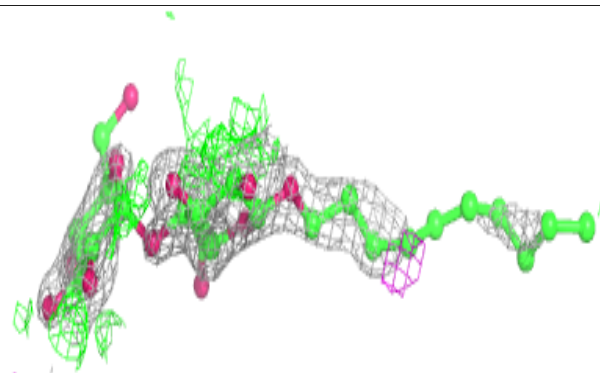
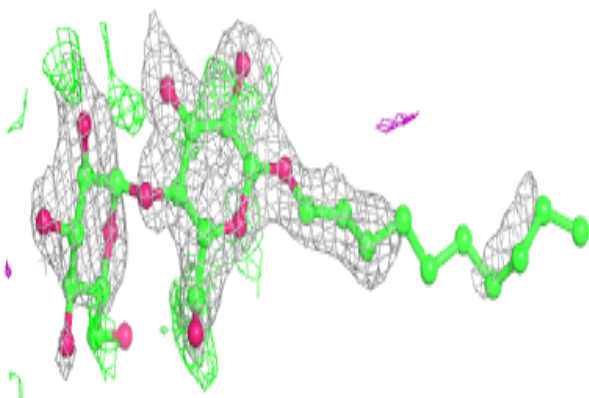


**Electron density around LFA C 624:**

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

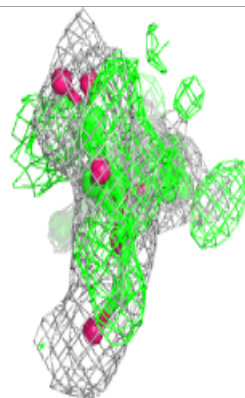
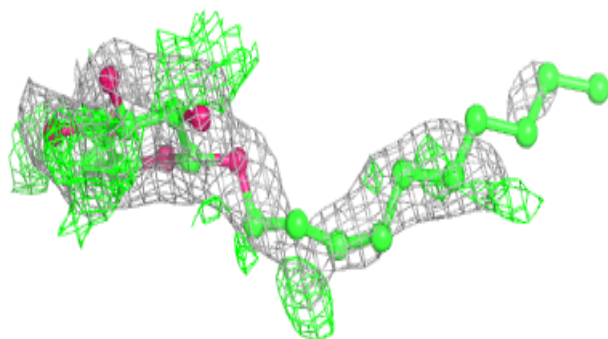
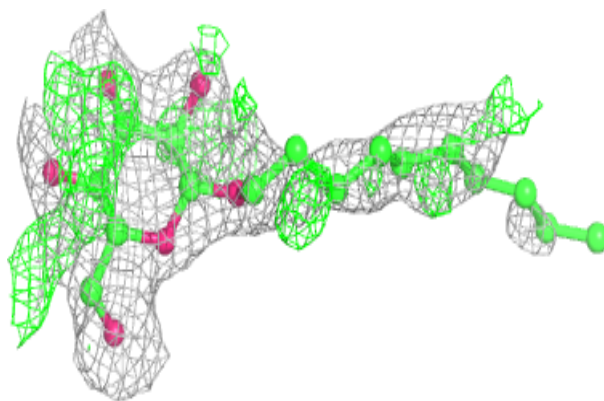
**Electron density around DMU C 714:**

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

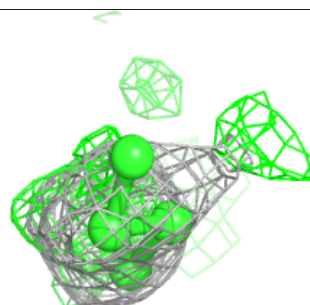
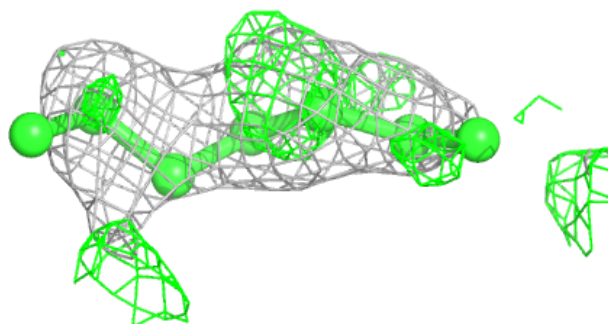
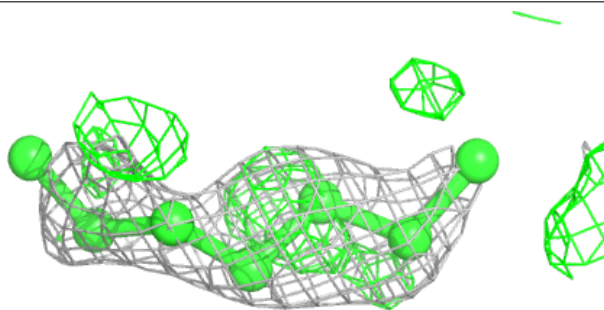


**Electron density around DMU G 713:**

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

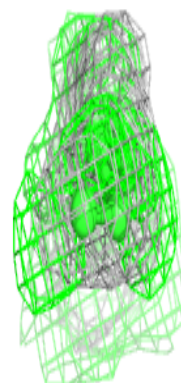
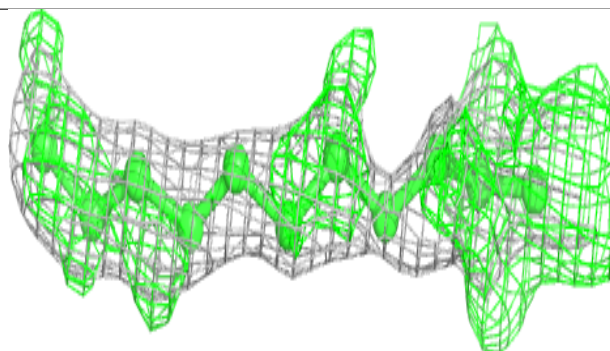
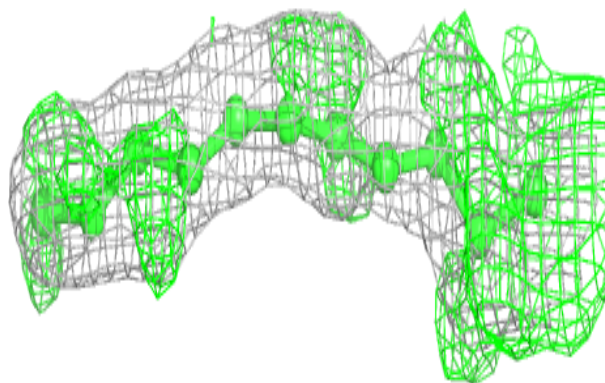
**Electron density around DMU C 721:**

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

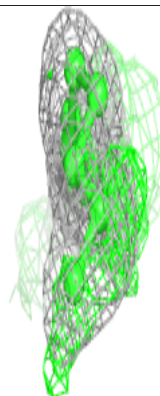
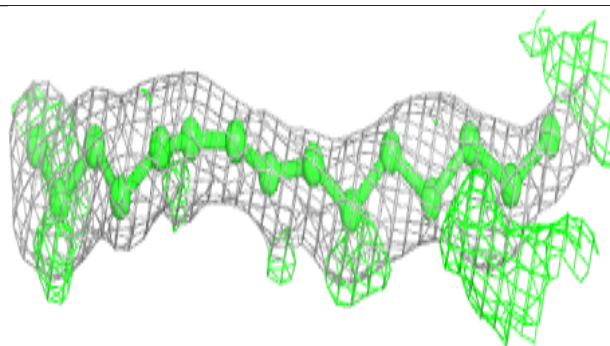
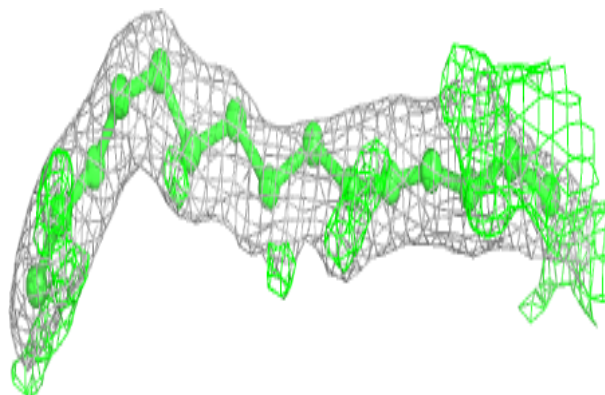


**Electron density around LFA G 622:**

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

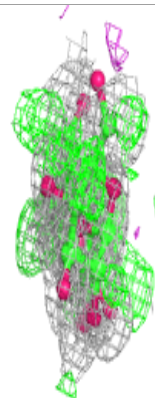
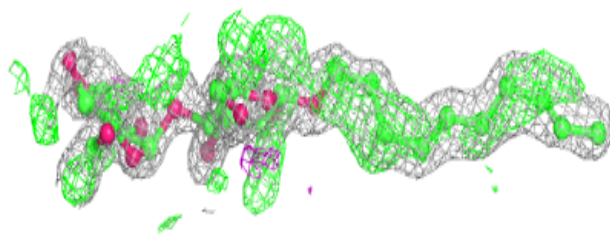
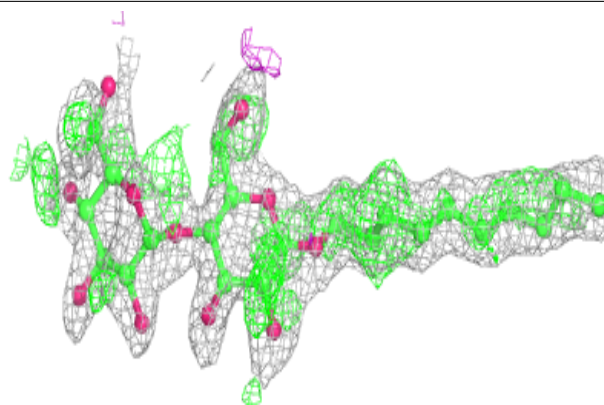
**Electron density around LFA P 625:**

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

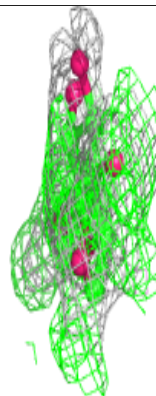
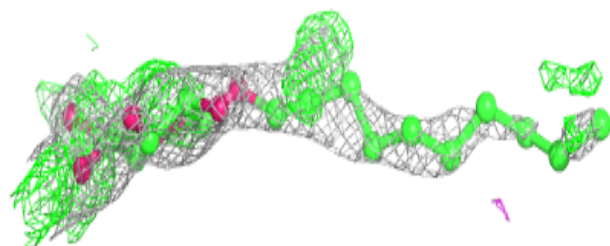
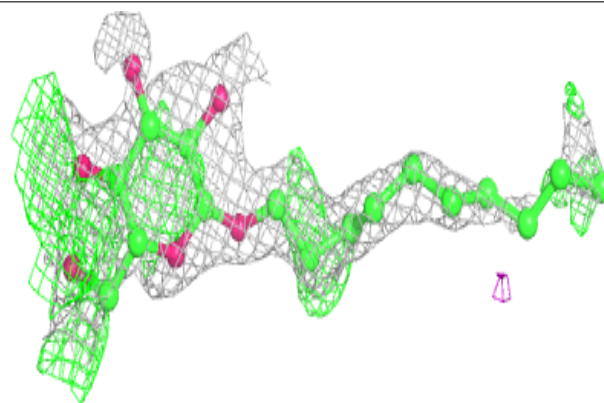


