



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:27 PM UTC

PDB ID : 9IKI / pdb_00009iki
Title : Bovine Heart Cytochrome c Oxidase in the Nitrous Oxide-bound Fully Reduced State
Authors : Muramoto, K.; Ide, T.; Shinzawa-Itoh, K.
Deposited on : 2024-06-27
Resolution : 1.75 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

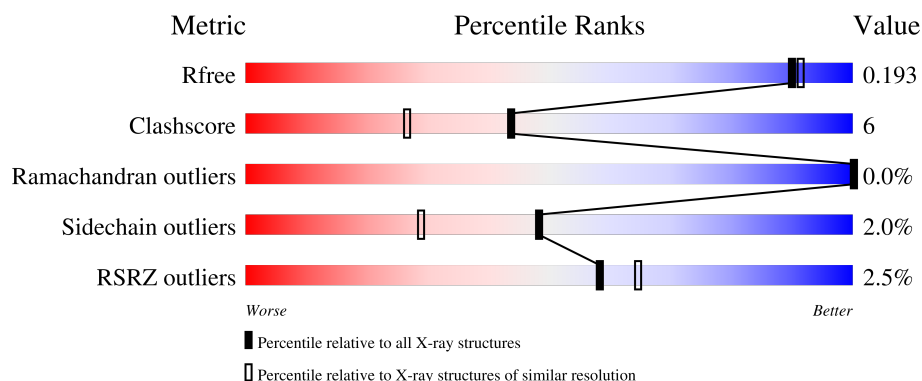
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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.



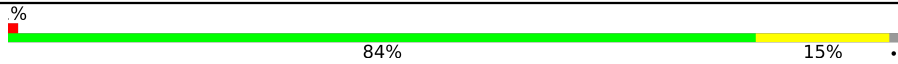
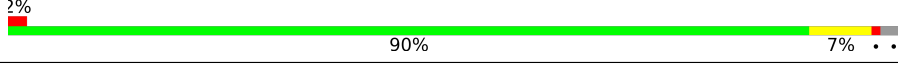
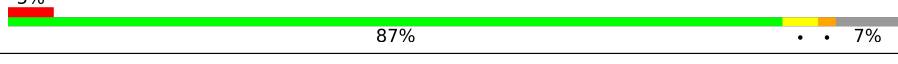
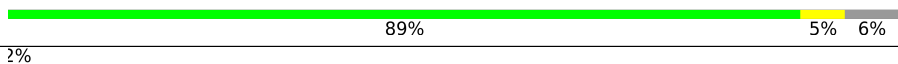
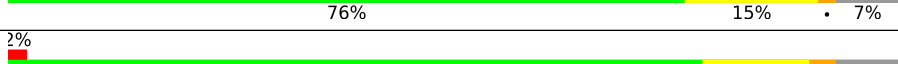
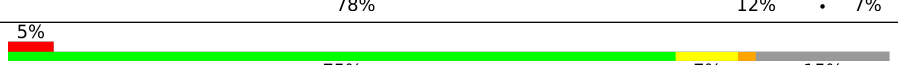
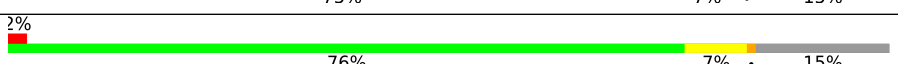
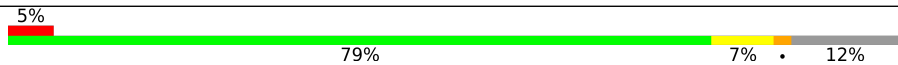
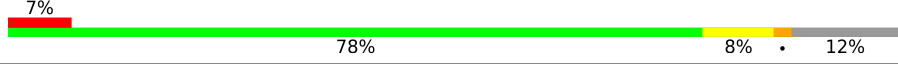
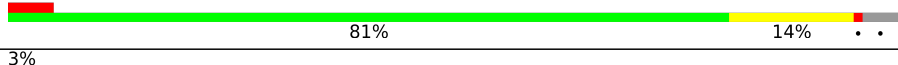
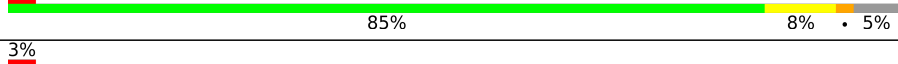
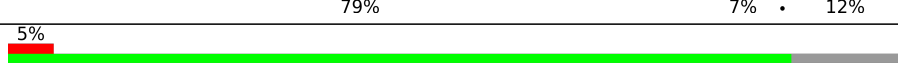
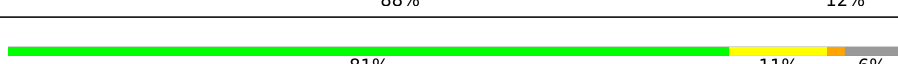
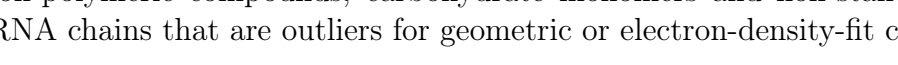
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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
19	LFA	P	310	-	-	-	X
26	CDL	C	304	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 33027 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

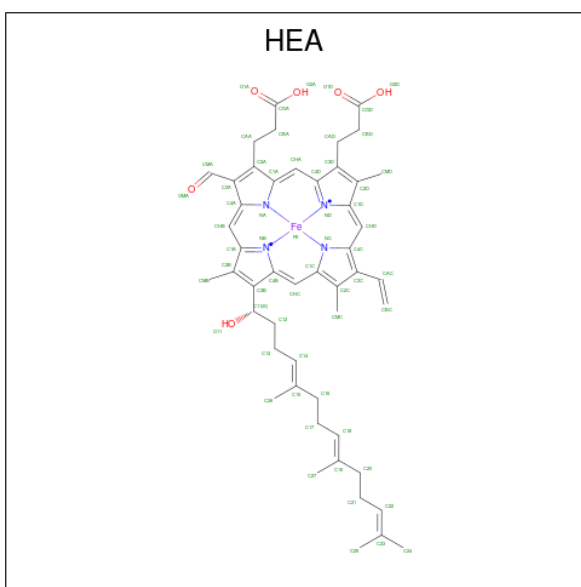
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

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



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

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

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

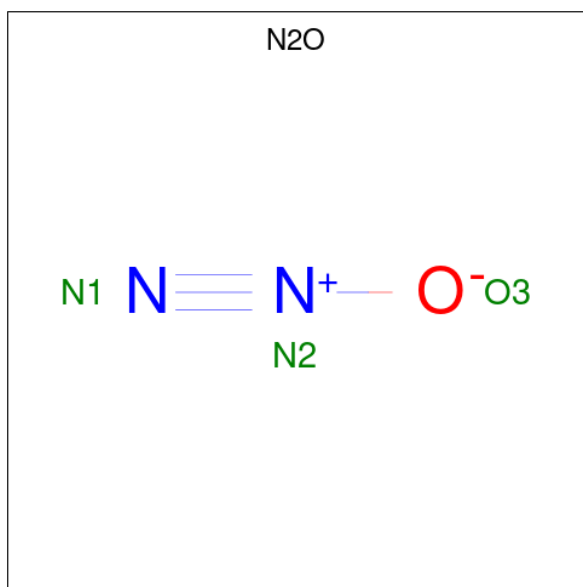
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

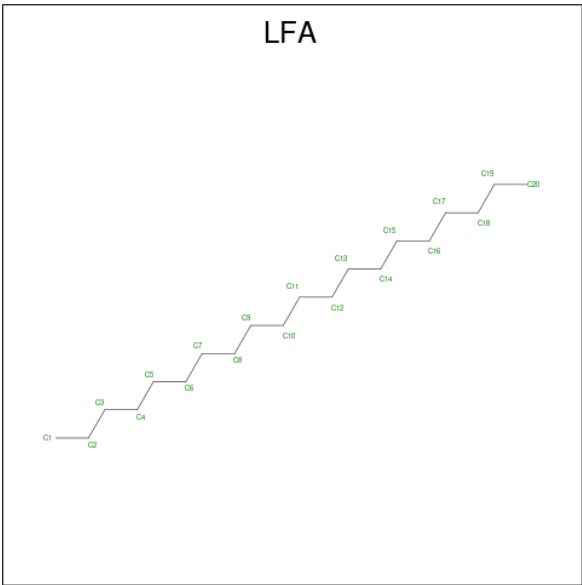
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total 1	Na 1	0	0
17	N	1	Total 1	Na 1	0	0

- Molecule 18 is NITROUS OXIDE (CCD ID: N2O) (formula: N₂O) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 19 is EICOSANE (CCD ID: LFA) (formula: C₂₀H₄₂).



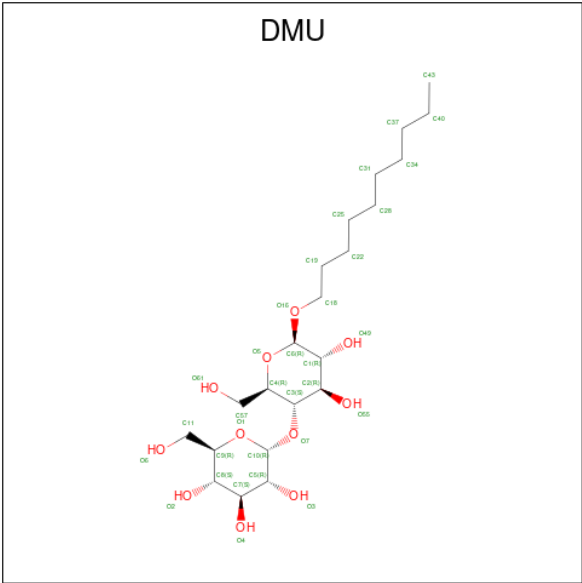
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	C	0	0
			14	14		
19	B	1	Total	C	0	0
			17	17		
19	C	1	Total	C	0	0
			11	11		
19	C	1	Total	C	0	0
			6	6		
19	C	1	Total	C	0	0
			18	18		
19	C	1	Total	C	0	0
			15	15		
19	C	1	Total	C	0	0
			11	11		
19	C	1	Total	C	0	0
			14	14		
19	C	1	Total	C	0	0
	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

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

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



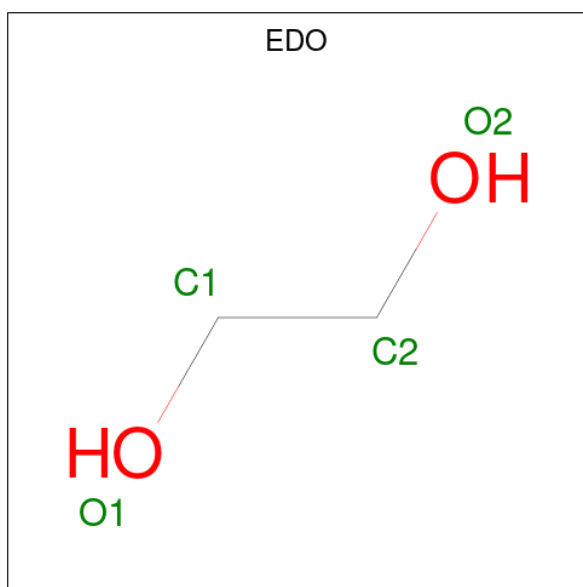
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C 7 7	0	0
20	A	1	Total C O 33 22 11	0	0
20	A	1	Total C O 11 10 1	0	0
20	B	1	Total C O 11 10 1	0	0
20	B	1	Total C O 11 10 1	0	0
20	B	1	Total C O 22 16 6	0	0
20	B	1	Total C O 22 16 6	0	0
20	C	1	Total C O 11 10 1	0	0
20	C	1	Total C O 33 22 11	0	0
20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

