



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:36 AM UTC

PDB ID : 9M56 / pdb_00009m56
Title : Bovine Heart Cytochrome c Oxidase in the Fully Reduced State
Authors : Muramoto, K.; Shinzawa-Itoh, K.
Deposited on : 2025-03-05
Resolution : 1.60 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

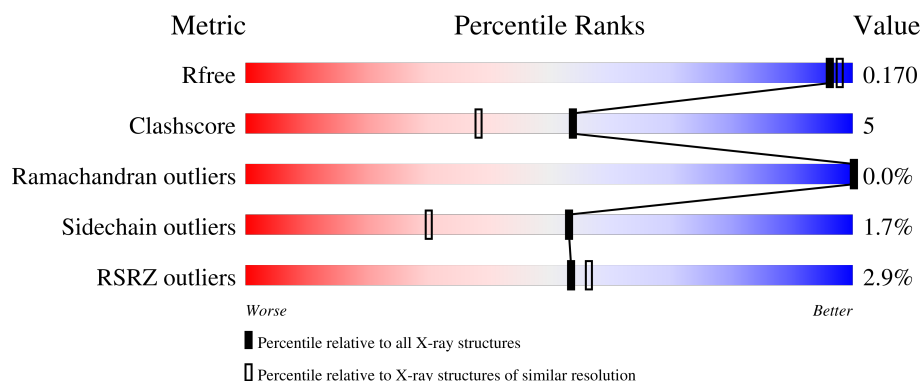
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

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



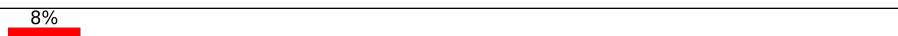
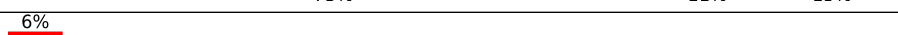
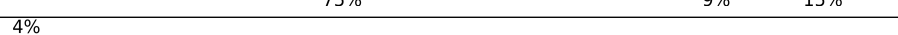
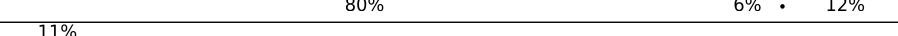
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	91%8% .
1	N	514	%91%8% .
2	B	227	5% 83%15% .
2	O	227	4% 84%14% .
3	C	261	87%12% .

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Mol	Chain	Length	Quality of chain
3	P	261	
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
19	LFA	P	311	-	-	-	X

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 33023 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			

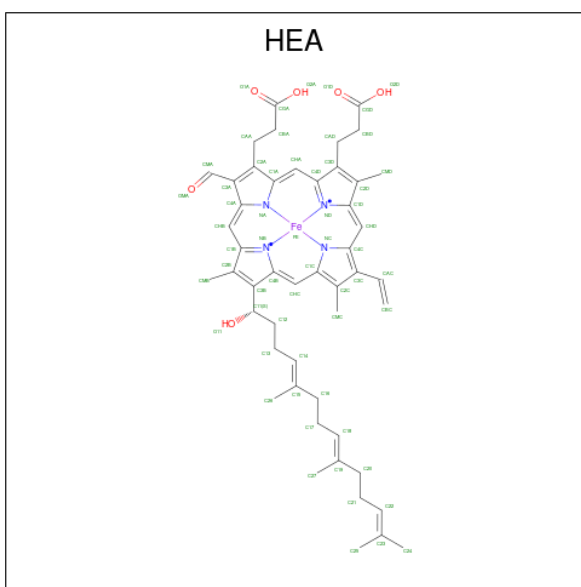
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

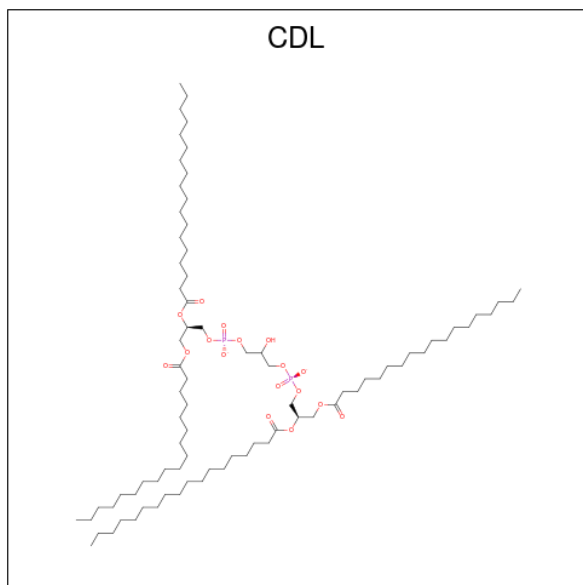
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

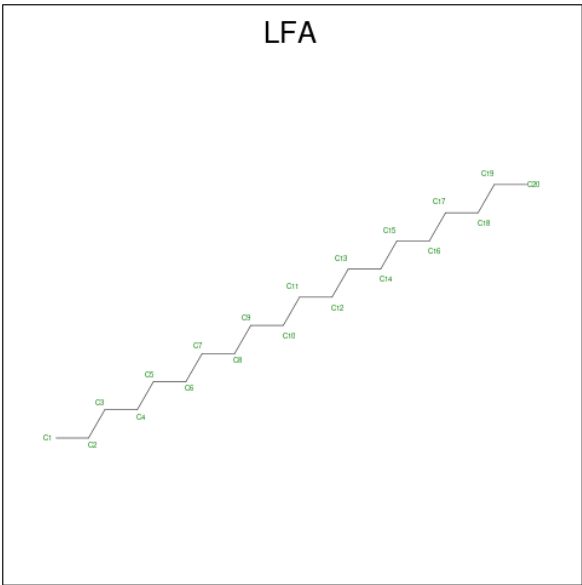
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 19 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



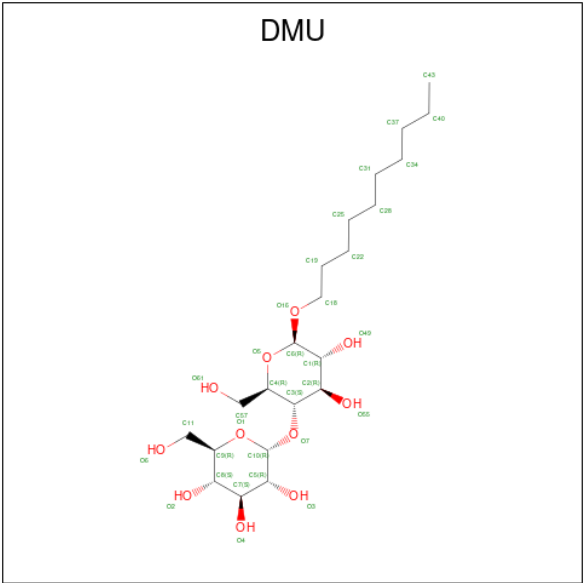
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	C	0	0
			14	14		
19	B	1	Total	C	0	0
			17	17		
19	C	1	Total	C	0	0
			11	11		
19	C	1	Total	C	0	0
			6	6		
19	C	1	Total	C	0	0
			18	18		
19	C	1	Total	C	0	0
			11	11		
19	C	1	Total	C	0	0
			14	14		
19	C	1	Total	C	0	0
			11	11		
19	C	1	Total	C	0	0
	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

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

- Molecule 20 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



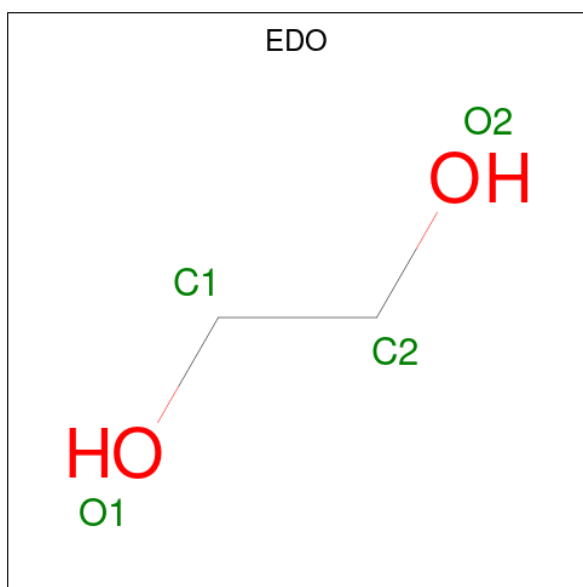
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C 7 7	0	0
20	A	1	Total C O 33 22 11	0	0
20	A	1	Total C O 11 10 1	0	0
20	B	1	Total C O 11 10 1	0	0
20	B	1	Total C O 11 10 1	0	0
20	B	1	Total C O 22 16 6	0	0
20	B	1	Total C O 22 16 6	0	0
20	C	1	Total C O 11 10 1	0	0
20	C	1	Total C O 33 22 11	0	0
20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

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

- Molecule 21 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



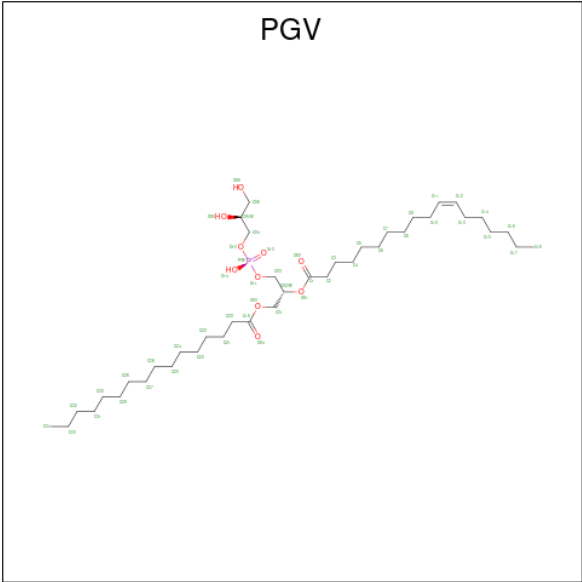
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	E	1	Total	C	O	0	0
			4	2	2		
21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

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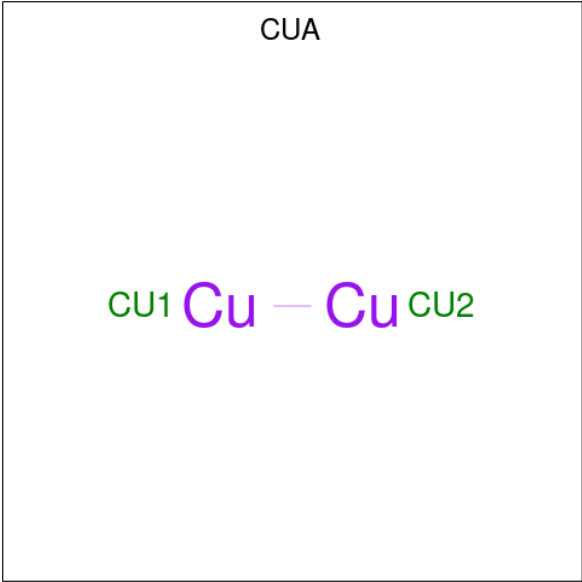
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	O	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21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

- Molecule 22 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



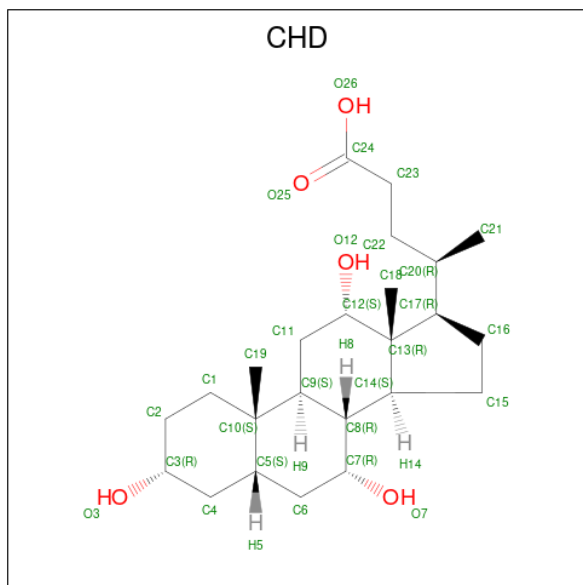
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	O	P	0	0
			51	40	10	1		
22	C	1	Total	C	O	P	0	0
			51	40	10	1		
22	N	1	Total	C	O	P	0	0
			51	40	10	1		
22	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 23 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

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



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

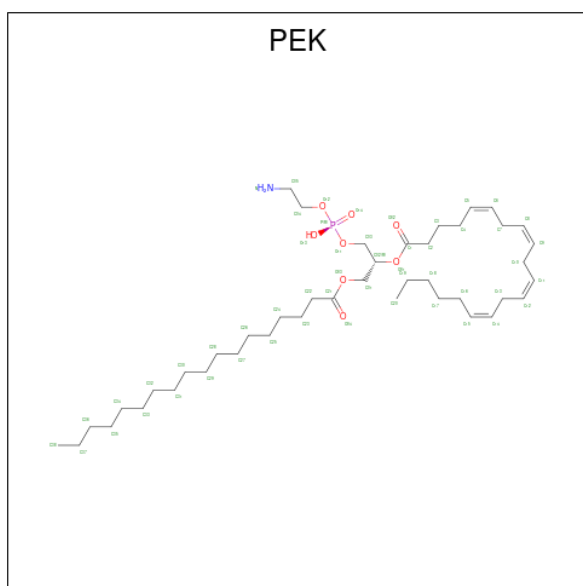
- Molecule 25 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

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

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 27 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
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	234	Total	O	0	11
			245	245		
28	B	169	Total	O	0	2
			171	171		
28	C	102	Total	O	0	1
			103	103		
28	D	139	Total	O	0	9
			148	148		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	E	107	Total 114	O 114	0	7
28	F	104	Total 111	O 111	0	7
28	G	48	Total 49	O 49	0	1
28	H	63	Total 63	O 63	0	0
28	I	39	Total 39	O 39	0	0
28	J	21	Total 21	O 21	0	0
28	K	22	Total 22	O 22	0	0
28	L	27	Total 29	O 29	0	2
28	M	21	Total 21	O 21	0	0
28	N	224	Total 234	O 234	0	10
28	O	142	Total 143	O 143	0	1
28	P	99	Total 100	O 100	0	1
28	Q	77	Total 81	O 81	0	4
28	R	88	Total 96	O 96	0	8
28	S	91	Total 97	O 97	0	6
28	T	36	Total 37	O 37	0	1
28	U	48	Total 48	O 48	0	0
28	V	25	Total 25	O 25	0	0
28	W	16	Total 16	O 16	0	0
28	X	18	Total 18	O 18	0	0
28	Y	25	Total 27	O 27	0	2

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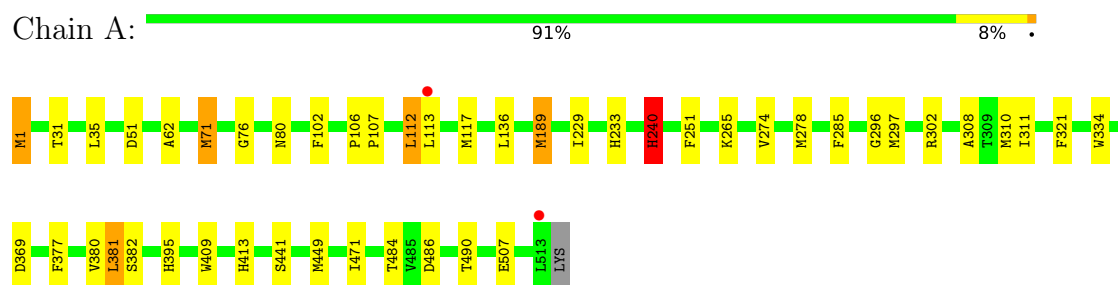
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	Z	18	Total	O	0	0
			18	18		

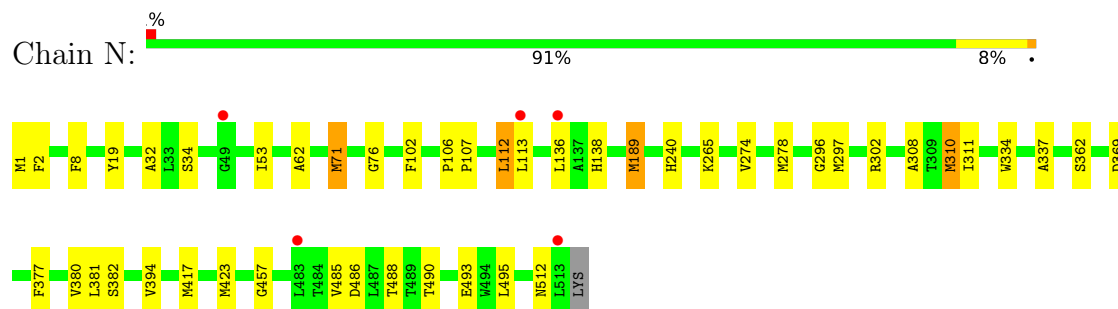
3 Residue-property plots [i](#)

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.

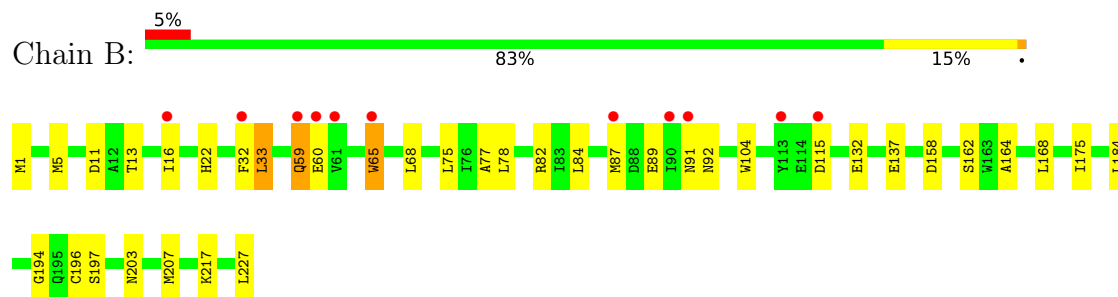
- Molecule 1: Cytochrome c oxidase subunit 1



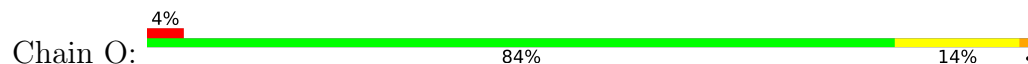
- Molecule 1: Cytochrome c oxidase subunit 1

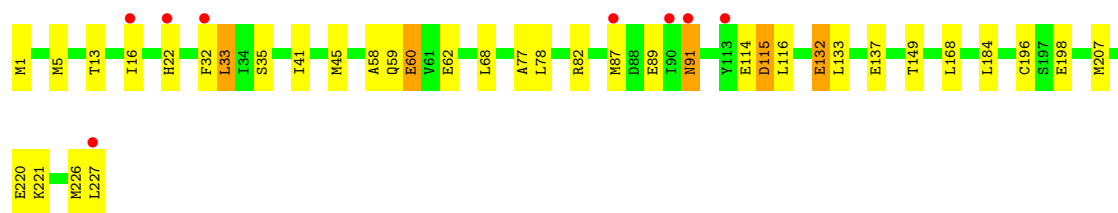


- Molecule 2: Cytochrome c oxidase subunit 2



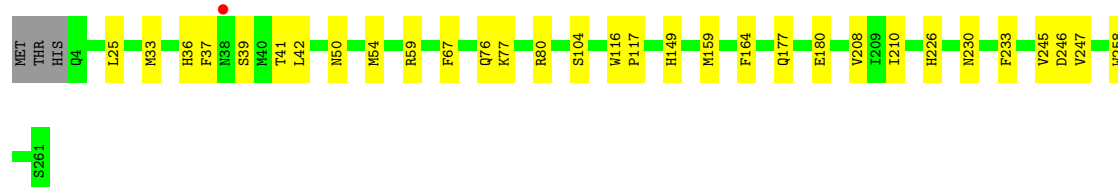
- Molecule 2: Cytochrome c oxidase subunit 2





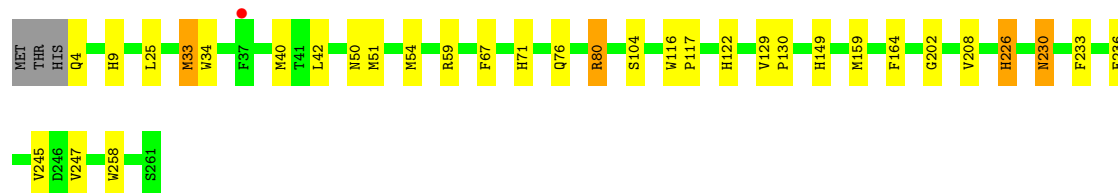
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 87% 12%



• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 86% 11%



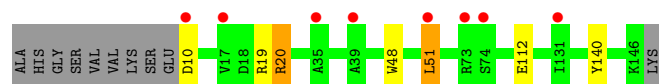
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 91% 5%



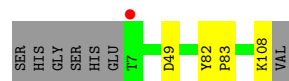
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q: 88% 5% 7%

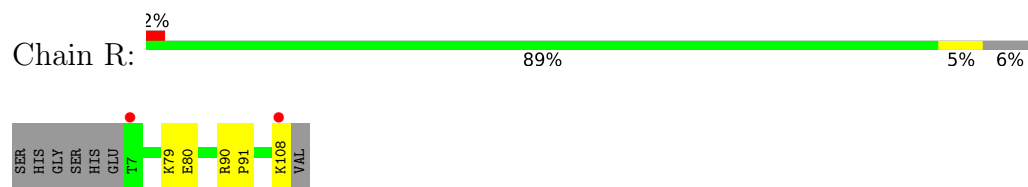


• Molecule 5: Cytochrome c oxidase subunit 5A

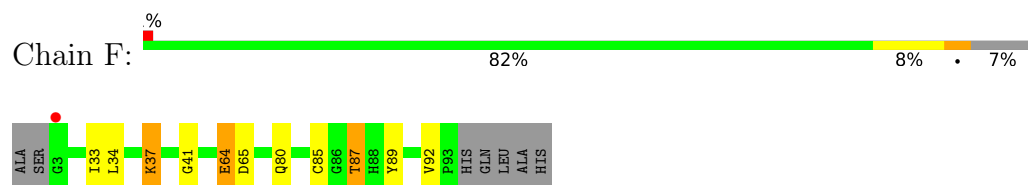
Chain E: 90% 6%



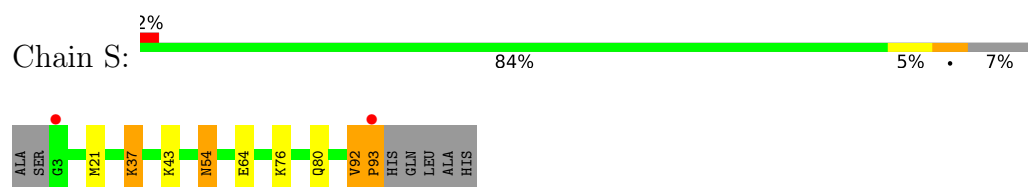
- Molecule 5: Cytochrome c oxidase subunit 5A



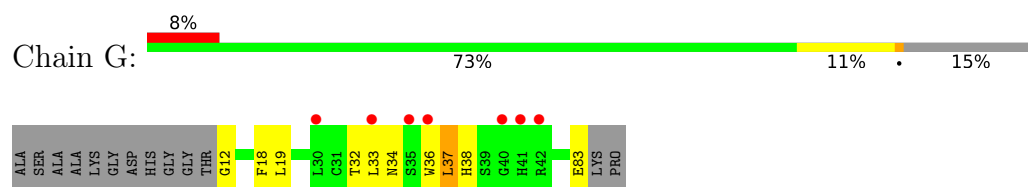
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



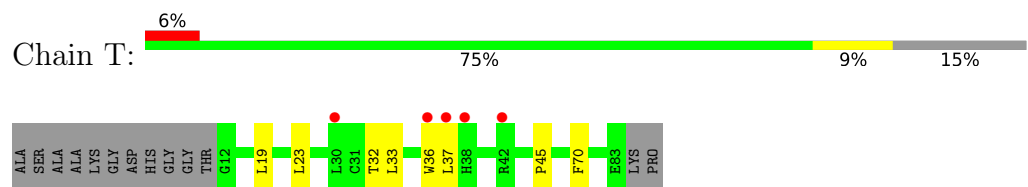
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



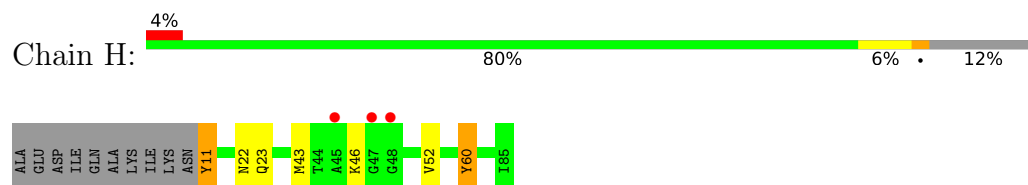
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



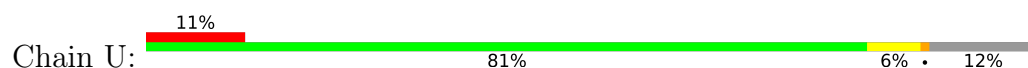
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

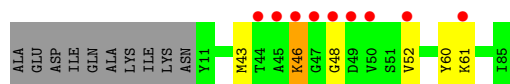


- Molecule 8: Cytochrome c oxidase subunit 6B1

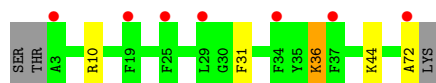
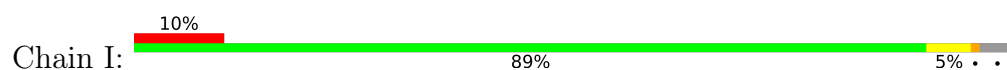


- Molecule 8: Cytochrome c oxidase subunit 6B1

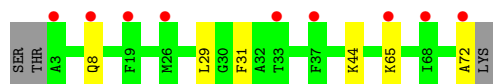
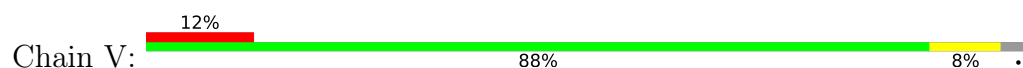




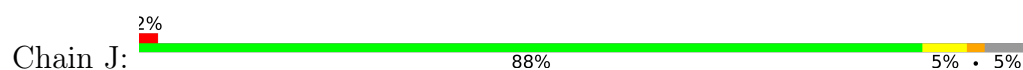
- Molecule 9: Cytochrome c oxidase subunit 6C



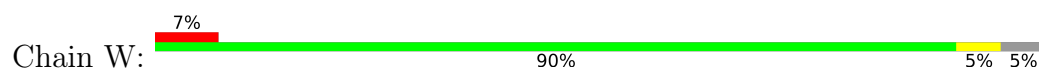
- Molecule 9: Cytochrome c oxidase subunit 6C



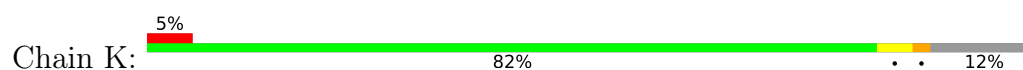
- Molecule 10: Cytochrome c oxidase subunit 7A1



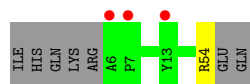
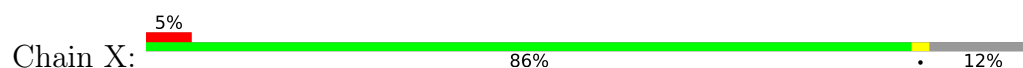
- Molecule 10: Cytochrome c oxidase subunit 7A1



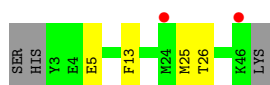
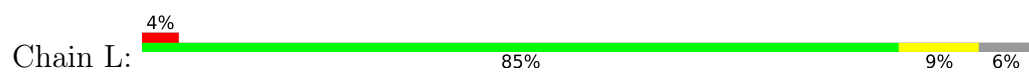
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



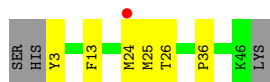
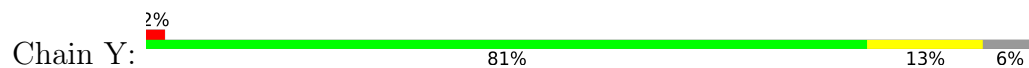
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



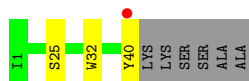
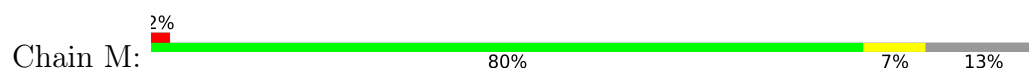
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



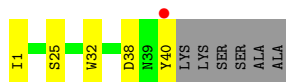
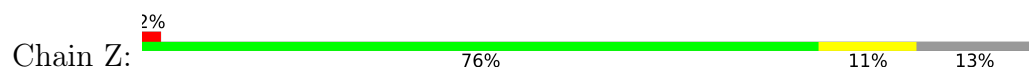
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.80Å 204.10Å 177.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.60 40.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.60) 100.0 (40.00-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.126 , 0.155 0.144 , 0.170	Depositor DCC
R_{free} test set	43303 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for l,k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33023	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: FME, LFA, HEA, UNX, PEK, PGV, ZN, CU, EDO, NA, DMU, MG, CUA, CDL, CHD

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	1.05	8/4259 (0.2%)	1.17	7/5816 (0.1%)
1	N	1.01	4/4259 (0.1%)	1.20	9/5816 (0.2%)
2	B	1.12	0/1908	1.25	9/2598 (0.3%)
2	O	1.09	4/1908 (0.2%)	1.23	2/2598 (0.1%)
3	C	1.01	1/2258 (0.0%)	1.13	3/3084 (0.1%)
3	P	1.00	3/2258 (0.1%)	1.15	5/3084 (0.2%)
4	D	1.08	2/1226 (0.2%)	1.16	4/1657 (0.2%)
4	Q	1.03	0/1182	1.28	4/1598 (0.3%)
5	E	1.04	1/843 (0.1%)	1.16	1/1145 (0.1%)
5	R	1.03	0/843	1.27	1/1145 (0.1%)
6	F	1.11	2/724 (0.3%)	1.18	0/983
6	S	1.13	3/724 (0.4%)	1.19	1/983 (0.1%)
7	G	1.07	0/633	1.19	1/864 (0.1%)
7	T	1.09	2/633 (0.3%)	1.16	0/864
8	H	1.04	1/648 (0.2%)	1.26	0/877
8	U	1.06	0/648	1.27	0/877
9	I	1.11	1/588 (0.2%)	1.37	1/781 (0.1%)
9	V	1.10	0/588	1.41	1/781 (0.1%)
10	J	1.02	0/451	1.26	1/610 (0.2%)
10	W	1.01	0/451	1.29	0/610
11	K	1.14	1/398 (0.3%)	1.30	1/546 (0.2%)
11	X	1.10	0/398	1.23	1/546 (0.2%)
12	L	1.14	1/372 (0.3%)	1.28	2/500 (0.4%)
12	Y	1.18	1/372 (0.3%)	1.24	2/500 (0.4%)
13	M	1.04	0/321	1.09	0/440
13	Z	1.01	0/321	1.23	0/440
All	All	1.06	35/29214 (0.1%)	1.21	56/39743 (0.1%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	1
All	All	0	3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	HIS	CE1-NE2	8.71	1.41	1.32
1	A	413	HIS	CE1-NE2	-8.39	1.24	1.32
11	K	10	HIS	CE1-NE2	8.20	1.40	1.32
4	D	21	ASP	CG-OD2	7.75	1.40	1.25
4	D	58	GLU	CD-OE1	7.12	1.38	1.25
12	L	5	GLU	C-O	6.76	1.32	1.23
1	A	189	MET	CG-SD	-6.71	1.64	1.80
1	A	189	MET	CB-CG	6.50	1.72	1.52
1	N	138	HIS	CE1-NE2	6.31	1.38	1.32
8	H	11	TYR	N-CA	6.10	1.57	1.46
2	O	59	GLN	C-O	6.01	1.31	1.24
3	P	71	HIS	CE1-NE2	5.96	1.38	1.32
3	P	9	HIS	CE1-NE2	5.90	1.38	1.32
7	T	32	THR	C-O	5.77	1.30	1.24
1	A	382	SER	C-O	5.75	1.30	1.24
6	F	34	LEU	C-O	5.75	1.30	1.23
6	S	93	PRO	C-O	5.68	1.34	1.23
2	O	198	GLU	C-O	5.59	1.30	1.23
1	N	71	MET	CG-SD	5.53	1.94	1.80
1	A	395	HIS	CE1-NE2	5.51	1.38	1.32
6	S	64	GLU	C-O	5.42	1.30	1.23
9	I	72	ALA	C-O	5.41	1.34	1.23
1	N	310	MET	CG-SD	-5.35	1.67	1.80
1	A	413	HIS	CG-ND1	-5.32	1.32	1.38
3	C	36	HIS	CE1-NE2	5.32	1.37	1.32
1	N	189	MET	CG-SD	-5.29	1.67	1.80
12	Y	3	TYR	N-CA	5.29	1.56	1.46
6	S	92	VAL	C-O	-5.18	1.17	1.24
2	O	132	GLU	CD-OE2	5.14	1.35	1.25
7	T	45	PRO	C-O	-5.14	1.18	1.23
5	E	49	ASP	CG-OD1	-5.13	1.15	1.25
1	A	381	LEU	C-O	-5.06	1.19	1.23
2	O	35	SER	C-O	5.04	1.29	1.24
3	P	226	HIS	CE1-NE2	5.03	1.37	1.32
6	F	64	GLU	C-O	5.03	1.29	1.23

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	71	MET	CG-SD-CE	-11.98	74.55	100.90
1	A	71	MET	CG-SD-CE	-11.36	75.90	100.90
9	V	72	ALA	CA-C-O	-10.47	103.00	120.80
1	N	240	HIS	CA-CB-CG	-10.22	103.58	113.80
4	D	58	GLU	CB-CG-CD	10.04	129.67	112.60
1	A	240	HIS	CA-CB-CG	-9.64	104.16	113.80
9	I	72	ALA	CA-C-O	-9.62	104.44	120.80
11	K	54	ARG	CA-C-O	-9.40	104.82	120.80
2	B	65	TRP	CB-CA-C	7.64	123.98	110.37
2	B	59	GLN	CB-CG-CD	7.37	125.13	112.60
12	L	25	MET	CA-C-N	7.13	130.17	120.54
12	L	25	MET	C-N-CA	7.13	130.17	120.54
2	B	115	ASP	CB-CA-C	7.08	123.08	112.03
3	C	80	ARG	CG-CD-NE	-6.88	96.87	112.00
10	J	7	GLU	CB-CA-C	6.72	122.27	110.85
2	B	184	LEU	N-CA-CB	-6.65	99.29	110.80
3	P	76	GLN	CG-CD-NE2	-6.64	106.44	116.40
1	A	382	SER	CA-C-O	-6.58	113.83	121.07
1	N	382	SER	CA-C-O	-6.52	114.16	121.00
1	A	102	PHE	CA-CB-CG	-6.43	107.37	113.80
3	P	80	ARG	CG-CD-NE	-6.40	97.93	112.00
1	N	102	PHE	CA-CB-CG	-6.18	107.62	113.80
6	S	93	PRO	CB-CA-C	6.16	121.80	110.10
2	B	82	ARG	CG-CD-NE	-6.12	98.53	112.00
2	B	158	ASP	CA-CB-CG	6.10	118.70	112.60
1	N	512	ASN	CB-CA-C	6.01	120.85	110.45
5	R	80	GLU	CB-CG-CD	5.99	122.78	112.60
4	D	20	ARG	NE-CZ-NH2	5.98	124.58	119.20
4	D	146	LYS	CA-C-O	-5.90	110.76	120.80
3	P	233	PHE	CA-CB-CG	-5.90	107.90	113.80
3	P	230	ASN	CA-CB-CG	-5.85	106.75	112.60
1	N	106	PRO	CB-CA-C	5.82	118.02	110.92
3	C	233	PHE	CA-CB-CG	-5.71	108.09	113.80
2	B	89	GLU	CA-C-O	-5.59	115.62	121.55
4	D	21	ASP	CA-CB-CG	5.55	118.15	112.60
12	Y	25	MET	CA-C-N	5.51	127.61	120.44
12	Y	25	MET	C-N-CA	5.51	127.61	120.44
1	N	493	GLU	CB-CG-CD	5.48	121.92	112.60
1	N	240	HIS	N-CA-CB	5.48	116.88	110.42
5	E	108	LYS	CA-C-O	-5.47	111.49	120.80
1	A	507	GLU	CB-CA-C	5.46	116.07	109.85
11	X	54	ARG	CA-C-O	-5.40	111.62	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	8	PHE	CA-CB-CG	5.40	119.20	113.80
4	Q	20	ARG	NE-CZ-NH1	5.34	126.84	121.50
3	P	122	HIS	CB-CA-C	5.33	116.20	110.65
1	A	106	PRO	CB-CA-C	5.33	117.42	110.92
2	B	11	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	251	PHE	CA-CB-CG	5.32	119.12	113.80
4	Q	20	ARG	CG-CD-NE	-5.30	100.35	112.00
7	G	83	GLU	CA-C-O	-5.27	111.83	120.80
3	C	76	GLN	CG-CD-NE2	-5.25	108.53	116.40
4	Q	140	TYR	CA-C-O	-5.18	112.88	119.31
2	O	184	LEU	N-CA-CB	-5.17	102.00	110.68
2	B	59	GLN	N-CA-CB	5.16	117.79	110.16
2	O	115	ASP	CB-CA-C	5.13	120.03	112.03
4	Q	20	ARG	NE-CZ-NH2	-5.09	114.62	119.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	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	40	0
1	N	4130	0	4102	44	0
2	B	1870	0	1870	27	0
2	O	1870	0	1870	29	0
3	C	2171	0	2080	31	0
3	P	2172	0	2081	25	0
4	D	1192	0	1178	7	0
4	Q	1148	0	1131	4	0
5	E	825	0	823	1	0
5	R	825	0	823	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	709	0	691	9	0
6	S	709	0	691	6	0
7	G	606	0	577	8	0
7	T	606	0	577	4	0
8	H	628	0	580	11	0
8	U	628	0	580	7	0
9	I	575	0	584	7	0
9	V	575	0	584	3	0
10	J	441	0	439	3	0
10	W	441	0	439	2	0
11	K	384	0	366	2	0
11	X	384	0	366	0	0
12	L	360	0	360	3	0
12	Y	360	0	360	8	0
13	M	311	0	321	2	0
13	Z	311	0	321	5	0
14	A	120	0	108	3	0
14	N	120	0	108	4	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	64	0	72	0	0
18	C	87	0	124	16	0
18	L	94	0	141	2	0
18	P	87	0	124	12	0
18	V	64	0	72	1	0
18	Y	94	0	141	8	0
19	A	14	0	27	6	0
19	B	17	0	33	0	0
19	C	114	0	204	10	0
19	G	14	0	27	7	0
19	N	14	0	27	5	0
19	O	28	0	54	0	0
19	P	114	0	201	7	0
19	T	25	0	48	7	0
20	A	51	0	76	2	0
20	B	66	0	104	0	0
20	C	172	0	231	2	0
20	D	33	0	40	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	G	33	0	52	0	0
20	H	33	0	29	1	0
20	J	11	0	21	0	0
20	L	22	0	31	1	0
20	M	41	0	56	0	0
20	N	73	0	77	0	0
20	O	66	0	104	1	0
20	P	172	0	231	3	0
20	Q	33	0	42	3	0
20	T	22	0	31	0	0
20	W	11	0	21	0	0
20	Y	22	0	31	2	0
20	Z	41	0	56	0	0
21	A	12	0	18	0	0
21	B	4	0	6	0	0
21	C	12	0	17	0	0
21	E	12	0	18	0	0
21	F	12	0	18	0	0
21	G	4	0	6	0	0
21	N	20	0	30	0	0
21	O	4	0	6	0	0
21	P	12	0	18	0	0
21	R	12	0	18	0	0
21	S	8	0	12	0	0
21	T	4	0	6	0	0
22	A	51	0	76	0	0
22	C	51	0	76	3	0
22	N	51	0	76	0	0
22	P	51	0	76	0	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	29	0	39	0	0
24	C	58	0	78	3	0
24	G	29	0	39	1	0
24	P	58	0	78	3	0
25	C	1	0	0	1	0
25	P	1	0	0	1	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	G	53	0	77	0	0
27	T	53	0	77	5	0
28	A	245	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	B	171	0	0	4	0
28	C	103	0	0	6	0
28	D	148	0	0	2	0
28	E	114	0	0	0	0
28	F	111	0	0	1	0
28	G	49	0	0	1	0
28	H	63	0	0	4	0
28	I	39	0	0	2	0
28	J	21	0	0	0	0
28	K	22	0	0	0	0
28	L	29	0	0	1	0
28	M	21	0	0	0	0
28	N	234	0	0	9	0
28	O	143	0	0	2	0
28	P	100	0	0	3	0
28	Q	81	0	0	2	0
28	R	96	0	0	1	0
28	S	97	0	0	1	0
28	T	37	0	0	0	0
28	U	48	0	0	0	0
28	V	25	0	0	0	0
28	W	16	0	0	0	0
28	X	18	0	0	0	0
28	Y	27	0	0	1	0
28	Z	18	0	0	0	0
All	All	33023	0	31505	308	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 (308) 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)
19:C:309:LFA:H12	28:C:481:HOH:O	1.35	1.21
1:A:112:LEU:HG	28:A:2018:HOH:O	1.34	1.20
1:A:31:THR:O	1:A:35:LEU:HD23	1.45	1.16
1:N:112:LEU:HG	28:N:3015:HOH:O	1.47	1.13
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.29	1.10
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:HE3	1.42	1.01
1:A:112:LEU:O	1:A:112:LEU:HD23	1.68	0.94
3:P:4:GLN:N	28:P:403:HOH:O	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.03	0.93
3:C:245:VAL:C	3:C:246[B]:ASP:CA	2.42	0.92
8:H:43:MET:HE1	8:U:52:VAL:HG11	1.51	0.92
20:A:609:DMU:O6	28:A:1803:HOH:O	1.88	0.91
7:G:19:LEU:HD23	19:G:106:LFA:H61	1.52	0.88
1:N:423[B]:MET:HE2	1:N:457:GLY:HA2	1.54	0.88
1:A:112:LEU:HD23	1:A:112:LEU:C	1.99	0.87
1:A:278[A]:MET:HE1	19:T:101:LFA:H51	1.54	0.87
2:O:89:GLU:O	2:O:91:ASN:OD1	1.92	0.86
1:N:112:LEU:HD23	1:N:112:LEU:C	2.01	0.85
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.57	0.85
3:P:149:HIS:NE2	19:P:313:LFA:H11	1.92	0.84
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.21	0.81
18:L:101:CDL:O1	28:L:222[B]:HOH:O	2.00	0.80
8:H:52:VAL:HG21	8:U:43:MET:HE1	1.62	0.80
1:N:417[B]:MET:CE	28:N:2966:HOH:O	2.31	0.78
3:P:67:PHE:CE2	18:P:305:CDL:O1	2.38	0.76
6:F:37:LYS:HG2	28:F:295:HOH:O	1.84	0.75
8:H:43:MET:CE	8:U:52:VAL:HG11	2.17	0.75
24:C:301:CHD:O25	19:C:309:LFA:H13	1.86	0.75
1:A:31:THR:O	1:A:35:LEU:CD2	2.32	0.75
27:T:102:PEK:H71	27:T:102:PEK:H32	1.69	0.75
6:S:76:LYS:CE	6:S:93:PRO:HG2	2.17	0.74
1:N:274:VAL:HG12	1:N:278[A]:MET:HE2	1.69	0.74
2:B:16[A]:ILE:CG2	2:B:87[A]:MET:HE3	2.15	0.74
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:CE	2.17	0.74
2:B:16[B]:ILE:HG23	28:B:515:HOH:O	1.87	0.74
1:A:136[B]:LEU:HD11	28:A:2028:HOH:O	1.89	0.72
1:N:417[B]:MET:HE1	28:N:2966:HOH:O	1.90	0.72
7:G:19:LEU:CD2	19:G:106:LFA:H61	2.21	0.70
2:B:22[B]:HIS:CE1	9:I:44:LYS:CE	2.75	0.69
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:HG2	1.75	0.69
1:N:278[B]:MET:HE1	19:N:606:LFA:H52	1.73	0.68
3:P:59:ARG:HG3	18:P:305:CDL:HA4	1.75	0.68
1:A:112:LEU:C	1:A:112:LEU:CD2	2.66	0.68
1:N:112:LEU:HD23	1:N:112:LEU:O	1.92	0.68
18:C:304:CDL:HB61	18:C:304:CDL:HB21	1.75	0.68
8:H:23:GLN:CD	28:H:201:HOH:O	2.36	0.68
8:H:52:VAL:HG12	8:U:46:LYS:CG	2.18	0.68
3:P:33[B]:MET:CE	3:P:42:LEU:HD12	2.24	0.67
1:A:278[A]:MET:CE	19:T:101:LFA:H51	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:PHE:CE2	18:C:304:CDL:O1	2.48	0.67
3:C:33[A]:MET:HE3	3:C:39:SER:OG	1.94	0.67
25:P:303:UNX:UNK	28:P:495:HOH:O	1.74	0.67
18:P:305:CDL:H121	18:P:305:CDL:HA62	1.77	0.67
1:A:297[B]:MET:SD	1:A:302:ARG:HG2	2.34	0.67
3:C:33[B]:MET:HG3	3:C:37:PHE:HB2	1.78	0.66
25:C:302:UNX:UNK	28:C:495:HOH:O	1.74	0.66
1:N:423[B]:MET:HE2	1:N:457:GLY:CA	2.25	0.66
1:N:310:MET:HE1	2:O:77:ALA:HB2	1.78	0.65
28:Q:315:HOH:O	5:R:108:LYS:HD3	1.95	0.65
3:C:180[B]:GLU:HG2	28:C:405:HOH:O	1.97	0.65
4:D:42:GLU:OE2	28:D:301:HOH:O	2.14	0.64
3:P:51[B]:MET:HE3	18:P:305:CDL:H873	1.80	0.64
19:A:607:LFA:H12	19:T:101:LFA:H11	1.79	0.64
19:G:106:LFA:H51	1:N:278[A]:MET:HE1	1.79	0.64
3:C:33[B]:MET:CA	3:C:33[B]:MET:HE2	1.99	0.63
7:T:19:LEU:HD23	19:T:101:LFA:H61	1.78	0.63
3:C:149:HIS:NE2	19:C:312:LFA:H11	2.14	0.63
18:Y:101:CDL:H362	18:Y:101:CDL:H711	1.81	0.62
7:G:34:ASN:O	7:G:38:HIS:HD2	1.81	0.62
1:N:136[B]:LEU:HD11	28:N:3022:HOH:O	2.00	0.61
1:N:278[B]:MET:SD	19:N:606:LFA:H51	2.41	0.61
4:Q:112:GLU:OE2	28:Q:301:HOH:O	2.16	0.61
3:C:33[A]:MET:HE2	3:C:42:LEU:H	1.66	0.61
1:N:486:ASP:OD2	4:Q:19:ARG:NE	2.33	0.61
3:C:33[A]:MET:HE1	3:C:41:THR:HB	1.81	0.61
18:C:304:CDL:HB21	18:C:304:CDL:HB32	1.83	0.60
3:P:164:PHE:CD1	24:P:306:CHD:H192	2.36	0.60
18:P:305:CDL:H752	10:W:27:THR:HG21	1.82	0.60
24:C:305:CHD:H162	24:C:305:CHD:H231	1.83	0.60
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.84	0.60
19:C:313:LFA:H21	19:C:314:LFA:H71	1.83	0.60
1:N:362[A]:SER:HA	2:O:87[A]:MET:HE1	1.82	0.60
1:N:297[B]:MET:SD	1:N:302:ARG:CG	2.90	0.59
1:A:51:ASP:OD2	1:A:441:SER:OG	2.18	0.59
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:CG	2.31	0.59
3:C:33[A]:MET:CE	3:C:42:LEU:H	2.14	0.59
3:C:104:SER:OG	28:C:403:HOH:O	2.07	0.58
3:C:59:ARG:HB2	18:C:304:CDL:OA9	2.03	0.58
1:N:113[A]:LEU:HD12	18:Y:101:CDL:C87	2.34	0.57
1:A:278[B]:MET:HE1	19:A:607:LFA:H52	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:C:304:CDL:H752	10:J:27:THR:HG21	1.87	0.57
28:N:2950:HOH:O	19:P:310:LFA:H41	2.04	0.57
18:C:304:CDL:HB61	18:C:304:CDL:CB2	2.35	0.56
27:T:102:PEK:H32	27:T:102:PEK:C7	2.36	0.56
2:B:13:THR:HB	2:B:168:LEU:HD23	1.88	0.56
3:C:54[A]:MET:HE1	22:C:303:PGV:H141	1.88	0.56
1:A:274:VAL:HG12	1:A:278[A]:MET:HE2	1.88	0.56
8:U:43:MET:O	8:U:48:GLY:N	2.38	0.56
18:Y:101:CDL:H711	18:Y:101:CDL:C36	2.36	0.56
3:C:258:TRP:CE2	19:C:307:LFA:H32	2.41	0.56
8:H:23:GLN:NE2	28:H:201:HOH:O	2.38	0.55
4:D:86:MET:HE1	11:K:22:ALA:HB2	1.89	0.55
18:C:304:CDL:HB21	18:C:304:CDL:CB3	2.37	0.55
4:D:58:GLU:HG3	28:D:371[A]:HOH:O	2.06	0.54
2:O:60:GLU:CD	2:O:60:GLU:H	2.15	0.54
19:C:309:LFA:C1	28:C:481:HOH:O	2.17	0.54
3:C:247:VAL:HG11	19:C:313:LFA:H71	1.89	0.54
18:C:304:CDL:HA62	18:C:304:CDL:H121	1.89	0.54
4:D:17[B]:VAL:HG22	4:D:19:ARG:HG3	1.90	0.54
18:P:305:CDL:HA62	18:P:305:CDL:C12	2.37	0.54
24:P:306:CHD:H162	24:P:306:CHD:H231	1.90	0.53
1:N:112:LEU:C	1:N:112:LEU:CD2	2.75	0.53
2:O:114:GLU:HG3	2:O:227:LEU:CD2	2.39	0.53
18:P:305:CDL:H121	18:P:305:CDL:CA6	2.39	0.53
2:O:22[B]:HIS:CE1	9:V:44:LYS:HE2	2.43	0.53
3:P:50:ASN:ND2	3:P:54[A]:MET:HE2	2.24	0.53
1:A:310:MET:HE1	2:B:77:ALA:HB2	1.91	0.53
2:B:84:LEU:O	2:B:87[B]:MET:HB2	2.09	0.53
6:F:64:GLU:O	6:F:65:ASP:HB2	2.09	0.53
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.90	0.52
18:C:304:CDL:OA3	18:C:304:CDL:H1	1.97	0.52
28:N:2979:HOH:O	4:Q:20:ARG:HG2	2.08	0.52
5:R:90:ARG:NH1	28:R:303:HOH:O	2.39	0.52
3:C:164:PHE:CD1	24:C:305:CHD:H192	2.44	0.52
18:C:304:CDL:HB22	10:J:8:LYS:HE3	1.92	0.52
6:F:92:VAL:HG23	6:F:92:VAL:O	2.08	0.52
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.40	0.52
18:C:304:CDL:CA3	18:C:304:CDL:OB9	2.58	0.51
1:N:417[B]:MET:HE2	28:N:2966:HOH:O	2.02	0.51
14:N:601:HEA:HBC1	14:N:601:HEA:HMC1	1.92	0.51
6:F:87[A]:THR:HG22	6:F:89:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:247:VAL:CG1	19:C:313:LFA:H71	2.41	0.51
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.41	0.51
6:S:54:ASN:HD22	6:S:54:ASN:C	2.19	0.51
1:A:308:ALA:O	1:A:311[B]:ILE:HG12	2.11	0.51
18:C:304:CDL:CA5	18:C:304:CDL:OB4	2.60	0.50
18:P:305:CDL:HB61	18:P:305:CDL:HB22	1.94	0.50
2:B:227:LEU:HD21	28:B:526:HOH:O	2.11	0.50
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.41	0.50
2:O:16[B]:ILE:HG23	28:O:500:HOH:O	2.11	0.50
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.94	0.50
4:D:127:LYS:HD2	28:I:136:HOH:O	2.12	0.49
18:C:304:CDL:H531	18:C:304:CDL:HB4	1.94	0.49
28:N:2950:HOH:O	19:P:310:LFA:C4	2.61	0.49
2:O:16[A]:ILE:HG21	2:O:87[A]:MET:HG2	1.92	0.49
2:B:33:LEU:HD13	9:I:31:PHE:CD2	2.48	0.49
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.48	0.49
2:O:32[B]:PHE:CD2	9:V:31:PHE:CZ	3.00	0.49
3:P:116:TRP:HA	3:P:117:PRO:C	2.38	0.49
28:A:1993:HOH:O	6:F:37:LYS:HE3	2.13	0.49
3:P:33[B]:MET:HE2	3:P:42:LEU:HD12	1.94	0.49
3:P:104:SER:OG	28:P:404:HOH:O	2.20	0.48
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.12	0.48
1:N:308:ALA:O	1:N:311[B]:ILE:HG12	2.12	0.48
12:Y:26:THR:CG2	20:Y:102:DMU:H26	2.43	0.48
7:T:23:LEU:HB2	19:T:101:LFA:C9	2.44	0.48
3:P:247:VAL:HG11	19:P:314:LFA:H71	1.95	0.48
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.96	0.48
12:L:13:PHE:HB3	18:L:101:CDL:H512	1.95	0.48
3:C:116:TRP:HA	3:C:117:PRO:C	2.38	0.47
1:A:486:ASP:HB3	28:A:1999[B]:HOH:O	2.15	0.47
1:A:189:MET:HE3	19:A:607:LFA:H31	1.95	0.47
3:C:41:THR:HG23	20:C:319:DMU:H15	1.96	0.47
20:Q:201:DMU:O55	20:Q:201:DMU:H36	2.14	0.47
8:H:23:GLN:NE2	28:H:202:HOH:O	2.46	0.47
1:N:278[B]:MET:SD	19:N:606:LFA:C5	3.02	0.47
18:C:304:CDL:OB9	18:C:304:CDL:OA5	2.32	0.47
3:P:80:ARG:NH2	3:P:236:GLU:OE1	2.44	0.47
19:G:106:LFA:H11	19:N:606:LFA:H12	1.95	0.47
3:P:33[B]:MET:HE2	3:P:33[B]:MET:HB2	1.60	0.47
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.97	0.47
8:H:11:TYR:N	28:H:204:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:24:MET:HG3	28:Y:216:HOH:O	2.14	0.47
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.68	0.47
1:A:334:TRP:HB2	20:D:201:DMU:C57	2.45	0.46
3:C:226:HIS:HE1	18:C:304:CDL:H111	1.80	0.46
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.96	0.46
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.97	0.46
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.97	0.46
1:N:381:LEU:HB2	14:N:602:HEA:CAC	2.46	0.46
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.96	0.46
18:P:305:CDL:HB32	18:P:305:CDL:HB21	1.97	0.46
12:Y:26:THR:HG21	20:Y:102:DMU:H26	1.96	0.46
1:A:484:THR:HG22	28:A:2019:HOH:O	2.15	0.46
1:N:377:PHE:O	1:N:381:LEU:HB3	2.15	0.46
1:A:321:PHE:CD2	2:B:65:TRP:HB2	2.51	0.46
7:G:32:THR:O	7:G:36:TRP:HB2	2.15	0.46
20:D:201:DMU:H36	20:D:201:DMU:O55	2.15	0.46
18:Y:101:CDL:OA5	18:Y:101:CDL:OA8	2.34	0.46
1:A:278[B]:MET:SD	19:A:607:LFA:C5	3.04	0.45
3:P:258:TRP:CE2	19:P:308:LFA:H32	2.50	0.45
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.98	0.45
3:C:33[B]:MET:HE1	20:C:323:DMU:H12	1.98	0.45
7:G:18:PHE:CE1	19:G:106:LFA:H71	2.51	0.45
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.99	0.45
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.98	0.45
1:N:2:PHE:HE2	18:Y:101:CDL:H712	1.81	0.45
2:O:91:ASN:HB2	2:O:149:THR:HG21	1.97	0.45
28:A:1900:HOH:O	3:C:77:LYS:HE3	2.16	0.45
18:C:304:CDL:CA5	18:C:304:CDL:OA8	2.63	0.45
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.97	0.45
3:C:50:ASN:ND2	3:C:54[A]:MET:HE2	2.32	0.45
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.98	0.45
2:O:58:ALA:O	2:O:62:GLU:HG3	2.16	0.45
1:A:71:MET:HB3	1:A:71:MET:HE2	1.87	0.44
1:A:297[B]:MET:HG2	1:A:302:ARG:HG3	1.99	0.44
2:B:22[B]:HIS:CE1	28:B:424:HOH:O	2.71	0.44
3:P:67:PHE:HE2	18:P:305:CDL:O1	1.99	0.44
3:P:149:HIS:NE2	19:P:313:LFA:C1	2.73	0.44
1:A:381:LEU:HB2	14:A:602:HEA:CAC	2.47	0.44
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.99	0.44
1:A:297[B]:MET:SD	1:A:302:ARG:CG	3.06	0.44
1:N:423[B]:MET:HE3	1:N:457:GLY:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:34:SER:HB2	14:N:601:HEA:C2B	2.48	0.44
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	2.00	0.44
19:C:307:LFA:H31	24:P:302:CHD:H61	2.00	0.44
2:O:33:LEU:HD13	9:V:31:PHE:CD2	2.53	0.44
12:L:26:THR:HG23	13:M:25:SER:HB3	2.00	0.44
1:A:1:FME:HE2	1:A:1:FME:HA	1.99	0.44
2:B:217:LYS:HE2	28:B:555:HOH:O	2.17	0.44
2:O:13:THR:HB	2:O:168:LEU:HD23	2.00	0.44
1:A:240:HIS:CD2	1:A:240:HIS:C	2.96	0.43
1:A:334:TRP:CZ3	20:A:608:DMU:H19	2.53	0.43
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.17	0.43
24:G:102:CHD:H12	24:G:102:CHD:H212	1.99	0.43
1:N:485:VAL:HG12	13:Z:1:ILE:HG13	1.99	0.43
3:P:258:TRP:CZ2	19:P:308:LFA:H32	2.52	0.43
3:C:33[A]:MET:CE	3:C:41:THR:HB	2.48	0.43
9:I:36:LYS:HE3	9:I:36:LYS:HA	2.00	0.43
1:N:423[B]:MET:CE	1:N:457:GLY:N	2.81	0.43
3:C:33[B]:MET:HE2	3:C:33[B]:MET:N	2.32	0.43
13:M:32:TRP:CZ3	13:M:40:TYR:OH	2.70	0.43
1:A:76:GLY:O	1:A:80:ASN:HB2	2.19	0.43
3:P:226:HIS:HE1	18:P:305:CDL:H111	1.84	0.43
20:P:319:DMU:H26	10:W:38:LEU:HD23	2.00	0.43
1:N:362[A]:SER:OG	2:O:87[A]:MET:HE2	2.18	0.43
1:N:189:MET:HE3	19:N:606:LFA:H31	2.01	0.43
1:A:285:PHE:CD2	19:A:607:LFA:H121	2.54	0.43
28:C:501:HOH:O	6:F:33:ILE:HD13	2.19	0.43
7:T:70[B]:PHE:HB2	27:T:102:PEK:H041	2.00	0.43
12:L:26:THR:HG21	20:L:102:DMU:C37	2.49	0.42
3:P:51[B]:MET:HE3	18:P:305:CDL:C87	2.48	0.42
18:Y:101:CDL:H142	18:Y:101:CDL:OB9	2.19	0.42
7:G:37:LEU:HD12	7:G:37:LEU:HA	1.95	0.42
8:H:22:ASN:ND2	20:H:101:DMU:O3	2.52	0.42
1:N:488:THR:HB	1:N:495:LEU:HD13	2.01	0.42
6:S:21[B]:MET:HE2	6:S:21[B]:MET:HB2	1.76	0.42
2:B:16[A]:ILE:HD12	2:B:87[A]:MET:HG3	2.00	0.42
4:D:17[B]:VAL:CG2	4:D:19:ARG:HG3	2.49	0.42
3:P:129:VAL:N	3:P:130:PRO:CD	2.81	0.42
20:P:324:DMU:O3	20:P:324:DMU:C2	2.68	0.42
1:A:113[B]:LEU:HD11	1:A:117[B]:MET:SD	2.59	0.42
9:I:10:ARG:CD	28:I:127:HOH:O	2.68	0.42
12:Y:26:THR:HG23	13:Z:25:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:101:CDL:C41	18:Y:101:CDL:H801	2.49	0.42
2:B:196:CYS:HB2	2:B:207:MET:HG3	2.00	0.42
27:T:102:PEK:C15	27:T:102:PEK:C11	2.97	0.42
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:SD	2.58	0.42
2:B:22[B]:HIS:HE1	9:I:44:LYS:CE	2.27	0.42
2:B:164:ALA:O	2:B:194:GLY:HA3	2.20	0.42
1:N:377:PHE:HA	1:N:380:VAL:HG12	2.01	0.42
3:C:210:ILE:HD13	22:C:303:PGV:H312	2.02	0.42
1:A:229:ILE:HD11	2:B:175:ILE:HD13	2.00	0.42
1:A:377:PHE:HA	1:A:380:VAL:HG12	2.01	0.42
6:S:37:LYS:HG3	28:S:211:HOH:O	2.20	0.42
2:O:60:GLU:CD	2:O:60:GLU:N	2.77	0.41
2:O:116:LEU:HD13	2:O:226:MET:CG	2.48	0.41
18:V:101:CDL:C52	18:V:101:CDL:H312	2.49	0.41
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:CG	2.50	0.41
19:G:106:LFA:H122	1:N:278[B]:MET:HE3	2.02	0.41
3:P:208:VAL:HG22	3:P:245:VAL:CG1	2.51	0.41
1:A:409:TRP:HB3	1:A:471:ILE:HG12	2.01	0.41
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	3.08	0.41
2:O:82:ARG:HA	20:O:303:DMU:H30	2.02	0.41
6:F:85:CYS:SG	6:F:87[B]:THR:OG1	2.71	0.41
12:Y:26:THR:HG23	13:Z:25:SER:HB3	2.01	0.41
1:N:53:ILE:HG12	28:N:2982:HOH:O	2.20	0.41
2:O:1:FME:HE1	2:O:133:LEU:CD2	2.50	0.41
3:P:34:TRP:CD1	3:P:40:MET:HG2	2.56	0.41
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.56	0.41
3:C:54[A]:MET:HE1	22:C:303:PGV:C14	2.51	0.41
7:G:12:GLY:HA3	28:G:242:HOH:O	2.20	0.41
20:P:324:DMU:C2	20:P:324:DMU:H38	2.33	0.41
3:C:149:HIS:NE2	19:C:312:LFA:C1	2.81	0.41
7:G:18:PHE:CD1	19:G:106:LFA:H71	2.56	0.41
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	2.02	0.41
1:N:71:MET:HB3	1:N:71:MET:HE2	1.86	0.41
1:A:278[B]:MET:SD	19:A:607:LFA:H52	2.61	0.41
2:B:162:SER:HB3	2:B:197:SER:C	2.46	0.41
2:O:220:GLU:OE1	28:O:402:HOH:O	2.22	0.41
6:S:92:VAL:O	6:S:92:VAL:HG23	2.21	0.41
2:O:41:ILE:O	2:O:45:MET:HG2	2.21	0.41
2:O:114:GLU:HG3	2:O:227:LEU:HD21	2.03	0.41
3:C:208:VAL:HG22	3:C:245:VAL:CG1	2.51	0.40
4:D:86:MET:CE	11:K:22:ALA:HB2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:23:LEU:HB2	19:T:101:LFA:H92	2.03	0.40
1:A:377:PHE:O	1:A:381:LEU:HB3	2.21	0.40
10:J:31:LEU:HD12	10:J:31:LEU:HA	1.94	0.40
1:N:19:TYR:CD1	1:N:76:GLY:HA3	2.56	0.40
3:P:202:GLY:HA3	27:T:102:PEK:H21	2.03	0.40
12:Y:13:PHE:HB3	18:Y:101:CDL:H512	2.02	0.40
1:A:449:MET:SD	2:B:5:MET:HG2	2.62	0.40
8:H:60:TYR:CD1	8:H:60:TYR:C	3.00	0.40
1:N:334:TRP:HB2	20:Q:201:DMU:C57	2.52	0.40
1:N:334:TRP:HB2	20:Q:201:DMU:H29	2.03	0.40
2:O:5:MET:HE2	2:O:5:MET:HB3	1.90	0.40
19:T:101:LFA:H92	19:T:101:LFA:H121	1.94	0.40
8:U:43:MET:HE2	8:U:43:MET:HA	2.03	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%)	511 (97%)	15 (3%)	0	100	100
1	N	526/514 (102%)	515 (98%)	11 (2%)	0	100	100
2	B	230/227 (101%)	225 (98%)	4 (2%)	1 (0%)	30	14
2	O	230/227 (101%)	224 (97%)	6 (3%)	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%)	133 (98%)	3 (2%)	0	100	100
5	E	100/109 (92%)	100 (100%)	0	0	100	100
5	R	100/109 (92%)	100 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	91/98 (93%)	91 (100%)	0	0	100	100
6	S	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
7	G	71/85 (84%)	67 (94%)	4 (6%)	0	100	100
7	T	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
8	H	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
8	U	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
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%)	47 (100%)	0	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%)	3421 (98%)	66 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	92	ASN