**Electron density around DMU A 745:**

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

**Electron density around DMU L 747:**

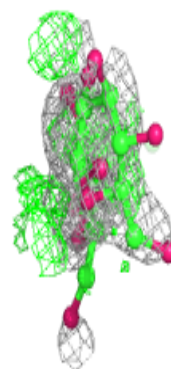
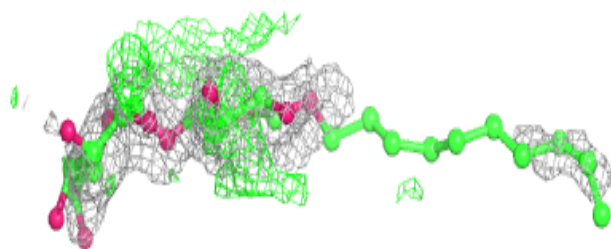
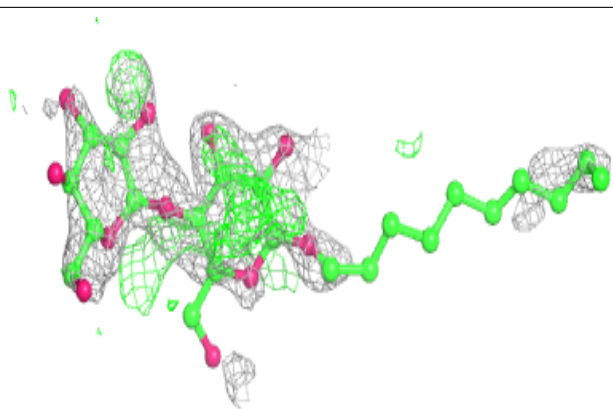
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



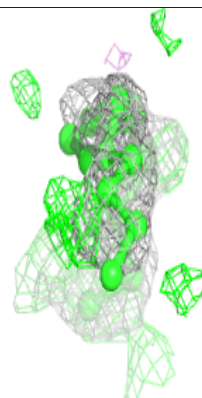
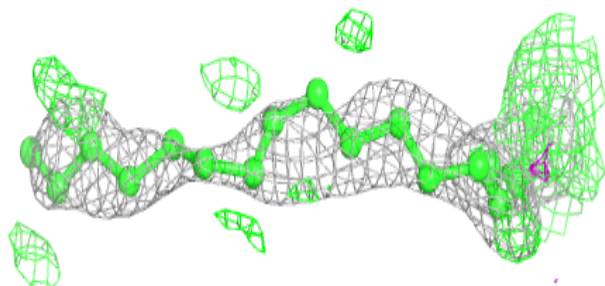
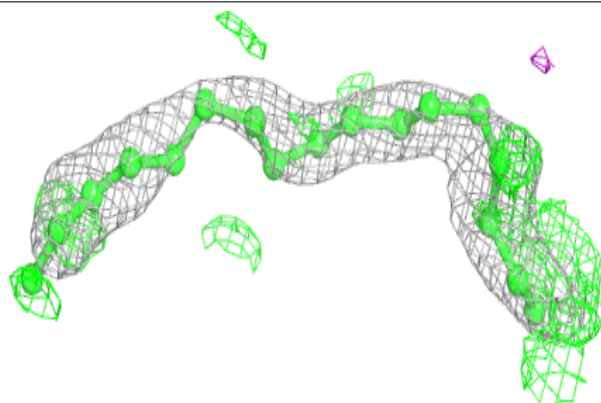


**Electron density around DMU P 734:**

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

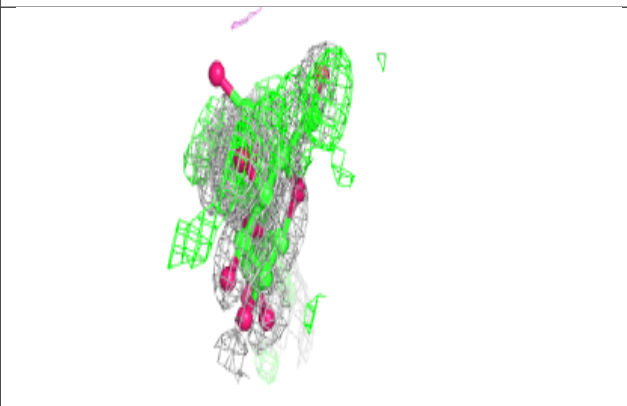
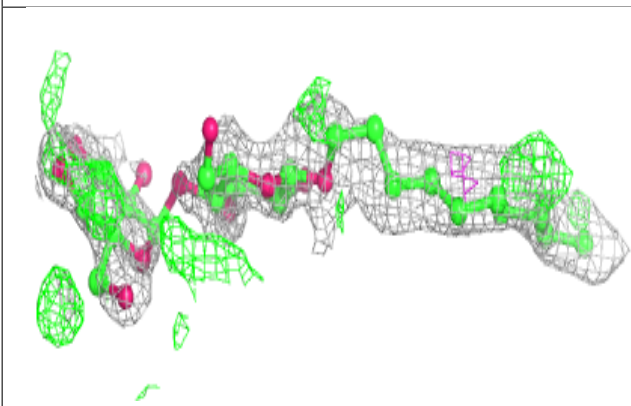
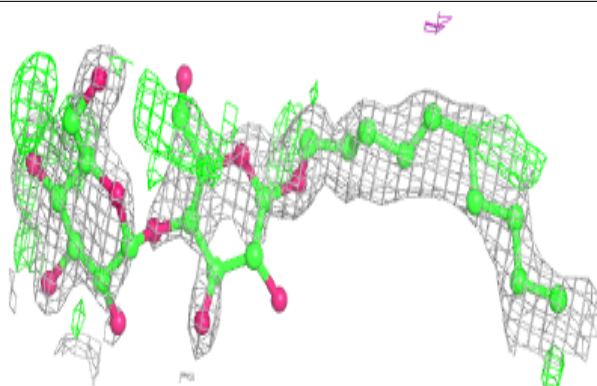
**Electron density around LFA G 621:**

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

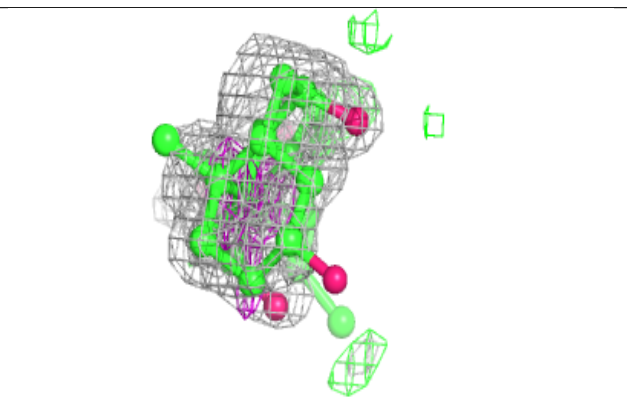
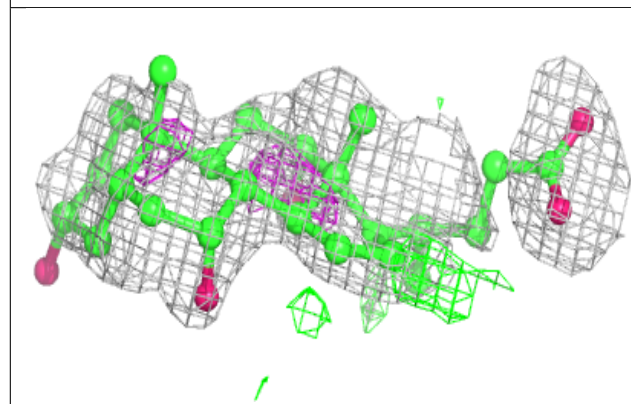
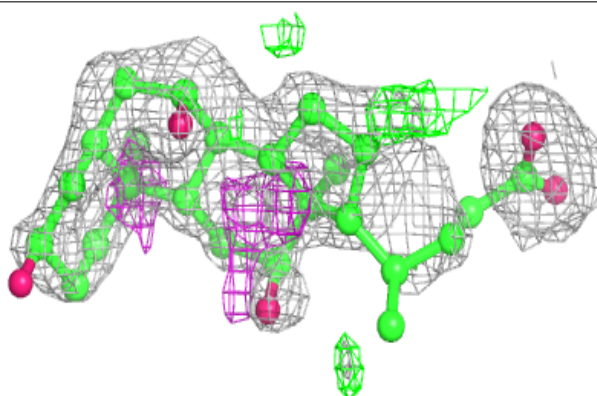


**Electron density around DMU C 715 (A):**

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

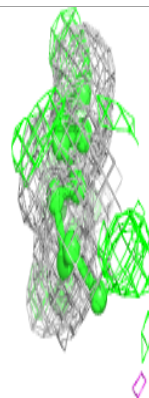
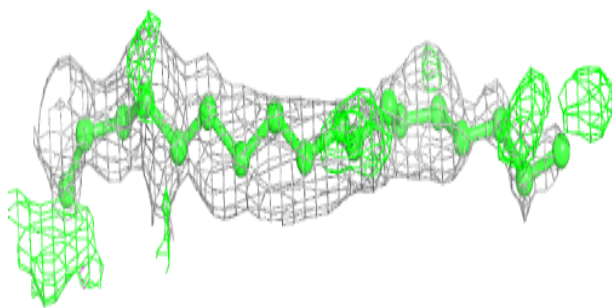
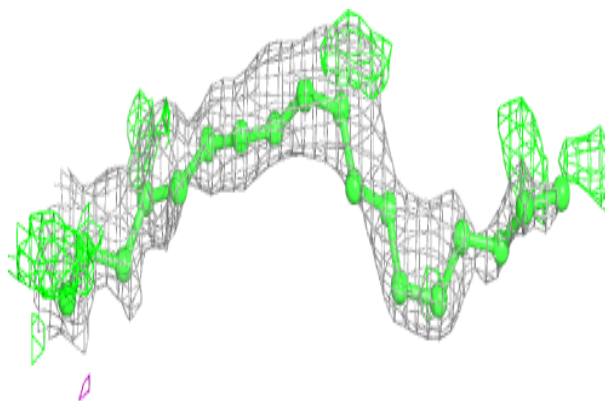
**Electron density around CHD P 271:**

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

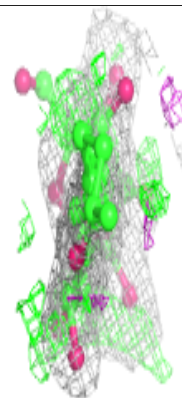
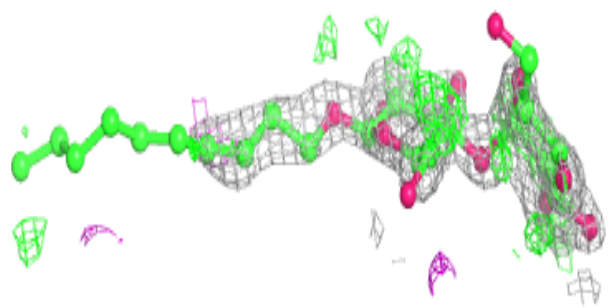
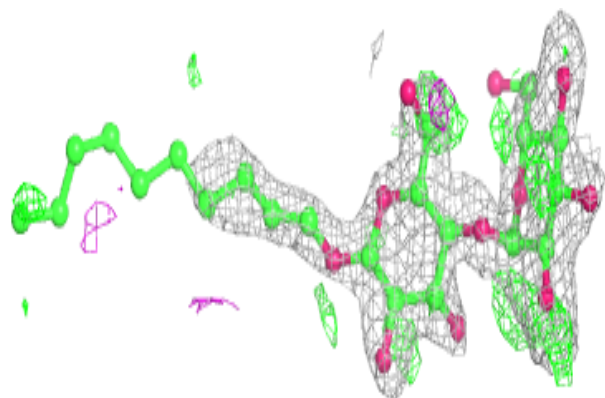


**Electron density around LFA C 716 (B):**

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

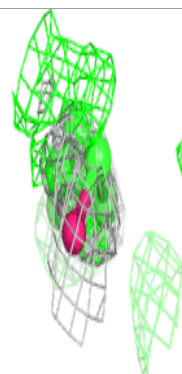
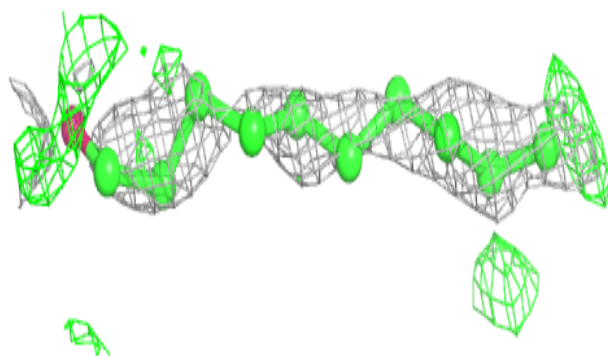
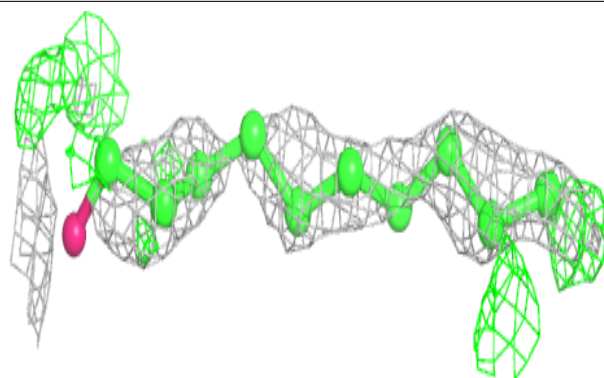
**Electron density around DMU P 714:**