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

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



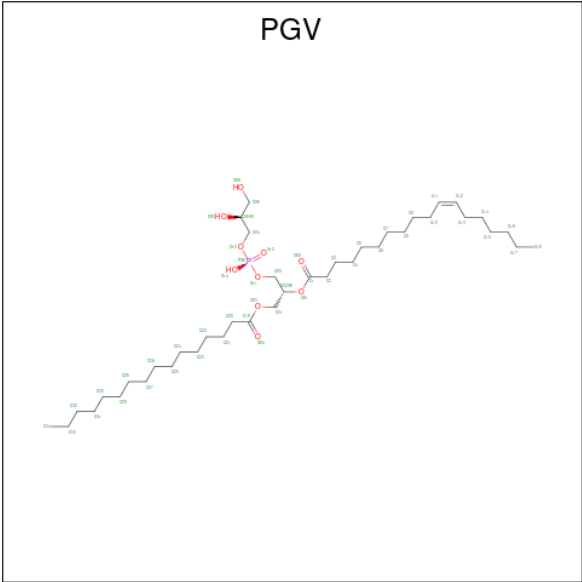
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	A	1	Total	C	O	0	0
			4	2	2		
21	B	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21	C	1	Total	C	O	0	0
			4	2	2		
21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

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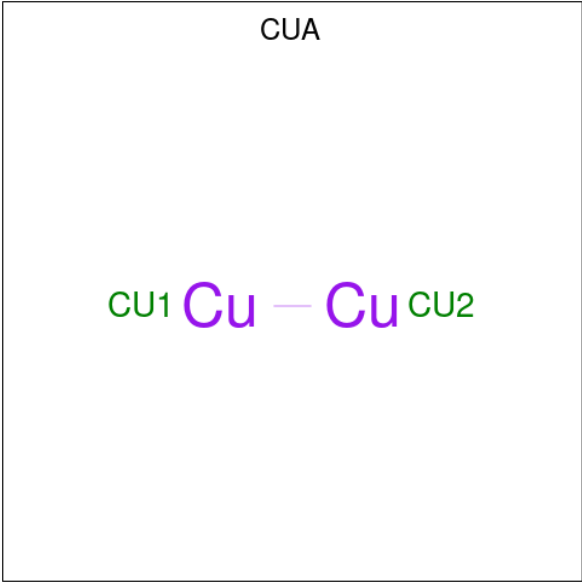
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4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

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



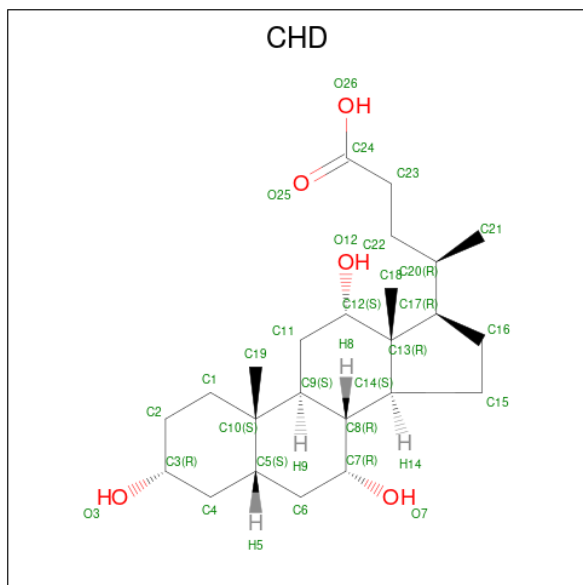
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	O	P	0	0
			51	40	10	1		
22	C	1	Total	C	O	P	0	0
			51	40	10	1		
22	N	1	Total	C	O	P	0	0
			51	40	10	1		
22	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



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

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

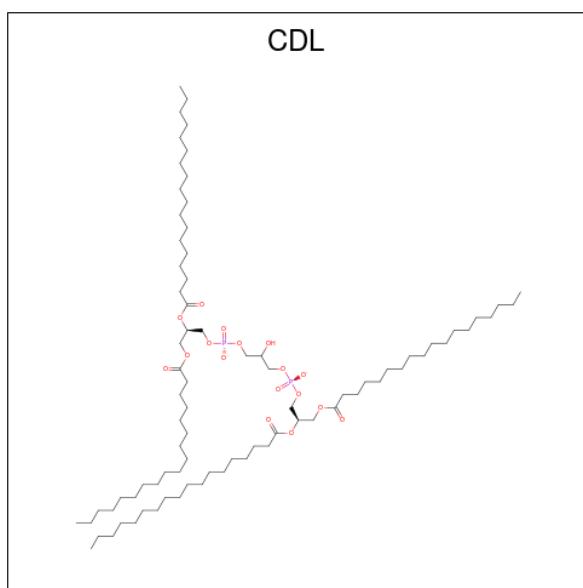


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	O	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0

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

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

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

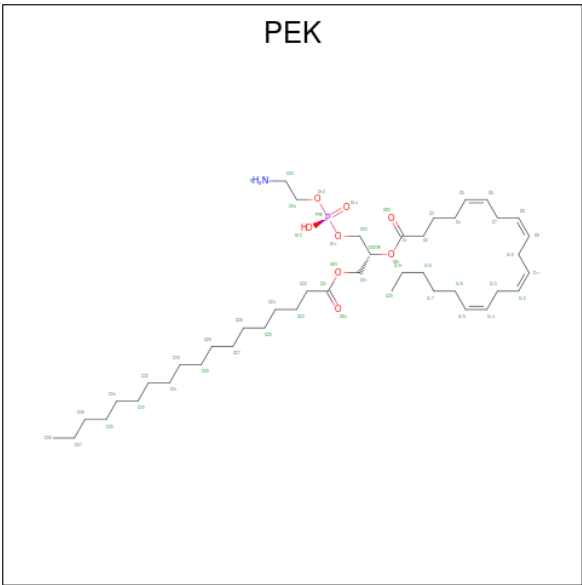


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			87	68	17	2		
26	I	1	Total	C	O	P	0	0
			64	45	17	2		
26	L	1	Total	C	O	P	0	0
			94	75	17	2		
26	N	1	Total	C	O	P	0	0
			64	45	17	2		
26	P	1	Total	C	O	P	0	0
			87	68	17	2		
26	Y	1	Total	C	O	P	0	0
			94	75	17	2		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 28 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: $C_{43}H_{78}NO_8P$).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	235	Total	O	0	11
			246	246		
29	B	167	Total	O	0	2
			169	169		
29	C	107	Total	O	0	1
			108	108		
29	D	136	Total	O	0	8
			144	144		
29	E	108	Total	O	0	8
			116	116		
29	F	103	Total	O	0	7
			110	110		
29	G	43	Total	O	0	1
			44	44		
29	H	62	Total	O	0	0
			62	62		
29	I	41	Total	O	0	0
			41	41		
29	J	20	Total	O	0	0
			20	20		

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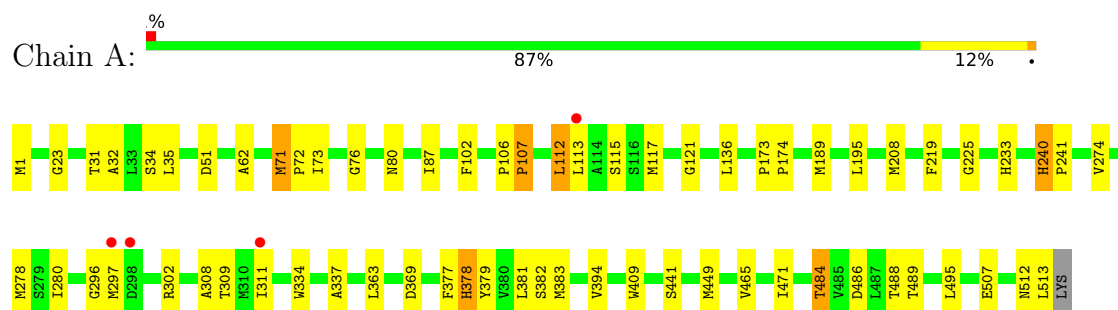
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	K	21	Total 21	O 21	0	0
29	L	26	Total 28	O 28	0	2
29	M	21	Total 21	O 21	0	0
29	N	221	Total 231	O 231	0	10
29	O	147	Total 148	O 148	0	1
29	P	101	Total 102	O 102	0	1
29	Q	78	Total 83	O 83	0	5
29	R	87	Total 93	O 93	0	6
29	S	91	Total 98	O 98	0	7
29	T	40	Total 41	O 41	0	1
29	U	51	Total 51	O 51	0	0
29	V	22	Total 22	O 22	0	0
29	W	15	Total 15	O 15	0	0
29	X	17	Total 17	O 17	0	0
29	Y	24	Total 26	O 26	0	2
29	Z	17	Total 17	O 17	0	0

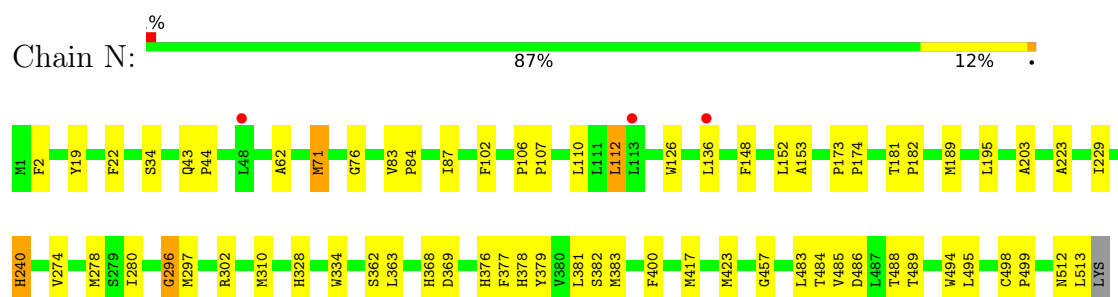
3 Residue-property plots

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.