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%)	81	70
1	N	440/426 (103%)	438 (100%)	2 (0%)	81	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	215/210 (102%)	208 (97%)	7 (3%)	33	12
2	O	215/210 (102%)	208 (97%)	7 (3%)	33	12
3	C	232/226 (103%)	230 (99%)	2 (1%)	70	55
3	P	232/226 (103%)	228 (98%)	4 (2%)	53	30
4	D	128/129 (99%)	128 (100%)	0	100	100
4	Q	122/129 (95%)	120 (98%)	2 (2%)	55	33
5	E	89/95 (94%)	89 (100%)	0	100	100
5	R	89/95 (94%)	88 (99%)	1 (1%)	65	46
6	F	78/81 (96%)	74 (95%)	4 (5%)	21	5
6	S	78/81 (96%)	74 (95%)	4 (5%)	21	5
7	G	63/69 (91%)	61 (97%)	2 (3%)	34	12
7	T	63/69 (91%)	60 (95%)	3 (5%)	23	6
8	H	67/75 (89%)	65 (97%)	2 (3%)	36	13
8	U	67/75 (89%)	64 (96%)	3 (4%)	24	7
9	I	55/58 (95%)	54 (98%)	1 (2%)	51	28
9	V	55/58 (95%)	52 (94%)	3 (6%)	19	4
10	J	47/50 (94%)	46 (98%)	1 (2%)	47	23
10	W	47/50 (94%)	46 (98%)	1 (2%)	47	23
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	17
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%)	34 (100%)	0	100	100
13	Z	34/38 (90%)	33 (97%)	1 (3%)	37	14
All	All	3042/3086 (99%)	2989 (98%)	53 (2%)	53	30

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	A	369	ASP
2	B	33	LEU
2	B	59	GLN
2	B	60	GLU

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Mol	Chain	Res	Type
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
3	C	159	MET
3	C	230	ASN
6	F	37	LYS
6	F	80	GLN
6	F	87[A]	THR
6	F	87[B]	THR
7	G	33	LEU
7	G	37	LEU
8	H	46	LYS
8	H	60	TYR
9	I	36	LYS
10	J	7	GLU
11	K	54	ARG
1	N	112	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	115	ASP
2	O	221	LYS
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	43	LYS
6	S	54	ASN
6	S	80	GLN
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
8	U	46	LYS
8	U	60	TYR

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Mol	Chain	Res	Type
8	U	61	LYS
9	V	8	GLN
9	V	29	LEU
9	V	65	LYS
10	W	50	LEU
13	Z	38	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	422	ASN
2	B	52	HIS
2	B	59	GLN
2	B	203	ASN
3	C	50	ASN
3	C	56	GLN
3	C	76	GLN
4	D	119	GLN
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	91	ASN
2	O	92	ASN
3	P	50	ASN
4	Q	109	HIS
4	Q	119	GLN
5	R	94	ASN
6	S	54	ASN
8	U	22	ASN
10	W	29	ASN
11	X	35	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	O	1	2	8,9,10	0.69	0	8,9,11	0.89	0
1	FME	A	1	1	8,9,10	0.50	0	8,9,11	0.88	1 (12%)
2	FME	B	1	2	8,9,10	1.33	1 (12%)	8,9,11	1.13	1 (12%)
1	FME	N	1	1	8,9,10	0.68	0	8,9,11	1.04	1 (12%)

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	-	3/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-3.29	1.64	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-2.64	104.78	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	O-C-CA	-2.21	119.08	124.77
1	A	1	FME	C-CA-N	2.00	113.36	109.50

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 131 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 121 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	DMU	C	315	-	34,34,34	0.85	1 (2%)	45,45,45	1.36	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	DMU	C	316	-	6,6,34	0.28	0	5,5,45	0.46	0
18	CDL	P	305	-	86,86,99	0.59	0	92,98,111	0.88	8 (8%)
19	LFA	P	313	-	10,10,19	0.27	0	9,9,18	0.30	0
20	DMU	D	201	-	34,34,34	1.50	7 (20%)	45,45,45	1.46	5 (11%)
23	CUA	O	304	2	0,1,1	-	-	-	-	-
18	CDL	Y	101	-	93,93,99	0.40	0	99,105,111	0.50	0
20	DMU	L	102	-	22,22,34	0.62	0	27,27,45	1.06	1 (3%)
20	DMU	O	305	-	10,10,34	0.13	0	9,9,45	0.63	0
27	PEK	T	102	-	52,52,52	0.77	2 (3%)	55,57,57	1.07	3 (5%)
21	EDO	F	104	-	3,3,3	0.10	0	2,2,2	0.25	0
20	DMU	O	307	-	22,22,34	0.72	1 (4%)	27,27,45	1.21	4 (14%)
19	LFA	C	310	-	10,10,19	0.18	0	9,9,18	0.09	0
19	LFA	C	308	-	5,5,19	0.22	0	4,4,18	0.15	0
19	LFA	C	314	-	12,12,19	0.20	0	11,11,18	0.12	0
19	LFA	O	302	-	10,10,19	0.26	0	9,9,18	0.15	0
20	DMU	G	103	-	10,10,34	0.34	0	9,9,45	0.56	0
21	EDO	A	612	-	3,3,3	0.57	0	2,2,2	0.27	0
24	CHD	G	102	-	32,32,32	0.73	0	51,51,51	0.74	0
19	LFA	C	324	-	14,14,19	0.26	0	13,13,18	0.13	0
20	DMU	Q	201	-	34,34,34	1.28	5 (14%)	45,45,45	1.67	9 (20%)
21	EDO	R	201	-	3,3,3	0.15	0	2,2,2	0.20	0
21	EDO	R	202	-	3,3,3	0.28	0	2,2,2	0.28	0
20	DMU	Y	102	-	22,22,34	0.63	0	27,27,45	1.19	2 (7%)
14	HEA	N	601	1	67,67,67	1.64	17 (25%)	81,103,103	2.21	25 (30%)
20	DMU	M	101	-	34,34,34	1.06	2 (5%)	45,45,45	0.97	2 (4%)
19	LFA	C	312	-	10,10,19	0.23	0	9,9,18	0.25	0
20	DMU	P	307	-	10,10,34	0.27	0	9,9,45	0.68	0
19	LFA	P	308	-	10,10,19	0.24	0	9,9,18	0.21	0
24	CHD	C	301	-	32,32,32	1.13	3 (9%)	51,51,51	0.83	2 (3%)
19	LFA	A	607	-	13,13,19	0.42	0	12,12,18	0.19	0
19	LFA	P	315	-	12,12,19	0.19	0	11,11,18	0.22	0
21	EDO	N	610	-	3,3,3	0.14	0	2,2,2	0.38	0
20	DMU	N	608	-	34,34,34	1.35	4 (11%)	45,45,45	1.26	5 (11%)
14	HEA	A	602	1	67,67,67	1.80	21 (31%)	81,103,103	2.32	29 (35%)
20	DMU	N	607	-	6,6,34	0.43	0	5,5,45	0.33	0
20	DMU	B	308	-	22,22,34	0.50	0	27,27,45	1.35	3 (11%)
20	DMU	C	317	-	22,22,34	0.68	1 (4%)	27,27,45	1.43	3 (11%)
24	CHD	B	306	-	32,32,32	0.78	1 (3%)	51,51,51	0.75	0
21	EDO	G	105	-	3,3,3	0.52	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	DMU	T	104	-	22,22,34	0.69	0	27,27,45	1.41	3 (11%)
21	EDO	F	101	-	3,3,3	0.33	0	2,2,2	0.15	0
27	PEK	G	101	-	52,52,52	0.66	1 (1%)	55,57,57	0.67	1 (1%)
20	DMU	P	319	-	34,34,34	0.83	2 (5%)	45,45,45	1.17	4 (8%)
19	LFA	C	309	-	17,17,19	0.25	0	16,16,18	0.19	0
19	LFA	P	301	-	14,14,19	0.13	0	13,13,18	0.11	0
20	DMU	B	303	-	10,10,34	0.29	0	9,9,45	0.56	0
19	LFA	B	307	-	16,16,19	0.29	0	15,15,18	0.18	0
23	CUA	B	301	2	0,1,1	-	-	-		
22	PGV	C	303	-	50,50,50	0.65	0	53,56,56	1.08	3 (5%)
19	LFA	C	313	-	14,14,19	0.21	0	13,13,18	0.41	0
19	LFA	G	106	-	13,13,19	0.58	0	12,12,18	0.40	0
21	EDO	E	202	-	3,3,3	0.24	0	2,2,2	0.17	0
19	LFA	T	103	-	10,10,19	0.22	0	9,9,18	0.24	0
19	LFA	C	311	-	13,13,19	0.23	0	12,12,18	0.10	0
22	PGV	P	304	-	50,50,50	0.72	0	53,56,56	1.04	4 (7%)
20	DMU	O	303	-	22,22,34	0.68	1 (4%)	27,27,45	1.55	4 (14%)
20	DMU	C	323	-	34,34,34	0.81	0	45,45,45	1.16	3 (6%)
21	EDO	P	322	-	3,3,3	0.39	0	2,2,2	0.15	0
21	EDO	N	611	-	3,3,3	0.64	0	2,2,2	0.31	0
21	EDO	O	308	-	3,3,3	0.10	0	2,2,2	0.35	0
21	EDO	F	103	-	3,3,3	0.49	0	2,2,2	0.16	0
20	DMU	B	302	-	10,10,34	0.21	0	9,9,45	0.66	0
21	EDO	A	611	-	3,3,3	0.17	0	2,2,2	0.26	0
20	DMU	M	102	-	7,7,34	0.36	0	6,6,45	0.45	0
19	LFA	O	301	-	16,16,19	0.19	0	15,15,18	0.17	0
20	DMU	P	324	-	34,34,34	0.64	0	45,45,45	1.42	4 (8%)
21	EDO	C	322	-	3,3,3	0.88	0	2,2,2	0.82	0
21	EDO	E	203	-	3,3,3	0.11	0	2,2,2	0.06	0
24	CHD	C	305	-	32,32,32	0.63	0	51,51,51	1.40	7 (13%)
21	EDO	E	201	-	3,3,3	0.17	0	2,2,2	0.12	0
14	HEA	A	601	1	67,67,67	1.69	13 (19%)	81,103,103	2.15	24 (29%)
19	LFA	P	309	-	5,5,19	0.21	0	4,4,18	0.10	0
20	DMU	A	609	-	34,34,34	1.18	4 (11%)	45,45,45	1.34	8 (17%)
21	EDO	N	613	-	3,3,3	0.66	0	2,2,2	0.02	0
19	LFA	C	307	-	10,10,19	0.25	0	9,9,18	0.25	0
14	HEA	N	602	1	67,67,67	1.83	20 (29%)	81,103,103	2.53	30 (37%)
20	DMU	C	306	-	10,10,34	0.41	0	9,9,45	0.55	0
21	EDO	A	610	-	3,3,3	0.61	0	2,2,2	0.58	0
20	DMU	A	614	-	10,10,34	0.35	0	9,9,45	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	LFA	P	311	-	10,10,19	0.14	0	9,9,18	0.10	0
20	DMU	N	615	-	34,34,34	0.90	1 (2%)	45,45,45	1.39	5 (11%)
22	PGV	N	614	-	50,50,50	0.75	1 (2%)	53,56,56	1.20	2 (3%)
24	CHD	P	306	-	32,32,32	0.69	0	51,51,51	1.38	8 (15%)
20	DMU	O	306	-	10,10,34	0.34	0	9,9,45	0.55	0
21	EDO	S	102	-	3,3,3	0.38	0	2,2,2	0.47	0
20	DMU	A	608	-	6,6,34	0.53	0	5,5,45	0.34	0
21	EDO	N	612	-	3,3,3	0.27	0	2,2,2	0.22	0
21	EDO	T	105	-	3,3,3	0.38	0	2,2,2	0.17	0
21	EDO	P	321	-	3,3,3	0.19	0	2,2,2	0.08	0
21	EDO	C	321	-	3,3,3	0.33	0	2,2,2	0.16	0
21	EDO	C	320	-	3,3,3	0.15	0	2,2,2	0.11	0
20	DMU	Z	101	-	34,34,34	1.08	2 (5%)	45,45,45	1.13	3 (6%)
21	EDO	S	103	-	3,3,3	0.19	0	2,2,2	0.23	0
24	CHD	P	302	-	32,32,32	0.99	2 (6%)	51,51,51	0.78	1 (1%)
18	CDL	L	101	-	93,93,99	0.45	0	99,105,111	0.55	1 (1%)
20	DMU	C	318	-	34,34,34	0.92	3 (8%)	45,45,45	1.22	3 (6%)
19	LFA	P	312	-	13,13,19	0.14	0	12,12,18	0.10	0
19	LFA	P	314	-	14,14,19	0.44	0	13,13,18	0.25	0
20	DMU	P	317	-	6,6,34	0.28	0	5,5,45	0.49	0
18	CDL	A	606	-	63,63,99	0.45	0	69,75,111	0.94	3 (4%)
19	LFA	P	310	-	17,17,19	0.22	0	16,16,18	0.14	0
18	CDL	V	101	-	63,63,99	0.44	0	69,75,111	0.88	4 (5%)
20	DMU	P	318	-	22,22,34	0.88	1 (4%)	27,27,45	1.40	3 (11%)
20	DMU	H	101	-	34,34,34	1.12	5 (14%)	45,45,45	1.45	8 (17%)
20	DMU	P	316	-	34,34,34	0.93	2 (5%)	45,45,45	1.70	8 (17%)
20	DMU	J	101	-	10,10,34	0.17	0	9,9,45	0.60	0
21	EDO	R	203	-	3,3,3	0.20	0	2,2,2	0.24	0
20	DMU	C	319	-	34,34,34	0.68	0	45,45,45	1.35	5 (11%)
20	DMU	P	320	-	34,34,34	0.86	2 (5%)	45,45,45	1.19	4 (8%)
19	LFA	T	101	-	13,13,19	0.75	0	12,12,18	0.49	0
21	EDO	B	305	-	3,3,3	0.10	0	2,2,2	0.22	0
21	EDO	P	323	-	3,3,3	0.43	0	2,2,2	0.74	0
18	CDL	C	304	-	86,86,99	0.55	0	92,98,111	1.17	10 (10%)
20	DMU	Z	102	-	7,7,34	0.27	0	6,6,45	0.68	0
20	DMU	W	101	-	10,10,34	0.20	0	9,9,45	0.59	0
20	DMU	G	104	-	22,22,34	0.81	1 (4%)	27,27,45	0.98	1 (3%)
19	LFA	N	606	-	13,13,19	0.31	0	12,12,18	0.50	0
20	DMU	B	304	-	22,22,34	0.90	1 (4%)	27,27,45	1.06	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PGV	A	613	-	50,50,50	0.68	0	53,56,56	1.06	2 (3%)
21	EDO	N	609	-	3,3,3	0.51	0	2,2,2	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	C	315	-	-	11/19/59/59	0/2/2/2
20	DMU	C	316	-	-	3/4/4/59	-
18	CDL	P	305	-	-	53/97/97/110	-
19	LFA	P	313	-	-	5/8/8/17	-
20	DMU	D	201	-	-	8/19/59/59	0/2/2/2
18	CDL	Y	101	-	-	51/104/104/110	-
20	DMU	L	102	-	-	9/13/33/59	0/1/1/2
20	DMU	O	305	-	-	5/8/8/59	-
27	PEK	T	102	-	-	19/56/56/56	-
21	EDO	F	104	-	-	0/1/1/1	-
20	DMU	O	307	-	-	4/13/33/59	0/1/1/2
19	LFA	C	310	-	-	6/8/8/17	-
19	LFA	C	308	-	-	1/3/3/17	-
19	LFA	C	314	-	-	3/10/10/17	-
19	LFA	O	302	-	-	4/8/8/17	-
20	DMU	G	103	-	-	4/8/8/59	-
21	EDO	A	612	-	-	0/1/1/1	-
24	CHD	G	102	-	-	2/9/74/74	0/4/4/4
19	LFA	C	324	-	-	8/12/12/17	-
20	DMU	Q	201	-	-	8/19/59/59	0/2/2/2
21	EDO	R	201	-	-	1/1/1/1	-
21	EDO	R	202	-	-	0/1/1/1	-
20	DMU	Y	102	-	-	10/13/33/59	0/1/1/2
14	HEA	N	601	1	-	3/36/76/76	-
20	DMU	M	101	-	-	5/19/59/59	0/2/2/2
19	LFA	C	312	-	-	3/8/8/17	-
20	DMU	P	307	-	-	4/8/8/59	-
19	LFA	P	308	-	-	4/8/8/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
19	LFA	A	607	-	-	4/11/11/17	-
19	LFA	P	315	-	-	5/10/10/17	-
21	EDO	N	610	-	-	0/1/1/1	-
20	DMU	N	608	-	-	6/19/59/59	0/2/2/2
14	HEA	A	602	1	-	6/36/76/76	-
20	DMU	N	607	-	-	1/4/4/59	-
20	DMU	B	308	-	-	9/13/33/59	0/1/1/2
20	DMU	C	317	-	-	8/13/33/59	0/1/1/2
24	CHD	B	306	-	-	2/9/74/74	0/4/4/4
21	EDO	G	105	-	-	0/1/1/1	-
20	DMU	T	104	-	-	7/13/33/59	0/1/1/2
21	EDO	F	101	-	-	0/1/1/1	-
27	PEK	G	101	-	-	13/56/56/56	-
20	DMU	P	319	-	-	14/19/59/59	0/2/2/2
19	LFA	C	309	-	-	11/15/15/17	-
19	LFA	P	301	-	-	7/12/12/17	-
20	DMU	B	303	-	-	5/8/8/59	-
19	LFA	B	307	-	-	9/14/14/17	-
22	PGV	C	303	-	-	14/55/55/55	-
19	LFA	C	313	-	-	3/12/12/17	-
19	LFA	G	106	-	-	5/11/11/17	-
21	EDO	E	202	-	-	0/1/1/1	-
19	LFA	T	103	-	-	4/8/8/17	-
19	LFA	C	311	-	-	5/11/11/17	-
22	PGV	P	304	-	-	8/55/55/55	-
20	DMU	O	303	-	-	4/13/33/59	0/1/1/2
20	DMU	C	323	-	-	4/19/59/59	0/2/2/2
21	EDO	P	322	-	-	0/1/1/1	-
21	EDO	N	611	-	-	0/1/1/1	-
21	EDO	O	308	-	-	0/1/1/1	-
21	EDO	F	103	-	-	0/1/1/1	-
20	DMU	B	302	-	-	3/8/8/59	-
21	EDO	A	611	-	-	1/1/1/1	-
20	DMU	M	102	-	-	3/5/5/59	-
19	LFA	O	301	-	-	7/14/14/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	P	324	-	-	7/19/59/59	0/2/2/2
21	EDO	C	322	-	-	1/1/1/1	-
21	EDO	E	203	-	-	0/1/1/1	-
24	CHD	C	305	-	-	8/9/74/74	0/4/4/4
21	EDO	E	201	-	-	0/1/1/1	-
14	HEA	A	601	1	-	4/36/76/76	-
19	LFA	P	309	-	-	1/3/3/17	-
20	DMU	A	609	-	-	6/19/59/59	0/2/2/2
21	EDO	N	613	-	-	0/1/1/1	-
19	LFA	C	307	-	-	6/8/8/17	-
14	HEA	N	602	1	-	5/36/76/76	-
20	DMU	C	306	-	-	2/8/8/59	-
21	EDO	A	610	-	-	0/1/1/1	-
20	DMU	A	614	-	-	3/8/8/59	-
19	LFA	P	311	-	-	6/8/8/17	-
20	DMU	N	615	-	-	8/19/59/59	0/2/2/2
22	PGV	N	614	-	-	9/55/55/55	-
24	CHD	P	306	-	-	8/9/74/74	0/4/4/4
20	DMU	O	306	-	-	4/8/8/59	-
21	EDO	S	102	-	-	0/1/1/1	-
20	DMU	A	608	-	-	3/4/4/59	-
21	EDO	N	612	-	-	1/1/1/1	-
21	EDO	T	105	-	-	0/1/1/1	-
21	EDO	P	321	-	-	1/1/1/1	-
21	EDO	C	321	-	-	0/1/1/1	-
21	EDO	C	320	-	-	0/1/1/1	-
20	DMU	Z	101	-	-	8/19/59/59	0/2/2/2
21	EDO	S	103	-	-	0/1/1/1	-
24	CHD	P	302	-	-	2/9/74/74	0/4/4/4
18	CDL	L	101	-	-	46/104/104/110	-
20	DMU	C	318	-	-	11/19/59/59	0/2/2/2
19	LFA	P	312	-	-	7/11/11/17	-
19	LFA	P	314	-	-	5/12/12/17	-
20	DMU	P	317	-	-	2/4/4/59	-
18	CDL	A	606	-	-	33/74/74/110	-
19	LFA	P	310	-	-	10/15/15/17	-
18	CDL	V	101	-	-	45/74/74/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	P	318	-	-	8/13/33/59	0/1/1/2
20	DMU	H	101	-	-	9/19/59/59	0/2/2/2
20	DMU	P	316	-	-	8/19/59/59	0/2/2/2
20	DMU	J	101	-	-	4/8/8/59	-
21	EDO	R	203	-	-	0/1/1/1	-
20	DMU	C	319	-	-	11/19/59/59	0/2/2/2
20	DMU	P	320	-	-	8/19/59/59	0/2/2/2
19	LFA	T	101	-	-	5/11/11/17	-
21	EDO	B	305	-	-	0/1/1/1	-
21	EDO	P	323	-	-	0/1/1/1	-
18	CDL	C	304	-	-	45/97/97/110	-
20	DMU	Z	102	-	-	2/5/5/59	-
20	DMU	W	101	-	-	4/8/8/59	-
20	DMU	G	104	-	-	5/13/33/59	0/1/1/2
19	LFA	N	606	-	-	4/11/11/17	-
20	DMU	B	304	-	-	8/13/33/59	0/1/1/2
22	PGV	A	613	-	-	12/55/55/55	-
21	EDO	N	609	-	-	0/1/1/1	-

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	CHB-C4A	5.23	1.48	1.38
14	A	601	HEA	C3A-C2A	4.10	1.46	1.37
20	N	608	DMU	O16-C6	-4.07	1.33	1.40
14	A	601	HEA	C4B-NB	-3.95	1.33	1.40
14	N	601	HEA	C1D-ND	-3.94	1.33	1.40
14	N	602	HEA	C3D-C2D	3.93	1.45	1.36
14	N	602	HEA	C1A-C2A	3.92	1.52	1.45
14	A	602	HEA	C3B-C2B	3.84	1.43	1.34
20	D	201	DMU	O49-C1	-3.84	1.33	1.43
20	Z	101	DMU	O3-C5	-3.74	1.33	1.43
14	A	602	HEA	CHD-C1D	3.70	1.45	1.38
14	A	601	HEA	C3D-C2D	3.64	1.44	1.36
14	N	601	HEA	C4D-ND	-3.63	1.31	1.38
14	N	602	HEA	C3B-C2B	3.58	1.42	1.34
20	A	609	DMU	O7-C10	3.53	1.51	1.41
24	C	301	CHD	O26-C24	-3.46	1.19	1.30
27	G	101	PEK	C23-C22	-3.44	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	601	HEA	C3A-C2A	3.40	1.44	1.37
24	P	302	CHD	O26-C24	-3.37	1.19	1.30
14	N	602	HEA	C1C-NC	-3.34	1.33	1.39
20	P	318	DMU	O16-C6	3.33	1.45	1.40
14	A	601	HEA	C1B-NB	-3.31	1.32	1.38
14	N	602	HEA	FE-NC	3.29	2.06	1.95
14	A	602	HEA	C1D-ND	-3.27	1.34	1.40
20	H	101	DMU	O5-C6	-3.26	1.33	1.41
14	A	602	HEA	C4D-ND	-3.21	1.32	1.38
14	A	602	HEA	CBD-CAD	-3.20	1.40	1.51
14	A	602	HEA	C3D-C2D	3.20	1.43	1.36
14	A	601	HEA	C1D-ND	-3.20	1.34	1.40
14	A	602	HEA	CHB-C4A	3.16	1.44	1.38
14	N	601	HEA	C16-C17	-3.16	1.43	1.53
14	A	601	HEA	C12-C11	-3.15	1.47	1.53
14	N	601	HEA	CHB-C4A	3.15	1.44	1.38
14	A	602	HEA	C1C-NC	-3.14	1.33	1.39
14	A	602	HEA	C3A-C2A	3.12	1.44	1.37
14	A	602	HEA	FE-NC	3.11	2.05	1.95
14	A	601	HEA	CHB-C4A	3.04	1.44	1.38
14	N	602	HEA	C1D-ND	-3.04	1.35	1.40
24	P	302	CHD	C22-C23	-3.03	1.43	1.52
14	N	602	HEA	CHC-C4B	3.02	1.44	1.38
24	C	301	CHD	C22-C23	-3.01	1.43	1.52
20	P	320	DMU	C7-C5	-2.92	1.44	1.52
20	N	608	DMU	C7-C5	-2.90	1.44	1.52
14	N	601	HEA	FE-NC	2.90	2.04	1.95
27	T	102	PEK	C2-C1	2.87	1.59	1.50
27	T	102	PEK	C23-C22	-2.85	1.41	1.52
14	A	601	HEA	CHA-C1A	2.83	1.43	1.38
20	P	319	DMU	O3-C5	2.83	1.50	1.43
24	C	301	CHD	O25-C24	2.82	1.31	1.22
14	A	602	HEA	C1B-NB	-2.82	1.33	1.38
20	H	101	DMU	O16-C6	-2.82	1.35	1.40
20	N	608	DMU	C10-C5	-2.81	1.44	1.52
14	A	601	HEA	C16-C17	-2.81	1.44	1.53
14	A	602	HEA	CHA-C1A	2.80	1.43	1.38
14	N	602	HEA	C3A-C2A	2.79	1.43	1.37
14	N	601	HEA	C4C-NC	-2.78	1.34	1.39
20	D	201	DMU	O3-C5	-2.78	1.36	1.43
20	D	201	DMU	O61-C57	2.75	1.54	1.42
20	Q	201	DMU	C10-C5	-2.75	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	CMA-C3A	2.73	1.51	1.45
20	D	201	DMU	O55-C2	2.71	1.49	1.43
14	N	601	HEA	C1B-NB	-2.71	1.33	1.38
20	D	201	DMU	O5-C6	-2.71	1.34	1.41
14	N	601	HEA	C3B-C2B	2.70	1.40	1.34
20	Q	201	DMU	O16-C6	-2.70	1.35	1.40
14	A	602	HEA	C4C-NC	-2.68	1.34	1.39
14	N	602	HEA	C4D-ND	-2.67	1.33	1.38
20	M	101	DMU	O3-C5	-2.65	1.36	1.43
14	N	602	HEA	C1C-C2C	2.65	1.49	1.43
14	N	601	HEA	FE-ND	2.65	2.03	1.94
14	N	602	HEA	CHD-C1D	2.64	1.43	1.38
20	P	316	DMU	O1-C10	2.63	1.48	1.41
14	A	602	HEA	C1C-C2C	2.59	1.49	1.43
14	A	602	HEA	FE-NB	2.56	2.02	1.94
14	A	602	HEA	FE-ND	2.54	2.02	1.94
20	C	318	DMU	C7-C5	-2.53	1.45	1.52
14	A	601	HEA	FE-ND	2.53	2.02	1.94
20	N	615	DMU	C7-C5	-2.50	1.45	1.52
14	N	602	HEA	C3C-C4C	2.49	1.50	1.42
20	A	609	DMU	O7-C3	2.49	1.50	1.43
14	N	602	HEA	C1B-NB	-2.47	1.34	1.38
14	A	602	HEA	C3C-C4C	2.45	1.49	1.42
20	D	201	DMU	C10-C5	-2.44	1.45	1.52
20	P	320	DMU	C10-C5	-2.44	1.45	1.52
20	C	318	DMU	O5-C6	-2.42	1.35	1.41
14	N	602	HEA	C4C-NC	-2.41	1.35	1.39
14	N	602	HEA	FE-ND	2.41	2.02	1.94
14	A	602	HEA	O1A-CGA	2.37	1.29	1.22
20	N	608	DMU	O1-C10	2.37	1.47	1.41
14	A	602	HEA	CHC-C4B	2.37	1.43	1.38
20	C	315	DMU	O5-C6	-2.36	1.35	1.41
14	A	602	HEA	CHC-C1C	2.35	1.44	1.39
14	A	601	HEA	CHD-C1D	2.32	1.43	1.38
20	Z	101	DMU	C10-C5	-2.32	1.45	1.52
14	N	601	HEA	CHC-C4B	2.30	1.43	1.38
20	A	609	DMU	O16-C6	-2.29	1.36	1.40
20	A	609	DMU	O3-C5	-2.29	1.37	1.43
14	N	601	HEA	C4B-NB	-2.25	1.36	1.40
20	H	101	DMU	C10-C5	-2.25	1.45	1.52
20	O	307	DMU	C6-C1	-2.24	1.46	1.52
20	P	316	DMU	O5-C6	-2.22	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	P	319	DMU	C7-C5	-2.21	1.46	1.52
14	N	601	HEA	C12-C13	2.20	1.60	1.53
20	C	318	DMU	O3-C5	2.20	1.48	1.43
14	A	601	HEA	FE-NB	2.18	2.01	1.94
20	C	317	DMU	O16-C6	2.18	1.43	1.40
14	A	601	HEA	C3B-C2B	2.14	1.39	1.34
14	N	601	HEA	C26-C15	-2.14	1.45	1.50
14	N	601	HEA	C11-C3B	-2.13	1.48	1.51
14	A	602	HEA	C1A-C2A	2.11	1.48	1.45
14	N	601	HEA	O11-C11	2.10	1.47	1.42
20	Q	201	DMU	O3-C5	-2.10	1.37	1.43
14	N	602	HEA	CHA-C1A	2.09	1.42	1.38
20	H	101	DMU	C7-C5	-2.09	1.46	1.52
20	Q	201	DMU	O55-C2	2.09	1.48	1.43
14	N	601	HEA	C3D-C2D	2.08	1.41	1.36
20	D	201	DMU	C7-C5	-2.08	1.46	1.52
24	B	306	CHD	O26-C24	-2.07	1.24	1.30
22	N	614	PGV	O01-C1	2.07	1.40	1.34
14	N	602	HEA	CBD-CAD	-2.07	1.44	1.51
14	N	602	HEA	C11-C3B	-2.05	1.48	1.51
20	B	304	DMU	O16-C6	2.04	1.43	1.40
20	O	303	DMU	C3-C4	-2.04	1.48	1.53
20	M	101	DMU	C6-C1	-2.03	1.46	1.52
20	G	104	DMU	C6-C1	-2.02	1.46	1.52
20	H	101	DMU	O2-C8	2.01	1.47	1.43
20	Q	201	DMU	O49-C1	-2.00	1.38	1.43

All (273) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	C3D-C4D-ND	8.29	118.37	110.35
20	P	316	DMU	O16-C6-C1	7.36	119.45	108.27
14	N	601	HEA	C3C-C4C-NC	6.99	115.68	109.80
14	N	602	HEA	C3D-C4D-ND	6.95	117.07	110.35
14	A	602	HEA	C2B-C1B-NB	6.79	117.75	109.90
14	N	602	HEA	C2B-C1B-NB	6.39	117.30	109.90
20	Q	201	DMU	O16-C6-C1	6.28	117.81	108.27
14	N	602	HEA	C3C-C4C-NC	6.26	115.07	109.80
14	A	602	HEA	C3D-C4D-ND	6.22	116.36	110.35
20	D	201	DMU	O16-C6-C1	6.14	117.59	108.27
14	N	601	HEA	C13-C12-C11	-6.02	104.77	114.39
14	A	601	HEA	C13-C12-C11	-5.96	104.88	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	CHB-C1B-C2B	-5.65	116.11	125.03
20	C	315	DMU	O16-C6-C1	5.49	116.62	108.27
14	A	601	HEA	C3C-C4C-NC	5.48	114.42	109.80
14	N	601	HEA	C2B-C1B-NB	5.36	116.09	109.90
14	A	601	HEA	CHA-C4D-C3D	-5.34	116.99	124.77
20	H	101	DMU	O16-C6-C1	5.34	116.38	108.27
14	N	601	HEA	C3D-C4D-ND	5.28	115.45	110.35
20	O	303	DMU	O5-C6-C1	5.19	121.03	110.37
14	N	602	HEA	C2D-C1D-ND	5.12	115.73	109.84
14	A	602	HEA	C2D-C1D-ND	5.11	115.72	109.84
27	T	102	PEK	O01-C1-O02	-5.11	111.76	123.70
14	N	602	HEA	C3B-C4B-NB	5.10	115.70	109.84
20	P	324	DMU	C10-C5-C7	5.06	120.66	110.01
20	T	104	DMU	O16-C6-C1	4.85	115.63	108.27
20	P	318	DMU	O5-C6-C1	4.78	120.19	110.37
24	P	306	CHD	C17-C13-C14	-4.78	95.32	100.11
14	A	602	HEA	C3C-C4C-NC	4.74	113.79	109.80
18	A	606	CDL	CA4-OA6-CA5	4.69	129.02	117.80
20	P	320	DMU	O16-C6-C1	4.68	115.38	108.27
20	Z	101	DMU	O16-C6-C1	4.67	115.36	108.27
20	C	317	DMU	O5-C6-C1	4.65	119.92	110.37
14	N	602	HEA	CHA-C4D-C3D	-4.49	118.23	124.77
20	P	324	DMU	O16-C6-C1	4.41	114.97	108.27
14	A	602	HEA	C3B-C4B-NB	4.41	114.90	109.84
14	A	602	HEA	CHA-C4D-C3D	-4.38	118.38	124.77
14	N	601	HEA	C4D-C3D-C2D	-4.29	100.65	106.89
20	N	615	DMU	O16-C6-C1	4.24	114.71	108.27
14	N	602	HEA	CAD-C3D-C4D	4.24	132.08	124.70
18	C	304	CDL	OA4-PA1-OA5	-4.22	88.43	107.57
14	A	602	HEA	CMD-C2D-C1D	4.16	131.54	125.03
18	C	304	CDL	OA6-CA5-C11	-4.14	102.52	111.48
14	A	601	HEA	C4D-C3D-C2D	-4.13	100.89	106.89
20	C	323	DMU	O16-C6-C1	4.10	114.50	108.27
14	N	602	HEA	C2C-C1C-NC	4.09	116.70	110.14
20	C	318	DMU	O16-C6-C1	4.06	114.44	108.27
14	N	602	HEA	C3A-C2A-C1A	-4.03	103.23	107.05
18	C	304	CDL	OA5-PA1-OA3	3.99	124.75	108.94
22	N	614	PGV	O03-C19-O04	-3.98	113.68	123.63
24	C	305	CHD	C5-C6-C7	3.96	119.10	114.40
14	N	602	HEA	CMD-C2D-C1D	3.95	131.21	125.03
14	N	602	HEA	C4B-NB-C1B	-3.93	100.55	105.21
14	N	602	HEA	C3C-C2C-C1C	-3.92	102.55	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601	HEA	CHB-C1B-C2B	-3.90	118.87	125.03
14	N	601	HEA	C3C-C2C-C1C	-3.84	102.64	107.17
14	A	601	HEA	C3C-C2C-C1C	-3.84	102.64	107.17
22	A	613	PGV	O03-C19-O04	-3.83	114.04	123.63
14	N	601	HEA	C2A-C1A-NA	3.83	114.02	110.32
20	N	615	DMU	C10-C5-C7	3.80	118.01	110.01
20	N	608	DMU	C10-O1-C9	3.79	121.12	113.72
14	N	601	HEA	C2C-C1C-NC	3.73	116.12	110.14
14	A	602	HEA	C3C-C2C-C1C	-3.72	102.78	107.17
18	A	606	CDL	OA6-CA4-CA6	3.71	121.65	108.34
14	A	602	HEA	C4B-NB-C1B	-3.68	100.84	105.21
14	N	602	HEA	C1D-C2D-C3D	-3.68	103.11	106.98
22	C	303	PGV	O03-C19-O04	-3.63	114.56	123.63
20	B	308	DMU	O16-C6-C1	3.62	113.77	108.27
18	V	101	CDL	OA6-CA5-C11	3.60	119.28	111.48
14	A	601	HEA	C3B-C4B-NB	3.60	113.98	109.84
20	C	319	DMU	O16-C6-C1	3.60	113.74	108.27
24	C	305	CHD	C6-C7-C8	3.58	115.41	111.50
18	C	304	CDL	OA4-PA1-OA3	3.55	128.96	112.44
14	A	601	HEA	C2C-C1C-NC	3.55	115.83	110.14
14	N	601	HEA	C3B-C4B-NB	3.53	113.89	109.84
20	P	319	DMU	O16-C6-C1	3.52	113.61	108.27
24	C	305	CHD	C17-C13-C14	-3.49	96.61	100.11
20	C	318	DMU	C10-C5-C7	3.49	117.35	110.01
20	B	308	DMU	O5-C6-C1	3.47	117.49	110.37
14	A	602	HEA	C4D-C3D-C2D	-3.46	101.85	106.89
24	P	306	CHD	C16-C17-C20	3.46	117.41	112.18
20	L	102	DMU	O5-C6-O16	3.44	118.18	110.04
14	A	601	HEA	CAD-C3D-C4D	3.43	130.67	124.70
14	A	602	HEA	C2C-C1C-NC	3.40	115.59	110.14
27	T	102	PEK	O02-C1-C2	3.38	137.01	123.78
20	A	609	DMU	O3-C5-C7	3.38	118.34	110.38
14	N	602	HEA	C4D-C3D-C2D	-3.37	101.98	106.89
20	Y	102	DMU	O5-C6-O16	3.37	118.01	110.04
20	C	317	DMU	C18-O16-C6	-3.36	107.95	113.68
24	C	305	CHD	C14-C13-C12	3.30	110.43	107.42
24	C	305	CHD	C16-C17-C20	3.29	117.16	112.18
20	M	101	DMU	O16-C6-C1	3.27	113.24	108.27
14	N	602	HEA	C4A-CHB-C1B	-3.26	119.09	126.02
14	A	602	HEA	CMB-C2B-C1B	3.26	130.12	125.03
18	V	101	CDL	OA6-CA4-CA3	3.26	120.03	108.34
20	O	303	DMU	O16-C6-C1	3.24	113.20	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	C1B-C2B-C3B	-3.22	103.07	106.80
20	P	316	DMU	C10-C5-C7	3.22	116.78	110.01
20	T	104	DMU	C18-O16-C6	-3.18	108.25	113.68
22	P	304	PGV	C27-C26-C25	-3.17	98.32	114.37
14	A	601	HEA	C26-C15-C16	3.16	120.72	115.23
20	P	320	DMU	C10-C5-C7	3.15	116.64	110.01
18	C	304	CDL	OA7-CA5-C11	3.15	136.10	123.78
14	A	602	HEA	CHB-C1B-C2B	-3.14	120.07	125.03
20	C	319	DMU	C10-C5-C7	3.13	116.59	110.01
14	N	601	HEA	C26-C15-C16	3.12	120.65	115.23
14	A	602	HEA	C1D-C2D-C3D	-3.11	103.71	106.98
14	N	601	HEA	CHA-C4D-C3D	-3.11	120.24	124.77
14	N	601	HEA	O11-C11-C3B	-3.10	105.57	111.26
20	P	319	DMU	C10-C5-C7	3.10	116.53	110.01
20	Q	201	DMU	C6-O5-C4	-3.07	107.73	113.72
14	N	601	HEA	C3A-C2A-C1A	-3.05	104.16	107.05
20	Q	201	DMU	C10-O1-C9	3.04	119.66	113.72
20	A	609	DMU	O1-C10-C5	-3.04	104.13	110.37
14	N	602	HEA	CHC-C1C-C2C	-3.01	118.69	127.43
14	N	601	HEA	C4C-C3C-C2C	-3.01	103.56	107.30
20	Q	201	DMU	O1-C9-C8	2.97	115.05	109.70
14	N	602	HEA	C4C-C3C-C2C	-2.94	103.65	107.30
14	A	602	HEA	CHC-C1C-C2C	-2.91	118.97	127.43
14	A	601	HEA	C2D-C1D-ND	2.91	113.19	109.84
20	H	101	DMU	C7-C8-C9	-2.89	104.98	110.23
18	P	305	CDL	OA4-PA1-OA2	-2.89	94.48	107.57
20	P	316	DMU	O5-C6-O16	-2.86	103.28	110.04
14	A	601	HEA	CHB-C1B-C2B	-2.86	120.52	125.03
20	P	316	DMU	O1-C9-C11	2.85	113.50	106.44
20	H	101	DMU	C18-O16-C6	-2.81	108.88	113.68
20	Q	201	DMU	C11-C9-C8	-2.80	106.15	113.02
14	A	602	HEA	O1D-CGD-CBD	-2.79	114.24	123.09
24	P	306	CHD	C14-C13-C12	2.79	109.96	107.42
14	N	602	HEA	C1B-C2B-C3B	-2.78	103.58	106.80
20	D	201	DMU	C10-O1-C9	2.77	119.13	113.72
20	N	615	DMU	C10-O7-C3	-2.77	111.42	117.98
14	A	601	HEA	C3A-C2A-C1A	-2.76	104.43	107.05
20	H	101	DMU	O5-C6-C1	2.76	116.03	110.37
20	N	615	DMU	O3-C5-C10	2.76	116.64	110.08
20	G	104	DMU	O16-C6-C1	2.75	112.45	108.27
18	V	101	CDL	OA6-CA4-CA6	-2.74	98.50	108.34
14	A	601	HEA	CHC-C1C-C2C	-2.73	119.51	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	C1D-ND-C4D	-2.73	101.98	105.21
14	N	602	HEA	C4B-C3B-C2B	-2.72	102.87	107.44
20	P	316	DMU	O7-C3-C2	2.71	114.13	107.23
20	A	609	DMU	O5-C6-O16	2.70	116.43	110.04
20	B	304	DMU	O5-C6-C1	2.70	115.91	110.37
20	C	317	DMU	C6-C1-C2	2.69	115.68	110.01
22	P	304	PGV	C22-C21-C20	-2.68	103.27	113.13
14	N	602	HEA	CMB-C2B-C1B	2.68	129.22	125.03
18	P	305	CDL	OA5-PA1-OA3	2.66	119.50	108.94
18	C	304	CDL	OA4-PA1-OA2	-2.66	95.49	107.57
14	A	601	HEA	C2B-C1B-NB	2.65	112.96	109.90
14	N	601	HEA	C1B-C2B-C3B	-2.65	103.73	106.80
20	P	316	DMU	C57-C4-C3	-2.63	105.98	113.38
14	A	602	HEA	C3A-C2A-C1A	-2.63	104.56	107.05
20	Y	102	DMU	O5-C6-C1	2.63	115.77	110.37
20	N	615	DMU	C18-O16-C6	-2.63	109.20	113.68
20	P	318	DMU	C6-C1-C2	2.62	115.53	110.01
20	M	101	DMU	O3-C5-C7	2.62	116.56	110.38
20	P	324	DMU	C10-O1-C9	-2.62	108.61	113.72
20	C	319	DMU	O3-C5-C10	2.61	116.30	110.08
20	B	308	DMU	C6-O5-C4	2.60	118.80	113.72
14	N	601	HEA	O11-C11-C12	2.60	116.03	109.14
20	C	315	DMU	C6-O5-C4	2.59	118.79	113.72
20	P	318	DMU	C18-O16-C6	-2.59	109.25	113.68
20	O	307	DMU	O5-C6-C1	2.58	115.67	110.37
20	C	319	DMU	O5-C6-C1	2.57	115.64	110.37
22	C	303	PGV	C24-C23-C22	2.56	127.31	114.37
18	C	304	CDL	OB6-CB5-C51	2.55	117.00	111.48
20	H	101	DMU	C10-C5-C7	2.55	115.37	110.01
14	A	601	HEA	C1D-ND-C4D	-2.55	102.19	105.21
20	C	315	DMU	C10-C5-C7	2.54	115.36	110.01
20	P	319	DMU	O3-C5-C10	2.54	116.13	110.08
20	D	201	DMU	C10-C5-C7	2.54	115.35	110.01
27	T	102	PEK	C2-C3-C4	2.54	118.89	113.35
14	N	602	HEA	CAD-CBD-CGD	-2.52	106.98	113.67
20	C	315	DMU	O3-C5-C10	2.50	116.04	110.08
20	O	303	DMU	C6-C1-C2	2.50	115.27	110.01
20	N	608	DMU	C7-C8-C9	2.49	114.74	110.23
18	C	304	CDL	O1-C1-CB2	2.48	118.25	109.70
14	N	602	HEA	C21-C20-C19	2.48	121.39	113.19
20	P	320	DMU	O5-C6-C1	2.47	115.45	110.37
14	A	601	HEA	C13-C14-C15	-2.47	121.97	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	C4A-C3A-C2A	-2.46	104.68	106.81
14	N	601	HEA	C4C-NC-C1C	-2.46	101.81	105.82
20	H	101	DMU	C2-C3-C4	-2.46	105.48	110.93
20	N	608	DMU	O5-C6-C1	2.46	115.42	110.37
14	A	602	HEA	C4B-C3B-C2B	-2.44	103.33	107.44
14	N	602	HEA	C4C-NC-C1C	-2.44	101.85	105.82
14	N	602	HEA	O1D-CGD-CBD	-2.44	115.37	123.09
14	A	602	HEA	C1D-ND-C4D	-2.43	102.32	105.21
22	C	303	PGV	C25-C24-C23	2.41	126.54	114.37
20	Q	201	DMU	C2-C3-C4	-2.40	105.61	110.93
27	G	101	PEK	O13-P-O14	2.39	123.56	112.44
20	Q	201	DMU	C57-C4-C3	2.39	120.09	113.38
18	L	101	CDL	OB4-PB2-OB2	2.38	118.35	107.57
20	H	101	DMU	O7-C3-C2	2.37	113.26	107.23
20	H	101	DMU	O3-C5-C10	2.37	115.72	110.08
14	N	601	HEA	C4B-NB-C1B	-2.37	102.41	105.21
14	A	602	HEA	CBD-CAD-C3D	2.35	119.03	112.53
18	C	304	CDL	OB5-PB2-OB3	2.34	118.19	108.94
22	A	613	PGV	C25-C24-C23	2.33	126.17	114.37
20	N	608	DMU	O5-C6-O16	2.32	115.54	110.04
24	C	301	CHD	C18-C13-C12	2.32	111.38	109.06
20	P	320	DMU	C10-O7-C3	-2.32	112.48	117.98
20	O	307	DMU	O5-C6-O16	2.31	115.50	110.04
14	A	602	HEA	CHD-C1D-C2D	-2.30	120.42	126.95
18	P	305	CDL	O1-C1-CB2	2.30	117.63	109.70
14	A	601	HEA	O11-C11-C3B	-2.29	107.05	111.26
14	A	602	HEA	C4C-C3C-C2C	-2.29	104.45	107.30
22	P	304	PGV	O03-C19-O04	-2.29	117.90	123.63
20	D	201	DMU	C2-C3-C4	-2.29	105.86	110.93
14	A	601	HEA	CMC-C2C-C1C	2.28	128.90	125.42
24	P	302	CHD	C22-C20-C17	-2.28	105.61	110.33
14	N	602	HEA	CBD-CAD-C3D	2.25	118.76	112.53
14	N	602	HEA	CHC-C4B-C3B	-2.25	120.14	125.80
20	Q	201	DMU	O3-C5-C7	2.24	115.65	110.38
14	N	601	HEA	C26-C15-C14	-2.24	117.88	123.63
14	A	601	HEA	C4B-C3B-C2B	-2.23	103.69	107.44
14	A	601	HEA	C2A-C1A-NA	2.23	112.47	110.32
24	P	306	CHD	C16-C17-C13	-2.23	101.38	103.54
20	Z	101	DMU	C10-C5-C7	2.22	114.68	110.01
20	P	316	DMU	O3-C5-C10	2.22	115.36	110.08
20	A	609	DMU	O3-C5-C10	2.19	115.31	110.08
20	O	307	DMU	C57-C4-C3	-2.19	107.64	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P	305	CDL	OA8-CA6-CA4	-2.19	102.09	108.40
20	P	324	DMU	O7-C10-O1	-2.19	104.94	110.69
22	N	614	PGV	O03-C01-C02	2.19	114.70	108.40
20	C	323	DMU	O3-C5-C7	2.19	115.53	110.38
14	N	602	HEA	C2A-C1A-NA	2.18	112.43	110.32
20	A	609	DMU	O7-C3-C4	2.18	115.19	109.48
14	A	601	HEA	C4C-C3C-C2C	-2.18	104.59	107.30
20	O	303	DMU	C57-C4-C3	-2.18	107.67	113.02
20	A	609	DMU	O7-C10-C5	2.17	113.44	108.09
20	N	608	DMU	O1-C9-C8	2.17	113.62	109.70
18	P	305	CDL	OA4-PA1-OA3	2.16	122.49	112.44
14	N	601	HEA	C25-C23-C24	2.15	119.55	114.59
24	P	306	CHD	C18-C13-C14	2.15	114.58	111.20
18	P	305	CDL	OA4-PA1-OA5	-2.15	97.83	107.57
14	N	601	HEA	C4B-C3B-C2B	-2.15	103.83	107.44
18	P	305	CDL	OA2-PA1-OA3	2.13	117.38	108.94
22	P	304	PGV	O14-P-O13	2.13	122.35	112.44
24	P	306	CHD	C6-C7-C8	2.13	113.82	111.50
14	N	601	HEA	C2D-C1D-ND	2.12	112.28	109.84
14	A	602	HEA	CAD-C3D-C4D	2.12	128.39	124.70
18	P	305	CDL	OB5-PB2-OB3	2.12	117.33	108.94
20	A	609	DMU	C10-C5-C7	2.11	114.45	110.01
20	C	315	DMU	O5-C6-O16	-2.11	105.07	110.04
14	A	602	HEA	CHA-C1A-C2A	-2.10	121.54	124.86
24	P	306	CHD	C18-C13-C12	-2.10	106.95	109.06
24	C	301	CHD	C22-C20-C17	-2.10	105.98	110.33
14	A	601	HEA	C1B-C2B-C3B	-2.10	104.37	106.80
14	A	602	HEA	CHB-C1B-NB	-2.10	122.17	124.42
24	P	306	CHD	C14-C8-C7	-2.09	109.07	111.85
24	C	305	CHD	O25-C24-C23	-2.09	116.46	123.09
20	C	323	DMU	C10-C5-C7	2.09	114.41	110.01
18	A	606	CDL	OA5-PA1-OA3	2.09	117.21	108.94
20	Q	201	DMU	C10-C5-C7	2.08	114.39	110.01
20	Z	101	DMU	O3-C5-C7	2.07	115.26	110.38
14	N	602	HEA	C27-C19-C20	2.07	118.82	115.23
20	P	316	DMU	C6-O5-C4	2.07	117.76	113.72
20	C	318	DMU	C10-O1-C9	-2.07	109.68	113.72
20	T	104	DMU	C57-C4-C3	-2.06	107.96	113.02
20	C	319	DMU	O5-C6-O16	2.05	114.88	110.04
14	N	601	HEA	CHC-C1C-C2C	-2.04	121.49	127.43
20	A	609	DMU	C10-O7-C3	-2.04	113.15	117.98
14	A	601	HEA	C4C-NC-C1C	-2.03	102.51	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	CAD-CBD-CGD	-2.02	108.30	113.67
14	A	602	HEA	C26-C15-C16	2.02	118.73	115.23
20	O	307	DMU	C18-O16-C6	-2.02	110.23	113.68
18	V	101	CDL	OA6-CA5-OA7	-2.02	118.99	123.70
14	N	601	HEA	CAD-C3D-C2D	2.01	131.64	127.87
24	C	305	CHD	C9-C8-C7	2.00	114.38	111.86
20	D	201	DMU	C57-C4-C3	2.00	119.01	113.38
20	P	319	DMU	C10-O1-C9	-2.00	109.81	113.72
18	C	304	CDL	CA6-CA4-CA3	2.00	116.45	111.78

There are no chirality outliers.