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

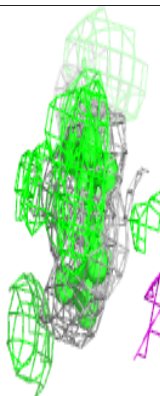
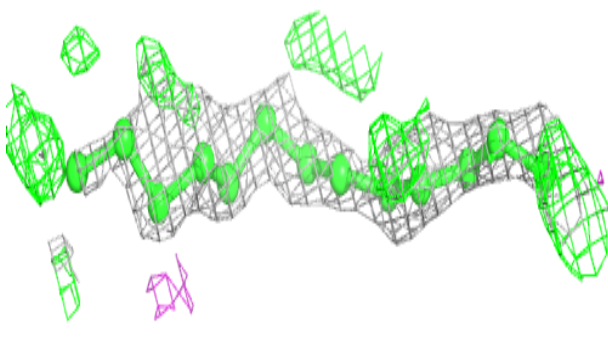
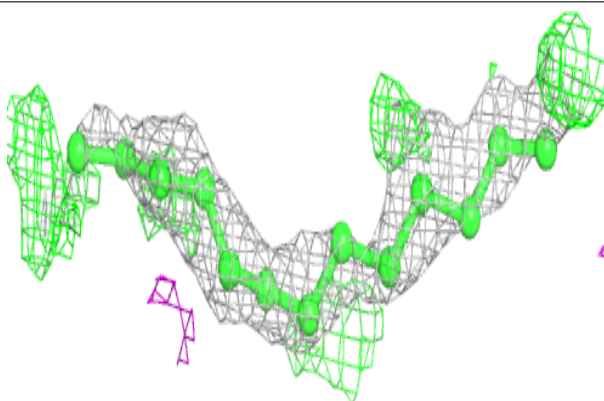


**Electron density around DMU B 731:**

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

**Electron density around LFA C 626:**

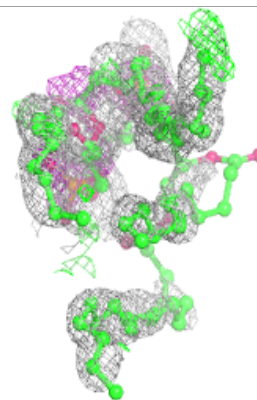
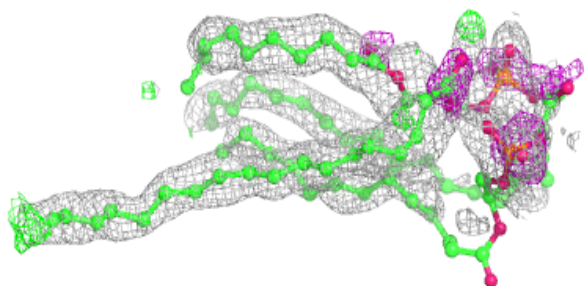
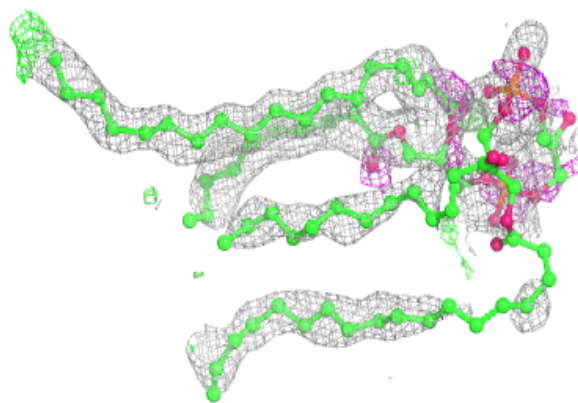
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



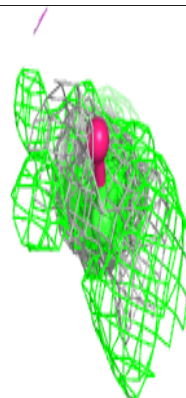
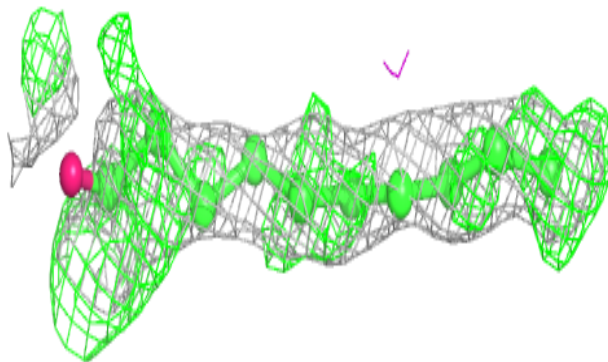
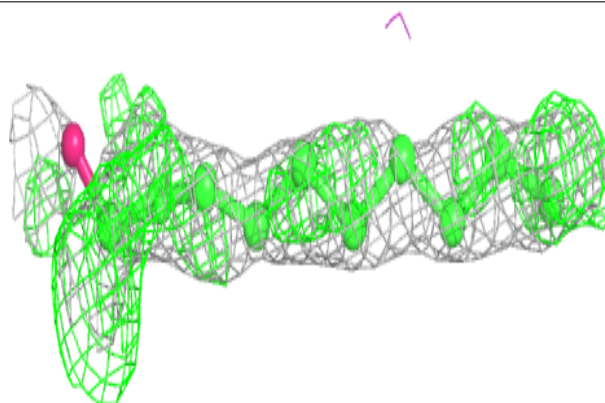


**Electron density around CDL C 270:**

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

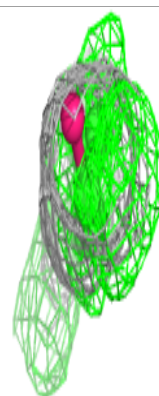
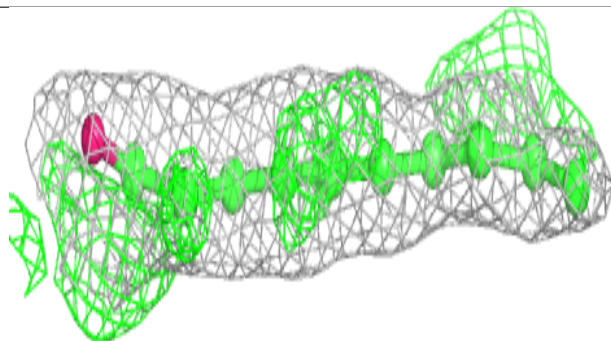
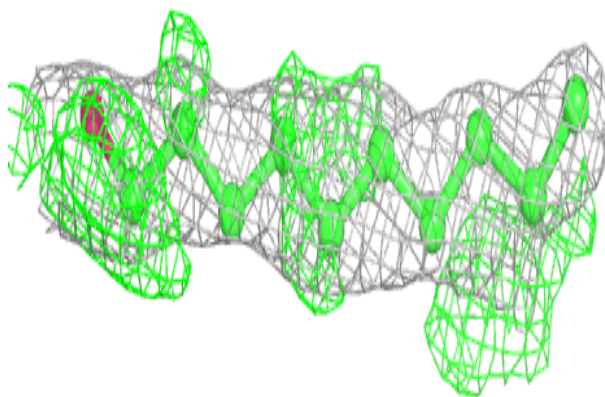
**Electron density around DMU O 731:**

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

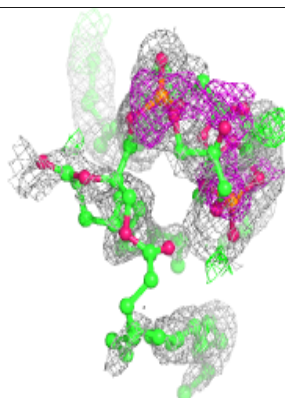
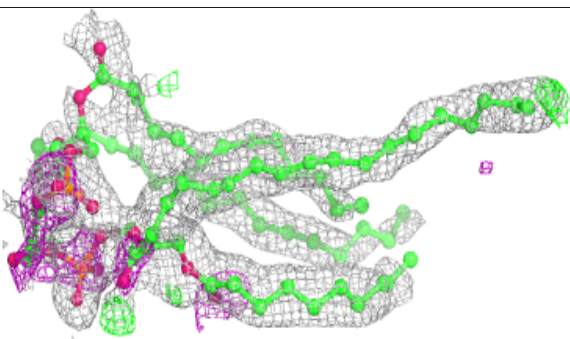
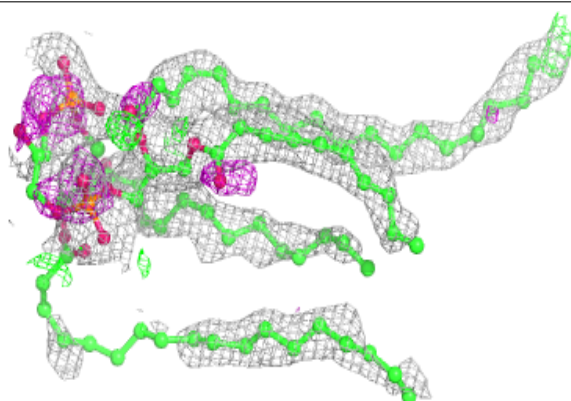


**Electron density around DMU P 272:**

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

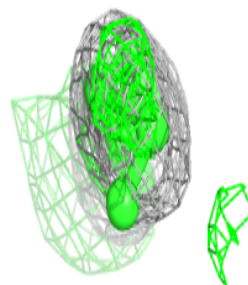
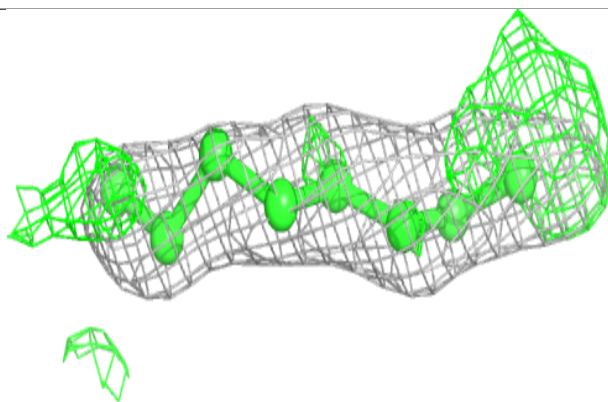
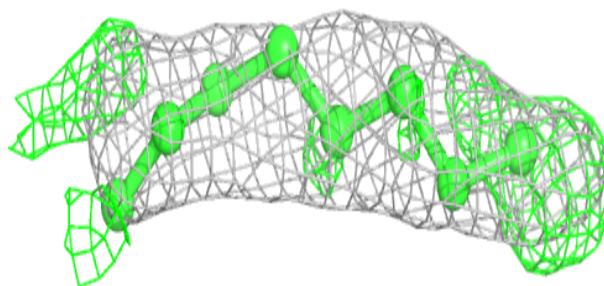
**Electron density around CDL P 270:**

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

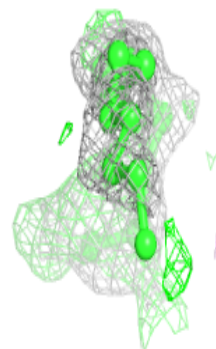
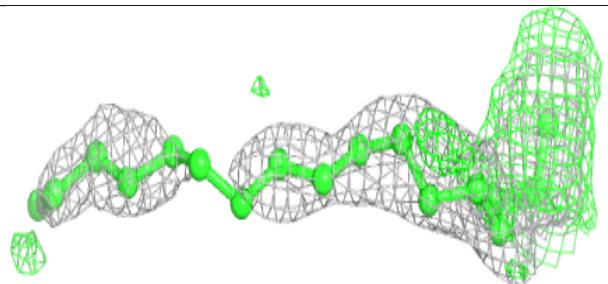
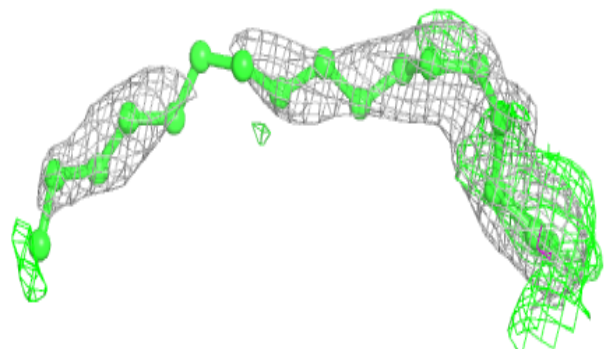