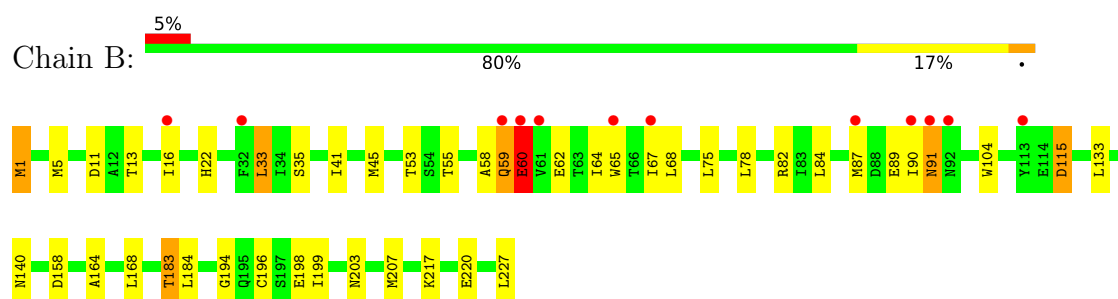
• Molecule 1: Cytochrome c oxidase subunit 1



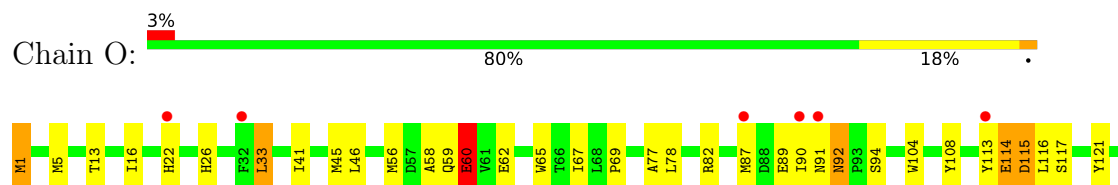
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2

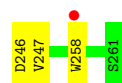
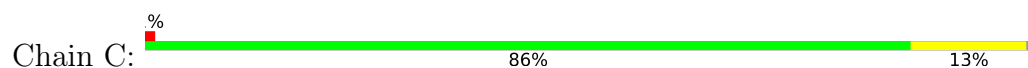


• Molecule 2: Cytochrome c oxidase subunit 2

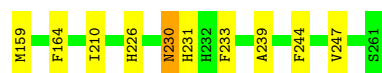
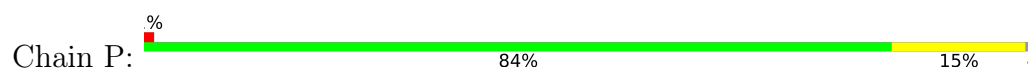




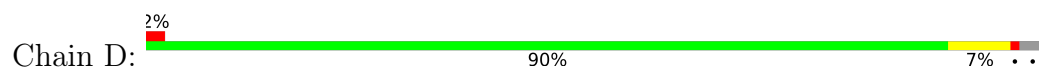
• Molecule 3: Cytochrome c oxidase subunit 3



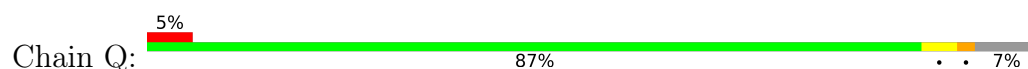
• Molecule 3: Cytochrome c oxidase subunit 3



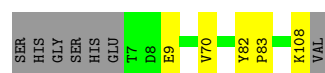
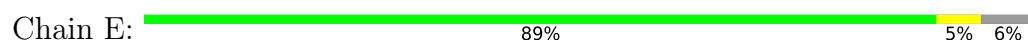
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



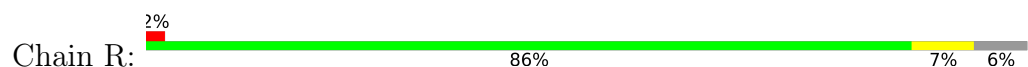
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



• Molecule 5: Cytochrome c oxidase subunit 5A

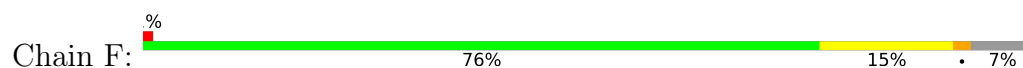


• Molecule 5: Cytochrome c oxidase subunit 5A

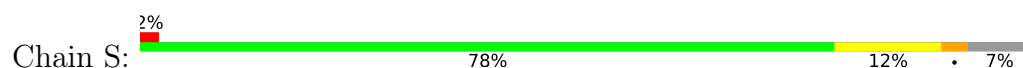




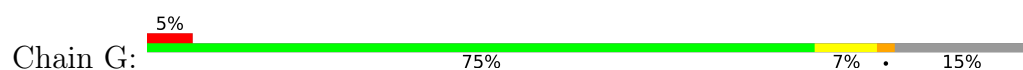
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



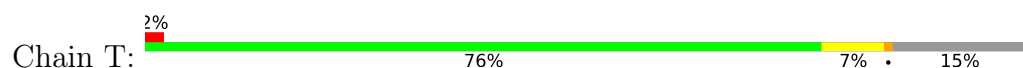
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



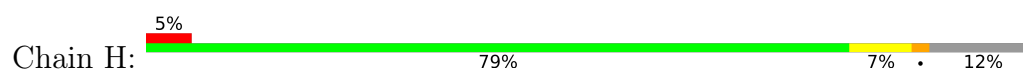
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



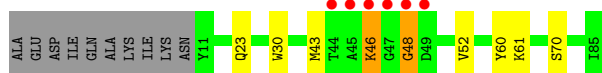
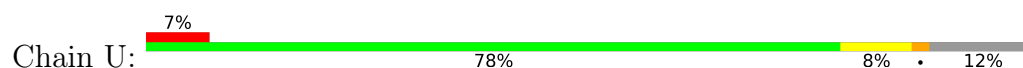
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



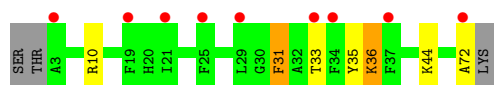
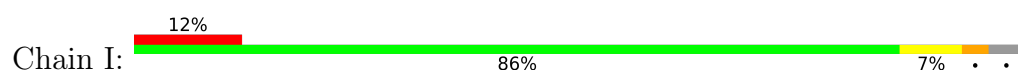
- Molecule 8: Cytochrome c oxidase subunit 6B1



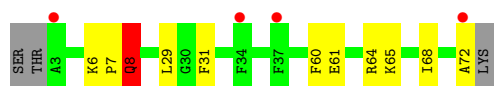
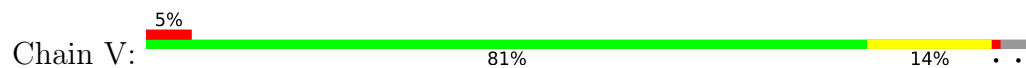
- Molecule 8: Cytochrome c oxidase subunit 6B1



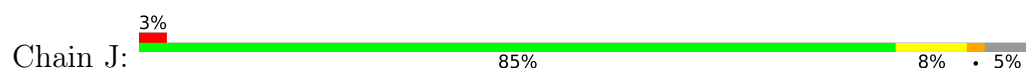
- Molecule 9: Cytochrome c oxidase subunit 6C



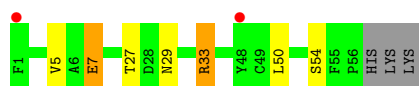
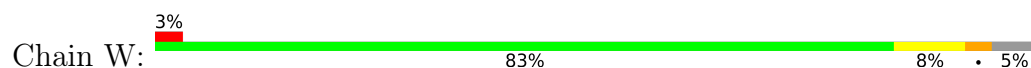
- Molecule 9: Cytochrome c oxidase subunit 6C



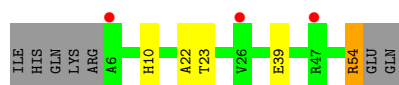
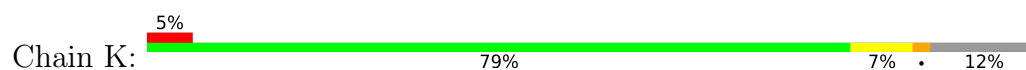
- Molecule 10: Cytochrome c oxidase subunit 7A1



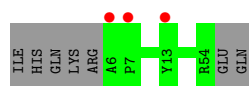
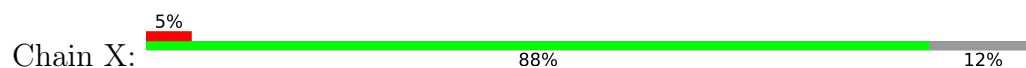
- Molecule 10: Cytochrome c oxidase subunit 7A1



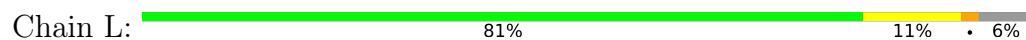
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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

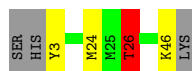


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



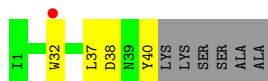
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:  85% 6% • 6%



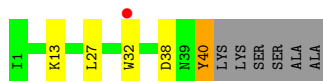
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:  78% 9% 13%



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

Chain Z:  76% 9% • 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.90Å 204.00Å 177.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.75 40.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.75) 100.0 (40.00-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.153 , 0.189 (Not available) , 0.193	Depositor DCC
R_{free} test set	32776 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.779	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33027	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 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, LFA, CDL, PGV, PEK, N2O, HEA, EDO, UNX, NA, DMU, CUA, CHD, CU, ZN, MG

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	1.17	4/4259 (0.1%)	1.30	9/5816 (0.2%)
1	N	1.16	6/4259 (0.1%)	1.31	13/5816 (0.2%)
2	B	1.25	4/1908 (0.2%)	1.40	15/2598 (0.6%)
2	O	1.22	7/1908 (0.4%)	1.35	5/2598 (0.2%)
3	C	1.15	2/2258 (0.1%)	1.26	3/3084 (0.1%)
3	P	1.18	4/2258 (0.2%)	1.27	8/3084 (0.3%)
4	D	1.18	2/1226 (0.2%)	1.36	2/1657 (0.1%)
4	Q	1.16	2/1182 (0.2%)	1.39	3/1598 (0.2%)
5	E	1.16	0/843	1.33	2/1145 (0.2%)
5	R	1.22	0/843	1.37	2/1145 (0.2%)
6	F	1.17	0/724	1.35	0/983
6	S	1.31	4/724 (0.6%)	1.34	3/983 (0.3%)
7	G	1.27	3/633 (0.5%)	1.30	0/864
7	T	1.24	2/633 (0.3%)	1.32	0/864
8	H	1.14	2/648 (0.3%)	1.42	0/877
8	U	1.13	1/648 (0.2%)	1.41	0/877
9	I	1.25	1/588 (0.2%)	1.46	2/781 (0.3%)
9	V	1.19	0/588	1.50	3/781 (0.4%)
10	J	1.15	0/451	1.29	1/610 (0.2%)
10	W	1.21	0/451	1.36	3/610 (0.5%)
11	K	1.20	2/398 (0.5%)	1.45	2/546 (0.4%)
11	X	1.15	0/398	1.32	0/546
12	L	1.12	0/372	1.41	4/500 (0.8%)
12	Y	1.14	1/372 (0.3%)	1.37	1/500 (0.2%)
13	M	1.11	0/321	1.35	0/440
13	Z	1.09	0/321	1.40	0/440
All	All	1.18	47/29214 (0.2%)	1.34	81/39743 (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	1
1	N	0	1
6	S	0	1
All	All	0	3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	198	GLU	C-O	9.10	1.34	1.23
2	B	198	GLU	C-O	8.24	1.33	1.23
2	O	60	GLU	CD-OE1	8.13	1.40	1.25
4	D	58	GLU	CD-OE1	7.83	1.40	1.25
2	B	90	ILE	C-O	7.57	1.32	1.24
3	P	38	ASN	C-O	7.56	1.33	1.23
1	A	174	PRO	C-O	-7.46	1.15	1.24
2	O	60	GLU	CD-OE2	7.25	1.39	1.25
6	S	64	GLU	C-O	7.25	1.32	1.23
1	N	203	ALA	C-O	7.21	1.32	1.24
3	P	71	HIS	CE1-NE2	6.88	1.39	1.32
2	O	90	ILE	C-O	6.86	1.32	1.24
1	A	233	HIS	CE1-NE2	6.79	1.39	1.32
7	G	12	GLY	N-CA	-6.68	1.34	1.45
3	C	34	TRP	C-O	-6.67	1.16	1.24
1	N	400	PHE	C-O	6.52	1.31	1.24
2	B	60	GLU	CD-OE1	6.50	1.37	1.25
9	I	31	PHE	C-O	6.34	1.31	1.24
11	K	39	GLU	C-O	-6.33	1.16	1.24
2	O	113	TYR	C-O	-6.32	1.16	1.24
7	G	37	LEU	C-O	-6.11	1.16	1.24
7	T	12	GLY	N-CA	-6.08	1.35	1.45
1	N	240	HIS	N-CA	5.96	1.51	1.46
1	N	174	PRO	C-O	-5.88	1.17	1.24
11	K	10	HIS	CE1-NE2	5.81	1.38	1.32
1	N	223	ALA	C-O	-5.70	1.17	1.24
8	H	69	VAL	C-O	-5.70	1.17	1.24
4	Q	61	ARG	C-O	-5.69	1.16	1.24
6	S	3	GLY	C-O	5.63	1.34	1.23
2	O	56	MET	C-O	5.59	1.30	1.23
8	H	44	THR	C-O	5.54	1.30	1.24
7	T	45	PRO	C-O	-5.53	1.17	1.23
6	S	75	HIS	CE1-NE2	5.46	1.38	1.32
1	A	378	HIS	CD2-NE2	-5.44	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	115	ASP	CG-OD2	5.37	1.35	1.25
6	S	92	VAL	C-O	-5.36	1.17	1.24
1	A	107	PRO	C-O	-5.36	1.17	1.24
3	P	34	TRP	C-O	-5.34	1.18	1.24
12	Y	3	TYR	N-CA	5.34	1.56	1.46
2	O	26	HIS	CE1-NE2	5.29	1.37	1.32
7	G	41	HIS	CE1-NE2	5.13	1.37	1.32
1	N	376	HIS	CE1-NE2	5.11	1.37	1.32
3	C	70	HIS	CE1-NE2	5.07	1.37	1.32
4	Q	10	ASP	N-CA	5.06	1.55	1.46
3	P	231	HIS	C-O	5.04	1.29	1.24
8	U	70	SER	C-O	5.02	1.29	1.24
4	D	15	SER	CA-CB	-5.01	1.45	1.53

