



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2025 – 01:07 PM JST

PDB ID : 9KUK / pdb_00009kuk
Title : Bovine Heart Cytochrome c Oxidase in the Xenon-bound Fully Oxidized State under Aerobic Condition
Authors : Muramoto, K.; Shinzawa-Itoh, K.
Deposited on : 2024-12-04
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

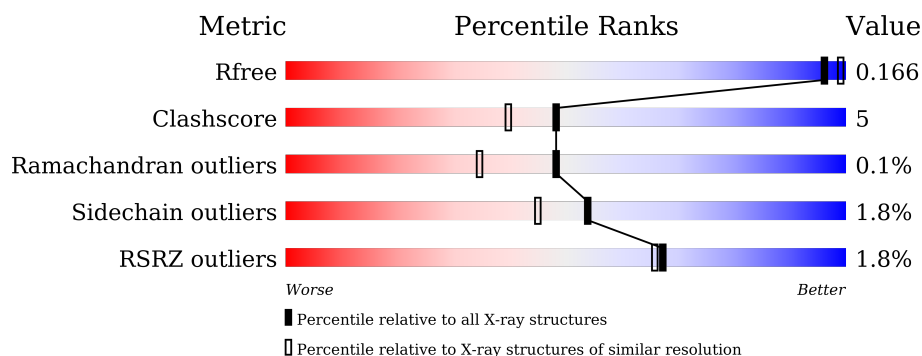
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



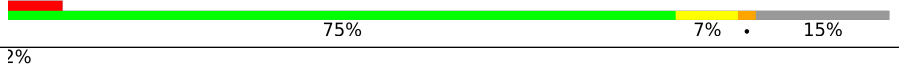

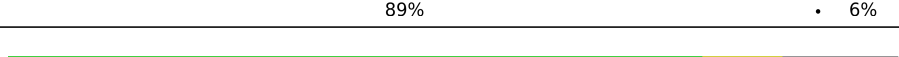
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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>90%</div> <div>9%</div> <div>.</div> </div>
1	N	514	<div> <div></div> <div>90%</div> <div>9%</div> <div></div> </div>
2	B	227	<div> <div>5%</div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div>
2	O	227	<div> <div>2%</div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div>
3	C	261	<div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div>
3	P	261	<div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	LFA	P	311	-	-	-	X
23	XE	B	301	-	-	X	-
23	XE	O	303	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33061 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

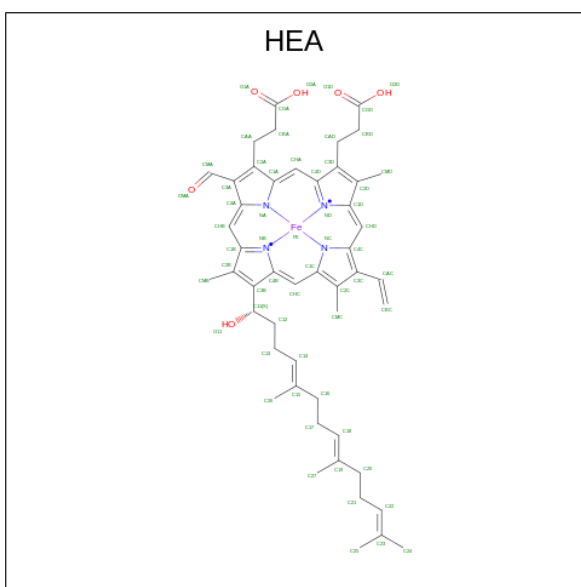
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

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



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

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

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

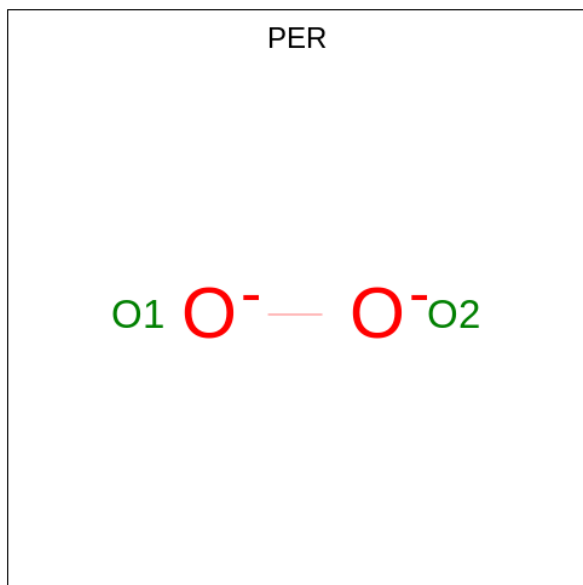
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

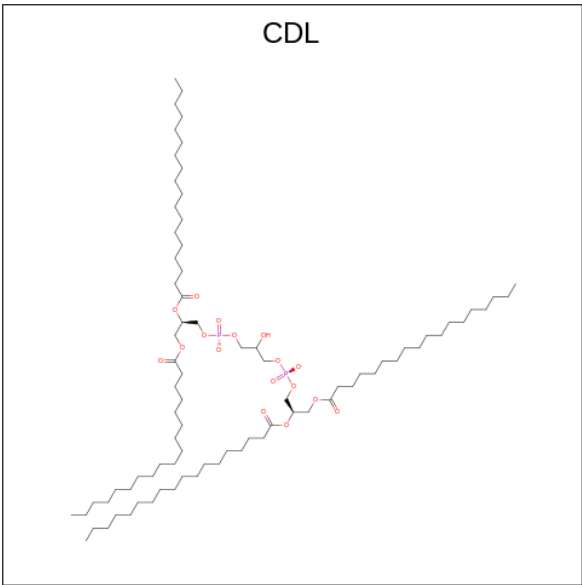
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total 1	Na 1	0	0
17	N	1	Total 1	Na 1	0	0

- Molecule 18 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



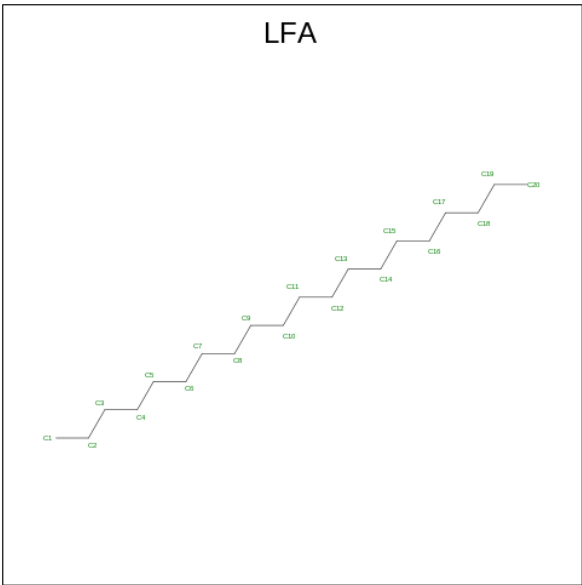
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total 2	O 2	0	0
18	N	1	Total 2	O 2	0	0

- Molecule 19 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 20 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



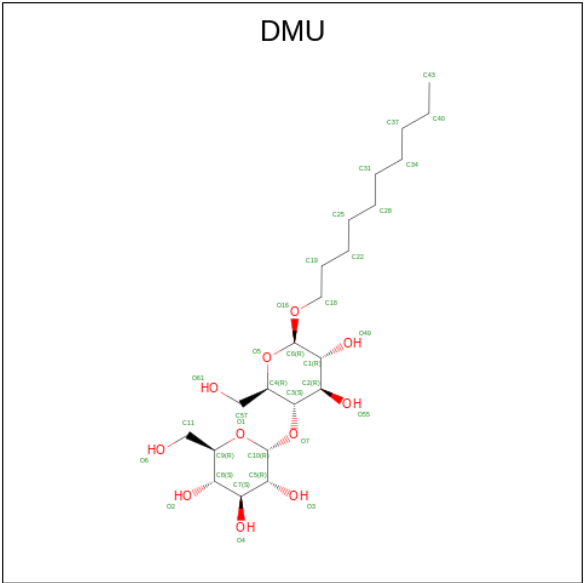
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	C	0	0
			14	14		
20	A	1	Total	C	0	0
			14	14		
20	B	1	Total	C	0	0
			17	17		
20	C	1	Total	C	0	0
			11	11		
20	C	1	Total	C	0	0
			6	6		
20	C	1	Total	C	0	0
			18	18		
20	C	1	Total	C	0	0
			11	11		
20	C	1	Total	C	0	0
			14	14		
20	C	1	Total	C	0	0
	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

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

- Molecule 21 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



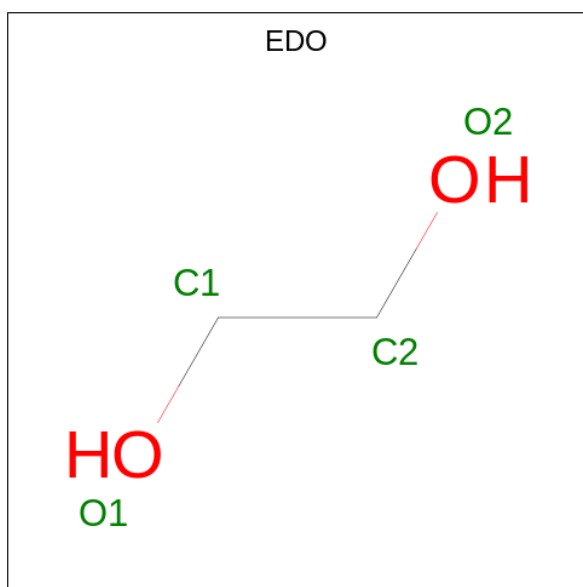
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 7 7	0	0
21	A	1	Total C O 33 22 11	0	0
21	A	1	Total C O 33 22 11	0	0
21	A	1	Total C O 11 10 1	0	0
21	B	1	Total C O 11 10 1	0	0
21	B	1	Total C O 11 10 1	0	0
21	B	1	Total C O 22 16 6	0	0
21	B	1	Total C O 22 16 6	0	0
21	C	1	Total C O 11 10 1	0	0
21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

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

- Molecule 22 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 23 is XENON (CCD ID: XE) (formula: Xe) (labeled as "Ligand of Interest" by depositor).

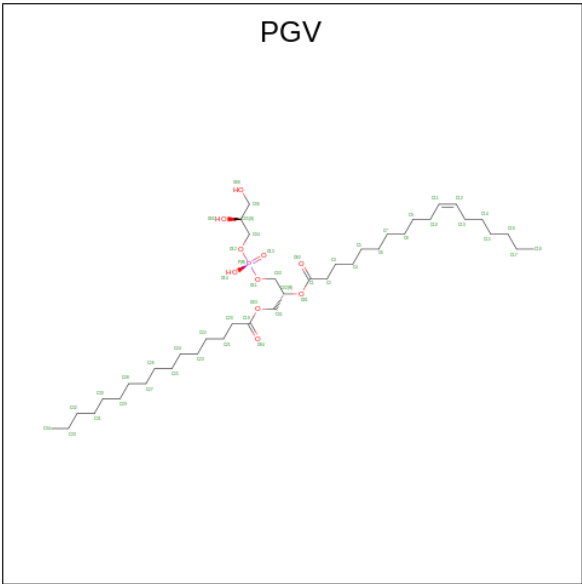
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	5	Total Xe 5 5	0	0
23	B	1	Total Xe 1 1	0	0
23	C	1	Total Xe 1 1	0	0
23	N	5	Total Xe 5 5	0	0

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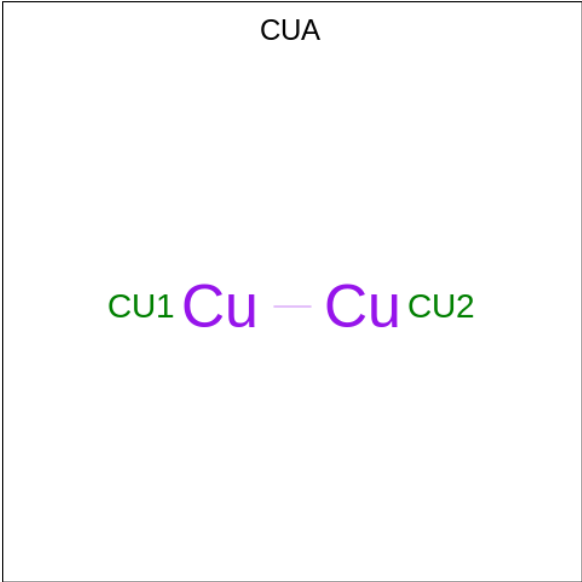
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	O	1	Total	Xe	0	0
			1	1		
23	P	1	Total	Xe	0	0
			1	1		

- Molecule 24 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



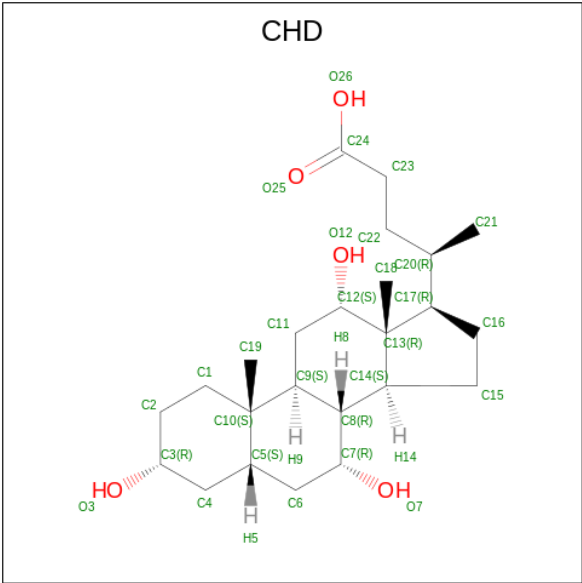
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	O	P	0	0
			51	40	10	1		
24	C	1	Total	C	O	P	0	0
			51	40	10	1		
24	N	1	Total	C	O	P	0	0
			51	40	10	1		
24	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 25 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 26 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



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

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

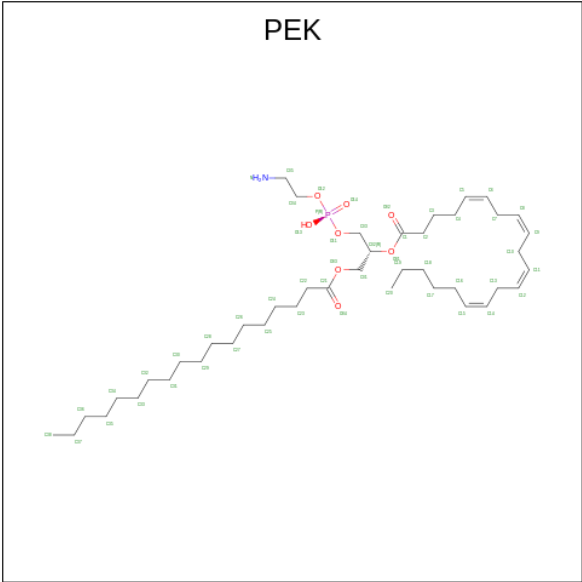
- Molecule 27 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

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

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

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

- Molecule 29 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	246	Total	O	0	11
			257	257		
30	B	177	Total	O	0	2
			179	179		
30	C	101	Total	O	0	1
			102	102		
30	D	139	Total	O	0	9
			148	148		
30	E	110	Total	O	0	7
			117	117		
30	F	97	Total	O	0	7
			104	104		
30	G	45	Total	O	0	1
			46	46		
30	H	58	Total	O	0	0
			58	58		
30	I	37	Total	O	0	0
			37	37		
30	J	21	Total	O	0	0
			21	21		

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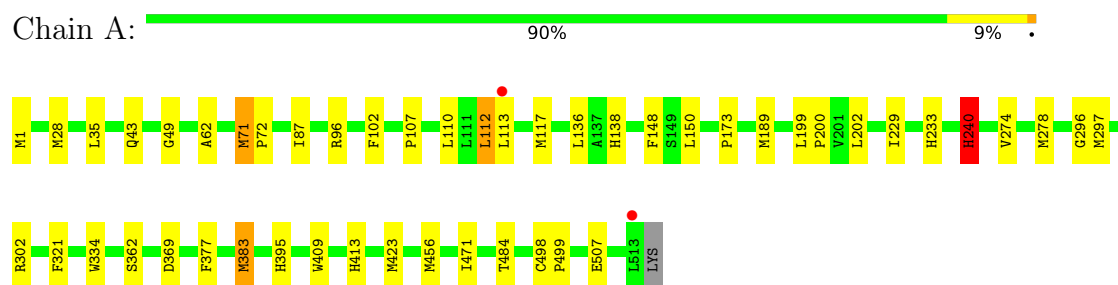
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	21	Total 21	O 21	0	0
30	L	25	Total 27	O 27	0	2
30	M	20	Total 20	O 20	0	0
30	N	226	Total 236	O 236	0	10
30	O	146	Total 147	O 147	0	1
30	P	101	Total 102	O 102	0	1
30	Q	78	Total 82	O 82	0	4
30	R	89	Total 97	O 97	0	8
30	S	86	Total 92	O 92	0	6
30	T	37	Total 38	O 38	0	1
30	U	49	Total 49	O 49	0	0
30	V	23	Total 23	O 23	0	0
30	W	15	Total 15	O 15	0	0
30	X	17	Total 17	O 17	0	0
30	Y	24	Total 26	O 26	0	2
30	Z	17	Total 17	O 17	0	0

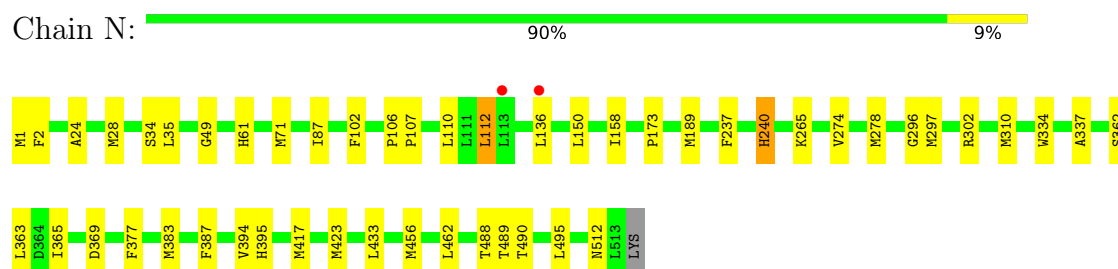
3 Residue-property plots [i](#)

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

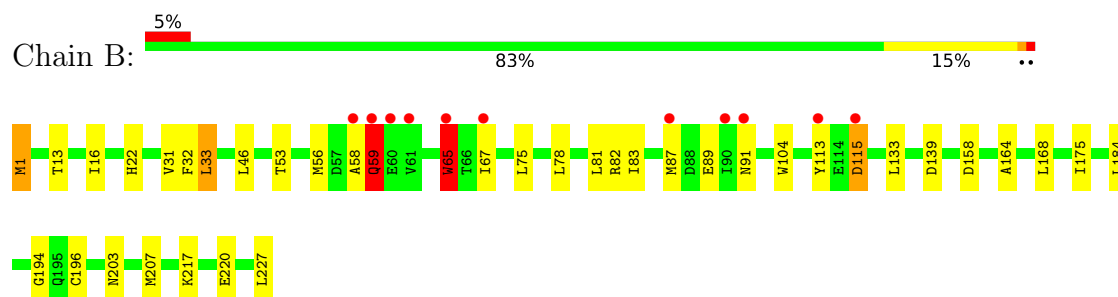
- Molecule 1: Cytochrome c oxidase subunit 1



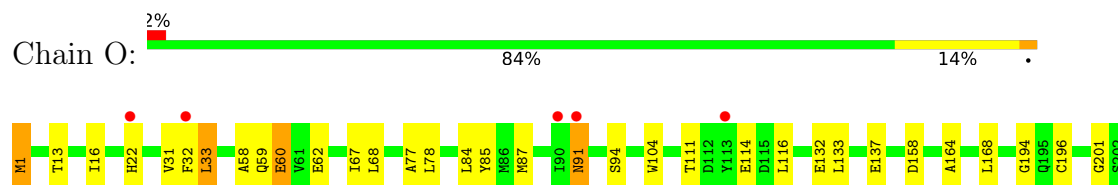
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2





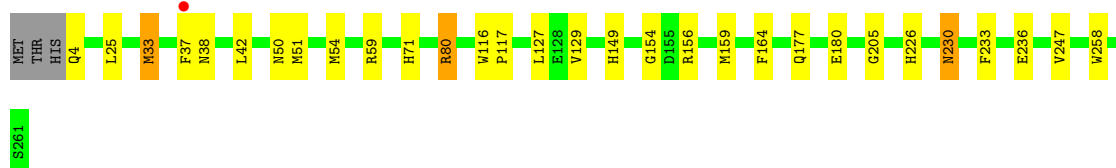
- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 87% 12% .



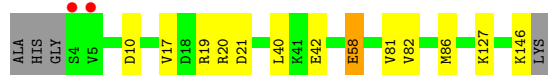
- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 87% 10% ..



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

Chain D: 88% 8% ..



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

Chain Q: 88% 7% ..



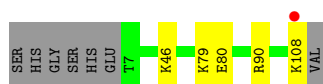
- Molecule 5: Cytochrome c oxidase subunit 5A

Chain E: 89% 5% 6%

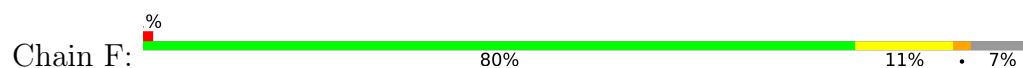


- Molecule 5: Cytochrome c oxidase subunit 5A

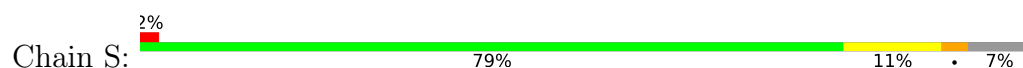
Chain R: 89% 5% 6%



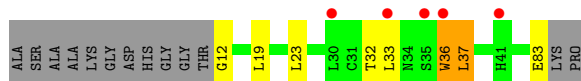
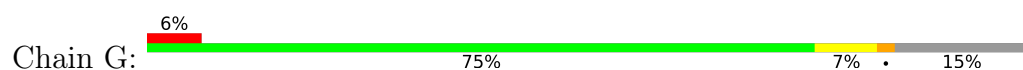
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



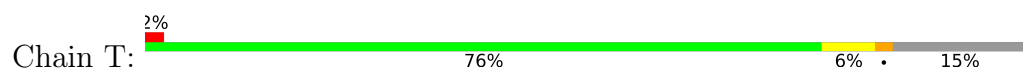
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



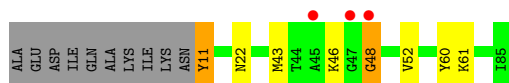
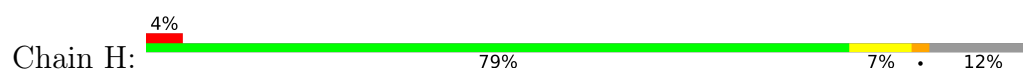
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



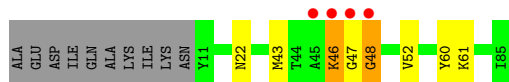
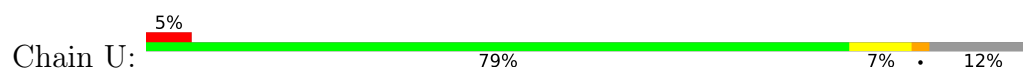
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



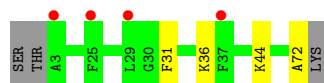
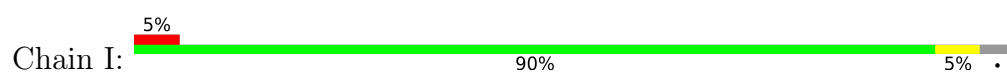
- Molecule 8: Cytochrome c oxidase subunit 6B1



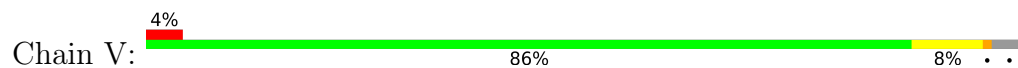
- Molecule 8: Cytochrome c oxidase subunit 6B1



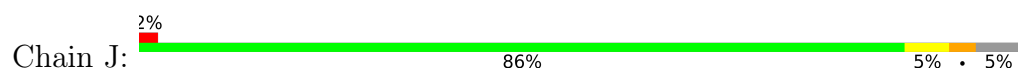
- Molecule 9: Cytochrome c oxidase subunit 6C



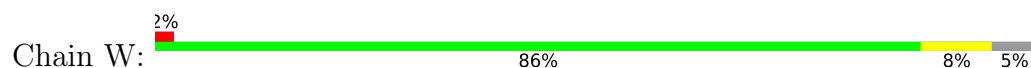
- Molecule 9: Cytochrome c oxidase subunit 6C



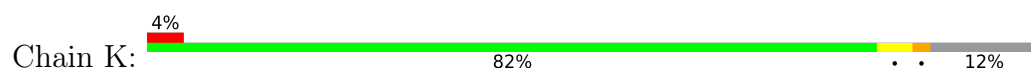
- Molecule 10: Cytochrome c oxidase subunit 7A1



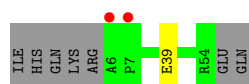
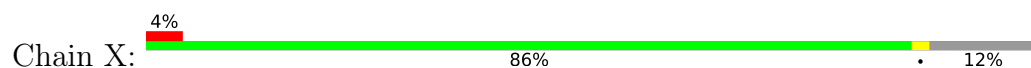
- Molecule 10: Cytochrome c oxidase subunit 7A1



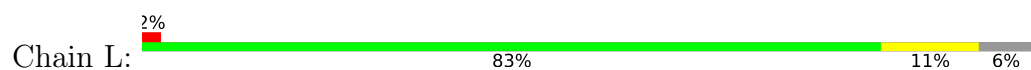
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial




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

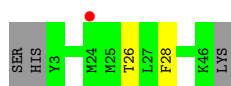


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial




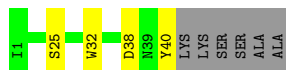
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:  2% 89% 6%




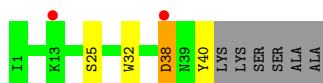
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:  78% 9% 13%



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

Chain Z:  4% 78% 7% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.90Å 204.00Å 178.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 40.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.80) 100.0 (40.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.120 , 0.156 0.137 , 0.166	Depositor DCC
R_{free} test set	30181 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33061	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.06	7/4259 (0.2%)	1.17	8/5816 (0.1%)
1	N	1.05	4/4259 (0.1%)	1.17	6/5816 (0.1%)
2	B	1.12	2/1908 (0.1%)	1.27	15/2598 (0.6%)
2	O	1.09	0/1908	1.25	4/2598 (0.2%)
3	C	1.03	1/2258 (0.0%)	1.14	3/3084 (0.1%)
3	P	1.03	1/2258 (0.0%)	1.15	3/3084 (0.1%)
4	D	1.10	2/1226 (0.2%)	1.17	5/1657 (0.3%)
4	Q	1.07	0/1182	1.29	0/1598
5	E	1.06	2/843 (0.2%)	1.17	2/1145 (0.2%)
5	R	1.01	0/843	1.26	1/1145 (0.1%)
6	F	1.08	1/724 (0.1%)	1.20	0/983
6	S	1.15	3/724 (0.4%)	1.20	1/983 (0.1%)
7	G	1.08	1/633 (0.2%)	1.19	1/864 (0.1%)
7	T	1.11	0/633	1.22	0/864
8	H	1.06	1/648 (0.2%)	1.32	0/877
8	U	1.07	0/648	1.25	0/877
9	I	1.13	0/588	1.39	1/781 (0.1%)
9	V	1.08	0/588	1.41	1/781 (0.1%)
10	J	1.08	0/451	1.30	2/610 (0.3%)
10	W	1.05	0/451	1.31	2/610 (0.3%)
11	K	1.19	1/398 (0.3%)	1.36	1/546 (0.2%)
11	X	1.12	0/398	1.27	0/546
12	L	1.11	1/372 (0.3%)	1.23	3/500 (0.6%)
12	Y	1.12	0/372	1.20	0/500
13	M	1.07	0/321	1.11	0/440
13	Z	1.05	0/321	1.43	0/440
All	All	1.07	27/29214 (0.1%)	1.22	59/39743 (0.1%)

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

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	N	0	1
All	All	0	4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	MET	C-O	8.40	1.34	1.24
11	K	10	HIS	CE1-NE2	8.05	1.40	1.32
3	P	71	HIS	CE1-NE2	7.20	1.39	1.32
1	A	233	HIS	CE1-NE2	7.13	1.39	1.32
1	A	49	GLY	C-O	7.13	1.33	1.23
4	D	58	GLU	CD-OE1	7.02	1.38	1.25
1	A	395	HIS	CE1-NE2	6.55	1.39	1.32
1	N	49	GLY	C-O	6.26	1.30	1.23
1	A	189	MET	CB-CG	6.14	1.70	1.52
3	C	36	HIS	CE1-NE2	6.12	1.38	1.32
8	H	11	TYR	N-CA	6.12	1.57	1.46
1	N	61	HIS	CE1-NE2	6.06	1.38	1.32
2	B	113	TYR	C-O	-5.93	1.16	1.24
1	N	189	MET	CG-SD	-5.88	1.66	1.80
6	S	64	GLU	C-O	5.88	1.30	1.23
1	N	395	HIS	CE1-NE2	5.79	1.38	1.32
2	B	65	TRP	NE1-CE2	-5.61	1.31	1.37
4	D	21	ASP	CG-OD2	5.58	1.35	1.25
6	F	64	GLU	C-O	5.57	1.30	1.23
6	S	93	PRO	C-O	5.39	1.34	1.23
1	A	413	HIS	CG-ND1	-5.24	1.32	1.38
6	S	3	GLY	C-O	5.20	1.33	1.23
5	E	108	LYS	C-O	5.14	1.33	1.23
7	G	12	GLY	N-CA	-5.13	1.37	1.45
5	E	49	ASP	CG-OD1	-5.12	1.15	1.25
12	L	5	GLU	CD-OE2	-5.05	1.15	1.25
1	A	138	HIS	CE1-NE2	5.01	1.37	1.32

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	65	TRP	CB-CG-CD1	-12.57	108.04	126.90
1	N	240	HIS	CA-CB-CG	-11.25	102.55	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	HIS	CA-CB-CG	-11.06	102.74	113.80
2	B	65	TRP	CA-CB-CG	10.19	132.95	113.60
9	V	72	ALA	CA-C-O	-9.72	104.28	120.80
11	K	54	ARG	CA-C-O	-9.69	104.33	120.80
4	D	58	GLU	CB-CG-CD	8.96	127.83	112.60
9	I	72	ALA	CA-C-O	-8.17	106.92	120.80
3	C	80	ARG	CG-CD-NE	-7.48	95.53	112.00
2	B	89	GLU	CA-C-N	7.20	131.28	120.77
2	B	89	GLU	C-N-CA	7.20	131.28	120.77
10	J	27	THR	CA-CB-OG1	-6.85	99.33	109.60
1	A	43	GLN	CB-CA-C	6.73	120.01	108.91
1	A	102	PHE	CA-CB-CG	-6.72	107.08	113.80
1	N	377	PHE	CA-CB-CG	6.52	120.32	113.80
2	B	59	GLN	CB-CG-CD	6.42	123.52	112.60
2	B	82	ARG	CG-CD-NE	-6.37	97.98	112.00
6	S	93	PRO	CB-CA-C	6.31	122.08	110.10
1	N	102	PHE	CA-CB-CG	-6.22	107.58	113.80
3	P	80	ARG	CG-CD-NE	-6.09	98.60	112.00
2	B	65	TRP	CB-CG-CD2	6.07	135.30	126.80
2	B	65	TRP	N-CA-CB	6.06	120.60	110.41
4	D	20	ARG	NE-CZ-NH2	5.98	124.58	119.20
3	P	233	PHE	CA-CB-CG	-5.97	107.83	113.80
1	A	96	ARG	CB-CA-C	5.91	121.51	110.70
2	B	184	LEU	N-CA-CB	-5.90	100.59	110.80
10	J	7	GLU	CB-CA-C	5.83	120.76	110.85
5	E	108	LYS	CA-C-O	-5.72	111.08	120.80
2	B	158	ASP	CA-CB-CG	5.70	118.30	112.60
4	D	20	ARG	NE-CZ-NH1	-5.70	115.80	121.50
3	C	233	PHE	CA-CB-CG	-5.69	108.11	113.80
3	C	76	GLN	CG-CD-NE2	-5.61	107.98	116.40
4	D	21	ASP	CA-CB-CG	5.59	118.19	112.60
12	L	25	MET	CA-C-N	5.56	128.05	120.54
12	L	25	MET	C-N-CA	5.56	128.05	120.54
1	A	377	PHE	CA-CB-CG	5.55	119.35	113.80
2	B	139	ASP	CA-CB-CG	5.55	118.15	112.60
10	W	25	GLY	CA-C-N	5.55	127.99	120.38
10	W	25	GLY	C-N-CA	5.55	127.99	120.38
2	B	115	ASP	CB-CA-C	5.51	120.63	112.03
1	A	71	MET	CG-SD-CE	-5.49	88.82	100.90
1	A	507	GLU	CB-CA-C	5.45	116.06	109.85
5	R	80	GLU	CB-CG-CD	5.42	121.81	112.60
2	B	65	TRP	CB-CA-C	-5.39	99.22	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	85	TYR	CB-CA-C	5.34	119.92	110.85
1	N	512	ASN	CB-CA-C	5.31	119.63	110.45
3	P	230	ASN	CA-CB-CG	-5.25	107.35	112.60
2	B	65	TRP	CG-CD2-CE3	5.24	139.14	133.90
1	N	71	MET	CG-SD-CE	-5.23	89.39	100.90
5	E	80	GLU	CB-CG-CD	5.17	121.38	112.60
12	L	16	GLU	CB-CG-CD	5.11	121.29	112.60
7	G	83	GLU	CA-C-O	-5.05	112.21	120.80
1	N	106	PRO	CB-CA-C	5.05	117.08	110.92
2	O	158	ASP	CB-CA-C	5.04	120.45	110.42
2	B	59	GLN	N-CA-CB	5.03	117.61	110.16
2	O	201	GLY	CA-C-N	5.03	127.27	120.38
2	O	201	GLY	C-N-CA	5.03	127.27	120.38
4	D	146	LYS	CA-C-O	-5.00	112.29	120.80
1	A	383	MET	O-C-N	-5.00	116.47	122.27

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
1	A	383	MET	Mainchain
1	N	296	GLY	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	45	0
1	N	4130	0	4102	49	0
2	B	1870	0	1870	32	0
2	O	1870	0	1870	33	0
3	C	2171	0	2080	29	0
3	P	2172	0	2081	27	0
4	D	1192	0	1178	8	0
4	Q	1148	0	1131	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	825	0	823	1	0
5	R	825	0	823	3	0
6	F	709	0	691	11	0
6	S	709	0	691	9	0
7	G	606	0	577	4	0
7	T	606	0	577	7	0
8	H	628	0	580	13	0
8	U	628	0	580	14	0
9	I	575	0	584	4	0
9	V	575	0	584	7	0
10	J	441	0	439	5	0
10	W	441	0	439	4	0
11	K	384	0	366	1	0
11	X	384	0	366	1	0
12	L	360	0	360	4	0
12	Y	360	0	360	5	0
13	M	311	0	321	3	0
13	Z	311	0	321	5	0
14	A	129	0	88	4	0
14	N	129	0	88	7	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	1	0
19	A	64	0	72	0	0
19	C	87	0	124	18	0
19	L	94	0	141	4	0
19	P	87	0	124	14	0
19	V	64	0	72	1	0
19	Y	94	0	141	4	0
20	A	28	0	54	8	0
20	B	17	0	33	1	0
20	C	114	0	202	6	0
20	G	14	0	27	6	0
20	N	31	0	60	5	0
20	O	11	0	21	2	0
20	P	114	0	202	8	0
20	T	11	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A	84	0	106	3	0
21	B	66	0	104	2	0
21	C	172	0	228	6	0
21	D	33	0	42	3	0
21	G	22	0	31	0	0
21	J	11	0	21	0	0
21	L	22	0	31	1	0
21	M	41	0	56	0	0
21	N	51	0	76	1	0
21	O	66	0	104	0	0
21	P	172	0	228	6	0
21	Q	33	0	42	1	0
21	T	22	0	31	1	0
21	U	33	0	27	1	0
21	W	11	0	21	0	0
21	Y	22	0	31	1	0
21	Z	41	0	56	0	0
22	A	16	0	24	1	0
22	B	4	0	6	0	0
22	C	12	0	17	0	0
22	E	12	0	18	0	0
22	F	8	0	12	0	0
22	G	4	0	6	0	0
22	N	20	0	30	0	0
22	O	4	0	6	0	0
22	P	12	0	18	0	0
22	R	12	0	18	0	0
22	S	8	0	12	0	0
22	T	4	0	6	0	0
23	A	5	0	0	2	0
23	B	1	0	0	3	0
23	C	1	0	0	0	0
23	N	5	0	0	1	0
23	O	1	0	0	3	0
23	P	1	0	0	0	0
24	A	51	0	76	0	0
24	C	51	0	76	1	0
24	N	51	0	76	2	0
24	P	51	0	76	0	0
25	B	2	0	0	0	0
25	O	2	0	0	0	0
26	B	29	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	C	58	0	78	1	0
26	G	29	0	39	1	0
26	P	58	0	78	3	0
27	C	1	0	0	1	0
27	P	1	0	0	0	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	G	53	0	77	0	0
29	T	53	0	77	4	0
30	A	257	0	0	9	0
30	B	179	0	0	5	0
30	C	102	0	0	3	0
30	D	148	0	0	2	0
30	E	117	0	0	0	0
30	F	104	0	0	1	0
30	G	46	0	0	0	0
30	H	58	0	0	1	0
30	I	37	0	0	1	0
30	J	21	0	0	0	0
30	K	21	0	0	0	0
30	L	27	0	0	0	0
30	M	20	0	0	0	0
30	N	236	0	0	7	0
30	O	147	0	0	1	0
30	P	102	0	0	3	0
30	Q	82	0	0	2	0
30	R	97	0	0	2	0
30	S	92	0	0	0	0
30	T	38	0	0	1	0
30	U	49	0	0	2	0
30	V	23	0	0	2	0
30	W	15	0	0	0	0
30	X	17	0	0	0	0
30	Y	26	0	0	0	0
30	Z	17	0	0	0	0
All	All	33061	0	31466	336	0

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

All (336) 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)
18:N:608:PER:O2	18:N:608:PER:O1	1.58	1.18
1:A:112:LEU:HG	30:A:2035:HOH:O	1.38	1.18
18:A:606:PER:O2	18:A:606:PER:O1	1.60	1.16
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.19	1.13
8:H:52:VAL:HG12	8:U:46:LYS:CG	1.80	1.11
1:N:112:LEU:HG	30:N:909:HOH:O	1.50	1.10
8:H:43:MET:HE1	8:U:52:VAL:HG11	1.37	1.06
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:HE3	1.38	1.05
3:P:4:GLN:N	30:P:403:HOH:O	1.91	1.03
1:A:35:LEU:HD21	30:A:2008:HOH:O	1.63	0.98
1:A:35:LEU:CD2	30:A:2008:HOH:O	2.15	0.95
3:C:245:VAL:C	3:C:246[B]:ASP:CA	2.41	0.92
8:H:52:VAL:CG1	8:U:46:LYS:HG2	1.99	0.92
2:O:22[B]:HIS:CE1	9:V:44:LYS:HE2	2.04	0.92
3:P:149:HIS:NE2	20:P:313:LFA:H11	1.88	0.89
20:G:105:LFA:H11	20:N:609:LFA:H12	1.55	0.87
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.14	0.87
1:A:136[B]:LEU:HD11	30:A:2040:HOH:O	1.74	0.85
21:P:324:DMU:H38	21:P:324:DMU:H28	0.89	0.85
19:P:305:CDL:H121	19:P:305:CDL:HA62	1.60	0.83
1:A:112:LEU:C	1:A:112:LEU:HD23	2.03	0.83
6:F:37:LYS:HG2	30:F:289:HOH:O	1.79	0.83
1:A:113[B]:LEU:HD11	1:A:117[B]:MET:SD	2.21	0.81
1:A:112:LEU:HD23	1:A:112:LEU:O	1.80	0.81
27:C:302:UNX:UNK	30:C:490:HOH:O	1.60	0.80
21:A:611:DMU:O6	30:A:1804:HOH:O	2.01	0.79
1:A:297[B]:MET:SD	1:A:302:ARG:HG2	2.22	0.79
8:H:43:MET:CE	8:U:52:VAL:HG11	2.15	0.77
1:N:274:VAL:HG12	1:N:278[A]:MET:HE2	1.67	0.76
1:N:112:LEU:HD23	1:N:112:LEU:O	1.86	0.75
1:N:278[B]:MET:HE1	20:N:609:LFA:H52	1.68	0.74
1:N:136[B]:LEU:HD11	30:N:924:HOH:O	1.87	0.74
4:D:42:GLU:OE2	30:D:301:HOH:O	2.07	0.73
3:P:51[B]:MET:HE3	19:P:305:CDL:H873	1.69	0.73
8:H:52:VAL:HG21	8:U:43:MET:HE1	1.70	0.73
2:B:16[B]:ILE:HG23	30:B:522:HOH:O	1.88	0.72
1:A:274:VAL:HG12	1:A:278[A]:MET:HE2	1.70	0.72
1:N:297[B]:MET:SD	1:N:302:ARG:CG	2.77	0.72
2:O:84:LEU:HA	2:O:87[A]:MET:HE2	1.72	0.71
9:V:8:GLN:OE1	30:V:201:HOH:O	2.09	0.71
4:Q:112:GLU:OE2	30:Q:301:HOH:O	2.10	0.70
1:N:278[B]:MET:SD	20:N:609:LFA:H51	2.32	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:THR:HG22	30:A:2030:HOH:O	1.92	0.69
21:P:324:DMU:O3	21:P:324:DMU:O55	1.98	0.69
2:B:31:VAL:CG2	23:B:301:XE:XE	3.19	0.69
21:C:323:DMU:H20	10:J:50:LEU:HB2	1.75	0.69
7:G:19:LEU:HD23	20:G:105:LFA:H61	1.74	0.69
3:C:33[A]:MET:HE3	3:C:39:SER:OG	1.94	0.68
30:A:1919:HOH:O	3:C:77:LYS:HE3	1.95	0.67
3:C:33[B]:MET:HG3	3:C:37:PHE:HB2	1.77	0.67
1:A:297[B]:MET:SD	1:A:302:ARG:CG	2.83	0.66
19:Y:101:CDL:OA5	19:Y:101:CDL:OA8	2.14	0.66
19:C:304:CDL:OA3	19:C:304:CDL:H1	1.91	0.66
8:H:52:VAL:HG12	8:U:46:LYS:HG3	1.73	0.66
2:B:31:VAL:HG22	23:B:301:XE:XE	2.75	0.65
3:C:33[A]:MET:HE2	3:C:42:LEU:H	1.60	0.65
29:T:101:PEK:H32	29:T:101:PEK:H71	1.79	0.65
2:O:22[B]:HIS:CE1	9:V:44:LYS:CE	2.78	0.65
7:T:33:LEU:HD22	7:T:37:LEU:HD22	1.78	0.64
4:D:10:ASP:OD2	30:D:302:HOH:O	2.14	0.64
3:C:33[A]:MET:CE	3:C:42:LEU:H	2.11	0.64
2:B:13:THR:HB	2:B:168:LEU:HD23	1.81	0.63
2:B:16[A]:ILE:HD12	2:B:87[A]:MET:HG2	1.81	0.62
1:N:112:LEU:HD23	1:N:112:LEU:C	2.24	0.62
3:C:67:PHE:CE2	19:C:304:CDL:O1	2.52	0.62
2:B:31:VAL:HG23	23:B:301:XE:XE	2.79	0.61
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.31	0.61
1:A:112:LEU:C	1:A:112:LEU:CD2	2.73	0.61
3:C:51[B]:MET:HE2	19:C:304:CDL:H861	1.82	0.61
2:O:59:GLN:NE2	20:O:301:LFA:H31	2.16	0.60
3:C:164:PHE:CD1	26:C:305:CHD:H192	2.36	0.60
19:C:304:CDL:H752	10:J:27:THR:HG21	1.84	0.60
2:O:91:ASN:C	2:O:91:ASN:HD22	2.08	0.60
30:N:874:HOH:O	4:Q:20:ARG:HG2	2.01	0.60
1:A:28:MET:CE	14:A:601[A]:HEA:H271	2.32	0.60
3:C:38:ASN:ND2	21:C:318:DMU:O4	2.34	0.59
19:C:304:CDL:HB61	19:C:304:CDL:CB2	2.32	0.59
3:P:33[B]:MET:HE3	3:P:42:LEU:HD12	1.83	0.59
7:T:12:GLY:HA3	30:T:231:HOH:O	2.01	0.59
19:C:304:CDL:HA62	19:C:304:CDL:H121	1.84	0.59
20:P:310:LFA:C3	30:U:206:HOH:O	2.50	0.59
19:C:304:CDL:HB21	19:C:304:CDL:HB32	1.83	0.59
19:L:101:CDL:OB9	19:L:101:CDL:H122	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:LEU:HD12	21:B:309:DMU:H11	1.84	0.59
1:A:278[B]:MET:HE1	20:A:608:LFA:H52	1.86	0.58
3:C:180[B]:GLU:HG2	30:C:429:HOH:O	2.03	0.58
3:P:156:ARG:HE	26:P:306:CHD:C24	2.17	0.58
8:H:46:LYS:HE2	8:H:46:LYS:O	2.04	0.58
21:C:323:DMU:H10	10:J:53:ALA:HB2	1.86	0.57
1:N:28:MET:CE	14:N:603[A]:HEA:C27	2.83	0.57
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.86	0.57
19:C:304:CDL:CA3	19:C:304:CDL:OB9	2.53	0.57
1:N:365:ILE:HD11	30:N:707:HOH:O	2.04	0.57
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.87	0.57
1:A:110:LEU:HD21	21:C:323:DMU:H24	1.87	0.56
1:A:278[B]:MET:SD	20:A:608:LFA:H51	2.45	0.56
20:N:601:LFA:H42	2:O:67:ILE:HD11	1.87	0.56
3:P:205:GLY:HA3	29:T:101:PEK:H182	1.87	0.56
3:P:33[B]:MET:CE	3:P:42:LEU:HD12	2.36	0.56
2:O:31:VAL:CG2	23:O:303:XE:XE	3.32	0.56
1:A:1:FME:HE2	1:A:1:FME:HA	1.87	0.56
5:R:46:LYS:NZ	30:R:303:HOH:O	2.38	0.55
2:O:32[B]:PHE:CD2	9:V:31:PHE:CZ	2.94	0.55
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:CE	2.23	0.55
2:O:16[A]:ILE:HG21	2:O:87[A]:MET:HG2	1.89	0.55
3:C:59:ARG:HB2	19:C:304:CDL:OA9	2.06	0.55
3:P:59:ARG:HG3	19:P:305:CDL:HA4	1.88	0.55
1:N:28:MET:HE2	14:N:603[A]:HEA:H273	1.87	0.55
2:B:16[A]:ILE:CG2	2:B:87[A]:MET:HE3	2.26	0.55
20:A:609:LFA:C6	7:T:19:LEU:HD23	2.37	0.54
6:S:54:ASN:HD22	6:S:54:ASN:C	2.16	0.54
2:O:33:LEU:HD13	9:V:31:PHE:CD2	2.43	0.54
3:P:258:TRP:CE2	20:P:308:LFA:H32	2.42	0.54
1:A:278[A]:MET:SD	20:A:609:LFA:H51	2.48	0.54
3:C:33[B]:MET:CA	3:C:33[B]:MET:HE2	2.07	0.54
1:N:362[A]:SER:HA	2:O:87[A]:MET:HE1	1.89	0.54
2:O:31:VAL:HG23	23:O:303:XE:XE	2.86	0.54
19:C:304:CDL:CA5	19:C:304:CDL:OB4	2.56	0.54
19:Y:101:CDL:C41	19:Y:101:CDL:H801	2.38	0.53
1:N:112:LEU:C	1:N:112:LEU:CD2	2.81	0.53
3:C:54[A]:MET:HE1	24:C:303:PGV:H141	1.90	0.53
19:P:305:CDL:H121	19:P:305:CDL:CA6	2.35	0.53
19:C:304:CDL:HB61	19:C:304:CDL:HB22	1.90	0.53
8:U:46:LYS:HE2	8:U:47:GLY:C	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:LEU:HD21	30:B:501:HOH:O	2.09	0.53
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:CG	2.39	0.53
8:H:43:MET:O	8:H:48:GLY:N	2.42	0.53
29:T:101:PEK:H32	29:T:101:PEK:C7	2.39	0.52
3:P:38:ASN:ND2	21:P:319:DMU:O4	2.42	0.52
1:A:278[A]:MET:CE	20:A:609:LFA:H51	2.40	0.52
19:C:304:CDL:HB61	19:C:304:CDL:HB21	1.91	0.52
1:N:28:MET:HE2	14:N:603[A]:HEA:C27	2.40	0.52
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.45	0.51
1:N:28:MET:CE	14:N:603[A]:HEA:H271	2.40	0.51
3:C:258:TRP:CE2	20:C:307:LFA:H32	2.45	0.51
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.91	0.51
30:C:500:HOH:O	6:F:33:ILE:HD13	2.11	0.51
3:P:59:ARG:HB2	19:P:305:CDL:OA9	2.11	0.51
2:B:56:MET:HB3	21:B:305:DMU:H7	1.93	0.51
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.11	0.51
20:A:608:LFA:H12	20:A:609:LFA:H11	1.93	0.51
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.93	0.51
3:P:247:VAL:HG11	20:P:314:LFA:H71	1.92	0.51
20:A:609:LFA:H62	7:T:19:LEU:HD23	1.92	0.51
3:C:149:HIS:NE2	20:C:312:LFA:H21	2.26	0.50
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.93	0.50
6:F:92:VAL:HG23	6:F:92:VAL:O	2.10	0.50
1:N:362[B]:SER:O	2:O:87[B]:MET:HE1	2.11	0.50
19:P:305:CDL:O1	10:W:8:LYS:HD2	2.11	0.50
3:P:164:PHE:CD1	26:P:306:CHD:H192	2.46	0.50
6:F:64:GLU:O	6:F:65:ASP:HB2	2.12	0.50
8:H:11:TYR:N	30:H:101:HOH:O	2.43	0.50
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:HG2	1.93	0.50
3:P:116:TRP:HA	3:P:117:PRO:C	2.37	0.50
6:F:85:CYS:SG	6:F:87[B]:THR:OG1	2.65	0.50
3:P:51[B]:MET:CE	19:P:305:CDL:H873	2.42	0.50
8:U:46:LYS:HE2	8:U:48:GLY:N	2.27	0.49
2:B:1:FME:HE1	2:B:133:LEU:HD22	1.93	0.49
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.94	0.49
2:B:220:GLU:OE1	30:B:402:HOH:O	2.20	0.49
1:A:28:MET:HE2	14:A:601[A]:HEA:C27	2.42	0.49
1:A:240:HIS:C	1:A:240:HIS:CD2	2.90	0.49
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	3.00	0.49
12:L:26:THR:HG21	21:L:102:DMU:H26	1.94	0.49
2:O:31:VAL:HG22	23:O:303:XE:XE	2.89	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:28:PHE:CD1	19:Y:101:CDL:H532	2.47	0.49
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.48	0.49
3:C:39:SER:HB2	21:C:318:DMU:O55	2.12	0.49
30:P:420:HOH:O	6:S:3:GLY:HA3	2.13	0.49
1:A:297[B]:MET:CG	1:A:302:ARG:HG3	2.43	0.49
8:H:46:LYS:O	8:H:46:LYS:CE	2.61	0.49
19:L:101:CDL:C73	19:L:101:CDL:H362	2.43	0.48
21:D:201:DMU:H36	21:D:201:DMU:O55	2.13	0.48
1:N:297[B]:MET:CG	1:N:302:ARG:HG3	2.43	0.48
21:Q:201:DMU:O55	21:Q:201:DMU:H36	2.12	0.48
1:N:110:LEU:CD2	21:P:324:DMU:H24	2.43	0.48
1:N:110:LEU:HD21	21:P:324:DMU:H24	1.94	0.48
30:N:922[B]:HOH:O	4:Q:19:ARG:HD2	2.12	0.48
1:N:24:ALA:HB2	14:N:603[B]:HEA:H253	1.95	0.48
2:B:33:LEU:HD13	9:I:31:PHE:CD2	2.49	0.48
12:Y:26:THR:HG21	21:Y:102:DMU:H20	1.95	0.48
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.47
24:N:622:PGV:H183	29:T:101:PEK:H331	1.95	0.47
1:A:28:MET:CE	14:A:601[A]:HEA:C27	2.92	0.47
19:C:304:CDL:HB21	19:C:304:CDL:CB3	2.44	0.47
1:N:240:HIS:C	1:N:240:HIS:CD2	2.92	0.47
1:A:321:PHE:CD2	2:B:65:TRP:HB3	2.49	0.47
3:P:80:ARG:NH2	3:P:236:GLU:OE1	2.44	0.47
1:A:136[B]:LEU:CD1	30:A:2040:HOH:O	2.48	0.47
14:N:604:HEA:HBC1	14:N:604:HEA:HMC3	1.96	0.47
20:P:310:LFA:C5	30:U:206:HOH:O	2.62	0.47
2:B:53:THR:O	30:B:403:HOH:O	2.20	0.47
8:U:46:LYS:CD	8:U:46:LYS:O	2.62	0.47
7:G:23:LEU:HB2	20:G:105:LFA:H91	1.97	0.47
2:O:59:GLN:HE22	20:O:301:LFA:H13	1.79	0.47
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.44	0.47
1:N:150:LEU:HD23	23:N:617:XE:XE	2.93	0.47
1:N:362[A]:SER:OG	2:O:87[A]:MET:CE	2.63	0.47
2:O:58:ALA:O	2:O:62:GLU:HG3	2.15	0.47
3:P:50:ASN:ND2	3:P:54[A]:MET:HE2	2.29	0.47
30:Q:318:HOH:O	5:R:108:LYS:HD3	2.15	0.47
1:N:297[B]:MET:SD	1:N:302:ARG:HG3	2.53	0.47
1:N:334:TRP:CE3	21:N:610:DMU:H19	2.49	0.47
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.97	0.46
1:N:310:MET:HE1	2:O:77:ALA:HB2	1.97	0.46
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:G:105:LFA:H31	1:N:278[A]:MET:SD	2.56	0.46
9:V:8:GLN:HG3	30:V:223:HOH:O	2.14	0.46
6:F:87[A]:THR:HG22	6:F:89:TYR:CE1	2.51	0.46
3:C:116:TRP:HA	3:C:117:PRO:C	2.40	0.46
21:A:622:DMU:O3	8:H:22:ASN:ND2	2.48	0.46
19:C:304:CDL:OB4	19:C:304:CDL:OA6	2.33	0.46
19:P:305:CDL:OB4	19:P:305:CDL:CA5	2.64	0.46
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.45	0.46
4:D:17[B]:VAL:HG22	4:D:19:ARG:HG3	1.98	0.46
1:A:362[B]:SER:O	2:B:87[B]:MET:HE1	2.16	0.46
19:L:101:CDL:H362	19:L:101:CDL:H731	1.96	0.46
1:A:334:TRP:HB2	21:D:201:DMU:C57	2.46	0.45
1:N:136[B]:LEU:CD1	30:N:924:HOH:O	2.55	0.45
3:P:226:HIS:HE1	19:P:305:CDL:H111	1.81	0.45
1:A:297[B]:MET:HG2	1:A:302:ARG:HG3	1.97	0.45
1:N:488:THR:HB	1:N:495:LEU:HD13	1.98	0.45
1:A:297[B]:MET:SD	1:A:302:ARG:HG3	2.57	0.45
26:G:102:CHD:H12	26:G:102:CHD:H212	1.97	0.45
6:S:21[B]:MET:HE2	6:S:21[B]:MET:HB2	1.80	0.45
1:N:417[B]:MET:CE	30:N:876:HOH:O	2.64	0.45
6:S:64:GLU:O	6:S:65:ASP:HB2	2.15	0.45
1:N:2:PHE:CE2	19:Y:101:CDL:H712	2.52	0.45
19:P:305:CDL:OA3	19:P:305:CDL:H1	2.14	0.45
8:U:47:GLY:C	8:U:48:GLY:O	2.60	0.45
1:A:113[B]:LEU:CD1	1:A:117[B]:MET:SD	2.99	0.45
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.52	0.45
1:N:87:ILE:O	1:N:173:PRO:HD3	2.16	0.44
14:N:604:HEA:HBC1	14:N:604:HEA:CMC	2.47	0.44
2:O:16[B]:ILE:HG23	30:O:503:HOH:O	2.17	0.44
2:O:111:THR:HA	2:O:114:GLU:O	2.17	0.44
21:P:324:DMU:O3	21:P:324:DMU:C2	2.65	0.44
30:P:501:HOH:O	6:S:33:ILE:HD13	2.16	0.44
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.98	0.44
8:H:52:VAL:HA	8:U:46:LYS:HG2	1.98	0.44
3:C:258:TRP:NE1	20:C:307:LFA:H12	2.32	0.44
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.99	0.44
3:P:247:VAL:CG1	20:P:314:LFA:H71	2.47	0.44
1:A:334:TRP:CE3	21:A:610:DMU:H19	2.53	0.44
2:B:22[B]:HIS:CE1	9:I:44:LYS:CE	3.00	0.44
1:N:158:ILE:HD13	24:N:622:PGV:H331	2.00	0.44
7:G:32:THR:O	7:G:36:TRP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:22[B]:HIS:HE1	9:V:44:LYS:HE2	1.74	0.44
3:P:33[B]:MET:HG3	3:P:37:PHE:HB2	1.99	0.44
3:P:129:VAL:HG11	3:P:180[B]:GLU:HG2	2.00	0.44
2:O:13:THR:HB	2:O:168:LEU:HD23	2.00	0.44
20:A:609:LFA:H61	7:T:19:LEU:HD23	2.00	0.44
4:D:81:VAL:HG11	21:D:201:DMU:H11	2.00	0.44
20:G:105:LFA:H51	1:N:278[A]:MET:HE1	1.99	0.44
7:T:37:LEU:HD12	7:T:37:LEU:HA	1.90	0.43
20:G:105:LFA:H121	20:G:105:LFA:H92	1.86	0.43
1:N:362[A]:SER:OG	2:O:87[A]:MET:HE2	2.19	0.43
8:U:22:ASN:ND2	21:U:101:DMU:O3	2.50	0.43
2:B:83:ILE:O	2:B:87[A]:MET:HG3	2.19	0.43
20:P:314:LFA:C1	20:P:315:LFA:H71	2.48	0.43
19:C:304:CDL:HB22	10:J:8:LYS:HE3	2.01	0.43
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.01	0.43
3:C:33[A]:MET:HG2	3:C:39:SER:O	2.18	0.43
5:E:82:TYR:HB3	5:E:83:PRO:HD3	2.01	0.43
12:Y:26:THR:HG23	13:Z:25:SER:HB2	1.99	0.43
1:A:28:MET:HE2	14:A:601[A]:HEA:H271	2.00	0.43
2:B:67:ILE:HD11	20:B:308:LFA:H42	2.00	0.43
4:D:82:VAL:HG12	4:D:86:MET:HE2	2.01	0.43
4:D:127:LYS:HD2	30:I:135:HOH:O	2.18	0.43
1:A:150:LEU:HD23	23:A:616:XE:XE	2.97	0.43
2:O:60:GLU:CD	2:O:60:GLU:H	2.25	0.43
2:O:116:LEU:HD13	2:O:226:MET:CG	2.49	0.42
3:C:177:GLN:OE1	3:C:177:GLN:HA	2.19	0.42
19:C:304:CDL:OB9	19:C:304:CDL:OA5	2.37	0.42
1:N:433:LEU:HD11	19:V:101:CDL:OA7	2.19	0.42
19:P:305:CDL:OB2	10:W:8:LYS:HE3	2.19	0.42
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.20	0.42
1:N:297[B]:MET:HB3	1:N:302:ARG:CD	2.49	0.42
1:N:383:MET:O	1:N:387:PHE:HB2	2.19	0.42
4:D:86:MET:HE1	11:K:22:ALA:HB2	2.02	0.42
12:L:26:THR:HG23	13:M:25:SER:HB3	2.02	0.42
2:B:83:ILE:O	2:B:87[B]:MET:HB2	2.19	0.42
2:O:164:ALA:O	2:O:194:GLY:HA3	2.19	0.42
3:P:177:GLN:OE1	3:P:177:GLN:HA	2.19	0.42
1:A:423[B]:MET:HE2	1:A:456:MET:HB2	2.01	0.42
6:F:21[B]:MET:HE2	6:F:21[B]:MET:HB2	1.80	0.42
1:N:278[B]:MET:SD	20:N:609:LFA:C5	3.04	0.42
19:P:305:CDL:C75	10:W:27:THR:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:26:THR:HG23	13:M:25:SER:CB	2.50	0.42
20:C:313:LFA:H21	20:C:314:LFA:H71	2.02	0.42
1:N:35:LEU:HD11	1:N:462:LEU:HD13	2.02	0.42
1:A:409:TRP:HB3	1:A:471:ILE:HG12	2.02	0.42
3:C:39:SER:CB	21:C:318:DMU:O55	2.68	0.42
22:A:613:EDO:H12	2:B:58:ALA:HB3	2.01	0.41
26:B:307:CHD:H212	26:B:307:CHD:H12	2.01	0.41
13:M:32:TRP:CZ3	13:M:40:TYR:OH	2.73	0.41
1:N:489:THR:HA	6:S:71:TRP:O	2.20	0.41
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.01	0.41
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.73	0.41
12:L:13:PHE:HB3	19:L:101:CDL:H512	2.02	0.41
19:P:305:CDL:H751	10:W:27:THR:HG21	2.02	0.41
7:T:50:TYR:HB3	7:T:52:HIS:CE1	2.55	0.41
3:C:33[B]:MET:HE2	3:C:33[B]:MET:N	2.34	0.41
30:A:2016:HOH:O	6:F:37:LYS:HE3	2.20	0.41
3:C:149:HIS:NE2	20:C:312:LFA:C1	2.84	0.41
1:A:199:LEU:N	1:A:200:PRO:CD	2.84	0.41
3:C:33[A]:MET:HE1	3:C:41:THR:HB	2.02	0.41
20:C:307:LFA:H31	26:P:302:CHD:H61	2.03	0.41
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:HG3	2.02	0.41
3:C:144[A]:ILE:HD13	3:C:239:ALA:HA	2.02	0.41
19:C:304:CDL:CB2	10:J:8:LYS:HE3	2.51	0.41
3:P:33[B]:MET:HB2	3:P:33[B]:MET:HE2	1.10	0.41
6:S:92:VAL:O	6:S:92:VAL:HG23	2.21	0.41
13:Z:38:ASP:OD1	13:Z:38:ASP:C	2.62	0.41
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.03	0.41
1:A:202:LEU:HD23	23:A:617:XE:XE	2.99	0.41
2:B:59:GLN:NE2	2:B:59:GLN:O	2.54	0.41
6:F:53:THR:HG23	6:F:55:LYS:H	1.85	0.41
1:N:237:PHE:CZ	20:P:310:LFA:H171	2.56	0.41
1:N:423[B]:MET:HE2	1:N:456:MET:HB2	2.03	0.41
4:Q:107:ILE:HD13	11:X:39:GLU:HB2	2.03	0.41
3:P:127:LEU:HD22	21:T:103:DMU:H14	2.03	0.41
1:A:498:CYS:HA	1:A:499:PRO:HA	1.94	0.40
2:B:217:LYS:CE	30:B:558:HOH:O	2.69	0.40
8:U:46:LYS:O	8:U:46:LYS:CE	2.69	0.40
1:A:87:ILE:O	1:A:173:PRO:HD3	2.21	0.40
7:G:37:LEU:HD12	7:G:37:LEU:HA	1.94	0.40
6:S:19:GLU:OE1	6:S:31:TYR:OH	2.25	0.40
1:A:148:PHE:HB3	3:C:28:THR:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:90:ARG:NH1	30:R:304:HOH:O	2.41	0.40
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.56	0.40
19:C:304:CDL:H121	19:C:304:CDL:CA6	2.51	0.40
3:P:51[B]:MET:HE3	19:P:305:CDL:C87	2.44	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	526/514 (102%)	513 (98%)	13 (2%)	0	100	100
1	N	526/514 (102%)	512 (97%)	14 (3%)	0	100	100
2	B	230/227 (101%)	224 (97%)	6 (3%)	0	100	100
2	O	230/227 (101%)	225 (98%)	5 (2%)	0	100	100
3	C	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
3	P	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	136/147 (92%)	132 (97%)	4 (3%)	0	100	100
5	E	100/109 (92%)	100 (100%)	0	0	100	100
5	R	100/109 (92%)	100 (100%)	0	0	100	100
6	F	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
6	S	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
7	G	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
7	T	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
8	H	73/85 (86%)	71 (97%)	1 (1%)	1 (1%)	9	2
8	U	73/85 (86%)	70 (96%)	2 (3%)	1 (1%)	9	2

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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%)	41 (98%)	1 (2%)	0	100	100
12	Y	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
13	M	38/46 (83%)	38 (100%)	0	0	100	100
13	Z	38/46 (83%)	38 (100%)	0	0	100	100
All	All	3488/3614 (96%)	3417 (98%)	69 (2%)	2 (0%)	48	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	438 (100%)	2 (0%)	86	86
1	N	440/426 (103%)	437 (99%)	3 (1%)	81	79
2	B	215/210 (102%)	208 (97%)	7 (3%)	33	21
2	O	215/210 (102%)	208 (97%)	7 (3%)	33	21
3	C	232/226 (103%)	230 (99%)	2 (1%)	75	72
3	P	232/226 (103%)	228 (98%)	4 (2%)	56	47
4	D	128/129 (99%)	128 (100%)	0	100	100
4	Q	122/129 (95%)	120 (98%)	2 (2%)	58	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	89/95 (94%)	89 (100%)	0	100	100
5	R	89/95 (94%)	88 (99%)	1 (1%)	70	65
6	F	78/81 (96%)	75 (96%)	3 (4%)	28	16
6	S	78/81 (96%)	75 (96%)	3 (4%)	28	16
7	G	63/69 (91%)	60 (95%)	3 (5%)	21	10
7	T	63/69 (91%)	60 (95%)	3 (5%)	21	10
8	H	67/75 (89%)	65 (97%)	2 (3%)	36	24
8	U	67/75 (89%)	64 (96%)	3 (4%)	23	11
9	I	55/58 (95%)	54 (98%)	1 (2%)	54	45
9	V	55/58 (95%)	51 (93%)	4 (7%)	11	3
10	J	47/50 (94%)	46 (98%)	1 (2%)	48	38
10	W	47/50 (94%)	45 (96%)	2 (4%)	25	12
11	K	39/46 (85%)	38 (97%)	1 (3%)	41	29
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	37/40 (92%)	37 (100%)	0	100	100
12	Y	37/40 (92%)	37 (100%)	0	100	100
13	M	34/38 (90%)	33 (97%)	1 (3%)	37	26
13	Z	34/38 (90%)	33 (97%)	1 (3%)	37	26
All	All	3042/3086 (99%)	2986 (98%)	56 (2%)	54	45

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	A	369	ASP
2	B	33	LEU
2	B	59	GLN
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
3	C	159	MET
3	C	230	ASN
6	F	80	GLN
6	F	87[A]	THR