**Electron density around DMU Z 746:**

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

**Electron density around LFA T 621:**

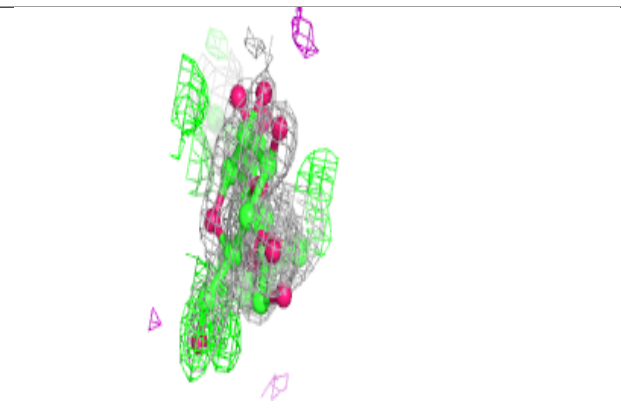
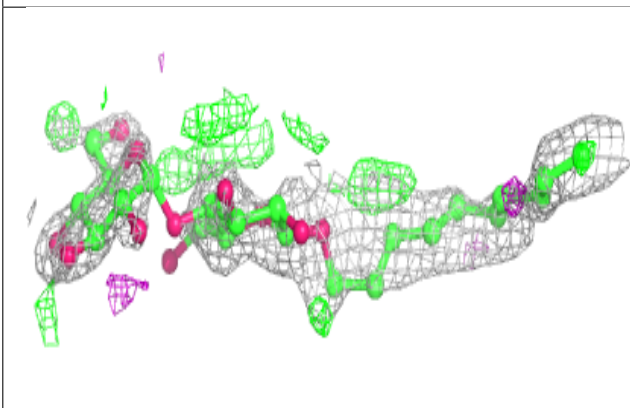
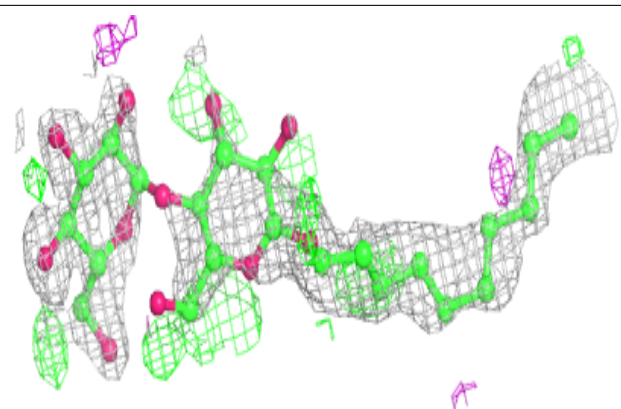
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



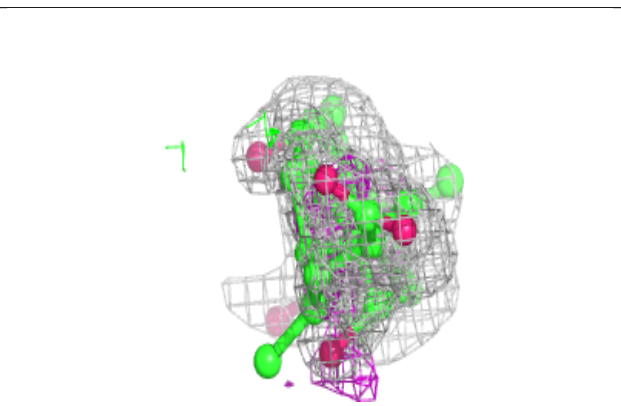
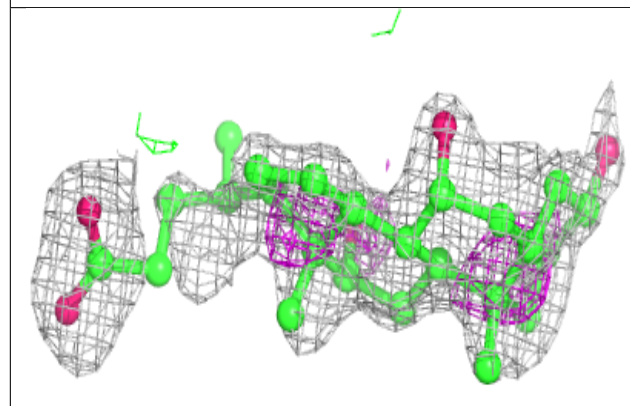
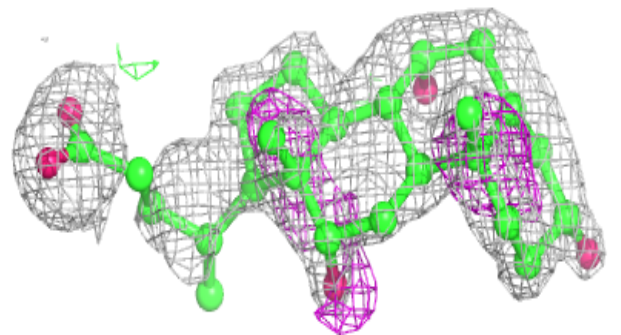


**Electron density around DMU P 715 (A):**

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

**Electron density around CHD C 271:**

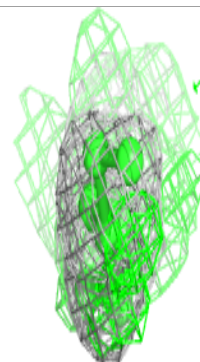
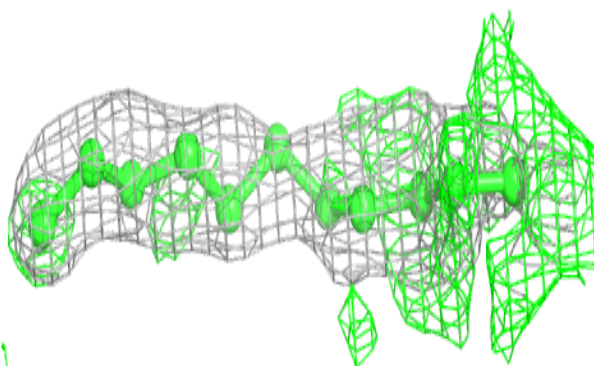
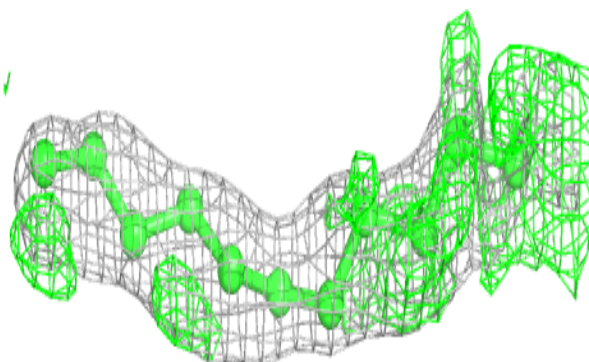
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



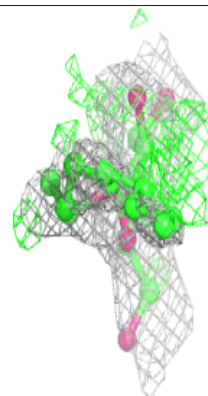
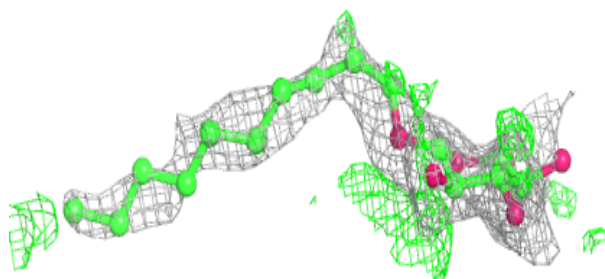
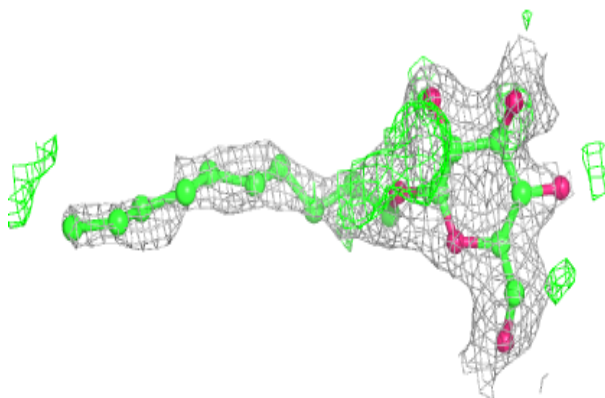


**Electron density around LFA T 622:**

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

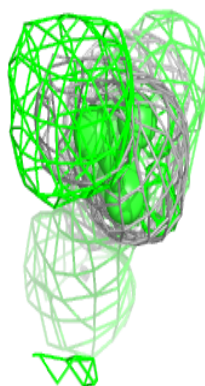
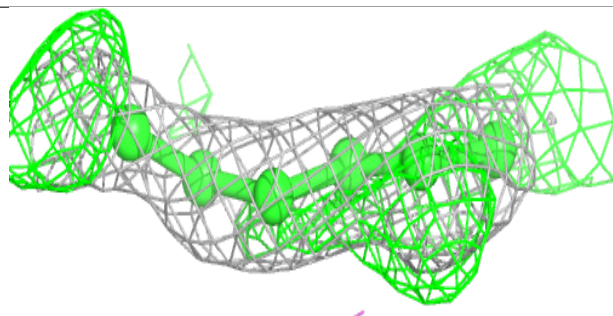
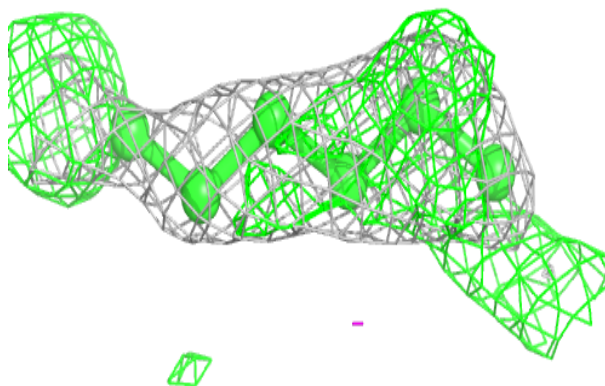
**Electron density around DMU T 713:**

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

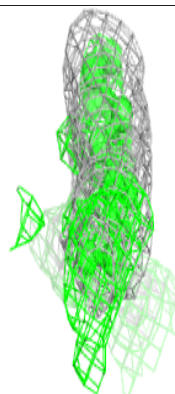
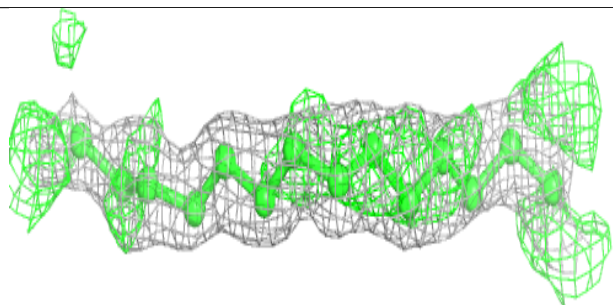
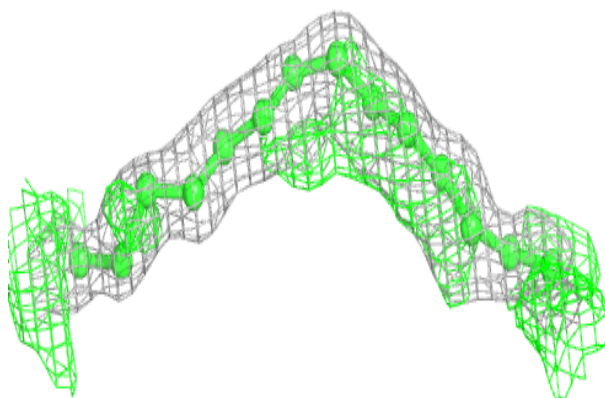