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	HIS	CA-CB-CG	-10.22	103.58	113.80
9	I	72	ALA	CA-C-O	-10.09	103.64	120.80
1	N	240	HIS	CA-CB-CG	-9.68	104.12	113.80
2	B	183	THR	CA-CB-OG1	-9.53	95.31	109.60
4	Q	146	LYS	CA-C-O	-9.29	105.01	120.80
1	A	71	MET	CG-SD-CE	-9.07	80.94	100.90
9	V	72	ALA	CA-C-O	-9.01	105.49	120.80
4	D	146	LYS	CA-C-O	-8.62	106.14	120.80
2	B	115	ASP	CB-CA-C	8.41	125.15	112.03
5	E	108	LYS	CA-C-O	-8.21	106.84	120.80
1	N	71	MET	CG-SD-CE	-8.16	82.94	100.90
3	P	80	ARG	CG-CD-NE	-8.03	94.33	112.00
3	C	80	ARG	CG-CD-NE	-7.92	94.58	112.00
1	A	484	THR	CA-CB-OG1	-7.51	98.34	109.60
2	B	59	GLN	CB-CG-CD	7.48	125.31	112.60
3	C	233	PHE	CA-CB-CG	-7.18	106.62	113.80
4	Q	10	ASP	CA-CB-CG	7.13	119.73	112.60
4	D	58	GLU	CB-CG-CD	7.06	124.61	112.60
11	K	54	ARG	CA-C-O	-6.95	108.98	120.80
12	L	26	THR	CA-CB-OG1	-6.87	99.30	109.60
12	L	25	MET	CA-C-N	6.77	130.19	120.79
12	L	25	MET	C-N-CA	6.77	130.19	120.79
2	O	91	ASN	CA-CB-CG	-6.72	105.88	112.60
3	P	233	PHE	CA-CB-CG	-6.72	107.08	113.80
2	B	65	TRP	CB-CA-C	6.55	122.04	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	76	GLN	CG-CD-NE2	-6.52	106.62	116.40
9	I	33	THR	CA-CB-OG1	-6.50	99.85	109.60
4	Q	20	ARG	CG-CD-NE	-6.49	97.72	112.00
9	V	8	GLN	N-CA-CB	6.42	119.52	109.69
3	P	122	HIS	CB-CA-C	6.17	117.06	110.65
1	A	102	PHE	CA-CB-CG	-6.14	107.66	113.80
2	B	82	ARG	CG-CD-NE	-6.11	98.57	112.00
1	A	513	LEU	CA-C-O	-5.98	110.63	120.80
2	B	59	GLN	N-CA-CB	5.94	118.95	110.16
1	A	507	GLU	CB-CA-C	5.91	116.59	109.85
2	B	199	ILE	N-CA-CB	5.87	117.24	110.49
2	B	184	LEU	N-CA-CB	-5.86	100.97	110.81
10	W	7	GLU	CB-CA-C	5.77	120.66	110.85
1	N	513	LEU	CA-C-O	-5.76	111.00	120.80
12	Y	26	THR	CA-CB-OG1	-5.75	100.97	109.60
3	C	45	ILE	N-CA-C	-5.72	104.83	110.67
3	P	230	ASN	CA-CB-CG	-5.71	106.89	112.60
2	O	89	GLU	CB-CA-C	-5.69	102.14	110.06
10	W	5	VAL	CA-C-O	-5.66	115.06	120.95
10	J	7	GLU	CB-CA-C	5.62	120.40	110.85
12	L	46	LYS	CA-C-O	-5.57	111.33	120.80
2	B	158	ASP	CA-CB-CG	5.56	118.16	112.60
11	K	23	THR	CA-CB-OG1	-5.56	101.26	109.60
1	N	512	ASN	CB-CA-C	5.53	120.02	110.45
5	R	78	HIS	CA-C-N	5.51	128.43	120.38
5	R	78	HIS	C-N-CA	5.51	128.43	120.38
1	A	280	ILE	N-CA-C	-5.50	105.01	110.62
3	P	35	PHE	CA-CB-CG	5.49	119.29	113.80
10	W	33	ARG	CB-CG-CD	5.47	123.89	111.30
1	A	512	ASN	CB-CA-C	5.47	119.92	110.45
1	A	489	THR	CA-CB-OG1	-5.46	101.41	109.60
6	S	3	GLY	CA-C-N	5.42	132.04	121.41
6	S	3	GLY	C-N-CA	5.42	132.04	121.41
1	N	102	PHE	CA-CB-CG	-5.36	108.44	113.80
1	N	240	HIS	N-CA-CB	5.32	116.69	110.42
2	O	114	GLU	CA-C-O	-5.25	115.25	121.66
2	B	11	ASP	CA-CB-CG	5.24	117.84	112.60
3	P	76	GLN	OE1-CD-NE2	5.23	127.83	122.60
1	N	106	PRO	CB-CA-C	5.19	117.25	110.92
2	O	115	ASP	CB-CA-C	5.16	119.86	112.12
9	V	7	PRO	CA-C-O	-5.14	115.74	122.12
2	B	89	GLU	CA-C-N	5.12	127.94	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	89	GLU	C-N-CA	5.12	127.94	120.98
5	E	9	GLU	CB-CG-CD	5.12	121.30	112.60
2	O	158	ASP	CA-CB-CG	5.09	117.69	112.60
1	N	126	TRP	CA-C-N	5.09	128.04	120.31
1	N	126	TRP	C-N-CA	5.09	128.04	120.31
2	B	55	THR	CA-CB-OG1	-5.08	101.98	109.60
1	N	280	ILE	N-CA-C	-5.07	105.45	110.62
2	B	89	GLU	CA-C-O	-5.05	116.20	121.55
1	N	153	ALA	CA-C-N	5.05	125.54	119.94
1	N	153	ALA	C-N-CA	5.05	125.54	119.94
6	S	3	GLY	O-C-N	5.05	131.08	123.00
2	B	64	ILE	N-CA-C	-5.05	105.47	110.62
3	P	94	PHE	CA-CB-CG	-5.03	108.77	113.80
1	N	368	HIS	CA-CB-CG	-5.03	108.77	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	GLY	Mainchain
1	N	296	GLY	Mainchain
6	S	92	VAL	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4102	54	0
1	N	4130	0	4102	60	0
2	B	1870	0	1870	35	0
2	O	1870	0	1870	36	0
3	C	2171	0	2080	32	0
3	P	2172	0	2081	26	0
4	D	1192	0	1178	7	0
4	Q	1148	0	1131	5	0
5	E	825	0	823	1	0
5	R	825	0	823	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	709	0	691	14	0
6	S	709	0	691	9	0
7	G	606	0	577	5	0
7	T	606	0	577	3	0
8	H	628	0	580	12	0
8	U	628	0	580	8	0
9	I	575	0	584	6	0
9	V	575	0	584	5	0
10	J	441	0	439	6	0
10	W	441	0	439	3	0
11	K	384	0	366	1	0
11	X	384	0	366	0	0
12	L	360	0	360	3	0
12	Y	360	0	360	5	0
13	M	311	0	321	2	0
13	Z	311	0	321	2	0
14	A	120	0	108	6	0
14	N	120	0	108	4	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	3	0	0	0	0
18	N	3	0	0	0	0
19	A	14	0	27	7	0
19	B	17	0	33	4	0
19	C	129	0	234	9	0
19	G	14	0	27	5	0
19	N	14	0	27	5	0
19	O	28	0	54	4	0
19	P	85	0	145	6	0
19	T	39	0	75	6	0
20	A	51	0	75	3	0
20	B	66	0	104	0	0
20	C	194	0	261	5	0
20	D	33	0	41	2	0
20	G	11	0	21	0	0
20	H	33	0	29	1	0
20	J	11	0	21	0	0
20	L	22	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	M	41	0	56	0	0
20	N	40	0	54	0	0
20	O	66	0	104	1	0
20	P	172	0	231	2	0
20	Q	33	0	42	3	0
20	T	22	0	31	1	0
20	U	33	0	26	0	0
20	W	11	0	21	0	0
20	Z	63	0	87	4	0
21	A	16	0	24	1	0
21	B	4	0	6	0	0
21	C	12	0	17	0	0
21	D	4	0	6	0	0
21	E	8	0	12	0	0
21	F	8	0	12	0	0
21	G	4	0	6	0	0
21	N	20	0	29	1	0
21	O	4	0	6	0	0
21	P	12	0	18	0	0
21	R	12	0	18	0	0
21	S	8	0	12	0	0
21	T	4	0	6	0	0
22	A	51	0	76	0	0
22	C	51	0	76	2	0
22	N	51	0	76	2	0
22	P	51	0	76	1	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	29	0	39	0	0
24	C	58	0	78	2	0
24	O	29	0	39	1	0
24	P	58	0	78	5	0
25	C	1	0	0	1	0
25	P	1	0	0	1	0
26	C	87	0	124	24	0
26	I	64	0	72	3	0
26	L	94	0	141	4	0
26	N	64	0	72	6	0
26	P	87	0	124	16	0
26	Y	94	0	141	10	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	G	53	0	77	0	0
28	T	53	0	77	4	0
29	A	246	0	0	10	0
29	B	169	0	0	6	0
29	C	108	0	0	5	0
29	D	144	0	0	3	0
29	E	116	0	0	0	0
29	F	110	0	0	1	0
29	G	44	0	0	1	0
29	H	62	0	0	6	0
29	I	41	0	0	2	0
29	J	20	0	0	0	0
29	K	21	0	0	0	0
29	L	28	0	0	1	0
29	M	21	0	0	0	0
29	N	231	0	0	7	0
29	O	148	0	0	3	0
29	P	102	0	0	4	0
29	Q	83	0	0	3	0
29	R	93	0	0	2	0
29	S	98	0	0	1	0
29	T	41	0	0	1	0
29	U	51	0	0	2	0
29	V	22	0	0	1	0
29	W	15	0	0	0	0
29	X	17	0	0	0	0
29	Y	26	0	0	2	0
29	Z	17	0	0	0	0
All	All	33027	0	31507	384	0