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Mol	Chain	Res	Type
6	F	87[B]	THR
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
8	H	60	TYR
8	H	61	LYS
9	I	36	LYS
10	J	7	GLU
11	K	54	ARG
13	M	38	ASP
1	N	112	LEU
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	94	SER
2	O	226	MET
3	P	33[A]	MET
3	P	33[B]	MET
3	P	159	MET
3	P	230	ASN
4	Q	10	ASP
4	Q	51	LEU
5	R	79	LYS
6	S	37	LYS
6	S	54	ASN
6	S	80	GLN
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
8	U	46	LYS
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	29	LEU
9	V	61	GLU
9	V	65	LYS
10	W	7	GLU
10	W	50	LEU

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Mol	Chain	Res	Type
13	Z	38	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	170	ASN
1	A	422	ASN
2	B	52	HIS
3	C	38	ASN
3	C	50	ASN
3	C	56	GLN
3	C	76	GLN
4	D	119	GLN
4	D	143	ASN
5	E	94	ASN
6	F	54	ASN
7	G	38	HIS
8	H	22	ASN
8	H	37	HIS
10	J	29	ASN
11	K	35	GLN
1	N	170	ASN
1	N	422	ASN
2	O	59	GLN
2	O	91	ASN
3	P	38	ASN
3	P	50	ASN
3	P	56	GLN
4	Q	32	ASN
4	Q	76	ASN
4	Q	101	HIS
4	Q	109	HIS
4	Q	119	GLN
4	Q	143	ASN
5	R	94	ASN
6	S	54	ASN
8	U	22	ASN
8	U	28	ASN
8	U	31	GLN
8	U	32	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
2	FME	O	1	2	8,9,10	0.87	1 (12%)	7,9,11	1.12	0
1	FME	A	1	1	8,9,10	0.43	0	7,9,11	0.92	0
2	FME	B	1	2	8,9,10	1.41	1 (12%)	7,9,11	1.41	1 (14%)
1	FME	N	1	1	8,9,10	0.68	0	7,9,11	1.14	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	0/7/9/11	-
1	FME	A	1	1	-	2/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-3.43	1.63	1.81
2	O	1	FME	CG-SD	-2.09	1.70	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-3.30	103.78	112.95
1	N	1	FME	O-C-CA	-2.23	118.94	124.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 149 ligands modelled in this entry, 22 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	$\# Z > 2$
21	DMU	C	323	-	34,34,34	0.77	0	45,45,45	1.22	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	DMU	T	103	-	22,22,34	0.56	0	27,27,45	1.51	2 (7%)
21	DMU	P	316	-	34,34,34	0.83	0	45,45,45	1.41	5 (11%)
21	DMU	Z	101	-	34,34,34	0.92	2 (5%)	45,45,45	1.03	3 (6%)
21	DMU	C	318	-	34,34,34	0.96	2 (5%)	45,45,45	1.24	4 (8%)
19	CDL	Y	101	-	93,93,99	0.36	0	99,105,111	0.49	1 (1%)
22	EDO	A	612	-	3,3,3	0.34	0	2,2,2	0.23	0
21	DMU	O	307	-	22,22,34	0.70	1 (4%)	27,27,45	1.32	4 (14%)
14	HEA	A	602	1,18	57,67,67	1.78	14 (24%)	61,103,103	2.39	24 (39%)
22	EDO	E	203	-	3,3,3	0.10	0	2,2,2	0.20	0
25	CUA	B	302	2	0,1,1	-	-	-	-	-
24	PGV	N	622	-	50,50,50	0.72	2 (4%)	53,56,56	1.14	3 (5%)
22	EDO	O	308	-	3,3,3	0.08	0	2,2,2	0.31	0
22	EDO	S	103	-	3,3,3	0.10	0	2,2,2	0.14	0
21	DMU	O	306	-	10,10,34	0.49	0	9,9,45	0.48	0
22	EDO	P	322	-	3,3,3	0.20	0	2,2,2	0.11	0
26	CHD	B	307	-	32,32,32	0.68	0	51,51,51	0.70	0
25	CUA	O	304	2	0,1,1	-	-	-	-	-
20	LFA	C	313	-	14,14,19	0.28	0	13,13,18	0.41	0
21	DMU	M	101	-	34,34,34	1.14	3 (8%)	45,45,45	1.07	3 (6%)
20	LFA	P	314	-	14,14,19	0.46	0	13,13,18	0.26	0
21	DMU	O	305	-	10,10,34	0.25	0	9,9,45	0.51	0
20	LFA	N	609	-	13,13,19	0.23	0	12,12,18	0.39	0
22	EDO	T	104	-	3,3,3	0.27	0	2,2,2	0.08	0
22	EDO	A	615	-	3,3,3	0.26	0	2,2,2	0.28	0
22	EDO	G	104	-	3,3,3	0.35	0	2,2,2	0.13	0
26	CHD	P	306	-	32,32,32	0.82	1 (3%)	51,51,51	1.18	5 (9%)
20	LFA	C	314	-	12,12,19	0.22	0	11,11,18	0.22	0
21	DMU	C	316	-	6,6,34	0.21	0	5,5,45	0.62	0
21	DMU	Y	102	-	22,22,34	0.66	1 (4%)	27,27,45	0.89	1 (3%)
14	HEA	N	603[B]	-	57,67,67	1.86	14 (24%)	61,103,103	2.43	24 (39%)
21	DMU	W	101	-	10,10,34	0.17	0	9,9,45	0.61	0
22	EDO	F	103	-	3,3,3	0.20	0	2,2,2	0.24	0
22	EDO	N	616	-	3,3,3	0.50	0	2,2,2	0.45	0
20	LFA	P	301	-	14,14,19	0.14	0	13,13,18	0.13	0
21	DMU	O	302	-	22,22,34	0.82	1 (4%)	27,27,45	1.28	3 (11%)
21	DMU	P	307	-	10,10,34	0.31	0	9,9,45	0.64	0
29	PEK	T	101	-	52,52,52	0.73	2 (3%)	55,57,57	1.05	3 (5%)
14	HEA	A	601[A]	-	57,67,67	1.98	15 (26%)	61,103,103	2.32	18 (29%)
20	LFA	C	325	-	14,14,19	0.16	0	13,13,18	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	DMU	C	317	-	22,22,34	0.54	0	27,27,45	1.50	4 (14%)
22	EDO	R	201	-	3,3,3	0.14	0	2,2,2	0.06	0
19	CDL	V	101	-	63,63,99	0.50	0	69,75,111	0.96	5 (7%)
21	DMU	P	317	-	6,6,34	0.21	0	5,5,45	0.55	0
22	EDO	N	612	-	3,3,3	0.39	0	2,2,2	0.20	0
22	EDO	N	615	-	3,3,3	0.30	0	2,2,2	0.13	0
18	PER	A	606	15,14	0,1,1	-	-	-		
20	LFA	B	308	-	16,16,19	0.40	0	15,15,18	0.18	0
29	PEK	G	101	-	52,52,52	0.54	1 (1%)	55,57,57	0.63	0
22	EDO	R	203	-	3,3,3	0.37	0	2,2,2	0.46	0
22	EDO	F	102	-	3,3,3	0.29	0	2,2,2	0.17	0
22	EDO	P	321	-	3,3,3	0.26	0	2,2,2	0.09	0
20	LFA	P	313	-	10,10,19	0.25	0	9,9,18	0.23	0
22	EDO	N	613	-	3,3,3	0.09	0	2,2,2	0.23	0
21	DMU	L	102	-	22,22,34	0.69	0	27,27,45	1.02	1 (3%)
20	LFA	P	310	-	17,17,19	0.23	0	16,16,18	0.20	0
22	EDO	E	202	-	3,3,3	0.21	0	2,2,2	0.14	0
14	HEA	N	604	1,18	57,67,67	1.52	11 (19%)	61,103,103	2.33	26 (42%)
22	EDO	N	614	-	3,3,3	0.38	0	2,2,2	0.27	0
24	PGV	C	303	-	50,50,50	0.60	0	53,56,56	1.11	3 (5%)
18	PER	N	608	15,14	0,1,1	-	-	-		
24	PGV	A	621	-	50,50,50	0.70	0	53,56,56	1.16	3 (5%)
21	DMU	A	622	-	34,34,34	0.98	2 (5%)	45,45,45	1.26	5 (11%)
21	DMU	B	304	-	10,10,34	0.41	0	9,9,45	0.48	0
14	HEA	A	601[B]	-	57,67,67	1.98	15 (26%)	61,103,103	2.32	20 (32%)
22	EDO	C	322	-	3,3,3	0.98	0	2,2,2	0.92	0
19	CDL	A	607	-	63,63,99	0.52	0	69,75,111	0.99	4 (5%)
20	LFA	G	105	-	13,13,19	0.73	0	12,12,18	0.41	0
21	DMU	D	201	-	34,34,34	1.35	5 (14%)	45,45,45	1.46	5 (11%)
21	DMU	B	309	-	22,22,34	0.79	0	27,27,45	1.42	3 (11%)
20	LFA	N	601	-	16,16,19	0.32	0	15,15,18	0.28	0
22	EDO	C	321	-	3,3,3	0.19	0	2,2,2	0.29	0
20	LFA	P	312	-	13,13,19	0.15	0	12,12,18	0.12	0
22	EDO	A	614	-	3,3,3	0.61	0	2,2,2	0.26	0
26	CHD	C	305	-	32,32,32	0.68	0	51,51,51	1.57	8 (15%)
21	DMU	G	103	-	22,22,34	0.58	0	27,27,45	1.14	2 (7%)
22	EDO	C	320	-	3,3,3	0.13	0	2,2,2	0.16	0
22	EDO	S	102	-	3,3,3	0.54	0	2,2,2	0.34	0
20	LFA	A	609	-	13,13,19	0.77	0	12,12,18	0.56	0
22	EDO	B	306	-	3,3,3	0.19	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LFA	T	102	-	10,10,19	0.22	0	9,9,18	0.16	0
21	DMU	A	610	-	6,6,34	0.61	0	5,5,45	0.35	0
20	LFA	C	310	-	10,10,19	0.23	0	9,9,18	0.15	0
22	EDO	P	323	-	3,3,3	0.36	0	2,2,2	0.95	0
20	LFA	P	309	-	5,5,19	0.29	0	4,4,18	0.08	0
21	DMU	Z	102	-	7,7,34	0.41	0	6,6,45	0.39	0
21	DMU	P	320	-	34,34,34	0.93	1 (2%)	45,45,45	1.31	4 (8%)
21	DMU	N	611	-	34,34,34	1.39	6 (17%)	45,45,45	1.16	3 (6%)
14	HEA	N	603[A]	-	57,67,67	1.86	14 (24%)	61,103,103	2.46	21 (34%)
20	LFA	P	308	-	10,10,19	0.18	0	9,9,18	0.14	0
19	CDL	C	304	-	86,86,99	0.56	0	92,98,111	1.21	10 (10%)
21	DMU	J	101	-	10,10,34	0.18	0	9,9,45	0.67	0
21	DMU	B	303	-	10,10,34	0.19	0	9,9,45	0.58	0
21	DMU	C	306	-	10,10,34	0.39	0	9,9,45	0.46	0
20	LFA	C	311	-	13,13,19	0.19	0	12,12,18	0.15	0
20	LFA	P	315	-	12,12,19	0.21	0	11,11,18	0.27	0
22	EDO	E	201	-	3,3,3	0.09	0	2,2,2	0.20	0
21	DMU	A	623	-	10,10,34	0.24	0	9,9,45	0.59	0
21	DMU	C	319	-	34,34,34	0.76	1 (2%)	45,45,45	1.35	7 (15%)
20	LFA	C	312	-	10,10,19	0.25	0	9,9,18	0.26	0
20	LFA	C	309	-	17,17,19	0.22	0	16,16,18	0.27	0
20	LFA	P	311	-	10,10,19	0.13	0	9,9,18	0.09	0
21	DMU	P	318	-	22,22,34	0.90	1 (4%)	27,27,45	1.32	4 (14%)
21	DMU	M	102	-	7,7,34	0.30	0	6,6,45	0.75	0
21	DMU	C	315	-	34,34,34	0.80	1 (2%)	45,45,45	1.49	7 (15%)
21	DMU	P	319	-	34,34,34	0.96	3 (8%)	45,45,45	1.09	2 (4%)
26	CHD	C	301	-	32,32,32	1.00	2 (6%)	51,51,51	0.73	1 (1%)
26	CHD	G	102	-	32,32,32	0.68	0	51,51,51	0.82	0
26	CHD	P	302	-	32,32,32	0.91	2 (6%)	51,51,51	0.65	0
24	PGV	P	304	-	50,50,50	0.90	3 (6%)	53,56,56	0.98	5 (9%)
21	DMU	N	610	-	6,6,34	0.38	0	5,5,45	0.35	0
20	LFA	C	308	-	5,5,19	0.21	0	4,4,18	0.07	0
21	DMU	Q	201	-	34,34,34	1.30	6 (17%)	45,45,45	1.57	7 (15%)
21	DMU	P	324	-	34,34,34	0.72	0	45,45,45	1.47	4 (8%)
19	CDL	L	101	-	93,93,99	0.40	0	99,105,111	0.60	2 (2%)
21	DMU	B	305	-	22,22,34	1.00	1 (4%)	27,27,45	1.20	4 (14%)
22	EDO	A	613	-	3,3,3	0.28	0	2,2,2	0.30	0
20	LFA	A	608	-	13,13,19	0.46	0	12,12,18	0.20	0
20	LFA	O	301	-	10,10,19	0.28	0	9,9,18	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	DMU	A	611	-	34,34,34	1.12	2 (5%)	45,45,45	1.22	5 (11%)
22	EDO	R	202	-	3,3,3	0.09	0	2,2,2	0.20	0
19	CDL	P	305	-	86,86,99	0.52	0	92,98,111	0.99	6 (6%)
21	DMU	N	602	-	10,10,34	0.37	0	9,9,45	0.53	0
20	LFA	C	307	-	10,10,19	0.24	0	9,9,18	0.18	0
21	DMU	U	101	-	34,34,34	0.94	2 (5%)	45,45,45	1.29	5 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	DMU	C	323	-	-	7/19/59/59	0/2/2/2
21	DMU	T	103	-	-	8/13/33/59	0/1/1/2
21	DMU	P	316	-	-	10/19/59/59	0/2/2/2
21	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
21	DMU	C	318	-	-	12/19/59/59	0/2/2/2
19	CDL	Y	101	-	-	55/104/104/110	-
22	EDO	A	612	-	-	0/1/1/1	-
21	DMU	O	307	-	-	6/13/33/59	0/1/1/2
14	HEA	A	602	1,18	-	4/32/76/76	-
22	EDO	E	203	-	-	0/1/1/1	-
24	PGV	N	622	-	-	9/55/55/55	-
22	EDO	O	308	-	-	0/1/1/1	-
22	EDO	S	103	-	-	0/1/1/1	-
21	DMU	O	306	-	-	5/8/8/59	-
22	EDO	P	322	-	-	0/1/1/1	-
26	CHD	B	307	-	-	2/9/74/74	0/4/4/4
20	LFA	C	313	-	-	4/12/12/17	-
21	DMU	M	101	-	-	3/19/59/59	0/2/2/2
20	LFA	P	314	-	-	5/12/12/17	-
21	DMU	O	305	-	-	5/8/8/59	-
20	LFA	N	609	-	-	3/11/11/17	-
22	EDO	T	104	-	-	0/1/1/1	-
22	EDO	A	615	-	-	0/1/1/1	-
22	EDO	G	104	-	-	0/1/1/1	-
26	CHD	P	306	-	-	5/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LFA	C	314	-	-	4/10/10/17	-
21	DMU	C	316	-	-	3/4/4/59	-
21	DMU	Y	102	-	-	10/13/33/59	0/1/1/2
14	HEA	N	603[B]	-	-	2/32/76/76	-
21	DMU	W	101	-	-	7/8/8/59	-
22	EDO	F	103	-	-	0/1/1/1	-
22	EDO	N	616	-	-	0/1/1/1	-
20	LFA	P	301	-	-	8/12/12/17	-
21	DMU	O	302	-	-	7/13/33/59	0/1/1/2
21	DMU	P	307	-	-	2/8/8/59	-
29	PEK	T	101	-	-	20/56/56/56	-
14	HEA	A	601[A]	-	-	6/32/76/76	-
20	LFA	C	325	-	-	6/12/12/17	-
21	DMU	C	317	-	-	8/13/33/59	0/1/1/2
22	EDO	R	201	-	-	1/1/1/1	-
19	CDL	V	101	-	-	43/74/74/110	-
21	DMU	P	317	-	-	1/4/4/59	-
22	EDO	N	612	-	-	0/1/1/1	-
22	EDO	N	615	-	-	0/1/1/1	-
20	LFA	B	308	-	-	9/14/14/17	-
29	PEK	G	101	-	-	9/56/56/56	-
22	EDO	R	203	-	-	1/1/1/1	-
22	EDO	F	102	-	-	0/1/1/1	-
22	EDO	P	321	-	-	1/1/1/1	-
20	LFA	P	313	-	-	2/8/8/17	-
22	EDO	N	613	-	-	0/1/1/1	-
21	DMU	L	102	-	-	8/13/33/59	0/1/1/2
20	LFA	P	310	-	-	8/15/15/17	-
22	EDO	E	202	-	-	0/1/1/1	-
14	HEA	N	604	1,18	-	4/32/76/76	-
22	EDO	N	614	-	-	0/1/1/1	-
24	PGV	C	303	-	-	11/55/55/55	-
24	PGV	A	621	-	-	12/55/55/55	-
21	DMU	A	622	-	-	4/19/59/59	0/2/2/2
21	DMU	B	304	-	-	5/8/8/59	-
14	HEA	A	601[B]	-	-	5/32/76/76	-
22	EDO	C	322	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CDL	A	607	-	-	33/74/74/110	-
20	LFA	G	105	-	-	5/11/11/17	-
21	DMU	D	201	-	-	7/19/59/59	0/2/2/2
21	DMU	B	309	-	-	9/13/33/59	0/1/1/2
20	LFA	N	601	-	-	11/14/14/17	-
22	EDO	C	321	-	-	0/1/1/1	-
20	LFA	P	312	-	-	6/11/11/17	-
22	EDO	A	614	-	-	0/1/1/1	-
26	CHD	C	305	-	-	8/9/74/74	0/4/4/4
21	DMU	G	103	-	-	7/13/33/59	0/1/1/2
22	EDO	C	320	-	-	1/1/1/1	-
22	EDO	S	102	-	-	0/1/1/1	-
20	LFA	A	609	-	-	5/11/11/17	-
22	EDO	B	306	-	-	0/1/1/1	-
20	LFA	T	102	-	-	5/8/8/17	-
21	DMU	A	610	-	-	3/4/4/59	-
20	LFA	C	310	-	-	7/8/8/17	-
22	EDO	P	323	-	-	0/1/1/1	-
20	LFA	P	309	-	-	1/3/3/17	-
21	DMU	Z	102	-	-	3/5/5/59	-
21	DMU	P	320	-	-	10/19/59/59	0/2/2/2
21	DMU	N	611	-	-	7/19/59/59	0/2/2/2
14	HEA	N	603[A]	-	-	6/32/76/76	-
20	LFA	P	308	-	-	7/8/8/17	-
19	CDL	C	304	-	-	49/97/97/110	-
21	DMU	J	101	-	-	5/8/8/59	-
21	DMU	B	303	-	-	3/8/8/59	-
21	DMU	C	306	-	-	3/8/8/59	-
20	LFA	C	311	-	-	5/11/11/17	-
20	LFA	P	315	-	-	5/10/10/17	-
22	EDO	E	201	-	-	0/1/1/1	-
21	DMU	A	623	-	-	3/8/8/59	-
21	DMU	C	319	-	-	10/19/59/59	0/2/2/2
20	LFA	C	312	-	-	3/8/8/17	-
20	LFA	C	309	-	-	7/15/15/17	-
20	LFA	P	311	-	-	5/8/8/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	DMU	P	318	-	-	6/13/33/59	0/1/1/2
21	DMU	M	102	-	-	4/5/5/59	-
21	DMU	C	315	-	-	12/19/59/59	0/2/2/2
21	DMU	P	319	-	-	13/19/59/59	0/2/2/2
26	CHD	C	301	-	-	2/9/74/74	0/4/4/4
26	CHD	G	102	-	-	2/9/74/74	0/4/4/4
26	CHD	P	302	-	-	2/9/74/74	0/4/4/4
24	PGV	P	304	-	-	9/55/55/55	-
21	DMU	N	610	-	-	4/4/4/59	-
20	LFA	C	308	-	-	1/3/3/17	-
21	DMU	Q	201	-	-	8/19/59/59	0/2/2/2
21	DMU	P	324	-	-	6/19/59/59	0/2/2/2
19	CDL	L	101	-	-	52/104/104/110	-
21	DMU	B	305	-	-	10/13/33/59	0/1/1/2
22	EDO	A	613	-	-	1/1/1/1	-
20	LFA	A	608	-	-	3/11/11/17	-
20	LFA	O	301	-	-	4/8/8/17	-
21	DMU	A	611	-	-	7/19/59/59	0/2/2/2
22	EDO	R	202	-	-	0/1/1/1	-
19	CDL	P	305	-	-	53/97/97/110	-
21	DMU	N	602	-	-	3/8/8/59	-
20	LFA	C	307	-	-	4/8/8/17	-
21	DMU	U	101	-	-	4/19/59/59	0/2/2/2

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	603[A]	HEA	C1D-ND	-4.99	1.31	1.40
14	N	603[B]	HEA	C1D-ND	-4.99	1.31	1.40
14	A	601[A]	HEA	C3A-C2A	4.93	1.47	1.40
14	A	601[B]	HEA	C3A-C2A	4.93	1.47	1.40
14	A	601[A]	HEA	C1D-ND	-4.84	1.32	1.40
14	A	601[B]	HEA	C1D-ND	-4.84	1.32	1.40
14	A	601[A]	HEA	C16-C17	-4.56	1.38	1.53
14	A	601[B]	HEA	C16-C17	-4.56	1.38	1.53
14	A	601[A]	HEA	C3D-C2D	4.53	1.46	1.36
14	A	601[B]	HEA	C3D-C2D	4.53	1.46	1.36
21	N	611	DMU	O16-C6	-4.10	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	M	101	DMU	O3-C5	-4.01	1.33	1.43
14	A	602	HEA	CHD-C1D	3.94	1.45	1.35
14	A	601[A]	HEA	C1B-NB	-3.93	1.30	1.38
14	A	601[B]	HEA	C1B-NB	-3.93	1.30	1.38
14	A	602	HEA	C3B-C2B	3.93	1.43	1.34
14	N	603[A]	HEA	C4B-NB	-3.70	1.33	1.40
14	N	603[B]	HEA	C4B-NB	-3.70	1.33	1.40
14	A	602	HEA	C1D-ND	-3.65	1.34	1.40
14	N	604	HEA	C4B-NB	-3.64	1.34	1.40
14	N	604	HEA	C3B-C2B	3.62	1.42	1.34
14	N	603[A]	HEA	C3B-C2B	3.60	1.42	1.34
14	N	603[B]	HEA	C3B-C2B	3.60	1.42	1.34
14	A	602	HEA	C4D-ND	-3.58	1.31	1.38
14	A	601[A]	HEA	C4B-NB	-3.52	1.34	1.40
14	A	601[B]	HEA	C4B-NB	-3.52	1.34	1.40
21	P	320	DMU	C10-C5	-3.50	1.42	1.52
14	N	603[A]	HEA	C3C-C2C	3.49	1.45	1.40
14	N	603[B]	HEA	C3C-C2C	3.49	1.45	1.40
14	N	603[A]	HEA	C4D-ND	-3.46	1.31	1.38
14	N	603[B]	HEA	C4D-ND	-3.46	1.31	1.38
26	C	301	CHD	O26-C24	-3.45	1.19	1.30
14	N	603[A]	HEA	C16-C17	-3.44	1.42	1.53
14	N	603[B]	HEA	C16-C17	-3.44	1.42	1.53
14	A	602	HEA	C3A-C2A	3.44	1.45	1.40
14	A	602	HEA	C1B-NB	-3.43	1.31	1.38
14	N	604	HEA	CHD-C1D	3.43	1.43	1.35
14	N	603[A]	HEA	CHC-C4B	3.42	1.43	1.35
14	N	603[B]	HEA	CHC-C4B	3.42	1.43	1.35
14	A	602	HEA	C4B-NB	-3.41	1.34	1.40
21	C	318	DMU	C7-C5	-3.39	1.43	1.52
14	N	603[A]	HEA	C1B-NB	-3.39	1.31	1.38
14	N	603[B]	HEA	C1B-NB	-3.39	1.31	1.38
14	A	602	HEA	C2A-C1A	3.36	1.50	1.42
14	N	604	HEA	C3D-C2D	3.33	1.43	1.36
21	P	318	DMU	O16-C6	3.30	1.45	1.40
14	N	603[A]	HEA	C3A-C2A	3.20	1.44	1.40
14	N	603[B]	HEA	C3A-C2A	3.20	1.44	1.40
14	N	604	HEA	C1D-ND	-3.19	1.34	1.40
21	Z	101	DMU	O3-C5	-3.18	1.35	1.43
14	A	601[A]	HEA	C3B-C2B	3.18	1.41	1.34
14	A	601[B]	HEA	C3B-C2B	3.18	1.41	1.34
24	P	304	PGV	O03-C19	3.17	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	319	DMU	O3-C5	3.16	1.50	1.43
14	A	601[A]	HEA	C3C-C2C	3.13	1.44	1.40
14	A	601[B]	HEA	C3C-C2C	3.13	1.44	1.40
26	P	302	CHD	C22-C23	-3.09	1.43	1.52
29	T	101	PEK	C2-C1	3.08	1.59	1.50
14	A	601[A]	HEA	CHD-C1D	3.08	1.42	1.35
14	A	601[B]	HEA	CHD-C1D	3.08	1.42	1.35
14	A	602	HEA	C3D-C2D	3.07	1.43	1.36
21	A	611	DMU	O7-C10	3.04	1.50	1.41
21	D	201	DMU	O5-C6	-3.02	1.34	1.41
21	U	101	DMU	C7-C5	-3.01	1.44	1.52
14	N	604	HEA	C3A-C2A	2.99	1.44	1.40
14	N	603[A]	HEA	CHD-C1D	2.98	1.42	1.35
14	N	603[B]	HEA	CHD-C1D	2.98	1.42	1.35
21	Q	201	DMU	C10-C5	-2.95	1.44	1.52
14	A	602	HEA	CHC-C4B	2.94	1.42	1.35
14	N	604	HEA	C2A-C1A	2.91	1.49	1.42
29	G	101	PEK	C23-C22	-2.88	1.41	1.52
14	A	602	HEA	C18-C19	2.87	1.39	1.33
21	D	201	DMU	O55-C2	2.87	1.49	1.43
14	N	604	HEA	CHC-C4B	2.83	1.42	1.35
29	T	101	PEK	C23-C22	-2.81	1.41	1.52
26	C	301	CHD	C22-C23	-2.76	1.44	1.52
21	D	201	DMU	C10-C5	-2.74	1.44	1.52
26	P	302	CHD	O26-C24	-2.74	1.21	1.30
14	N	604	HEA	C1B-NB	-2.70	1.33	1.38
21	N	611	DMU	C7-C5	-2.68	1.45	1.52
26	P	306	CHD	O25-C24	2.67	1.31	1.22
21	Q	201	DMU	O5-C6	-2.66	1.35	1.41
14	N	603[A]	HEA	C4B-C3B	2.66	1.49	1.44
14	N	603[B]	HEA	C4B-C3B	2.66	1.49	1.44
14	A	601[A]	HEA	CHC-C4B	2.63	1.41	1.35
14	A	601[B]	HEA	CHC-C4B	2.63	1.41	1.35
21	B	305	DMU	O16-C6	2.58	1.44	1.40
21	N	611	DMU	C10-C5	-2.56	1.45	1.52
24	N	622	PGV	O01-C1	2.56	1.41	1.34
14	A	601[A]	HEA	C2A-C1A	2.51	1.48	1.42
14	A	601[B]	HEA	C2A-C1A	2.51	1.48	1.42
21	A	622	DMU	C10-C5	-2.50	1.45	1.52
14	A	601[A]	HEA	CMC-C2C	-2.50	1.46	1.51
14	A	601[B]	HEA	CMC-C2C	-2.50	1.46	1.51
14	A	601[A]	HEA	C4D-ND	-2.48	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[B]	HEA	C4D-ND	-2.48	1.33	1.38
21	C	319	DMU	O55-C2	-2.47	1.37	1.43
14	A	601[A]	HEA	C16-C15	2.45	1.56	1.51
14	A	601[B]	HEA	C16-C15	2.45	1.56	1.51
21	Q	201	DMU	C7-C5	-2.44	1.46	1.52
14	A	601[A]	HEA	O1D-CGD	2.42	1.30	1.22
14	A	601[B]	HEA	O1D-CGD	2.42	1.30	1.22
21	M	101	DMU	C10-C5	-2.41	1.45	1.52
21	P	319	DMU	C7-C5	-2.40	1.46	1.52
14	N	603[A]	HEA	C3D-C2D	2.40	1.41	1.36
14	N	603[B]	HEA	C3D-C2D	2.40	1.41	1.36
14	N	604	HEA	C4D-ND	-2.39	1.33	1.38
14	N	603[A]	HEA	C4C-NC	-2.39	1.31	1.36
14	N	603[B]	HEA	C4C-NC	-2.39	1.31	1.36
21	N	611	DMU	O1-C10	2.35	1.47	1.41
24	P	304	PGV	O01-C02	-2.34	1.40	1.46
21	D	201	DMU	O3-C5	-2.32	1.37	1.43
21	D	201	DMU	O61-C57	2.31	1.52	1.42
14	N	603[A]	HEA	C2A-C1A	2.31	1.47	1.42
14	N	603[B]	HEA	C2A-C1A	2.31	1.47	1.42
21	Q	201	DMU	O3-C5	-2.31	1.37	1.43
21	U	101	DMU	C6-C1	-2.30	1.45	1.52
21	C	315	DMU	O5-C6	-2.28	1.36	1.41
21	M	101	DMU	C7-C5	-2.26	1.46	1.52
21	A	611	DMU	O16-C6	-2.26	1.36	1.40
24	P	304	PGV	O03-C01	-2.22	1.40	1.45
21	O	307	DMU	C6-C1	-2.20	1.46	1.52
21	Q	201	DMU	O16-C6	-2.19	1.36	1.40
21	C	318	DMU	O3-C5	2.17	1.48	1.43
21	O	302	DMU	C3-C4	-2.16	1.48	1.53
21	Z	101	DMU	C10-C5	-2.14	1.46	1.52
14	A	602	HEA	CBD-CGD	2.14	1.55	1.50
21	A	622	DMU	C7-C5	-2.14	1.46	1.52
21	Q	201	DMU	O55-C2	2.12	1.48	1.43
21	N	611	DMU	C6-C1	-2.11	1.46	1.52
24	N	622	PGV	O03-C01	2.10	1.49	1.45
21	N	611	DMU	O5-C6	-2.06	1.36	1.41
21	P	319	DMU	C6-C1	-2.05	1.46	1.52
14	A	602	HEA	C1C-NC	-2.04	1.32	1.36
21	Y	102	DMU	C6-C1	-2.02	1.46	1.52
14	A	602	HEA	O1A-CGA	2.01	1.28	1.22
14	N	604	HEA	C18-C19	2.01	1.37	1.33

All (292) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	603[A]	HEA	C3D-C4D-ND	7.40	117.52	110.36
14	N	603[B]	HEA	C3D-C4D-ND	7.40	117.52	110.36
21	P	316	DMU	O16-C6-C1	6.27	118.09	108.30
21	Q	201	DMU	O16-C6-C1	5.95	117.59	108.30
14	N	604	HEA	C3D-C4D-ND	5.88	116.05	110.36
14	A	601[A]	HEA	C3D-C4D-ND	5.80	115.97	110.36
14	A	601[B]	HEA	C3D-C4D-ND	5.80	115.97	110.36
21	C	315	DMU	O16-C6-C1	5.76	117.30	108.30
21	D	201	DMU	O16-C6-C1	5.70	117.20	108.30
14	A	602	HEA	C3B-C4B-NB	5.67	116.55	109.84
21	T	103	DMU	O16-C6-C1	5.55	116.96	108.30
19	C	304	CDL	OA6-CA5-C11	-5.54	99.56	111.50
21	B	309	DMU	O16-C6-C1	5.48	116.87	108.30
21	C	323	DMU	O16-C6-C1	5.39	116.72	108.30
14	N	603[A]	HEA	C27-C19-C20	5.39	124.33	115.27
14	A	602	HEA	C2B-C1B-NB	5.38	116.32	109.88
14	A	601[A]	HEA	C3C-C4C-NC	5.32	116.08	109.21
14	A	601[B]	HEA	C3C-C4C-NC	5.32	116.08	109.21
14	N	603[A]	HEA	C2B-C1B-NB	5.31	116.25	109.88
14	N	603[B]	HEA	C2B-C1B-NB	5.31	116.25	109.88
26	C	305	CHD	C14-C13-C12	5.24	112.28	107.40
14	A	601[A]	HEA	C27-C19-C20	5.19	124.00	115.27
14	A	602	HEA	C3D-C4D-ND	5.00	115.20	110.36
21	C	317	DMU	O5-C6-C1	4.97	120.87	110.35
26	C	305	CHD	C17-C13-C14	-4.83	95.22	100.09
21	P	324	DMU	C10-C5-C7	4.83	120.05	110.00
14	N	604	HEA	C3B-C4B-NB	4.80	115.52	109.84
21	M	101	DMU	O16-C6-C1	4.74	115.70	108.30
14	N	604	HEA	CHB-C1B-C2B	-4.73	117.59	124.98
14	A	602	HEA	C2D-C1D-ND	4.65	115.35	109.84
24	A	621	PGV	O03-C19-O04	-4.65	111.87	123.59
21	P	318	DMU	O5-C6-C1	4.59	120.06	110.35
21	P	324	DMU	O16-C6-C1	4.56	115.42	108.30
14	N	603[A]	HEA	C13-C12-C11	-4.54	107.53	114.35
14	N	603[B]	HEA	C13-C12-C11	-4.54	107.53	114.35
24	C	303	PGV	C27-C26-C25	-4.52	91.46	114.42
14	N	603[A]	HEA	C2D-C1D-ND	4.52	115.19	109.84
14	N	603[B]	HEA	C2D-C1D-ND	4.52	115.19	109.84
14	A	601[A]	HEA	C2D-C1D-ND	4.51	115.19	109.84
14	A	601[B]	HEA	C2D-C1D-ND	4.51	115.19	109.84
19	A	607	CDL	OA6-CA4-CA6	4.51	124.72	108.40
14	A	601[A]	HEA	CHA-C4D-C3D	-4.47	118.26	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601[B]	HEA	CHA-C4D-C3D	-4.47	118.26	124.84
14	N	603[A]	HEA	C3B-C4B-NB	4.47	115.14	109.84
14	N	603[B]	HEA	C3B-C4B-NB	4.47	115.14	109.84
14	A	601[A]	HEA	C2B-C1B-NB	4.43	115.19	109.88
14	A	601[B]	HEA	C2B-C1B-NB	4.43	115.19	109.88
14	A	601[A]	HEA	C3B-C4B-NB	4.40	115.05	109.84
14	A	601[B]	HEA	C3B-C4B-NB	4.40	115.05	109.84
14	N	604	HEA	C2B-C1B-NB	4.39	115.14	109.88
24	N	622	PGV	O03-C19-O04	-4.36	112.59	123.59
14	N	603[A]	HEA	C4D-C3D-C2D	-4.35	100.56	106.90
14	N	603[B]	HEA	C4D-C3D-C2D	-4.35	100.56	106.90
14	N	604	HEA	C2D-C1D-ND	4.34	114.98	109.84
21	A	622	DMU	O16-C6-C1	4.28	114.98	108.30
21	P	320	DMU	C10-C5-C7	4.18	118.70	110.00
14	N	603[A]	HEA	C3C-C4C-NC	4.17	114.60	109.21
14	N	603[B]	HEA	C3C-C4C-NC	4.17	114.60	109.21
14	N	604	HEA	CAD-C3D-C4D	4.16	131.93	124.66
14	N	603[A]	HEA	CHB-C1B-C2B	-4.15	118.50	124.98
14	N	603[B]	HEA	CHB-C1B-C2B	-4.15	118.50	124.98
14	A	602	HEA	C3C-C4C-NC	4.04	114.43	109.21
29	T	101	PEK	O01-C1-O02	-4.04	113.95	123.70
21	P	320	DMU	O16-C6-C1	3.97	114.49	108.30
21	C	318	DMU	O16-C6-C1	3.94	114.46	108.30
14	A	602	HEA	CAD-CBD-CGD	-3.94	105.12	113.60
14	N	604	HEA	CAD-CBD-CGD	-3.90	105.20	113.60
14	N	604	HEA	CMD-C2D-C1D	3.88	130.94	125.04
19	C	304	CDL	OA7-CA5-C11	3.88	138.86	123.73
21	Z	101	DMU	O16-C6-C1	3.88	114.36	108.30
14	N	604	HEA	CBA-CAA-C2A	-3.84	106.13	112.60
21	O	302	DMU	O5-C6-C1	3.83	118.46	110.35
29	T	101	PEK	O02-C1-C2	3.82	138.64	123.73
21	U	101	DMU	O16-C6-C1	3.81	114.26	108.30
21	C	315	DMU	C6-O5-C4	3.77	121.09	113.69
14	N	604	HEA	CHA-C4D-C3D	-3.76	119.32	124.84
26	C	305	CHD	C16-C17-C20	3.72	117.91	112.15
19	C	304	CDL	OA5-PA1-OA3	3.72	123.59	109.07
21	C	319	DMU	O16-C6-C1	3.71	114.10	108.30
14	A	601[A]	HEA	C13-C12-C11	-3.70	108.79	114.35
14	A	601[B]	HEA	C13-C12-C11	-3.70	108.79	114.35
26	C	305	CHD	C6-C7-C8	3.65	115.38	111.48
21	P	319	DMU	C10-C5-C7	3.63	117.56	110.00
14	A	601[A]	HEA	C4D-C3D-C2D	-3.61	101.63	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601[B]	HEA	C4D-C3D-C2D	-3.61	101.63	106.90
21	G	103	DMU	O16-C6-C1	3.61	113.94	108.30
21	U	101	DMU	C10-C5-C7	3.61	117.51	110.00
21	L	102	DMU	O5-C6-O16	3.58	118.46	109.97
19	P	305	CDL	OA4-PA1-OA5	-3.57	91.16	107.75
14	A	602	HEA	CMD-C2D-C1D	3.57	130.47	125.04
14	A	601[A]	HEA	C4B-C3B-C2B	-3.54	101.37	107.41
14	A	601[B]	HEA	C4B-C3B-C2B	-3.54	101.37	107.41
24	N	622	PGV	O03-C19-C20	3.53	122.97	111.91
14	A	601[A]	HEA	C1D-C2D-C3D	-3.52	103.25	106.96
14	A	601[B]	HEA	C1D-C2D-C3D	-3.52	103.25	106.96
14	N	603[A]	HEA	CHA-C4D-C3D	-3.47	119.73	124.84
14	N	603[B]	HEA	CHA-C4D-C3D	-3.47	119.73	124.84
14	A	602	HEA	CHA-C4D-C3D	-3.46	119.75	124.84
14	A	601[B]	HEA	C27-C19-C20	3.46	121.09	115.27
14	A	602	HEA	CMC-C2C-C3C	3.43	131.09	124.68
24	C	303	PGV	O03-C19-O04	-3.41	115.00	123.59
19	A	607	CDL	CA4-OA6-CA5	3.40	126.15	117.79
29	T	101	PEK	C2-C3-C4	3.39	119.27	113.23
19	A	607	CDL	OA5-PA1-OA3	3.34	122.13	109.07
19	P	305	CDL	OA4-PA1-OA2	-3.34	92.22	107.75
19	C	304	CDL	OB6-CB5-C51	3.33	118.67	111.50
14	A	601[A]	HEA	CHB-C1B-C2B	-3.32	119.79	124.98
14	A	601[B]	HEA	CHB-C1B-C2B	-3.32	119.79	124.98
21	T	103	DMU	C18-O16-C6	-3.31	108.35	113.84
24	A	621	PGV	O03-C19-C20	3.29	122.25	111.91
14	A	602	HEA	C4D-C3D-C2D	-3.29	102.10	106.90
19	L	101	CDL	OB4-PB2-OB2	3.27	122.92	107.75
14	A	602	HEA	C1B-C2B-C3B	-3.23	102.94	106.80
19	V	101	CDL	OA6-CA4-CA3	3.21	120.03	108.40
14	A	602	HEA	CHB-C1B-C2B	-3.20	119.98	124.98
21	Y	102	DMU	O5-C6-O16	3.19	117.52	109.97
21	Q	201	DMU	C10-O1-C9	3.18	119.94	113.69
14	A	601[B]	HEA	C20-C19-C18	-3.16	114.72	121.12
14	A	602	HEA	C4B-C3B-C2B	-3.16	102.01	107.41
14	A	602	HEA	C1D-C2D-C3D	-3.15	103.64	106.96
14	N	604	HEA	C3C-C4C-NC	3.14	113.27	109.21
21	U	101	DMU	O3-C5-C10	3.13	117.66	110.05
14	N	604	HEA	C1D-C2D-C3D	-3.12	103.68	106.96
14	N	603[A]	HEA	C4B-C3B-C2B	-3.09	102.14	107.41
14	N	603[B]	HEA	C4B-C3B-C2B	-3.09	102.14	107.41
14	A	602	HEA	C20-C19-C18	-3.06	114.93	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601[A]	HEA	CMD-C2D-C1D	3.06	129.70	125.04
14	A	601[B]	HEA	CMD-C2D-C1D	3.06	129.70	125.04
14	A	602	HEA	OMA-CMA-C3A	-3.04	118.29	124.91
14	N	604	HEA	C4D-C3D-C2D	-3.04	102.47	106.90
26	P	306	CHD	C5-C6-C7	3.03	117.81	114.46
19	P	305	CDL	OA2-PA1-OA3	3.03	120.90	109.07
21	C	315	DMU	O5-C6-O16	-3.00	102.86	109.97
19	V	101	CDL	OA6-CA5-C11	2.97	117.91	111.50
21	C	315	DMU	C10-C5-C7	2.95	116.14	110.00
21	C	317	DMU	C2-C3-C4	-2.95	104.98	110.24
26	P	306	CHD	C15-C14-C13	2.93	106.42	103.55
14	A	602	HEA	C4B-NB-C1B	-2.92	102.05	105.07
14	N	603[A]	HEA	C1B-C2B-C3B	-2.92	103.31	106.80
14	N	603[B]	HEA	C1B-C2B-C3B	-2.92	103.31	106.80
21	U	101	DMU	C10-O7-C3	-2.91	110.75	117.96
21	C	318	DMU	C8-C7-C5	-2.91	105.75	110.82
21	P	320	DMU	O5-C6-C1	2.90	116.49	110.35
26	P	306	CHD	C6-C7-C8	2.90	114.58	111.48
21	C	318	DMU	C10-C5-C7	2.90	116.03	110.00
21	D	201	DMU	O3-C5-C7	2.87	116.99	110.35
21	P	316	DMU	O7-C3-C2	2.87	114.91	107.28
21	C	319	DMU	C10-C5-C7	2.86	115.96	110.00
21	A	622	DMU	O5-C6-C1	2.86	116.41	110.35
21	C	319	DMU	O5-C6-C1	2.86	116.41	110.35
21	O	302	DMU	O16-C6-C1	2.86	112.77	108.30
21	O	302	DMU	C6-C1-C2	2.86	115.94	110.00
14	A	601[A]	HEA	C4A-CHB-C1B	2.85	126.32	122.56
14	A	601[B]	HEA	C4A-CHB-C1B	2.85	126.32	122.56
14	N	604	HEA	C1B-C2B-C3B	-2.85	103.39	106.80
14	A	602	HEA	C4A-CHB-C1B	2.84	126.31	122.56
21	N	611	DMU	C10-O1-C9	2.84	119.26	113.69
14	A	602	HEA	CAD-C3D-C4D	2.83	129.61	124.66
21	Q	201	DMU	C6-O5-C4	-2.82	108.15	113.69
14	A	601[A]	HEA	C26-C15-C16	2.82	120.01	115.27
14	A	601[B]	HEA	C26-C15-C16	2.82	120.01	115.27
21	O	307	DMU	C57-C4-C3	-2.80	106.45	113.00
19	C	304	CDL	OB5-PB2-OB3	2.80	120.00	109.07
21	Q	201	DMU	O1-C9-C8	2.77	114.73	109.69
21	A	611	DMU	C10-O7-C3	-2.77	111.12	117.96
19	C	304	CDL	OA4-PA1-OA5	-2.76	94.91	107.75
21	B	305	DMU	O5-C6-C1	2.76	116.20	110.35
19	V	101	CDL	OA8-CA6-CA4	2.75	116.44	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	319	DMU	O3-C5-C7	2.74	116.69	110.35
14	N	603[B]	HEA	C20-C19-C18	-2.74	115.57	121.12
14	N	604	HEA	C4B-C3B-C2B	-2.74	102.73	107.41
21	A	611	DMU	C18-O16-C6	2.73	118.37	113.84
14	A	602	HEA	CBA-CAA-C2A	-2.72	108.03	112.60
21	C	317	DMU	C18-O16-C6	-2.71	109.35	113.84
26	P	306	CHD	C18-C13-C12	-2.71	106.31	109.07
14	N	604	HEA	C20-C19-C18	-2.71	115.64	121.12
14	N	604	HEA	C27-C19-C20	2.68	119.78	115.27
21	O	307	DMU	O5-C6-O16	2.67	116.30	109.97
21	O	307	DMU	O5-C6-C1	2.67	116.00	110.35
14	N	603[A]	HEA	C1D-C2D-C3D	-2.67	104.15	106.96
14	N	603[B]	HEA	C1D-C2D-C3D	-2.67	104.15	106.96
14	N	603[A]	HEA	C4D-CHA-C1A	2.66	126.07	122.56
14	N	603[B]	HEA	C4D-CHA-C1A	2.66	126.07	122.56
14	A	602	HEA	C13-C12-C11	-2.65	110.36	114.35
14	A	601[A]	HEA	CAD-C3D-C4D	2.65	129.29	124.66
14	A	601[B]	HEA	CAD-C3D-C4D	2.65	129.29	124.66
21	C	319	DMU	O3-C5-C10	2.64	116.45	110.05
21	C	315	DMU	C18-O16-C6	-2.61	109.51	113.84
21	C	323	DMU	C10-C5-C7	2.60	115.41	110.00
21	D	201	DMU	C10-O1-C9	2.59	118.78	113.69
21	B	305	DMU	C3-C2-C1	-2.59	106.30	110.82
21	D	201	DMU	C10-C5-C7	2.59	115.39	110.00
19	L	101	CDL	OB5-PB2-OB3	-2.59	98.96	109.07
24	P	304	PGV	C22-C21-C20	-2.59	103.90	113.19
21	O	307	DMU	O16-C6-C1	-2.57	104.30	108.30
14	A	601[B]	HEA	C21-C22-C23	-2.56	118.99	127.75
19	P	305	CDL	OA5-PA1-OA3	2.56	119.06	109.07
21	A	622	DMU	C10-C5-C7	2.56	115.32	110.00
14	A	602	HEA	CHC-C4B-NB	-2.55	121.23	124.38
19	P	305	CDL	OA8-CA6-CA4	-2.53	101.07	108.43
21	Z	101	DMU	O3-C5-C7	2.52	116.19	110.35
21	Q	201	DMU	C2-C3-C4	-2.52	105.15	110.93
24	P	304	PGV	O03-C19-O04	-2.52	117.24	123.59
21	N	611	DMU	O5-C6-O16	2.51	115.91	109.97
14	N	604	HEA	CHB-C1B-NB	2.50	127.15	124.43
14	N	603[A]	HEA	C1D-ND-C4D	-2.49	102.50	105.07
14	N	603[B]	HEA	C1D-ND-C4D	-2.49	102.50	105.07
19	C	304	CDL	OA4-PA1-OA3	2.49	124.55	112.24
24	C	303	PGV	O01-C1-O02	-2.49	117.69	123.70
21	B	305	DMU	C6-O5-C4	2.48	118.56	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	CMB-C2B-C1B	2.47	128.80	125.04
14	N	603[A]	HEA	C4A-CHB-C1B	2.47	125.81	122.56
14	N	603[B]	HEA	C4A-CHB-C1B	2.47	125.81	122.56
24	P	304	PGV	C27-C26-C25	-2.47	101.91	114.42
21	A	611	DMU	C10-C5-C7	2.44	115.08	110.00
21	P	318	DMU	C6-C1-C2	2.44	115.07	110.00
21	P	324	DMU	C10-O1-C9	-2.44	108.91	113.69
21	Z	101	DMU	O5-C6-C1	2.43	115.50	110.35
14	N	603[B]	HEA	C27-C19-C20	2.43	119.36	115.27
26	C	305	CHD	C16-C17-C13	-2.42	101.17	103.55
21	C	317	DMU	C6-C1-C2	2.41	115.01	110.00
21	D	201	DMU	C2-C3-C4	-2.41	105.41	110.93
19	C	304	CDL	OA4-PA1-OA2	-2.40	96.58	107.75
19	C	304	CDL	O1-C1-CB2	2.40	117.98	109.56
14	N	603[B]	HEA	C25-C23-C24	2.38	119.87	114.60
14	A	601[B]	HEA	C25-C23-C24	2.37	119.85	114.60
14	A	601[A]	HEA	CHC-C4B-NB	-2.36	121.46	124.38
14	A	601[B]	HEA	CHC-C4B-NB	-2.36	121.46	124.38
21	M	101	DMU	O5-C6-C1	2.36	115.34	110.35
14	N	604	HEA	C13-C12-C11	-2.36	110.81	114.35
14	N	603[A]	HEA	CMB-C2B-C1B	2.33	128.59	125.04
14	N	603[B]	HEA	CMB-C2B-C1B	2.33	128.59	125.04
21	A	622	DMU	C18-O16-C6	-2.32	109.99	113.84
14	N	604	HEA	CMC-C2C-C3C	2.31	129.00	124.68
14	N	604	HEA	CMB-C2B-C1B	2.31	128.55	125.04
26	P	306	CHD	C16-C17-C13	2.31	105.81	103.55
14	A	601[A]	HEA	C27-C19-C18	-2.29	117.80	123.68
21	Q	201	DMU	O3-C5-C7	2.29	115.64	110.35
26	C	301	CHD	C22-C20-C17	-2.28	105.58	110.28
26	C	305	CHD	C18-C13-C12	-2.27	106.76	109.07
21	C	315	DMU	O3-C5-C10	2.27	115.55	110.05
14	N	604	HEA	C21-C20-C19	2.25	120.37	112.98
21	B	309	DMU	O5-C6-O16	2.24	115.28	109.97
14	N	604	HEA	CHD-C1D-C2D	-2.24	120.53	126.72
21	P	316	DMU	C10-C5-C7	2.23	114.64	110.00
14	N	603[B]	HEA	C21-C20-C19	-2.23	105.64	112.98
14	N	603[A]	HEA	O1A-CGA-CBA	-2.22	115.95	123.08
14	N	603[B]	HEA	O1A-CGA-CBA	-2.22	115.95	123.08
21	Q	201	DMU	C11-C9-C8	-2.21	107.82	113.00
19	V	101	CDL	OA4-PA1-OA5	2.21	118.00	107.75
21	N	611	DMU	O5-C6-C1	2.19	114.98	110.35
21	A	611	DMU	O3-C5-C7	2.19	115.41	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	604	HEA	C1D-ND-C4D	-2.18	102.82	105.07
21	P	319	DMU	O16-C6-C1	2.18	111.70	108.30
26	C	305	CHD	C5-C6-C7	2.17	116.86	114.46
19	V	101	CDL	OA6-CA4-CA6	-2.17	100.54	108.40
21	A	611	DMU	O5-C6-O16	2.16	115.10	109.97
21	C	319	DMU	C2-C3-C4	-2.16	105.97	110.93
21	M	101	DMU	C10-C5-C7	2.16	114.50	110.00
24	N	622	PGV	O01-C1-O02	-2.16	118.48	123.70
14	N	603[A]	HEA	CMC-C2C-C3C	2.16	128.71	124.68
14	N	603[B]	HEA	CMC-C2C-C3C	2.16	128.71	124.68
21	C	323	DMU	O3-C5-C7	2.16	115.33	110.35
14	N	604	HEA	CHC-C4B-C3B	-2.15	120.27	125.80
14	N	603[A]	HEA	CMD-C2D-C1D	2.15	128.31	125.04
14	N	603[B]	HEA	CMD-C2D-C1D	2.15	128.31	125.04
14	N	604	HEA	OMA-CMA-C3A	-2.14	120.24	124.91
21	C	318	DMU	O3-C5-C10	2.14	115.25	110.05
21	B	305	DMU	O5-C6-O16	2.14	115.05	109.97
21	P	318	DMU	C18-O16-C6	-2.12	110.32	113.84
21	P	324	DMU	O7-C10-O1	-2.11	104.77	110.67
24	P	304	PGV	O01-C1-O02	-2.11	118.61	123.70
21	B	309	DMU	O5-C6-C1	2.11	114.81	110.35
14	N	603[A]	HEA	O11-C11-C12	2.09	115.26	109.42
14	N	603[B]	HEA	O11-C11-C12	2.09	115.26	109.42
19	C	304	CDL	CA6-CA4-CA3	2.08	116.71	111.79
21	P	316	DMU	O3-C5-C7	2.08	115.16	110.35
21	P	316	DMU	C6-O5-C4	2.08	117.77	113.69
21	G	103	DMU	O5-C6-O16	2.08	114.89	109.97
19	A	607	CDL	OA2-PA1-OA3	-2.07	100.98	109.07
21	P	320	DMU	C8-C7-C5	-2.05	107.25	110.82
14	A	602	HEA	C4D-CHA-C1A	2.04	125.25	122.56
26	C	305	CHD	C14-C8-C7	-2.04	109.10	111.81
21	A	622	DMU	O3-C5-C10	2.04	115.00	110.05
21	C	315	DMU	O5-C6-C1	2.04	114.66	110.35
24	A	621	PGV	C25-C24-C23	2.03	124.73	114.42
24	P	304	PGV	O14-P-O13	2.03	122.28	112.24
19	Y	101	CDL	OB4-PB2-OB3	2.03	122.26	112.24
21	P	318	DMU	C2-C3-C4	-2.01	106.65	110.24
21	U	101	DMU	O5-C6-O16	2.01	114.73	109.97
19	P	305	CDL	OB4-PB2-OB3	2.01	122.16	112.24
21	C	319	DMU	C10-O1-C9	-2.00	109.75	113.69

There are no chirality outliers.

All (804) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C18-C19-C20-C21
14	A	601[B]	HEA	C18-C19-C20-C21
14	A	601[B]	HEA	C27-C19-C20-C21
19	A	607	CDL	C1-CA2-OA2-PA1
19	A	607	CDL	CA3-OA5-PA1-OA2
19	A	607	CDL	CB2-OB2-PB2-OB3
19	A	607	CDL	CB3-OB5-PB2-OB3
19	A	607	CDL	CB3-OB5-PB2-OB4
19	A	607	CDL	C51-CB5-OB6-CB4
19	C	304	CDL	O1-C1-CB2-OB2
19	C	304	CDL	C1-CA2-OA2-PA1
19	C	304	CDL	CA3-OA5-PA1-OA2
19	C	304	CDL	CB3-OB5-PB2-OB4
19	C	304	CDL	OB7-CB5-OB6-CB4
19	C	304	CDL	C51-CB5-OB6-CB4
19	L	101	CDL	CB2-C1-CA2-OA2
19	L	101	CDL	CA2-OA2-PA1-OA3
19	L	101	CDL	CA3-OA5-PA1-OA3
19	L	101	CDL	C11-CA5-OA6-CA4
19	L	101	CDL	CB2-OB2-PB2-OB3
19	L	101	CDL	C51-CB5-OB6-CB4
19	P	305	CDL	O1-C1-CB2-OB2
19	P	305	CDL	CA2-C1-CB2-OB2
19	P	305	CDL	C1-CA2-OA2-PA1
19	P	305	CDL	CA3-OA5-PA1-OA3
19	P	305	CDL	OA7-CA5-OA6-CA4
19	P	305	CDL	C11-CA5-OA6-CA4
19	P	305	CDL	CB2-OB2-PB2-OB4
19	P	305	CDL	OB7-CB5-OB6-CB4
19	V	101	CDL	OA6-CA4-CA6-OA8
19	V	101	CDL	CB2-OB2-PB2-OB3
19	V	101	CDL	CB3-OB5-PB2-OB4
19	Y	101	CDL	CA2-OA2-PA1-OA3
19	Y	101	CDL	CB2-OB2-PB2-OB3
19	Y	101	CDL	CB3-OB5-PB2-OB3
19	Y	101	CDL	CB3-OB5-PB2-OB4
19	Y	101	CDL	C51-CB5-OB6-CB4
21	B	305	DMU	C1-C6-O16-C18
21	B	305	DMU	O5-C6-O16-C18
21	B	309	DMU	O5-C6-O16-C18
21	B	309	DMU	C19-C18-O16-C6
21	C	318	DMU	C1-C6-O16-C18

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Mol	Chain	Res	Type	Atoms
21	C	318	DMU	O5-C6-O16-C18
21	C	318	DMU	C19-C18-O16-C6
21	D	201	DMU	C19-C18-O16-C6
21	G	103	DMU	C19-C18-O16-C6
21	L	102	DMU	C19-C18-O16-C6
21	N	611	DMU	O5-C6-O16-C18
21	O	302	DMU	C19-C18-O16-C6
21	O	307	DMU	C19-C18-O16-C6
21	Q	201	DMU	O5-C6-O16-C18
21	T	103	DMU	C1-C6-O16-C18
21	U	101	DMU	C1-C6-O16-C18
21	Y	102	DMU	O5-C6-O16-C18
21	Y	102	DMU	C19-C18-O16-C6
26	C	305	CHD	C13-C17-C20-C21
26	C	305	CHD	C13-C17-C20-C22
26	C	305	CHD	C16-C17-C20-C21
29	T	101	PEK	C11-C12-C13-C14
29	T	101	PEK	C12-C13-C14-C15
19	Y	101	CDL	OA9-CA7-OA8-CA6
19	A	607	CDL	OA7-CA5-OA6-CA4
19	A	607	CDL	OB7-CB5-OB6-CB4
19	L	101	CDL	OA7-CA5-OA6-CA4
19	L	101	CDL	OB7-CB5-OB6-CB4
19	Y	101	CDL	OB7-CB5-OB6-CB4
19	A	607	CDL	C11-CA5-OA6-CA4
19	C	304	CDL	C11-CA5-OA6-CA4
19	P	305	CDL	C51-CB5-OB6-CB4
21	C	315	DMU	O6-C11-C9-C8
26	C	305	CHD	C16-C17-C20-C22
21	P	324	DMU	O6-C11-C9-O1
14	A	601[A]	HEA	C27-C19-C20-C21
20	C	309	LFA	C12-C13-C14-C15
19	Y	101	CDL	C31-CA7-OA8-CA6
21	P	320	DMU	O6-C11-C9-O1
21	B	309	DMU	C3-C4-C57-O61
19	C	304	CDL	OA7-CA5-OA6-CA4
19	V	101	CDL	OA7-CA5-OA6-CA4
19	L	101	CDL	OA9-CA7-OA8-CA6
21	O	302	DMU	O5-C4-C57-O61
21	A	611	DMU	O6-C11-C9-C8
21	C	319	DMU	O6-C11-C9-C8
19	A	607	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
19	C	304	CDL	O1-C1-CA2-OA2
19	L	101	CDL	O1-C1-CA2-OA2
19	C	304	CDL	C31-CA7-OA8-CA6
19	L	101	CDL	C31-CA7-OA8-CA6
21	C	315	DMU	O6-C11-C9-O1
21	C	318	DMU	O5-C4-C57-O61
21	L	102	DMU	O5-C4-C57-O61
21	Q	201	DMU	O6-C11-C9-C8
19	V	101	CDL	C11-CA5-OA6-CA4
19	Y	101	CDL	C11-CA5-OA6-CA4
20	P	301	LFA	C2-C3-C4-C5
21	P	316	DMU	O5-C4-C57-O61
21	P	320	DMU	O6-C11-C9-C8
20	C	309	LFA	C11-C10-C9-C8
21	C	315	DMU	O5-C4-C57-O61
21	P	319	DMU	O6-C11-C9-O1
21	L	102	DMU	C3-C4-C57-O61
21	O	302	DMU	C3-C4-C57-O61
26	P	306	CHD	C17-C20-C22-C23
19	P	305	CDL	C31-CA7-OA8-CA6
21	A	611	DMU	O6-C11-C9-O1
21	C	318	DMU	O6-C11-C9-O1
21	T	103	DMU	O5-C4-C57-O61
20	G	105	LFA	C9-C10-C11-C12
24	A	621	PGV	C26-C27-C28-C29
14	N	603[A]	HEA	C27-C19-C20-C21
21	P	324	DMU	O6-C11-C9-C8
14	N	603[A]	HEA	C18-C19-C20-C21
26	P	306	CHD	C21-C20-C22-C23
21	B	309	DMU	O5-C4-C57-O61
21	U	101	DMU	O5-C4-C57-O61
21	N	611	DMU	O6-C11-C9-C8
14	A	601[A]	HEA	C15-C16-C17-C18
14	N	603[A]	HEA	C15-C16-C17-C18
20	P	311	LFA	C5-C6-C7-C8
21	C	318	DMU	C3-C4-C57-O61
19	A	607	CDL	C78-C79-C80-C81
20	P	310	LFA	C11-C10-C9-C8
19	A	607	CDL	CA2-C1-CB2-OB2
19	Y	101	CDL	OA7-CA5-OA6-CA4
19	C	304	CDL	OA9-CA7-OA8-CA6
19	C	304	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
19	V	101	CDL	C31-CA7-OA8-CA6
21	T	103	DMU	C3-C4-C57-O61
20	C	325	LFA	C9-C10-C11-C12
21	C	315	DMU	C3-C4-C57-O61
21	Q	201	DMU	O6-C11-C9-O1
21	P	316	DMU	C3-C4-C57-O61
19	C	304	CDL	CA7-C31-C32-C33
20	P	301	LFA	C7-C8-C9-C10
21	C	319	DMU	O6-C11-C9-O1
21	B	305	DMU	C3-C4-C57-O61
19	P	305	CDL	OA9-CA7-OA8-CA6
21	C	318	DMU	O6-C11-C9-C8
19	V	101	CDL	CA7-C31-C32-C33
19	C	304	CDL	C51-C52-C53-C54
21	P	316	DMU	C31-C34-C37-C40
21	P	320	DMU	C4-C3-O7-C10
19	C	304	CDL	CB5-C51-C52-C53
24	A	621	PGV	C23-C24-C25-C26
24	C	303	PGV	C28-C29-C30-C31
21	P	319	DMU	O5-C4-C57-O61
19	C	304	CDL	CB7-C71-C72-C73
19	P	305	CDL	CB5-C51-C52-C53
29	T	101	PEK	C1-C2-C3-C4
22	R	201	EDO	O1-C1-C2-O2
20	P	301	LFA	C10-C11-C12-C13
19	C	304	CDL	OB9-CB7-OB8-CB6
21	N	611	DMU	O16-C18-C19-C22
19	V	101	CDL	OA9-CA7-OA8-CA6
21	P	319	DMU	C3-C4-C57-O61
21	T	103	DMU	O5-C6-O16-C18
21	C	317	DMU	O16-C18-C19-C22
21	L	102	DMU	O16-C18-C19-C22
21	N	611	DMU	O6-C11-C9-O1
19	Y	101	CDL	O1-C1-CA2-OA2
21	C	318	DMU	O16-C18-C19-C22
21	Y	102	DMU	O16-C18-C19-C22
21	B	309	DMU	O16-C18-C19-C22
29	T	101	PEK	C7-C8-C9-C10
26	C	305	CHD	C21-C20-C22-C23
21	G	103	DMU	O16-C18-C19-C22
19	A	607	CDL	CB2-OB2-PB2-OB5
19	A	607	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
19	L	101	CDL	CA2-OA2-PA1-OA5
19	L	101	CDL	CA3-OA5-PA1-OA2
19	L	101	CDL	CB2-OB2-PB2-OB5
19	P	305	CDL	CA3-OA5-PA1-OA2
19	V	101	CDL	CB3-OB5-PB2-OB2
19	Y	101	CDL	CA2-OA2-PA1-OA5
19	Y	101	CDL	CB2-OB2-PB2-OB5
19	Y	101	CDL	CB3-OB5-PB2-OB2
21	P	320	DMU	O1-C10-O7-C3
19	P	305	CDL	CB7-C71-C72-C73
19	Y	101	CDL	CB2-C1-CA2-OA2
20	N	601	LFA	C5-C6-C7-C8
20	P	312	LFA	C11-C10-C9-C8
21	Z	101	DMU	O16-C18-C19-C22
20	N	601	LFA	C7-C8-C9-C10
19	L	101	CDL	C34-C35-C36-C37
20	P	312	LFA	C10-C11-C12-C13
21	C	315	DMU	C28-C31-C34-C37
19	V	101	CDL	C12-C13-C14-C15
19	V	101	CDL	C76-C77-C78-C79
19	Y	101	CDL	C16-C17-C18-C19
19	Y	101	CDL	C77-C78-C79-C80
20	C	309	LFA	C3-C4-C5-C6
20	N	601	LFA	C13-C14-C15-C16
21	C	316	DMU	C28-C31-C34-C37
21	C	318	DMU	C31-C34-C37-C40
21	M	102	DMU	C25-C28-C31-C34
21	P	319	DMU	C25-C28-C31-C34
21	Z	101	DMU	C22-C25-C28-C31
24	A	621	PGV	C29-C30-C31-C32
29	T	101	PEK	C22-C23-C24-C25
19	Y	101	CDL	C75-C76-C77-C78
20	A	609	LFA	C11-C10-C9-C8
20	G	105	LFA	C3-C4-C5-C6
20	P	311	LFA	C7-C8-C9-C10
21	P	319	DMU	C31-C34-C37-C40
21	T	103	DMU	C25-C28-C31-C34
21	Z	102	DMU	C31-C34-C37-C40
29	G	101	PEK	C16-C17-C18-C19
21	W	101	DMU	O16-C18-C19-C22
19	V	101	CDL	C17-C18-C19-C20
19	Y	101	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
21	O	305	DMU	C25-C28-C31-C34
24	C	303	PGV	C7-C8-C9-C10
19	C	304	CDL	C35-C36-C37-C38
20	O	301	LFA	C2-C3-C4-C5
20	P	310	LFA	C13-C14-C15-C16
21	C	315	DMU	C19-C22-C25-C28
21	C	317	DMU	C28-C31-C34-C37
21	G	103	DMU	C22-C25-C28-C31
21	P	318	DMU	C31-C34-C37-C40
29	T	101	PEK	C26-C27-C28-C29
19	P	305	CDL	O1-C1-CA2-OA2
19	V	101	CDL	O1-C1-CB2-OB2
19	L	101	CDL	C58-C59-C60-C61
20	B	308	LFA	C13-C14-C15-C16
20	C	312	LFA	C5-C6-C7-C8
21	O	305	DMU	C22-C25-C28-C31
21	Y	102	DMU	C1-C6-O16-C18
21	G	103	DMU	C3-C4-C57-O61
20	P	313	LFA	C1-C2-C3-C4
20	T	102	LFA	C3-C4-C5-C6
21	A	611	DMU	C31-C34-C37-C40
21	P	320	DMU	C2-C3-O7-C10
20	P	301	LFA	C11-C12-C13-C14
20	P	312	LFA	C3-C4-C5-C6
19	L	101	CDL	C18-C19-C20-C21
19	P	305	CDL	C73-C74-C75-C76
19	Y	101	CDL	C19-C20-C21-C22
20	C	311	LFA	C11-C10-C9-C8
20	P	310	LFA	C3-C4-C5-C6
21	A	623	DMU	C19-C22-C25-C28
19	L	101	CDL	C37-C38-C39-C40
19	L	101	CDL	C59-C60-C61-C62
21	P	317	DMU	C28-C31-C34-C37
21	C	317	DMU	C19-C22-C25-C28
21	C	319	DMU	C31-C34-C37-C40
21	A	611	DMU	C3-C4-C57-O61
19	P	305	CDL	CA7-C31-C32-C33
19	V	101	CDL	C74-C75-C76-C77
19	Y	101	CDL	C61-C62-C63-C64
20	B	308	LFA	C10-C11-C12-C13
20	N	601	LFA	C11-C12-C13-C14
20	P	301	LFA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	P	312	LFA	C4-C5-C6-C7
21	C	316	DMU	C31-C34-C37-C40
21	C	318	DMU	C19-C22-C25-C28
21	G	103	DMU	C19-C22-C25-C28
21	L	102	DMU	C25-C28-C31-C34
21	L	102	DMU	C31-C34-C37-C40
24	N	622	PGV	C14-C15-C16-C17
19	L	101	CDL	C72-C73-C74-C75
19	Y	101	CDL	C73-C74-C75-C76
20	B	308	LFA	C11-C12-C13-C14
24	P	304	PGV	C7-C8-C9-C10
24	P	304	PGV	C30-C31-C32-C33
21	C	306	DMU	C18-C19-C22-C25
19	A	607	CDL	C19-C20-C21-C22
19	Y	101	CDL	C63-C64-C65-C66
21	C	323	DMU	C28-C31-C34-C37
19	C	304	CDL	C13-C14-C15-C16
20	C	325	LFA	C4-C5-C6-C7
20	P	310	LFA	C4-C5-C6-C7
20	P	311	LFA	C2-C3-C4-C5
21	C	319	DMU	C19-C22-C25-C28
21	M	101	DMU	C22-C25-C28-C31
24	C	303	PGV	C14-C15-C16-C17
24	C	303	PGV	C30-C31-C32-C33
19	Y	101	CDL	C12-C13-C14-C15
20	C	309	LFA	C5-C6-C7-C8
21	B	305	DMU	C19-C18-O16-C6
21	Q	201	DMU	C19-C18-O16-C6
19	A	607	CDL	C12-C13-C14-C15
19	A	607	CDL	C17-C18-C19-C20
19	V	101	CDL	C78-C79-C80-C81
20	C	313	LFA	C4-C5-C6-C7
21	B	303	DMU	C19-C22-C25-C28
21	C	317	DMU	C31-C34-C37-C40
21	C	319	DMU	C25-C28-C31-C34
19	L	101	CDL	C22-C23-C24-C25
20	N	601	LFA	C6-C7-C8-C9
20	P	301	LFA	C9-C10-C11-C12
19	C	304	CDL	C33-C34-C35-C36
19	L	101	CDL	CA5-C11-C12-C13
21	B	309	DMU	C31-C34-C37-C40
21	P	318	DMU	C22-C25-C28-C31