All (789) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	CDL	C1-CA2-OA2-PA1
18	A	606	CDL	CA3-OA5-PA1-OA2
18	A	606	CDL	CA3-OA5-PA1-OA3
18	A	606	CDL	CB3-OB5-PB2-OB2
18	A	606	CDL	CB3-OB5-PB2-OB3
18	A	606	CDL	CB3-OB5-PB2-OB4
18	A	606	CDL	C51-CB5-OB6-CB4
18	C	304	CDL	O1-C1-CB2-OB2
18	C	304	CDL	C1-CA2-OA2-PA1
18	C	304	CDL	CA3-OA5-PA1-OA2
18	C	304	CDL	CB3-OB5-PB2-OB4
18	C	304	CDL	OB7-CB5-OB6-CB4
18	C	304	CDL	C51-CB5-OB6-CB4
18	L	101	CDL	CB2-C1-CA2-OA2
18	L	101	CDL	CA2-OA2-PA1-OA3
18	L	101	CDL	CA2-OA2-PA1-OA4
18	L	101	CDL	CA2-OA2-PA1-OA5
18	L	101	CDL	C11-CA5-OA6-CA4
18	L	101	CDL	CB2-OB2-PB2-OB3
18	L	101	CDL	CB2-OB2-PB2-OB4
18	L	101	CDL	CB2-OB2-PB2-OB5
18	L	101	CDL	C51-CB5-OB6-CB4
18	P	305	CDL	C1-CA2-OA2-PA1
18	P	305	CDL	CA2-OA2-PA1-OA3
18	P	305	CDL	CA2-OA2-PA1-OA5
18	P	305	CDL	CA3-OA5-PA1-OA2
18	P	305	CDL	CA3-OA5-PA1-OA3
18	P	305	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
18	V	101	CDL	CA3-OA5-PA1-OA2
18	V	101	CDL	CA3-OA5-PA1-OA4
18	V	101	CDL	C11-CA5-OA6-CA4
18	V	101	CDL	CB2-OB2-PB2-OB3
18	V	101	CDL	CB2-OB2-PB2-OB5
18	V	101	CDL	CB3-OB5-PB2-OB2
18	V	101	CDL	CB3-OB5-PB2-OB3
18	V	101	CDL	CB3-OB5-PB2-OB4
18	V	101	CDL	OB7-CB5-OB6-CB4
18	Y	101	CDL	CA2-OA2-PA1-OA3
18	Y	101	CDL	CA2-OA2-PA1-OA5
18	Y	101	CDL	C11-CA5-OA6-CA4
18	Y	101	CDL	CB2-OB2-PB2-OB3
18	Y	101	CDL	CB3-OB5-PB2-OB2
18	Y	101	CDL	OB6-CB4-CB6-OB8
18	Y	101	CDL	C51-CB5-OB6-CB4
20	B	308	DMU	O5-C6-O16-C18
20	D	201	DMU	C19-C18-O16-C6
20	O	307	DMU	C19-C18-O16-C6
20	Q	201	DMU	O5-C6-O16-C18
20	Y	102	DMU	C1-C6-O16-C18
24	C	305	CHD	C13-C17-C20-C21
24	C	305	CHD	C13-C17-C20-C22
24	C	305	CHD	C16-C17-C20-C22
24	P	306	CHD	C13-C17-C20-C21
24	P	306	CHD	C13-C17-C20-C22
24	P	306	CHD	C16-C17-C20-C21
27	G	101	PEK	C11-C12-C13-C14
27	T	102	PEK	C11-C10-C9-C8
27	T	102	PEK	C12-C13-C14-C15
18	Y	101	CDL	OA9-CA7-OA8-CA6
24	C	305	CHD	C16-C17-C20-C21
20	O	303	DMU	O5-C4-C57-O61
18	A	606	CDL	OB7-CB5-OB6-CB4
18	L	101	CDL	OA7-CA5-OA6-CA4
18	L	101	CDL	OB7-CB5-OB6-CB4
18	P	305	CDL	OA7-CA5-OA6-CA4
18	V	101	CDL	OA7-CA5-OA6-CA4
18	Y	101	CDL	OA7-CA5-OA6-CA4
18	Y	101	CDL	OB7-CB5-OB6-CB4
18	V	101	CDL	C31-CA7-OA8-CA6
18	C	304	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
18	P	305	CDL	C11-CA5-OA6-CA4
18	P	305	CDL	C51-CB5-OB6-CB4
18	V	101	CDL	C51-CB5-OB6-CB4
24	P	306	CHD	C16-C17-C20-C22
20	L	102	DMU	C3-C4-C57-O61
20	C	319	DMU	O5-C4-C57-O61
20	T	104	DMU	O5-C4-C57-O61
18	Y	101	CDL	C31-CA7-OA8-CA6
18	P	305	CDL	O1-C1-CB2-OB2
18	Y	101	CDL	O1-C1-CB2-OB2
18	C	304	CDL	C31-CA7-OA8-CA6
20	C	317	DMU	O5-C4-C57-O61
20	C	318	DMU	O6-C11-C9-O1
20	C	319	DMU	O6-C11-C9-O1
20	P	320	DMU	O6-C11-C9-O1
20	P	318	DMU	O5-C4-C57-O61
20	C	319	DMU	C3-C4-C57-O61
19	C	324	LFA	C9-C10-C11-C12
20	O	303	DMU	C3-C4-C57-O61
19	P	308	LFA	C7-C8-C9-C10
18	V	101	CDL	OA9-CA7-OA8-CA6
18	C	304	CDL	OA7-CA5-OA6-CA4
20	B	308	DMU	O5-C4-C57-O61
20	A	609	DMU	O6-C11-C9-C8
20	P	320	DMU	O6-C11-C9-C8
20	T	104	DMU	C3-C4-C57-O61
20	C	315	DMU	O6-C11-C9-O1
20	B	304	DMU	O5-C6-O16-C18
20	A	609	DMU	O6-C11-C9-O1
20	L	102	DMU	O5-C4-C57-O61
20	N	608	DMU	O6-C11-C9-C8
19	C	309	LFA	C11-C10-C9-C8
18	C	304	CDL	OA9-CA7-OA8-CA6
18	A	606	CDL	OA7-CA5-OA6-CA4
18	C	304	CDL	CB2-C1-CA2-OA2
18	Y	101	CDL	CB2-C1-CA2-OA2
18	C	304	CDL	C71-CB7-OB8-CB6
19	P	301	LFA	C2-C3-C4-C5
19	P	311	LFA	C5-C6-C7-C8
22	A	613	PGV	C26-C27-C28-C29
19	T	101	LFA	C9-C10-C11-C12
20	P	318	DMU	C3-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
22	C	303	PGV	C28-C29-C30-C31
20	B	304	DMU	C1-C6-O16-C18
20	C	318	DMU	C1-C6-O16-C18
20	N	615	DMU	C1-C6-O16-C18
20	T	104	DMU	C1-C6-O16-C18
18	C	304	CDL	CB5-C51-C52-C53
18	L	101	CDL	O1-C1-CA2-OA2
18	P	305	CDL	O1-C1-CA2-OA2
18	Y	101	CDL	O1-C1-CA2-OA2
20	C	319	DMU	O6-C11-C9-C8
18	P	305	CDL	CB5-C51-C52-C53
19	C	309	LFA	C12-C13-C14-C15
18	P	305	CDL	C31-CA7-OA8-CA6
18	L	101	CDL	CB7-C71-C72-C73
19	P	301	LFA	C7-C8-C9-C10
20	C	318	DMU	O16-C18-C19-C22
20	C	317	DMU	C3-C4-C57-O61
20	L	102	DMU	O16-C18-C19-C22
20	N	615	DMU	O5-C4-C57-O61
22	N	614	PGV	C26-C27-C28-C29
18	C	304	CDL	CA7-C31-C32-C33
19	B	307	LFA	C9-C10-C11-C12
20	P	319	DMU	O6-C11-C9-O1
20	C	317	DMU	O16-C18-C19-C22
20	Y	102	DMU	O16-C18-C19-C22
22	A	613	PGV	C23-C24-C25-C26
18	A	606	CDL	CA5-C11-C12-C13
18	C	304	CDL	CB7-C71-C72-C73
18	V	101	CDL	CA5-C11-C12-C13
18	C	304	CDL	OB9-CB7-OB8-CB6
20	P	319	DMU	O16-C18-C19-C22
20	D	201	DMU	O6-C11-C9-O1
20	H	101	DMU	O5-C4-C57-O61
20	G	104	DMU	O16-C18-C19-C22
18	V	101	CDL	CA7-C31-C32-C33
20	C	318	DMU	O5-C6-O16-C18
20	N	608	DMU	O5-C6-O16-C18
20	N	615	DMU	O5-C6-O16-C18
20	T	104	DMU	O5-C6-O16-C18
20	C	318	DMU	O6-C11-C9-C8
18	C	304	CDL	O1-C1-CA2-OA2
18	V	101	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
18	Y	101	CDL	CA5-C11-C12-C13
20	P	319	DMU	C3-C4-C57-O61
27	T	102	PEK	C7-C8-C9-C10
20	B	308	DMU	C3-C4-C57-O61
19	C	312	LFA	C1-C2-C3-C4
18	V	101	CDL	CA2-C1-CB2-OB2
18	L	101	CDL	C31-CA7-OA8-CA6
20	P	319	DMU	O5-C4-C57-O61
18	A	606	CDL	C11-CA5-OA6-CA4
20	P	319	DMU	C1-C6-O16-C18
20	N	608	DMU	O6-C11-C9-O1
20	N	608	DMU	O16-C18-C19-C22
19	P	313	LFA	C1-C2-C3-C4
20	P	320	DMU	C4-C3-O7-C10
19	P	310	LFA	C11-C10-C9-C8
20	P	318	DMU	C18-C19-C22-C25
20	Y	102	DMU	O5-C6-O16-C18
18	P	305	CDL	OA9-CA7-OA8-CA6
18	P	305	CDL	C11-C12-C13-C14
18	Y	101	CDL	C79-C80-C81-C82
19	G	106	LFA	C11-C10-C9-C8
20	P	319	DMU	C28-C31-C34-C37
20	C	315	DMU	O6-C11-C9-C8
20	B	303	DMU	C18-C19-C22-C25
19	B	307	LFA	C13-C14-C15-C16
27	T	102	PEK	C13-C14-C15-C16
18	A	606	CDL	C17-C18-C19-C20
19	P	310	LFA	C5-C6-C7-C8
19	P	311	LFA	C7-C8-C9-C10
18	C	304	CDL	C35-C36-C37-C38
19	P	312	LFA	C3-C4-C5-C6
19	T	101	LFA	C5-C6-C7-C8
20	C	318	DMU	C19-C18-O16-C6
20	L	102	DMU	C19-C18-O16-C6
20	B	303	DMU	C19-C22-C25-C28
19	P	312	LFA	C10-C11-C12-C13
18	P	305	CDL	C56-C57-C58-C59
22	N	614	PGV	C14-C15-C16-C17
19	B	307	LFA	C4-C5-C6-C7
27	T	102	PEK	C22-C23-C24-C25
18	A	606	CDL	C75-C76-C77-C78
18	V	101	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
20	B	304	DMU	C31-C34-C37-C40
27	T	102	PEK	C1-C2-C3-C4
18	Y	101	CDL	C16-C17-C18-C19
22	C	303	PGV	C7-C8-C9-C10
27	G	101	PEK	C16-C17-C18-C19
19	B	307	LFA	C7-C8-C9-C10
18	L	101	CDL	OA9-CA7-OA8-CA6
18	A	606	CDL	C78-C79-C80-C81
19	O	301	LFA	C5-C6-C7-C8
20	G	104	DMU	C28-C31-C34-C37
27	T	102	PEK	C26-C27-C28-C29
18	Y	101	CDL	C13-C14-C15-C16
18	L	101	CDL	C37-C38-C39-C40
18	V	101	CDL	C73-C74-C75-C76
19	P	310	LFA	C13-C14-C15-C16
20	P	316	DMU	C28-C31-C34-C37
20	P	320	DMU	C2-C3-O7-C10
18	C	304	CDL	C51-C52-C53-C54
19	C	312	LFA	C5-C6-C7-C8
19	O	302	LFA	C5-C6-C7-C8
20	C	315	DMU	C19-C22-C25-C28
20	C	317	DMU	C22-C25-C28-C31
20	C	318	DMU	C31-C34-C37-C40
22	P	304	PGV	C24-C25-C26-C27
20	C	315	DMU	C28-C31-C34-C37
27	G	101	PEK	C34-C35-C36-C37
20	D	201	DMU	O16-C18-C19-C22
22	C	303	PGV	C13-C14-C15-C16
18	C	304	CDL	C22-C23-C24-C25
27	T	102	PEK	C17-C18-C19-C20
20	L	102	DMU	C31-C34-C37-C40
20	P	317	DMU	C31-C34-C37-C40
19	P	313	LFA	C4-C5-C6-C7
18	C	304	CDL	C71-C72-C73-C74
18	Y	101	CDL	C63-C64-C65-C66
19	O	301	LFA	C13-C14-C15-C16
20	J	101	DMU	C25-C28-C31-C34
19	C	309	LFA	C5-C6-C7-C8
19	P	301	LFA	C4-C5-C6-C7
18	C	304	CDL	C75-C76-C77-C78
18	V	101	CDL	C17-C18-C19-C20
19	G	106	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	O	307	DMU	C34-C37-C40-C43
18	L	101	CDL	C14-C15-C16-C17
18	V	101	CDL	C76-C77-C78-C79
20	G	104	DMU	C25-C28-C31-C34
20	Z	101	DMU	C22-C25-C28-C31
20	O	306	DMU	C18-C19-C22-C25
20	P	324	DMU	O16-C18-C19-C22
20	L	102	DMU	C25-C28-C31-C34
20	P	318	DMU	C31-C34-C37-C40
27	G	101	PEK	C26-C27-C28-C29
22	C	303	PGV	C14-C15-C16-C17
19	P	301	LFA	C9-C10-C11-C12
22	P	304	PGV	C12-C13-C14-C15
27	G	101	PEK	C15-C16-C17-C18
27	T	102	PEK	C2-C3-C4-C5
27	G	101	PEK	C28-C29-C30-C31
19	P	310	LFA	C4-C5-C6-C7
18	Y	101	CDL	C71-C72-C73-C74
24	C	305	CHD	C21-C20-C22-C23
24	P	306	CHD	C21-C20-C22-C23
19	C	311	LFA	C11-C10-C9-C8
20	A	608	DMU	C28-C31-C34-C37
18	Y	101	CDL	C51-C52-C53-C54
18	Y	101	CDL	C61-C62-C63-C64
18	Y	101	CDL	C76-C77-C78-C79
20	C	316	DMU	C28-C31-C34-C37
22	A	613	PGV	C29-C30-C31-C32
22	C	303	PGV	C22-C23-C24-C25
20	P	307	DMU	O16-C18-C19-C22
19	C	309	LFA	C1-C2-C3-C4
20	A	609	DMU	C31-C34-C37-C40
19	P	301	LFA	C6-C7-C8-C9
18	L	101	CDL	C72-C73-C74-C75
18	V	101	CDL	C78-C79-C80-C81
19	P	314	LFA	C2-C3-C4-C5
20	B	304	DMU	O16-C18-C19-C22
18	C	304	CDL	C33-C34-C35-C36
18	L	101	CDL	C34-C35-C36-C37
22	P	304	PGV	C7-C8-C9-C10
20	P	316	DMU	C18-C19-C22-C25
22	C	303	PGV	C24-C25-C26-C27
19	C	310	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	C	311	LFA	C4-C5-C6-C7
19	N	606	LFA	C10-C11-C12-C13
18	L	101	CDL	C17-C18-C19-C20
18	P	305	CDL	C52-C53-C54-C55
19	P	312	LFA	C5-C6-C7-C8
19	C	324	LFA	C6-C7-C8-C9
18	V	101	CDL	C1-CA2-OA2-PA1
19	A	607	LFA	C9-C10-C11-C12
20	L	102	DMU	C22-C25-C28-C31
22	C	303	PGV	C25-C26-C27-C28
20	G	103	DMU	O16-C18-C19-C22
20	W	101	DMU	O16-C18-C19-C22
20	M	101	DMU	C22-C25-C28-C31
18	P	305	CDL	CA2-C1-CB2-OB2
20	P	318	DMU	C28-C31-C34-C37
19	C	309	LFA	C3-C4-C5-C6
20	N	608	DMU	C31-C34-C37-C40
19	P	310	LFA	C3-C4-C5-C6
20	B	308	DMU	O16-C18-C19-C22
20	Y	102	DMU	C18-C19-C22-C25
20	C	317	DMU	C19-C22-C25-C28
20	C	315	DMU	C18-C19-C22-C25
22	N	614	PGV	C12-C13-C14-C15
22	P	304	PGV	C27-C28-C29-C30
18	L	101	CDL	C13-C14-C15-C16
20	W	101	DMU	C25-C28-C31-C34
20	C	317	DMU	C31-C34-C37-C40
20	B	302	DMU	O16-C18-C19-C22
20	B	303	DMU	O16-C18-C19-C22
22	P	304	PGV	C30-C31-C32-C33
18	C	304	CDL	C23-C24-C25-C26
20	B	302	DMU	C18-C19-C22-C25
18	A	606	CDL	C19-C20-C21-C22
19	P	313	LFA	C3-C4-C5-C6
18	P	305	CDL	C53-C54-C55-C56
19	C	324	LFA	C7-C8-C9-C10
18	V	101	CDL	C31-C32-C33-C34
18	L	101	CDL	CB3-CB4-CB6-OB8
18	Y	101	CDL	CB3-CB4-CB6-OB8
20	C	323	DMU	O16-C18-C19-C22
18	Y	101	CDL	C21-C22-C23-C24
19	T	103	LFA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	A	613	PGV	C12-C13-C14-C15
20	C	316	DMU	C34-C37-C40-C43
18	P	305	CDL	C71-CB7-OB8-CB6
20	O	305	DMU	O16-C18-C19-C22
18	L	101	CDL	C80-C81-C82-C83
20	P	320	DMU	C22-C25-C28-C31
19	P	308	LFA	C3-C4-C5-C6
20	C	315	DMU	O5-C4-C57-O61
18	P	305	CDL	C54-C55-C56-C57
19	C	307	LFA	C3-C4-C5-C6
20	A	614	DMU	C19-C22-C25-C28
18	C	304	CDL	CA4-CA3-OA5-PA1
22	N	614	PGV	C30-C31-C32-C33
20	P	316	DMU	O6-C11-C9-O1
20	Y	102	DMU	O5-C4-C57-O61
20	Z	101	DMU	O6-C11-C9-C8
20	C	316	DMU	C31-C34-C37-C40
22	N	614	PGV	C29-C30-C31-C32
20	C	319	DMU	C18-C19-C22-C25
20	P	316	DMU	O5-C4-C57-O61
18	V	101	CDL	C72-C73-C74-C75
19	C	307	LFA	C4-C5-C6-C7
19	C	308	LFA	C2-C3-C4-C5
20	B	303	DMU	C28-C31-C34-C37
20	M	101	DMU	C25-C28-C31-C34
20	O	306	DMU	O16-C18-C19-C22
20	C	319	DMU	C22-C25-C28-C31
20	O	306	DMU	C19-C22-C25-C28
27	G	101	PEK	C25-C26-C27-C28
27	T	102	PEK	C4-C5-C6-C7
19	O	301	LFA	C11-C12-C13-C14
20	G	103	DMU	C34-C37-C40-C43
19	P	311	LFA	C11-C10-C9-C8
18	Y	101	CDL	C57-C58-C59-C60
20	N	615	DMU	C18-C19-C22-C25
19	N	606	LFA	C6-C7-C8-C9
20	C	319	DMU	C19-C22-C25-C28
20	P	320	DMU	C25-C28-C31-C34
18	L	101	CDL	C84-C85-C86-C87
19	C	324	LFA	C12-C13-C14-C15
19	O	301	LFA	C14-C15-C16-C17
20	B	308	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
19	C	310	LFA	C6-C7-C8-C9
19	P	314	LFA	C6-C7-C8-C9
20	Y	102	DMU	C19-C22-C25-C28
18	C	304	CDL	C13-C14-C15-C16
19	C	324	LFA	C3-C4-C5-C6
20	P	316	DMU	C19-C22-C25-C28
18	Y	101	CDL	C84-C85-C86-C87
19	C	310	LFA	C11-C10-C9-C8
20	L	102	DMU	C34-C37-C40-C43
20	P	319	DMU	C34-C37-C40-C43
18	L	101	CDL	CB5-C51-C52-C53
18	Y	101	CDL	C73-C74-C75-C76
18	A	606	CDL	OA6-CA4-CA6-OA8
18	L	101	CDL	OB6-CB4-CB6-OB8
18	V	101	CDL	OA6-CA4-CA6-OA8
19	P	308	LFA	C11-C10-C9-C8
18	Y	101	CDL	C80-C81-C82-C83
20	P	319	DMU	C4-C3-O7-C10
18	A	606	CDL	C16-C17-C18-C19
19	C	324	LFA	C4-C5-C6-C7
19	P	310	LFA	C14-C15-C16-C17
20	O	305	DMU	C25-C28-C31-C34
20	A	614	DMU	O16-C18-C19-C22
19	P	312	LFA	C4-C5-C6-C7
19	C	311	LFA	C10-C11-C12-C13
22	C	303	PGV	C30-C31-C32-C33
20	A	608	DMU	C25-C28-C31-C34
20	H	101	DMU	C19-C22-C25-C28
20	P	319	DMU	C25-C28-C31-C34
18	A	606	CDL	C20-C21-C22-C23
20	P	319	DMU	C2-C3-O7-C10
20	P	324	DMU	C2-C3-O7-C10
20	P	324	DMU	C4-C3-O7-C10
18	Y	101	CDL	C64-C65-C66-C67
19	B	307	LFA	C14-C15-C16-C17
19	C	312	LFA	C11-C10-C9-C8
18	L	101	CDL	C74-C75-C76-C77
18	P	305	CDL	C73-C74-C75-C76
18	Y	101	CDL	C58-C59-C60-C61
20	C	318	DMU	C2-C3-O7-C10
22	A	613	PGV	C30-C31-C32-C33
20	C	318	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
20	Z	101	DMU	C34-C37-C40-C43
20	Z	101	DMU	O6-C11-C9-O1
20	M	102	DMU	C34-C37-C40-C43
18	P	305	CDL	C20-C21-C22-C23
18	Y	101	CDL	C32-C33-C34-C35
19	O	301	LFA	C11-C10-C9-C8
20	B	308	DMU	C19-C18-O16-C6
20	H	101	DMU	C19-C18-O16-C6
20	P	318	DMU	C19-C18-O16-C6
20	P	320	DMU	C19-C18-O16-C6
18	P	305	CDL	C75-C76-C77-C78
19	P	315	LFA	C6-C7-C8-C9
18	P	305	CDL	C57-C58-C59-C60
18	Y	101	CDL	C22-C23-C24-C25
19	C	310	LFA	C7-C8-C9-C10
20	Y	102	DMU	C25-C28-C31-C34
20	Z	101	DMU	C25-C28-C31-C34
20	D	201	DMU	C4-C3-O7-C10
20	P	319	DMU	O1-C10-O7-C3
18	V	101	CDL	C18-C19-C20-C21
18	P	305	CDL	C35-C36-C37-C38
20	L	102	DMU	C1-C6-O16-C18
22	N	614	PGV	C31-C32-C33-C34
20	O	303	DMU	C22-C25-C28-C31
19	C	309	LFA	C15-C16-C17-C18
20	C	315	DMU	C34-C37-C40-C43
18	L	101	CDL	C72-C71-CB7-OB8
19	C	313	LFA	C4-C5-C6-C7
20	W	101	DMU	C34-C37-C40-C43
19	B	307	LFA	C1-C2-C3-C4
18	Y	101	CDL	CA7-C31-C32-C33
20	C	318	DMU	C4-C3-O7-C10
19	C	310	LFA	C1-C2-C3-C4
18	P	305	CDL	OB9-CB7-OB8-CB6
18	P	305	CDL	C33-C34-C35-C36
19	A	607	LFA	C6-C7-C8-C9
20	C	315	DMU	C4-C3-O7-C10
18	Y	101	CDL	C59-C60-C61-C62
19	B	307	LFA	C11-C12-C13-C14
22	A	613	PGV	C11-C10-C9-C8
22	N	614	PGV	C11-C10-C9-C8
20	B	308	DMU	C31-C34-C37-C40

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Mol	Chain	Res	Type	Atoms
19	P	314	LFA	C9-C10-C11-C12
18	P	305	CDL	CB3-CB4-CB6-OB8
18	V	101	CDL	CA3-CA4-CA6-OA8
20	T	104	DMU	C25-C28-C31-C34
19	O	302	LFA	C2-C3-C4-C5
20	O	305	DMU	C18-C19-C22-C25
19	C	314	LFA	C1-C2-C3-C4
20	P	324	DMU	C25-C28-C31-C34
27	G	101	PEK	C17-C18-C19-C20
18	P	305	CDL	OA5-CA3-CA4-OA6
18	C	304	CDL	C18-C19-C20-C21
18	L	101	CDL	C58-C59-C60-C61
20	B	303	DMU	C22-C25-C28-C31
20	Q	201	DMU	C4-C3-O7-C10
19	C	324	LFA	C10-C11-C12-C13
22	A	613	PGV	C28-C29-C30-C31
18	L	101	CDL	C57-C58-C59-C60
18	C	304	CDL	OB6-CB4-CB6-OB8
19	O	302	LFA	C1-C2-C3-C4
27	G	101	PEK	C9-C10-C11-C12
27	T	102	PEK	C11-C12-C13-C14
19	C	310	LFA	C3-C4-C5-C6
19	P	301	LFA	C11-C12-C13-C14
20	P	317	DMU	C28-C31-C34-C37
18	A	606	CDL	C71-C72-C73-C74
18	A	606	CDL	C77-C78-C79-C80
19	P	314	LFA	C11-C10-C9-C8
18	A	606	CDL	C71-CB7-OB8-CB6
27	G	101	PEK	C29-C30-C31-C32
20	B	304	DMU	C34-C37-C40-C43
18	L	101	CDL	C19-C20-C21-C22
19	P	311	LFA	C6-C7-C8-C9
22	A	613	PGV	C31-C32-C33-C34
18	Y	101	CDL	C19-C20-C21-C22
18	L	101	CDL	C51-C52-C53-C54
18	A	606	CDL	C12-C13-C14-C15
18	Y	101	CDL	CA2-C1-CB2-OB2
20	M	102	DMU	C31-C34-C37-C40
20	C	306	DMU	O16-C18-C19-C22
22	P	304	PGV	C14-C15-C16-C17
18	A	606	CDL	C13-C14-C15-C16
19	P	311	LFA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
18	Y	101	CDL	C38-C39-C40-C41
20	D	201	DMU	C2-C3-O7-C10
19	C	324	LFA	C5-C6-C7-C8
19	N	606	LFA	C7-C8-C9-C10
20	C	315	DMU	C2-C3-O7-C10
27	G	101	PEK	C13-C14-C15-C16
19	P	314	LFA	C5-C6-C7-C8
18	P	305	CDL	CA7-C31-C32-C33
19	C	307	LFA	C6-C7-C8-C9
22	A	613	PGV	C15-C16-C17-C18
18	L	101	CDL	C21-C22-C23-C24
19	P	310	LFA	C11-C12-C13-C14
22	P	304	PGV	C11-C12-C13-C14
19	P	310	LFA	C1-C2-C3-C4
20	C	319	DMU	O16-C18-C19-C22
20	C	319	DMU	C28-C31-C34-C37
18	P	305	CDL	C21-C22-C23-C24
20	H	101	DMU	C25-C28-C31-C34
18	P	305	CDL	C71-C72-C73-C74
20	B	308	DMU	C25-C28-C31-C34
20	O	305	DMU	C22-C25-C28-C31
20	Z	102	DMU	C22-C25-C28-C31
18	A	606	CDL	CA7-C31-C32-C33
20	C	318	DMU	C19-C22-C25-C28
20	M	101	DMU	O16-C18-C19-C22
18	L	101	CDL	C59-C60-C61-C62
27	T	102	PEK	C10-C11-C12-C13
19	P	301	LFA	C1-C2-C3-C4
18	C	304	CDL	C73-C74-C75-C76
20	O	305	DMU	C19-C22-C25-C28
18	A	606	CDL	OB9-CB7-OB8-CB6
18	L	101	CDL	C76-C77-C78-C79
19	P	310	LFA	C7-C8-C9-C10
19	T	103	LFA	C6-C7-C8-C9
20	G	103	DMU	C19-C22-C25-C28
20	H	101	DMU	C28-C31-C34-C37
18	C	304	CDL	C20-C21-C22-C23
19	T	103	LFA	C7-C8-C9-C10
19	B	307	LFA	C11-C10-C9-C8
20	P	316	DMU	C34-C37-C40-C43
20	B	304	DMU	C19-C18-O16-C6
20	G	104	DMU	C19-C18-O16-C6

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Mol	Chain	Res	Type	Atoms
20	Y	102	DMU	C19-C18-O16-C6
20	P	324	DMU	O1-C10-O7-C3
18	C	304	CDL	C12-C11-CA5-OA6
20	H	101	DMU	O6-C11-C9-O1
18	A	606	CDL	C15-C16-C17-C18
18	P	305	CDL	OA5-CA3-CA4-CA6
20	H	101	DMU	C22-C25-C28-C31
19	C	311	LFA	C5-C6-C7-C8
19	O	301	LFA	C1-C2-C3-C4
19	C	314	LFA	C6-C7-C8-C9
18	C	304	CDL	C77-C78-C79-C80
20	H	101	DMU	C3-C4-C57-O61
20	N	615	DMU	C3-C4-C57-O61
19	P	313	LFA	C11-C10-C9-C8
18	V	101	CDL	OA5-CA3-CA4-OA6
27	T	102	PEK	C2-C1-O01-C02
20	N	615	DMU	C22-C25-C28-C31
18	L	101	CDL	C22-C23-C24-C25
18	P	305	CDL	C23-C24-C25-C26
20	Y	102	DMU	C22-C25-C28-C31
18	P	305	CDL	OB6-CB4-CB6-OB8
18	Y	101	CDL	OA6-CA4-CA6-OA8
20	Q	201	DMU	C25-C28-C31-C34
18	C	304	CDL	CB3-CB4-CB6-OB8
18	P	305	CDL	CA3-CA4-CA6-OA8
18	Y	101	CDL	CA3-CA4-CA6-OA8
18	C	304	CDL	C79-C80-C81-C82
18	P	305	CDL	C13-C14-C15-C16
20	D	201	DMU	C19-C22-C25-C28
19	C	307	LFA	C11-C10-C9-C8
20	J	101	DMU	C34-C37-C40-C43
20	M	102	DMU	C22-C25-C28-C31
24	P	306	CHD	C17-C20-C22-C23
18	P	305	CDL	C18-C19-C20-C21
18	A	606	CDL	CA2-OA2-PA1-OA3
18	C	304	CDL	CA3-OA5-PA1-OA3
18	L	101	CDL	CA3-OA5-PA1-OA3
18	V	101	CDL	CA3-OA5-PA1-OA3
18	V	101	CDL	CB2-OB2-PB2-OB4
18	Y	101	CDL	CA2-OA2-PA1-OA4
18	Y	101	CDL	CB2-OB2-PB2-OB4
18	Y	101	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
20	P	319	DMU	O6-C11-C9-C8
19	P	311	LFA	C4-C5-C6-C7
20	N	615	DMU	C19-C22-C25-C28
18	P	305	CDL	CA4-CA3-OA5-PA1
22	C	303	PGV	C02-C03-O11-P
22	P	304	PGV	C02-C03-O11-P
20	T	104	DMU	C34-C37-C40-C43
20	C	319	DMU	C34-C37-C40-C43
20	P	318	DMU	C22-C25-C28-C31
19	C	314	LFA	C11-C10-C9-C8
19	G	106	LFA	C9-C10-C11-C12
20	Q	201	DMU	C2-C3-O7-C10
20	C	317	DMU	C25-C28-C31-C34
19	P	309	LFA	C1-C2-C3-C4
20	Q	201	DMU	O6-C11-C9-C8
19	P	312	LFA	C1-C2-C3-C4
20	P	320	DMU	C19-C22-C25-C28
19	C	309	LFA	C2-C3-C4-C5
19	G	106	LFA	C6-C7-C8-C9
20	P	324	DMU	C5-C10-O7-C3
27	T	102	PEK	O02-C1-O01-C02
20	J	101	DMU	C31-C34-C37-C40
20	Y	102	DMU	C31-C34-C37-C40
18	V	101	CDL	C16-C17-C18-C19
27	G	101	PEK	C27-C28-C29-C30
19	G	106	LFA	C1-C2-C3-C4
19	T	103	LFA	C3-C4-C5-C6
20	J	101	DMU	C18-C19-C22-C25
18	C	304	CDL	C59-C60-C61-C62
18	P	305	CDL	C74-C75-C76-C77
20	D	201	DMU	O5-C6-O16-C18
20	P	318	DMU	C19-C22-C25-C28
22	C	303	PGV	C21-C22-C23-C24
18	P	305	CDL	C80-C81-C82-C83
18	V	101	CDL	C12-C13-C14-C15
20	B	302	DMU	C31-C34-C37-C40
20	C	317	DMU	C19-C18-O16-C6
20	O	303	DMU	C19-C18-O16-C6
20	Z	101	DMU	O16-C18-C19-C22
18	L	101	CDL	OB5-CB3-CB4-OB6
18	L	101	CDL	C36-C37-C38-C39
18	Y	101	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
14	A	602	HEA	C4D-C3D-CAD-CBD
19	B	307	LFA	C6-C7-C8-C9
18	Y	101	CDL	OB9-CB7-OB8-CB6
18	V	101	CDL	C74-C75-C76-C77
20	C	306	DMU	C28-C31-C34-C37
18	L	101	CDL	C15-C16-C17-C18
18	V	101	CDL	C19-C20-C21-C22
20	A	609	DMU	C2-C3-O7-C10
20	Z	102	DMU	C31-C34-C37-C40
20	N	615	DMU	C25-C28-C31-C34
19	C	313	LFA	C9-C10-C11-C12
20	P	307	DMU	C18-C19-C22-C25
19	C	313	LFA	C2-C3-C4-C5
27	T	102	PEK	C29-C30-C31-C32
14	A	602	HEA	CAD-CBD-CGD-O1D
20	B	304	DMU	C3-C4-C57-O61
18	P	305	CDL	C12-C11-CA5-OA6
18	A	606	CDL	CA6-CA4-OA6-CA5
22	N	614	PGV	C23-C24-C25-C26
24	G	102	CHD	C22-C23-C24-O25
21	P	321	EDO	O1-C1-C2-O2
24	B	306	CHD	C22-C23-C24-O26
18	L	101	CDL	C72-C71-CB7-OB9
14	A	601	HEA	CAD-CBD-CGD-O1D
20	C	315	DMU	O1-C10-O7-C3
19	C	307	LFA	C7-C8-C9-C10
18	V	101	CDL	C52-C51-CB5-OB6
27	T	102	PEK	C30-C31-C32-C33
20	A	609	DMU	C4-C3-O7-C10
14	A	602	HEA	CAD-CBD-CGD-O2D
14	N	602	HEA	CAA-CBA-CGA-O1A
14	N	602	HEA	CAD-CBD-CGD-O1D
24	C	305	CHD	C22-C23-C24-O25
14	N	601	HEA	CAD-CBD-CGD-O1D
24	B	306	CHD	C22-C23-C24-O25
24	G	102	CHD	C22-C23-C24-O26
20	A	614	DMU	C25-C28-C31-C34
24	P	306	CHD	C22-C23-C24-O25
18	Y	101	CDL	C12-C13-C14-C15
19	P	310	LFA	C12-C13-C14-C15
20	P	319	DMU	C5-C10-O7-C3
18	P	305	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
24	C	305	CHD	C22-C23-C24-O26
19	P	308	LFA	C2-C3-C4-C5
27	T	102	PEK	C32-C33-C34-C35
20	Z	101	DMU	C19-C22-C25-C28
14	A	602	HEA	CAA-CBA-CGA-O1A
18	C	304	CDL	CA2-C1-CB2-OB2
20	P	307	DMU	C31-C34-C37-C40
20	Q	201	DMU	O5-C4-C57-O61
18	L	101	CDL	C77-C78-C79-C80
20	O	306	DMU	C25-C28-C31-C34
20	G	103	DMU	C31-C34-C37-C40
20	A	609	DMU	C3-C4-C57-O61
18	C	304	CDL	C52-C53-C54-C55
19	A	607	LFA	C7-C8-C9-C10
20	N	608	DMU	C19-C22-C25-C28
14	N	602	HEA	CAA-CBA-CGA-O2A
14	N	602	HEA	CAD-CBD-CGD-O2D
22	C	303	PGV	C05-C04-O12-P
20	C	315	DMU	C5-C10-O7-C3
18	V	101	CDL	C52-C51-CB5-OB7
24	C	305	CHD	C17-C20-C22-C23
20	G	104	DMU	C22-C25-C28-C31
24	P	306	CHD	C22-C23-C24-O26
21	A	611	EDO	O1-C1-C2-O2
21	R	201	EDO	O1-C1-C2-O2
20	B	304	DMU	C18-C19-C22-C25
18	C	304	CDL	C72-C71-CB7-OB8
20	P	324	DMU	C28-C31-C34-C37
14	A	601	HEA	CAD-CBD-CGD-O2D
27	G	101	PEK	C10-C11-C12-C13
18	V	101	CDL	C13-C14-C15-C16
22	A	613	PGV	O03-C19-C20-C21
20	M	101	DMU	C34-C37-C40-C43
14	A	602	HEA	CAA-CBA-CGA-O2A
22	N	614	PGV	O03-C19-C20-C21
24	P	302	CHD	C22-C23-C24-O26
20	O	307	DMU	C22-C25-C28-C31
20	O	307	DMU	C18-C19-C22-C25
20	P	307	DMU	C22-C25-C28-C31
18	L	101	CDL	C78-C79-C80-C81
20	H	101	DMU	C18-C19-C22-C25
20	A	608	DMU	C31-C34-C37-C40

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Mol	Chain	Res	Type	Atoms
18	V	101	CDL	C20-C21-C22-C23
19	P	313	LFA	C6-C7-C8-C9
20	C	323	DMU	O1-C10-O7-C3
24	P	302	CHD	C22-C23-C24-O25
18	V	101	CDL	C15-C16-C17-C18
19	P	315	LFA	C2-C3-C4-C5
19	P	312	LFA	C7-C8-C9-C10
27	T	102	PEK	C15-C16-C17-C18
19	O	302	LFA	C6-C7-C8-C9
19	P	315	LFA	C5-C6-C7-C8
18	P	305	CDL	C77-C78-C79-C80
19	A	607	LFA	C2-C3-C4-C5
19	T	101	LFA	C11-C10-C9-C8
18	Y	101	CDL	OA5-CA3-CA4-OA6
19	T	101	LFA	C6-C7-C8-C9
19	C	309	LFA	C7-C8-C9-C10
18	L	101	CDL	C73-C74-C75-C76
19	O	301	LFA	C6-C7-C8-C9
22	A	613	PGV	C14-C15-C16-C17
18	C	304	CDL	C55-C56-C57-C58
19	N	606	LFA	C2-C3-C4-C5
20	C	323	DMU	C31-C34-C37-C40
21	C	322	EDO	O1-C1-C2-O2
24	C	301	CHD	C22-C23-C24-O25
18	A	606	CDL	C32-C31-CA7-OA8
18	V	101	CDL	C72-C71-CB7-OB8
18	Y	101	CDL	OA5-CA3-CA4-CA6
14	A	602	HEA	C2D-C3D-CAD-CBD
18	P	305	CDL	C72-C73-C74-C75
20	Z	101	DMU	C28-C31-C34-C37
22	C	303	PGV	C9-C10-C11-C12
19	P	315	LFA	C3-C4-C5-C6
20	D	201	DMU	O6-C11-C9-C8
18	P	305	CDL	C1-CB2-OB2-PB2
20	Q	201	DMU	O1-C10-O7-C3
20	P	319	DMU	O5-C6-O16-C18
20	M	101	DMU	C19-C22-C25-C28
18	P	305	CDL	C52-C51-CB5-OB6
18	A	606	CDL	C72-C71-CB7-OB8
20	T	104	DMU	C28-C31-C34-C37
18	C	304	CDL	C12-C11-CA5-OA7
22	C	303	PGV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
18	C	304	CDL	C52-C51-CB5-OB6
18	P	305	CDL	C72-C71-CB7-OB8
14	N	601	HEA	CAD-CBD-CGD-O2D
18	P	305	CDL	C14-C15-C16-C17
24	C	301	CHD	C22-C23-C24-O26
20	W	101	DMU	C22-C25-C28-C31
20	B	308	DMU	C18-C19-C22-C25
18	L	101	CDL	C56-C57-C58-C59
19	C	311	LFA	C3-C4-C5-C6
18	V	101	CDL	CB4-CB3-OB5-PB2
19	P	312	LFA	C11-C10-C9-C8
18	P	305	CDL	C55-C56-C57-C58
20	C	319	DMU	C31-C34-C37-C40
20	N	607	DMU	C31-C34-C37-C40
21	N	612	EDO	O1-C1-C2-O2
22	A	613	PGV	C13-C14-C15-C16
18	A	606	CDL	C18-C19-C20-C21
19	C	309	LFA	C13-C14-C15-C16
18	Y	101	CDL	C83-C84-C85-C86
19	T	101	LFA	C10-C11-C12-C13
18	A	606	CDL	C32-C31-CA7-OA9
18	Y	101	CDL	C60-C61-C62-C63
18	C	304	CDL	C1-CB2-OB2-PB2
14	N	602	HEA	C26-C15-C16-C17
19	C	309	LFA	C6-C7-C8-C9
18	A	606	CDL	C72-C71-CB7-OB9
18	Y	101	CDL	C71-CB7-OB8-CB6
19	C	309	LFA	C11-C12-C13-C14
18	L	101	CDL	C32-C31-CA7-OA8
18	P	305	CDL	C52-C51-CB5-OB7
22	C	303	PGV	C29-C30-C31-C32
18	V	101	CDL	C72-C71-CB7-OB9
20	P	316	DMU	C3-C4-C57-O61
18	P	305	CDL	C72-C71-CB7-OB9
20	P	316	DMU	C4-C3-O7-C10
14	N	601	HEA	CAA-CBA-CGA-O2A
20	C	323	DMU	C18-C19-C22-C25
19	C	307	LFA	C2-C3-C4-C5
18	C	304	CDL	C52-C51-CB5-OB7
19	P	315	LFA	C1-C2-C3-C4
18	C	304	CDL	C36-C37-C38-C39
14	A	601	HEA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
18	V	101	CDL	C32-C33-C34-C35
14	A	601	HEA	CAA-CBA-CGA-O2A
27	T	102	PEK	O01-C1-C2-C3
18	V	101	CDL	C71-CB7-OB8-CB6
20	Q	201	DMU	C5-C10-O7-C3

There are no ring outliers.

41 monomers are involved in 116 short contacts:

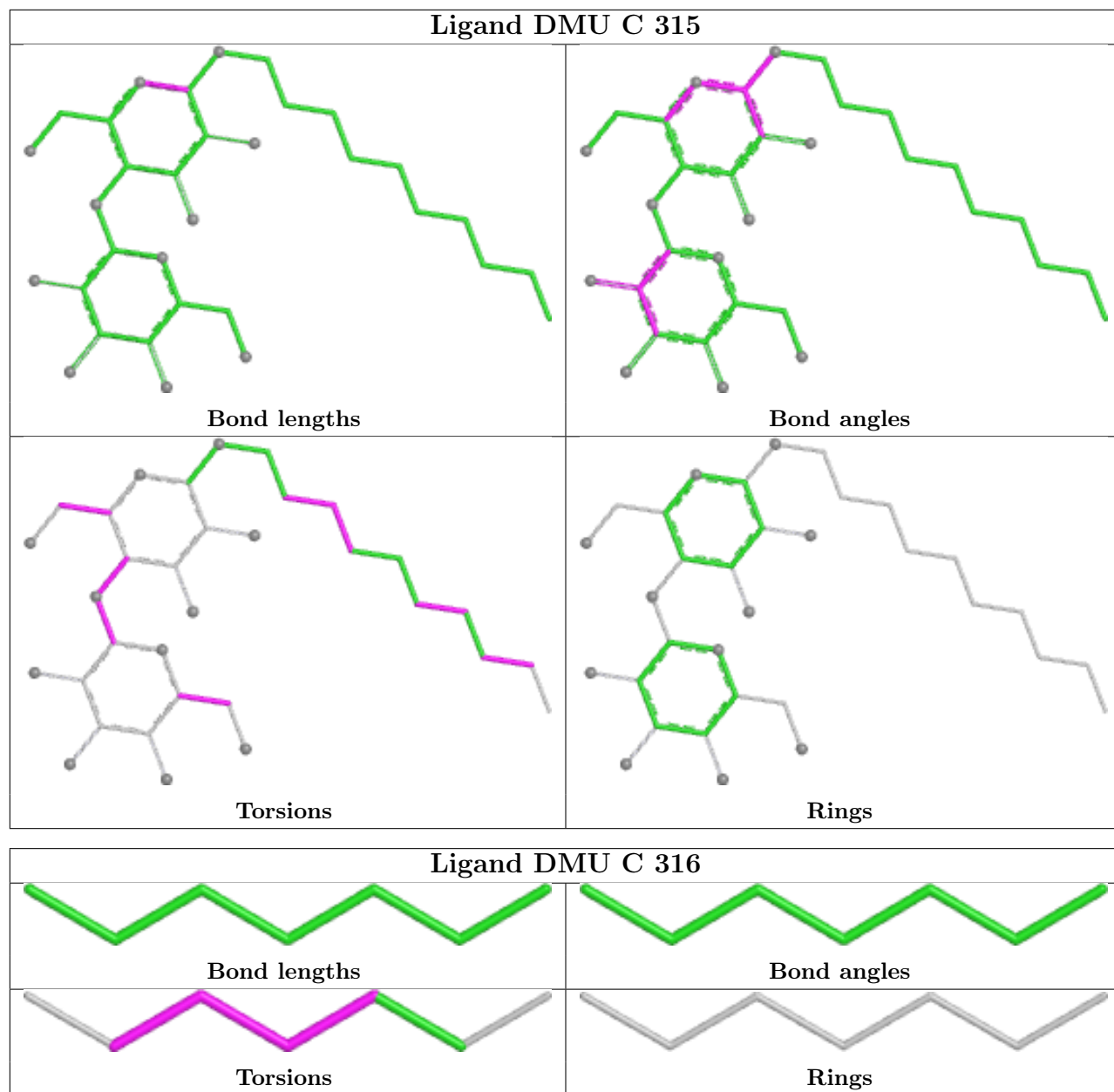
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	P	305	CDL	12	0
19	P	313	LFA	2	0
20	D	201	DMU	2	0
18	Y	101	CDL	8	0
20	L	102	DMU	1	0
27	T	102	PEK	5	0
19	C	314	LFA	1	0
24	G	102	CHD	1	0
20	Q	201	DMU	3	0
20	Y	102	DMU	2	0
14	N	601	HEA	3	0
19	C	312	LFA	2	0
19	P	308	LFA	2	0
24	C	301	CHD	1	0
19	A	607	LFA	6	0
14	A	602	HEA	1	0
20	P	319	DMU	1	0
19	C	309	LFA	3	0
22	C	303	PGV	3	0
19	C	313	LFA	3	0
19	G	106	LFA	7	0
20	O	303	DMU	1	0
20	C	323	DMU	1	0
20	P	324	DMU	2	0
24	C	305	CHD	2	0
14	A	601	HEA	2	0
20	A	609	DMU	1	0
19	C	307	LFA	2	0
14	N	602	HEA	1	0
24	P	306	CHD	2	0
20	A	608	DMU	1	0
24	P	302	CHD	1	0