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

All (384) 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	29:N:914:HOH:O	1.15	1.28
1:A:112:LEU:HG	29:A:922:HOH:O	1.13	1.28
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:HE3	1.23	1.11
19:C:309:LFA:H12	29:H:228:HOH:O	1.46	1.11
2:B:16[A]:ILE:CG2	2:B:87[A]:MET:HE3	1.82	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:4:GLN:N	29:P:402:HOH:O	1.88	1.04
26:C:304:CDL:HA62	26:C:304:CDL:H121	1.41	1.03
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.42	0.98
26:Y:101:CDL:O1	29:Y:218[B]:HOH:O	1.82	0.97
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:CE	1.96	0.95
3:C:245:VAL:C	3:C:246[B]:ASP:CA	2.41	0.93
20:A:609:DMU:O6	29:A:706:HOH:O	1.88	0.91
24:P:305:CHD:H231	24:P:305:CHD:H162	1.51	0.91
1:N:112:LEU:HD23	1:N:112:LEU:C	1.96	0.90
2:B:16[B]:ILE:HG23	29:B:521:HOH:O	1.71	0.89
26:Y:101:CDL:H142	26:Y:101:CDL:OB9	1.72	0.89
26:L:101:CDL:O1	29:L:216[B]:HOH:O	1.91	0.88
1:N:417[B]:MET:CE	29:N:869:HOH:O	2.21	0.87
1:N:417[B]:MET:HE1	29:N:869:HOH:O	1.71	0.87
26:P:304:CDL:HA62	26:P:304:CDL:H121	1.54	0.87
26:C:304:CDL:HB21	26:C:304:CDL:HB32	1.53	0.86
2:B:16[A]:ILE:HD12	2:B:87[A]:MET:HG3	1.57	0.86
7:G:19:LEU:HD23	19:G:104:LFA:H61	1.58	0.85
4:D:42:GLU:OE2	29:D:301:HOH:O	1.95	0.84
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.18	0.84
1:A:112:LEU:C	1:A:112:LEU:HD23	2.02	0.84
1:N:274:VAL:HG12	1:N:278[A]:MET:HE2	1.62	0.82
4:Q:112:GLU:OE2	29:Q:301:HOH:O	1.97	0.82
26:C:304:CDL:H121	26:C:304:CDL:CA6	2.11	0.80
1:A:112:LEU:HD23	1:A:112:LEU:O	1.83	0.79
25:C:302:UNX:UNK	29:C:501:HOH:O	1.62	0.79
6:S:76:LYS:CE	6:S:93:PRO:HG2	2.13	0.79
29:A:818:HOH:O	3:C:77:LYS:HE3	1.84	0.78
1:N:112:LEU:HD23	1:N:112:LEU:O	1.84	0.78
1:A:278[A]:MET:HE1	19:T:101:LFA:H51	1.67	0.77
12:Y:24:MET:HG3	29:Y:213:HOH:O	1.85	0.76
26:C:304:CDL:HB21	26:C:304:CDL:CB3	2.16	0.75
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.69	0.75
8:H:23:GLN:NE2	29:H:201:HOH:O	2.18	0.75
19:P:309:LFA:H41	29:U:214:HOH:O	1.87	0.75
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:CG	2.18	0.74
3:C:33[A]:MET:HE3	3:C:39:SER:OG	1.88	0.73
3:C:258:TRP:CE2	19:C:307:LFA:H32	2.24	0.72
3:P:33[B]:MET:CE	3:P:42:LEU:HD12	2.19	0.72
19:G:104:LFA:H51	1:N:278[A]:MET:HE1	1.72	0.71
19:G:104:LFA:H11	19:N:608:LFA:H12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:D:201:DMU:H36	20:D:201:DMU:O55	1.90	0.70
26:P:304:CDL:H121	26:P:304:CDL:CA6	2.21	0.70
1:A:274:VAL:HG12	1:A:278[A]:MET:HE2	1.74	0.70
1:A:31:THR:O	1:A:35:LEU:CD2	2.41	0.69
19:C:309:LFA:C1	29:H:228:HOH:O	2.16	0.69
1:N:423[B]:MET:HA	26:N:606:CDL:H782	1.75	0.69
8:H:46:LYS:HE2	8:H:46:LYS:O	1.93	0.68
1:A:136[B]:LEU:HD11	29:A:928:HOH:O	1.93	0.68
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:HG2	1.76	0.67
3:P:50:ASN:HD22	3:P:51[A]:MET:HE2	1.59	0.67
1:N:423[A]:MET:HA	26:N:606:CDL:H782	1.76	0.67
3:C:180[A]:GLU:OE2	29:C:403:HOH:O	2.11	0.67
3:C:33[A]:MET:CE	3:C:42:LEU:H	2.08	0.67
20:Q:201:DMU:O55	20:Q:201:DMU:H36	1.95	0.66
1:N:483:LEU:O	29:N:703:HOH:O	2.11	0.66
1:A:31:THR:O	1:A:35:LEU:HD23	1.95	0.66
2:B:220:GLU:OE1	29:B:402:HOH:O	2.12	0.66
7:G:19:LEU:CD2	19:G:104:LFA:H61	2.26	0.66
6:F:87[A]:THR:HG22	6:F:89:TYR:CE1	2.30	0.66
1:N:112:LEU:C	1:N:112:LEU:CD2	2.68	0.65
2:B:67:ILE:CD1	19:B:307:LFA:H61	2.27	0.65
19:P:309:LFA:C4	29:U:214:HOH:O	2.42	0.65
1:A:113[B]:LEU:HD11	1:A:117[B]:MET:SD	2.37	0.64
6:F:37:LYS:HG2	29:F:297:HOH:O	1.97	0.64
25:P:302:UNX:UNK	29:P:497:HOH:O	1.78	0.64
12:Y:26:THR:CG2	20:Z:102:DMU:H26	2.27	0.64
2:O:60:GLU:CD	2:O:60:GLU:H	2.05	0.64
19:A:607:LFA:H12	19:T:101:LFA:H11	1.78	0.64
26:N:606:CDL:H711	26:N:606:CDL:C52	2.29	0.64
8:H:23:GLN:NE2	29:H:202:HOH:O	2.30	0.63
8:H:22:ASN:ND2	20:H:101:DMU:O3	2.31	0.63
2:B:16[A]:ILE:HG22	2:B:87[A]:MET:HE3	1.76	0.63
3:P:51[B]:MET:HE3	26:P:304:CDL:H873	1.79	0.63
1:N:297[B]:MET:SD	1:N:302:ARG:CG	2.87	0.62
2:B:84:LEU:O	2:B:87[B]:MET:HB2	1.99	0.62
1:N:22:PHE:HA	26:Y:101:CDL:H802	1.81	0.62
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:HG3	1.82	0.62
6:S:76:LYS:HE2	6:S:93:PRO:HG2	1.81	0.62
1:A:297[B]:MET:SD	1:A:302:ARG:HG2	2.39	0.62
1:A:112:LEU:C	1:A:112:LEU:CD2	2.73	0.62
2:B:16[A]:ILE:HD12	2:B:87[A]:MET:CG	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:12:GLY:HA3	29:G:238:HOH:O	1.98	0.62
2:B:227:LEU:HD21	29:B:518:HOH:O	1.99	0.61
26:C:304:CDL:HB61	26:C:304:CDL:CB2	2.30	0.61
26:P:304:CDL:HB61	26:P:304:CDL:HB22	1.82	0.61
1:N:423[B]:MET:HE2	1:N:457:GLY:HA2	1.82	0.61
2:O:67:ILE:HD11	19:O:302:LFA:H42	1.83	0.60
3:P:133:ASN:ND2	29:P:404:HOH:O	2.22	0.60
26:P:304:CDL:HA62	26:P:304:CDL:C12	2.27	0.60
3:C:247:VAL:HG11	19:C:314:LFA:H71	1.84	0.60
8:H:23:GLN:HG3	29:H:241:HOH:O	2.02	0.60
26:L:101:CDL:H381	26:L:101:CDL:H722	1.83	0.59
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.37	0.59
2:O:16[A]:ILE:HG21	2:O:87[A]:MET:HG2	1.84	0.59
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.03	0.59
28:T:102:PEK:H71	28:T:102:PEK:H32	1.83	0.59
26:Y:101:CDL:H362	26:Y:101:CDL:H711	1.84	0.59
26:C:304:CDL:OA3	26:C:304:CDL:H1	2.01	0.59
3:C:104:SER:OG	29:C:404:HOH:O	2.14	0.59
3:P:149:HIS:NE2	19:P:311:LFA:H11	2.18	0.59
26:Y:101:CDL:H711	26:Y:101:CDL:C36	2.33	0.59
26:C:304:CDL:HB21	26:C:304:CDL:HB61	1.84	0.59
7:T:19:LEU:HD23	19:T:101:LFA:H61	1.83	0.59
8:U:43:MET:O	8:U:48:GLY:N	2.36	0.58
2:B:67:ILE:HD11	19:B:307:LFA:H42	1.85	0.58
8:H:43:MET:CE	8:U:52:VAL:HG11	2.34	0.58
12:Y:26:THR:HG21	20:Z:102:DMU:H26	1.85	0.58
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.34	0.57
13:Z:27:LEU:HD22	20:Z:101:DMU:H14	1.86	0.57
3:C:33[A]:MET:HE1	3:C:41:THR:HB	1.85	0.57
4:D:10:ASP:OD2	29:D:302:HOH:O	2.17	0.57
4:Q:73:ARG:NH1	29:Q:303:HOH:O	2.36	0.57
2:B:13:THR:HB	2:B:168:LEU:HD23	1.87	0.57
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.05	0.57
1:A:278[B]:MET:SD	19:A:607:LFA:H52	2.45	0.57
1:A:278[B]:MET:HE1	19:A:607:LFA:H52	1.86	0.56
1:A:51:ASP:OD2	1:A:441:SER:OG	2.22	0.56
29:Q:320:HOH:O	5:R:108:LYS:HD3	2.06	0.56
20:C:325:DMU:H20	10:J:50:LEU:HB2	1.87	0.56
8:H:43:MET:HE1	8:U:52:VAL:HG11	1.88	0.56
21:A:611:EDO:H12	2:B:58:ALA:HB3	1.88	0.55
24:C:305:CHD:H162	24:C:305:CHD:H231	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:8:GLN:NE2	29:V:101:HOH:O	2.38	0.55
8:H:52:VAL:CG1	8:U:46:LYS:HG2	2.29	0.55
1:N:87:ILE:O	1:N:173:PRO:HD3	2.06	0.55
3:C:33[B]:MET:HE3	3:C:42:LEU:HD12	1.87	0.55
6:S:19:GLU:OE1	6:S:31:TYR:OH	2.12	0.55
29:A:885:HOH:O	6:F:37:LYS:CE	2.55	0.55
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.42	0.55
1:N:486:ASP:OD2	4:Q:19:ARG:NE	2.40	0.55
26:C:304:CDL:OA5	26:C:304:CDL:OB9	2.24	0.55
1:A:112:LEU:CG	29:A:922:HOH:O	1.99	0.54
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.88	0.54
1:A:486:ASP:HB3	29:A:913[B]:HOH:O	2.07	0.54
2:B:60:GLU:H	2:B:60:GLU:CD	2.15	0.54