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Mol	Chain	Res	Type	Atoms
21	Z	101	DMU	C25-C28-C31-C34
19	C	304	CDL	C23-C24-C25-C26
21	P	319	DMU	O6-C11-C9-C8
19	A	607	CDL	C75-C76-C77-C78
19	P	305	CDL	C75-C76-C77-C78
21	M	101	DMU	C19-C22-C25-C28
24	P	304	PGV	C12-C13-C14-C15
21	G	103	DMU	C18-C19-C22-C25
19	P	305	CDL	C56-C57-C58-C59
19	V	101	CDL	CA2-C1-CB2-OB2
20	P	312	LFA	C6-C7-C8-C9
21	A	610	DMU	C28-C31-C34-C37
21	B	304	DMU	C19-C22-C25-C28
21	C	323	DMU	O16-C18-C19-C22
21	P	320	DMU	C19-C22-C25-C28
21	O	306	DMU	C18-C19-C22-C25
19	C	304	CDL	C75-C76-C77-C78
20	A	608	LFA	C6-C7-C8-C9
20	C	325	LFA	C7-C8-C9-C10
29	G	101	PEK	C34-C35-C36-C37
19	A	607	CDL	CA5-C11-C12-C13
20	P	314	LFA	C5-C6-C7-C8
26	C	305	CHD	C17-C20-C22-C23
19	V	101	CDL	C73-C74-C75-C76
20	P	308	LFA	C7-C8-C9-C10
20	P	314	LFA	C6-C7-C8-C9
21	Y	102	DMU	C31-C34-C37-C40
19	Y	101	CDL	OB9-CB7-OB8-CB6
21	G	103	DMU	O5-C4-C57-O61
19	C	304	CDL	C22-C23-C24-C25
20	C	312	LFA	C1-C2-C3-C4
20	P	310	LFA	C12-C13-C14-C15
24	C	303	PGV	C13-C14-C15-C16
29	G	101	PEK	C26-C27-C28-C29
21	C	317	DMU	C25-C28-C31-C34
29	T	101	PEK	C15-C16-C17-C18
19	A	607	CDL	C71-CB7-OB8-CB6
19	V	101	CDL	C71-CB7-OB8-CB6
19	Y	101	CDL	C71-CB7-OB8-CB6
21	O	302	DMU	O16-C18-C19-C22
19	C	304	CDL	C71-C72-C73-C74
19	P	305	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
20	P	308	LFA	C4-C5-C6-C7
20	P	311	LFA	C6-C7-C8-C9
21	P	318	DMU	C19-C22-C25-C28
24	P	304	PGV	C24-C25-C26-C27
19	L	101	CDL	C80-C81-C82-C83
19	V	101	CDL	CB7-C71-C72-C73
19	L	101	CDL	C75-C76-C77-C78
19	P	305	CDL	C53-C54-C55-C56
21	P	307	DMU	C31-C34-C37-C40
21	W	101	DMU	C25-C28-C31-C34
21	U	101	DMU	O5-C6-O16-C18
20	C	310	LFA	C3-C4-C5-C6
20	T	102	LFA	C4-C5-C6-C7
21	O	305	DMU	C19-C22-C25-C28
20	B	308	LFA	C4-C5-C6-C7
20	O	301	LFA	C5-C6-C7-C8
21	O	307	DMU	C1-C6-O16-C18
19	L	101	CDL	OB6-CB4-CB6-OB8
21	B	305	DMU	O5-C4-C57-O61
24	A	621	PGV	C12-C13-C14-C15
24	N	622	PGV	C11-C10-C9-C8
29	T	101	PEK	C2-C3-C4-C5
20	C	311	LFA	C4-C5-C6-C7
20	P	308	LFA	C6-C7-C8-C9
21	C	319	DMU	O16-C18-C19-C22
21	J	101	DMU	C28-C31-C34-C37
24	N	622	PGV	C26-C27-C28-C29
21	B	309	DMU	C18-C19-C22-C25
19	C	304	CDL	C14-C15-C16-C17
20	N	601	LFA	C9-C10-C11-C12
29	T	101	PEK	C10-C11-C12-C13
19	Y	101	CDL	C53-C54-C55-C56
20	B	308	LFA	C12-C13-C14-C15
19	P	305	CDL	C54-C55-C56-C57
21	C	315	DMU	C18-C19-C22-C25
21	C	319	DMU	C18-C19-C22-C25
29	G	101	PEK	C28-C29-C30-C31
21	Y	102	DMU	C18-C19-C22-C25
19	V	101	CDL	CB2-OB2-PB2-OB5
21	C	317	DMU	C3-C4-C57-O61
20	C	309	LFA	C2-C3-C4-C5
19	V	101	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
19	C	304	CDL	C72-C73-C74-C75
21	L	102	DMU	C22-C25-C28-C31
21	P	320	DMU	C22-C25-C28-C31
19	P	305	CDL	C33-C34-C35-C36
19	P	305	CDL	C52-C53-C54-C55
19	Y	101	CDL	C57-C58-C59-C60
19	Y	101	CDL	C80-C81-C82-C83
20	C	307	LFA	C3-C4-C5-C6
21	A	611	DMU	O5-C4-C57-O61
19	P	305	CDL	CB3-CB4-CB6-OB8
19	V	101	CDL	CA3-CA4-CA6-OA8
21	A	610	DMU	C25-C28-C31-C34
21	B	304	DMU	C28-C31-C34-C37
21	Y	102	DMU	O5-C4-C57-O61
21	A	623	DMU	C18-C19-C22-C25
19	P	305	CDL	C35-C36-C37-C38
19	Y	101	CDL	C84-C85-C86-C87
20	C	314	LFA	C1-C2-C3-C4
21	N	602	DMU	C34-C37-C40-C43
21	W	101	DMU	C34-C37-C40-C43
21	B	303	DMU	O16-C18-C19-C22
21	P	307	DMU	O16-C18-C19-C22
19	L	101	CDL	C36-C37-C38-C39
19	V	101	CDL	C79-C80-C81-C82
20	B	308	LFA	C1-C2-C3-C4
21	C	318	DMU	C34-C37-C40-C43
21	L	102	DMU	C34-C37-C40-C43
21	Y	102	DMU	C34-C37-C40-C43
19	L	101	CDL	C84-C85-C86-C87
19	V	101	CDL	OB9-CB7-OB8-CB6
19	Y	101	CDL	C64-C65-C66-C67
21	C	315	DMU	C25-C28-C31-C34
19	L	101	CDL	C12-C13-C14-C15
19	Y	101	CDL	C76-C77-C78-C79
20	P	313	LFA	C3-C4-C5-C6
21	P	318	DMU	C18-C19-C22-C25
19	L	101	CDL	C77-C78-C79-C80
20	C	310	LFA	C7-C8-C9-C10
21	C	315	DMU	C34-C37-C40-C43
21	C	323	DMU	C22-C25-C28-C31
29	G	101	PEK	C15-C16-C17-C18
21	C	316	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
21	D	201	DMU	O6-C11-C9-O1
20	C	310	LFA	C11-C10-C9-C8
21	Q	201	DMU	C4-C3-O7-C10
20	C	310	LFA	C1-C2-C3-C4
20	P	315	LFA	C3-C4-C5-C6
21	N	610	DMU	C34-C37-C40-C43
19	A	607	CDL	CA6-CA4-OA6-CA5
21	P	316	DMU	O6-C11-C9-O1
21	O	305	DMU	O16-C18-C19-C22
21	O	306	DMU	O16-C18-C19-C22
21	P	319	DMU	C34-C37-C40-C43
21	P	320	DMU	C5-C10-O7-C3
20	C	308	LFA	C3-C4-C5-C6
19	A	607	CDL	C18-C19-C20-C21
19	V	101	CDL	C19-C20-C21-C22
20	P	308	LFA	C3-C4-C5-C6
22	C	320	EDO	O1-C1-C2-O2
21	P	319	DMU	C4-C3-O7-C10
21	P	319	DMU	O16-C18-C19-C22
21	C	306	DMU	C31-C34-C37-C40
21	M	102	DMU	C22-C25-C28-C31
19	L	101	CDL	C74-C75-C76-C77
20	P	310	LFA	C14-C15-C16-C17
21	O	307	DMU	C34-C37-C40-C43
19	A	607	CDL	OB9-CB7-OB8-CB6
19	L	101	CDL	CB5-C51-C52-C53
20	B	308	LFA	C14-C15-C16-C17
21	C	306	DMU	O16-C18-C19-C22
19	A	607	CDL	C16-C17-C18-C19
19	Y	101	CDL	CB5-C51-C52-C53
21	B	309	DMU	C34-C37-C40-C43
19	Y	101	CDL	C22-C23-C24-C25
21	A	610	DMU	C34-C37-C40-C43
19	L	101	CDL	C24-C25-C26-C27
20	C	310	LFA	C6-C7-C8-C9
20	P	308	LFA	C11-C10-C9-C8
20	T	102	LFA	C6-C7-C8-C9
21	A	622	DMU	C25-C28-C31-C34
29	T	101	PEK	C4-C5-C6-C7
21	J	101	DMU	O16-C18-C19-C22
19	V	101	CDL	C77-C78-C79-C80
20	C	307	LFA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	J	101	DMU	C25-C28-C31-C34
19	A	607	CDL	CB7-C71-C72-C73
19	C	304	CDL	C79-C80-C81-C82
21	P	319	DMU	C2-C3-O7-C10
19	L	101	CDL	C56-C57-C58-C59
20	C	307	LFA	C4-C5-C6-C7
21	P	320	DMU	C28-C31-C34-C37
19	P	305	CDL	C59-C60-C61-C62
29	G	101	PEK	C25-C26-C27-C28
19	Y	101	CDL	CA7-C31-C32-C33
20	C	310	LFA	C4-C5-C6-C7
20	C	310	LFA	C5-C6-C7-C8
20	C	311	LFA	C5-C6-C7-C8
20	P	315	LFA	C10-C11-C12-C13
19	C	304	CDL	CA4-CA3-OA5-PA1
19	V	101	CDL	C1-CA2-OA2-PA1
29	T	101	PEK	C14-C15-C16-C17
19	P	305	CDL	C13-C14-C15-C16
19	Y	101	CDL	C38-C39-C40-C41
21	C	317	DMU	C19-C18-O16-C6
21	P	318	DMU	C19-C18-O16-C6
19	L	101	CDL	C31-C32-C33-C34
19	L	101	CDL	C76-C77-C78-C79
21	B	304	DMU	O16-C18-C19-C22
21	D	201	DMU	C4-C3-O7-C10
21	U	101	DMU	C3-C4-C57-O61
19	C	304	CDL	CB3-CB4-CB6-OB8
19	L	101	CDL	CB3-CB4-CB6-OB8
21	B	303	DMU	C18-C19-C22-C25
19	Y	101	CDL	C59-C60-C61-C62
20	N	601	LFA	C11-C10-C9-C8
24	P	304	PGV	C11-C12-C13-C14
19	V	101	CDL	C18-C19-C20-C21
29	T	101	PEK	C11-C10-C9-C8
19	V	101	CDL	C32-C33-C34-C35
19	V	101	CDL	C31-C32-C33-C34
20	P	308	LFA	C2-C3-C4-C5
20	P	312	LFA	C1-C2-C3-C4
19	Y	101	CDL	OA5-CA3-CA4-OA6
21	N	602	DMU	O16-C18-C19-C22
19	P	305	CDL	C76-C77-C78-C79
19	A	607	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
20	P	315	LFA	C9-C10-C11-C12
24	P	304	PGV	C27-C28-C29-C30
19	A	607	CDL	C15-C16-C17-C18
19	C	304	CDL	OB6-CB4-CB6-OB8
21	Q	201	DMU	O5-C4-C57-O61
20	C	314	LFA	C11-C10-C9-C8
19	P	305	CDL	C12-C11-CA5-OA6
19	C	304	CDL	C18-C19-C20-C21
20	C	325	LFA	C6-C7-C8-C9
19	P	305	CDL	CA4-CA3-OA5-PA1
24	C	303	PGV	C02-C03-O11-P
24	P	304	PGV	C02-C03-O11-P
21	J	101	DMU	C18-C19-C22-C25
24	A	621	PGV	C11-C10-C9-C8
20	N	601	LFA	C1-C2-C3-C4
26	P	306	CHD	C20-C22-C23-C24
19	Y	101	CDL	C31-C32-C33-C34
22	P	321	EDO	O1-C1-C2-O2
21	Y	102	DMU	C25-C28-C31-C34
20	P	315	LFA	C2-C3-C4-C5
24	A	621	PGV	C31-C32-C33-C34
19	Y	101	CDL	C79-C80-C81-C82
20	A	609	LFA	C6-C7-C8-C9
20	N	601	LFA	C14-C15-C16-C17
29	G	101	PEK	C29-C30-C31-C32
19	L	101	CDL	C15-C16-C17-C18
21	C	317	DMU	O5-C4-C57-O61
19	C	304	CDL	C77-C78-C79-C80
21	B	305	DMU	C31-C34-C37-C40
19	P	305	CDL	C57-C58-C59-C60
21	Z	102	DMU	C22-C25-C28-C31
21	M	101	DMU	C25-C28-C31-C34
19	L	101	CDL	C62-C63-C64-C65
21	B	305	DMU	C18-C19-C22-C25
24	C	303	PGV	C29-C30-C31-C32
20	A	608	LFA	C9-C10-C11-C12
21	Q	201	DMU	C2-C3-O7-C10
19	P	305	CDL	CA3-CA4-CA6-OA8
19	Y	101	CDL	C23-C24-C25-C26
20	P	314	LFA	C4-C5-C6-C7
19	V	101	CDL	OB5-CB3-CB4-OB6
29	G	101	PEK	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
20	B	308	LFA	C6-C7-C8-C9
21	P	316	DMU	C19-C22-C25-C28
19	C	304	CDL	CB2-C1-CA2-OA2
19	P	305	CDL	C18-C19-C20-C21
21	N	611	DMU	C34-C37-C40-C43
21	A	622	DMU	C1-C6-O16-C18
19	A	607	CDL	OA6-CA4-CA6-OA8
19	Y	101	CDL	OB6-CB4-CB6-OB8
19	L	101	CDL	C52-C53-C54-C55
24	N	622	PGV	C12-C13-C14-C15
20	G	105	LFA	C10-C11-C12-C13
21	D	201	DMU	O16-C18-C19-C22
24	N	622	PGV	C15-C16-C17-C18
21	C	323	DMU	O1-C10-O7-C3
19	P	305	CDL	C21-C22-C23-C24
21	O	307	DMU	O16-C18-C19-C22
19	C	304	CDL	C52-C53-C54-C55
24	N	622	PGV	C29-C30-C31-C32
20	C	325	LFA	C10-C11-C12-C13
21	O	306	DMU	C19-C22-C25-C28
20	C	312	LFA	C11-C10-C9-C8
20	C	314	LFA	C10-C11-C12-C13
21	C	323	DMU	C5-C10-O7-C3
20	A	609	LFA	C2-C3-C4-C5
20	N	601	LFA	C4-C5-C6-C7
21	C	319	DMU	C28-C31-C34-C37
19	A	607	CDL	CA3-OA5-PA1-OA3
19	A	607	CDL	CB2-OB2-PB2-OB4
19	C	304	CDL	CA3-OA5-PA1-OA3
19	L	101	CDL	CA2-OA2-PA1-OA4
19	V	101	CDL	CA3-OA5-PA1-OA4
19	V	101	CDL	CB2-OB2-PB2-OB4
19	V	101	CDL	CB3-OB5-PB2-OB3
19	Y	101	CDL	CA2-OA2-PA1-OA4
19	Y	101	CDL	CB2-OB2-PB2-OB4
19	Y	101	CDL	OA5-CA3-CA4-CA6
21	D	201	DMU	C2-C3-O7-C10
21	W	101	DMU	C31-C34-C37-C40
21	Z	101	DMU	C34-C37-C40-C43
24	N	622	PGV	C31-C32-C33-C34
20	A	608	LFA	C7-C8-C9-C10
20	N	609	LFA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	C	304	CDL	CA2-C1-CB2-OB2
21	Q	201	DMU	C34-C37-C40-C43
19	C	304	CDL	C84-C85-C86-C87
19	C	304	CDL	C12-C11-CA5-OA6
19	L	101	CDL	CA3-CA4-CA6-OA8
19	Y	101	CDL	CA3-CA4-CA6-OA8
19	L	101	CDL	OA6-CA4-CA6-OA8
19	P	305	CDL	OB6-CB4-CB6-OB8
19	Y	101	CDL	OA6-CA4-CA6-OA8
20	C	309	LFA	C13-C14-C15-C16
21	P	319	DMU	C28-C31-C34-C37
20	A	609	LFA	C11-C12-C13-C14
21	P	324	DMU	O16-C18-C19-C22
20	P	315	LFA	C6-C7-C8-C9
19	P	305	CDL	C71-CB7-OB8-CB6
19	A	607	CDL	C71-C72-C73-C74
19	P	305	CDL	C72-C73-C74-C75
19	L	101	CDL	C72-C71-CB7-OB8
21	T	103	DMU	C22-C25-C28-C31
19	Y	101	CDL	C13-C14-C15-C16
19	P	305	CDL	OB9-CB7-OB8-CB6
20	P	314	LFA	C9-C10-C11-C12
20	G	105	LFA	C11-C10-C9-C8
20	P	311	LFA	C11-C10-C9-C8
19	C	304	CDL	C78-C79-C80-C81
21	N	610	DMU	C25-C28-C31-C34
19	V	101	CDL	C72-C73-C74-C75
29	T	101	PEK	C29-C30-C31-C32
19	V	101	CDL	C15-C16-C17-C18
20	C	314	LFA	C5-C6-C7-C8
20	G	105	LFA	C5-C6-C7-C8
21	C	319	DMU	C34-C37-C40-C43
20	O	301	LFA	C1-C2-C3-C4
21	D	201	DMU	C19-C22-C25-C28
21	M	102	DMU	C28-C31-C34-C37
21	B	304	DMU	C22-C25-C28-C31
20	C	309	LFA	C14-C15-C16-C17
19	C	304	CDL	C16-C17-C18-C19
19	P	305	CDL	OA5-CA3-CA4-OA6
19	Y	101	CDL	C18-C19-C20-C21
29	T	101	PEK	C17-C18-C19-C20
29	T	101	PEK	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
21	P	316	DMU	C4-C3-O7-C10
21	O	302	DMU	C1-C6-O16-C18
19	C	304	CDL	C55-C56-C57-C58
19	L	101	CDL	C51-C52-C53-C54
19	Y	101	CDL	CA5-C11-C12-C13
20	C	313	LFA	C2-C3-C4-C5
19	C	304	CDL	C17-C18-C19-C20
20	P	308	LFA	C1-C2-C3-C4
21	N	610	DMU	C28-C31-C34-C37
21	C	323	DMU	C31-C34-C37-C40
19	P	305	CDL	C20-C21-C22-C23
14	A	602	HEA	CAA-CBA-CGA-O1A
19	Y	101	CDL	C32-C33-C34-C35
21	W	101	DMU	C22-C25-C28-C31
29	G	101	PEK	C32-C33-C34-C35
19	Y	101	CDL	C21-C22-C23-C24
24	C	303	PGV	C22-C23-C24-C25
19	P	305	CDL	C11-C12-C13-C14
19	L	101	CDL	C60-C61-C62-C63
21	P	324	DMU	C19-C22-C25-C28
19	L	101	CDL	C64-C65-C66-C67
20	N	609	LFA	C2-C3-C4-C5
24	A	621	PGV	C28-C29-C30-C31
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
14	A	601[B]	HEA	CAD-CBD-CGD-O1D
21	D	201	DMU	O5-C6-O16-C18
21	P	324	DMU	O1-C10-O7-C3
20	B	308	LFA	C11-C10-C9-C8
26	G	102	CHD	C22-C23-C24-O25
19	V	101	CDL	OB6-CB4-CB6-OB8
19	V	101	CDL	C20-C21-C22-C23
24	N	622	PGV	O03-C19-C20-C21
21	A	623	DMU	C25-C28-C31-C34
26	C	305	CHD	C22-C23-C24-O25
22	R	203	EDO	O1-C1-C2-O2
19	Y	101	CDL	C58-C59-C60-C61
26	P	306	CHD	C22-C23-C24-O26
21	P	316	DMU	C22-C25-C28-C31
21	C	323	DMU	C18-C19-C22-C25
26	B	307	CHD	C22-C23-C24-O25
26	B	307	CHD	C22-C23-C24-O26
20	C	311	LFA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	N	603[A]	HEA	CAD-CBD-CGD-O1D
14	N	603[B]	HEA	CAD-CBD-CGD-O1D
21	B	309	DMU	C25-C28-C31-C34
20	T	102	LFA	C7-C8-C9-C10
21	A	622	DMU	C19-C22-C25-C28
14	N	604	HEA	CAA-CBA-CGA-O1A
26	P	306	CHD	C22-C23-C24-O25
21	P	324	DMU	C5-C10-O7-C3
21	Z	102	DMU	C34-C37-C40-C43
21	B	305	DMU	C34-C37-C40-C43
14	N	604	HEA	CAA-CBA-CGA-O2A
26	G	102	CHD	C22-C23-C24-O26
21	B	304	DMU	C18-C19-C22-C25
21	P	320	DMU	C18-C19-C22-C25
20	C	313	LFA	C11-C12-C13-C14
26	C	305	CHD	C22-C23-C24-O26
19	C	304	CDL	C12-C13-C14-C15
19	Y	101	CDL	C54-C55-C56-C57
14	A	602	HEA	CAD-CBD-CGD-O1D
21	P	319	DMU	C5-C10-O7-C3
20	C	311	LFA	C10-C11-C12-C13
29	T	101	PEK	O02-C1-O01-C02
14	A	602	HEA	CAA-CBA-CGA-O2A
19	P	305	CDL	C80-C81-C82-C83
21	Z	101	DMU	O6-C11-C9-C8
21	O	302	DMU	C34-C37-C40-C43
29	T	101	PEK	C13-C14-C15-C16
21	C	315	DMU	O1-C10-O7-C3
14	A	602	HEA	CAD-CBD-CGD-O2D
19	P	305	CDL	C23-C24-C25-C26
20	N	609	LFA	C11-C12-C13-C14
24	A	621	PGV	C13-C14-C15-C16
24	A	621	PGV	O03-C19-C20-C21
20	P	314	LFA	C2-C3-C4-C5
21	N	610	DMU	C31-C34-C37-C40
22	A	613	EDO	O1-C1-C2-O2
21	P	316	DMU	C2-C3-O7-C10
26	C	301	CHD	C22-C23-C24-O26
19	P	305	CDL	C12-C11-CA5-OA7
24	C	303	PGV	C24-C25-C26-C27
24	C	303	PGV	C25-C26-C27-C28
21	P	318	DMU	C28-C31-C34-C37

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Mol	Chain	Res	Type	Atoms
29	T	101	PEK	C34-C35-C36-C37
14	N	604	HEA	CAD-CBD-CGD-O2D
20	C	325	LFA	C1-C2-C3-C4
21	B	305	DMU	C19-C22-C25-C28
21	O	307	DMU	C18-C19-C22-C25
19	C	304	CDL	C20-C21-C22-C23
19	L	101	CDL	C73-C74-C75-C76
20	P	301	LFA	C4-C5-C6-C7
21	O	302	DMU	C18-C19-C22-C25
19	L	101	CDL	C53-C54-C55-C56
21	C	315	DMU	C5-C10-O7-C3
21	O	307	DMU	O5-C6-O16-C18
19	C	304	CDL	C73-C74-C75-C76
19	V	101	CDL	CB4-CB3-OB5-PB2
26	P	302	CHD	C22-C23-C24-O26
21	O	305	DMU	C31-C34-C37-C40
20	O	301	LFA	C7-C8-C9-C10
14	N	604	HEA	CAD-CBD-CGD-O1D
24	A	621	PGV	C15-C16-C17-C18
19	P	305	CDL	CA2-OA2-PA1-OA5
20	P	309	LFA	C1-C2-C3-C4
19	C	304	CDL	C52-C51-CB5-OB6
20	P	310	LFA	C11-C12-C13-C14
21	W	101	DMU	C19-C22-C25-C28
20	N	601	LFA	C3-C4-C5-C6
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
14	A	601[B]	HEA	CAD-CBD-CGD-O2D
19	P	305	CDL	C52-C51-CB5-OB6
21	T	103	DMU	C18-C19-C22-C25
21	P	319	DMU	O1-C10-O7-C3
19	V	101	CDL	CA5-C11-C12-C13
14	A	601[A]	HEA	C12-C11-C3B-C2B
14	A	601[B]	HEA	C12-C11-C3B-C2B
21	B	305	DMU	O16-C18-C19-C22
21	N	611	DMU	C19-C22-C25-C28
21	P	316	DMU	O1-C10-O7-C3
19	L	101	CDL	C21-C22-C23-C24
19	V	101	CDL	C72-C71-CB7-OB8
20	C	307	LFA	C1-C2-C3-C4
19	V	101	CDL	C16-C17-C18-C19
26	P	302	CHD	C22-C23-C24-O25
20	P	301	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	W	101	DMU	C28-C31-C34-C37
26	C	301	CHD	C22-C23-C24-O25
21	J	101	DMU	C34-C37-C40-C43
21	C	318	DMU	C5-C10-O7-C3
20	C	313	LFA	C1-C2-C3-C4
21	O	306	DMU	C25-C28-C31-C34
24	P	304	PGV	C9-C10-C11-C12
14	N	603[A]	HEA	C19-C20-C21-C22
14	N	603[A]	HEA	CAD-CBD-CGD-O2D
14	N	603[B]	HEA	CAD-CBD-CGD-O2D
19	Y	101	CDL	C72-C73-C74-C75
19	P	305	CDL	C52-C51-CB5-OB7
19	V	101	CDL	C72-C71-CB7-OB9
24	N	622	PGV	C22-C23-C24-C25
21	M	102	DMU	C34-C37-C40-C43
21	N	611	DMU	C31-C34-C37-C40
21	P	316	DMU	C5-C10-O7-C3
21	A	611	DMU	C4-C3-O7-C10
21	Y	102	DMU	C22-C25-C28-C31
19	L	101	CDL	C17-C18-C19-C20
19	L	101	CDL	C78-C79-C80-C81
19	P	305	CDL	C72-C71-CB7-OB8
24	C	303	PGV	C05-C04-O12-P
24	P	304	PGV	C05-C04-O12-P
21	A	611	DMU	C2-C3-O7-C10
19	C	304	CDL	C52-C51-CB5-OB7
29	T	101	PEK	C3-C4-C5-C6
19	A	607	CDL	CA2-OA2-PA1-OA3
19	L	101	CDL	CA3-OA5-PA1-OA4
19	P	305	CDL	CB2-OB2-PB2-OB3
19	P	305	CDL	C55-C56-C57-C58
19	P	305	CDL	C78-C79-C80-C81
20	P	310	LFA	C5-C6-C7-C8
20	T	102	LFA	C11-C10-C9-C8
21	T	103	DMU	C19-C22-C25-C28
21	C	319	DMU	C22-C25-C28-C31
24	A	621	PGV	C30-C31-C32-C33
19	A	607	CDL	C72-C71-CB7-OB8
29	T	101	PEK	O01-C1-C2-C3
21	N	602	DMU	C19-C22-C25-C28
19	P	305	CDL	C72-C71-CB7-OB9
21	A	622	DMU	C19-C18-O16-C6

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Mol	Chain	Res	Type	Atoms
24	A	621	PGV	C14-C15-C16-C17
19	C	304	CDL	C34-C35-C36-C37
19	C	304	CDL	C72-C71-CB7-OB8
21	C	315	DMU	C4-C3-O7-C10
20	A	609	LFA	C5-C6-C7-C8
21	O	306	DMU	C28-C31-C34-C37

There are no ring outliers.

52 monomers are involved in 127 short contacts:

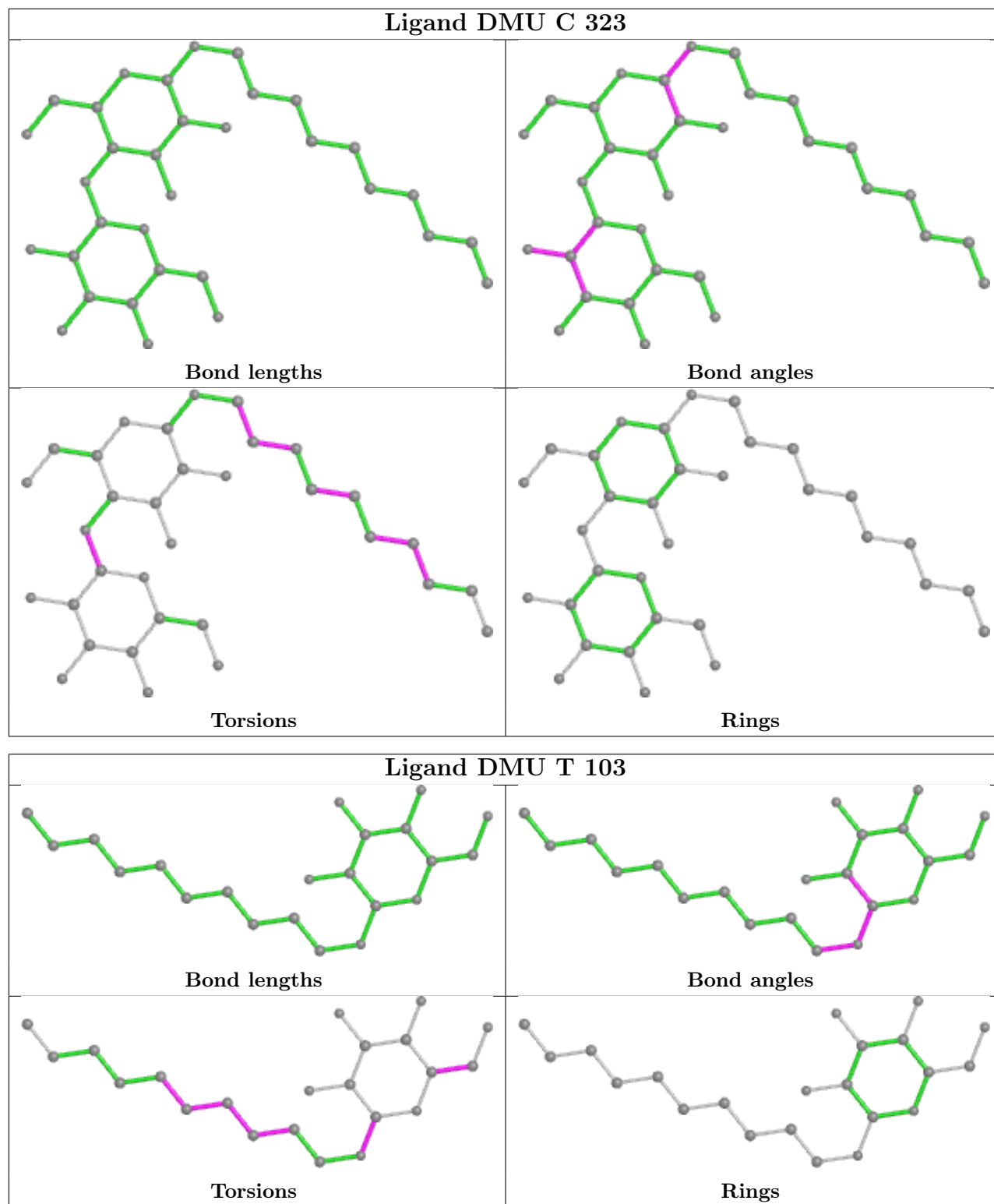
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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21	T	103	DMU	1	0
21	C	318	DMU	3	0
19	Y	101	CDL	4	0
24	N	622	PGV	2	0
26	B	307	CHD	1	0
20	C	313	LFA	1	0
20	P	314	LFA	3	0
20	N	609	LFA	4	0
26	P	306	CHD	2	0
20	C	314	LFA	1	0
21	Y	102	DMU	1	0
14	N	603[B]	HEA	1	0
29	T	101	PEK	4	0
14	A	601[A]	HEA	4	0
19	V	101	CDL	1	0
18	A	606	PER	1	0
20	B	308	LFA	1	0
20	P	313	LFA	1	0
21	L	102	DMU	1	0
20	P	310	LFA	3	0
14	N	604	HEA	2	0
24	C	303	PGV	1	0
18	N	608	PER	1	0
21	A	622	DMU	1	0
20	G	105	LFA	6	0
21	D	201	DMU	3	0
21	B	309	DMU	1	0
20	N	601	LFA	1	0
26	C	305	CHD	1	0
20	A	609	LFA	6	0

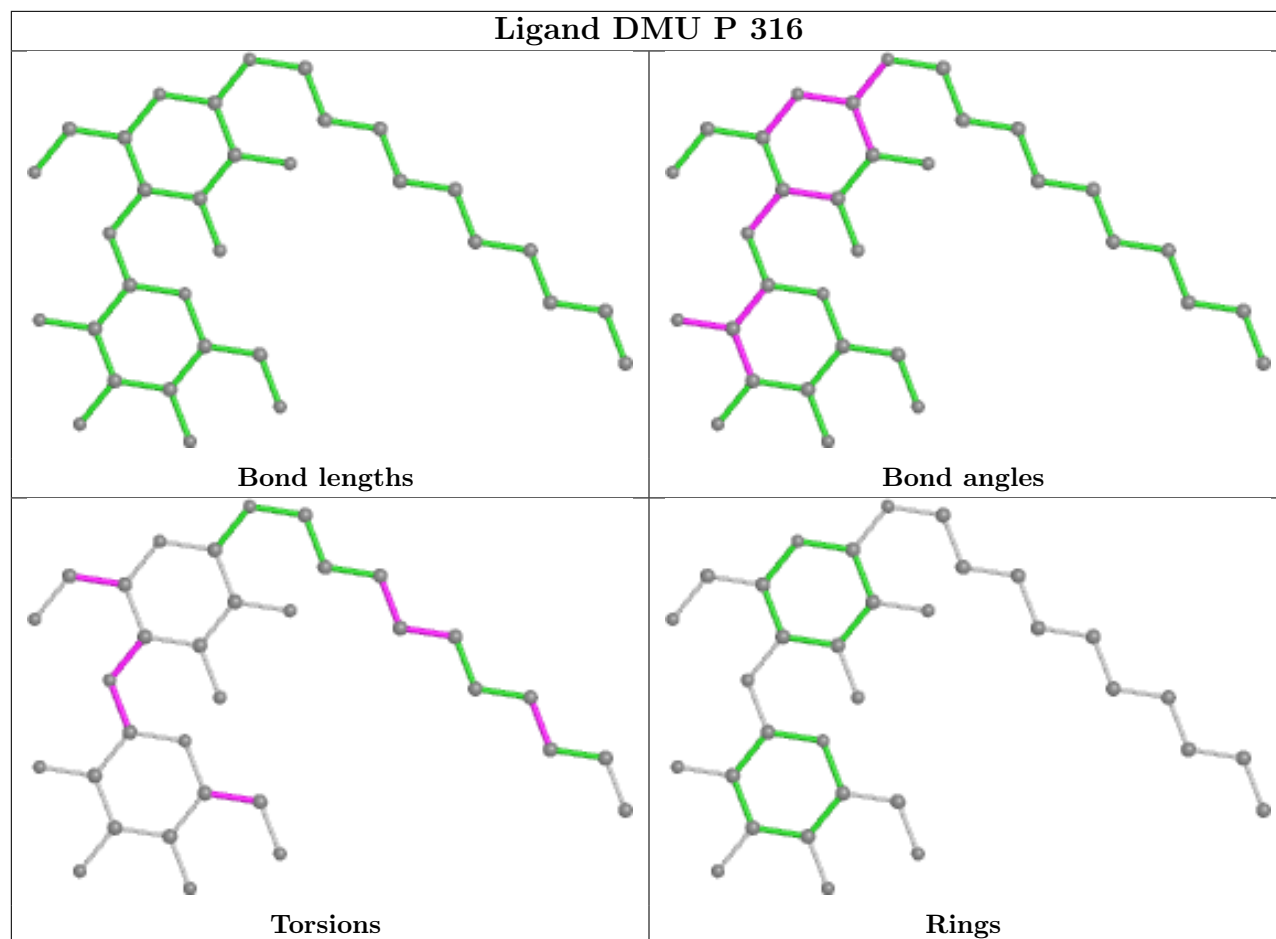
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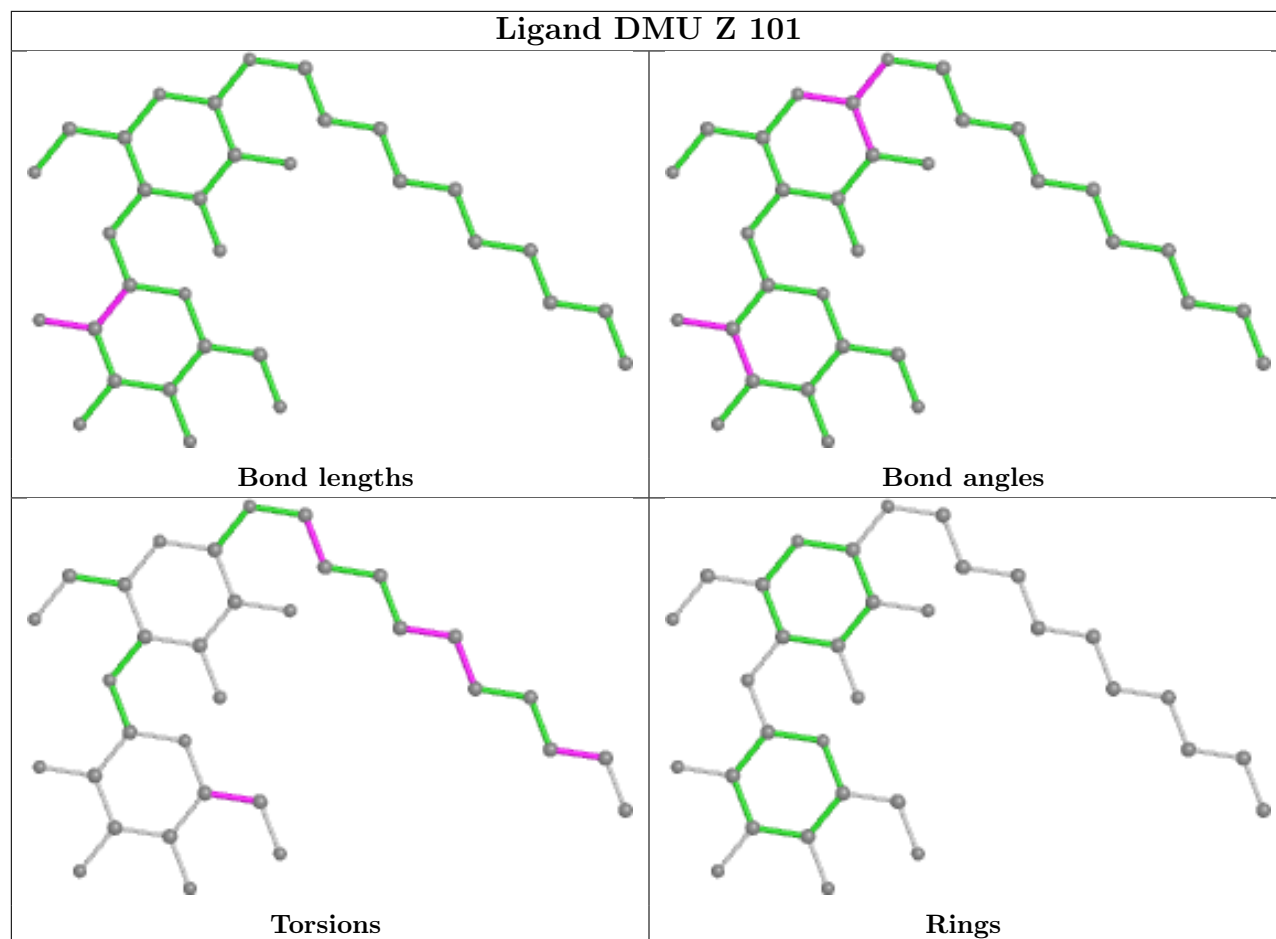
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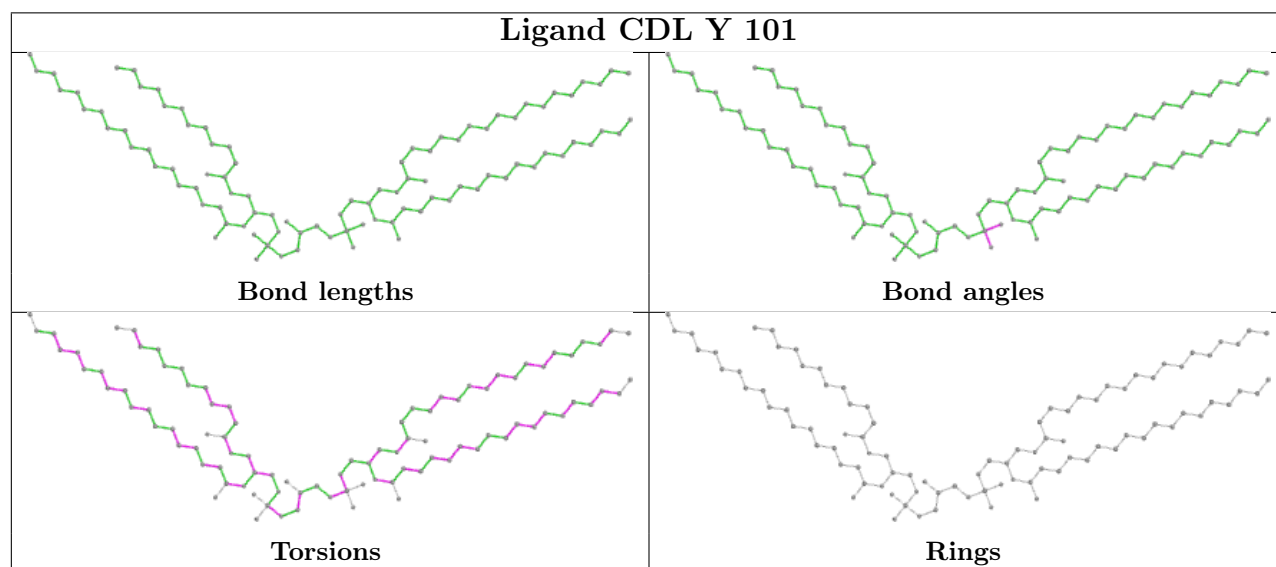
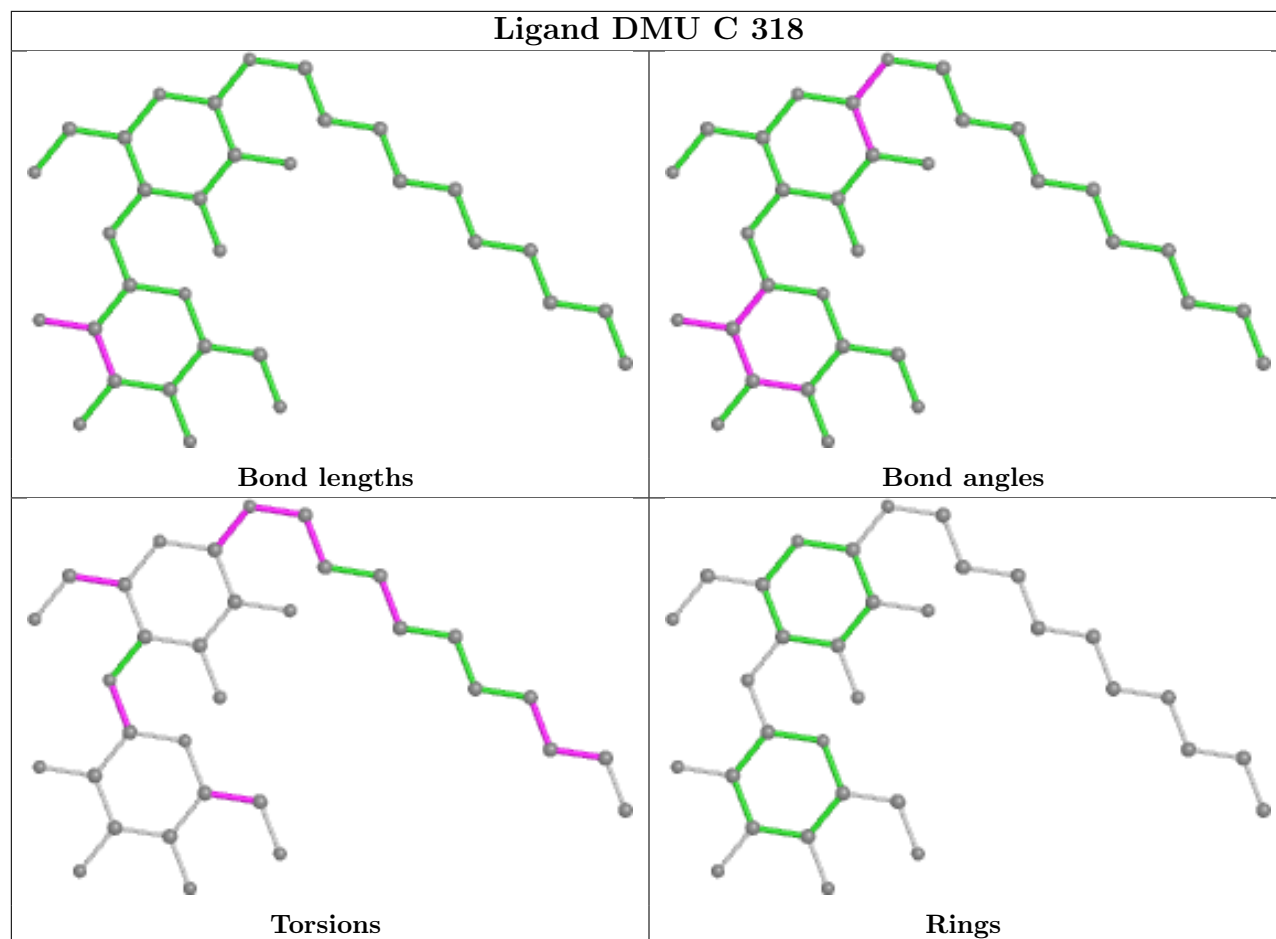
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	610	DMU	1	0
14	N	603[A]	HEA	4	0
20	P	308	LFA	1	0
19	C	304	CDL	18	0
20	P	315	LFA	1	0
20	C	312	LFA	2	0
21	P	319	DMU	1	0
26	G	102	CHD	1	0
26	P	302	CHD	1	0
21	N	610	DMU	1	0
21	Q	201	DMU	1	0
21	P	324	DMU	5	0
19	L	101	CDL	4	0
21	B	305	DMU	1	0
22	A	613	EDO	1	0
20	A	608	LFA	3	0
20	O	301	LFA	2	0
21	A	611	DMU	1	0
19	P	305	CDL	14	0
20	C	307	LFA	3	0
21	U	101	DMU	1	0

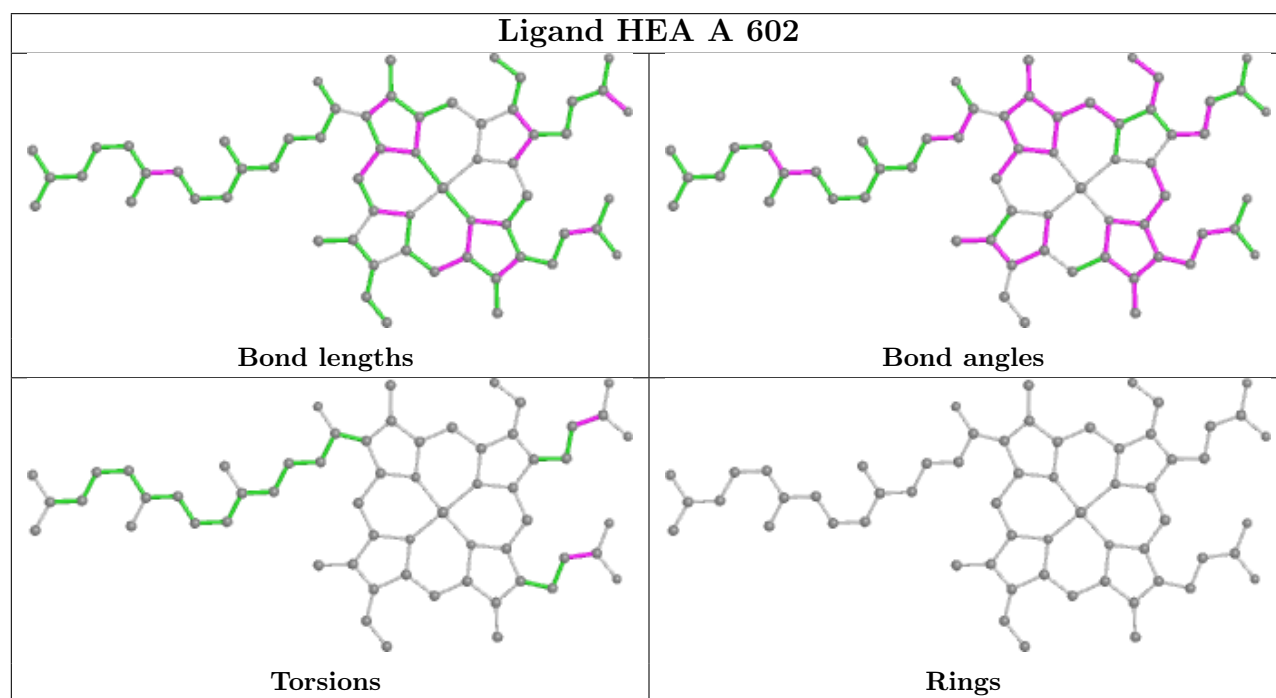
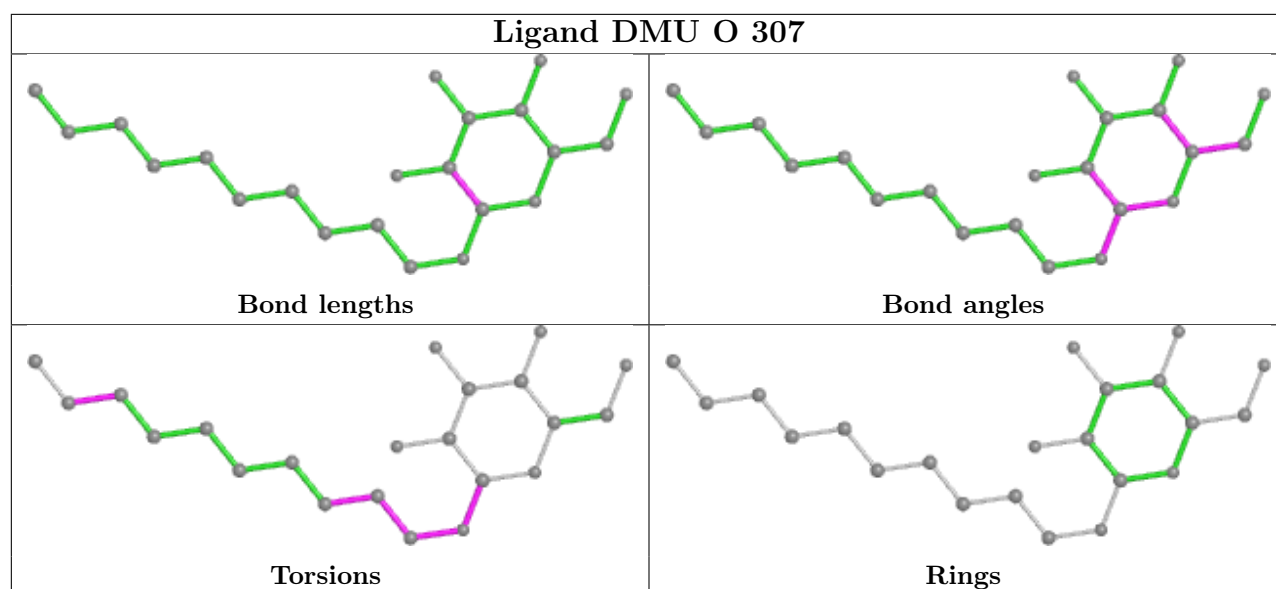
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

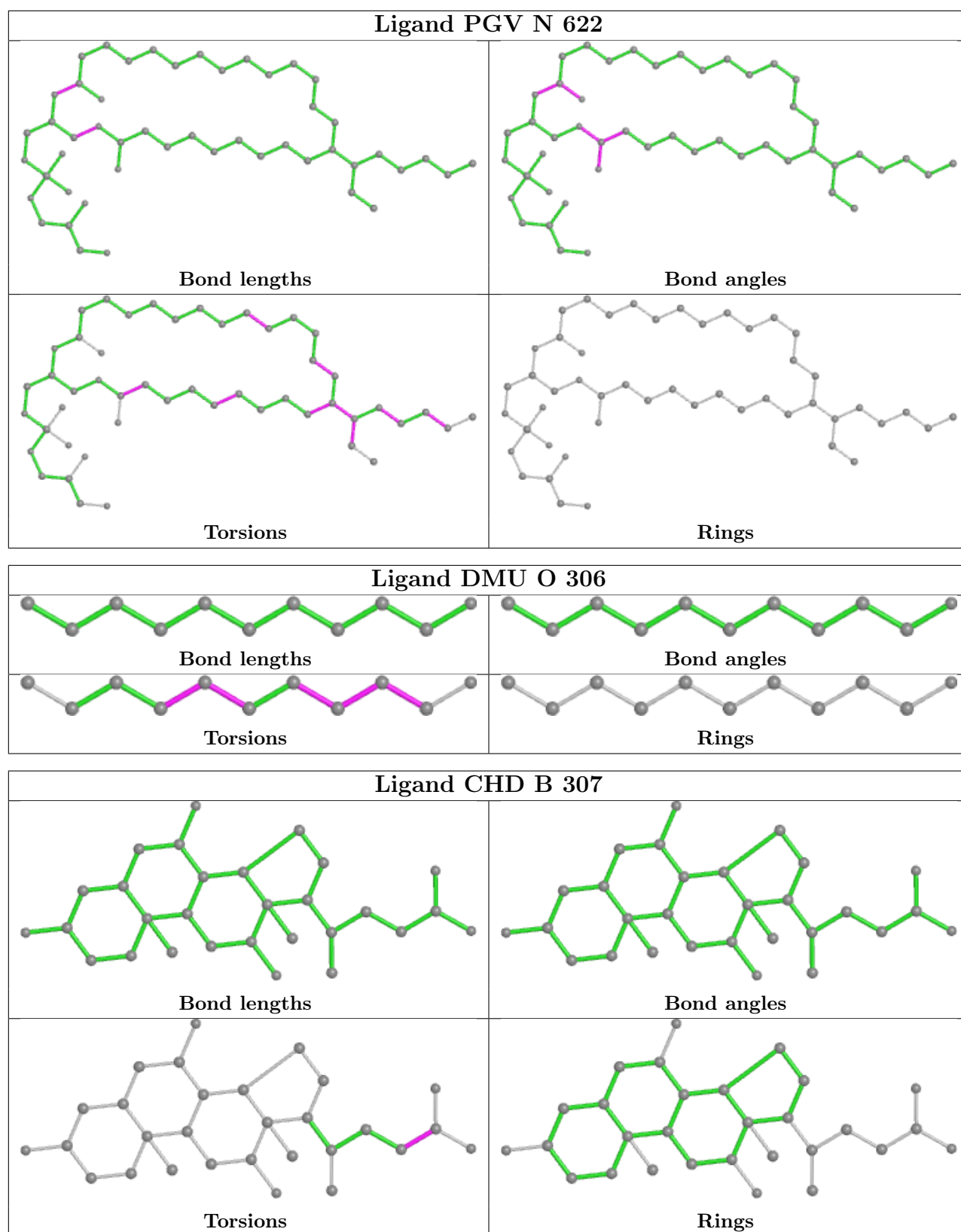


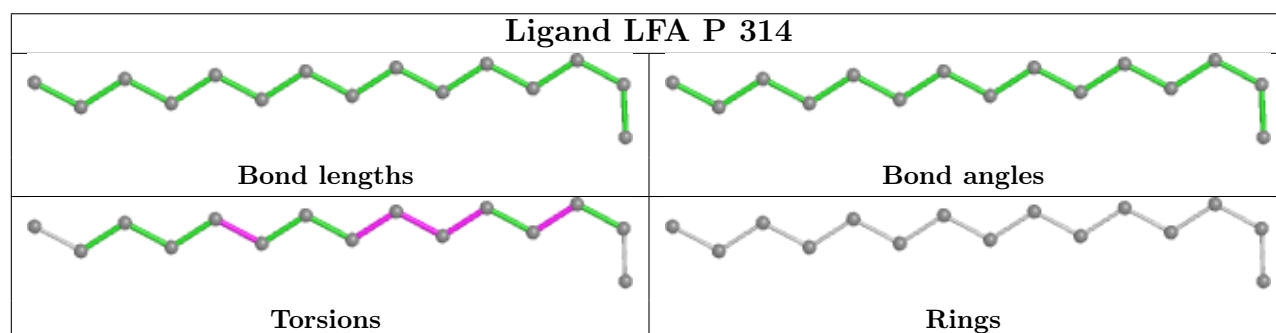
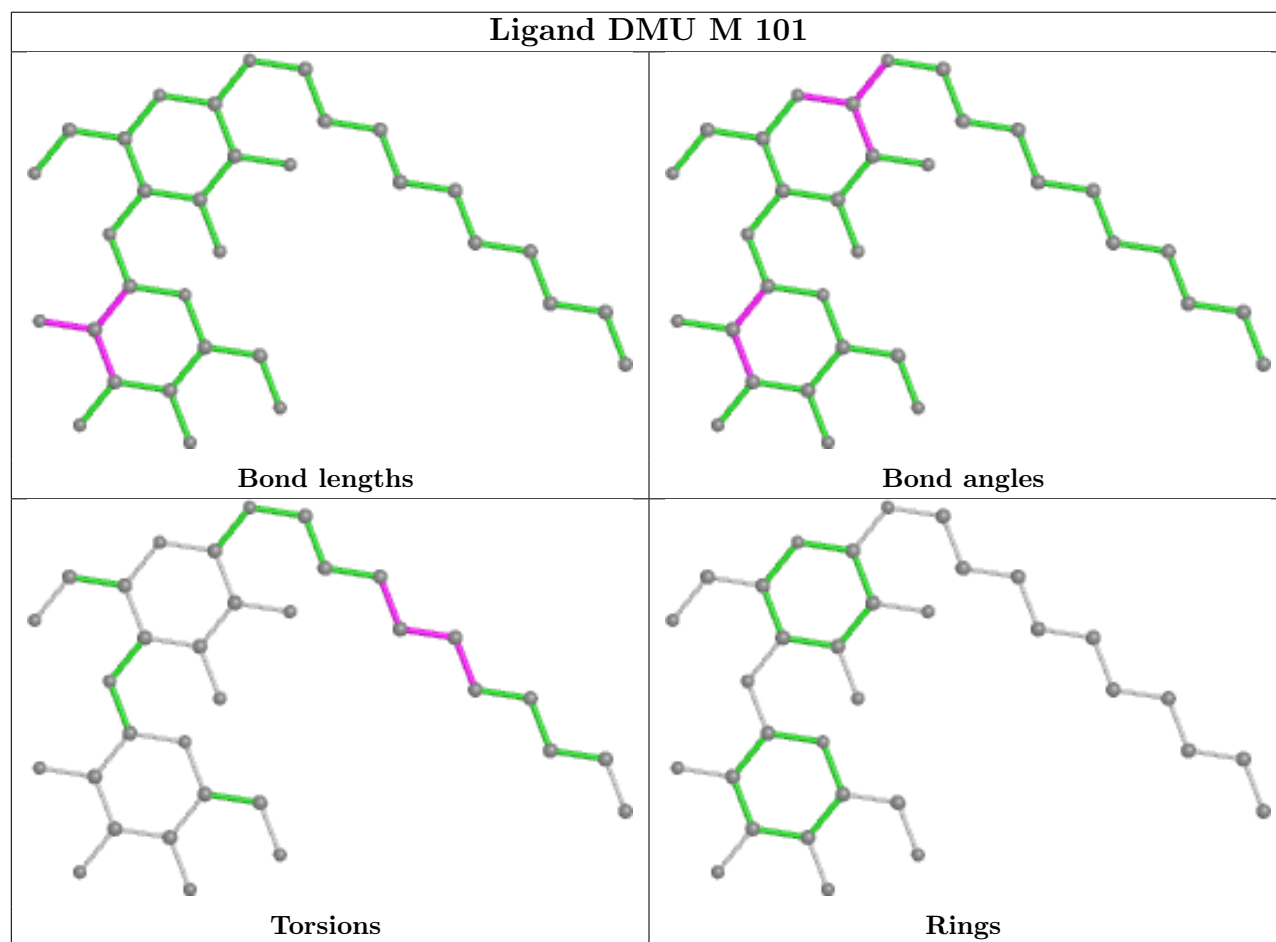
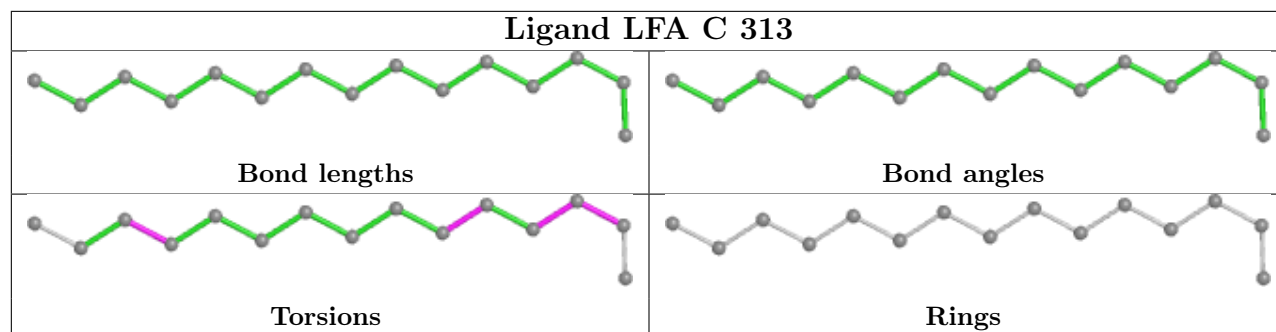