**Electron density around LFA P 612:**

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

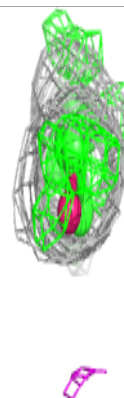
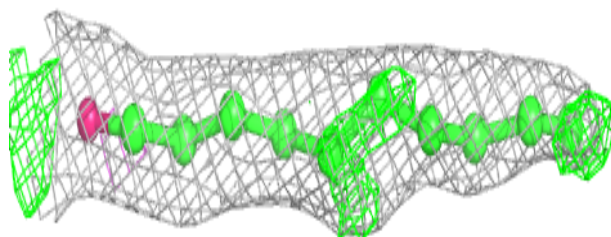
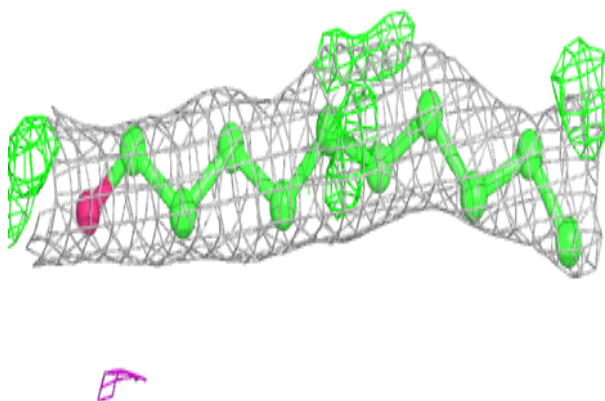
**Electron density around LFA N 627:**

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

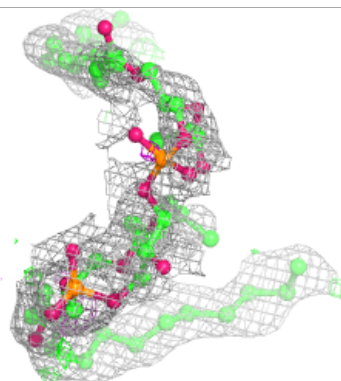
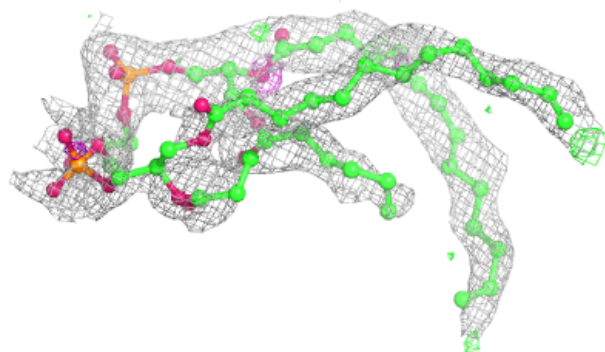
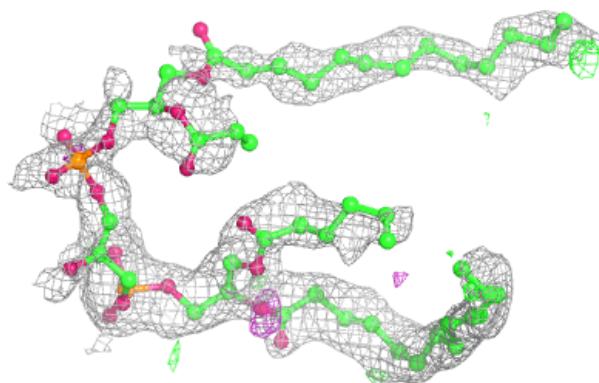


**Electron density around DMU C 272:**

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

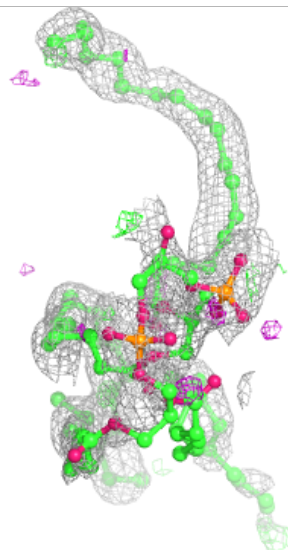
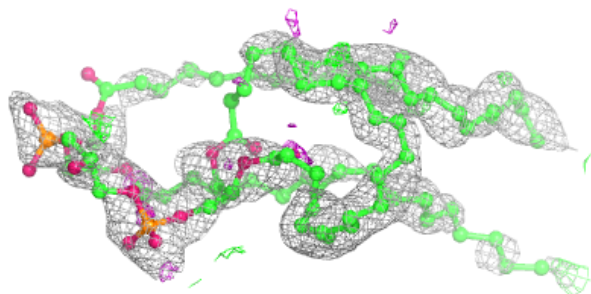
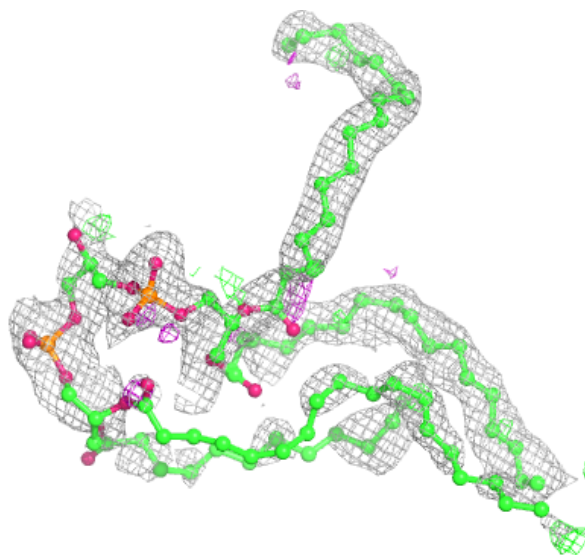
**Electron density around CDL N 522:**

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



**Electron density around CDL N 521:**

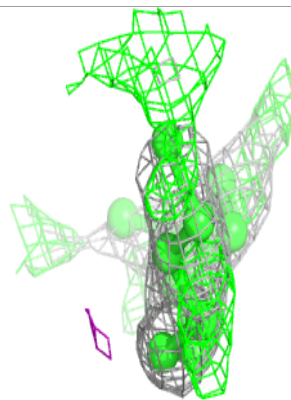
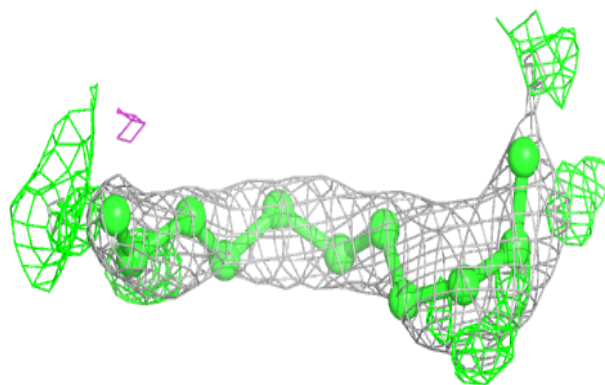
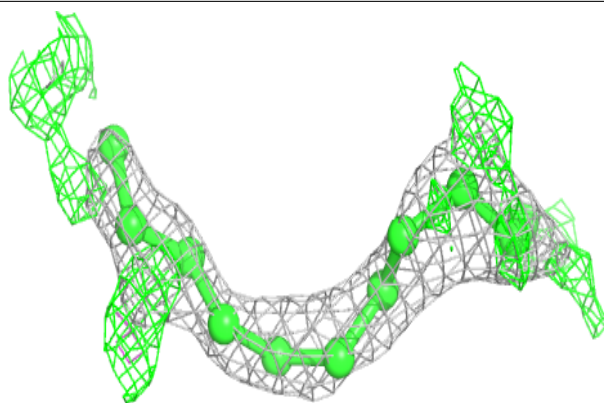
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



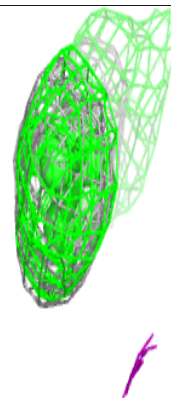
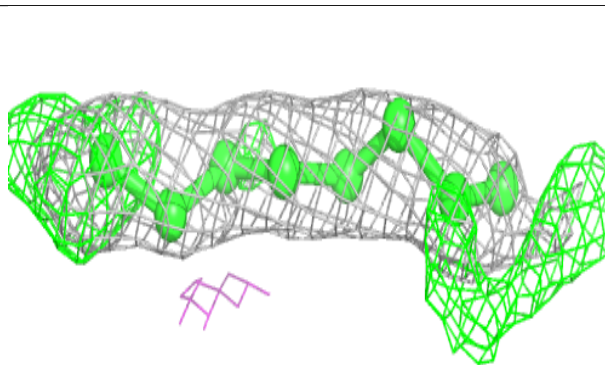
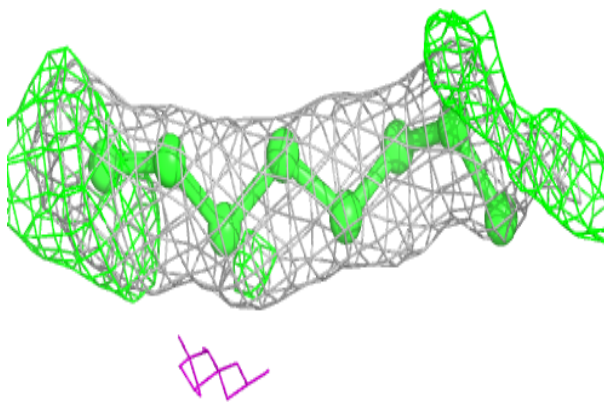


**Electron density around LFA C 611:**

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

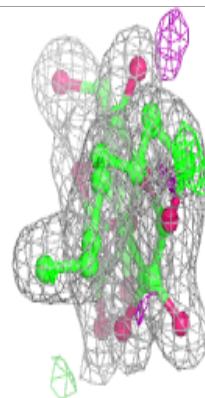
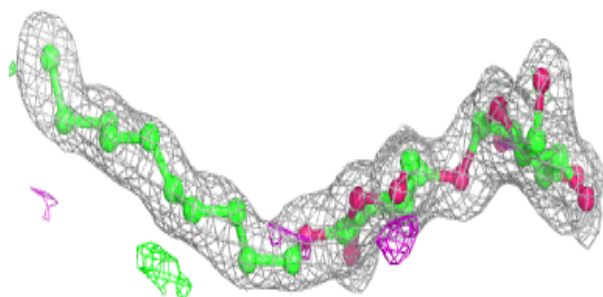
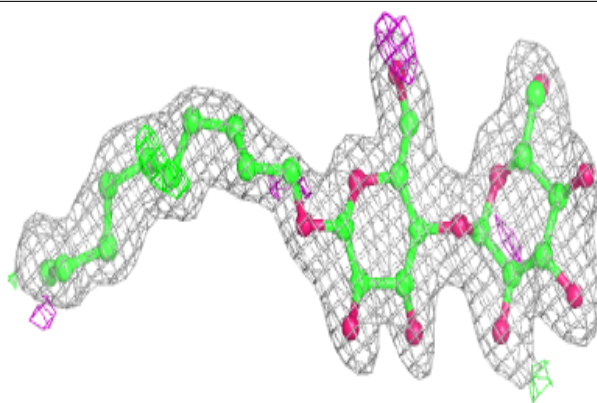
**Electron density around DMU M 746:**

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

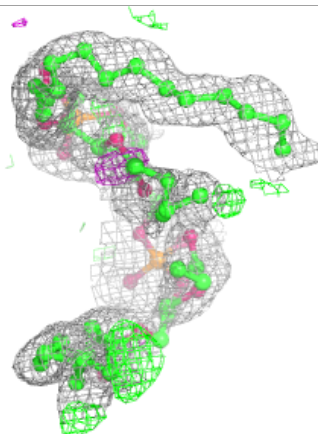
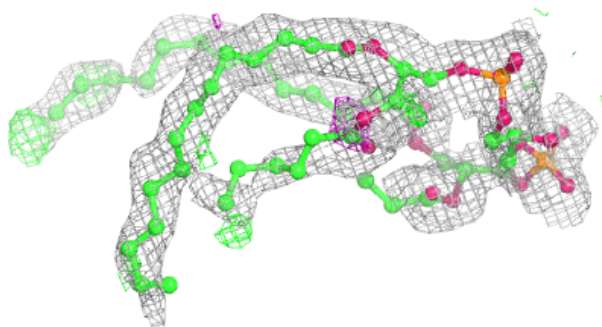
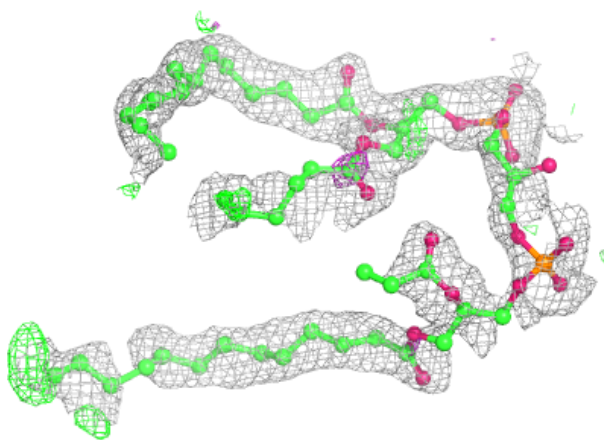