1:N:136[B]:LEU:HD11	29:N:919:HOH:O	2.07	0.54
1:A:309:THR:HG22	14:A:602:HEA:HMB2	1.90	0.54
3:C:59:ARG:HB2	26:C:304:CDL:OA9	2.08	0.54
2:B:67:ILE:HD11	19:B:307:LFA:H61	1.88	0.54
2:B:140:ASN:HB3	29:B:520:HOH:O	2.06	0.54
9:I:10:ARG:CD	29:I:216:HOH:O	2.56	0.54
1:N:310:MET:HE1	2:O:77:ALA:HB2	1.89	0.54
1:A:278[A]:MET:CE	19:T:101:LFA:H51	2.38	0.53
26:C:304:CDL:H752	10:J:27:THR:HG21	1.90	0.53
1:N:34:SER:HB2	14:N:601:HEA:C2B	2.38	0.53
1:N:488:THR:HB	1:N:495:LEU:HD13	1.89	0.53
1:A:484:THR:HG22	29:A:924:HOH:O	2.09	0.53
26:I:101:CDL:OA4	29:I:201:HOH:O	2.18	0.53
26:P:304:CDL:H752	10:W:27:THR:HG21	1.90	0.53
24:P:305:CHD:H231	24:P:305:CHD:C16	2.33	0.53
26:I:101:CDL:C1	26:I:101:CDL:OA3	2.56	0.53
22:N:616:PGV:H183	28:T:102:PEK:H331	1.89	0.53
3:P:104:SER:OG	29:P:403:HOH:O	2.19	0.53
26:N:606:CDL:C52	26:N:606:CDL:H312	2.38	0.53
2:O:16[B]:ILE:HG23	29:O:506:HOH:O	2.09	0.53
29:C:507:HOH:O	6:F:33:ILE:HD13	2.09	0.52
5:R:90:ARG:NH1	29:R:303:HOH:O	2.25	0.52
8:H:52:VAL:HG21	8:U:43:MET:HE1	1.92	0.52
13:M:32:TRP:CZ3	13:M:40:TYR:OH	2.62	0.52
1:N:362[A]:SER:HA	2:O:87[A]:MET:HE1	1.92	0.52
1:A:189:MET:HE3	19:A:607:LFA:H31	1.91	0.52
2:O:82:ARG:HA	20:O:304:DMU:H30	1.92	0.52
29:N:855:HOH:O	4:Q:20:ARG:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:164:PHE:CD1	24:P:305:CHD:H192	2.44	0.52
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.90	0.52
1:N:278[B]:MET:HE1	19:N:608:LFA:H52	1.92	0.52
2:B:22[B]:HIS:CE1	9:I:44:LYS:CE	2.92	0.52
19:C:314:LFA:H21	19:C:315:LFA:H71	1.91	0.52
2:O:58:ALA:O	2:O:62:GLU:HG3	2.10	0.51
6:F:10:GLU:OE2	6:F:25:ARG:NH2	2.41	0.51
1:A:31:THR:O	1:A:35:LEU:HD22	2.09	0.51
8:H:23:GLN:CD	29:H:201:HOH:O	2.52	0.51
26:Y:101:CDL:OB9	26:Y:101:CDL:C14	2.54	0.51
26:Y:101:CDL:HB22	26:Y:101:CDL:HA32	1.91	0.51
3:C:33[A]:MET:HE1	3:C:42:LEU:H	1.74	0.51
3:P:51[B]:MET:CE	26:P:304:CDL:H873	2.40	0.51
1:N:362[A]:SER:OG	2:O:87[A]:MET:CE	2.59	0.51
6:S:37:LYS:HG3	29:S:209:HOH:O	2.11	0.50
2:O:60:GLU:CD	2:O:60:GLU:N	2.68	0.50
3:C:180[B]:GLU:HG2	29:C:424:HOH:O	2.11	0.50
3:C:41:THR:HG23	20:C:320:DMU:H15	1.93	0.50
2:O:67:ILE:HD13	19:O:302:LFA:H62	1.94	0.50
29:A:885:HOH:O	6:F:37:LYS:HE2	2.09	0.50
1:N:334:TRP:HB2	20:Q:201:DMU:H29	1.93	0.50
1:A:87:ILE:O	1:A:173:PRO:HD3	2.11	0.49
3:P:116:TRP:HA	3:P:117:PRO:C	2.37	0.49
1:N:484:THR:OG1	29:N:705[A]:HOH:O	2.20	0.49
26:C:304:CDL:HB22	10:J:8:LYS:HE3	1.93	0.49
2:O:92:ASN:ND2	29:O:406:HOH:O	2.46	0.49
12:Y:26:THR:HG22	20:Z:102:DMU:H26	1.93	0.49
3:C:67:PHE:CE2	26:C:304:CDL:O1	2.65	0.49
26:C:304:CDL:OB9	26:C:304:CDL:CA3	2.61	0.49
26:C:304:CDL:CA5	26:C:304:CDL:OA8	2.61	0.49
26:P:304:CDL:OA8	26:P:304:CDL:CA5	2.60	0.49
6:F:85:CYS:SG	6:F:87[B]:THR:OG1	2.68	0.48
1:A:1:FME:HE2	1:A:1:FME:HA	1.95	0.48
2:O:13:THR:HB	2:O:168:LEU:HD23	1.95	0.48
1:N:494:TRP:O	21:N:615:EDO:H22	2.14	0.48
3:P:67:PHE:CE2	26:P:304:CDL:O1	2.66	0.48
1:N:362[A]:SER:OG	2:O:87[A]:MET:HE2	2.13	0.48
3:C:37:PHE:CE2	20:C:325:DMU:H13	2.49	0.48
20:C:325:DMU:H11	10:J:49:CYS:HB3	1.94	0.48
4:D:86:MET:HE1	11:K:22:ALA:HB2	1.94	0.48
1:A:240:HIS:C	1:A:240:HIS:CD2	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:59:GLN:NE2	19:O:303:LFA:H31	2.28	0.48
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.43	0.48
2:B:91:ASN:OD1	2:B:183:THR:HG21	2.14	0.48
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.66	0.48
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.48	0.48
1:A:334:TRP:CZ3	20:A:608:DMU:H19	2.49	0.47
26:C:304:CDL:H531	26:C:304:CDL:HB4	1.96	0.47
2:O:121:TYR:O	2:O:138:VAL:HA	2.14	0.47
2:O:67:ILE:CD1	19:O:302:LFA:H62	2.45	0.47
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.50	0.47
6:F:92:VAL:HG23	6:F:92:VAL:O	2.14	0.47
1:A:76:GLY:O	1:A:80:ASN:HB2	2.15	0.47
1:A:308:ALA:O	1:A:311[B]:ILE:HG12	2.14	0.47
2:B:60:GLU:CD	2:B:60:GLU:N	2.73	0.47
1:A:278[B]:MET:SD	19:A:607:LFA:C5	3.03	0.47
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.97	0.46
1:N:423[B]:MET:HE3	1:N:457:GLY:N	2.30	0.46
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.96	0.46
2:B:58:ALA:O	2:B:62:GLU:HG3	2.14	0.46
3:C:33[A]:MET:HE2	3:C:42:LEU:H	1.78	0.46
1:N:334:TRP:HB2	20:Q:201:DMU:C57	2.45	0.46
3:C:16:TRP:N	3:C:17:PRO:CD	2.79	0.46
28:T:102:PEK:H32	28:T:102:PEK:C7	2.45	0.46
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.39	0.46
1:A:297[B]:MET:SD	1:A:302:ARG:CG	3.04	0.46
29:A:818:HOH:O	3:C:77:LYS:CE	2.55	0.46
22:C:303:PGV:H12	22:C:303:PGV:H161	1.97	0.46
26:P:304:CDL:HB31	26:P:304:CDL:H512	1.98	0.46
4:D:16:TYR:OH	4:D:18:ASP:OD1	2.33	0.46
4:D:82:VAL:HG12	4:D:86:MET:HE2	1.98	0.46
1:A:449:MET:SD	2:B:5:MET:HG2	2.56	0.46
3:C:116:TRP:HA	3:C:117:PRO:C	2.40	0.46
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.97	0.46
19:G:104:LFA:H51	1:N:278[A]:MET:CE	2.43	0.46
3:C:33[A]:MET:HG2	3:C:39:SER:O	2.16	0.45
26:C:304:CDL:HB4	26:C:304:CDL:C52	2.46	0.45
1:A:23:GLY:HA3	1:A:73:ILE:HG13	1.98	0.45
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.97	0.45
7:G:34:ASN:O	7:G:38:HIS:HD2	2.00	0.45
2:B:67:ILE:HD13	19:B:307:LFA:H61	1.98	0.45
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:220:GLU:OE1	29:O:402:HOH:O	2.21	0.45
1:N:240:HIS:C	1:N:240:HIS:CD2	2.94	0.45
26:N:606:CDL:C52	26:N:606:CDL:C31	2.95	0.45
24:O:301:CHD:H212	24:O:301:CHD:H12	1.97	0.45
3:P:144[A]:ILE:HD13	3:P:239:ALA:HA	1.99	0.45
26:C:304:CDL:H751	26:C:304:CDL:H711	1.99	0.45
1:N:71:MET:HE1	1:N:195:LEU:HD21	1.98	0.45
3:P:33[B]:MET:HB2	3:P:33[B]:MET:HE2	1.48	0.45
7:T:37:LEU:HD12	7:T:37:LEU:HA	1.87	0.45
3:P:59:ARG:HG3	26:P:304:CDL:HA4	1.99	0.44
1:N:2:PHE:HE2	26:Y:101:CDL:H712	1.81	0.44
6:S:54:ASN:HD22	6:S:54:ASN:C	2.26	0.44
1:A:379:TYR:CZ	1:A:383:MET:HE1	2.52	0.44
2:B:33:LEU:HD13	9:I:31:PHE:CD2	2.51	0.44
5:R:46:LYS:NZ	29:R:305:HOH:O	2.50	0.44
26:Y:101:CDL:HB22	26:Y:101:CDL:CA3	2.47	0.44
1:A:378:HIS:HA	1:A:382:SER:HB2	2.00	0.44
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.99	0.44
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:CG	2.47	0.44
2:B:53:THR:O	29:B:403:HOH:O	2.21	0.44
1:N:328:HIS:HB2	2:O:45:MET:SD	2.58	0.44
26:P:304:CDL:OA3	26:P:304:CDL:H1	2.14	0.44
3:C:59:ARG:HG3	26:C:304:CDL:HA4	2.00	0.44
3:C:258:TRP:CD2	19:C:307:LFA:H32	2.52	0.44
2:O:65:TRP:O	2:O:69:PRO:HG2	2.18	0.44
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.99	0.44
1:A:278[B]:MET:CE	19:A:607:LFA:H52	2.47	0.44
1:N:278[B]:MET:SD	19:N:608:LFA:H52	2.57	0.44
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.99	0.44
1:A:308:ALA:HA	20:A:615:DMU:H23	2.00	0.44
6:F:51:SER:HB2	6:F:91:LEU:HD11	2.00	0.44
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	2.00	0.44
20:T:105:DMU:O7	29:T:201:HOH:O	2.20	0.44
26:L:101:CDL:OB9	26:L:101:CDL:H122	2.18	0.43
2:B:1:FME:HE1	2:B:133:LEU:HD22	2.01	0.43
22:N:616:PGV:H343	28:T:102:PEK:H382	1.99	0.43
10:W:29:ASN:O	10:W:33:ARG:HG3	2.19	0.43
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.01	0.43