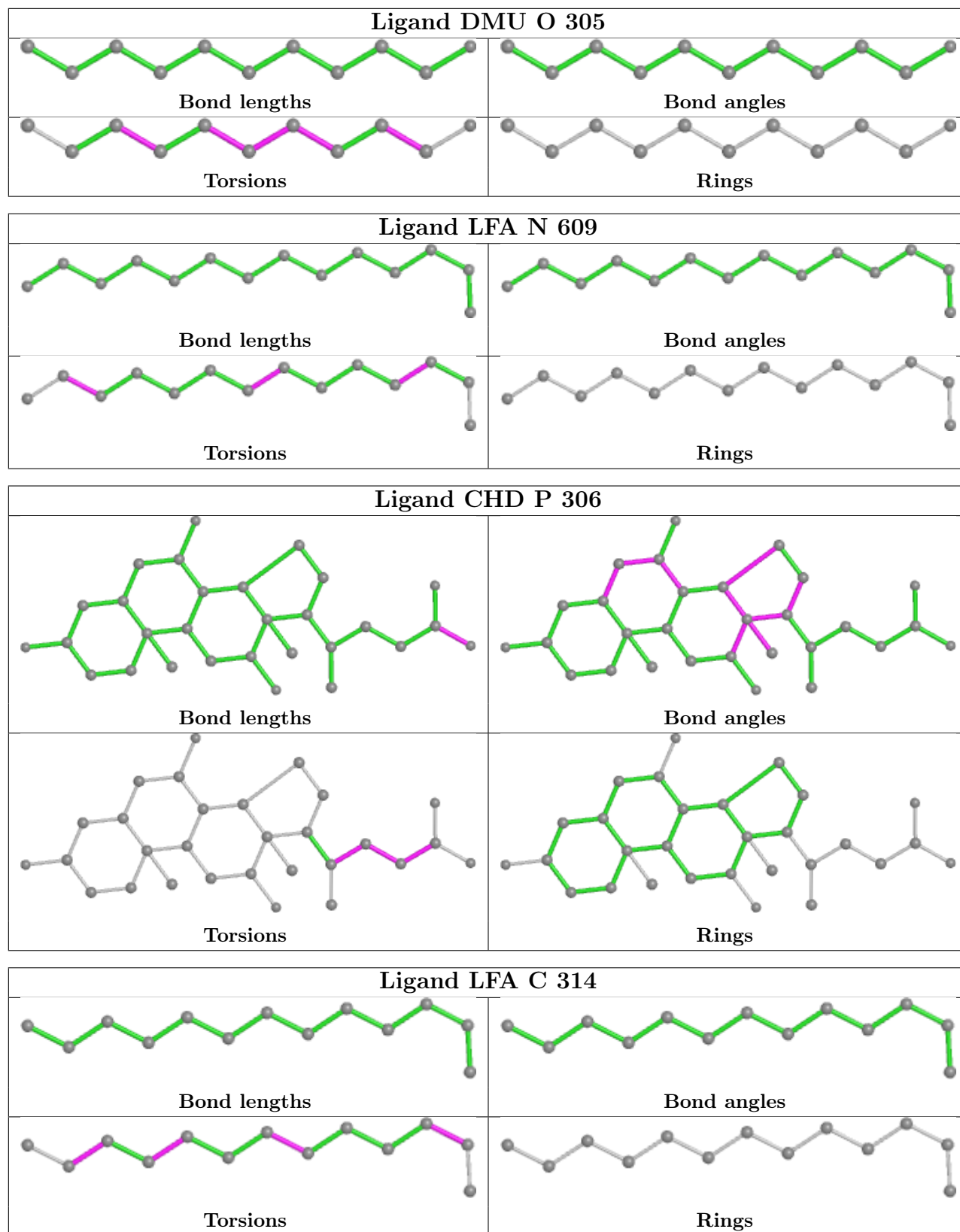


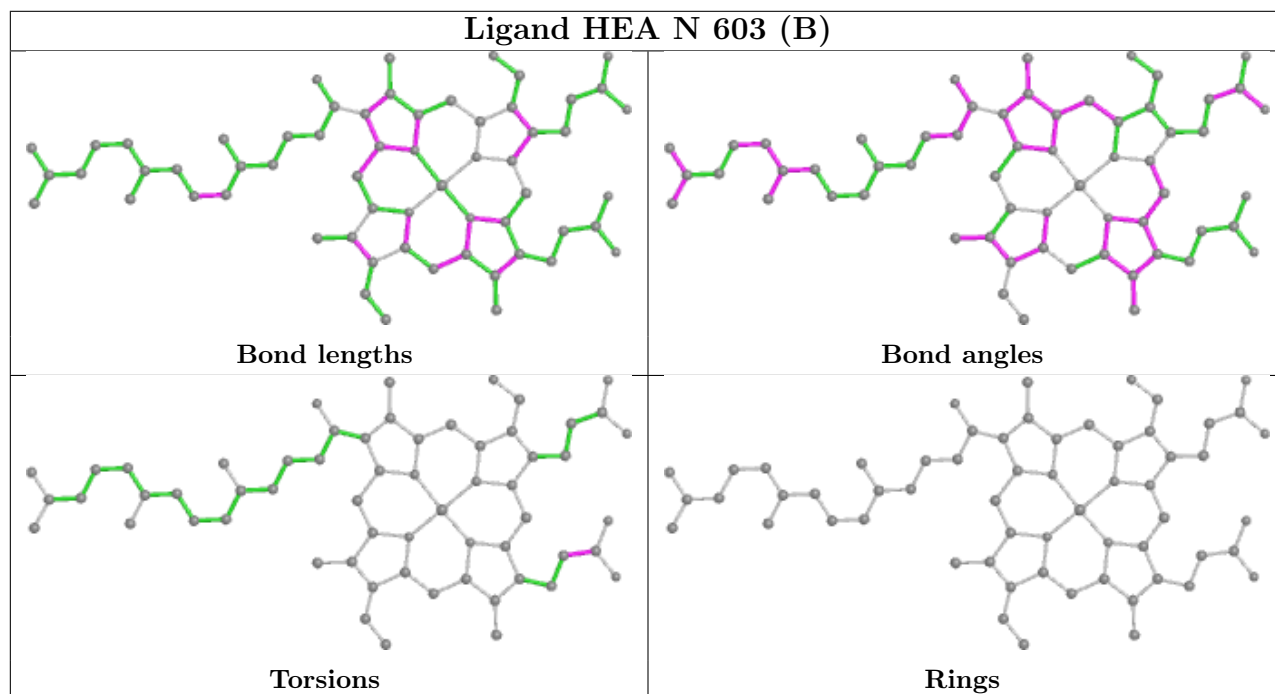
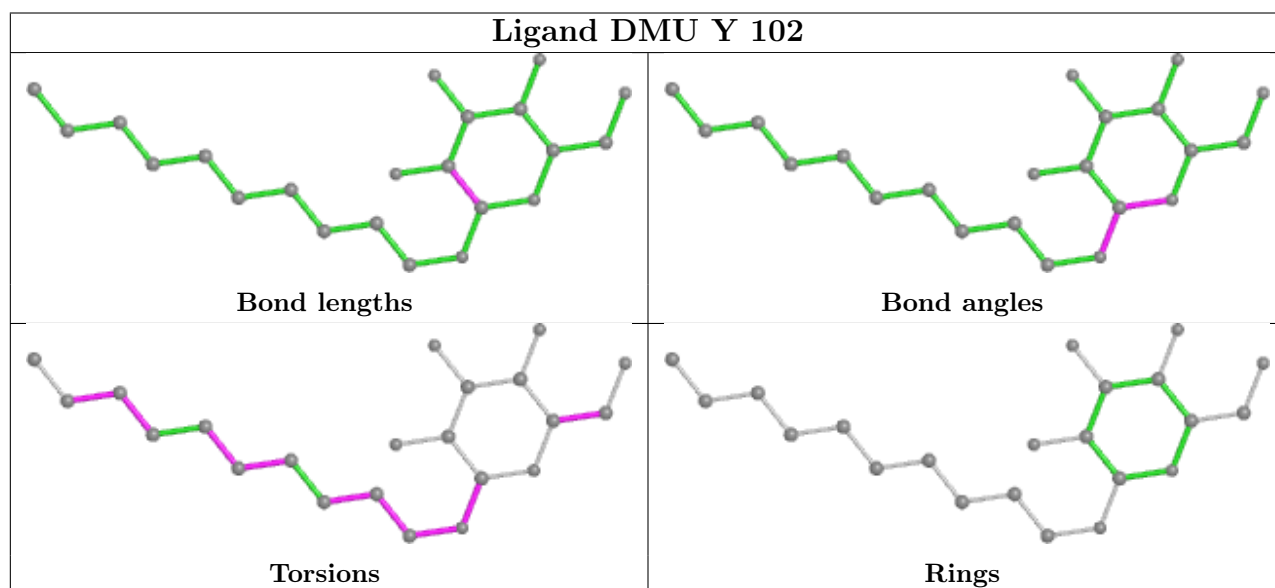
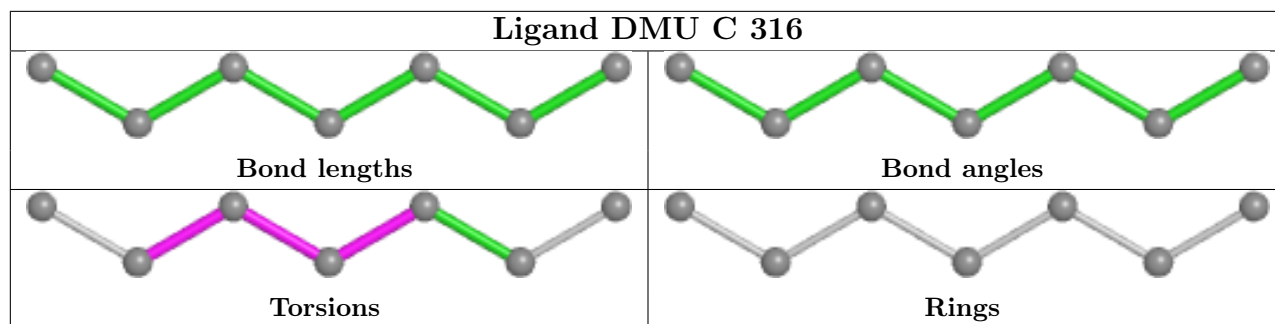


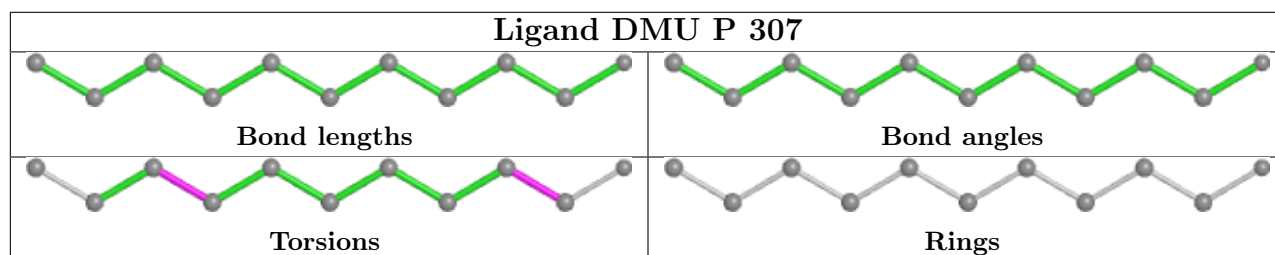
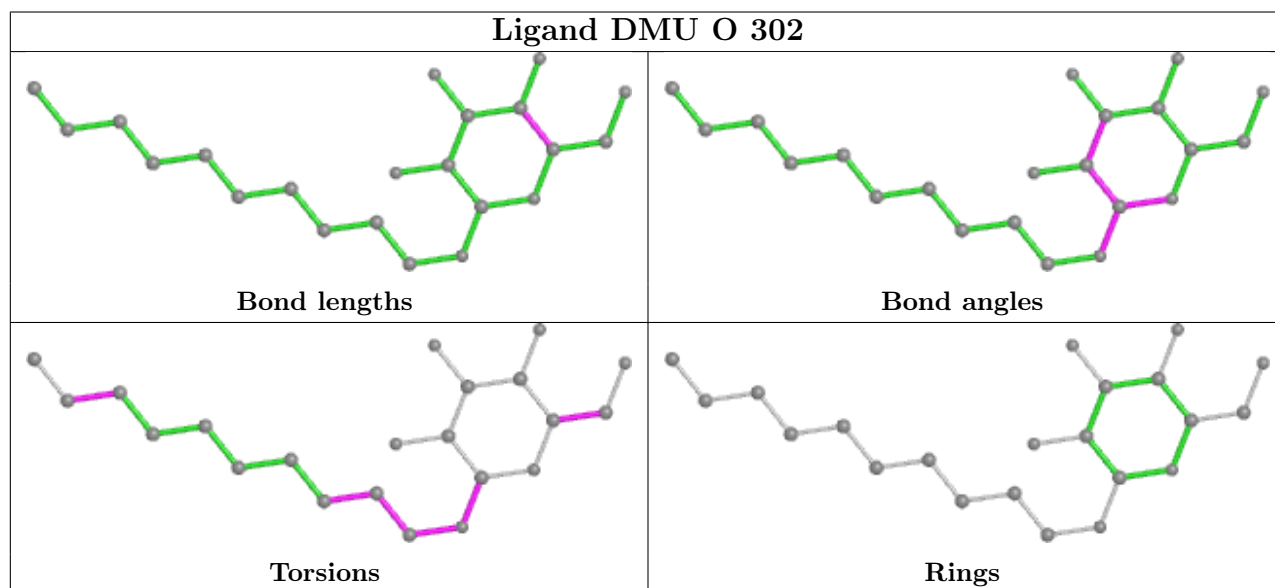
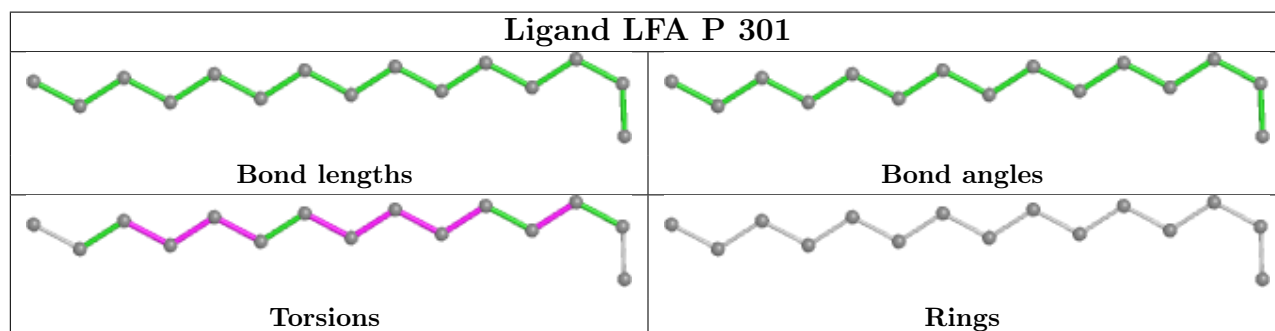
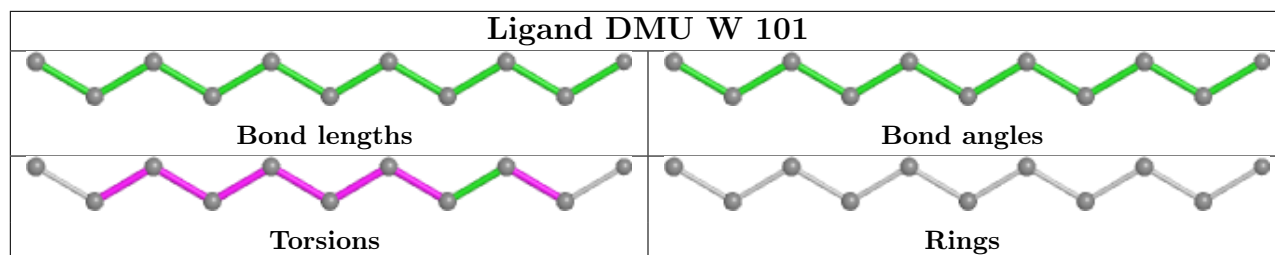


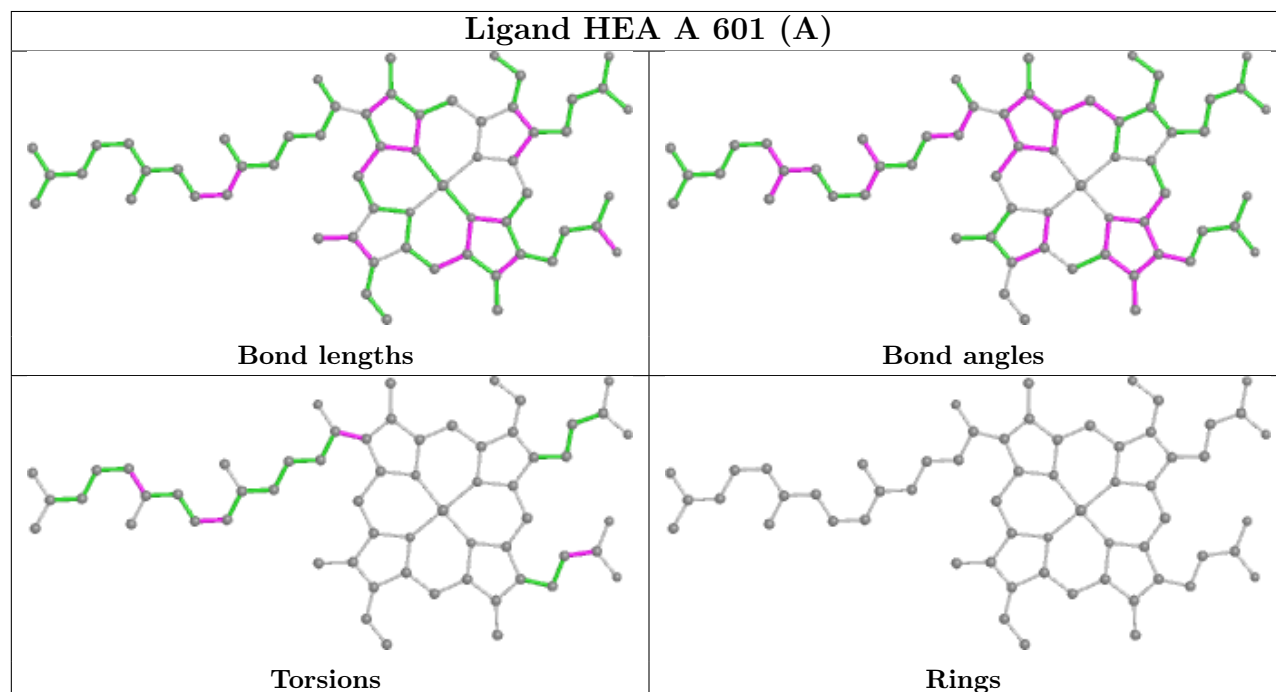
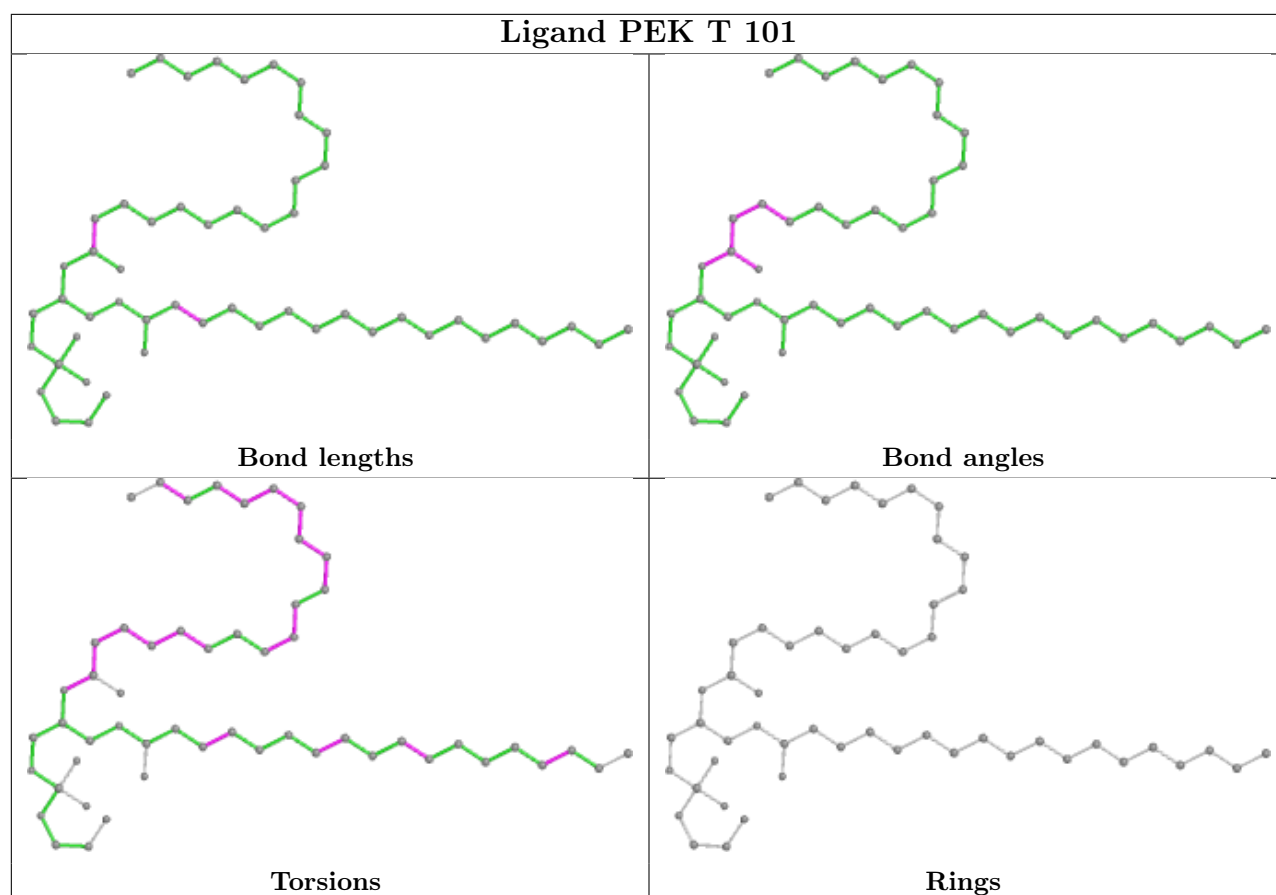


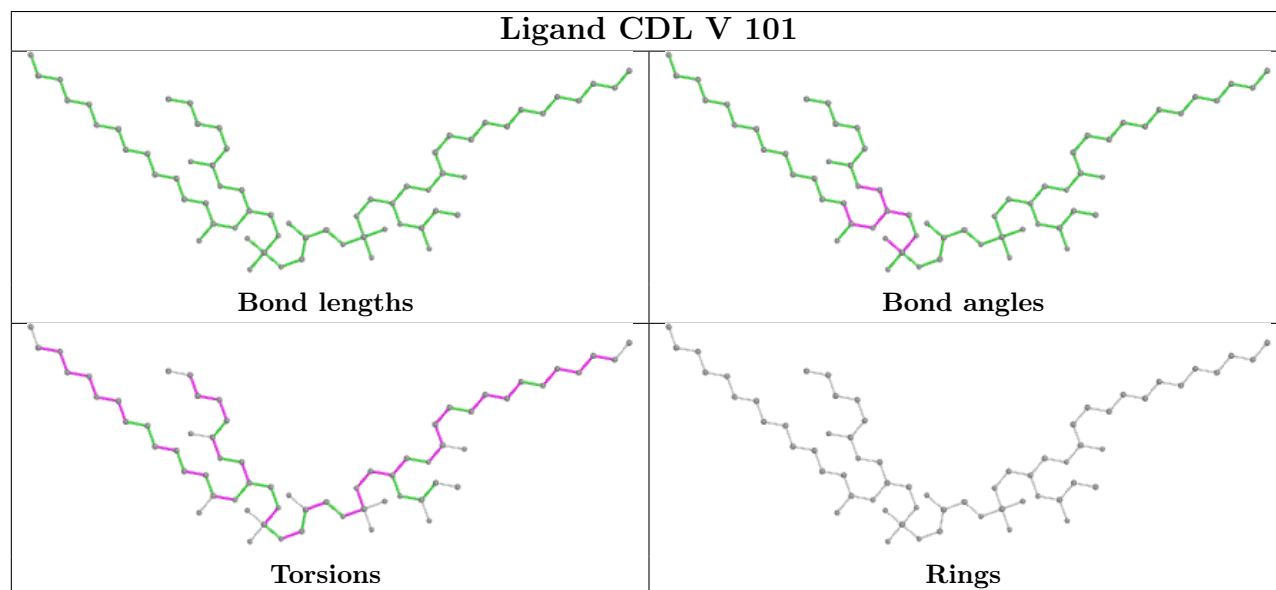
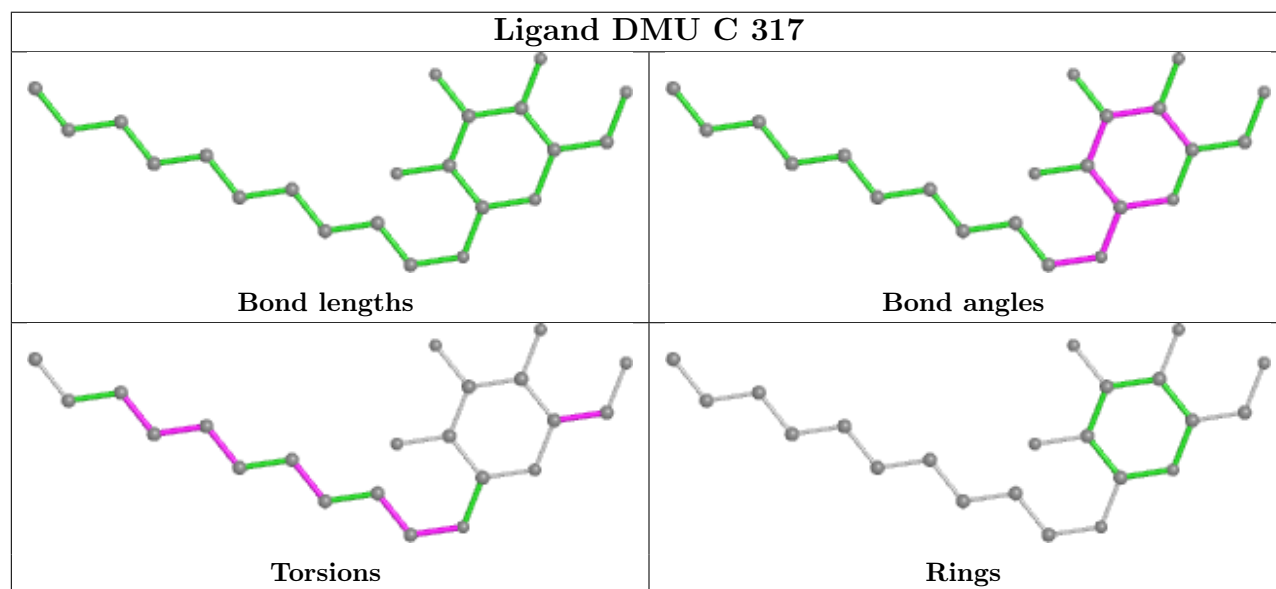
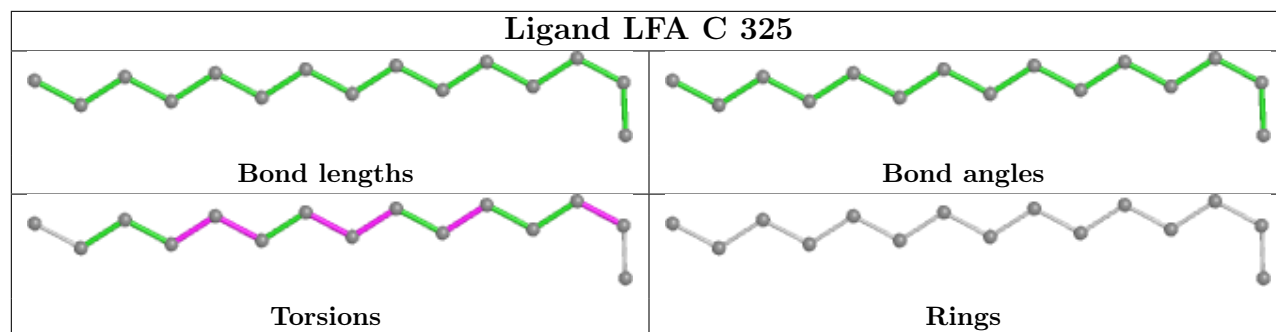


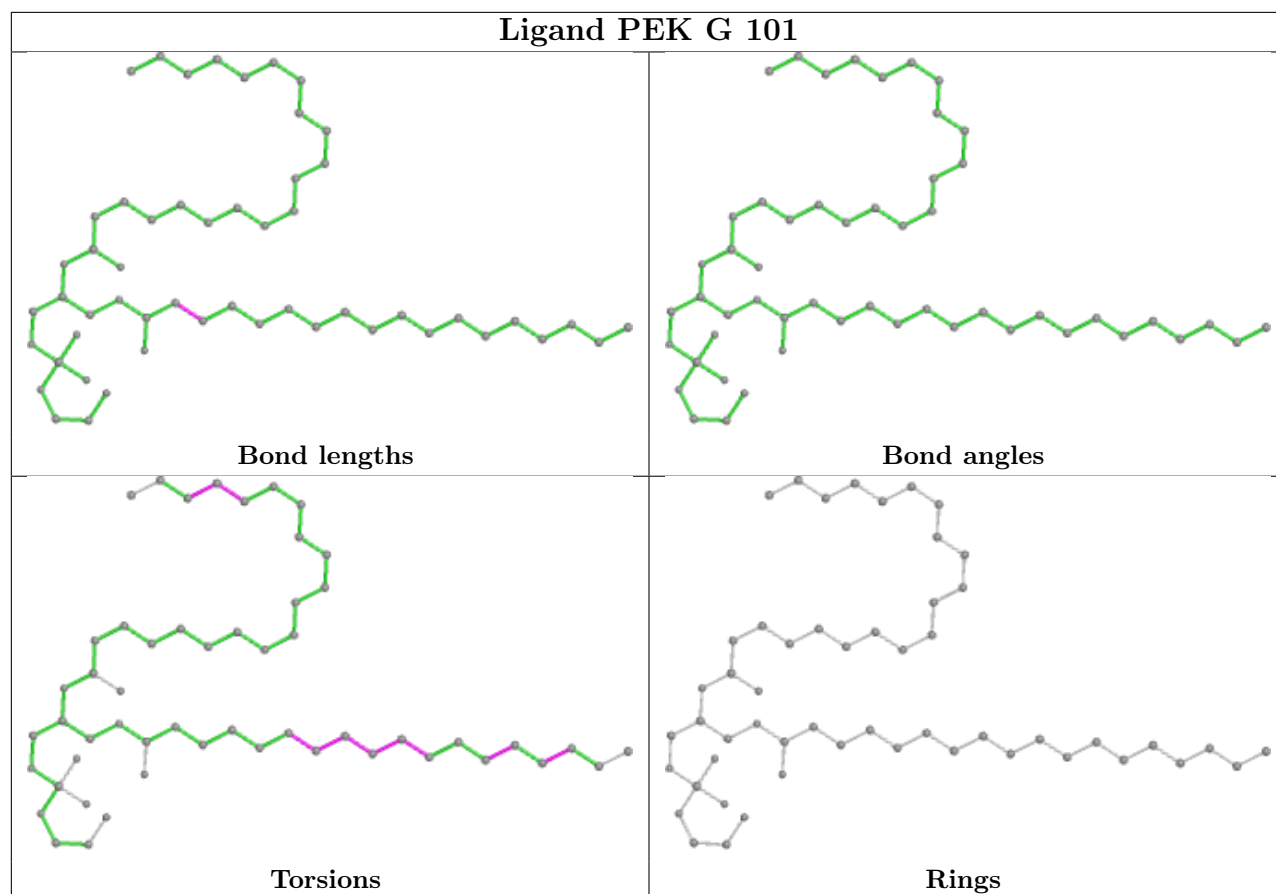
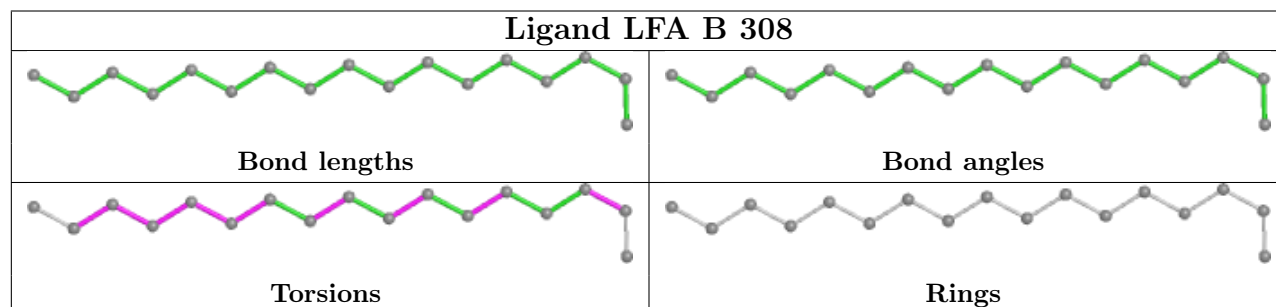
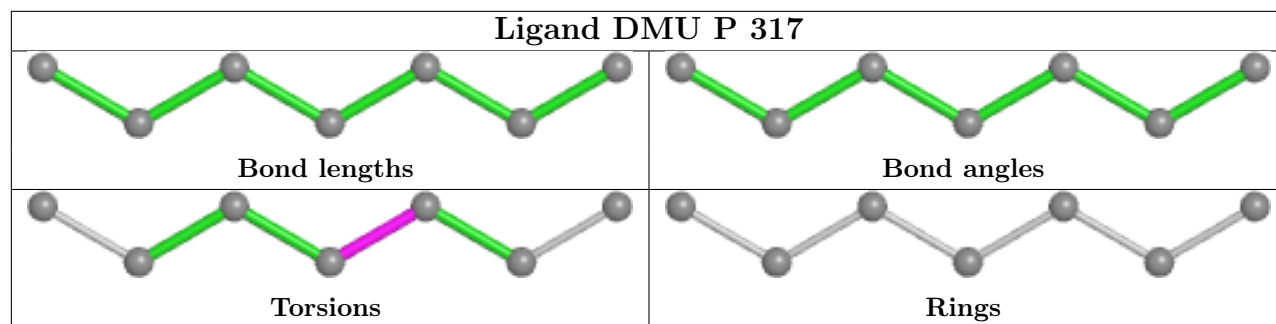


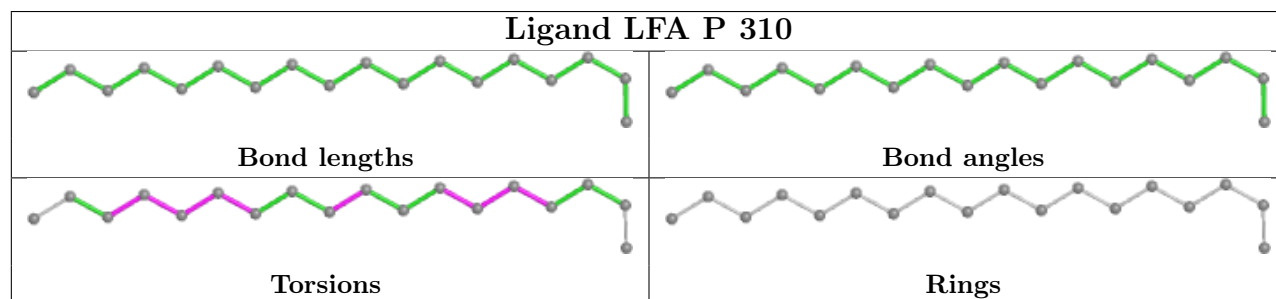
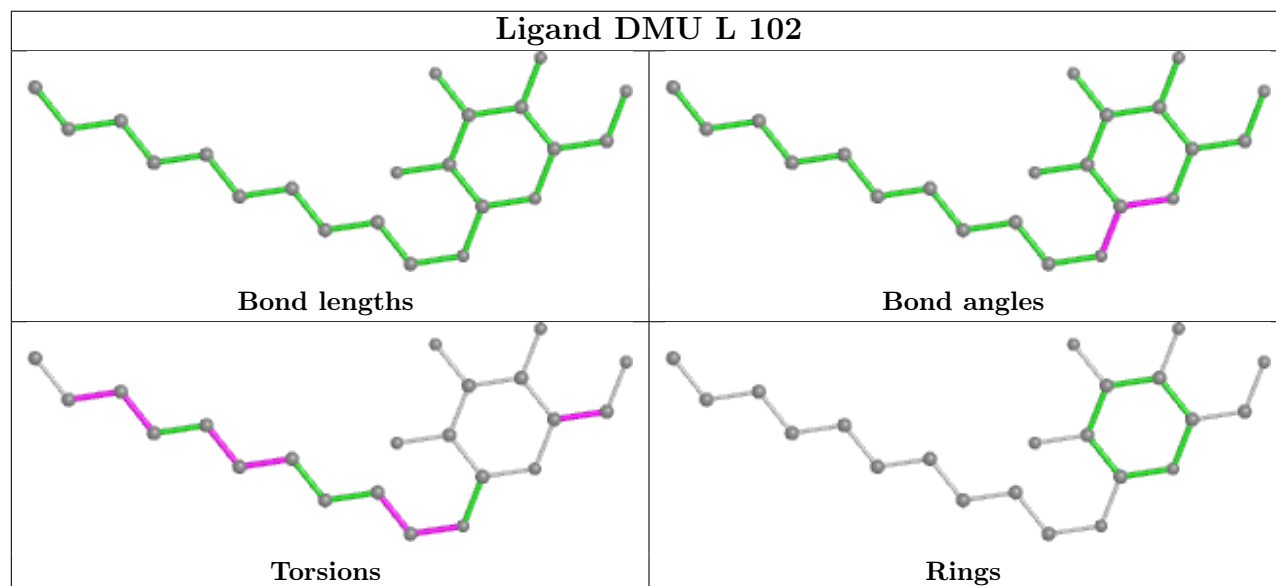
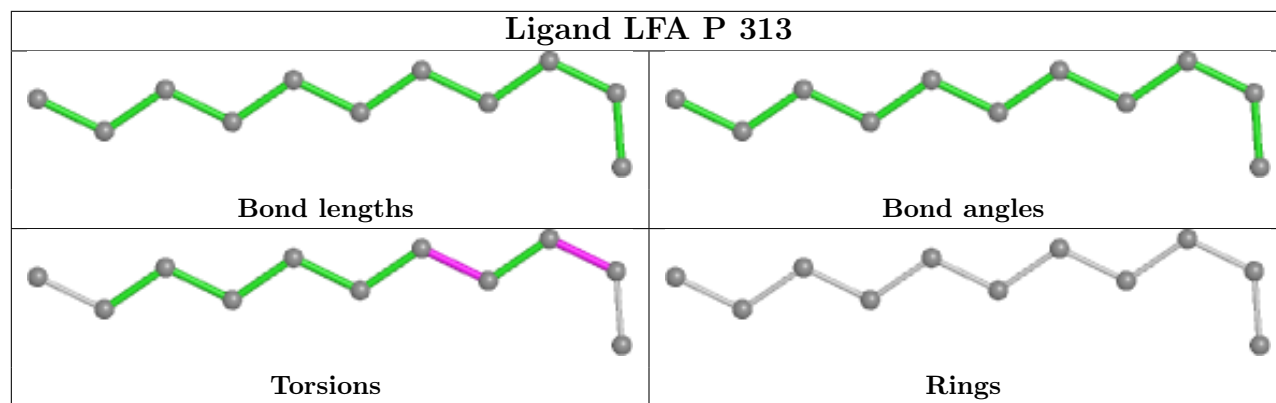


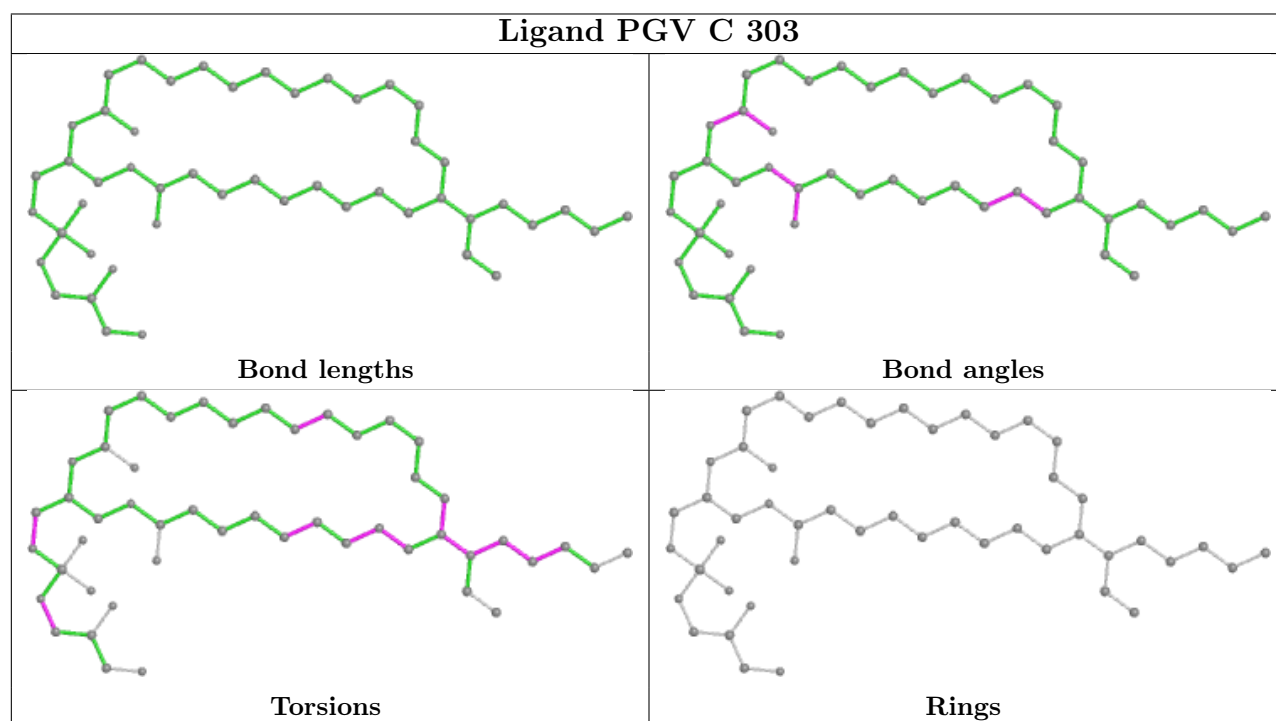
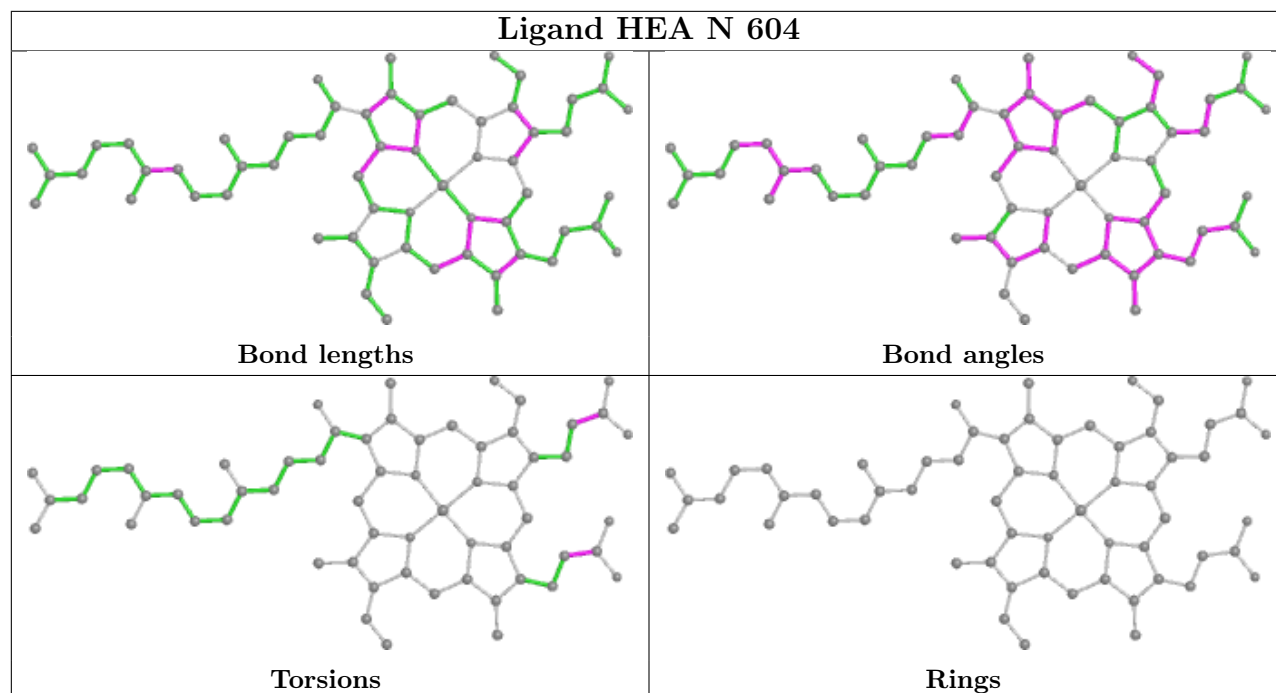


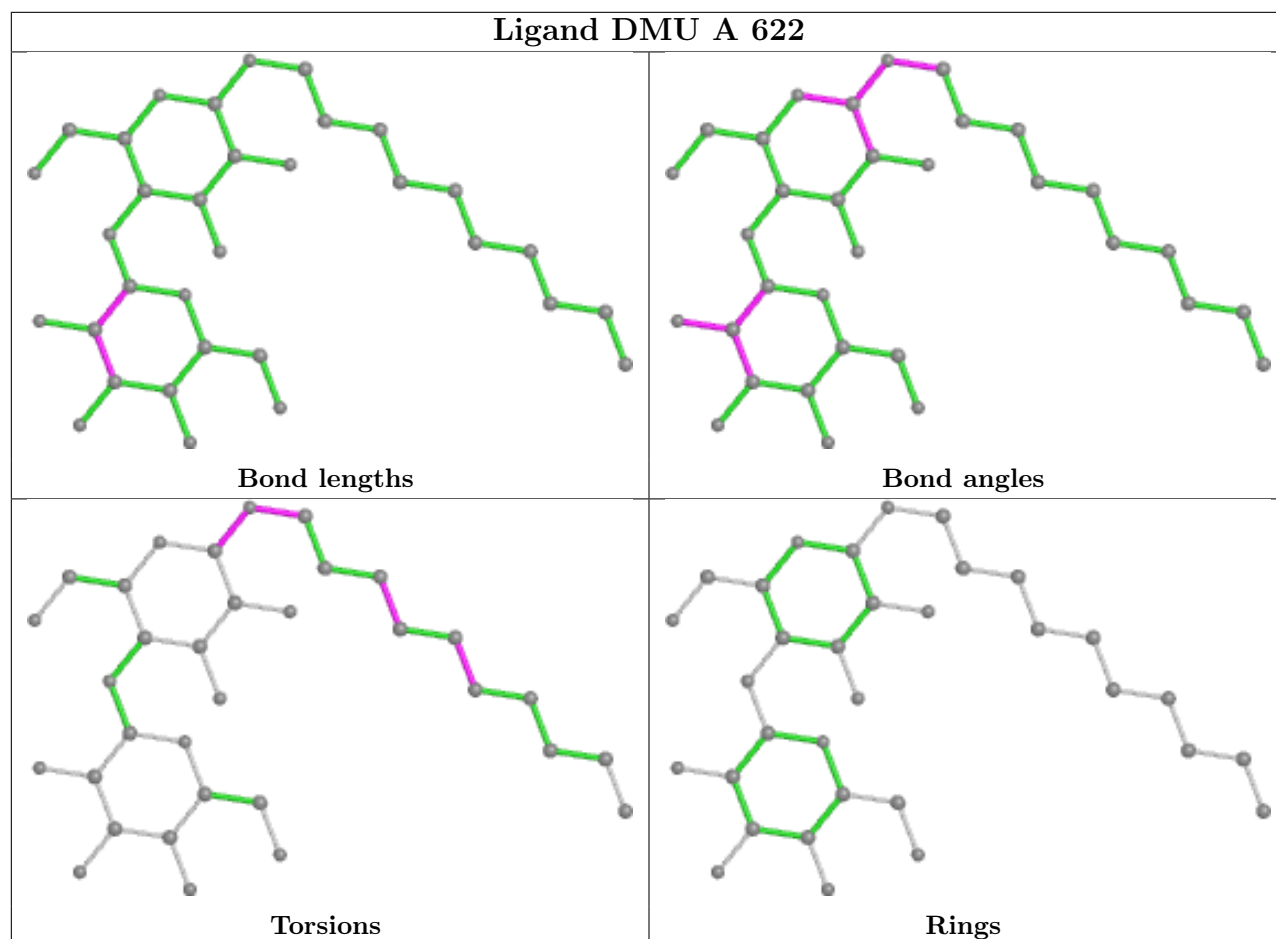
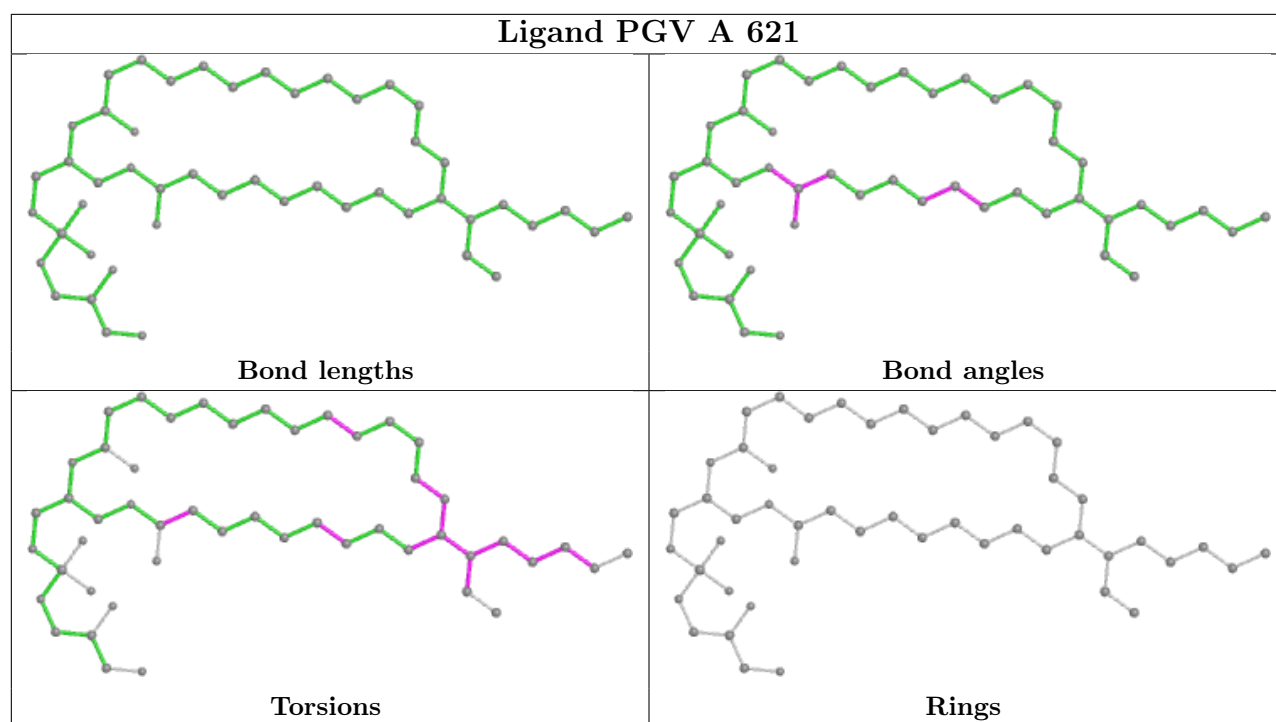


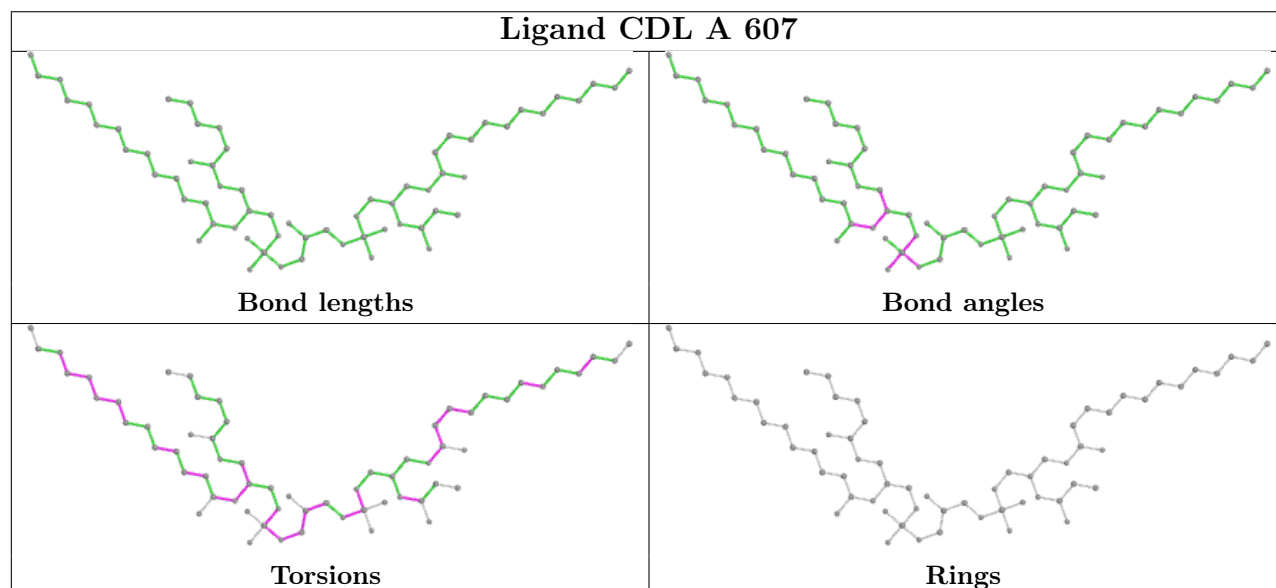
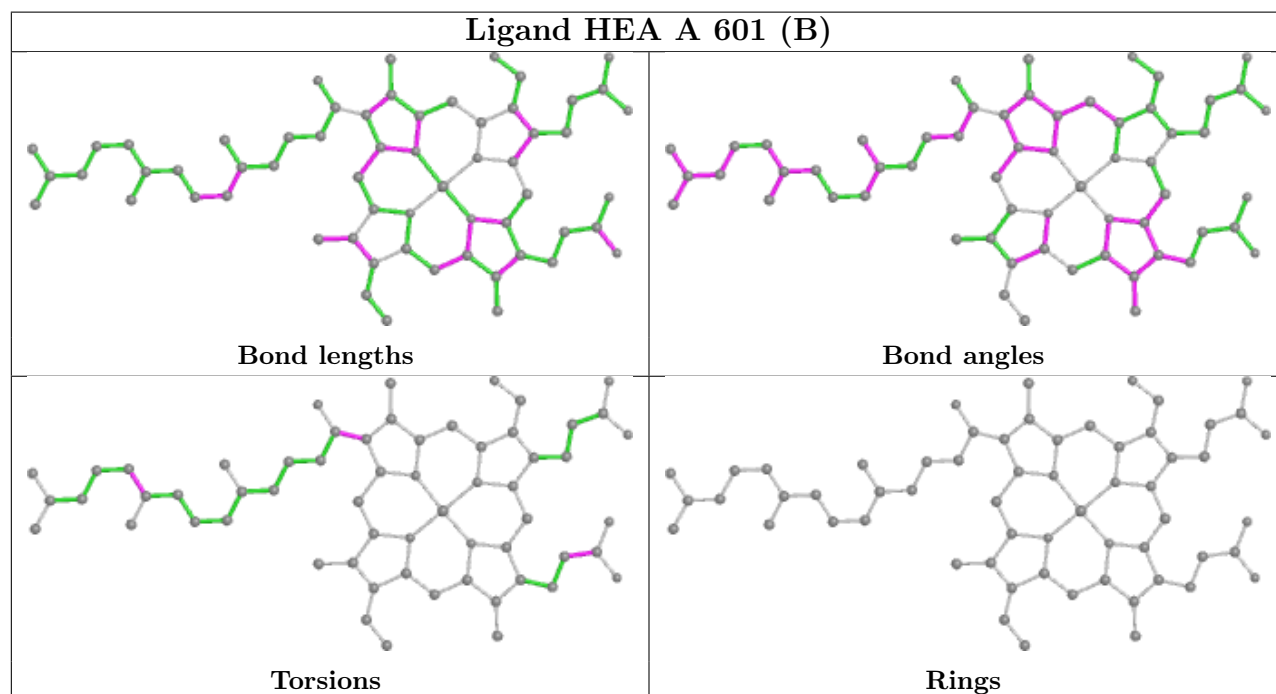
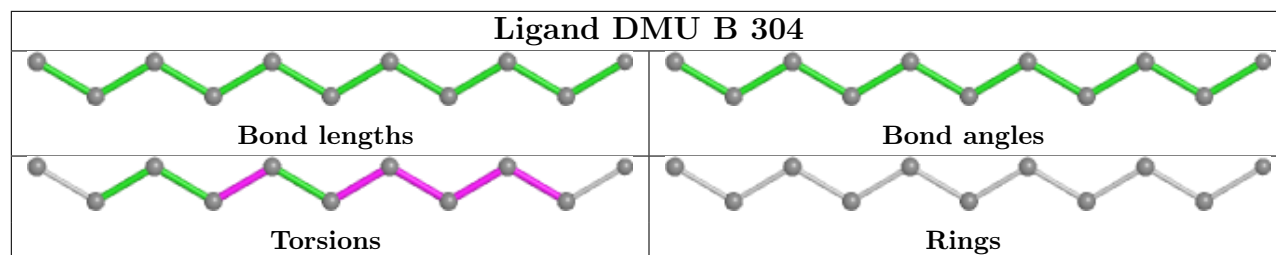


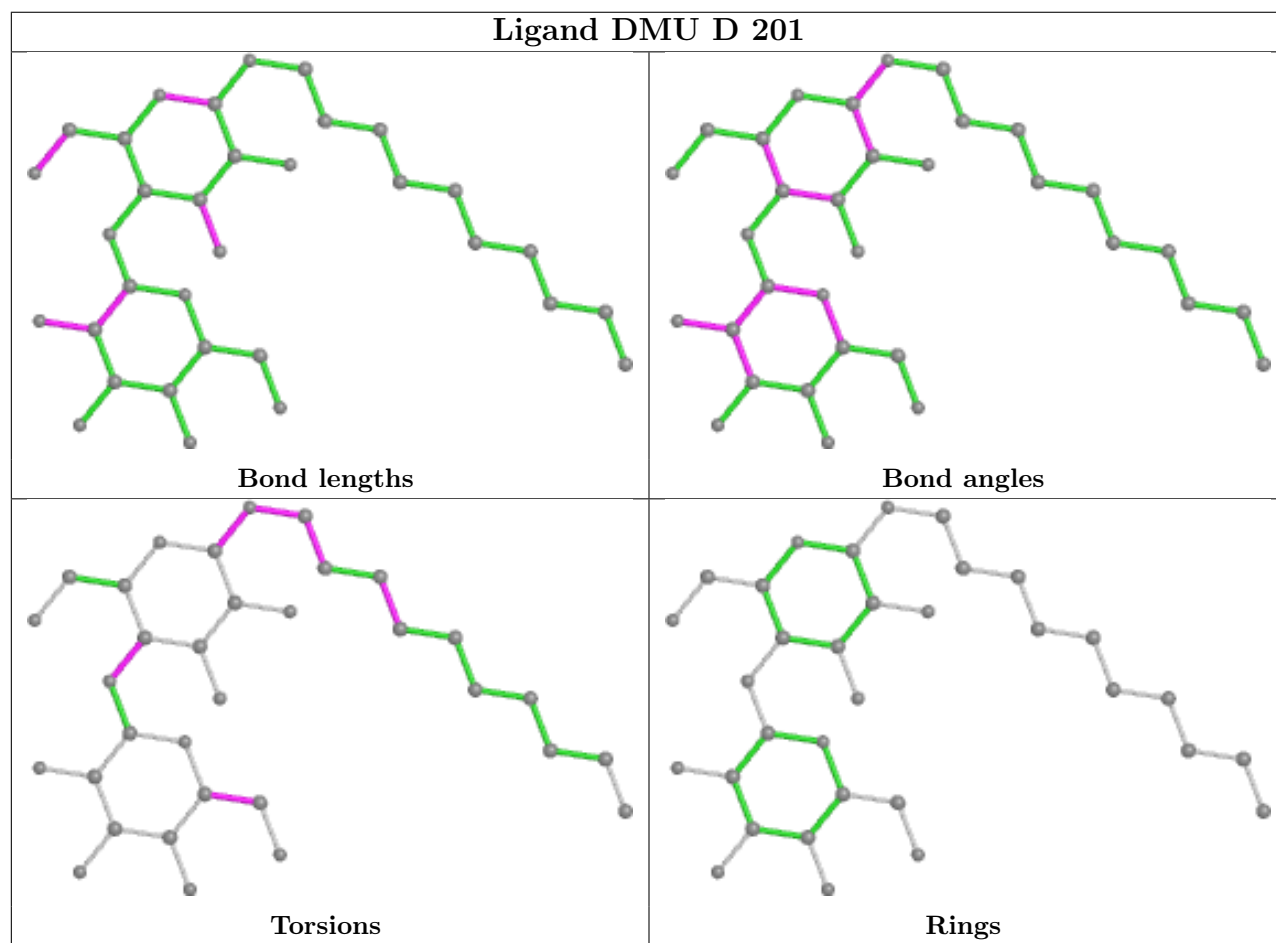
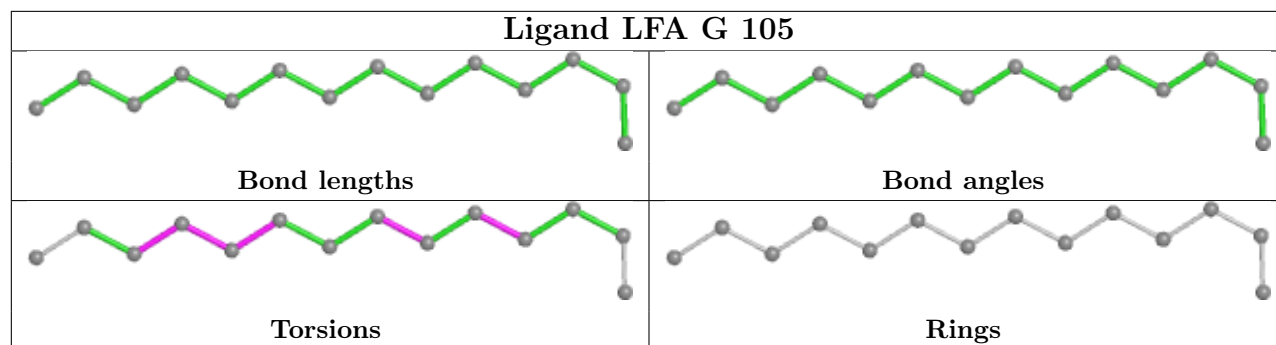