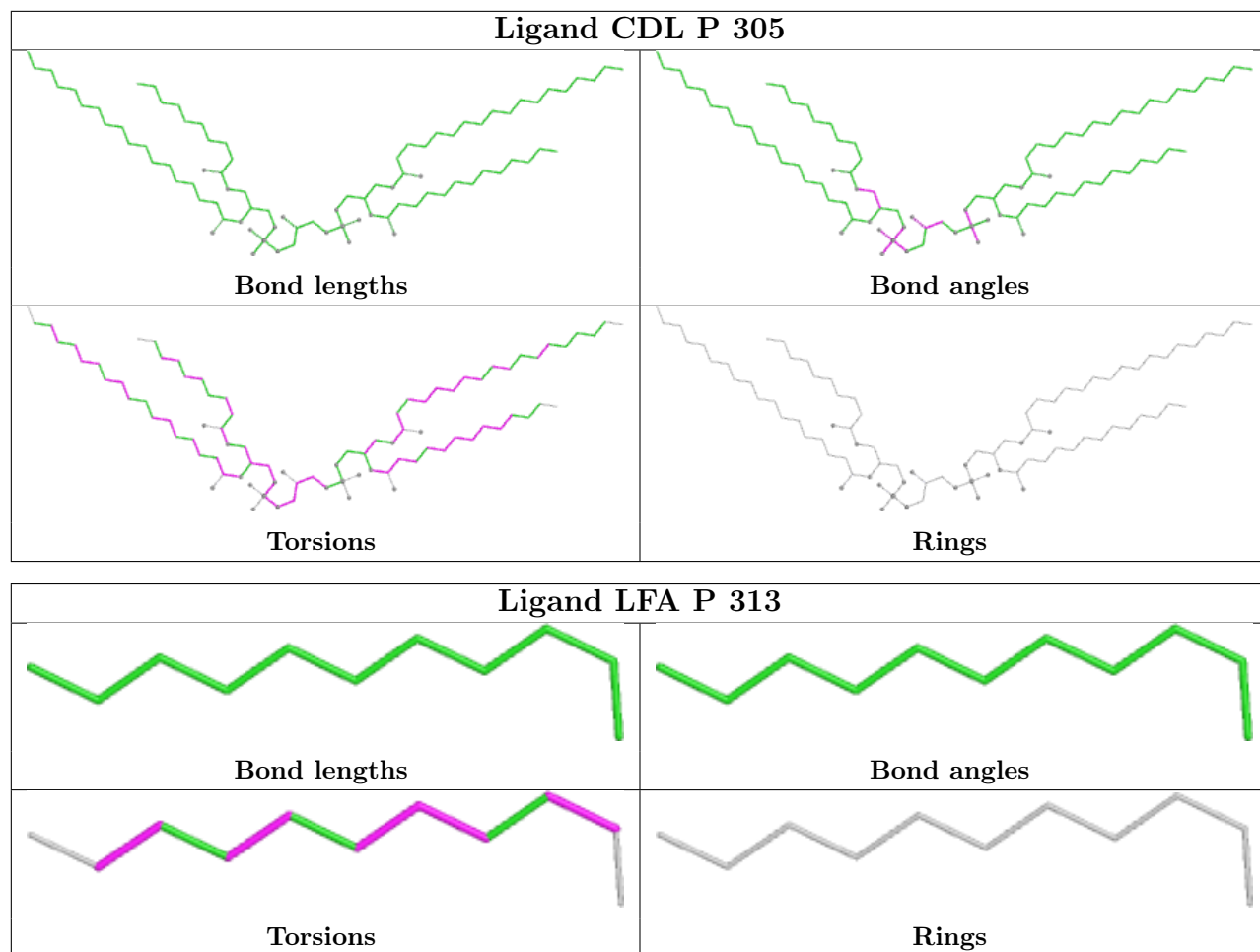
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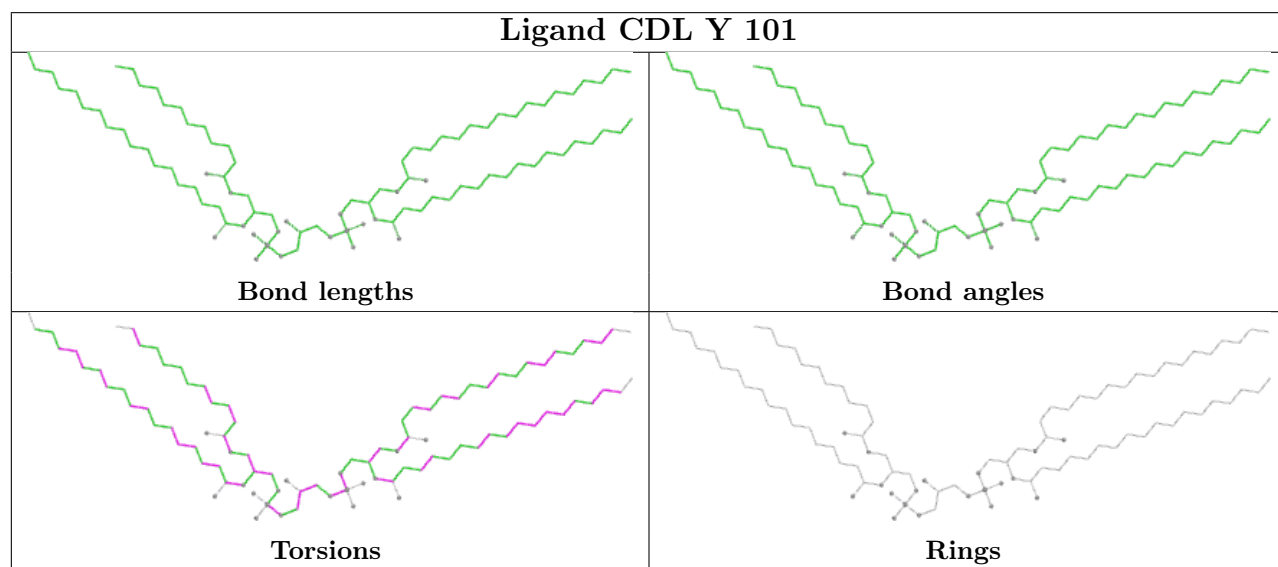
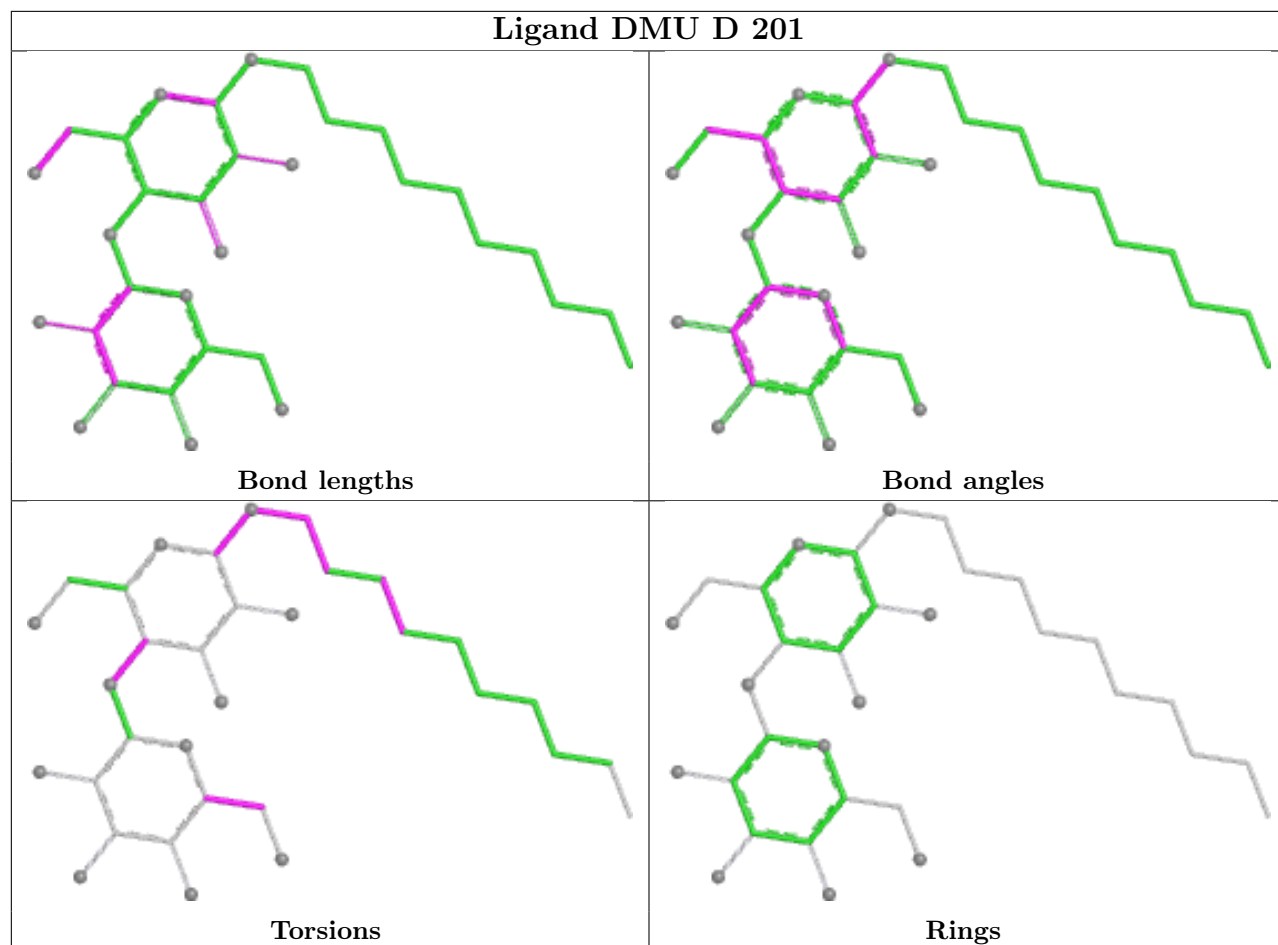
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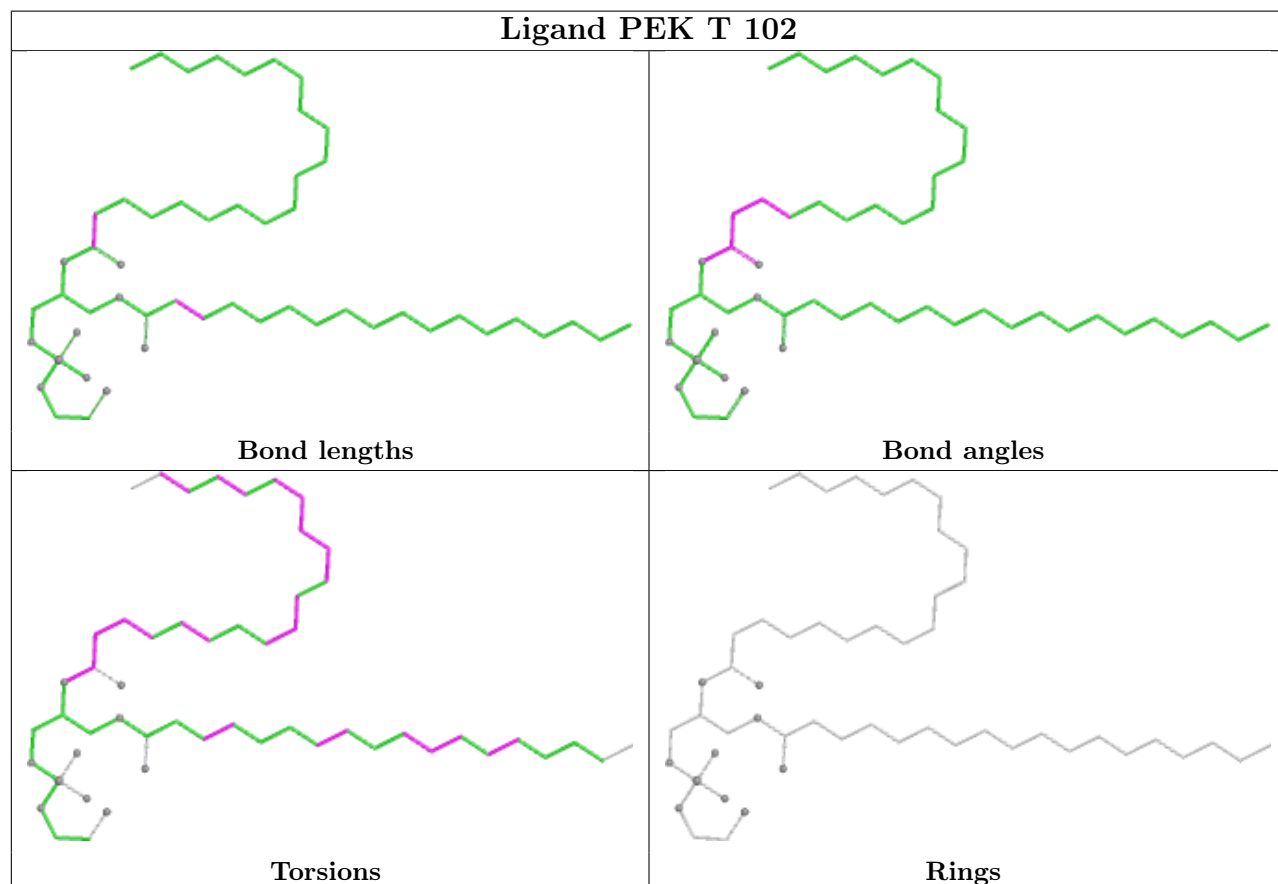
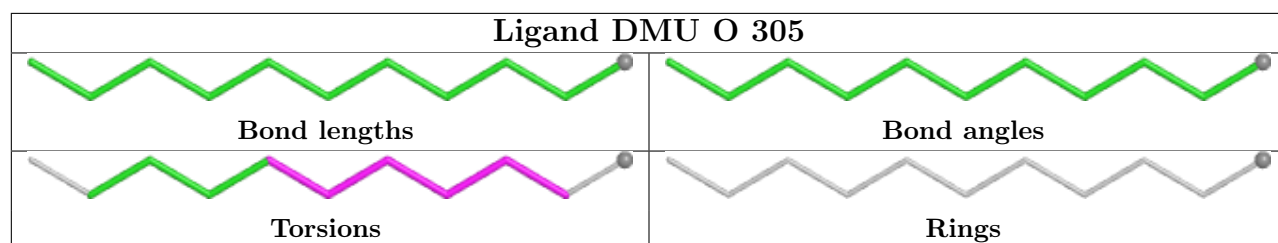
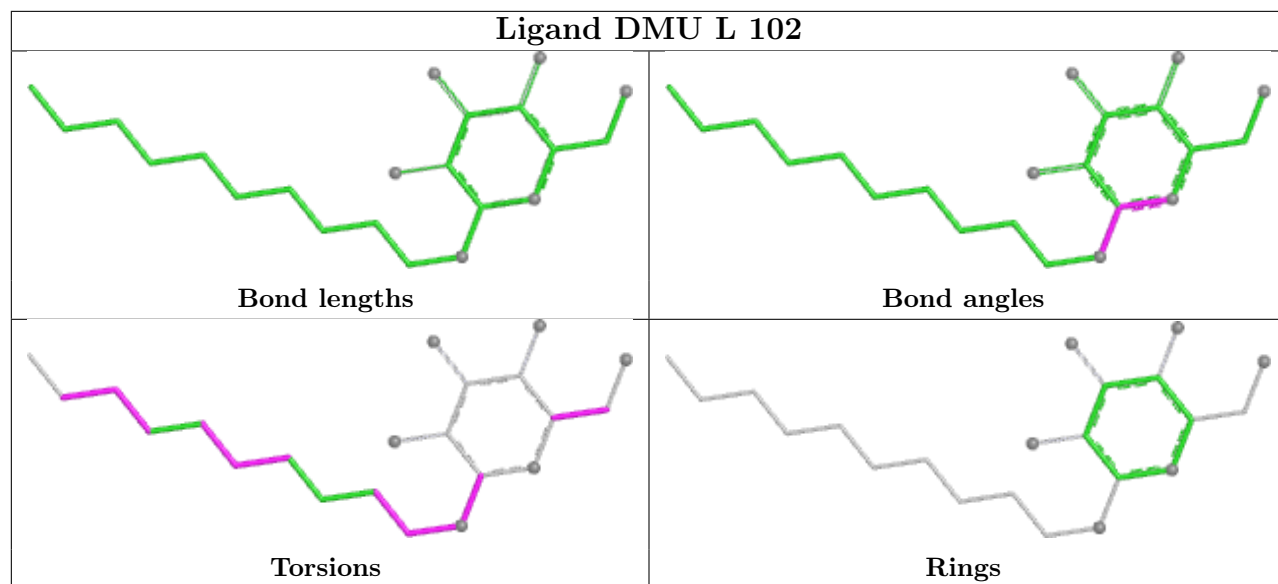
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	L	101	CDL	2	0
19	P	314	LFA	1	0
19	P	310	LFA	2	0
18	V	101	CDL	1	0
20	H	101	DMU	1	0
20	C	319	DMU	1	0
19	T	101	LFA	7	0
18	C	304	CDL	16	0
19	N	606	LFA	5	0

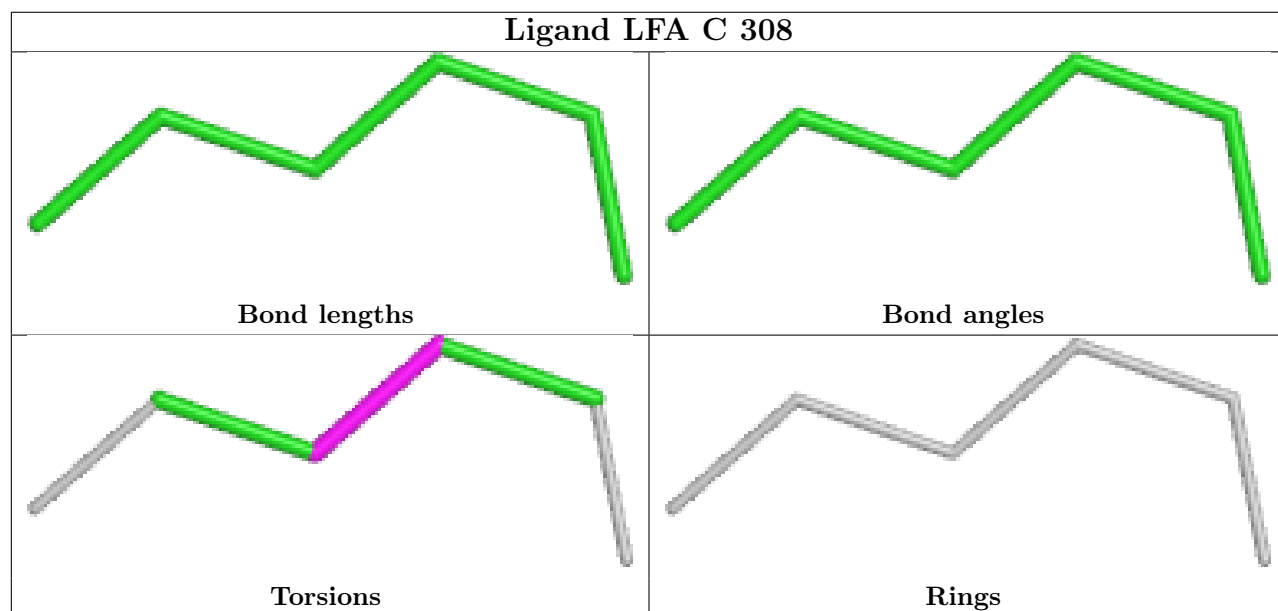
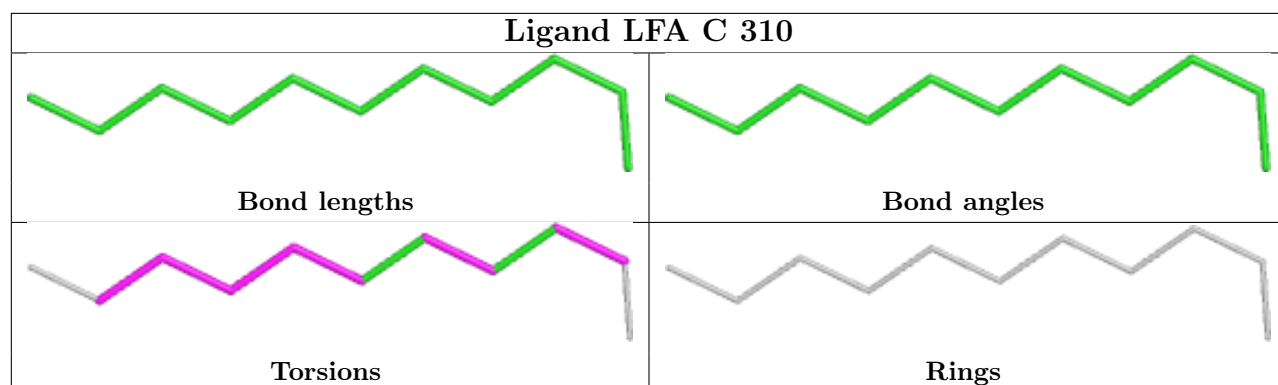
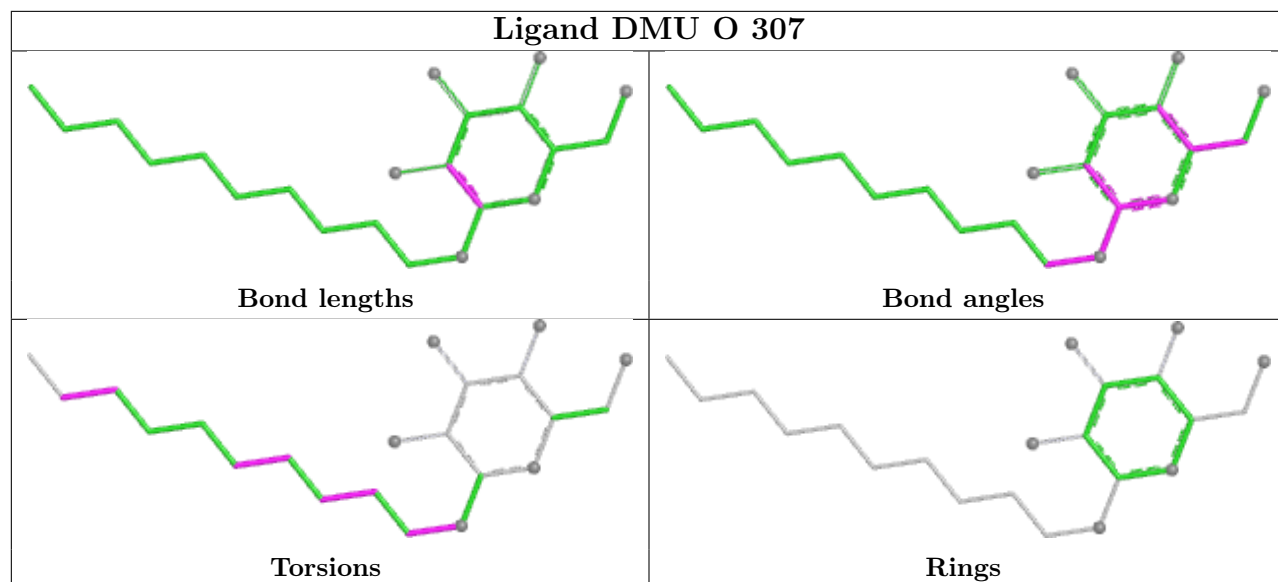
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

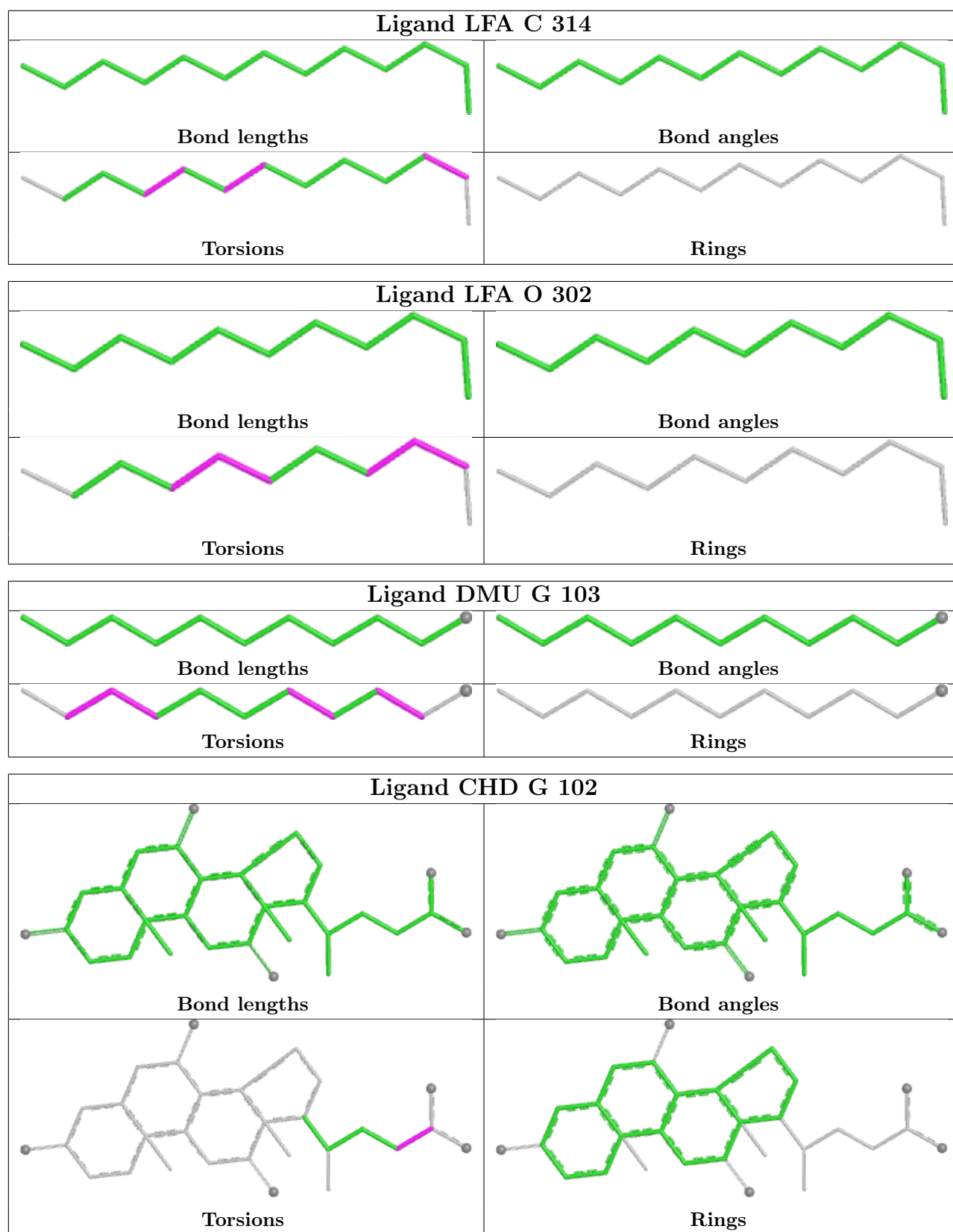


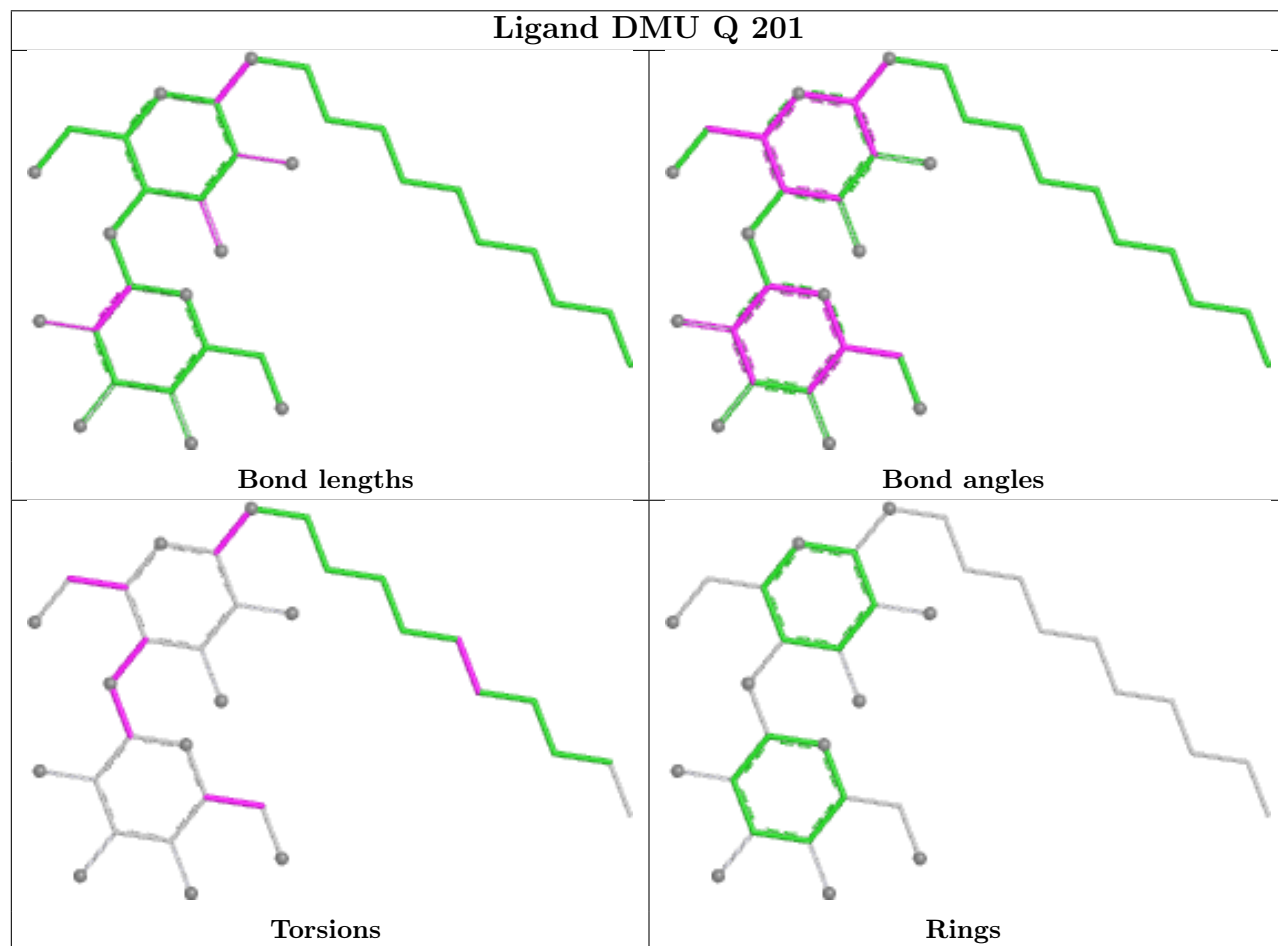
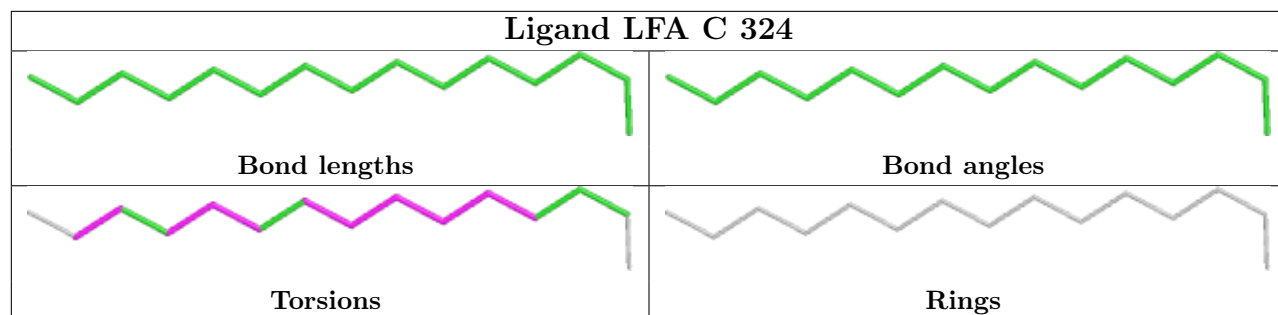


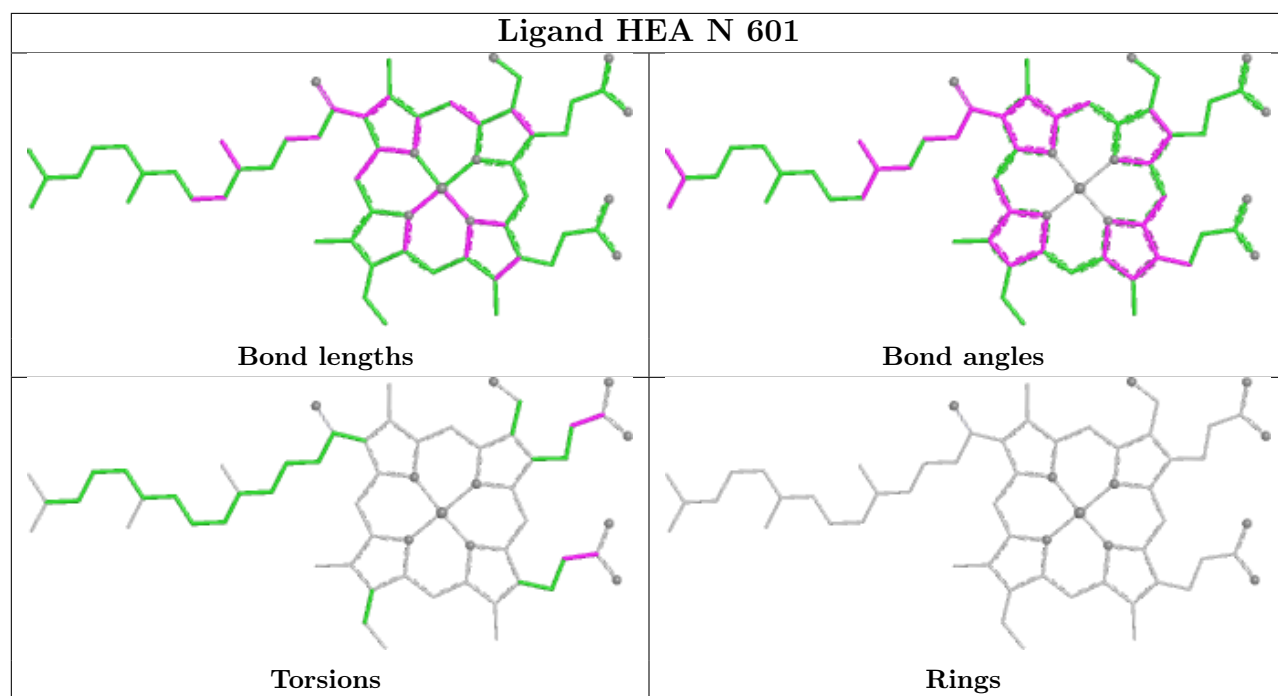
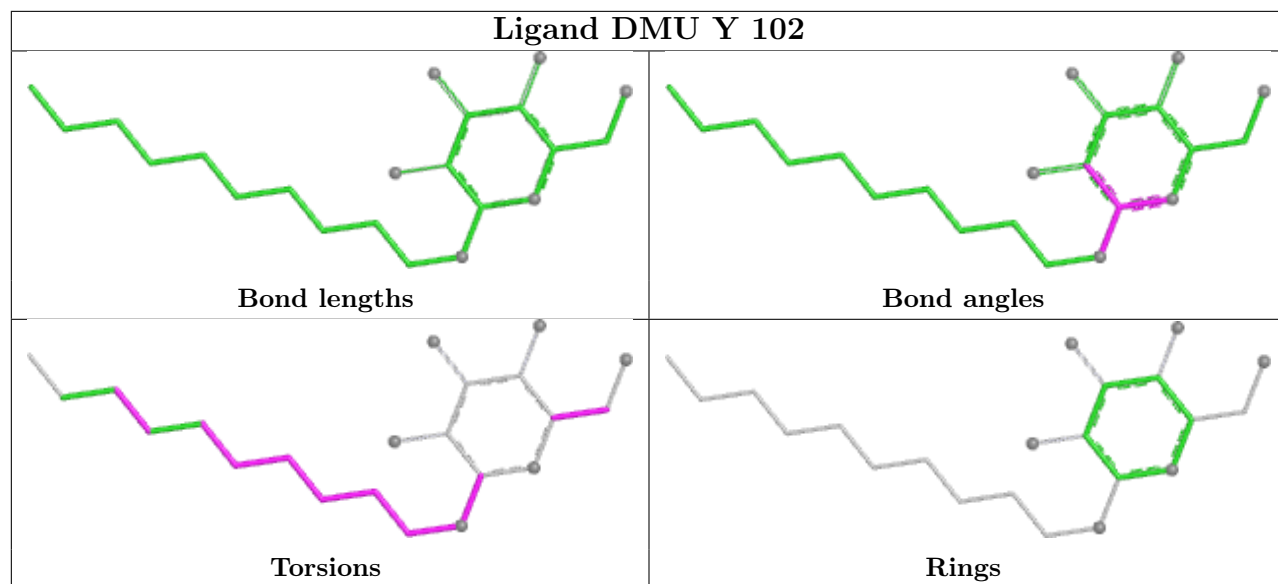


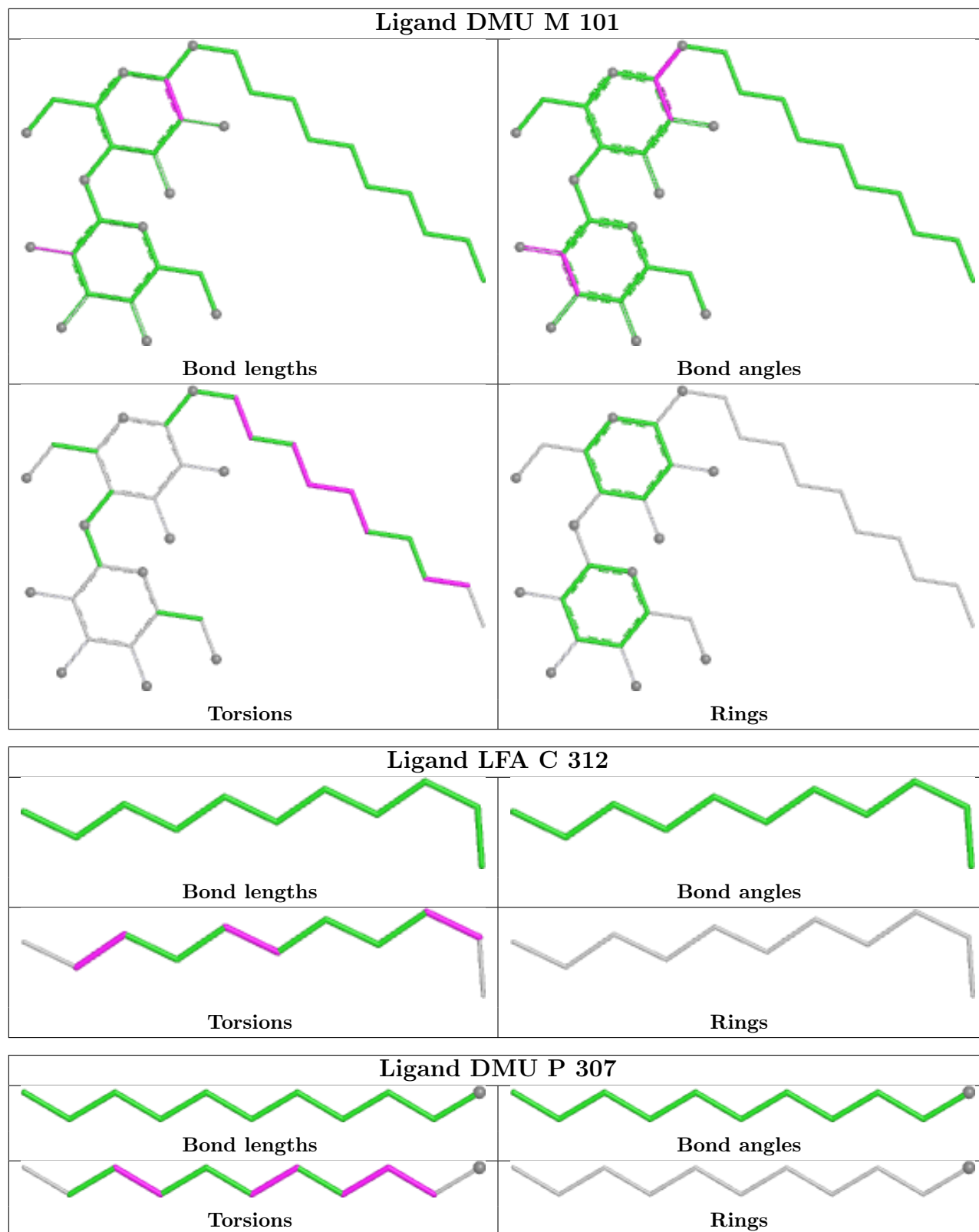


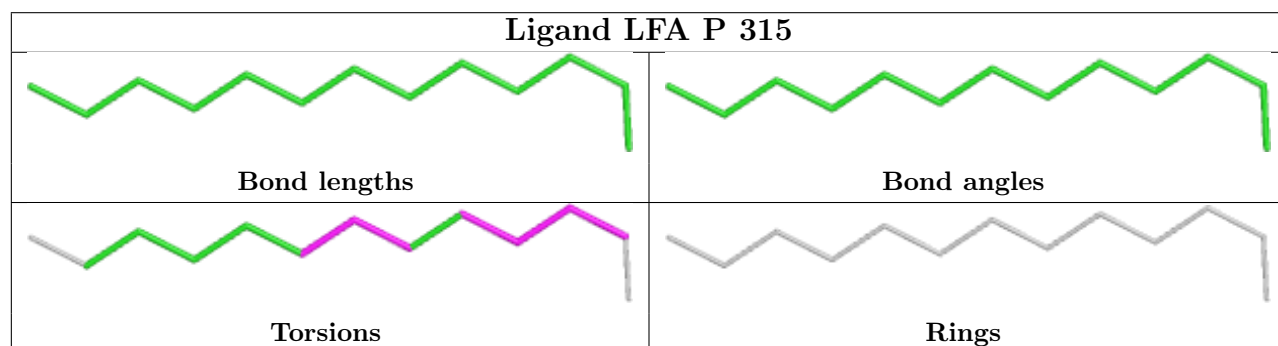
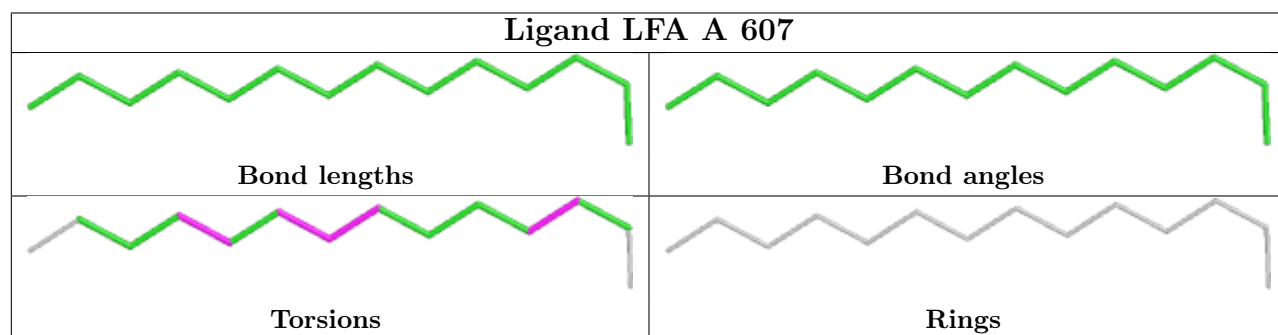
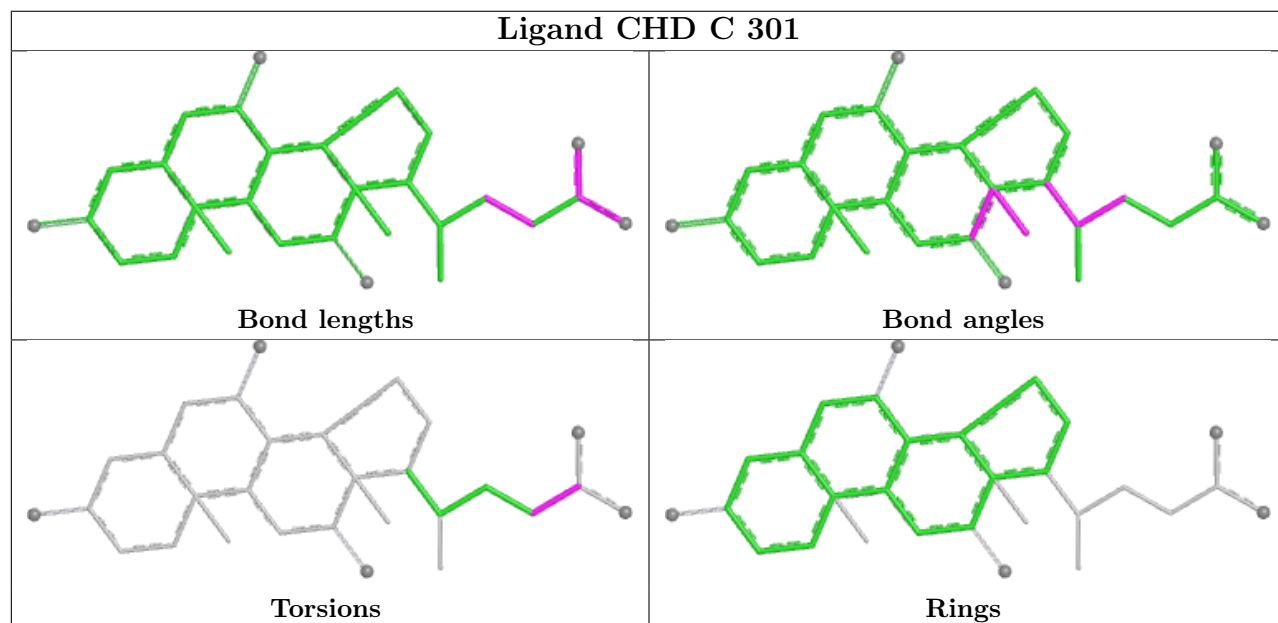
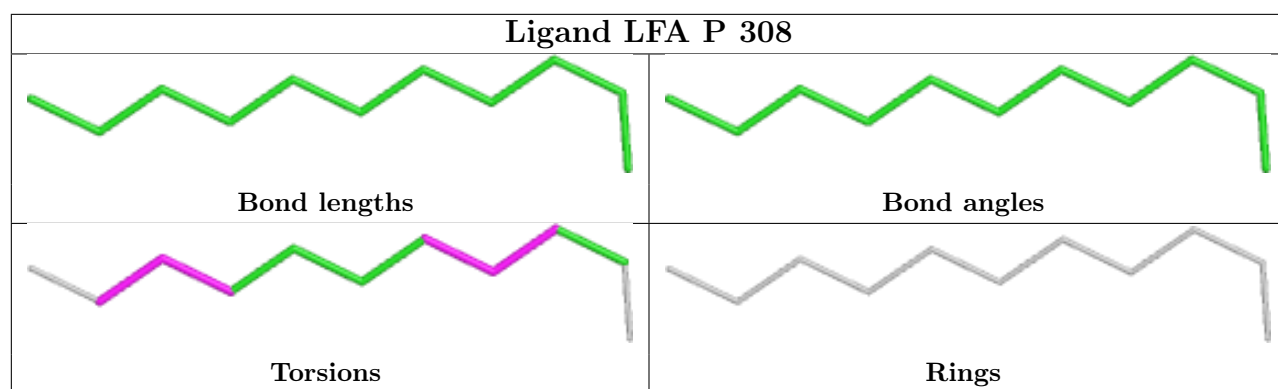


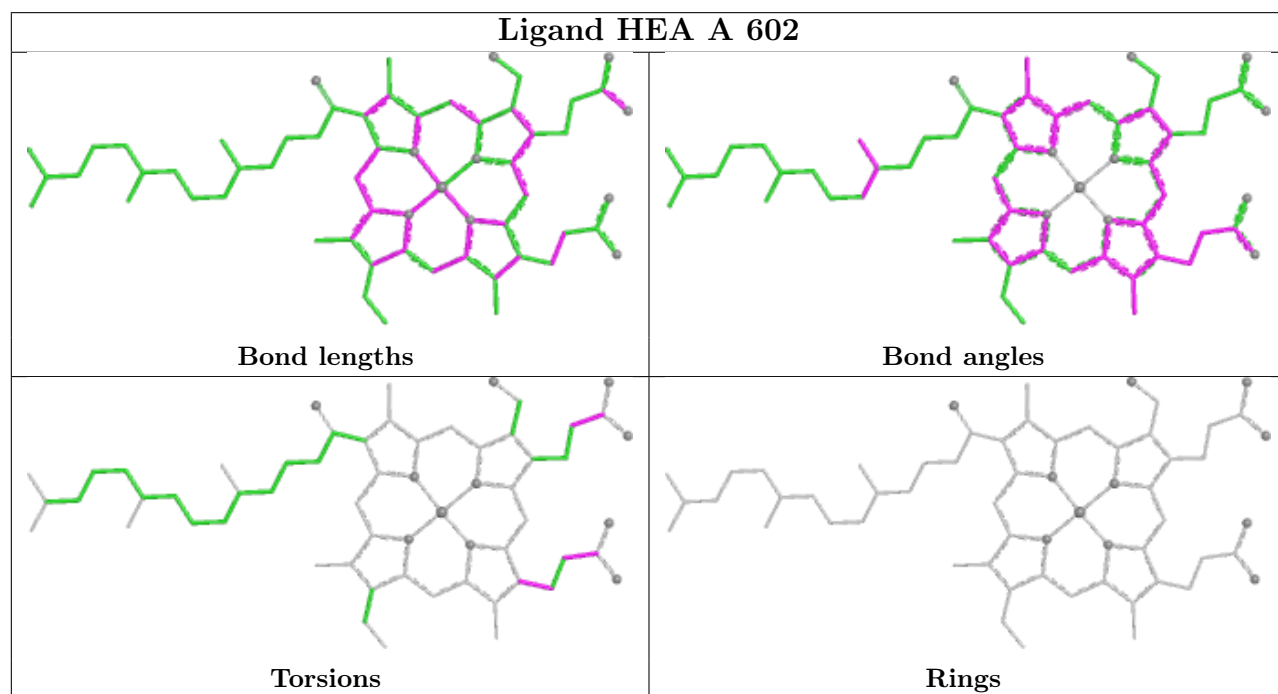
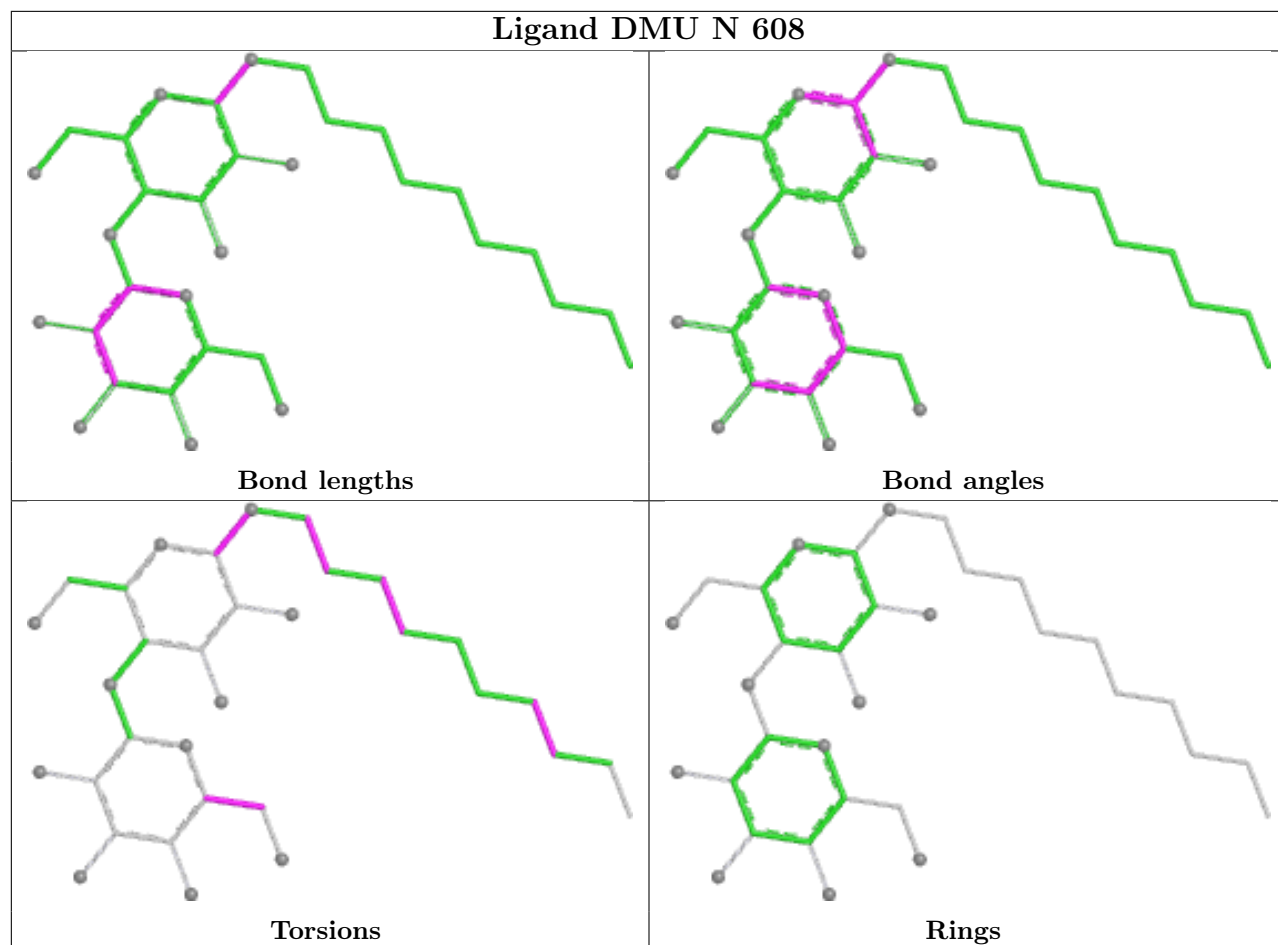


