



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:40 PM UTC

PDB ID : 9KUL / pdb_00009kul
Title : Bovine Heart Cytochrome c Oxidase in the Xenon-bound Fully Oxidized State under Anaerobic Condition
Authors : Muramoto, K.; Shinzawa-Itoh, K.
Deposited on : 2024-12-04
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
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

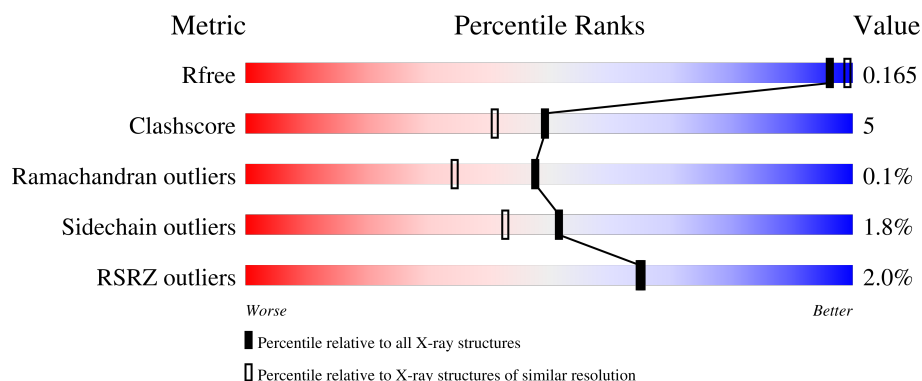
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

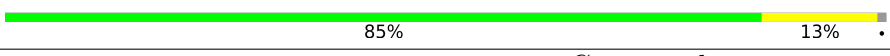
The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	514	
1	N	514	
2	B	227	
2	O	227	
3	C	261	

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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
20	LFA	P	311	-	-	-	X
23	XE	B	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	XE	N	618	-	-	X	-
23	XE	O	304	-	-	X	-

2 Entry composition [i](#)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

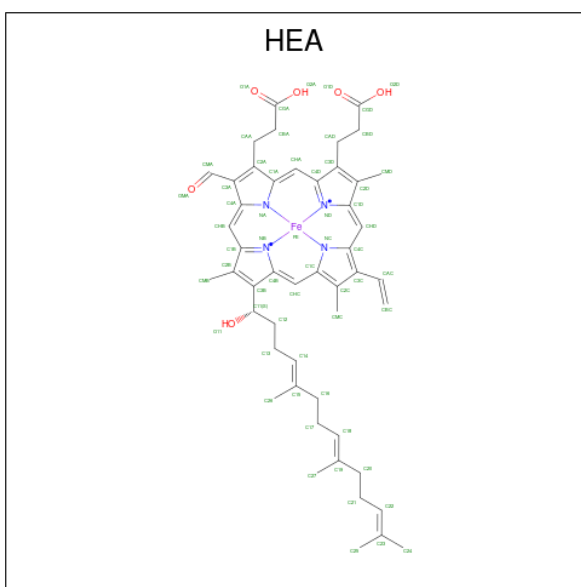
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

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



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

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

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

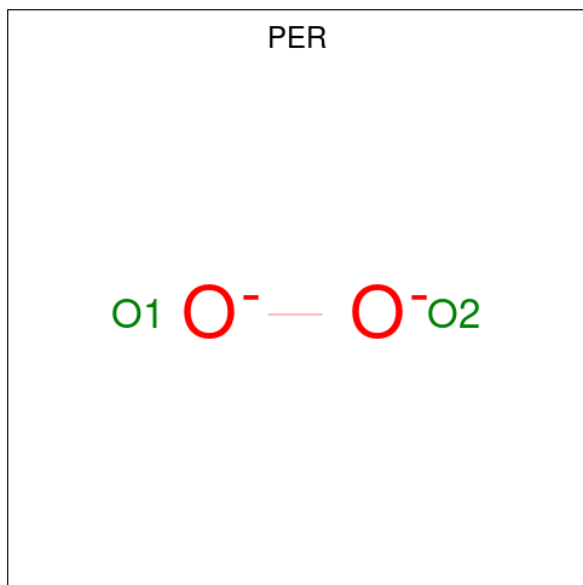
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

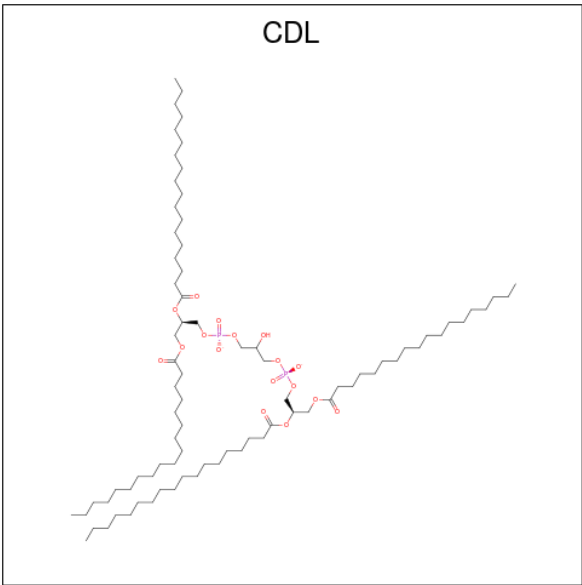
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total 1	Na 1	0	0
17	N	1	Total 1	Na 1	0	0

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



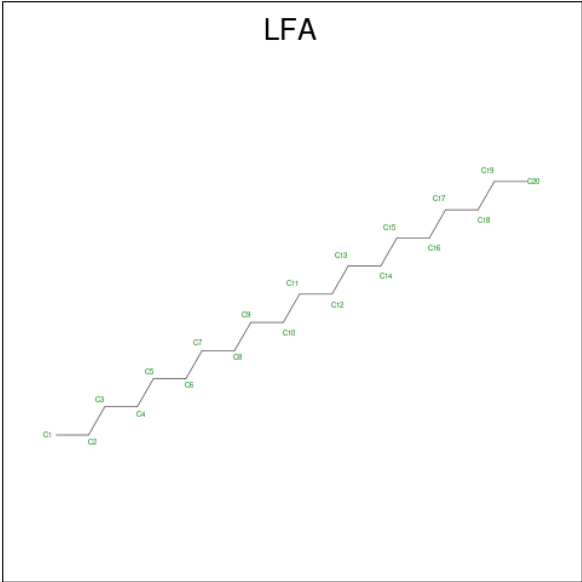
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total 2	O 2	0	0
18	N	1	Total 2	O 2	0	0

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



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

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



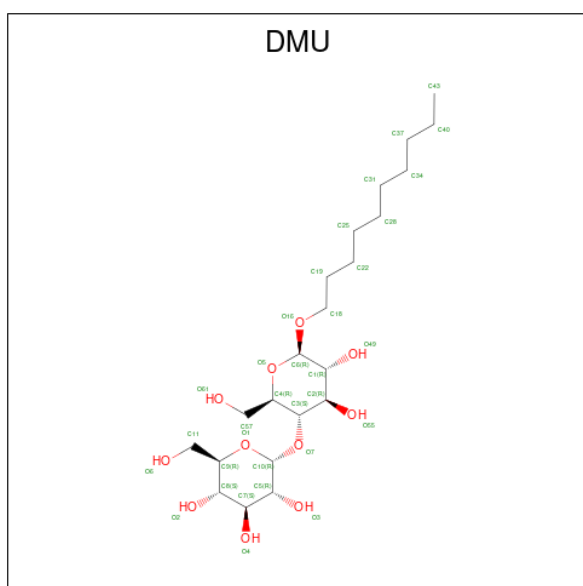
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	C	0	0
			14	14		
20	A	1	Total	C	0	0
			14	14		
20	B	1	Total	C	0	0
			17	17		
20	C	1	Total	C	0	0
			11	11		
20	C	1	Total	C	0	0
			6	6		
20	C	1	Total	C	0	0
			18	18		
20	C	1	Total	C	0	0
			11	11		
20	C	1	Total	C	0	0
			14	14		
20	C	1	Total	C	0	0
	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

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

- Molecule 21 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



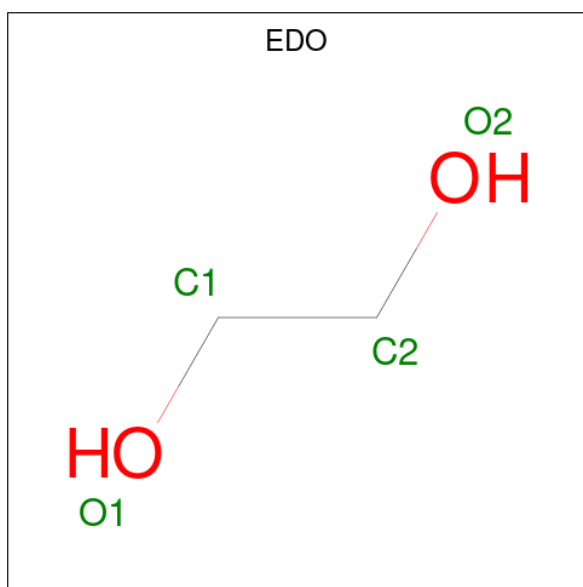
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 7 7	0	0
21	A	1	Total C O 33 22 11	0	0
21	A	1	Total C O 33 22 11	0	0
21	A	1	Total C O 11 10 1	0	0
21	B	1	Total C O 11 10 1	0	0
21	B	1	Total C O 11 10 1	0	0
21	B	1	Total C O 22 16 6	0	0
21	B	1	Total C O 22 16 6	0	0
21	C	1	Total C O 11 10 1	0	0
21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

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

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



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

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

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

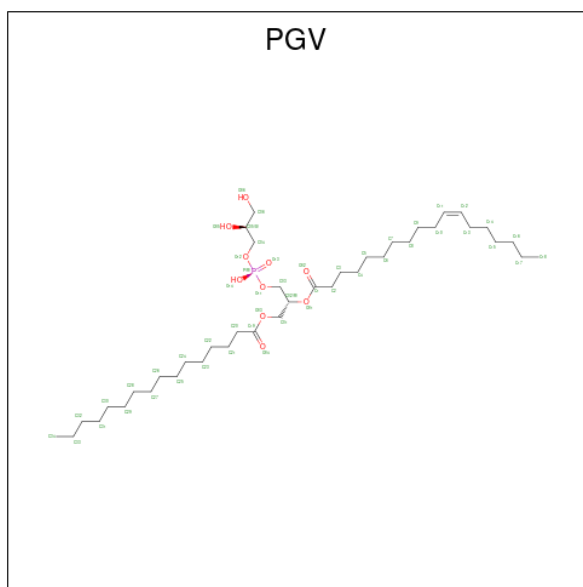
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	5	Total Xe 5 5	0	0
23	B	1	Total Xe 1 1	0	0
23	C	1	Total Xe 1 1	0	0
23	N	5	Total Xe 5 5	0	0

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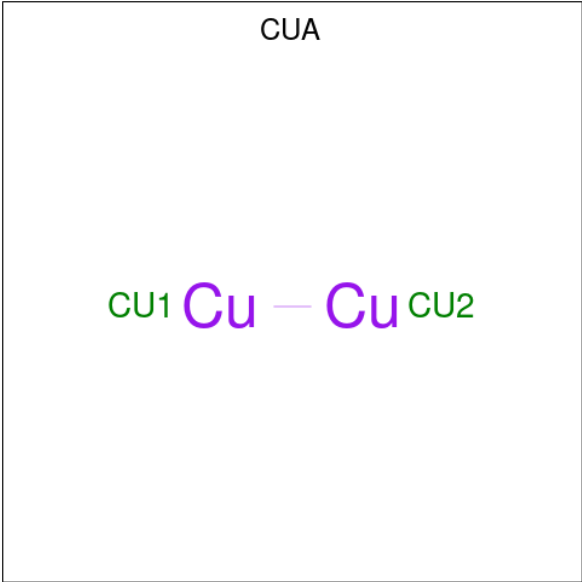
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	O	1	Total	Xe	0	0
			1	1		
23	P	1	Total	Xe	0	0
			1	1		

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



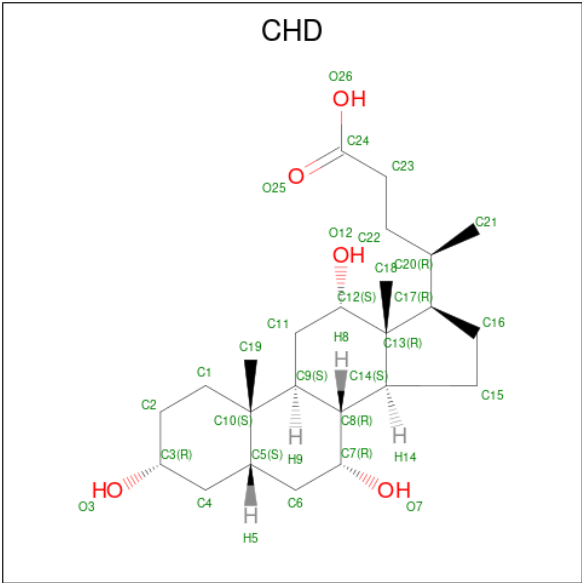
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	O	P	0	0
			51	40	10	1		
24	C	1	Total	C	O	P	0	0
			51	40	10	1		
24	N	1	Total	C	O	P	0	0
			51	40	10	1		
24	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



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

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



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

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

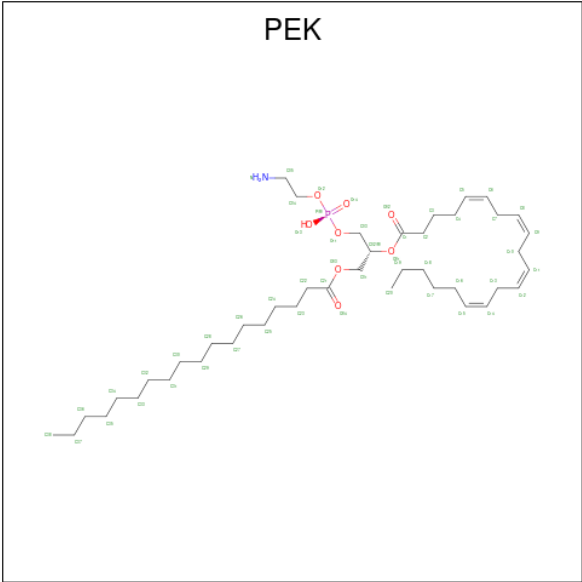
- Molecule 27 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

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

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

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

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



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	245	Total	O	0	11
			256	256		
30	B	178	Total	O	0	2
			180	180		
30	C	101	Total	O	0	1
			102	102		
30	D	139	Total	O	0	9
			148	148		
30	E	109	Total	O	0	7
			116	116		
30	F	98	Total	O	0	7
			105	105		
30	G	44	Total	O	0	1
			45	45		
30	H	58	Total	O	0	0
			58	58		
30	I	37	Total	O	0	0
			37	37		
30	J	21	Total	O	0	0
			21	21		

Continued on next page...

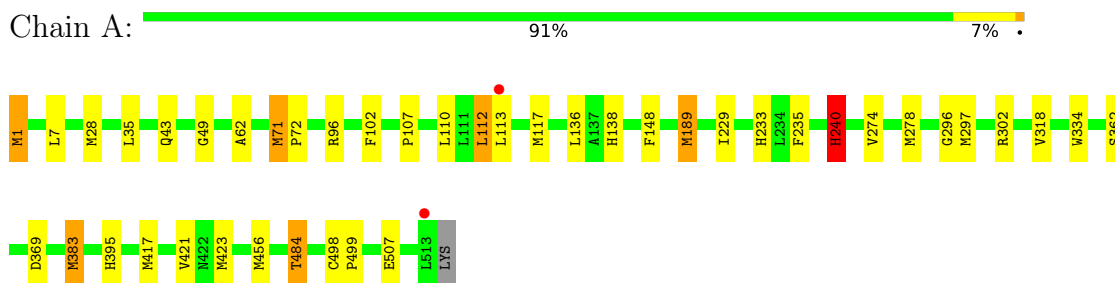
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	21	Total 21	O 21	0	0
30	L	24	Total 26	O 26	0	2
30	M	21	Total 21	O 21	0	0
30	N	229	Total 239	O 239	0	10
30	O	147	Total 148	O 148	0	1
30	P	99	Total 100	O 100	0	1
30	Q	78	Total 83	O 83	0	5
30	R	86	Total 93	O 93	0	7
30	S	89	Total 95	O 95	0	6
30	T	36	Total 37	O 37	0	1
30	U	47	Total 47	O 47	0	0
30	V	25	Total 25	O 25	0	0
30	W	15	Total 15	O 15	0	0
30	X	18	Total 18	O 18	0	0
30	Y	23	Total 25	O 25	0	2
30	Z	17	Total 17	O 17	0	0

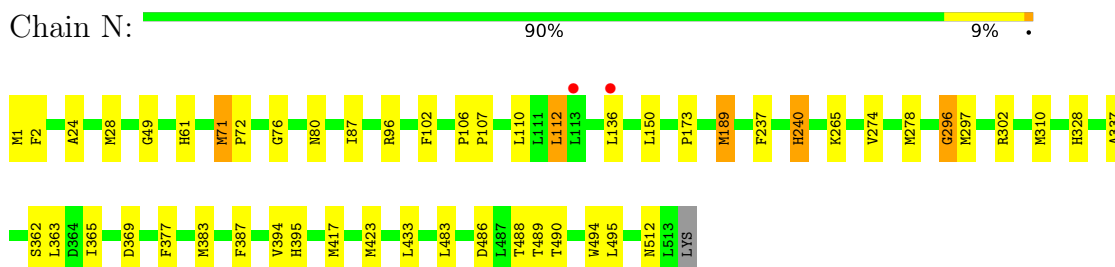
3 Residue-property plots

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

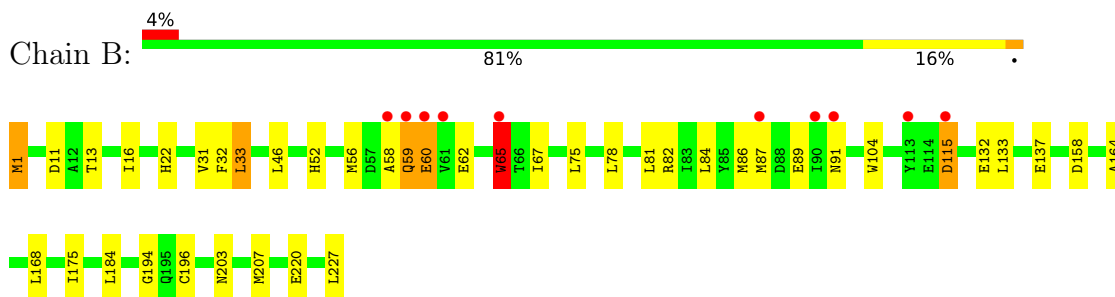
• Molecule 1: Cytochrome c oxidase subunit 1



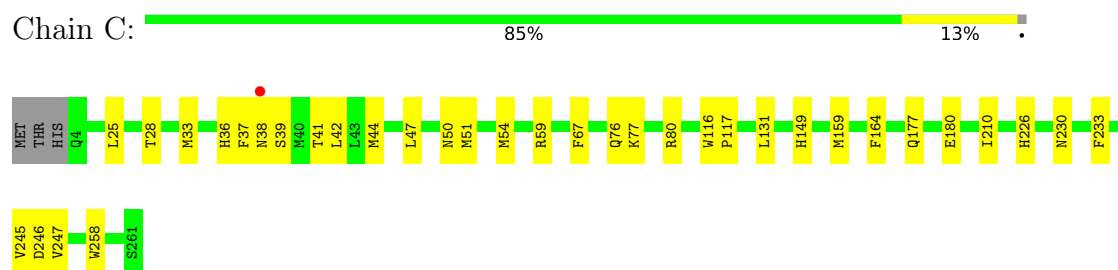
• Molecule 1: Cytochrome c oxidase subunit 1



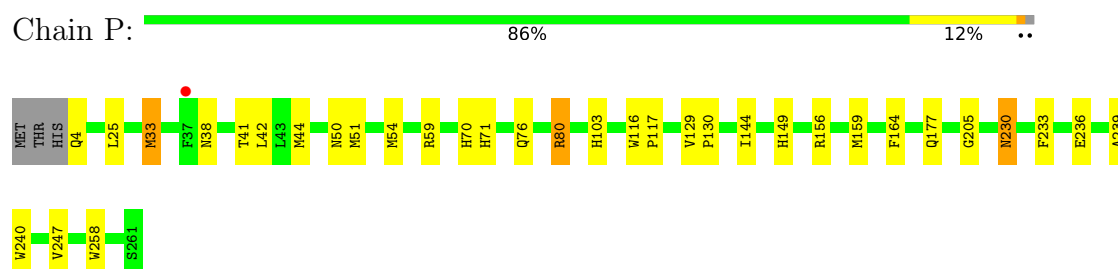
• Molecule 2: Cytochrome c oxidase subunit 2



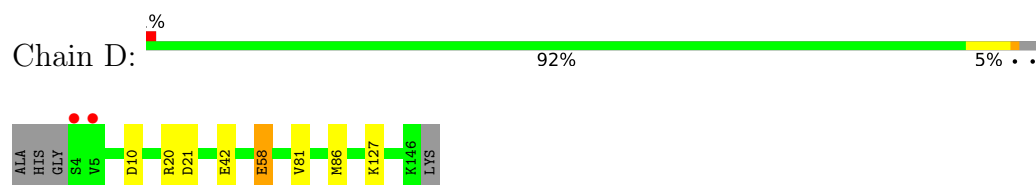
- Molecule 3: Cytochrome c oxidase subunit 3



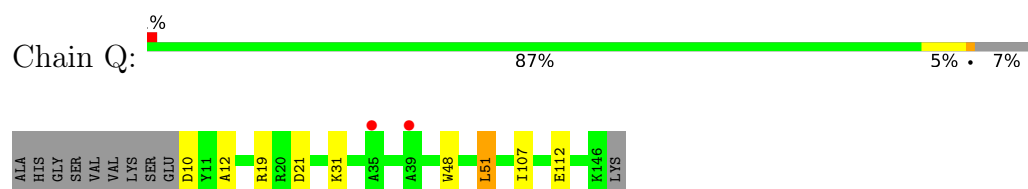
- Molecule 3: Cytochrome c oxidase subunit 3



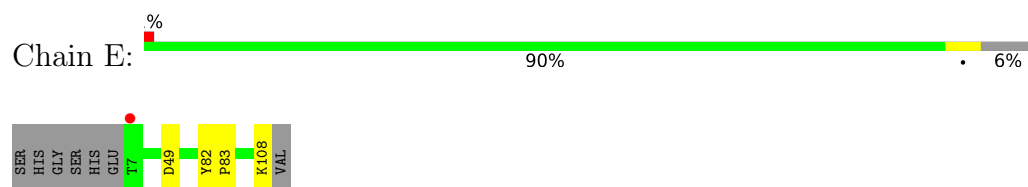
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



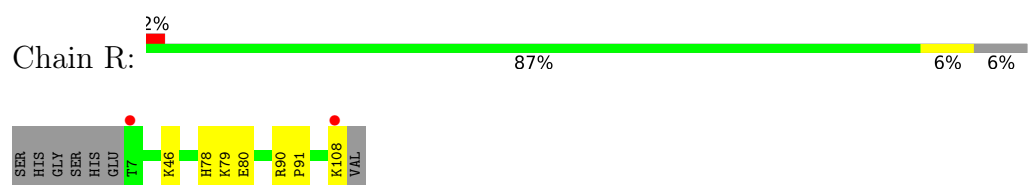
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



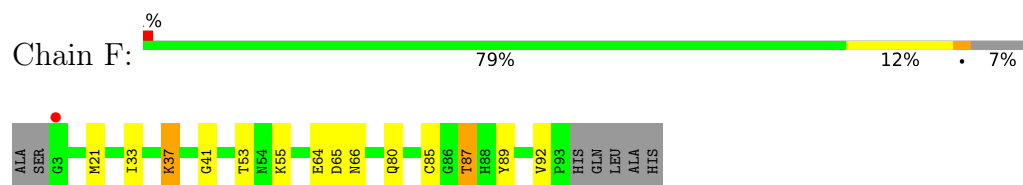
- Molecule 5: Cytochrome c oxidase subunit 5A



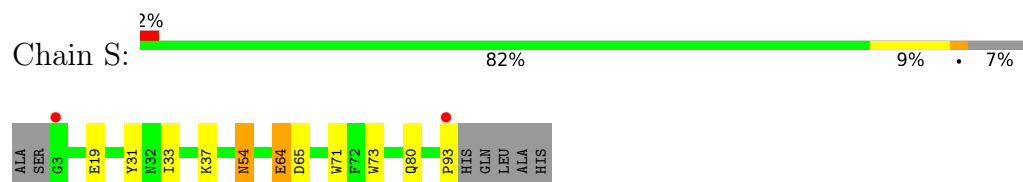
- Molecule 5: Cytochrome c oxidase subunit 5A



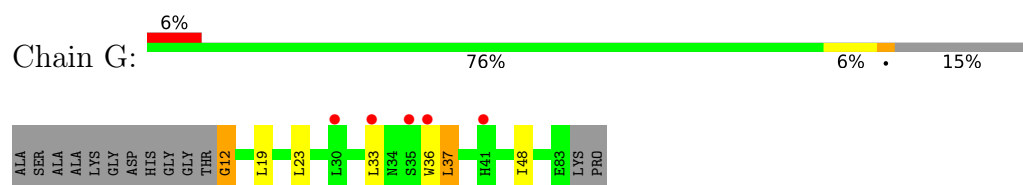
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



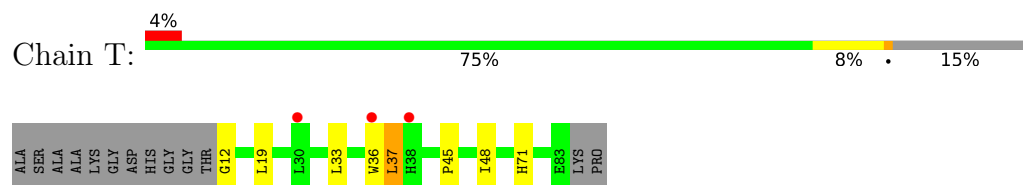
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



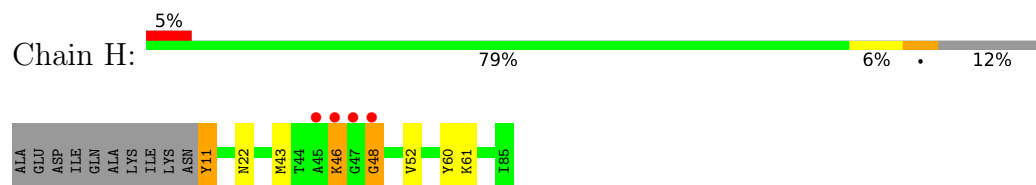
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



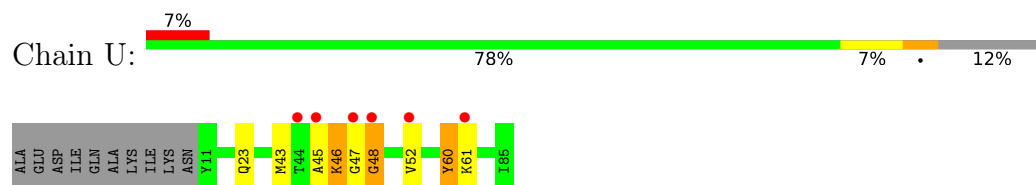
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



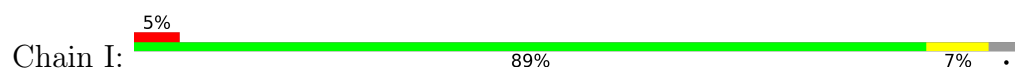
- Molecule 8: Cytochrome c oxidase subunit 6B1

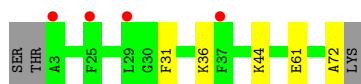


- Molecule 8: Cytochrome c oxidase subunit 6B1

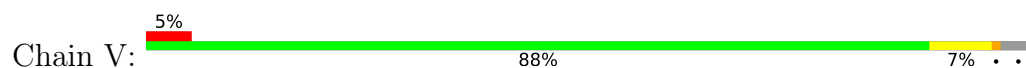


- Molecule 9: Cytochrome c oxidase subunit 6C

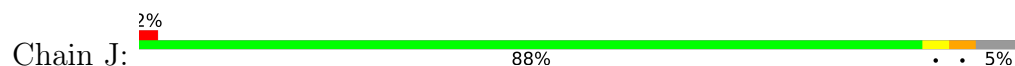




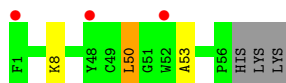
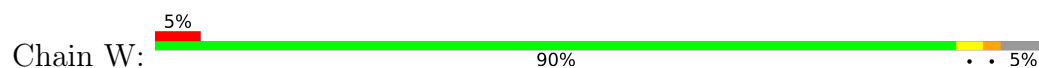
- Molecule 9: Cytochrome c oxidase subunit 6C



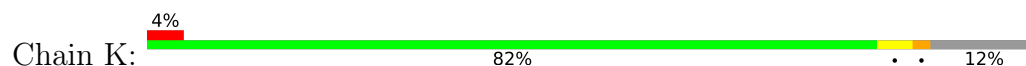
- Molecule 10: Cytochrome c oxidase subunit 7A1



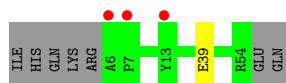
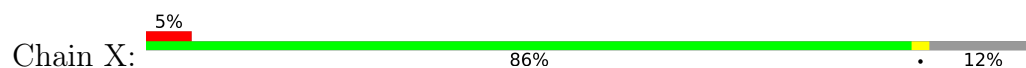
- Molecule 10: Cytochrome c oxidase subunit 7A1



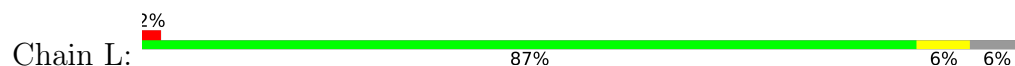
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



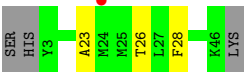
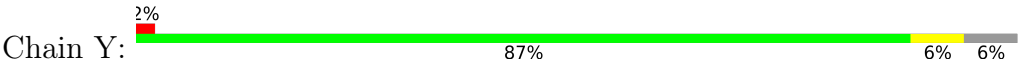
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



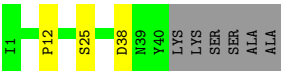
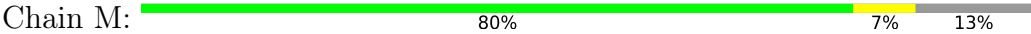
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



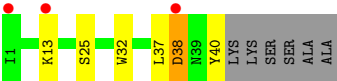
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



• 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	181.90Å 204.00Å 178.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 40.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.80) 100.0 (40.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.42 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.120 , 0.155 0.138 , 0.165	Depositor DCC
R_{free} test set	30183 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33061	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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, ZN, CHD, PEK, HEA, LFA, PGV, XE, MG, DMU, CUA, CDL, UNX, PER, NA, CU, EDO

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	1.08	7/4259 (0.2%)	1.16	9/5816 (0.2%)
1	N	1.06	6/4259 (0.1%)	1.18	9/5816 (0.2%)
2	B	1.12	0/1908	1.32	15/2598 (0.6%)
2	O	1.11	2/1908 (0.1%)	1.24	1/2598 (0.0%)
3	C	1.03	1/2258 (0.0%)	1.14	3/3084 (0.1%)
3	P	1.04	3/2258 (0.1%)	1.15	4/3084 (0.1%)
4	D	1.12	2/1226 (0.2%)	1.18	3/1657 (0.2%)
4	Q	1.04	0/1182	1.27	0/1598
5	E	1.07	1/843 (0.1%)	1.19	1/1145 (0.1%)
5	R	1.01	0/843	1.28	3/1145 (0.3%)
6	F	1.11	1/724 (0.1%)	1.19	0/983
6	S	1.17	2/724 (0.3%)	1.20	1/983 (0.1%)
7	G	1.09	2/633 (0.3%)	1.20	0/864
7	T	1.10	3/633 (0.5%)	1.23	0/864
8	H	1.08	1/648 (0.2%)	1.32	0/877
8	U	1.05	0/648	1.28	0/877
9	I	1.15	1/588 (0.2%)	1.40	1/781 (0.1%)
9	V	1.07	0/588	1.44	1/781 (0.1%)
10	J	1.08	0/451	1.26	2/610 (0.3%)
10	W	1.04	0/451	1.30	0/610
11	K	1.17	1/398 (0.3%)	1.32	1/546 (0.2%)
11	X	1.11	0/398	1.29	0/546
12	L	1.10	0/372	1.23	3/500 (0.6%)
12	Y	1.11	0/372	1.21	0/500
13	M	1.08	0/321	1.09	0/440
13	Z	1.06	0/321	1.46	4/440 (0.9%)
All	All	1.08	33/29214 (0.1%)	1.22	61/39743 (0.2%)

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

sidechain that are expected to be planar.

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

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	383	MET	C-O	10.65	1.37	1.24
1	A	49	GLY	C-O	9.04	1.33	1.23
1	A	395	HIS	CE1-NE2	8.15	1.40	1.32
1	N	395	HIS	CE1-NE2	7.91	1.40	1.32
3	P	71	HIS	CE1-NE2	7.85	1.40	1.32
4	D	58	GLU	CD-OE1	7.83	1.40	1.25
8	H	11	TYR	N-CA	7.70	1.60	1.46
1	N	49	GLY	C-O	7.49	1.32	1.23
11	K	10	HIS	CE1-NE2	7.05	1.39	1.32
4	D	21	ASP	CG-OD2	6.69	1.38	1.25
1	A	189	MET	CB-CG	6.40	1.71	1.52
6	S	64	GLU	C-O	6.37	1.31	1.23
1	N	189	MET	CG-SD	-6.04	1.65	1.80
6	S	93	PRO	C-O	6.02	1.35	1.23
7	T	45	PRO	C-O	-5.86	1.17	1.23
1	A	233	HIS	CE1-NE2	5.79	1.38	1.32
1	N	61	HIS	CE1-NE2	5.77	1.38	1.32
1	N	483	LEU	C-O	5.76	1.31	1.24
5	E	49	ASP	CG-OD1	-5.46	1.15	1.25
3	P	70	HIS	CE1-NE2	5.39	1.38	1.32
3	C	36	HIS	CE1-NE2	5.36	1.38	1.32
3	P	103	HIS	CE1-NE2	5.34	1.37	1.32
7	T	48	ILE	N-CA	5.22	1.50	1.45
7	G	48	ILE	N-CA	5.21	1.50	1.45
2	O	198	GLU	C-O	5.20	1.29	1.23
1	A	138	HIS	CE1-NE2	5.12	1.37	1.32
7	T	71	HIS	CE1-NE2	5.10	1.37	1.32
1	A	189	MET	CG-SD	-5.08	1.68	1.80
2	O	60	GLU	CD-OE2	5.08	1.34	1.25
7	G	12	GLY	N-CA	-5.05	1.37	1.45
1	N	328	HIS	CE1-NE2	5.04	1.37	1.32
6	F	66	ASN	C-O	5.04	1.29	1.23
9	I	61	GLU	CD-OE2	-5.02	1.15	1.25

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	65	TRP	CB-CG-CD1	-16.31	102.44	126.90
1	N	240	HIS	CA-CB-CG	-10.86	102.94	113.80
1	A	240	HIS	CA-CB-CG	-10.77	103.03	113.80
2	B	65	TRP	CA-CB-CG	10.35	133.27	113.60
4	D	58	GLU	CB-CG-CD	9.45	128.67	112.60
9	V	72	ALA	CA-C-O	-9.28	105.02	120.80
9	I	72	ALA	CA-C-O	-8.98	105.53	120.80
2	B	65	TRP	CB-CG-CD2	7.78	137.70	126.80
13	Z	38	ASP	CA-CB-CG	7.48	120.08	112.60
2	B	59	GLN	CB-CG-CD	7.38	125.14	112.60
3	C	80	ARG	CG-CD-NE	-7.26	96.03	112.00
2	B	82	ARG	CG-CD-NE	-6.92	96.77	112.00
1	N	102	PHE	CA-CB-CG	-6.80	107.00	113.80
1	A	102	PHE	CA-CB-CG	-6.71	107.09	113.80
2	B	65	TRP	CB-CA-C	-6.44	97.13	109.95
2	B	89	GLU	CA-C-N	6.41	130.12	120.77
2	B	89	GLU	C-N-CA	6.41	130.12	120.77
2	B	115	ASP	CB-CA-C	6.36	121.96	112.03
1	A	43	GLN	CB-CA-C	6.29	119.29	108.91
1	N	377	PHE	CA-CB-CG	6.21	120.01	113.80
1	A	96	ARG	CB-CA-C	6.20	122.05	110.70
3	P	233	PHE	CA-CB-CG	-6.16	107.64	113.80
4	D	20	ARG	NE-CZ-NH2	6.16	124.74	119.20
2	B	184	LEU	N-CA-CB	-6.14	100.17	110.80
3	C	76	GLN	CG-CD-NE2	-6.12	107.23	116.40
1	A	71	MET	CG-SD-CE	-6.11	87.46	100.90
3	P	80	ARG	CG-CD-NE	-6.10	98.59	112.00
11	K	54	ARG	CA-C-O	-5.97	110.66	120.80
2	B	59	GLN	N-CA-CB	5.95	118.69	110.07
1	N	96	ARG	CB-CA-C	5.91	121.52	110.70
5	E	108	LYS	CA-C-O	-5.86	110.84	120.80
10	J	27	THR	CA-CB-OG1	-5.83	100.86	109.60
2	B	115	ASP	CA-CB-CG	-5.79	106.81	112.60
2	B	11	ASP	CA-CB-CG	5.79	118.39	112.60
6	S	93	PRO	CB-CA-C	5.75	121.03	110.10
12	L	16	GLU	CB-CG-CD	5.71	122.30	112.60
3	P	230	ASN	CA-CB-CG	-5.69	106.91	112.60
4	D	20	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	N	71	MET	CG-SD-CE	-5.64	88.48	100.90
2	O	92	ASN	CB-CA-C	5.64	115.51	110.44
2	B	65	TRP	CG-CD2-CE3	5.53	139.43	133.90
12	L	25	MET	CA-C-N	5.50	127.97	120.54
12	L	25	MET	C-N-CA	5.50	127.97	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	106	PRO	CB-CA-C	5.47	117.59	110.92
3	C	233	PHE	CA-CB-CG	-5.46	108.33	113.80
13	Z	37	LEU	O-C-N	5.45	127.90	122.12
13	Z	38	ASP	CA-C-N	5.42	127.55	120.28
13	Z	38	ASP	C-N-CA	5.42	127.55	120.28
10	J	7	GLU	CB-CA-C	5.38	119.99	110.85
1	A	484	THR	CA-CB-OG1	-5.33	101.61	109.60
1	A	507	GLU	CB-CA-C	5.33	115.92	109.85
1	N	512	ASN	CB-CA-C	5.26	119.55	110.45
2	B	158	ASP	CA-CB-CG	5.25	117.85	112.60
1	N	237	PHE	CA-CB-CG	-5.23	108.57	113.80
1	A	240	HIS	N-CA-CB	5.12	116.47	110.42
1	A	235	PHE	CA-CB-CG	-5.08	108.72	113.80
5	R	80	GLU	CB-CG-CD	5.07	121.21	112.60
5	R	78	HIS	CA-C-N	5.05	127.56	120.28
5	R	78	HIS	C-N-CA	5.05	127.56	120.28
3	P	76	GLN	CG-CD-NE2	-5.03	108.86	116.40
1	N	240	HIS	N-CA-CB	5.00	116.32	110.42

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	296	GLY	Mainchain
1	A	383	MET	Mainchain
1	N	296	GLY	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4102	48	0
1	N	4130	0	4102	52	0
2	B	1870	0	1870	31	0
2	O	1870	0	1870	29	0
3	C	2171	0	2080	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	2172	0	2081	25	0
4	D	1192	0	1178	6	0
4	Q	1148	0	1131	7	0
5	E	825	0	823	1	0
5	R	825	0	823	4	0
6	F	709	0	691	12	0
6	S	709	0	691	6	0
7	G	606	0	577	4	0
7	T	606	0	577	4	0
8	H	628	0	580	14	0
8	U	628	0	580	13	0
9	I	575	0	584	4	0
9	V	575	0	584	6	0
10	J	441	0	439	4	0
10	W	441	0	439	5	0
11	K	384	0	366	1	0
11	X	384	0	366	1	0
12	L	360	0	360	2	0
12	Y	360	0	360	7	0
13	M	311	0	321	3	0
13	Z	311	0	321	5	0
14	A	129	0	88	4	0
14	N	129	0	88	7	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	1	0
19	A	64	0	72	0	0
19	C	87	0	124	19	0
19	L	94	0	141	6	0
19	P	87	0	124	8	0
19	V	64	0	72	2	0
19	Y	94	0	141	5	0
20	A	28	0	54	9	0
20	B	17	0	33	1	0
20	C	114	0	204	5	0
20	G	14	0	27	6	0
20	N	14	0	27	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	O	28	0	54	1	0
20	P	114	0	203	9	0
20	T	11	0	21	0	0
21	A	84	0	105	2	0
21	B	66	0	104	3	0
21	C	194	0	259	6	0
21	D	33	0	41	3	0
21	J	11	0	21	0	0
21	L	22	0	31	0	0
21	M	41	0	56	1	0
21	N	84	0	102	0	0
21	O	66	0	104	1	0
21	P	172	0	228	8	0
21	Q	33	0	41	1	0
21	T	22	0	31	0	0
21	W	11	0	21	0	0
21	Z	63	0	87	4	0
22	A	16	0	24	0	0
22	B	4	0	6	0	0
22	C	12	0	17	0	0
22	E	12	0	18	0	0
22	F	8	0	12	0	0
22	G	4	0	6	0	0
22	N	20	0	30	1	0
22	O	4	0	6	0	0
22	P	12	0	18	0	0
22	R	12	0	18	0	0
22	S	8	0	12	0	0
22	T	4	0	6	0	0
23	A	5	0	0	1	0
23	B	1	0	0	3	0
23	C	1	0	0	0	0
23	N	5	0	0	3	0
23	O	1	0	0	3	0
23	P	1	0	0	0	0
24	A	51	0	76	0	0
24	C	51	0	76	1	0
24	N	51	0	76	1	0
24	P	51	0	76	0	0
25	B	2	0	0	0	0
25	O	2	0	0	0	0
26	B	29	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	C	58	0	78	2	0
26	G	29	0	39	1	0
26	P	58	0	78	2	0
27	C	1	0	0	1	0
27	P	1	0	0	1	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	G	53	0	77	0	0
29	T	53	0	77	4	0
30	A	256	0	0	11	0
30	B	180	0	0	3	0
30	C	102	0	0	4	0
30	D	148	0	0	3	0
30	E	116	0	0	0	0
30	F	105	0	0	1	0
30	G	45	0	0	1	0
30	H	58	0	0	1	0
30	I	37	0	0	1	0
30	J	21	0	0	0	0
30	K	21	0	0	0	0
30	L	26	0	0	1	0
30	M	21	0	0	0	0
30	N	239	0	0	10	0
30	O	148	0	0	1	0
30	P	100	0	0	3	0
30	Q	83	0	0	3	0
30	R	93	0	0	2	0
30	S	95	0	0	0	0
30	T	37	0	0	1	0
30	U	47	0	0	0	0
30	V	25	0	0	2	0
30	W	15	0	0	0	0
30	X	18	0	0	0	0
30	Y	25	0	0	1	0
30	Z	17	0	0	0	0
All	All	33061	0	31465	333	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 (333) 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)
1:N:112:LEU:HG	30:N:3017:HOH:O	1.30	1.29
1:A:112:LEU:HG	30:A:2034:HOH:O	1.08	1.25
18:N:607:PER:O2	18:N:607:PER:O1	1.58	1.18
18:A:606:PER:O2	18:A:606:PER:O1	1.60	1.16
1:A:35:LEU:HD21	30:A:2007:HOH:O	1.46	1.12
1:A:35:LEU:CD2	30:A:2007:HOH:O	1.98	1.10
3:P:4:GLN:N	30:P:402:HOH:O	1.90	1.05
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.33	1.05
4:Q:21:ASP:OD2	30:Q:301:HOH:O	1.74	1.04
1:N:112:LEU:HD22	23:N:618:XE:XE	2.36	1.04
8:H:43:MET:HE1	8:U:52:VAL:HG11	1.39	1.02
8:H:52:VAL:HG12	8:U:46:LYS:CG	1.90	1.01
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:HE3	1.45	0.97
1:A:112:LEU:HD22	23:A:618:XE:XE	2.44	0.96
20:G:104:LFA:H11	20:N:608:LFA:H12	1.48	0.96
2:O:22[B]:HIS:CE1	9:V:44:LYS:HE2	2.06	0.91
3:C:245:VAL:C	3:C:246[B]:ASP:CA	2.43	0.91
1:A:136[B]:LEU:HD11	30:A:2039:HOH:O	1.72	0.88
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.13	0.87
21:C:324:DMU:H20	10:J:50:LEU:HB2	1.56	0.87
1:A:297[B]:MET:SD	1:A:302:ARG:HG2	2.15	0.86
3:P:149:HIS:NE2	20:P:313:LFA:H11	1.92	0.85
1:A:112:LEU:O	1:A:112:LEU:HD23	1.80	0.82
27:C:302:UNX:UNK	30:C:490:HOH:O	1.59	0.81
8:H:52:VAL:HG21	8:U:43:MET:HE1	1.62	0.81
8:H:52:VAL:CG1	8:U:46:LYS:HG2	2.11	0.78
21:A:611:DMU:O6	30:A:1805:HOH:O	2.03	0.77
29:T:101:PEK:H32	29:T:101:PEK:H71	1.67	0.77
2:O:84:LEU:HA	2:O:87[A]:MET:HE2	1.67	0.76
8:H:43:MET:CE	8:U:52:VAL:HG11	2.16	0.76
1:N:136[B]:LEU:HD11	30:N:3027:HOH:O	1.84	0.76
1:A:113[B]:LEU:HD11	1:A:117[B]:MET:SD	2.27	0.75
4:Q:112:GLU:OE2	30:Q:302:HOH:O	2.04	0.75
19:P:305:CDL:H121	19:P:305:CDL:HA62	1.68	0.75
1:N:278[B]:MET:HE1	20:N:608:LFA:H52	1.69	0.75
9:V:8:GLN:OE1	30:V:201:HOH:O	2.05	0.74
1:N:297[B]:MET:SD	1:N:302:ARG:CG	2.76	0.73
1:A:297[B]:MET:SD	1:A:302:ARG:CG	2.77	0.73
2:B:16[B]:ILE:HG23	30:B:524:HOH:O	1.89	0.71
1:N:112:LEU:HD23	1:N:112:LEU:O	1.89	0.71
3:P:156:ARG:HE	26:P:306:CHD:C24	2.04	0.71
27:P:303:UNX:UNK	30:P:495:HOH:O	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180[B]:GLU:HG2	30:C:427:HOH:O	1.92	0.70
2:O:22[B]:HIS:HE1	9:V:44:LYS:HE2	1.53	0.69
3:C:33[A]:MET:HE3	3:C:39:SER:OG	1.92	0.69
4:D:42:GLU:OE2	30:D:301:HOH:O	2.11	0.69
6:F:37:LYS:HG2	30:F:290:HOH:O	1.92	0.69
3:C:33[B]:MET:HG3	3:C:37:PHE:HB2	1.75	0.68
1:A:484:THR:HG22	30:A:2028:HOH:O	1.93	0.68
12:Y:26:THR:HG21	21:Z:102:DMU:H26	1.76	0.68
1:N:274:VAL:HG12	1:N:278[A]:MET:HE2	1.74	0.68
8:H:52:VAL:HG12	8:U:46:LYS:HG3	1.75	0.67
8:H:46:LYS:HE2	8:H:46:LYS:O	1.96	0.66
19:C:304:CDL:HB21	19:C:304:CDL:HB32	1.77	0.66
4:D:10:ASP:OD2	30:D:302:HOH:O	2.13	0.65
1:A:112:LEU:HD21	30:A:2025:HOH:O	1.95	0.65
8:H:46:LYS:O	8:H:46:LYS:CE	2.45	0.65
2:B:81:LEU:HD12	21:B:309:DMU:H11	1.79	0.65
3:C:180[A]:GLU:OE2	30:C:403:HOH:O	2.14	0.64
3:C:33[A]:MET:CE	3:C:42:LEU:H	2.11	0.64
3:C:33[A]:MET:HE2	3:C:42:LEU:H	1.62	0.64
19:C:304:CDL:HB61	19:C:304:CDL:CB2	2.27	0.64
1:A:274:VAL:HG12	1:A:278[A]:MET:HE2	1.79	0.64
1:A:28:MET:CE	14:A:601[A]:HEA:H271	2.28	0.64
3:C:149:HIS:NE2	20:C:312:LFA:H11	2.13	0.63
3:P:258:TRP:CE2	20:P:308:LFA:H32	2.33	0.63
3:C:51[B]:MET:HE2	19:C:304:CDL:H861	1.79	0.63
21:C:324:DMU:H10	10:J:53:ALA:HB2	1.81	0.62
2:B:31:VAL:CG2	23:B:301:XE:XE	3.26	0.62
2:B:13:THR:HB	2:B:168:LEU:HD23	1.82	0.61
2:B:16[A]:ILE:HD11	2:B:86:MET:HG2	1.83	0.61
1:A:278[B]:MET:SD	20:A:608:LFA:H51	2.41	0.60
2:B:31:VAL:HG22	23:B:301:XE:XE	2.80	0.60
20:A:608:LFA:H12	20:A:609:LFA:H11	1.84	0.60
19:L:101:CDL:OB9	19:L:101:CDL:H122	2.02	0.60
1:N:112:LEU:CD2	23:N:618:XE:XE	3.23	0.59
19:C:304:CDL:H752	10:J:27:THR:HG21	1.84	0.59
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.32	0.59
2:B:33:LEU:HD13	9:I:31:PHE:CD2	2.37	0.59
3:C:38:ASN:ND2	21:C:318:DMU:O4	2.35	0.59
1:A:278[B]:MET:HE1	20:A:608:LFA:H52	1.84	0.59
3:P:33[B]:MET:HE3	3:P:42:LEU:HD12	1.84	0.59
29:T:101:PEK:H32	29:T:101:PEK:C7	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:C	1:A:112:LEU:CD2	2.76	0.58
7:G:23:LEU:HB2	20:G:104:LFA:H91	1.86	0.58
20:A:609:LFA:H62	7:T:19:LEU:HD23	1.84	0.58
3:P:50:ASN:ND2	3:P:54[A]:MET:HE2	2.17	0.58
5:R:46:LYS:NZ	30:R:303:HOH:O	2.35	0.58
1:A:110:LEU:HD21	21:C:324:DMU:H24	1.86	0.58
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:CE	2.28	0.58
19:C:304:CDL:HB21	19:C:304:CDL:HB61	1.85	0.57
3:C:67:PHE:CE2	19:C:304:CDL:O1	2.57	0.57
1:N:112:LEU:HD21	30:N:3016:HOH:O	2.04	0.57
19:C:304:CDL:HA62	19:C:304:CDL:H121	1.85	0.57
1:A:278[A]:MET:CE	20:A:609:LFA:H51	2.34	0.57
2:O:91:ASN:C	2:O:91:ASN:HD22	2.11	0.57
30:A:1914:HOH:O	3:C:77:LYS:HE3	2.04	0.57
12:Y:26:THR:CG2	21:Z:102:DMU:H26	2.35	0.57
19:P:305:CDL:OB4	19:P:305:CDL:CA5	2.54	0.56
19:Y:101:CDL:C41	19:Y:101:CDL:H801	2.35	0.56
1:N:365:ILE:HD11	30:N:2807:HOH:O	2.05	0.56
1:N:112:LEU:HD23	1:N:112:LEU:C	2.31	0.56
6:F:92:VAL:HG23	6:F:92:VAL:O	2.05	0.55
19:C:304:CDL:HB61	19:C:304:CDL:HB22	1.88	0.55
8:H:43:MET:O	8:H:48:GLY:N	2.40	0.55
13:M:12:PRO:HG3	21:M:102:DMU:H16	1.88	0.55
3:P:205:GLY:HA3	29:T:101:PEK:H182	1.88	0.55
1:A:112:LEU:O	1:A:112:LEU:CD2	2.52	0.55
30:A:2016:HOH:O	6:F:37:LYS:HE3	2.06	0.55
1:N:28:MET:HE2	14:N:602[A]:HEA:H273	1.88	0.55
19:C:304:CDL:OA3	19:C:304:CDL:H1	1.95	0.55
21:P:324:DMU:O55	21:P:324:DMU:O3	2.25	0.55
1:A:112:LEU:HD23	1:A:112:LEU:C	2.31	0.54
2:B:227:LEU:HD21	30:B:500:HOH:O	2.08	0.54
20:A:609:LFA:C6	7:T:19:LEU:HD23	2.37	0.54
2:O:33:LEU:HD13	9:V:31:PHE:CD2	2.42	0.54
1:A:1:FME:HE2	1:A:1:FME:HA	1.88	0.54
30:C:500:HOH:O	6:F:33:ILE:HD13	2.07	0.54
8:U:46:LYS:HE2	8:U:47:GLY:C	2.33	0.54
1:N:28:MET:CE	14:N:602[A]:HEA:C27	2.86	0.54
2:B:31:VAL:HG23	23:B:301:XE:XE	2.86	0.54
8:U:47:GLY:C	8:U:48:GLY:O	2.50	0.54
3:C:164:PHE:CD1	26:C:305:CHD:H192	2.43	0.54
19:C:304:CDL:HB21	19:C:304:CDL:CB3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:164:PHE:CD1	26:P:306:CHD:H192	2.43	0.54
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.44	0.53
21:P:324:DMU:O3	21:P:324:DMU:C2	2.57	0.53
7:T:12:GLY:HA3	30:T:231:HOH:O	2.08	0.53
1:A:28:MET:HE2	14:A:601[A]:HEA:C27	2.38	0.53
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.90	0.53
2:O:32[B]:PHE:CD2	9:V:31:PHE:CZ	2.97	0.53
6:S:54:ASN:HD22	6:S:54:ASN:C	2.17	0.53
6:F:64:GLU:O	6:F:65:ASP:HB2	2.09	0.52
24:N:621:PGV:H183	29:T:101:PEK:H331	1.92	0.52
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:HG2	1.90	0.52
1:A:28:MET:CE	14:A:601[A]:HEA:C27	2.87	0.52
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.90	0.52
3:C:59:ARG:HB2	19:C:304:CDL:OA9	2.10	0.52
1:N:112:LEU:CD2	1:N:112:LEU:C	2.83	0.52
1:N:278[B]:MET:SD	20:N:608:LFA:H51	2.50	0.52
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.92	0.52
21:P:324:DMU:H10	10:W:53:ALA:HB2	1.91	0.52
1:N:136[B]:LEU:CD1	30:N:3027:HOH:O	2.49	0.51
7:G:19:LEU:HD23	20:G:104:LFA:H61	1.91	0.51
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:CG	2.41	0.51
1:A:297[B]:MET:CG	1:A:302:ARG:HG3	2.41	0.51
2:O:60:GLU:CD	2:O:60:GLU:H	2.18	0.51
3:P:116:TRP:HA	3:P:117:PRO:C	2.36	0.51
19:P:305:CDL:O1	10:W:8:LYS:HD2	2.10	0.51
1:N:28:MET:HE2	14:N:602[A]:HEA:C27	2.41	0.51
1:N:110:LEU:HD21	21:P:324:DMU:H24	1.93	0.50
2:O:67:ILE:HD11	20:O:301:LFA:H42	1.93	0.50
3:P:41:THR:HA	3:P:44[B]:MET:HE2	1.93	0.50
2:O:16[A]:ILE:HG21	2:O:87[A]:MET:HG2	1.93	0.50
1:A:7:LEU:HD21	19:L:101:CDL:H352	1.92	0.50
2:B:220:GLU:OE1	30:B:402:HOH:O	2.19	0.50
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.47	0.50
19:L:101:CDL:C73	19:L:101:CDL:H362	2.41	0.50
2:O:16[B]:ILE:HG23	30:O:504:HOH:O	2.12	0.49
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.94	0.49
1:N:28:MET:CE	14:N:602[A]:HEA:H271	2.42	0.49
3:P:80:ARG:NH2	3:P:236:GLU:OE1	2.44	0.49
19:L:101:CDL:H362	19:L:101:CDL:H731	1.93	0.49
1:A:240:HIS:C	1:A:240:HIS:CD2	2.90	0.49
1:A:297[B]:MET:SD	1:A:302:ARG:HG3	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:64:GLU:O	6:S:65:ASP:HB2	2.11	0.49
3:C:258:TRP:CE2	20:C:307:LFA:H32	2.47	0.49
2:B:16[A]:ILE:CG2	2:B:87[A]:MET:HE3	2.30	0.49
1:N:110:LEU:CD2	21:P:324:DMU:H24	2.43	0.49
13:Z:13:LYS:NZ	21:Z:102:DMU:O61	2.31	0.49
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.94	0.49
1:A:278[A]:MET:SD	20:A:609:LFA:H51	2.52	0.49
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.43	0.48
21:A:622:DMU:O3	8:H:22:ASN:ND2	2.46	0.48
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.95	0.48
4:D:81:VAL:HG11	21:D:201:DMU:H11	1.94	0.48
1:N:488:THR:HB	1:N:495:LEU:HD13	1.95	0.48
30:N:2816:HOH:O	20:P:310:LFA:C5	2.61	0.48
2:O:31:VAL:CG2	23:O:304:XE:XE	3.39	0.48
8:H:52:VAL:HA	8:U:46:LYS:HG2	1.95	0.48
1:N:297[B]:MET:SD	1:N:302:ARG:HG3	2.52	0.48
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.96	0.48
3:C:131:LEU:CD2	21:C:323:DMU:H18	2.44	0.48
20:G:104:LFA:H51	1:N:278[A]:MET:HE1	1.94	0.48
1:N:417[B]:MET:CE	30:N:2988:HOH:O	2.61	0.48
19:C:304:CDL:CA5	19:C:304:CDL:OB4	2.62	0.48
19:C:304:CDL:OB4	19:C:304:CDL:OA6	2.31	0.48
21:Q:201:DMU:O55	21:Q:201:DMU:H36	2.13	0.48
2:B:1:FME:HE1	2:B:133:LEU:HD22	1.95	0.47
2:O:31:VAL:HG23	23:O:304:XE:XE	2.92	0.47
30:N:2816:HOH:O	20:P:310:LFA:C4	2.63	0.47
3:C:149:HIS:NE2	20:C:312:LFA:C1	2.77	0.47
26:C:305:CHD:H162	26:C:305:CHD:H231	1.96	0.47
4:D:86:MET:HE1	11:K:22:ALA:HB2	1.96	0.47
21:D:201:DMU:H36	21:D:201:DMU:O55	2.14	0.47
6:F:85:CYS:SG	6:F:87[B]:THR:OG1	2.68	0.47
1:N:362[A]:SER:HA	2:O:87[A]:MET:HE1	1.95	0.47
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.97	0.47
1:A:136[B]:LEU:CD1	30:A:2039:HOH:O	2.47	0.47
3:C:67:PHE:HE2	19:C:304:CDL:H1O1	1.58	0.47
1:N:278[B]:MET:CE	20:N:608:LFA:H52	2.42	0.47
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.67	0.47
30:A:1998:HOH:O	20:C:309:LFA:C4	2.63	0.47
1:N:362[B]:SER:O	2:O:87[B]:MET:HE1	2.15	0.47
1:A:297[B]:MET:HG2	1:A:302:ARG:HG3	1.96	0.47
2:O:58:ALA:O	2:O:62:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:26:THR:HG23	13:Z:25:SER:HB2	1.96	0.47
1:A:334:TRP:HB2	21:D:201:DMU:C57	2.45	0.46
1:N:2:PHE:CE2	19:Y:101:CDL:H712	2.50	0.46
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.96	0.46
1:N:240:HIS:C	1:N:240:HIS:CD2	2.93	0.46
5:R:90:ARG:NH1	30:R:304:HOH:O	2.40	0.46
8:U:46:LYS:HG3	8:U:48:GLY:H	1.79	0.46
1:N:278[B]:MET:SD	20:N:608:LFA:C5	3.03	0.46
9:V:8:GLN:HG3	30:V:225:HOH:O	2.13	0.46
1:N:24:ALA:HB2	14:N:602[B]:HEA:H253	1.96	0.46
1:N:189:MET:HE3	20:N:608:LFA:H31	1.98	0.46
3:P:33[B]:MET:HB2	3:P:33[B]:MET:HE2	1.19	0.46
21:P:324:DMU:O3	21:P:324:DMU:H2	2.15	0.46
3:P:59:ARG:HB2	19:P:305:CDL:OA9	2.16	0.46
19:Y:101:CDL:O1	30:Y:219[B]:HOH:O	2.21	0.46
8:H:46:LYS:O	8:H:46:LYS:HE3	2.15	0.46
1:A:189:MET:HE3	20:A:608:LFA:H31	1.98	0.46
3:C:41:THR:HA	3:C:44[B]:MET:HE2	1.98	0.46
8:H:11:TYR:N	30:H:102:HOH:O	2.49	0.46
1:A:423[B]:MET:HE2	1:A:456:MET:HB2	1.98	0.45
3:C:33[B]:MET:CA	3:C:33[B]:MET:HE2	2.11	0.45
19:L:101:CDL:H362	19:L:101:CDL:H711	1.97	0.45
2:B:164:ALA:O	2:B:194:GLY:HA3	2.16	0.45
6:F:87[A]:THR:HG22	6:F:89:TYR:CE1	2.52	0.45
2:O:116:LEU:HD13	2:O:226:MET:CG	2.47	0.45
1:A:28:MET:HE2	14:A:601[A]:HEA:H271	1.97	0.45
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.51	0.45
3:P:247:VAL:HG11	20:P:314:LFA:H71	1.99	0.45
1:A:362[B]:SER:O	2:B:87[B]:MET:HE1	2.17	0.45
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	3.04	0.45
3:C:116:TRP:HA	3:C:117:PRO:C	2.41	0.45
12:L:26:THR:HG23	13:M:25:SER:CB	2.47	0.45
3:P:51[B]:MET:HE3	19:P:305:CDL:H873	1.99	0.45
3:P:149:HIS:NE2	20:P:313:LFA:C1	2.74	0.45
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.98	0.45
12:Y:28:PHE:CD1	19:Y:101:CDL:H532	2.52	0.45
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.17	0.44
3:C:210:ILE:HD13	24:C:303:PGV:H312	1.99	0.44
2:B:56:MET:HB3	21:B:305:DMU:H7	2.00	0.44
3:P:240:TRP:CZ2	20:P:315:LFA:H31	2.53	0.44
3:P:177:GLN:OE1	3:P:177:GLN:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:107:ILE:HD13	11:X:39:GLU:HB2	1.99	0.44
20:G:104:LFA:H121	20:G:104:LFA:H92	1.70	0.44
12:L:26:THR:HG23	13:M:25:SER:HB3	2.00	0.44
19:C:304:CDL:CA3	19:C:304:CDL:OB9	2.66	0.44
4:D:127:LYS:HD2	30:I:136:HOH:O	2.17	0.44
1:N:87:ILE:O	1:N:173:PRO:HD3	2.17	0.44
3:C:226:HIS:HE1	19:C:304:CDL:H111	1.81	0.44
3:P:247:VAL:CG1	20:P:314:LFA:H71	2.48	0.44
30:P:499:HOH:O	6:S:33:ILE:HD13	2.17	0.43
26:G:102:CHD:H12	26:G:102:CHD:H212	2.00	0.43
3:C:41:THR:HG23	21:C:319:DMU:H15	2.00	0.43
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.19	0.43
1:N:310:MET:HE1	2:O:77:ALA:HB2	2.01	0.43
1:A:318:VAL:HG22	2:B:65:TRP:HD1	1.84	0.43
12:Y:23:ALA:HA	21:Z:102:DMU:H21	2.00	0.43
1:N:486:ASP:OD2	4:Q:19:ARG:NE	2.52	0.43
20:G:104:LFA:H31	1:N:278[A]:MET:SD	2.59	0.43
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.01	0.43
2:O:13:THR:HB	2:O:168:LEU:HD23	2.01	0.42
6:S:19:GLU:OE1	6:S:31:TYR:OH	2.29	0.42
2:B:58:ALA:O	2:B:62:GLU:HG3	2.19	0.42
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.54	0.42
2:O:5:MET:HE2	2:O:5:MET:HB3	1.87	0.42
2:O:60:GLU:CD	2:O:60:GLU:N	2.76	0.42
1:N:494:TRP:O	22:N:615:EDO:H22	2.19	0.42
3:P:258:TRP:CZ2	20:P:308:LFA:H32	2.54	0.42
19:C:304:CDL:H121	19:C:304:CDL:CA6	2.49	0.42
1:N:417[B]:MET:HE2	30:N:2988:HOH:O	2.19	0.42
6:F:21[B]:MET:HE2	6:F:21[B]:MET:HB2	1.82	0.42
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	2.01	0.42
30:N:3021[B]:HOH:O	4:Q:19:ARG:HD3	2.19	0.42
3:P:38:ASN:HD21	21:P:320:DMU:H41	1.84	0.42
1:A:297[B]:MET:HB3	1:A:302:ARG:CD	2.50	0.42
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.20	0.42
14:N:603:HEA:HBC1	14:N:603:HEA:HMC3	2.02	0.42
2:O:31:VAL:HG22	23:O:304:XE:XE	2.97	0.42
2:B:60:GLU:H	2:B:60:GLU:CD	2.27	0.42
5:R:90:ARG:HB3	5:R:91:PRO:HD3	2.01	0.42
1:A:278[B]:MET:SD	20:A:608:LFA:C5	3.06	0.42
1:A:297[B]:MET:O	1:A:302:ARG:NE	2.37	0.42
7:G:37:LEU:HD23	21:O:303:DMU:H10	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:150:LEU:HD23	23:N:616:XE:XE	2.98	0.42
3:P:33[B]:MET:CE	3:P:42:LEU:HD12	2.49	0.42
3:P:129:VAL:N	3:P:130:PRO:CD	2.83	0.42
2:B:84:LEU:O	2:B:87[B]:MET:HB2	2.20	0.42
2:B:132:GLU:HB3	2:B:137:GLU:HG3	2.01	0.42
14:N:603:HEA:HBC1	14:N:603:HEA:CMC	2.50	0.42
2:O:111:THR:HA	2:O:114:GLU:O	2.19	0.42
19:P:305:CDL:HA22	10:W:8:LYS:HZ1	1.84	0.42
2:B:22[B]:HIS:CE1	9:I:44:LYS:CE	3.02	0.41
6:F:21[B]:MET:HB3	6:F:21[B]:MET:HE3	1.82	0.41
19:L:101:CDL:O1	30:L:221[B]:HOH:O	2.19	0.41
2:B:196:CYS:HB2	2:B:207:MET:HG3	2.02	0.41
7:G:12:GLY:HA3	30:G:238:HOH:O	2.20	0.41
1:N:489:THR:HA	6:S:71:TRP:O	2.21	0.41
30:Q:313:HOH:O	5:R:108:LYS:HD3	2.20	0.41
1:N:297[B]:MET:CG	1:N:302:ARG:HG3	2.50	0.41
3:C:247:VAL:CG1	20:C:313:LFA:H71	2.51	0.41
4:D:58:GLU:HG3	30:D:363[A]:HOH:O	2.20	0.41
1:N:423[B]:MET:HA	19:V:101:CDL:H782	2.03	0.41
8:U:60:TYR:CD1	8:U:60:TYR:C	2.98	0.41
1:N:383:MET:O	1:N:387:PHE:HB2	2.20	0.41
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.03	0.41
1:A:498:CYS:HA	1:A:499:PRO:HA	1.93	0.41
2:B:67:ILE:HD11	20:B:308:LFA:H42	2.03	0.41
19:C:304:CDL:C52	19:C:304:CDL:HB4	2.50	0.41
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.55	0.41
3:C:177:GLN:OE1	3:C:177:GLN:HA	2.20	0.41
19:Y:101:CDL:OA5	19:Y:101:CDL:OA8	2.38	0.41
1:A:148:PHE:HB3	3:C:28:THR:HB	2.02	0.41
6:F:53:THR:HG23	6:F:55:LYS:H	1.85	0.41
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.02	0.41
19:P:305:CDL:HA22	10:W:8:LYS:NZ	2.36	0.41
19:C:304:CDL:C75	10:J:27:THR:HG21	2.51	0.40
19:P:305:CDL:OA3	19:P:305:CDL:H1	2.17	0.40
1:A:297[B]:MET:HB3	1:A:302:ARG:HD3	2.03	0.40
21:P:324:DMU:H20	10:W:50:LEU:HB2	2.03	0.40
7:T:37:LEU:HD12	7:T:37:LEU:HA	1.91	0.40
1:A:417[A]:MET:HE3	1:A:421:VAL:CG1	2.51	0.40
2:B:52:HIS:CE1	21:B:305:DMU:H29	2.56	0.40
3:C:50:ASN:ND2	3:C:54[A]:MET:HE2	2.36	0.40
3:P:144[A]:ILE:HD13	3:P:239:ALA:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:76:GLY:O	1:N:80:ASN:HB2	2.22	0.40
1:N:433:LEU:HD11	19:V:101:CDL:OA7	2.21	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%)	512 (97%)	14 (3%)	0	100	100
1	N	526/514 (102%)	511 (97%)	15 (3%)	0	100	100
2	B	230/227 (101%)	222 (96%)	8 (4%)	0	100	100
2	O	230/227 (101%)	225 (98%)	5 (2%)	0	100	100
3	C	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
3	P	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	136/147 (92%)	132 (97%)	4 (3%)	0	100	100
5	E	100/109 (92%)	100 (100%)	0	0	100	100
5	R	100/109 (92%)	100 (100%)	0	0	100	100
6	F	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
6	S	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
7	G	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
7	T	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
8	H	73/85 (86%)	71 (97%)	1 (1%)	1 (1%)	9	2
8	U	73/85 (86%)	70 (96%)	1 (1%)	2 (3%)	4	0
9	I	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
9	V	68/73 (93%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	54/59 (92%)	54 (100%)	0	0	100	100
10	W	54/59 (92%)	54 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	42/47 (89%)	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%)	36 (95%)	1 (3%)	1 (3%)	4	0
All	All	3488/3614 (96%)	3411 (98%)	73 (2%)	4 (0%)	48	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	48	GLY
8	U	48	GLY
13	Z	38	ASP
8	U	45	ALA