**Electron density around DMU N 526:**

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

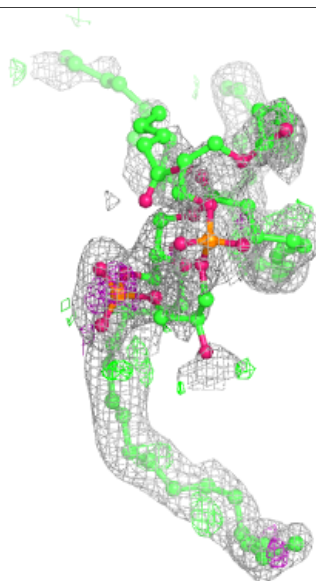
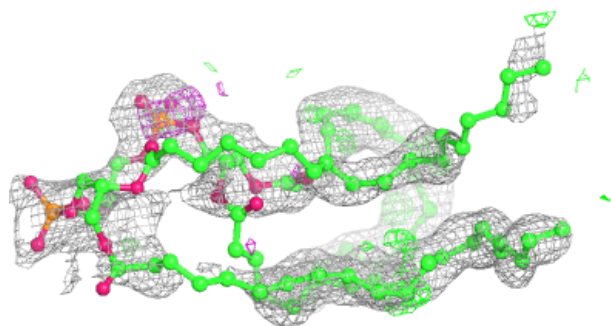
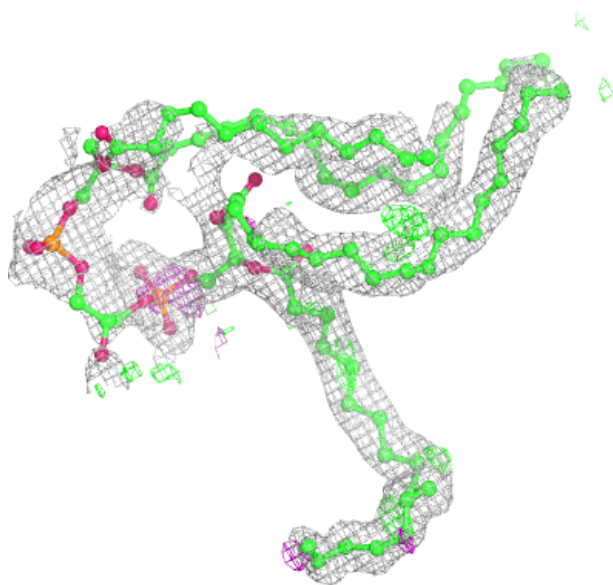
**Electron density around CDL A 522:**

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



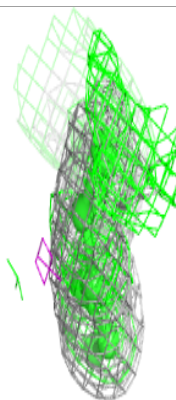
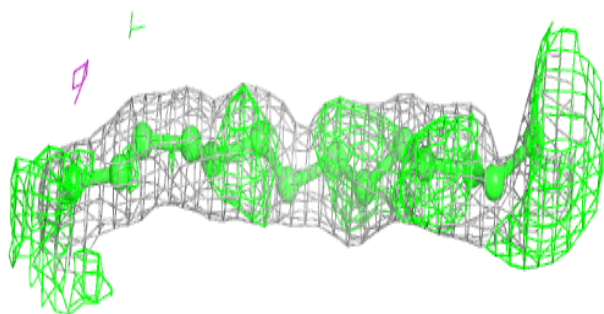
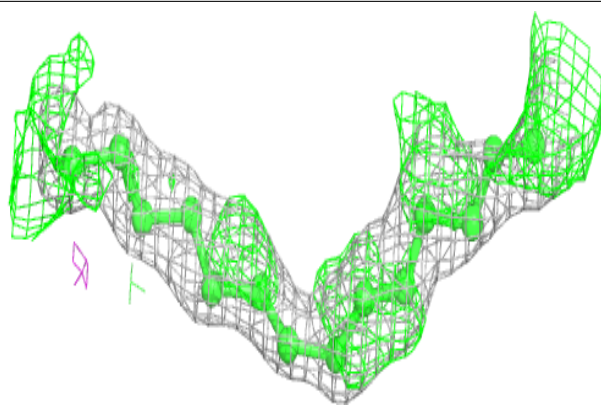
**Electron density around CDL A 521:**

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

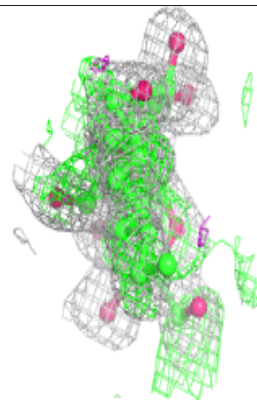
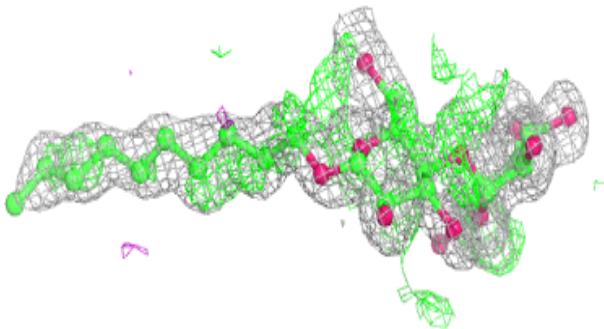
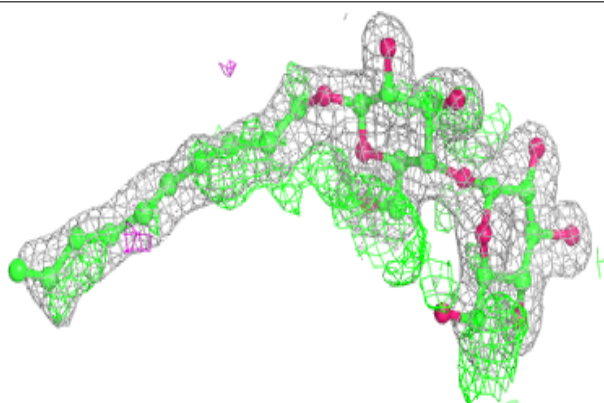


**Electron density around LFA A 627:**

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

**Electron density around DMU A 744:**

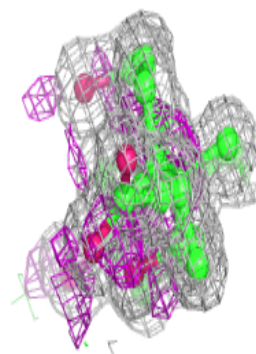
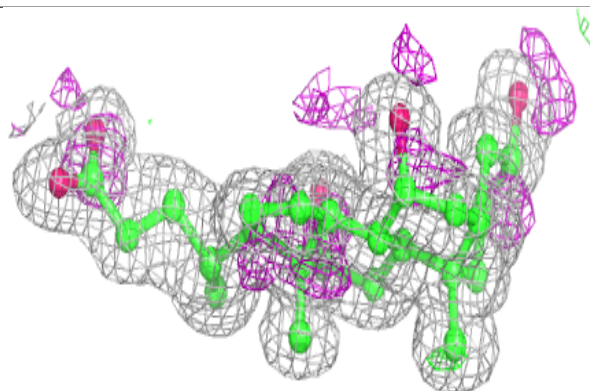
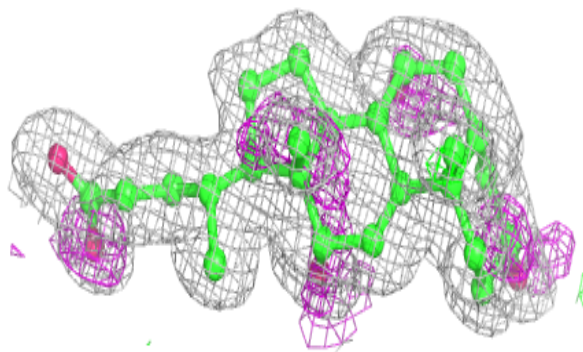
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



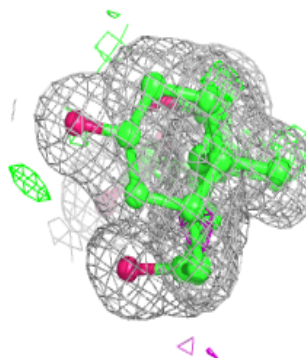
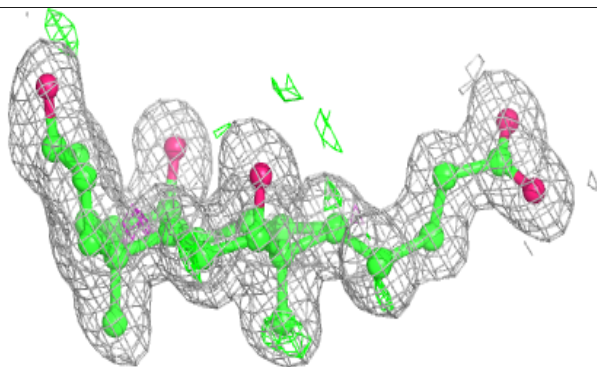
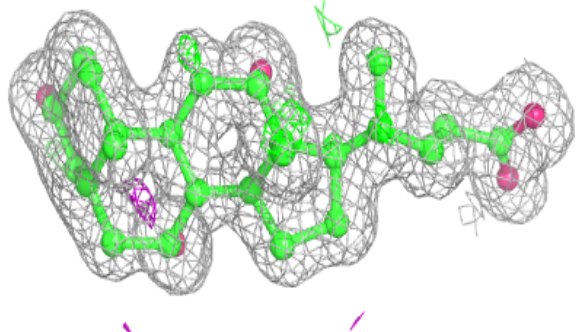


**Electron density around CHD A 525:**

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

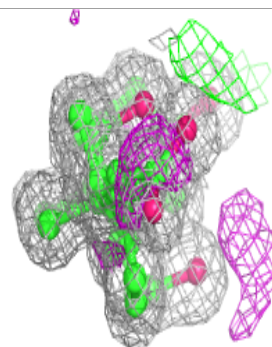
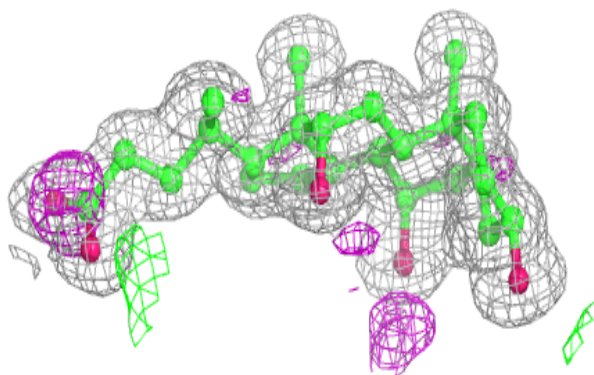
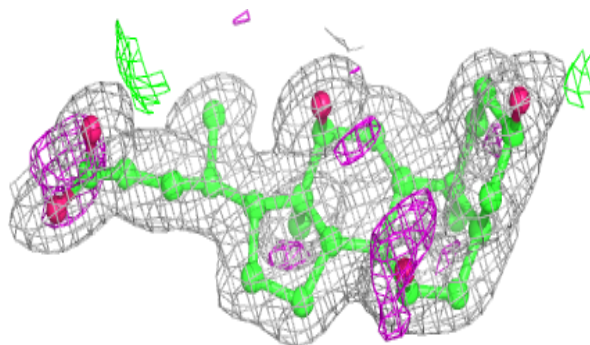
**Electron density around CHD G 86:**