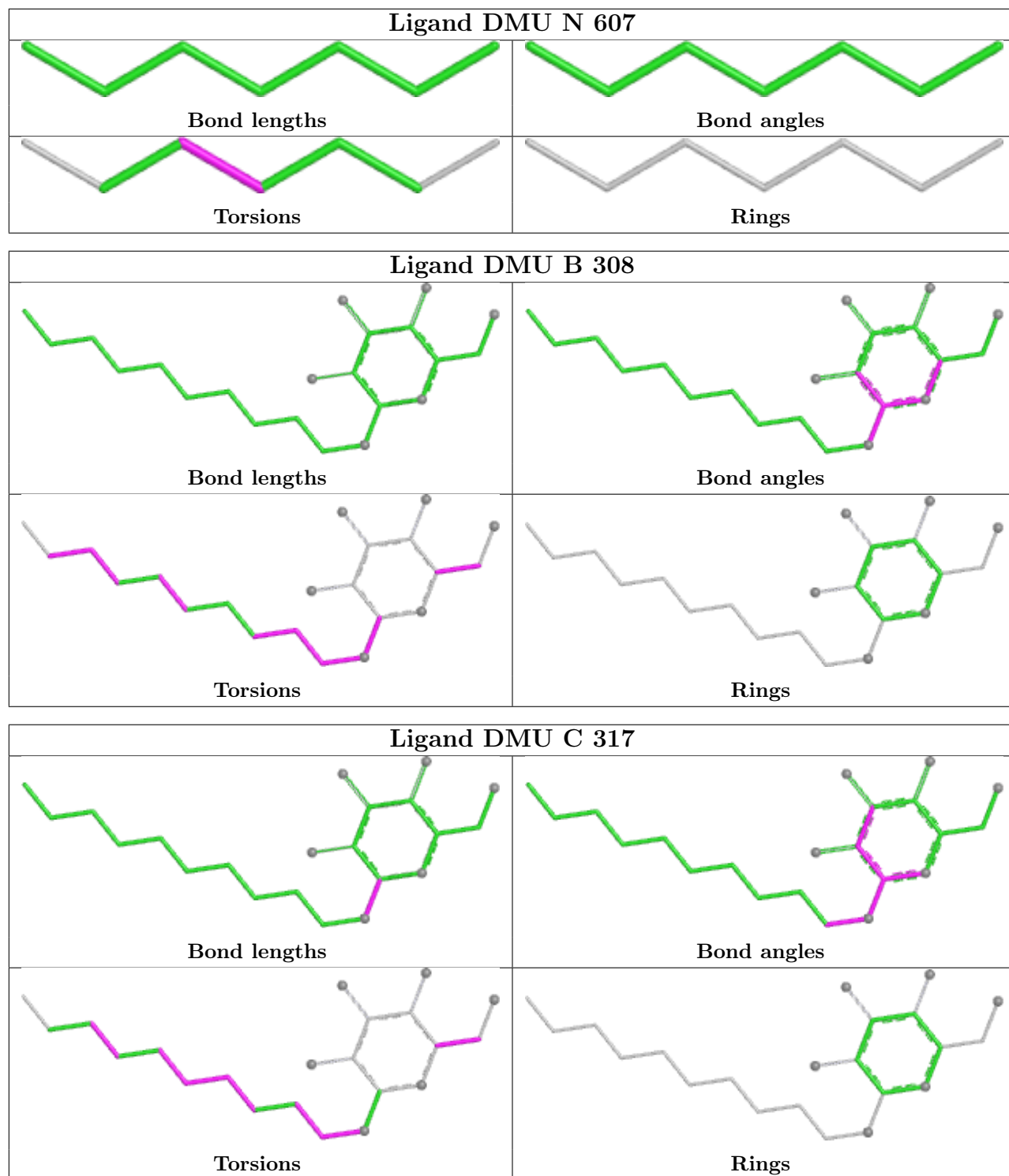


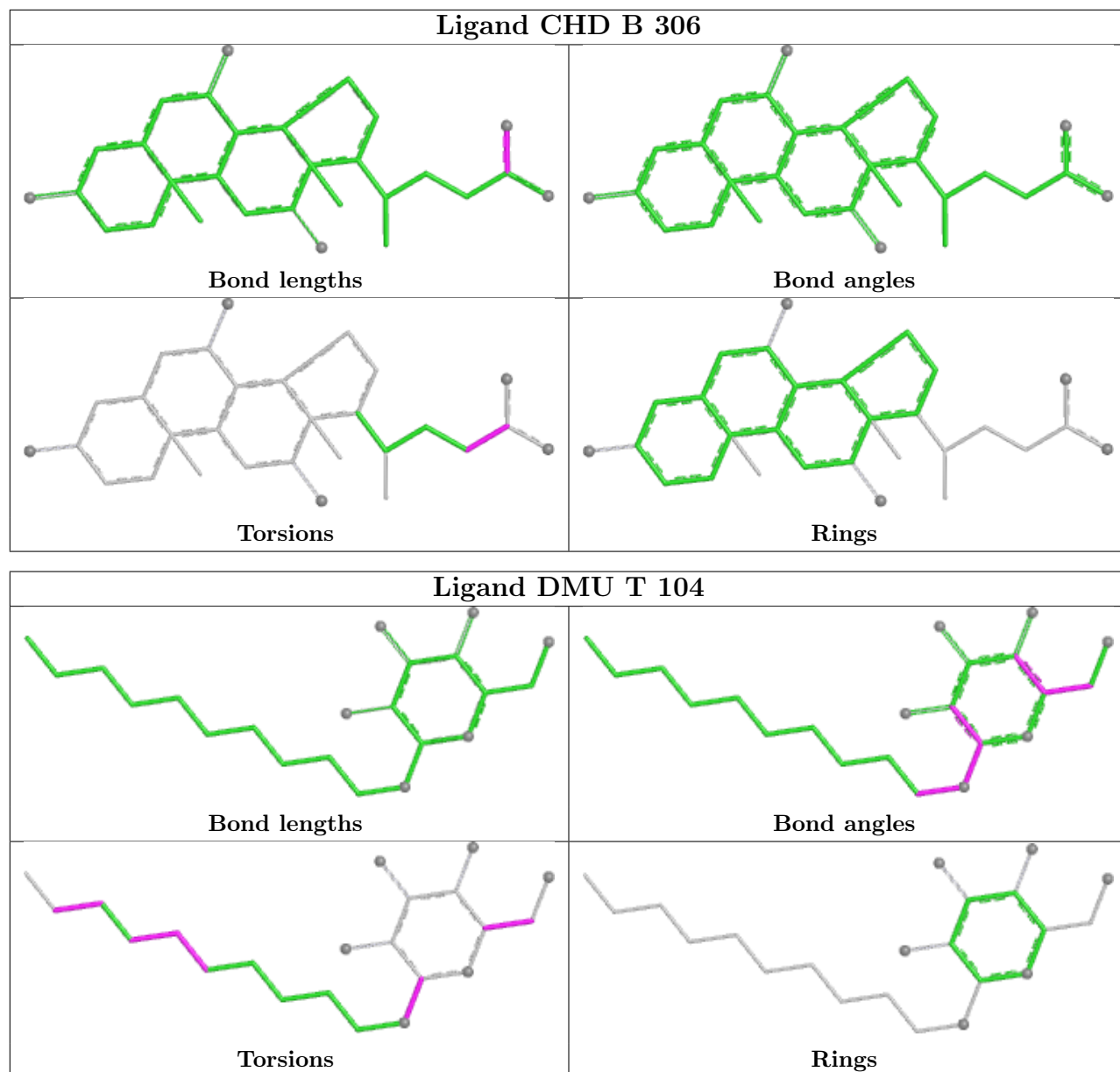


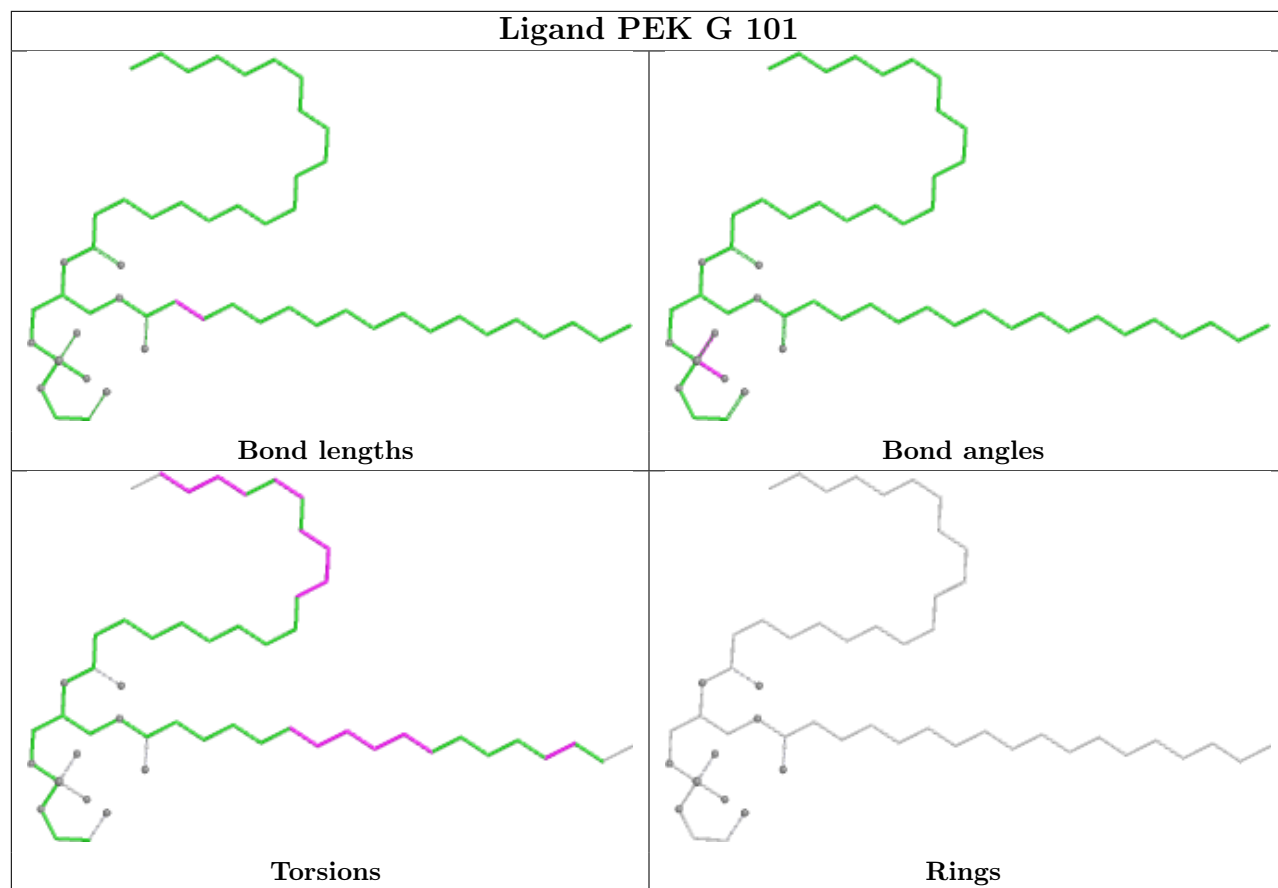


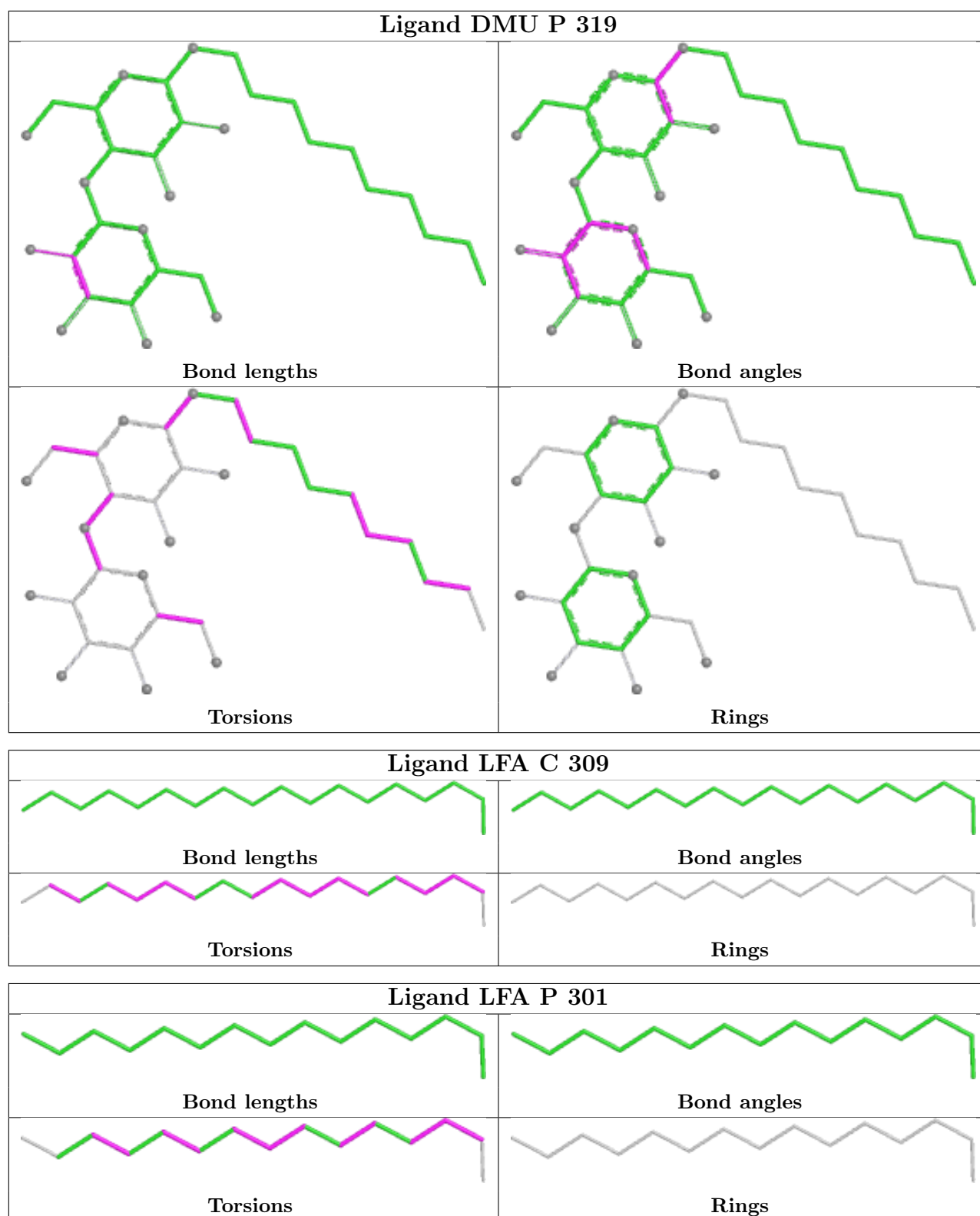


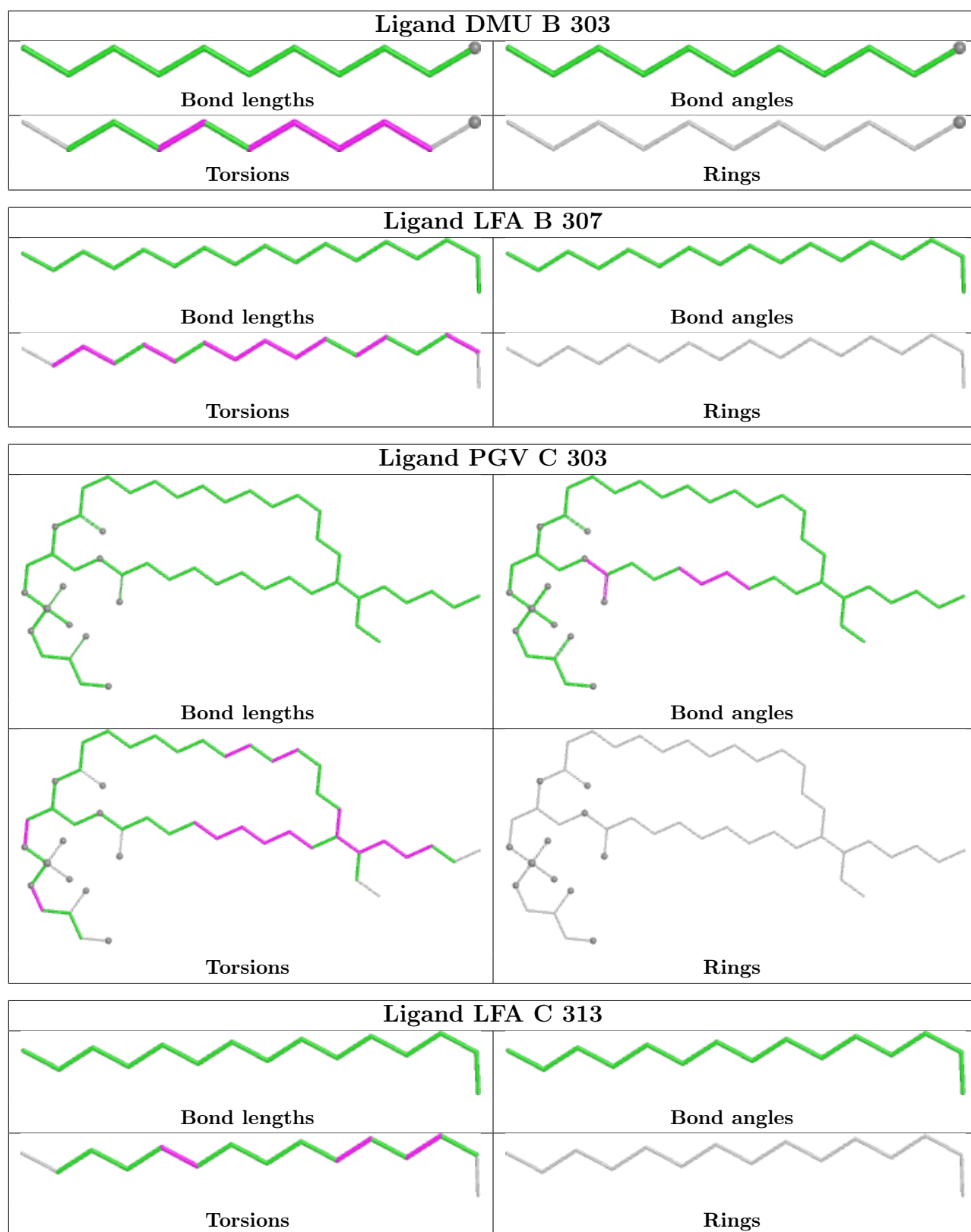


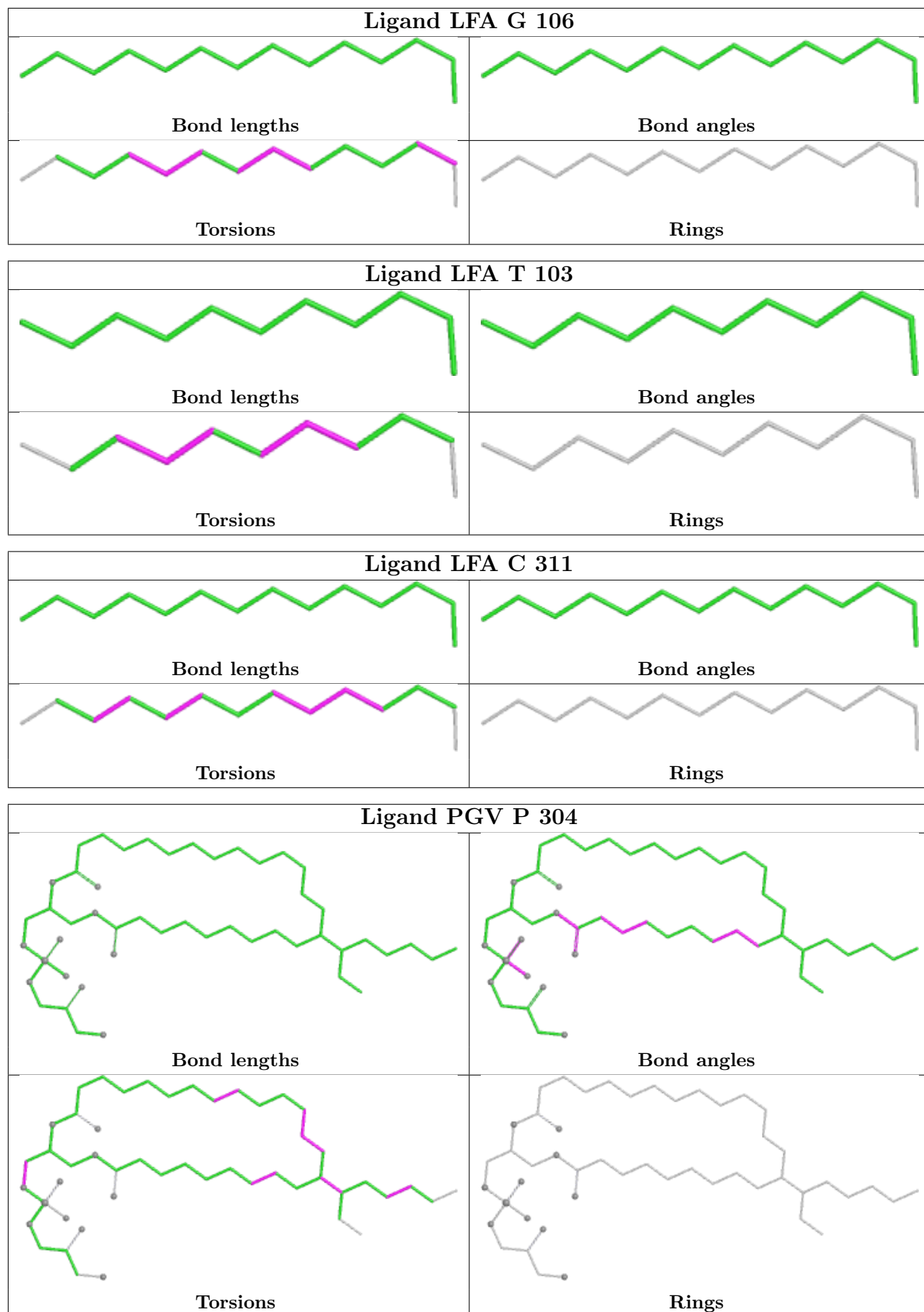


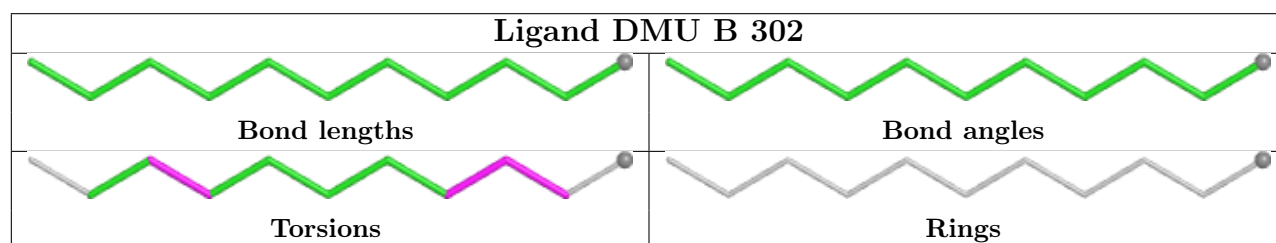
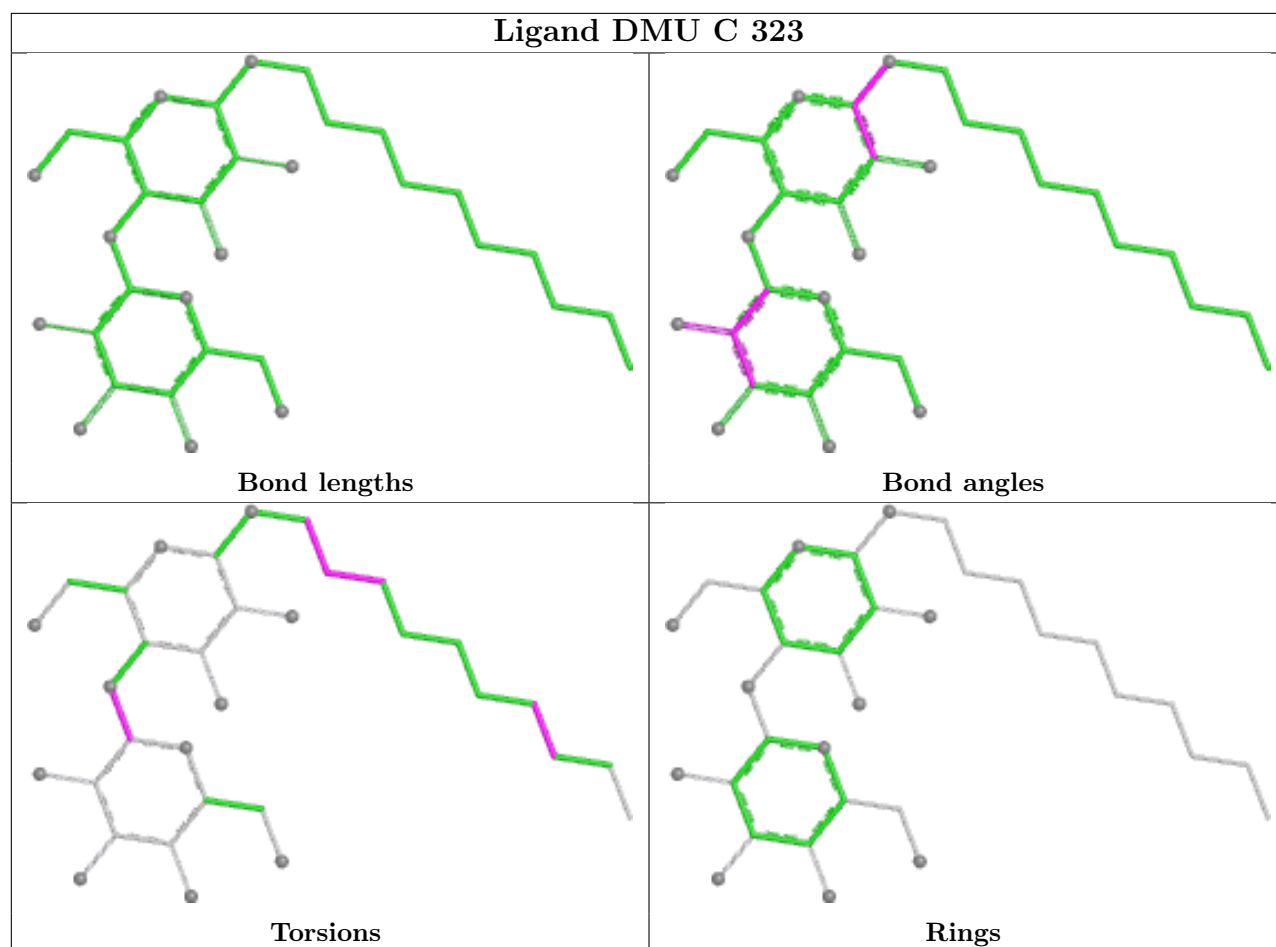
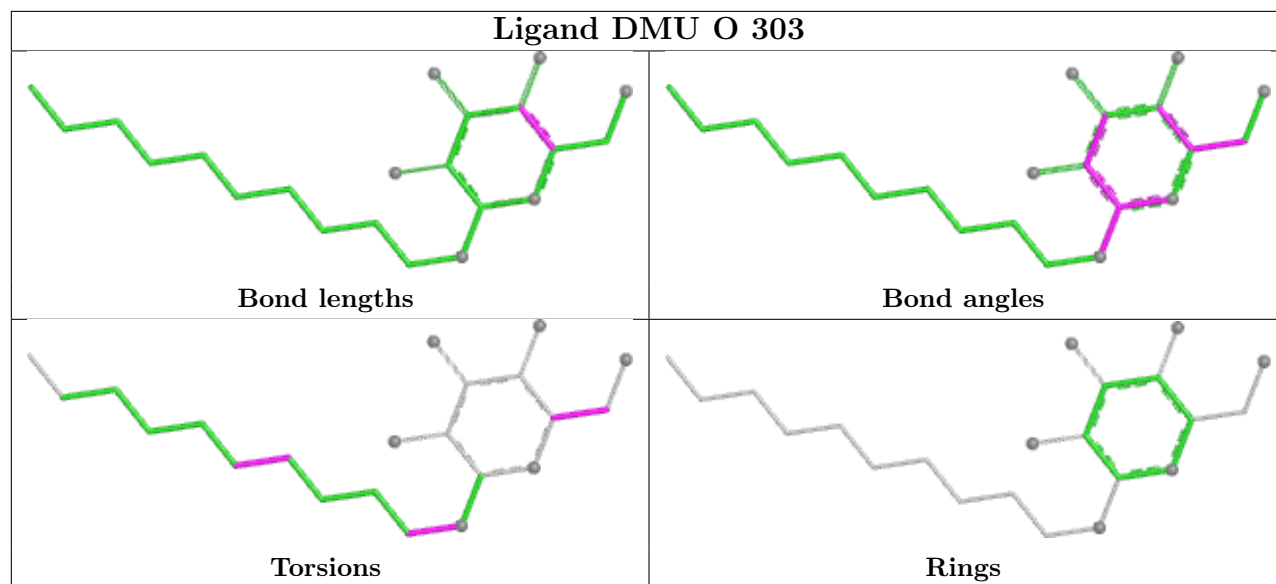


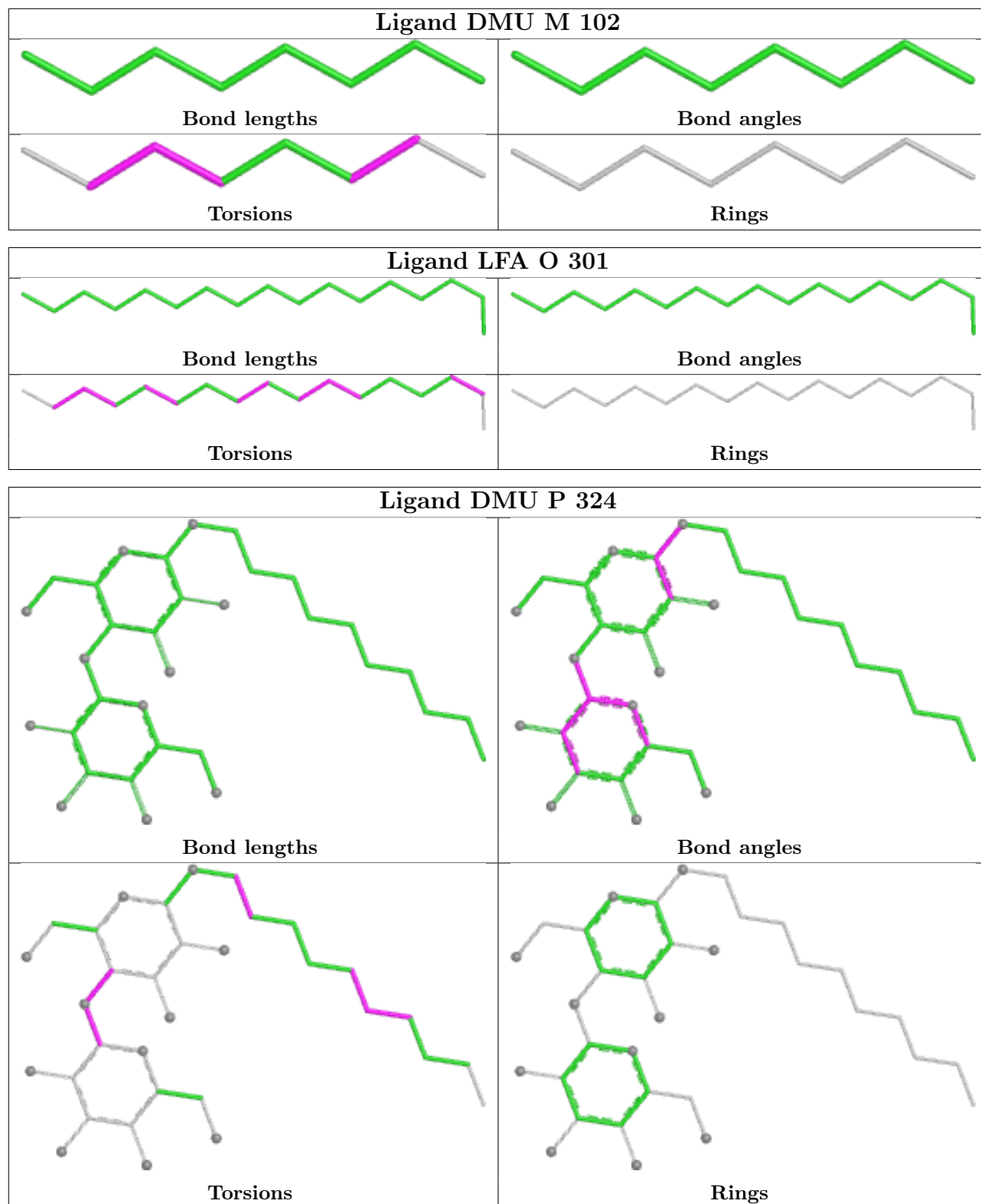


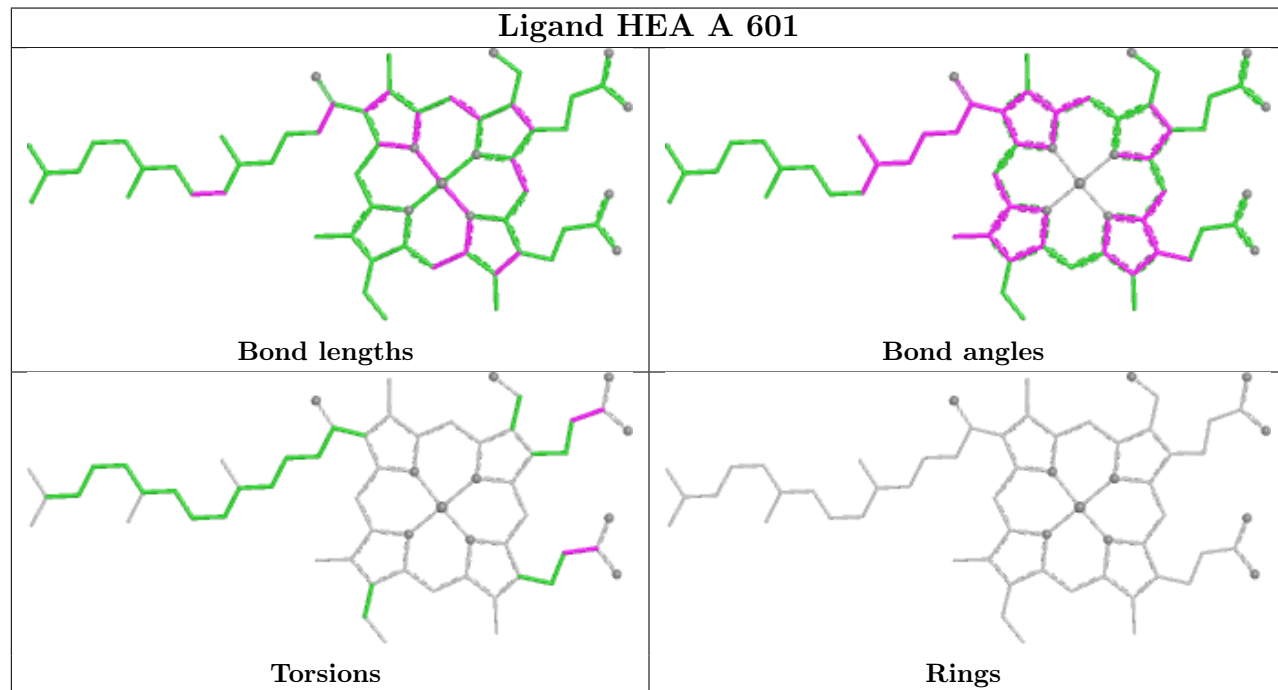
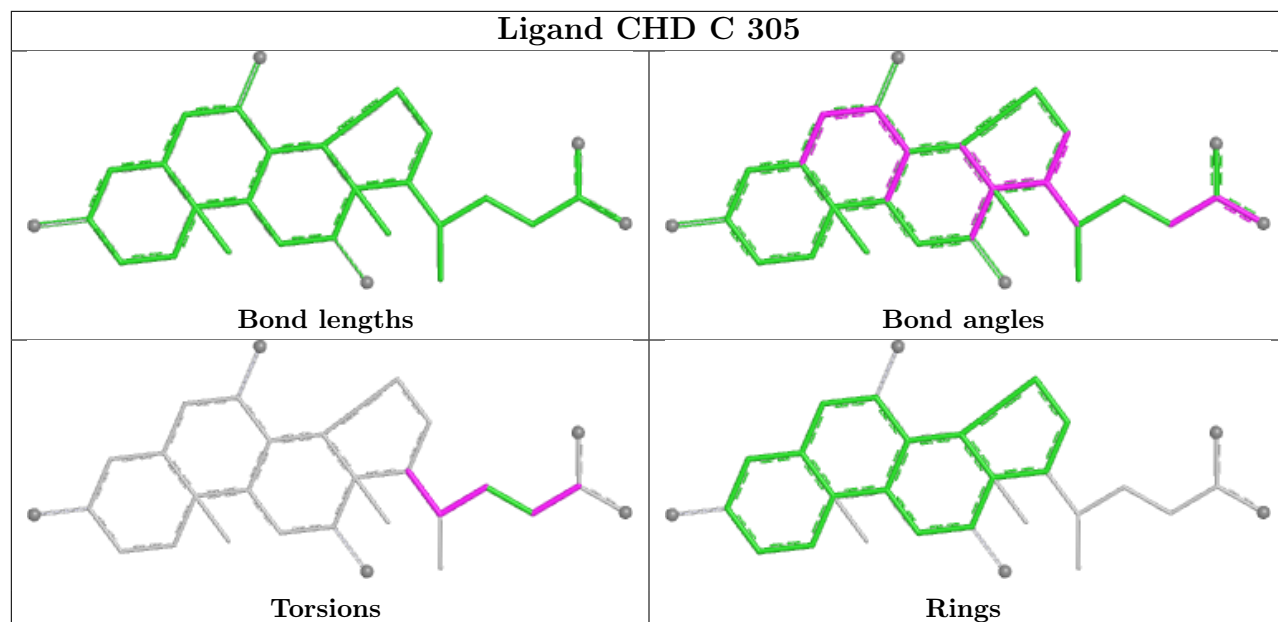


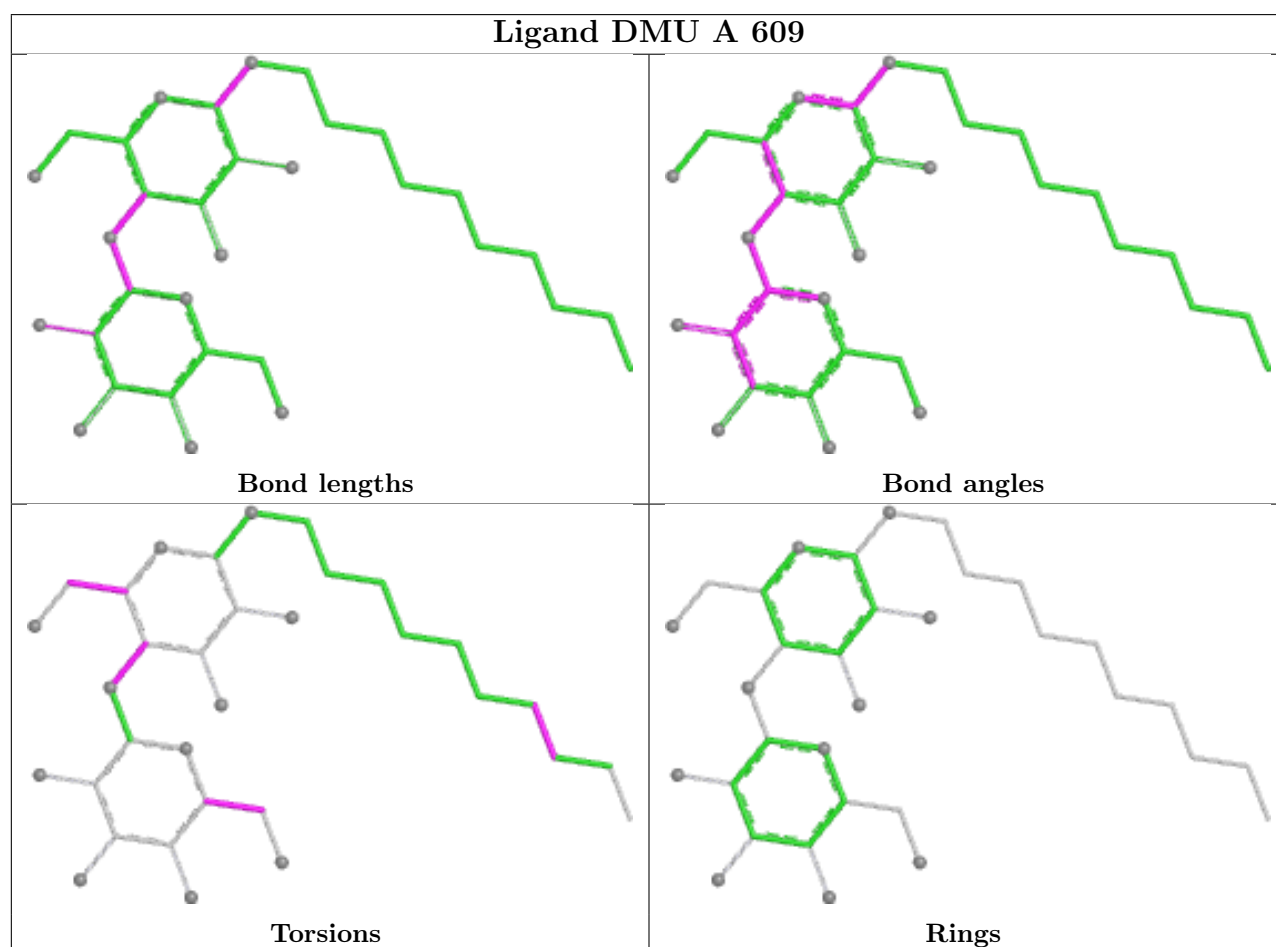
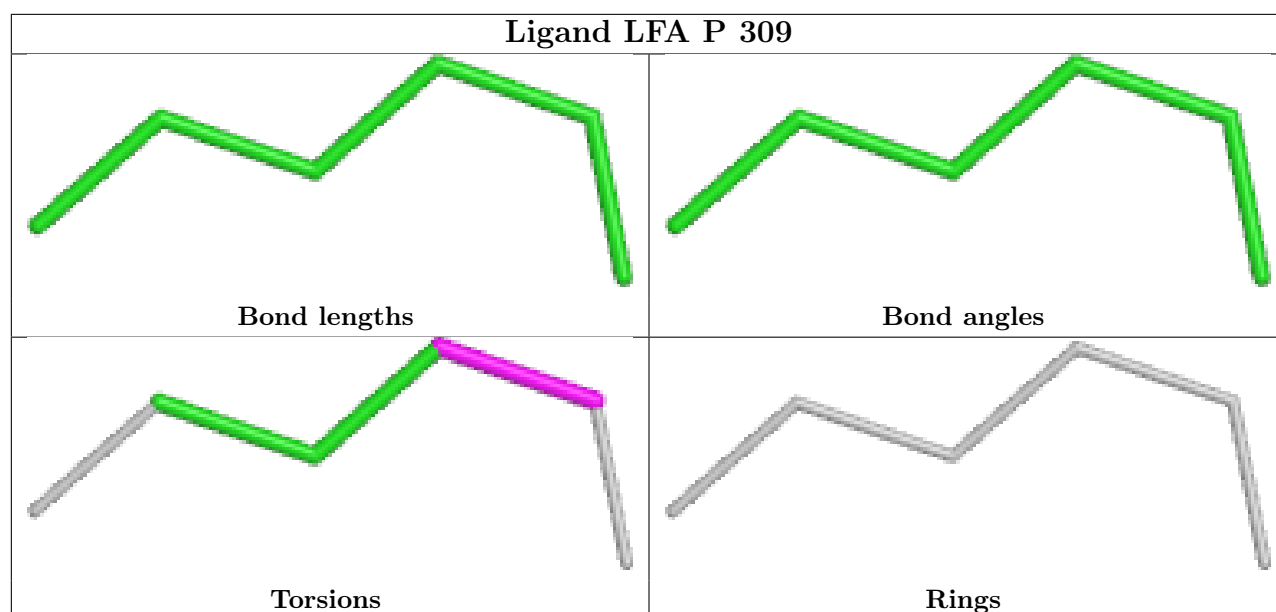


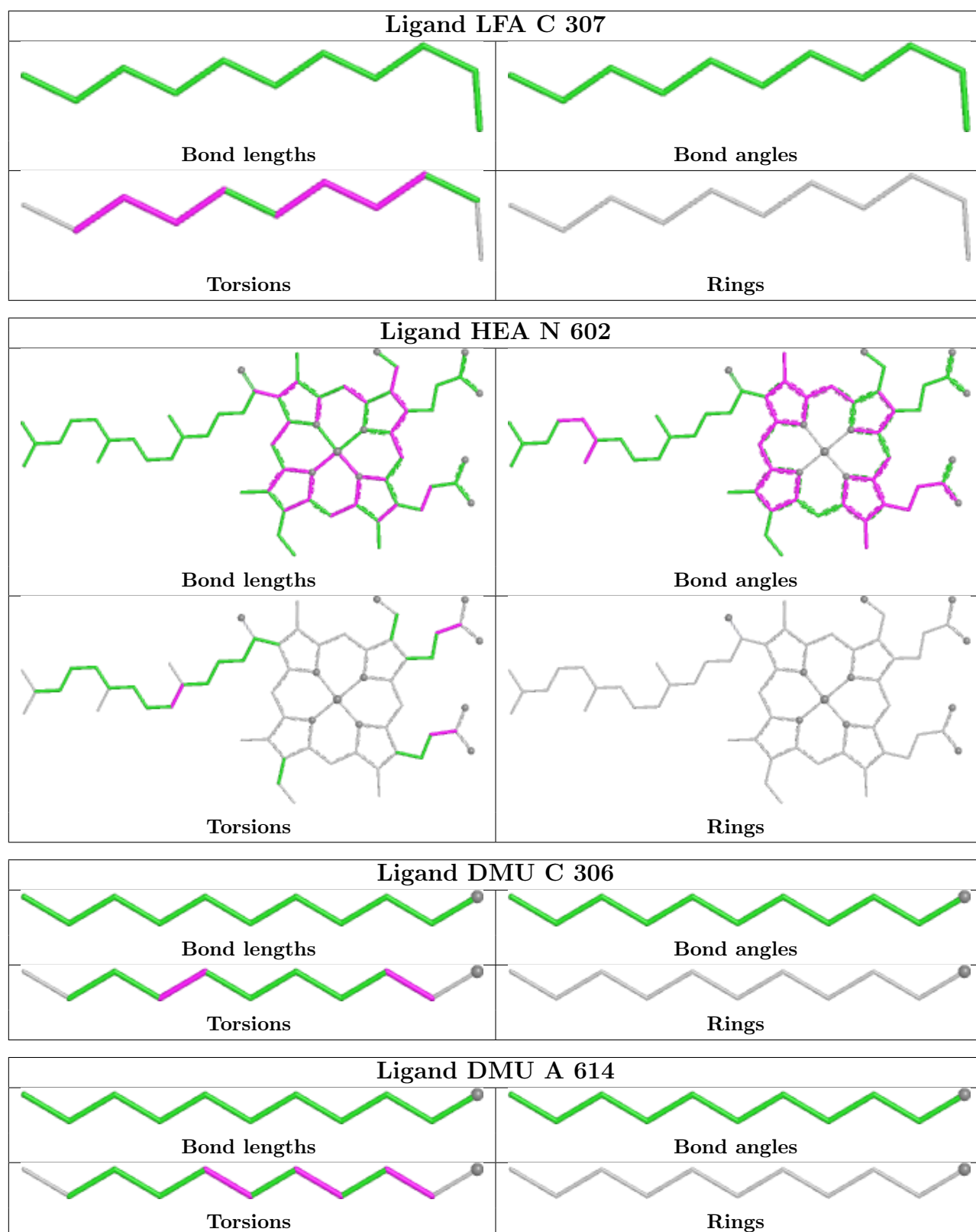


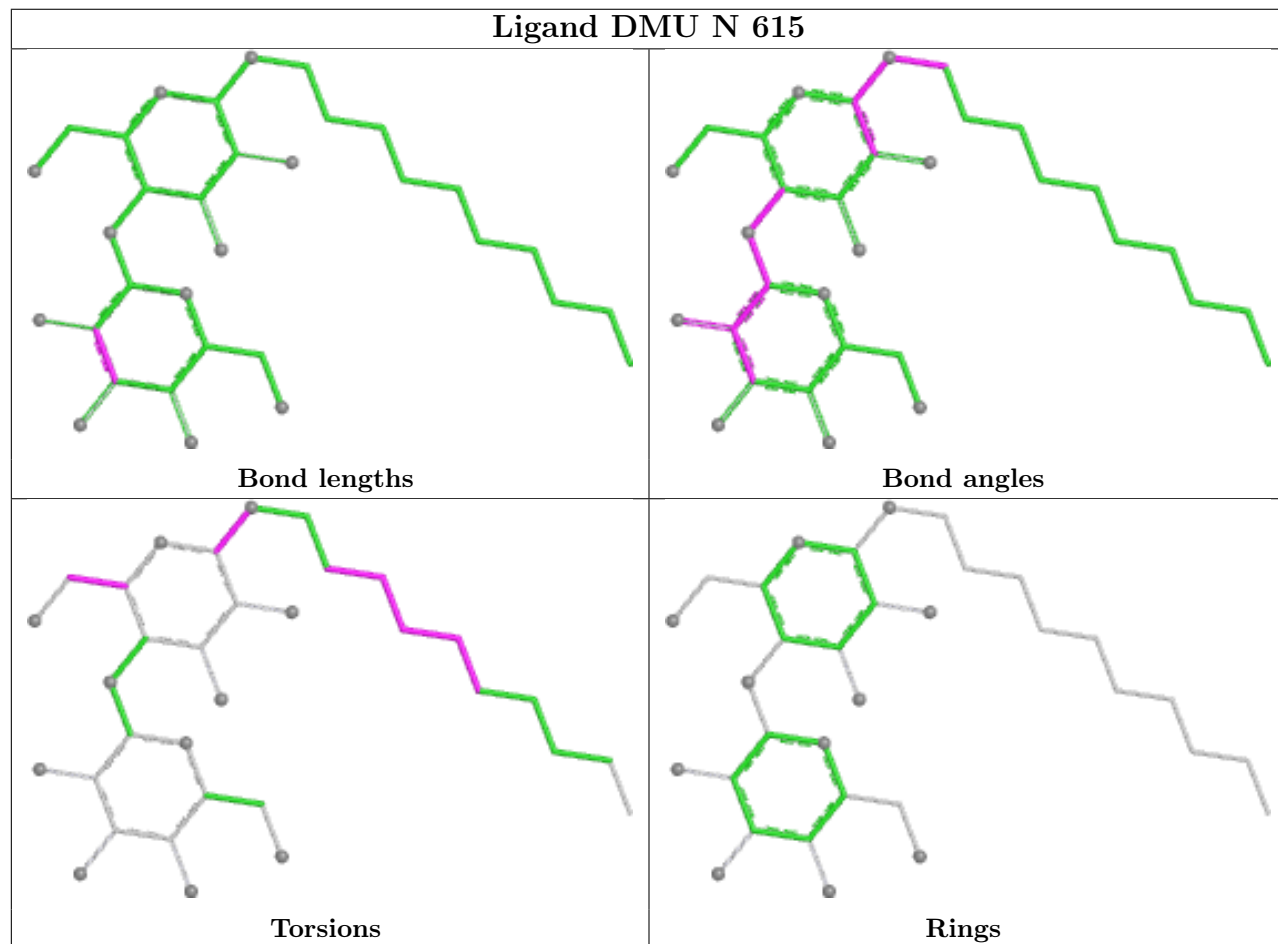
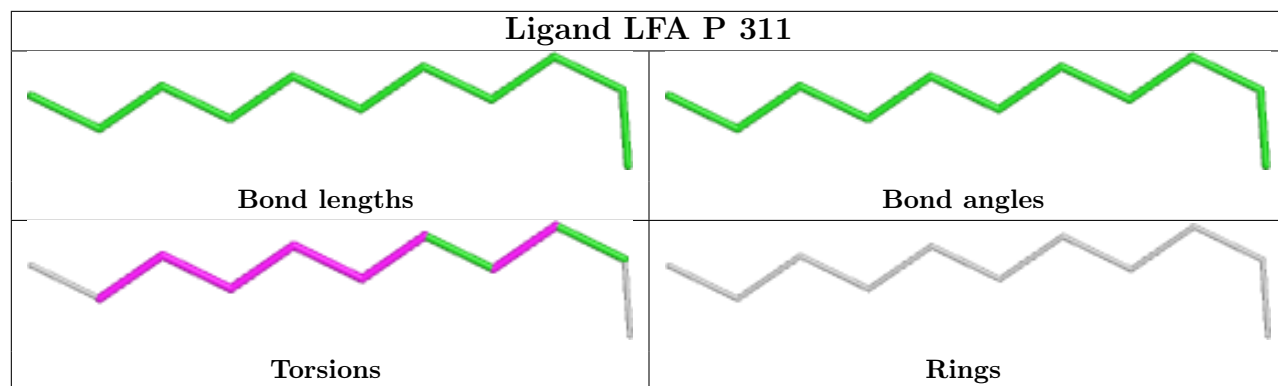