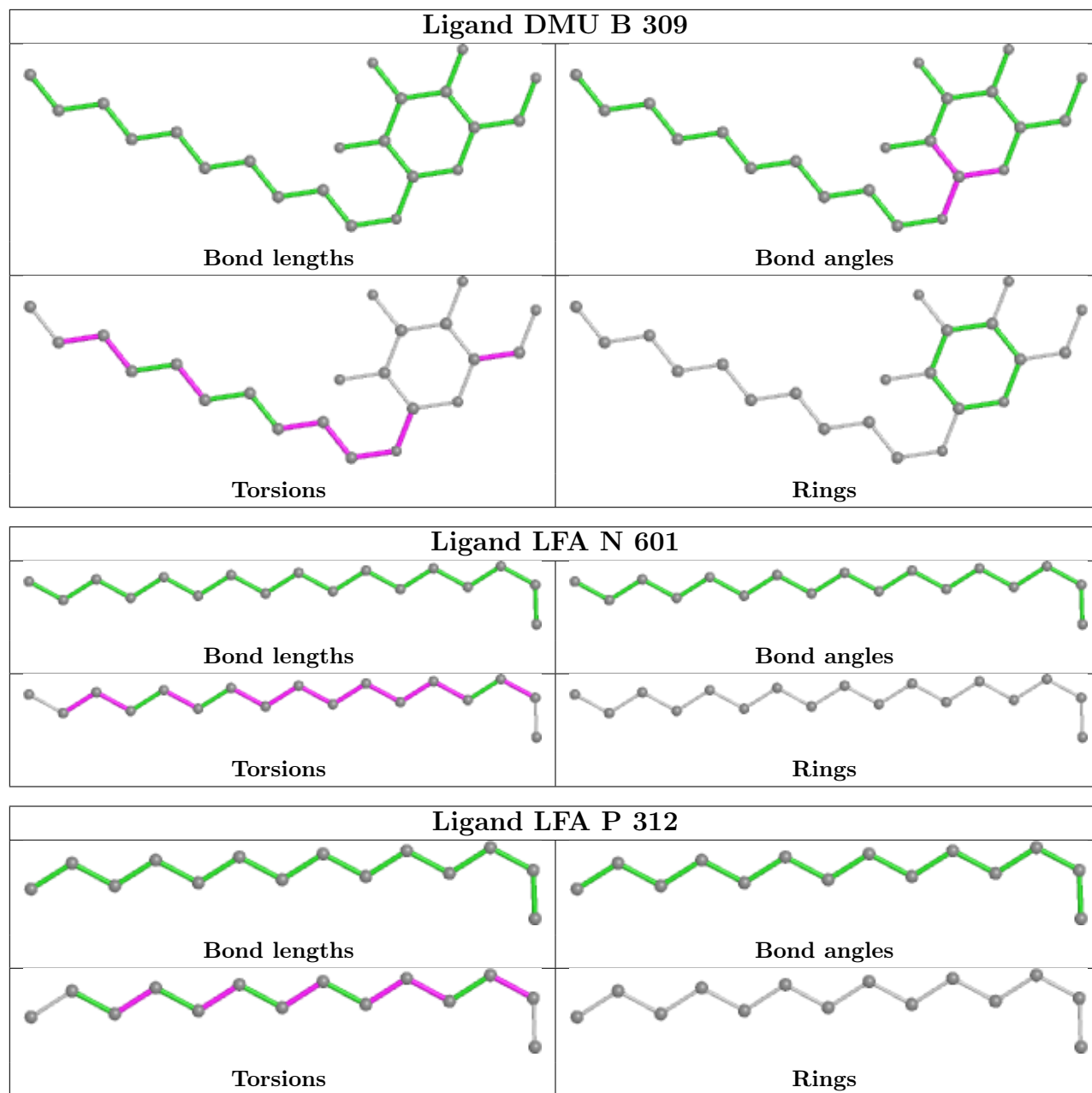


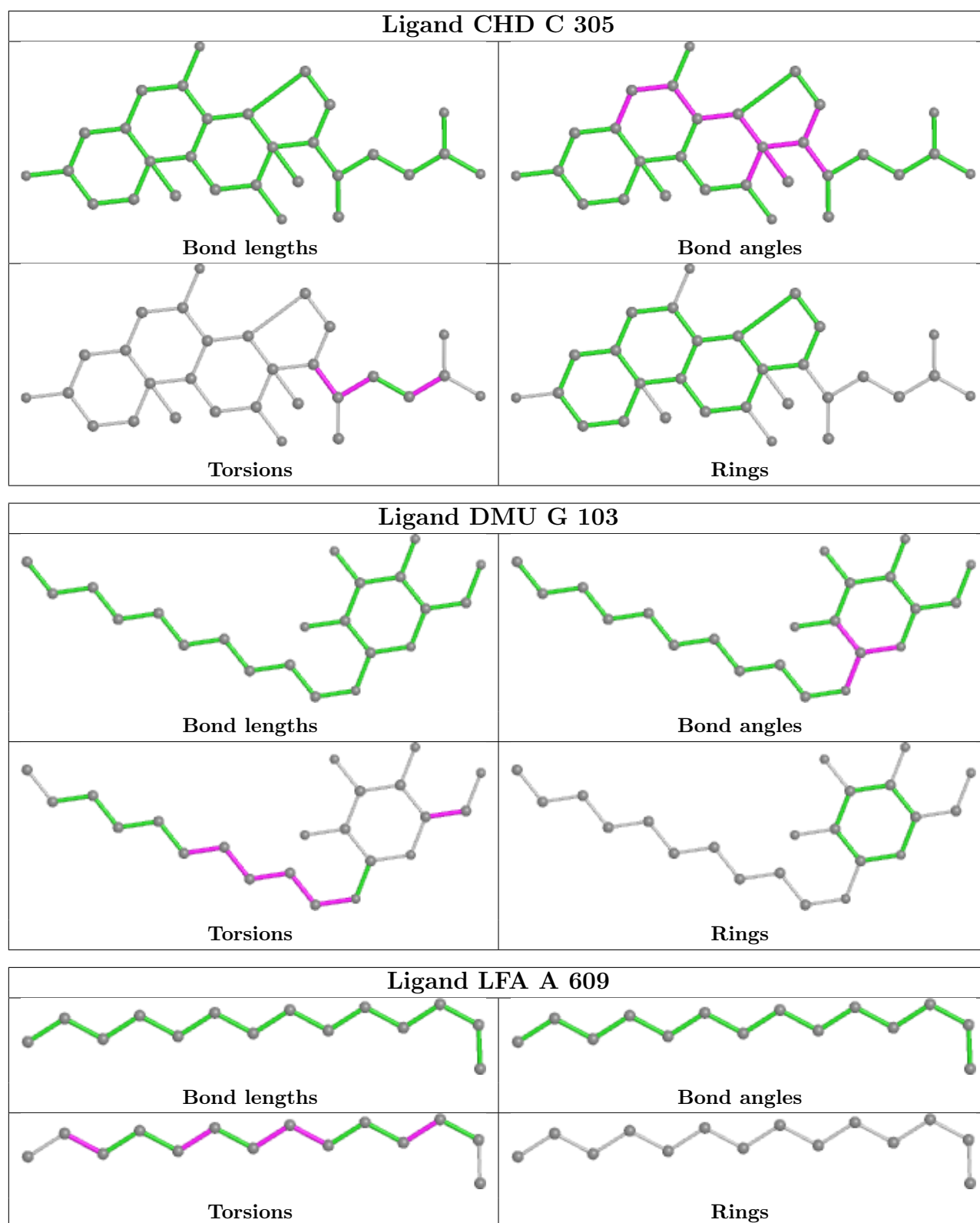


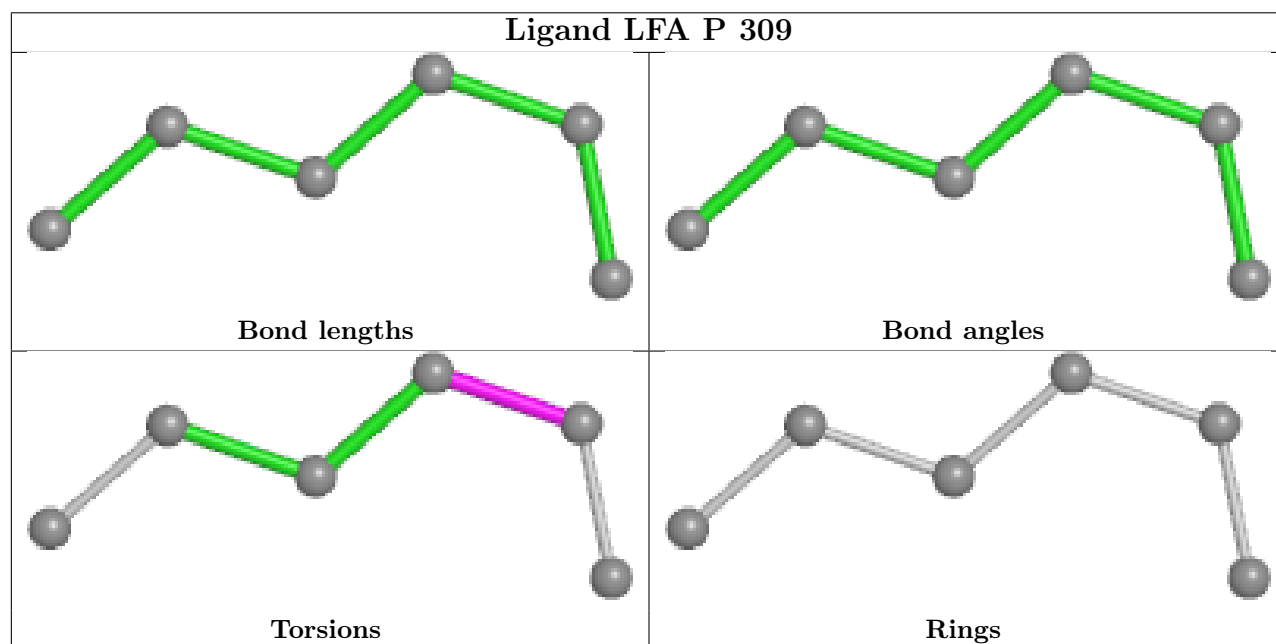
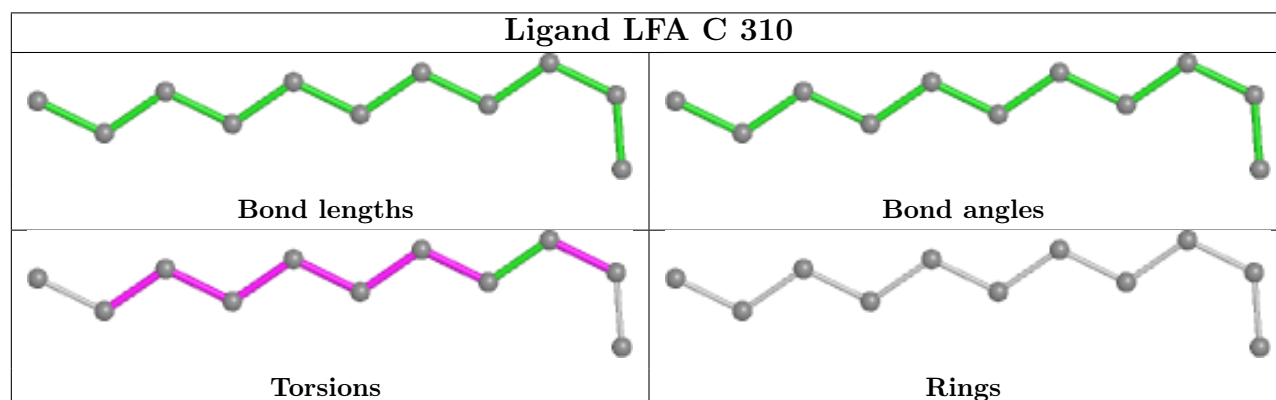
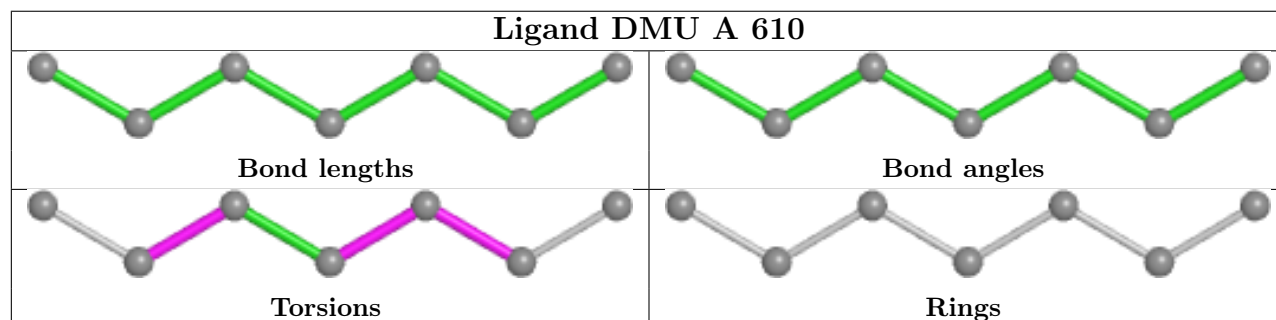
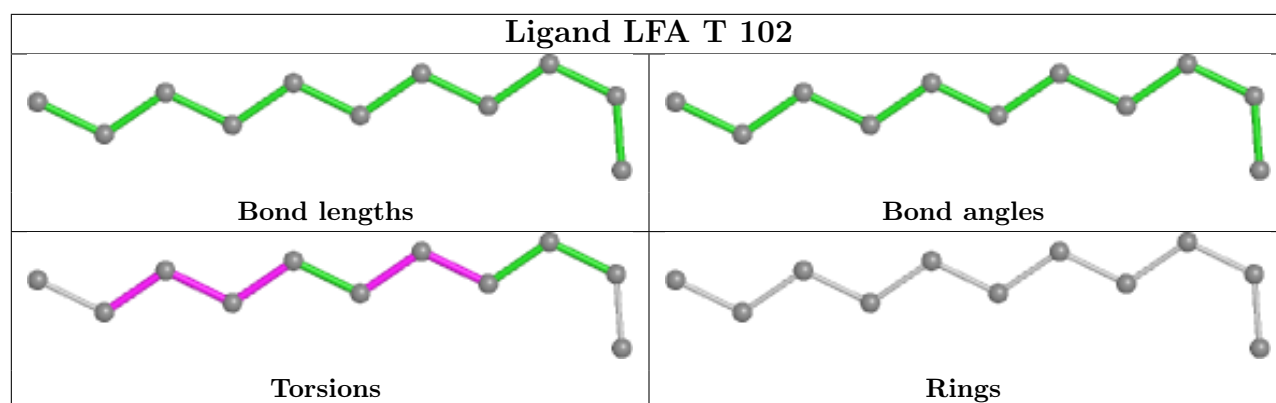


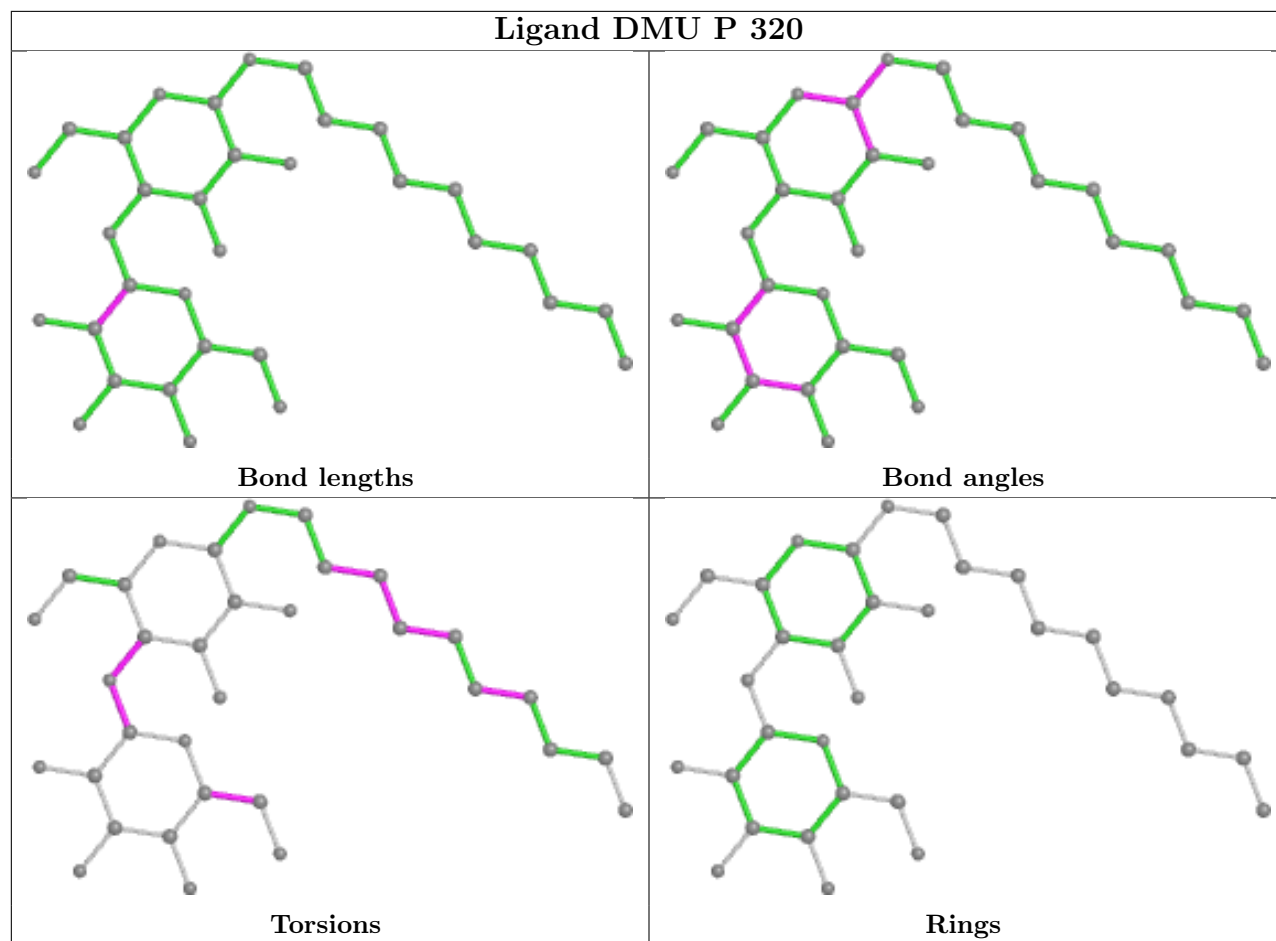
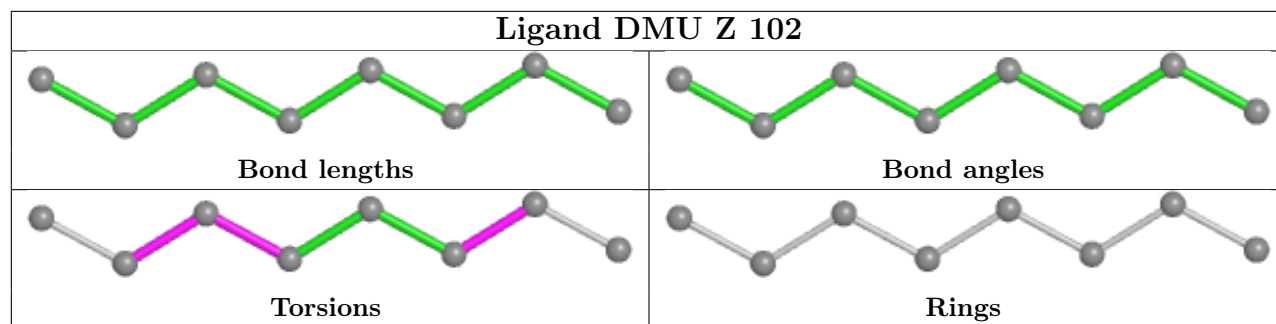


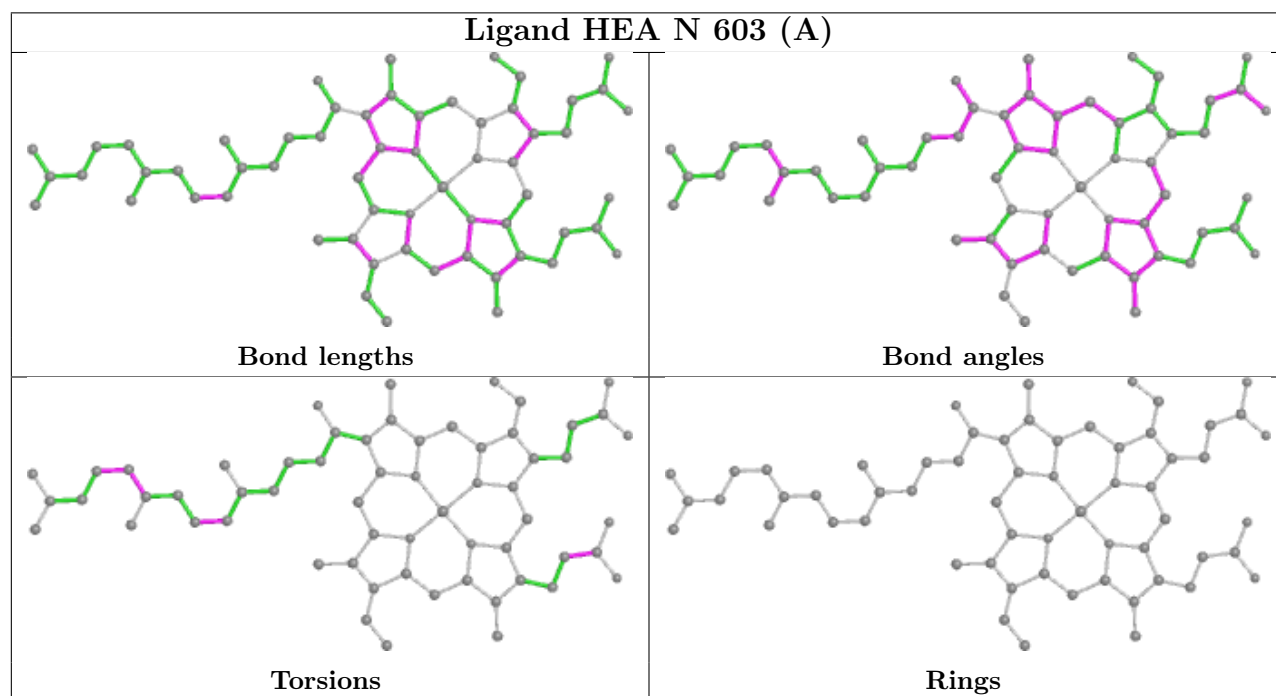
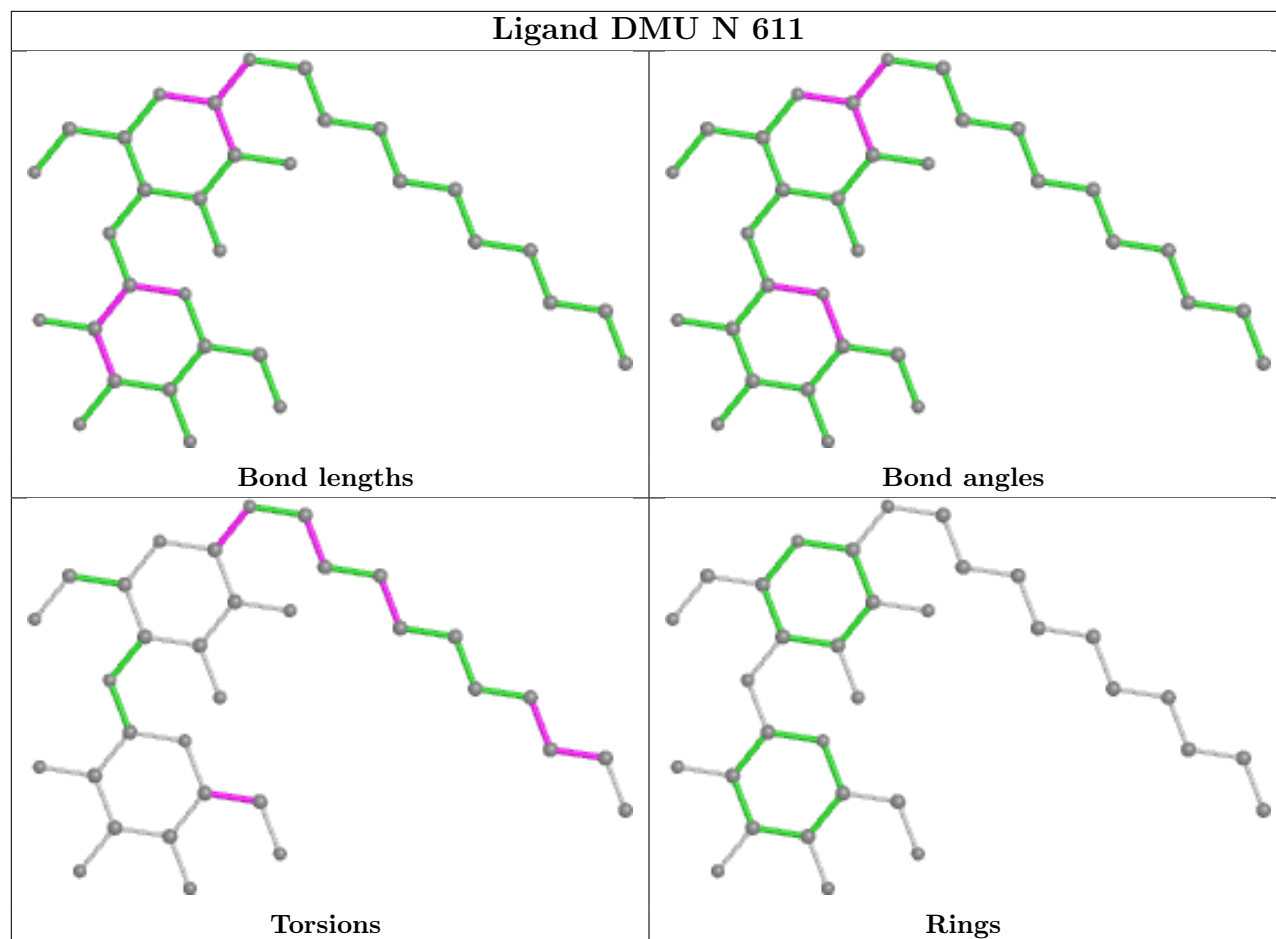


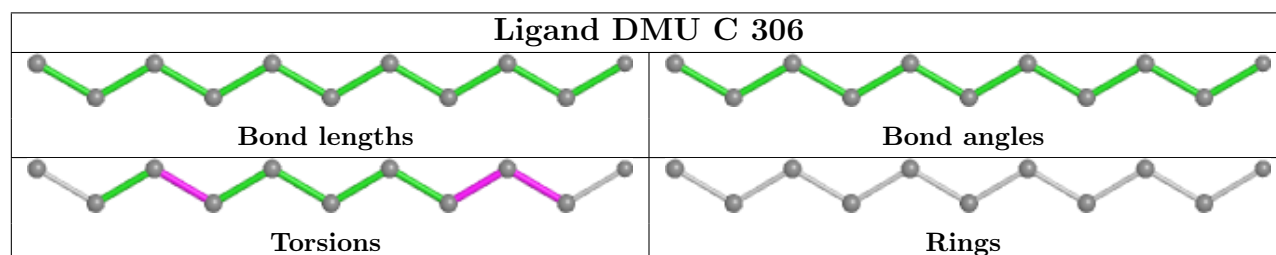
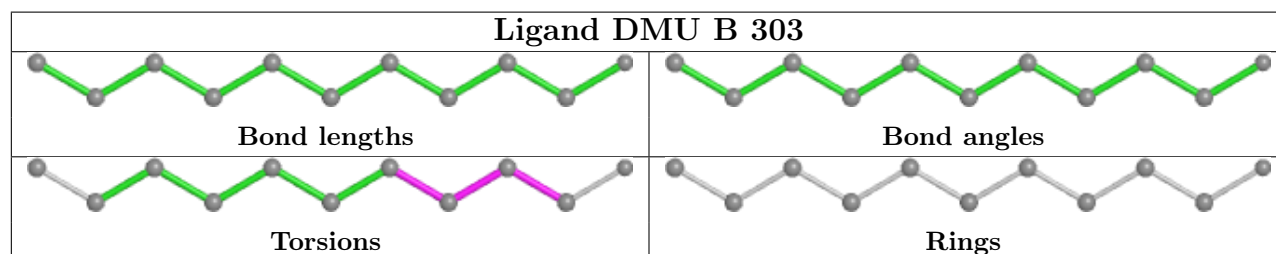
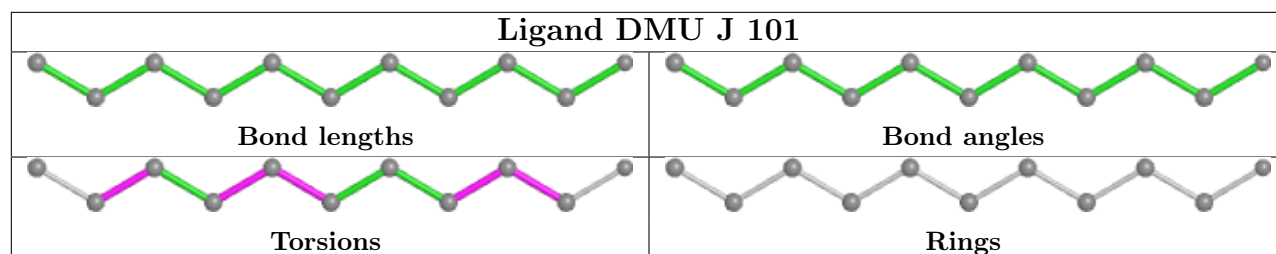
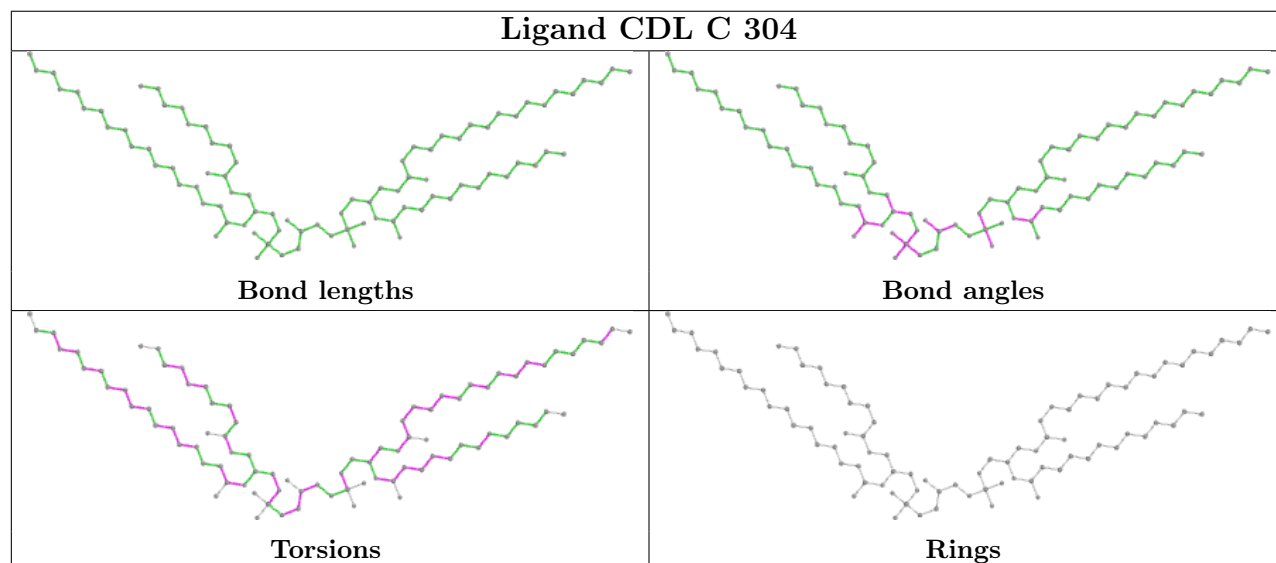
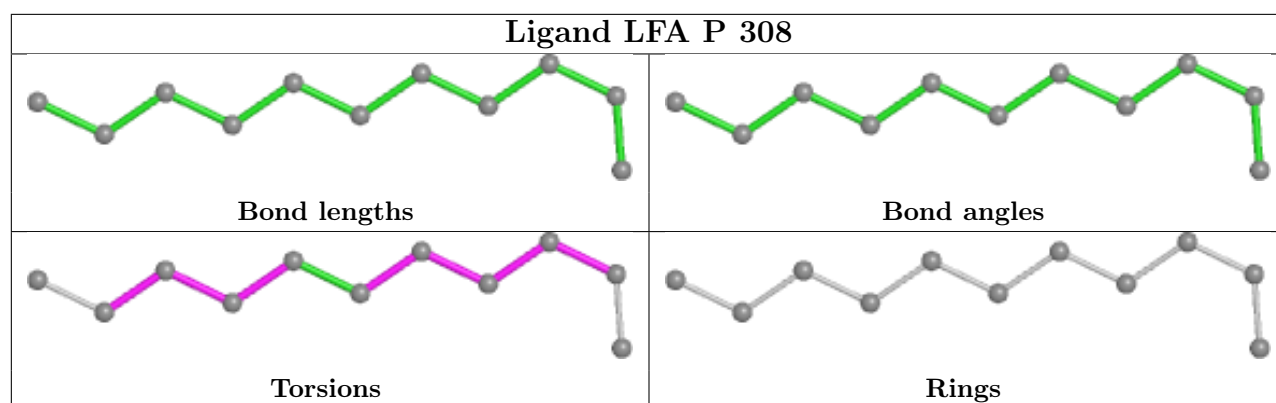


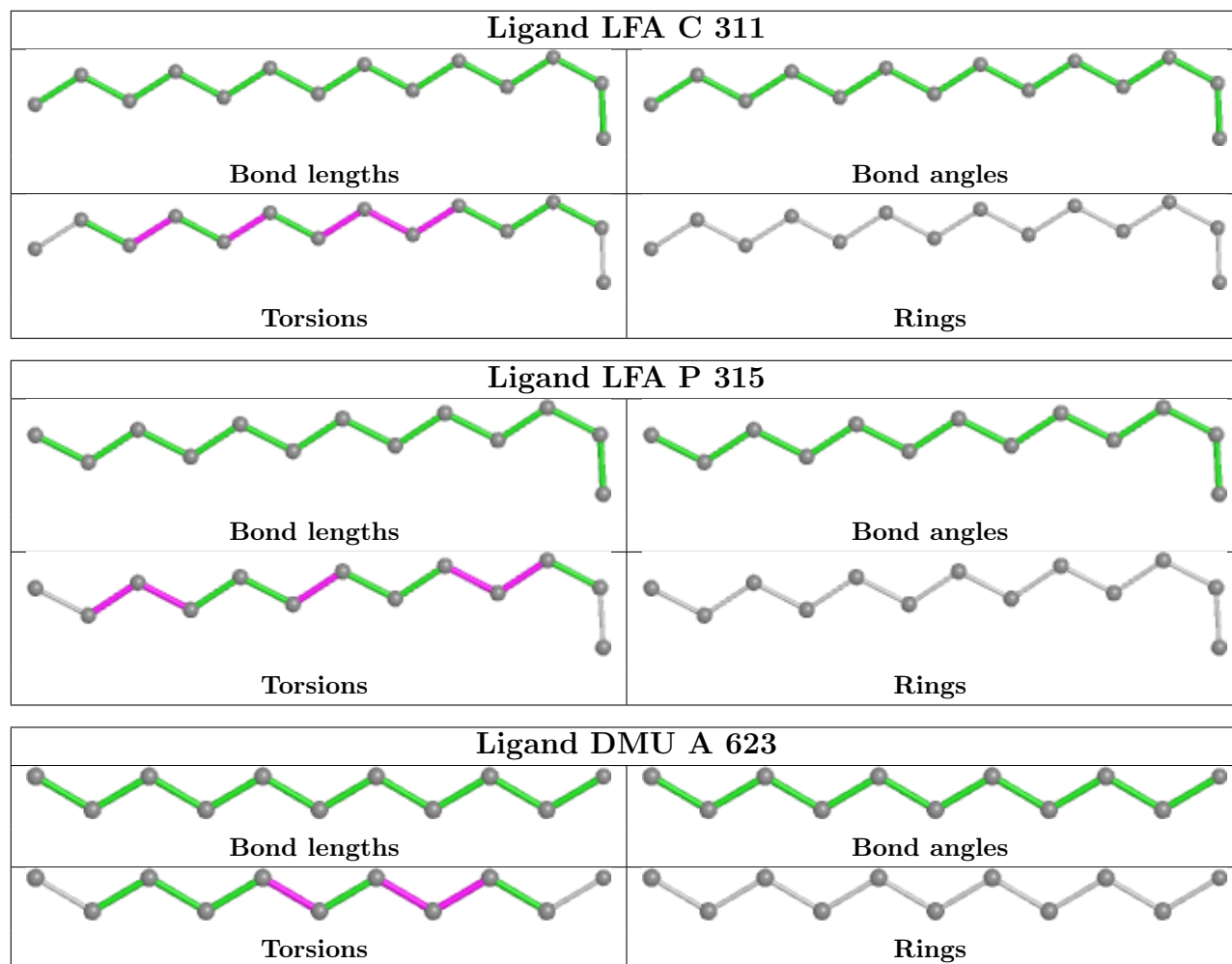


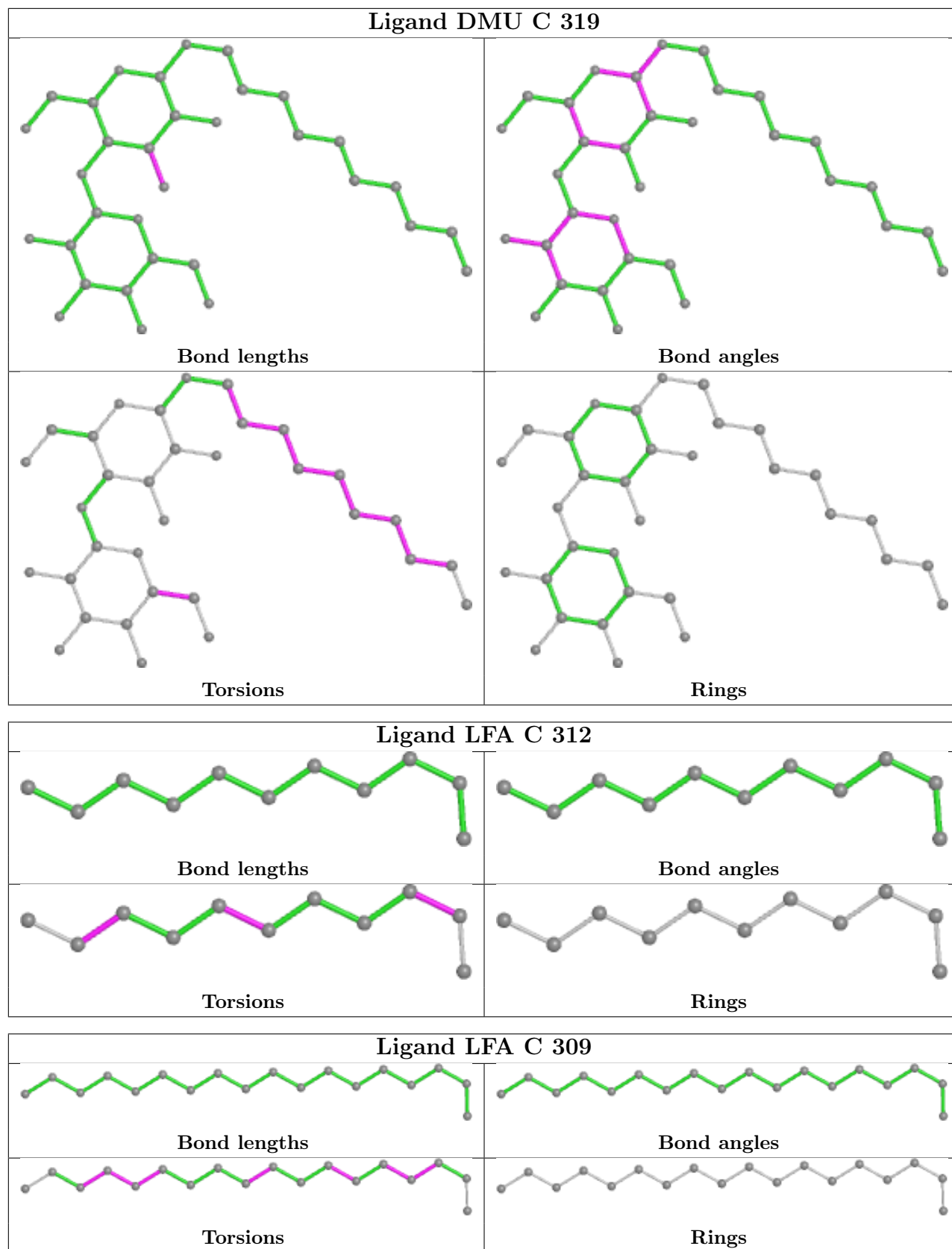


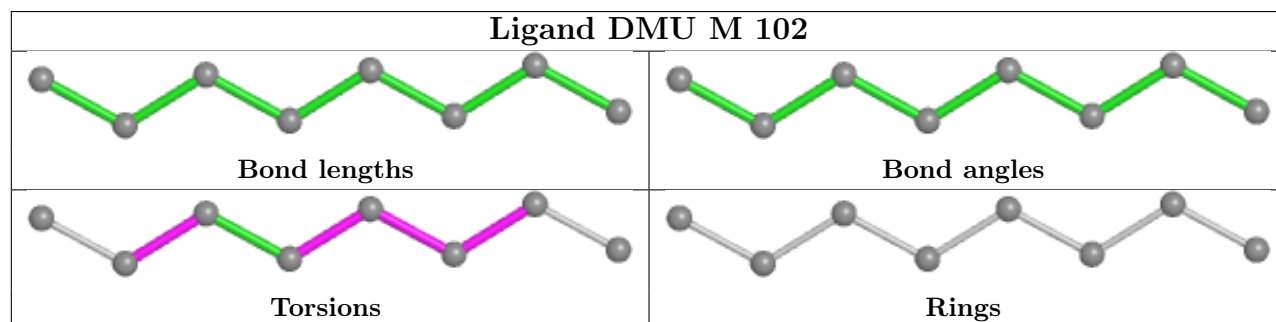
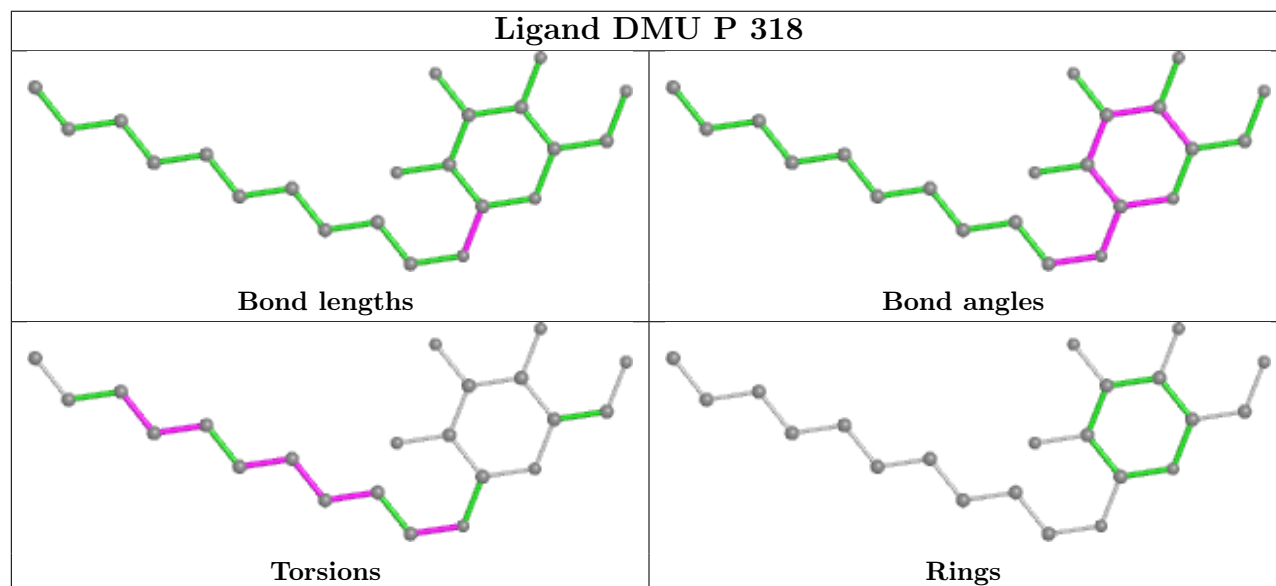
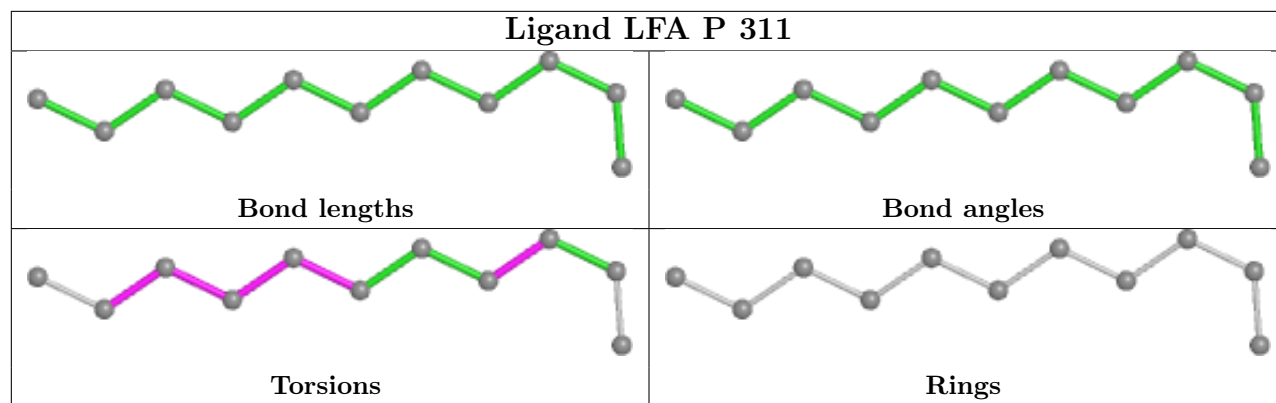


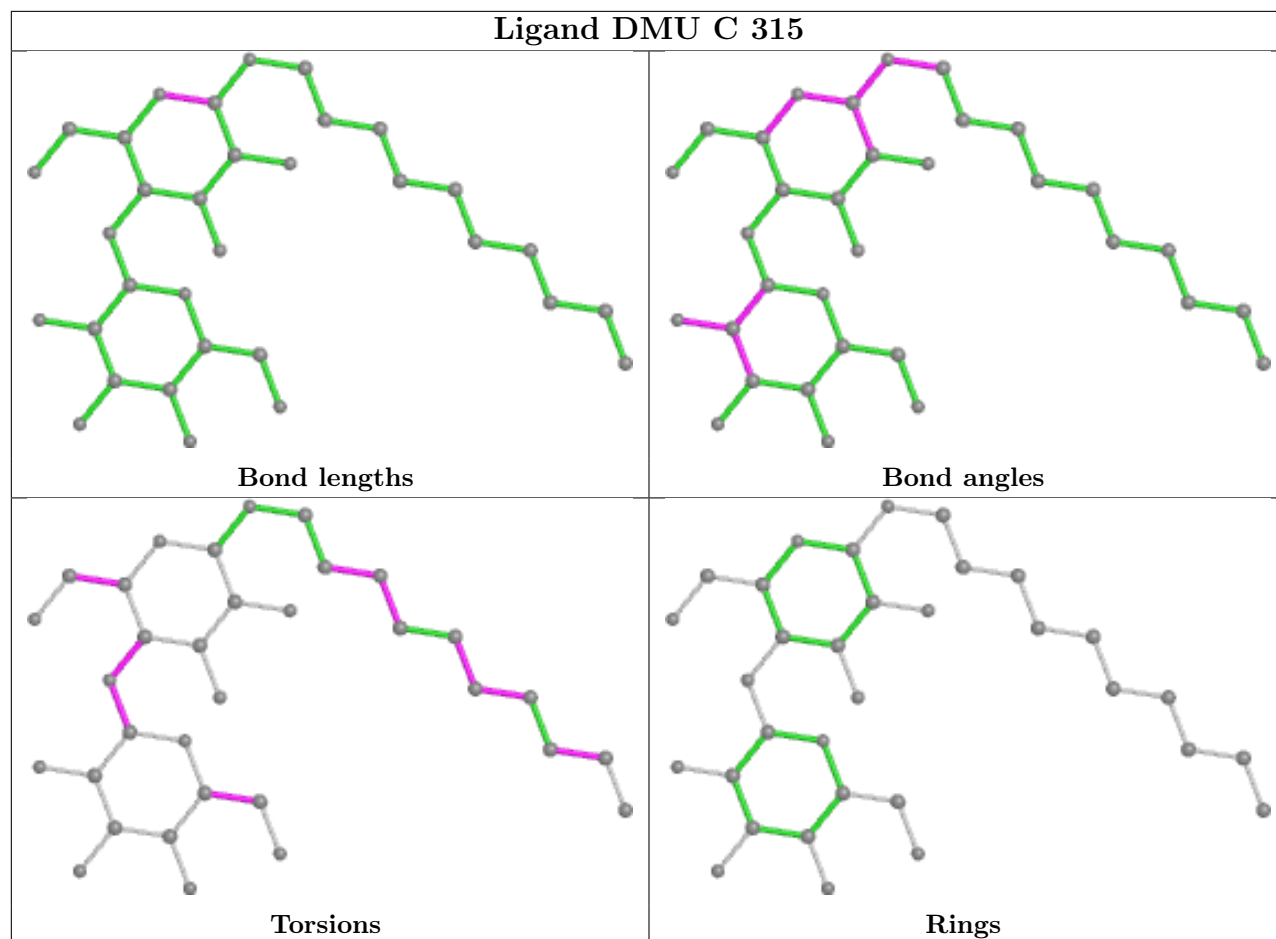


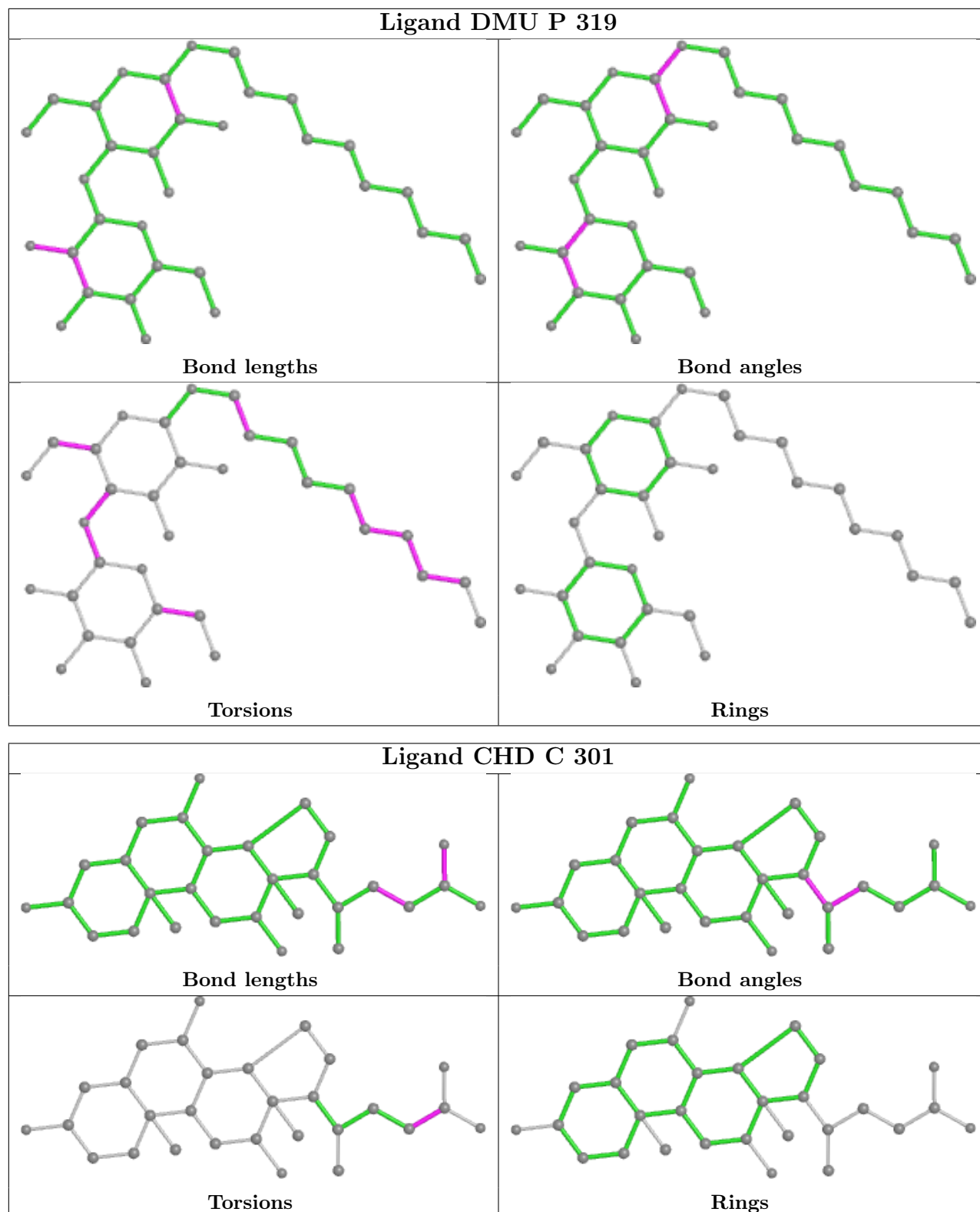


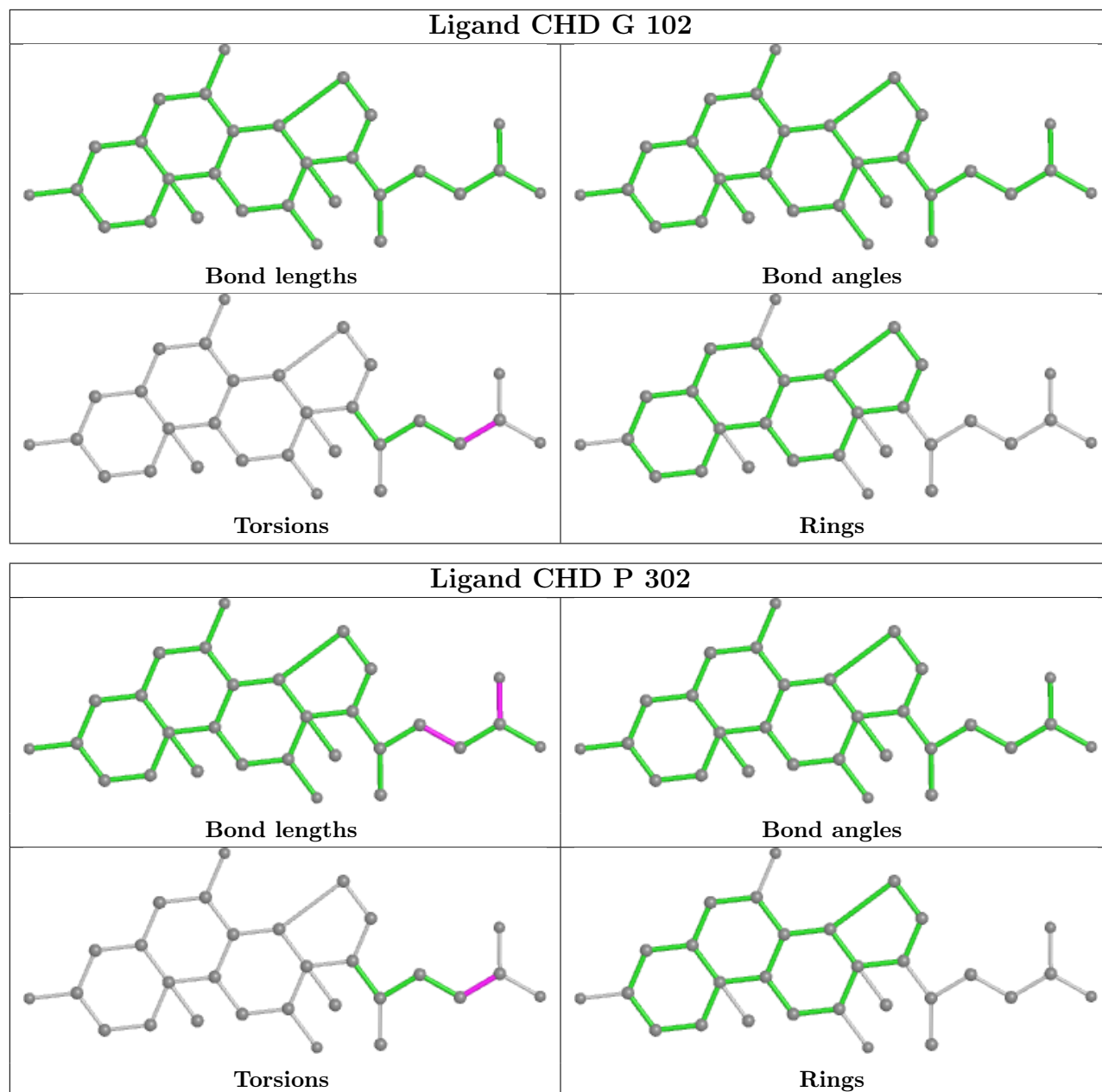


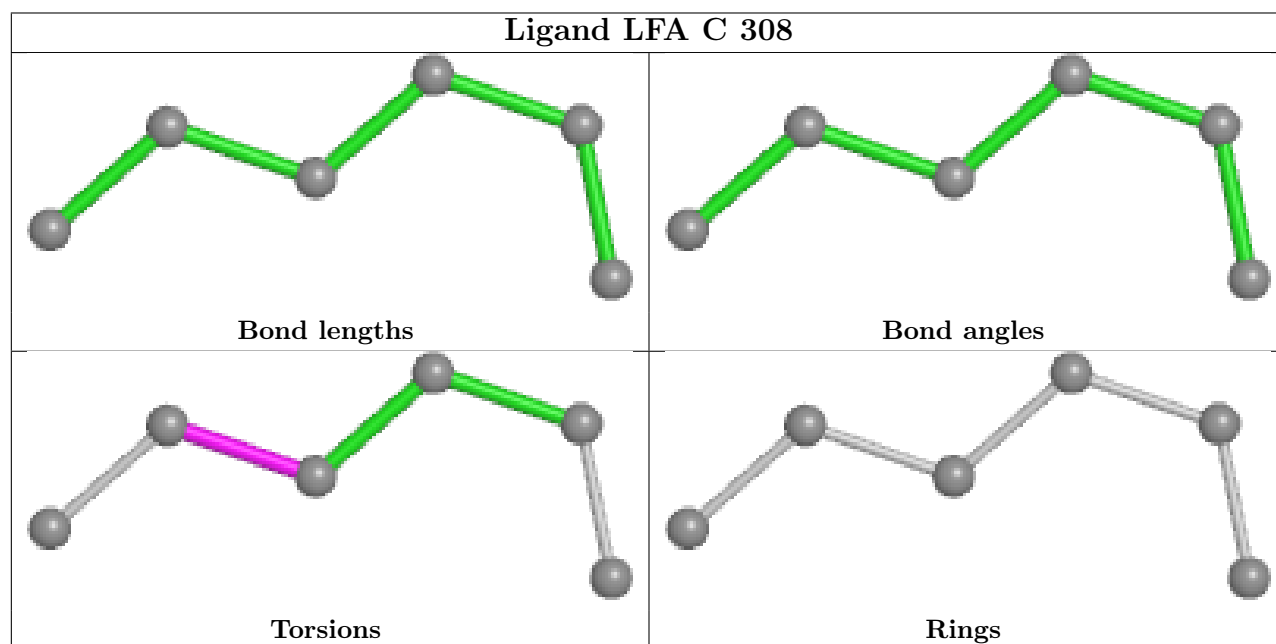
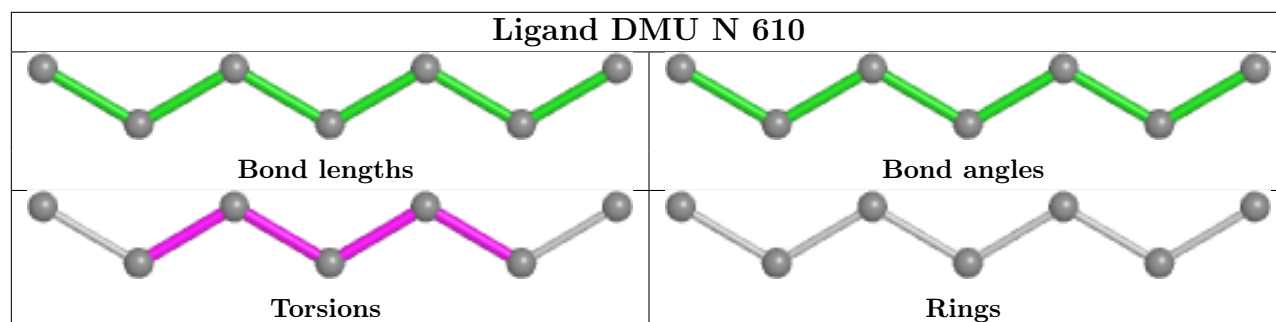
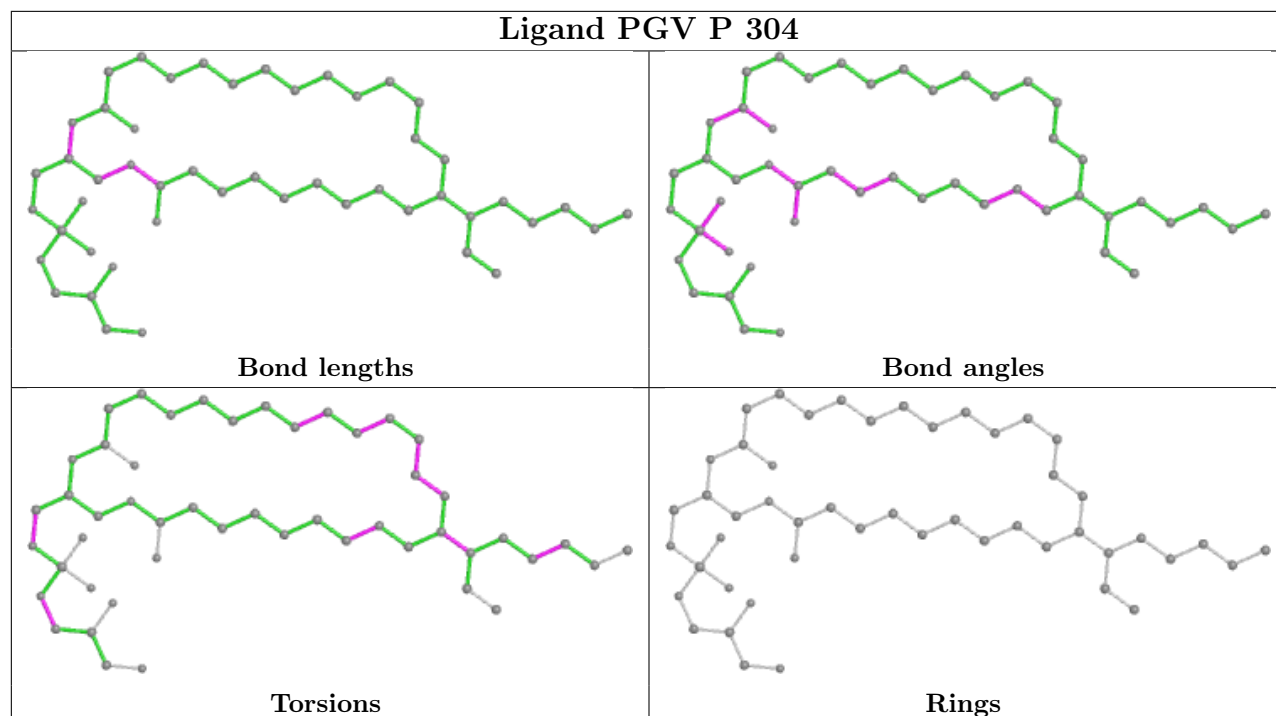


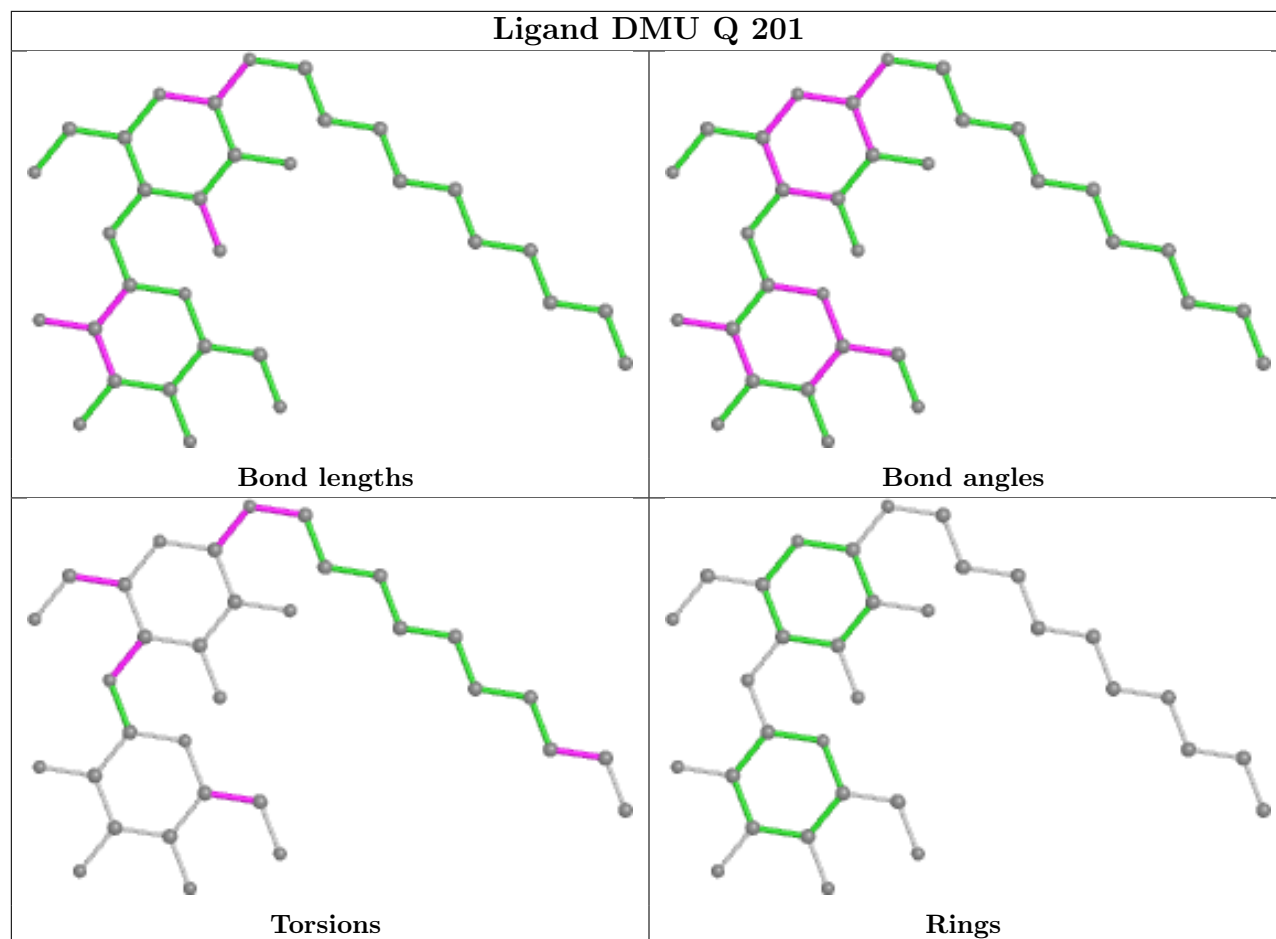


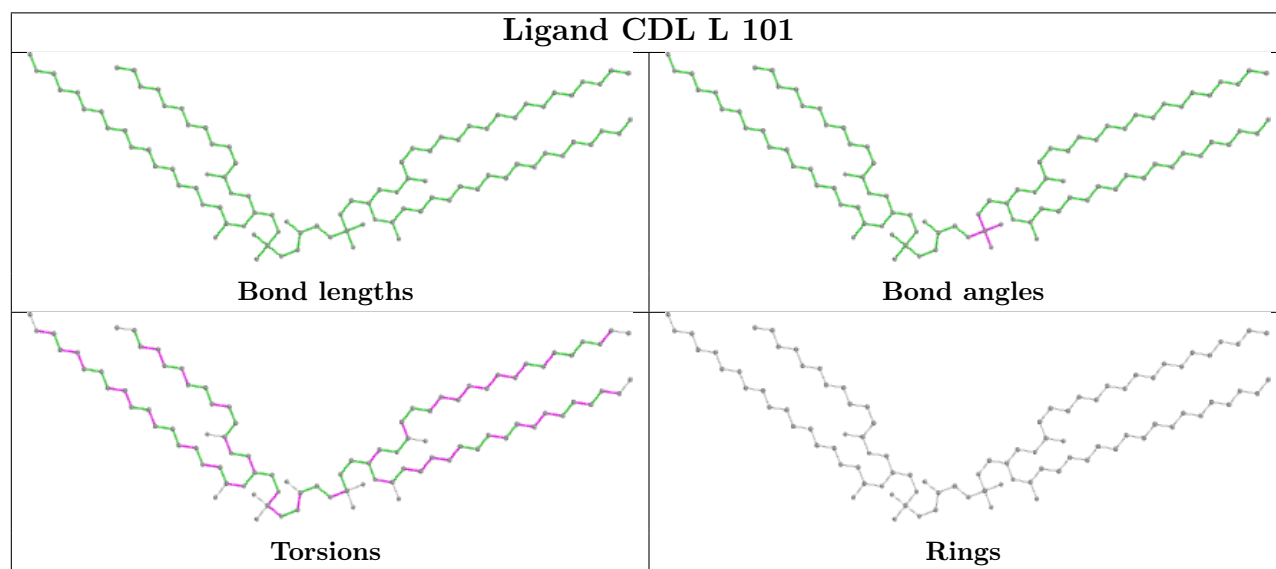
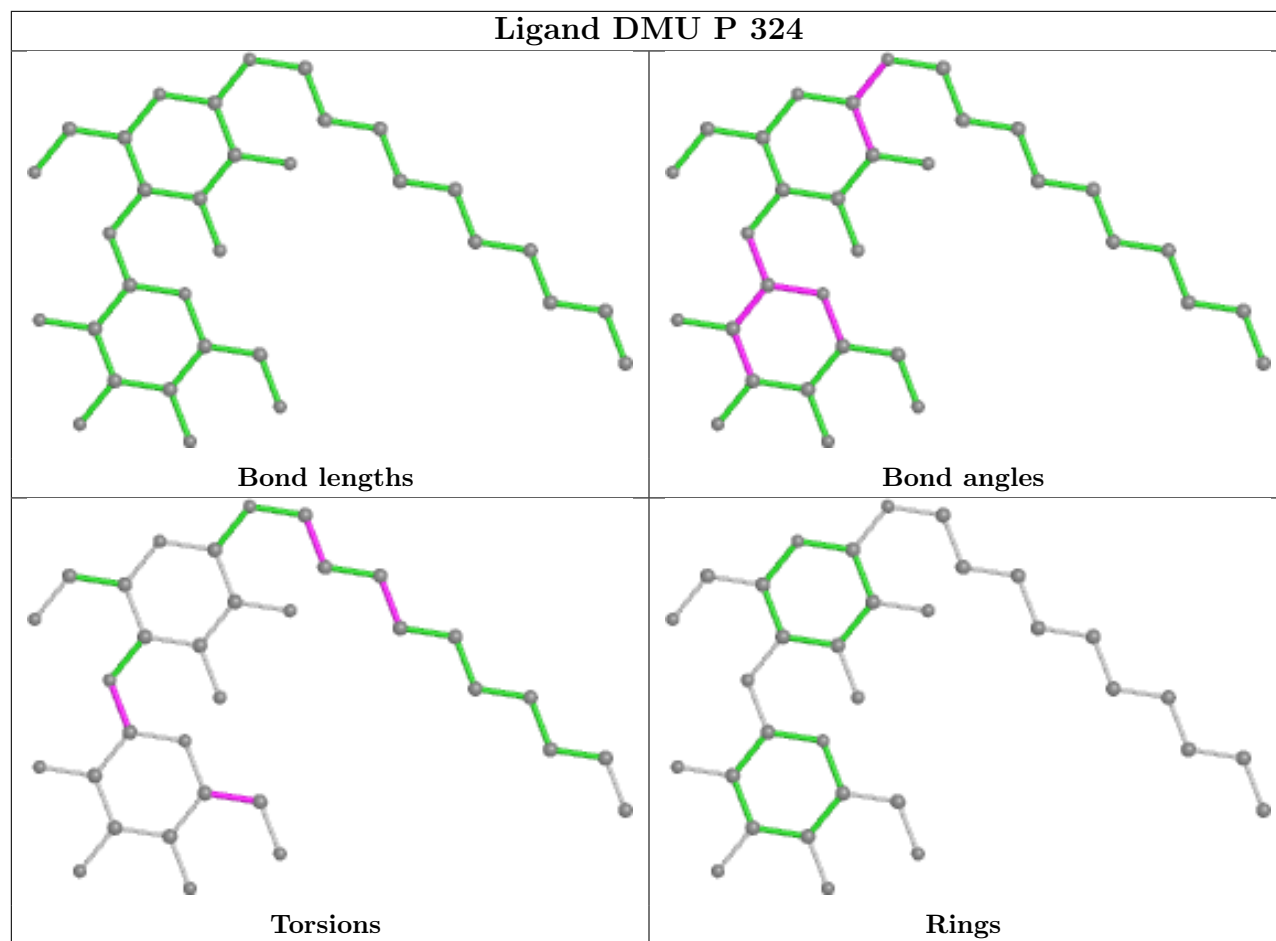