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

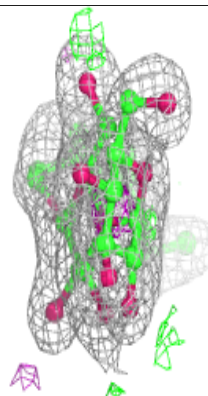
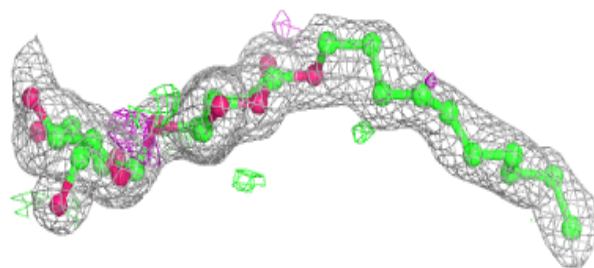
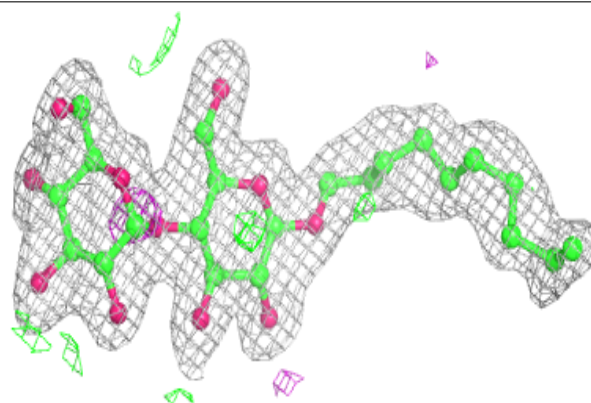


**Electron density around CHD N 525:**

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

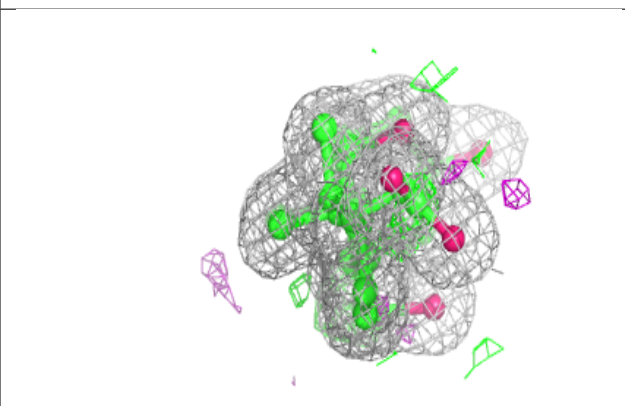
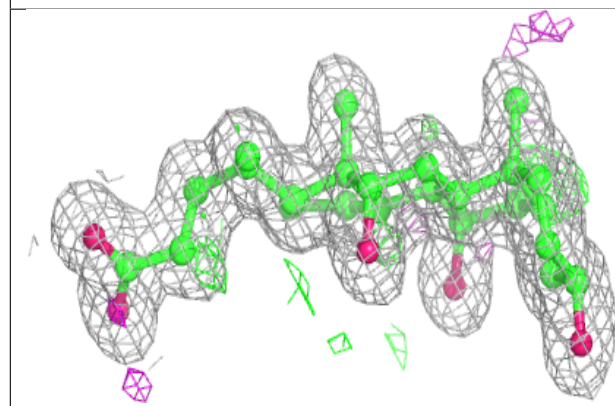
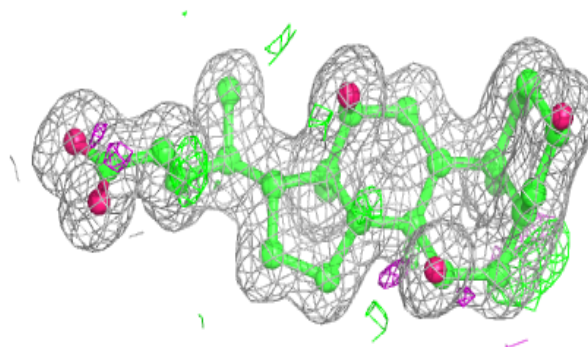
**Electron density around DMU A 526:**

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

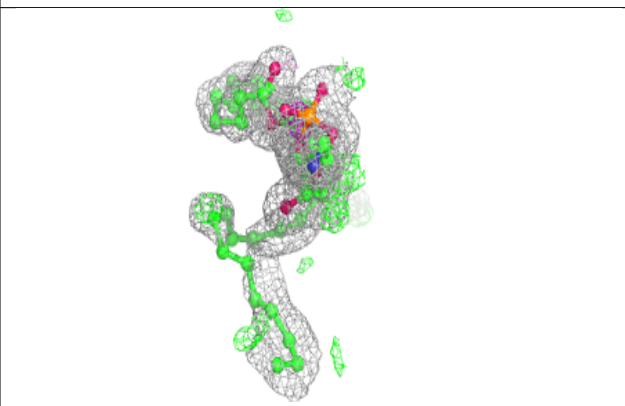
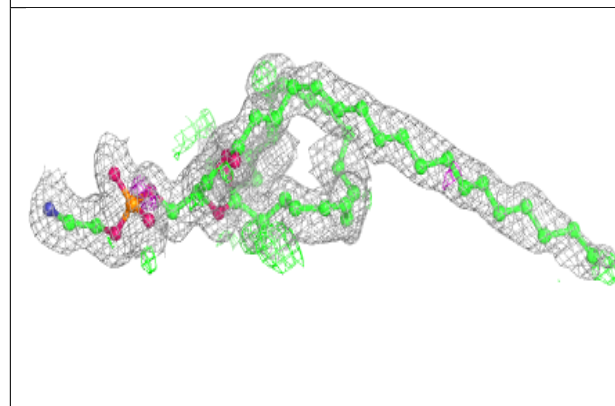
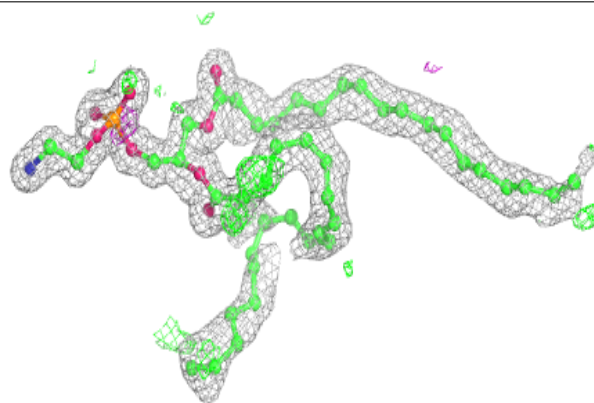


**Electron density around CHD T 86:**

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

**Electron density around PEK P 264:**

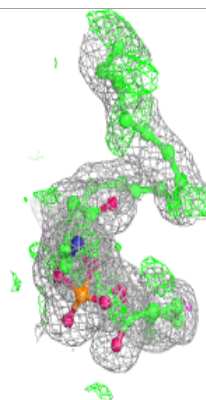
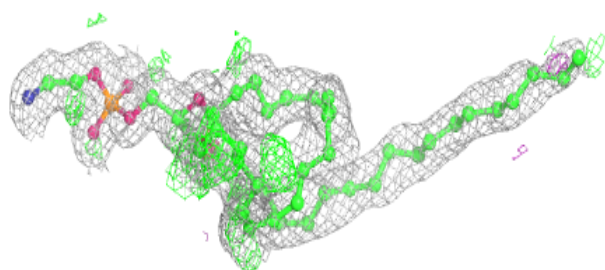
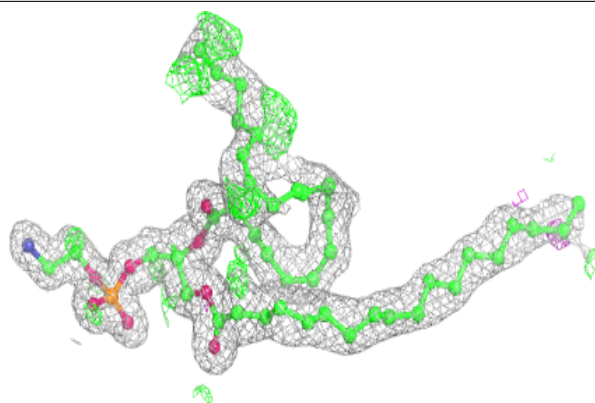
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



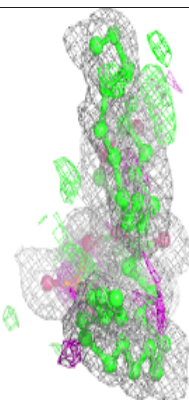
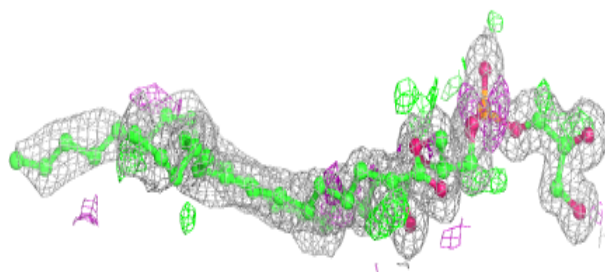
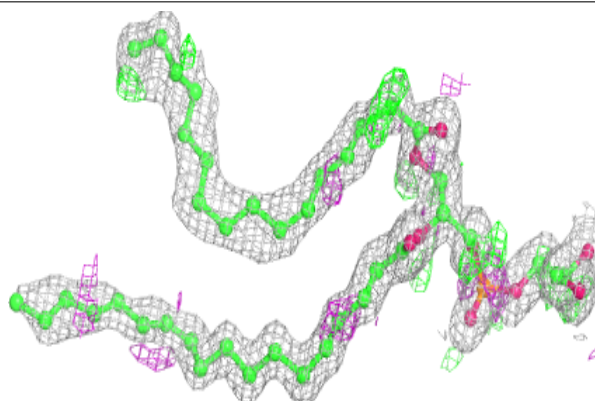


**Electron density around PEK C 264:**

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

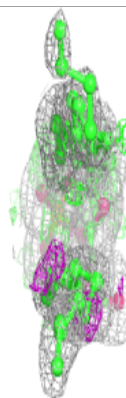
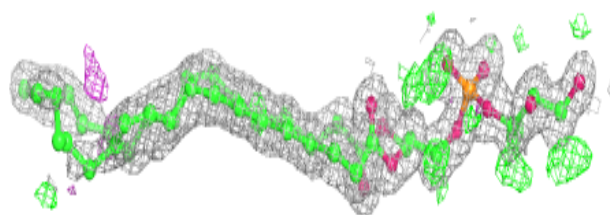
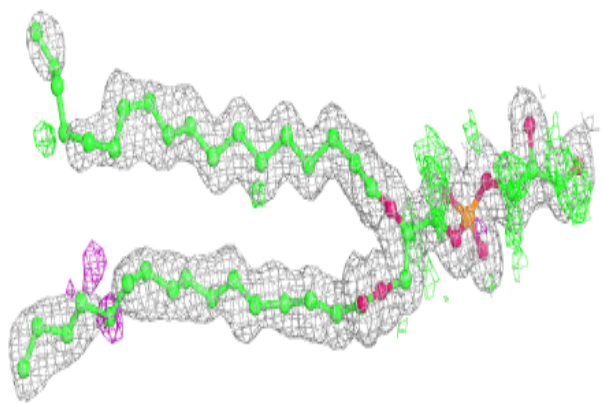
**Electron density around PGV C 266:**

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

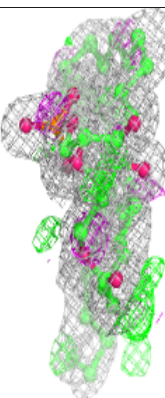
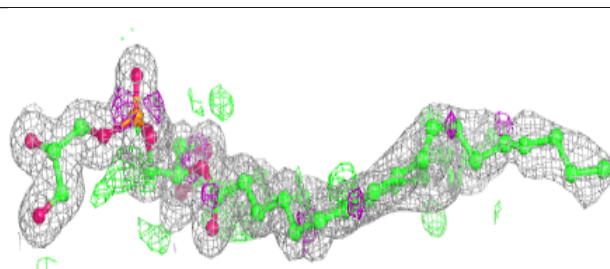
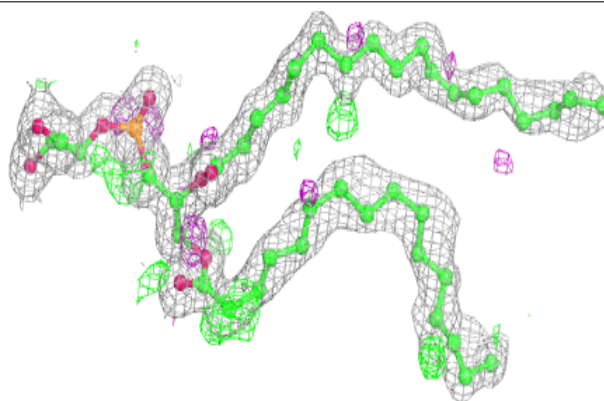