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	80
1	N	440/426 (103%)	437 (99%)	3 (1%)	76	73
2	B	215/210 (102%)	207 (96%)	8 (4%)	30	18
2	O	215/210 (102%)	209 (97%)	6 (3%)	38	26
3	C	232/226 (103%)	230 (99%)	2 (1%)	70	67
3	P	232/226 (103%)	228 (98%)	4 (2%)	53	45
4	D	128/129 (99%)	128 (100%)	0	100	100
4	Q	122/129 (95%)	119 (98%)	3 (2%)	42	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	89/95 (94%)	89 (100%)	0	100	100
5	R	89/95 (94%)	88 (99%)	1 (1%)	65	60
6	F	78/81 (96%)	74 (95%)	4 (5%)	21	9
6	S	78/81 (96%)	75 (96%)	3 (4%)	29	17
7	G	63/69 (91%)	60 (95%)	3 (5%)	23	11
7	T	63/69 (91%)	60 (95%)	3 (5%)	23	11
8	H	67/75 (89%)	64 (96%)	3 (4%)	24	12
8	U	67/75 (89%)	64 (96%)	3 (4%)	24	12
9	I	55/58 (95%)	54 (98%)	1 (2%)	51	43
9	V	55/58 (95%)	52 (94%)	3 (6%)	19	8
10	J	47/50 (94%)	46 (98%)	1 (2%)	47	36
10	W	47/50 (94%)	46 (98%)	1 (2%)	47	36
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	28
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	37/40 (92%)	37 (100%)	0	100	100
12	Y	37/40 (92%)	37 (100%)	0	100	100
13	M	34/38 (90%)	33 (97%)	1 (3%)	37	25
13	Z	34/38 (90%)	34 (100%)	0	100	100
All	All	3042/3086 (99%)	2986 (98%)	56 (2%)	51	43

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

Mol	Chain	Res	Type
1	A	112	LEU
1	A	369	ASP
2	B	33	LEU
2	B	59	GLN
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
3	C	159	MET
3	C	230	ASN
6	F	37	LYS

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Mol	Chain	Res	Type
6	F	80	GLN
6	F	87[A]	THR
6	F	87[B]	THR
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
8	H	46	LYS
8	H	60	TYR
8	H	61	LYS
9	I	36	LYS
10	J	7	GLU
11	K	54	ARG
13	M	38	ASP
1	N	112	LEU
1	N	363	LEU
1	N	369	ASP
2	O	33	LEU
2	O	60	GLU
2	O	68	LEU
2	O	78	LEU
2	O	91	ASN
2	O	226	MET
3	P	33[A]	MET
3	P	33[B]	MET
3	P	159	MET
3	P	230	ASN
4	Q	10	ASP
4	Q	31	LYS
4	Q	51	LEU
5	R	79	LYS
6	S	37	LYS
6	S	54	ASN
6	S	80	GLN
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
8	U	46	LYS
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	29	LEU
9	V	65	LYS

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Mol	Chain	Res	Type
10	W	50	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	170	ASN
1	A	422	ASN
1	A	503	HIS
2	B	52	HIS
3	C	38	ASN
3	C	50	ASN
3	C	76	GLN
3	C	230	ASN
4	D	119	GLN
4	D	143	ASN
5	E	94	ASN
6	F	54	ASN
7	G	38	HIS
8	H	22	ASN
8	H	37	HIS
10	J	29	ASN
11	K	35	GLN
1	N	170	ASN
1	N	422	ASN
2	O	10	GLN
2	O	91	ASN
3	P	38	ASN
3	P	50	ASN
3	P	56	GLN
4	Q	76	ASN
4	Q	109	HIS
4	Q	119	GLN
5	R	94	ASN
6	S	54	ASN
8	U	12	GLN
8	U	22	ASN
8	U	28	ASN
8	U	32	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	0.88	1 (12%)	8,9,11	1.02	1 (12%)
1	FME	A	1	1	8,9,10	0.53	0	8,9,11	0.96	1 (12%)
2	FME	B	1	2	8,9,10	1.36	1 (12%)	8,9,11	1.09	1 (12%)
1	FME	N	1	1	8,9,10	0.69	0	8,9,11	1.13	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	-	2/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-3.25	1.64	1.81
2	O	1	FME	CG-SD	-2.07	1.70	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-2.62	104.87	112.87
1	N	1	FME	O-C-CA	-2.43	118.52	124.77
1	A	1	FME	C-CA-N	2.08	113.52	109.50
2	O	1	FME	O-C-CA	-2.05	119.51	124.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 149 ligands modelled in this entry, 22 are monoatomic and 2 are unknown - leaving 125 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	DMU	N	622	-	34,34,34	0.90	2 (5%)	45,45,45	1.32	4 (8%)
22	EDO	E	203	-	3,3,3	0.18	0	2,2,2	0.11	0
21	DMU	D	201	-	34,34,34	1.28	6 (17%)	45,45,45	1.45	5 (11%)
22	EDO	S	102	-	3,3,3	0.58	0	2,2,2	0.33	0
22	EDO	B	306	-	3,3,3	0.27	0	2,2,2	0.16	0
20	LFA	N	608	-	13,13,19	0.36	0	12,12,18	0.41	0
19	CDL	L	101	-	93,93,99	0.44	0	99,105,111	0.63	2 (2%)
14	HEA	N	603	1,18	67,67,67	1.78	20 (29%)	81,103,103	2.42	33 (40%)
21	DMU	J	101	-	10,10,34	0.14	0	9,9,45	0.67	0
21	DMU	N	609	-	6,6,34	0.45	0	5,5,45	0.31	0
20	LFA	P	308	-	10,10,19	0.36	0	9,9,18	0.26	0
22	EDO	R	201	-	3,3,3	0.21	0	2,2,2	0.11	0
26	CHD	P	302	-	32,32,32	1.02	2 (6%)	51,51,51	0.70	0
20	LFA	C	308	-	5,5,19	0.28	0	4,4,18	0.16	0
20	LFA	P	301	-	14,14,19	0.16	0	13,13,18	0.14	0
22	EDO	R	202	-	3,3,3	0.09	0	2,2,2	0.13	0
21	DMU	C	324	-	34,34,34	0.78	0	45,45,45	1.26	4 (8%)
22	EDO	P	323	-	3,3,3	0.28	0	2,2,2	0.71	0
21	DMU	P	307	-	10,10,34	0.36	0	9,9,45	0.59	0
21	DMU	N	601	-	10,10,34	0.38	0	9,9,45	0.50	0
22	EDO	C	321	-	3,3,3	0.20	0	2,2,2	0.15	0
24	PGV	N	621	-	50,50,50	0.76	1 (2%)	53,56,56	1.26	3 (5%)
14	HEA	A	602	1,18	67,67,67	1.89	20 (29%)	81,103,103	2.31	26 (32%)
20	LFA	P	312	-	13,13,19	0.19	0	12,12,18	0.15	0
20	LFA	C	309	-	17,17,19	0.23	0	16,16,18	0.26	0
21	DMU	C	316	-	6,6,34	0.16	0	5,5,45	0.63	0
22	EDO	A	614	-	3,3,3	0.60	0	2,2,2	0.20	0
21	DMU	O	303	-	22,22,34	1.23	2 (9%)	27,27,45	1.36	3 (11%)
22	EDO	R	203	-	3,3,3	0.39	0	2,2,2	0.28	0
14	HEA	A	601[B]	-	67,67,67	2.00	21 (31%)	81,103,103	2.30	25 (30%)
21	DMU	O	307	-	10,10,34	0.48	0	9,9,45	0.48	0
14	HEA	N	602[A]	-	67,67,67	1.91	21 (31%)	81,103,103	2.47	33 (40%)
22	EDO	N	615	-	3,3,3	0.55	0	2,2,2	0.24	0
22	EDO	F	102	-	3,3,3	0.23	0	2,2,2	0.24	0
14	HEA	A	601[A]	-	67,67,67	2.00	21 (31%)	81,103,103	2.26	22 (27%)
22	EDO	A	615	-	3,3,3	0.44	0	2,2,2	0.21	0
26	CHD	G	102	-	32,32,32	0.71	0	51,51,51	0.81	0
22	EDO	O	309	-	3,3,3	0.16	0	2,2,2	0.18	0
21	DMU	W	101	-	10,10,34	0.22	0	9,9,45	0.58	0
20	LFA	C	307	-	10,10,19	0.29	0	9,9,18	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	DMU	Q	201	-	34,34,34	1.31	6 (17%)	45,45,45	1.61	8 (17%)
26	CHD	B	307	-	32,32,32	0.78	0	51,51,51	0.74	0
21	DMU	P	318	-	22,22,34	0.94	2 (9%)	27,27,45	1.37	3 (11%)
22	EDO	N	611	-	3,3,3	0.42	0	2,2,2	0.25	0
21	DMU	B	303	-	10,10,34	0.21	0	9,9,45	0.56	0
21	DMU	Z	102	-	22,22,34	0.74	0	27,27,45	0.99	1 (3%)
21	DMU	Z	103	-	7,7,34	0.30	0	6,6,45	0.42	0
21	DMU	P	324	-	34,34,34	0.81	1 (2%)	45,45,45	1.71	8 (17%)
21	DMU	C	323	-	22,22,34	0.64	0	27,27,45	1.06	1 (3%)
20	LFA	C	326	-	14,14,19	0.17	0	13,13,18	0.10	0
22	EDO	F	103	-	3,3,3	0.15	0	2,2,2	0.26	0
21	DMU	P	320	-	34,34,34	1.03	2 (5%)	45,45,45	1.32	5 (11%)
20	LFA	O	302	-	10,10,19	0.34	0	9,9,18	0.17	0
21	DMU	A	611	-	34,34,34	1.09	2 (5%)	45,45,45	1.20	5 (11%)
20	LFA	P	314	-	14,14,19	0.53	0	13,13,18	0.24	0
20	LFA	T	102	-	10,10,19	0.19	0	9,9,18	0.16	0
21	DMU	A	622	-	34,34,34	1.08	4 (11%)	45,45,45	1.23	5 (11%)
20	LFA	P	310	-	17,17,19	0.19	0	16,16,18	0.17	0
21	DMU	P	317	-	6,6,34	0.22	0	5,5,45	0.50	0
20	LFA	P	309	-	5,5,19	0.28	0	4,4,18	0.16	0
20	LFA	P	311	-	10,10,19	0.15	0	9,9,18	0.09	0
19	CDL	Y	101	-	93,93,99	0.40	0	99,105,111	0.55	1 (1%)
29	PEK	T	101	-	52,52,52	0.77	2 (3%)	55,57,57	1.05	3 (5%)
20	LFA	G	104	-	13,13,19	1.04	2 (15%)	12,12,18	0.49	0
21	DMU	L	102	-	22,22,34	0.72	0	27,27,45	1.02	1 (3%)
19	CDL	V	101	-	63,63,99	0.51	0	69,75,111	0.99	5 (7%)
22	EDO	A	612	-	3,3,3	0.39	0	2,2,2	0.28	0
20	LFA	C	311	-	13,13,19	0.21	0	12,12,18	0.13	0
21	DMU	A	623	-	10,10,34	0.28	0	9,9,45	0.56	0
18	PER	N	607	15,14	1,1,1	1.11	0	-		
26	CHD	C	305	-	32,32,32	0.67	0	51,51,51	1.50	5 (9%)
21	DMU	P	316	-	34,34,34	0.86	2 (5%)	45,45,45	1.57	8 (17%)
21	DMU	B	305	-	22,22,34	1.13	1 (4%)	27,27,45	1.26	4 (14%)
22	EDO	E	201	-	3,3,3	0.14	0	2,2,2	0.13	0
22	EDO	C	322	-	3,3,3	0.76	0	2,2,2	0.85	0
22	EDO	N	612	-	3,3,3	0.11	0	2,2,2	0.27	0
20	LFA	C	312	-	10,10,19	0.25	0	9,9,18	0.14	0
22	EDO	E	202	-	3,3,3	0.14	0	2,2,2	0.04	0
24	PGV	A	621	-	50,50,50	0.76	0	53,56,56	1.23	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	DMU	M	102	-	7,7,34	0.37	0	6,6,45	0.81	0
21	DMU	A	610	-	6,6,34	0.58	0	5,5,45	0.35	0
24	PGV	C	303	-	50,50,50	0.64	0	53,56,56	1.10	2 (3%)
25	CUA	B	302	2	0,1,1	-	-	-	-	-
22	EDO	C	320	-	3,3,3	0.13	0	2,2,2	0.37	0
19	CDL	C	304	-	86,86,99	0.61	1 (1%)	92,98,111	1.24	10 (10%)
21	DMU	O	306	-	10,10,34	0.19	0	9,9,45	0.57	0
21	DMU	C	315	-	34,34,34	0.80	1 (2%)	45,45,45	1.51	6 (13%)
21	DMU	Z	101	-	34,34,34	1.02	2 (5%)	45,45,45	1.07	4 (8%)
22	EDO	T	104	-	3,3,3	0.27	0	2,2,2	0.16	0
20	LFA	C	314	-	12,12,19	0.23	0	11,11,18	0.25	0
29	PEK	G	101	-	52,52,52	0.54	1 (1%)	55,57,57	0.64	0
21	DMU	B	304	-	10,10,34	0.53	0	9,9,45	0.44	0
21	DMU	N	610	-	34,34,34	1.41	6 (17%)	45,45,45	1.20	4 (8%)
21	DMU	T	103	-	22,22,34	0.53	0	27,27,45	1.57	2 (7%)
18	PER	A	606	15,14	1,1,1	1.27	0	-	-	-
22	EDO	P	321	-	3,3,3	0.24	0	2,2,2	0.03	0
21	DMU	C	317	-	22,22,34	0.48	0	27,27,45	1.54	4 (14%)
20	LFA	B	308	-	16,16,19	0.40	0	15,15,18	0.19	0
22	EDO	S	103	-	3,3,3	0.09	0	2,2,2	0.32	0
24	PGV	P	304	-	50,50,50	0.92	3 (6%)	53,56,56	0.98	4 (7%)
26	CHD	C	301	-	32,32,32	1.00	3 (9%)	51,51,51	0.79	1 (1%)
26	CHD	P	306	-	32,32,32	0.86	1 (3%)	51,51,51	1.07	3 (5%)
21	DMU	M	101	-	34,34,34	1.10	3 (8%)	45,45,45	1.04	3 (6%)
21	DMU	B	309	-	22,22,34	1.07	1 (4%)	27,27,45	1.45	3 (11%)
19	CDL	P	305	-	86,86,99	0.59	1 (1%)	92,98,111	1.10	8 (8%)
20	LFA	A	608	-	13,13,19	0.62	0	12,12,18	0.21	0
20	LFA	A	609	-	13,13,19	0.85	0	12,12,18	0.74	0
22	EDO	N	614	-	3,3,3	0.29	0	2,2,2	0.11	0
21	DMU	C	306	-	10,10,34	0.42	0	9,9,45	0.50	0
22	EDO	N	613	-	3,3,3	0.25	0	2,2,2	0.12	0
21	DMU	P	319	-	34,34,34	1.13	3 (8%)	45,45,45	1.07	3 (6%)
22	EDO	A	613	-	3,3,3	0.14	0	2,2,2	0.29	0
19	CDL	A	607	-	63,63,99	0.58	0	69,75,111	1.05	5 (7%)
22	EDO	G	103	-	3,3,3	0.30	0	2,2,2	0.13	0
21	DMU	C	319	-	34,34,34	0.81	1 (2%)	45,45,45	1.18	5 (11%)
20	LFA	O	301	-	16,16,19	0.35	0	15,15,18	0.29	0
20	LFA	P	313	-	10,10,19	0.26	0	9,9,18	0.25	0
20	LFA	P	315	-	12,12,19	0.25	0	11,11,18	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	DMU	O	308	-	22,22,34	0.69	1 (4%)	27,27,45	1.33	4 (14%)
20	LFA	C	313	-	14,14,19	0.32	0	13,13,18	0.33	0
22	EDO	P	322	-	3,3,3	0.40	0	2,2,2	0.17	0
14	HEA	N	602[B]	-	67,67,67	1.90	21 (31%)	81,103,103	2.44	34 (41%)
25	CUA	O	305	2	0,1,1	-	-	-	-	-
20	LFA	C	310	-	10,10,19	0.20	0	9,9,18	0.16	0
21	DMU	C	318	-	34,34,34	0.90	2 (5%)	45,45,45	1.36	5 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	DMU	N	622	-	-	4/19/59/59	0/2/2/2
22	EDO	E	203	-	-	0/1/1/1	-
21	DMU	D	201	-	-	5/19/59/59	0/2/2/2
22	EDO	S	102	-	-	0/1/1/1	-
22	EDO	B	306	-	-	0/1/1/1	-
20	LFA	N	608	-	-	3/11/11/17	-
19	CDL	L	101	-	-	49/104/104/110	-
14	HEA	N	603	1,18	-	4/36/76/76	-
21	DMU	J	101	-	-	4/8/8/59	-
21	DMU	N	609	-	-	2/4/4/59	-
20	LFA	P	308	-	-	7/8/8/17	-
22	EDO	R	201	-	-	1/1/1/1	-
26	CHD	P	302	-	-	2/9/74/74	0/4/4/4
20	LFA	C	308	-	-	1/3/3/17	-
20	LFA	P	301	-	-	8/12/12/17	-
22	EDO	R	202	-	-	0/1/1/1	-
21	DMU	C	324	-	-	6/19/59/59	0/2/2/2
22	EDO	P	323	-	-	0/1/1/1	-
21	DMU	P	307	-	-	2/8/8/59	-
21	DMU	N	601	-	-	5/8/8/59	-
22	EDO	C	321	-	-	0/1/1/1	-
24	PGV	N	621	-	-	8/55/55/55	-
14	HEA	A	602	1,18	-	4/36/76/76	-
20	LFA	P	312	-	-	5/11/11/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LFA	C	309	-	-	8/15/15/17	-
21	DMU	C	316	-	-	2/4/4/59	-
22	EDO	A	614	-	-	0/1/1/1	-
21	DMU	O	303	-	-	9/13/33/59	0/1/1/2
22	EDO	R	203	-	-	0/1/1/1	-
14	HEA	A	601[B]	-	-	4/36/76/76	-
21	DMU	O	307	-	-	3/8/8/59	-
14	HEA	N	602[A]	-	-	5/36/76/76	-
22	EDO	N	615	-	-	0/1/1/1	-
22	EDO	F	102	-	-	0/1/1/1	-
14	HEA	A	601[A]	-	-	6/36/76/76	-
22	EDO	A	615	-	-	0/1/1/1	-
26	CHD	G	102	-	-	2/9/74/74	0/4/4/4
22	EDO	O	309	-	-	0/1/1/1	-
21	DMU	W	101	-	-	4/8/8/59	-
20	LFA	C	307	-	-	4/8/8/17	-
21	DMU	Q	201	-	-	9/19/59/59	0/2/2/2
26	CHD	B	307	-	-	2/9/74/74	0/4/4/4
21	DMU	P	318	-	-	7/13/33/59	0/1/1/2
22	EDO	N	611	-	-	0/1/1/1	-
21	DMU	B	303	-	-	3/8/8/59	-
21	DMU	Z	102	-	-	10/13/33/59	0/1/1/2
21	DMU	Z	103	-	-	2/5/5/59	-
21	DMU	P	324	-	-	13/19/59/59	0/2/2/2
21	DMU	C	323	-	-	11/13/33/59	0/1/1/2
20	LFA	C	326	-	-	7/12/12/17	-
22	EDO	F	103	-	-	0/1/1/1	-
21	DMU	P	320	-	-	8/19/59/59	0/2/2/2
20	LFA	O	302	-	-	3/8/8/17	-
21	DMU	A	611	-	-	8/19/59/59	0/2/2/2
20	LFA	P	314	-	-	5/12/12/17	-
20	LFA	T	102	-	-	3/8/8/17	-
21	DMU	A	622	-	-	6/19/59/59	0/2/2/2
20	LFA	P	310	-	-	7/15/15/17	-
21	DMU	P	317	-	-	2/4/4/59	-
20	LFA	P	309	-	-	1/3/3/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LFA	P	311	-	-	6/8/8/17	-
19	CDL	Y	101	-	-	60/104/104/110	-
29	PEK	T	101	-	-	20/56/56/56	-
20	LFA	G	104	-	-	6/11/11/17	-
21	DMU	L	102	-	-	10/13/33/59	0/1/1/2
19	CDL	V	101	-	-	39/74/74/110	-
22	EDO	A	612	-	-	0/1/1/1	-
20	LFA	C	311	-	-	6/11/11/17	-
21	DMU	A	623	-	-	4/8/8/59	-
26	CHD	C	305	-	-	8/9/74/74	0/4/4/4
21	DMU	P	316	-	-	8/19/59/59	0/2/2/2
21	DMU	B	305	-	-	8/13/33/59	0/1/1/2
22	EDO	E	201	-	-	0/1/1/1	-
22	EDO	C	322	-	-	0/1/1/1	-
22	EDO	N	612	-	-	0/1/1/1	-
20	LFA	C	312	-	-	3/8/8/17	-
22	EDO	E	202	-	-	0/1/1/1	-
24	PGV	A	621	-	-	11/55/55/55	-
21	DMU	M	102	-	-	5/5/5/59	-
21	DMU	A	610	-	-	3/4/4/59	-
24	PGV	C	303	-	-	12/55/55/55	-
22	EDO	C	320	-	-	0/1/1/1	-
19	CDL	C	304	-	-	47/97/97/110	-
21	DMU	O	306	-	-	6/8/8/59	-
21	DMU	C	315	-	-	13/19/59/59	0/2/2/2
21	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
22	EDO	T	104	-	-	0/1/1/1	-
20	LFA	C	314	-	-	4/10/10/17	-
29	PEK	G	101	-	-	11/56/56/56	-
21	DMU	B	304	-	-	4/8/8/59	-
21	DMU	N	610	-	-	6/19/59/59	0/2/2/2
21	DMU	T	103	-	-	7/13/33/59	0/1/1/2
22	EDO	S	103	-	-	0/1/1/1	-
22	EDO	P	321	-	-	1/1/1/1	-
21	DMU	C	317	-	-	7/13/33/59	0/1/1/2
20	LFA	B	308	-	-	8/14/14/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PGV	P	304	-	-	9/55/55/55	-
26	CHD	C	301	-	-	2/9/74/74	0/4/4/4
26	CHD	P	306	-	-	5/9/74/74	0/4/4/4
21	DMU	M	101	-	-	3/19/59/59	0/2/2/2
21	DMU	B	309	-	-	9/13/33/59	0/1/1/2
19	CDL	P	305	-	-	46/97/97/110	-
20	LFA	A	608	-	-	5/11/11/17	-
20	LFA	A	609	-	-	4/11/11/17	-
22	EDO	N	614	-	-	0/1/1/1	-
21	DMU	C	306	-	-	3/8/8/59	-
22	EDO	N	613	-	-	0/1/1/1	-
21	DMU	P	319	-	-	13/19/59/59	0/2/2/2
22	EDO	A	613	-	-	1/1/1/1	-
19	CDL	A	607	-	-	37/74/74/110	-
22	EDO	G	103	-	-	0/1/1/1	-
21	DMU	C	319	-	-	11/19/59/59	0/2/2/2
20	LFA	O	301	-	-	12/14/14/17	-
20	LFA	P	313	-	-	3/8/8/17	-
20	LFA	P	315	-	-	4/10/10/17	-
21	DMU	O	308	-	-	3/13/33/59	0/1/1/2
20	LFA	C	313	-	-	3/12/12/17	-
22	EDO	P	322	-	-	0/1/1/1	-
14	HEA	N	602[B]	-	-	2/36/76/76	-
20	LFA	C	310	-	-	7/8/8/17	-
21	DMU	C	318	-	-	15/19/59/59	0/2/2/2

All (191) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[A]	HEA	C1D-ND	-5.74	1.30	1.40
14	A	601[B]	HEA	C1D-ND	-5.74	1.30	1.40
14	N	602[A]	HEA	C1D-ND	-4.93	1.31	1.40
14	N	602[B]	HEA	C1D-ND	-4.93	1.31	1.40
14	A	601[A]	HEA	C16-C17	-4.53	1.38	1.53
14	A	601[B]	HEA	C16-C17	-4.53	1.38	1.53
21	P	319	DMU	O3-C5	4.53	1.54	1.43
14	N	602[A]	HEA	C4C-NC	-4.48	1.31	1.39
14	N	602[B]	HEA	C4C-NC	-4.48	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	610	DMU	O16-C6	-4.33	1.33	1.40
21	O	303	DMU	C43-C40	4.27	1.80	1.50
14	A	601[A]	HEA	C3D-C2D	4.17	1.45	1.36
14	A	601[B]	HEA	C3D-C2D	4.17	1.45	1.36
14	A	601[A]	HEA	C3A-C2A	4.12	1.46	1.37
14	A	601[B]	HEA	C3A-C2A	4.12	1.46	1.37
14	N	603	HEA	C3B-C2B	4.12	1.44	1.34
14	A	602	HEA	C3A-C2A	4.04	1.46	1.37
14	A	602	HEA	C1D-ND	-4.01	1.33	1.40
14	N	603	HEA	C4B-NB	-3.95	1.33	1.40
14	A	602	HEA	C1C-NC	-3.88	1.32	1.39
14	N	602[A]	HEA	C16-C17	-3.83	1.41	1.53
14	N	602[B]	HEA	C16-C17	-3.83	1.41	1.53
14	N	603	HEA	C1D-ND	-3.82	1.33	1.40
14	A	602	HEA	C3B-C2B	3.81	1.43	1.34
14	A	601[A]	HEA	C1B-NB	-3.67	1.31	1.38
14	A	601[B]	HEA	C1B-NB	-3.67	1.31	1.38
14	N	602[A]	HEA	C3B-C2B	3.65	1.43	1.34
14	N	602[B]	HEA	C3B-C2B	3.65	1.43	1.34
21	B	305	DMU	O16-C6	3.64	1.46	1.40
14	N	602[A]	HEA	C4B-NB	-3.62	1.34	1.40
14	N	602[B]	HEA	C4B-NB	-3.62	1.34	1.40
14	A	602	HEA	C4D-ND	-3.61	1.31	1.38
14	A	601[A]	HEA	C4B-NB	-3.53	1.34	1.40
14	A	601[B]	HEA	C4B-NB	-3.53	1.34	1.40
14	A	601[A]	HEA	C4C-NC	-3.52	1.33	1.39
14	A	601[B]	HEA	C4C-NC	-3.52	1.33	1.39
26	P	302	CHD	C22-C23	-3.51	1.42	1.52
14	N	603	HEA	C3A-C2A	3.47	1.45	1.37
14	N	602[A]	HEA	C1B-NB	-3.44	1.32	1.38
14	N	602[B]	HEA	C1B-NB	-3.44	1.32	1.38
14	N	602[A]	HEA	C4D-ND	-3.44	1.32	1.38
14	N	602[B]	HEA	C4D-ND	-3.44	1.32	1.38
21	M	101	DMU	O3-C5	-3.44	1.34	1.43
14	A	602	HEA	FE-NB	3.39	2.05	1.94
21	P	318	DMU	O16-C6	3.36	1.45	1.40
14	A	602	HEA	C3D-C2D	3.36	1.44	1.36
21	P	320	DMU	C7-C5	-3.35	1.43	1.52
26	C	301	CHD	O26-C24	-3.34	1.19	1.30
14	A	601[A]	HEA	C11-C3B	-3.34	1.47	1.51
14	A	601[B]	HEA	C11-C3B	-3.34	1.47	1.51
14	A	602	HEA	C1C-C2C	3.33	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	603	HEA	C3D-C2D	3.29	1.43	1.36
26	P	302	CHD	O26-C24	-3.29	1.19	1.30
14	A	602	HEA	CHB-C4A	3.26	1.44	1.38
14	A	602	HEA	C4C-NC	-3.24	1.33	1.39
14	A	602	HEA	FE-ND	3.24	2.04	1.94
14	N	603	HEA	C1B-NB	-3.23	1.32	1.38
14	N	603	HEA	CHB-C4A	3.23	1.44	1.38
29	T	101	PEK	C2-C1	3.22	1.60	1.50
14	A	601[A]	HEA	FE-ND	3.18	2.04	1.94
14	A	601[B]	HEA	FE-ND	3.18	2.04	1.94
14	A	601[A]	HEA	C3B-C2B	3.16	1.41	1.34
14	A	601[B]	HEA	C3B-C2B	3.16	1.41	1.34
14	N	602[A]	HEA	CHB-C4A	3.11	1.44	1.38
14	N	602[B]	HEA	CHB-C4A	3.11	1.44	1.38
14	N	603	HEA	CHD-C1D	3.09	1.44	1.38
21	D	201	DMU	O5-C6	-3.09	1.33	1.41
14	N	602[A]	HEA	C11-C3B	-3.09	1.47	1.51
14	N	602[B]	HEA	C11-C3B	-3.09	1.47	1.51
21	N	622	DMU	C7-C5	-3.06	1.44	1.52
29	T	101	PEK	C23-C22	-3.05	1.41	1.52
14	N	602[A]	HEA	C3A-C2A	3.04	1.44	1.37
14	N	602[B]	HEA	C3A-C2A	3.04	1.44	1.37
21	Z	101	DMU	O3-C5	-3.03	1.35	1.43
14	N	603	HEA	C4D-ND	-3.02	1.32	1.38
21	Q	201	DMU	C10-C5	-2.98	1.43	1.52
14	A	602	HEA	C1A-C2A	2.97	1.50	1.45
14	A	602	HEA	CHD-C1D	2.95	1.44	1.38
14	N	603	HEA	C11-C3B	-2.94	1.47	1.51
14	A	601[A]	HEA	FE-NB	2.92	2.03	1.94
14	A	601[B]	HEA	FE-NB	2.92	2.03	1.94
24	P	304	PGV	O03-C19	2.91	1.41	1.33
14	A	602	HEA	C1B-NB	-2.90	1.33	1.38
21	P	320	DMU	C10-C5	-2.89	1.44	1.52
21	A	611	DMU	O7-C10	2.88	1.49	1.41
26	C	301	CHD	C22-C23	-2.86	1.44	1.52
14	A	602	HEA	C4B-NB	-2.85	1.35	1.40
21	D	201	DMU	O3-C5	-2.85	1.35	1.43
14	N	602[A]	HEA	FE-NC	2.82	2.04	1.95
14	N	602[B]	HEA	FE-NC	2.82	2.04	1.95
14	N	602[A]	HEA	FE-ND	2.82	2.03	1.94
14	N	602[B]	HEA	FE-ND	2.82	2.03	1.94
29	G	101	PEK	C23-C22	-2.79	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	G	104	LFA	C10-C9	-2.76	1.38	1.51
21	Q	201	DMU	O3-C5	-2.74	1.36	1.43
21	A	611	DMU	O16-C6	-2.61	1.35	1.40
21	C	318	DMU	C7-C5	-2.61	1.45	1.52
21	N	610	DMU	C7-C5	-2.56	1.45	1.52
21	A	622	DMU	C7-C5	-2.56	1.45	1.52
14	N	603	HEA	C3C-C4C	2.55	1.50	1.42
21	A	622	DMU	C10-C5	-2.54	1.45	1.52
21	Q	201	DMU	O16-C6	-2.52	1.36	1.40
14	N	603	HEA	C12-C11	2.50	1.57	1.53
14	A	601[A]	HEA	C16-C15	2.50	1.56	1.51
14	A	601[B]	HEA	C16-C15	2.50	1.56	1.51
24	P	304	PGV	O01-C02	-2.50	1.40	1.46
21	N	610	DMU	C10-C5	-2.47	1.45	1.52
26	P	306	CHD	O25-C24	2.46	1.30	1.22
21	C	318	DMU	O3-C5	2.45	1.49	1.43
14	A	602	HEA	CHC-C1C	2.43	1.44	1.39
21	Q	201	DMU	O5-C6	-2.41	1.35	1.41
21	N	610	DMU	C6-C1	-2.41	1.45	1.52
14	N	603	HEA	CHA-C1A	2.39	1.43	1.38
14	A	601[A]	HEA	C4D-ND	-2.37	1.34	1.38
14	A	601[B]	HEA	C4D-ND	-2.37	1.34	1.38
14	N	603	HEA	FE-ND	2.37	2.02	1.94
21	D	201	DMU	O55-C2	2.36	1.48	1.43
14	A	601[A]	HEA	CHB-C4A	2.35	1.43	1.38
14	A	601[B]	HEA	CHB-C4A	2.35	1.43	1.38
14	N	603	HEA	C1C-C2C	2.35	1.48	1.43
21	M	101	DMU	C10-C5	-2.34	1.45	1.52
14	N	602[A]	HEA	FE-NB	2.34	2.02	1.94
14	N	602[B]	HEA	FE-NB	2.34	2.02	1.94
21	A	622	DMU	O5-C6	-2.33	1.35	1.41
21	N	610	DMU	O1-C10	2.33	1.47	1.41
14	A	601[A]	HEA	O1D-CGD	2.33	1.29	1.22
14	A	601[B]	HEA	O1D-CGD	2.33	1.29	1.22
21	C	319	DMU	O55-C2	-2.32	1.37	1.43
21	C	315	DMU	O5-C6	-2.32	1.35	1.41
14	N	602[A]	HEA	C3D-C2D	2.31	1.41	1.36
14	N	602[B]	HEA	C3D-C2D	2.31	1.41	1.36
14	N	603	HEA	C1C-NC	-2.30	1.35	1.39
14	A	601[A]	HEA	CHD-C1D	2.30	1.43	1.38
14	A	601[B]	HEA	CHD-C1D	2.30	1.43	1.38
19	P	305	CDL	C31-CA7	-2.30	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	603	HEA	C4C-NC	-2.29	1.35	1.39
14	A	602	HEA	C18-C19	2.29	1.38	1.33
21	P	316	DMU	O5-C6	-2.27	1.36	1.41
14	N	602[A]	HEA	C4B-C3B	2.27	1.48	1.44
14	N	602[B]	HEA	C4B-C3B	2.27	1.48	1.44
21	O	308	DMU	C6-C1	-2.26	1.45	1.52
14	A	601[A]	HEA	CMC-C2C	-2.26	1.46	1.50
14	A	601[B]	HEA	CMC-C2C	-2.26	1.46	1.50
21	A	622	DMU	O16-C6	-2.26	1.36	1.40
20	G	104	LFA	C9-C8	-2.25	1.40	1.51
14	A	601[A]	HEA	C1C-C2C	2.24	1.48	1.43
14	A	601[B]	HEA	C1C-C2C	2.24	1.48	1.43
14	A	601[A]	HEA	CHA-C1A	2.22	1.42	1.38
14	A	601[B]	HEA	CHA-C1A	2.22	1.42	1.38
14	N	603	HEA	CHC-C4B	2.22	1.42	1.38
14	A	602	HEA	FE-NC	2.21	2.02	1.95
21	P	318	DMU	C3-C4	-2.20	1.48	1.53
21	P	319	DMU	C7-C5	-2.19	1.46	1.52
21	D	201	DMU	O61-C57	2.19	1.51	1.42
21	M	101	DMU	C7-C5	-2.19	1.46	1.52
21	P	319	DMU	O5-C6	-2.18	1.36	1.41
21	O	303	DMU	C3-C4	-2.17	1.48	1.53
14	N	602[A]	HEA	CHC-C1C	2.16	1.44	1.39
14	N	602[B]	HEA	CHC-C1C	2.16	1.44	1.39
14	N	602[A]	HEA	C4D-C3D	2.15	1.48	1.45
14	N	602[B]	HEA	C4D-C3D	2.15	1.48	1.45
24	N	621	PGV	O01-C1	2.12	1.40	1.34
21	B	309	DMU	C40-C37	2.11	1.64	1.51
14	N	602[A]	HEA	CHA-C1A	2.10	1.42	1.38
14	N	602[B]	HEA	CHA-C1A	2.10	1.42	1.38
21	D	201	DMU	C10-C5	-2.10	1.46	1.52
21	Q	201	DMU	C7-C5	-2.10	1.46	1.52
14	A	601[A]	HEA	C26-C15	-2.10	1.45	1.50
14	A	601[B]	HEA	C26-C15	-2.10	1.45	1.50
14	A	602	HEA	CHC-C4B	2.08	1.42	1.38
14	A	601[A]	HEA	FE-NC	2.08	2.02	1.95
14	A	601[B]	HEA	FE-NC	2.08	2.02	1.95
21	N	610	DMU	O6-C11	2.08	1.51	1.42
21	P	316	DMU	O1-C10	2.07	1.47	1.41
14	A	602	HEA	C11-C3B	-2.06	1.48	1.51
14	N	603	HEA	FE-NC	2.05	2.01	1.95
24	P	304	PGV	O03-C01	-2.05	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	324	DMU	O16-C6	2.05	1.43	1.40
21	D	201	DMU	O49-C1	-2.05	1.37	1.43
14	N	602[A]	HEA	C1C-NC	-2.04	1.35	1.39
14	N	602[B]	HEA	C1C-NC	-2.04	1.35	1.39
21	Q	201	DMU	O55-C2	2.04	1.48	1.43
21	N	622	DMU	C6-C1	-2.04	1.46	1.52
19	C	304	CDL	PA1-OA3	2.03	1.57	1.50
14	N	602[A]	HEA	CHC-C4B	2.02	1.42	1.38
14	N	602[B]	HEA	CHC-C4B	2.02	1.42	1.38
21	Z	101	DMU	C10-C5	-2.02	1.46	1.52
14	N	602[A]	HEA	C1D-C2D	2.01	1.48	1.44
14	N	602[B]	HEA	C1D-C2D	2.01	1.48	1.44
14	N	603	HEA	C1A-C2A	2.00	1.48	1.45
26	C	301	CHD	O25-C24	2.00	1.28	1.22

All (336) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602[A]	HEA	C3D-C4D-ND	7.82	117.91	110.35
14	N	602[B]	HEA	C3D-C4D-ND	7.82	117.91	110.35
14	A	601[A]	HEA	C3C-C4C-NC	6.56	115.32	109.80
14	A	601[B]	HEA	C3C-C4C-NC	6.56	115.32	109.80
21	T	103	DMU	O16-C6-C1	6.38	117.95	108.27
19	C	304	CDL	OA6-CA5-C11	-6.25	97.97	111.48
14	N	603	HEA	C3D-C4D-ND	6.16	116.31	110.35
14	A	601[A]	HEA	C3D-C4D-ND	6.09	116.24	110.35
14	A	601[B]	HEA	C3D-C4D-ND	6.09	116.24	110.35
21	C	315	DMU	O16-C6-C1	6.00	117.38	108.27
21	Q	201	DMU	O16-C6-C1	5.82	117.11	108.27
21	P	316	DMU	O16-C6-C1	5.79	117.06	108.27
21	C	324	DMU	O16-C6-C1	5.78	117.06	108.27
14	N	602[A]	HEA	C3C-C4C-NC	5.75	114.64	109.80
14	N	602[B]	HEA	C3C-C4C-NC	5.75	114.64	109.80
21	D	201	DMU	O16-C6-C1	5.73	116.98	108.27
21	B	309	DMU	O16-C6-C1	5.64	116.83	108.27
14	A	602	HEA	C3C-C4C-NC	5.52	114.45	109.80
14	N	602[A]	HEA	C27-C19-C20	5.48	124.74	115.23
14	A	602	HEA	C2B-C1B-NB	5.40	116.14	109.90
14	N	603	HEA	C2D-C1D-ND	5.25	115.88	109.84
14	N	602[A]	HEA	C2B-C1B-NB	5.18	115.89	109.90
14	N	602[B]	HEA	C2B-C1B-NB	5.18	115.89	109.90
14	A	602	HEA	C3C-C2C-C1C	-5.15	101.10	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	324	DMU	O16-C6-C1	5.12	116.04	108.27
14	A	602	HEA	C3B-C4B-NB	5.10	115.70	109.84
14	N	603	HEA	C3C-C2C-C1C	-5.06	101.20	107.17
21	P	324	DMU	C10-C5-C7	5.05	120.63	110.01
19	A	607	CDL	OA6-CA4-CA6	4.98	126.21	108.34
14	A	602	HEA	C2D-C1D-ND	4.91	115.48	109.84
14	N	603	HEA	C3B-C4B-NB	4.90	115.48	109.84
21	P	318	DMU	O5-C6-C1	4.89	120.42	110.37
14	N	602[A]	HEA	C2A-C1A-NA	4.87	115.03	110.32
14	N	602[B]	HEA	C2A-C1A-NA	4.87	115.03	110.32
21	C	317	DMU	O5-C6-C1	4.86	120.35	110.37
26	C	305	CHD	C17-C13-C14	-4.78	95.32	100.11
14	N	602[A]	HEA	C4D-C3D-C2D	-4.73	100.00	106.89
14	N	602[B]	HEA	C4D-C3D-C2D	-4.73	100.00	106.89
26	C	305	CHD	C14-C13-C12	4.72	111.73	107.42
14	N	603	HEA	C2A-C1A-NA	4.71	114.87	110.32
21	P	320	DMU	O16-C6-C1	4.69	115.40	108.27
14	A	601[A]	HEA	CHA-C4D-C3D	-4.68	117.95	124.77
14	A	601[B]	HEA	CHA-C4D-C3D	-4.68	117.95	124.77
24	C	303	PGV	C27-C26-C25	-4.67	90.78	114.37
24	A	621	PGV	O03-C19-O04	-4.67	111.96	123.63
14	A	601[A]	HEA	C2D-C1D-ND	4.66	115.19	109.84
14	A	601[B]	HEA	C2D-C1D-ND	4.66	115.19	109.84
14	N	602[A]	HEA	C13-C12-C11	-4.61	107.03	114.39
14	N	602[B]	HEA	C13-C12-C11	-4.61	107.03	114.39
14	N	603	HEA	C3A-C2A-C1A	-4.61	102.69	107.05
14	A	601[A]	HEA	C27-C19-C20	4.59	123.19	115.23
19	P	305	CDL	OA4-PA1-OA5	-4.51	87.12	107.57
29	T	101	PEK	O01-C1-O02	-4.48	113.22	123.70
14	N	603	HEA	C2C-C1C-NC	4.45	117.27	110.14
21	N	622	DMU	O16-C6-C1	4.44	115.01	108.27
21	M	101	DMU	O16-C6-C1	4.43	115.00	108.27
21	A	622	DMU	O16-C6-C1	4.41	114.97	108.27
14	N	602[A]	HEA	C2D-C1D-ND	4.39	114.89	109.84
14	N	602[B]	HEA	C2D-C1D-ND	4.39	114.89	109.84
14	N	603	HEA	C3C-C4C-NC	4.37	113.48	109.80
14	N	602[A]	HEA	C3C-C2C-C1C	-4.36	102.02	107.17
14	N	602[B]	HEA	C3C-C2C-C1C	-4.36	102.02	107.17
14	N	602[A]	HEA	CHB-C1B-C2B	-4.34	118.18	125.03
14	N	602[B]	HEA	CHB-C1B-C2B	-4.34	118.18	125.03
14	A	601[A]	HEA	C2B-C1B-NB	4.33	114.91	109.90
14	A	601[B]	HEA	C2B-C1B-NB	4.33	114.91	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	603	HEA	CHB-C1B-C2B	-4.30	118.23	125.03
14	N	603	HEA	CAD-C3D-C4D	4.30	132.19	124.70
24	N	621	PGV	O03-C19-O04	-4.30	112.87	123.63
14	A	601[A]	HEA	C3B-C4B-NB	4.29	114.77	109.84
14	A	601[B]	HEA	C3B-C4B-NB	4.29	114.77	109.84
14	A	602	HEA	C3A-C2A-C1A	-4.27	103.00	107.05
14	N	603	HEA	C2B-C1B-NB	4.27	114.83	109.90
21	P	324	DMU	C10-O1-C9	-4.26	105.41	113.72
14	N	602[A]	HEA	C3B-C4B-NB	4.25	114.72	109.84
14	N	602[B]	HEA	C3B-C4B-NB	4.25	114.72	109.84
14	N	603	HEA	CHA-C4D-C3D	-4.25	118.58	124.77
14	A	601[A]	HEA	C3C-C2C-C1C	-4.15	102.28	107.17
14	A	601[B]	HEA	C3C-C2C-C1C	-4.15	102.28	107.17
21	O	303	DMU	O5-C6-C1	4.11	118.81	110.37
14	N	603	HEA	CHB-C4A-NA	-4.08	120.01	124.45
14	A	602	HEA	C1D-C2D-C3D	-4.06	102.71	106.98
14	A	602	HEA	C3D-C4D-ND	4.02	114.24	110.35
14	A	601[A]	HEA	C13-C12-C11	-4.01	107.98	114.39
14	A	601[B]	HEA	C13-C12-C11	-4.01	107.98	114.39
19	C	304	CDL	OA7-CA5-C11	4.00	139.42	123.78
14	A	602	HEA	CMD-C2D-C1D	3.99	131.27	125.03
14	A	601[B]	HEA	C27-C19-C20	3.98	122.13	115.23
24	N	621	PGV	O03-C19-C20	3.91	123.77	111.83
26	C	305	CHD	C16-C17-C20	3.90	118.08	112.18
21	Z	101	DMU	O16-C6-C1	3.88	114.17	108.27
14	N	602[A]	HEA	C3A-C2A-C1A	-3.87	103.38	107.05
14	N	602[B]	HEA	C3A-C2A-C1A	-3.87	103.38	107.05
14	A	601[A]	HEA	C4D-C3D-C2D	-3.86	101.27	106.89
14	A	601[B]	HEA	C4D-C3D-C2D	-3.86	101.27	106.89
14	N	603	HEA	C1D-C2D-C3D	-3.81	102.97	106.98
14	A	602	HEA	C1B-C2B-C3B	-3.78	102.42	106.80
19	P	305	CDL	OA4-PA1-OA2	-3.78	90.43	107.57
19	L	101	CDL	OB4-PB2-OB2	3.74	124.53	107.57
14	A	602	HEA	C2A-C1A-NA	3.69	113.88	110.32
21	L	102	DMU	O5-C6-O16	3.68	118.74	110.04
14	A	601[A]	HEA	CHB-C1B-C2B	-3.67	119.24	125.03
14	A	601[B]	HEA	CHB-C1B-C2B	-3.67	119.24	125.03
24	C	303	PGV	O03-C19-O04	-3.66	114.48	123.63
21	C	318	DMU	O3-C5-C10	3.64	118.75	110.08
21	N	622	DMU	C10-C5-C7	3.63	117.65	110.01
19	V	101	CDL	OA6-CA4-CA3	3.62	121.34	108.34
14	A	602	HEA	C2C-C1C-NC	3.62	115.95	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	318	DMU	C1-C2-C3	3.59	117.84	109.68
26	P	306	CHD	C18-C13-C12	-3.58	105.47	109.06
14	A	602	HEA	CHA-C4D-C3D	-3.56	119.58	124.77
21	C	315	DMU	C6-O5-C4	3.55	120.65	113.72
19	P	305	CDL	OA2-PA1-OA3	3.55	122.99	108.94
14	A	601[A]	HEA	C3A-C2A-C1A	-3.49	103.74	107.05
14	A	601[B]	HEA	C3A-C2A-C1A	-3.49	103.74	107.05
29	T	101	PEK	O02-C1-C2	3.43	137.22	123.78
14	A	601[A]	HEA	C1D-C2D-C3D	-3.41	103.39	106.98
14	A	601[B]	HEA	C1D-C2D-C3D	-3.41	103.39	106.98
19	P	305	CDL	OA4-PA1-OA3	3.41	128.31	112.44
24	A	621	PGV	O03-C19-C20	3.39	122.16	111.83
14	A	601[A]	HEA	C4B-C3B-C2B	-3.38	101.75	107.44
14	A	601[B]	HEA	C4B-C3B-C2B	-3.38	101.75	107.44
21	C	317	DMU	C2-C3-C4	-3.38	104.10	110.23
21	Z	102	DMU	O5-C6-O16	3.36	117.99	110.04
14	A	601[A]	HEA	C2A-C1A-NA	3.36	113.56	110.32
14	A	601[B]	HEA	C2A-C1A-NA	3.36	113.56	110.32
14	N	603	HEA	CMD-C2D-C1D	3.32	130.22	125.03
14	N	602[A]	HEA	CHA-C4D-C3D	-3.30	119.95	124.77
14	N	602[B]	HEA	CHA-C4D-C3D	-3.30	119.95	124.77
14	N	603	HEA	CAD-CBD-CGD	-3.30	104.91	113.67
14	A	602	HEA	CHB-C1B-C2B	-3.28	119.84	125.03
14	A	601[B]	HEA	C20-C19-C18	-3.26	113.84	121.17
24	N	621	PGV	O01-C1-O02	-3.25	116.11	123.70
21	C	315	DMU	O5-C6-O16	-3.24	102.38	110.04
21	Q	201	DMU	C10-O1-C9	3.23	120.03	113.72
21	C	319	DMU	O16-C6-C1	3.23	113.17	108.27
26	C	305	CHD	C6-C7-C8	3.22	115.02	111.50
19	C	304	CDL	OA5-PA1-OA3	3.20	121.63	108.94
19	A	607	CDL	CA4-OA6-CA5	3.20	125.45	117.80
21	N	622	DMU	C10-O7-C3	-3.19	110.43	117.98
21	C	323	DMU	O16-C6-C1	3.17	113.09	108.27
14	N	603	HEA	C4D-C3D-C2D	-3.16	102.30	106.89
21	C	318	DMU	O16-C6-C1	3.15	113.06	108.27
14	A	602	HEA	CAD-CBD-CGD	-3.14	105.34	113.67
21	B	305	DMU	O5-C6-C1	3.12	116.77	110.37
14	N	603	HEA	C4B-C3B-C2B	-3.10	102.22	107.44
14	A	602	HEA	CHC-C1C-C2C	-3.08	118.50	127.43
14	N	602[A]	HEA	CHB-C4A-NA	-3.07	121.11	124.45
14	N	602[B]	HEA	CHB-C4A-NA	-3.07	121.11	124.45
14	A	602	HEA	CHB-C4A-NA	-3.06	121.13	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602[A]	HEA	C4B-C3B-C2B	-3.05	102.32	107.44
14	N	602[B]	HEA	C4B-C3B-C2B	-3.05	102.32	107.44
14	A	602	HEA	CMB-C2B-C1B	3.04	129.78	125.03
21	N	622	DMU	O3-C5-C10	3.03	117.31	110.08
21	P	316	DMU	C10-C5-C7	3.03	116.38	110.01
19	A	607	CDL	OA5-PA1-OA3	3.02	120.92	108.94
14	A	601[A]	HEA	C26-C15-C16	3.02	120.47	115.23
14	A	601[B]	HEA	C26-C15-C16	3.02	120.47	115.23
19	C	304	CDL	OB5-PB2-OB3	3.00	120.82	108.94
21	Q	201	DMU	C6-O5-C4	-2.98	107.89	113.72
21	C	315	DMU	C18-O16-C6	-2.97	108.60	113.68
14	N	602[A]	HEA	C2C-C1C-NC	2.97	114.90	110.14
14	N	602[B]	HEA	C2C-C1C-NC	2.97	114.90	110.14
21	T	103	DMU	C18-O16-C6	-2.97	108.61	113.68
21	N	610	DMU	O5-C6-O16	2.96	117.03	110.04
14	N	603	HEA	C1B-C2B-C3B	-2.92	103.42	106.80
14	N	603	HEA	C27-C19-C20	2.90	120.27	115.23
19	V	101	CDL	OA6-CA5-C11	2.90	117.76	111.48
21	C	315	DMU	C10-C5-C7	2.89	116.09	110.01
21	O	308	DMU	O5-C6-O16	2.89	116.87	110.04
21	O	303	DMU	O16-C6-C1	2.88	112.64	108.27
14	N	602[A]	HEA	C1B-C2B-C3B	-2.87	103.47	106.80
14	N	602[B]	HEA	C1B-C2B-C3B	-2.87	103.47	106.80
21	Q	201	DMU	O1-C9-C8	2.85	114.84	109.70
14	N	603	HEA	C4A-NA-C1A	-2.84	101.18	105.82
21	O	303	DMU	C6-C1-C2	2.84	115.97	110.01
21	D	201	DMU	C10-C5-C7	2.83	115.96	110.01
29	T	101	PEK	C2-C3-C4	2.82	119.51	113.35
21	P	320	DMU	O5-C6-C1	2.82	116.16	110.37
21	C	319	DMU	O3-C5-C7	2.82	117.01	110.38
24	P	304	PGV	C22-C21-C20	-2.80	102.85	113.13
19	V	101	CDL	OA8-CA6-CA4	2.79	116.45	108.40
14	A	602	HEA	CHC-C4B-NB	-2.79	120.92	124.37
19	C	304	CDL	O1-C1-CB2	2.79	119.33	109.70
14	A	601[A]	HEA	C4C-C3C-C2C	-2.78	103.84	107.30
14	A	601[B]	HEA	C4C-C3C-C2C	-2.78	103.84	107.30
19	C	304	CDL	OA4-PA1-OA5	-2.77	95.00	107.57
14	A	601[A]	HEA	CMC-C2C-C1C	2.76	129.63	125.42
14	A	601[B]	HEA	CMC-C2C-C1C	2.76	129.63	125.42
21	B	305	DMU	C6-O5-C4	2.76	119.12	113.72
14	N	602[A]	HEA	C4C-C3C-C2C	-2.76	103.87	107.30
14	N	602[B]	HEA	C4C-C3C-C2C	-2.76	103.87	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	324	DMU	O1-C9-C8	-2.75	104.74	109.70
21	P	316	DMU	O1-C9-C11	2.75	113.25	106.44
14	A	601[A]	HEA	CHB-C4A-NA	-2.74	121.47	124.45
14	A	601[B]	HEA	CHB-C4A-NA	-2.74	121.47	124.45
21	P	316	DMU	C6-O5-C4	2.73	119.05	113.72
21	N	610	DMU	C10-O1-C9	2.72	119.04	113.72
21	C	319	DMU	O5-C6-C1	2.71	115.94	110.37
19	C	304	CDL	OA4-PA1-OA3	2.70	125.01	112.44
14	A	601[B]	HEA	C21-C22-C23	-2.70	118.63	127.64
14	A	601[A]	HEA	C2C-C1C-NC	2.70	114.47	110.14
14	A	601[B]	HEA	C2C-C1C-NC	2.70	114.47	110.14
21	P	319	DMU	O3-C5-C10	2.69	116.48	110.08
19	V	101	CDL	OA6-CA4-CA6	-2.69	98.71	108.34
21	C	318	DMU	C6-C1-C2	2.68	115.64	110.01
14	A	602	HEA	C4D-C3D-C2D	-2.67	103.00	106.89
21	O	308	DMU	C57-C4-C3	-2.67	106.47	113.02
21	A	611	DMU	C10-O7-C3	-2.65	111.69	117.98
21	O	308	DMU	O16-C6-C1	-2.64	104.26	108.27
14	A	602	HEA	C4B-NB-C1B	-2.63	102.09	105.21
14	N	603	HEA	CHC-C1C-C2C	-2.63	119.80	127.43
21	Q	201	DMU	C2-C3-C4	-2.63	105.11	110.93
19	P	305	CDL	OA8-CA6-CA4	-2.62	100.84	108.40
14	N	602[B]	HEA	C20-C19-C18	-2.62	115.29	121.17
14	N	602[A]	HEA	CHA-C1A-NA	-2.62	121.60	124.45
14	N	602[B]	HEA	CHA-C1A-NA	-2.62	121.60	124.45
21	B	309	DMU	O5-C6-O16	2.61	116.20	110.04
14	A	601[A]	HEA	CAD-C3D-C4D	2.58	129.19	124.70
14	A	601[B]	HEA	CAD-C3D-C4D	2.58	129.19	124.70
14	N	602[A]	HEA	O11-C11-C3B	-2.58	106.53	111.26
14	N	602[B]	HEA	O11-C11-C3B	-2.58	106.53	111.26
14	A	602	HEA	C20-C19-C18	-2.57	115.39	121.17
26	C	305	CHD	C16-C17-C13	-2.56	101.06	103.54
21	M	101	DMU	O5-C6-C1	2.56	115.64	110.37
14	N	602[B]	HEA	C27-C19-C20	2.56	119.68	115.23
24	A	621	PGV	C25-C24-C23	2.54	127.23	114.37
19	C	304	CDL	OB6-CB5-C51	2.54	116.98	111.48
14	A	601[B]	HEA	C25-C23-C24	2.54	120.44	114.59
21	P	320	DMU	C8-C7-C5	-2.54	106.38	110.83
19	L	101	CDL	OB5-PB2-OB3	-2.52	98.93	108.94
21	Z	101	DMU	O5-C6-C1	2.52	115.55	110.37
19	C	304	CDL	OA4-PA1-OA2	-2.52	96.15	107.57
21	C	317	DMU	C18-O16-C6	-2.52	109.38	113.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	304	PGV	C27-C26-C25	-2.51	101.66	114.37
21	P	324	DMU	O7-C10-O1	-2.51	104.10	110.69
21	P	316	DMU	O7-C3-C2	2.49	113.57	107.23
21	P	319	DMU	C10-C5-C7	2.49	115.25	110.01
21	D	201	DMU	C2-C3-C4	-2.48	105.42	110.93
21	A	611	DMU	O3-C5-C7	2.48	116.23	110.38
21	A	622	DMU	O5-C6-C1	2.47	115.45	110.37
14	N	602[A]	HEA	C4A-NA-C1A	-2.47	101.79	105.82
14	N	602[B]	HEA	C4A-NA-C1A	-2.47	101.79	105.82
21	Z	101	DMU	O3-C5-C7	2.46	116.18	110.38
21	A	622	DMU	C10-O1-C9	2.45	118.50	113.72
14	N	602[A]	HEA	C1D-ND-C4D	-2.43	102.33	105.21
14	N	602[B]	HEA	C1D-ND-C4D	-2.43	102.33	105.21
14	A	602	HEA	C13-C12-C11	-2.43	110.51	114.39
21	D	201	DMU	C11-C9-C8	-2.41	107.11	113.02
21	P	316	DMU	C57-C4-C3	-2.40	106.62	113.38
14	N	603	HEA	CBA-CAA-C2A	-2.40	105.91	112.53
21	Q	201	DMU	O3-C5-C7	2.39	116.02	110.38
14	N	603	HEA	CHD-C1D-C2D	-2.38	120.18	126.95
14	A	602	HEA	C4B-C3B-C2B	-2.38	103.44	107.44
21	A	622	DMU	O3-C5-C10	2.38	115.75	110.08
21	P	318	DMU	C6-C1-C2	2.37	115.00	110.01
26	P	306	CHD	C15-C14-C13	2.37	105.84	103.54
21	C	319	DMU	O3-C5-C10	2.37	115.71	110.08
14	N	603	HEA	CMB-C2B-C1B	2.36	128.72	125.03
14	N	603	HEA	OMA-CMA-C3A	-2.35	120.32	125.62
21	C	318	DMU	O5-C6-C1	2.32	115.13	110.37
21	A	611	DMU	C10-C5-C7	2.31	114.87	110.01
14	N	602[A]	HEA	O1A-CGA-CBA	-2.31	115.78	123.09
14	N	602[B]	HEA	O1A-CGA-CBA	-2.31	115.78	123.09
14	A	602	HEA	CMC-C2C-C3C	2.30	131.96	126.55
14	N	602[A]	HEA	CMB-C2B-C1B	2.29	128.62	125.03
14	N	602[B]	HEA	CMB-C2B-C1B	2.29	128.62	125.03
24	P	304	PGV	O03-C19-O04	-2.29	117.89	123.63
14	N	603	HEA	C13-C12-C11	-2.29	110.73	114.39
19	Y	101	CDL	OB4-PB2-OB3	2.29	123.10	112.44
21	P	324	DMU	C7-C8-C9	-2.29	106.09	110.23
14	N	602[A]	HEA	CHC-C1C-C2C	-2.26	120.86	127.43
14	N	602[B]	HEA	CHC-C1C-C2C	-2.26	120.86	127.43
21	A	622	DMU	C10-C5-C7	2.25	114.73	110.01
14	N	603	HEA	C1D-ND-C4D	-2.25	102.55	105.21
19	P	305	CDL	OB4-PB2-OB3	2.24	122.89	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602[A]	HEA	CMC-C2C-C1C	2.24	128.83	125.42
14	N	602[B]	HEA	CMC-C2C-C1C	2.24	128.83	125.42
14	N	603	HEA	C20-C19-C18	-2.24	116.14	121.17
21	P	316	DMU	O5-C6-C1	2.23	114.96	110.37
14	N	603	HEA	C4C-NC-C1C	-2.23	102.19	105.82
21	Z	101	DMU	C10-O7-C3	-2.22	112.71	117.98
21	A	611	DMU	C18-O16-C6	2.22	117.47	113.68
21	B	309	DMU	C18-O16-C6	2.22	117.47	113.68
21	O	308	DMU	O5-C6-C1	2.21	114.92	110.37
14	N	603	HEA	CHC-C4B-C3B	-2.20	120.26	125.80
21	C	319	DMU	C10-C5-C7	2.18	114.60	110.01
21	P	319	DMU	O16-C6-C1	2.18	111.59	108.27
19	P	305	CDL	OA6-CA5-OA7	-2.18	118.61	123.70
14	A	601[A]	HEA	CHC-C1C-C2C	-2.18	121.11	127.43
14	A	601[B]	HEA	CHC-C1C-C2C	-2.18	121.11	127.43
14	N	603	HEA	CHB-C1B-NB	2.17	126.76	124.42
24	P	304	PGV	O01-C1-O02	-2.17	118.64	123.70
26	C	301	CHD	C22-C20-C17	-2.15	105.86	110.33
21	B	305	DMU	C3-C2-C1	-2.15	107.05	110.83
14	N	602[A]	HEA	C1D-C2D-C3D	-2.15	104.72	106.98
14	N	602[B]	HEA	C1D-C2D-C3D	-2.15	104.72	106.98
19	A	607	CDL	OA2-PA1-OA3	-2.14	100.44	108.94
14	A	602	HEA	OMA-CMA-C3A	-2.14	120.78	125.62
21	P	318	DMU	C2-C3-C4	-2.14	106.35	110.23
14	N	602[A]	HEA	CHA-C4D-ND	-2.14	122.12	124.42
14	N	602[B]	HEA	CHA-C4D-ND	-2.14	122.12	124.42
21	B	305	DMU	O5-C6-O16	2.13	115.08	110.04
21	N	610	DMU	O5-C6-C1	2.13	114.74	110.37
21	P	320	DMU	O3-C5-C7	2.12	115.38	110.38
14	N	602[A]	HEA	C25-C23-C24	2.12	119.48	114.59
21	N	610	DMU	O5-C4-C57	2.11	111.67	106.44
14	N	602[A]	HEA	O2D-CGD-CBD	2.11	120.67	114.00
14	N	602[B]	HEA	O2D-CGD-CBD	2.11	120.67	114.00
21	C	315	DMU	O3-C5-C10	2.11	115.10	110.08
19	A	607	CDL	OA6-CA4-CA3	-2.11	100.77	108.34
21	D	201	DMU	O3-C5-C7	2.09	115.31	110.38
19	C	304	CDL	OB4-PB2-OB3	2.09	122.17	112.44
26	P	306	CHD	C16-C17-C13	2.09	105.57	103.54
21	C	324	DMU	C10-C5-C7	2.09	114.40	110.01
21	M	101	DMU	C10-C5-C7	2.08	114.39	110.01
21	A	611	DMU	O5-C6-O16	2.07	114.94	110.04
14	N	602[B]	HEA	C21-C22-C23	-2.07	120.73	127.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	316	DMU	O5-C6-O16	-2.07	105.15	110.04
21	P	324	DMU	C11-C9-C8	2.07	118.11	113.02
14	N	602[B]	HEA	C21-C20-C19	-2.07	106.32	113.19
21	Q	201	DMU	O7-C3-C2	2.07	112.49	107.23
19	V	101	CDL	OA5-PA1-OA3	-2.06	100.76	108.94
21	C	324	DMU	O3-C5-C7	2.06	115.23	110.38
14	N	602[A]	HEA	O11-C11-C12	2.06	114.59	109.14
14	N	602[B]	HEA	O11-C11-C12	2.06	114.59	109.14
14	N	602[A]	HEA	O2A-CGA-CBA	2.05	120.47	114.00
14	N	602[B]	HEA	O2A-CGA-CBA	2.05	120.47	114.00
21	P	320	DMU	C10-O1-C9	-2.04	109.73	113.72
14	N	602[A]	HEA	C27-C19-C18	-2.03	118.41	123.63
14	N	603	HEA	C21-C20-C19	2.02	119.87	113.19
19	P	305	CDL	OA7-CA5-C11	2.02	131.66	123.78
21	P	324	DMU	O1-C9-C11	2.01	111.43	106.44
21	C	324	DMU	O3-C5-C10	2.01	114.87	110.08
21	C	317	DMU	C6-C1-C2	2.01	114.24	110.01
21	Q	201	DMU	C11-C9-C8	-2.00	108.11	113.02

There are no chirality outliers.