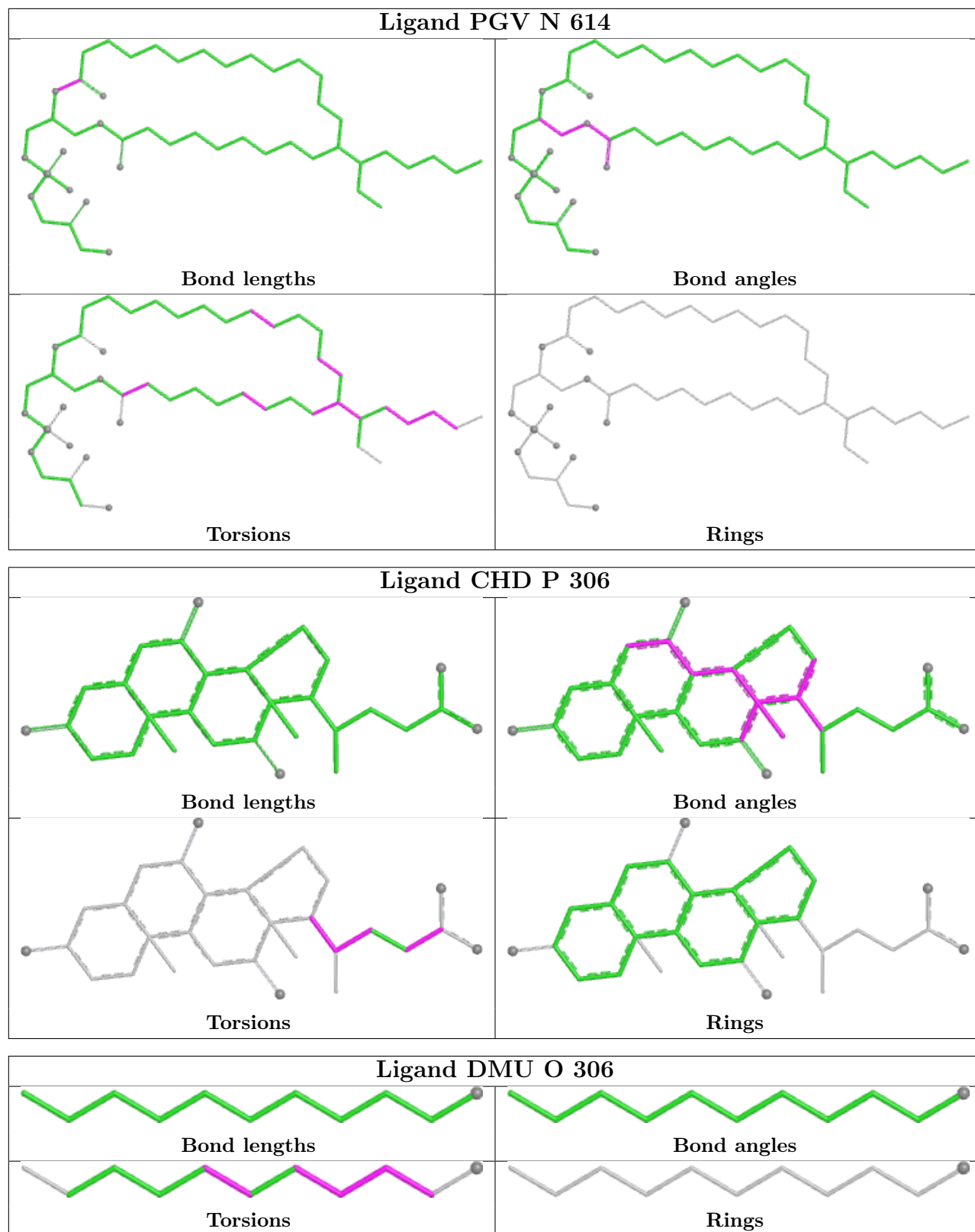


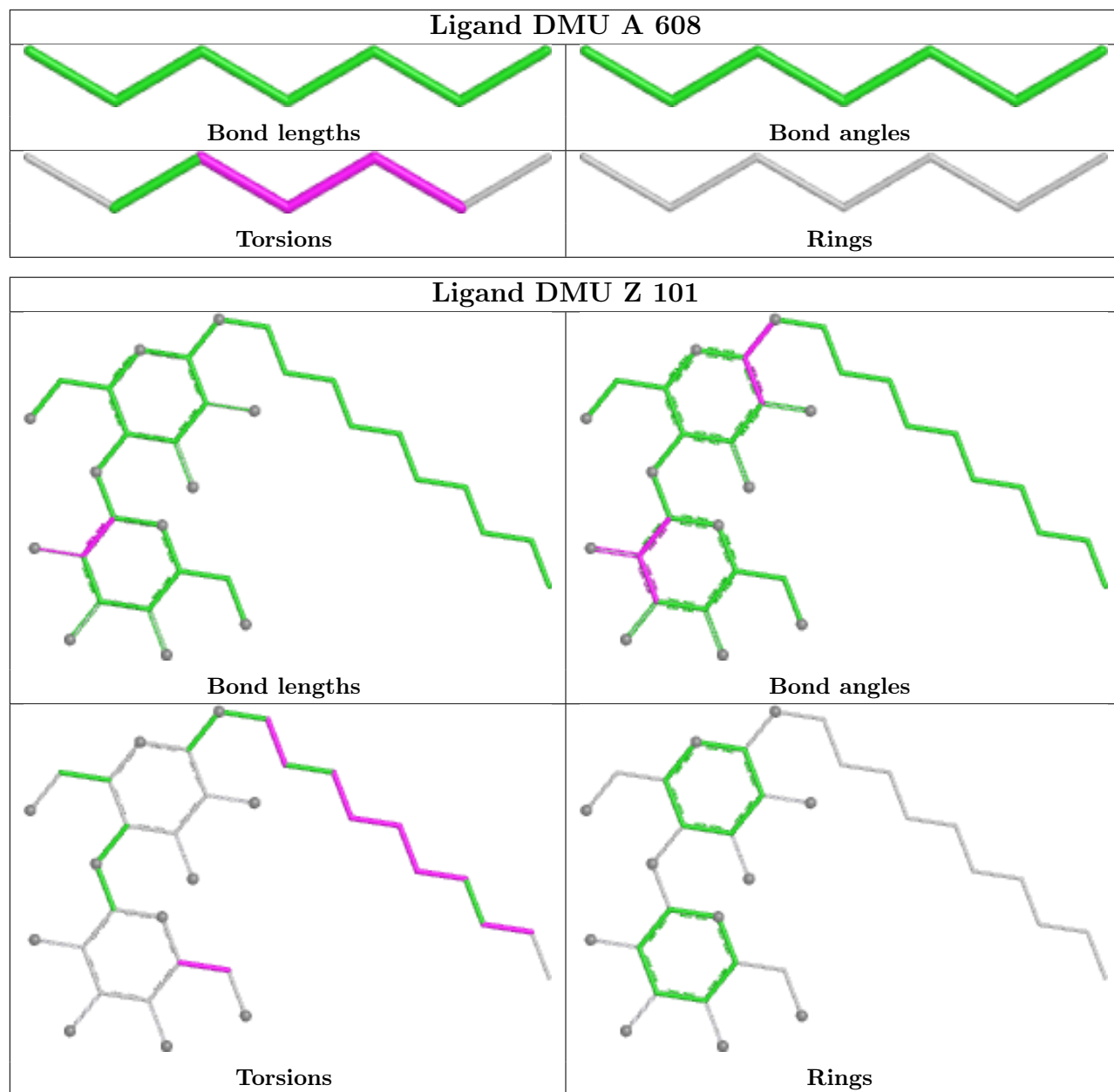


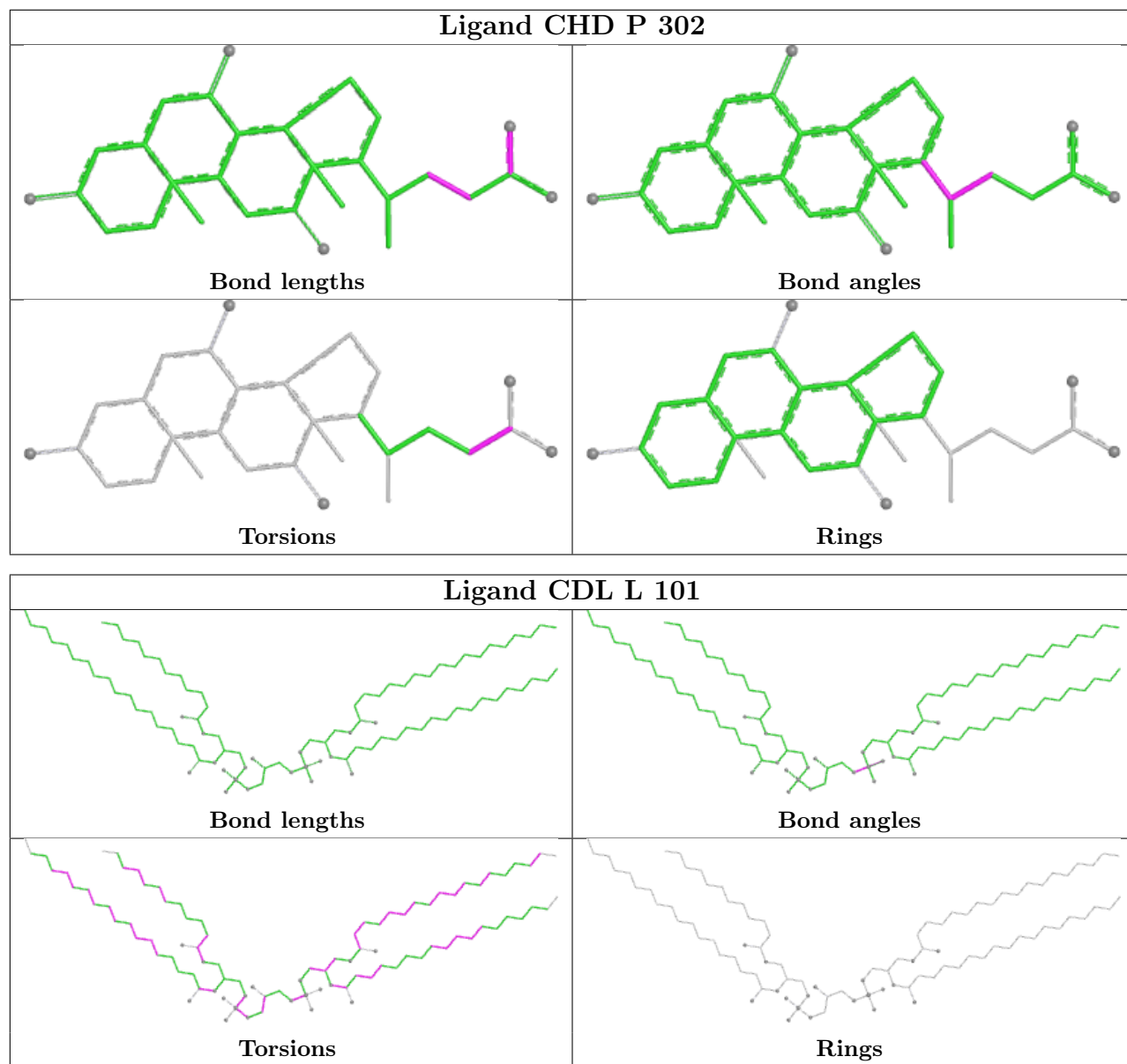


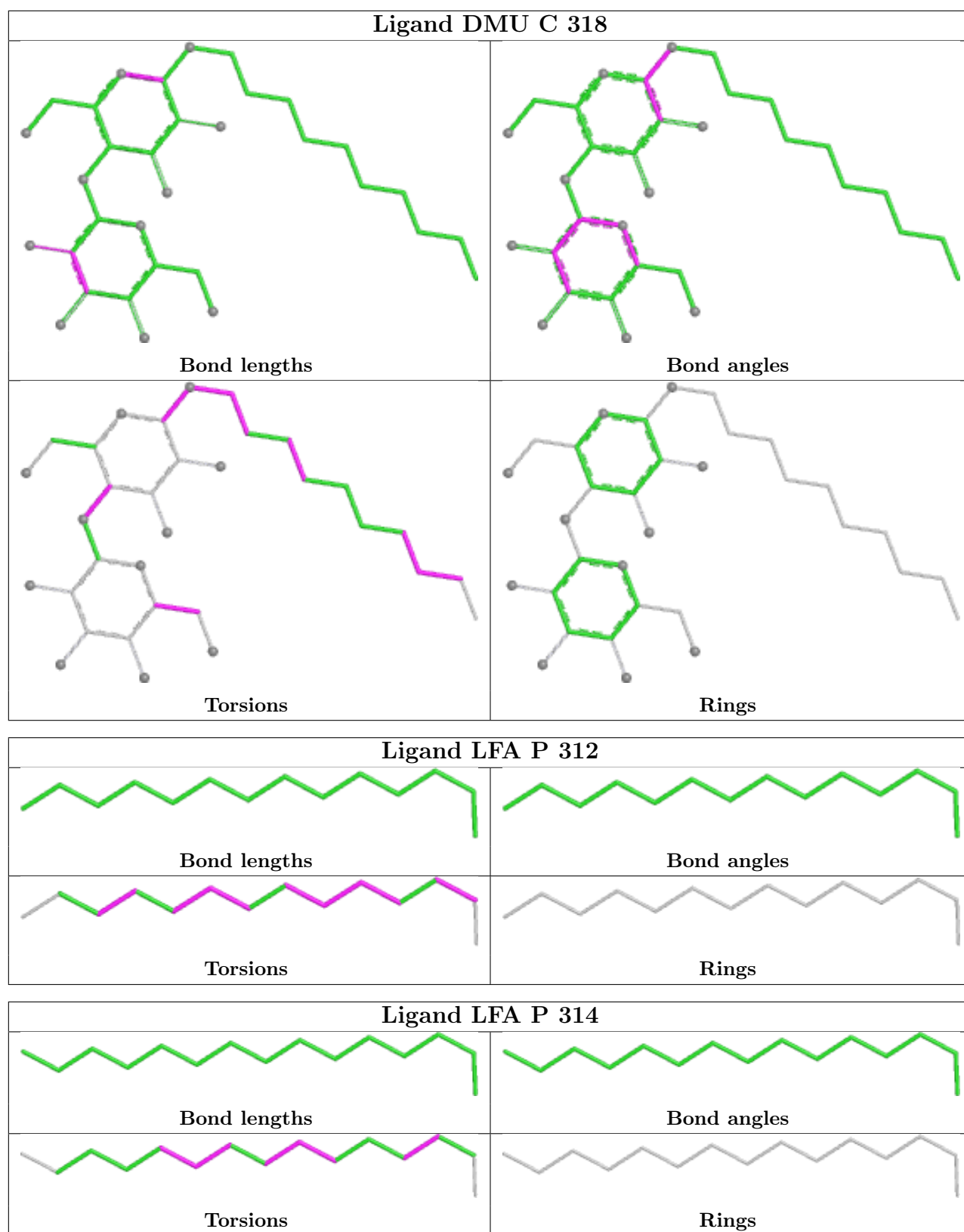


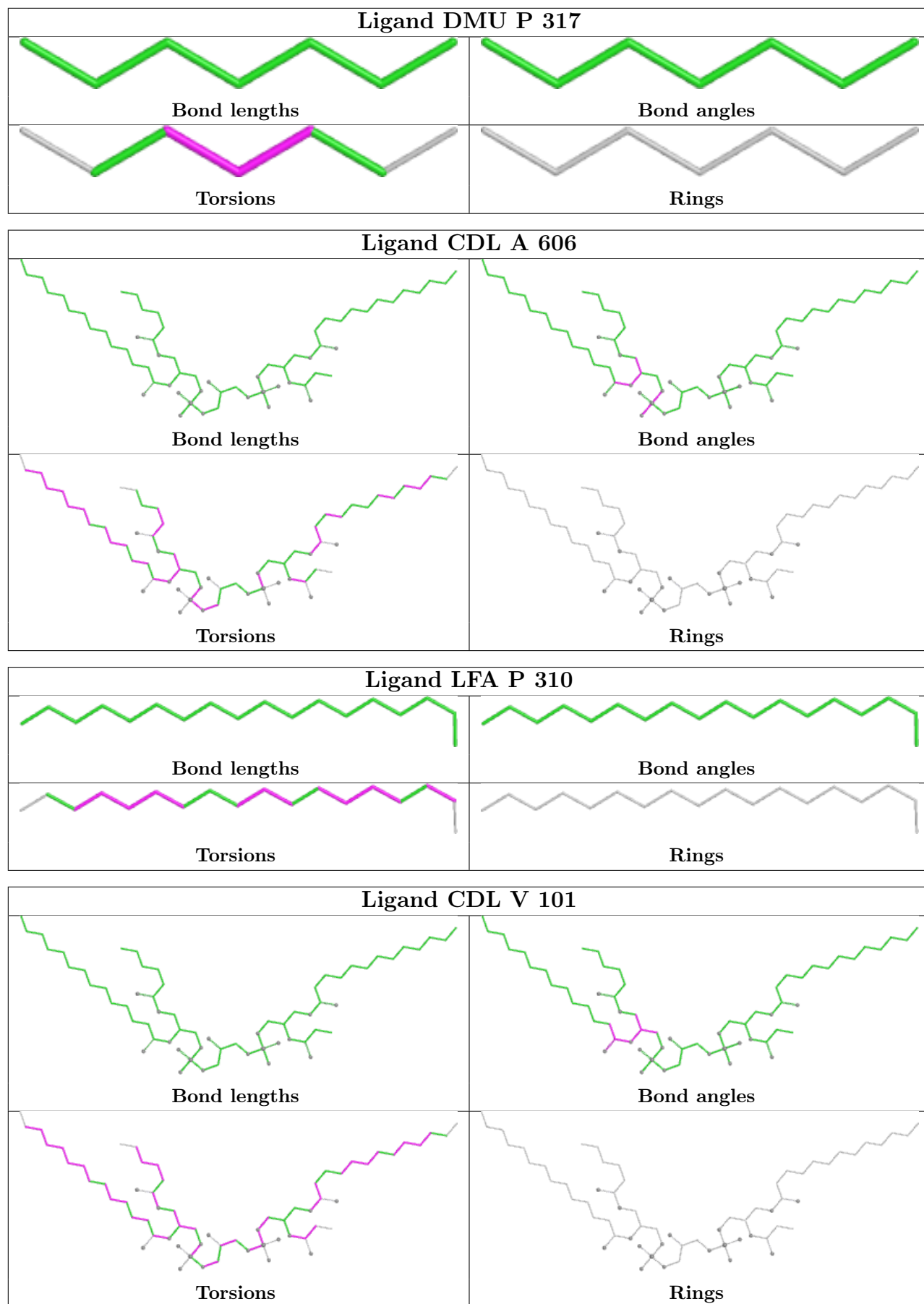


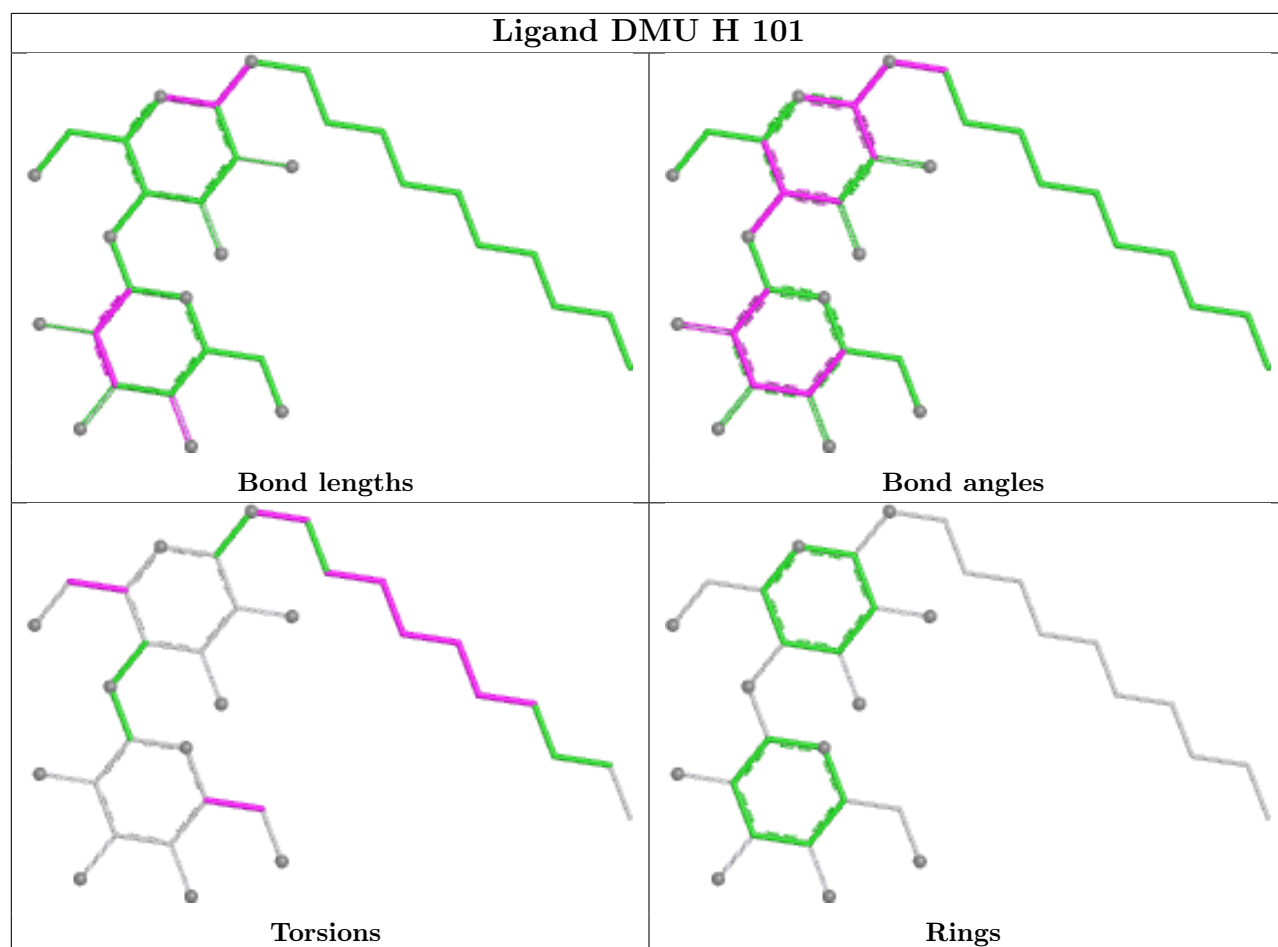
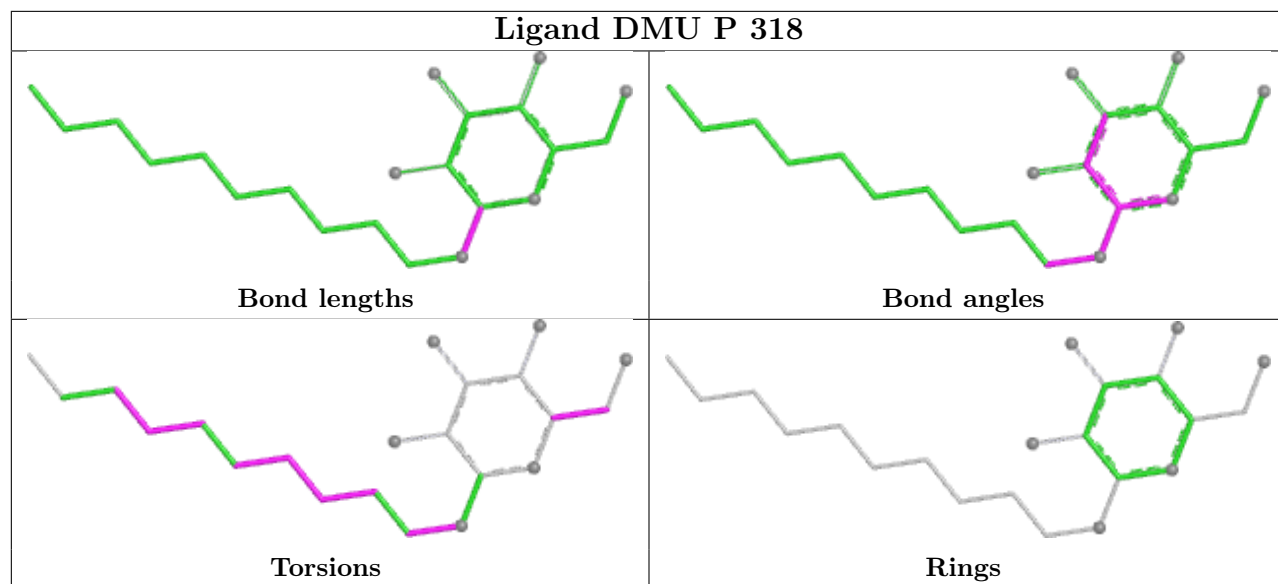


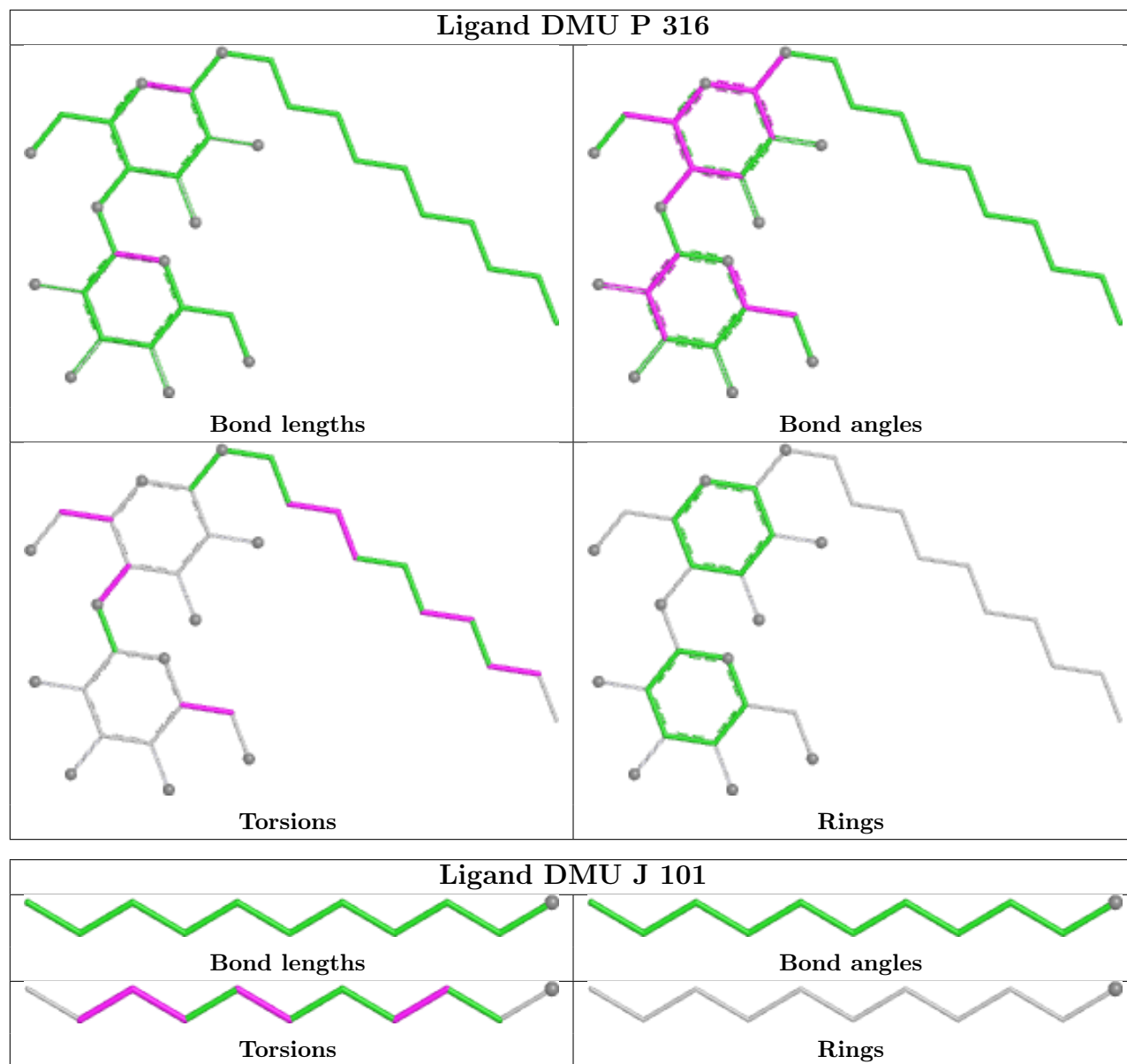


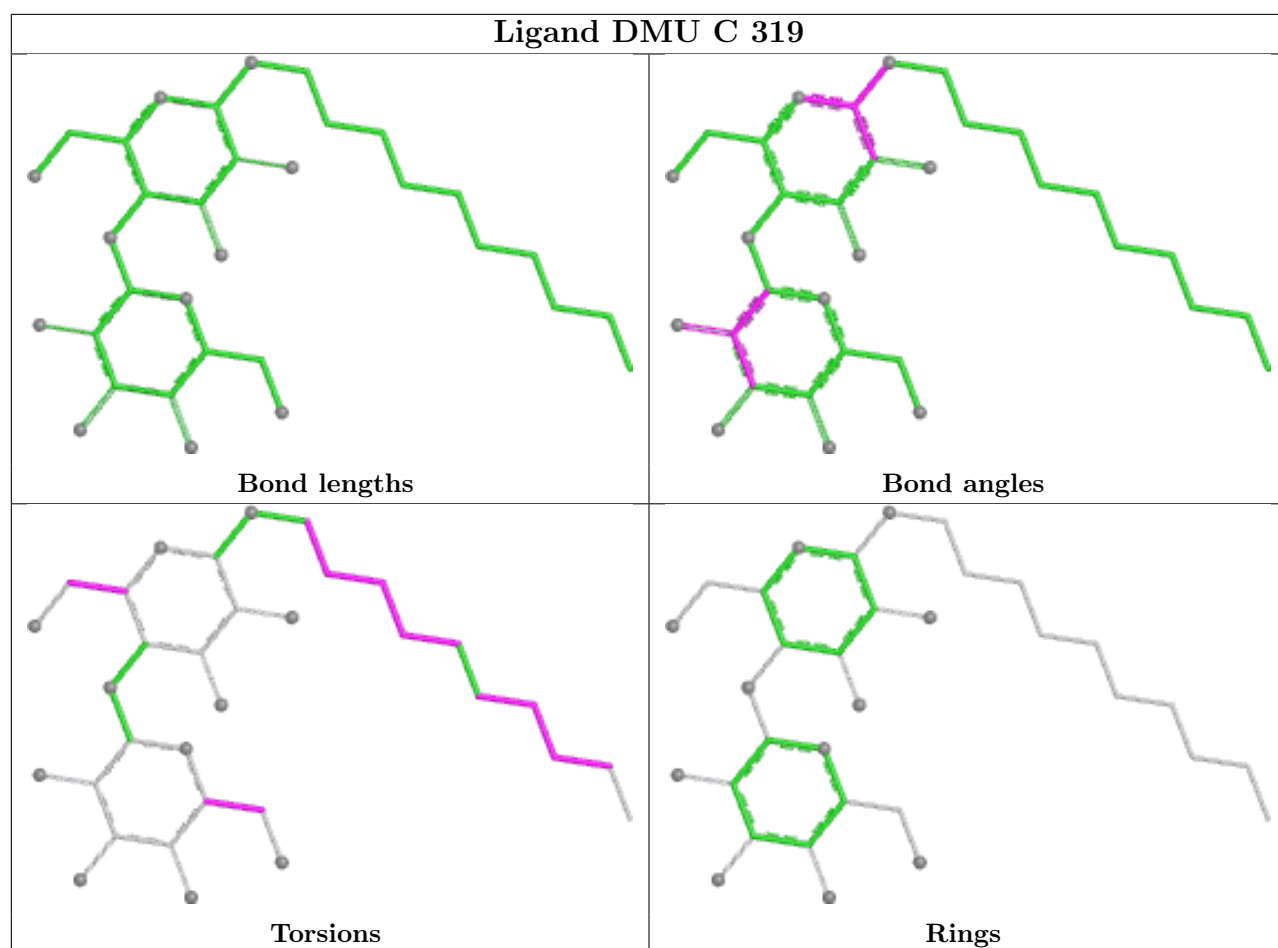


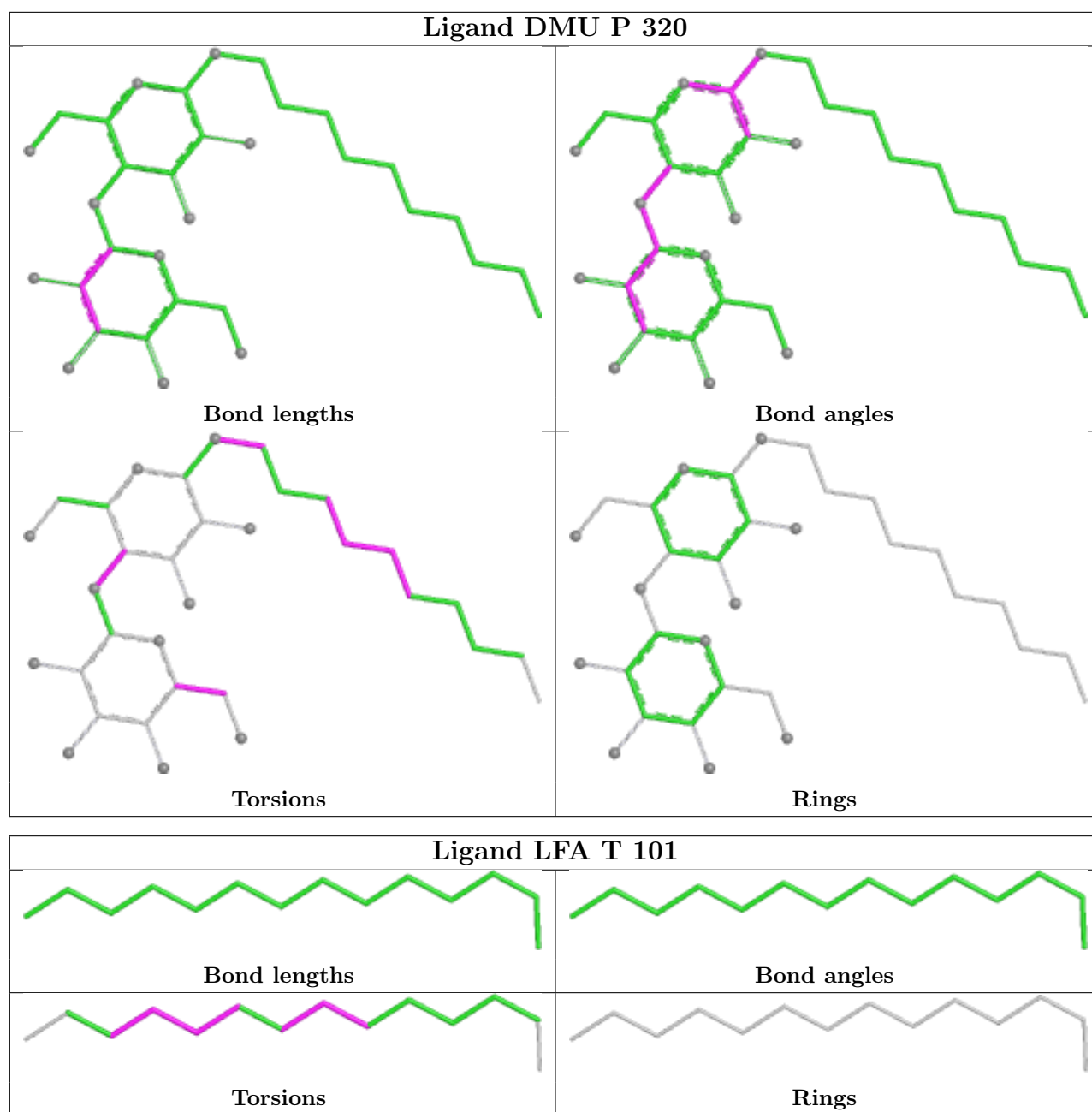


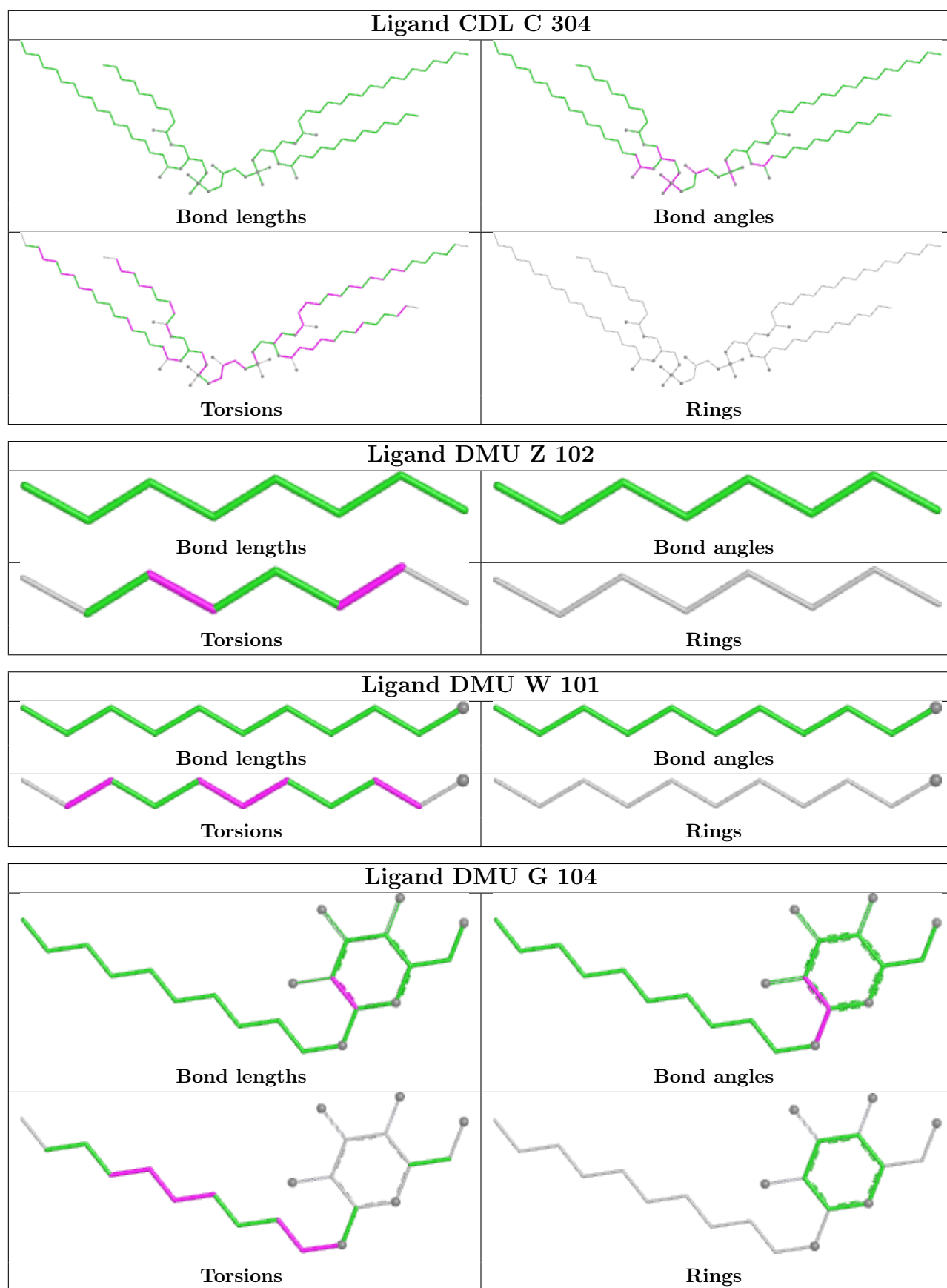


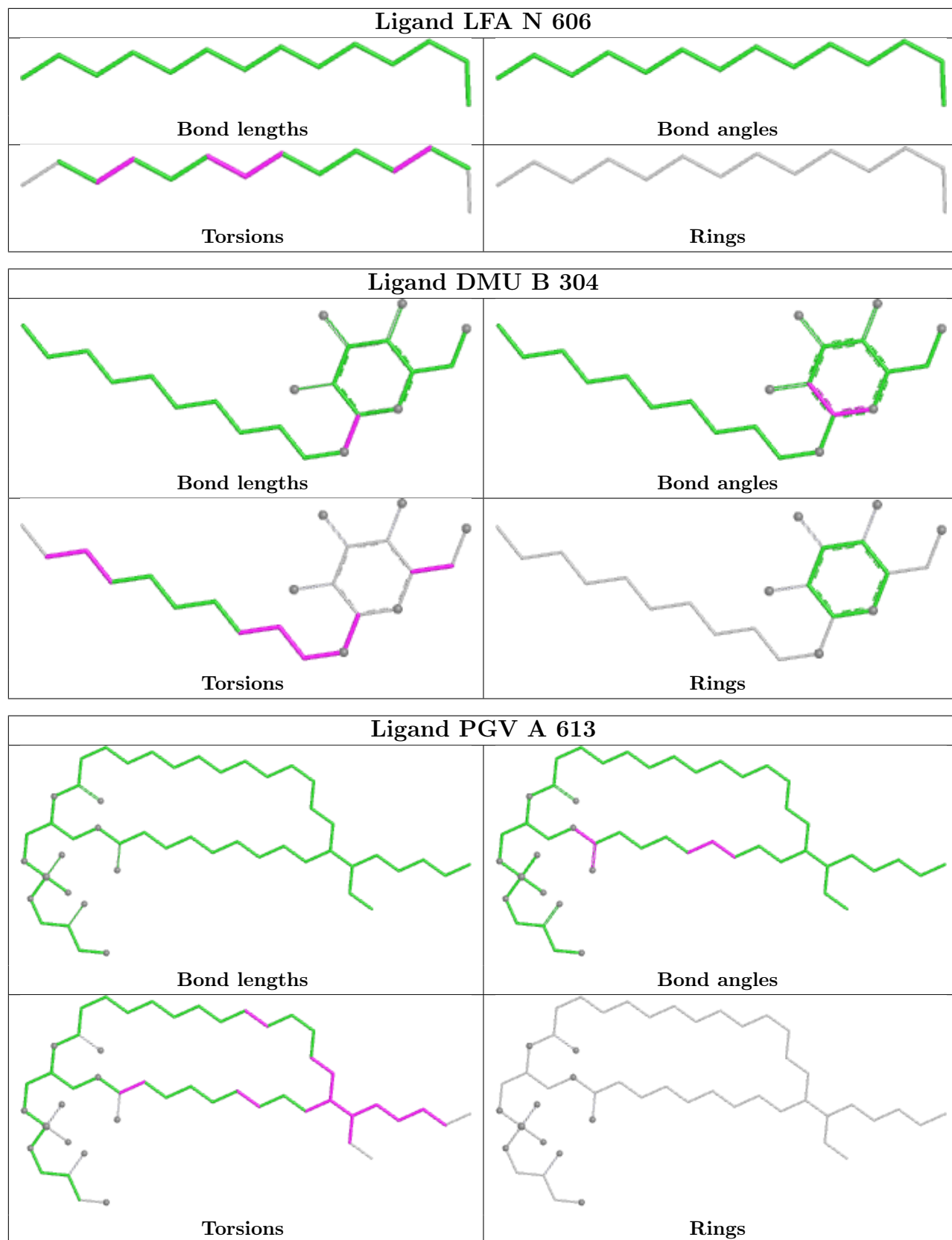












5.7 Other polymers [i](#)

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%)	-0.17	2 (0%)	88 91	16, 33, 41, 58	15 (2%)
1	N	512/514 (99%)	-0.07	5 (0%)	79 83	16, 35, 44, 62	15 (2%)
2	B	226/227 (99%)	0.25	11 (4%)	35 36	22, 39, 60, 89	5 (2%)
2	O	226/227 (99%)	0.25	8 (3%)	47 49	23, 44, 66, 96	5 (2%)
3	C	258/261 (98%)	-0.06	1 (0%)	88 91	17, 36, 46, 64	9 (3%)
3	P	258/261 (98%)	-0.06	1 (0%)	88 91	16, 36, 47, 68	9 (3%)
4	D	143/147 (97%)	0.12	2 (1%)	73 78	20, 42, 57, 73	1 (0%)
4	Q	137/147 (93%)	0.46	8 (5%)	29 29	24, 52, 79, 90	1 (0%)
5	E	102/109 (93%)	0.03	1 (0%)	79 83	35, 42, 56, 75	0
5	R	102/109 (93%)	0.19	2 (1%)	65 69	37, 50, 67, 85	0
6	F	91/98 (92%)	0.11	1 (1%)	78 82	20, 42, 65, 73	2 (2%)
6	S	91/98 (92%)	0.20	2 (2%)	62 66	19, 40, 63, 71	2 (2%)
7	G	72/85 (84%)	0.42	7 (9%)	13 13	21, 42, 82, 102	1 (1%)
7	T	72/85 (84%)	0.51	5 (6%)	23 23	22, 44, 75, 105	1 (1%)
8	H	75/85 (88%)	0.41	3 (4%)	42 44	36, 45, 90, 130	0
8	U	75/85 (88%)	0.53	9 (12%)	9 8	40, 47, 89, 124	0
9	I	70/73 (95%)	0.62	7 (10%)	12 12	39, 51, 77, 96	0
9	V	70/73 (95%)	0.72	9 (12%)	7 7	39, 58, 78, 102	0
10	J	56/59 (94%)	0.41	1 (1%)	67 71	37, 46, 73, 87	0
10	W	56/59 (94%)	0.55	4 (7%)	22 22	37, 48, 72, 89	0
11	K	49/56 (87%)	0.49	3 (6%)	27 27	39, 47, 64, 85	0
11	X	49/56 (87%)	0.86	3 (6%)	27 27	45, 55, 73, 103	0
12	L	44/47 (93%)	0.08	2 (4%)	38 40	33, 38, 51, 59	0
12	Y	44/47 (93%)	0.20	1 (2%)	61 64	38, 44, 59, 62	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	40/46 (86%)	0.23	1 (2%) 58 61	35, 39, 57, 75	0
13	Z	40/46 (86%)	0.55	1 (2%) 58 61	42, 48, 69, 82	0
All	All	3470/3614 (96%)	0.14	100 (2%) 53 56	16, 40, 66, 130	66 (1%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	36	TRP	6.8
2	O	113	TYR	5.6
1	N	113[A]	LEU	5.1
11	X	6	ALA	5.0
1	A	113[A]	LEU	4.9
6	S	3	GLY	4.9
2	O	90	ILE	4.8
2	B	59	GLN	4.8
11	K	6	ALA	4.8
8	U	48	GLY	4.7
6	S	93	PRO	4.4
2	B	87[A]	MET	4.4
7	G	36	TRP	4.0
10	J	1	PHE	4.0
10	W	1	PHE	4.0
9	V	3	ALA	3.9
2	B	91	ASN	3.8
8	U	45	ALA	3.8
2	B	90	ILE	3.8
6	F	3	GLY	3.8
8	H	48	GLY	3.7
9	V	37	PHE	3.6
8	H	45	ALA	3.5
3	P	37	PHE	3.5
7	G	33	LEU	3.4
9	I	3	ALA	3.3
9	I	37	PHE	3.2
4	Q	35	ALA	3.0
8	U	47	GLY	3.0
9	V	72	ALA	3.0
4	D	5	VAL	2.9
9	I	29	LEU	2.9
2	B	61	VAL	2.9
2	O	227	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
8	U	49	ASP	2.9
2	B	65	TRP	2.9
5	R	7	THR	2.8
2	O	32[A]	PHE	2.8
2	B	113	TYR	2.8
12	L	24	MET	2.8
8	H	47	GLY	2.8
3	C	38	ASN	2.7
11	X	7	PRO	2.7
2	O	87[A]	MET	2.7
4	Q	10	ASP	2.7
9	I	25	PHE	2.7
13	M	40	TYR	2.7
7	G	35	SER	2.7
4	D	4	SER	2.6
7	T	30	LEU	2.6
7	G	41	HIS	2.6
7	T	42	ARG	2.6
5	E	7	THR	2.6
2	B	60	GLU	2.6
9	I	19	PHE	2.5
7	T	37	LEU	2.5
13	Z	40	TYR	2.5
10	W	56	PRO	2.5
2	O	91	ASN	2.4
11	X	13	TYR	2.4
8	U	46	LYS	2.4
9	I	72	ALA	2.4
9	V	19	PHE	2.4
9	V	33	THR	2.4
11	K	47	ARG	2.4
1	N	513	LEU	2.3
10	W	48	TYR	2.3
7	G	42	ARG	2.3
7	G	40	GLY	2.3
8	U	61	LYS	2.3
8	U	44	THR	2.3
1	A	513	LEU	2.3
2	B	32[A]	PHE	2.3
2	B	16[A]	ILE	2.3
9	V	8	GLN	2.2
9	I	34	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	O	16[A]	ILE	2.2
7	T	38	HIS	2.2
11	K	26	VAL	2.2
4	Q	74	SER	2.2
5	R	108	LYS	2.2
1	N	483	LEU	2.2
2	B	115	ASP	2.2
4	Q	39	ALA	2.2
2	O	22[A]	HIS	2.2
4	Q	131	ILE	2.2
12	Y	24	MET	2.1
1	N	49	GLY	2.1
4	Q	51	LEU	2.1
7	G	30	LEU	2.1
9	V	68	ILE	2.1
4	Q	73	ARG	2.1
4	Q	17[A]	VAL	2.1
8	U	50	VAL	2.1
12	L	46	LYS	2.1
1	N	136[A]	LEU	2.1
8	U	52	VAL	2.1
10	W	52	TRP	2.1
9	V	65	LYS	2.1
9	V	26	MET	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	0.93	0.14	42,51,82,101	0
1	FME	N	1	10/11	0.95	0.13	45,50,81,99	0
2	FME	B	1	10/11	0.97	0.09	36,37,48,77	0
2	FME	O	1	10/11	0.97	0.09	40,43,52,76	0

6.3 Carbohydrates [i](#)

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
20	DMU	C	317	22/33	0.70	0.33	44,64,74,80	22
20	DMU	P	318	22/33	0.72	0.36	44,66,86,96	22
19	LFA	P	311	11/20	0.73	0.41	58,67,71,74	11
24	CHD	P	306	29/29	0.73	0.22	66,86,116,130	0
21	EDO	P	323	4/4	0.75	0.36	33,33,41,44	4
20	DMU	A	608	7/33	0.76	0.38	53,55,64,71	7
19	LFA	P	308	11/20	0.79	0.35	38,49,63,65	11
24	CHD	C	305	29/29	0.80	0.18	65,90,115,123	0
20	DMU	B	308	22/33	0.81	0.31	54,73,83,91	22
20	DMU	O	303	22/33	0.81	0.29	46,66,85,98	22
20	DMU	P	320	33/33	0.82	0.28	52,76,88,96	33
19	LFA	C	311	14/20	0.82	0.37	39,64,70,72	14
19	LFA	P	313	11/20	0.82	0.33	41,59,68,72	11
20	DMU	C	315	33/33	0.82	0.34	45,58,70,77	33
20	DMU	N	607	7/33	0.83	0.39	53,69,72,72	7
19	LFA	C	310	11/20	0.83	0.38	56,75,96,97	11
19	LFA	C	308	6/20	0.83	0.40	43,53,62,62	6
19	LFA	P	312	14/20	0.83	0.35	43,68,78,83	14
21	EDO	C	322	4/4	0.83	0.29	35,37,41,44	4
21	EDO	E	201	4/4	0.83	0.34	44,45,47,53	4
19	LFA	C	324	15/20	0.83	0.39	56,60,67,72	15
20	DMU	C	318	33/33	0.83	0.32	44,56,67,100	33
20	DMU	M	102	8/33	0.83	0.29	48,56,61,65	8
20	DMU	N	608	33/33	0.84	0.25	45,60,79,85	33
20	DMU	G	103	11/33	0.84	0.33	48,58,62,71	11
20	DMU	P	317	7/33	0.84	0.29	54,58,67,73	7
19	LFA	P	301	15/20	0.84	0.33	52,61,67,68	15
19	LFA	C	312	11/20	0.84	0.33	46,58,73,76	11
20	DMU	P	319	33/33	0.85	0.32	49,60,88,103	33
19	LFA	P	309	6/20	0.85	0.33	41,51,53,55	6
19	LFA	P	315	13/20	0.85	0.29	50,59,79,80	13
19	LFA	T	103	11/20	0.85	0.33	55,62,77,80	11
20	DMU	P	316	33/33	0.85	0.28	47,58,75,77	33
19	LFA	C	314	13/20	0.85	0.28	53,61,75,80	13
19	LFA	O	302	11/20	0.85	0.31	47,59,69,71	11
21	EDO	C	320	4/4	0.86	0.37	56,56,63,82	4
18	CDL	V	101	64/100	0.86	0.19	56,94,138,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	LFA	C	313	15/20	0.86	0.26	47,52,75,76	15
19	LFA	G	106	14/20	0.86	0.28	47,54,70,74	14
20	DMU	C	316	7/33	0.86	0.28	59,59,65,70	7
21	EDO	A	611	4/4	0.86	0.27	36,41,50,52	4
20	DMU	Q	201	33/33	0.87	0.22	41,60,72,79	33
20	DMU	W	101	11/33	0.87	0.35	64,70,76,83	11
20	DMU	Y	102	22/33	0.87	0.39	57,71,81,85	22
20	DMU	C	319	33/33	0.87	0.23	46,73,80,82	33
20	DMU	C	323	33/33	0.87	0.17	39,53,79,89	33
19	LFA	T	101	14/20	0.87	0.28	48,52,63,70	14
18	CDL	P	305	87/100	0.87	0.20	43,91,141,183	0
18	CDL	A	606	64/100	0.87	0.18	50,87,120,147	0
18	CDL	C	304	87/100	0.87	0.19	43,83,122,135	0
20	DMU	P	324	33/33	0.87	0.19	45,57,95,99	33
19	LFA	C	307	11/20	0.88	0.31	43,54,65,69	11
20	DMU	T	104	22/33	0.88	0.24	42,56,68,68	22
19	LFA	O	301	17/20	0.88	0.27	44,61,76,80	17
20	DMU	N	615	33/33	0.88	0.23	36,50,68,73	33
18	CDL	Y	101	94/100	0.88	0.17	53,91,141,152	0
20	DMU	A	609	33/33	0.88	0.20	39,54,62,68	33
20	DMU	A	614	11/33	0.88	0.34	52,65,68,70	11
20	DMU	B	302	11/33	0.88	0.29	48,57,66,80	11
21	EDO	N	610	4/4	0.88	0.22	37,39,50,51	4
20	DMU	B	304	22/33	0.88	0.22	47,70,80,89	22
20	DMU	H	101	33/33	0.88	0.22	37,49,57,70	33
19	LFA	P	310	18/20	0.88	0.24	35,53,61,64	18
19	LFA	B	307	17/20	0.89	0.28	43,63,75,79	17
19	LFA	C	309	18/20	0.89	0.23	32,47,62,63	18
19	LFA	A	607	14/20	0.89	0.27	38,50,70,75	14
19	LFA	P	314	15/20	0.89	0.21	44,52,66,69	15
20	DMU	G	104	22/33	0.90	0.27	44,59,68,73	22
19	LFA	N	606	14/20	0.90	0.25	36,49,67,68	14
20	DMU	J	101	11/33	0.90	0.35	65,71,82,92	11
21	EDO	A	610	4/4	0.90	0.17	27,31,32,35	4
20	DMU	Z	102	8/33	0.91	0.29	54,58,60,61	8
21	EDO	F	101	4/4	0.91	0.18	46,47,48,55	4
21	EDO	N	609	4/4	0.91	0.15	30,31,33,35	4
20	DMU	D	201	33/33	0.91	0.18	31,50,60,73	33
21	EDO	P	321	4/4	0.91	0.20	51,52,60,75	4
20	DMU	O	305	11/33	0.91	0.29	47,52,67,73	11
18	CDL	L	101	94/100	0.91	0.16	45,86,134,154	0
20	DMU	B	303	11/33	0.91	0.25	46,62,69,76	11

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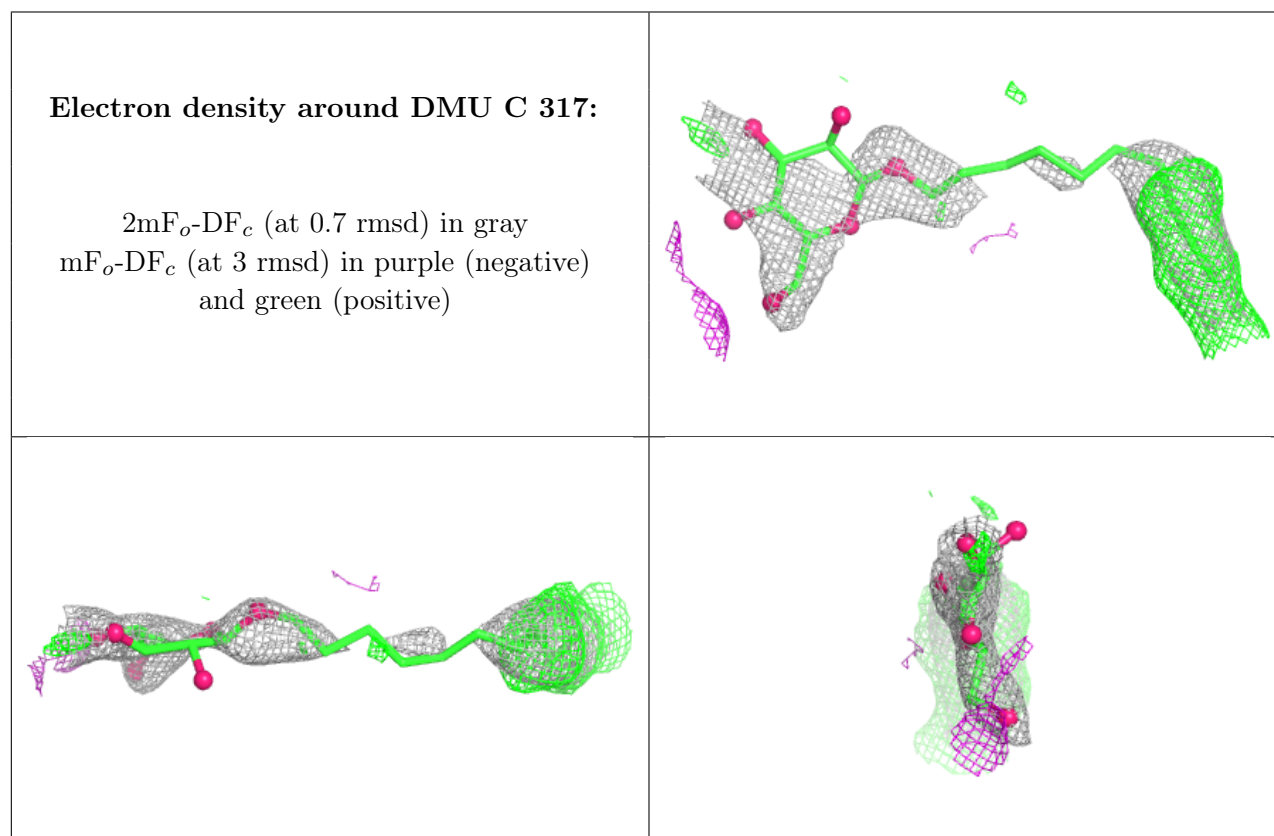
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	DMU	O	307	22/33	0.92	0.18	40,52,61,63	22
20	DMU	P	307	11/33	0.92	0.28	50,56,60,62	11
20	DMU	L	102	22/33	0.92	0.32	51,62,75,79	22
21	EDO	S	102	4/4	0.92	0.11	22,23,30,31	4
21	EDO	F	103	4/4	0.92	0.15	23,23,31,31	4
20	DMU	Z	101	33/33	0.92	0.11	50,58,83,86	0
20	DMU	C	306	11/33	0.93	0.24	56,60,68,71	11
21	EDO	N	613	4/4	0.93	0.23	34,34,34,37	4
21	EDO	R	203	4/4	0.93	0.20	45,47,57,59	4
20	DMU	O	306	11/33	0.95	0.25	51,57,63,63	11
20	DMU	M	101	33/33	0.95	0.09	43,53,69,78	0
21	EDO	E	202	4/4	0.95	0.15	37,37,38,38	4
21	EDO	E	203	4/4	0.95	0.17	38,40,47,47	4
21	EDO	C	321	4/4	0.95	0.15	37,37,40,41	4
27	PEK	T	102	53/53	0.95	0.13	37,57,103,130	0
21	EDO	R	201	4/4	0.96	0.29	67,69,70,70	4
21	EDO	N	612	4/4	0.96	0.12	36,38,39,42	4
21	EDO	A	612	4/4	0.96	0.18	28,28,29,29	4
24	CHD	C	301	29/29	0.96	0.08	34,38,42,46	0
21	EDO	O	308	4/4	0.96	0.10	33,34,34,36	4
21	EDO	G	105	4/4	0.96	0.12	33,36,37,41	4
27	PEK	G	101	53/53	0.96	0.12	35,55,109,130	0
21	EDO	N	611	4/4	0.96	0.18	29,31,32,33	4
22	PGV	N	614	51/51	0.97	0.09	32,42,74,85	0
24	CHD	B	306	29/29	0.97	0.07	31,35,40,47	0
21	EDO	P	322	4/4	0.97	0.15	37,40,41,42	4
21	EDO	R	202	4/4	0.97	0.11	38,40,41,41	4
24	CHD	P	302	29/29	0.97	0.07	34,38,43,47	0
21	EDO	S	103	4/4	0.97	0.11	33,36,37,41	4
25	UNX	P	303	1/1	0.97	0.24	44,44,44,44	0
21	EDO	T	105	4/4	0.97	0.09	34,37,38,40	4
22	PGV	C	303	51/51	0.97	0.10	32,41,104,118	0
24	CHD	G	102	29/29	0.98	0.06	31,35,39,46	0
21	EDO	F	104	4/4	0.98	0.07	33,36,36,39	4
22	PGV	P	304	51/51	0.98	0.09	32,42,91,112	0
25	UNX	C	302	1/1	0.98	0.17	44,44,44,44	0
17	NA	A	605	1/1	0.98	0.11	37,37,37,37	0
22	PGV	A	613	51/51	0.98	0.09	31,41,79,89	0
21	EDO	B	305	4/4	0.98	0.08	28,31,31,33	4
16	MG	N	604	1/1	0.99	0.03	35,35,35,35	0
14	HEA	A	601	60/60	0.99	0.06	28,30,44,52	0
17	NA	N	605	1/1	0.99	0.08	43,43,43,43	0

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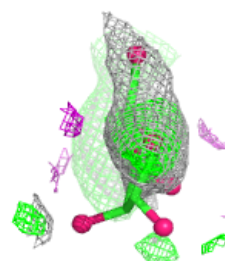
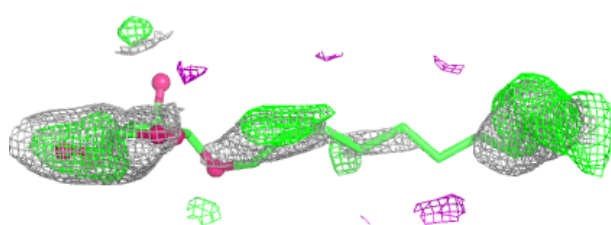
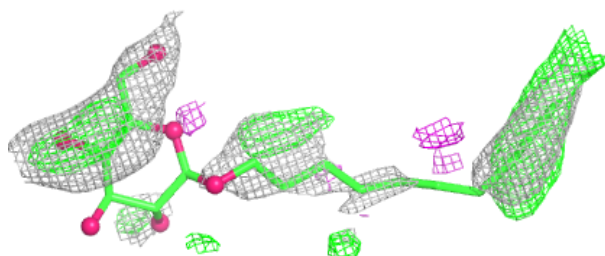
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	HEA	A	602	60/60	0.99	0.05	27,31,37,43	0
14	HEA	N	601	60/60	0.99	0.06	30,33,47,51	0
14	HEA	N	602	60/60	0.99	0.05	30,32,38,43	0
16	MG	A	604	1/1	1.00	0.03	32,32,32,32	0
15	CU	A	603	1/1	1.00	0.02	30,30,30,30	0
15	CU	N	603	1/1	1.00	0.01	32,32,32,32	0
26	ZN	F	102	1/1	1.00	0.01	37,37,37,37	0
26	ZN	S	101	1/1	1.00	0.02	37,37,37,37	0
23	CUA	B	301	2/2	1.00	0.02	32,32,32,32	0
23	CUA	O	304	2/2	1.00	0.02	35,35,35,35	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.