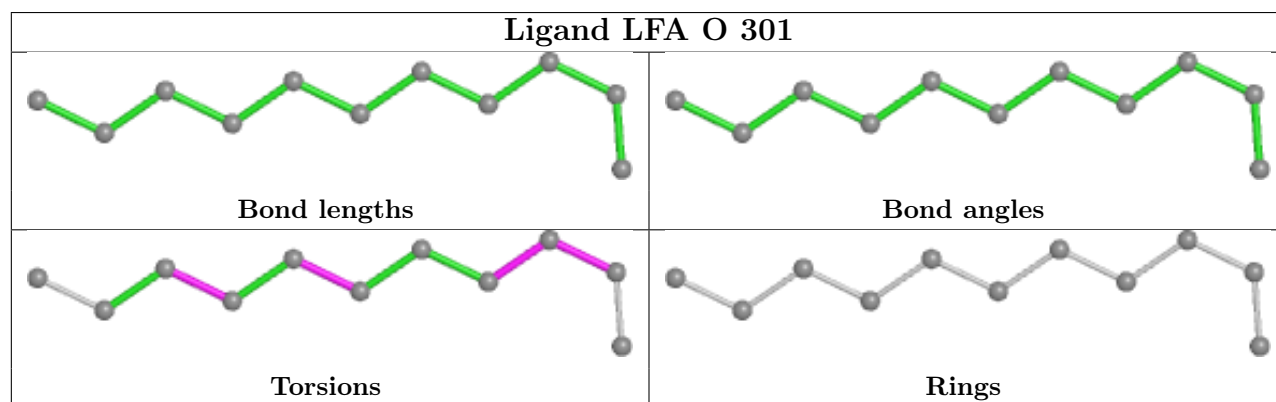
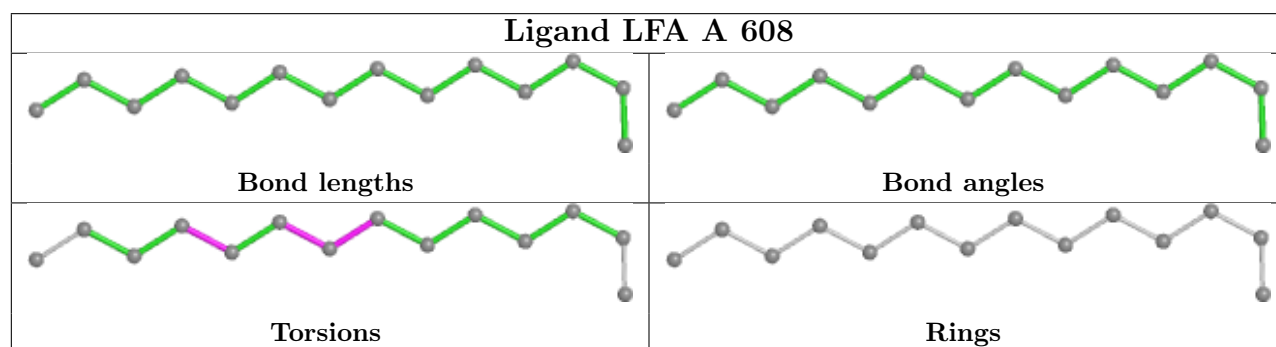
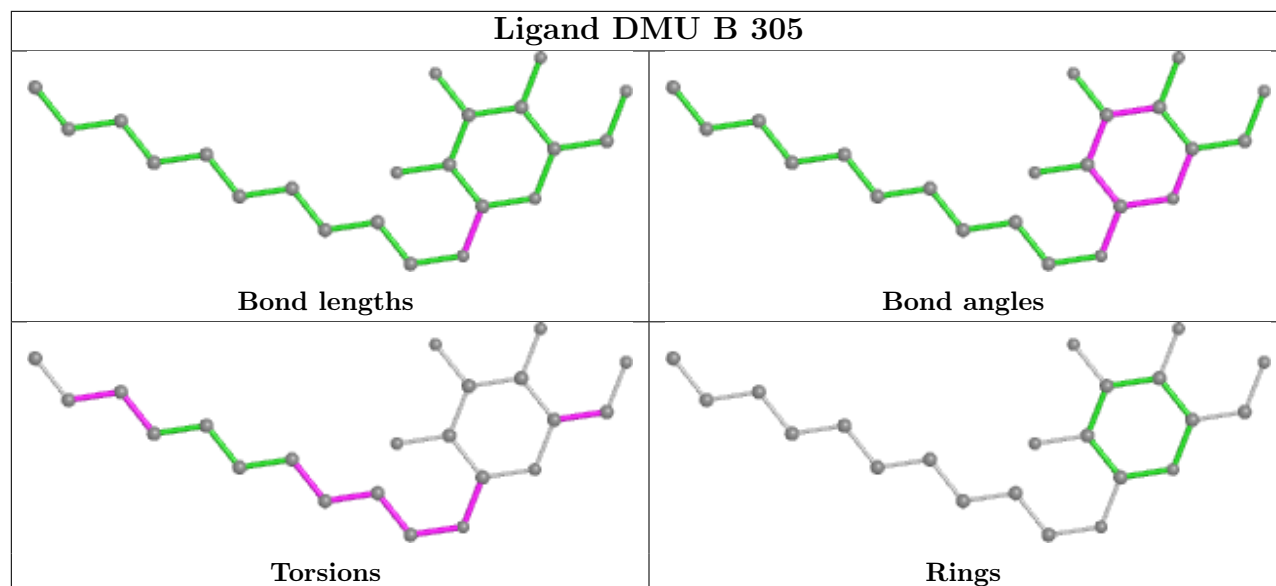


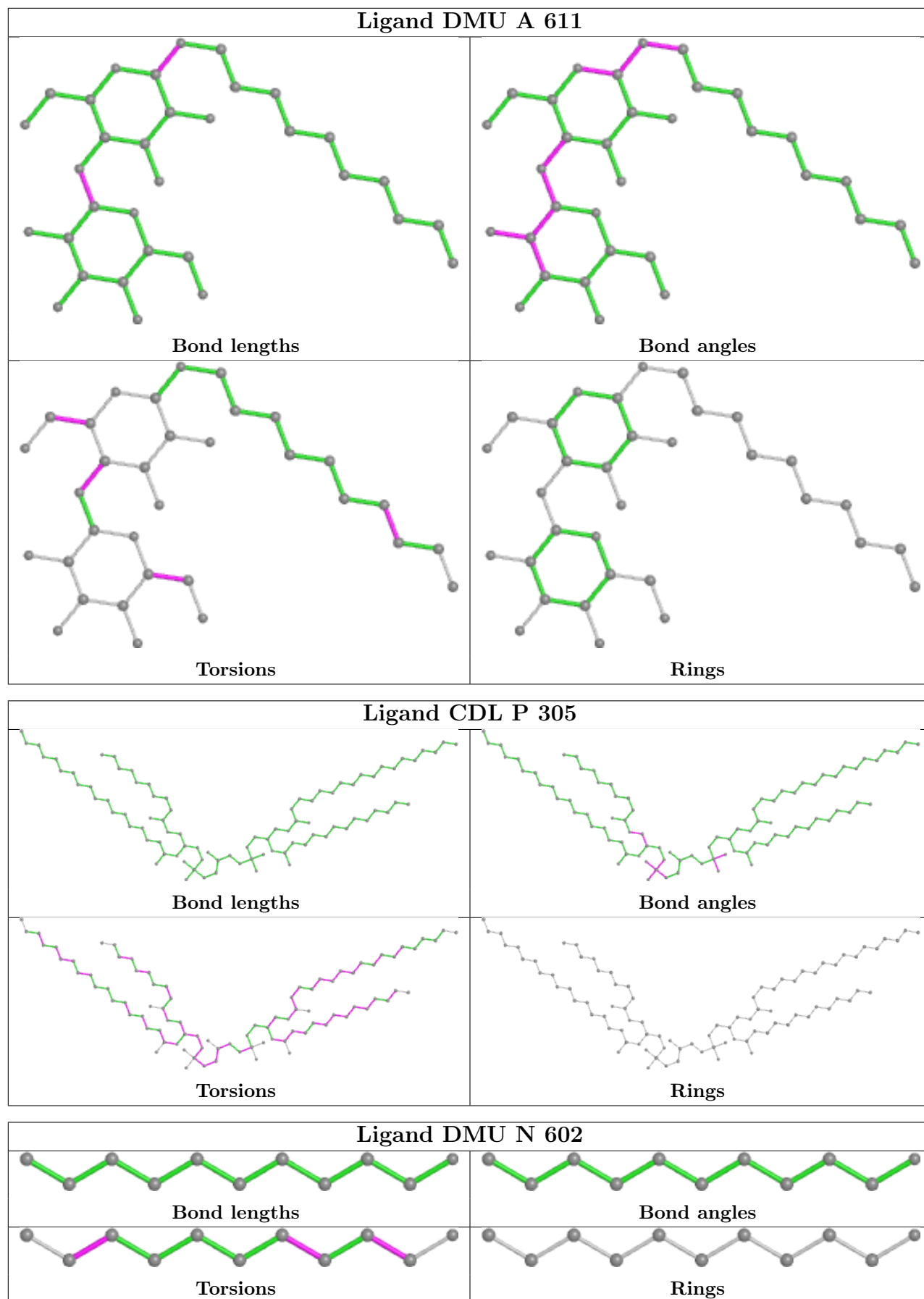


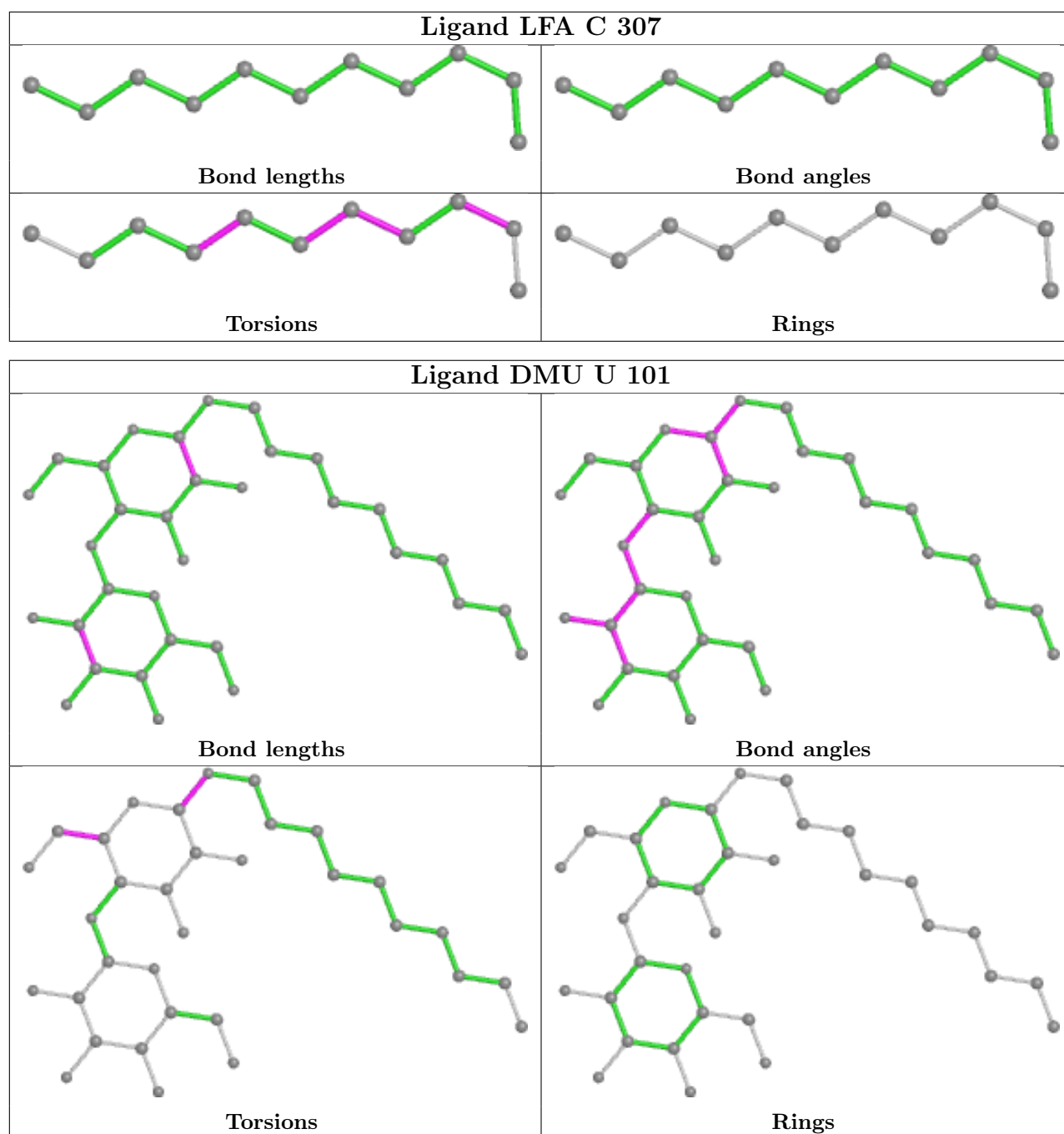












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	512/514 (99%)	-0.49	2 (0%) 89 88	15, 31, 38, 54	15 (2%)
1	N	512/514 (99%)	-0.41	2 (0%) 89 88	16, 33, 42, 54	15 (2%)
2	B	226/227 (99%)	-0.06	11 (4%) 36 33	20, 37, 57, 77	5 (2%)
2	O	226/227 (99%)	-0.03	5 (2%) 62 60	21, 41, 67, 92	5 (2%)
3	C	258/261 (98%)	-0.35	1 (0%) 89 88	15, 34, 44, 56	9 (3%)
3	P	258/261 (98%)	-0.34	1 (0%) 89 88	16, 35, 47, 65	9 (3%)
4	D	143/147 (97%)	-0.17	2 (1%) 73 72	19, 39, 54, 71	1 (0%)
4	Q	137/147 (93%)	0.20	3 (2%) 62 60	23, 50, 77, 89	1 (0%)
5	E	102/109 (93%)	-0.30	0 100 100	33, 40, 53, 70	0
5	R	102/109 (93%)	-0.09	1 (0%) 79 78	36, 48, 65, 78	0
6	F	91/98 (92%)	-0.13	1 (1%) 77 77	19, 40, 62, 74	2 (2%)
6	S	91/98 (92%)	-0.07	2 (2%) 62 60	18, 39, 60, 66	2 (2%)
7	G	72/85 (84%)	0.09	5 (6%) 24 21	20, 40, 82, 96	1 (1%)
7	T	72/85 (84%)	0.23	2 (2%) 55 53	21, 43, 76, 100	1 (1%)
8	H	75/85 (88%)	0.14	3 (4%) 43 40	34, 43, 83, 118	0
8	U	75/85 (88%)	0.21	4 (5%) 33 30	38, 46, 89, 117	0
9	I	70/73 (95%)	0.23	4 (5%) 30 28	36, 49, 73, 96	0
9	V	70/73 (95%)	0.36	3 (4%) 40 37	37, 55, 74, 104	0
10	J	56/59 (94%)	0.13	1 (1%) 67 66	35, 44, 67, 79	0
10	W	56/59 (94%)	0.19	1 (1%) 67 66	36, 47, 68, 84	0
11	K	49/56 (87%)	0.21	2 (4%) 42 39	38, 45, 60, 79	0
11	X	49/56 (87%)	0.57	2 (4%) 42 39	43, 53, 72, 101	0
12	L	44/47 (93%)	-0.19	1 (2%) 61 59	32, 36, 49, 61	0
12	Y	44/47 (93%)	-0.09	1 (2%) 61 59	36, 42, 57, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	40/46 (86%)	-0.03	0 100 100	34, 37, 54, 68	0
13	Z	40/46 (86%)	0.36	2 (5%) 35 32	40, 47, 70, 88	0
All	All	3470/3614 (96%)	-0.16	62 (1%) 67 66	15, 38, 63, 118	66 (1%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	36	TRP	6.5
11	X	6	ALA	4.5
2	O	113	TYR	4.4
2	B	59	GLN	4.4
6	S	3	GLY	4.1
8	H	45	ALA	4.0
6	S	93	PRO	3.9
8	U	47	GLY	3.7
8	U	45	ALA	3.5
11	K	6	ALA	3.5
7	G	36	TRP	3.5
10	J	1	PHE	3.5
9	V	37	PHE	3.2
6	F	3	GLY	3.2
2	B	61	VAL	3.1
2	O	90	ILE	3.0
8	H	48	GLY	3.0
8	U	48	GLY	3.0
10	W	1	PHE	3.0
7	T	38	HIS	3.0
2	O	91	ASN	2.9
9	V	3	ALA	2.9
1	N	136[A]	LEU	2.9
2	B	60	GLU	2.8
4	D	5	VAL	2.8
2	B	91	ASN	2.7
12	Y	24	MET	2.7
1	A	113[A]	LEU	2.7
4	D	4	SER	2.6
2	B	58	ALA	2.6
9	I	25	PHE	2.6
11	X	7	PRO	2.6
4	Q	35	ALA	2.6
9	I	3	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
8	U	46	LYS	2.5
2	B	65	TRP	2.5
2	B	113	TYR	2.4
7	G	35	SER	2.4
1	N	113[A]	LEU	2.4
3	C	38	ASN	2.4
13	Z	13	LYS	2.4
9	V	72	ALA	2.4
2	B	87[A]	MET	2.4
7	G	33	LEU	2.3
5	R	108	LYS	2.3
13	Z	38	ASP	2.3
9	I	37	PHE	2.3
11	K	47	ARG	2.2
2	B	115	ASP	2.2
2	B	67	ILE	2.2
2	O	32[A]	PHE	2.2
8	H	47	GLY	2.2
12	L	24	MET	2.2
4	Q	39	ALA	2.2
7	G	30	LEU	2.2
2	B	90	ILE	2.2
1	A	513	LEU	2.1
2	O	22[A]	HIS	2.1
9	I	29	LEU	2.0
3	P	37	PHE	2.0
7	G	41	HIS	2.0
4	Q	10	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	FME	A	1	10/11	0.94	0.12	41,49,80,95	0
1	FME	N	1	10/11	0.95	0.12	43,50,80,90	0
2	FME	B	1	10/11	0.97	0.09	32,37,47,87	0
2	FME	O	1	10/11	0.98	0.09	38,40,52,75	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
21	DMU	P	318	22/33	0.70	0.33	35,60,73,85	22
22	EDO	P	323	4/4	0.70	0.35	33,34,37,42	4
20	LFA	P	311	11/20	0.73	0.41	49,65,73,78	11
21	DMU	A	610	7/33	0.76	0.38	54,60,67,69	7
21	DMU	N	610	7/33	0.78	0.40	61,64,67,74	7
21	DMU	B	309	22/33	0.78	0.32	54,74,85,98	22
22	EDO	C	322	4/4	0.78	0.31	32,36,40,42	4
21	DMU	C	317	22/33	0.78	0.26	37,65,77,87	22
23	XE	A	618	1/1	0.78	0.25	48,48,48,48	1
21	DMU	C	318	33/33	0.79	0.34	40,55,70,94	33
21	DMU	O	302	22/33	0.80	0.29	50,62,83,96	22
22	EDO	A	613	4/4	0.81	0.31	36,44,47,48	4
23	XE	N	619	1/1	0.81	0.32	57,57,57,57	1
21	DMU	C	315	33/33	0.82	0.33	43,56,64,65	33
20	LFA	C	308	6/20	0.82	0.36	41,45,52,54	6
22	EDO	E	201	4/4	0.82	0.36	39,40,41,50	4
26	CHD	P	306	29/29	0.82	0.18	68,76,97,108	0
21	DMU	N	611	33/33	0.83	0.25	41,57,79,86	33
20	LFA	P	309	6/20	0.83	0.35	44,48,48,51	6
21	DMU	C	323	33/33	0.83	0.20	38,58,75,84	33
21	DMU	P	319	33/33	0.83	0.31	47,56,71,93	33
21	DMU	P	320	33/33	0.83	0.26	50,68,80,86	33
26	CHD	C	305	29/29	0.83	0.17	57,85,103,115	0
20	LFA	C	311	14/20	0.83	0.34	40,59,66,70	14
21	DMU	C	319	33/33	0.84	0.24	41,64,73,75	33
20	LFA	P	313	11/20	0.84	0.30	33,51,60,62	11
20	LFA	C	325	15/20	0.84	0.34	50,53,65,68	15
20	LFA	P	301	15/20	0.84	0.31	47,55,62,69	15
20	LFA	C	314	13/20	0.85	0.29	52,58,75,79	13
20	LFA	C	309	18/20	0.85	0.23	38,46,63,63	18
20	LFA	O	301	11/20	0.85	0.31	42,54,68,76	11
21	DMU	P	316	33/33	0.85	0.28	43,58,69,73	33

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	LFA	P	312	14/20	0.85	0.32	38,56,70,75	14
21	DMU	B	303	11/33	0.86	0.33	49,58,65,77	11
20	LFA	C	312	11/20	0.86	0.33	45,55,64,70	11
21	DMU	M	102	8/33	0.86	0.23	42,49,56,60	8
20	LFA	N	601	17/20	0.86	0.27	37,55,70,76	17
20	LFA	A	609	14/20	0.86	0.25	40,44,59,61	14
21	DMU	A	622	33/33	0.86	0.23	35,46,53,67	33
21	DMU	A	623	11/33	0.87	0.30	42,51,69,75	11
20	LFA	C	313	15/20	0.87	0.26	43,53,74,78	15
21	DMU	P	317	7/33	0.87	0.24	51,55,60,67	7
21	DMU	B	304	11/33	0.87	0.27	38,55,67,69	11
20	LFA	C	310	11/20	0.87	0.29	57,63,68,71	11
20	LFA	B	308	17/20	0.87	0.28	38,60,74,80	17
20	LFA	C	307	11/20	0.87	0.29	41,48,61,61	11
21	DMU	P	324	33/33	0.88	0.18	41,60,88,95	33
19	CDL	V	101	64/100	0.88	0.17	50,82,127,147	0
21	DMU	C	316	7/33	0.88	0.30	47,53,62,69	7
21	DMU	O	305	11/33	0.88	0.33	45,50,61,73	11
22	EDO	N	613	4/4	0.88	0.28	37,43,44,51	4
21	DMU	G	103	22/33	0.88	0.26	45,54,61,64	22
21	DMU	J	101	11/33	0.88	0.34	58,63,76,86	11
20	LFA	P	308	11/20	0.88	0.30	41,50,63,68	11
21	DMU	N	602	11/33	0.88	0.29	41,53,65,71	11
20	LFA	G	105	14/20	0.88	0.25	40,46,57,60	14
21	DMU	W	101	11/33	0.89	0.35	64,72,80,83	11
21	DMU	Y	102	22/33	0.89	0.34	53,62,73,80	22
20	LFA	A	608	14/20	0.89	0.23	36,43,70,79	14
20	LFA	P	315	13/20	0.89	0.22	46,54,71,78	13
19	CDL	C	304	87/100	0.89	0.18	41,80,116,127	0
19	CDL	P	305	87/100	0.89	0.18	39,83,128,160	0
22	EDO	P	321	4/4	0.89	0.22	50,51,56,68	4
20	LFA	P	310	18/20	0.89	0.23	40,50,56,57	18
19	CDL	A	607	64/100	0.89	0.16	50,81,119,133	0
19	CDL	Y	101	94/100	0.89	0.17	52,84,134,147	0
21	DMU	Q	201	33/33	0.89	0.20	38,51,64,74	33
21	DMU	U	101	33/33	0.89	0.22	34,48,65,68	33
20	LFA	P	314	15/20	0.90	0.19	42,47,55,59	15
21	DMU	L	102	22/33	0.90	0.30	46,59,67,71	22
21	DMU	O	307	22/33	0.90	0.18	35,52,58,58	22
21	DMU	T	103	22/33	0.90	0.20	43,54,67,70	22
21	DMU	A	611	33/33	0.90	0.18	35,47,61,65	33
20	LFA	T	102	11/20	0.90	0.27	51,56,68,73	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	DMU	D	201	33/33	0.90	0.18	28,48,60,76	33
22	EDO	A	612	4/4	0.90	0.15	27,29,31,32	4
21	DMU	B	305	22/33	0.90	0.21	40,69,83,91	22
19	CDL	L	101	94/100	0.91	0.15	43,81,124,142	0
20	LFA	N	609	14/20	0.91	0.23	37,50,68,69	14
21	DMU	Z	102	8/33	0.92	0.22	51,54,55,56	8
22	EDO	A	615	4/4	0.92	0.13	36,43,46,49	4
22	EDO	F	102	4/4	0.92	0.16	22,23,29,32	4
22	EDO	R	203	4/4	0.92	0.24	40,41,49,56	4
21	DMU	P	307	11/33	0.93	0.24	45,50,58,71	11
22	EDO	R	202	4/4	0.93	0.19	35,36,39,40	4
22	EDO	G	104	4/4	0.93	0.14	29,33,35,36	4
22	EDO	N	612	4/4	0.93	0.14	30,31,32,32	4
21	DMU	C	306	11/33	0.93	0.23	50,54,60,69	11
22	EDO	N	614	4/4	0.93	0.19	30,31,32,33	4
22	EDO	E	203	4/4	0.93	0.24	34,37,43,44	4
22	EDO	C	320	4/4	0.94	0.26	46,54,57,76	4
22	EDO	C	321	4/4	0.94	0.18	35,37,38,38	4
22	EDO	S	102	4/4	0.94	0.11	21,24,28,29	4
22	EDO	N	616	4/4	0.94	0.21	30,30,33,38	4
22	EDO	O	308	4/4	0.94	0.12	30,31,33,37	4
21	DMU	O	306	11/33	0.94	0.23	38,53,61,62	11
21	DMU	Z	101	33/33	0.94	0.10	51,58,72,76	0
22	EDO	E	202	4/4	0.95	0.20	31,33,35,35	4
26	CHD	C	301	29/29	0.95	0.08	32,36,41,43	0
27	UNX	P	303	1/1	0.95	0.29	45,45,45,45	0
21	DMU	M	101	33/33	0.96	0.08	45,52,66,73	0
22	EDO	R	201	4/4	0.96	0.25	57,59,65,68	4
23	XE	N	620	1/1	0.96	0.17	52,52,52,52	1
22	EDO	A	614	4/4	0.96	0.17	26,27,28,28	4
22	EDO	N	615	4/4	0.96	0.14	36,37,38,39	4
22	EDO	P	322	4/4	0.96	0.18	36,38,40,43	4
22	EDO	T	104	4/4	0.96	0.11	34,34,36,40	4
22	EDO	B	306	4/4	0.97	0.09	25,27,28,31	4
23	XE	A	619	1/1	0.97	0.10	49,49,49,49	1
26	CHD	P	302	29/29	0.97	0.07	33,37,42,45	0
24	PGV	N	622	51/51	0.97	0.09	31,45,76,79	0
27	UNX	C	302	1/1	0.97	0.18	44,44,44,44	0
26	CHD	B	307	29/29	0.97	0.06	31,34,38,49	0
29	PEK	G	101	53/53	0.97	0.11	34,53,94,116	0
29	PEK	T	101	53/53	0.97	0.11	36,55,97,109	0
26	CHD	G	102	29/29	0.98	0.06	30,33,36,44	0

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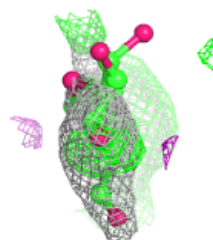
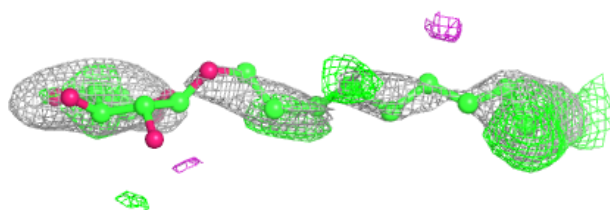
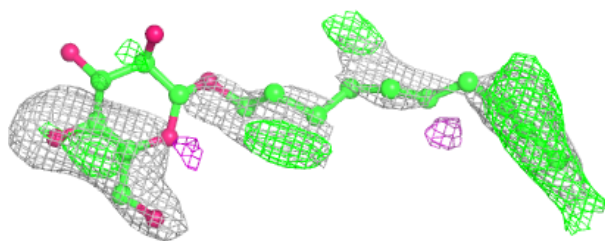
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	PGV	C	303	51/51	0.98	0.09	30,39,104,112	0
22	EDO	S	103	4/4	0.98	0.08	31,37,38,40	4
24	PGV	P	304	51/51	0.98	0.08	30,40,97,116	0
22	EDO	F	103	4/4	0.98	0.08	32,32,32,36	4
23	XE	P	325	1/1	0.98	0.06	49,49,49,49	1
24	PGV	A	621	51/51	0.98	0.09	29,44,79,87	0
14	HEA	A	601[B]	60/60	0.99	0.05	26,28,44,49	9
14	HEA	A	602	60/60	0.99	0.05	25,28,35,41	0
14	HEA	N	603[A]	60/60	0.99	0.06	28,31,44,50	9
14	HEA	N	603[B]	60/60	0.99	0.06	28,31,45,45	9
14	HEA	N	604	60/60	0.99	0.05	27,30,36,42	0
16	MG	A	604	1/1	0.99	0.03	31,31,31,31	0
16	MG	N	606	1/1	0.99	0.02	34,34,34,34	0
17	NA	A	605	1/1	0.99	0.05	34,34,34,34	0
18	PER	A	606	2/2	0.99	0.04	26,26,26,36	0
18	PER	N	608	2/2	0.99	0.07	29,29,29,38	0
14	HEA	A	601[A]	60/60	0.99	0.05	26,28,38,44	9
23	XE	A	620	1/1	1.00	0.11	52,52,52,52	1
23	XE	B	301	1/1	1.00	0.32	54,54,54,54	1
25	CUA	B	302	2/2	1.00	0.02	30,30,30,30	0
25	CUA	O	304	2/2	1.00	0.02	34,34,34,34	0
23	XE	C	324	1/1	1.00	0.06	51,51,51,51	1
23	XE	N	617	1/1	1.00	0.21	50,50,50,50	0
23	XE	N	618	1/1	1.00	0.27	49,49,49,49	1
17	NA	N	607	1/1	1.00	0.06	39,39,39,39	0
23	XE	A	616	1/1	1.00	0.23	49,49,49,49	0
23	XE	N	621	1/1	1.00	0.09	53,53,53,53	1
23	XE	O	303	1/1	1.00	0.27	51,51,51,51	1
23	XE	A	617	1/1	1.00	0.26	47,47,47,47	1
28	ZN	F	101	1/1	1.00	0.01	35,35,35,35	0
28	ZN	S	101	1/1	1.00	0.01	35,35,35,35	0
15	CU	N	605	1/1	1.00	0.02	30,30,30,30	0
15	CU	A	603	1/1	1.00	0.01	29,29,29,29	0

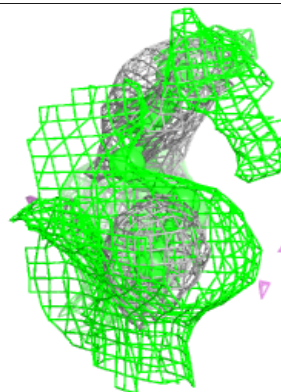
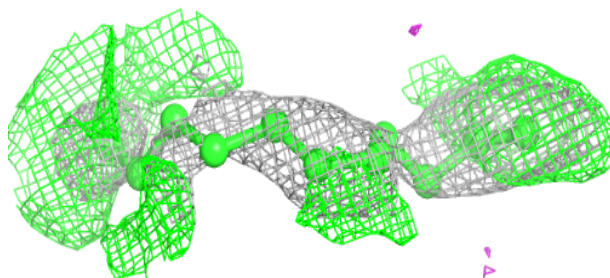
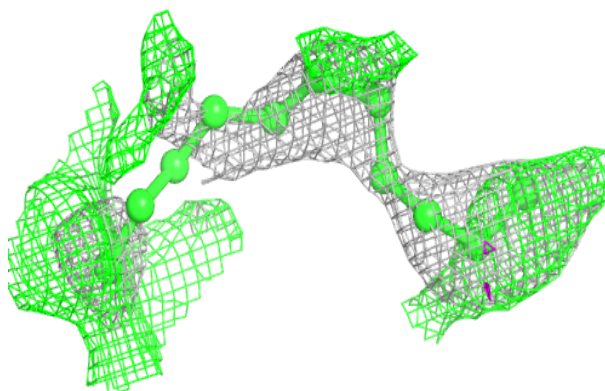
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU P 318:

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

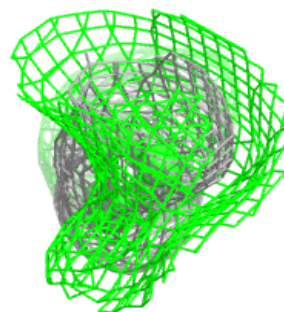
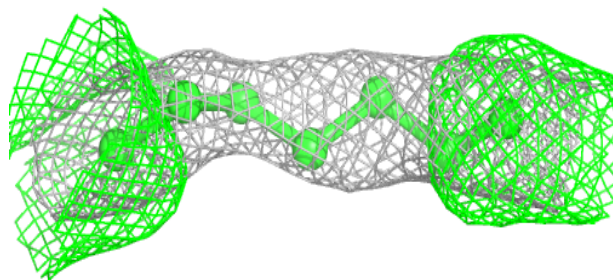
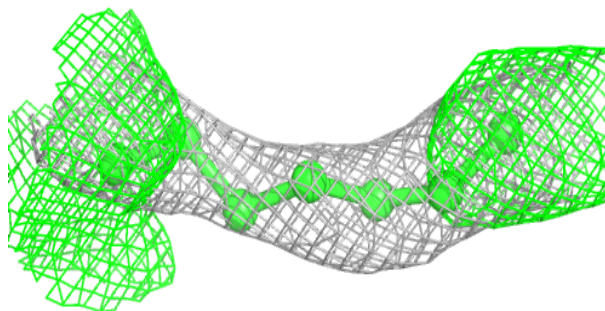
**Electron density around LFA P 311:**

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

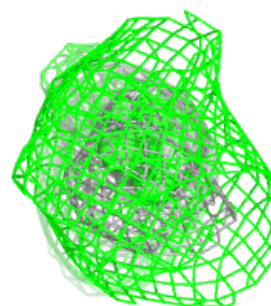
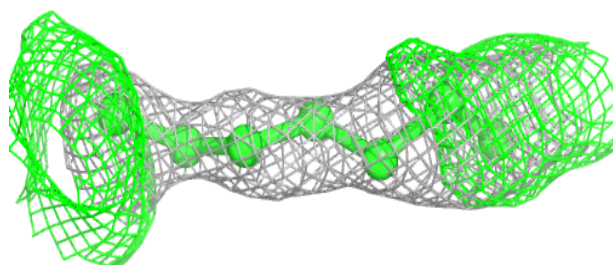
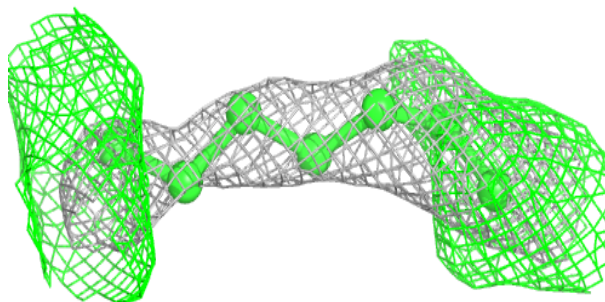


Electron density around DMU A 610:

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

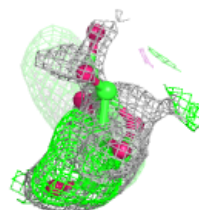
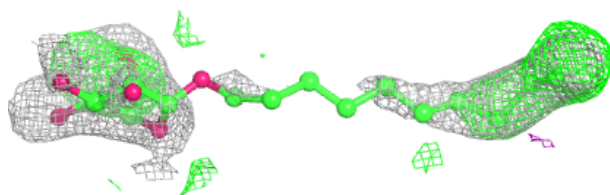
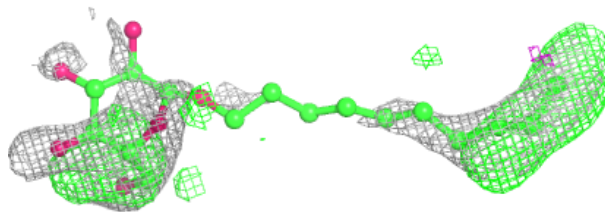
**Electron density around DMU N 610:**

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

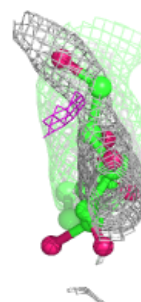
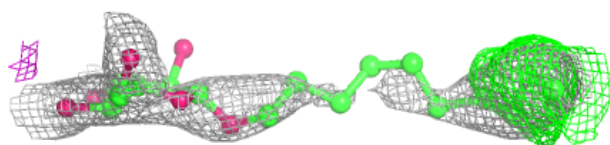
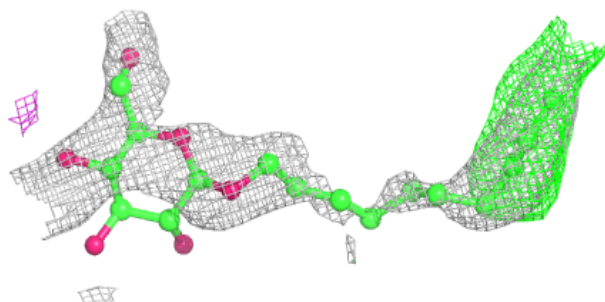


Electron density around DMU B 309:

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

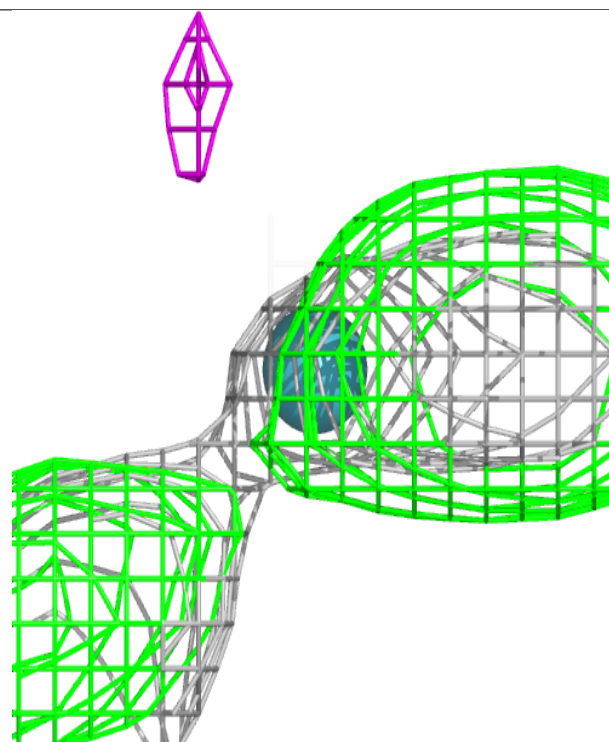
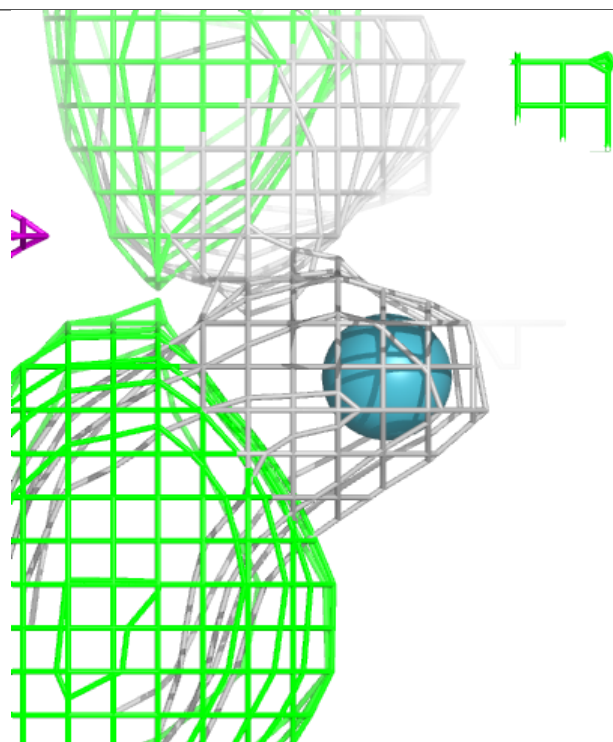
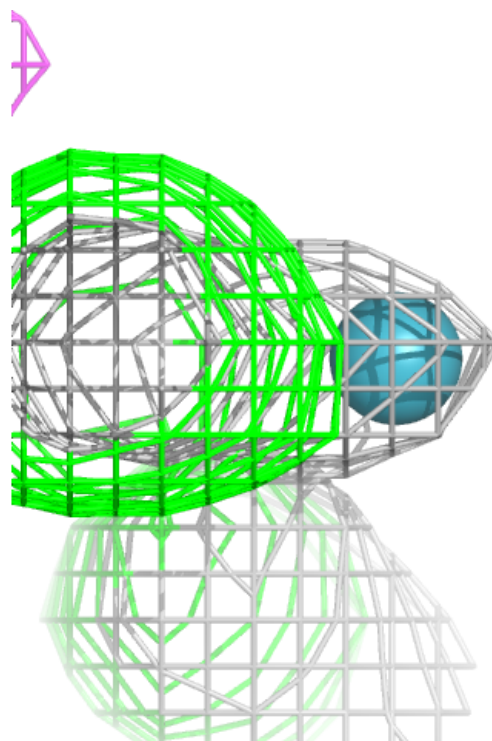
**Electron density around DMU C 317:**

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



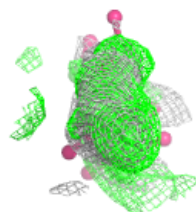
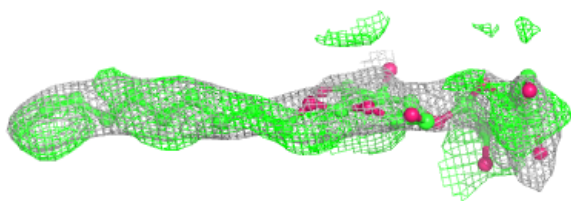
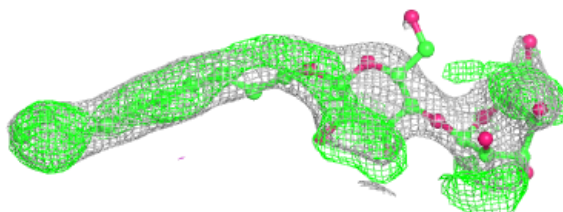
Electron density around XE A 618:

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

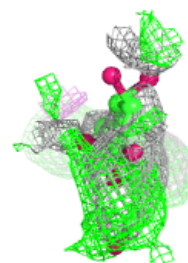
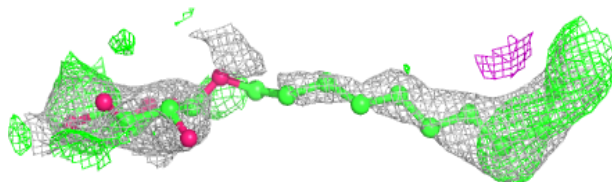
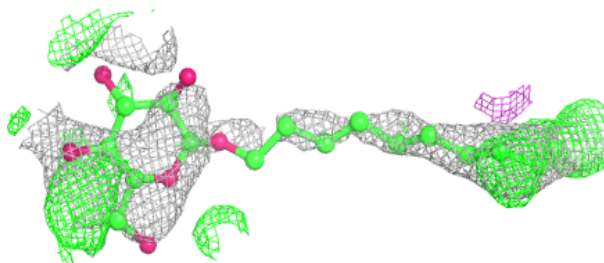


Electron density around DMU C 318:

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

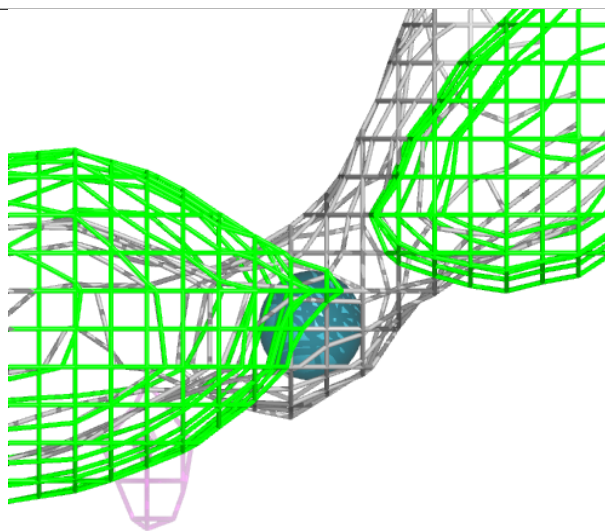
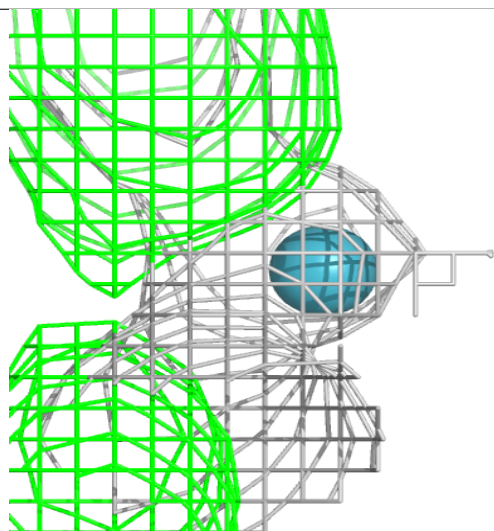
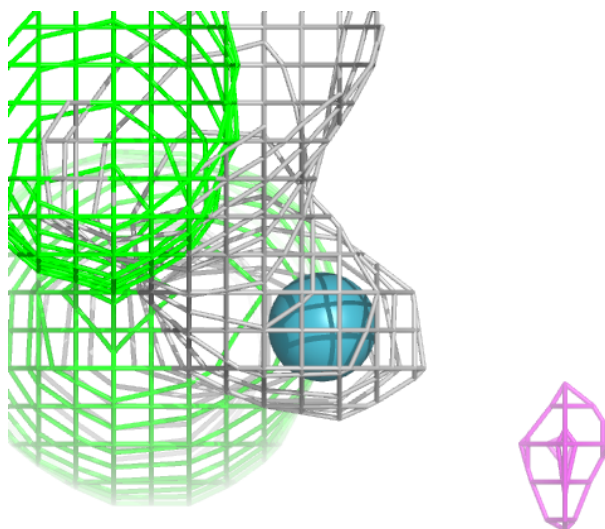
**Electron density around DMU O 302:**

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



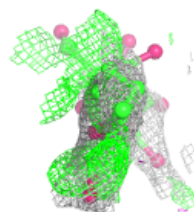
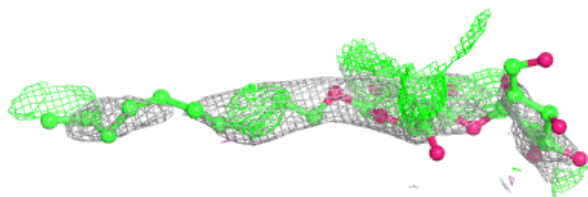
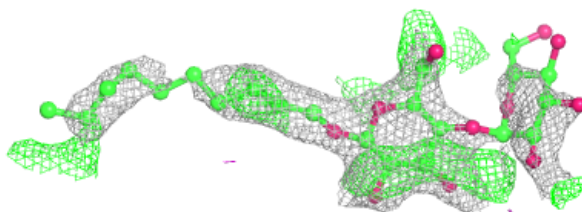
Electron density around XE N 619:

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

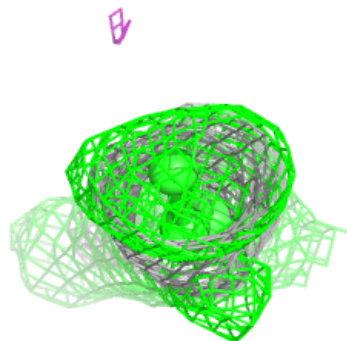
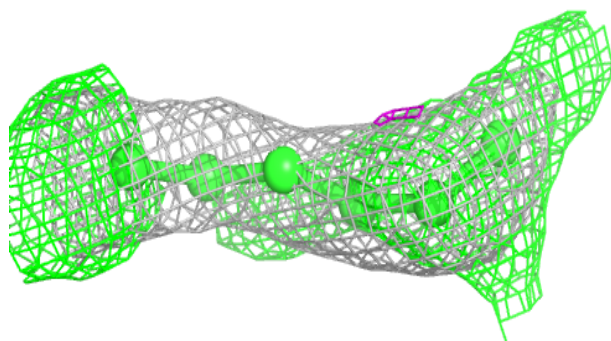
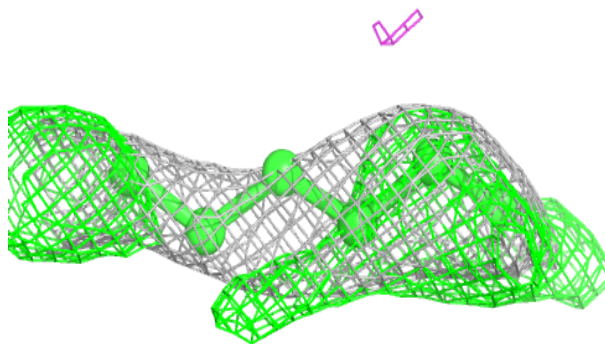


Electron density around DMU C 315:

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

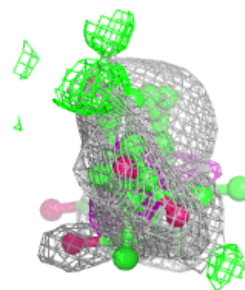
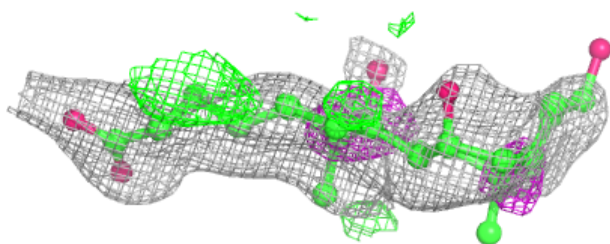
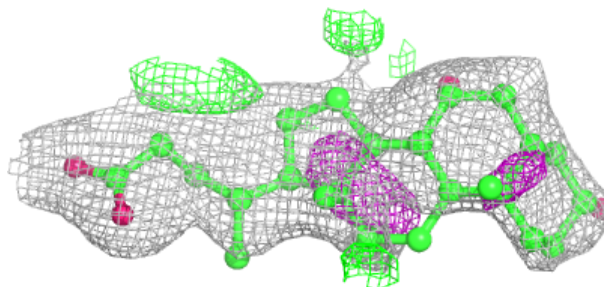
**Electron density around LFA C 308:**

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

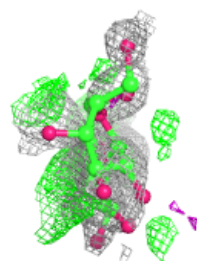
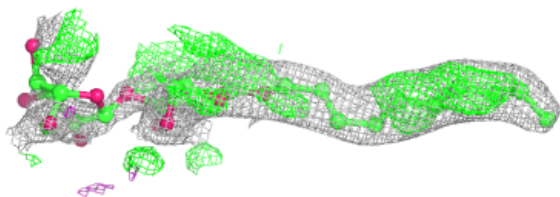
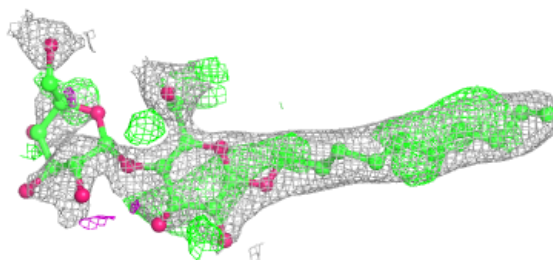


Electron density around CHD P 306:

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

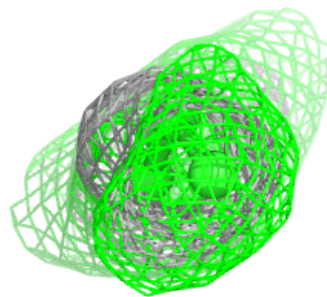
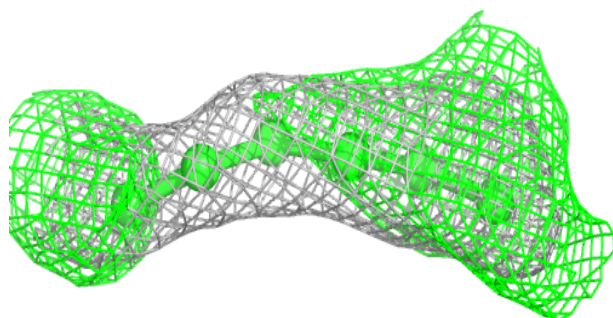
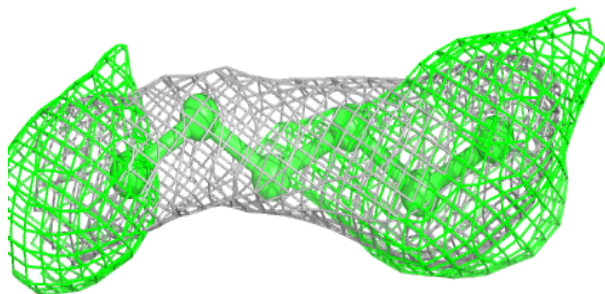
**Electron density around DMU N 611:**

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

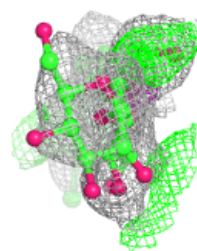
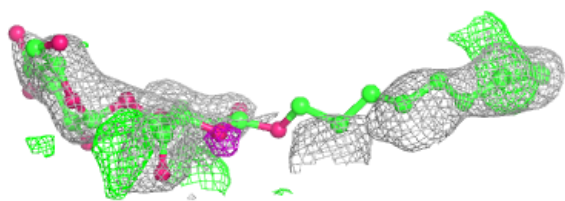
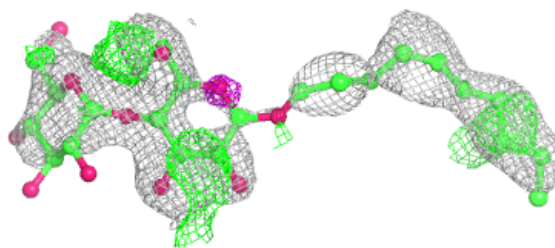


Electron density around LFA P 309:

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

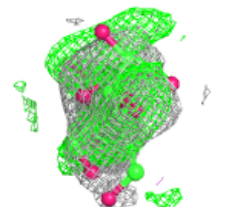
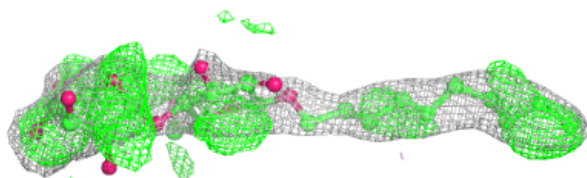
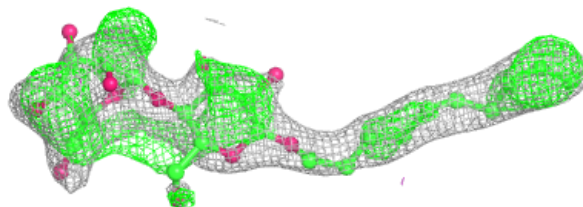
**Electron density around DMU C 323:**

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

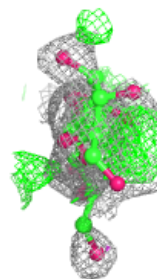
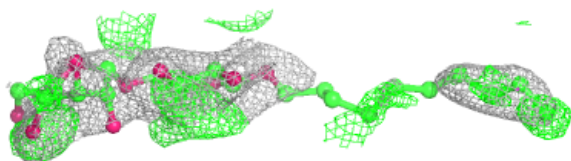
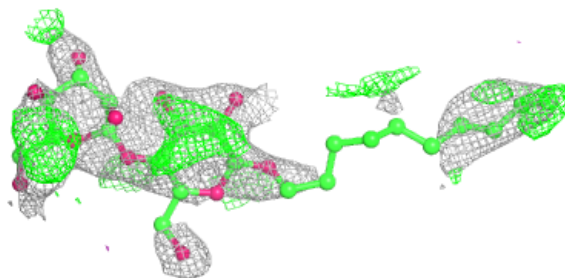


Electron density around DMU P 319:

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

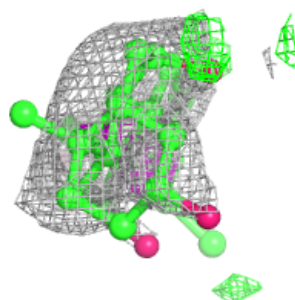
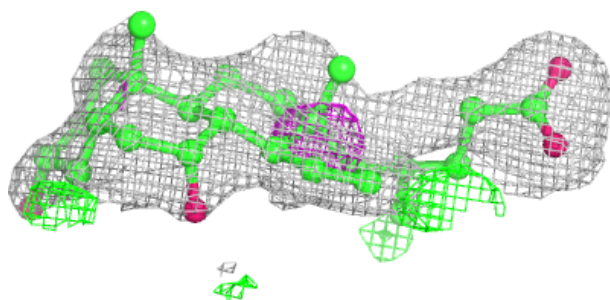
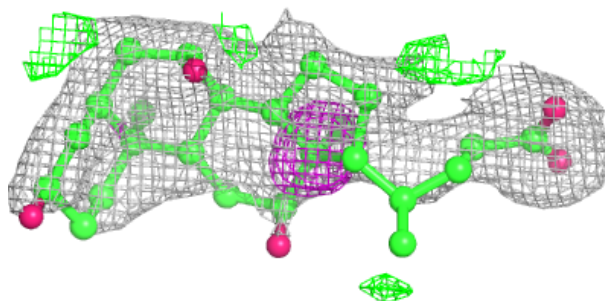
**Electron density around DMU P 320:**

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

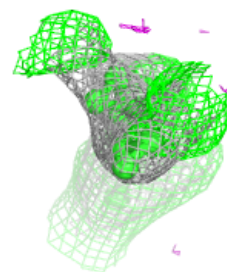
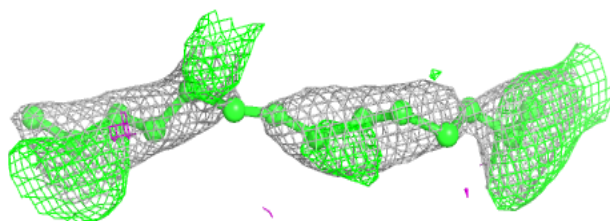
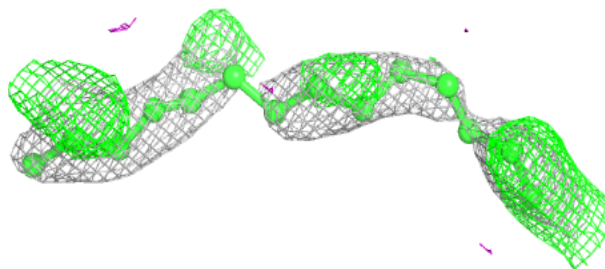


Electron density around CHD C 305:

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

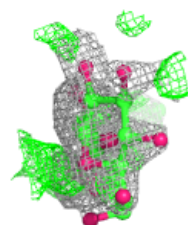
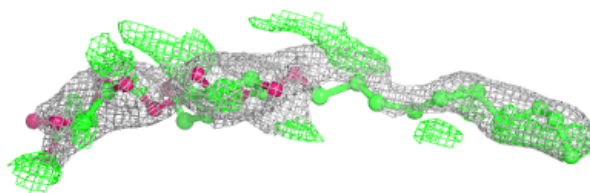
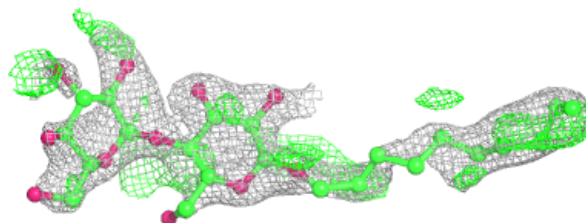
**Electron density around LFA C 311:**

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

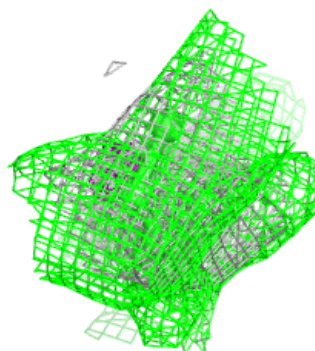
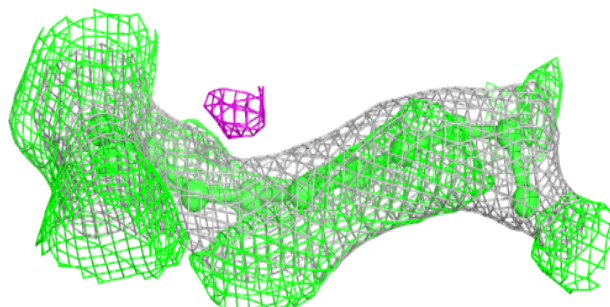
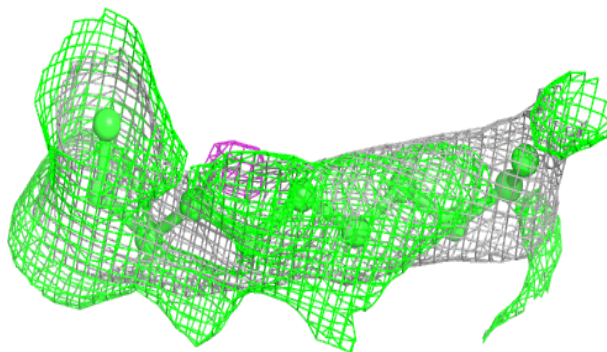


Electron density around DMU C 319:

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

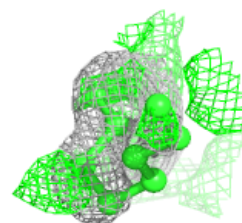
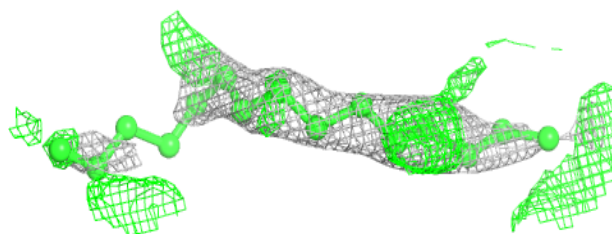
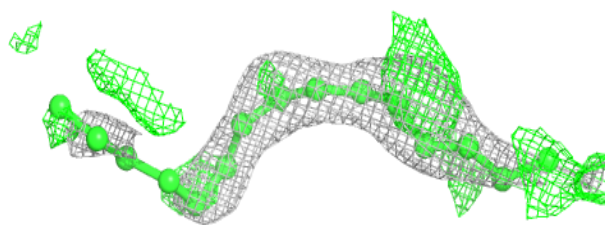
**Electron density around LFA P 313:**

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

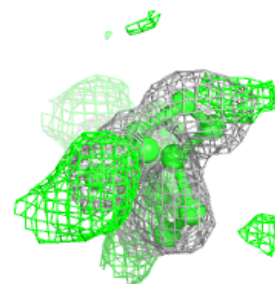
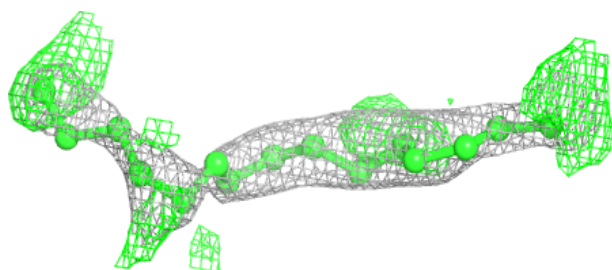
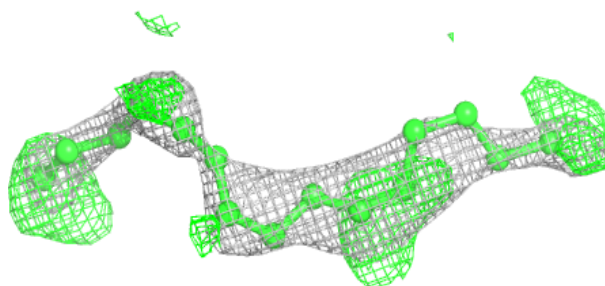


Electron density around LFA C 325:

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

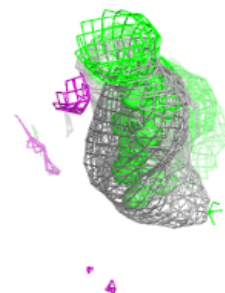
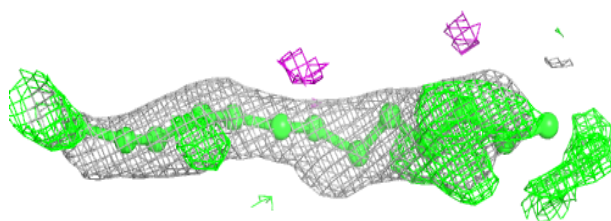
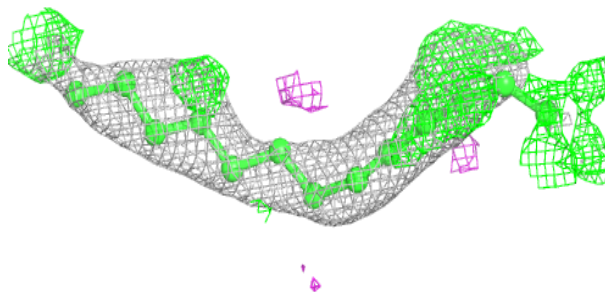
**Electron density around LFA P 301:**

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

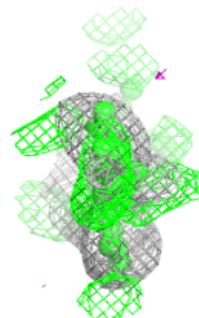
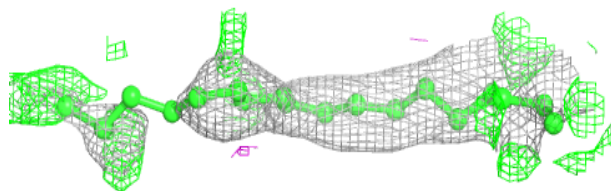
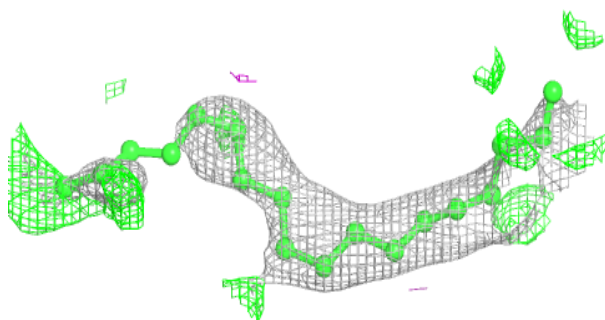