All (798) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C18-C19-C20-C21
14	A	601[A]	HEA	C27-C19-C20-C21
14	A	601[B]	HEA	C27-C19-C20-C21
19	A	607	CDL	C1-CA2-OA2-PA1
19	A	607	CDL	C11-CA5-OA6-CA4
19	A	607	CDL	CB2-OB2-PB2-OB3
19	A	607	CDL	CB2-OB2-PB2-OB5
19	A	607	CDL	CB3-OB5-PB2-OB2
19	A	607	CDL	CB3-OB5-PB2-OB3
19	A	607	CDL	CB3-OB5-PB2-OB4
19	A	607	CDL	C51-CB5-OB6-CB4
19	C	304	CDL	O1-C1-CB2-OB2
19	C	304	CDL	C1-CA2-OA2-PA1
19	C	304	CDL	CA3-OA5-PA1-OA2
19	C	304	CDL	CB3-OB5-PB2-OB4
19	C	304	CDL	OB7-CB5-OB6-CB4
19	C	304	CDL	C51-CB5-OB6-CB4
19	L	101	CDL	CB2-C1-CA2-OA2
19	L	101	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
19	L	101	CDL	CA2-OA2-PA1-OA4
19	L	101	CDL	CA2-OA2-PA1-OA5
19	L	101	CDL	CA3-OA5-PA1-OA2
19	L	101	CDL	CA3-OA5-PA1-OA3
19	L	101	CDL	CB2-OB2-PB2-OB3
19	L	101	CDL	CB2-OB2-PB2-OB5
19	L	101	CDL	C51-CB5-OB6-CB4
19	P	305	CDL	CA2-C1-CB2-OB2
19	P	305	CDL	C1-CA2-OA2-PA1
19	P	305	CDL	CA3-OA5-PA1-OA2
19	P	305	CDL	CA3-OA5-PA1-OA3
19	P	305	CDL	C11-CA5-OA6-CA4
19	P	305	CDL	CB2-OB2-PB2-OB4
19	P	305	CDL	OB7-CB5-OB6-CB4
19	V	101	CDL	CB3-OB5-PB2-OB2
19	V	101	CDL	CB3-OB5-PB2-OB3
19	V	101	CDL	CB3-OB5-PB2-OB4
19	Y	101	CDL	O1-C1-CB2-OB2
19	Y	101	CDL	CA3-OA5-PA1-OA2
19	Y	101	CDL	CA3-OA5-PA1-OA3
19	Y	101	CDL	C11-CA5-OA6-CA4
19	Y	101	CDL	CB2-OB2-PB2-OB3
19	Y	101	CDL	CB3-OB5-PB2-OB4
19	Y	101	CDL	C51-CB5-OB6-CB4
21	B	305	DMU	C1-C6-O16-C18
21	B	309	DMU	C19-C18-O16-C6
21	C	318	DMU	C1-C6-O16-C18
21	L	102	DMU	C19-C18-O16-C6
21	N	610	DMU	O5-C6-O16-C18
21	O	303	DMU	C19-C18-O16-C6
21	O	308	DMU	C19-C18-O16-C6
21	Z	102	DMU	C1-C6-O16-C18
26	C	305	CHD	C13-C17-C20-C21
26	C	305	CHD	C13-C17-C20-C22
26	C	305	CHD	C16-C17-C20-C21
29	T	101	PEK	C11-C12-C13-C14
29	T	101	PEK	C12-C13-C14-C15
19	Y	101	CDL	OA9-CA7-OA8-CA6
26	C	305	CHD	C16-C17-C20-C22
21	L	102	DMU	C3-C4-C57-O61
19	A	607	CDL	OA7-CA5-OA6-CA4
19	A	607	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
19	L	101	CDL	OB7-CB5-OB6-CB4
19	P	305	CDL	OA7-CA5-OA6-CA4
19	Y	101	CDL	OA7-CA5-OA6-CA4
19	P	305	CDL	C51-CB5-OB6-CB4
14	N	602[A]	HEA	C27-C19-C20-C21
14	A	601[B]	HEA	C18-C19-C20-C21
14	N	602[A]	HEA	C18-C19-C20-C21
21	T	103	DMU	O5-C4-C57-O61
21	B	309	DMU	C3-C4-C57-O61
21	L	102	DMU	O5-C4-C57-O61
19	V	101	CDL	OA7-CA5-OA6-CA4
19	Y	101	CDL	OB7-CB5-OB6-CB4
19	L	101	CDL	O1-C1-CA2-OA2
19	P	305	CDL	O1-C1-CB2-OB2
19	Y	101	CDL	C31-CA7-OA8-CA6
21	O	303	DMU	O5-C4-C57-O61
21	P	320	DMU	O6-C11-C9-O1
21	C	315	DMU	O6-C11-C9-C8
21	C	319	DMU	O6-C11-C9-C8
21	Q	201	DMU	O6-C11-C9-C8
21	Q	201	DMU	O6-C11-C9-O1
19	C	304	CDL	C11-CA5-OA6-CA4
19	V	101	CDL	C11-CA5-OA6-CA4
21	N	622	DMU	O5-C4-C57-O61
20	G	104	LFA	C9-C10-C11-C12
21	A	611	DMU	O6-C11-C9-C8
21	O	303	DMU	C3-C4-C57-O61
20	C	309	LFA	C12-C13-C14-C15
24	C	303	PGV	C28-C29-C30-C31
14	A	601[A]	HEA	C15-C16-C17-C18
14	N	602[A]	HEA	C15-C16-C17-C18
21	N	610	DMU	O6-C11-C9-C8
21	T	103	DMU	C3-C4-C57-O61
21	B	305	DMU	O5-C6-O16-C18
21	C	318	DMU	O5-C6-O16-C18
21	Q	201	DMU	O5-C6-O16-C18
21	Z	102	DMU	O5-C6-O16-C18
21	A	611	DMU	O6-C11-C9-O1
19	C	304	CDL	C31-CA7-OA8-CA6
19	P	305	CDL	C31-CA7-OA8-CA6
21	C	315	DMU	O5-C4-C57-O61
26	P	306	CHD	C17-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
21	B	309	DMU	O5-C4-C57-O61
24	A	621	PGV	C26-C27-C28-C29
19	C	304	CDL	OA7-CA5-OA6-CA4
19	C	304	CDL	CB2-C1-CA2-OA2
19	C	304	CDL	C71-CB7-OB8-CB6
19	L	101	CDL	C31-CA7-OA8-CA6
19	V	101	CDL	C31-CA7-OA8-CA6
20	C	309	LFA	C11-C10-C9-C8
20	P	301	LFA	C2-C3-C4-C5
20	P	310	LFA	C12-C13-C14-C15
21	P	316	DMU	C31-C34-C37-C40
21	C	315	DMU	C3-C4-C57-O61
21	N	622	DMU	C1-C6-O16-C18
21	T	103	DMU	C1-C6-O16-C18
19	A	607	CDL	C78-C79-C80-C81
21	C	315	DMU	O6-C11-C9-O1
21	P	320	DMU	C2-C3-O7-C10
19	P	305	CDL	CB5-C51-C52-C53
19	V	101	CDL	CA7-C31-C32-C33
21	J	101	DMU	C18-C19-C22-C25
19	C	304	CDL	OA9-CA7-OA8-CA6
19	C	304	CDL	OB9-CB7-OB8-CB6
19	L	101	CDL	OA9-CA7-OA8-CA6
19	P	305	CDL	OA9-CA7-OA8-CA6
19	L	101	CDL	C11-CA5-OA6-CA4
26	P	306	CHD	C21-C20-C22-C23
24	A	621	PGV	C23-C24-C25-C26
21	C	319	DMU	O6-C11-C9-O1
21	C	318	DMU	O6-C11-C9-O1
21	N	610	DMU	O6-C11-C9-O1
21	P	319	DMU	O6-C11-C9-O1
19	C	304	CDL	C57-C58-C59-C60
21	P	316	DMU	O5-C4-C57-O61
21	C	323	DMU	O16-C18-C19-C22
21	N	610	DMU	O16-C18-C19-C22
21	N	622	DMU	C3-C4-C57-O61
21	Z	102	DMU	O16-C18-C19-C22
21	P	320	DMU	C4-C3-O7-C10
19	Y	101	CDL	CA5-C11-C12-C13
19	V	101	CDL	OA9-CA7-OA8-CA6
21	Z	102	DMU	O5-C4-C57-O61
19	C	304	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
19	C	304	CDL	CB5-C51-C52-C53
19	V	101	CDL	CB7-C71-C72-C73
20	C	326	LFA	C9-C10-C11-C12
21	B	309	DMU	O5-C6-O16-C18
21	T	103	DMU	O5-C6-O16-C18
21	P	320	DMU	O6-C11-C9-C8
19	C	304	CDL	O1-C1-CA2-OA2
19	V	101	CDL	O1-C1-CB2-OB2
19	Y	101	CDL	O1-C1-CA2-OA2
19	C	304	CDL	CB7-C71-C72-C73
19	L	101	CDL	OA7-CA5-OA6-CA4
21	C	317	DMU	O16-C18-C19-C22
20	C	312	LFA	C1-C2-C3-C4
21	B	309	DMU	O16-C18-C19-C22
21	L	102	DMU	O16-C18-C19-C22
29	T	101	PEK	C7-C8-C9-C10
19	V	101	CDL	CA2-C1-CB2-OB2
19	Y	101	CDL	CB2-C1-CA2-OA2
20	P	301	LFA	C10-C11-C12-C13
21	P	319	DMU	C3-C4-C57-O61
21	C	318	DMU	O16-C18-C19-C22
20	P	308	LFA	C7-C8-C9-C10
21	C	319	DMU	C1-C6-O16-C18
21	O	303	DMU	C1-C6-O16-C18
29	T	101	PEK	C10-C11-C12-C13
19	L	101	CDL	CB5-C51-C52-C53
19	V	101	CDL	C1-CA2-OA2-PA1
21	C	319	DMU	O16-C18-C19-C22
26	C	305	CHD	C21-C20-C22-C23
21	C	323	DMU	C3-C4-C57-O61
20	P	311	LFA	C5-C6-C7-C8
20	P	313	LFA	C1-C2-C3-C4
21	N	622	DMU	O5-C6-O16-C18
19	C	304	CDL	C51-C52-C53-C54
20	P	310	LFA	C11-C10-C9-C8
21	P	319	DMU	C31-C34-C37-C40
24	C	303	PGV	C7-C8-C9-C10
19	V	101	CDL	C76-C77-C78-C79
19	V	101	CDL	C78-C79-C80-C81
20	C	311	LFA	C4-C5-C6-C7
21	C	323	DMU	C28-C31-C34-C37
29	T	101	PEK	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
19	V	101	CDL	C12-C13-C14-C15
19	V	101	CDL	C73-C74-C75-C76
20	O	301	LFA	C6-C7-C8-C9
20	P	301	LFA	C11-C12-C13-C14
21	C	315	DMU	C19-C22-C25-C28
19	L	101	CDL	C18-C19-C20-C21
19	Y	101	CDL	C16-C17-C18-C19
19	Y	101	CDL	C19-C20-C21-C22
19	Y	101	CDL	C73-C74-C75-C76
20	P	311	LFA	C7-C8-C9-C10
21	P	319	DMU	C25-C28-C31-C34
21	C	318	DMU	C19-C18-O16-C6
21	D	201	DMU	C19-C18-O16-C6
21	Q	201	DMU	C19-C18-O16-C6
21	Z	102	DMU	C19-C18-O16-C6
20	G	104	LFA	C3-C4-C5-C6
19	Y	101	CDL	C31-C32-C33-C34
19	Y	101	CDL	C77-C78-C79-C80
21	C	323	DMU	O5-C4-C57-O61
20	C	309	LFA	C5-C6-C7-C8
21	B	303	DMU	C19-C22-C25-C28
24	N	621	PGV	C26-C27-C28-C29
20	B	308	LFA	C13-C14-C15-C16
29	G	101	PEK	C16-C17-C18-C19
29	T	101	PEK	C1-C2-C3-C4
21	P	319	DMU	O5-C4-C57-O61
19	C	304	CDL	C71-C72-C73-C74
20	O	301	LFA	C13-C14-C15-C16
21	M	102	DMU	C25-C28-C31-C34
24	C	303	PGV	C13-C14-C15-C16
21	A	610	DMU	C28-C31-C34-C37
21	C	306	DMU	C18-C19-C22-C25
21	O	306	DMU	C22-C25-C28-C31
21	P	317	DMU	C28-C31-C34-C37
21	A	611	DMU	C3-C4-C57-O61
21	C	318	DMU	O5-C4-C57-O61
19	L	101	CDL	C52-C53-C54-C55
19	C	304	CDL	C72-C73-C74-C75
21	C	316	DMU	C28-C31-C34-C37
21	C	317	DMU	C28-C31-C34-C37
21	O	306	DMU	C25-C28-C31-C34
21	O	307	DMU	C18-C19-C22-C25

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Mol	Chain	Res	Type	Atoms
19	Y	101	CDL	C52-C53-C54-C55
21	A	623	DMU	C19-C22-C25-C28
24	C	303	PGV	C30-C31-C32-C33
21	C	317	DMU	C31-C34-C37-C40
21	Z	101	DMU	C22-C25-C28-C31
24	A	621	PGV	C29-C30-C31-C32
24	P	304	PGV	C7-C8-C9-C10
29	G	101	PEK	C34-C35-C36-C37
19	V	101	CDL	C17-C18-C19-C20
20	A	609	LFA	C11-C10-C9-C8
22	P	321	EDO	O1-C1-C2-O2
20	T	102	LFA	C3-C4-C5-C6
21	C	315	DMU	C28-C31-C34-C37
21	J	101	DMU	C25-C28-C31-C34
21	C	318	DMU	C31-C34-C37-C40
21	P	318	DMU	C31-C34-C37-C40
19	C	304	CDL	C35-C36-C37-C38
19	Y	101	CDL	C75-C76-C77-C78
19	L	101	CDL	C58-C59-C60-C61
20	C	312	LFA	C5-C6-C7-C8
19	Y	101	CDL	OB9-CB7-OB8-CB6
21	Z	101	DMU	O16-C18-C19-C22
19	Y	101	CDL	C63-C64-C65-C66
20	P	301	LFA	C7-C8-C9-C10
21	C	319	DMU	C25-C28-C31-C34
19	P	305	CDL	C54-C55-C56-C57
20	C	309	LFA	C3-C4-C5-C6
20	C	326	LFA	C10-C11-C12-C13
19	Y	101	CDL	C71-CB7-OB8-CB6
20	C	326	LFA	C4-C5-C6-C7
20	P	301	LFA	C6-C7-C8-C9
21	C	319	DMU	C31-C34-C37-C40
20	C	313	LFA	C4-C5-C6-C7
21	C	318	DMU	C19-C22-C25-C28
21	Z	102	DMU	C18-C19-C22-C25
20	B	308	LFA	C11-C12-C13-C14
24	P	304	PGV	C30-C31-C32-C33
19	A	607	CDL	C19-C20-C21-C22
19	P	305	CDL	C35-C36-C37-C38
20	B	308	LFA	C4-C5-C6-C7
21	P	318	DMU	C18-C19-C22-C25
19	P	305	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
24	N	621	PGV	C14-C15-C16-C17
20	O	301	LFA	C9-C10-C11-C12
20	O	302	LFA	C2-C3-C4-C5
20	T	102	LFA	C4-C5-C6-C7
21	O	303	DMU	O16-C18-C19-C22
19	V	101	CDL	C71-CB7-OB8-CB6
21	C	324	DMU	C22-C25-C28-C31
19	C	304	CDL	C75-C76-C77-C78
20	A	608	LFA	C6-C7-C8-C9
20	P	312	LFA	C10-C11-C12-C13
21	O	308	DMU	C34-C37-C40-C43
20	A	609	LFA	C6-C7-C8-C9
20	P	312	LFA	C4-C5-C6-C7
21	B	303	DMU	C18-C19-C22-C25
21	M	101	DMU	C19-C22-C25-C28
19	L	101	CDL	C59-C60-C61-C62
21	Z	103	DMU	C31-C34-C37-C40
21	B	309	DMU	C18-C19-C22-C25
19	Y	101	CDL	C61-C62-C63-C64
21	C	324	DMU	C28-C31-C34-C37
21	L	102	DMU	C22-C25-C28-C31
29	T	101	PEK	C22-C23-C24-C25
21	W	101	DMU	O16-C18-C19-C22
19	C	304	CDL	C23-C24-C25-C26
24	N	621	PGV	C29-C30-C31-C32
19	A	607	CDL	CA5-C11-C12-C13
21	O	303	DMU	C34-C37-C40-C43
19	L	101	CDL	C72-C73-C74-C75
19	V	101	CDL	C77-C78-C79-C80
21	P	316	DMU	O6-C11-C9-O1
19	C	304	CDL	C33-C34-C35-C36
19	L	101	CDL	C75-C76-C77-C78
21	C	315	DMU	C18-C19-C22-C25
20	P	310	LFA	C4-C5-C6-C7
21	T	103	DMU	C25-C28-C31-C34
21	A	611	DMU	C31-C34-C37-C40
19	V	101	CDL	OA6-CA4-CA6-OA8
24	A	621	PGV	C12-C13-C14-C15
20	C	314	LFA	C5-C6-C7-C8
21	Z	102	DMU	C31-C34-C37-C40
29	G	101	PEK	C28-C29-C30-C31
21	M	101	DMU	C22-C25-C28-C31

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Mol	Chain	Res	Type	Atoms
21	P	324	DMU	C4-C3-O7-C10
19	L	101	CDL	C37-C38-C39-C40
20	G	104	LFA	C11-C10-C9-C8
19	V	101	CDL	C74-C75-C76-C77
19	P	305	CDL	C75-C76-C77-C78
29	G	101	PEK	C26-C27-C28-C29
21	C	306	DMU	O16-C18-C19-C22
21	P	307	DMU	O16-C18-C19-C22
20	P	311	LFA	C6-C7-C8-C9
19	A	607	CDL	C12-C13-C14-C15
19	Y	101	CDL	C80-C81-C82-C83
20	P	308	LFA	C3-C4-C5-C6
21	P	320	DMU	C31-C34-C37-C40
21	Z	101	DMU	C25-C28-C31-C34
19	P	305	CDL	C53-C54-C55-C56
20	P	310	LFA	C3-C4-C5-C6
19	A	607	CDL	C76-C77-C78-C79
19	A	607	CDL	C17-C18-C19-C20
19	C	304	CDL	C22-C23-C24-C25
20	C	307	LFA	C3-C4-C5-C6
21	B	305	DMU	C31-C34-C37-C40
21	N	601	DMU	C19-C22-C25-C28
21	Q	201	DMU	C4-C3-O7-C10
21	A	623	DMU	C18-C19-C22-C25
21	C	323	DMU	C18-C19-C22-C25
19	Y	101	CDL	C13-C14-C15-C16
20	B	308	LFA	C10-C11-C12-C13
20	O	301	LFA	C11-C12-C13-C14
20	C	326	LFA	C7-C8-C9-C10
20	O	301	LFA	C11-C10-C9-C8
21	P	324	DMU	C22-C25-C28-C31
19	Y	101	CDL	C12-C13-C14-C15
20	C	310	LFA	C6-C7-C8-C9
24	P	304	PGV	C12-C13-C14-C15
29	T	101	PEK	C2-C3-C4-C5
20	P	312	LFA	C3-C4-C5-C6
21	B	303	DMU	O16-C18-C19-C22
21	O	306	DMU	O16-C18-C19-C22
21	O	307	DMU	O16-C18-C19-C22
21	P	324	DMU	O1-C10-O7-C3
19	P	305	CDL	CA7-C31-C32-C33
20	C	309	LFA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
21	C	317	DMU	C25-C28-C31-C34
19	A	607	CDL	C71-CB7-OB8-CB6
19	L	101	CDL	C12-C13-C14-C15
19	L	101	CDL	CB3-CB4-CB6-OB8
20	C	310	LFA	C5-C6-C7-C8
20	P	314	LFA	C5-C6-C7-C8
24	N	621	PGV	C11-C10-C9-C8
29	G	101	PEK	C15-C16-C17-C18
20	P	301	LFA	C4-C5-C6-C7
21	C	306	DMU	C31-C34-C37-C40
29	T	101	PEK	C17-C18-C19-C20
21	B	309	DMU	C31-C34-C37-C40
19	L	101	CDL	CA5-C11-C12-C13
20	C	311	LFA	C6-C7-C8-C9
21	C	323	DMU	C19-C22-C25-C28
21	B	304	DMU	C19-C22-C25-C28
21	P	320	DMU	C22-C25-C28-C31
20	P	308	LFA	C2-C3-C4-C5
19	P	305	CDL	C56-C57-C58-C59
19	V	101	CDL	OB9-CB7-OB8-CB6
19	Y	101	CDL	C76-C77-C78-C79
20	O	301	LFA	C4-C5-C6-C7
21	C	317	DMU	C19-C22-C25-C28
21	C	324	DMU	O16-C18-C19-C22
19	A	607	CDL	CA6-CA4-OA6-CA5
21	P	324	DMU	C2-C3-O7-C10
29	T	101	PEK	C15-C16-C17-C18
19	P	305	CDL	C13-C14-C15-C16
19	P	305	CDL	C71-C72-C73-C74
29	T	101	PEK	C4-C5-C6-C7
21	P	319	DMU	C4-C3-O7-C10
24	P	304	PGV	C24-C25-C26-C27
20	C	310	LFA	C3-C4-C5-C6
19	P	305	CDL	C71-CB7-OB8-CB6
21	C	319	DMU	C34-C37-C40-C43
21	P	318	DMU	C19-C22-C25-C28
21	P	319	DMU	C2-C3-O7-C10
19	L	101	CDL	C84-C85-C86-C87
20	A	608	LFA	C9-C10-C11-C12
20	P	314	LFA	C6-C7-C8-C9
19	P	305	CDL	C76-C77-C78-C79
20	C	310	LFA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
20	C	313	LFA	C2-C3-C4-C5
20	P	313	LFA	C3-C4-C5-C6
24	C	303	PGV	C25-C26-C27-C28
20	C	312	LFA	C11-C10-C9-C8
21	M	102	DMU	C22-C25-C28-C31
21	P	319	DMU	C34-C37-C40-C43
21	Z	102	DMU	C34-C37-C40-C43
19	Y	101	CDL	C57-C58-C59-C60
20	C	311	LFA	C10-C11-C12-C13
19	L	101	CDL	OB6-CB4-CB6-OB8
19	Y	101	CDL	C84-C85-C86-C87
21	C	315	DMU	C34-C37-C40-C43
20	C	326	LFA	C12-C13-C14-C15
21	N	609	DMU	C34-C37-C40-C43
21	Z	103	DMU	C22-C25-C28-C31
24	A	621	PGV	C30-C31-C32-C33
21	P	316	DMU	C3-C4-C57-O61
19	L	101	CDL	C22-C23-C24-C25
20	C	310	LFA	C1-C2-C3-C4
21	C	316	DMU	C31-C34-C37-C40
19	Y	101	CDL	C38-C39-C40-C41
20	C	308	LFA	C3-C4-C5-C6
21	A	611	DMU	O5-C4-C57-O61
20	C	314	LFA	C1-C2-C3-C4
20	B	308	LFA	C6-C7-C8-C9
19	Y	101	CDL	C64-C65-C66-C67
21	C	318	DMU	C34-C37-C40-C43
24	A	621	PGV	C31-C32-C33-C34
26	C	305	CHD	C17-C20-C22-C23
19	L	101	CDL	C74-C75-C76-C77
20	P	310	LFA	C1-C2-C3-C4
21	O	303	DMU	C31-C34-C37-C40
21	P	324	DMU	C3-C4-C57-O61
19	Y	101	CDL	C21-C22-C23-C24
21	Z	102	DMU	C25-C28-C31-C34
24	A	621	PGV	C28-C29-C30-C31
24	P	304	PGV	C11-C12-C13-C14
29	T	101	PEK	C14-C15-C16-C17
21	B	304	DMU	O16-C18-C19-C22
19	P	305	CDL	C57-C58-C59-C60
19	C	304	CDL	CA4-CA3-OA5-PA1
19	P	305	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
29	G	101	PEK	C25-C26-C27-C28
21	D	201	DMU	C4-C3-O7-C10
19	A	607	CDL	C15-C16-C17-C18
19	A	607	CDL	C16-C17-C18-C19
20	C	314	LFA	C11-C10-C9-C8
21	C	324	DMU	C31-C34-C37-C40
21	J	101	DMU	C34-C37-C40-C43
19	V	101	CDL	OB5-CB3-CB4-CB6
20	C	310	LFA	C4-C5-C6-C7
21	A	622	DMU	C25-C28-C31-C34
20	B	308	LFA	C14-C15-C16-C17
20	C	310	LFA	C11-C10-C9-C8
19	P	305	CDL	O1-C1-CA2-OA2
24	C	303	PGV	C14-C15-C16-C17
21	N	601	DMU	C34-C37-C40-C43
19	L	101	CDL	C80-C81-C82-C83
21	B	304	DMU	C28-C31-C34-C37
20	A	609	LFA	C2-C3-C4-C5
19	A	607	CDL	C18-C19-C20-C21
19	Y	101	CDL	C23-C24-C25-C26
20	B	308	LFA	C1-C2-C3-C4
21	O	307	DMU	C19-C22-C25-C28
19	A	607	CDL	CA2-C1-CB2-OB2
19	Y	101	CDL	C79-C80-C81-C82
19	C	304	CDL	CB3-CB4-CB6-OB8
19	P	305	CDL	CA3-CA4-CA6-OA8
19	P	305	CDL	CB3-CB4-CB6-OB8
19	V	101	CDL	CA3-CA4-CA6-OA8
20	P	311	LFA	C2-C3-C4-C5
21	A	610	DMU	C25-C28-C31-C34
19	A	607	CDL	OB9-CB7-OB8-CB6
21	P	324	DMU	O16-C18-C19-C22
21	C	319	DMU	C28-C31-C34-C37
20	P	312	LFA	C5-C6-C7-C8
19	V	101	CDL	C31-C32-C33-C34
19	Y	101	CDL	C53-C54-C55-C56
21	P	324	DMU	O6-C11-C9-C8
20	O	301	LFA	C14-C15-C16-C17
20	P	308	LFA	C5-C6-C7-C8
19	P	305	CDL	C82-C83-C84-C85
19	P	305	CDL	C33-C34-C35-C36
21	P	316	DMU	C19-C22-C25-C28

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Mol	Chain	Res	Type	Atoms
19	L	101	CDL	C76-C77-C78-C79
20	P	315	LFA	C9-C10-C11-C12
20	C	326	LFA	C6-C7-C8-C9
19	C	304	CDL	OB6-CB4-CB6-OB8
21	P	319	DMU	O6-C11-C9-C8
29	T	101	PEK	C11-C10-C9-C8
29	T	101	PEK	C9-C10-C11-C12
21	Q	201	DMU	C2-C3-O7-C10
21	P	324	DMU	C5-C10-O7-C3
19	P	305	CDL	CB7-C71-C72-C73
29	G	101	PEK	C29-C30-C31-C32
21	N	610	DMU	C31-C34-C37-C40
21	O	306	DMU	C19-C22-C25-C28
21	P	318	DMU	C22-C25-C28-C31
20	C	326	LFA	C11-C12-C13-C14
20	P	314	LFA	C9-C10-C11-C12
19	Y	101	CDL	CA7-C31-C32-C33
21	C	323	DMU	C22-C25-C28-C31
21	P	318	DMU	C28-C31-C34-C37
19	A	607	CDL	C71-C72-C73-C74
21	Q	201	DMU	C25-C28-C31-C34
24	A	621	PGV	C13-C14-C15-C16
21	L	102	DMU	C34-C37-C40-C43
19	V	101	CDL	C19-C20-C21-C22
20	C	307	LFA	C6-C7-C8-C9
19	C	304	CDL	C36-C37-C38-C39
19	C	304	CDL	CA2-C1-CB2-OB2
19	Y	101	CDL	CA2-C1-CB2-OB2
19	A	607	CDL	C73-C74-C75-C76
20	G	104	LFA	C10-C11-C12-C13
24	A	621	PGV	C11-C10-C9-C8
19	V	101	CDL	C32-C33-C34-C35
20	P	315	LFA	C10-C11-C12-C13
19	C	304	CDL	C73-C74-C75-C76
19	C	304	CDL	C13-C14-C15-C16
21	W	101	DMU	C28-C31-C34-C37
19	L	101	CDL	C15-C16-C17-C18
19	P	305	CDL	OB9-CB7-OB8-CB6
20	P	311	LFA	C11-C10-C9-C8
19	V	101	CDL	C20-C21-C22-C23
20	P	308	LFA	C11-C10-C9-C8
19	Y	101	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
21	C	315	DMU	C25-C28-C31-C34
21	B	305	DMU	C3-C4-C57-O61
20	P	314	LFA	C4-C5-C6-C7
19	P	305	CDL	C73-C74-C75-C76
19	V	101	CDL	OB5-CB3-CB4-OB6
19	Y	101	CDL	OA5-CA3-CA4-OA6
19	V	101	CDL	C18-C19-C20-C21
20	C	313	LFA	C9-C10-C11-C12
21	M	101	DMU	C25-C28-C31-C34
21	C	318	DMU	O6-C11-C9-C8
20	C	311	LFA	C11-C10-C9-C8
21	B	309	DMU	C28-C31-C34-C37
21	W	101	DMU	C25-C28-C31-C34
21	D	201	DMU	C2-C3-O7-C10
21	B	305	DMU	C18-C19-C22-C25
21	A	622	DMU	O6-C11-C9-O1
19	L	101	CDL	C36-C37-C38-C39
24	P	304	PGV	C27-C28-C29-C30
19	P	305	CDL	OB6-CB4-CB6-OB8
20	C	309	LFA	C4-C5-C6-C7
19	Y	101	CDL	C22-C23-C24-C25
21	L	102	DMU	C31-C34-C37-C40
21	Z	102	DMU	C22-C25-C28-C31
21	C	317	DMU	C1-C6-O16-C18
20	N	608	LFA	C6-C7-C8-C9
19	C	304	CDL	C12-C11-CA5-OA6
19	A	607	CDL	O1-C1-CA2-OA2
21	A	623	DMU	C25-C28-C31-C34
21	T	103	DMU	C22-C25-C28-C31
29	G	101	PEK	C27-C28-C29-C30
20	A	608	LFA	C7-C8-C9-C10
21	P	319	DMU	C28-C31-C34-C37
20	O	301	LFA	C5-C6-C7-C8
21	P	319	DMU	C5-C10-O7-C3
19	P	305	CDL	C59-C60-C61-C62
20	P	315	LFA	C1-C2-C3-C4
24	N	621	PGV	C15-C16-C17-C18
21	B	305	DMU	C19-C18-O16-C6
21	C	323	DMU	C19-C18-O16-C6
21	P	318	DMU	C19-C18-O16-C6
24	N	621	PGV	C12-C13-C14-C15
19	C	304	CDL	C79-C80-C81-C82

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Mol	Chain	Res	Type	Atoms
19	Y	101	CDL	C58-C59-C60-C61
19	Y	101	CDL	C32-C33-C34-C35
19	A	607	CDL	O1-C1-CB2-OB2
24	C	303	PGV	C02-C03-O11-P
24	P	304	PGV	C02-C03-O11-P
21	L	102	DMU	C19-C22-C25-C28
20	B	308	LFA	C12-C13-C14-C15
19	P	305	CDL	C21-C22-C23-C24
20	C	311	LFA	C3-C4-C5-C6
20	T	102	LFA	C5-C6-C7-C8
20	P	309	LFA	C1-C2-C3-C4
20	A	609	LFA	C11-C12-C13-C14
21	C	323	DMU	C34-C37-C40-C43
20	A	608	LFA	C2-C3-C4-C5
24	N	621	PGV	C31-C32-C33-C34
21	A	622	DMU	C22-C25-C28-C31
20	P	301	LFA	C9-C10-C11-C12
21	C	323	DMU	C25-C28-C31-C34
20	P	308	LFA	C6-C7-C8-C9
19	A	607	CDL	CA2-OA2-PA1-OA3
19	A	607	CDL	CA3-OA5-PA1-OA2
19	A	607	CDL	CA3-OA5-PA1-OA3
19	A	607	CDL	CB2-OB2-PB2-OB4
19	C	304	CDL	CA3-OA5-PA1-OA3
19	Y	101	CDL	CA3-OA5-PA1-OA4
19	Y	101	CDL	CB2-OB2-PB2-OB4
19	Y	101	CDL	CB2-OB2-PB2-OB5
19	Y	101	CDL	CB3-OB5-PB2-OB2
19	Y	101	CDL	CB3-OB5-PB2-OB3
19	L	101	CDL	C77-C78-C79-C80
19	V	101	CDL	C15-C16-C17-C18
20	O	302	LFA	C5-C6-C7-C8
21	B	305	DMU	O16-C18-C19-C22
19	V	101	CDL	C52-C51-CB5-OB6
21	P	324	DMU	C31-C34-C37-C40
21	P	316	DMU	C25-C28-C31-C34
24	C	303	PGV	C15-C16-C17-C18
19	C	304	CDL	C18-C19-C20-C21
19	C	304	CDL	C52-C53-C54-C55
19	P	305	CDL	C20-C21-C22-C23
20	C	309	LFA	C14-C15-C16-C17
21	P	324	DMU	C19-C22-C25-C28

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Mol	Chain	Res	Type	Atoms
21	P	319	DMU	O1-C10-O7-C3
21	P	307	DMU	C31-C34-C37-C40
21	B	304	DMU	C22-C25-C28-C31
20	O	302	LFA	C1-C2-C3-C4
21	N	601	DMU	C28-C31-C34-C37
21	N	601	DMU	O16-C18-C19-C22
21	P	316	DMU	O1-C10-O7-C3
21	L	102	DMU	C18-C19-C22-C25
20	C	307	LFA	C4-C5-C6-C7
20	O	301	LFA	C2-C3-C4-C5
19	V	101	CDL	OB6-CB4-CB6-OB8
19	P	305	CDL	C12-C11-CA5-OA6
21	C	318	DMU	C5-C10-O7-C3
21	B	305	DMU	C34-C37-C40-C43
21	P	320	DMU	C28-C31-C34-C37
19	L	101	CDL	C72-C71-CB7-OB8
19	L	101	CDL	C56-C57-C58-C59
21	A	622	DMU	C19-C22-C25-C28
29	G	101	PEK	C32-C33-C34-C35
22	A	613	EDO	O1-C1-C2-O2
22	R	201	EDO	O1-C1-C2-O2
21	T	103	DMU	C18-C19-C22-C25
19	Y	101	CDL	C72-C73-C74-C75
19	A	607	CDL	CB7-C71-C72-C73
19	A	607	CDL	C52-C51-CB5-OB6
21	C	317	DMU	C19-C18-O16-C6
21	J	101	DMU	O16-C18-C19-C22
21	P	319	DMU	C22-C25-C28-C31
19	P	305	CDL	CA4-CA3-OA5-PA1
21	O	303	DMU	C18-C19-C22-C25
19	P	305	CDL	C18-C19-C20-C21
20	P	315	LFA	C6-C7-C8-C9
21	Q	201	DMU	O5-C4-C57-O61
19	P	305	CDL	C78-C79-C80-C81
20	P	312	LFA	C7-C8-C9-C10
24	N	621	PGV	O03-C19-C20-C21
20	C	314	LFA	C10-C11-C12-C13
19	L	101	CDL	C62-C63-C64-C65
19	Y	101	CDL	OB6-CB4-CB6-OB8
19	V	101	CDL	C52-C51-CB5-OB7
21	N	610	DMU	C19-C22-C25-C28
21	W	101	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
21	C	318	DMU	O1-C10-O7-C3
29	T	101	PEK	C32-C33-C34-C35
19	Y	101	CDL	C1-CA2-OA2-PA1
19	L	101	CDL	C33-C34-C35-C36
21	Z	101	DMU	C34-C37-C40-C43
19	L	101	CDL	C60-C61-C62-C63
19	Y	101	CDL	C18-C19-C20-C21
29	T	101	PEK	C30-C31-C32-C33
26	G	102	CHD	C22-C23-C24-O25
19	C	304	CDL	C77-C78-C79-C80
21	M	102	DMU	C28-C31-C34-C37
20	O	301	LFA	C3-C4-C5-C6
19	C	304	CDL	C17-C18-C19-C20
21	C	315	DMU	O1-C10-O7-C3
21	A	622	DMU	C18-C19-C22-C25
26	B	307	CHD	C22-C23-C24-O25
24	C	303	PGV	C24-C25-C26-C27
14	A	602	HEA	CAD-CBD-CGD-O1D
26	C	305	CHD	C22-C23-C24-O25
21	C	318	DMU	C2-C3-O7-C10
24	P	304	PGV	C15-C16-C17-C18
20	C	309	LFA	C7-C8-C9-C10
21	C	315	DMU	C5-C10-O7-C3
21	P	316	DMU	C5-C10-O7-C3
20	A	608	LFA	C11-C10-C9-C8
19	L	101	CDL	C31-C32-C33-C34
19	Y	101	CDL	OA5-CA3-CA4-CA6
21	N	609	DMU	C31-C34-C37-C40
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
14	A	601[B]	HEA	CAD-CBD-CGD-O1D
14	A	602	HEA	CAD-CBD-CGD-O2D
26	B	307	CHD	C22-C23-C24-O26
26	P	306	CHD	C20-C22-C23-C24
20	C	307	LFA	C2-C3-C4-C5
19	A	607	CDL	OA6-CA4-CA6-OA8
14	A	602	HEA	CAA-CBA-CGA-O1A
26	G	102	CHD	C22-C23-C24-O26
21	C	324	DMU	O1-C10-O7-C3
29	G	101	PEK	C5-C6-C7-C8
29	G	101	PEK	C11-C12-C13-C14
20	N	608	LFA	C2-C3-C4-C5
21	N	601	DMU	C25-C28-C31-C34

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Mol	Chain	Res	Type	Atoms
21	B	309	DMU	C34-C37-C40-C43
21	C	324	DMU	C5-C10-O7-C3
20	G	104	LFA	C6-C7-C8-C9
20	P	310	LFA	C15-C16-C17-C18
21	A	623	DMU	C31-C34-C37-C40
19	L	101	CDL	C24-C25-C26-C27
14	A	602	HEA	CAA-CBA-CGA-O2A
21	A	622	DMU	C28-C31-C34-C37
20	C	311	LFA	C5-C6-C7-C8
20	P	301	LFA	C11-C10-C9-C8
20	P	313	LFA	C4-C5-C6-C7
21	A	610	DMU	C34-C37-C40-C43
21	A	611	DMU	C4-C3-O7-C10
14	N	603	HEA	CAA-CBA-CGA-O1A
26	C	301	CHD	C22-C23-C24-O26
26	P	306	CHD	C22-C23-C24-O26
24	A	621	PGV	O03-C19-C20-C21
20	G	104	LFA	C5-C6-C7-C8
14	N	602[A]	HEA	CAD-CBD-CGD-O1D
14	N	602[B]	HEA	CAD-CBD-CGD-O1D
21	P	324	DMU	O5-C4-C57-O61
14	N	603	HEA	CAD-CBD-CGD-O2D
29	T	101	PEK	C13-C14-C15-C16
21	P	324	DMU	C28-C31-C34-C37
26	C	305	CHD	C22-C23-C24-O26
19	L	101	CDL	C32-C33-C34-C35
21	A	611	DMU	C19-C22-C25-C28
26	P	302	CHD	C22-C23-C24-O26
21	C	319	DMU	C22-C25-C28-C31
19	V	101	CDL	CB4-CB3-OB5-PB2
14	N	603	HEA	CAA-CBA-CGA-O2A
19	Y	101	CDL	C34-C35-C36-C37
21	D	201	DMU	C28-C31-C34-C37
21	O	306	DMU	C31-C34-C37-C40
14	N	603	HEA	CAD-CBD-CGD-O1D
19	V	101	CDL	C72-C73-C74-C75
21	O	308	DMU	C1-C6-O16-C18
19	Y	101	CDL	C51-C52-C53-C54
19	L	101	CDL	C78-C79-C80-C81
21	P	324	DMU	O6-C11-C9-O1
26	C	301	CHD	C22-C23-C24-O25
29	T	101	PEK	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
21	A	611	DMU	C2-C3-O7-C10
21	D	201	DMU	O5-C6-O16-C18
26	P	306	CHD	C22-C23-C24-O25
26	P	302	CHD	C22-C23-C24-O25
19	Y	101	CDL	C14-C15-C16-C17
21	O	303	DMU	C28-C31-C34-C37
19	C	304	CDL	C78-C79-C80-C81
21	M	102	DMU	C31-C34-C37-C40
19	C	304	CDL	C52-C51-CB5-OB6
19	P	305	CDL	C72-C71-CB7-OB8
19	V	101	CDL	C72-C71-CB7-OB8
24	A	621	PGV	C15-C16-C17-C18
20	N	608	LFA	C7-C8-C9-C10
20	O	301	LFA	C7-C8-C9-C10
21	L	102	DMU	C28-C31-C34-C37
21	C	319	DMU	C18-C19-C22-C25
21	Q	201	DMU	C22-C25-C28-C31
19	Y	101	CDL	C60-C61-C62-C63
29	T	101	PEK	C2-C1-O01-C02
21	P	320	DMU	O5-C4-C57-O61
21	C	315	DMU	C4-C3-O7-C10
20	O	301	LFA	C1-C2-C3-C4
19	Y	101	CDL	C62-C63-C64-C65
19	Y	101	CDL	CB5-C51-C52-C53
14	A	601[A]	HEA	C16-C17-C18-C19
19	C	304	CDL	C12-C11-CA5-OA7
24	C	303	PGV	C22-C23-C24-C25
19	L	101	CDL	C64-C65-C66-C67
19	V	101	CDL	C75-C76-C77-C78
19	C	304	CDL	C55-C56-C57-C58
21	M	102	DMU	C34-C37-C40-C43
24	P	304	PGV	C28-C29-C30-C31
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
14	A	601[B]	HEA	CAD-CBD-CGD-O2D
20	P	310	LFA	C13-C14-C15-C16
21	C	319	DMU	O5-C6-O16-C18
21	C	323	DMU	C31-C34-C37-C40
19	L	101	CDL	C54-C55-C56-C57
19	A	607	CDL	C72-C71-CB7-OB8
19	P	305	CDL	C52-C51-CB5-OB6
21	C	315	DMU	C2-C3-O7-C10
19	C	304	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
21	P	318	DMU	C25-C28-C31-C34
21	C	318	DMU	C4-C3-O7-C10
19	A	607	CDL	C75-C76-C77-C78
20	P	314	LFA	C2-C3-C4-C5
19	C	304	CDL	C74-C75-C76-C77
21	O	306	DMU	C28-C31-C34-C37
19	L	101	CDL	C34-C35-C36-C37
24	C	303	PGV	C29-C30-C31-C32
24	C	303	PGV	C05-C04-O12-P
19	P	305	CDL	C72-C71-CB7-OB9
19	A	607	CDL	C13-C14-C15-C16
19	P	305	CDL	C52-C51-CB5-OB7
14	N	602[A]	HEA	CAD-CBD-CGD-O2D
14	N	602[B]	HEA	CAD-CBD-CGD-O2D
19	V	101	CDL	C72-C71-CB7-OB9
19	C	304	CDL	C52-C51-CB5-OB7
21	P	317	DMU	C34-C37-C40-C43
21	C	318	DMU	C3-C4-C57-O61
20	P	308	LFA	C1-C2-C3-C4
20	P	311	LFA	C4-C5-C6-C7
19	L	101	CDL	C32-C31-CA7-OA8
19	L	101	CDL	C32-C31-CA7-OA9
29	T	101	PEK	O01-C1-C2-C3

There are no ring outliers.

48 monomers are involved in 129 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	D	201	DMU	3	0
20	N	608	LFA	6	0
19	L	101	CDL	6	0
14	N	603	HEA	2	0
20	P	308	LFA	2	0
21	C	324	DMU	3	0
24	N	621	PGV	1	0
20	C	309	LFA	1	0
21	O	303	DMU	1	0
14	N	602[A]	HEA	4	0
22	N	615	EDO	1	0
14	A	601[A]	HEA	4	0
26	G	102	CHD	1	0
20	C	307	LFA	1	0

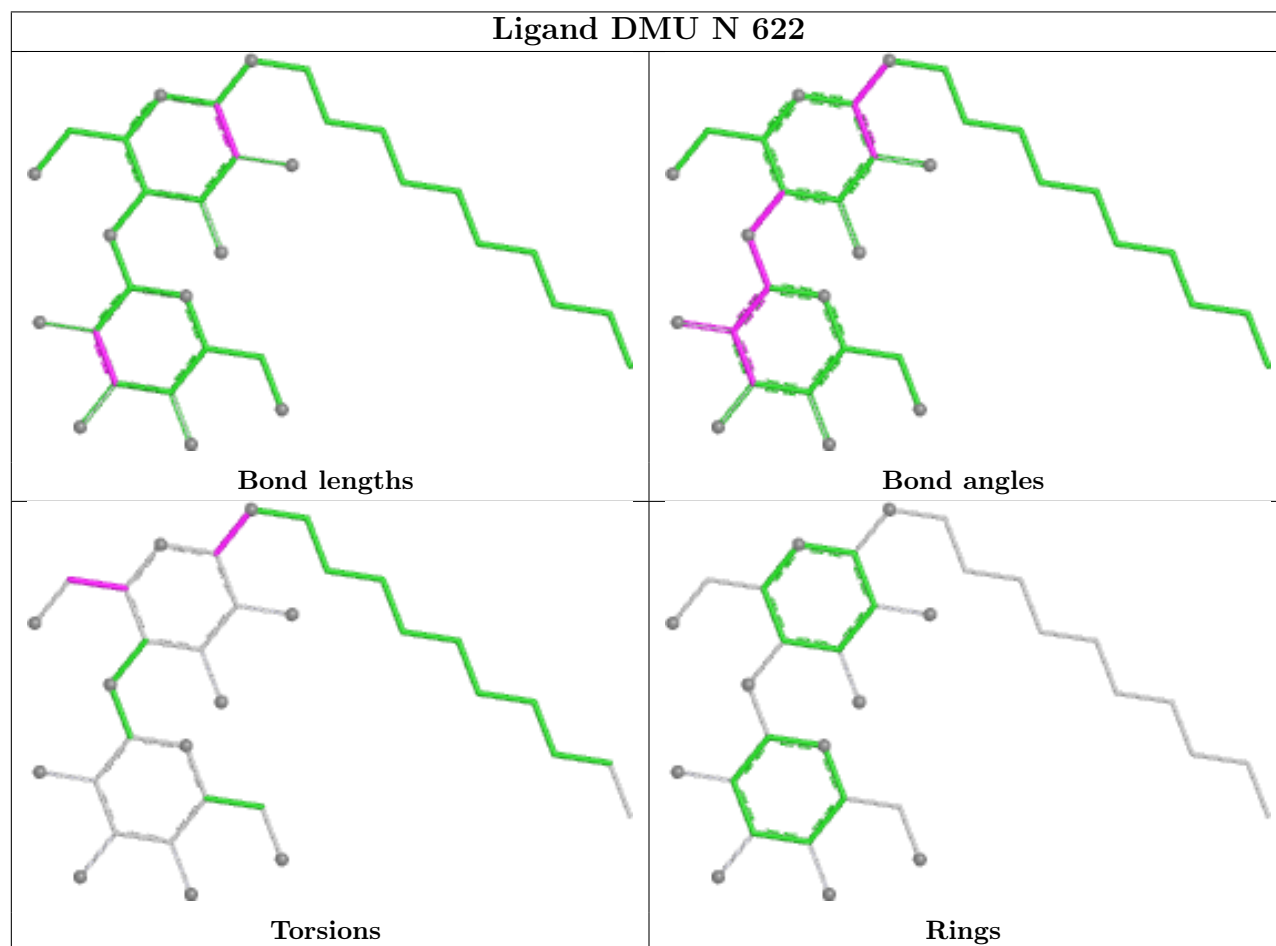
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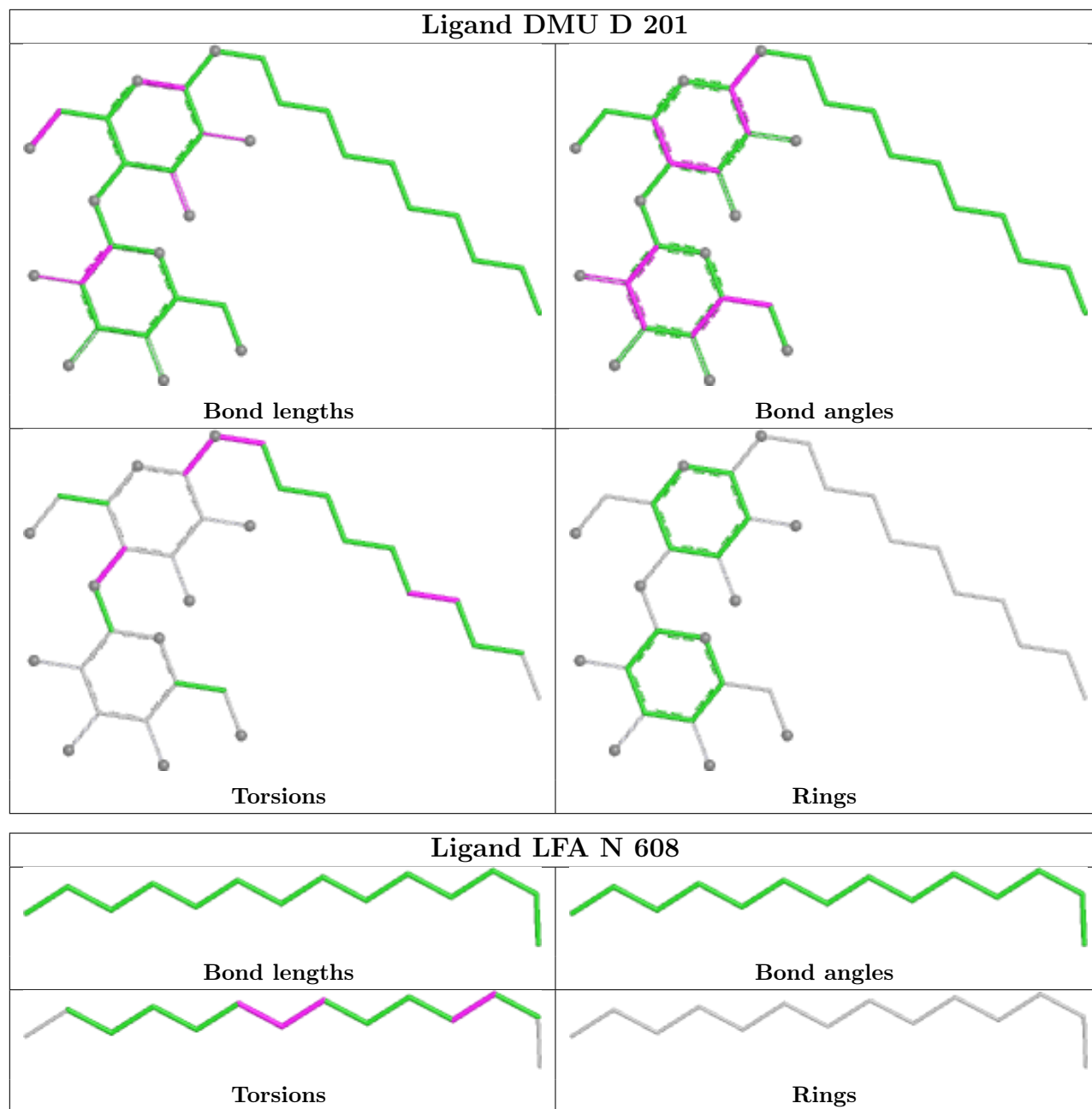
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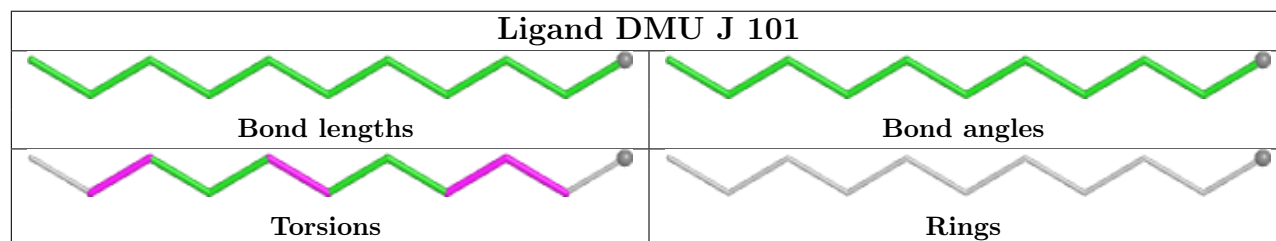
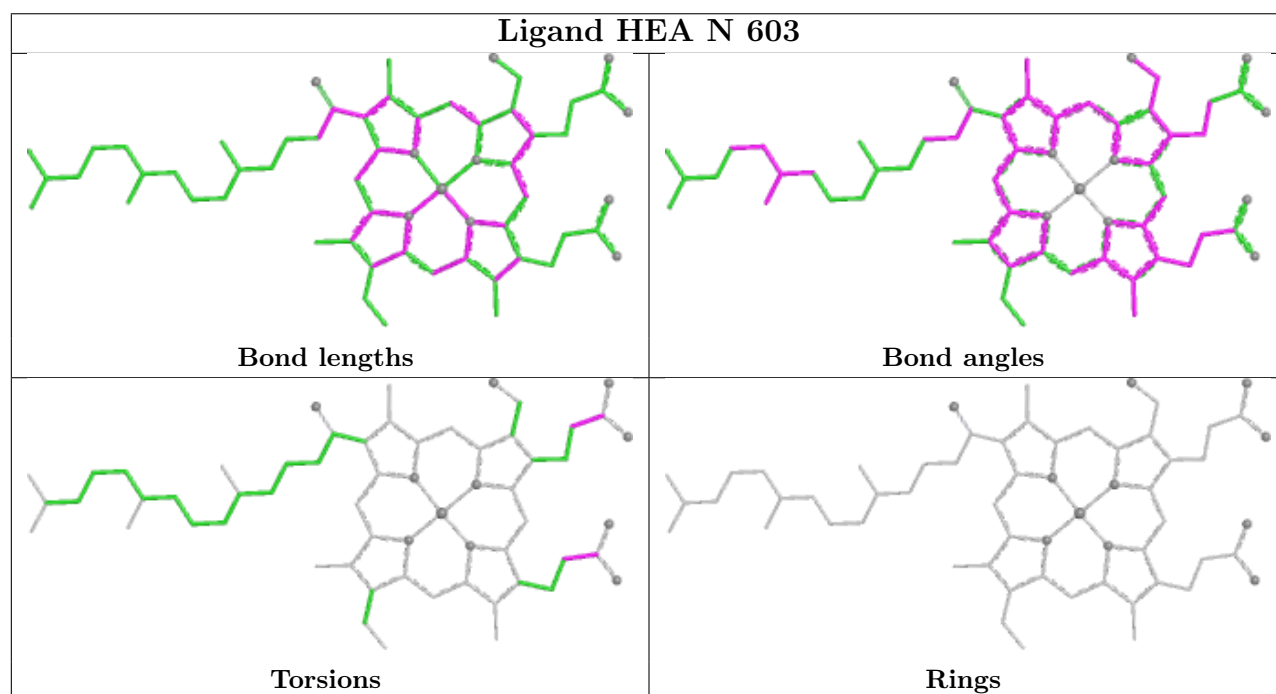
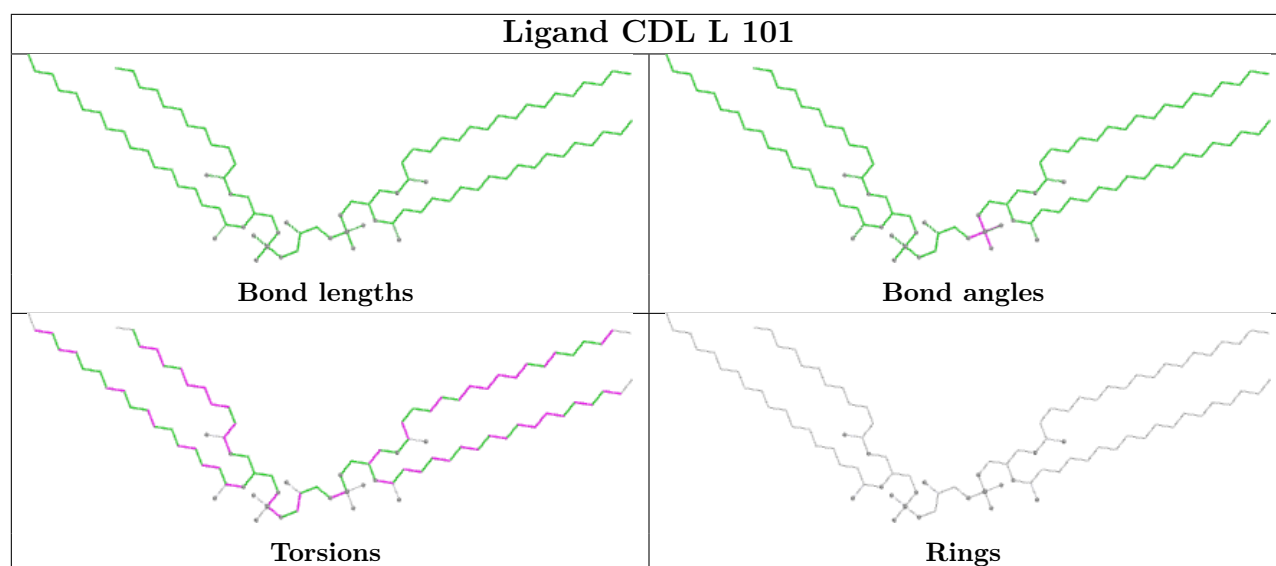
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	Q	201	DMU	1	0
21	Z	102	DMU	4	0
21	P	324	DMU	7	0
21	C	323	DMU	1	0
21	P	320	DMU	1	0
21	A	611	DMU	1	0
20	P	314	LFA	2	0
21	A	622	DMU	1	0
20	P	310	LFA	2	0
19	Y	101	CDL	5	0
29	T	101	PEK	4	0
20	G	104	LFA	6	0
19	V	101	CDL	2	0
18	N	607	PER	1	0
26	C	305	CHD	2	0
21	B	305	DMU	2	0
20	C	312	LFA	2	0
21	M	102	DMU	1	0
24	C	303	PGV	1	0
19	C	304	CDL	19	0
18	A	606	PER	1	0
20	B	308	LFA	1	0
26	P	306	CHD	2	0
21	B	309	DMU	1	0
19	P	305	CDL	8	0
20	A	608	LFA	5	0
20	A	609	LFA	5	0
21	C	319	DMU	1	0
20	O	301	LFA	1	0
20	P	313	LFA	2	0
20	P	315	LFA	1	0
20	C	313	LFA	1	0
14	N	602[B]	HEA	1	0
21	C	318	DMU	1	0

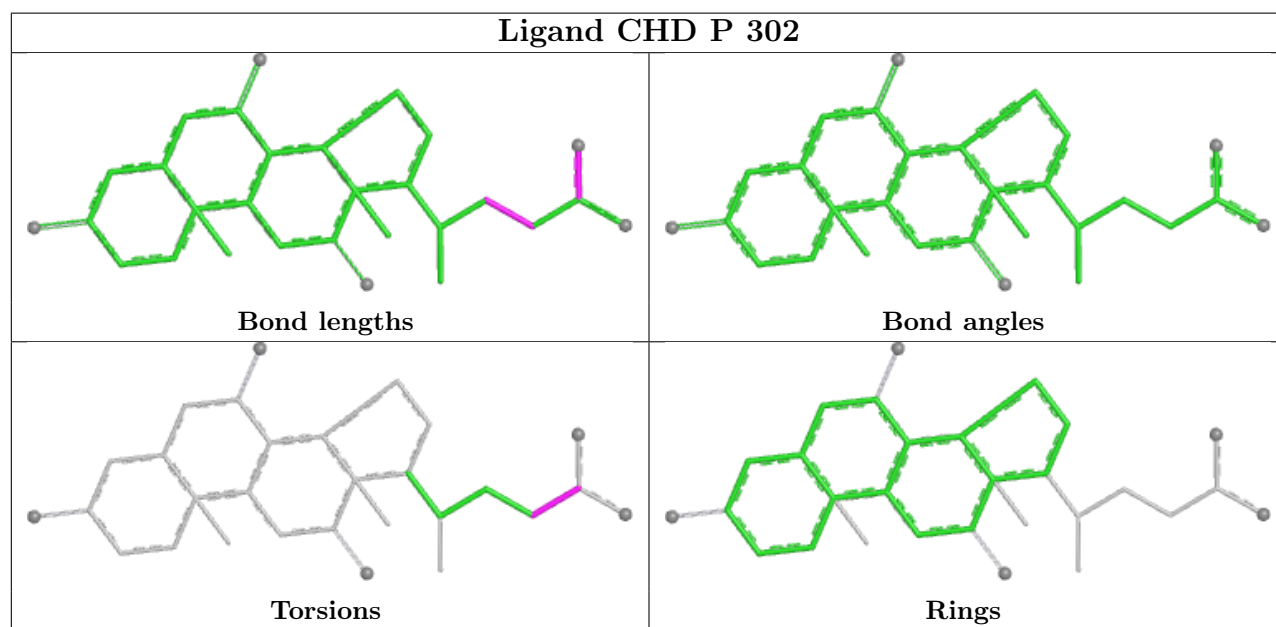
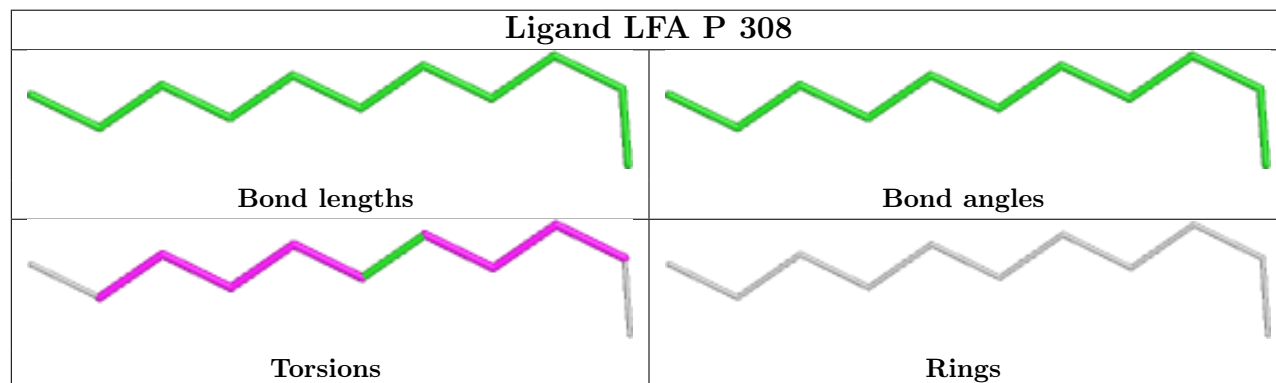
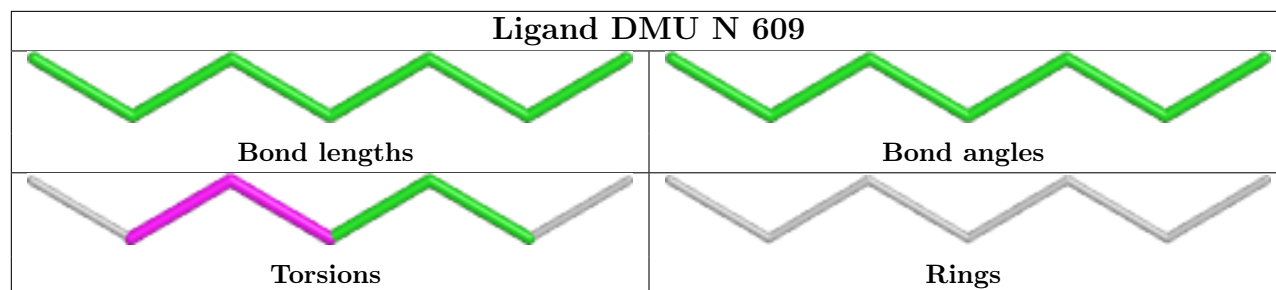
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

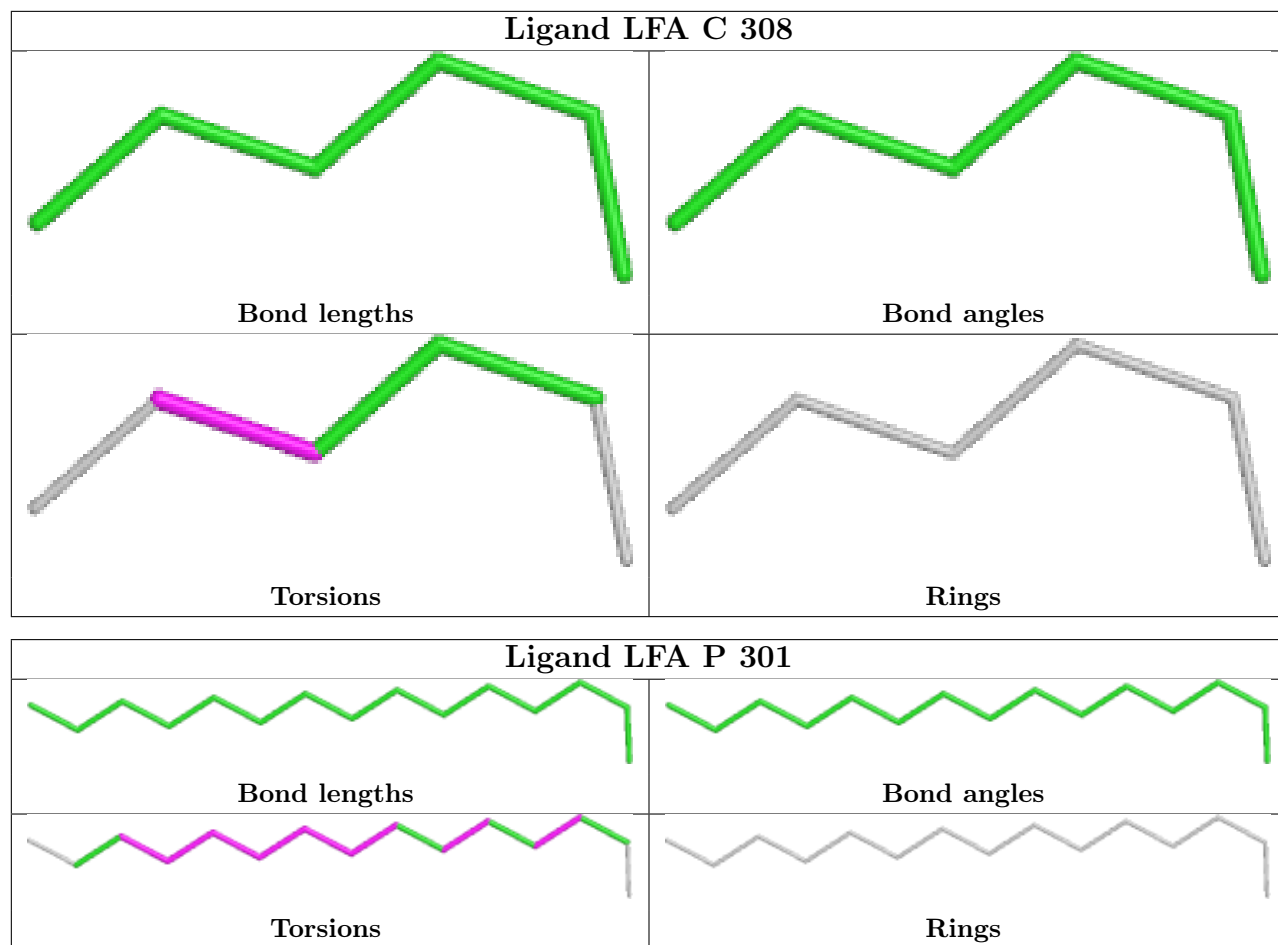
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