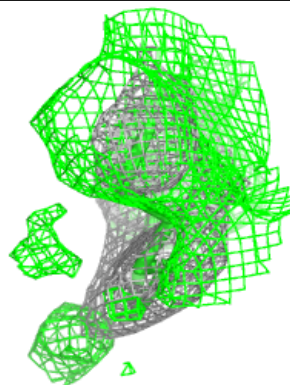
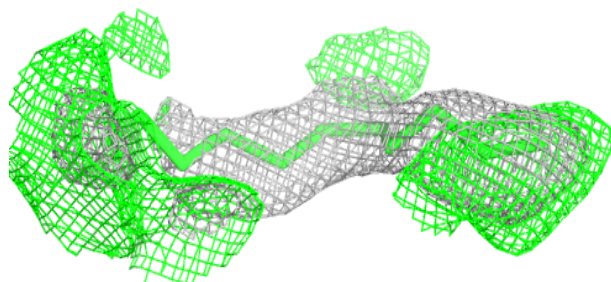
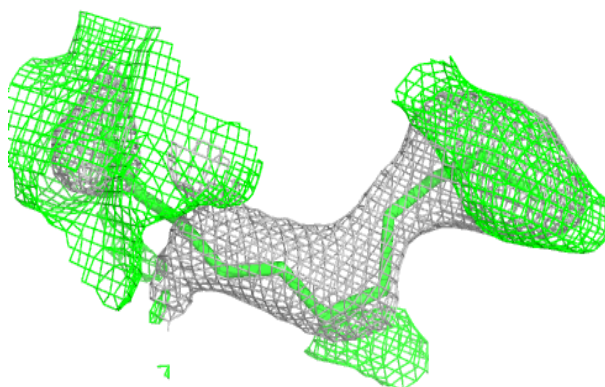


Electron density around DMU P 318:

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

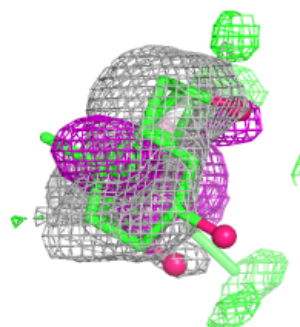
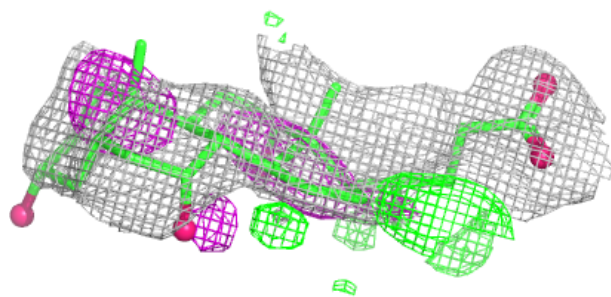
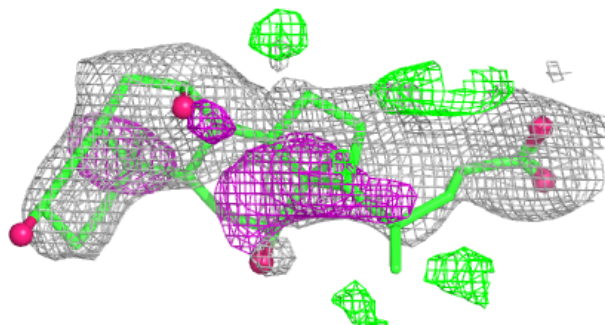
**Electron density around LFA P 311:**

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

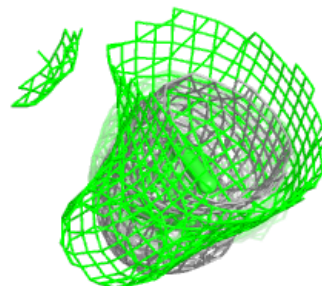
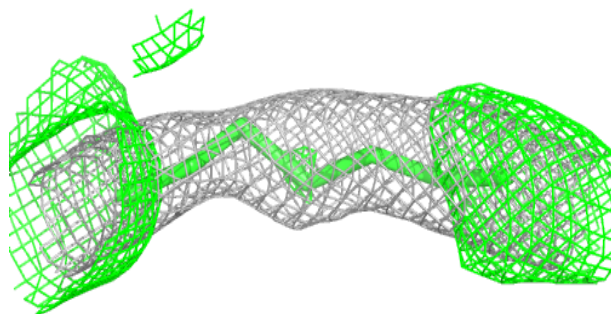
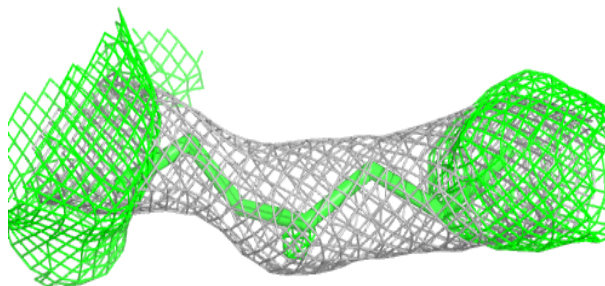


Electron density around CHD P 306:

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

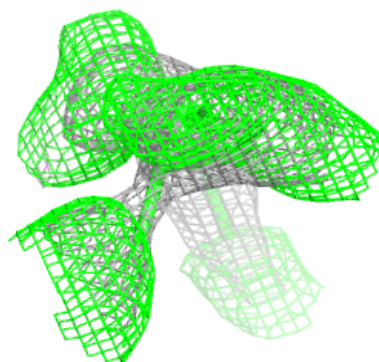
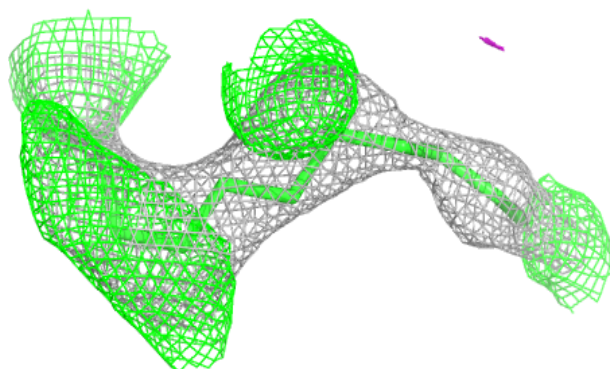
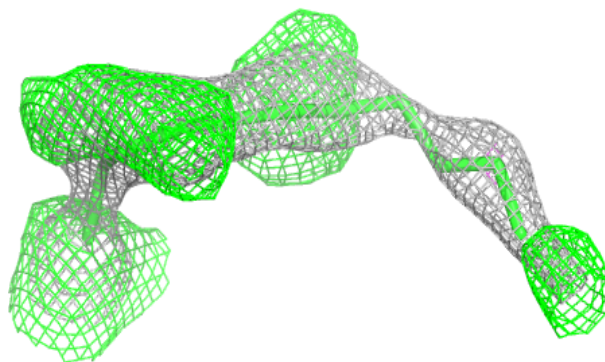
**Electron density around DMU A 608:**

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

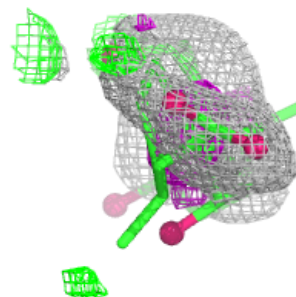
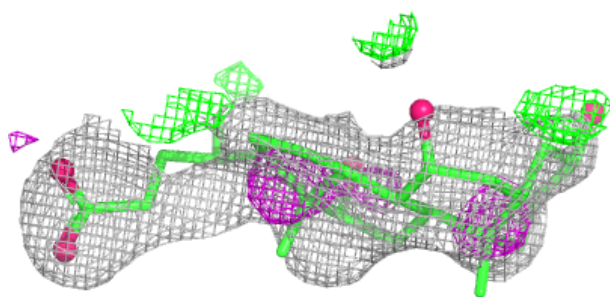
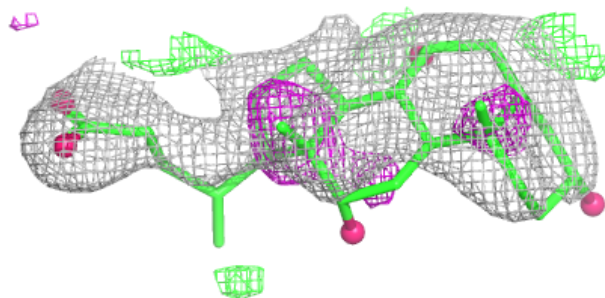


Electron density around LFA P 308:

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

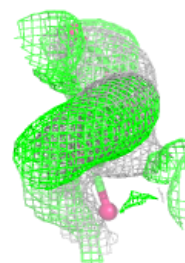
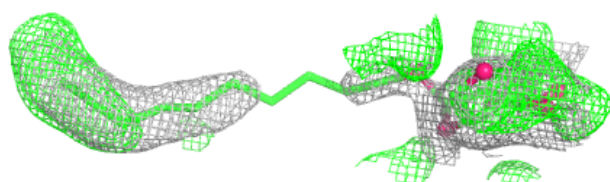
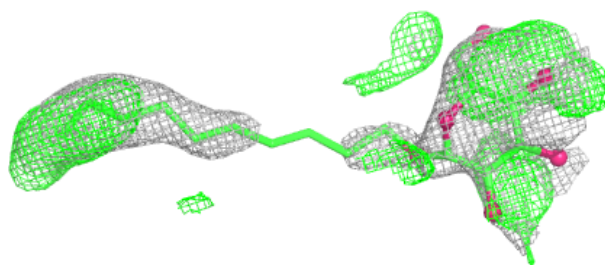
**Electron density around CHD C 305:**

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

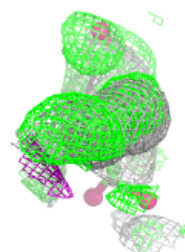
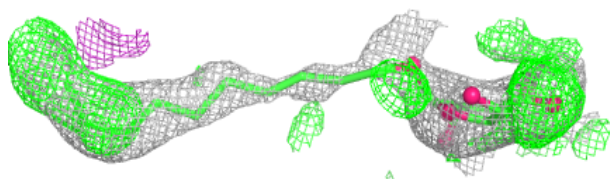
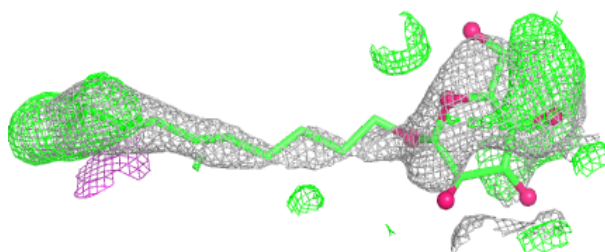


Electron density around DMU B 308:

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

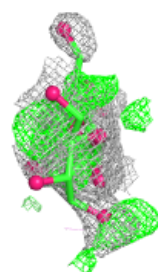
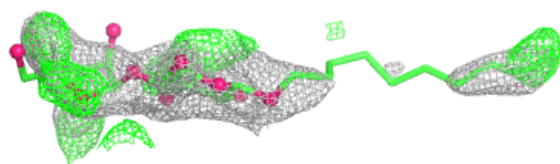
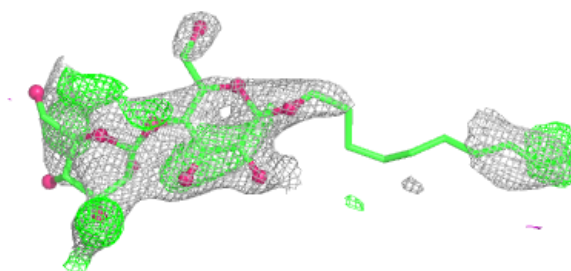
**Electron density around DMU O 303:**

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

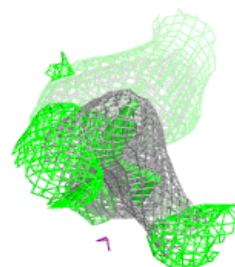
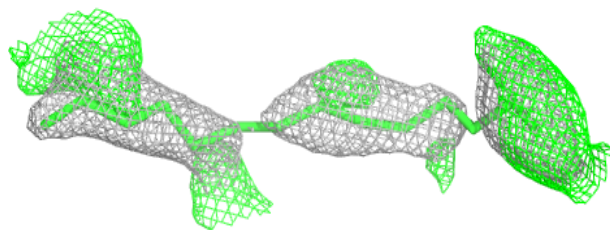
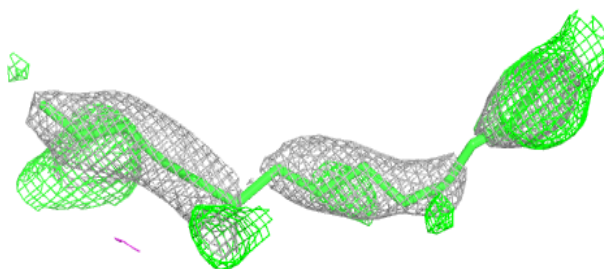


Electron density around DMU P 320:

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

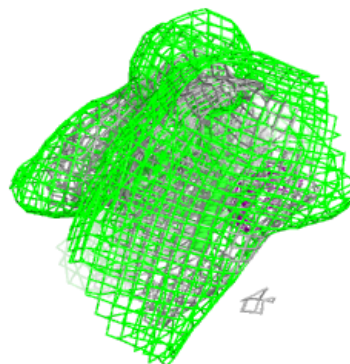
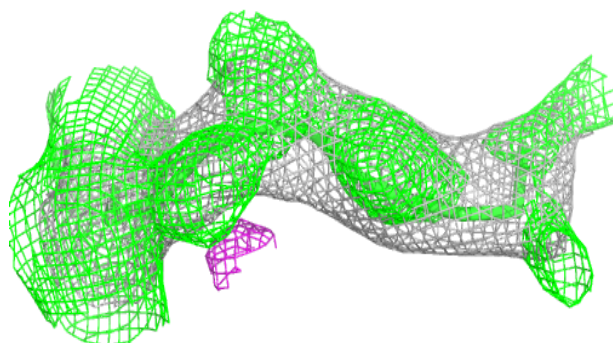
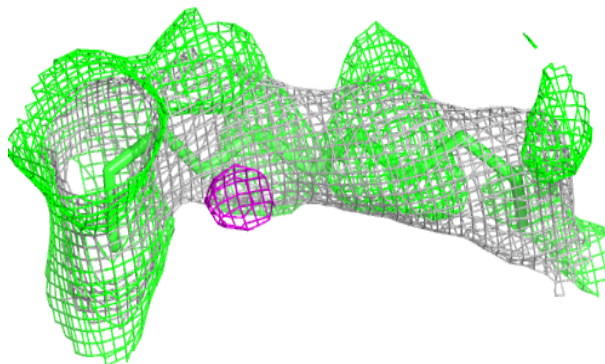
**Electron density around LFA C 311:**

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

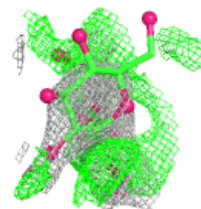
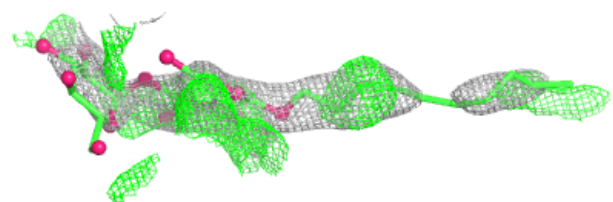
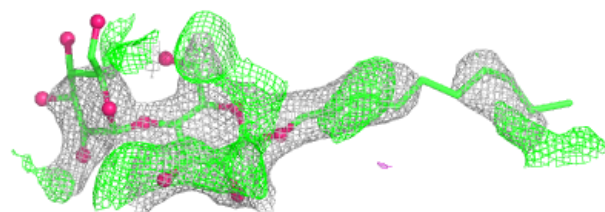


Electron density around LFA P 313:

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

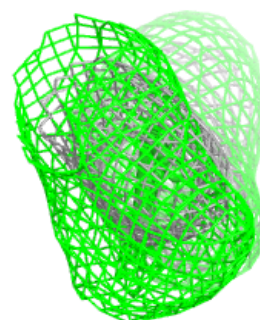
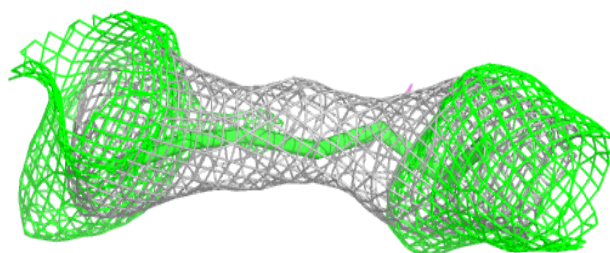
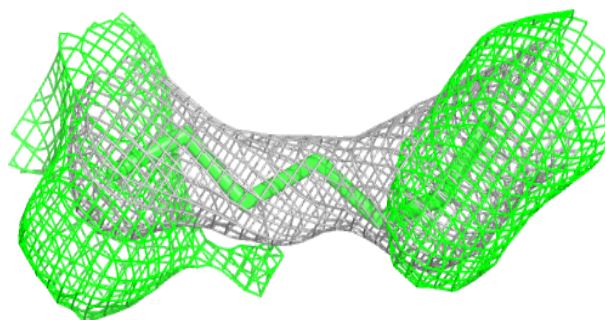
**Electron density around DMU C 315:**

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

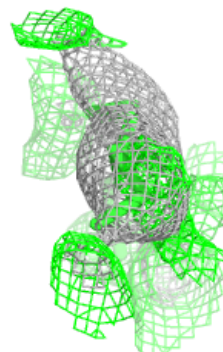
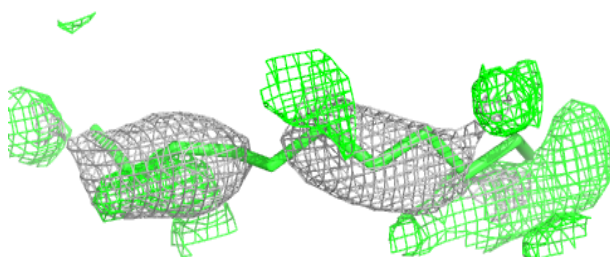
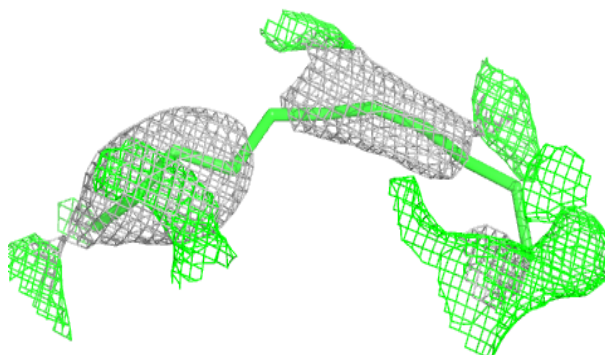


Electron density around DMU N 607:

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

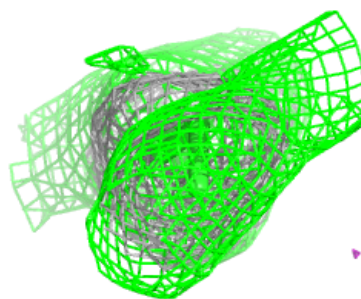
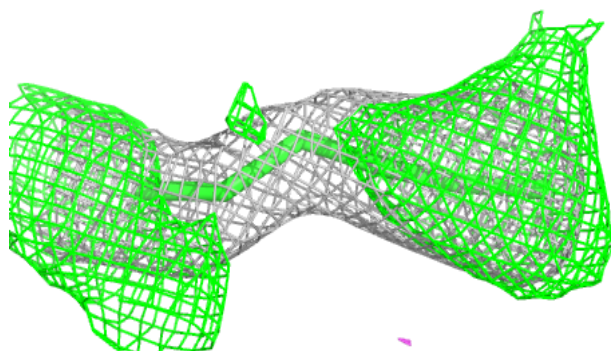
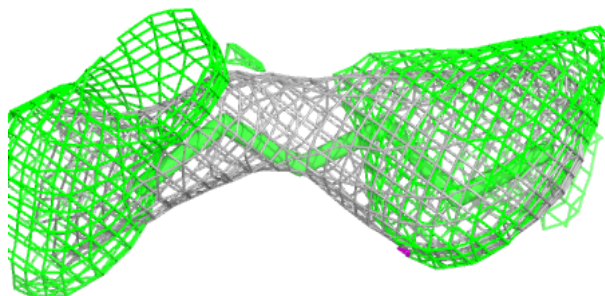
**Electron density around LFA C 310:**

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

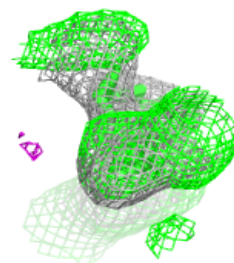
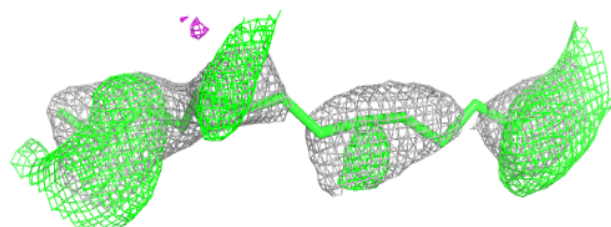
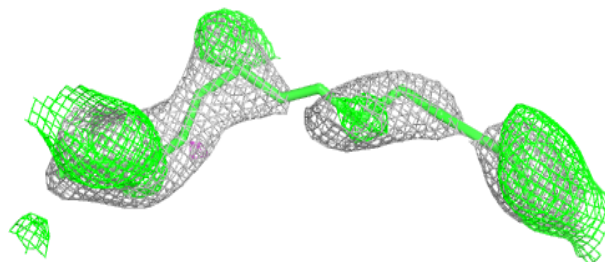


Electron density around LFA C 308:

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

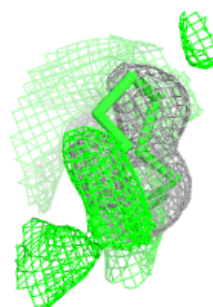
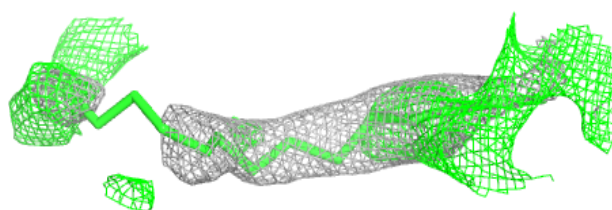
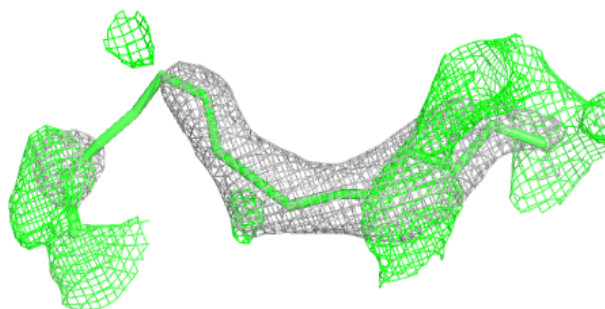
**Electron density around LFA P 312:**

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

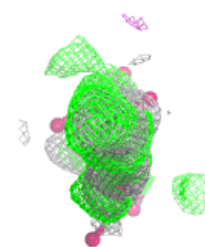
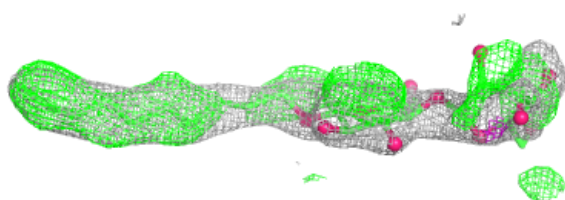
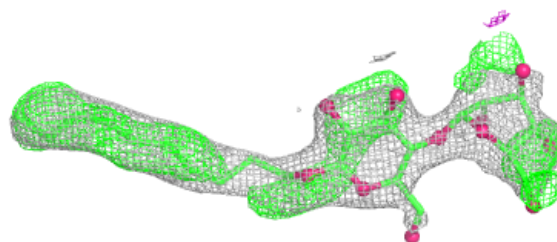


Electron density around LFA C 324:

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

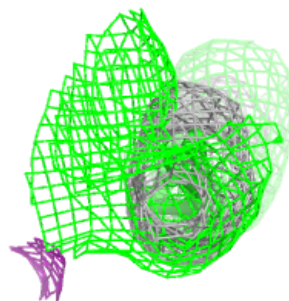
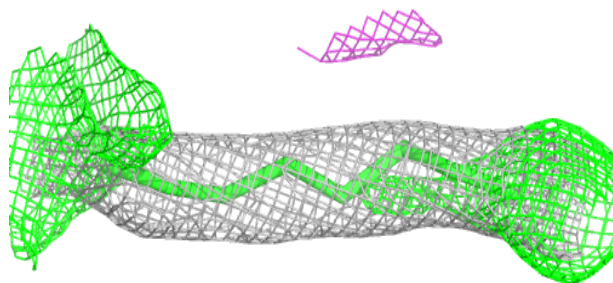
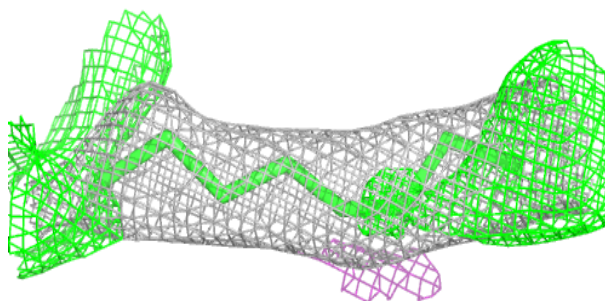
**Electron density around DMU C 318:**

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

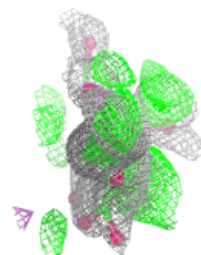
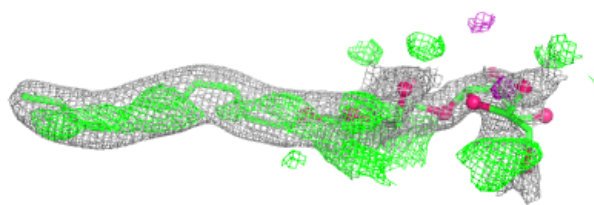
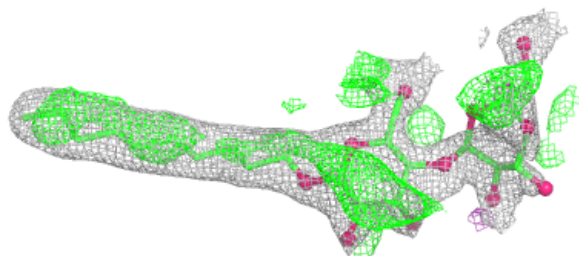


Electron density around DMU M 102:

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

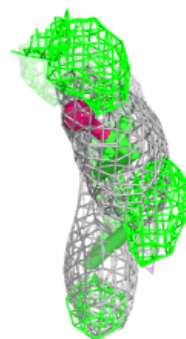
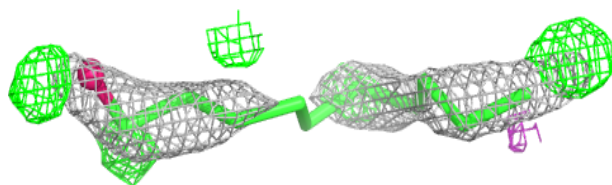
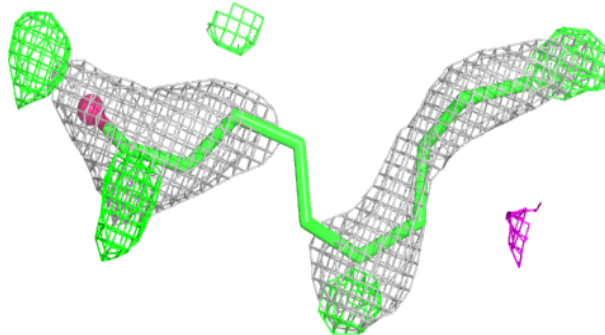
**Electron density around DMU N 608:**

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

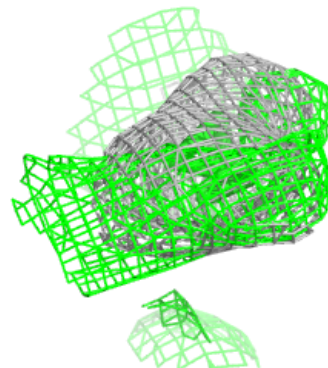
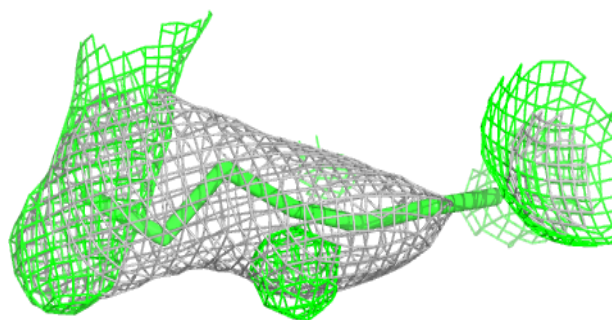
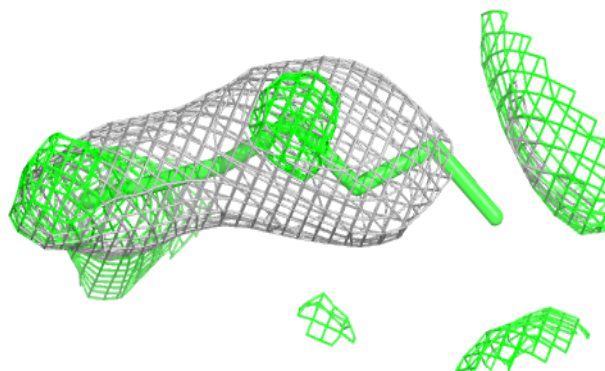


Electron density around DMU G 103:

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

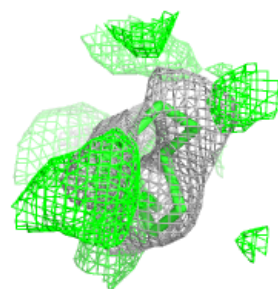
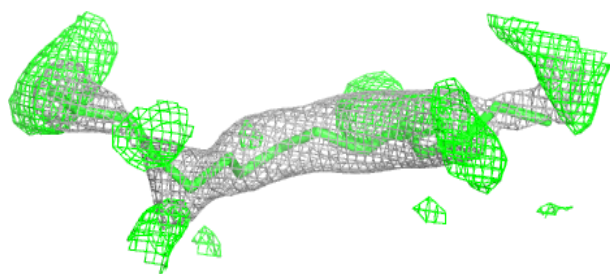
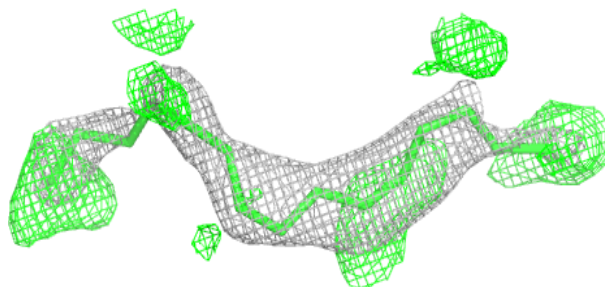
**Electron density around DMU P 317:**

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

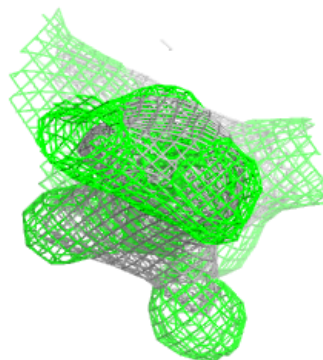
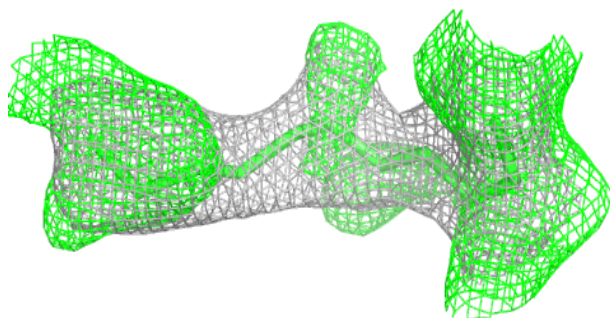
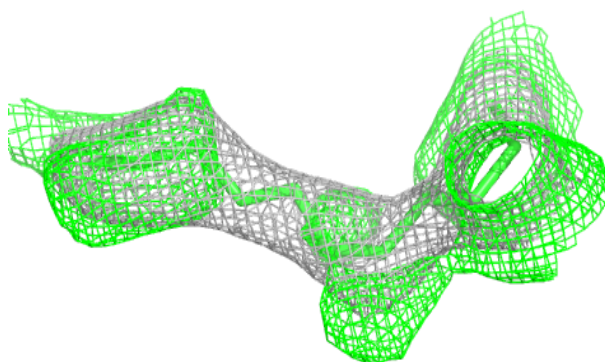


Electron density around LFA P 301:

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

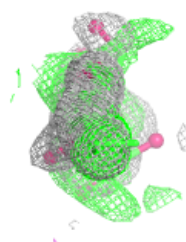
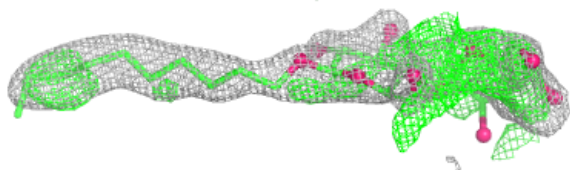
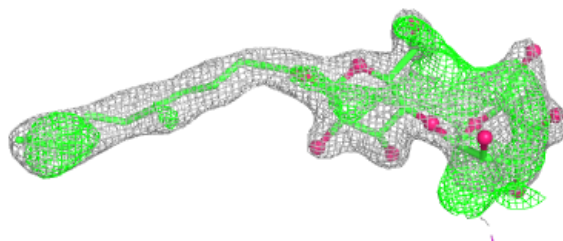
**Electron density around LFA C 312:**

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

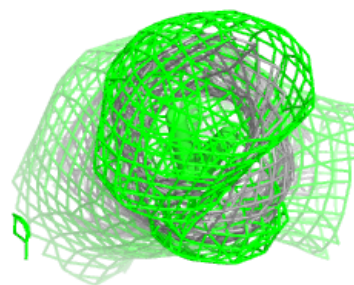
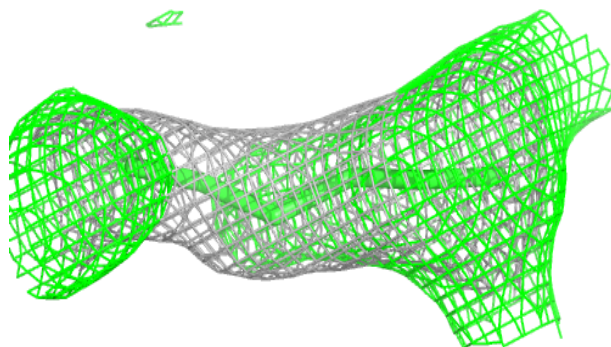
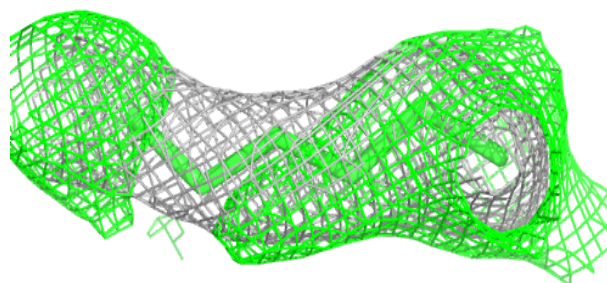


Electron density around DMU P 319:

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

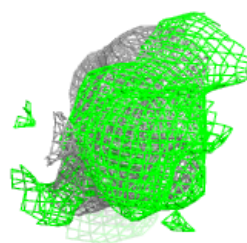
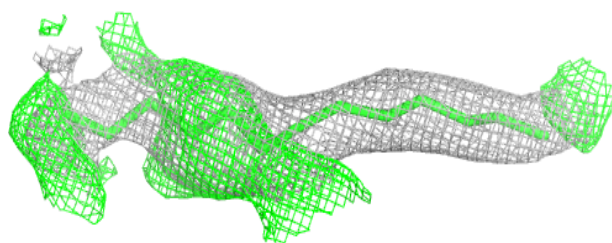
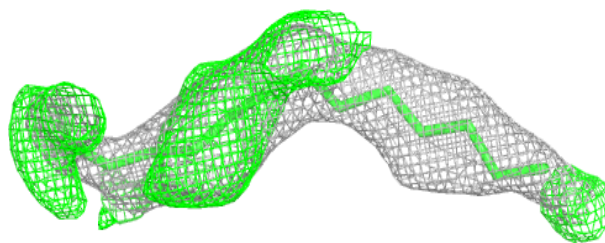
**Electron density around LFA P 309:**

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

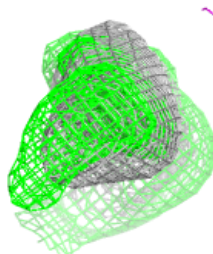
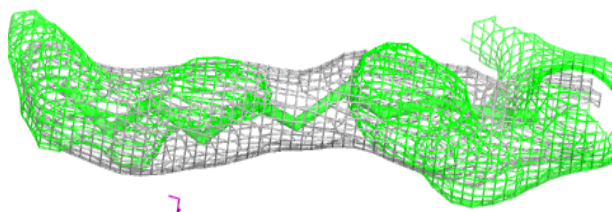
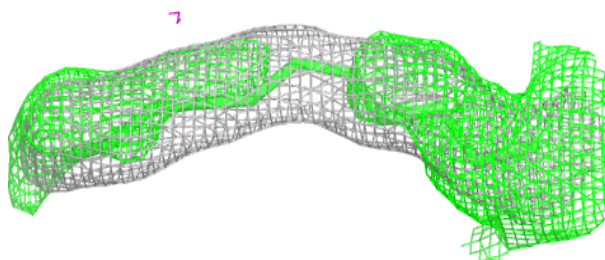


Electron density around LFA P 315:

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

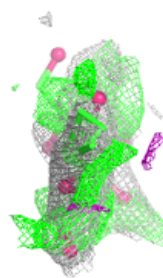
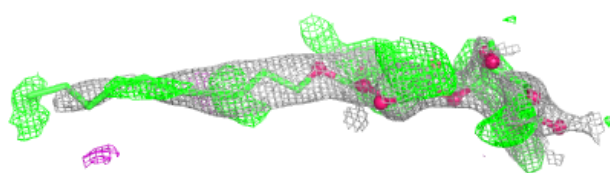
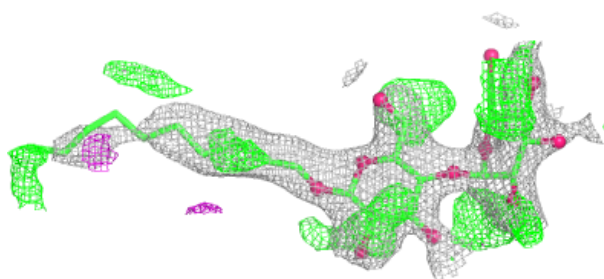
**Electron density around LFA T 103:**

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

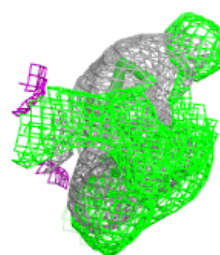
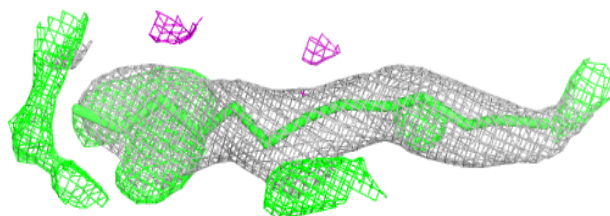
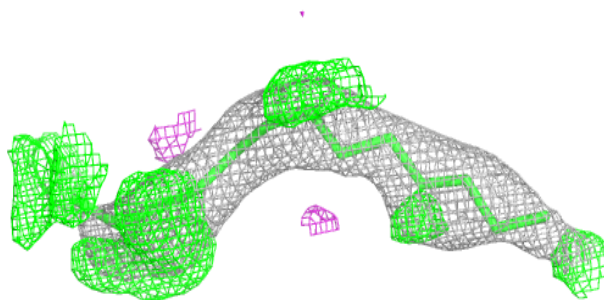


Electron density around DMU P 316:

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

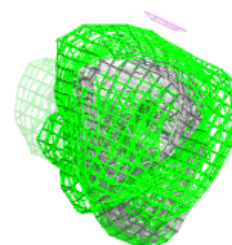
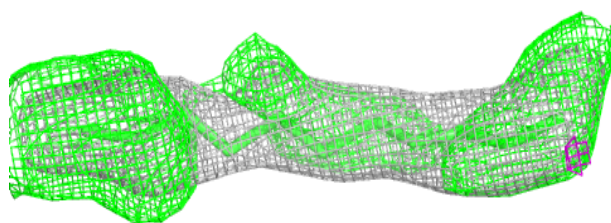
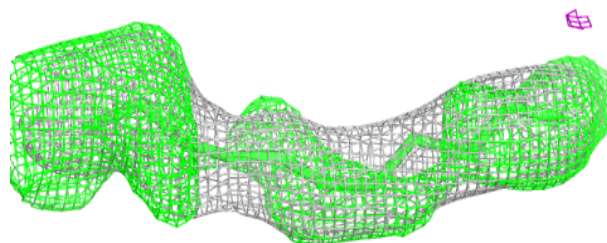
**Electron density around LFA C 314:**

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

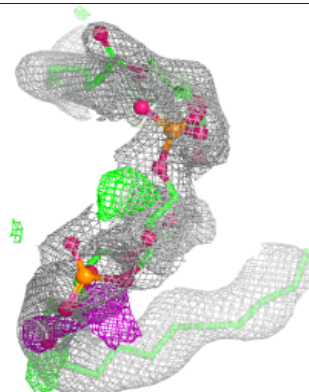
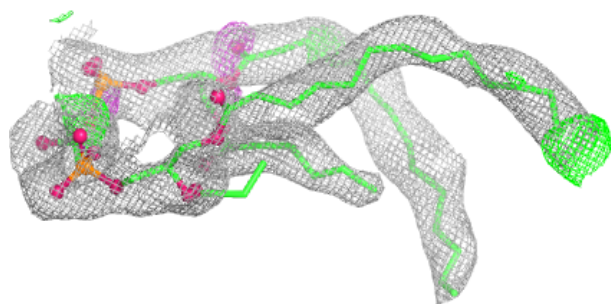
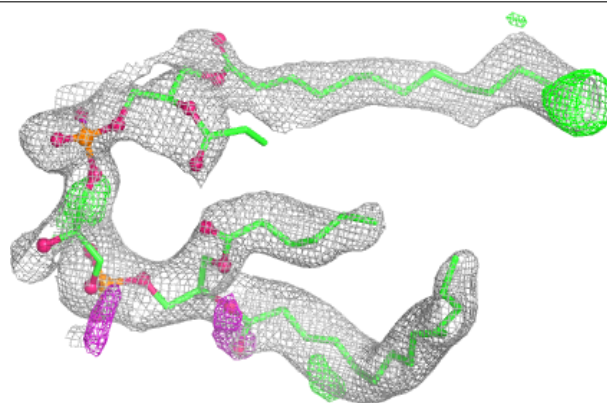


Electron density around LFA O 302:

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

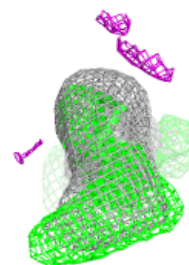
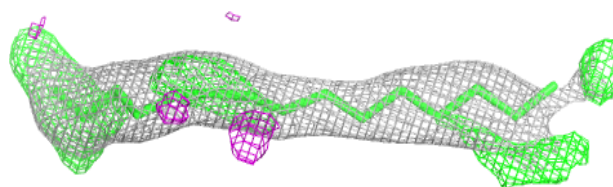
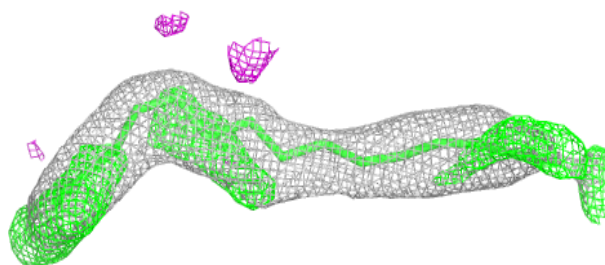
**Electron density around CDL V 101:**

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

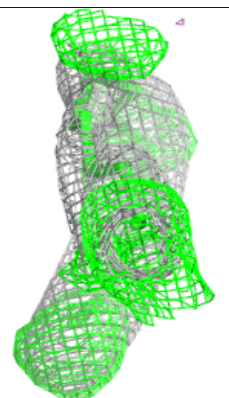
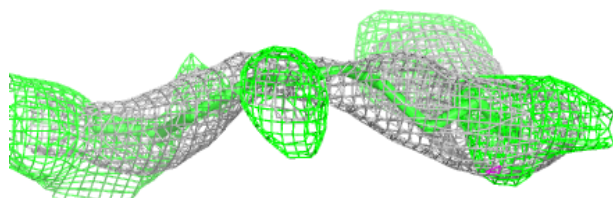
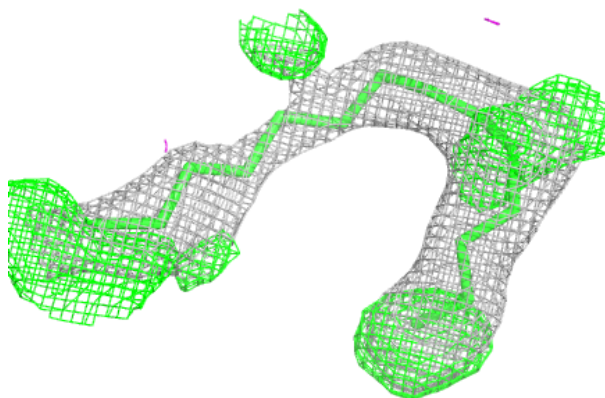


Electron density around LFA C 313:

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

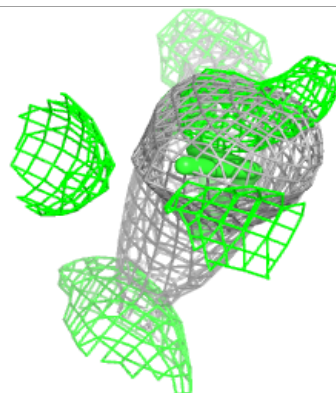
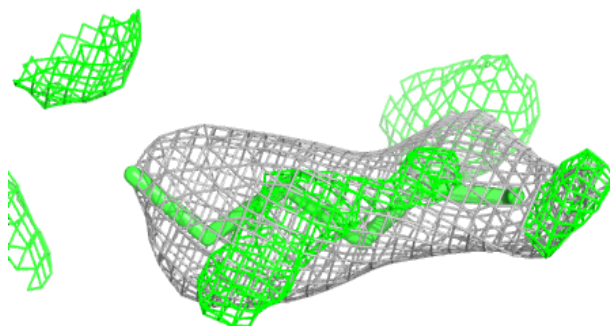
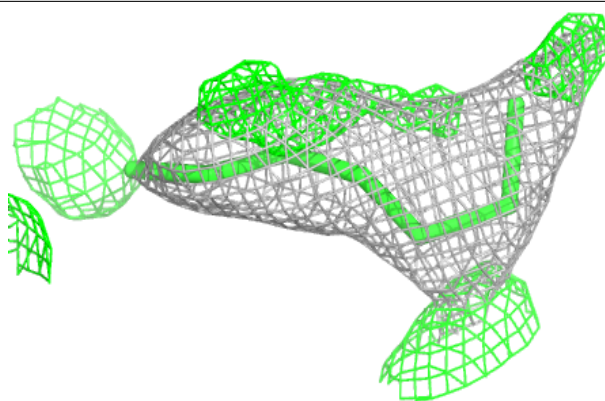
**Electron density around LFA G 106:**

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

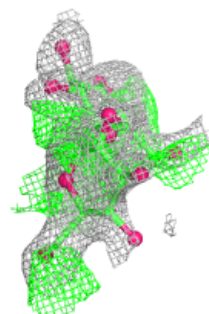
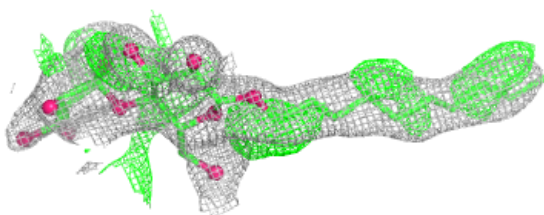
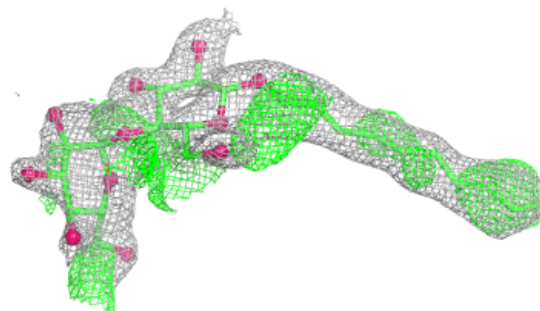


Electron density around DMU C 316:

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

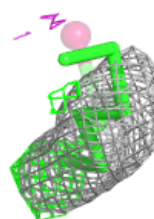
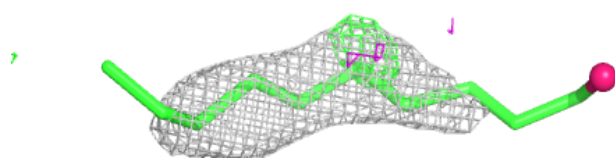
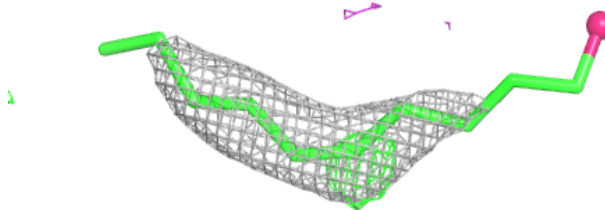
**Electron density around DMU Q 201:**

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

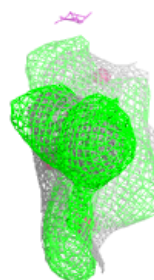
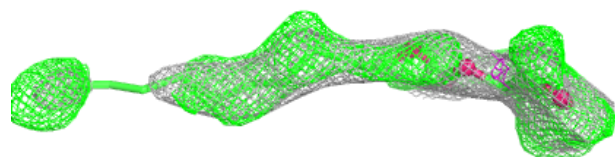
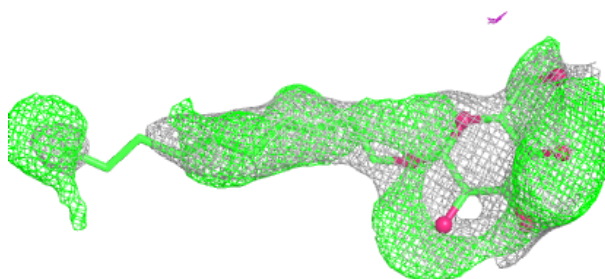


Electron density around DMU W 101:

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

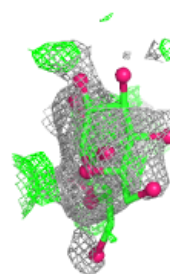
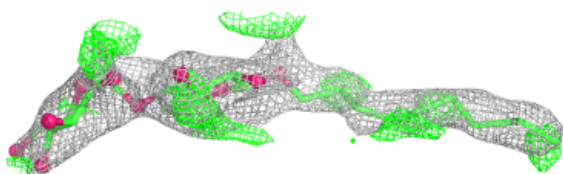
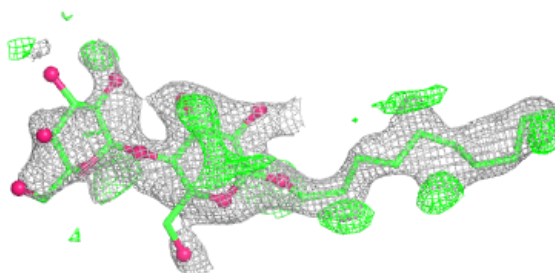
**Electron density around DMU Y 102:**

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

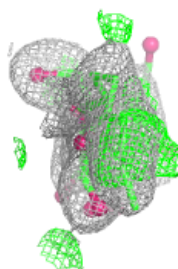
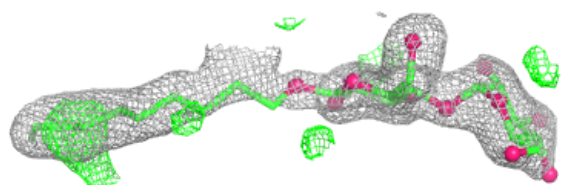
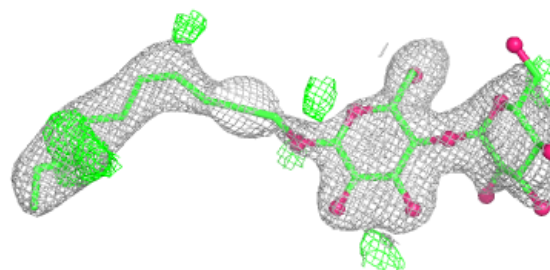


Electron density around DMU C 319:

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

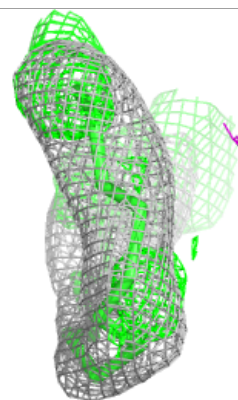
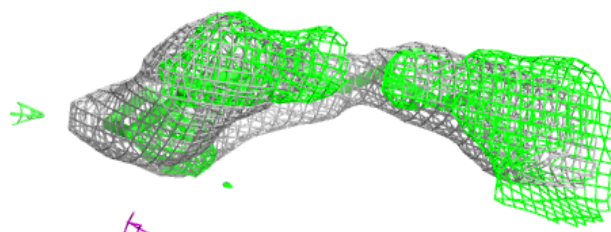
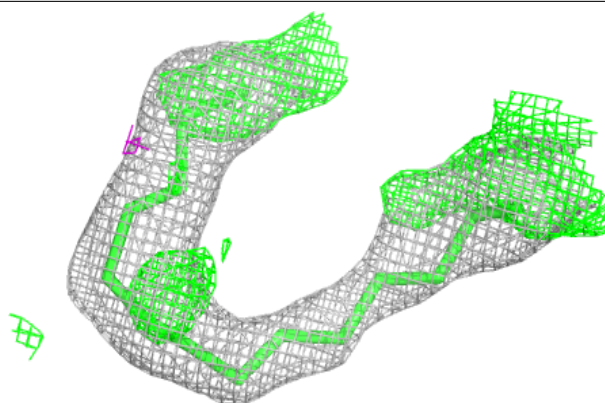
**Electron density around DMU C 323:**

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

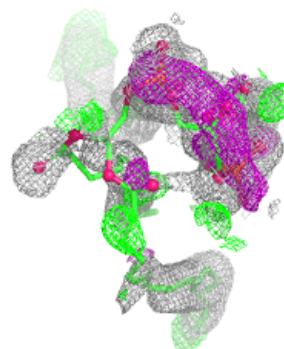
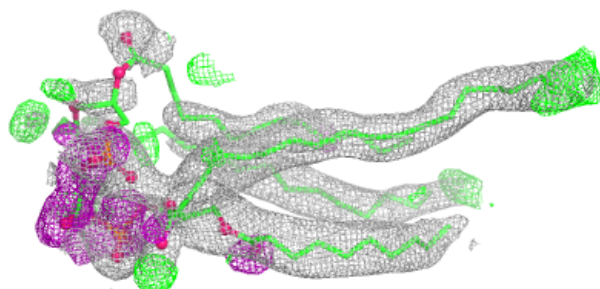
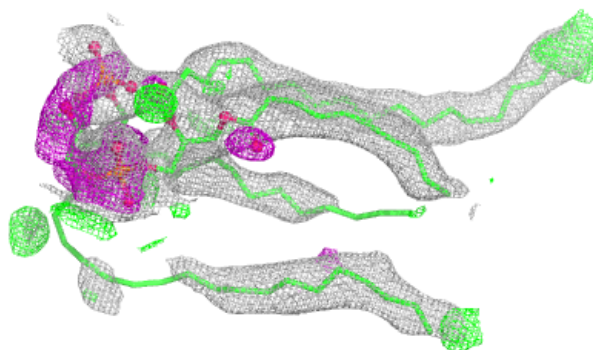


Electron density around LFA T 101:

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

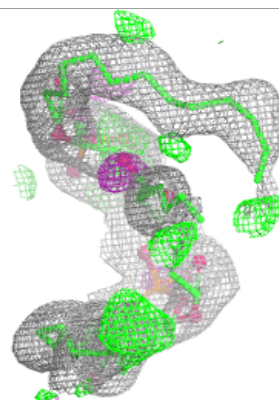
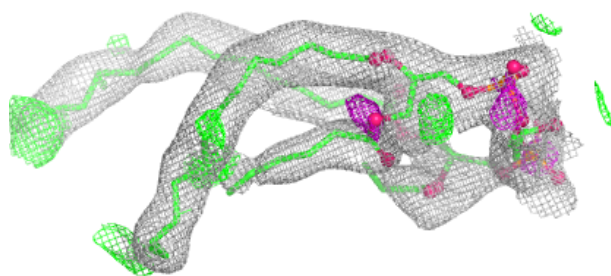
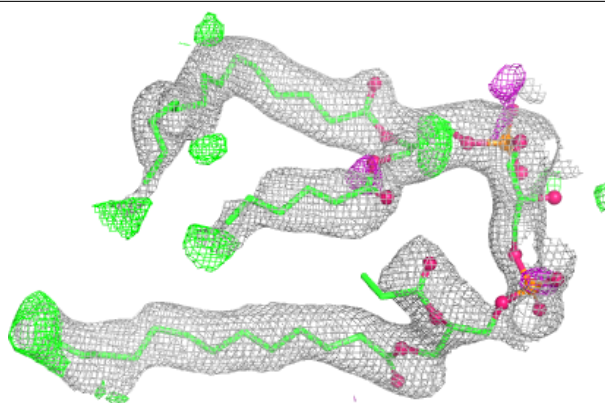
**Electron density around CDL P 305:**

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

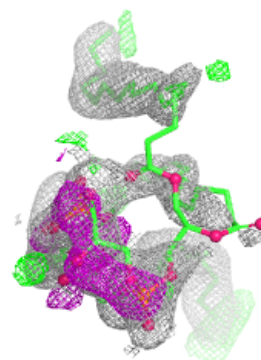
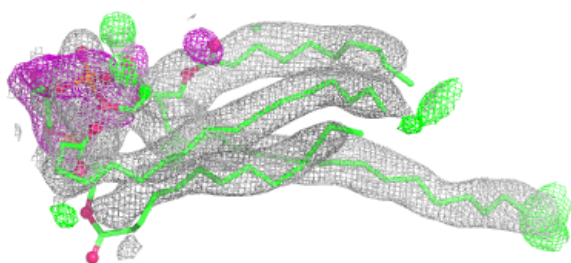
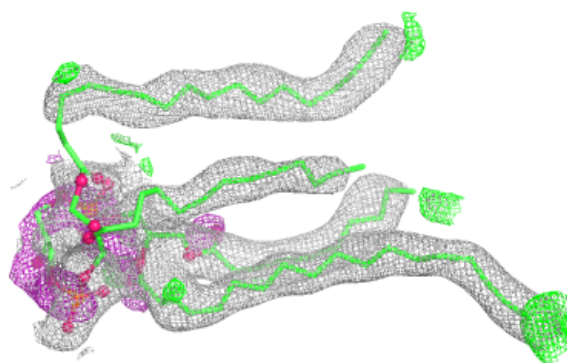


Electron density around CDL A 606:

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

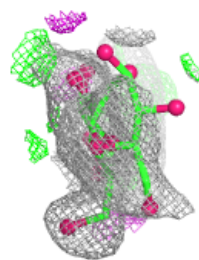
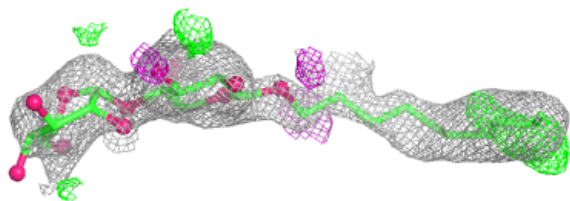
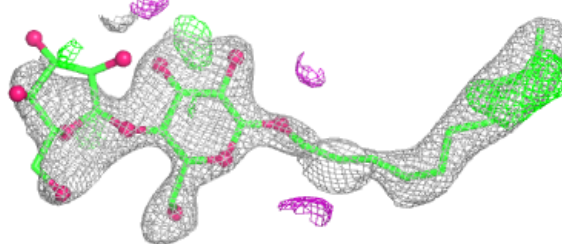
**Electron density around CDL C 304:**