Electron density around LFA C 314:

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

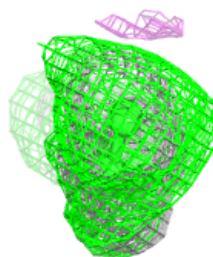
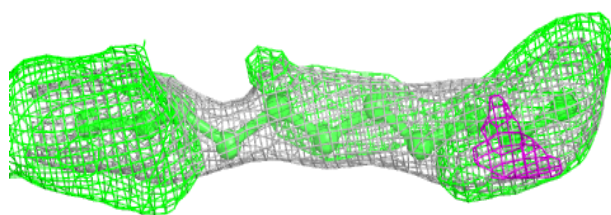
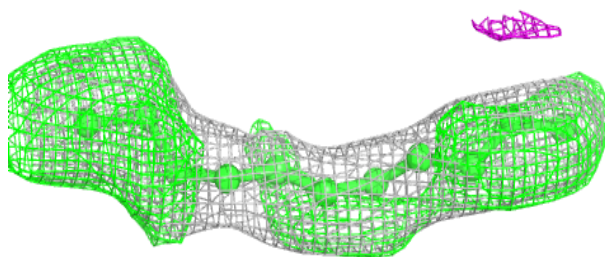
**Electron density around LFA C 309:**

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

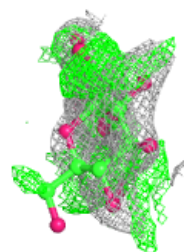
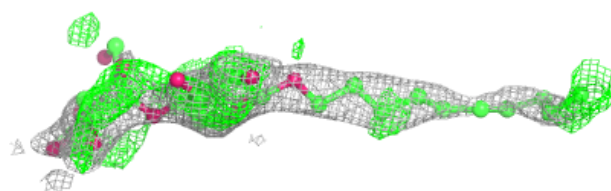
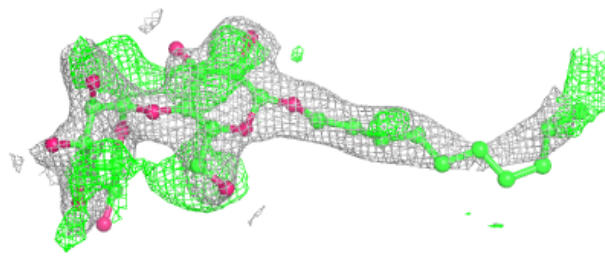


Electron density around LFA O 301:

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

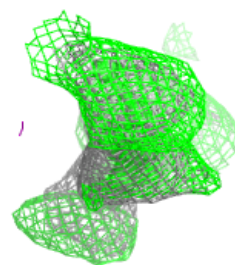
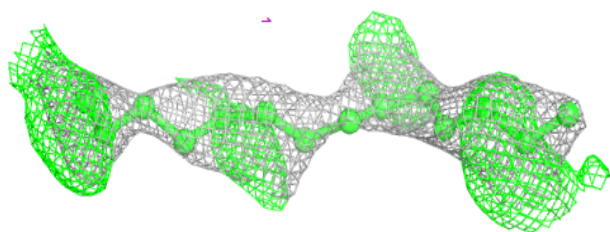
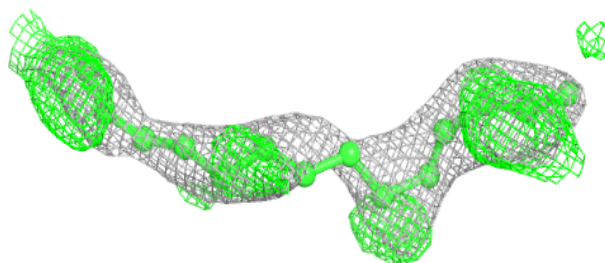
**Electron density around DMU P 316:**

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

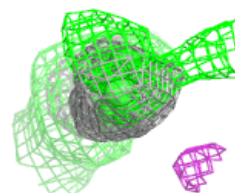
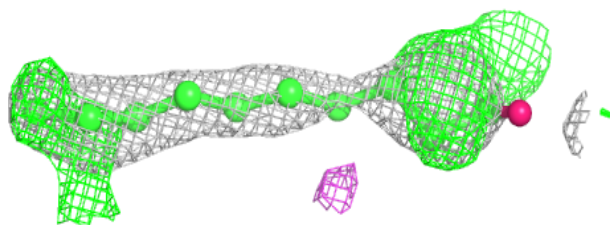
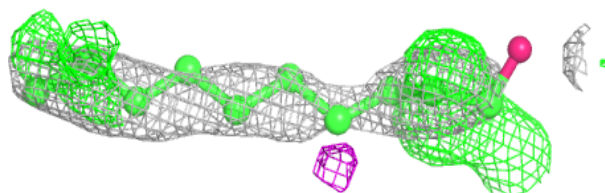


Electron density around LFA P 312:

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

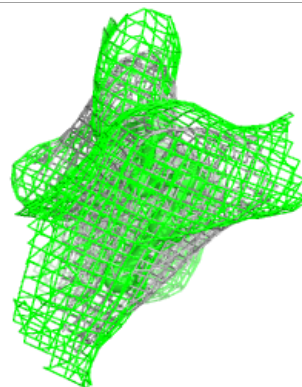
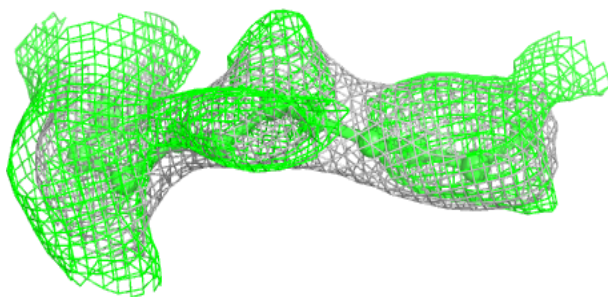
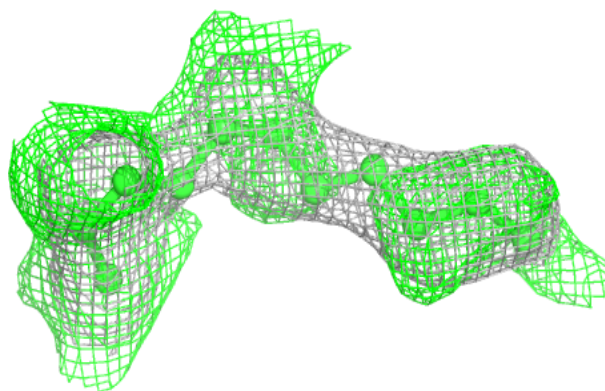
**Electron density around DMU B 303:**

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

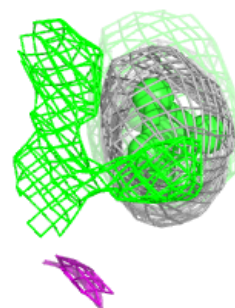
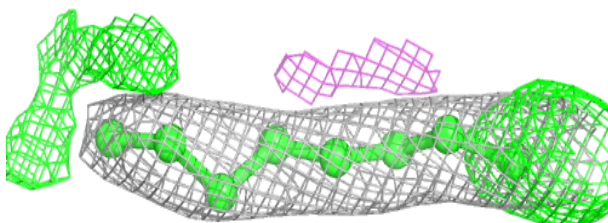
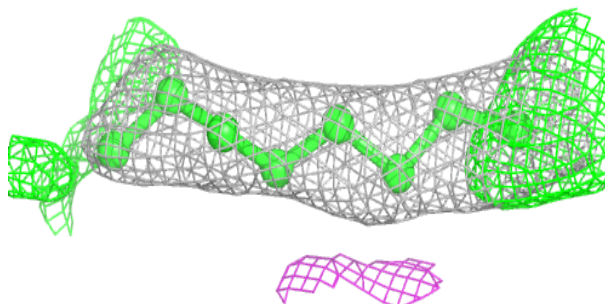


Electron density around LFA C 312:

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

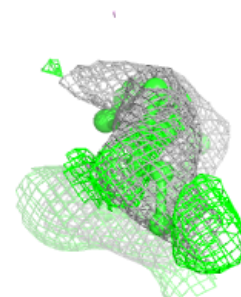
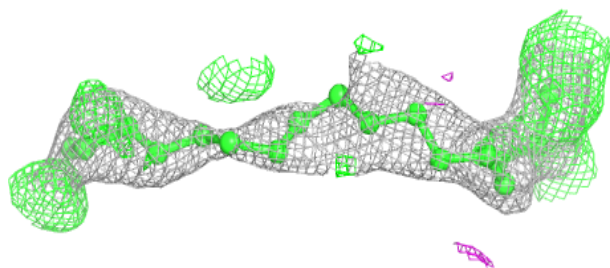
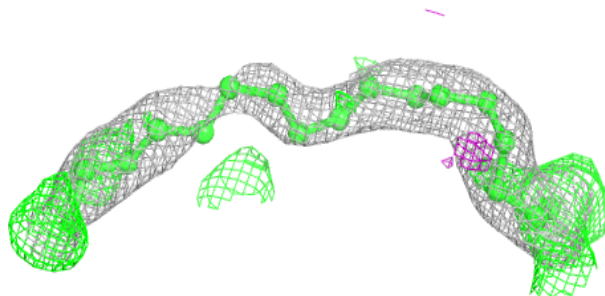
**Electron density around DMU M 102:**

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

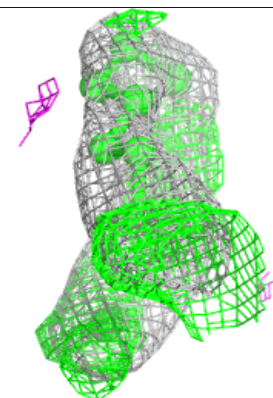
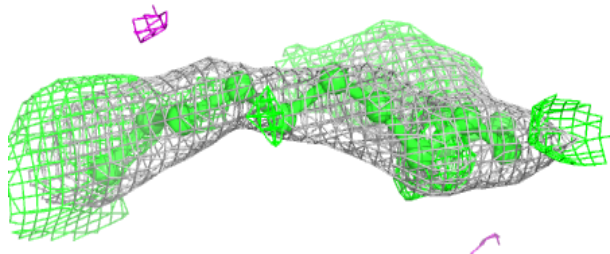
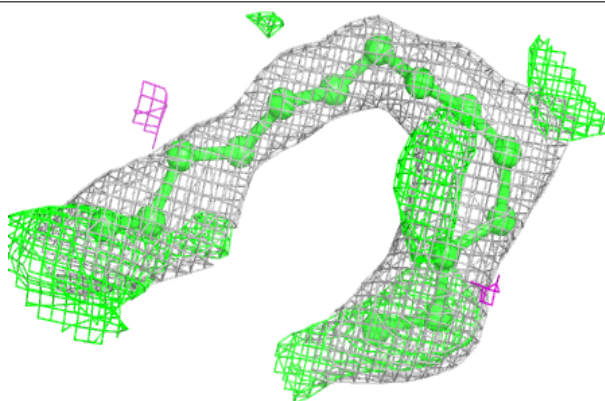


Electron density around LFA N 601:

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

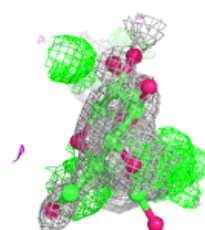
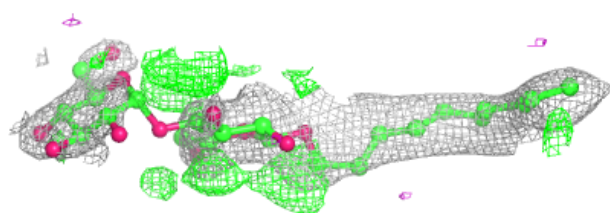
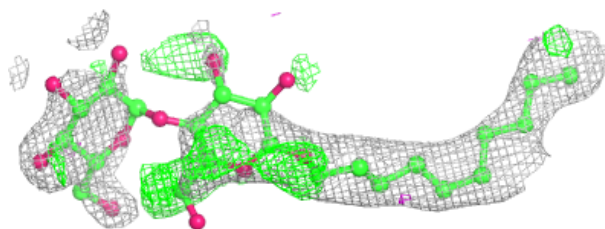
**Electron density around LFA A 609:**

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

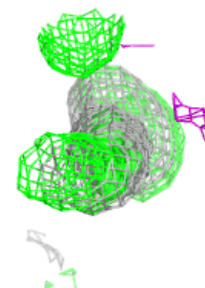
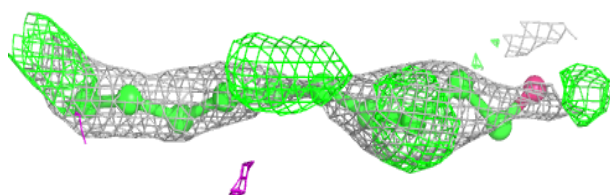
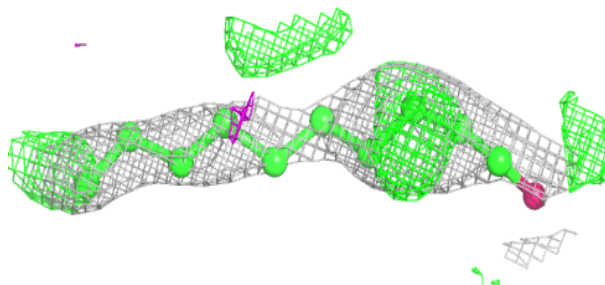


Electron density around DMU A 622:

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

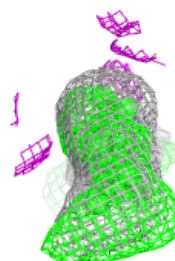
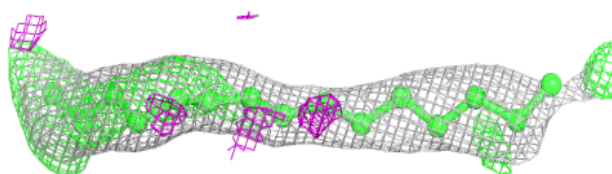
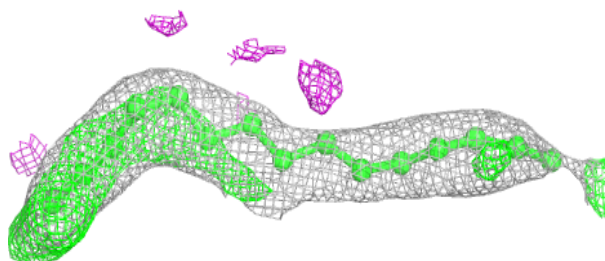
**Electron density around DMU A 623:**

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

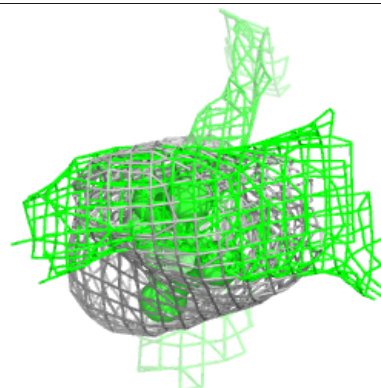
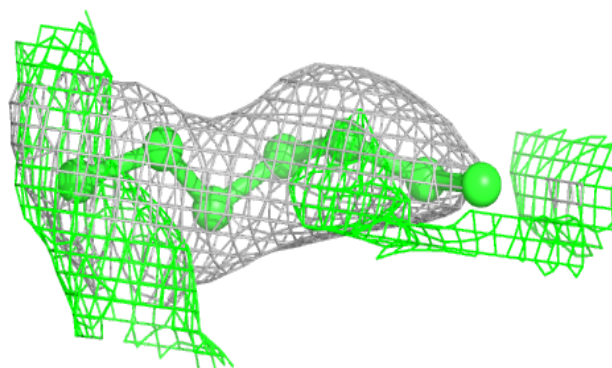
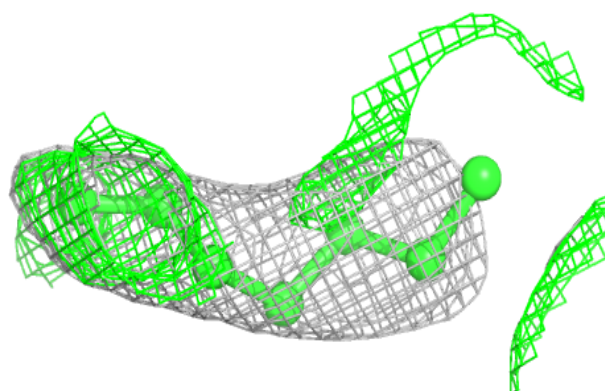


Electron density around LFA C 313:

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

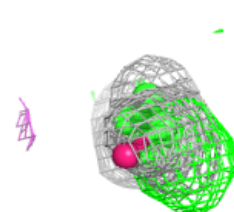
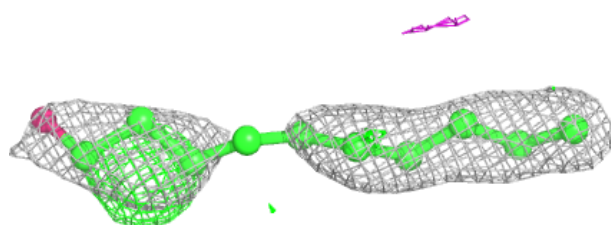
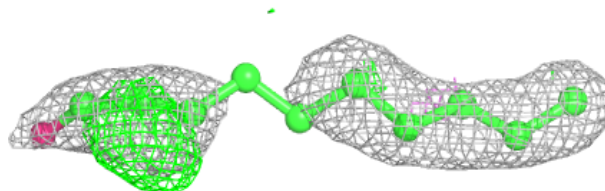
**Electron density around DMU P 317:**

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

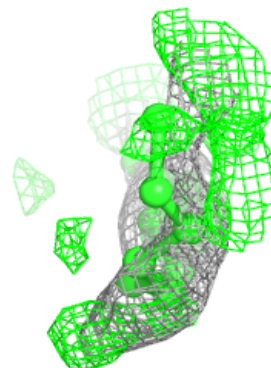
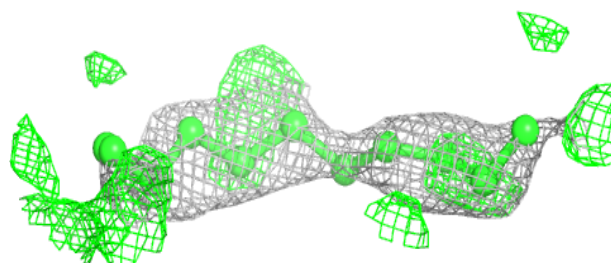
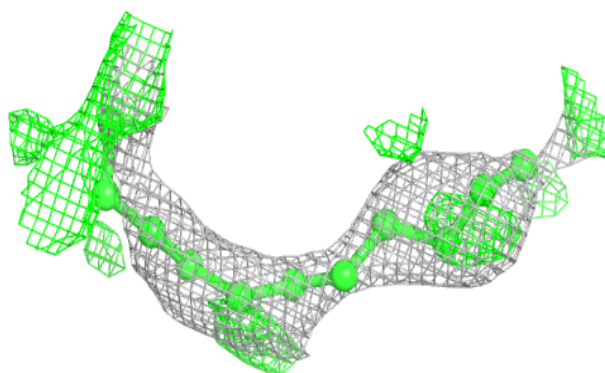


Electron density around DMU B 304:

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

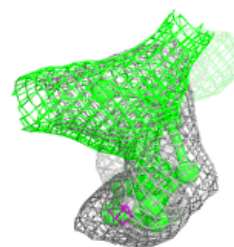
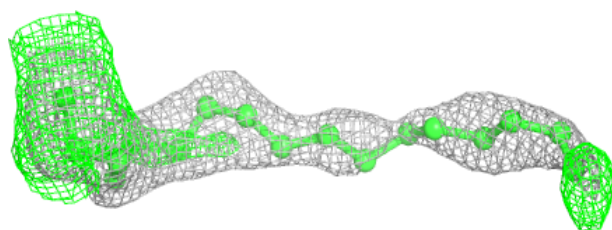
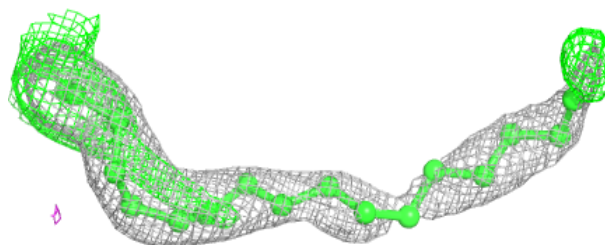
**Electron density around LFA C 310:**

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

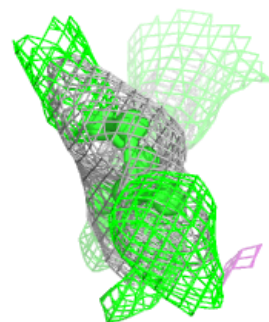
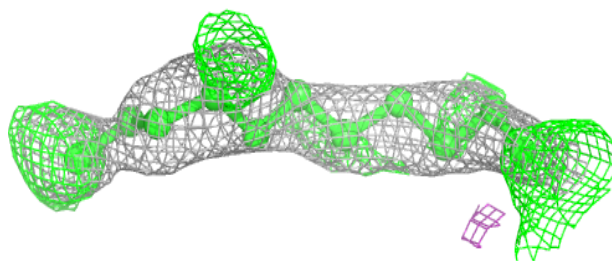
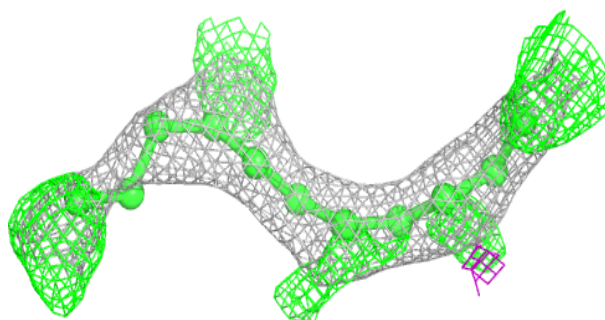


Electron density around LFA B 308:

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

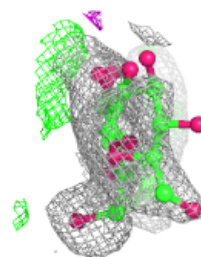
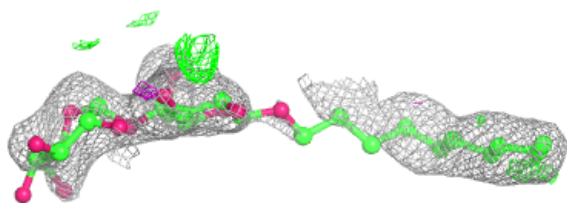
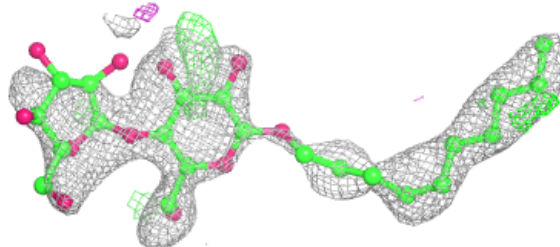
**Electron density around LFA C 307:**

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

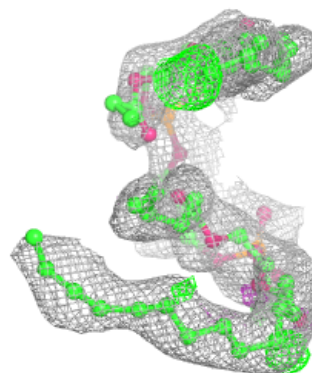
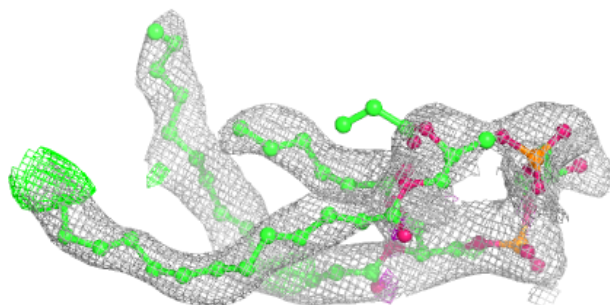
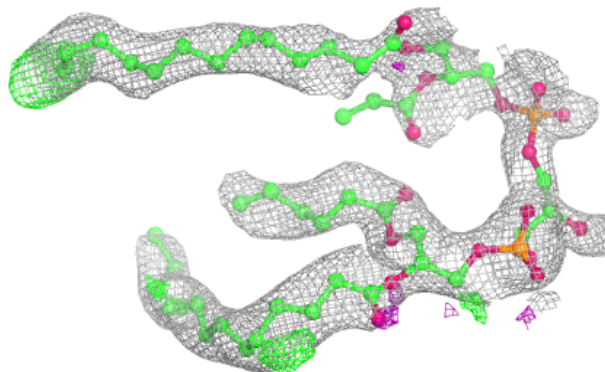


Electron density around DMU P 324:

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

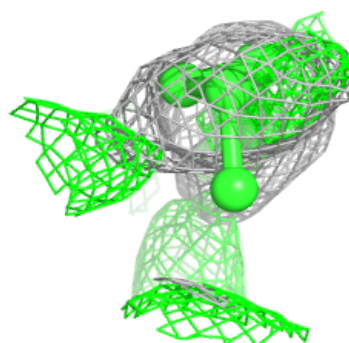
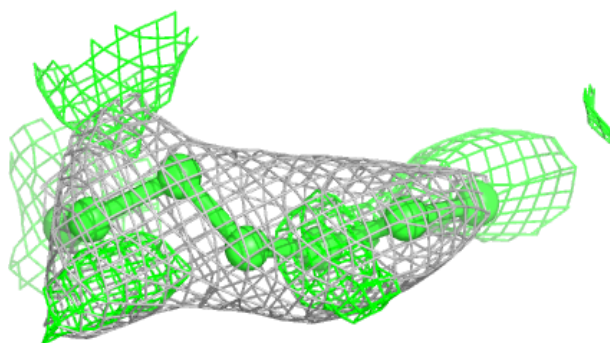
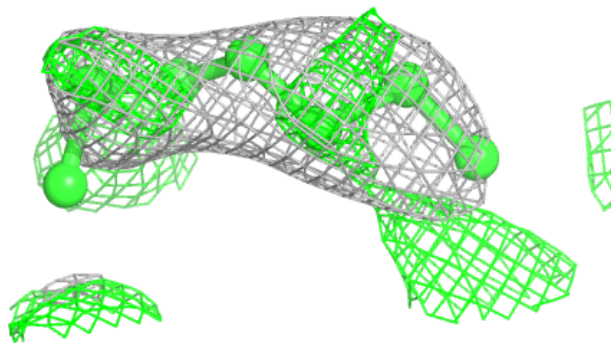
**Electron density around CDL V 101:**

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

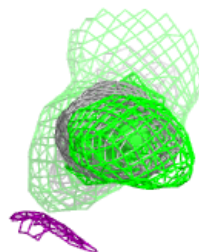
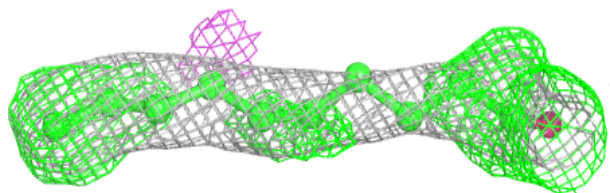
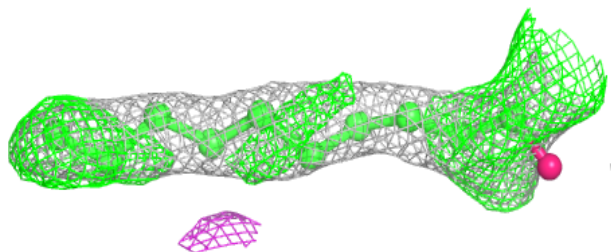


Electron density around DMU C 316:

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

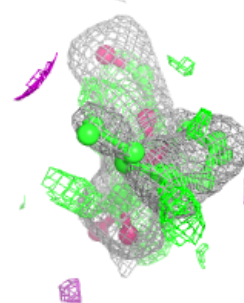
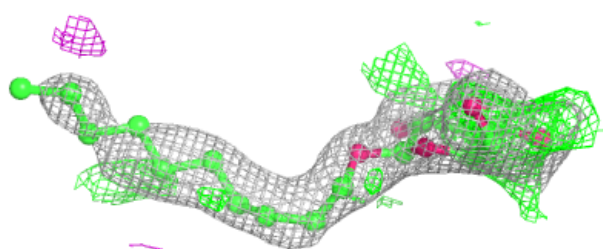
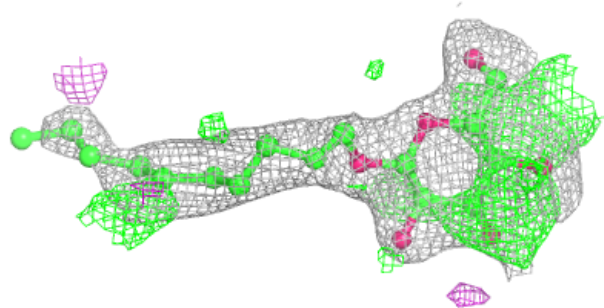
**Electron density around DMU O 305:**

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

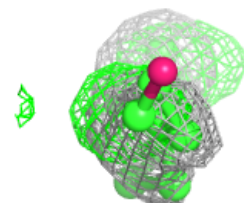
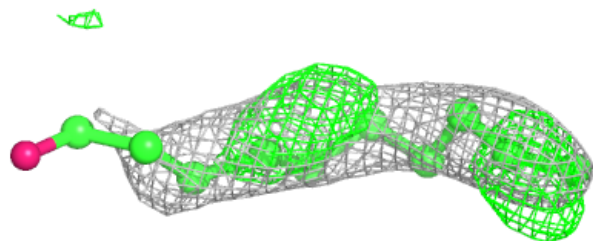
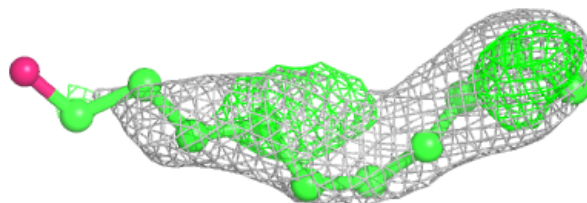


Electron density around DMU G 103:

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

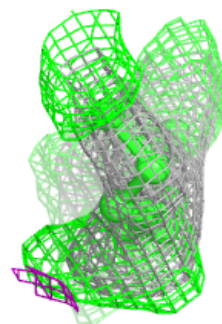
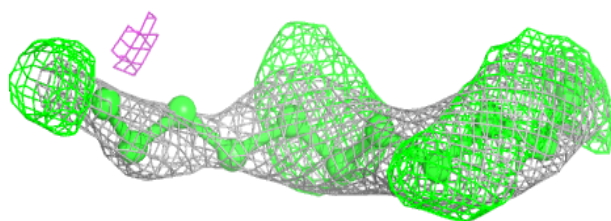
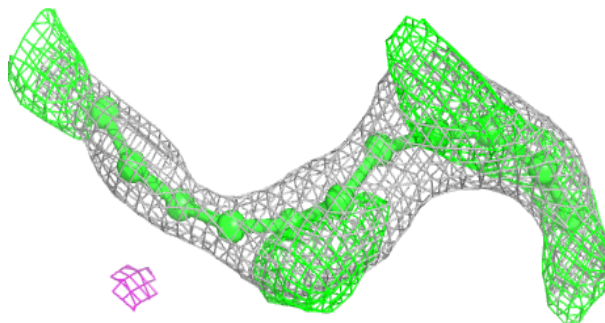
**Electron density around DMU J 101:**

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

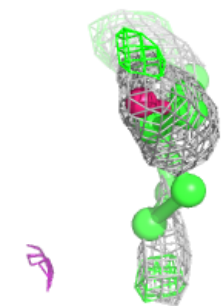
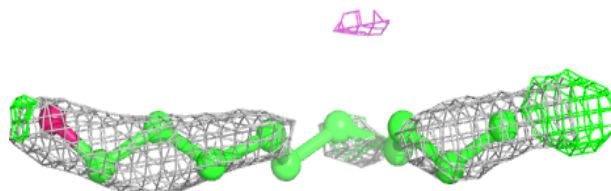
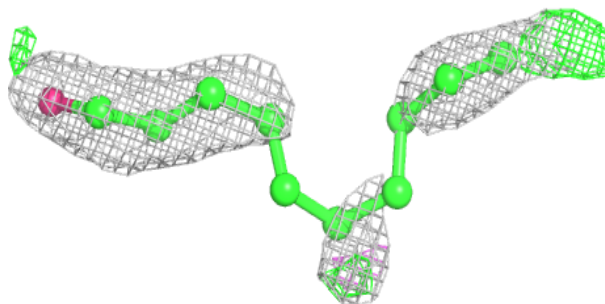


Electron density around LFA P 308:

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

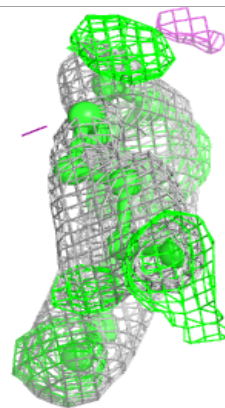
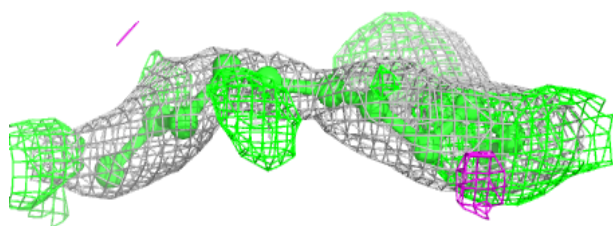
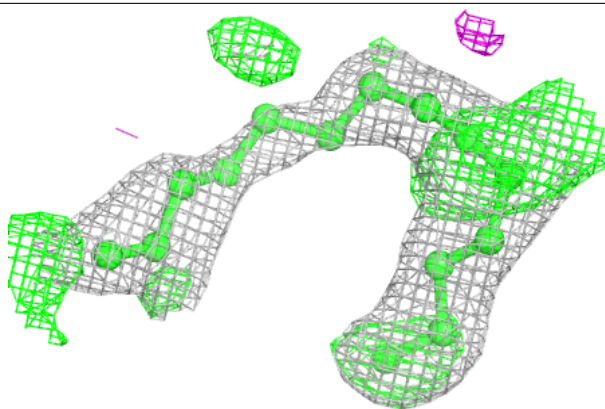
**Electron density around DMU N 602:**

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

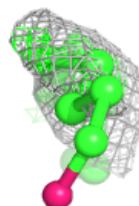
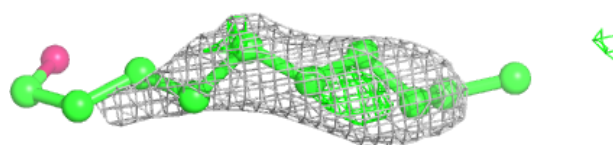
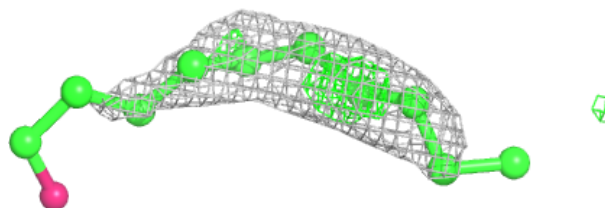


Electron density around LFA G 105:

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

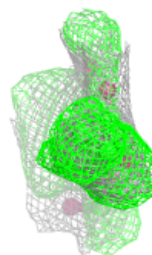
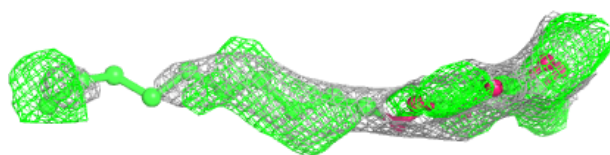
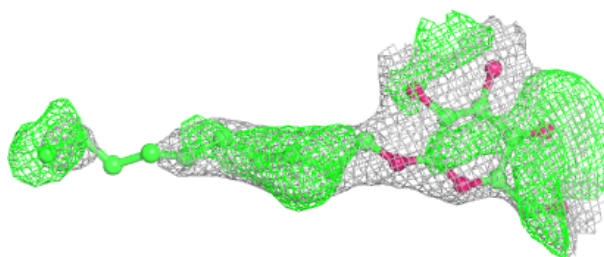
**Electron density around DMU W 101:**

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

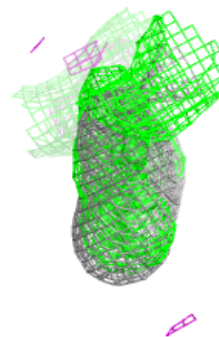
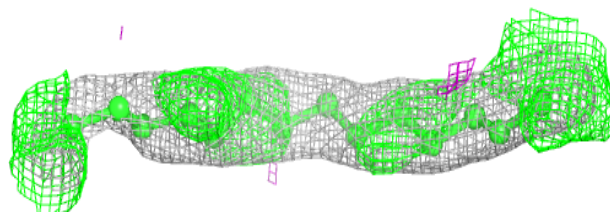
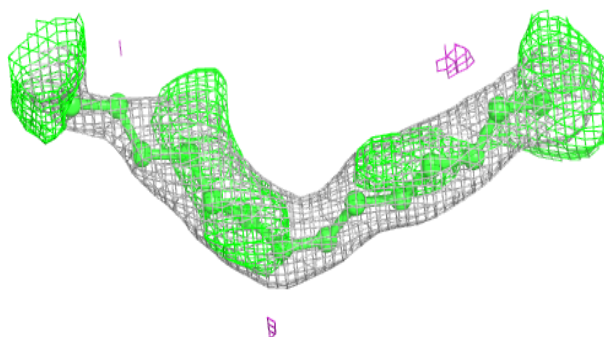


Electron density around DMU Y 102:

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

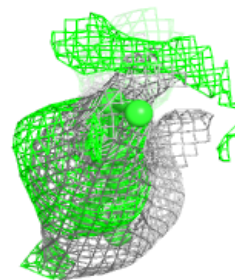
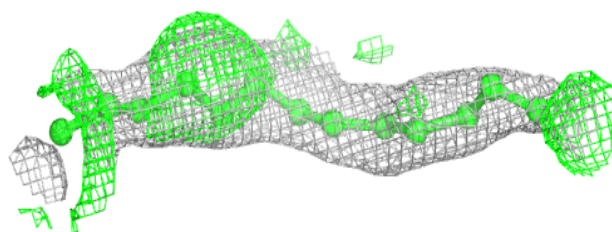
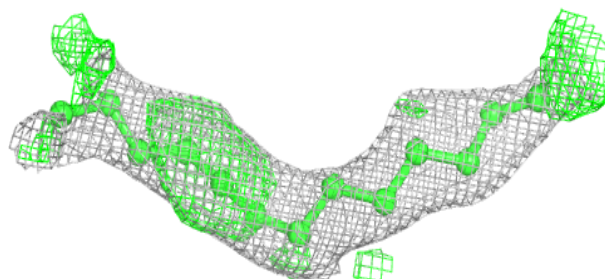
**Electron density around LFA A 608:**

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

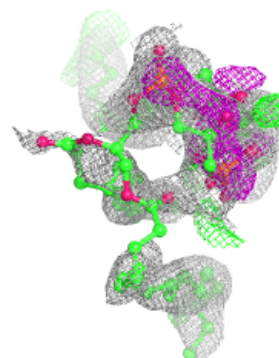
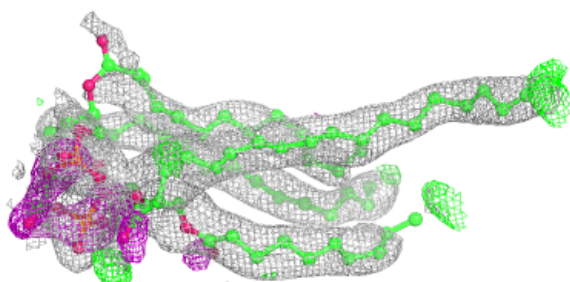
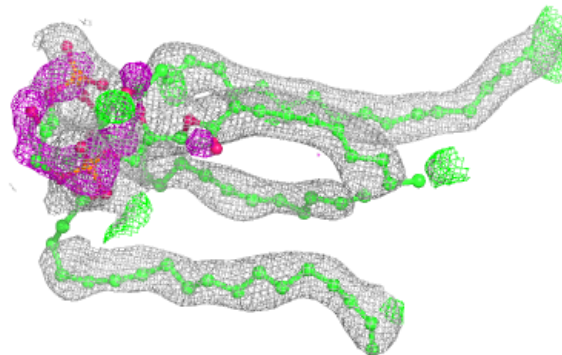


Electron density around LFA P 315:

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

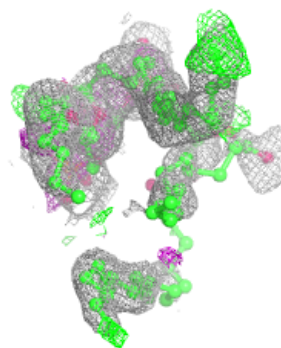
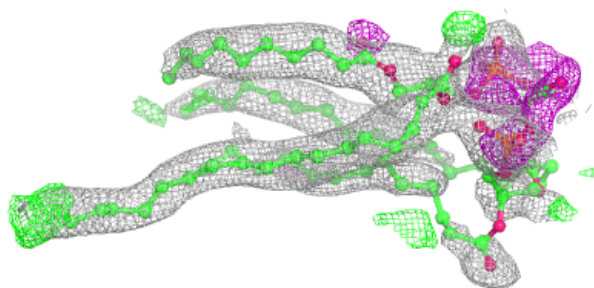
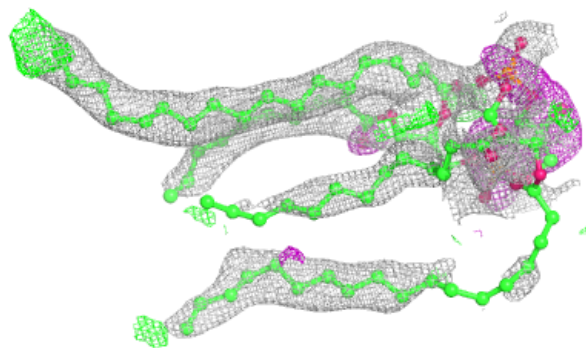
**Electron density around CDL C 304:**

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

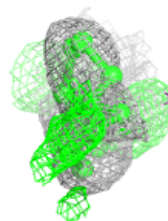
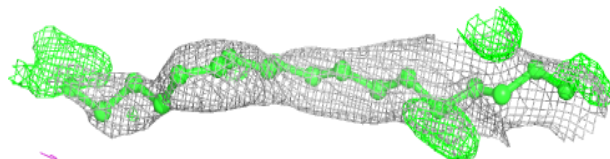
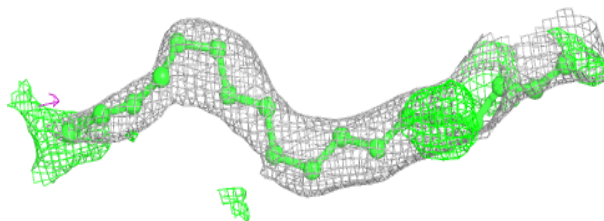


Electron density around CDL P 305:

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

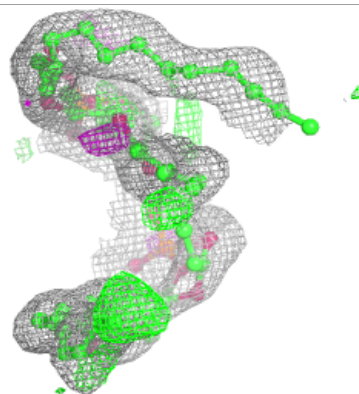
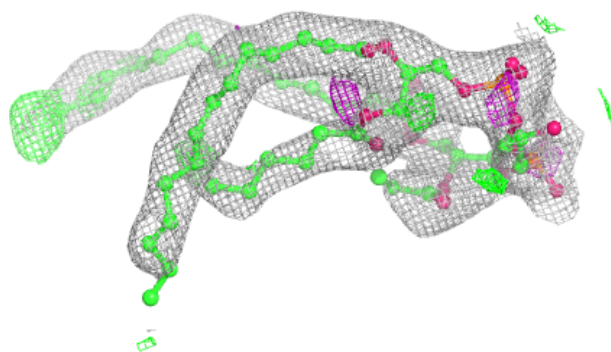
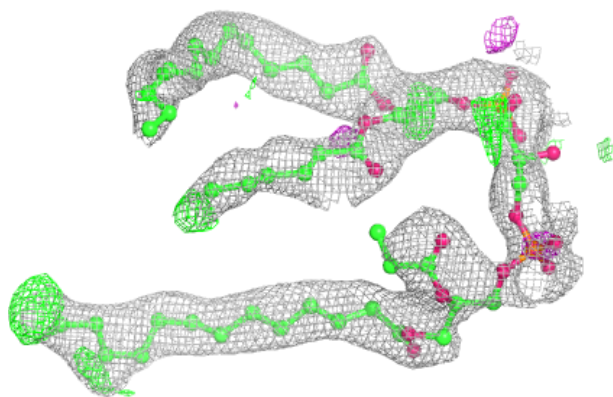
**Electron density around LFA P 310:**

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



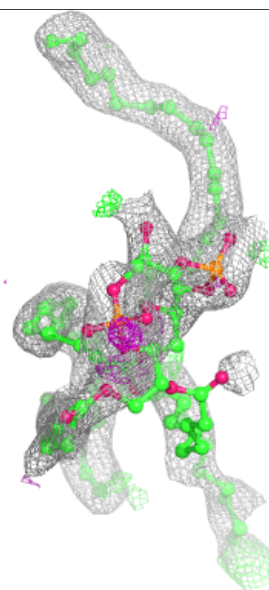
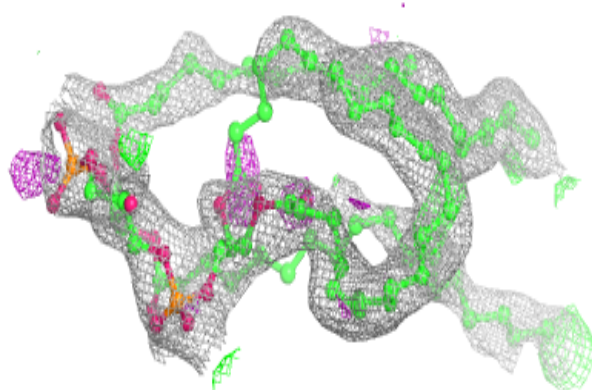
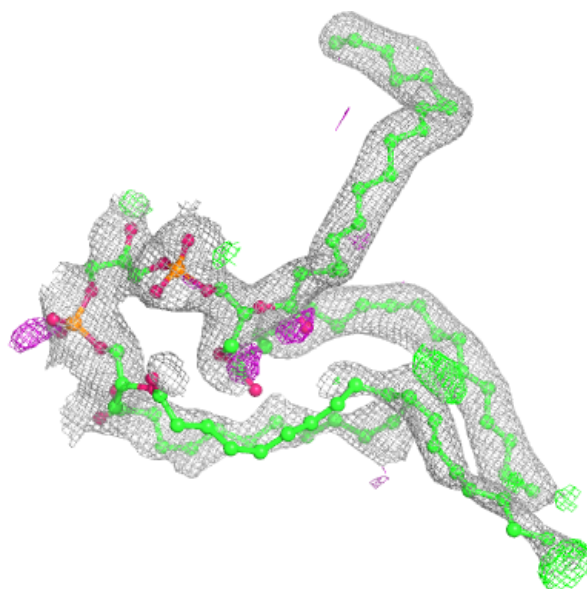
Electron density around CDL A 607:

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



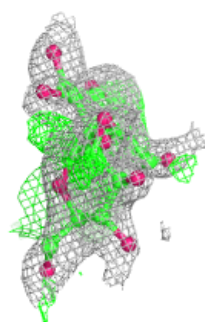
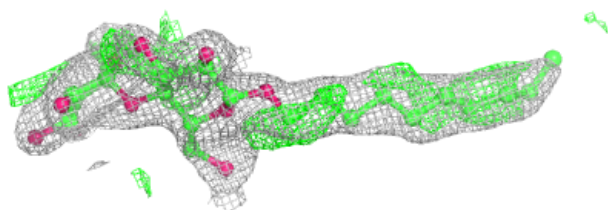
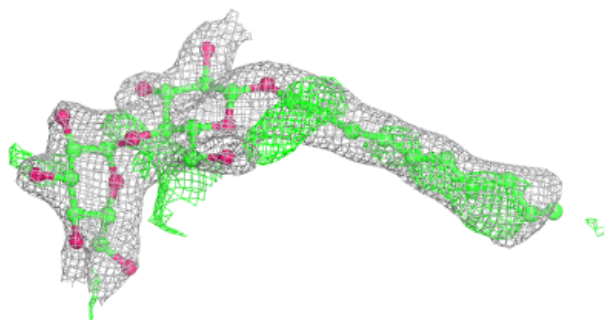
Electron density around CDL Y 101:

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

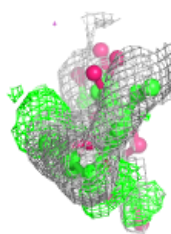
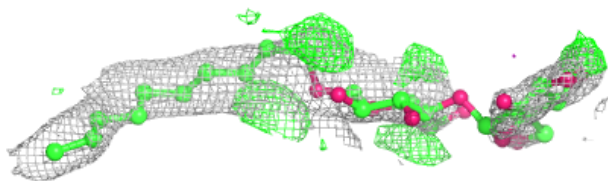
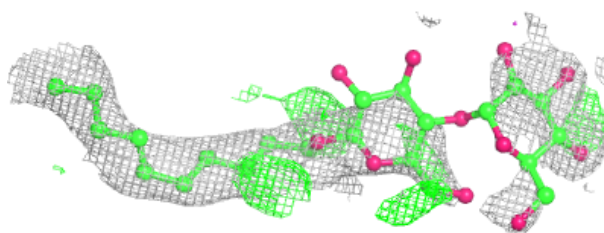


Electron density around DMU Q 201:

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

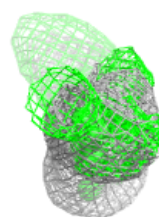
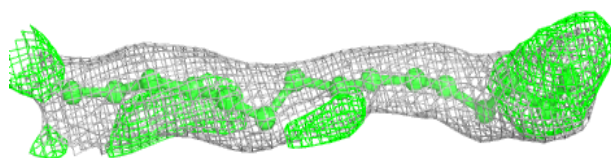
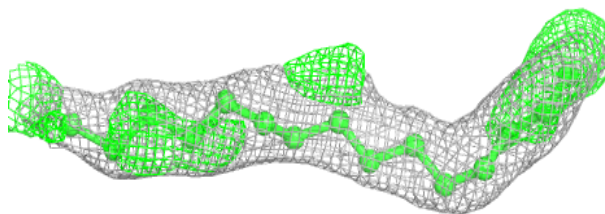
**Electron density around DMU U 101:**

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

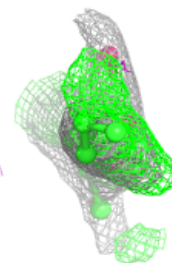
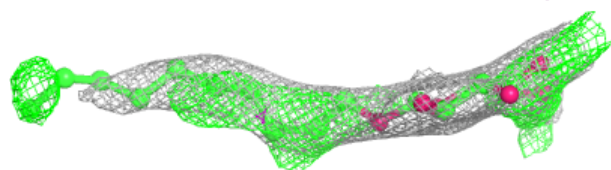
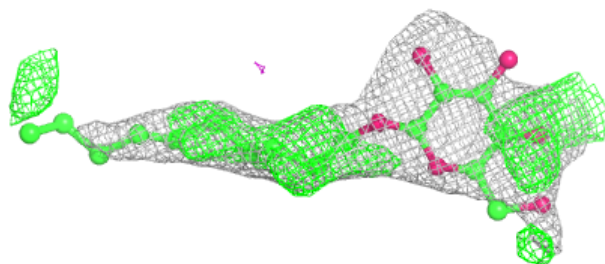


Electron density around LFA P 314:

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

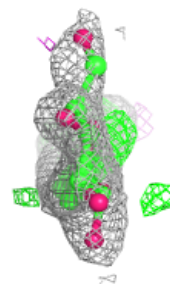
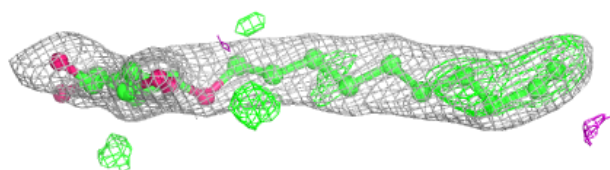
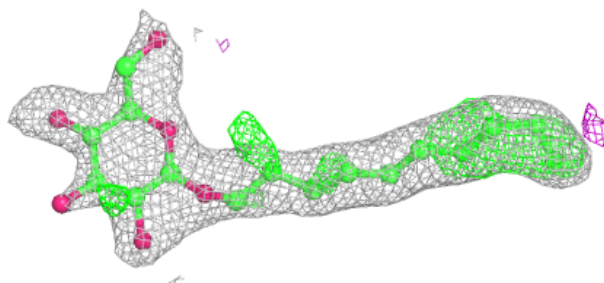
**Electron density around DMU L 102:**

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

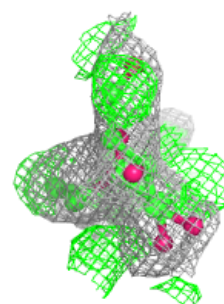
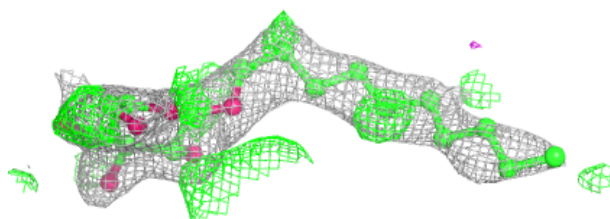
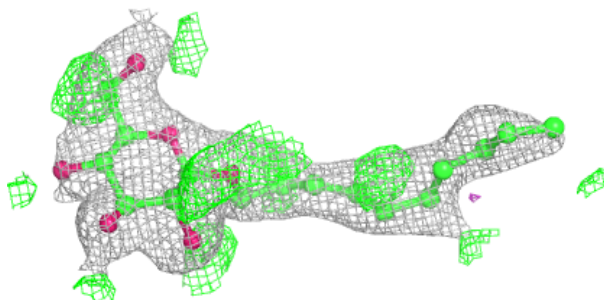


Electron density around DMU O 307:

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

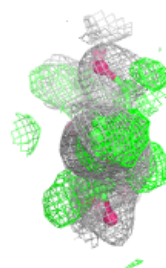
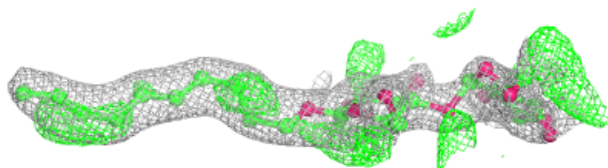
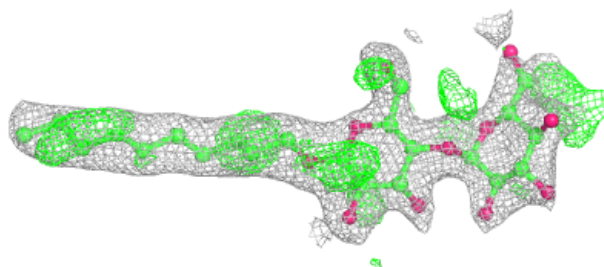
**Electron density around DMU T 103:**

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

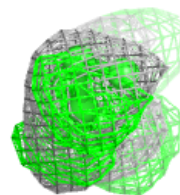
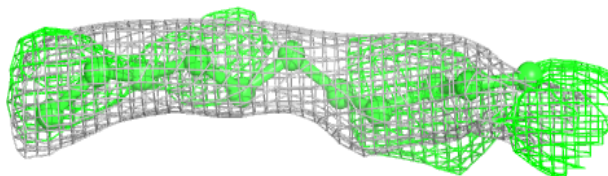
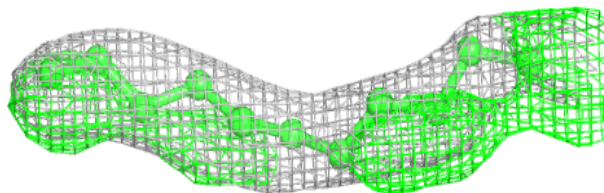


Electron density around DMU A 611:

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

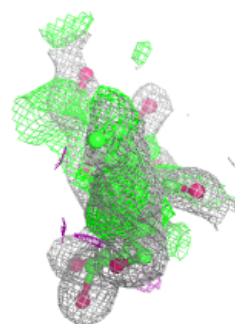
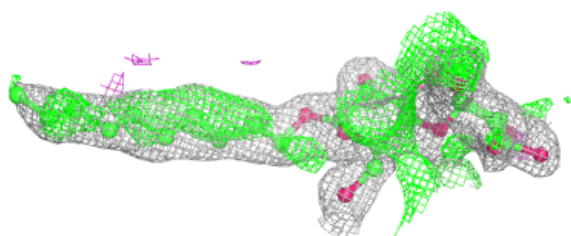
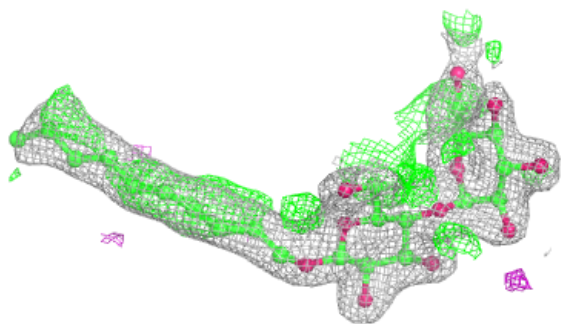
**Electron density around LFA T 102:**

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

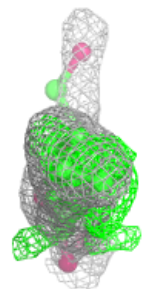
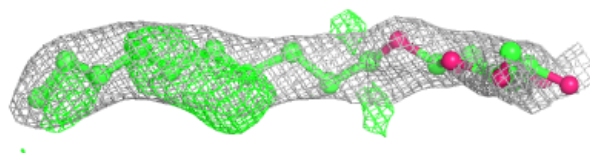
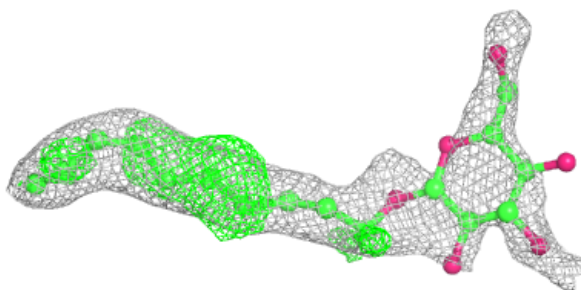


Electron density around DMU D 201:

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

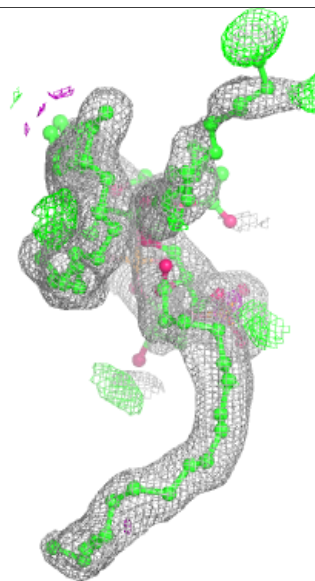
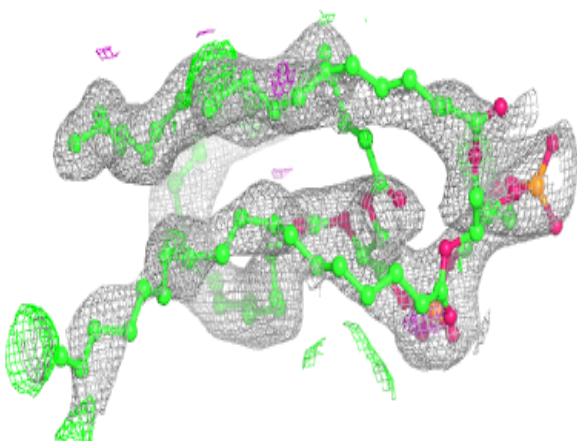
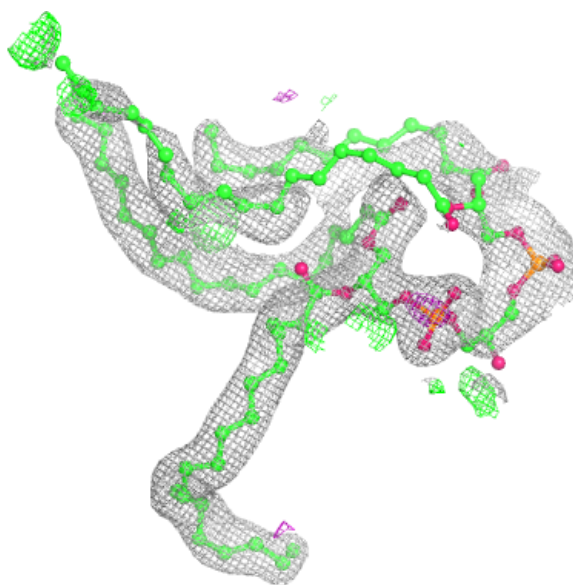
**Electron density around DMU B 305:**

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



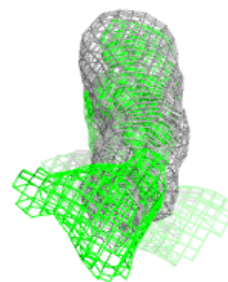
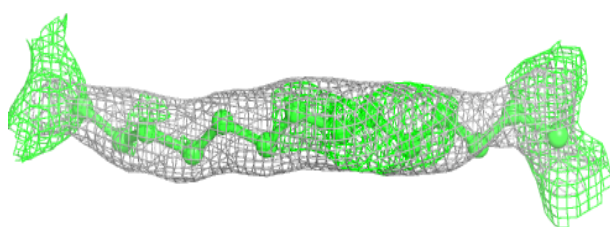
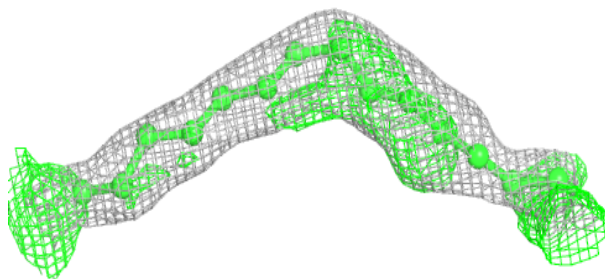
Electron density around CDL L 101:

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

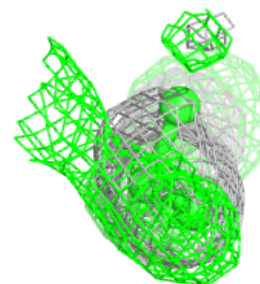
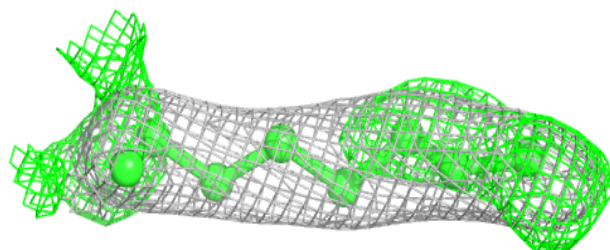
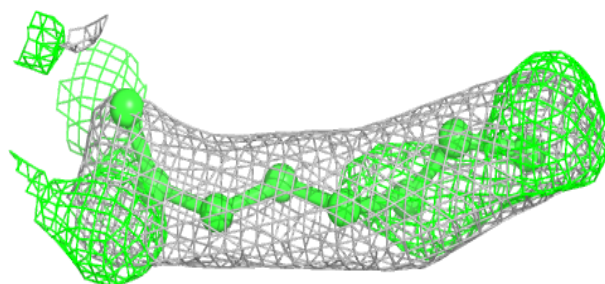


Electron density around LFA N 609:

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

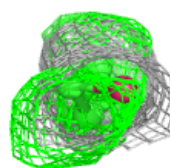
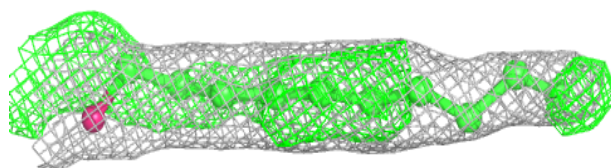
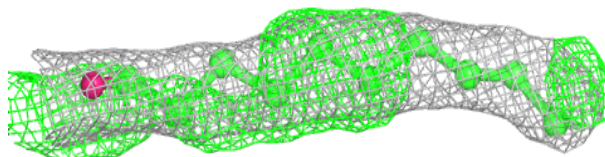
**Electron density around DMU Z 102:**

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

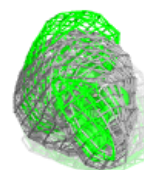
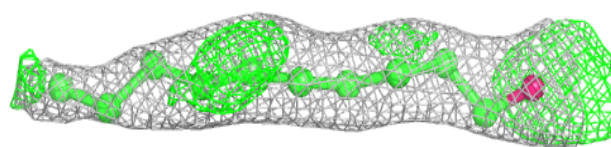
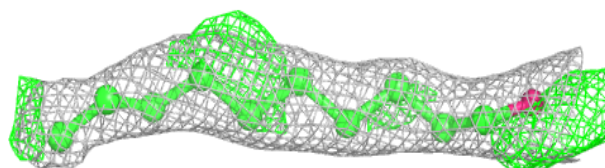


Electron density around DMU P 307:

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

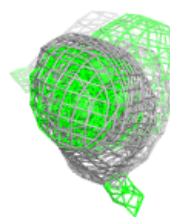
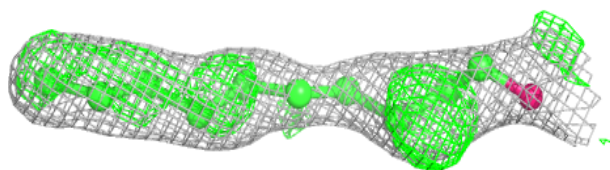
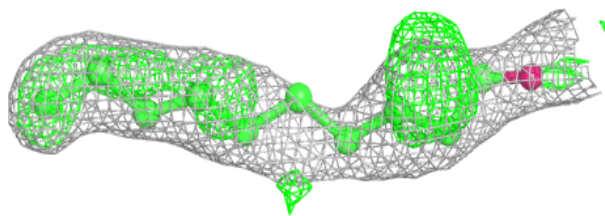
**Electron density around DMU C 306:**

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

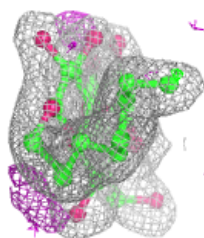
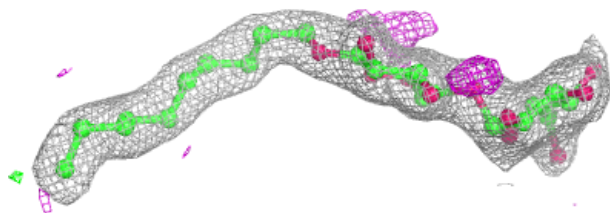
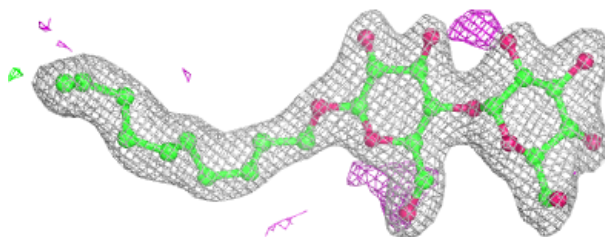