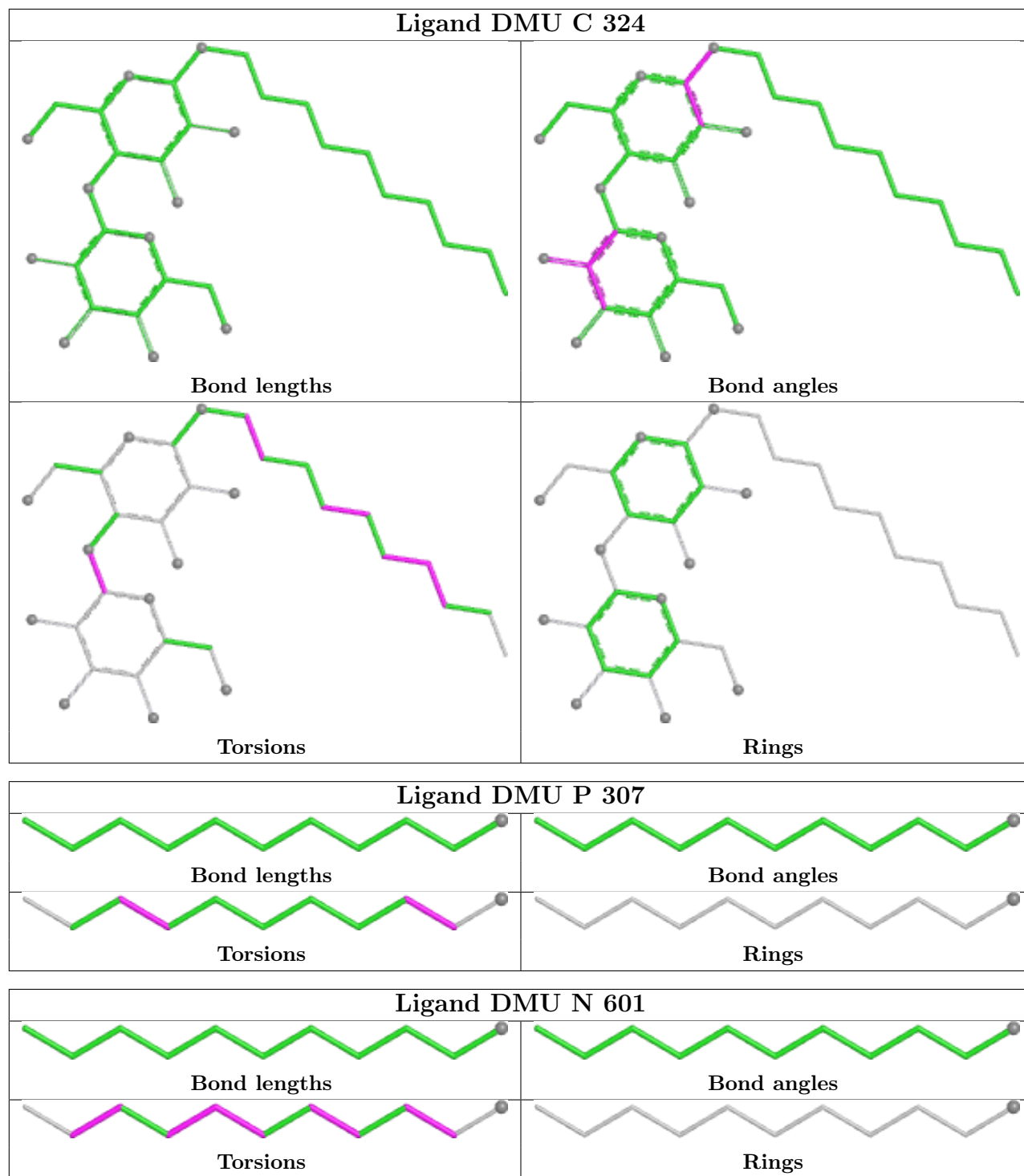


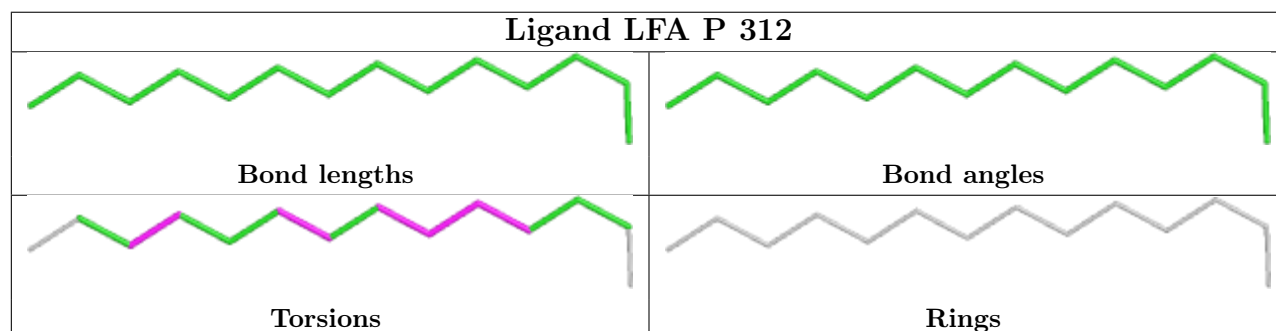
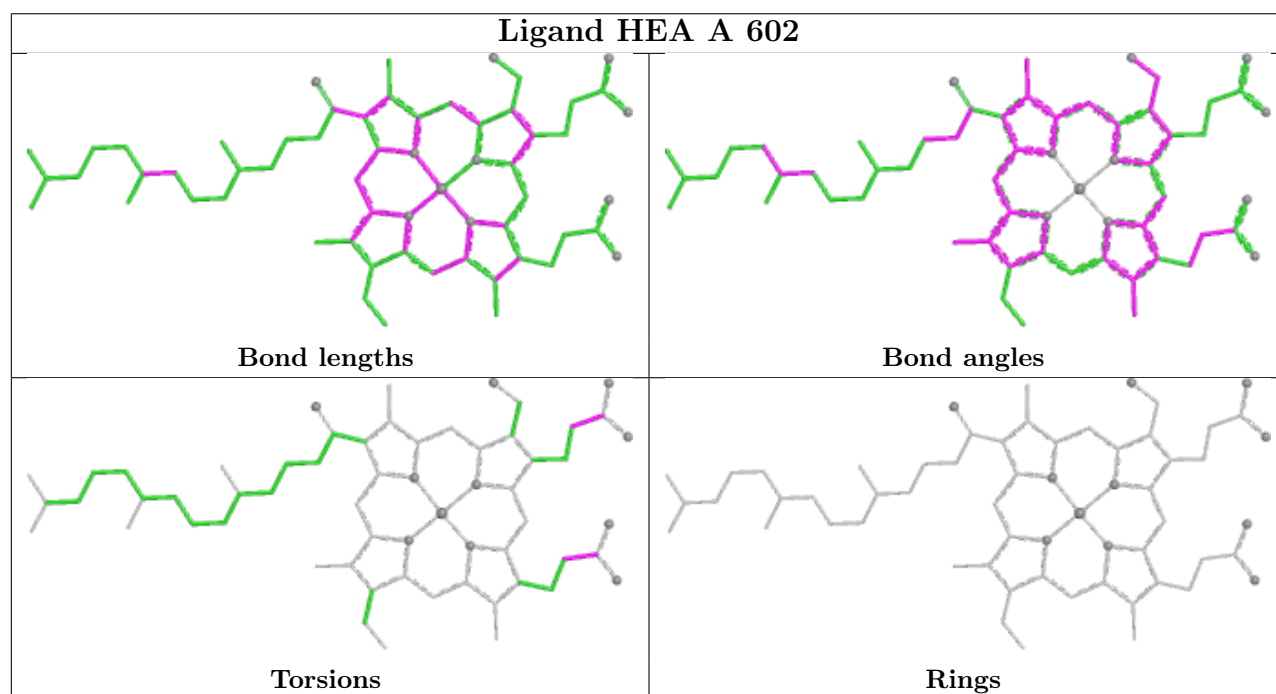
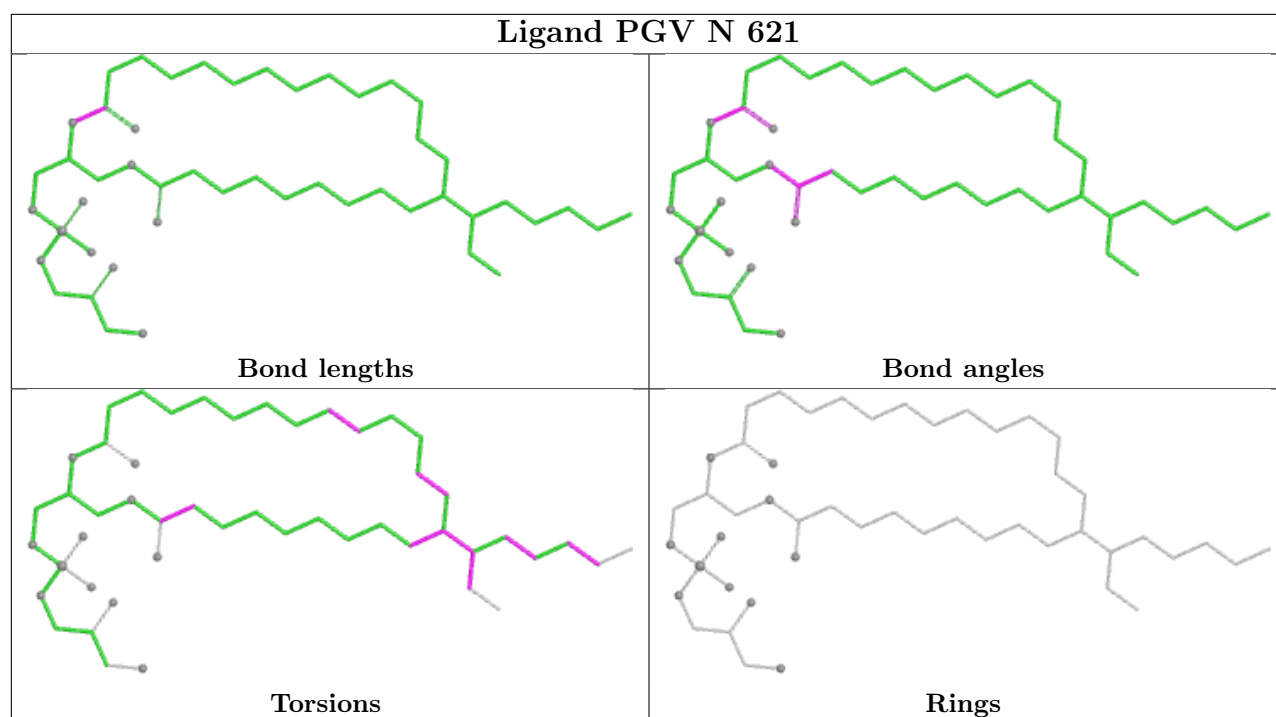


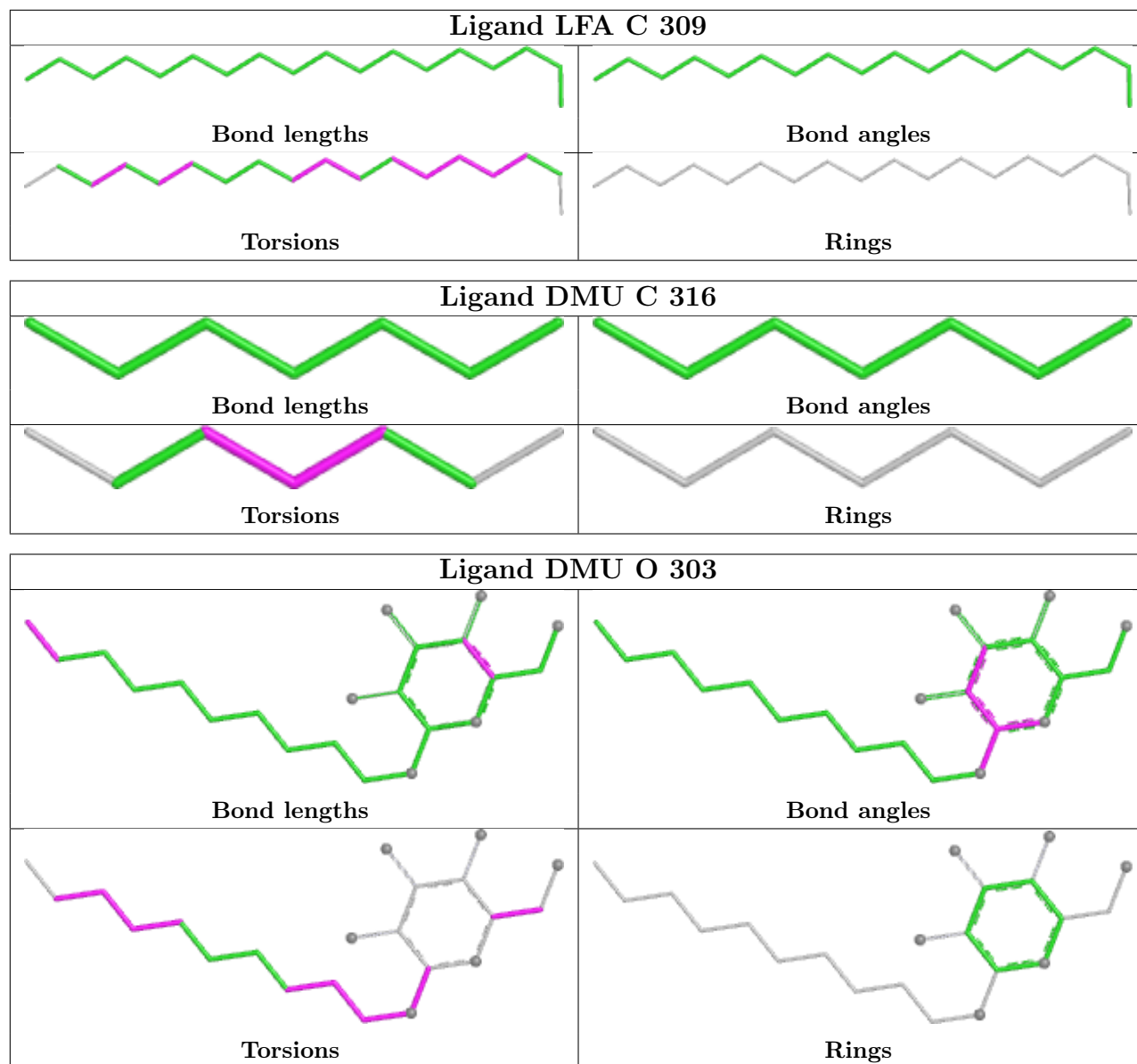


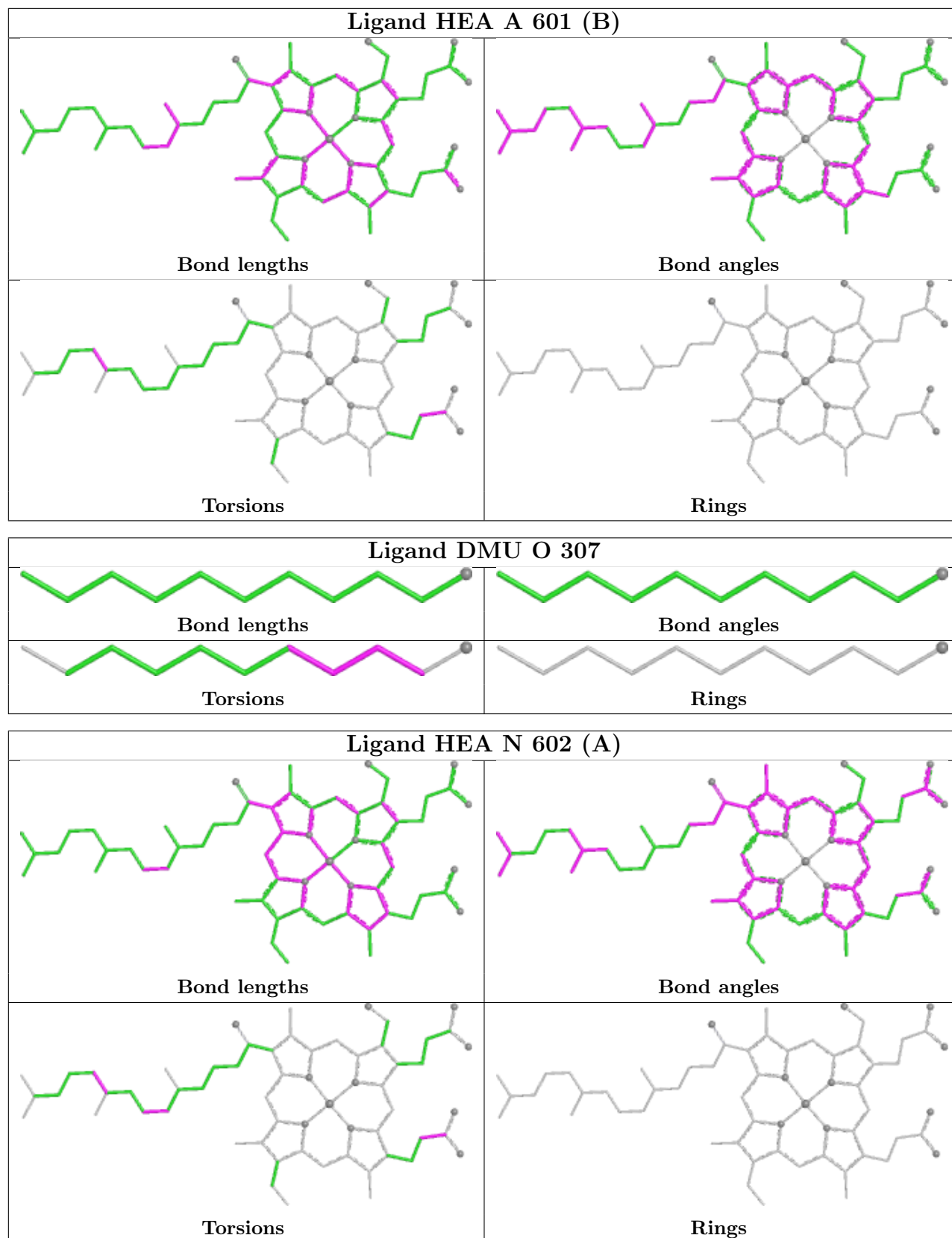


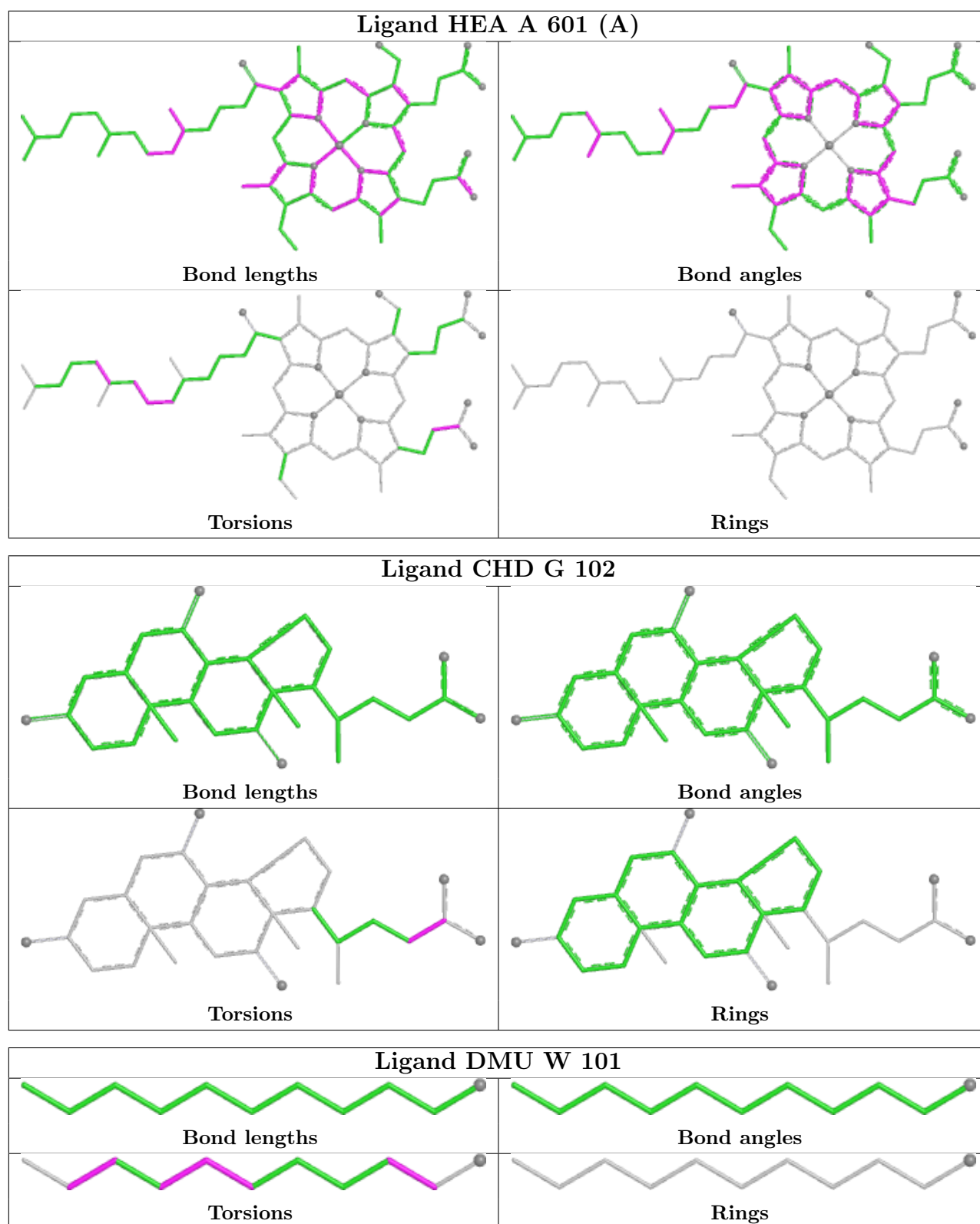


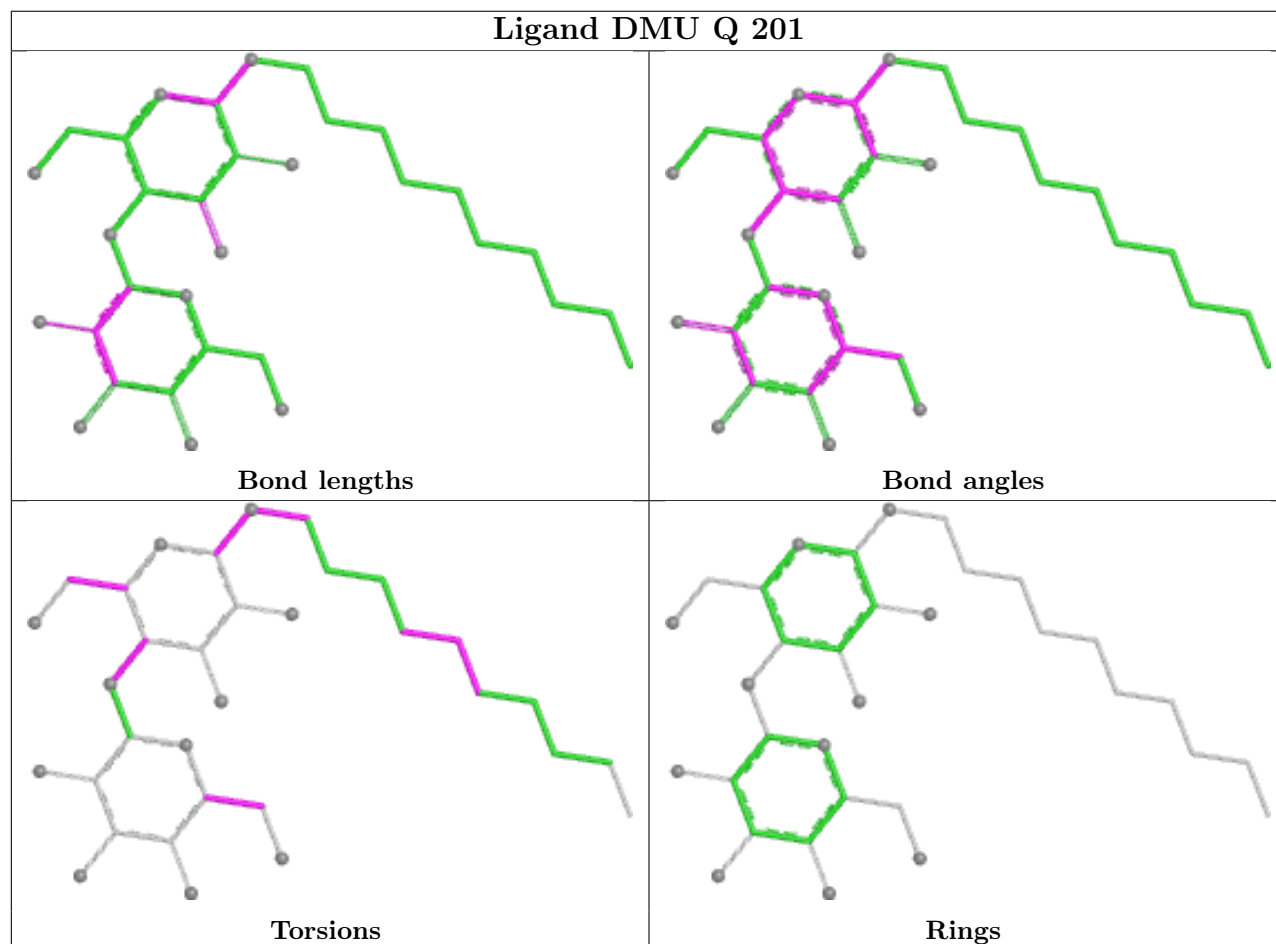
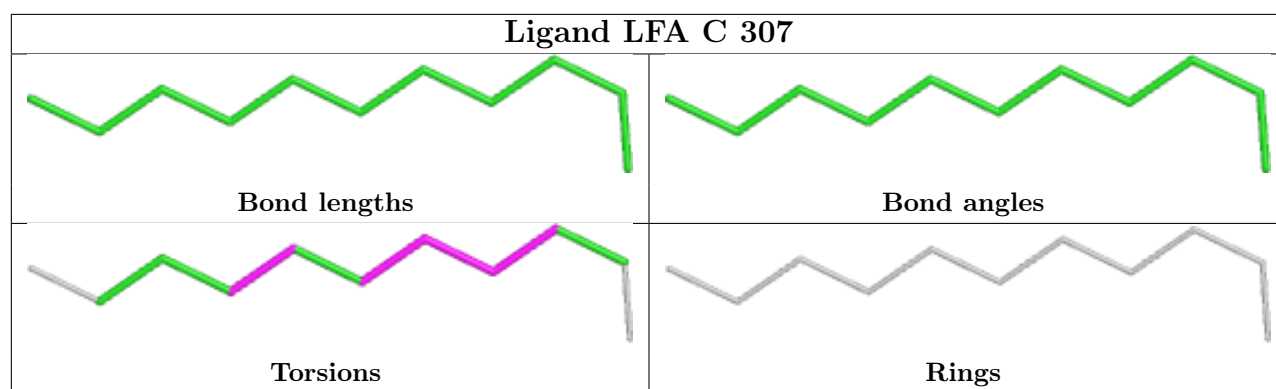


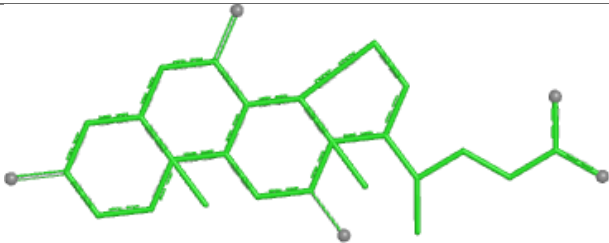
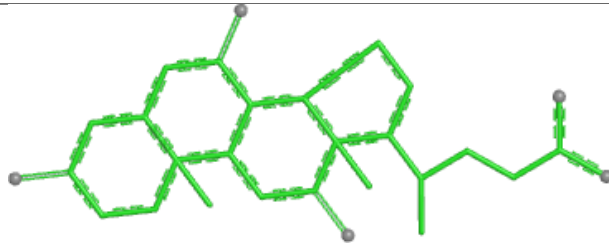
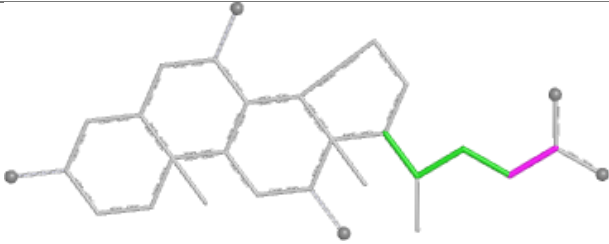
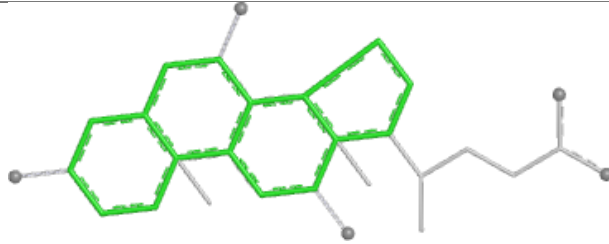


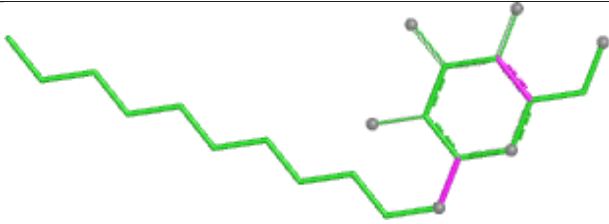
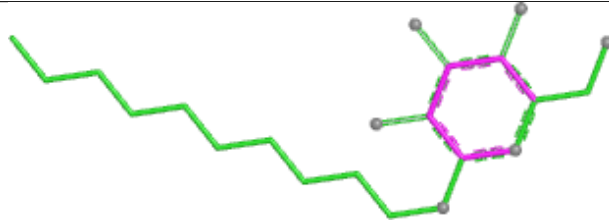




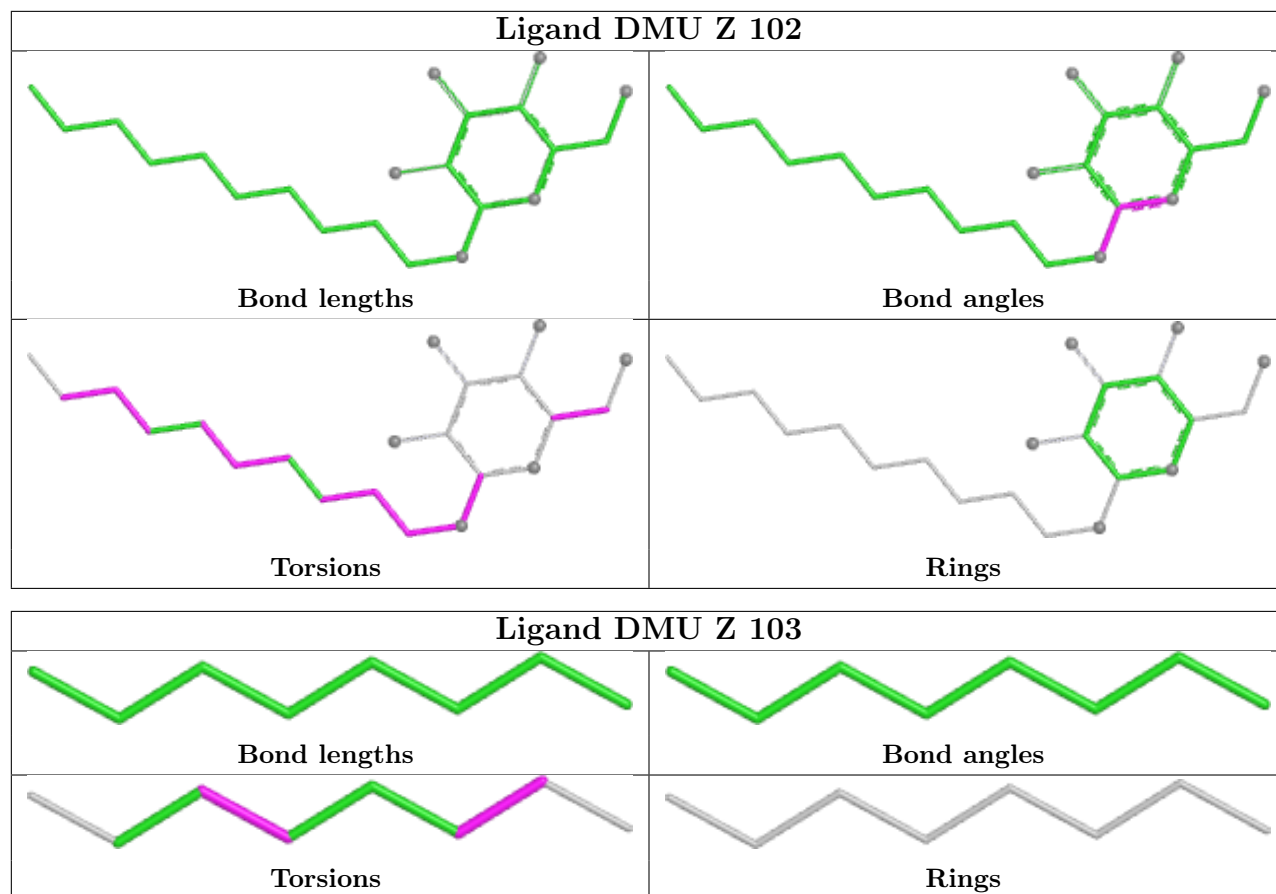


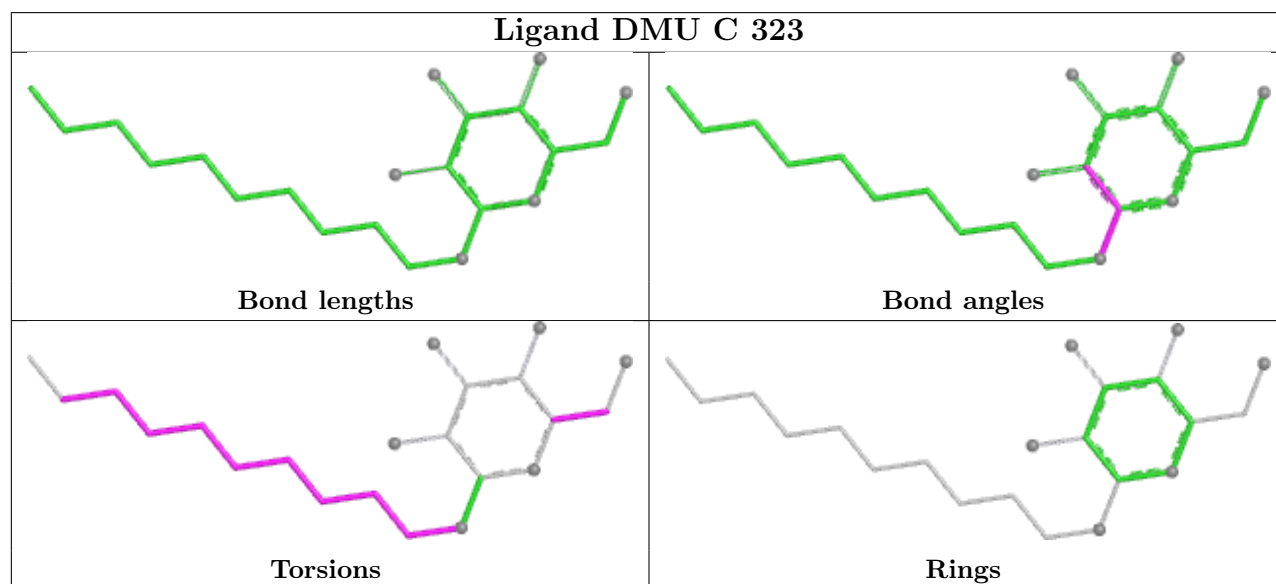
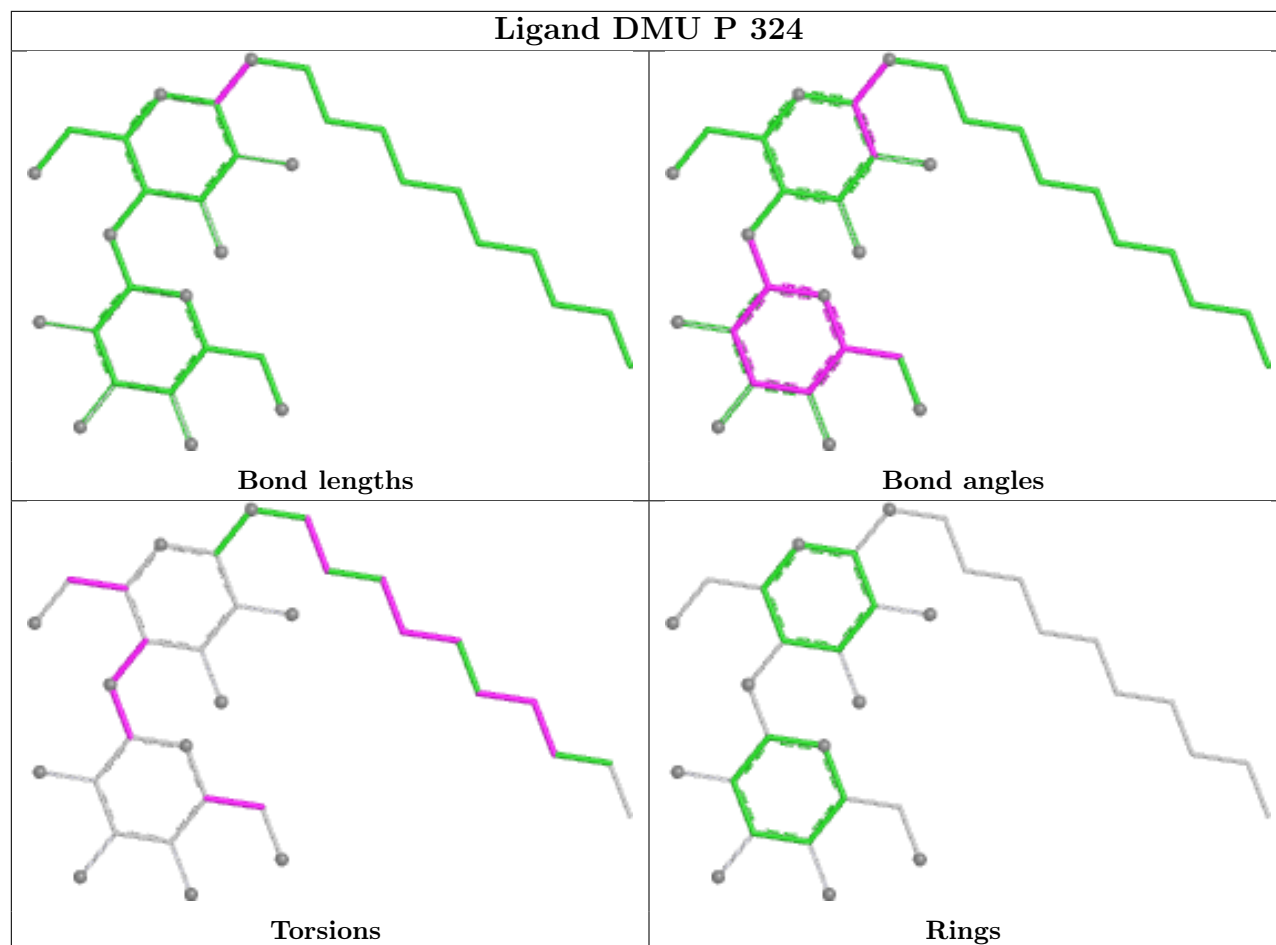


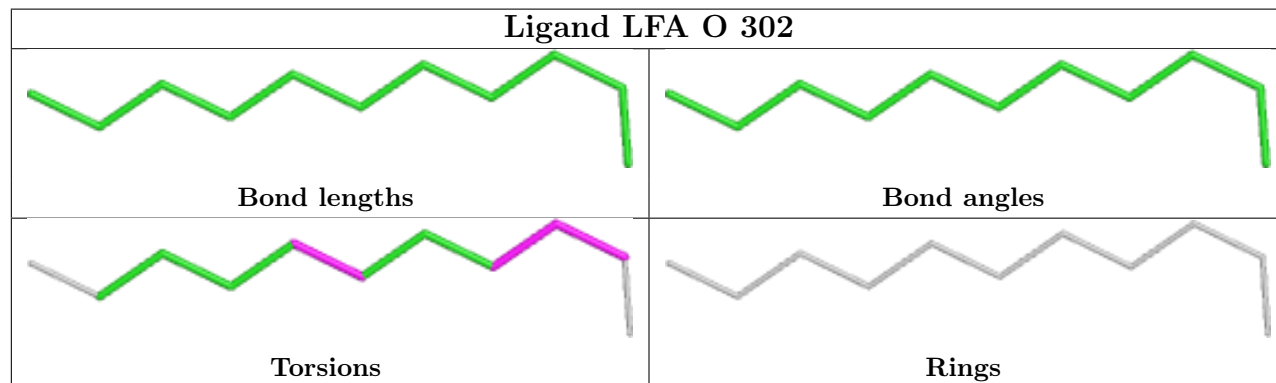
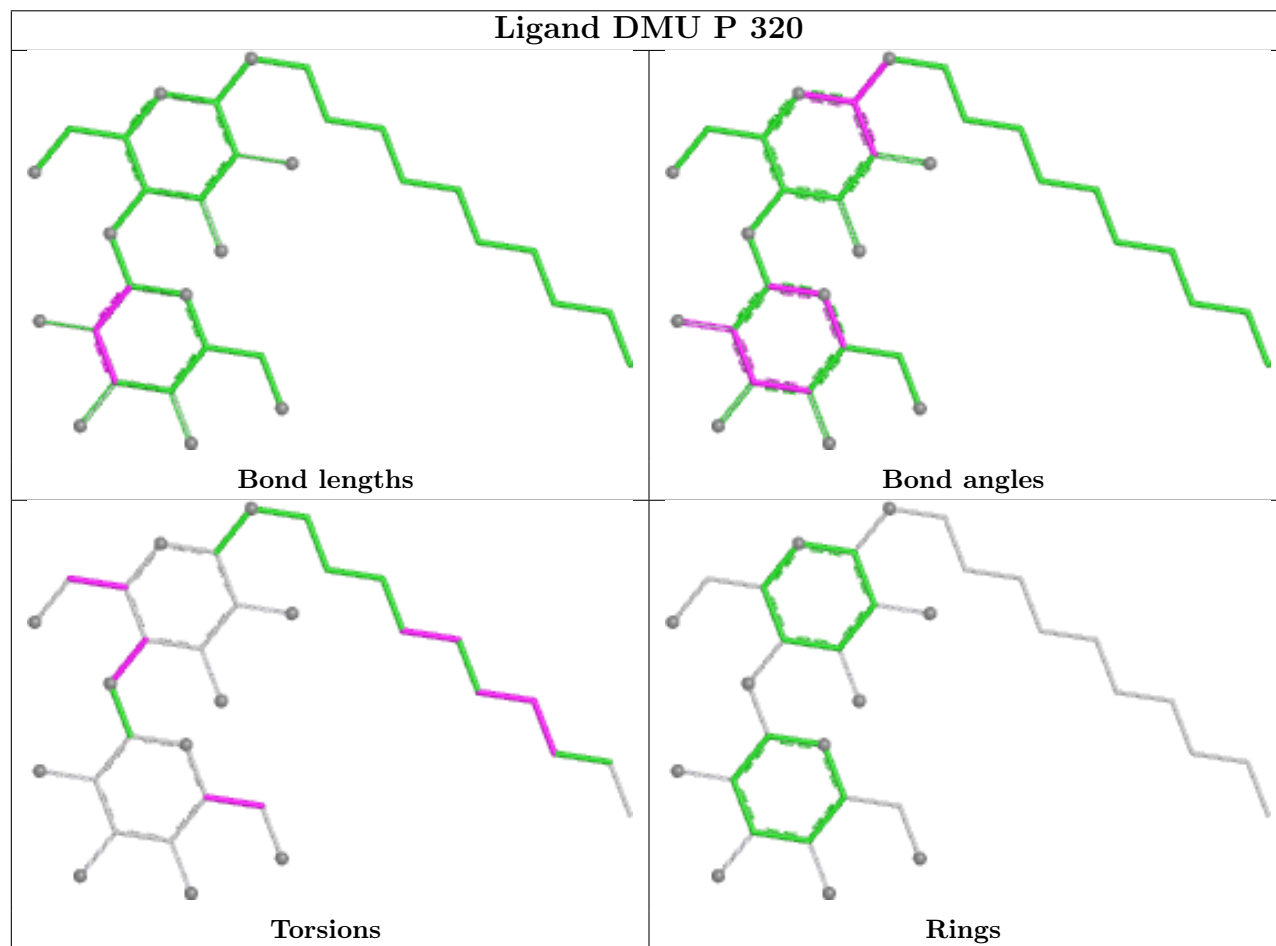
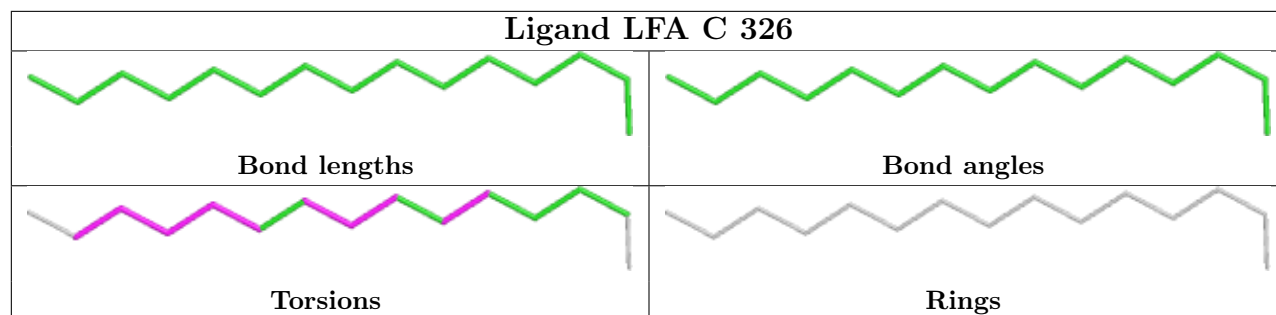
Ligand CHD B 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

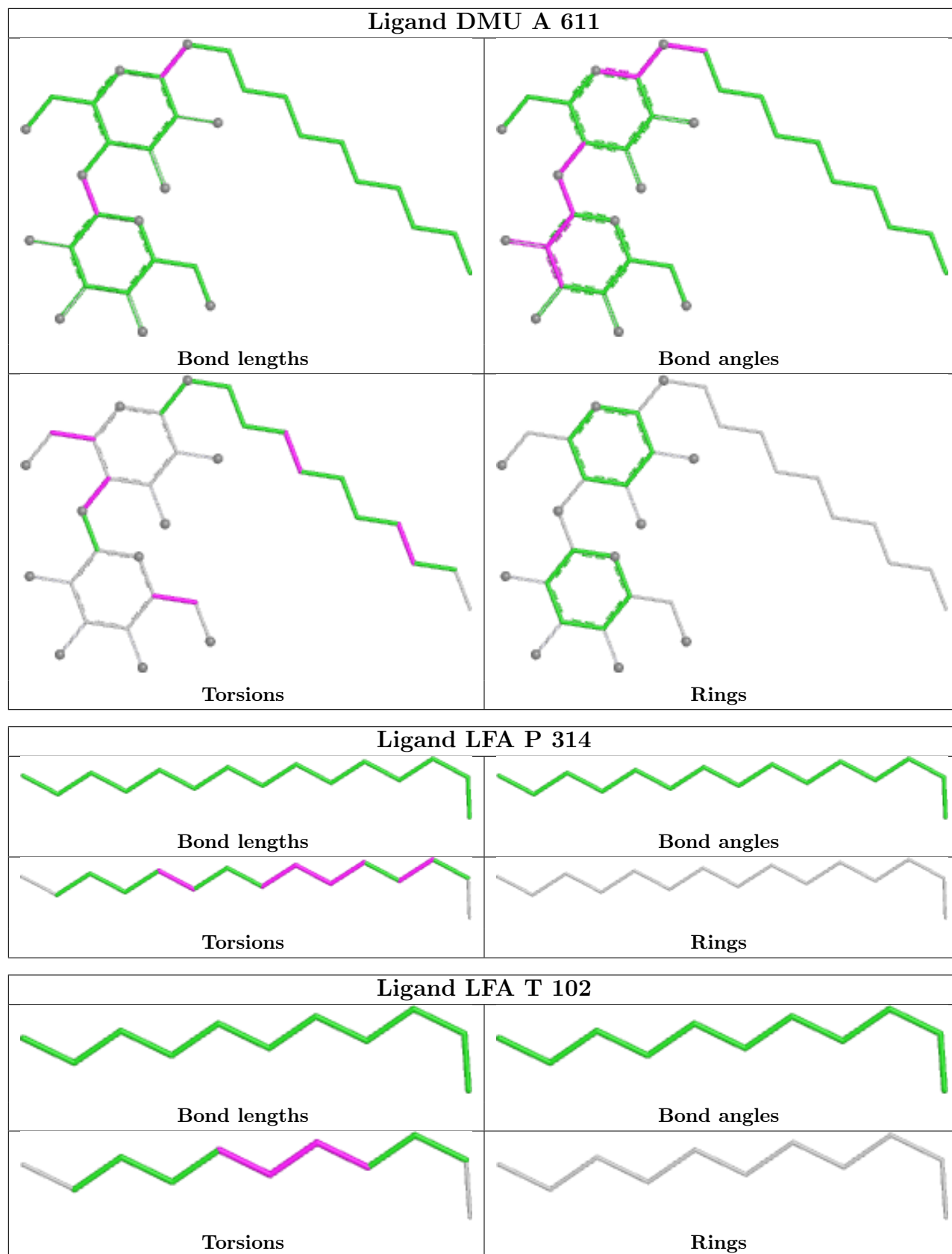
Ligand DMU P 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

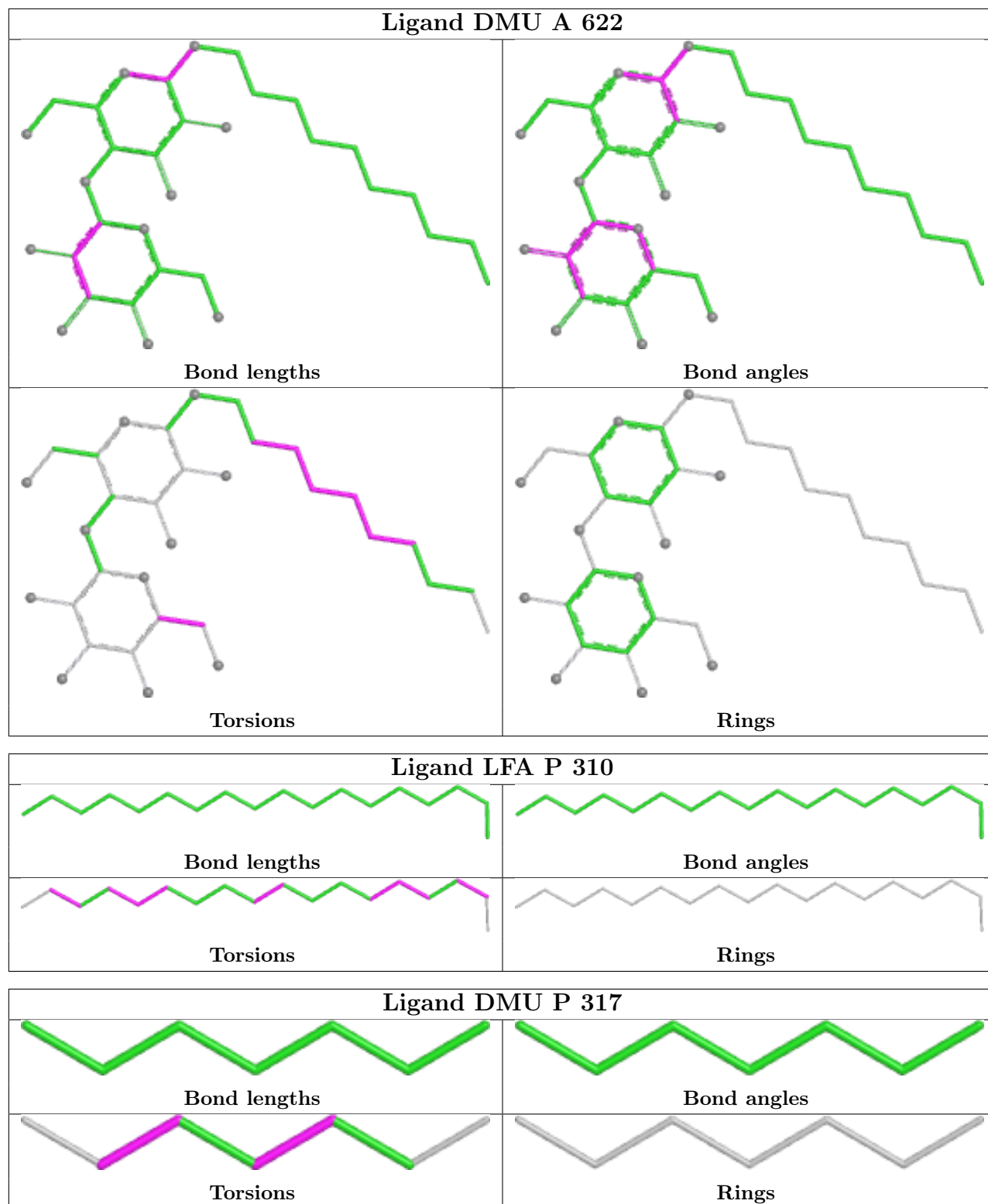
Ligand DMU B 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

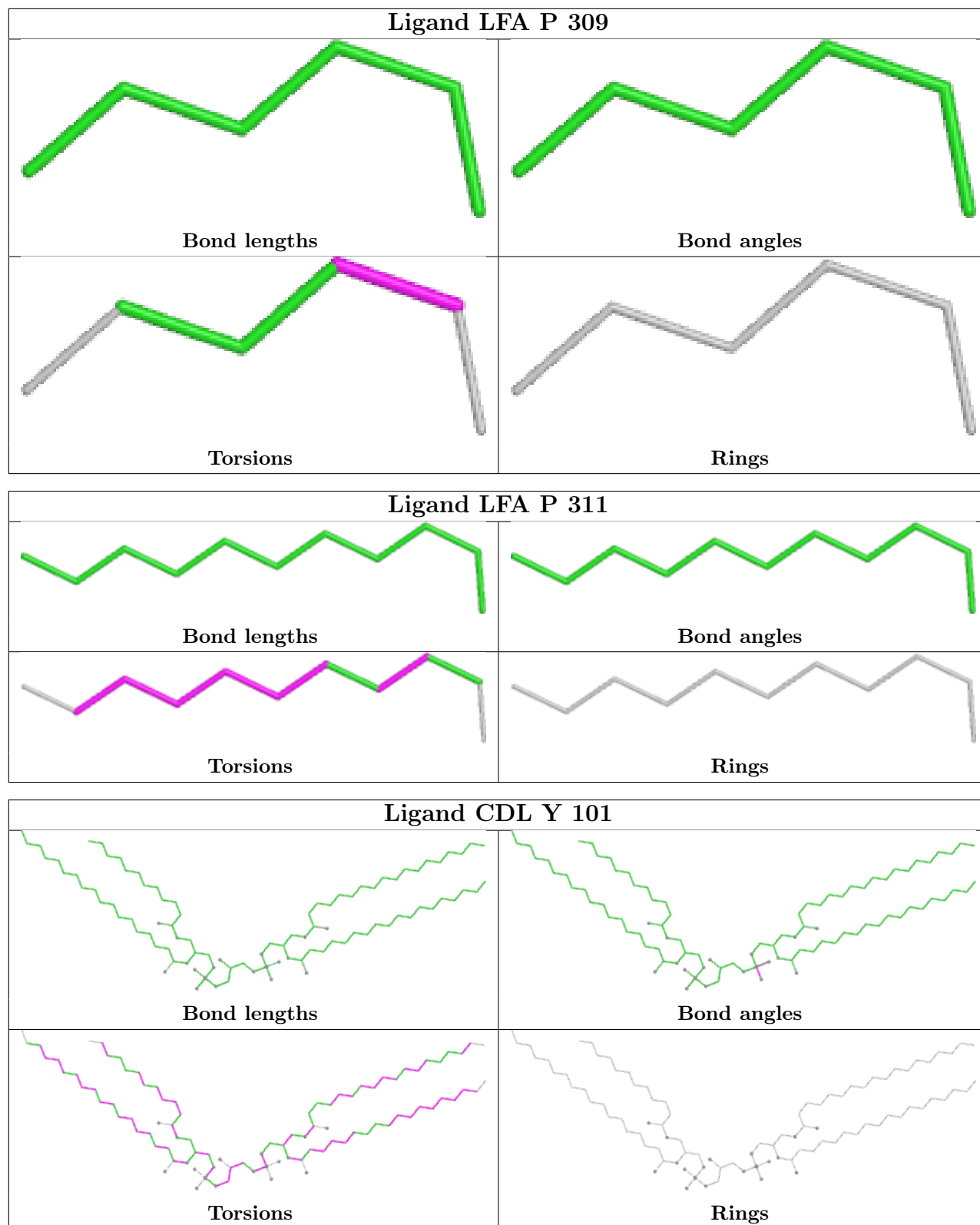


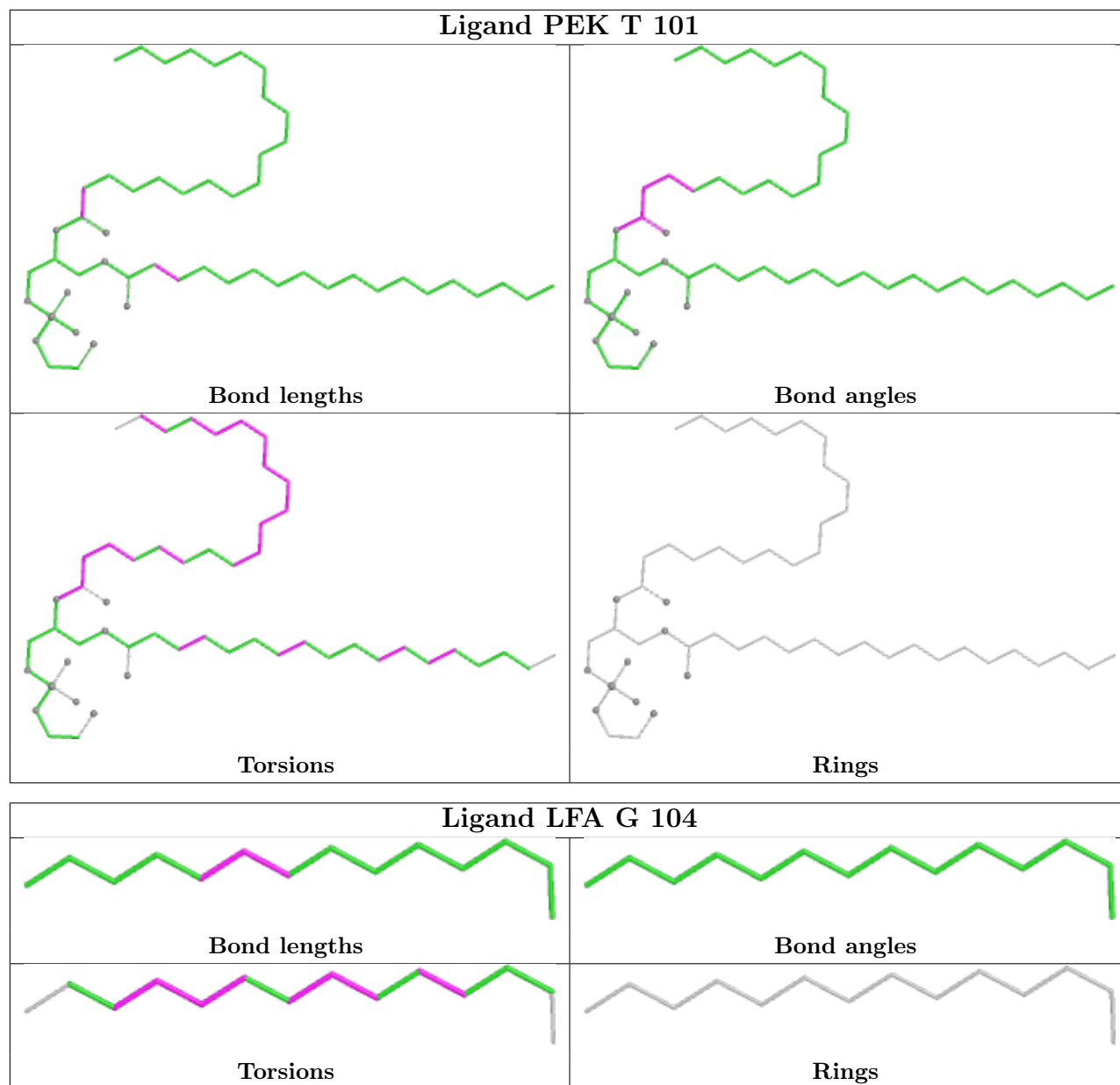


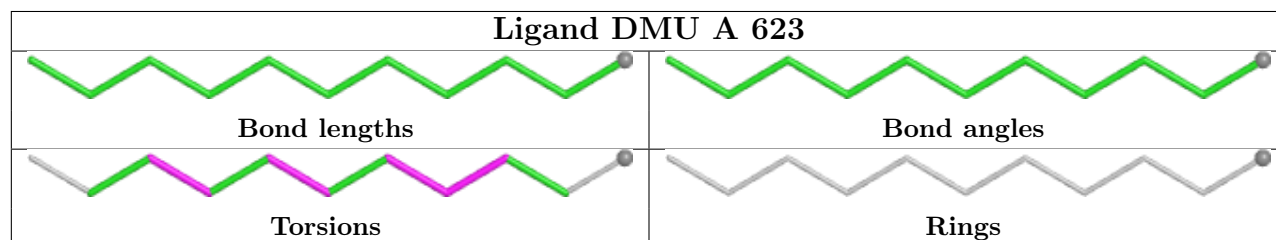
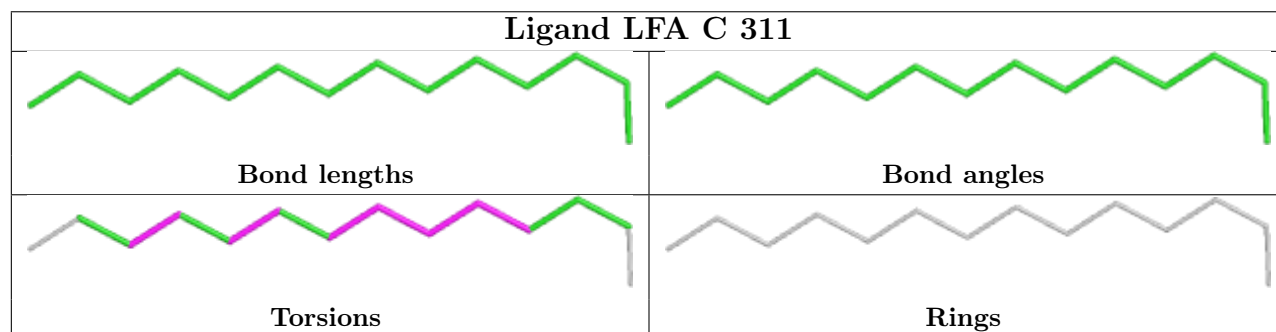
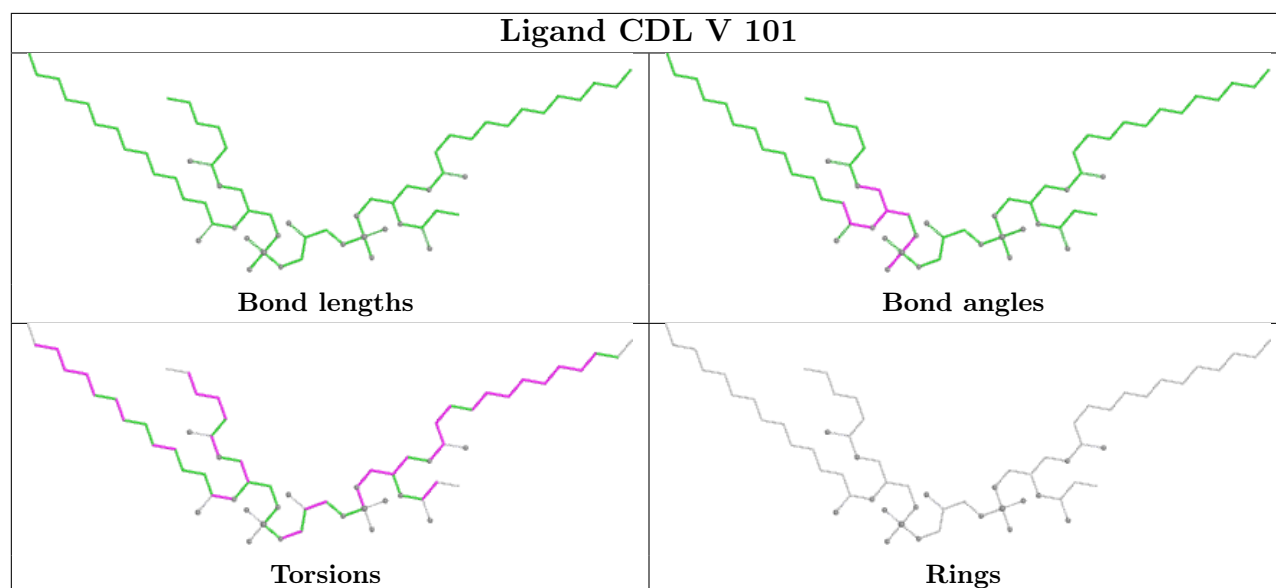
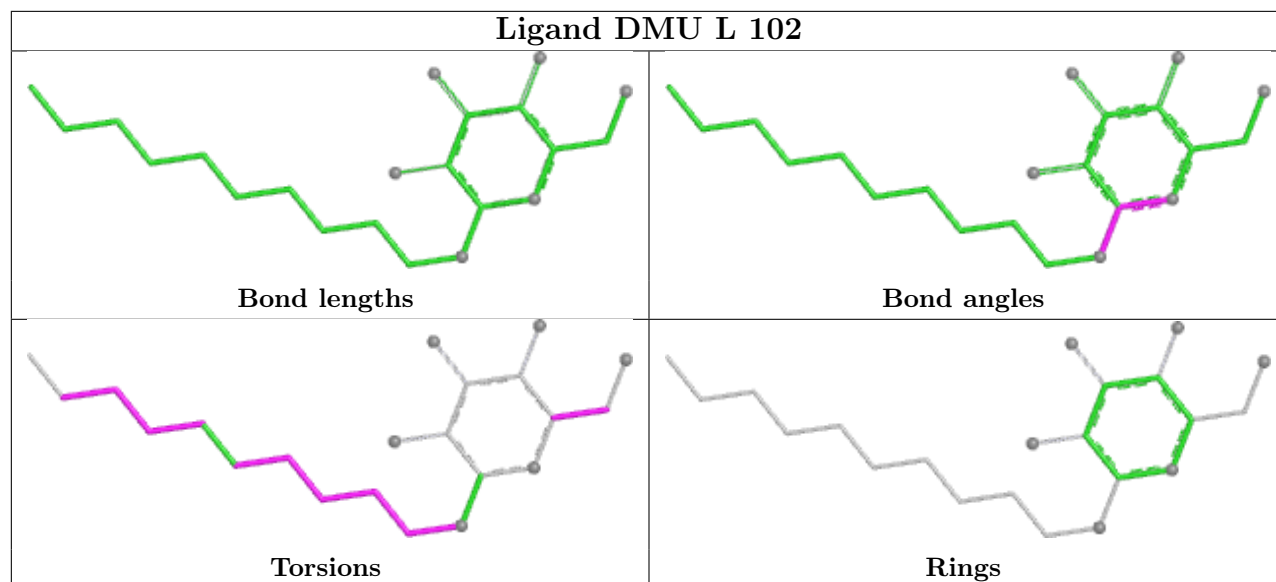