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

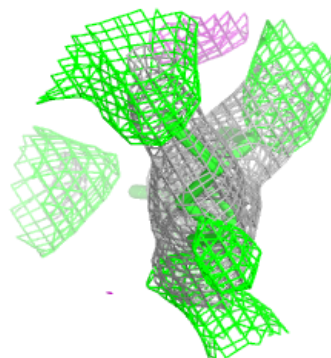
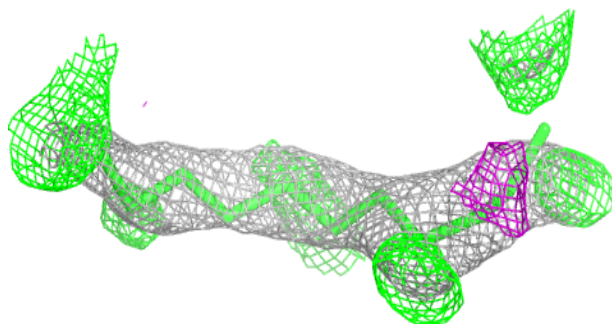
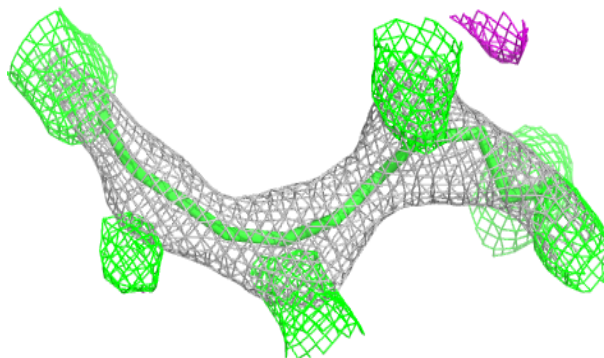


Electron density around DMU P 324:

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

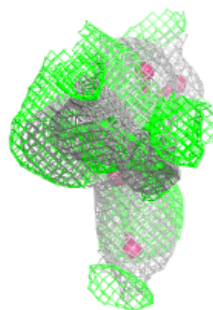
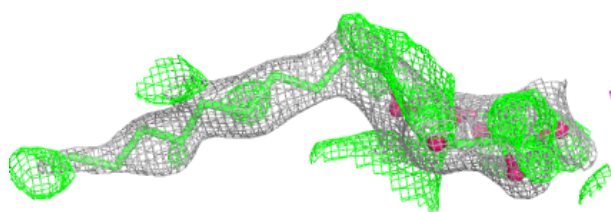
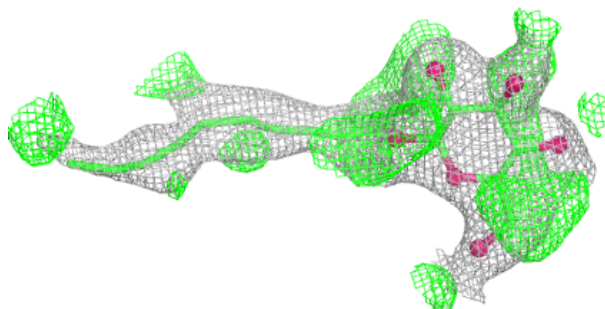
**Electron density around LFA C 307:**

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

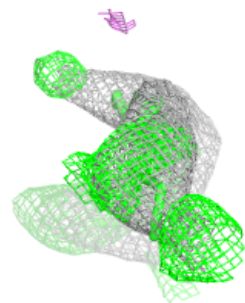
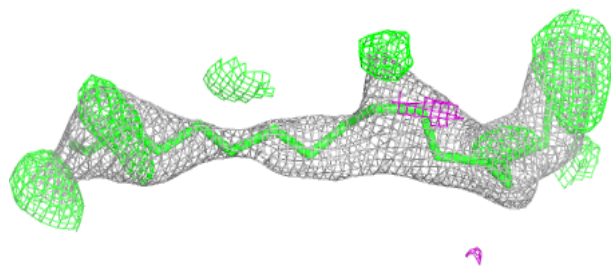
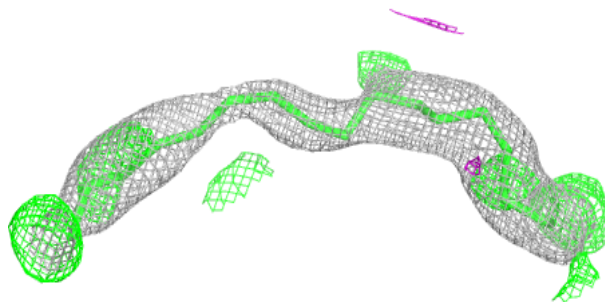


Electron density around DMU T 104:

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

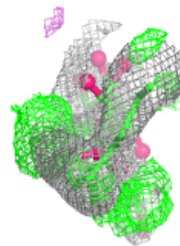
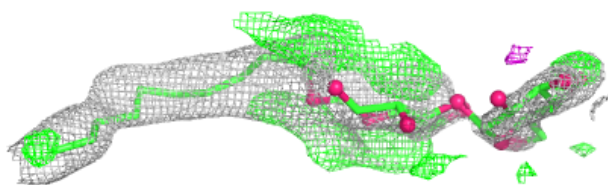
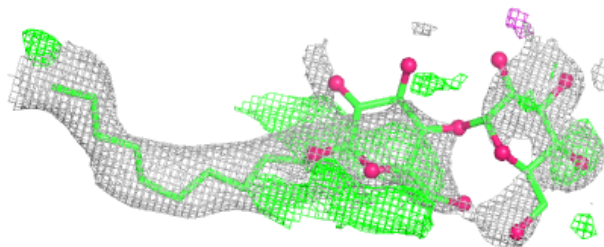
**Electron density around LFA O 301:**

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



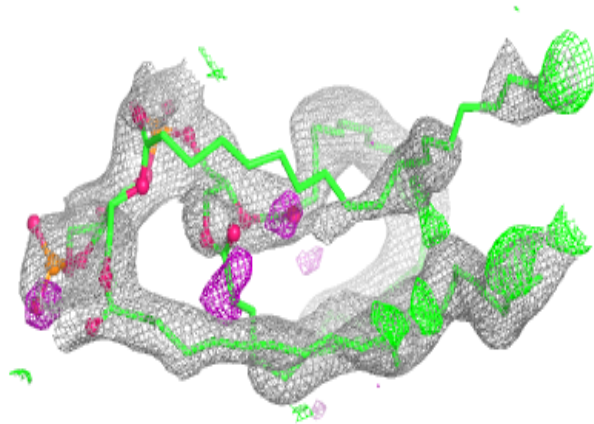
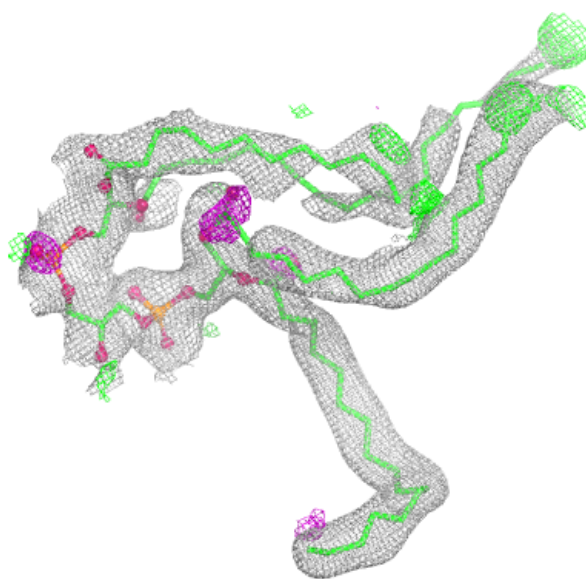
Electron density around DMU N 615:

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



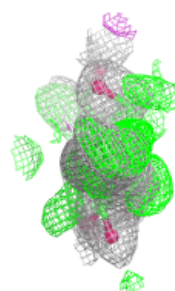
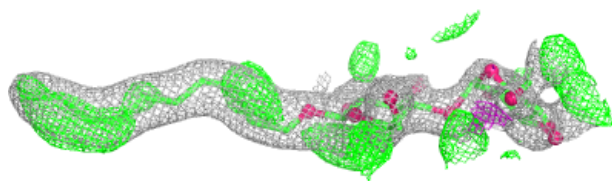
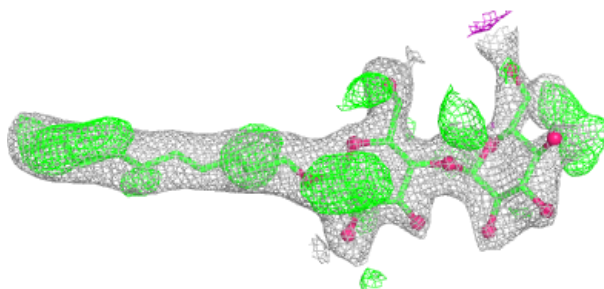
Electron density around CDL Y 101:

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

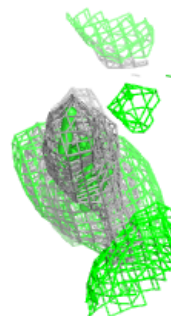
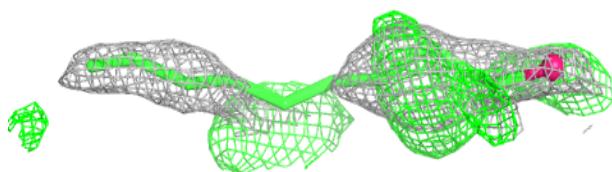
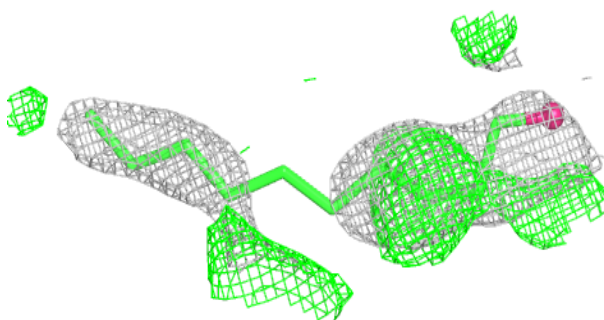


Electron density around DMU A 609:

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

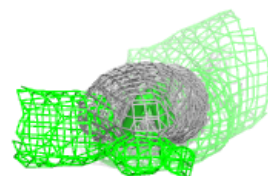
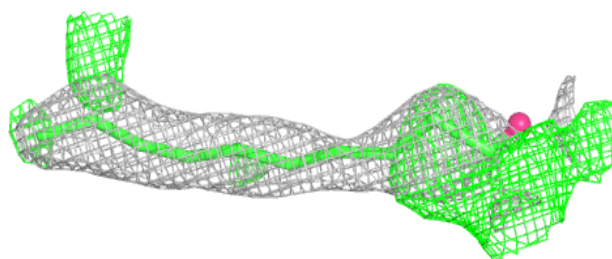
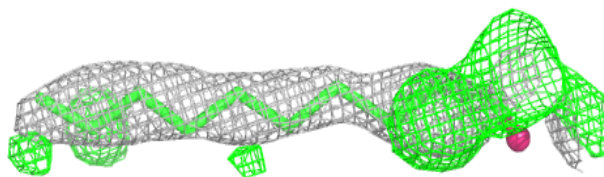
**Electron density around DMU A 614:**

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

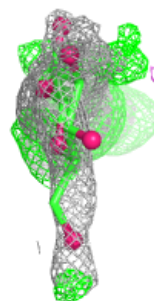
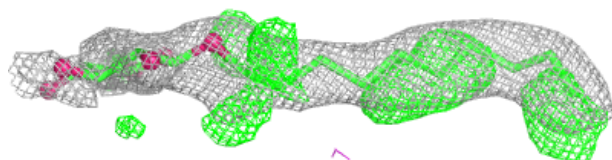
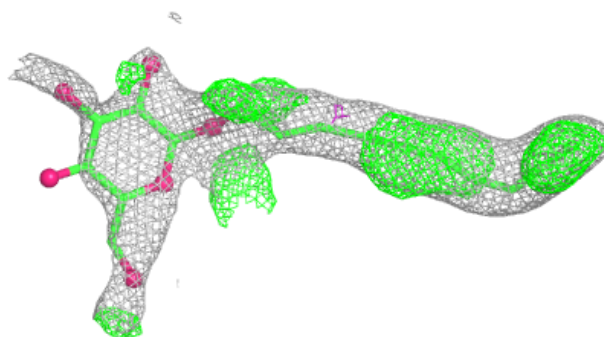


Electron density around DMU B 302:

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

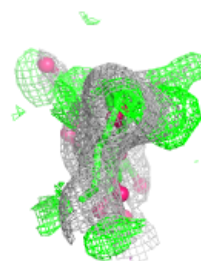
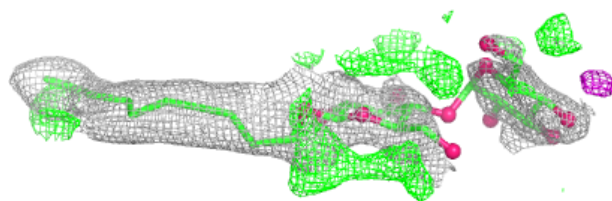
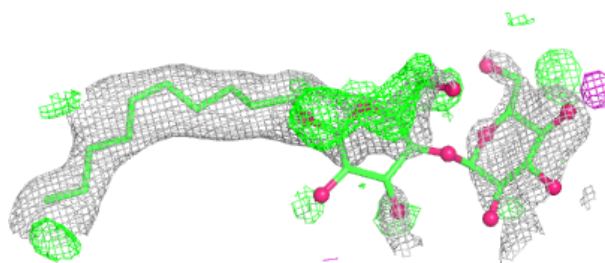
**Electron density around DMU B 304:**

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

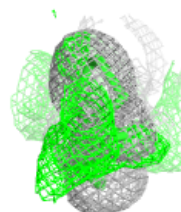
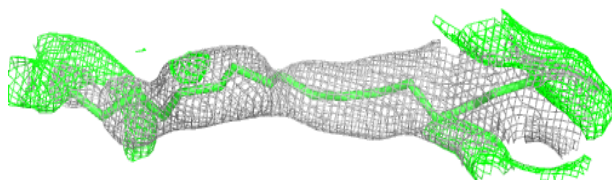
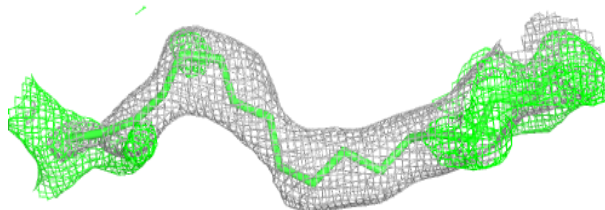


Electron density around DMU H 101:

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

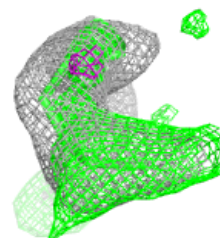
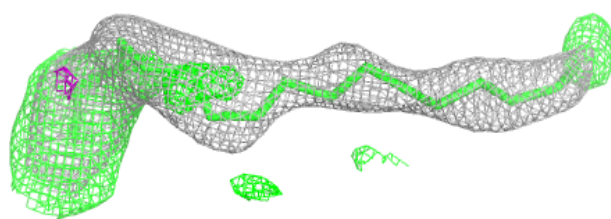
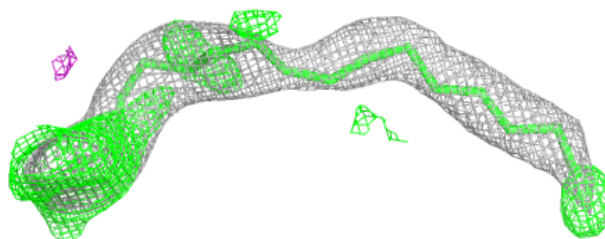
**Electron density around LFA P 310:**

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

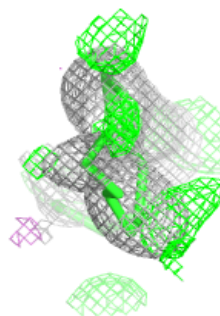
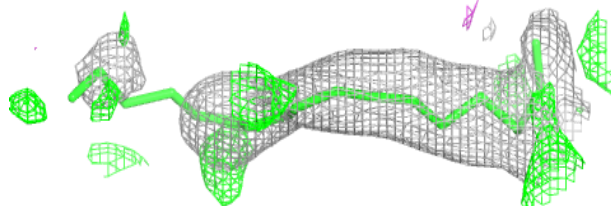
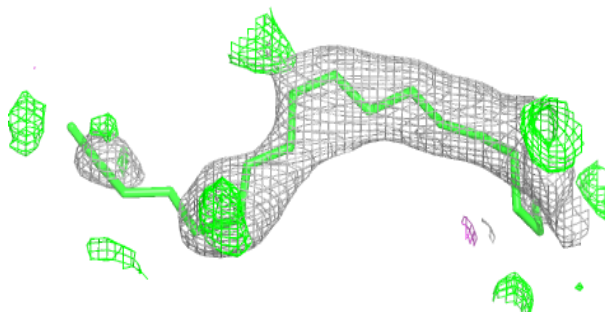


Electron density around LFA B 307:

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

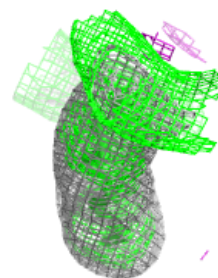
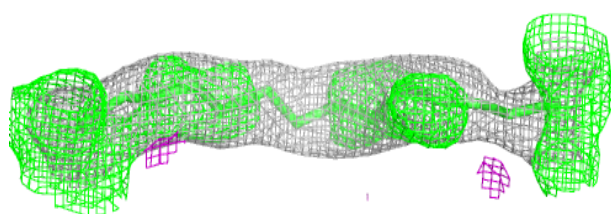
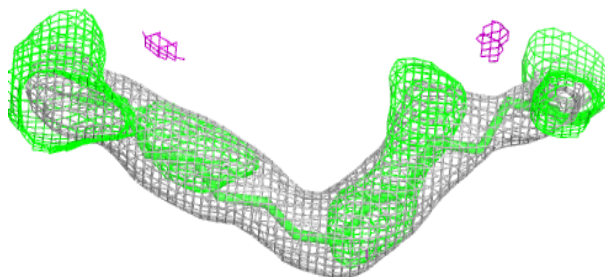
**Electron density around LFA C 309:**

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

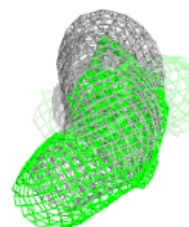
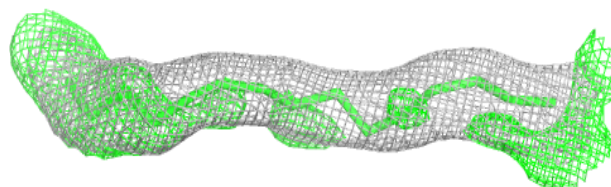
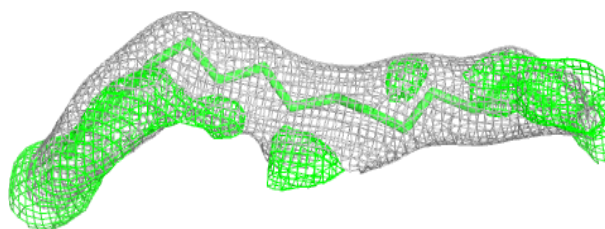


Electron density around LFA A 607:

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

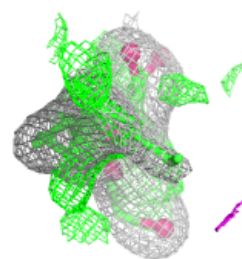
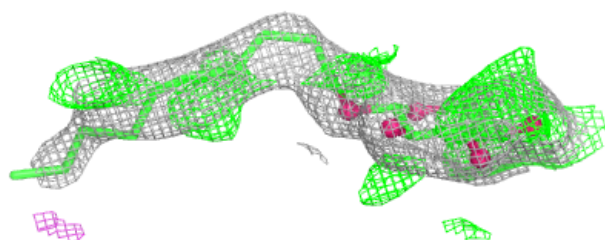
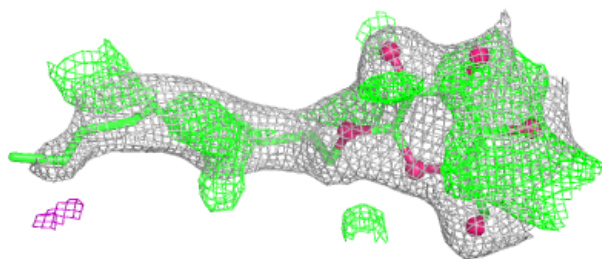
**Electron density around LFA P 314:**

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

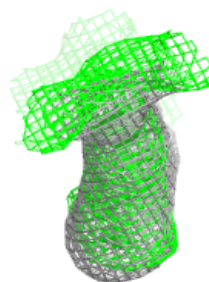
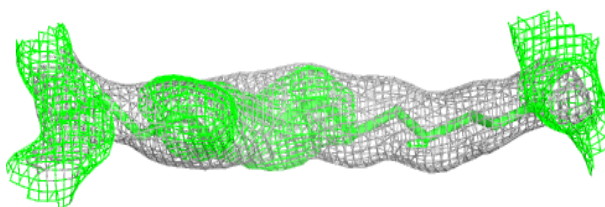
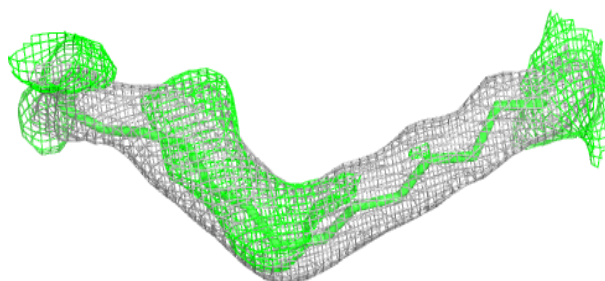


Electron density around DMU G 104:

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

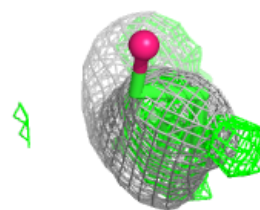
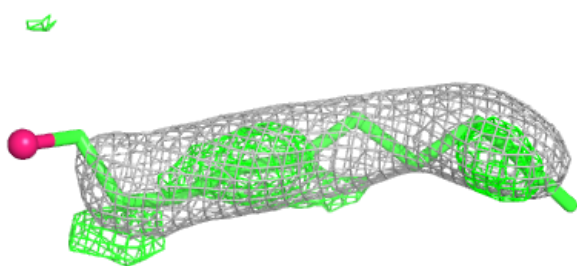
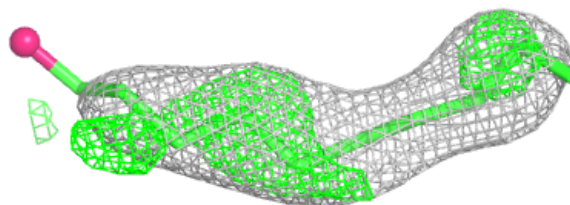
**Electron density around LFA N 606:**

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

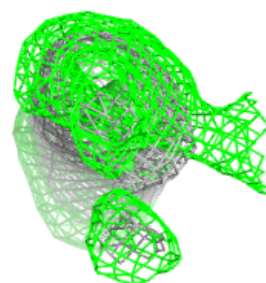
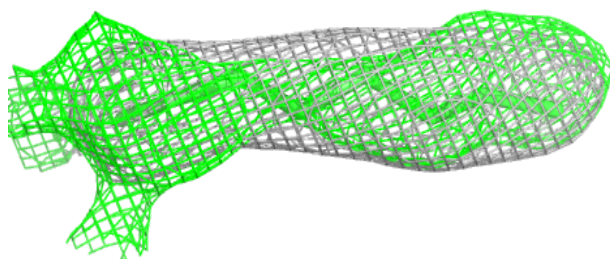
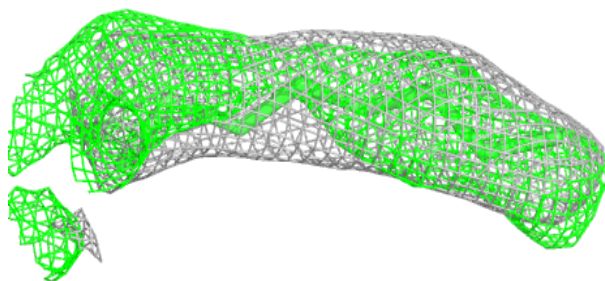


Electron density around DMU J 101:

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

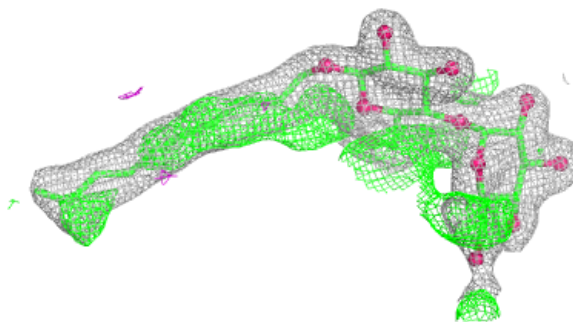
**Electron density around DMU Z 102:**

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

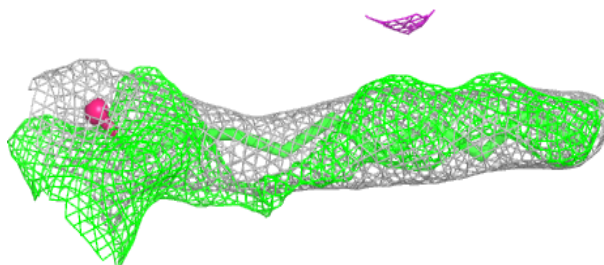


Electron density around DMU D 201:

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

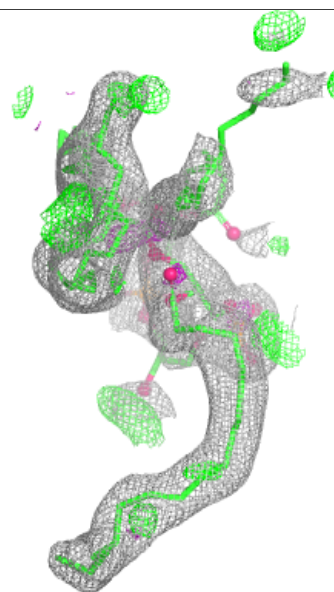
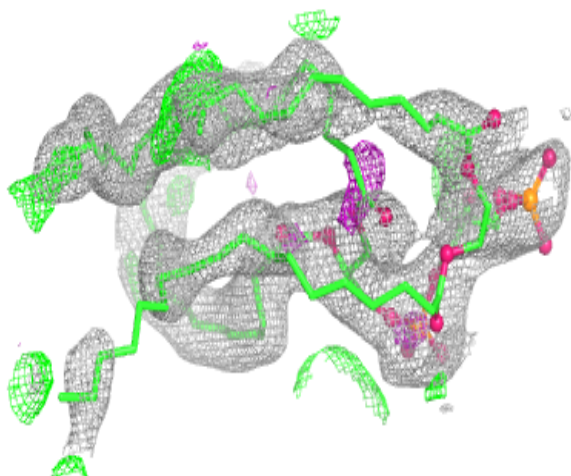
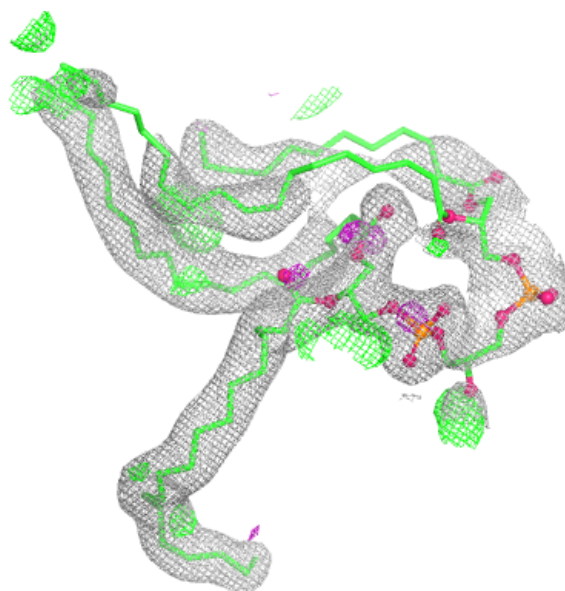
**Electron density around DMU O 305:**

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



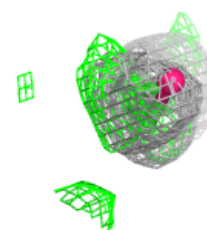
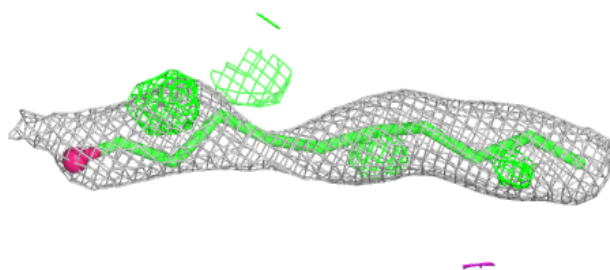
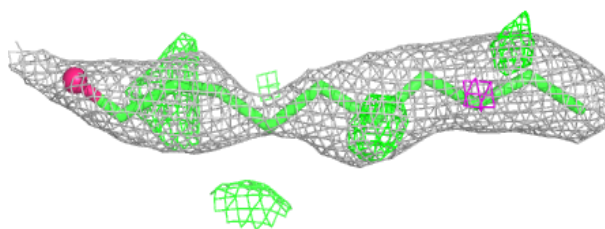
Electron density around CDL L 101:

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

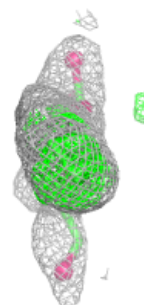
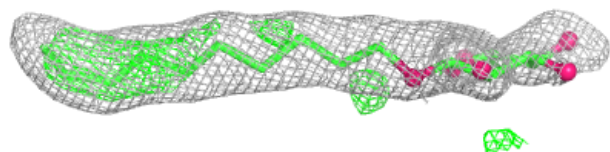
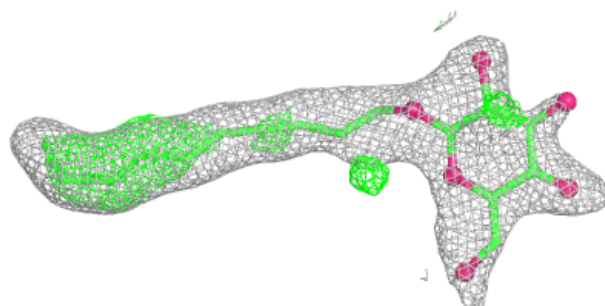


Electron density around DMU B 303:

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

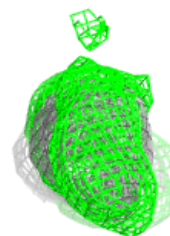
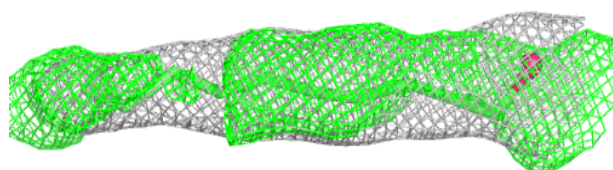
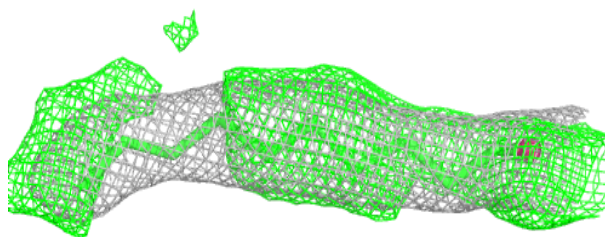
**Electron density around DMU O 307:**

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

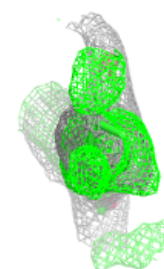
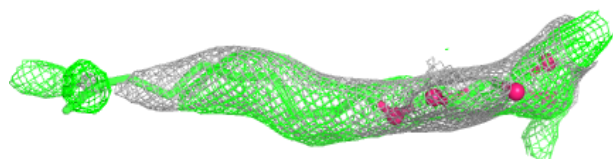
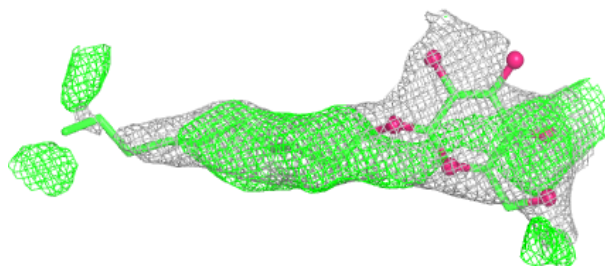


Electron density around DMU P 307:

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

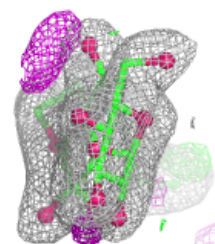
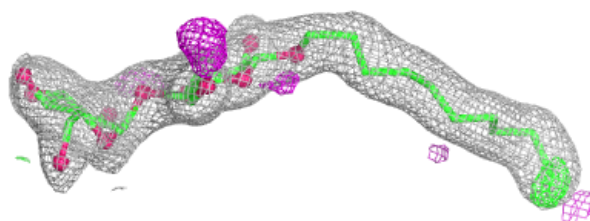
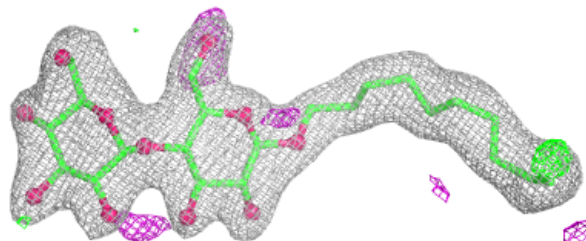
**Electron density around DMU L 102:**

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

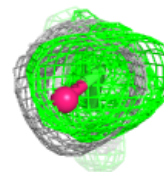
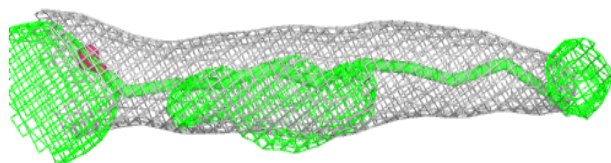
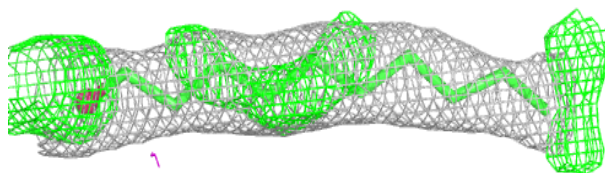


Electron density around DMU Z 101:

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

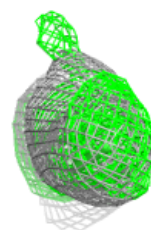
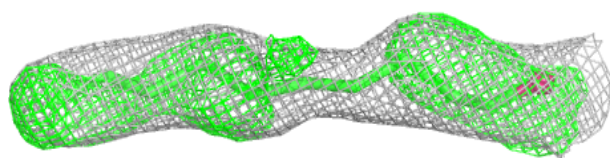
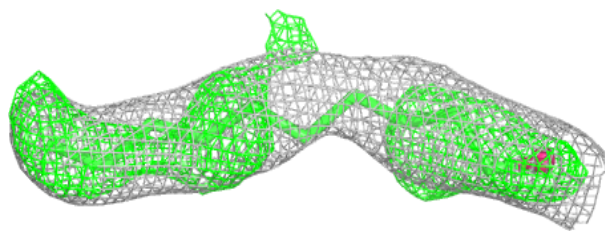
**Electron density around DMU C 306:**

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

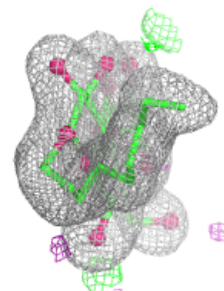
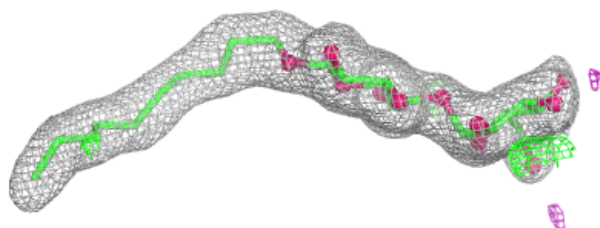
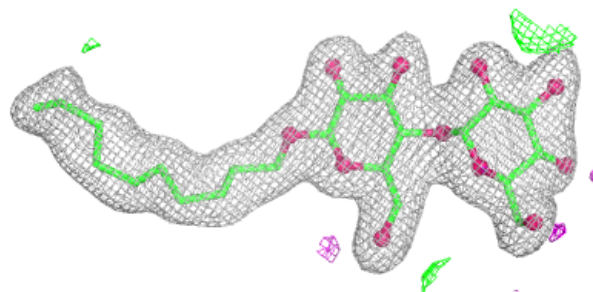


Electron density around DMU O 306:

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

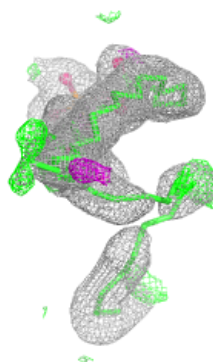
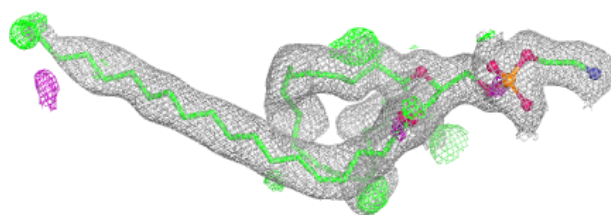
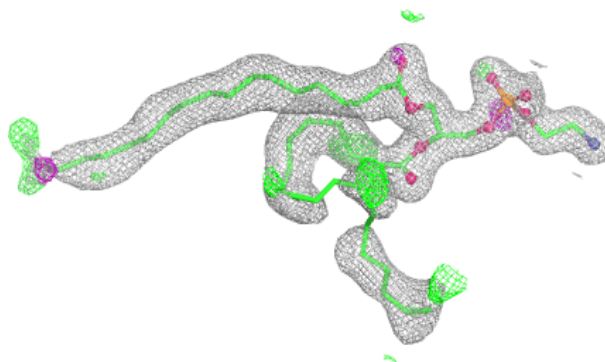
**Electron density around DMU M 101:**

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

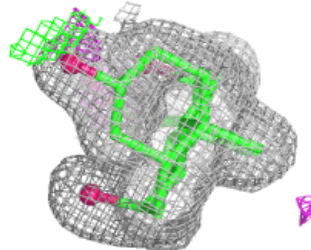
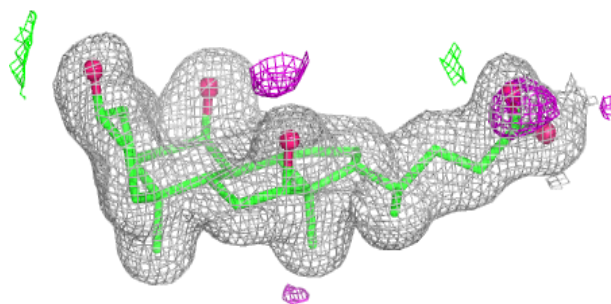
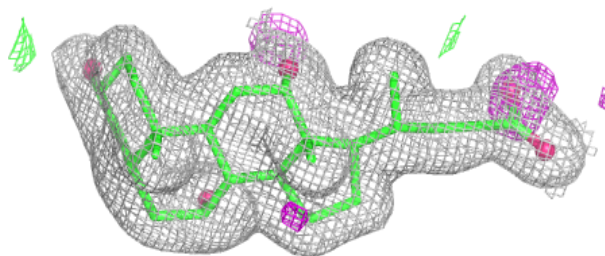


Electron density around PEK T 102:

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

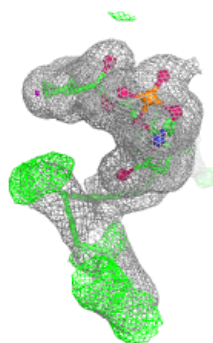
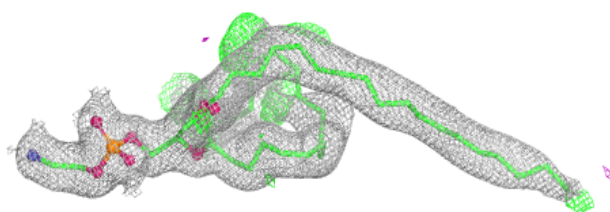
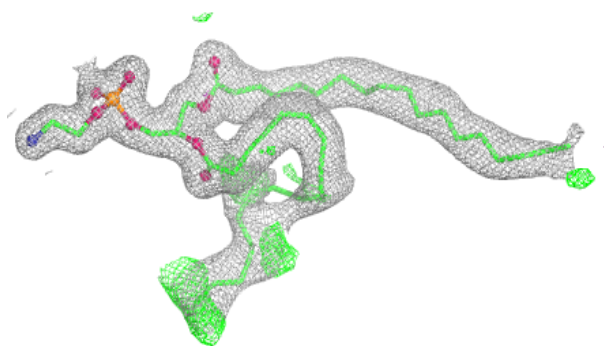
**Electron density around CHD C 301:**

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

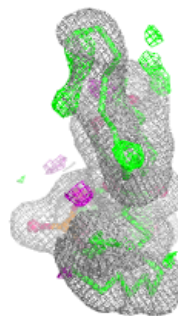
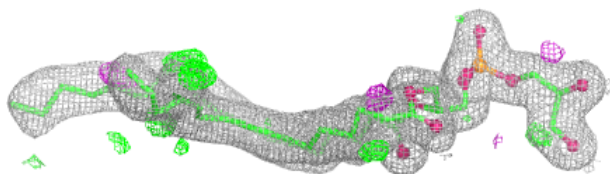
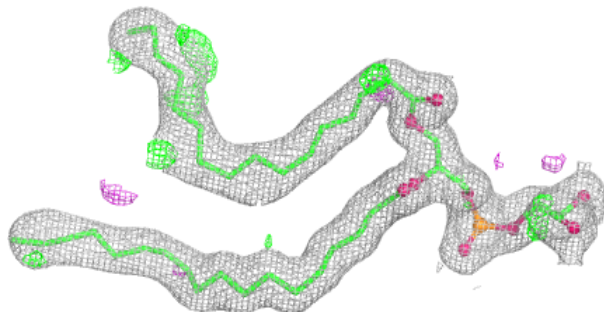


Electron density around PEK G 101:

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

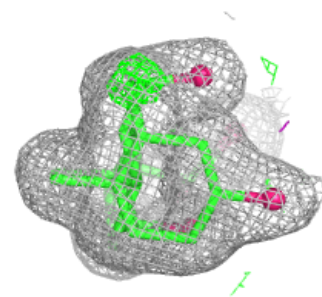
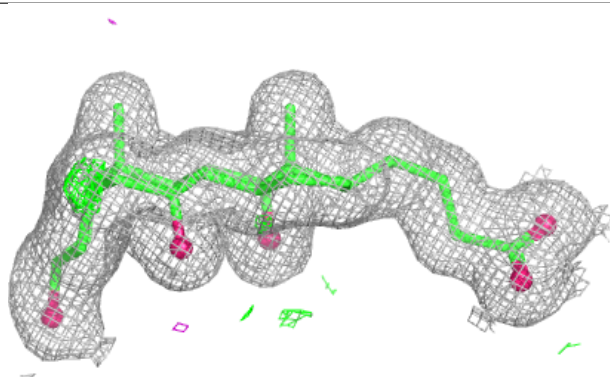
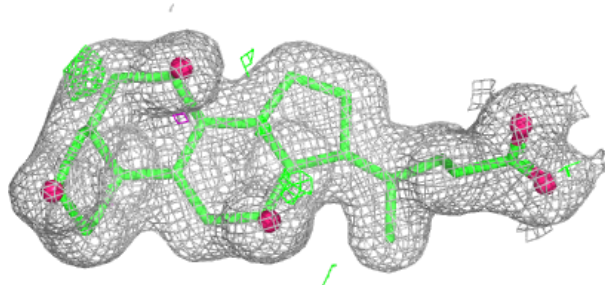
**Electron density around PGV N 614:**

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

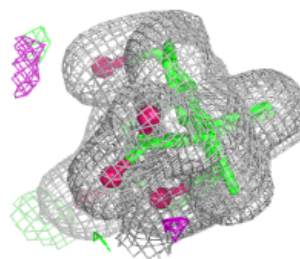
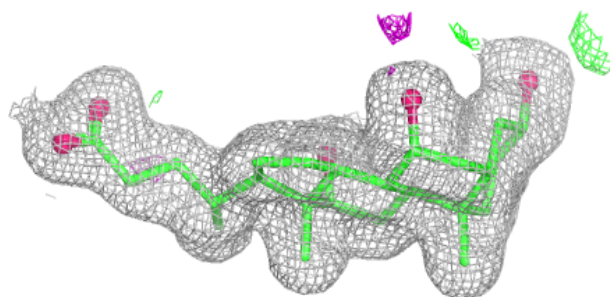
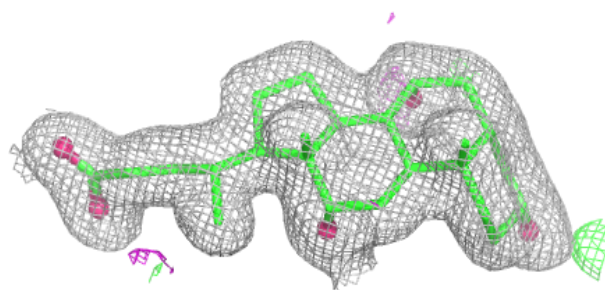


Electron density around CHD B 306:

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

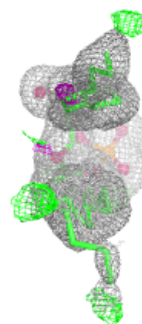
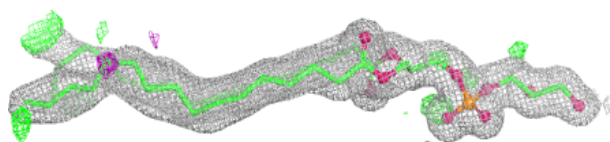
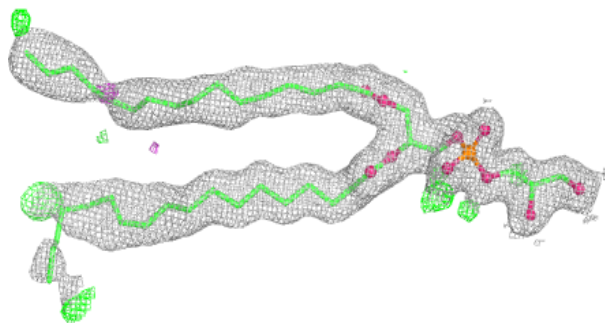
**Electron density around CHD P 302:**

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

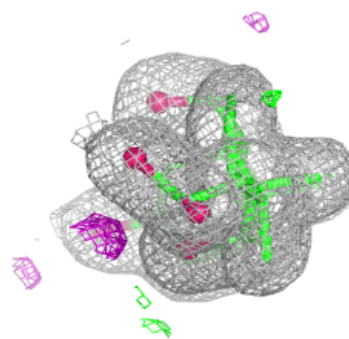
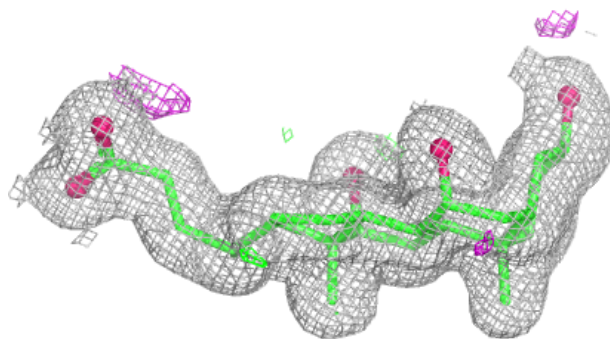
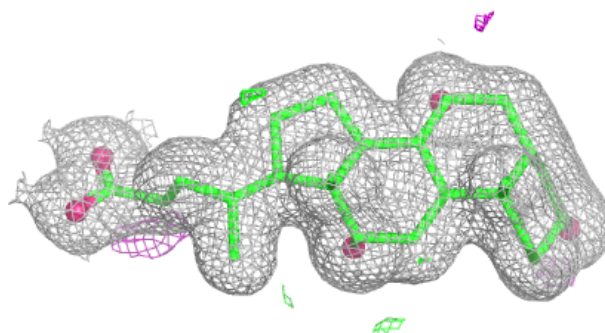


Electron density around PGV C 303:

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

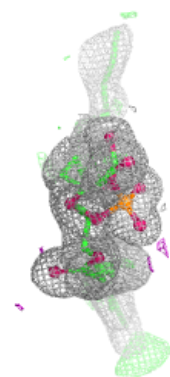
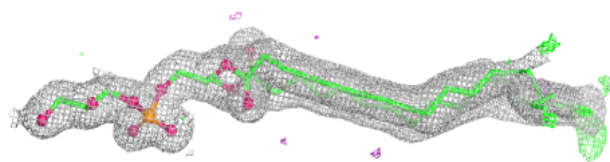
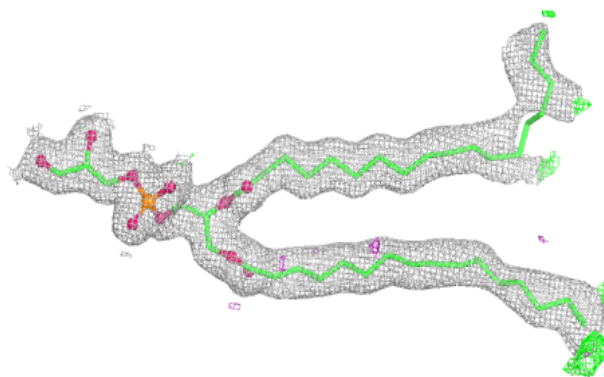
**Electron density around CHD G 102:**

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

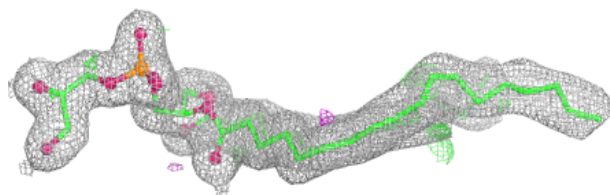
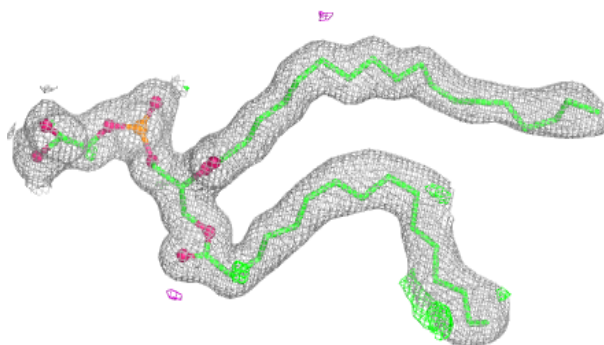


Electron density around PGV P 304:

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

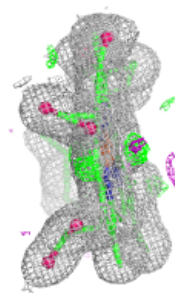
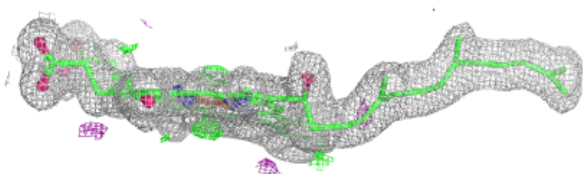
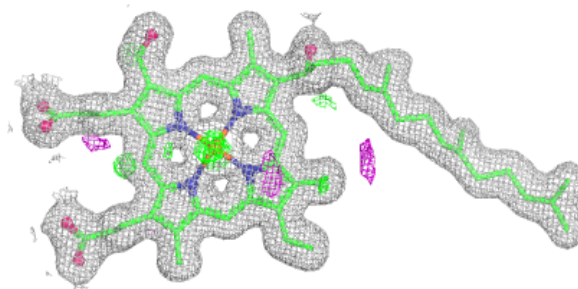
**Electron density around PGV A 613:**

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

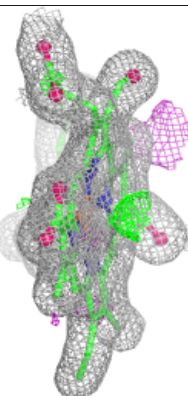
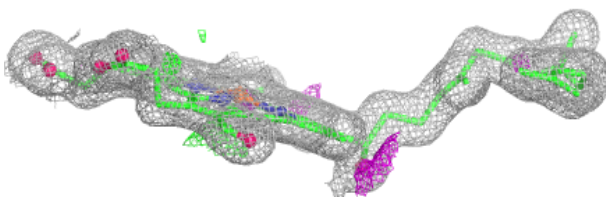
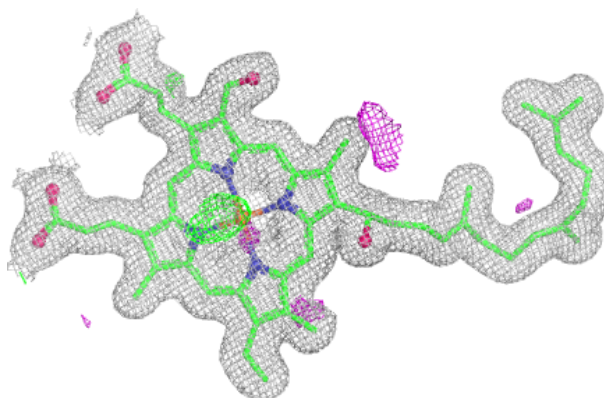


Electron density around HEA A 601:

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

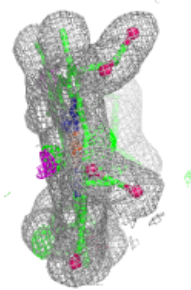
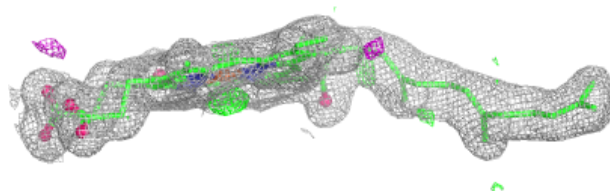
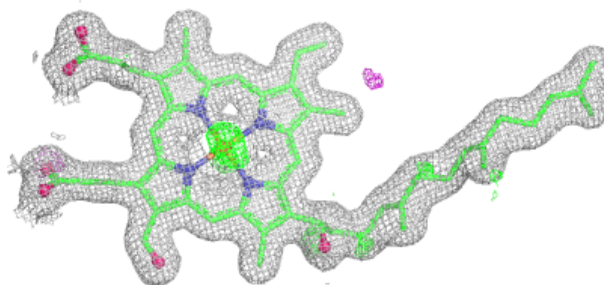
**Electron density around HEA A 602:**

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

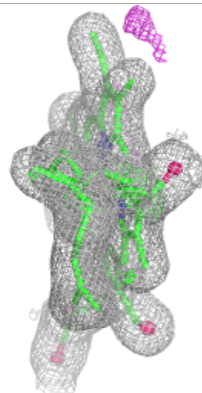
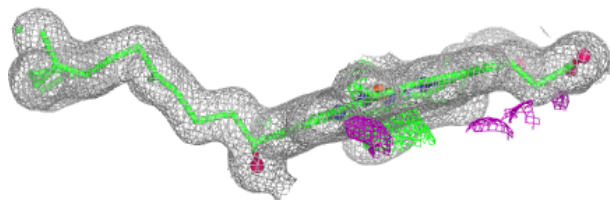
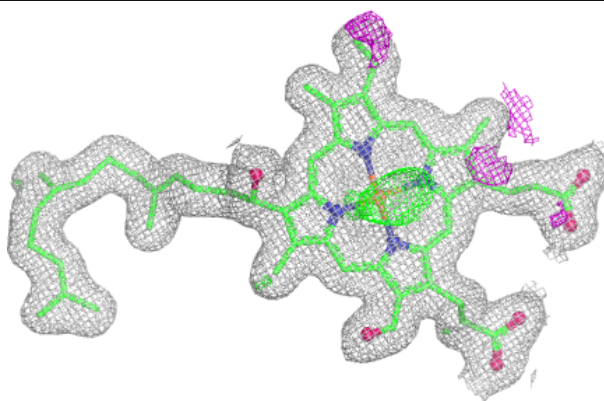


Electron density around HEA N 601:

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

**Electron density around HEA N 602:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.