3:C:226:HIS:HE1	26:C:304:CDL:H111	1.82	0.43
2:O:16[A]:ILE:HG21	2:O:87[A]:MET:CG	2.48	0.43
3:P:247:VAL:HG11	19:P:312:LFA:H71	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:THR:CG2	14:A:602:HEA:HMB2	2.48	0.43
3:C:144[A]:ILE:HD13	3:C:239:ALA:HA	2.00	0.43
1:N:377:PHE:O	1:N:381:LEU:HB3	2.18	0.43
26:P:304:CDL:CA6	26:P:304:CDL:C12	2.92	0.43
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	2.00	0.43
2:B:164:ALA:O	2:B:194:GLY:HA3	2.19	0.43
26:C:304:CDL:H612	26:C:304:CDL:H831	2.00	0.43
1:N:278[B]:MET:SD	19:N:608:LFA:C5	3.07	0.43
3:C:210:ILE:HD13	22:C:303:PGV:H312	1.99	0.43
19:C:307:LFA:H31	24:P:301:CHD:H61	2.01	0.43
26:I:101:CDL:OA3	26:I:101:CDL:H1	2.18	0.43
1:N:423[B]:MET:CE	1:N:457:GLY:N	2.81	0.43
19:A:607:LFA:H12	19:T:101:LFA:C1	2.46	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.19	0.43
6:F:64:GLU:O	6:F:65:ASP:HB2	2.19	0.42
1:N:378:HIS:HA	1:N:382:SER:HB2	2.01	0.42
3:P:33[A]:MET:HG2	3:P:39:SER:O	2.19	0.42
1:A:240:HIS:O	1:A:241:PRO:C	2.60	0.42
1:N:19:TYR:CD1	1:N:76:GLY:HA3	2.54	0.42
1:N:83:VAL:HB	1:N:84:PRO:HD3	2.01	0.42
1:N:189:MET:HE3	19:N:608:LFA:H31	2.02	0.42
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.54	0.42
1:N:423[B]:MET:HE2	1:N:457:GLY:CA	2.47	0.42
26:P:304:CDL:H151	26:P:304:CDL:H311	2.02	0.42
1:A:334:TRP:HB2	20:D:201:DMU:C57	2.49	0.42
6:F:13:ALA:CB	6:F:21[B]:MET:HE1	2.49	0.42
3:P:50:ASN:ND2	3:P:54[A]:MET:HE2	2.34	0.42
3:P:226:HIS:HE1	26:P:304:CDL:H111	1.85	0.42
7:T:23:LEU:HB2	19:T:101:LFA:H92	2.01	0.42
9:I:36:LYS:HE3	9:I:36:LYS:HA	2.02	0.42
1:N:43:GLN:HB2	1:N:44:PRO:HD2	2.01	0.42
1:N:498:CYS:HA	1:N:499:PRO:HA	1.92	0.42
1:N:379:TYR:CZ	1:N:383:MET:HE1	2.55	0.42
1:A:71:MET:HE1	1:A:195:LEU:HD21	2.02	0.42
2:B:41:ILE:O	2:B:45:MET:HG2	2.19	0.42
26:C:304:CDL:HB61	26:C:304:CDL:HB22	2.01	0.42
12:L:13:PHE:HB3	26:L:101:CDL:H512	2.02	0.42
3:C:33[B]:MET:HG3	3:C:37:PHE:HB2	2.02	0.42
1:N:148:PHE:HB3	3:P:28:THR:HB	2.02	0.42
1:N:181:THR:HA	1:N:182:PRO:HD3	1.93	0.42
1:N:381:LEU:HB2	14:N:602:HEA:CAC	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:210:ILE:HD13	22:P:303:PGV:H312	2.00	0.42
1:A:34:SER:HB2	14:A:601:HEA:C2B	2.49	0.41
1:A:297[A]:MET:HE3	1:A:297[A]:MET:HB2	1.85	0.41
1:N:377:PHE:CD2	14:N:602:HEA:HAD1	2.55	0.41
2:O:33:LEU:HD13	9:V:31:PHE:CD2	2.55	0.41
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.54	0.41
6:S:10:GLU:OE2	6:S:25:ARG:NH1	2.50	0.41
1:A:377:PHE:O	1:A:381:LEU:HB3	2.20	0.41
1:N:423[B]:MET:HA	26:N:606:CDL:C78	2.45	0.41
1:A:488:THR:HB	1:A:495:LEU:HD13	2.02	0.41
3:C:51[B]:MET:HE2	26:C:304:CDL:H872	2.02	0.41
5:R:44:GLU:OE1	9:V:6:LYS:NZ	2.46	0.41
3:C:149:HIS:NE2	19:C:313:LFA:H21	2.36	0.41
1:N:110:LEU:CD2	20:P:322:DMU:H24	2.50	0.41
3:P:244:PHE:HA	19:P:312:LFA:H41	2.02	0.41
26:Y:101:CDL:OA5	26:Y:101:CDL:OA8	2.38	0.41
1:A:115[A]:SER:O	1:A:121:GLY:HA2	2.21	0.41
3:P:127:LEU:HD21	19:P:307:LFA:H31	2.02	0.41
2:B:217:LYS:HD3	29:B:547:HOH:O	2.20	0.41
3:C:247:VAL:CG1	19:C:314:LFA:H71	2.49	0.41
4:D:104:TYR:O	29:D:303:HOH:O	2.22	0.41
2:O:108:TYR:O	2:O:117:SER:HA	2.21	0.41
1:A:409:TRP:HB3	1:A:471:ILE:HG12	2.02	0.41
3:P:22:LEU:O	3:P:26:LEU:HG	2.21	0.41
1:A:208[B]:MET:HG2	1:A:219:PHE:CE2	2.56	0.41
26:C:304:CDL:OA8	26:C:304:CDL:C11	2.68	0.41
9:I:35:TYR:CD1	9:I:35:TYR:C	2.99	0.41
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	2.02	0.41
1:A:32:ALA:HB3	12:L:36:PRO:HG2	2.03	0.41
1:A:465:VAL:HG21	14:A:601:HEA:H261	2.03	0.41
2:B:1:FME:HE2	2:B:1:FME:HB3	1.94	0.41
24:C:305:CHD:O25	10:J:1:PHE:N	2.53	0.41
1:N:363:LEU:HD23	1:N:363:LEU:HA	1.89	0.41
1:N:489:THR:HA	6:S:71:TRP:O	2.21	0.41
2:O:5:MET:HE2	2:O:5:MET:HB3	1.92	0.41
2:O:22[B]:HIS:ND1	2:O:22[B]:HIS:O	2.54	0.41
1:A:225:GLY:HA3	3:C:112:LEU:HD21	2.03	0.40
2:B:196:CYS:HB2	2:B:207:MET:HG3	2.02	0.40
6:F:55:LYS:HA	6:F:74:LEU:O	2.21	0.40
12:L:44:LEU:HD23	12:L:44:LEU:HA	1.94	0.40
2:O:114:GLU:HG3	2:O:227:LEU:CD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:324:DMU:H26	7:G:31:CYS:SG	2.62	0.40
8:H:60:TYR:CD1	8:H:60:TYR:C	2.99	0.40
3:P:63:ARG:HH21	26:P:304:CDL:PA1	2.44	0.40
20:P:322:DMU:O55	20:P:322:DMU:H36	2.21	0.40
2:O:1:FME:HE1	2:O:133:LEU:HD22	2.04	0.40
10:W:54:SER:O	12:Y:46:LYS:HE2	2.21	0.40
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.89	0.40
24:P:301:CHD:H12	24:P:301:CHD:H212	2.03	0.40
26:C:304:CDL:C75	10:J:27:THR:HG21	2.52	0.40
6:S:21[B]:MET:HE2	6:S:21[B]:MET:HB2	1.87	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%)	223 (97%)	7 (3%)	0	100	100
2	O	230/227 (101%)	223 (97%)	7 (3%)	0	100	100
3	C	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
3	P	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	136/147 (92%)	133 (98%)	3 (2%)	0	100	100
5	E	100/109 (92%)	100 (100%)	0	0	100	100
5	R	100/109 (92%)	99 (99%)	1 (1%)	0	100	100
6	F	91/98 (93%)	91 (100%)	0	0	100	100
6	S	91/98 (93%)	88 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	71/85 (84%)	67 (94%)	4 (6%)	0	100	100
7	T	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
8	H	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
8	U	73/85 (86%)	71 (97%)	1 (1%)	1 (1%)	9	2
9	I	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
9	V	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
10	J	54/59 (92%)	54 (100%)	0	0	100	100
10	W	54/59 (92%)	54 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
12	Y	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
13	M	38/46 (83%)	38 (100%)	0	0	100	100
13	Z	38/46 (83%)	38 (100%)	0	0	100	100
All	All	3488/3614 (96%)	3411 (98%)	76 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	U	48	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/426 (103%)	437 (99%)	3 (1%)	76	67
1	N	440/426 (103%)	436 (99%)	4 (1%)	70	60
2	B	215/210 (102%)	206 (96%)	9 (4%)	26	8
2	O	215/210 (102%)	209 (97%)	6 (3%)	38	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	232/226 (103%)	230 (99%)	2 (1%)	70	60
3	P	232/226 (103%)	230 (99%)	2 (1%)	70	60
4	D	128/129 (99%)	127 (99%)	1 (1%)	73	64
4	Q	122/129 (95%)	120 (98%)	2 (2%)	55	38
5	E	89/95 (94%)	88 (99%)	1 (1%)	65	52
5	R	89/95 (94%)	88 (99%)	1 (1%)	65	52
6	F	78/81 (96%)	75 (96%)	3 (4%)	29	10
6	S	78/81 (96%)	75 (96%)	3 (4%)	29	10
7	G	63/69 (91%)	61 (97%)	2 (3%)	34	14
7	T	63/69 (91%)	60 (95%)	3 (5%)	23	6
8	H	67/75 (89%)	65 (97%)	2 (3%)	36	16
8	U	67/75 (89%)	64 (96%)	3 (4%)	24	7
9	I	55/58 (95%)	54 (98%)	1 (2%)	51	33
9	V	55/58 (95%)	51 (93%)	4 (7%)	13	2
10	J	47/50 (94%)	46 (98%)	1 (2%)	47	27
10	W	47/50 (94%)	45 (96%)	2 (4%)	26	8
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	20
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	37/40 (92%)	36 (97%)	1 (3%)	39	19
12	Y	37/40 (92%)	36 (97%)	1 (3%)	39	19
13	M	34/38 (90%)	33 (97%)	1 (3%)	37	17
13	Z	34/38 (90%)	31 (91%)	3 (9%)	9	1
All	All	3042/3086 (99%)	2980 (98%)	62 (2%)	48	29