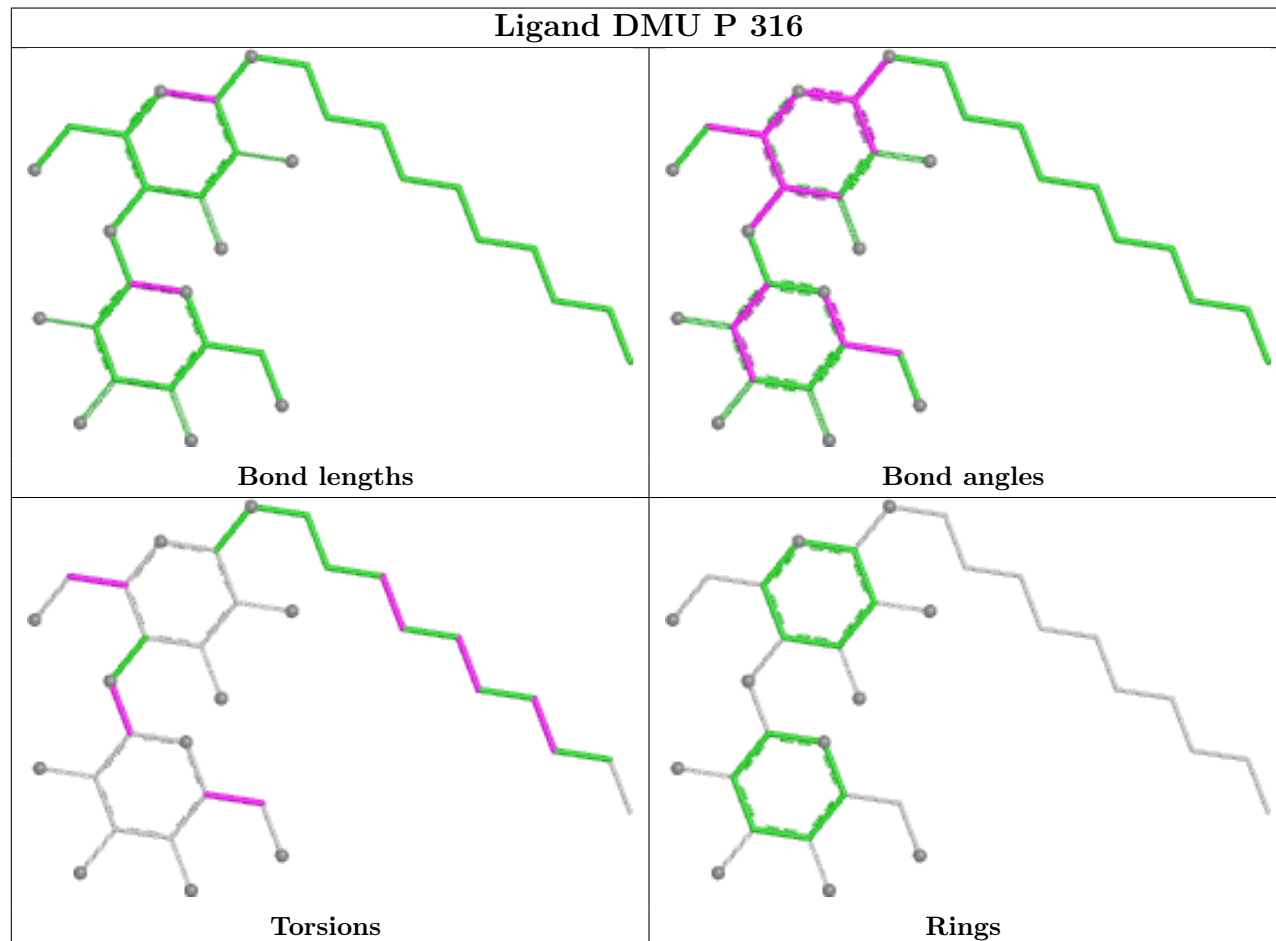
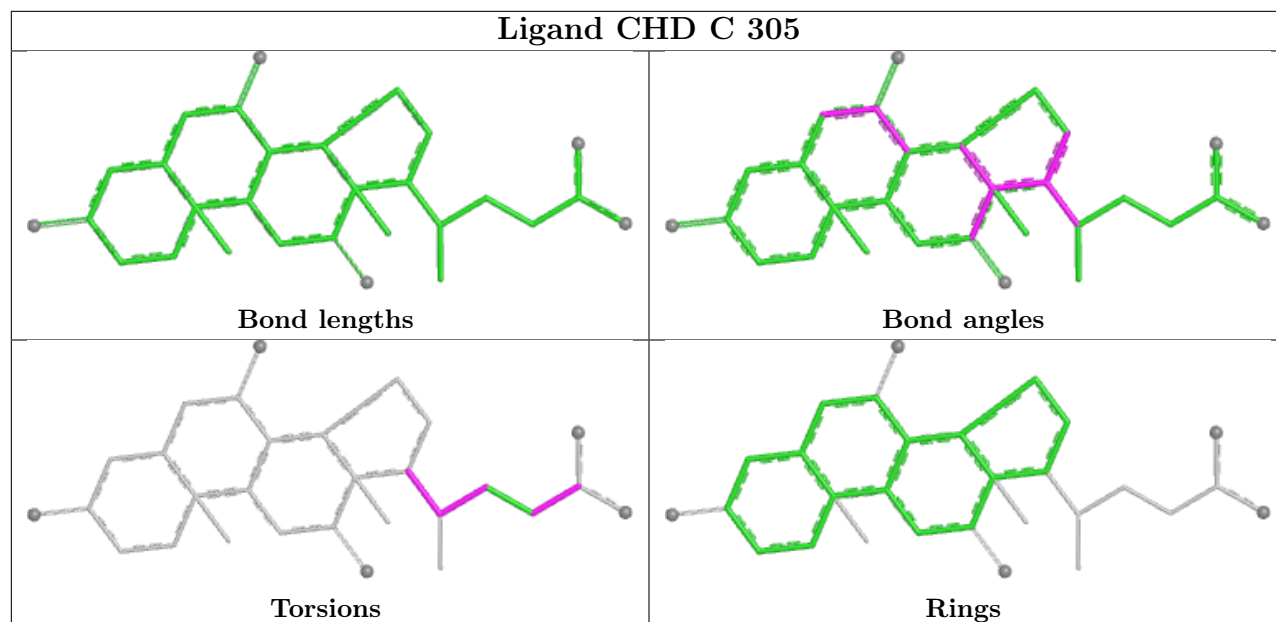


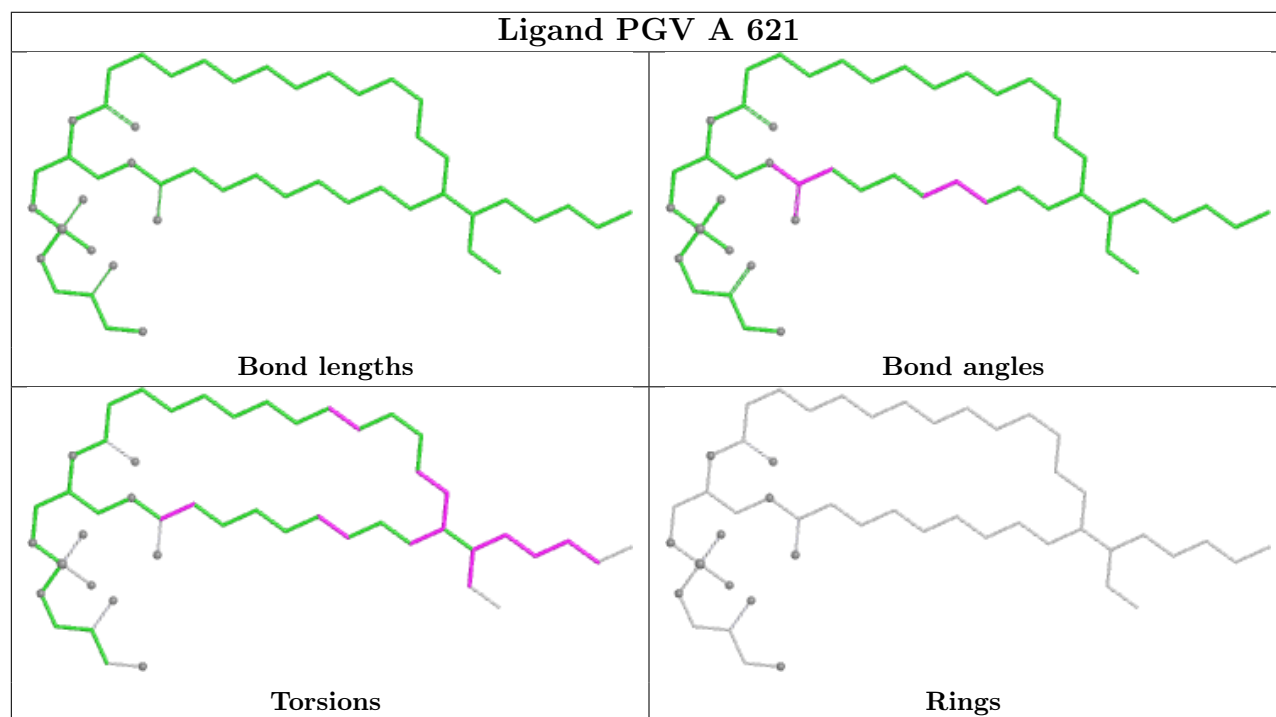
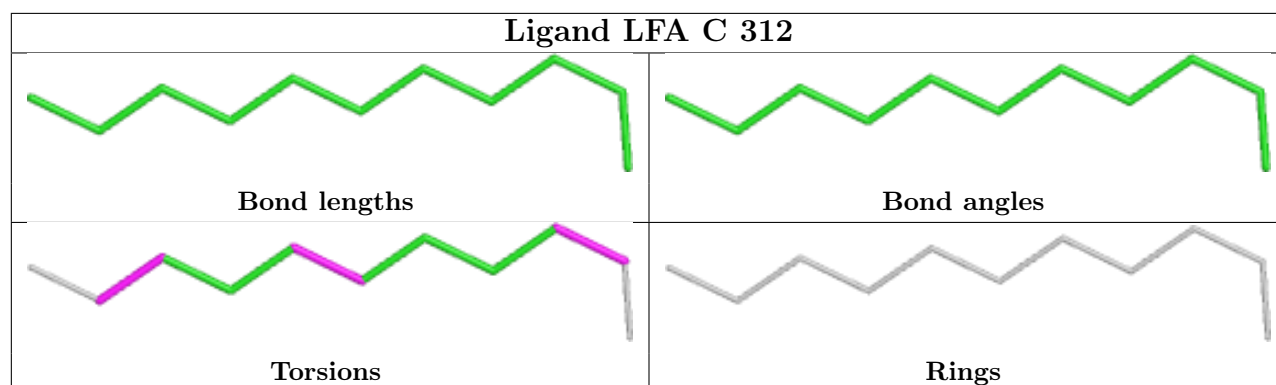
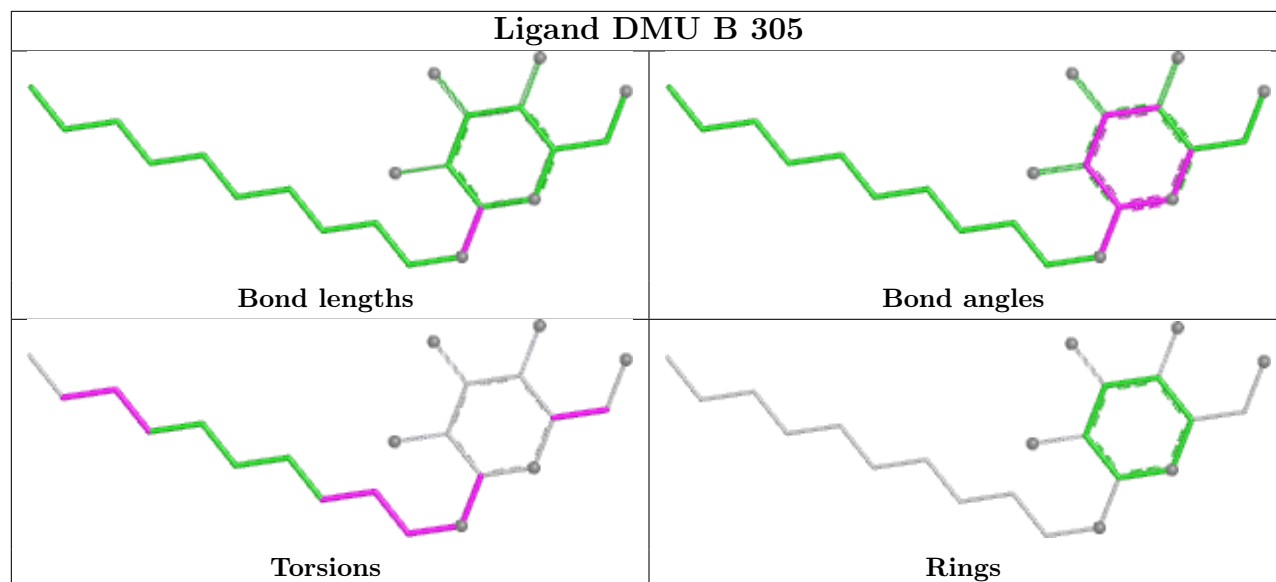


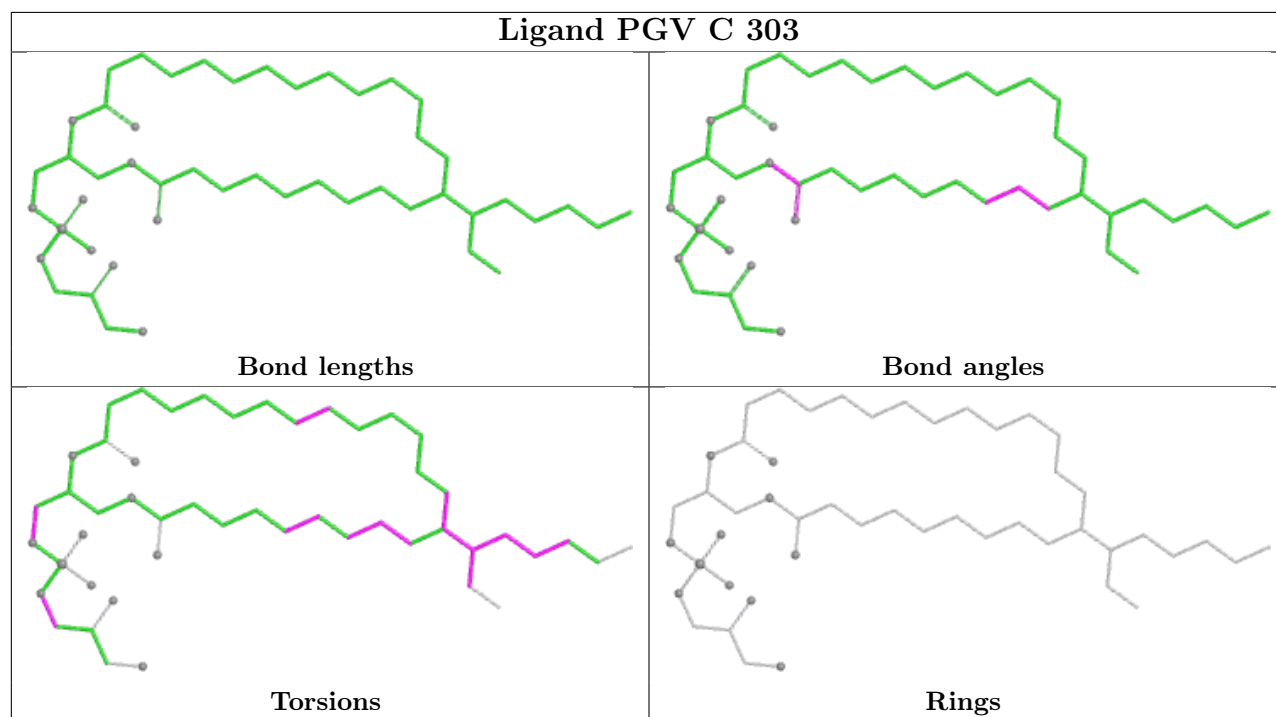
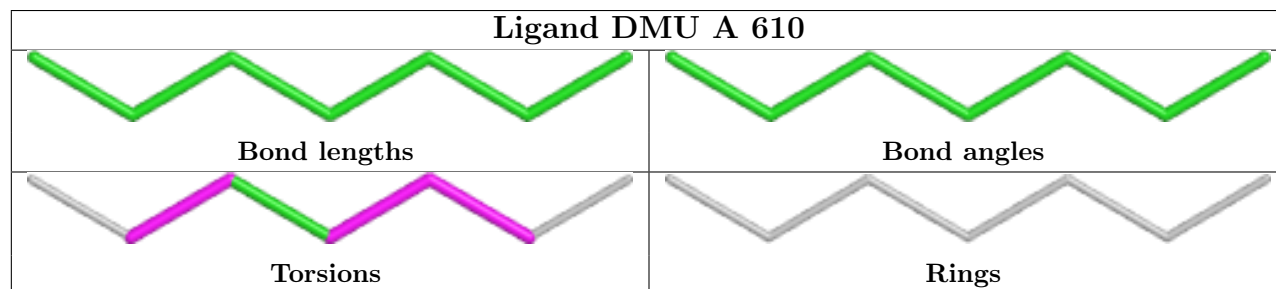
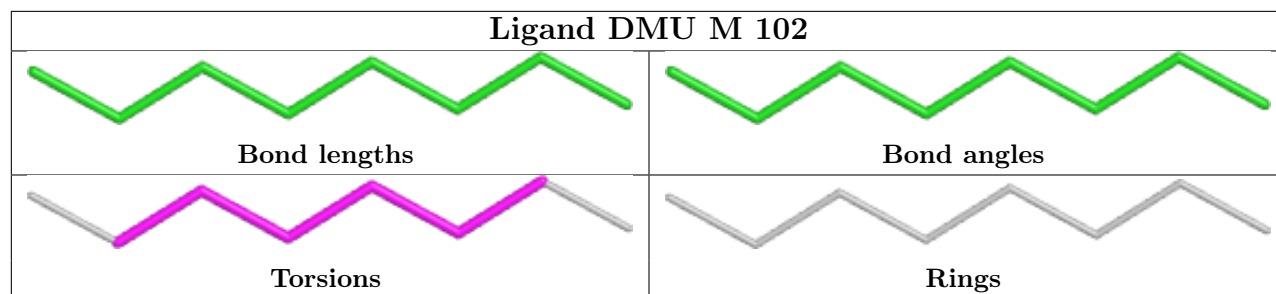


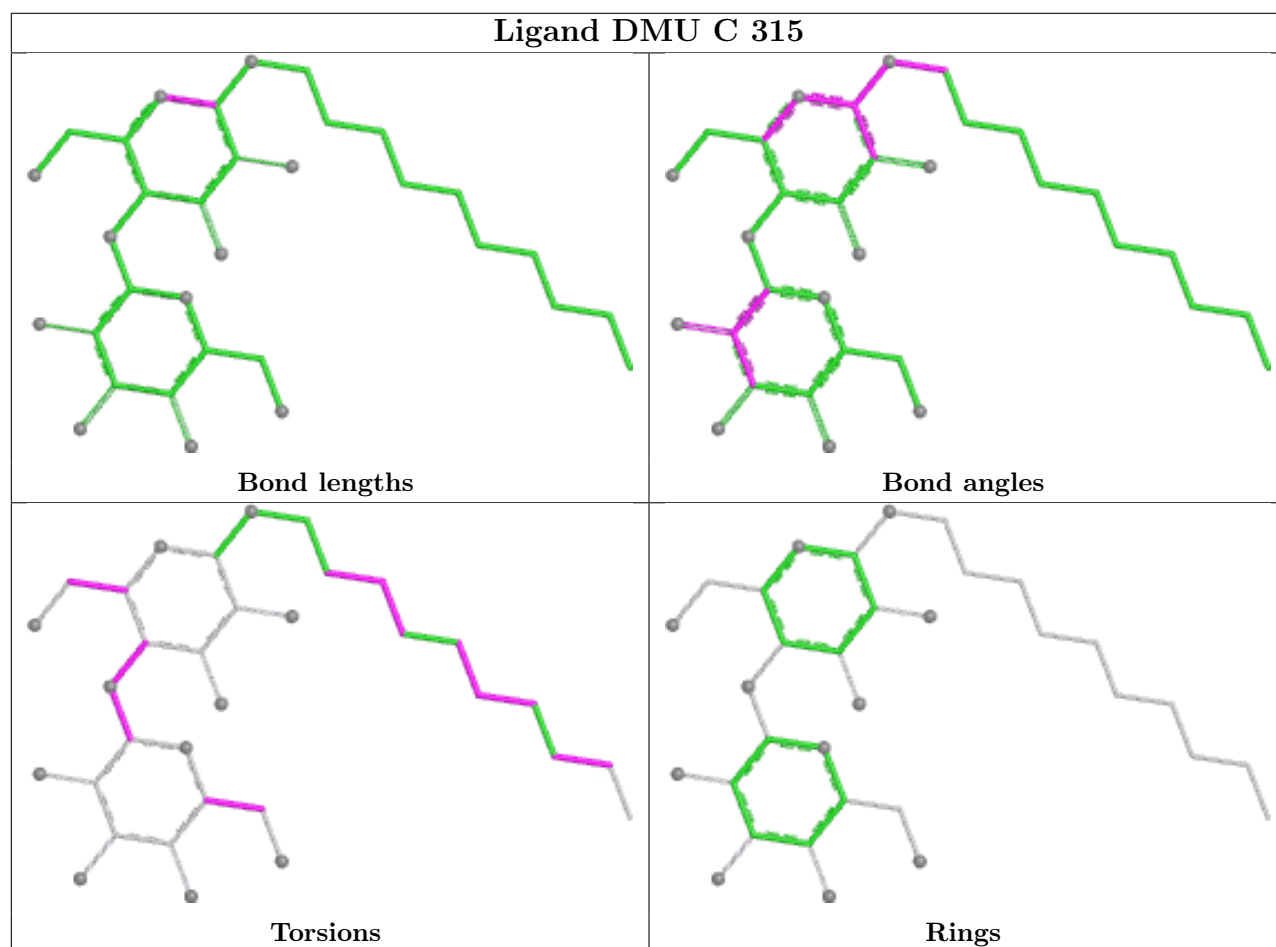
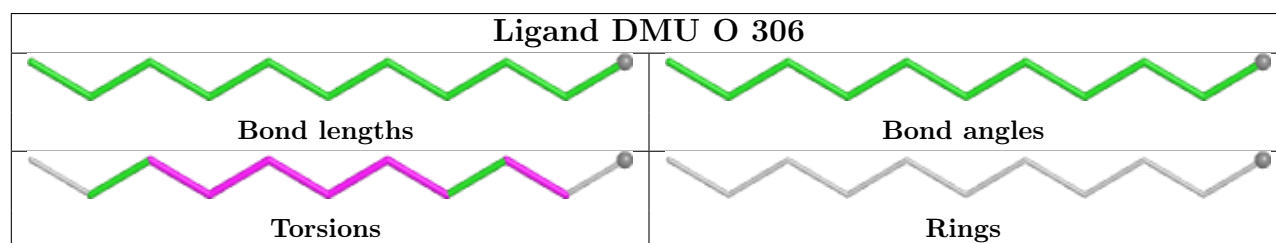
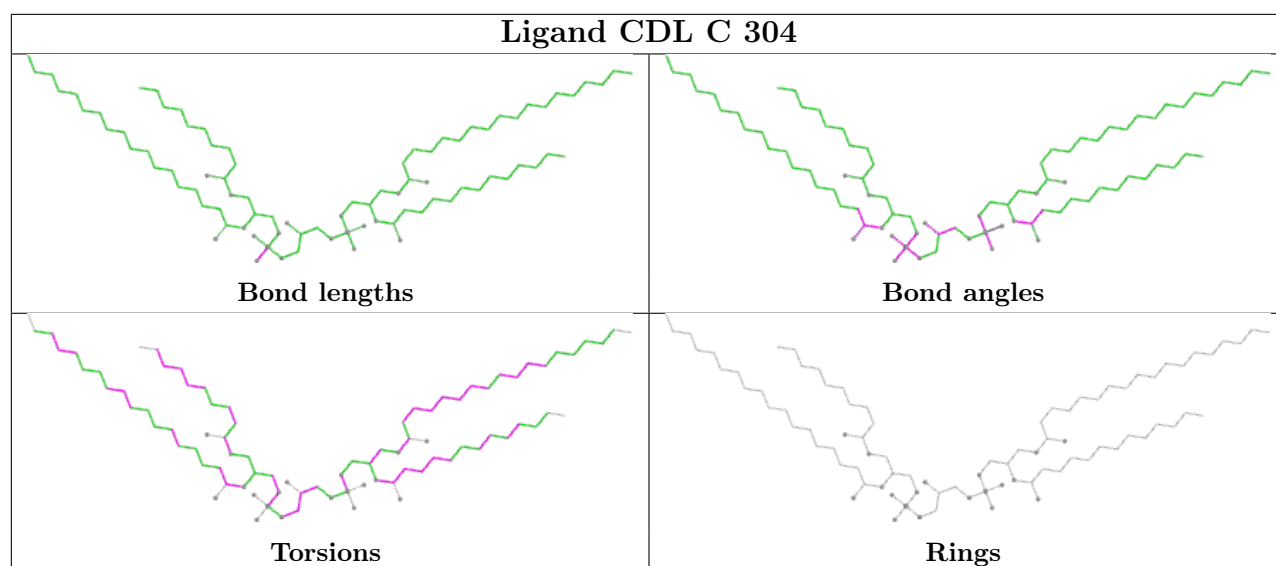


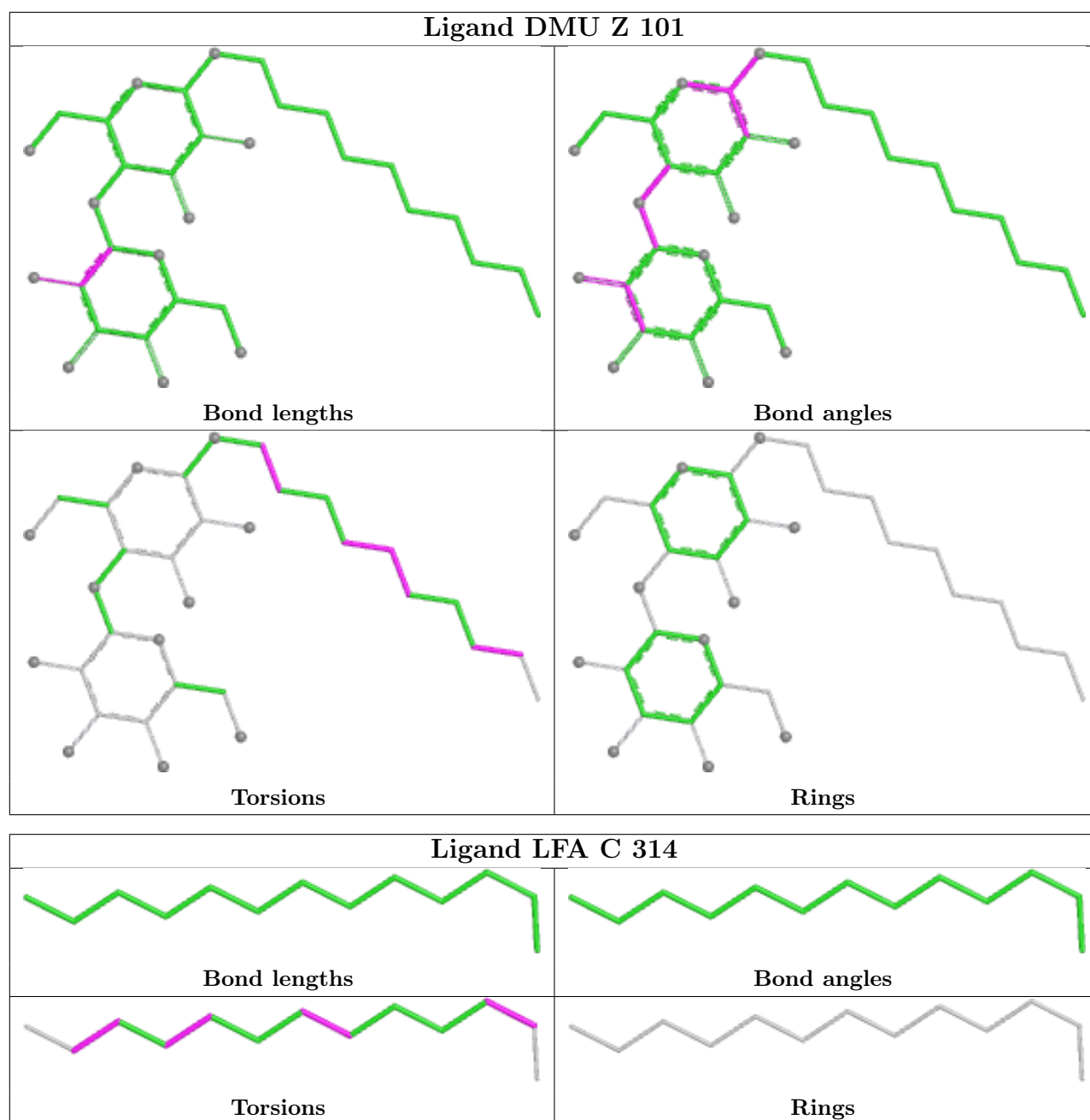


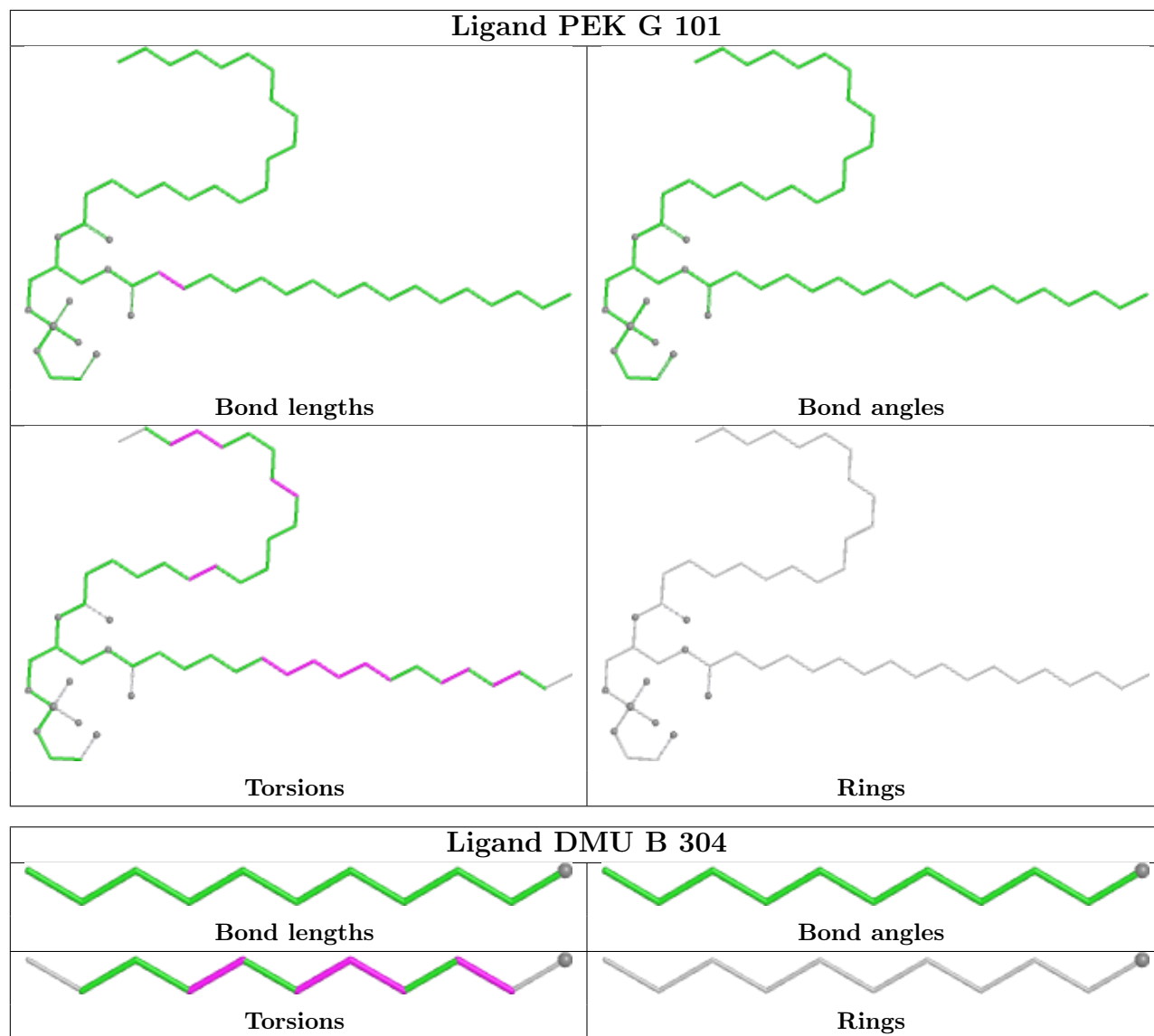


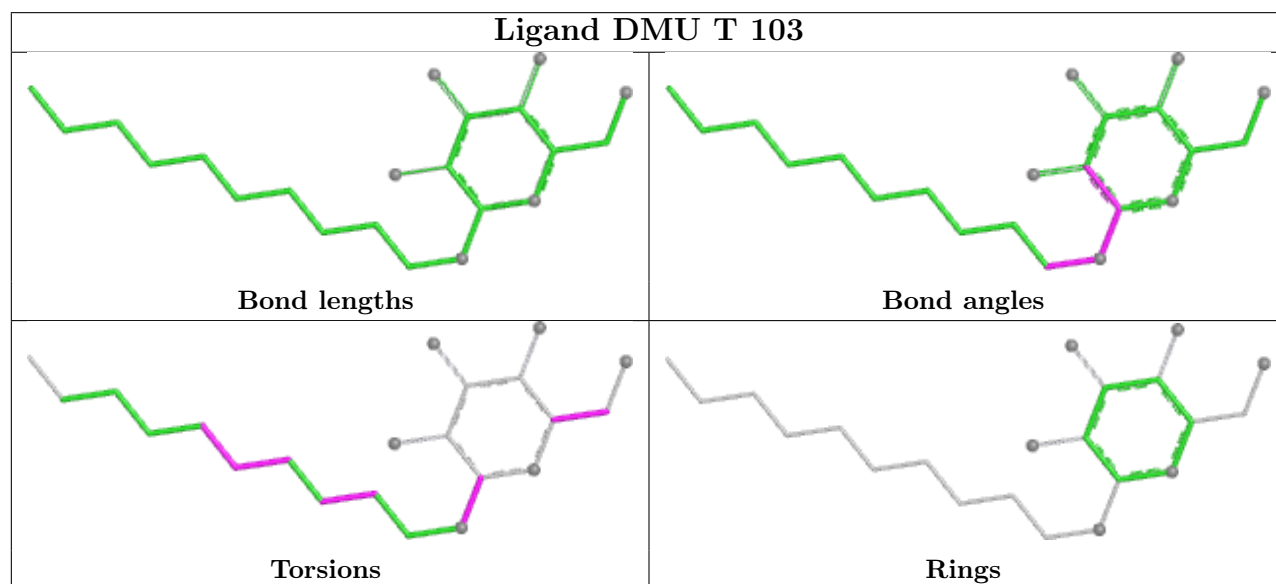
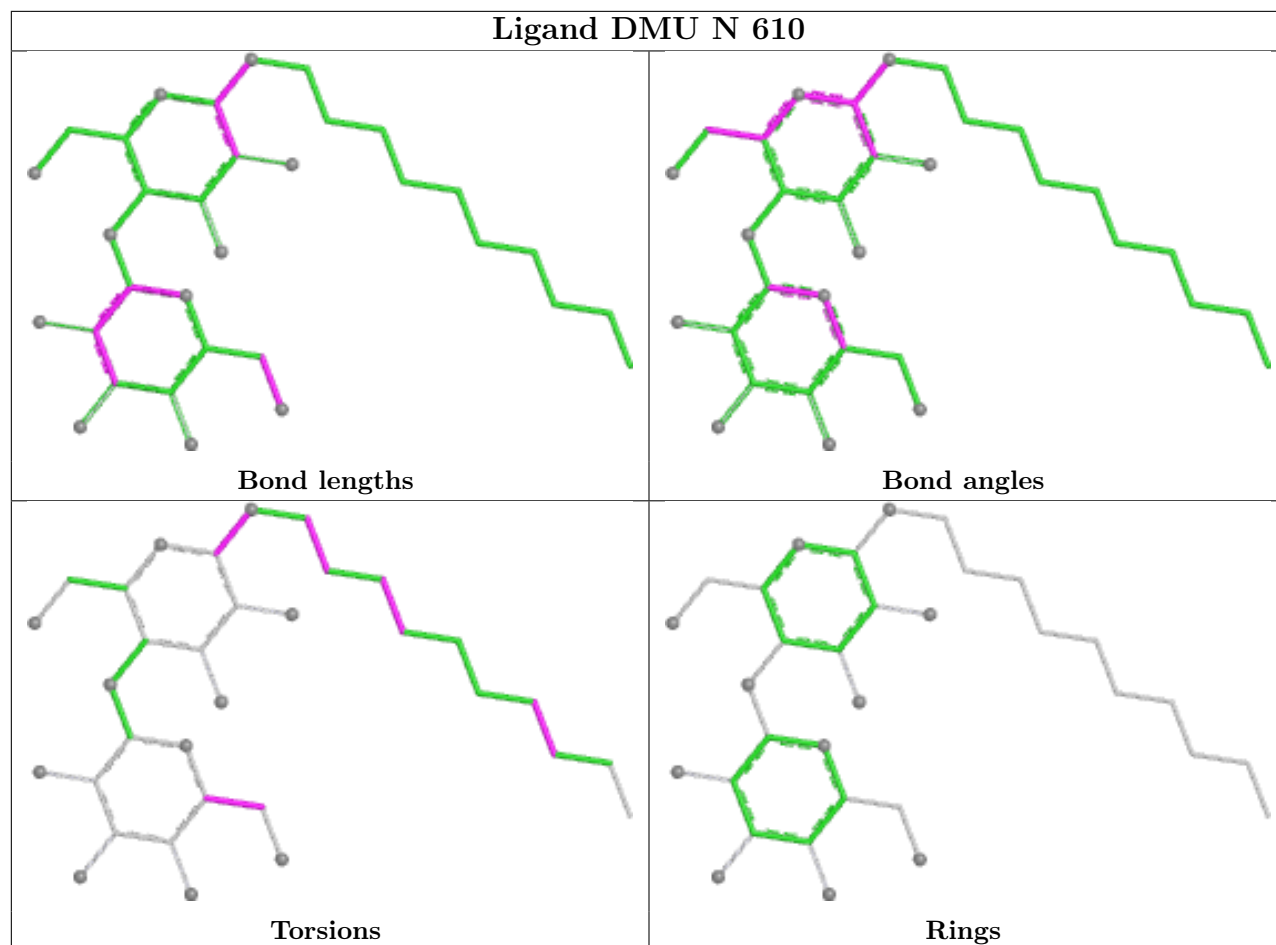


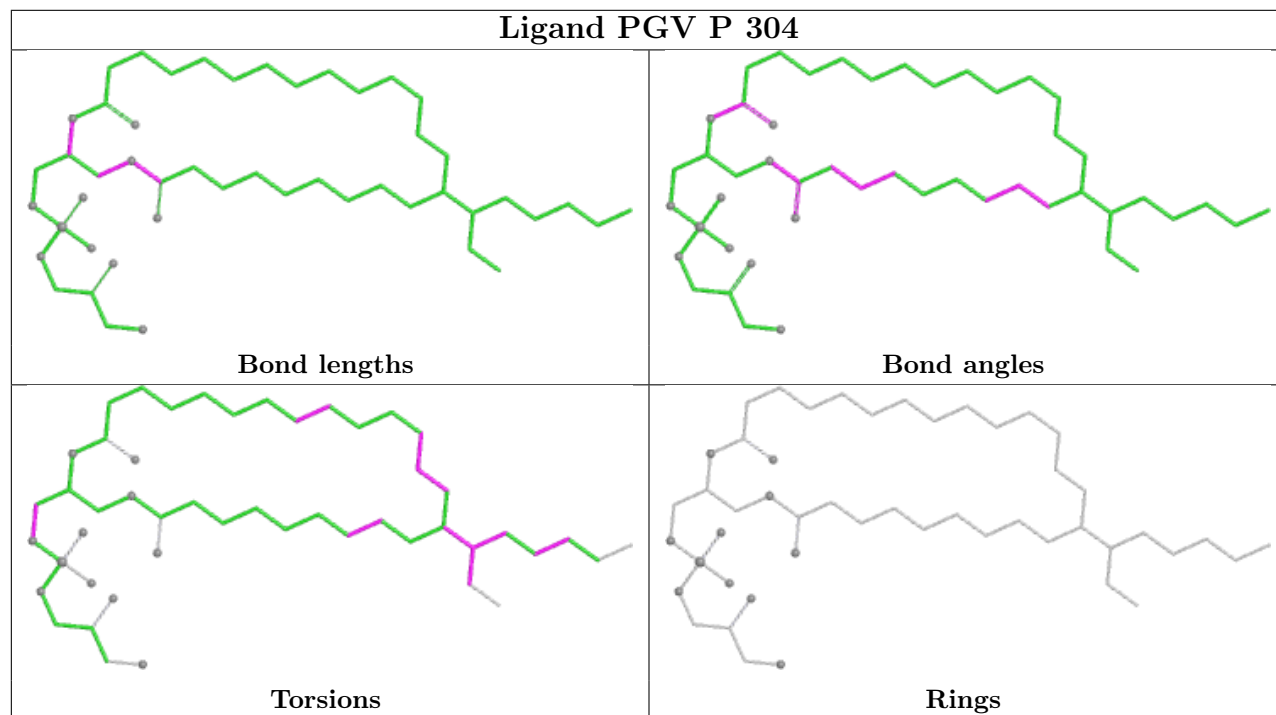
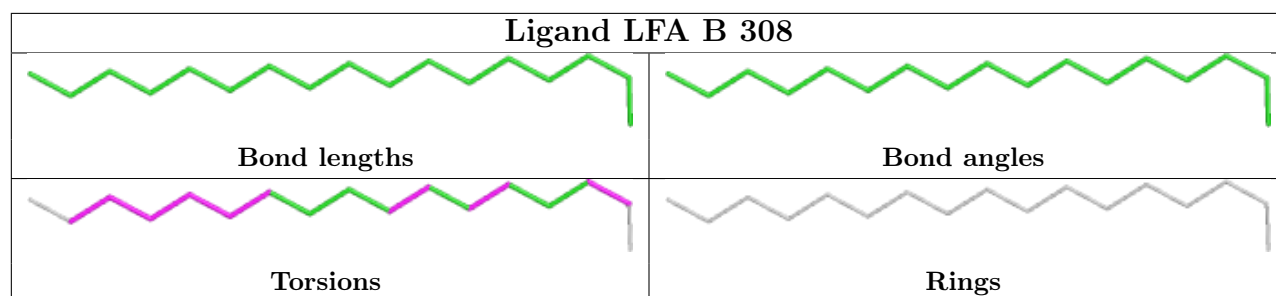
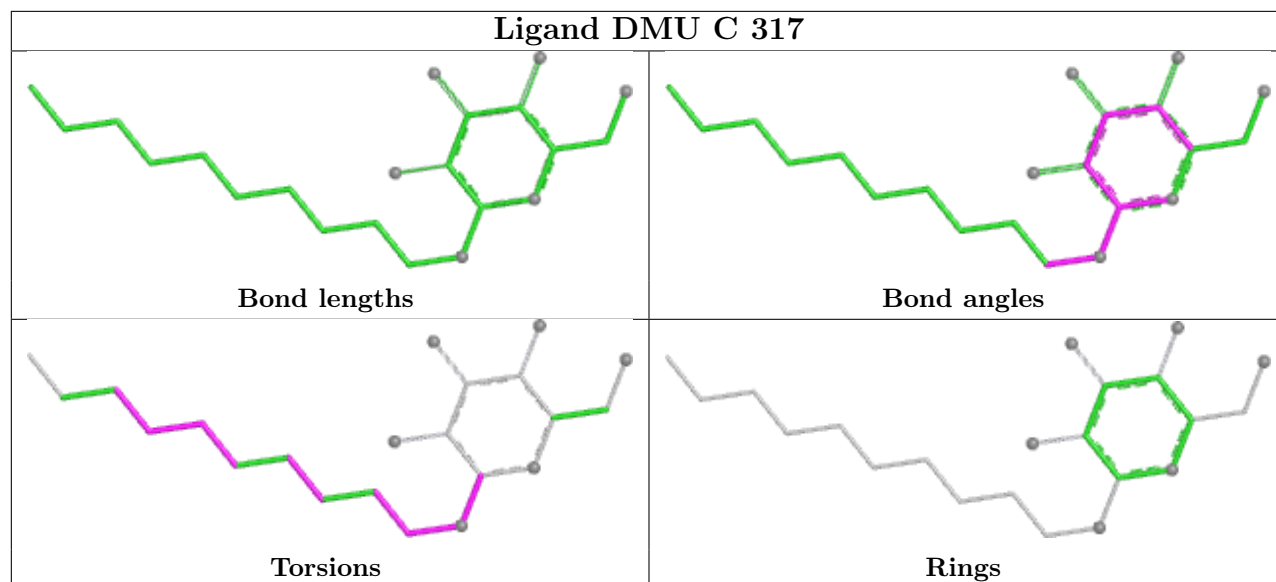


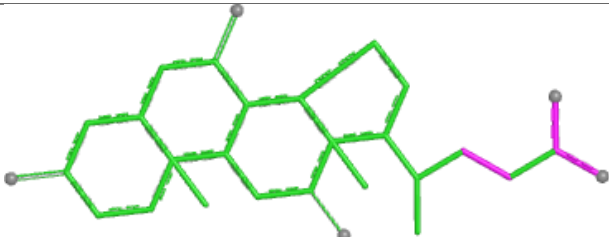
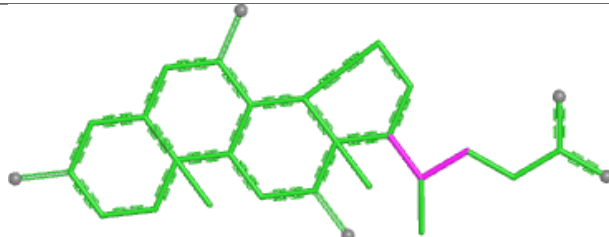
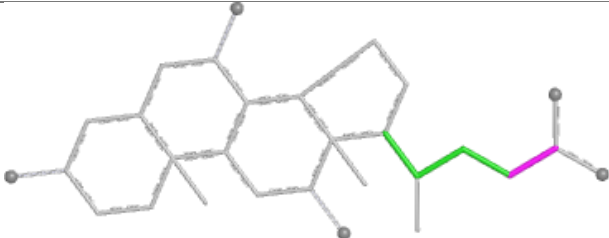
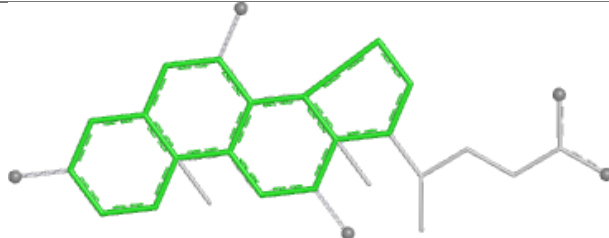


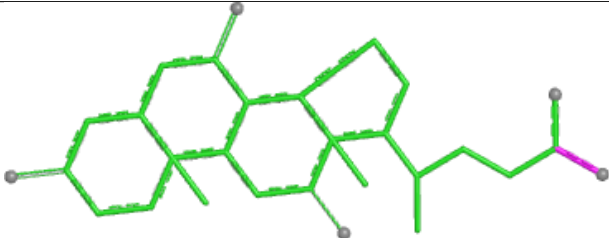
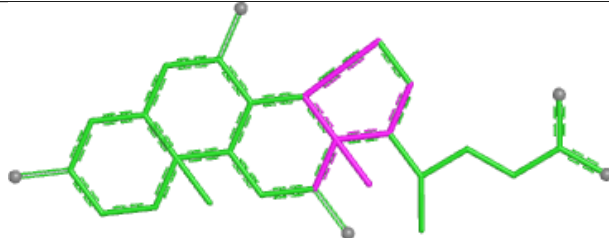
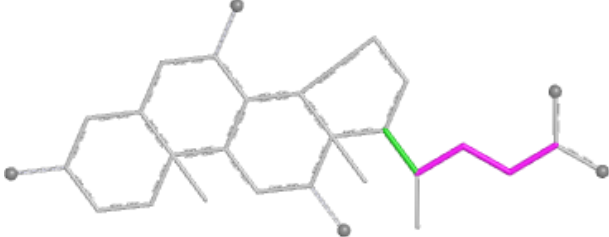
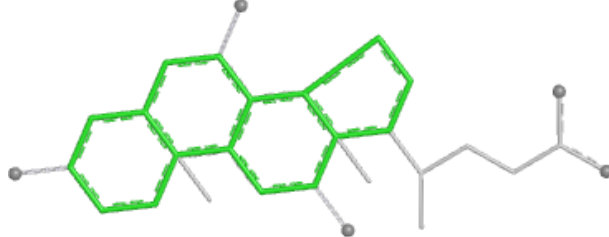


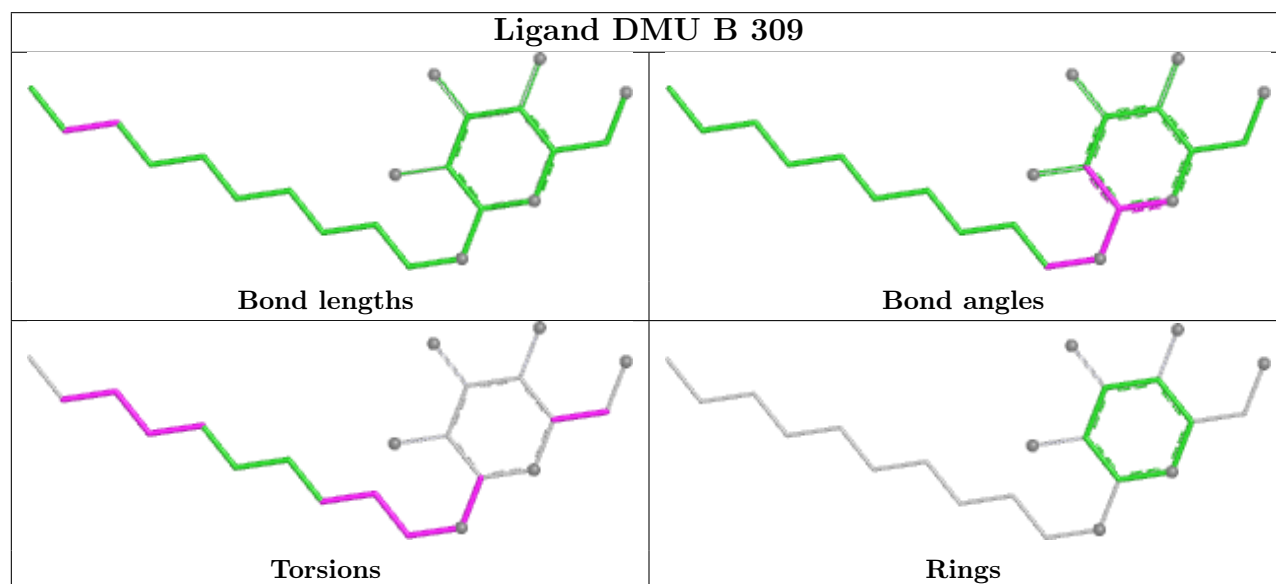
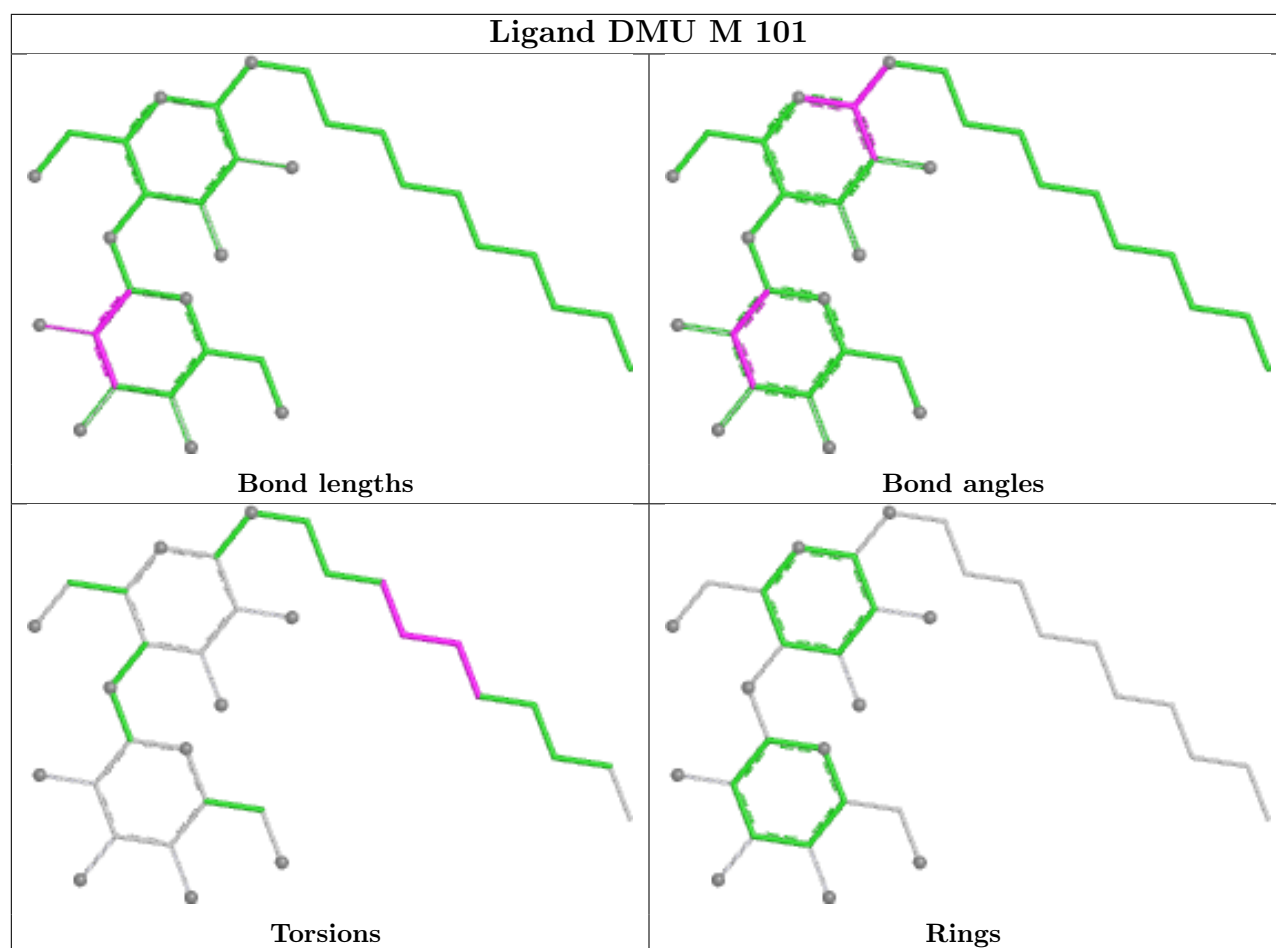


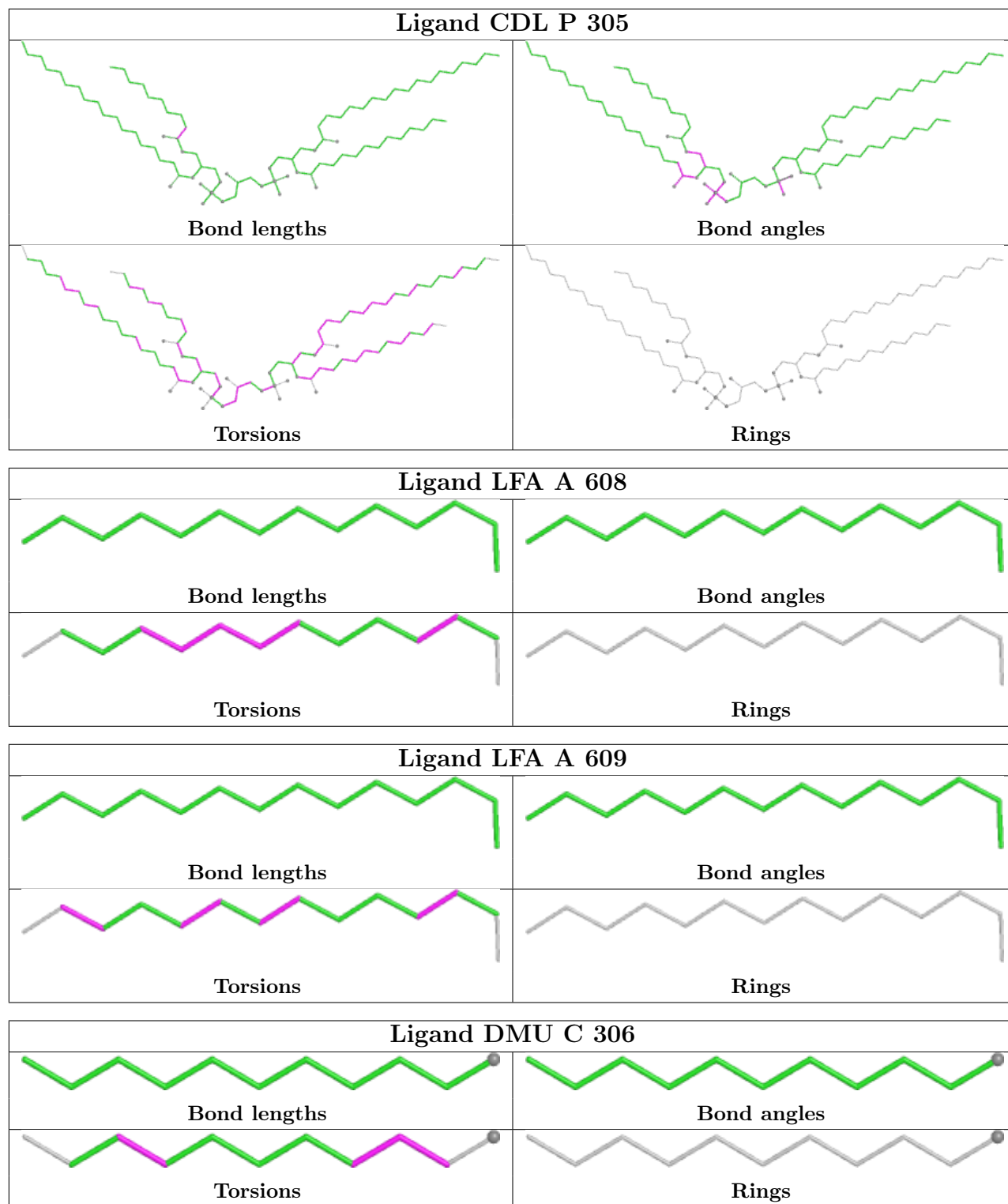


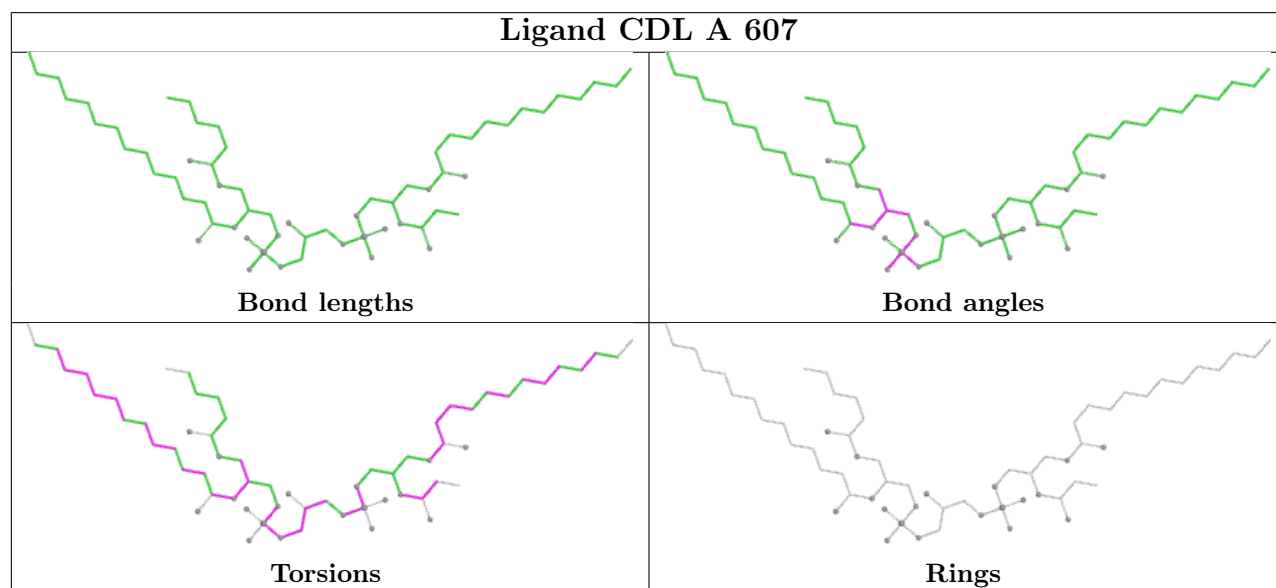
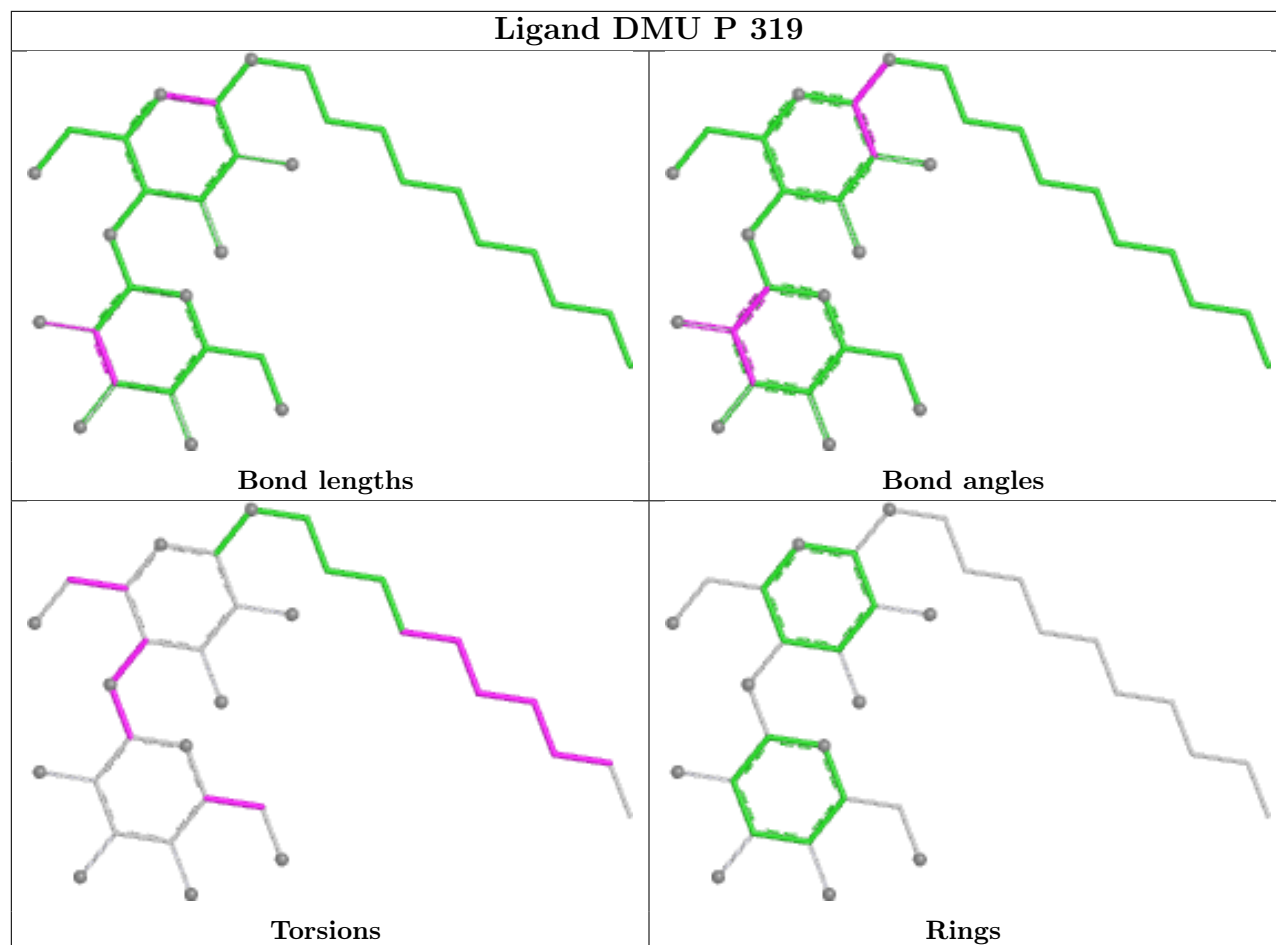