**Electron density around PGV C 267:**

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

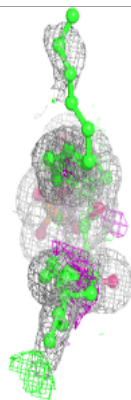
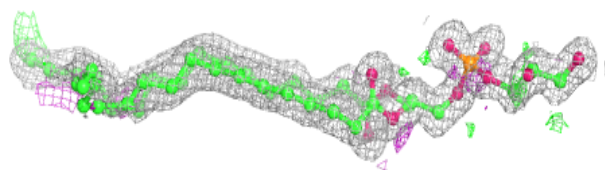
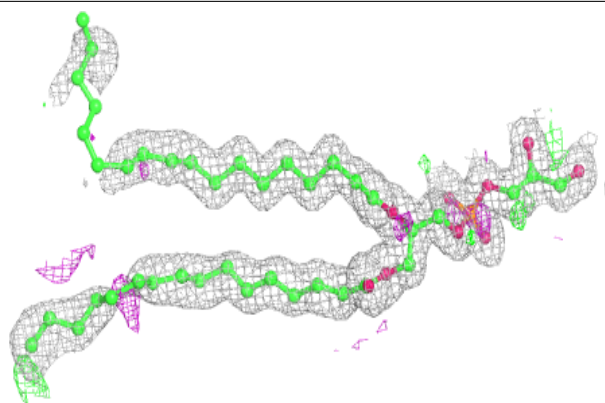
**Electron density around PGV P 266:**

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

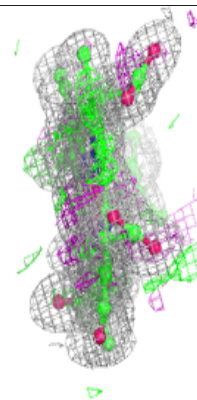
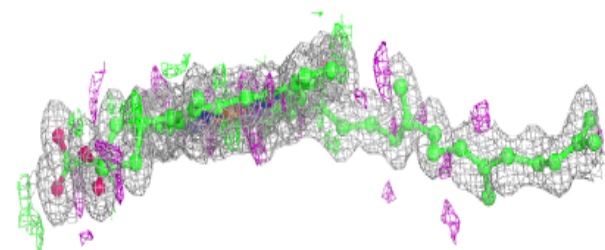
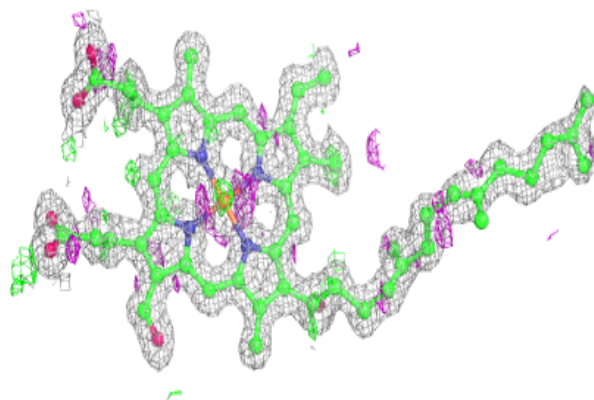


**Electron density around PGV P 267:**

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

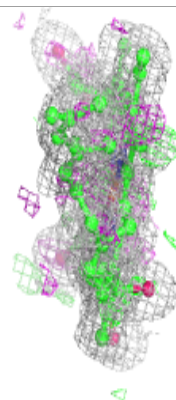
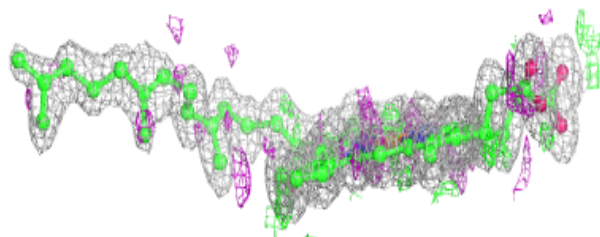
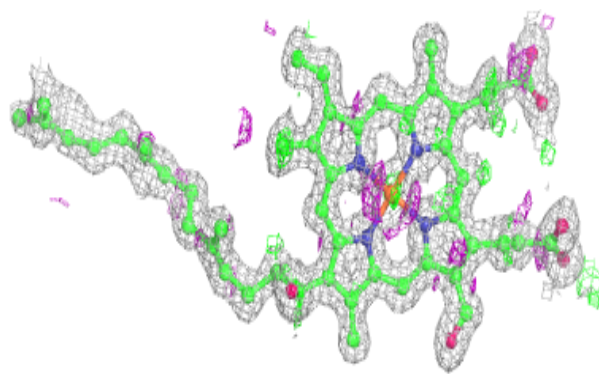
**Electron density around HEA A 515 (A):**

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

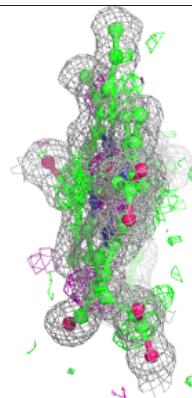
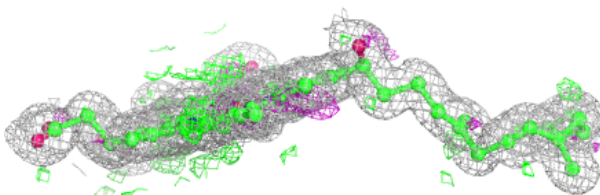
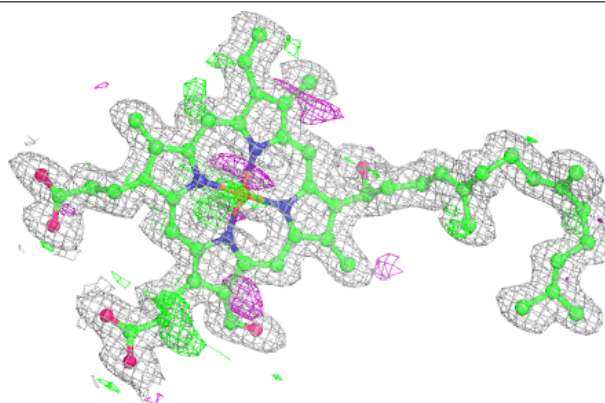


**Electron density around HEA A 515 (B):**

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

**Electron density around HEA A 516:**

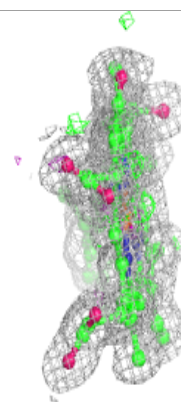
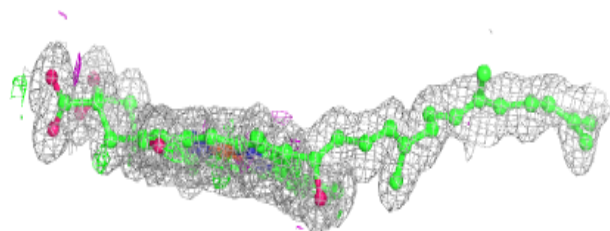
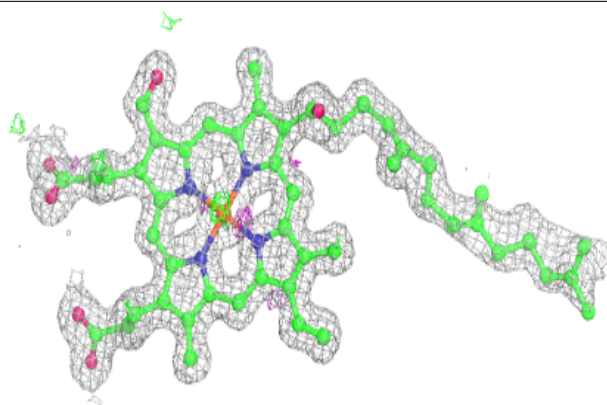
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



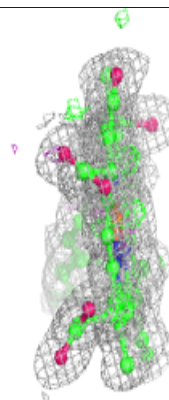
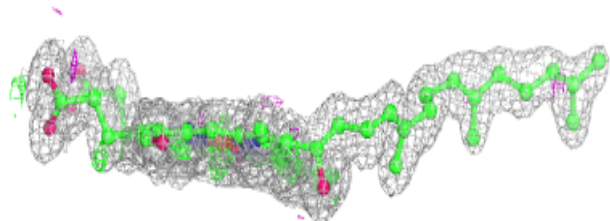
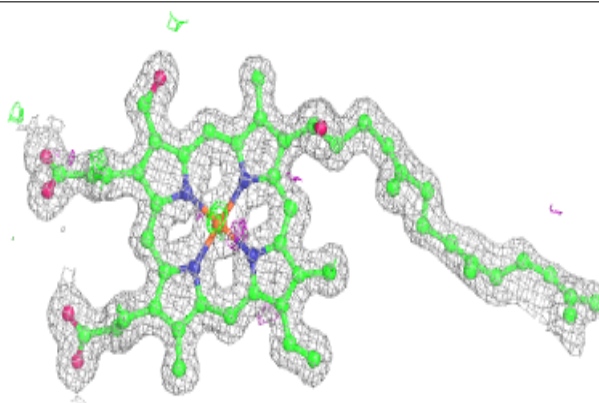


**Electron density around HEA N 515 (A):**

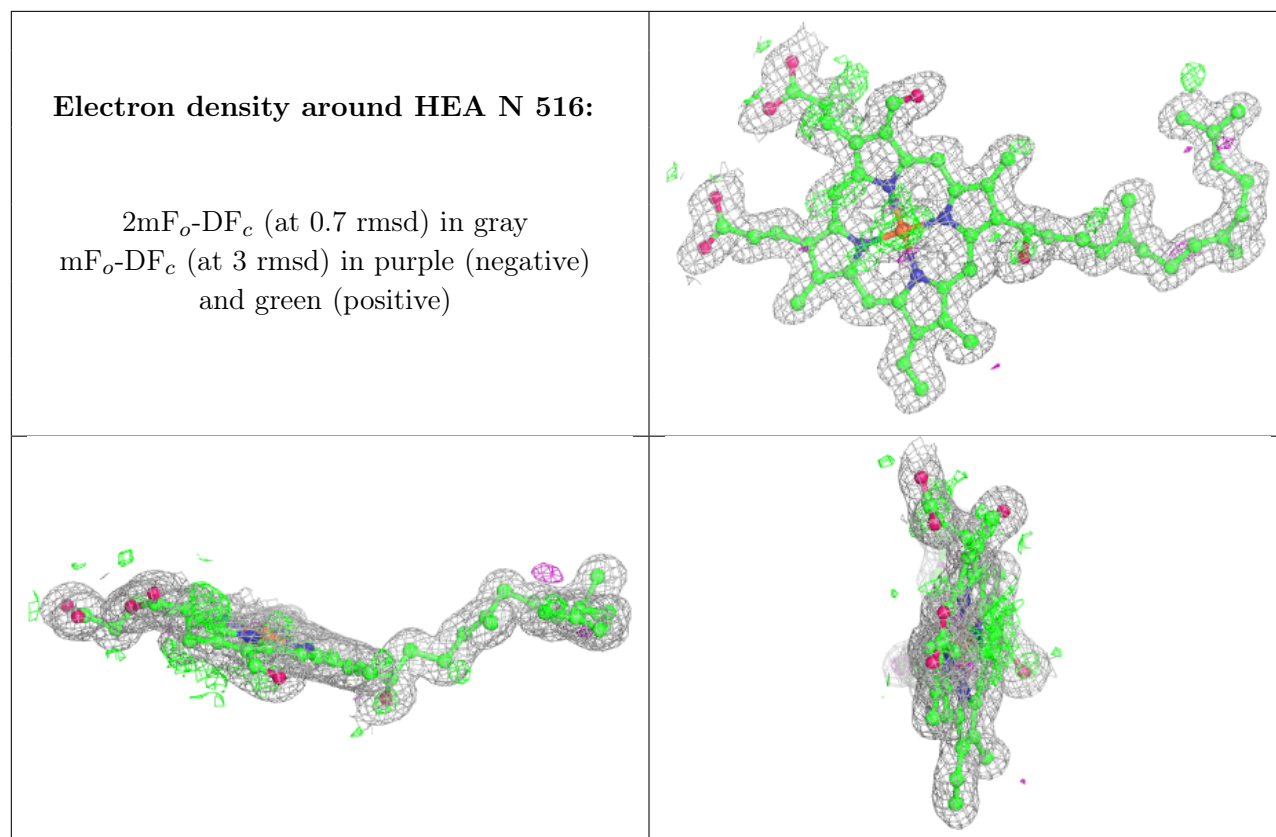
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

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

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.