Electron density around DMU O 306:

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

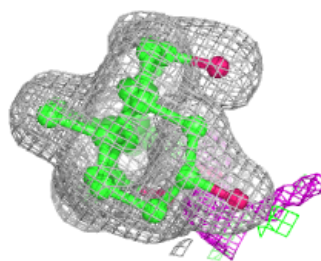
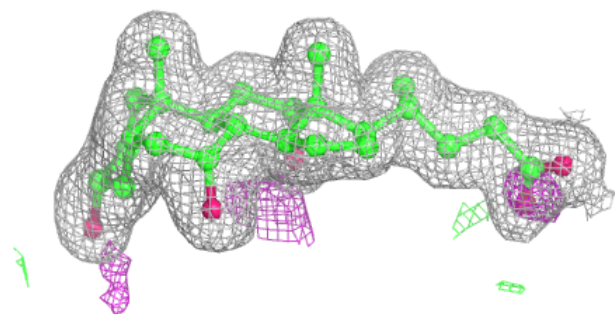
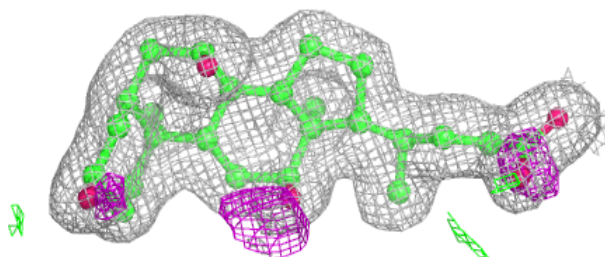
**Electron density around DMU Z 101:**

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

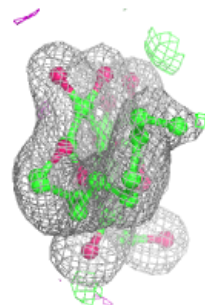
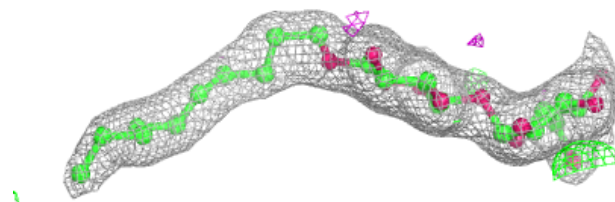
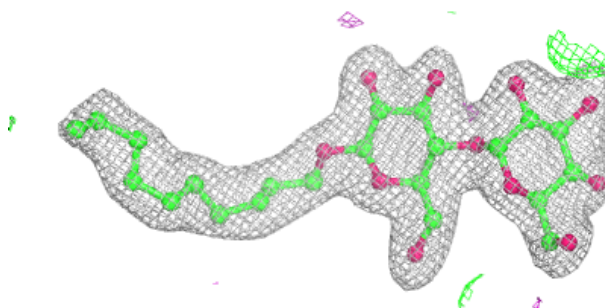


Electron density around CHD C 301:

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

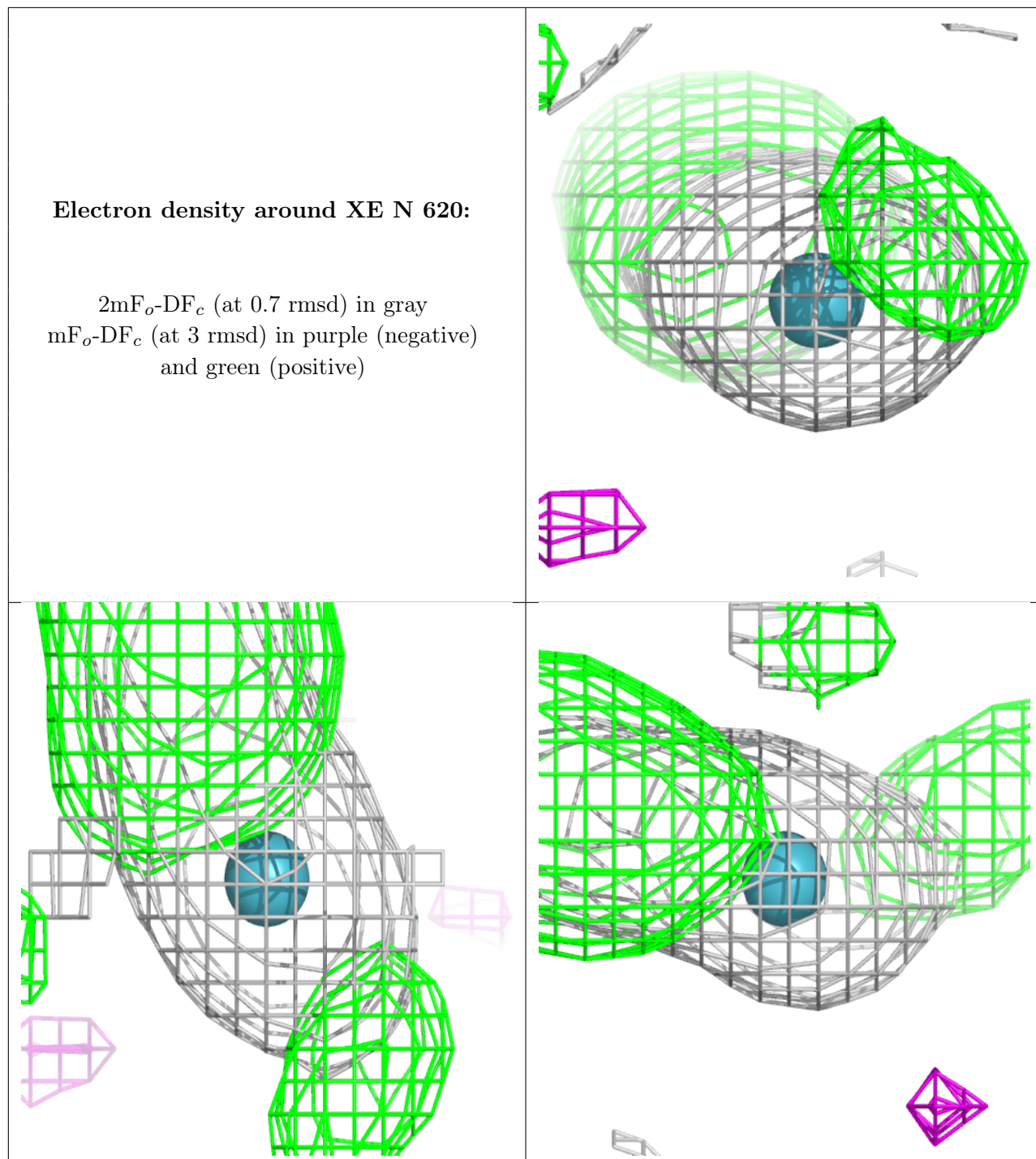
**Electron density around DMU M 101:**

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



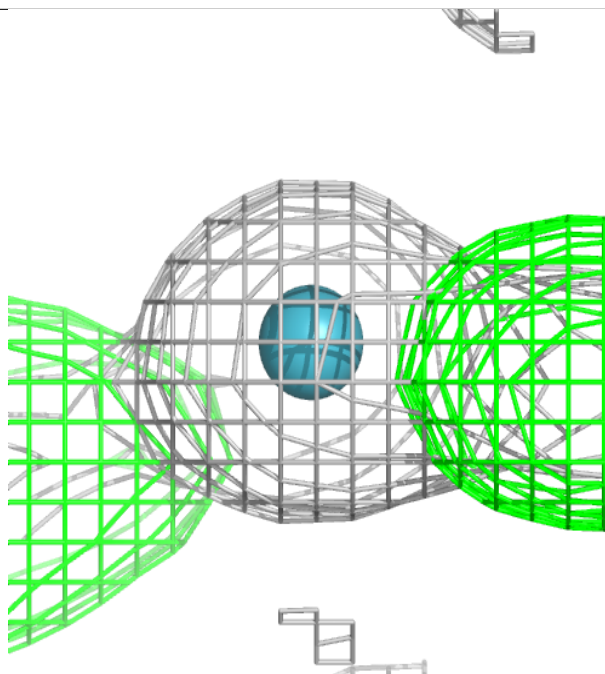
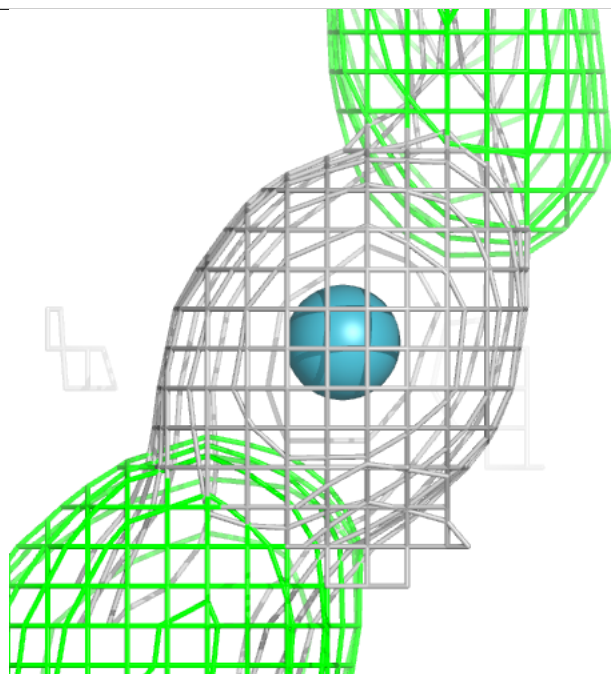
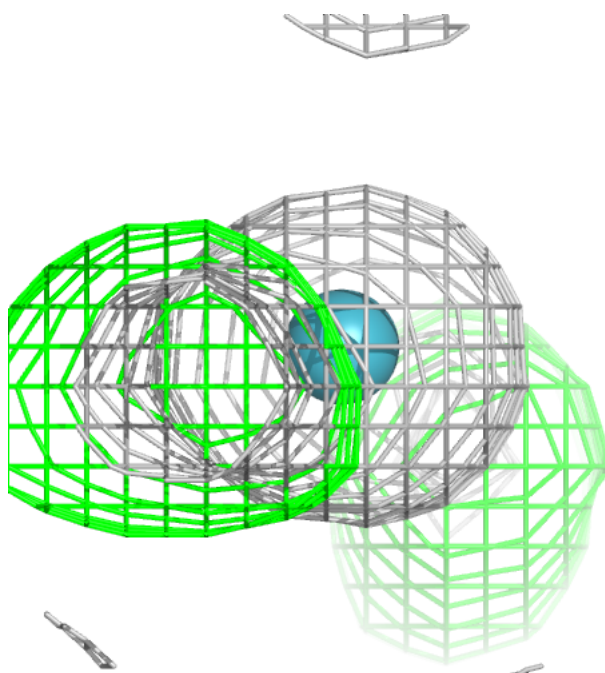
Electron density around XE N 620:

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



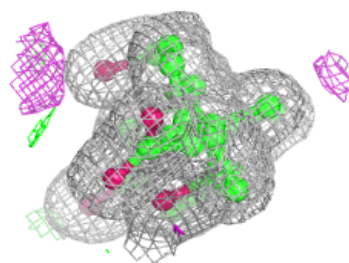
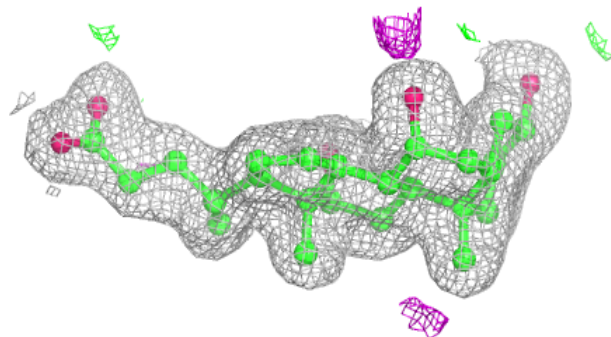
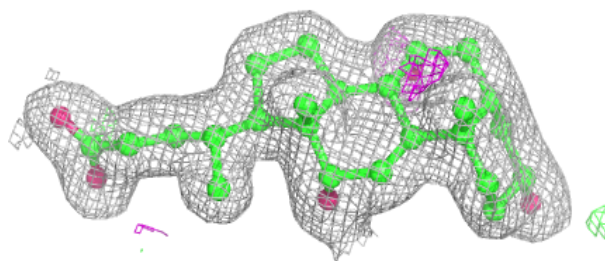
Electron density around XE A 619:

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

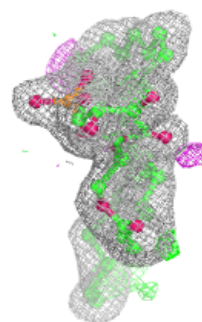
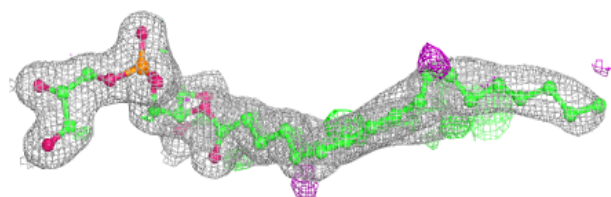
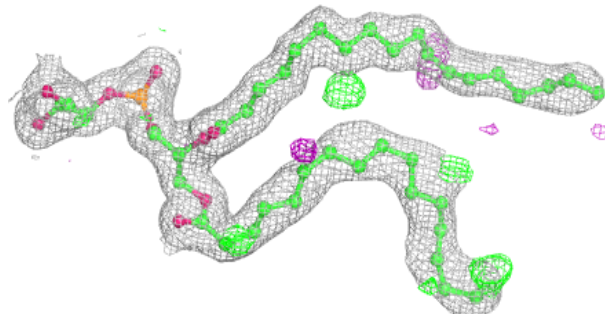


Electron density around CHD P 302:

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

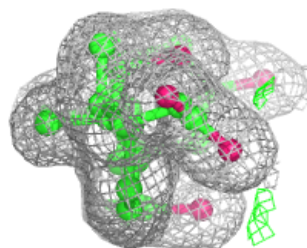
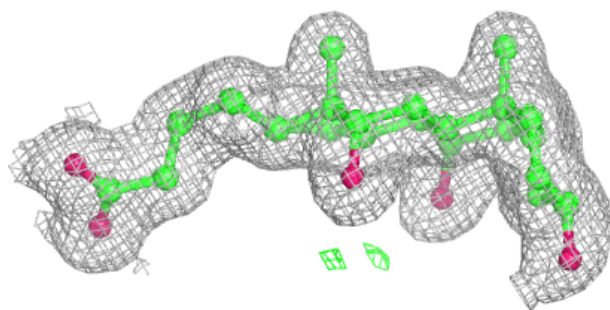
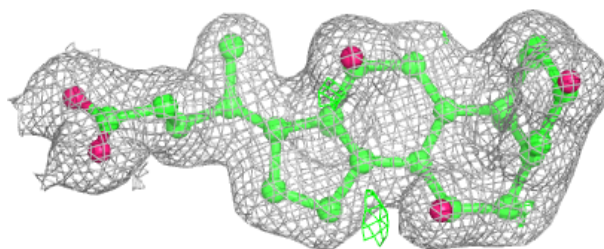
**Electron density around PGV N 622:**

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

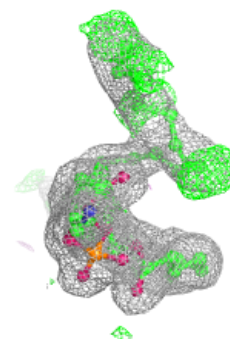
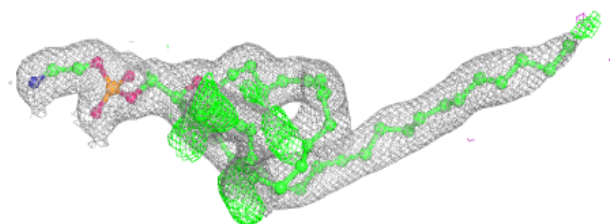
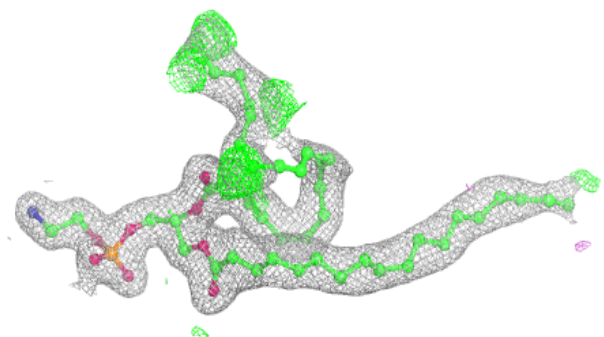


Electron density around CHD B 307:

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

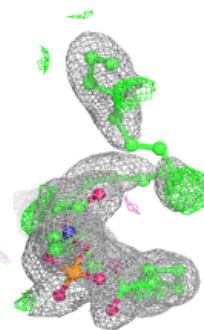
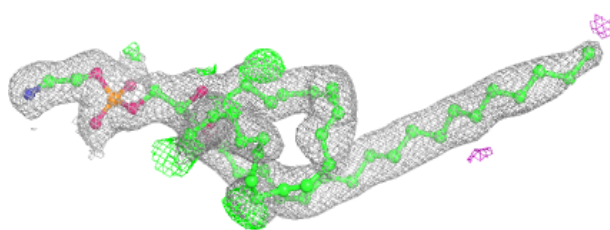
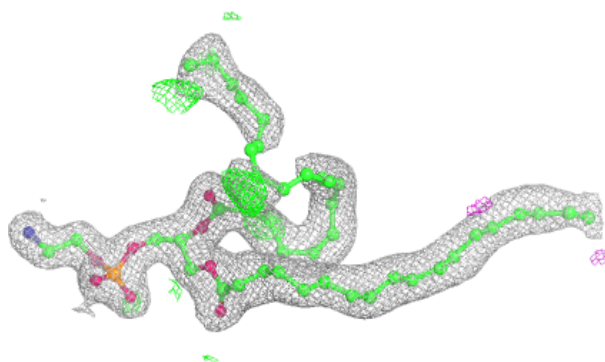
**Electron density around PEK G 101:**

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

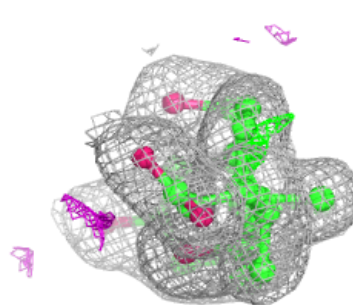
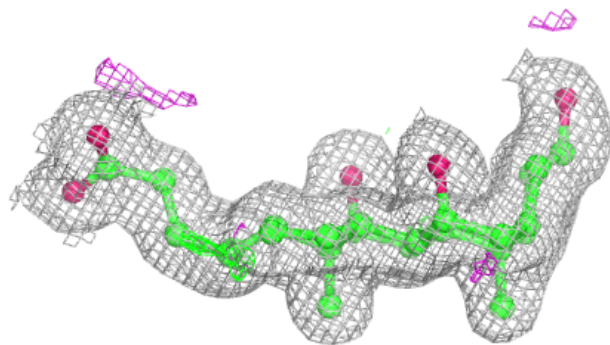
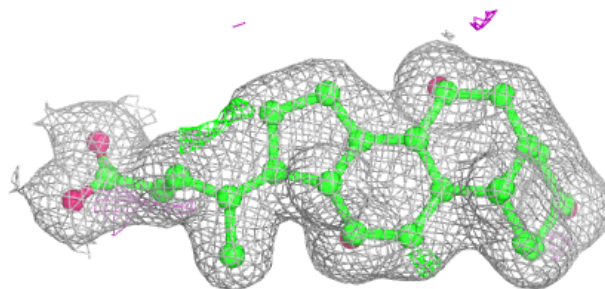


Electron density around PEK T 101:

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

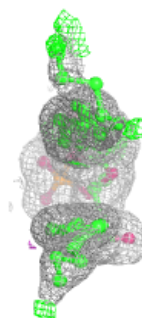
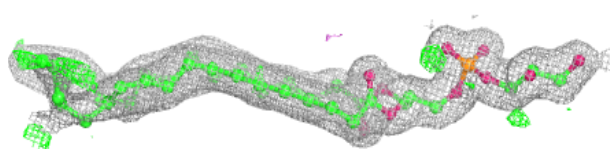
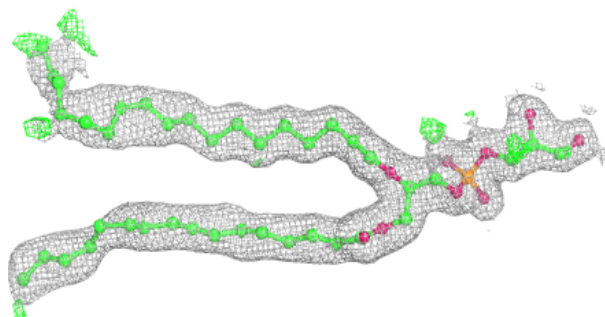
**Electron density around CHD G 102:**

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

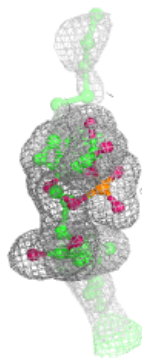
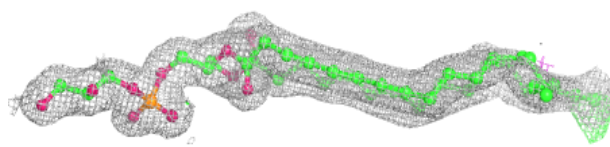
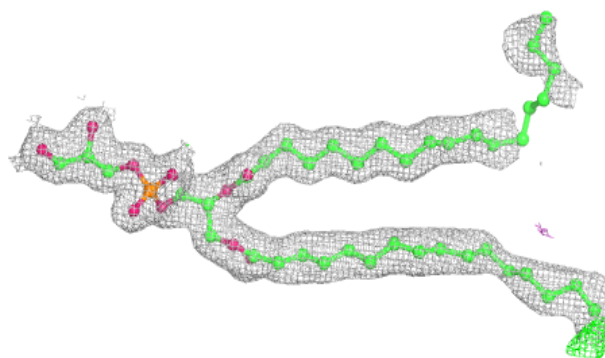


Electron density around PGV C 303:

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

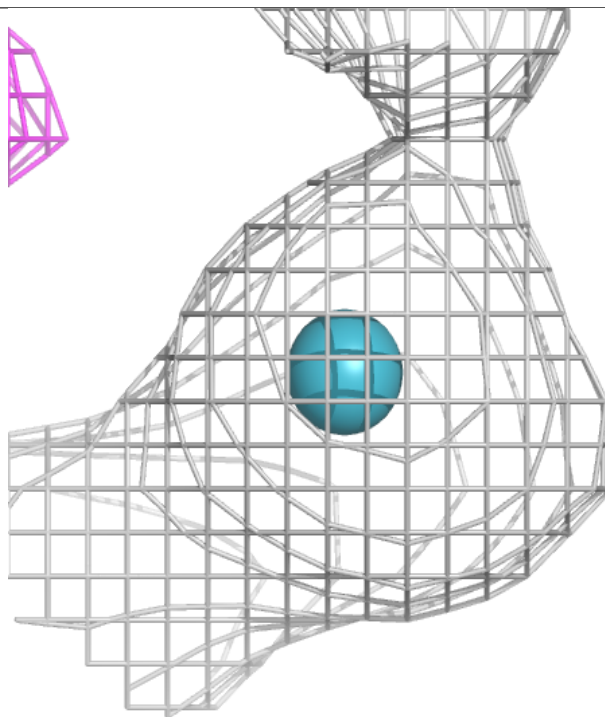
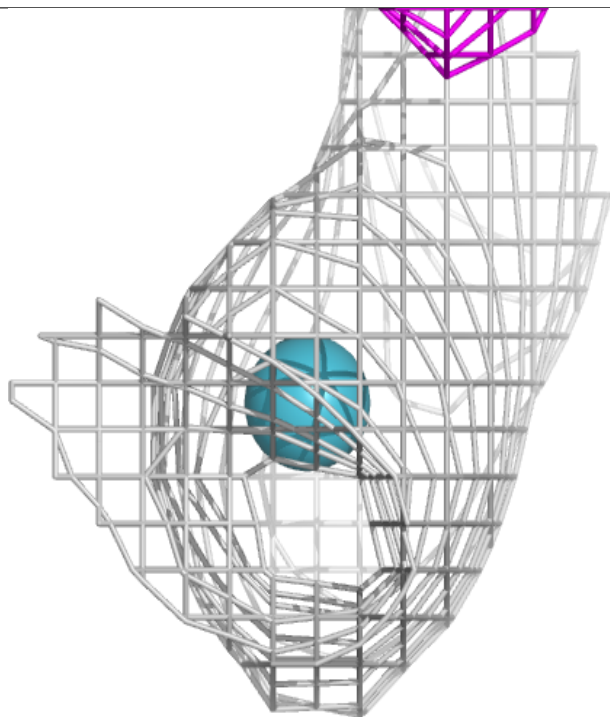
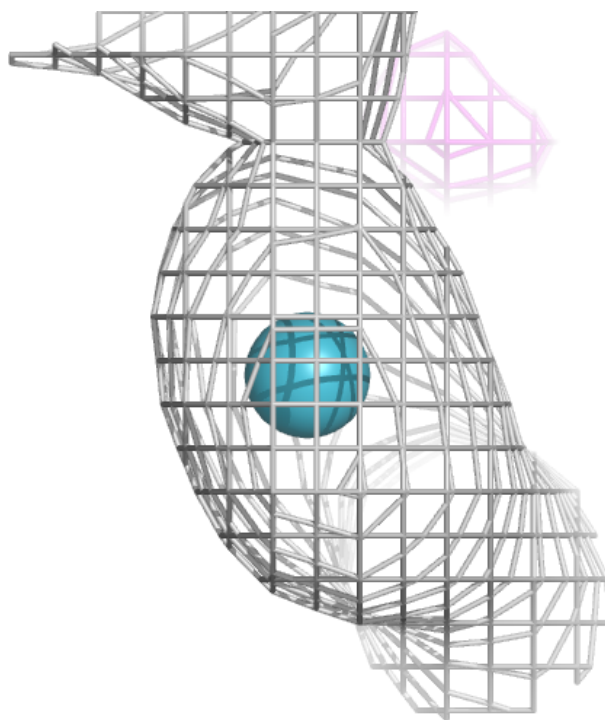
**Electron density around PGV P 304:**

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



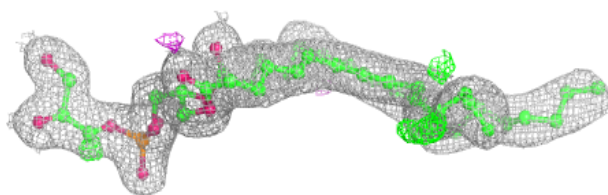
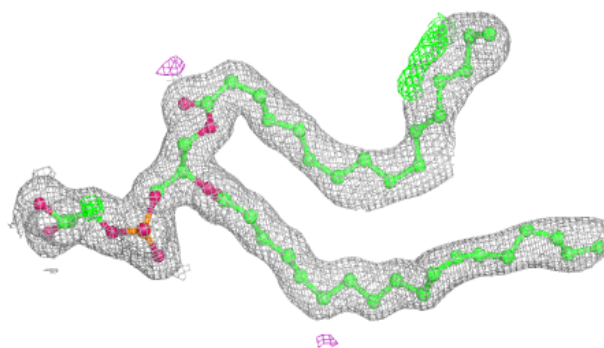
Electron density around XE P 325:

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

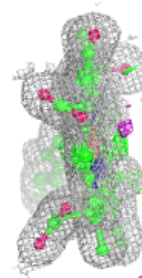
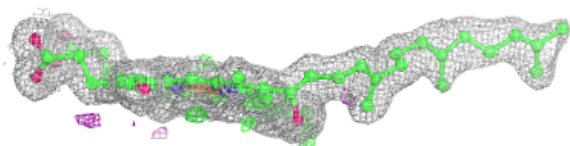
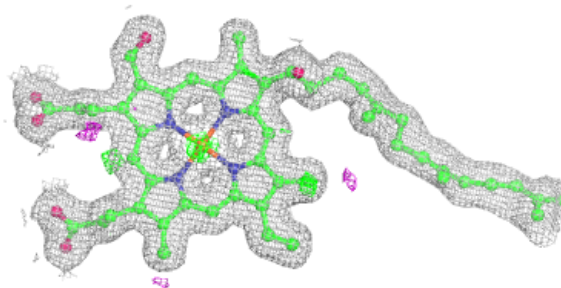


Electron density around PGV A 621:

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

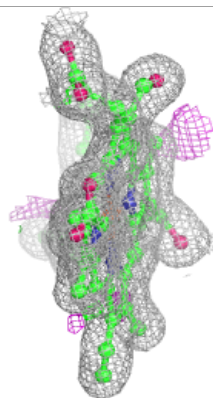
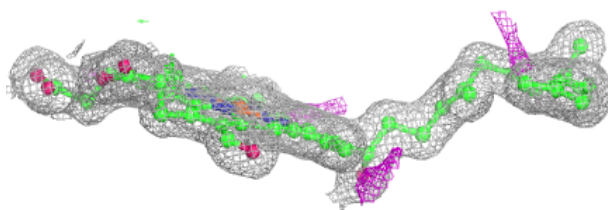
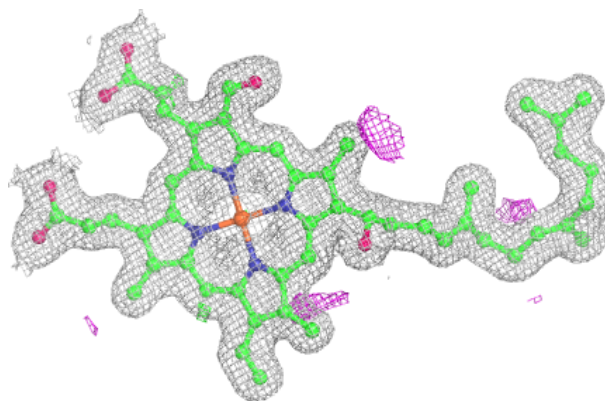
**Electron density around HEA A 601 (B):**

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

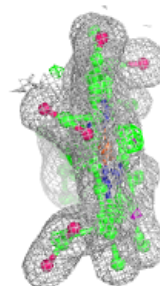
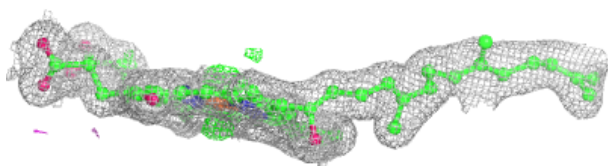
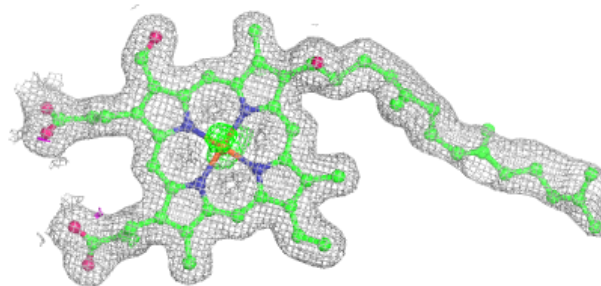


Electron density around HEA A 602:

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

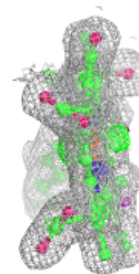
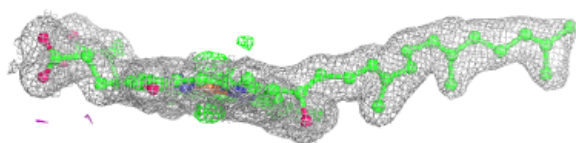
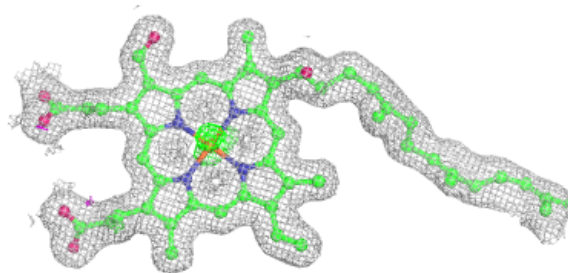
**Electron density around HEA N 603 (A):**

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

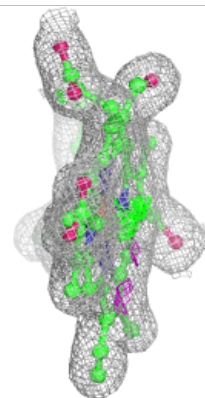
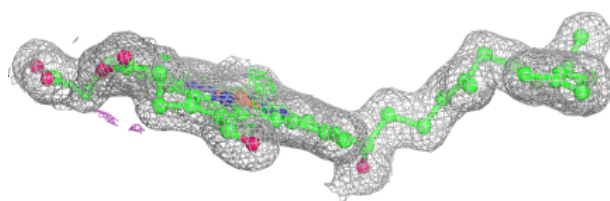
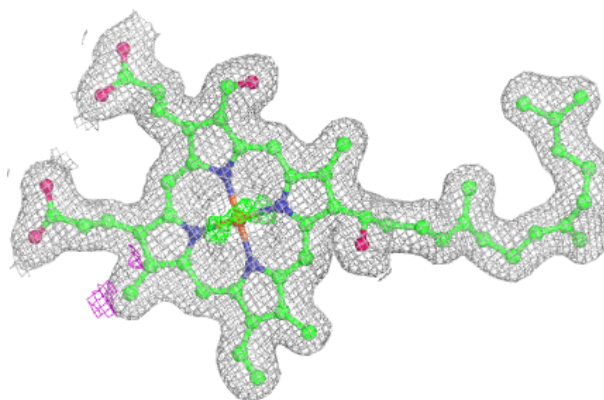


Electron density around HEA N 603 (B):

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

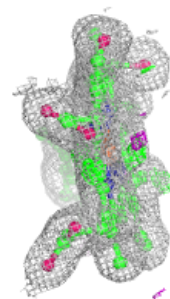
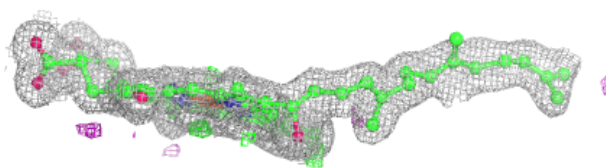
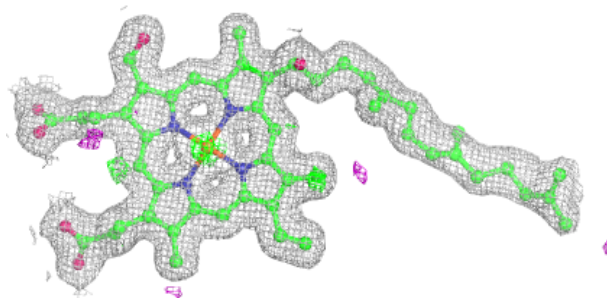
**Electron density around HEA N 604:**

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



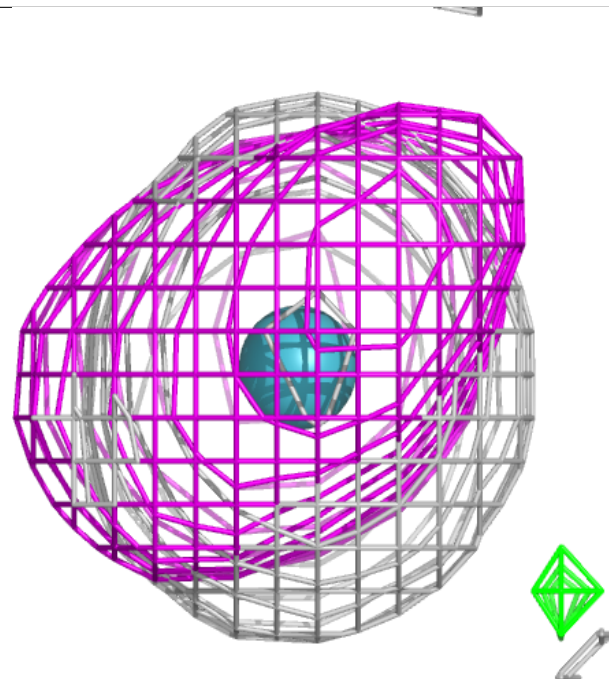
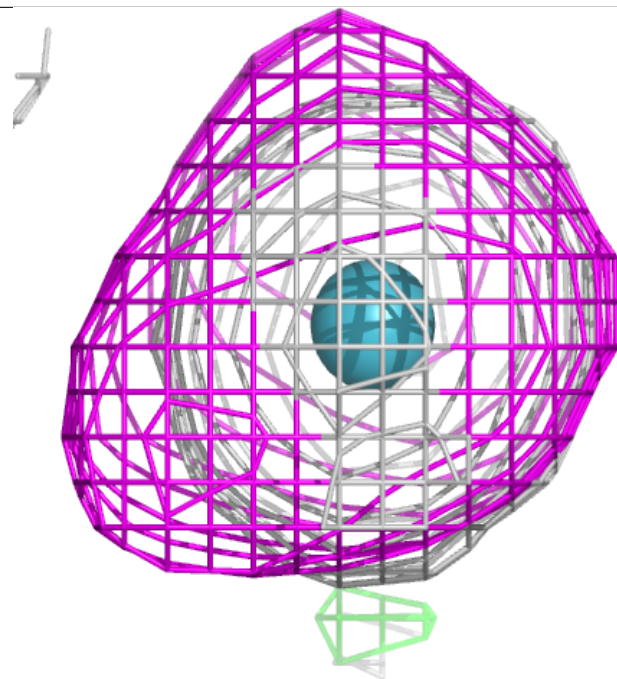
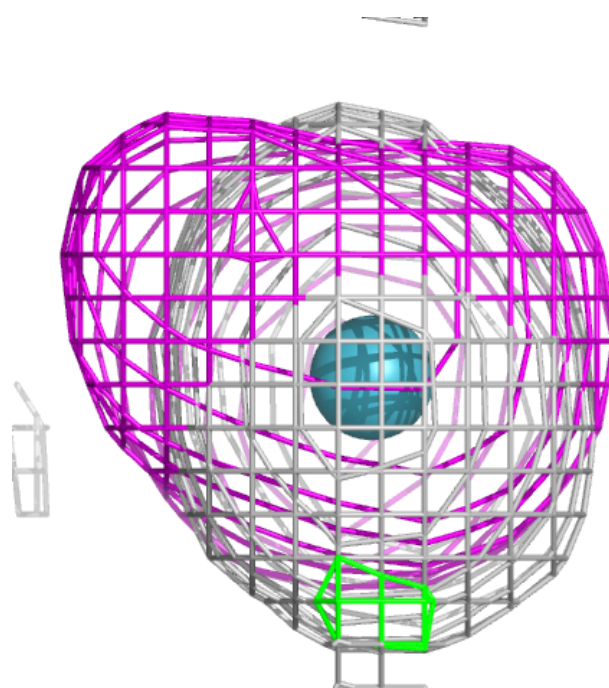
Electron density around HEA A 601 (A):

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



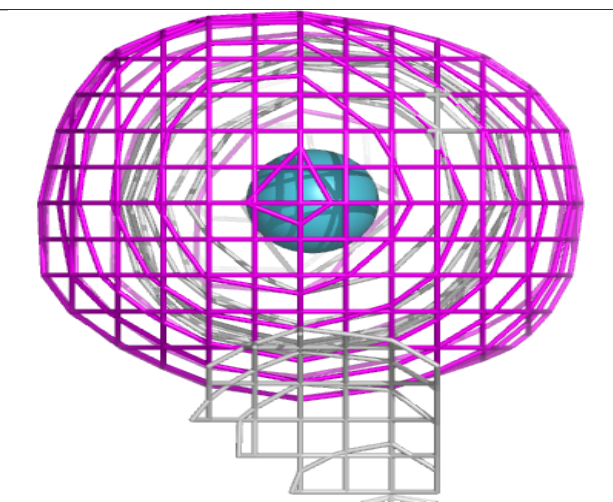
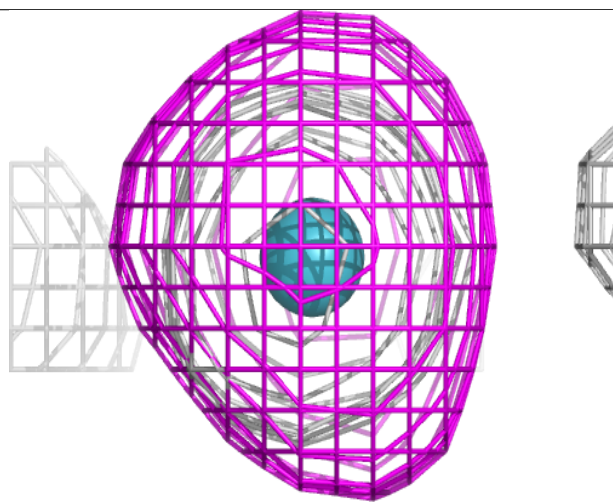
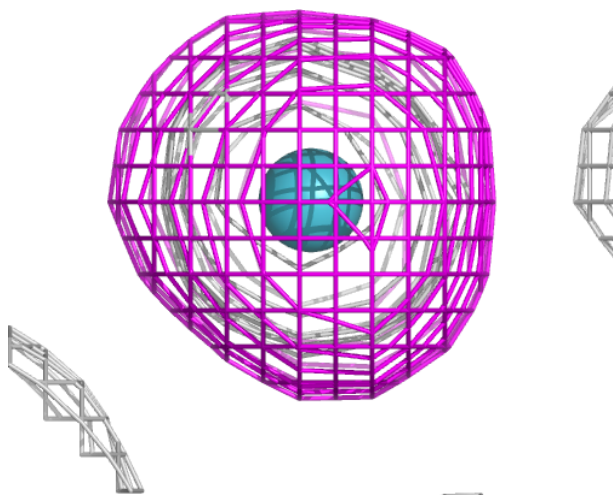
Electron density around XE A 620:

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



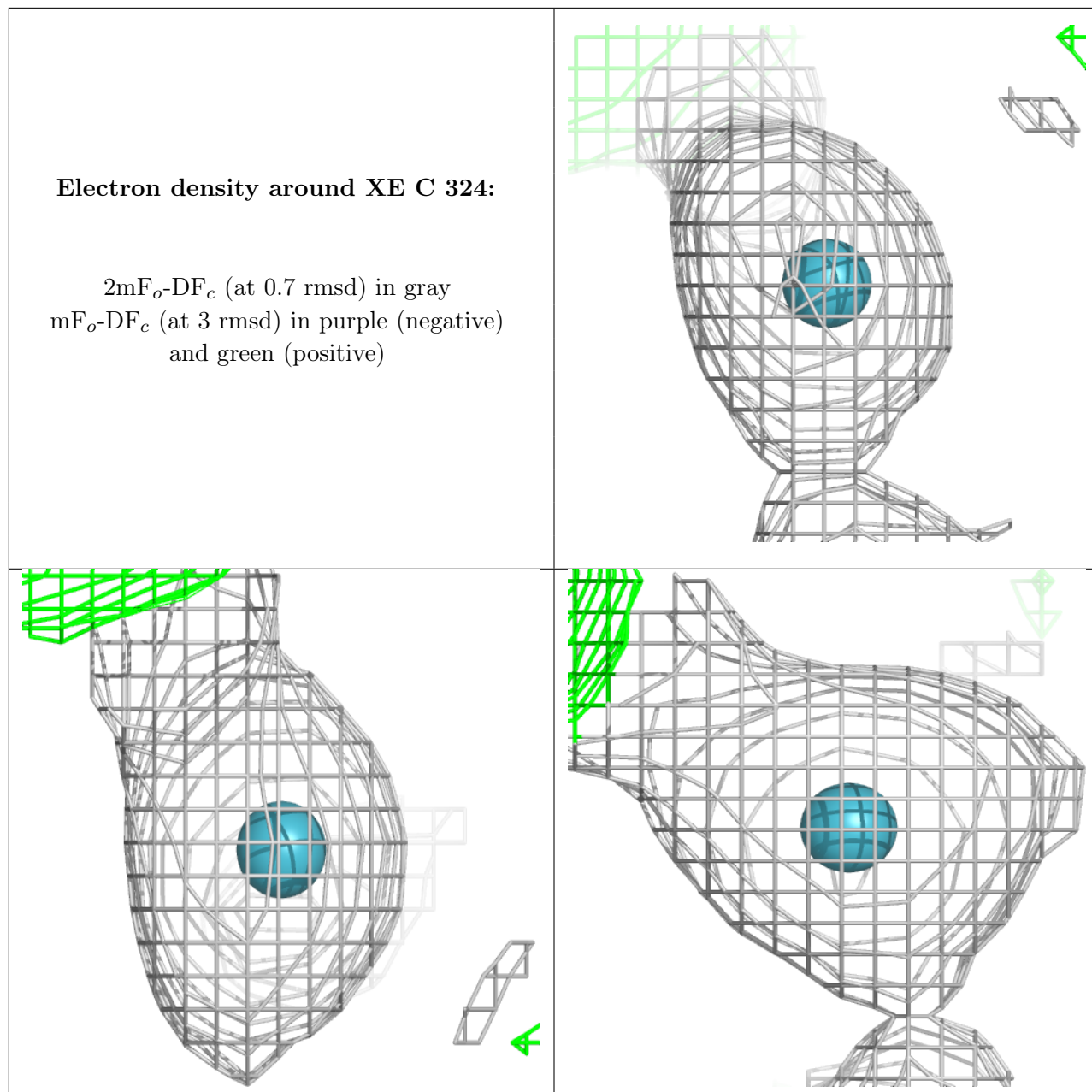
Electron density around XE B 301:

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



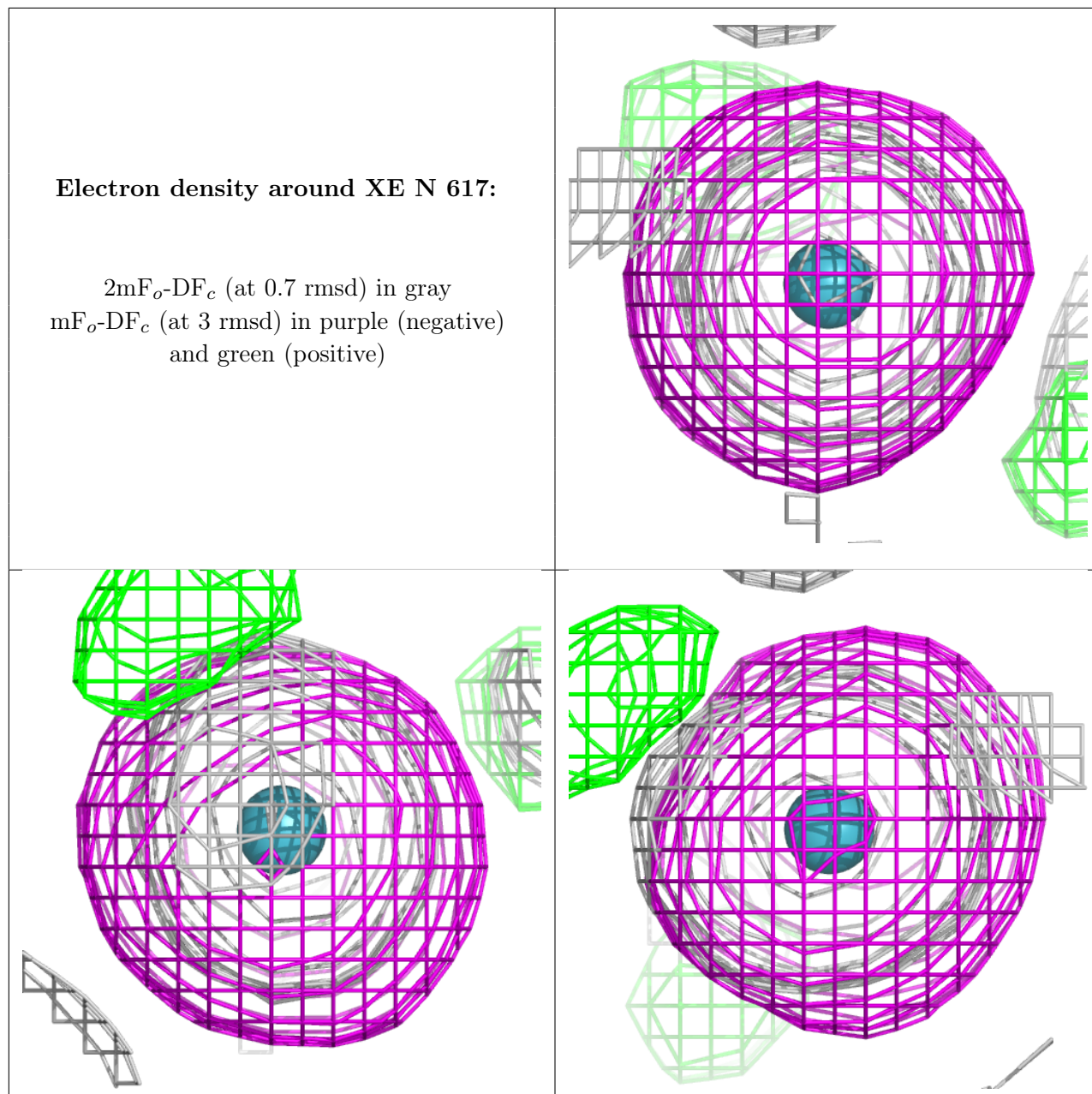
Electron density around XE C 324:

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



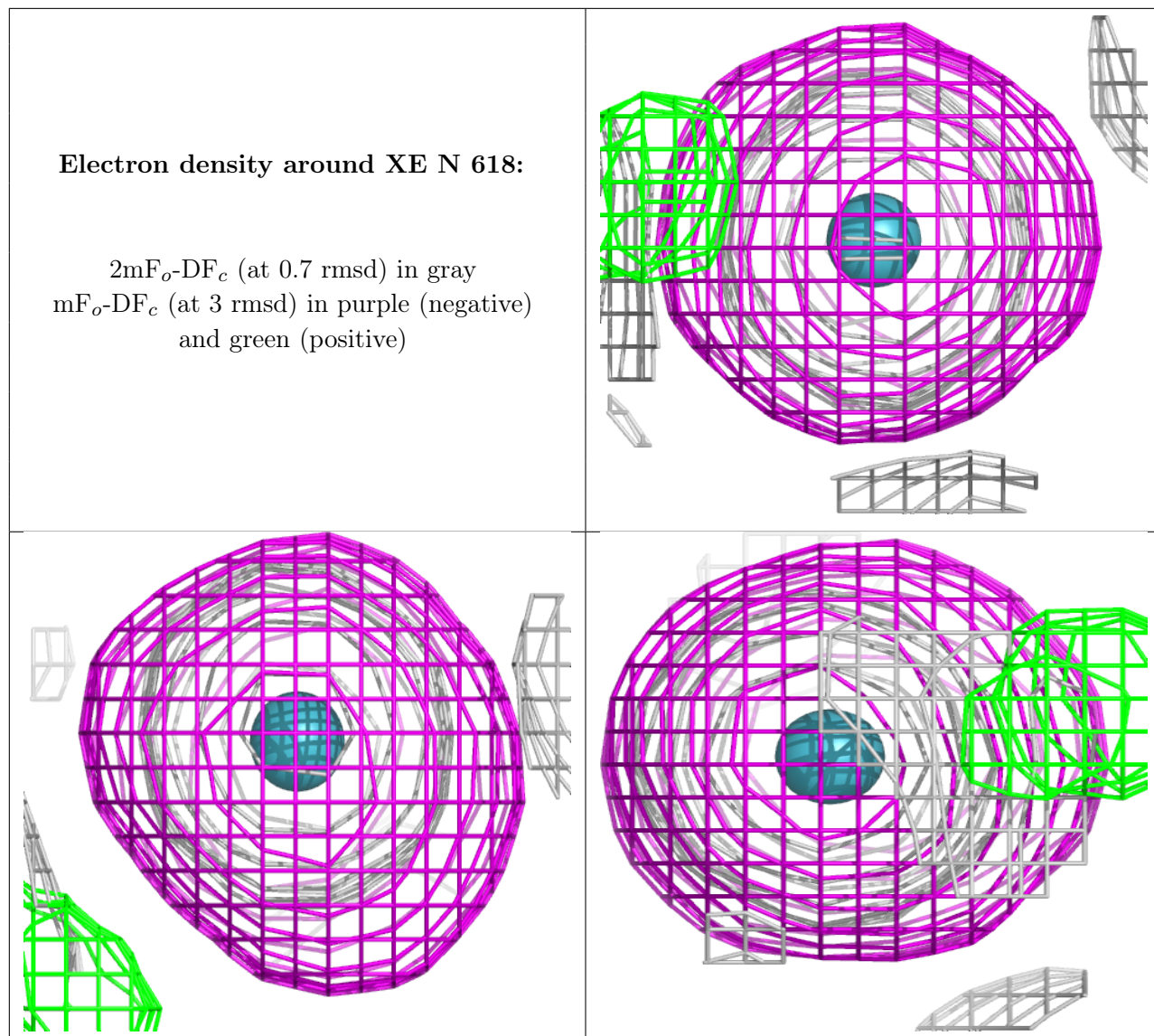
Electron density around XE N 617:

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



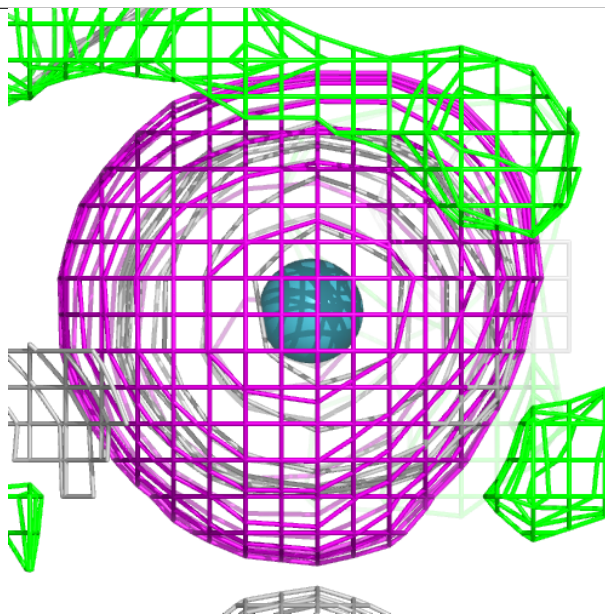
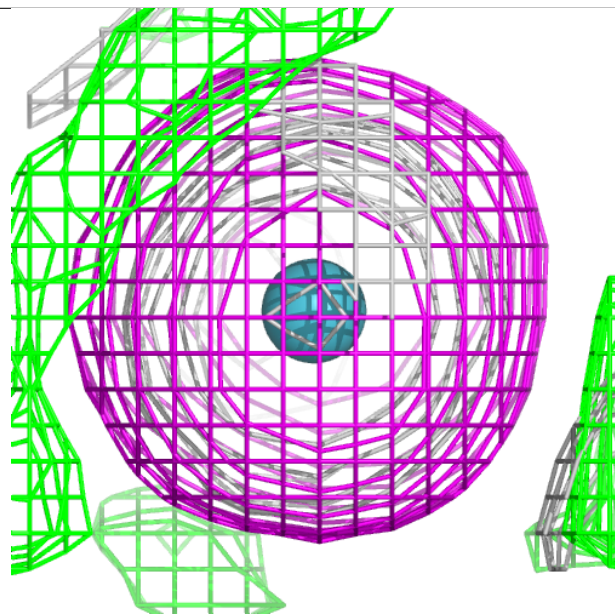
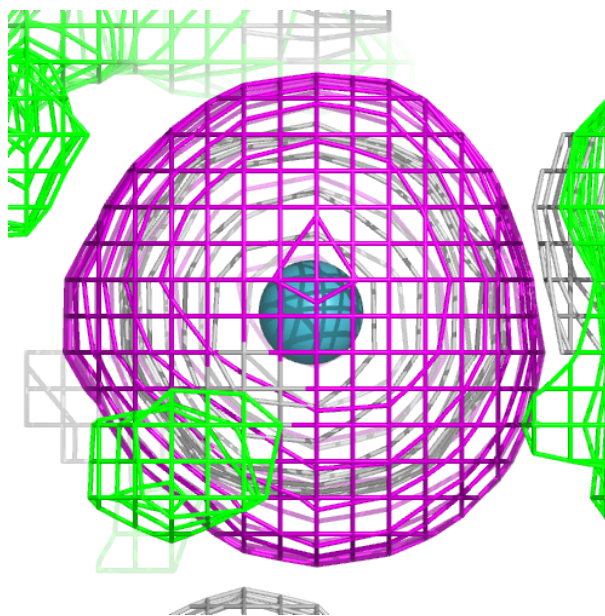
Electron density around XE N 618:

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



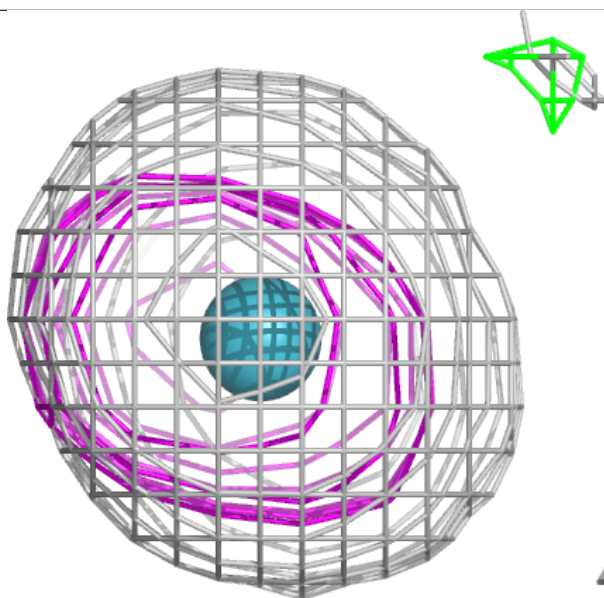
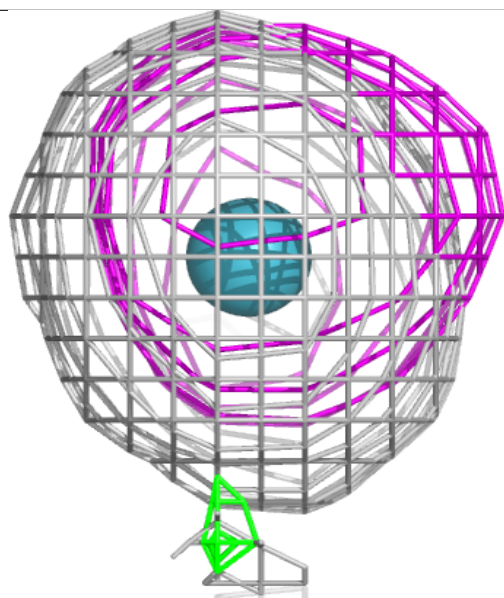
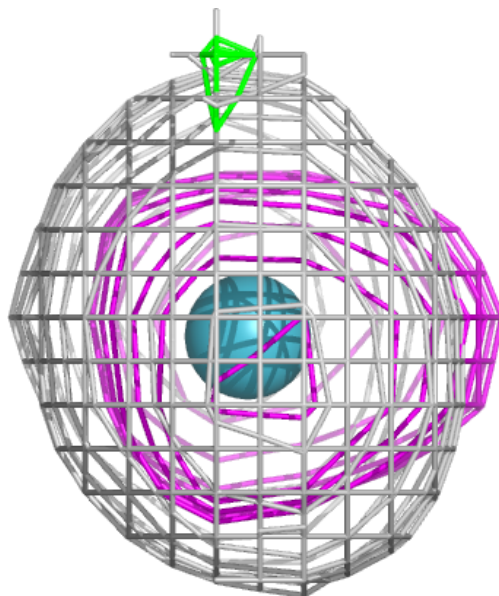
Electron density around XE A 616:

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



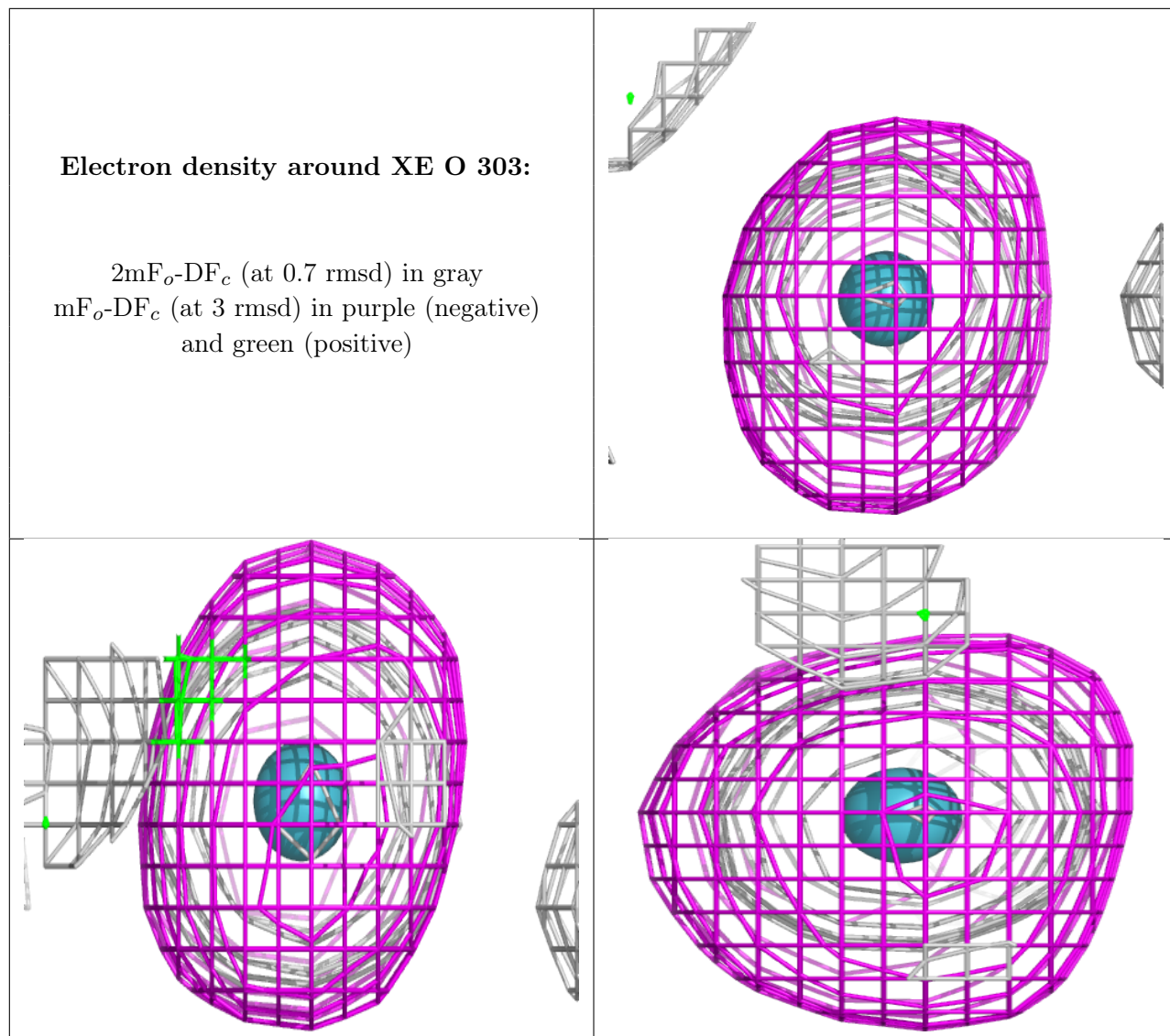
Electron density around XE N 621:

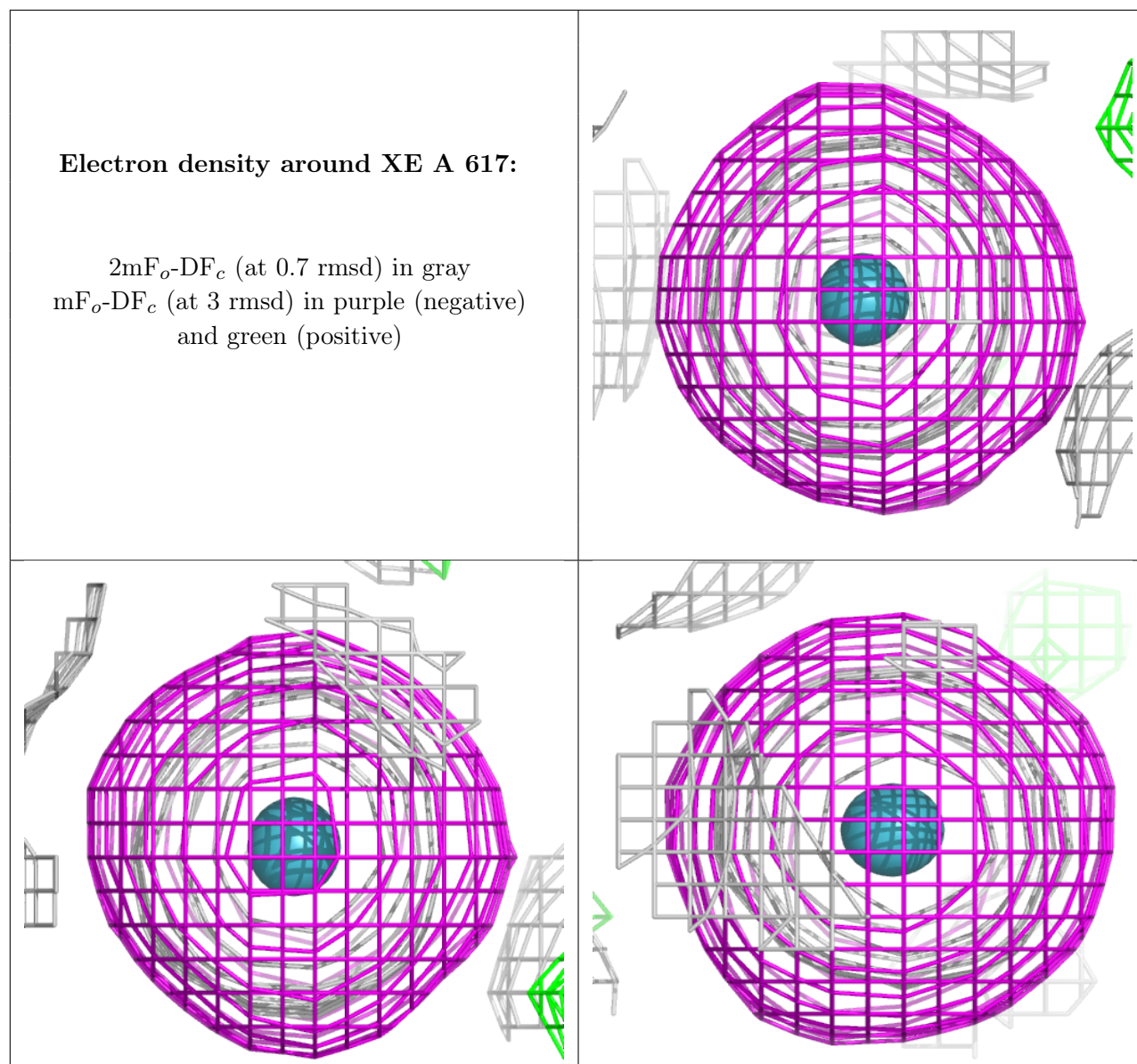
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around XE O 303:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.