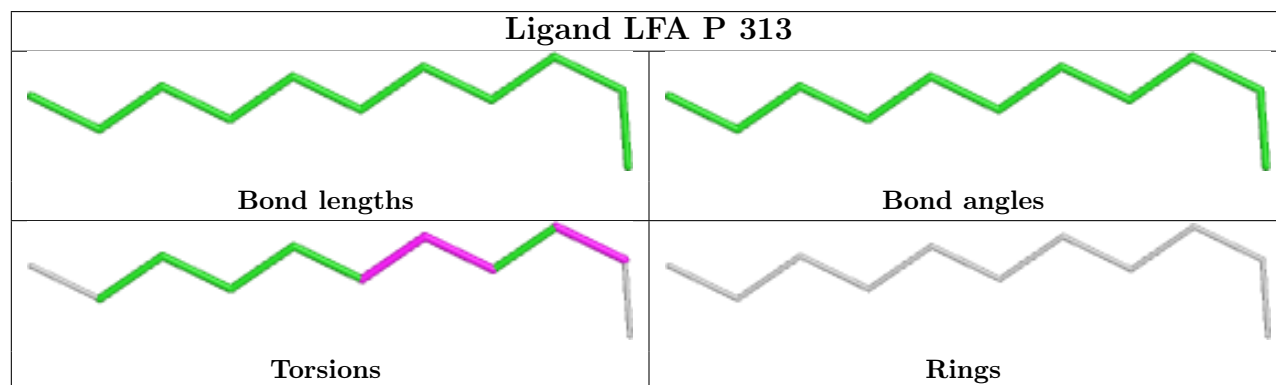
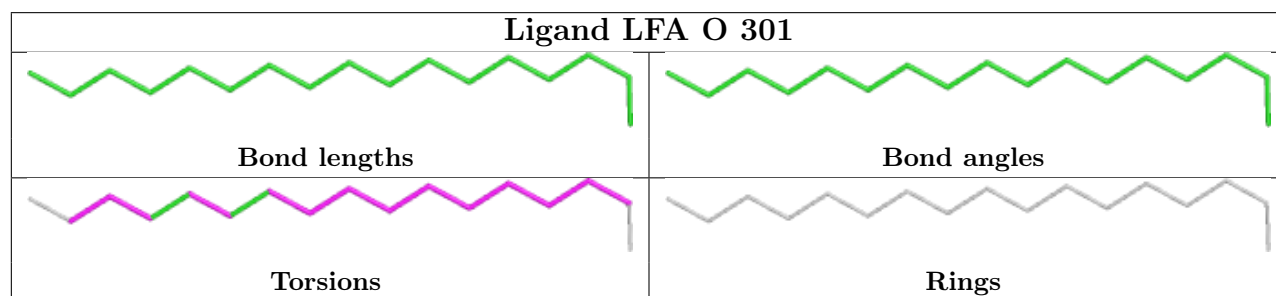
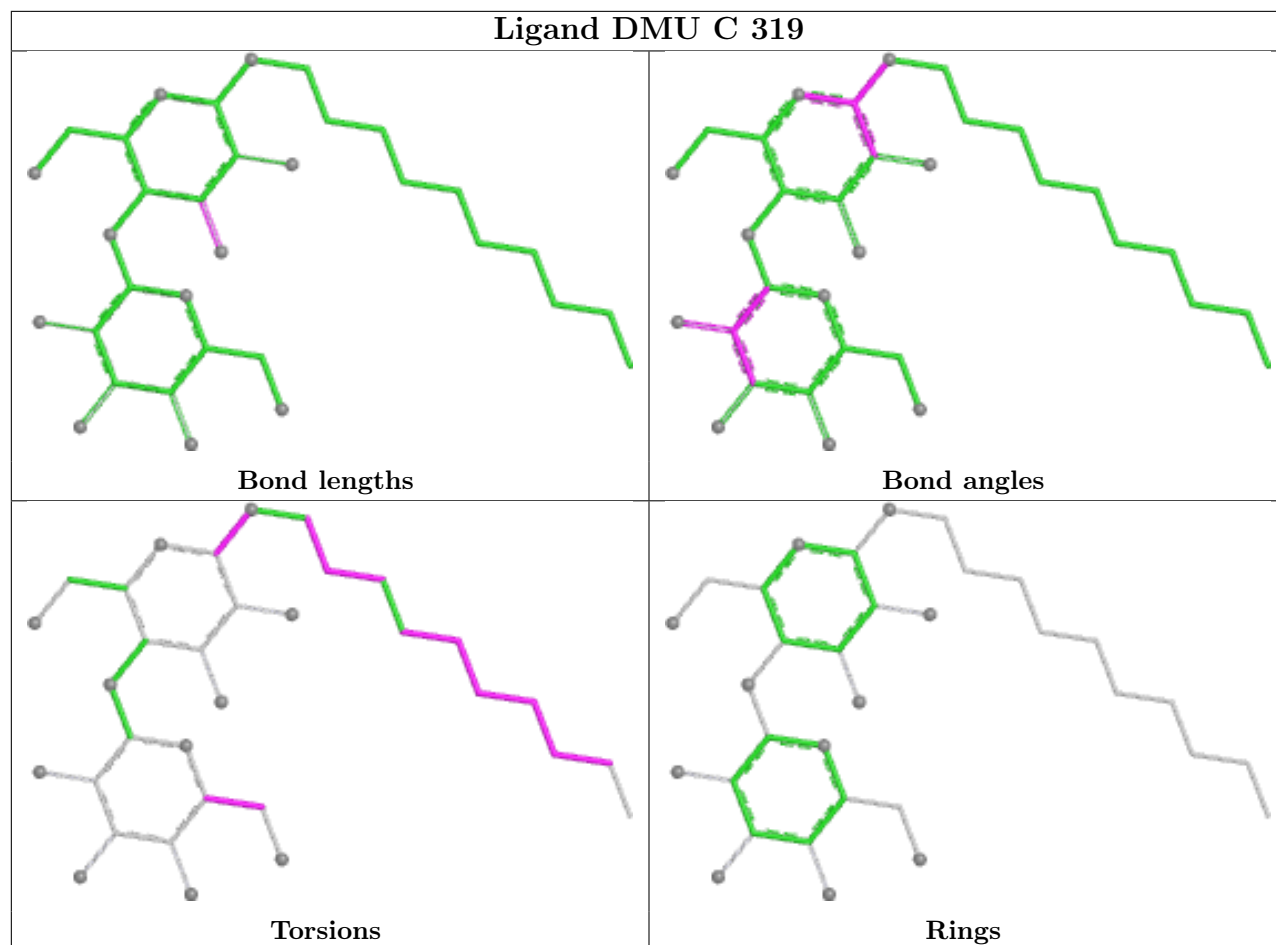
Ligand CHD C 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

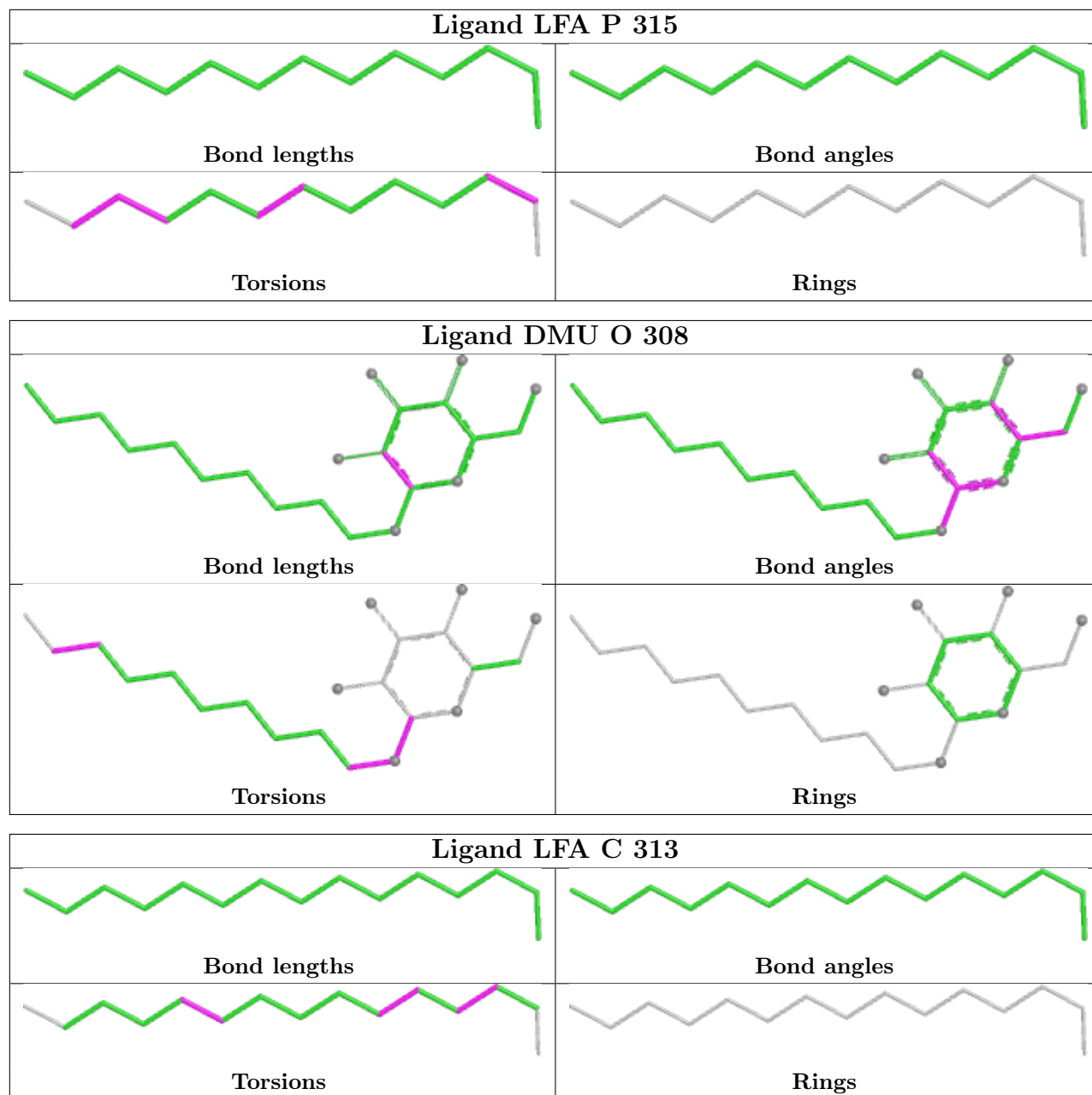
Ligand CHD P 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

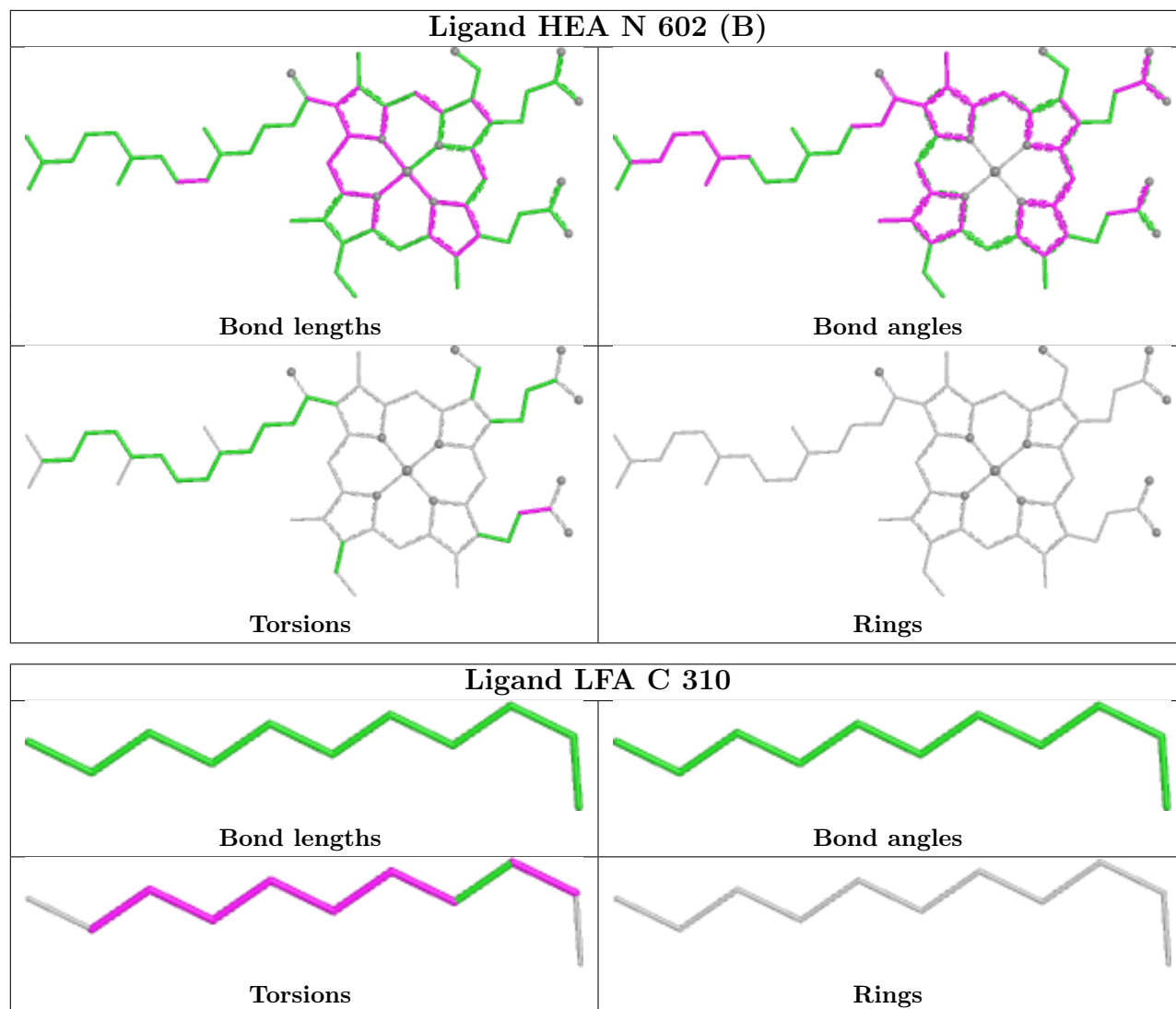


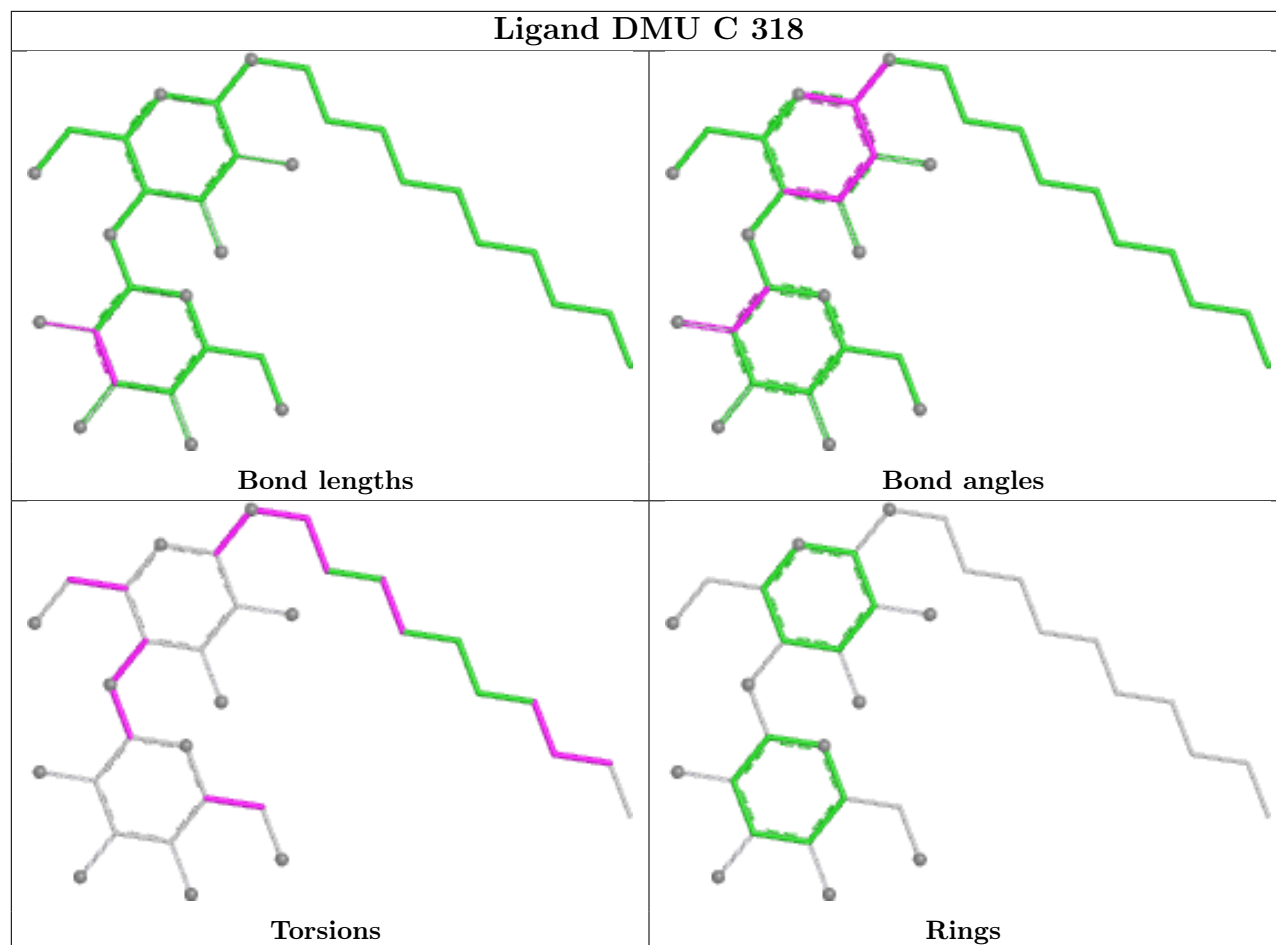












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	512/514 (99%)	-0.37	2 (0%) 88 89	15, 32, 39, 56	15 (2%)
1	N	512/514 (99%)	-0.30	2 (0%) 88 89	16, 34, 42, 56	15 (2%)
2	B	226/227 (99%)	0.05	10 (4%) 39 38	20, 37, 57, 75	5 (2%)
2	O	226/227 (99%)	0.09	5 (2%) 62 62	21, 42, 65, 94	5 (2%)
3	C	258/261 (98%)	-0.23	1 (0%) 88 89	16, 35, 45, 57	9 (3%)
3	P	258/261 (98%)	-0.23	1 (0%) 88 89	16, 36, 47, 64	9 (3%)
4	D	143/147 (97%)	-0.04	2 (1%) 73 73	19, 40, 54, 73	1 (0%)
4	Q	137/147 (93%)	0.31	2 (1%) 72 72	23, 51, 75, 86	1 (0%)
5	E	102/109 (93%)	-0.15	1 (0%) 79 80	34, 40, 55, 71	0
5	R	102/109 (93%)	0.01	2 (1%) 65 65	36, 49, 65, 80	0
6	F	91/98 (92%)	0.00	1 (1%) 78 78	19, 41, 62, 73	2 (2%)
6	S	91/98 (92%)	0.06	2 (2%) 62 62	18, 39, 61, 69	2 (2%)
7	G	72/85 (84%)	0.22	5 (6%) 23 21	20, 41, 77, 99	1 (1%)
7	T	72/85 (84%)	0.36	3 (4%) 40 40	21, 44, 76, 101	1 (1%)
8	H	75/85 (88%)	0.27	4 (5%) 32 31	35, 43, 85, 109	0
8	U	75/85 (88%)	0.34	6 (8%) 18 16	38, 46, 88, 112	0
9	I	70/73 (95%)	0.39	4 (5%) 29 28	37, 49, 72, 92	0
9	V	70/73 (95%)	0.50	4 (5%) 29 28	37, 56, 73, 103	0
10	J	56/59 (94%)	0.27	1 (1%) 67 68	36, 45, 67, 79	0
10	W	56/59 (94%)	0.34	3 (5%) 31 30	37, 47, 70, 82	0
11	K	49/56 (87%)	0.33	2 (4%) 41 41	38, 45, 60, 78	0
11	X	49/56 (87%)	0.66	3 (6%) 27 25	44, 53, 72, 98	0
12	L	44/47 (93%)	-0.08	1 (2%) 61 61	33, 37, 50, 60	0
12	Y	44/47 (93%)	0.02	1 (2%) 61 61	37, 43, 57, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	40/46 (86%)	0.07	0 100 100	34, 38, 55, 69	0
13	Z	40/46 (86%)	0.47	3 (7%) 20 18	40, 47, 69, 84	0
All	All	3470/3614 (96%)	-0.04	71 (2%) 65 65	15, 38, 63, 112	66 (1%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	36	TRP	6.6
2	O	113	TYR	4.8
8	H	45	ALA	4.6
6	S	3	GLY	4.5
2	B	59	GLN	4.2
6	S	93	PRO	4.2
7	G	36	TRP	4.1
11	X	6	ALA	3.8
9	V	37	PHE	3.8
8	U	47	GLY	3.7
9	V	3	ALA	3.7
8	U	45	ALA	3.7
6	F	3	GLY	3.7
8	H	48	GLY	3.6
1	A	113[A]	LEU	3.5
10	J	1	PHE	3.5
1	N	136[A]	LEU	3.5
7	T	38	HIS	3.5
8	U	48	GLY	3.4
2	B	60	GLU	3.2
2	O	91	ASN	3.2
4	D	5	VAL	3.1
11	K	6	ALA	3.0
10	W	1	PHE	2.9
9	I	3	ALA	2.9
12	Y	24	MET	2.9
5	E	7	THR	2.9
2	B	91	ASN	2.9
2	O	90	ILE	2.9
2	B	61	VAL	2.8
4	D	4	SER	2.7
9	I	25	PHE	2.7
2	O	32[A]	PHE	2.7
1	N	113[A]	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
7	G	30	LEU	2.6
2	B	113	TYR	2.6
2	B	65	TRP	2.6
4	Q	35	ALA	2.6
3	C	38	ASN	2.6
11	X	7	PRO	2.5
7	G	33	LEU	2.5
8	H	47	GLY	2.5
2	B	87[A]	MET	2.5
9	I	37	PHE	2.4
2	B	115	ASP	2.4
2	B	58	ALA	2.4
4	Q	39	ALA	2.4
12	L	24	MET	2.4
7	G	35	SER	2.4
1	A	513	LEU	2.4
5	R	108	LYS	2.4
13	Z	38	ASP	2.4
2	O	22[A]	HIS	2.4
9	V	72	ALA	2.3
8	H	46	LYS	2.3
7	T	30	LEU	2.3
2	B	90	ILE	2.3
8	U	52	VAL	2.3
8	U	61	LYS	2.3
11	K	47	ARG	2.2
3	P	37	PHE	2.2
5	R	7	THR	2.2
9	I	29	LEU	2.2
8	U	44	THR	2.2
10	W	48	TYR	2.1
7	G	41	HIS	2.1
13	Z	13	LYS	2.1
11	X	13	TYR	2.0
10	W	52	TRP	2.0
9	V	26	MET	2.0
13	Z	1	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	FME	A	1	10/11	0.94	0.12	41,50,83,93	0
1	FME	N	1	10/11	0.96	0.12	44,50,80,89	0
2	FME	B	1	10/11	0.97	0.09	33,37,47,89	0
2	FME	O	1	10/11	0.98	0.09	39,41,52,75	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	EDO	P	323	4/4	0.70	0.34	31,34,38,42	4
20	LFA	P	311	11/20	0.71	0.41	54,63,68,71	11
21	DMU	P	318	22/33	0.72	0.32	36,59,75,84	22
21	DMU	O	303	22/33	0.75	0.31	51,66,84,100	22
21	DMU	C	317	22/33	0.76	0.29	40,64,71,80	22
22	EDO	C	322	4/4	0.77	0.32	33,37,40,42	4
21	DMU	B	309	22/33	0.78	0.33	47,73,81,83	22
20	LFA	C	308	6/20	0.78	0.40	41,47,56,57	6
21	DMU	P	320	33/33	0.79	0.30	51,78,102,106	33
21	DMU	A	610	7/33	0.79	0.38	54,59,68,69	7
21	DMU	C	318	33/33	0.79	0.35	38,54,71,79	33
22	EDO	E	201	4/4	0.80	0.36	40,40,42,50	4
26	CHD	P	306	29/29	0.80	0.20	68,75,100,107	0
21	DMU	C	315	33/33	0.81	0.34	42,56,65,71	33
22	EDO	A	613	4/4	0.81	0.33	37,42,49,51	4
26	CHD	C	305	29/29	0.82	0.17	58,78,102,113	0
20	LFA	C	311	14/20	0.82	0.36	38,60,68,69	14
20	LFA	P	309	6/20	0.83	0.38	44,47,54,54	6
21	DMU	C	324	33/33	0.83	0.20	39,57,77,84	33
21	DMU	N	609	7/33	0.83	0.36	63,70,79,80	7
21	DMU	N	610	33/33	0.83	0.24	43,55,78,87	33
20	LFA	C	326	15/20	0.83	0.34	46,52,60,61	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	LFA	P	301	15/20	0.83	0.31	46,51,69,70	15
21	DMU	P	319	33/33	0.83	0.32	46,56,76,93	33
21	DMU	C	319	33/33	0.84	0.23	41,61,73,79	33
20	LFA	P	313	11/20	0.84	0.31	36,52,61,64	11
21	DMU	B	303	11/33	0.85	0.33	49,58,64,76	11
21	DMU	P	324	33/33	0.85	0.21	44,63,90,102	33
21	DMU	W	101	11/33	0.85	0.35	59,72,81,81	11
21	DMU	M	102	8/33	0.85	0.24	41,49,54,62	8
20	LFA	C	314	13/20	0.85	0.28	51,57,70,73	13
20	LFA	C	310	11/20	0.85	0.32	58,66,76,78	11
20	LFA	P	312	14/20	0.85	0.32	39,57,69,76	14
20	LFA	C	313	15/20	0.85	0.25	45,54,68,70	15
20	LFA	P	308	11/20	0.85	0.30	39,51,62,62	11
21	DMU	P	317	7/33	0.86	0.27	49,55,61,71	7
21	DMU	A	623	11/33	0.86	0.30	38,52,71,74	11
20	LFA	O	301	17/20	0.86	0.28	39,55,74,77	17
20	LFA	O	302	11/20	0.86	0.30	47,57,68,75	11
20	LFA	C	312	11/20	0.86	0.30	42,53,61,64	11
21	DMU	P	316	33/33	0.86	0.27	47,56,68,73	33
20	LFA	A	609	14/20	0.87	0.25	37,47,58,60	14
22	EDO	N	612	4/4	0.87	0.30	39,43,48,53	4
19	CDL	V	101	64/100	0.87	0.18	49,81,123,144	0
21	DMU	J	101	11/33	0.87	0.33	56,63,71,72	11
20	LFA	C	309	18/20	0.87	0.22	38,49,60,64	18
19	CDL	C	304	87/100	0.88	0.18	41,79,116,134	0
21	DMU	A	622	33/33	0.88	0.22	35,45,53,70	33
21	DMU	Q	201	33/33	0.88	0.20	38,51,63,74	33
20	LFA	B	308	17/20	0.88	0.27	39,57,72,79	17
22	EDO	A	612	4/4	0.88	0.17	27,30,32,33	4
20	LFA	C	307	11/20	0.88	0.28	42,48,59,66	11
21	DMU	B	304	11/33	0.88	0.27	34,56,68,69	11
19	CDL	P	305	87/100	0.88	0.19	40,81,132,164	0
19	CDL	A	607	64/100	0.88	0.17	49,78,115,131	0
20	LFA	G	104	14/20	0.88	0.26	35,46,61,64	14
23	XE	N	618	1/1	0.88	0.17	48,48,48,48	1
20	LFA	A	608	14/20	0.88	0.25	39,47,68,80	14
20	LFA	P	315	13/20	0.88	0.23	42,55,74,75	13
21	DMU	C	323	22/33	0.89	0.24	45,56,63,65	22
21	DMU	Z	102	22/33	0.89	0.34	55,62,74,78	22
21	DMU	O	306	11/33	0.89	0.32	46,51,64,75	11
21	DMU	A	611	33/33	0.89	0.18	35,48,59,68	33
20	LFA	P	314	15/20	0.89	0.20	41,48,56,61	15

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	LFA	P	310	18/20	0.89	0.23	42,49,59,59	18
21	DMU	N	601	11/33	0.89	0.30	48,63,69,71	11
20	LFA	T	102	11/20	0.89	0.28	50,58,67,76	11
22	EDO	R	203	4/4	0.89	0.27	42,45,53,57	4
23	XE	A	618	1/1	0.89	0.15	47,47,47,47	1
20	LFA	N	608	14/20	0.89	0.25	36,48,67,68	14
21	DMU	N	622	33/33	0.89	0.22	35,47,65,68	33
21	DMU	T	103	22/33	0.89	0.20	43,55,68,69	22
21	DMU	D	201	33/33	0.90	0.18	28,48,55,66	33
21	DMU	C	316	7/33	0.90	0.29	45,57,64,76	7
21	DMU	L	102	22/33	0.90	0.31	51,59,69,75	22
19	CDL	Y	101	94/100	0.90	0.17	51,86,128,150	0
21	DMU	B	305	22/33	0.90	0.21	40,68,86,87	22
22	EDO	P	321	4/4	0.90	0.24	51,52,55,71	4
21	DMU	P	307	11/33	0.91	0.26	44,50,59,73	11
22	EDO	C	320	4/4	0.91	0.29	49,54,60,74	4
21	DMU	O	308	22/33	0.91	0.19	37,48,56,58	22
21	DMU	C	306	11/33	0.92	0.23	51,56,61,69	11
19	CDL	L	101	94/100	0.92	0.15	43,81,126,145	0
22	EDO	A	615	4/4	0.92	0.17	40,45,48,49	4
22	EDO	F	102	4/4	0.92	0.17	24,24,30,33	4
22	EDO	N	615	4/4	0.93	0.20	31,31,34,40	4
22	EDO	E	203	4/4	0.93	0.24	34,38,44,45	4
21	DMU	Z	101	33/33	0.93	0.10	51,58,74,75	0
21	DMU	Z	103	8/33	0.93	0.23	51,54,56,57	8
22	EDO	R	202	4/4	0.94	0.19	37,38,40,40	4
22	EDO	E	202	4/4	0.94	0.23	35,35,36,38	4
22	EDO	S	102	4/4	0.94	0.12	23,25,29,30	4
22	EDO	N	613	4/4	0.94	0.20	30,32,33,35	4
21	DMU	O	307	11/33	0.94	0.23	35,52,60,61	11
22	EDO	C	321	4/4	0.94	0.18	37,37,39,40	4
22	EDO	N	611	4/4	0.94	0.13	30,30,33,33	4
22	EDO	R	201	4/4	0.95	0.27	57,60,62,69	4
22	EDO	O	309	4/4	0.95	0.13	31,33,35,39	4
26	CHD	C	301	29/29	0.95	0.08	33,37,41,42	0
22	EDO	A	614	4/4	0.95	0.17	27,27,30,30	4
22	EDO	G	103	4/4	0.95	0.13	31,33,35,37	4
22	EDO	N	614	4/4	0.96	0.15	36,39,40,40	4
21	DMU	M	101	33/33	0.96	0.08	44,52,66,73	0
22	EDO	T	104	4/4	0.96	0.11	35,36,38,41	4
22	EDO	P	322	4/4	0.96	0.18	36,37,41,43	4
27	UNX	C	302	1/1	0.96	0.17	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	UNX	P	303	1/1	0.96	0.27	45,45,45,45	0
29	PEK	G	101	53/53	0.96	0.12	33,55,91,117	0
29	PEK	T	101	53/53	0.96	0.11	38,54,99,110	0
26	CHD	P	302	29/29	0.97	0.07	34,37,41,44	0
24	PGV	N	621	51/51	0.97	0.10	32,45,78,86	0
26	CHD	B	307	29/29	0.97	0.07	31,34,40,49	0
22	EDO	B	306	4/4	0.97	0.10	26,27,29,32	4
24	PGV	A	621	51/51	0.97	0.09	30,44,77,84	0
26	CHD	G	102	29/29	0.97	0.06	30,33,37,45	0
22	EDO	F	103	4/4	0.98	0.09	32,33,35,35	4
24	PGV	P	304	51/51	0.98	0.09	31,40,88,114	0
23	XE	N	619	1/1	0.98	0.18	43,43,43,43	1
23	XE	P	325	1/1	0.98	0.05	49,49,49,49	1
22	EDO	S	103	4/4	0.98	0.08	33,37,40,41	4
24	PGV	C	303	51/51	0.98	0.09	30,39,100,113	0
14	HEA	A	601[A]	60/60	0.99	0.05	26,29,39,45	9
14	HEA	A	601[B]	60/60	0.99	0.05	26,29,44,46	9
14	HEA	A	602	60/60	0.99	0.05	26,28,36,42	0
14	HEA	N	602[A]	60/60	0.99	0.06	29,32,42,47	9
23	XE	A	619	1/1	0.99	0.11	39,39,39,39	1
14	HEA	N	602[B]	60/60	0.99	0.06	29,32,46,47	9
14	HEA	N	603	60/60	0.99	0.05	28,31,37,42	0
16	MG	A	604	1/1	0.99	0.03	32,32,32,32	0
17	NA	A	605	1/1	0.99	0.05	34,34,34,34	0
18	PER	A	606	2/2	0.99	0.05	27,27,27,37	0
18	PER	N	607	2/2	0.99	0.07	30,30,30,39	0
16	MG	N	605	1/1	1.00	0.02	34,34,34,34	0
15	CU	N	604	1/1	1.00	0.02	31,31,31,31	0
23	XE	A	620	1/1	1.00	0.06	46,46,46,46	1
25	CUA	B	302	2/2	1.00	0.02	31,31,31,31	0
25	CUA	O	305	2/2	1.00	0.02	34,34,34,35	0
23	XE	B	301	1/1	1.00	0.18	46,46,46,46	1
23	XE	C	325	1/1	1.00	0.02	44,44,44,44	1
23	XE	N	616	1/1	1.00	0.14	43,43,43,43	0
23	XE	N	617	1/1	1.00	0.18	42,42,42,42	1
17	NA	N	606	1/1	1.00	0.06	39,39,39,39	0
15	CU	A	603	1/1	1.00	0.01	29,29,29,29	0
23	XE	N	620	1/1	1.00	0.03	46,46,46,46	1
23	XE	O	304	1/1	1.00	0.17	46,46,46,46	1
28	ZN	F	101	1/1	1.00	0.01	36,36,36,36	0
28	ZN	S	101	1/1	1.00	0.01	36,36,36,36	0
23	XE	A	616	1/1	1.00	0.15	43,43,43,43	0

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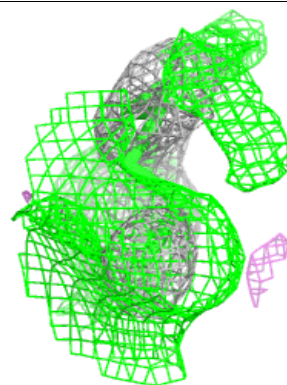
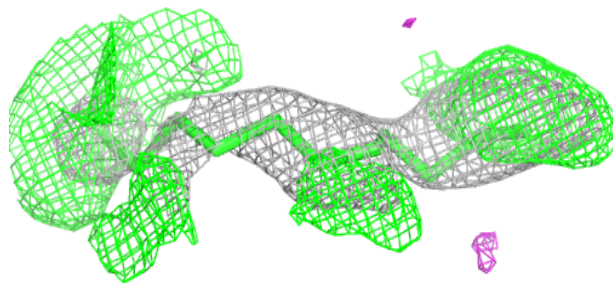
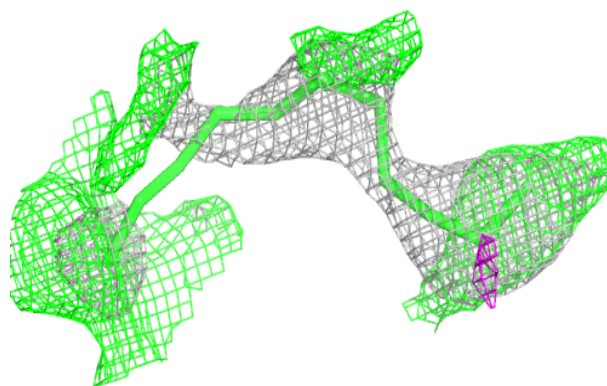
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	XE	A	617	1/1	1.00	0.18	42,42,42,42	1

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.

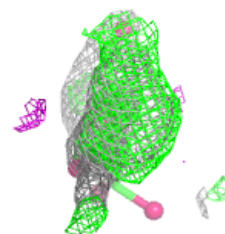
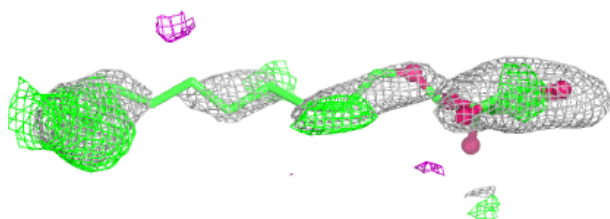
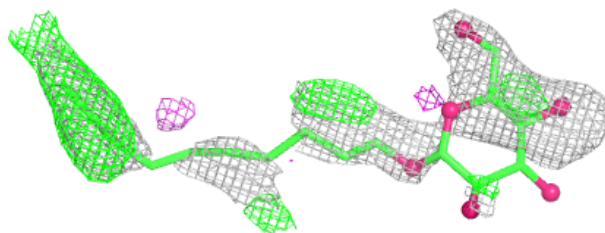
Electron density around LFA P 311:

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

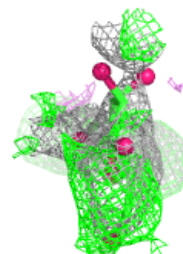
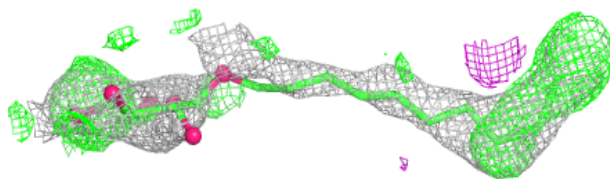
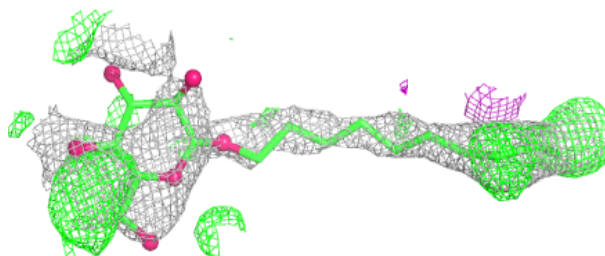


Electron density around DMU P 318:

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

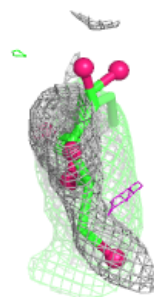
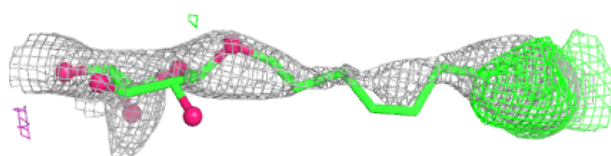
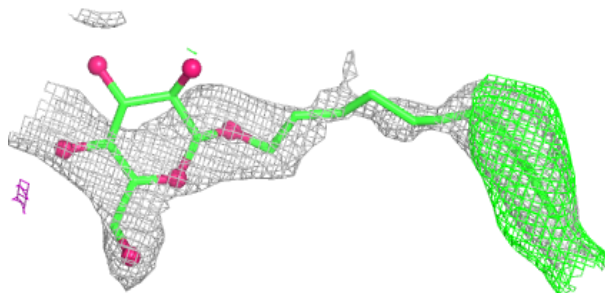
**Electron density around DMU O 303:**

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

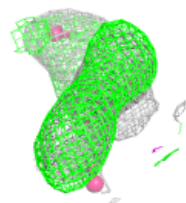
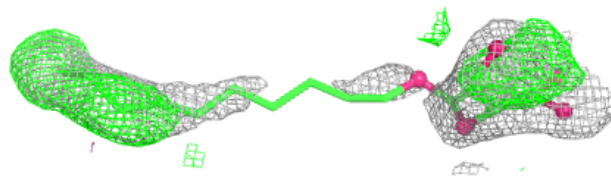
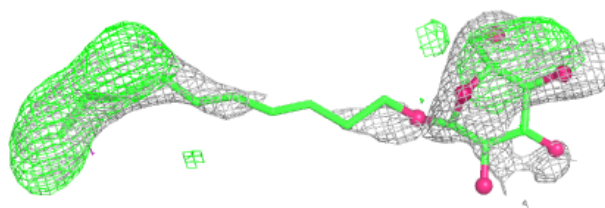


Electron density around DMU C 317:

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

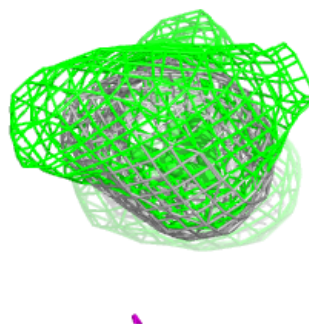
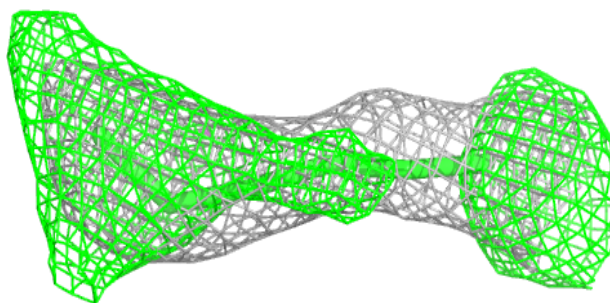
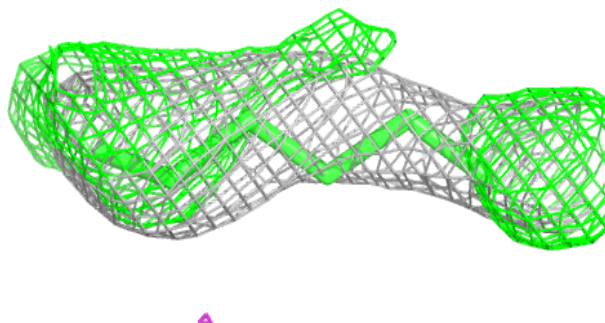
**Electron density around DMU B 309:**

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

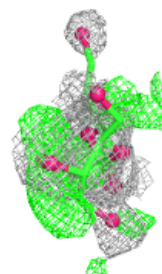
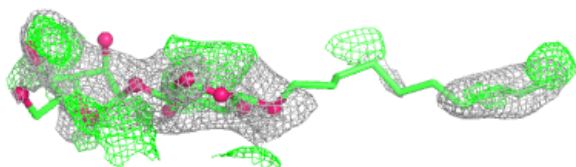
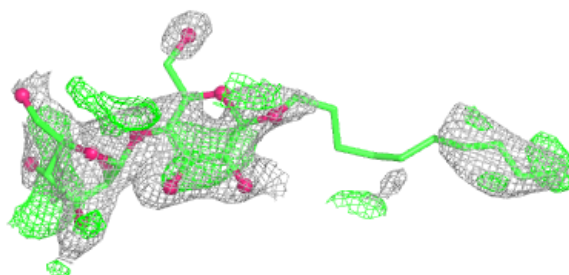


Electron density around LFA C 308:

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

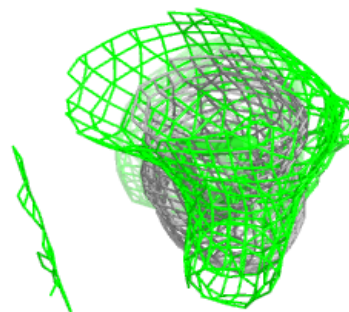
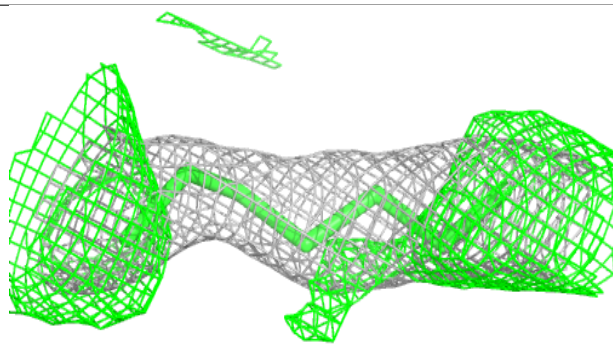
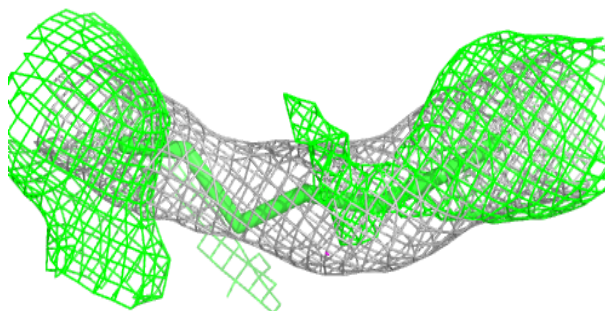
**Electron density around DMU P 320:**

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

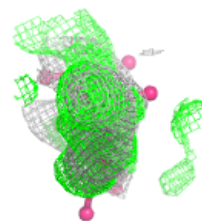
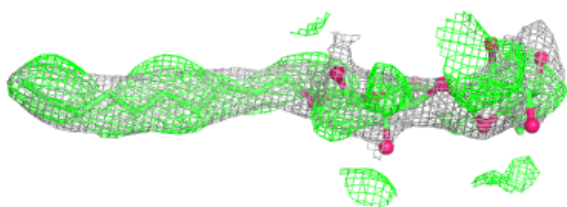
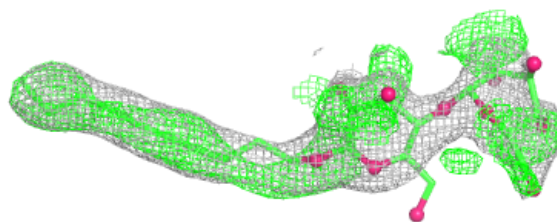


Electron density around DMU A 610:

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

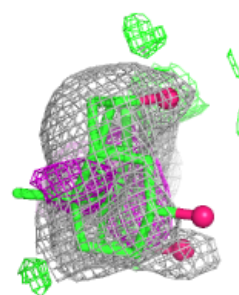
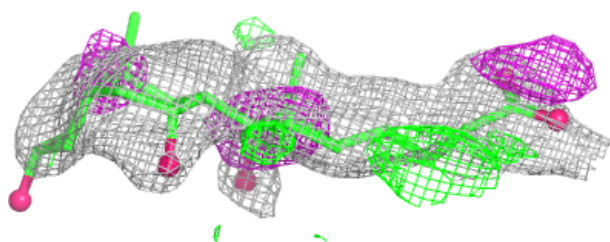
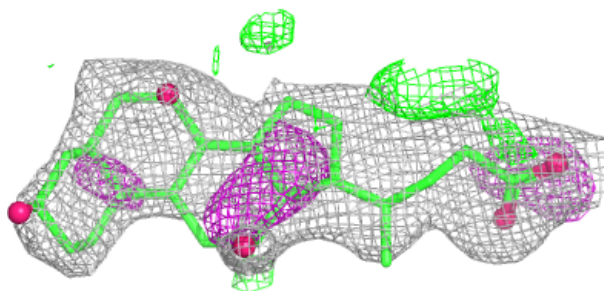
**Electron density around DMU C 318:**

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

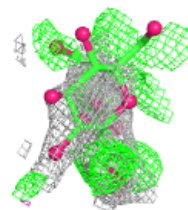
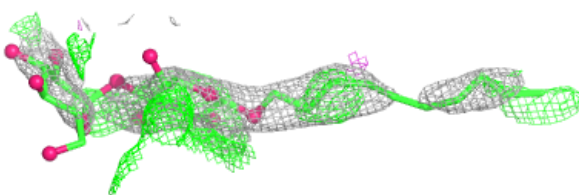
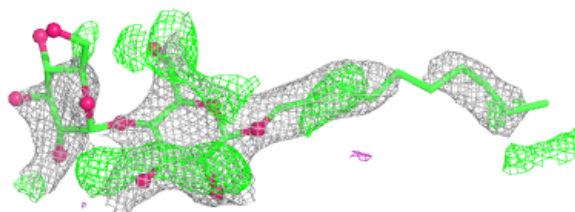


Electron density around CHD P 306:

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

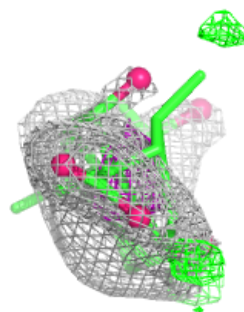
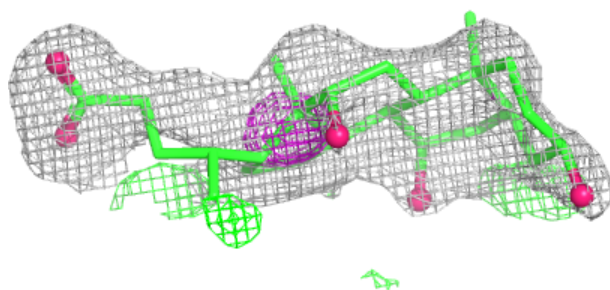
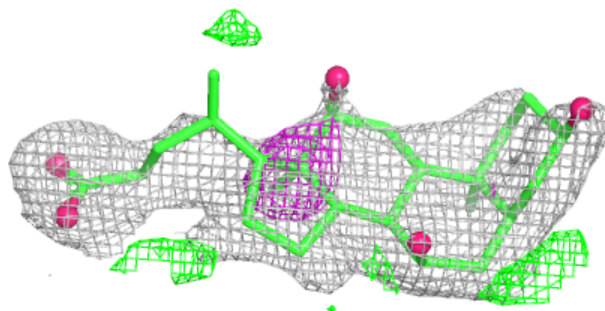
**Electron density around DMU C 315:**

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

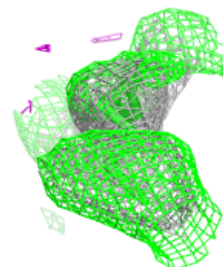
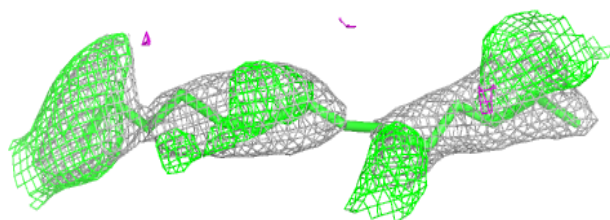
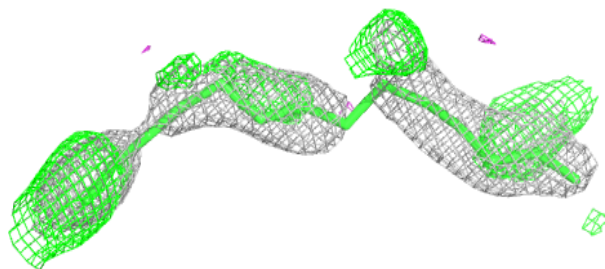


Electron density around CHD C 305:

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

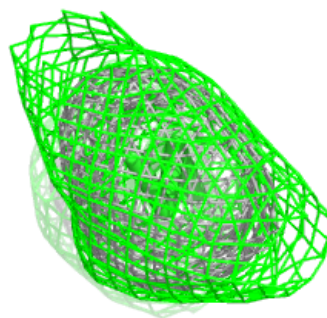
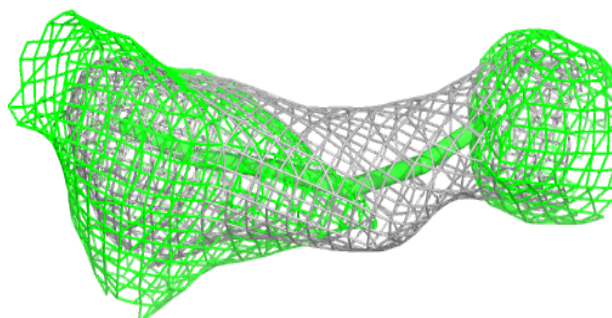
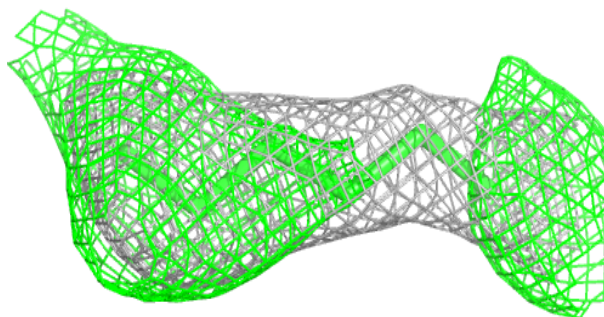
**Electron density around LFA C 311:**

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

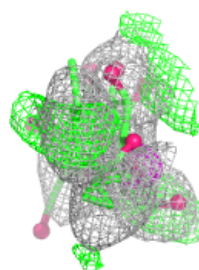
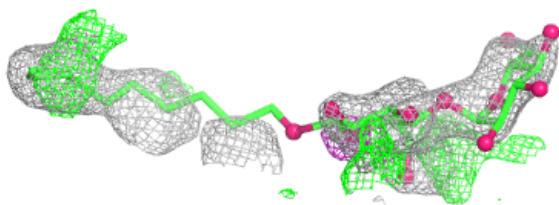
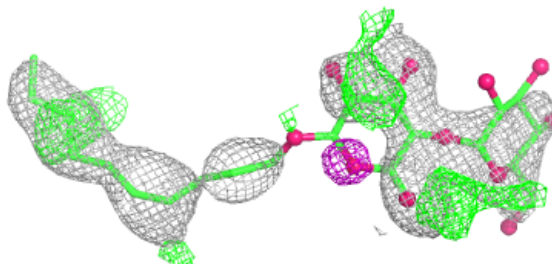


Electron density around LFA P 309:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

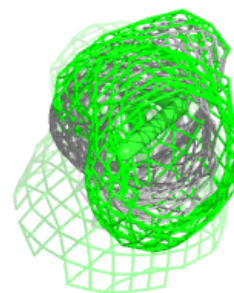
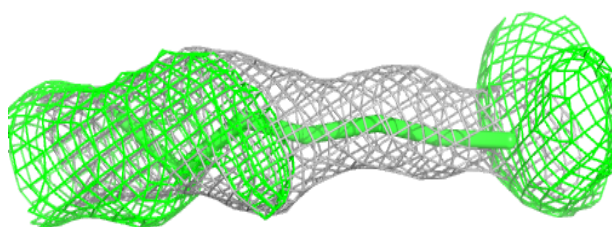
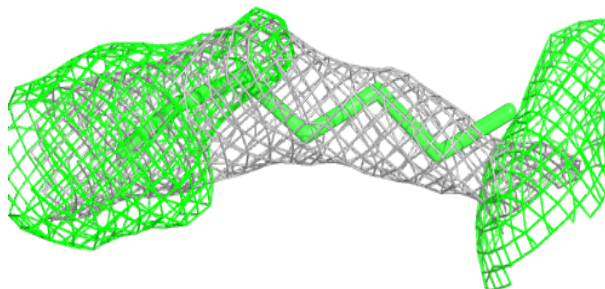
**Electron density around DMU C 324:**

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

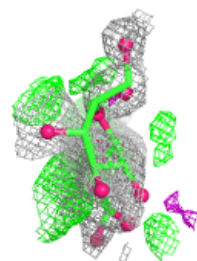
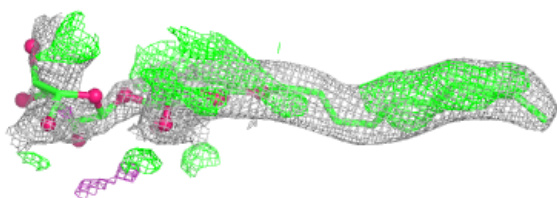
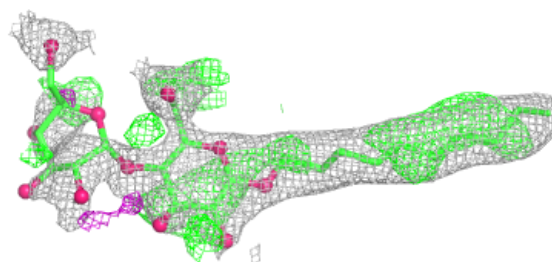


Electron density around DMU N 609:

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

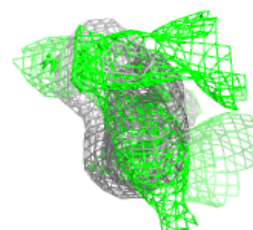
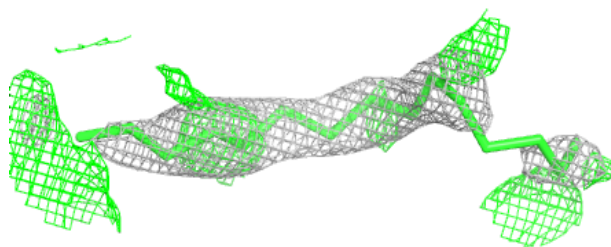
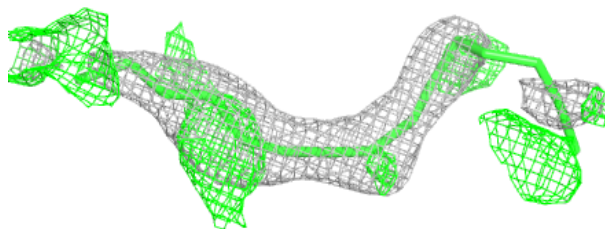
**Electron density around DMU N 610:**

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

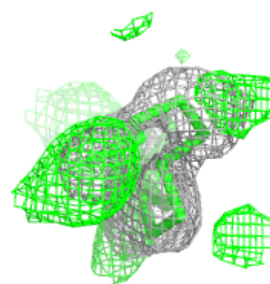
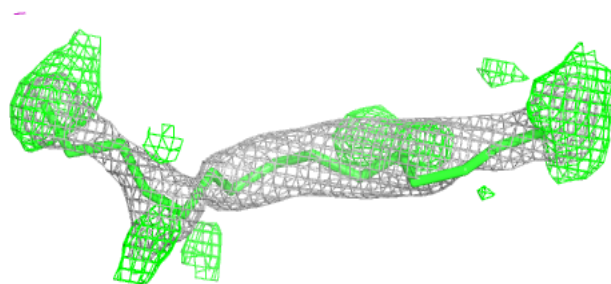
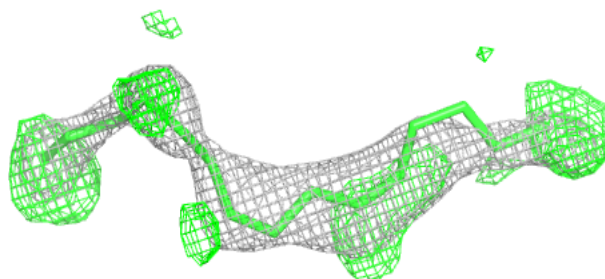


Electron density around LFA C 326:

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

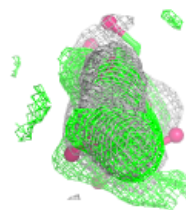
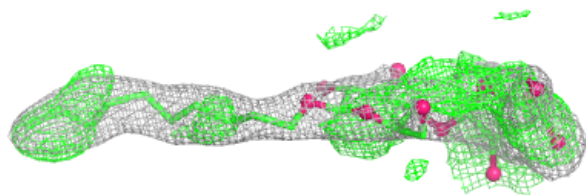
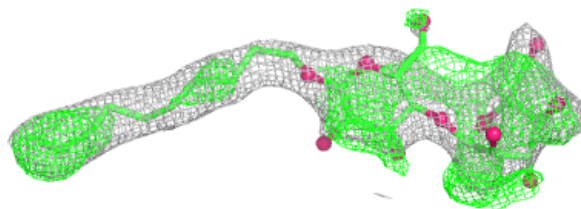
**Electron density around LFA P 301:**

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

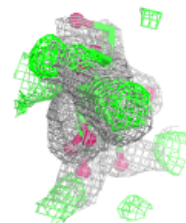
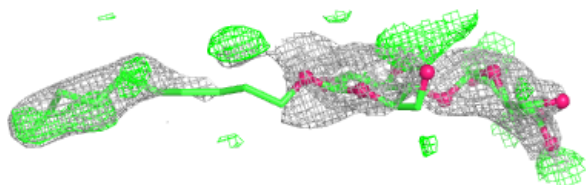
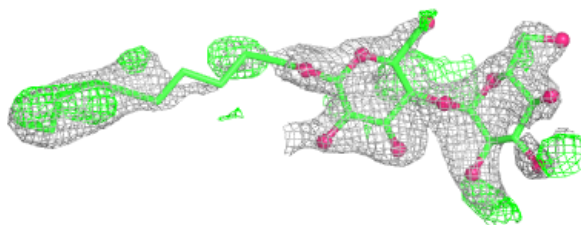


Electron density around DMU P 319:

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

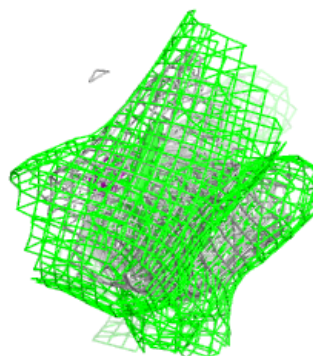
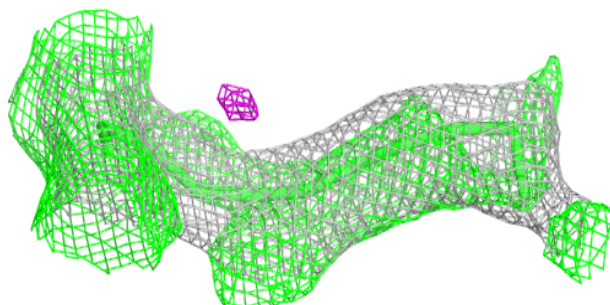
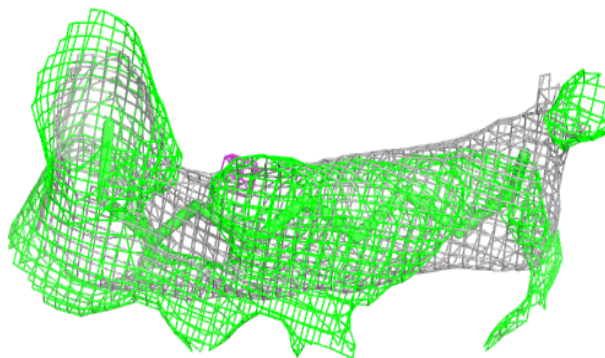
**Electron density around DMU C 319:**

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

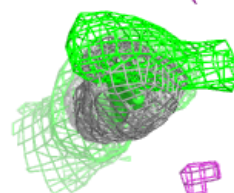
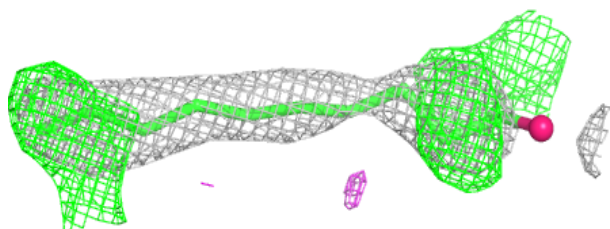
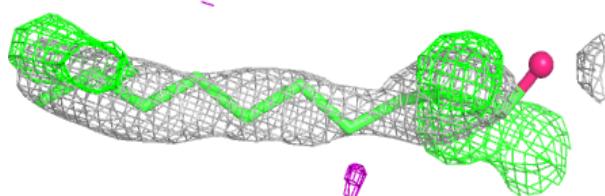


Electron density around LFA P 313:

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

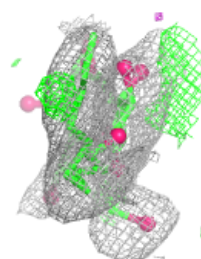
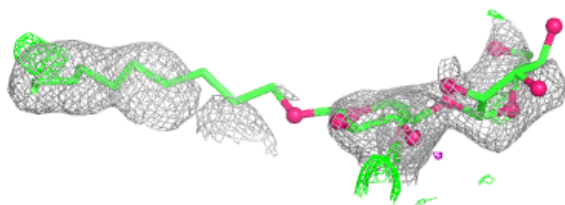
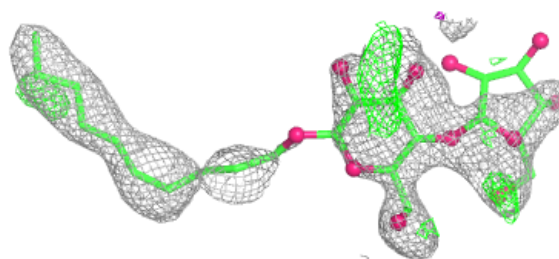
**Electron density around DMU B 303:**

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

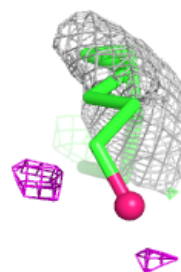
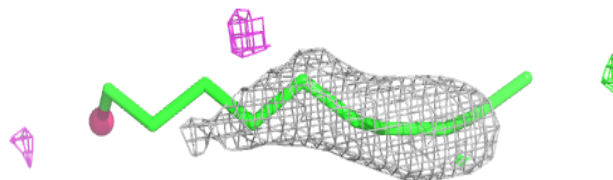
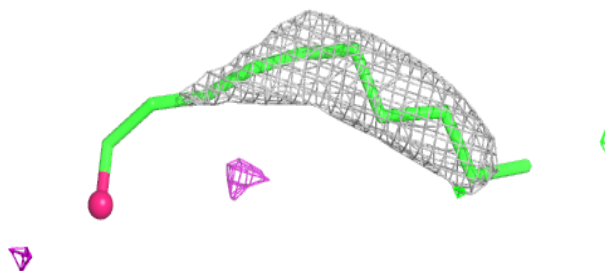


Electron density around DMU P 324:

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

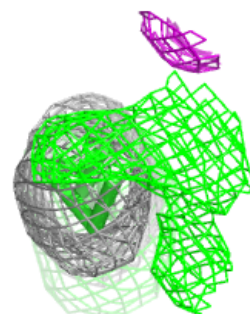
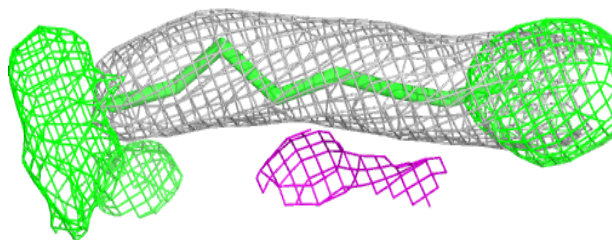
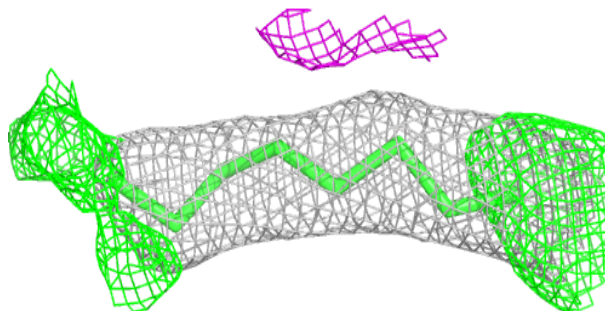
**Electron density around DMU W 101:**

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

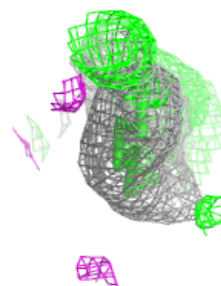
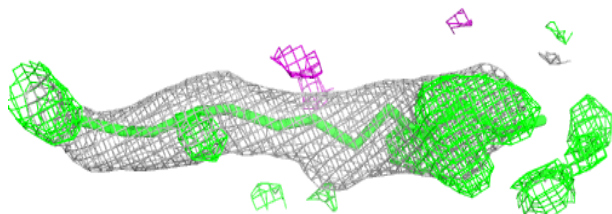
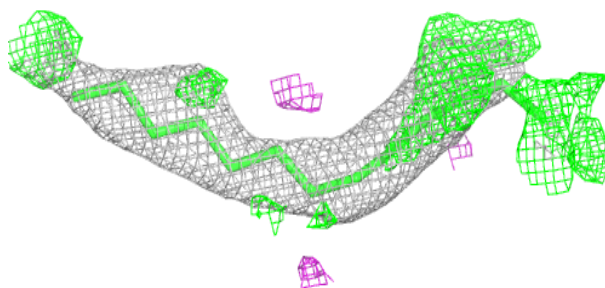


Electron density around DMU M 102:

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

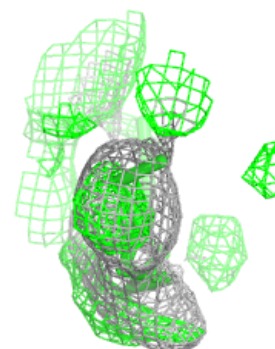
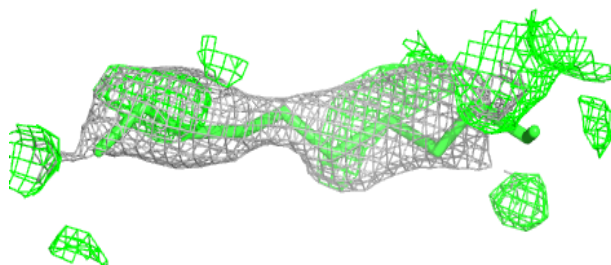
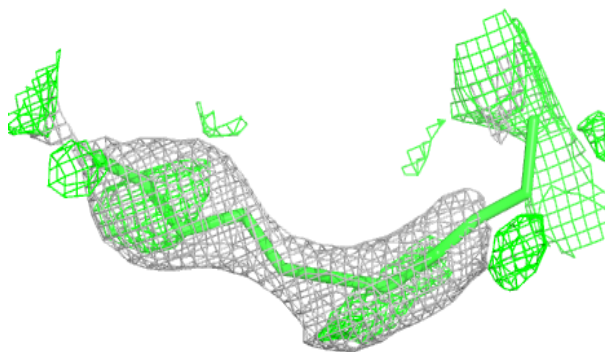
**Electron density around LFA C 314:**

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

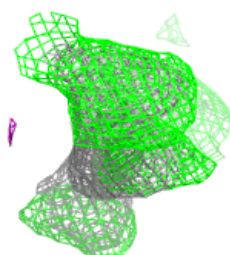
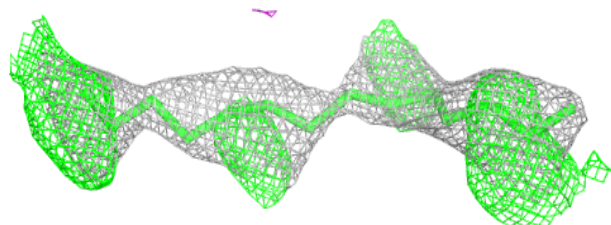
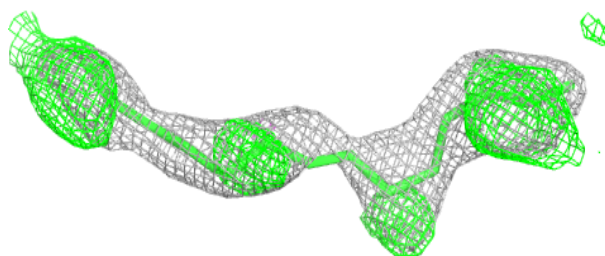


Electron density around LFA C 310:

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

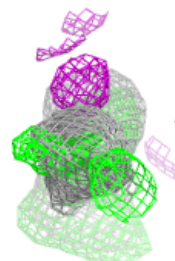
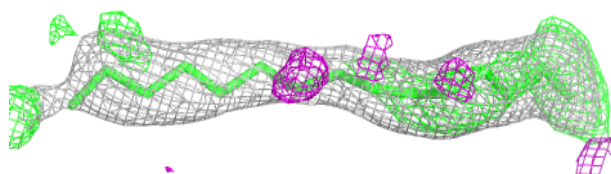
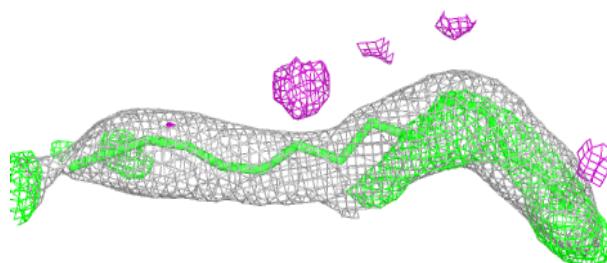
**Electron density around LFA P 312:**

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

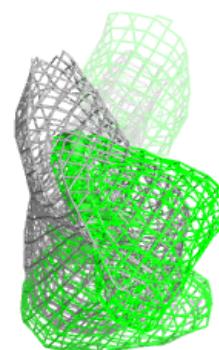
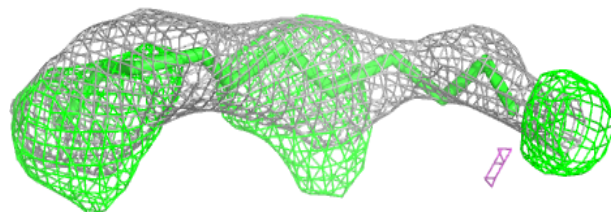
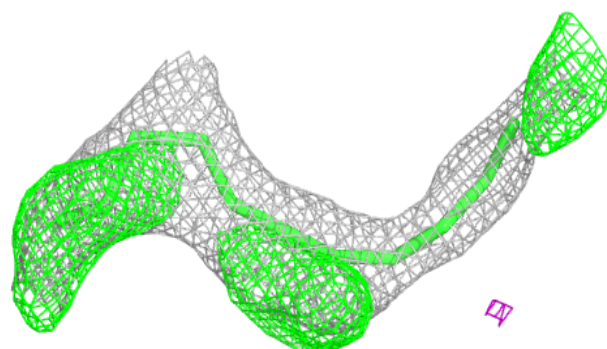


Electron density around LFA C 313:

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

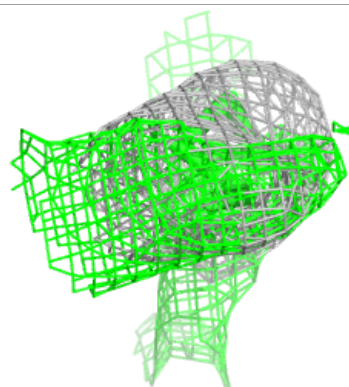
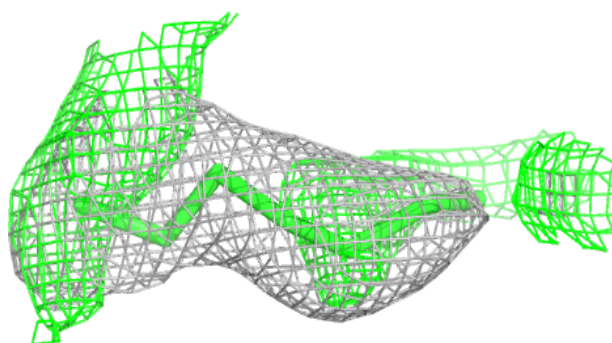
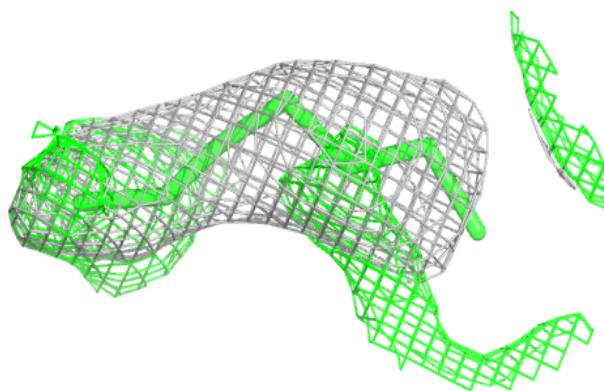
**Electron density around LFA P 308:**

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

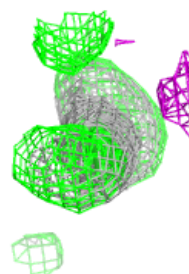
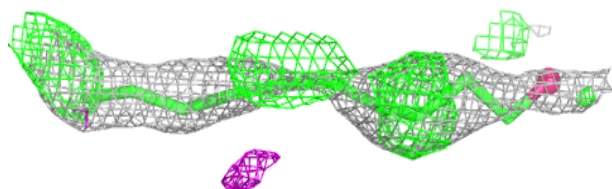
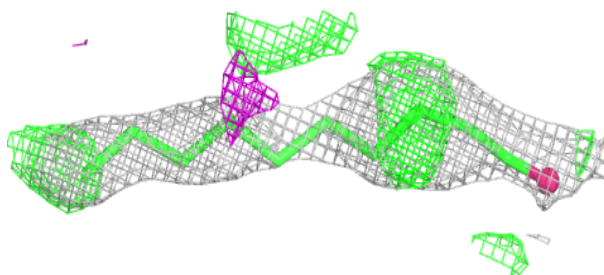


Electron density around DMU P 317:

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

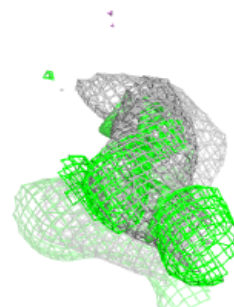
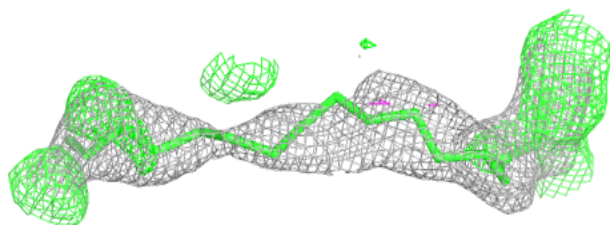
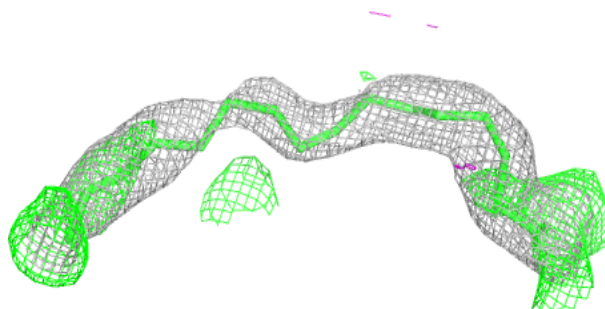
**Electron density around DMU A 623:**

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

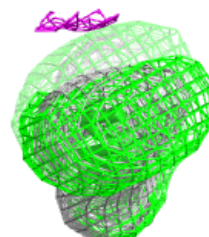
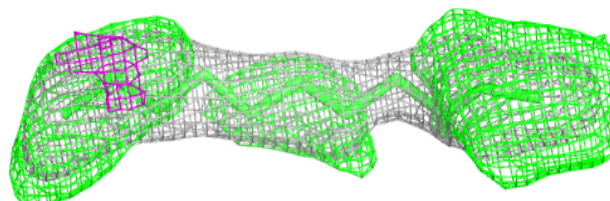
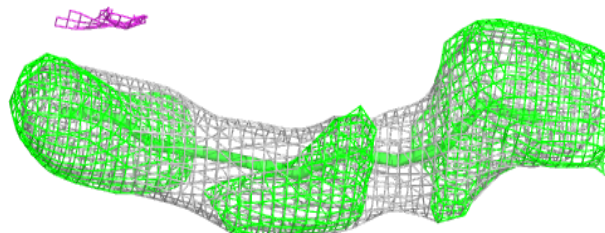


Electron density around LFA O 301:

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

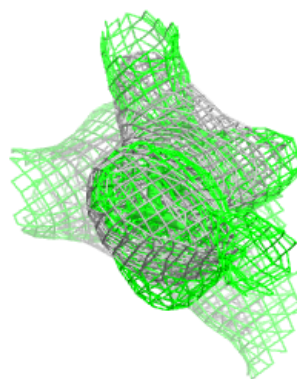
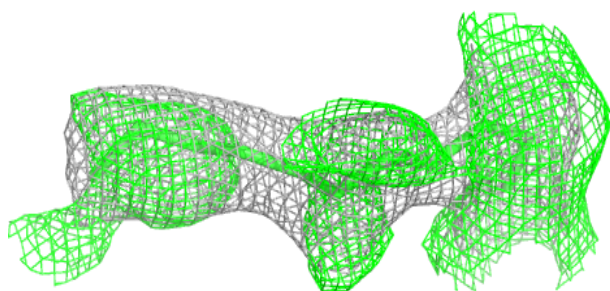
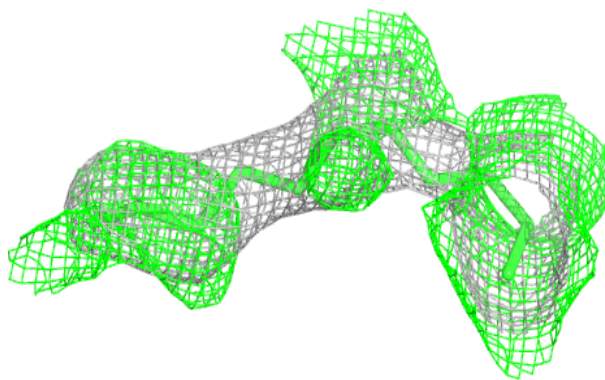
**Electron density around LFA O 302:**

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

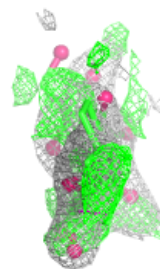
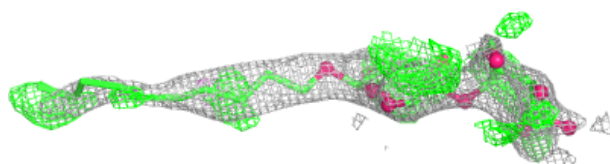
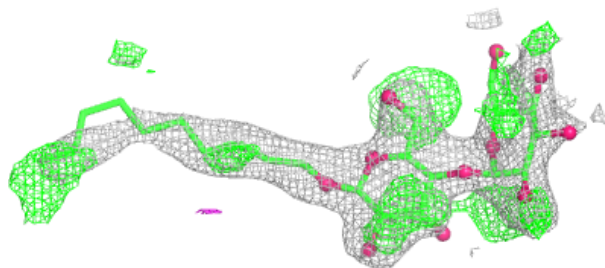


Electron density around LFA C 312:

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

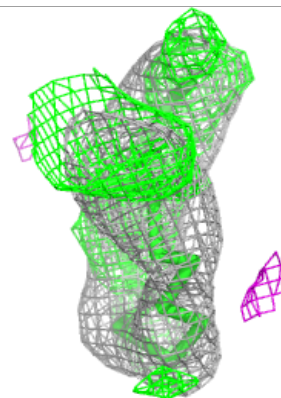
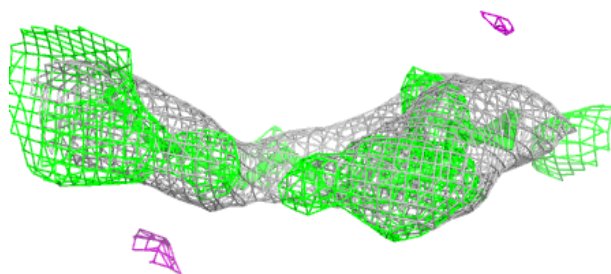
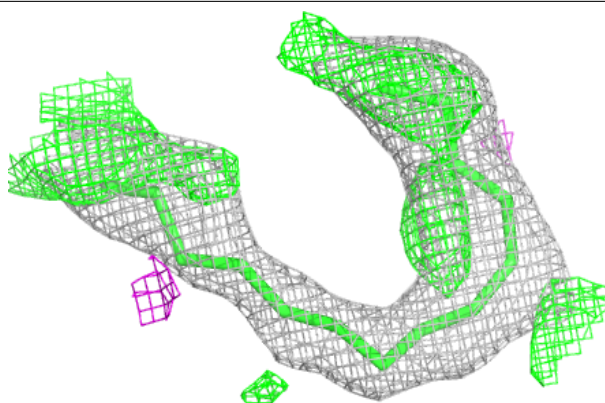
**Electron density around DMU P 316:**

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

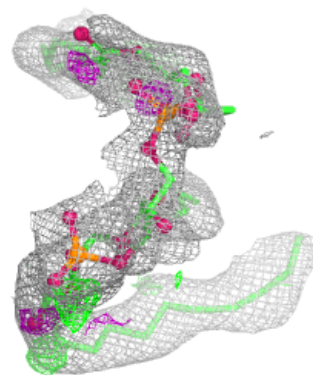
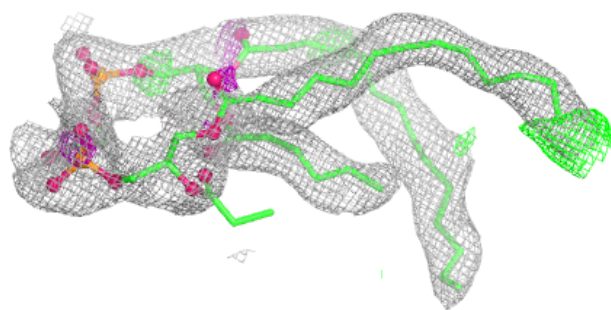
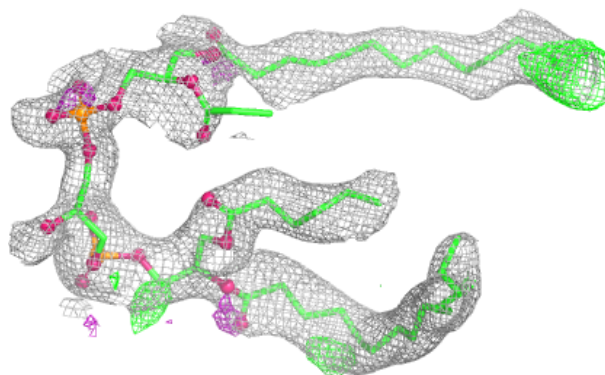


Electron density around LFA A 609:

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

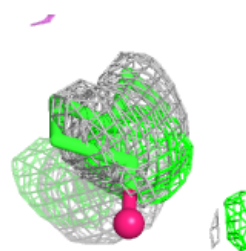
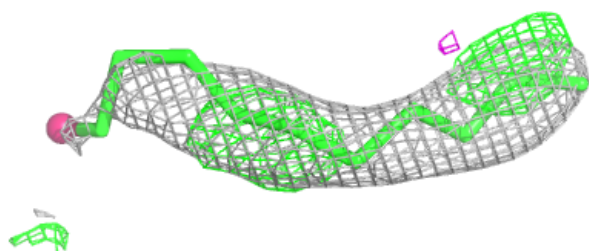
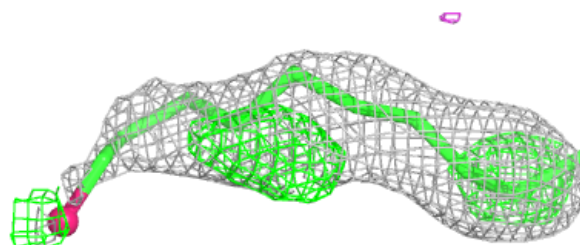
**Electron density around CDL V 101:**

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

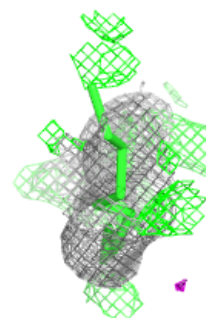
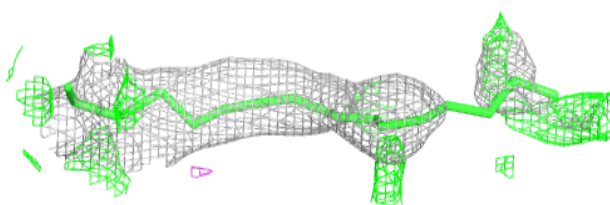
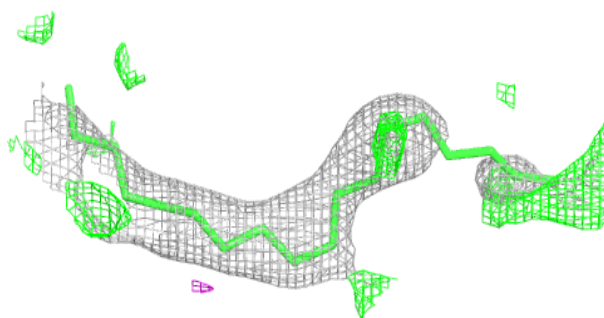


Electron density around DMU J 101:

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

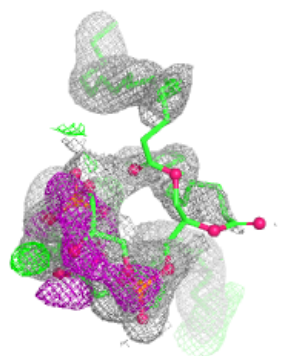
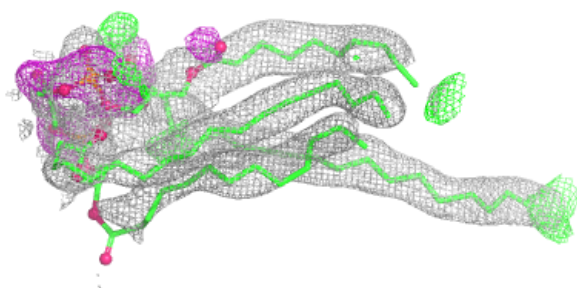
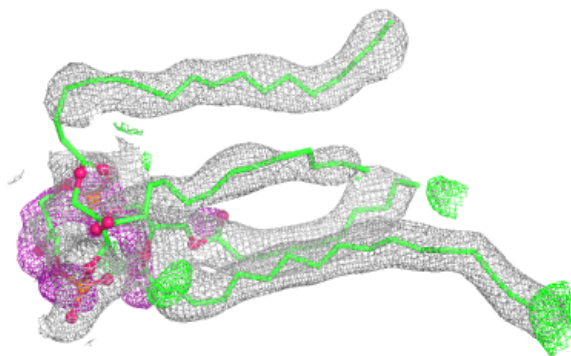
**Electron density around LFA C 309:**

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

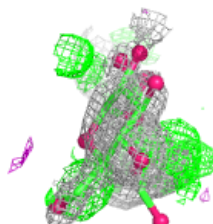
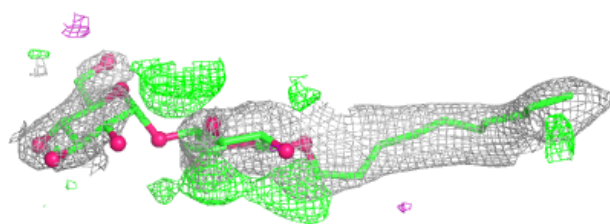
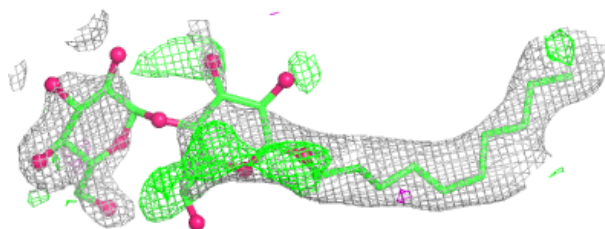


Electron density around CDL C 304:

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

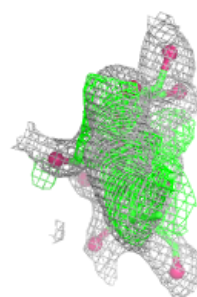
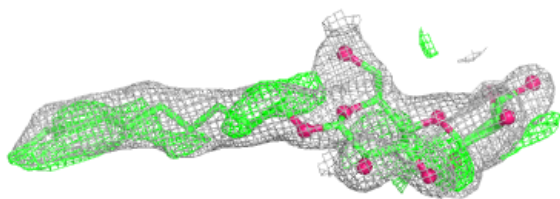
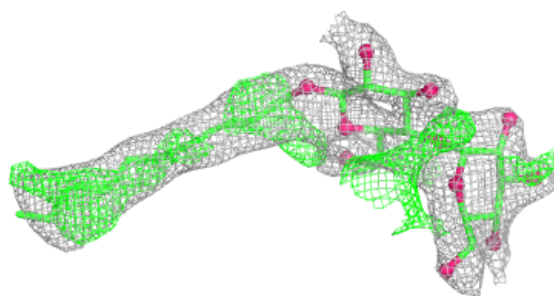
**Electron density around DMU A 622:**

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

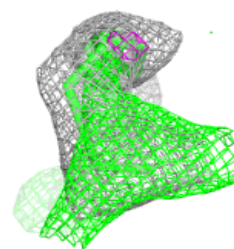
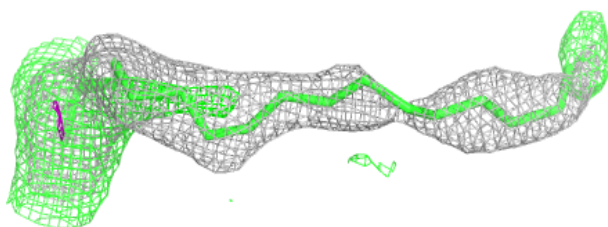
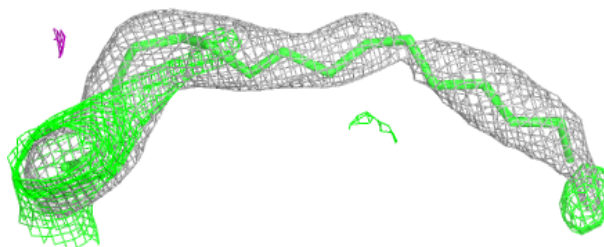


Electron density around DMU Q 201:

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

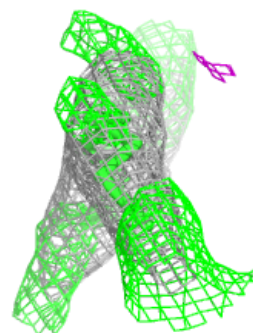
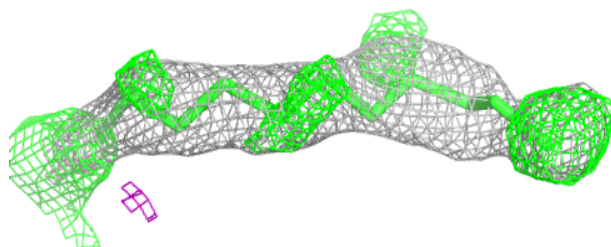
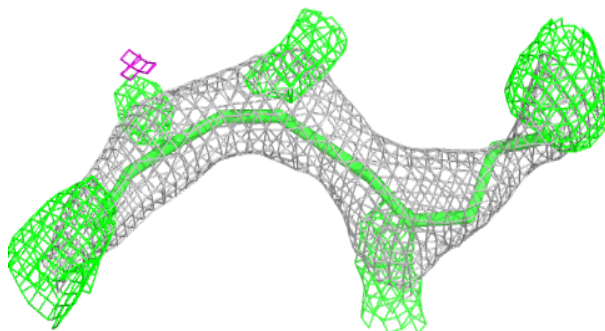
**Electron density around LFA B 308:**

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

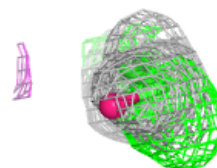
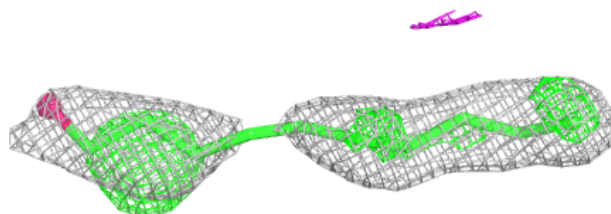
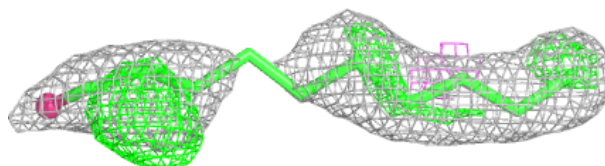


Electron density around LFA C 307:

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

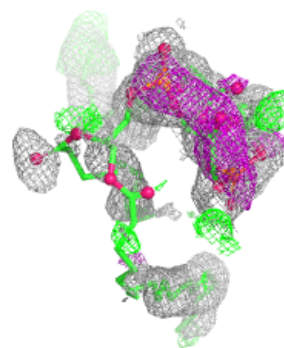
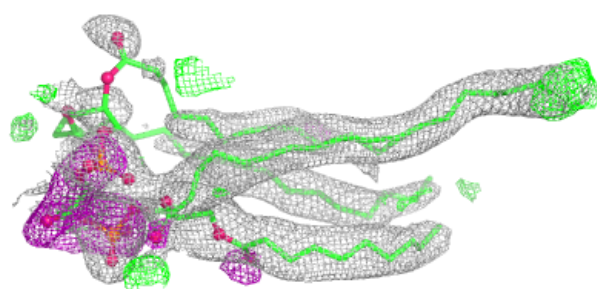
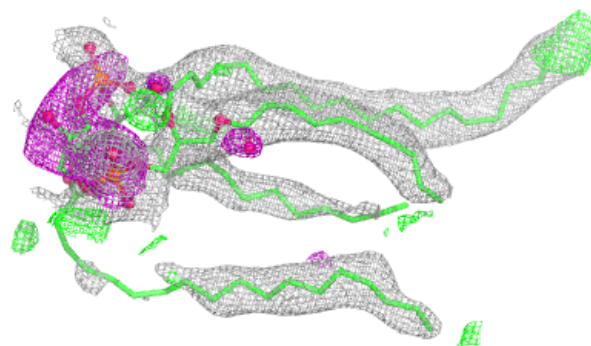
**Electron density around DMU B 304:**

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

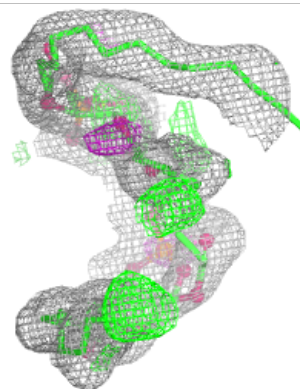
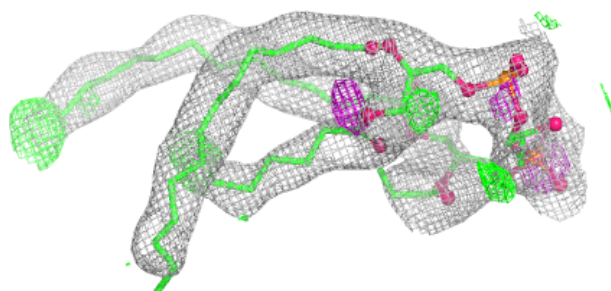
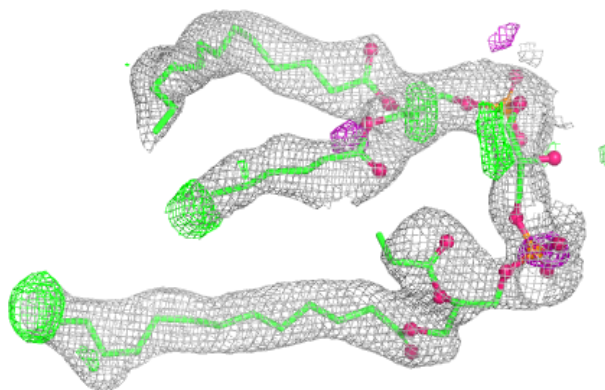


Electron density around CDL P 305:

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

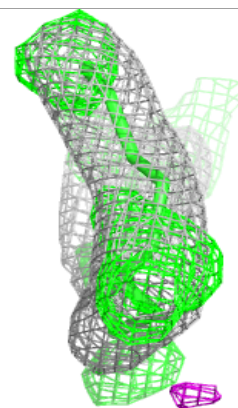
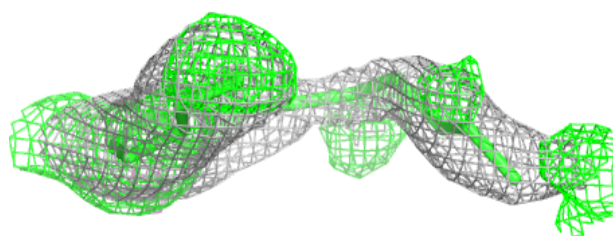
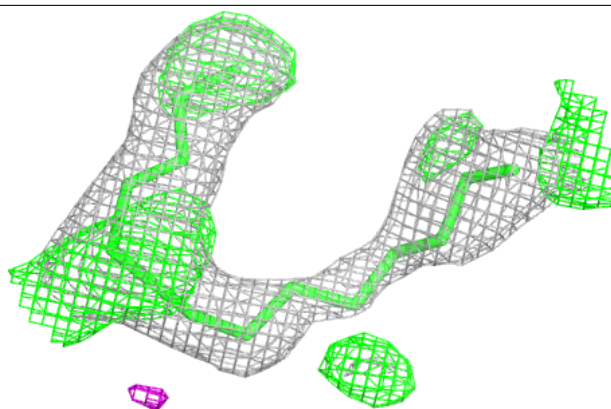
**Electron density around CDL A 607:**

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



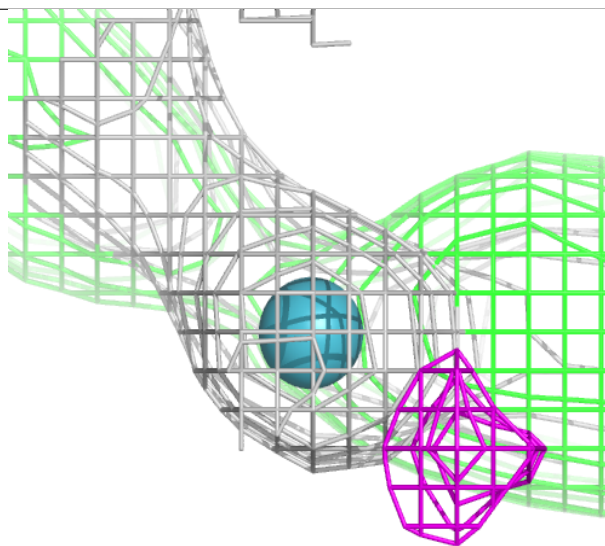
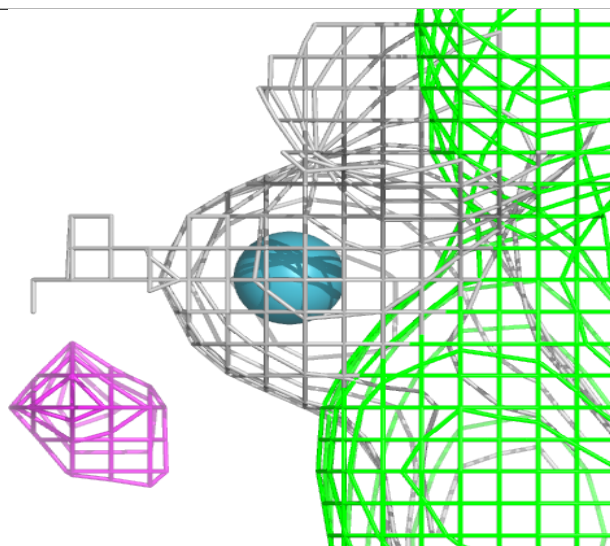
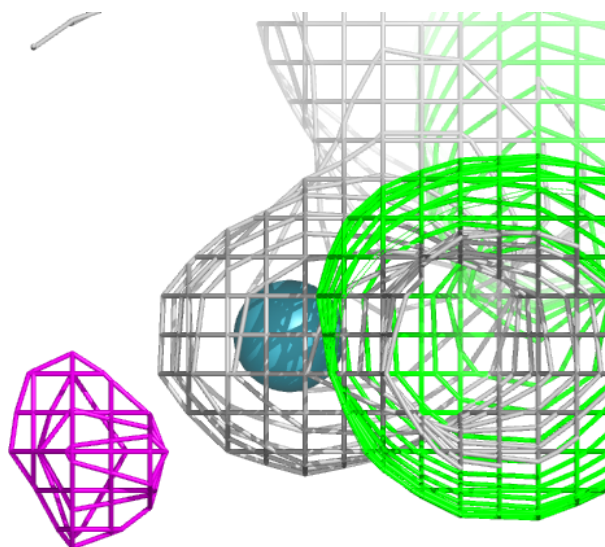
Electron density around LFA G 104:

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



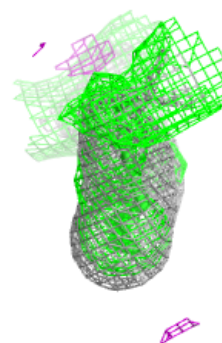
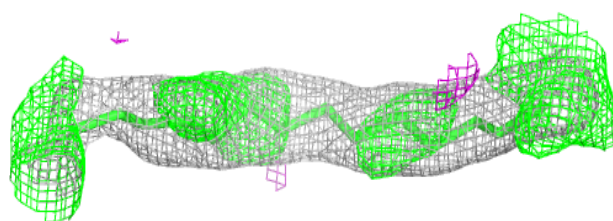
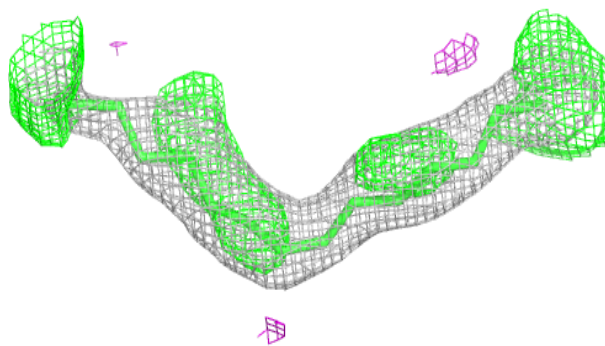
Electron density around XE N 618:

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

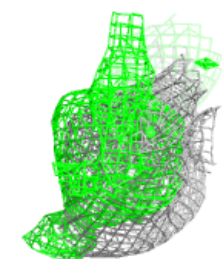
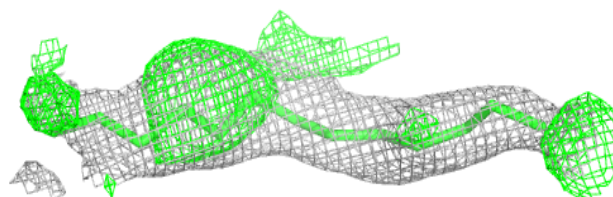
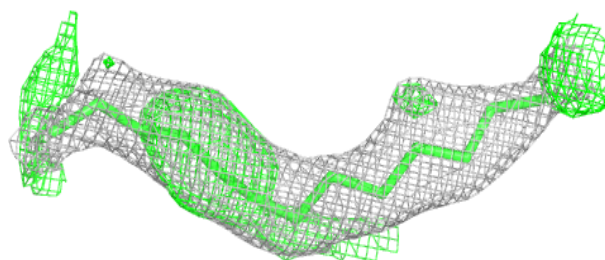


Electron density around LFA A 608:

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

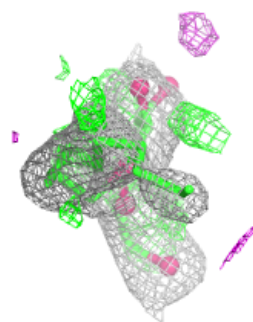
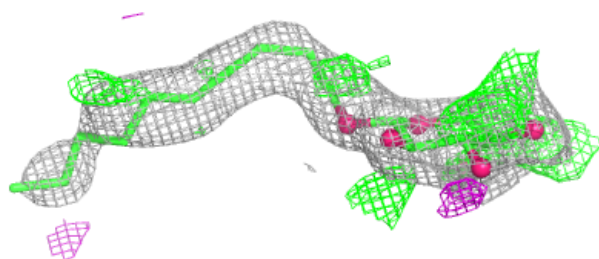
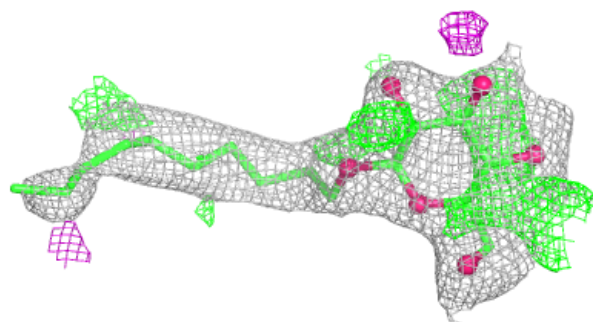
**Electron density around LFA P 315:**

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

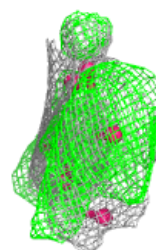
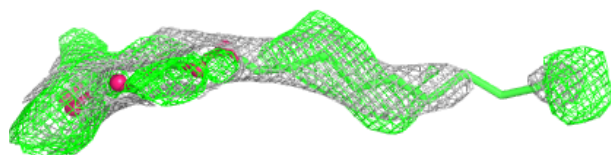
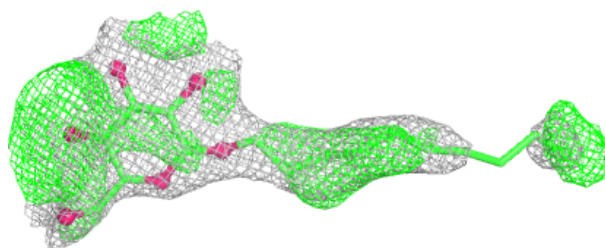


Electron density around DMU C 323:

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

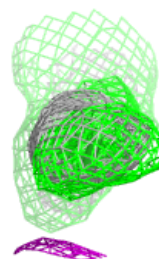
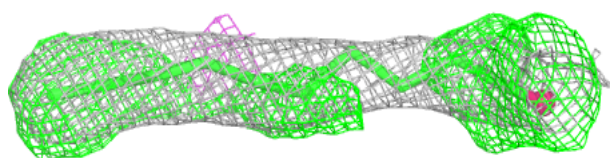
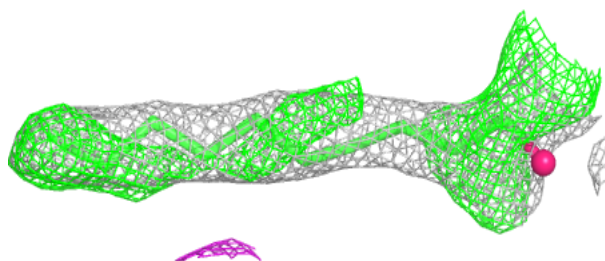
**Electron density around DMU Z 102:**

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

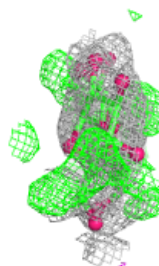
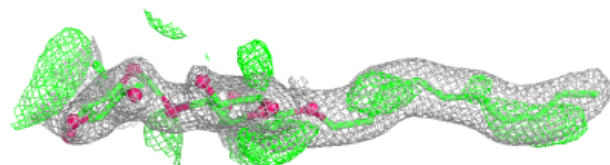
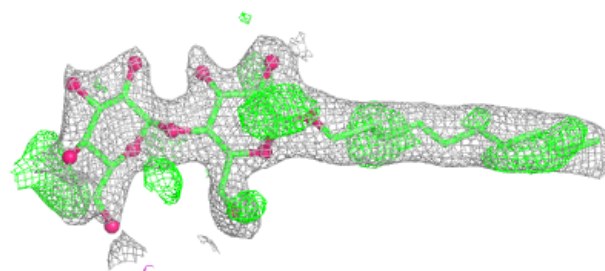


Electron density around DMU O 306:

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

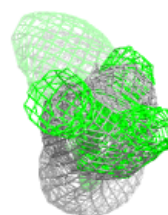
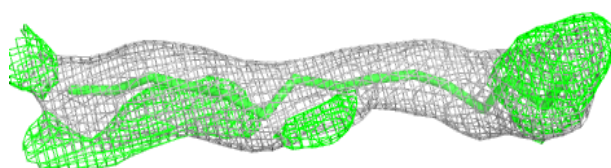
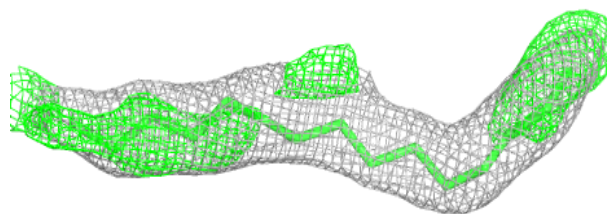
**Electron density around DMU A 611:**

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

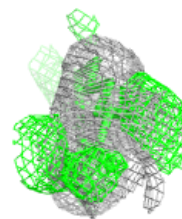
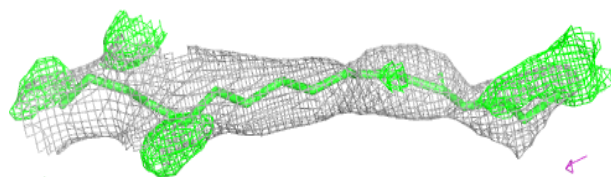
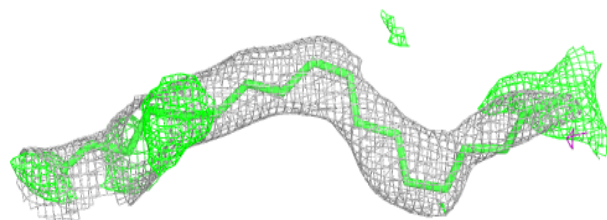


Electron density around LFA P 314:

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

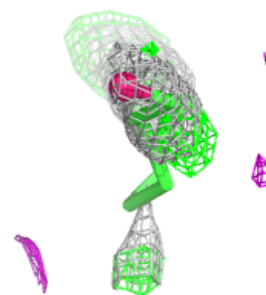
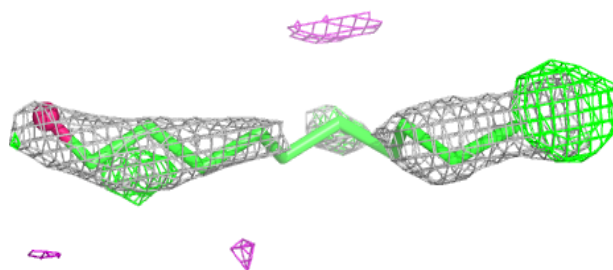
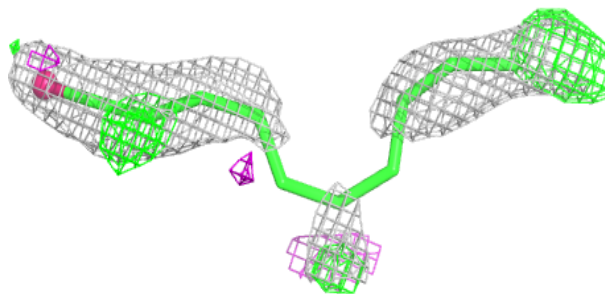
**Electron density around LFA P 310:**

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

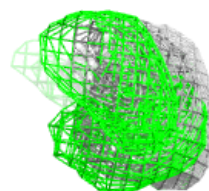
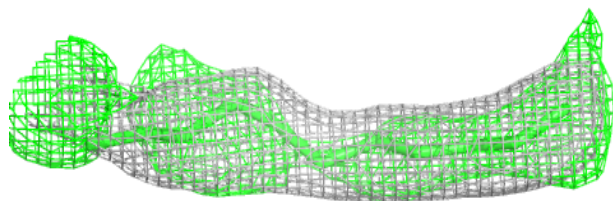
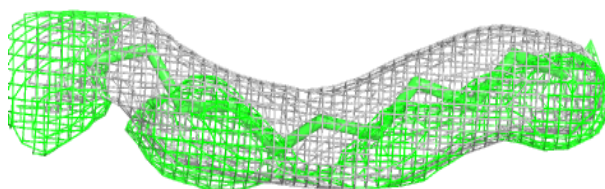


Electron density around DMU N 601:

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

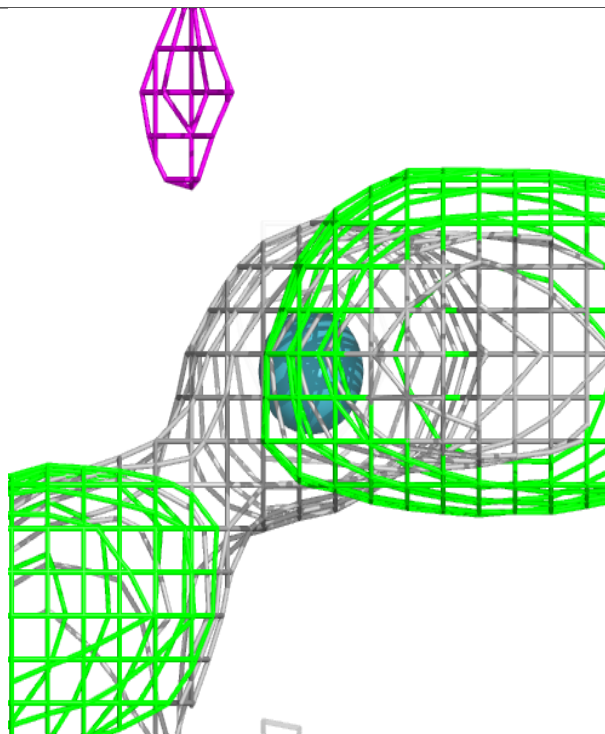
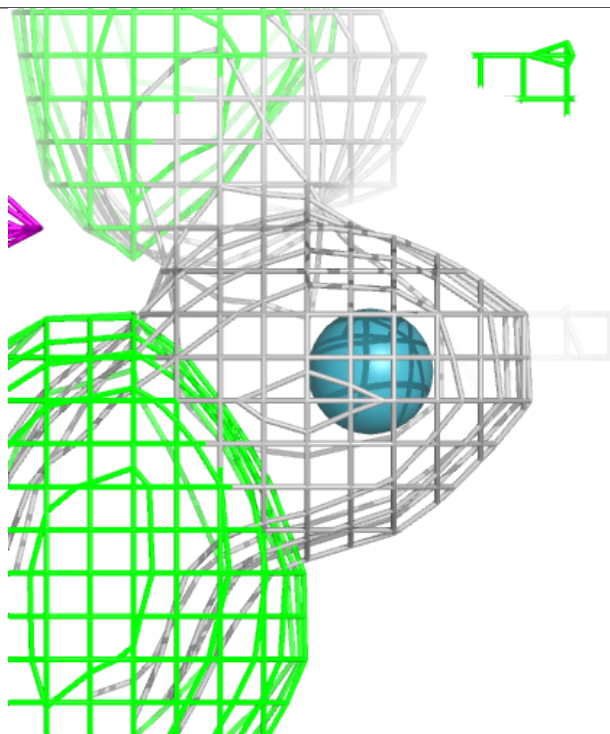
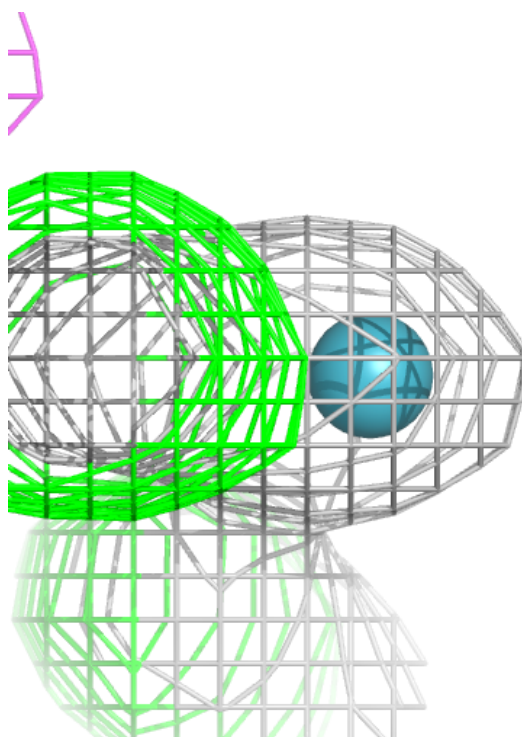
**Electron density around LFA T 102:**

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



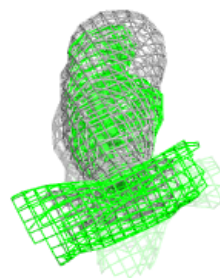
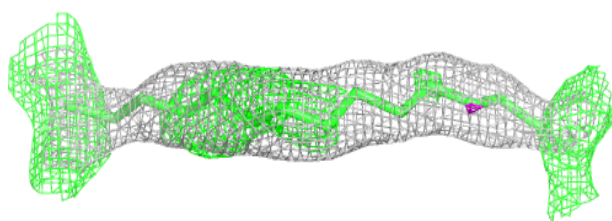
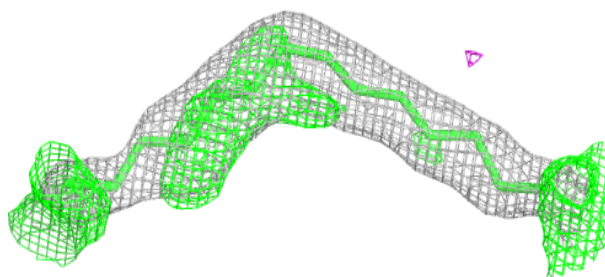
Electron density around XE A 618:

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

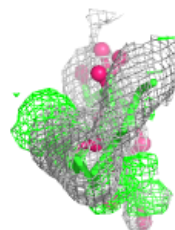
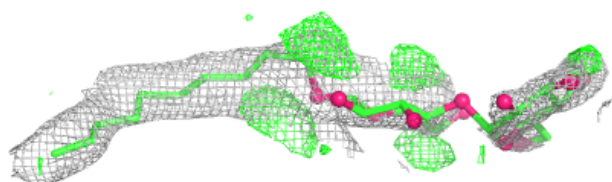
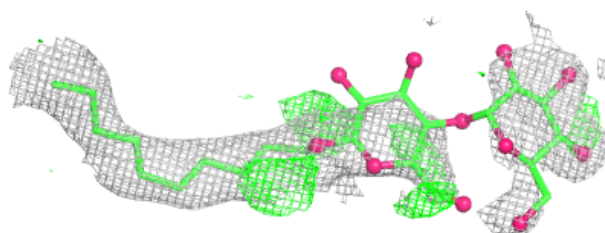


Electron density around LFA N 608:

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

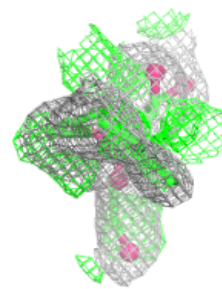
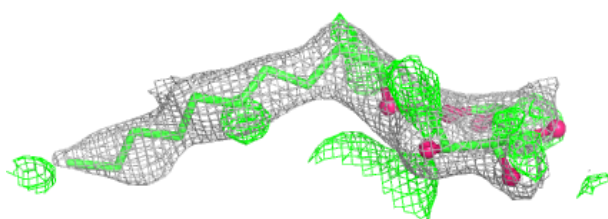
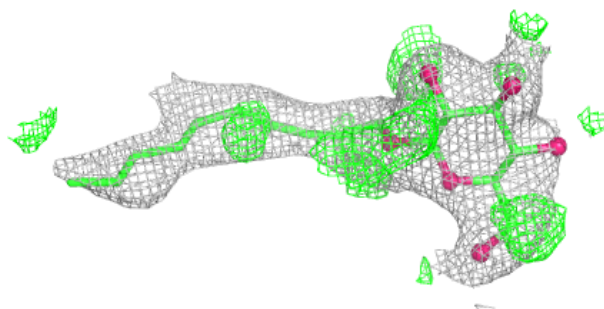
**Electron density around DMU N 622:**

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

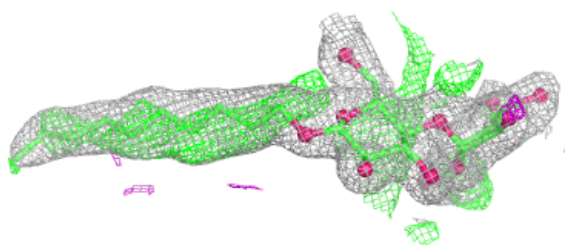
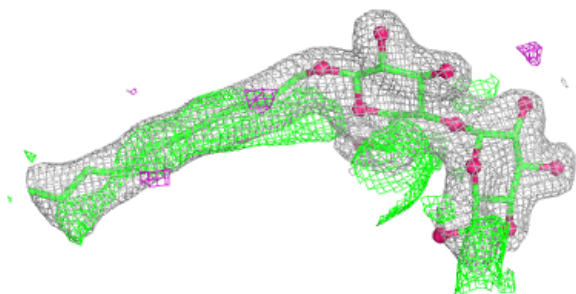


Electron density around DMU T 103:

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

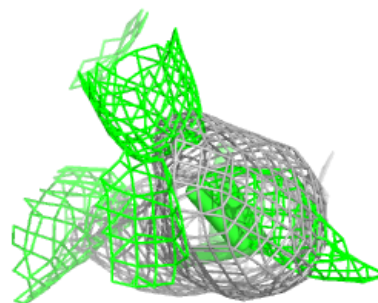
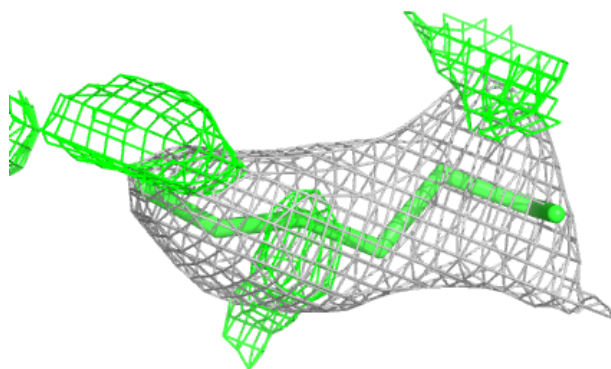
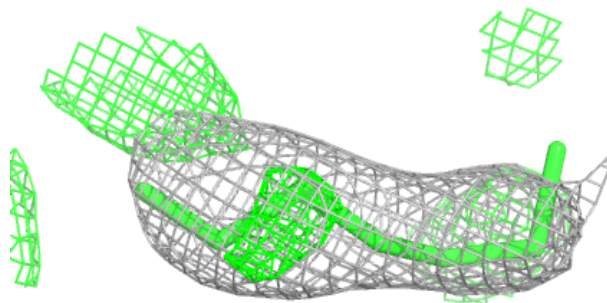
**Electron density around DMU D 201:**

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

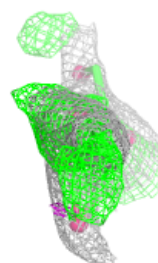
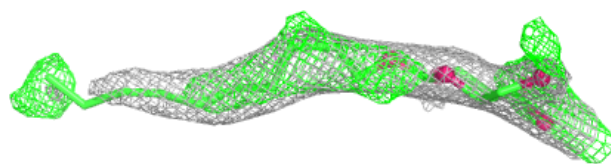
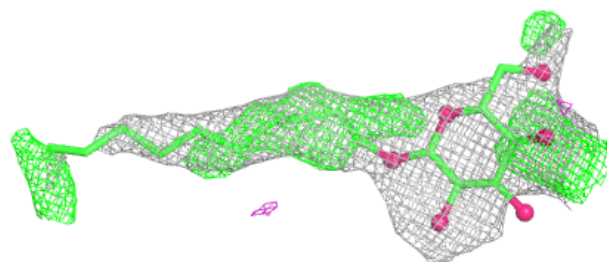


Electron density around DMU C 316:

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

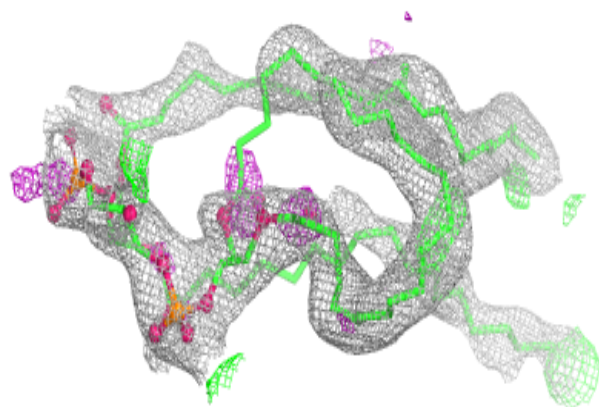
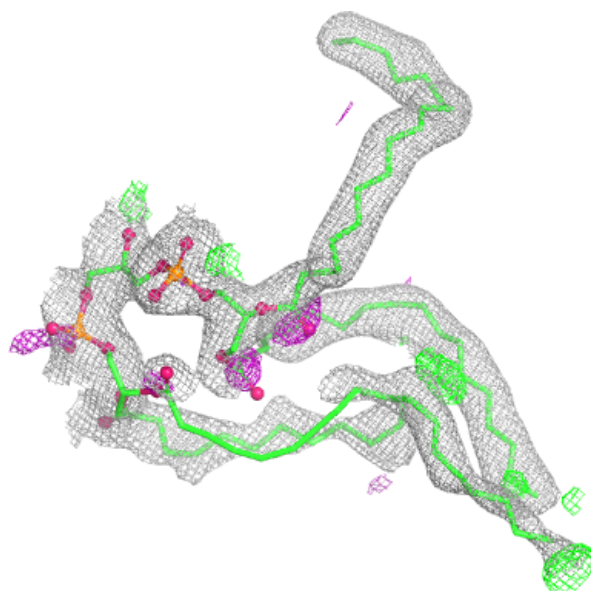
**Electron density around DMU L 102:**

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



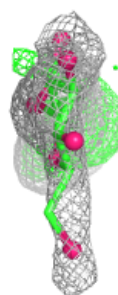
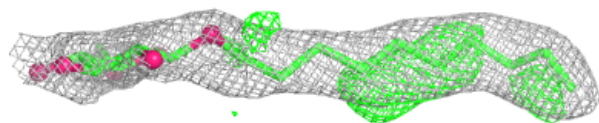
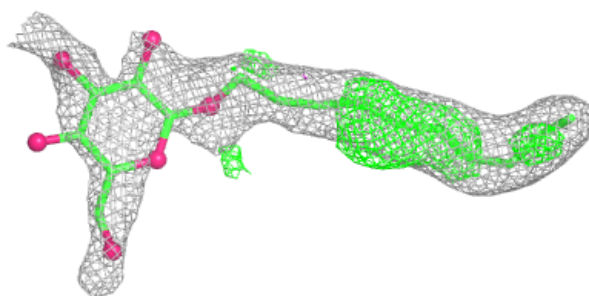
Electron density around CDL Y 101:

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

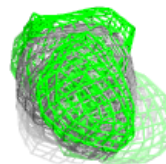
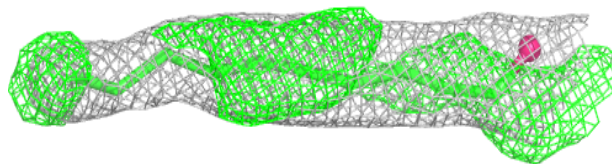
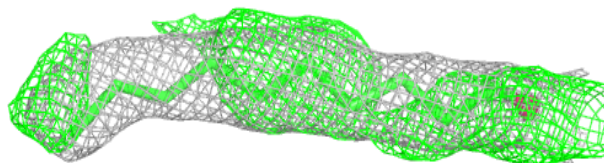


Electron density around DMU B 305:

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

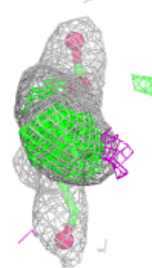
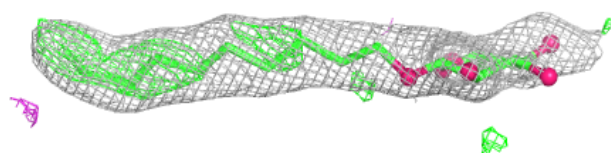
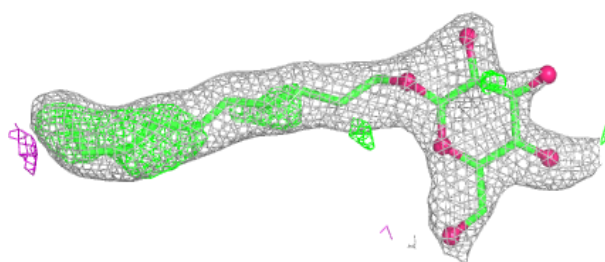
**Electron density around DMU P 307:**

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

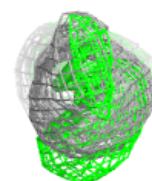
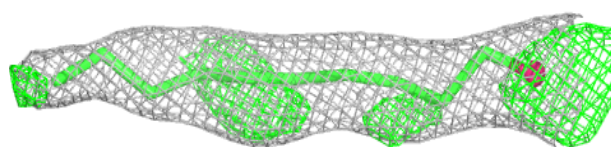
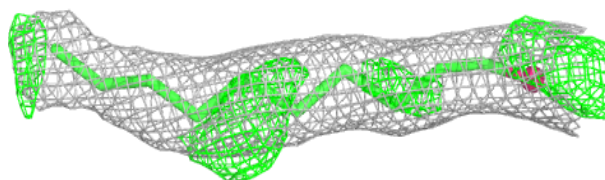


Electron density around DMU O 308:

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

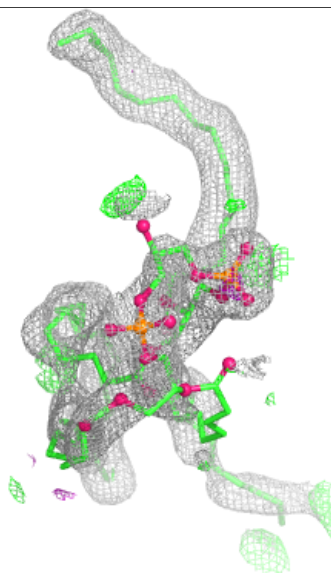
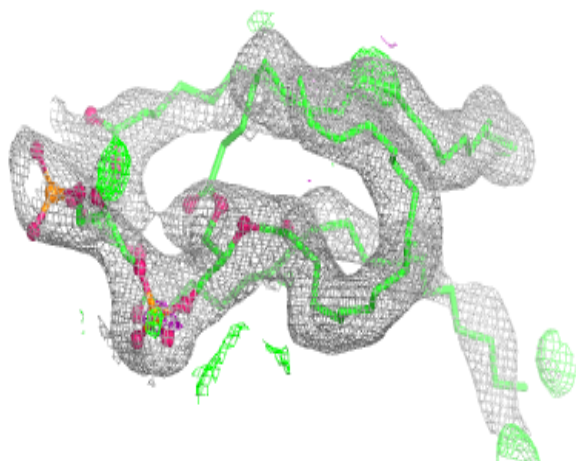
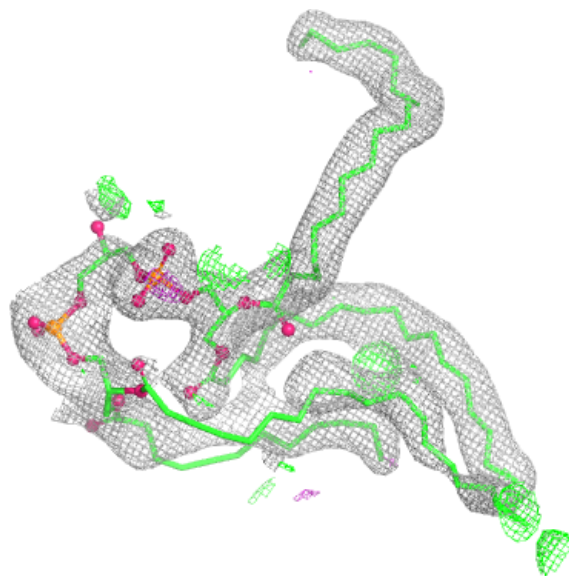
**Electron density around DMU C 306:**

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



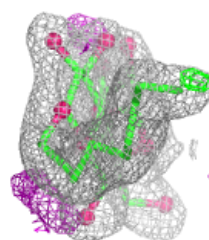
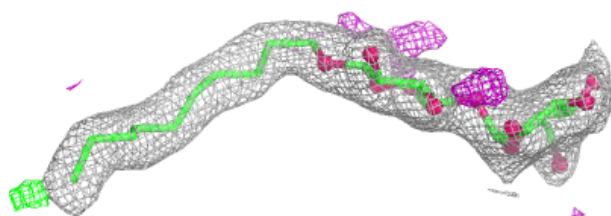
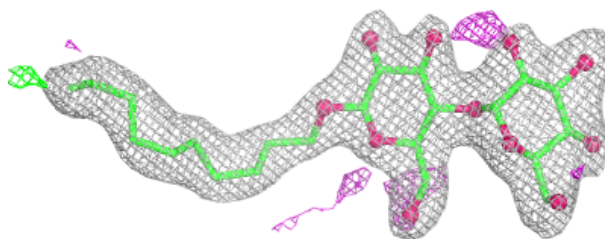
Electron density around CDL L 101:

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

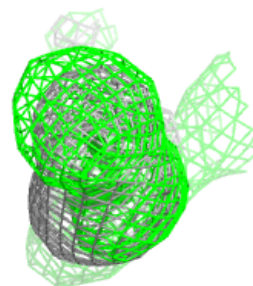
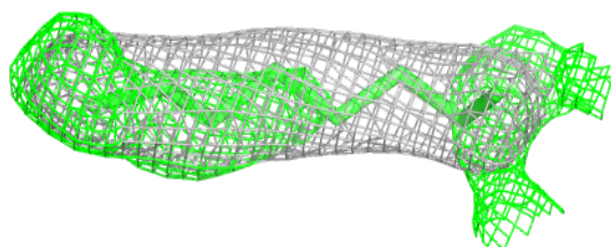
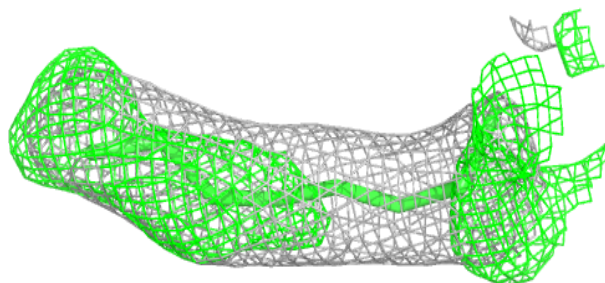


Electron density around DMU Z 101:

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

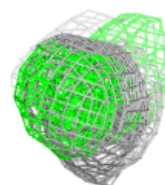
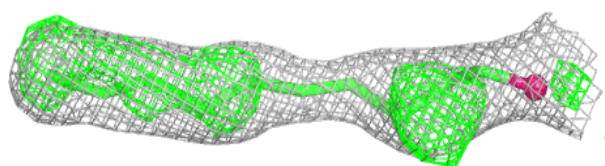
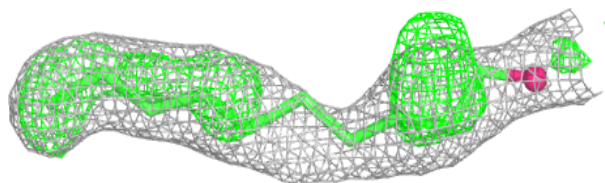
**Electron density around DMU Z 103:**

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

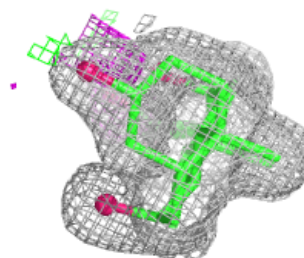
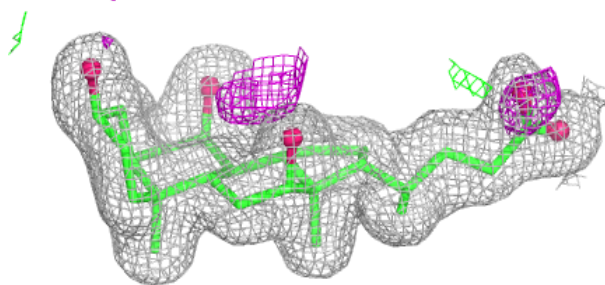
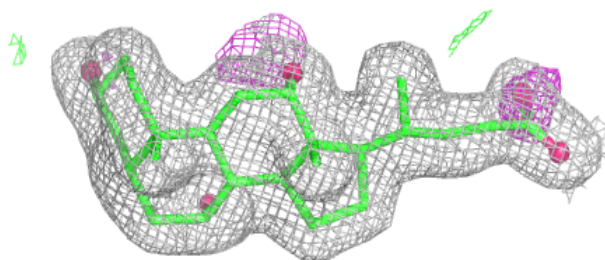


Electron density around DMU O 307:

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

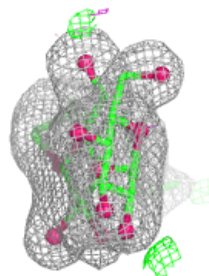
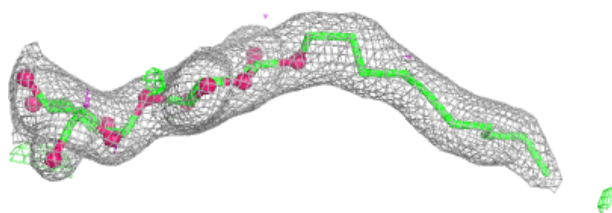
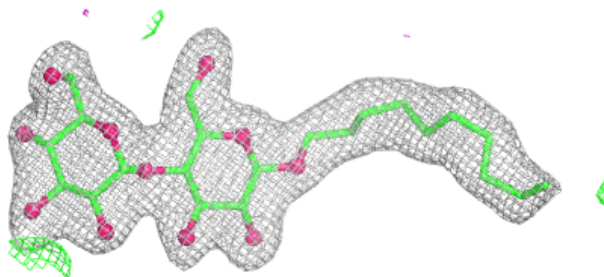
**Electron density around CHD C 301:**

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

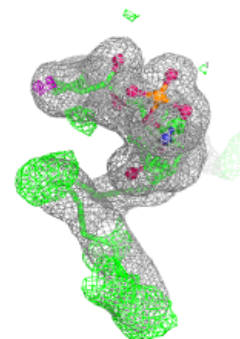
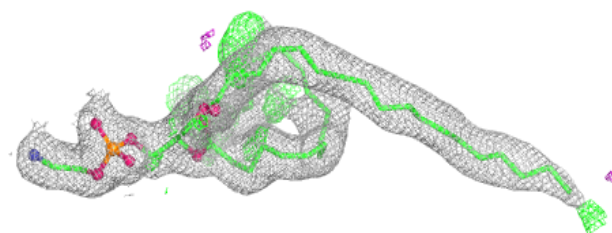
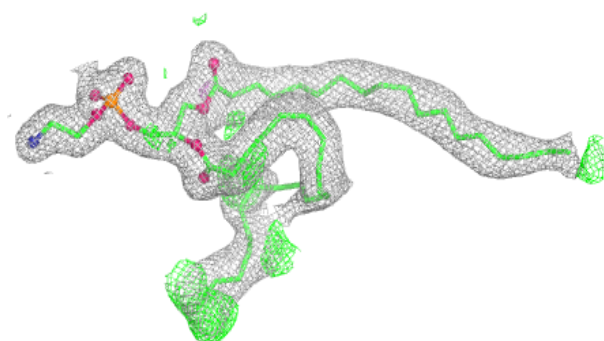


Electron density around DMU M 101:

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

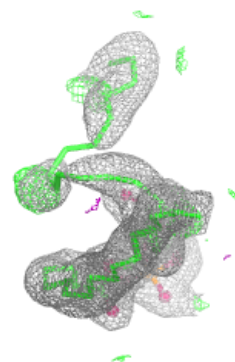
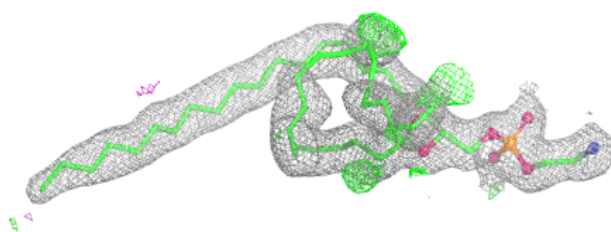
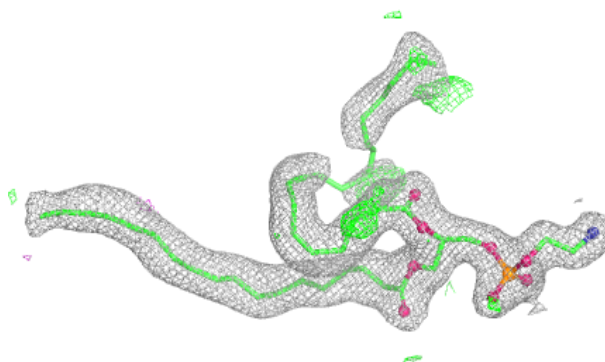
**Electron density around PEK G 101:**

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

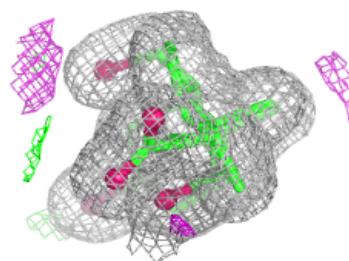
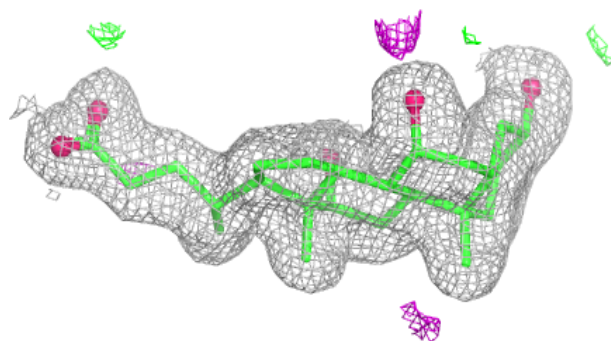
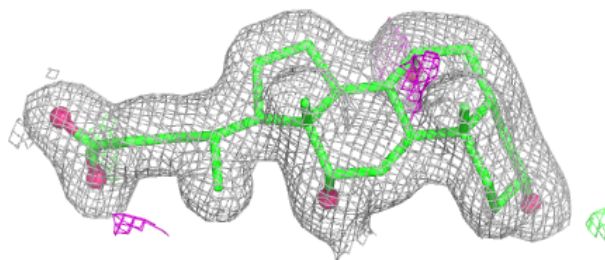


Electron density around PEK T 101:

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

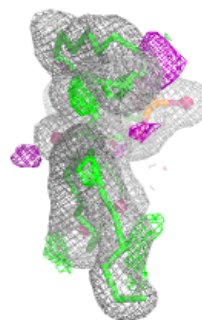
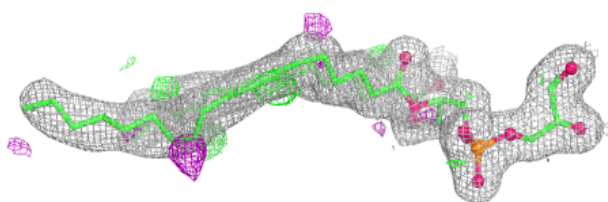
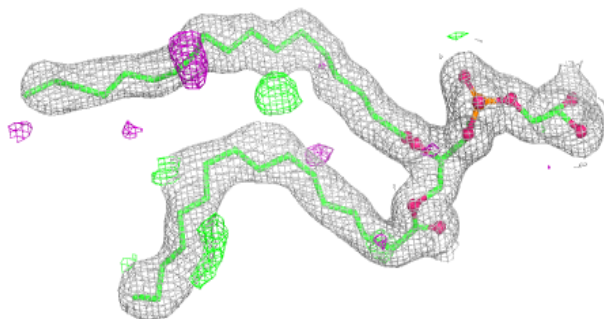
**Electron density around CHD P 302:**

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

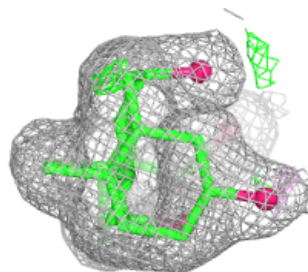
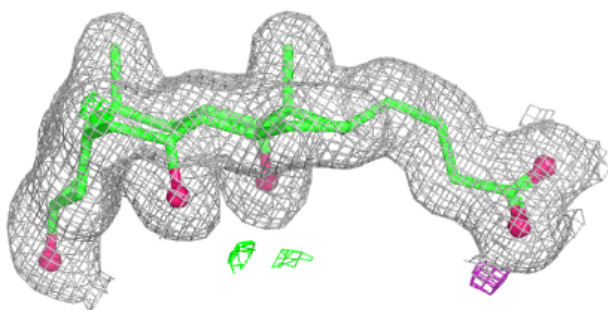
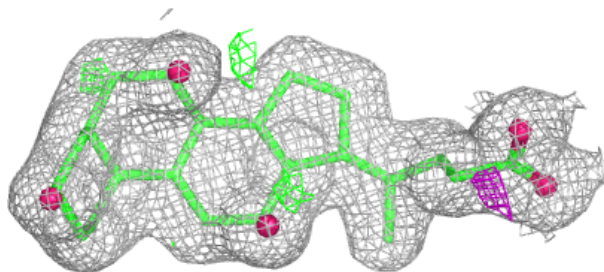


Electron density around PGV N 621:

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

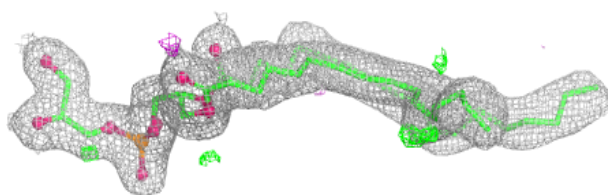
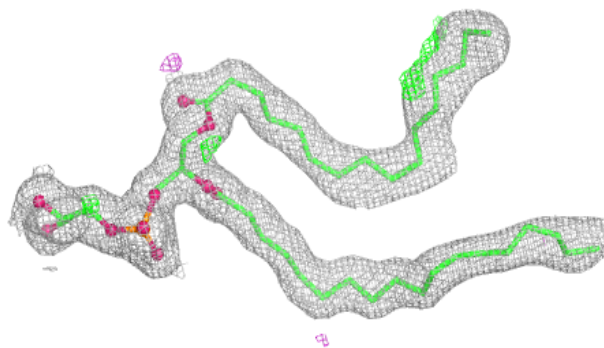
**Electron density around CHD B 307:**

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

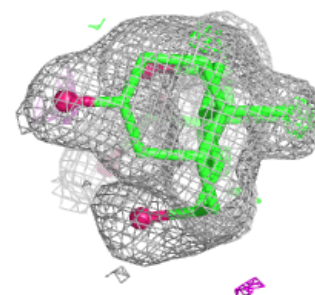
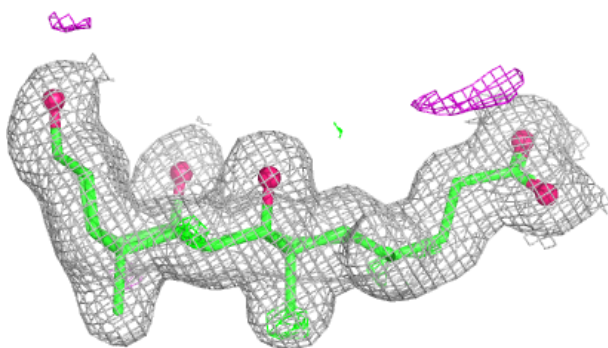
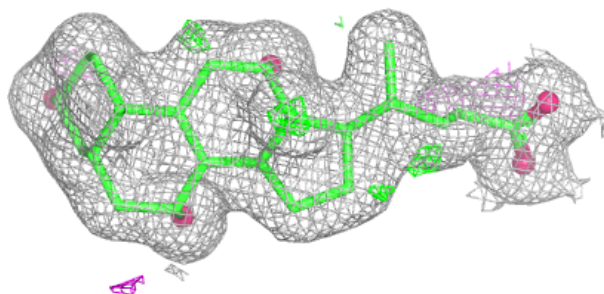


Electron density around PGV A 621:

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

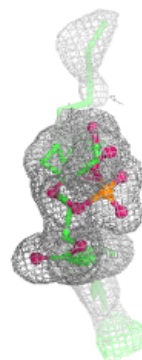
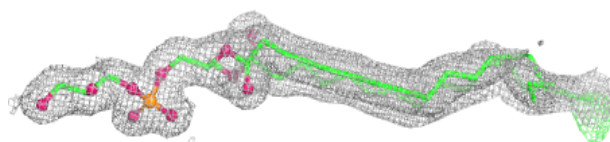
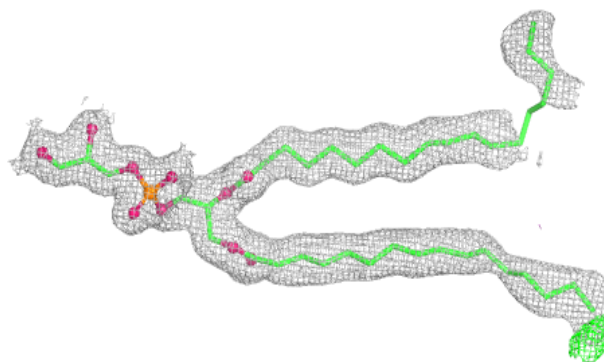
**Electron density around CHD G 102:**

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



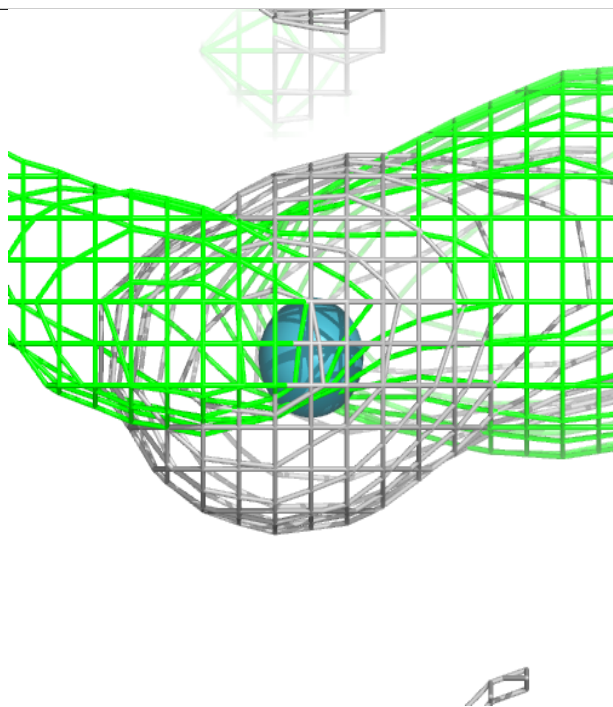
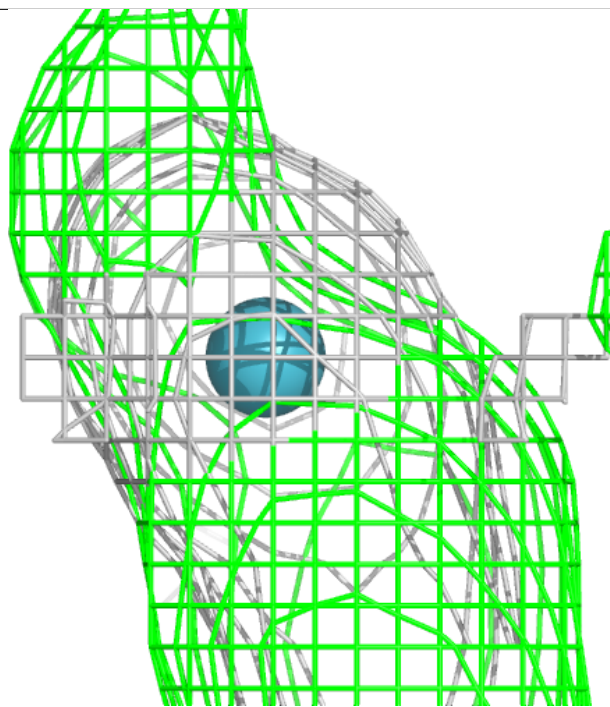
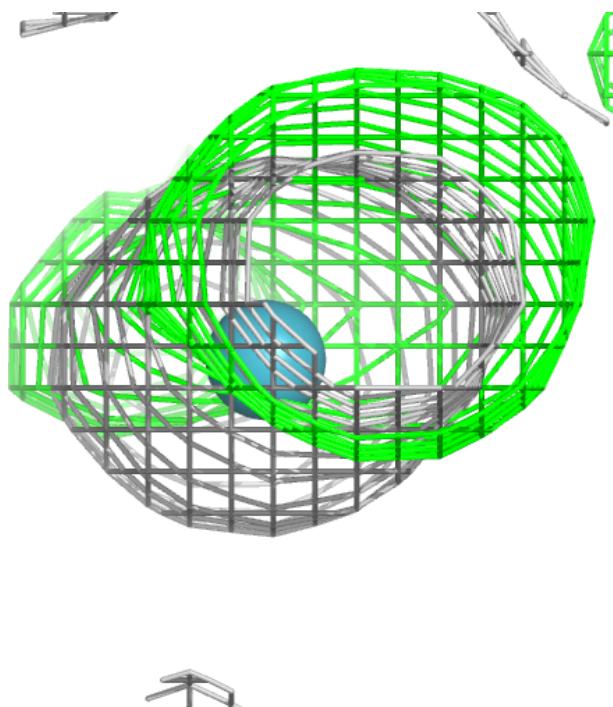
Electron density around PGV P 304:

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



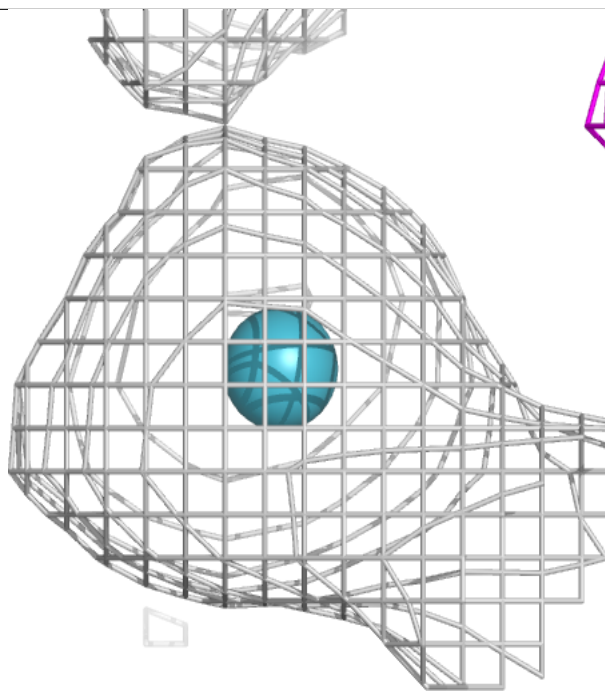
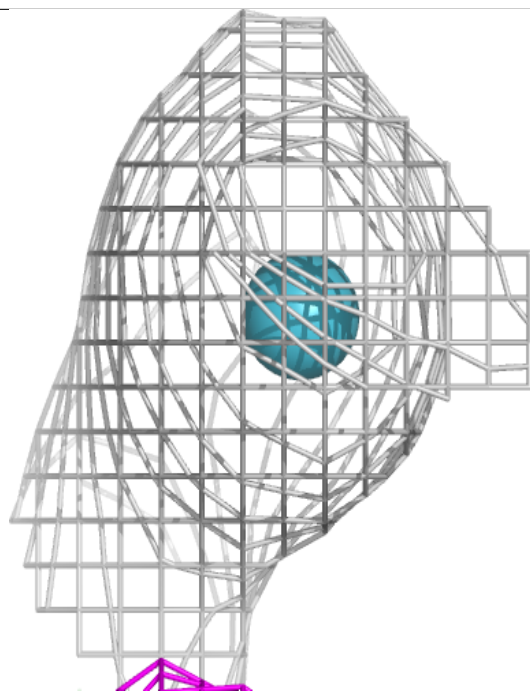
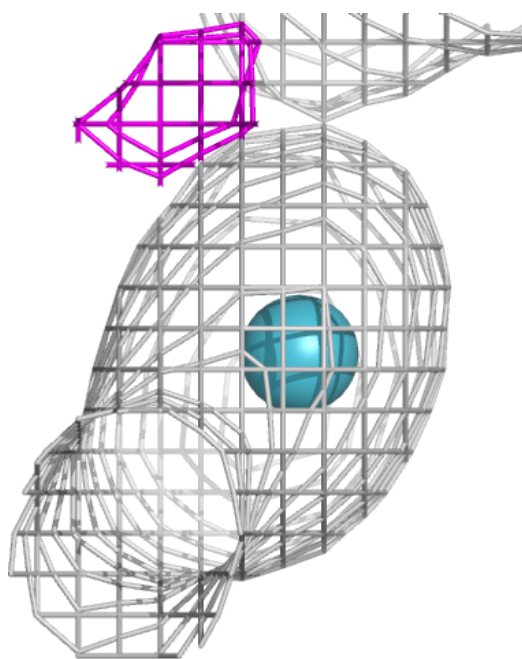
Electron density around XE N 619:

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



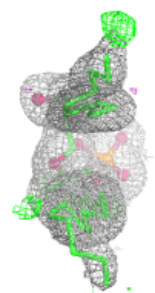
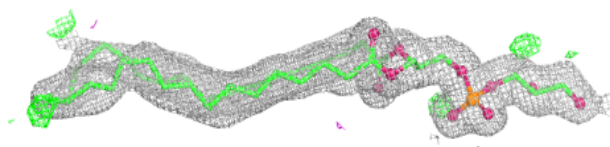
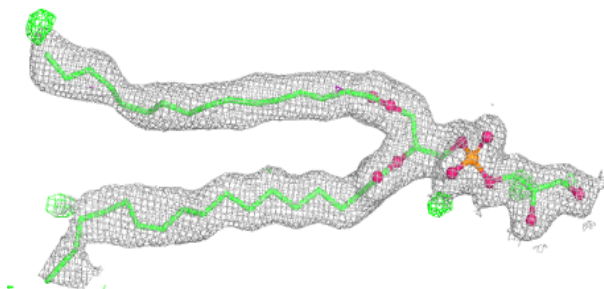
Electron density around XE P 325:

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

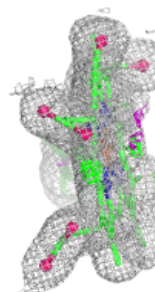
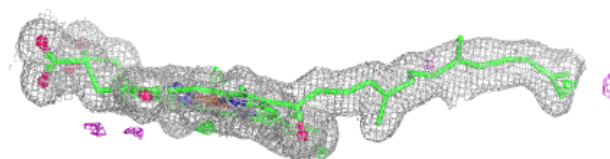
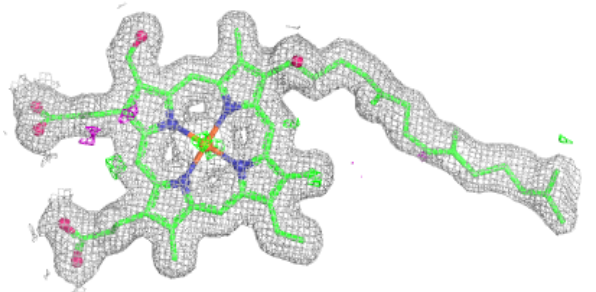


Electron density around PGV C 303:

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

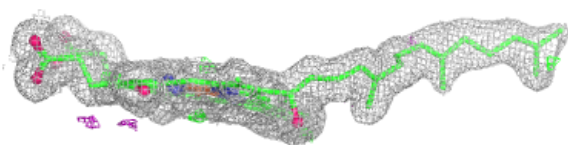
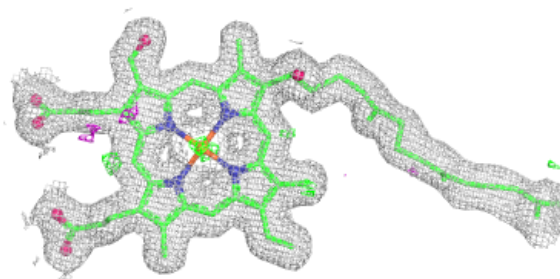
**Electron density around HEA A 601 (A):**

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

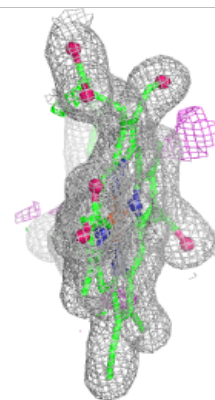
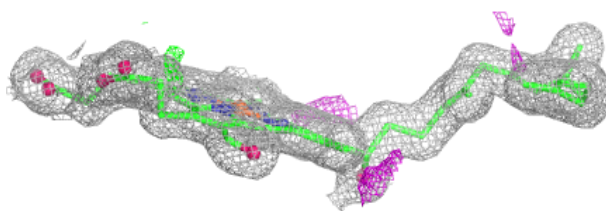
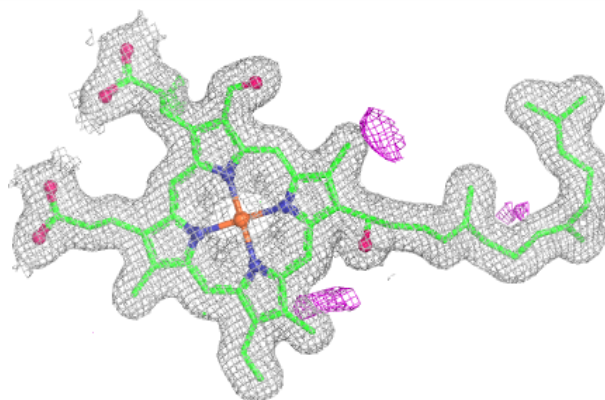


Electron density around HEA A 601 (B):

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

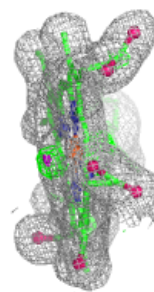
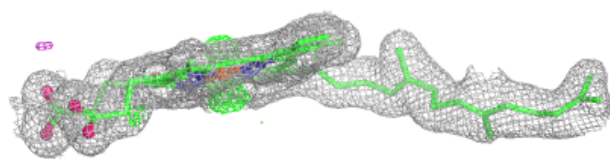
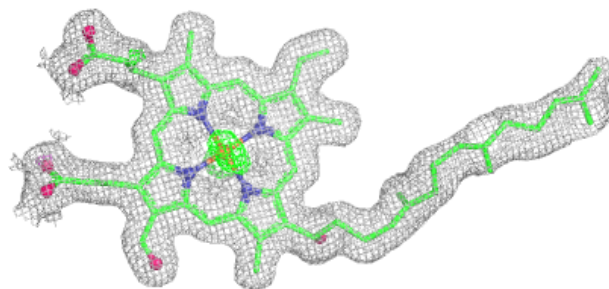
**Electron density around HEA A 602:**

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



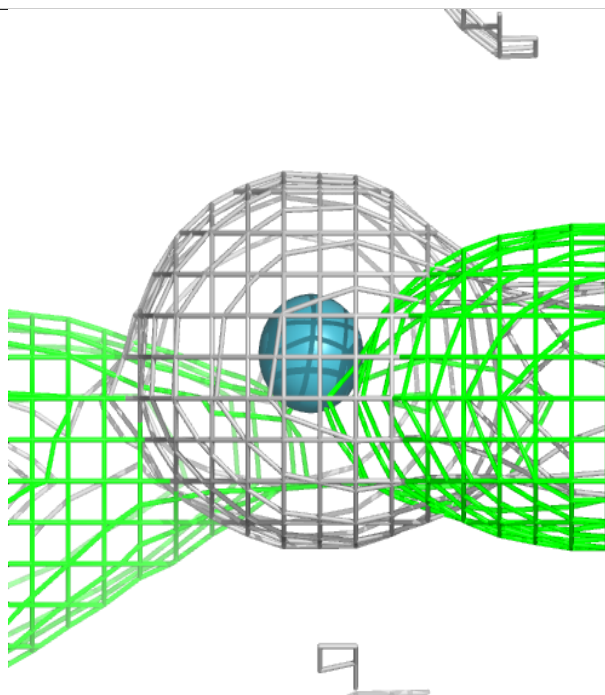
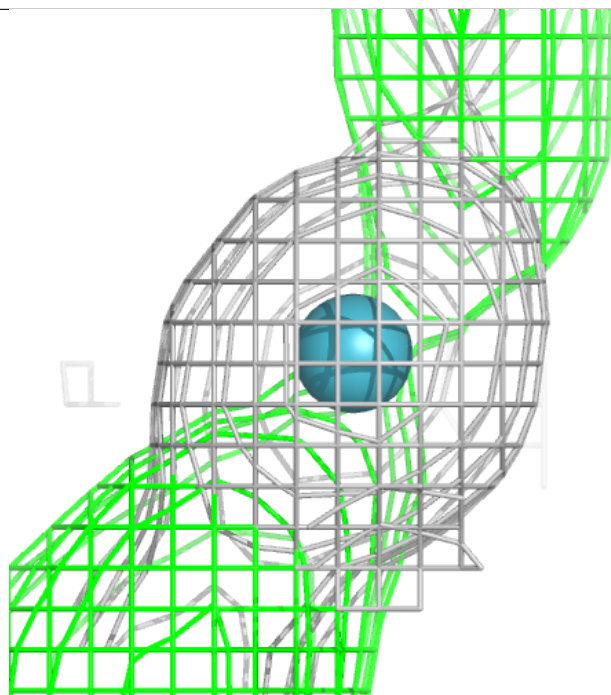
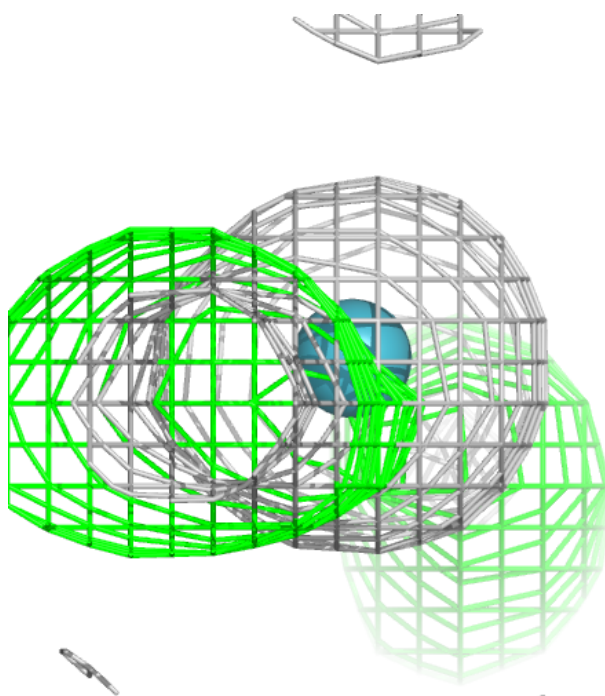
Electron density around HEA N 602 (A):

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



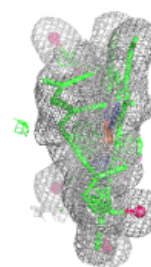
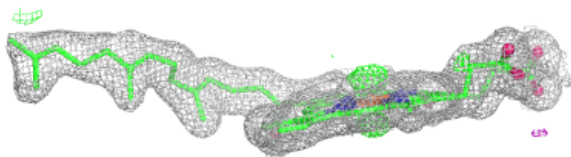
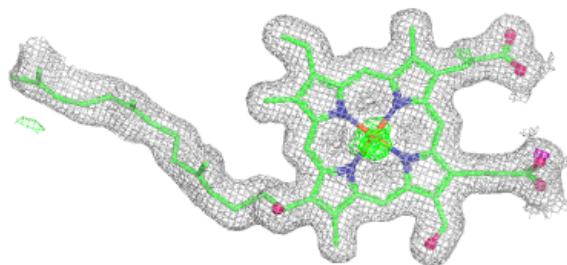
Electron density around XE A 619:

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

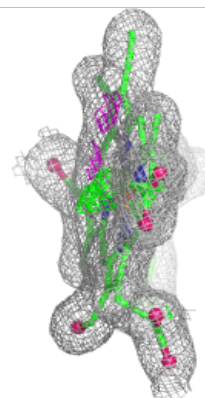
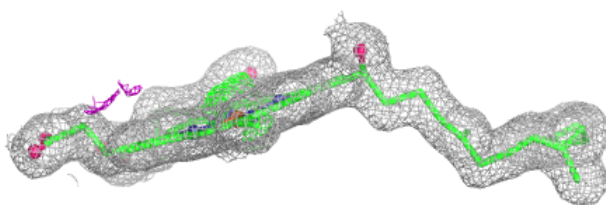
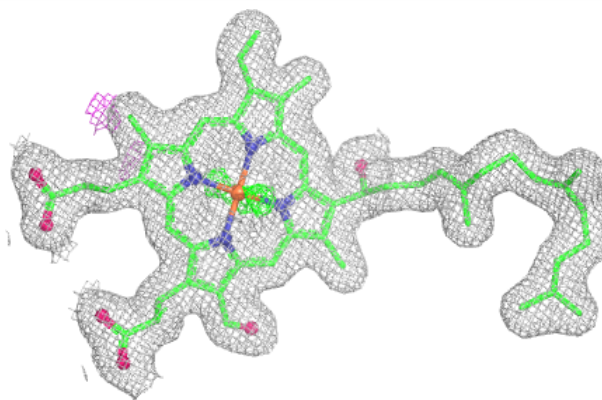


Electron density around HEA N 602 (B):

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

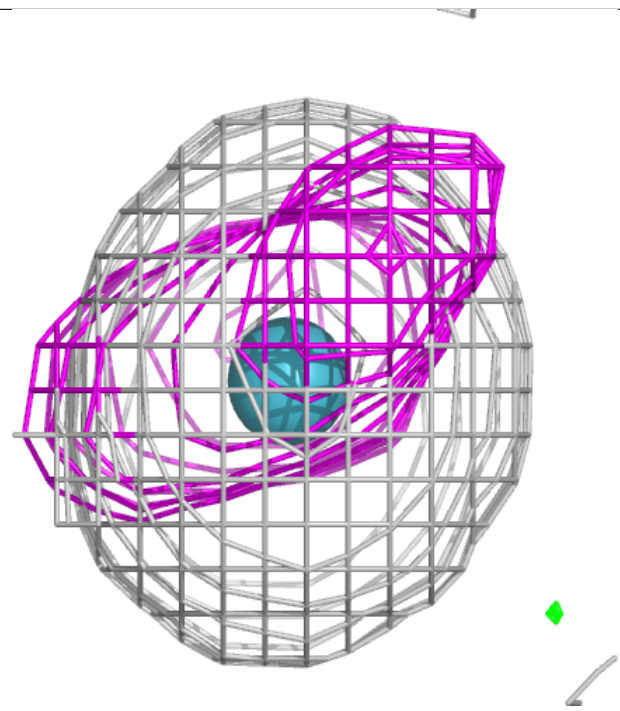
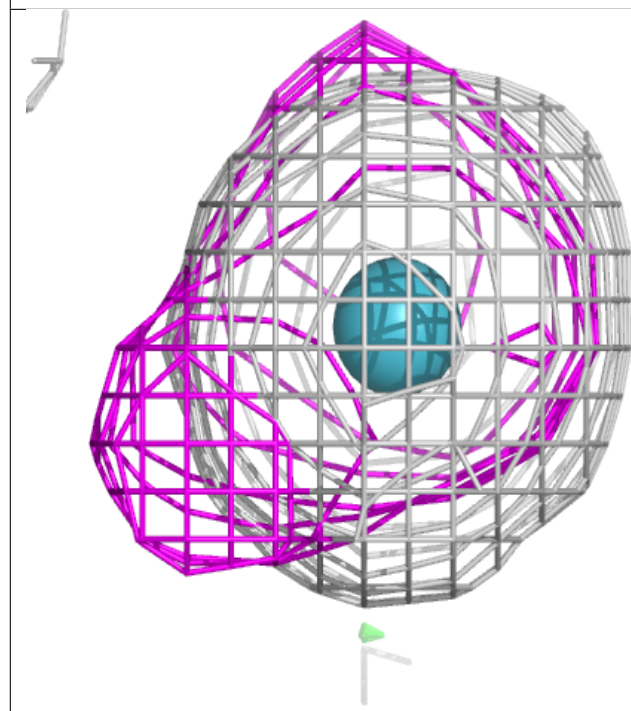
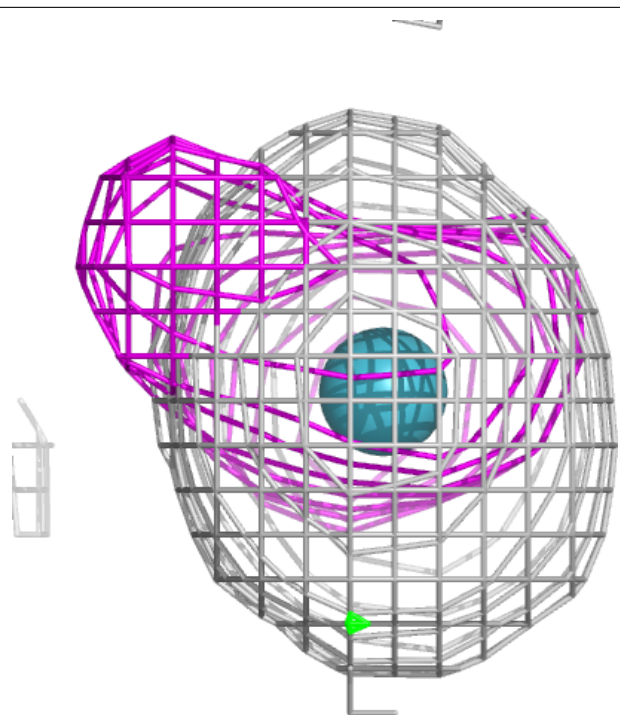
**Electron density around HEA N 603:**

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



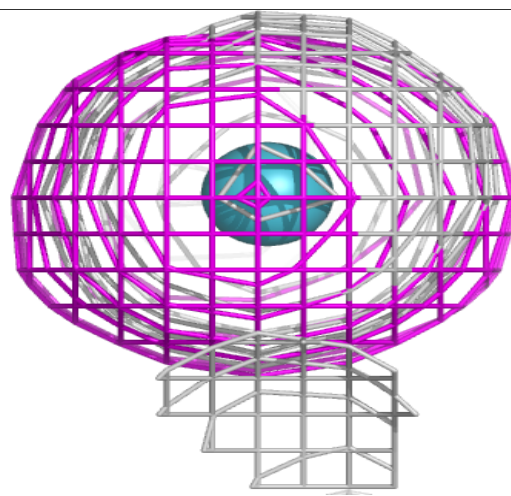
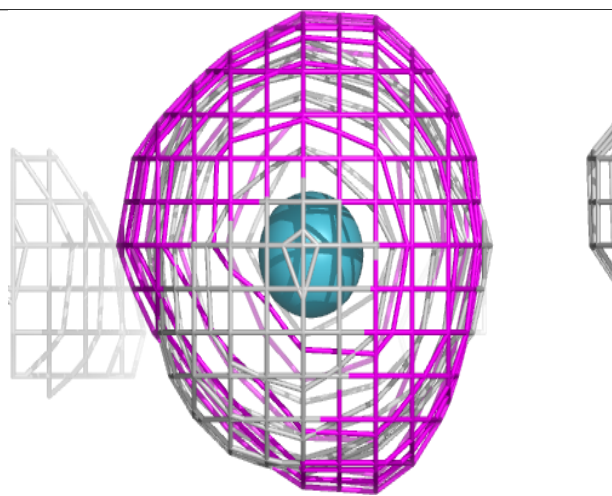
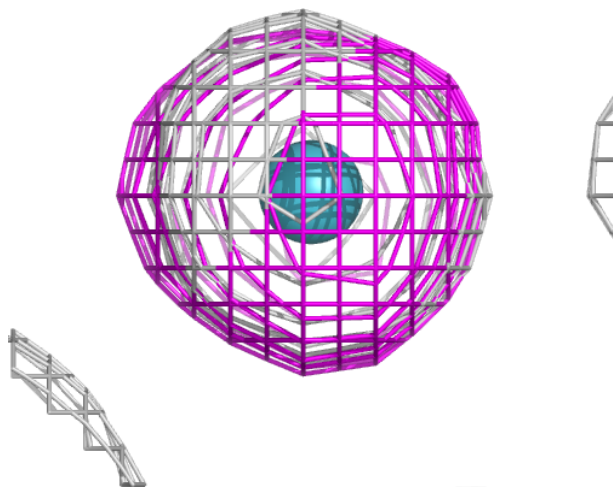
Electron density around XE A 620:

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



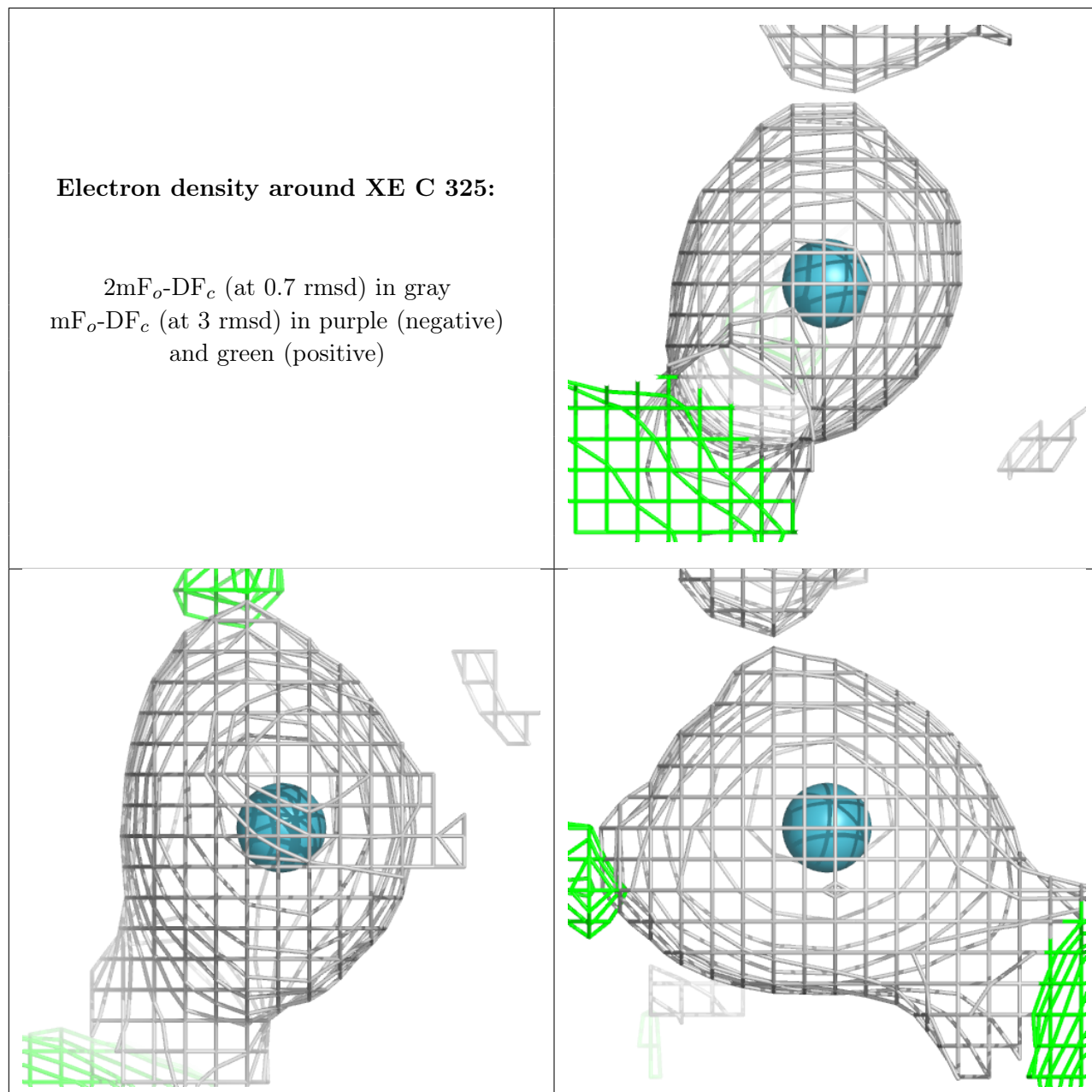
Electron density around XE B 301:

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



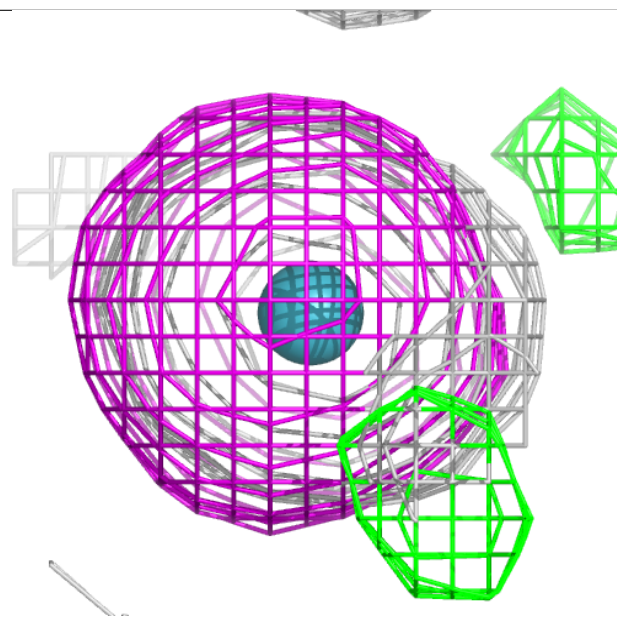
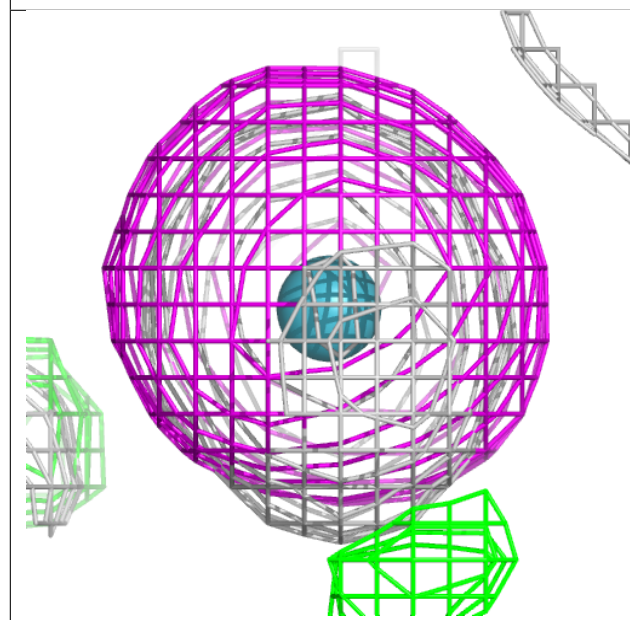
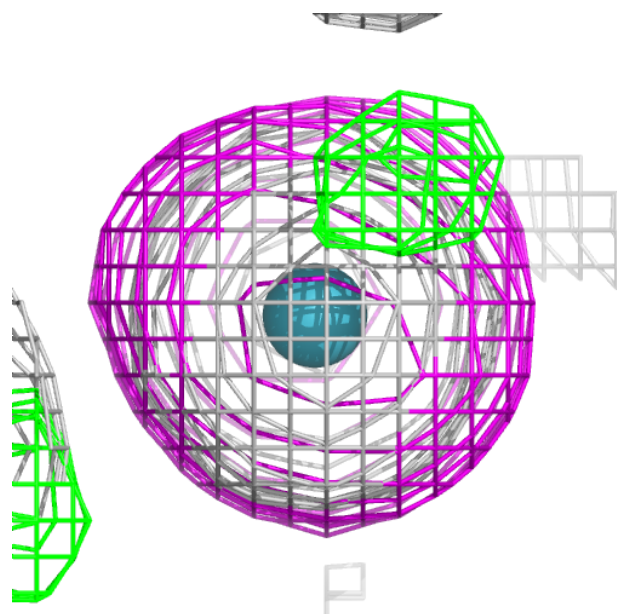
Electron density around XE C 325:

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



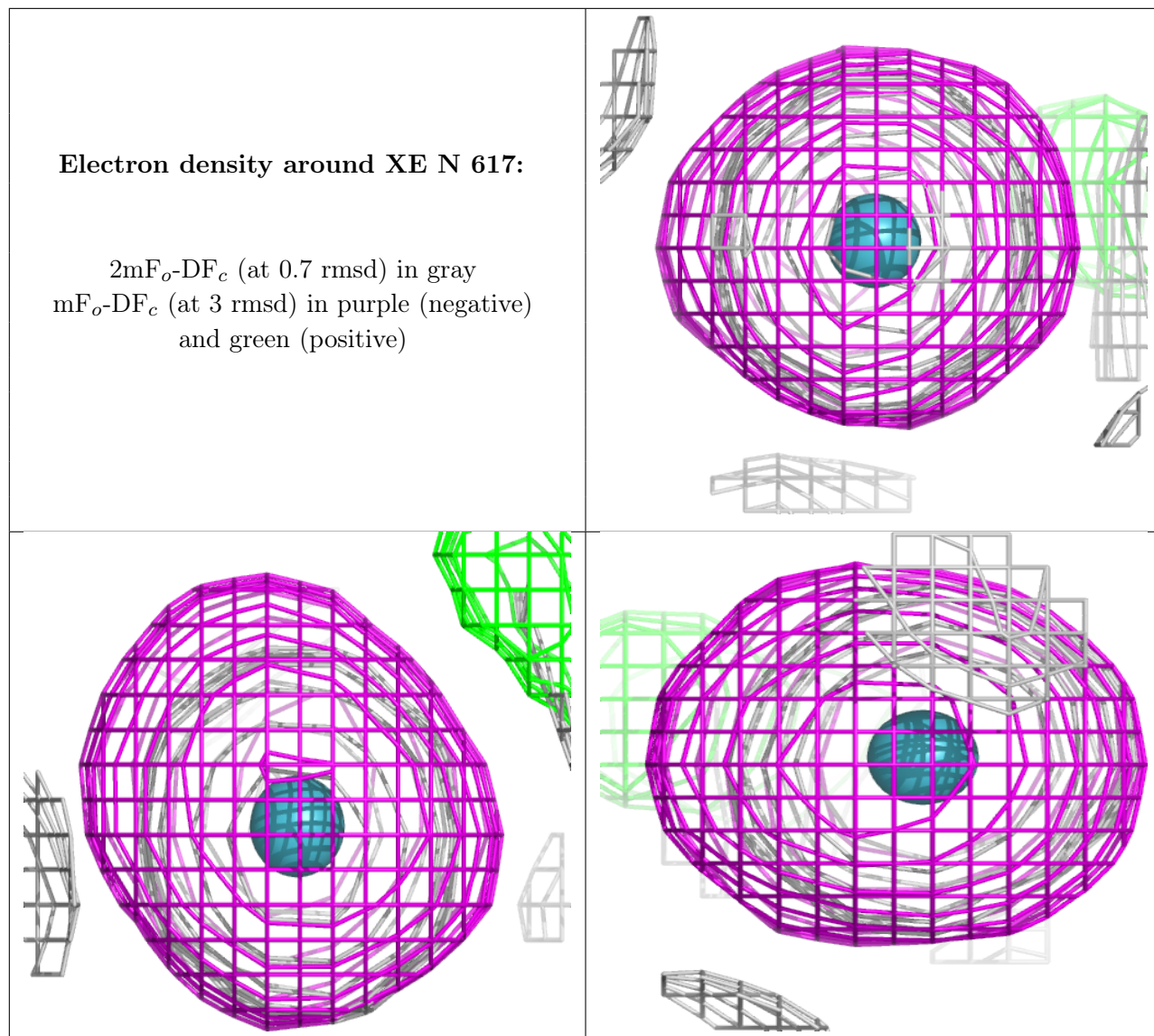
Electron density around XE N 616:

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



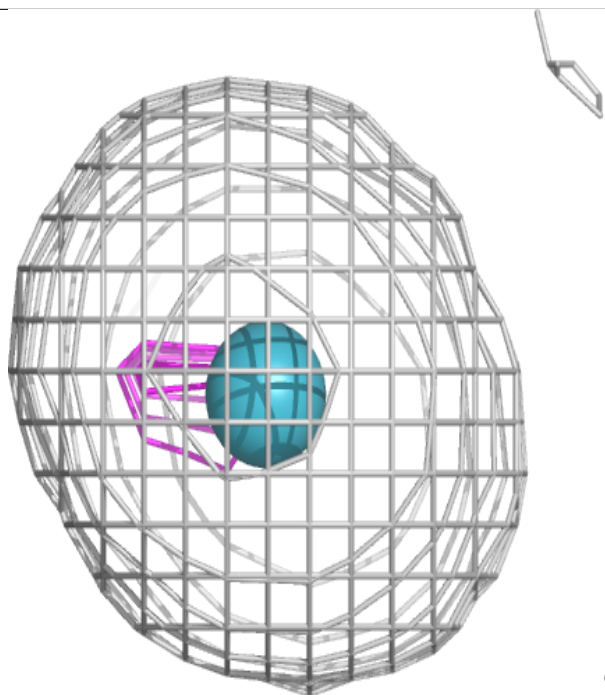
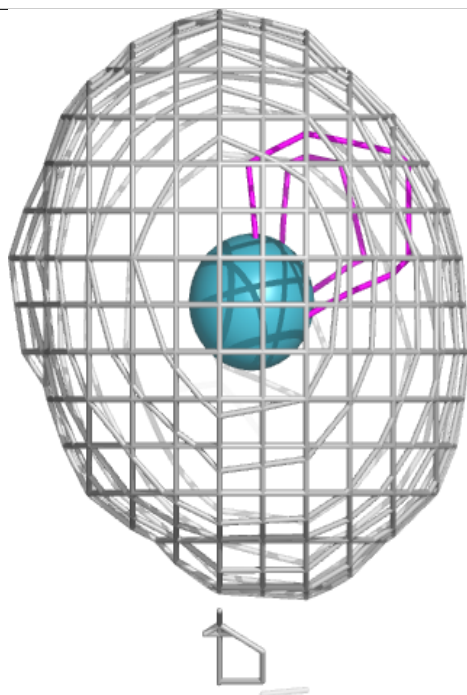
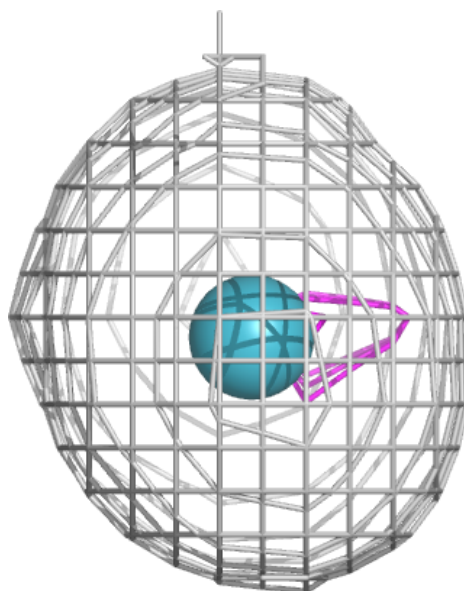
Electron density around XE N 617:

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



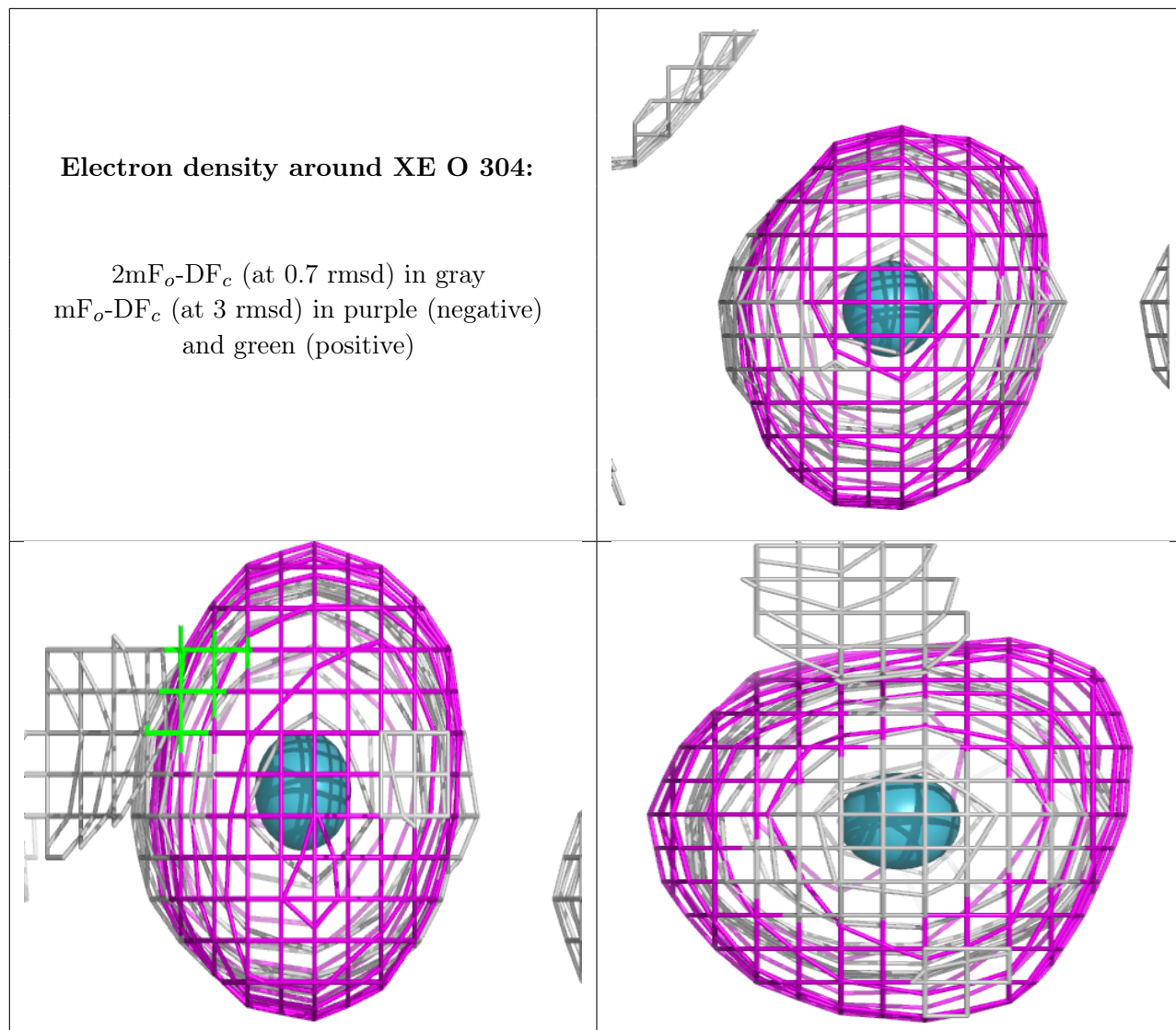
Electron density around XE N 620:

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



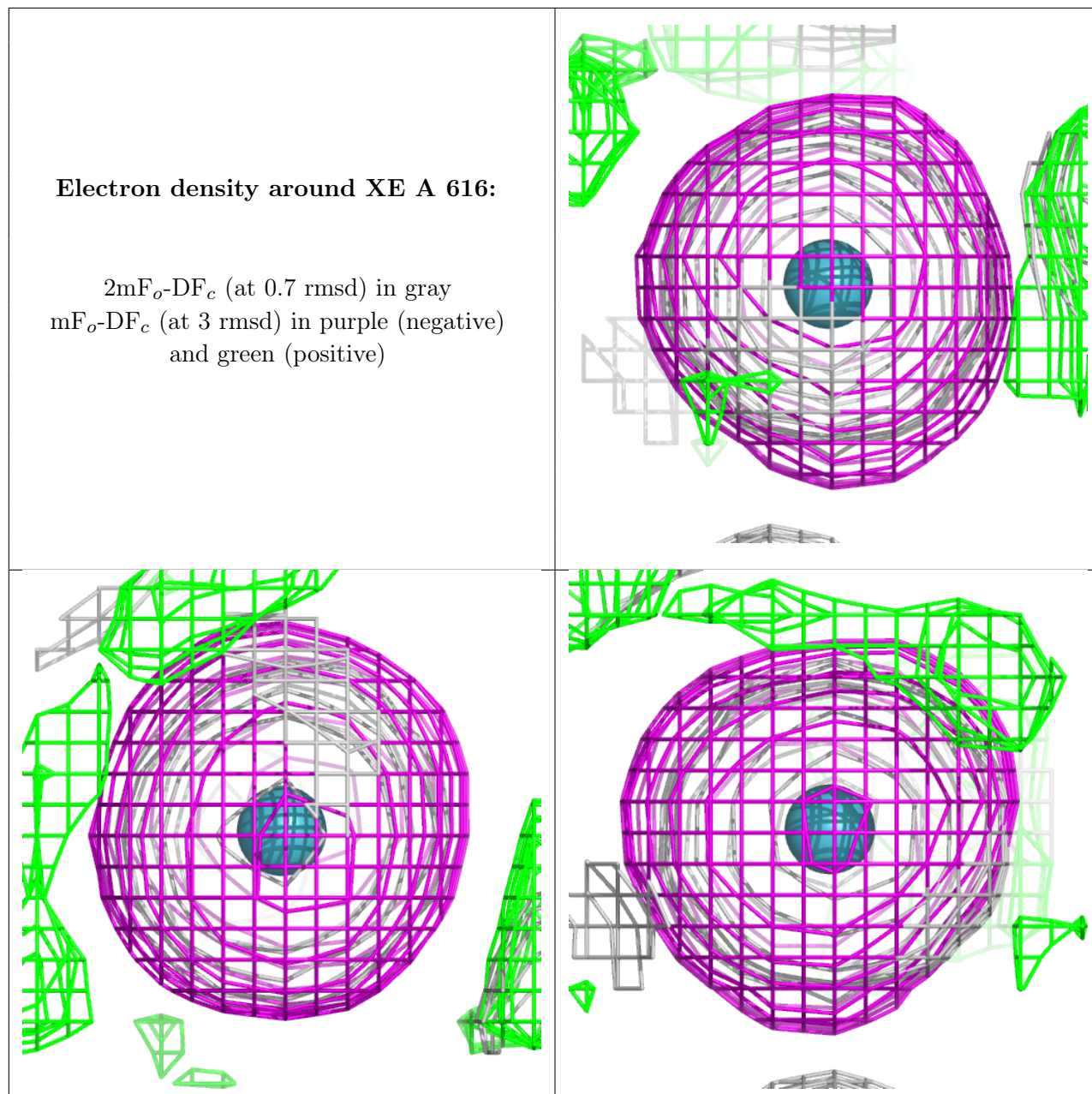
Electron density around XE O 304:

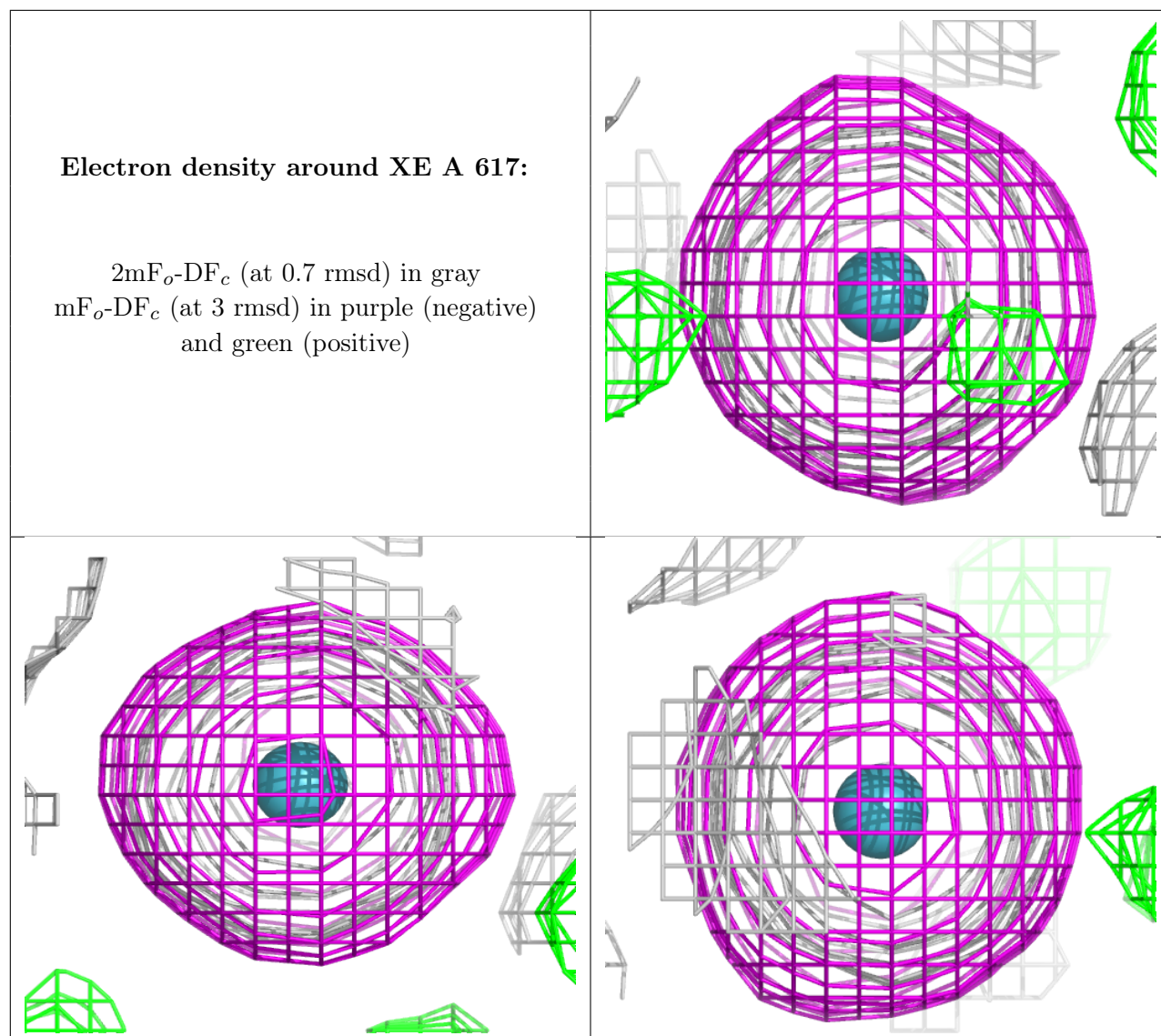
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around XE A 616:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.