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	A	363	LEU
1	A	369	ASP
2	B	33	LEU
2	B	35	SER
2	B	59	GLN
2	B	60	GLU

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Mol	Chain	Res	Type
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
3	C	159	MET
3	C	230	ASN
4	D	58	GLU
5	E	70	VAL
6	F	37	LYS
6	F	87[A]	THR
6	F	87[B]	THR
7	G	36	TRP
7	G	37	LEU
8	H	46	LYS
8	H	60	TYR
9	I	36	LYS
10	J	7	GLU
11	K	54	ARG
12	L	26	THR
13	M	38	ASP
1	N	112	LEU
1	N	152	LEU
1	N	369	ASP
1	N	485	VAL
2	O	33	LEU
2	O	60	GLU
2	O	78	LEU
2	O	92	ASN
2	O	94	SER
2	O	115	ASP
3	P	159	MET
3	P	230	ASN
4	Q	10	ASP
4	Q	51	LEU
5	R	79	LYS
6	S	37	LYS
6	S	43	LYS
6	S	54	ASN
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU

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Mol	Chain	Res	Type
8	U	46	LYS
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	29	LEU
9	V	65	LYS
9	V	68	ILE
10	W	7	GLU
10	W	50	LEU
12	Y	26	THR
13	Z	13	LYS
13	Z	38	ASP
13	Z	40	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	52	HIS
2	B	203	ASN
3	C	50	ASN
4	D	29	HIS
4	D	119	GLN
4	D	143	ASN
5	E	78	HIS
5	E	94	ASN
6	F	54	ASN
7	G	34	ASN
7	G	38	HIS
8	H	22	ASN
8	H	37	HIS
11	K	35	GLN
2	O	59	GLN
2	O	92	ASN
3	P	50	ASN
4	Q	76	ASN
4	Q	109	HIS
4	Q	119	GLN
4	Q	143	ASN
5	R	94	ASN
6	S	54	ASN
7	T	34	ASN
8	U	22	ASN

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Mol	Chain	Res	Type
8	U	37	HIS

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	B	1	2	8,9,10	1.01	1 (12%)	8,9,11	1.05	1 (12%)
1	FME	N	1	1	8,9,10	0.80	0	8,9,11	0.96	0
2	FME	O	1	2	8,9,10	0.71	0	8,9,11	1.00	1 (12%)
1	FME	A	1	1	8,9,10	0.58	0	8,9,11	1.03	0

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-2.39	1.69	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	O-C-CA	-2.13	119.30	124.77
2	B	1	FME	CG-CB-CA	-2.06	106.57	112.87

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 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 133 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 123 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
19	LFA	P	311	-	10,10,19	0.26	0	9,9,18	0.30	0
21	EDO	N	615	-	3,3,3	0.74	0	2,2,2	0.24	0
26	CDL	L	101	-	93,93,99	0.68	2 (2%)	99,105,111	0.92	8 (8%)
26	CDL	Y	101	-	93,93,99	0.60	0	99,105,111	0.84	6 (6%)
21	EDO	A	610	-	3,3,3	0.29	0	2,2,2	0.26	0
20	DMU	N	610	-	34,34,34	1.62	9 (26%)	45,45,45	1.15	3 (6%)
21	EDO	A	612	-	3,3,3	0.74	0	2,2,2	0.15	0
20	DMU	Z	101	-	34,34,34	1.01	3 (8%)	45,45,45	1.24	5 (11%)
21	EDO	C	322	-	3,3,3	0.45	0	2,2,2	0.05	0
21	EDO	N	614	-	3,3,3	0.24	0	2,2,2	0.11	0
20	DMU	B	303	-	10,10,34	0.30	0	9,9,45	0.73	0
20	DMU	P	316	-	22,22,34	0.87	2 (9%)	27,27,45	1.11	2 (7%)
21	EDO	R	203	-	3,3,3	0.62	0	2,2,2	0.35	0
21	EDO	T	106	-	3,3,3	0.26	0	2,2,2	0.11	0
20	DMU	C	317	-	6,6,34	0.38	0	5,5,45	0.45	0
24	CHD	P	301	-	32,32,32	0.94	1 (3%)	51,51,51	0.94	3 (5%)
20	DMU	C	324	-	22,22,34	0.84	1 (4%)	27,27,45	1.05	2 (7%)
14	HEA	N	602	1	67,67,67	2.18	23 (34%)	81,103,103	2.55	33 (40%)
21	EDO	F	102	-	3,3,3	0.35	0	2,2,2	0.18	0
24	CHD	C	305	-	32,32,32	0.82	1 (3%)	51,51,51	1.66	7 (13%)
21	EDO	A	611	-	3,3,3	0.32	0	2,2,2	0.29	0
20	DMU	P	306	-	10,10,34	0.31	0	9,9,45	0.66	0
20	DMU	C	320	-	34,34,34	0.89	1 (2%)	45,45,45	1.33	5 (11%)
24	CHD	B	306	-	32,32,32	0.84	0	51,51,51	0.91	2 (3%)
19	LFA	P	308	-	5,5,19	0.21	0	4,4,18	0.19	0
18	N2O	N	607	-	0,2,2	-	-	0,1,1	-	-
19	LFA	P	312	-	14,14,19	0.71	0	13,13,18	0.28	0
24	CHD	O	301	-	32,32,32	0.71	0	51,51,51	0.99	2 (3%)
19	LFA	P	313	-	12,12,19	0.35	0	11,11,18	0.31	0
21	EDO	G	103	-	3,3,3	0.16	0	2,2,2	0.09	0
20	DMU	C	319	-	34,34,34	0.99	3 (8%)	45,45,45	1.23	3 (6%)
21	EDO	P	319	-	3,3,3	0.32	0	2,2,2	0.21	0
20	DMU	L	102	-	22,22,34	0.72	0	27,27,45	0.98	1 (3%)
21	EDO	C	321	-	3,3,3	0.12	0	2,2,2	0.32	0
21	EDO	P	321	-	3,3,3	0.42	0	2,2,2	0.98	0
28	PEK	T	102	-	52,52,52	0.80	2 (3%)	55,57,57	1.03	4 (7%)
20	DMU	D	201	-	34,34,34	1.52	7 (20%)	45,45,45	1.41	5 (11%)
20	DMU	G	102	-	10,10,34	0.42	0	9,9,45	0.50	0
19	LFA	C	326	-	14,14,19	0.30	0	13,13,18	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	PGV	N	616	-	50,50,50	0.95	3 (6%)	53,56,56	1.31	4 (7%)
20	DMU	C	316	-	34,34,34	0.97	3 (8%)	45,45,45	1.58	6 (13%)
20	DMU	U	101	-	34,34,34	1.02	3 (8%)	45,45,45	1.50	5 (11%)
19	LFA	C	314	-	14,14,19	0.33	0	13,13,18	0.45	0
21	EDO	N	611	-	3,3,3	0.50	0	2,2,2	0.09	0
20	DMU	O	304	-	22,22,34	0.94	1 (4%)	27,27,45	1.52	4 (14%)
20	DMU	C	318	-	22,22,34	0.92	2 (9%)	27,27,45	1.27	4 (14%)
21	EDO	R	201	-	3,3,3	0.74	0	2,2,2	0.38	0
22	PGV	A	614	-	50,50,50	0.95	2 (4%)	53,56,56	1.21	3 (5%)
20	DMU	N	609	-	6,6,34	0.23	0	5,5,45	0.41	0
19	LFA	C	312	-	13,13,19	0.27	0	12,12,18	0.20	0
19	LFA	P	307	-	10,10,19	0.27	0	9,9,18	0.22	0
21	EDO	E	202	-	3,3,3	0.30	0	2,2,2	0.06	0
19	LFA	T	103	-	13,13,19	0.22	0	12,12,18	0.16	0
20	DMU	P	322	-	34,34,34	0.94	2 (5%)	45,45,45	1.71	9 (20%)
21	EDO	E	201	-	3,3,3	0.25	0	2,2,2	0.21	0
19	LFA	O	302	-	16,16,19	0.27	0	15,15,18	0.24	0
21	EDO	A	613	-	3,3,3	0.47	0	2,2,2	0.30	0
20	DMU	P	315	-	6,6,34	0.29	0	5,5,45	0.54	0
20	DMU	B	308	-	22,22,34	0.74	0	27,27,45	1.56	5 (18%)
14	HEA	N	601	1	67,67,67	1.97	22 (32%)	81,103,103	2.75	37 (45%)
21	EDO	S	103	-	3,3,3	0.39	0	2,2,2	0.17	0
19	LFA	C	308	-	5,5,19	0.31	0	4,4,18	0.21	0
28	PEK	G	101	-	52,52,52	0.73	1 (1%)	55,57,57	0.74	2 (3%)
20	DMU	P	314	-	34,34,34	0.86	2 (5%)	45,45,45	1.46	6 (13%)
19	LFA	O	303	-	10,10,19	0.31	0	9,9,18	0.20	0
19	LFA	C	313	-	10,10,19	0.38	0	9,9,18	0.24	0
20	DMU	B	302	-	10,10,34	0.24	0	9,9,45	0.57	0
21	EDO	D	202	-	3,3,3	0.22	0	2,2,2	0.16	0
20	DMU	P	317	-	34,34,34	1.09	3 (8%)	45,45,45	1.38	5 (11%)
20	DMU	W	101	-	10,10,34	0.24	0	9,9,45	0.57	0
24	CHD	P	305	-	32,32,32	0.87	0	51,51,51	1.73	10 (19%)
19	LFA	C	307	-	10,10,19	0.22	0	9,9,18	0.23	0
20	DMU	B	304	-	22,22,34	1.20	2 (9%)	27,27,45	1.19	3 (11%)
20	DMU	J	101	-	10,10,34	0.29	0	9,9,45	0.72	0
24	CHD	C	301	-	32,32,32	0.91	2 (6%)	51,51,51	0.87	1 (1%)
26	CDL	I	101	-	63,63,99	0.77	0	69,75,111	1.38	10 (14%)
20	DMU	T	105	-	22,22,34	0.74	0	27,27,45	1.71	4 (14%)
26	CDL	P	304	-	86,86,99	0.85	2 (2%)	92,98,111	1.49	14 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	DMU	C	306	-	10,10,34	0.28	0	9,9,45	0.61	0
21	EDO	S	102	-	3,3,3	0.41	0	2,2,2	0.51	0
19	LFA	G	104	-	13,13,19	0.60	0	12,12,18	0.28	0
19	LFA	C	311	-	10,10,19	0.26	0	9,9,18	0.17	0
20	DMU	A	608	-	6,6,34	0.65	0	5,5,45	0.34	0
21	EDO	N	612	-	3,3,3	0.22	0	2,2,2	0.19	0
20	DMU	H	101	-	34,34,34	1.20	5 (14%)	45,45,45	1.42	6 (13%)
20	DMU	C	325	-	34,34,34	0.94	1 (2%)	45,45,45	1.20	3 (6%)
23	CUA	O	305	2	0,1,1	-	-	-	-	-
21	EDO	F	103	-	3,3,3	0.39	0	2,2,2	0.47	0
19	LFA	P	310	-	10,10,19	0.25	0	9,9,18	0.13	0
20	DMU	Q	201	-	34,34,34	1.41	7 (20%)	45,45,45	1.66	7 (15%)
20	DMU	O	308	-	22,22,34	0.88	1 (4%)	27,27,45	1.40	4 (14%)
20	DMU	A	609	-	34,34,34	1.40	5 (14%)	45,45,45	1.21	6 (13%)
23	CUA	B	301	2	0,1,1	-	-	-	-	-
19	LFA	T	104	-	10,10,19	0.37	0	9,9,18	0.34	0
14	HEA	A	601	1	67,67,67	2.13	26 (38%)	81,103,103	2.48	28 (34%)
18	N2O	A	606	-	0,2,2	-	-	0,1,1	-	-
19	LFA	B	307	-	16,16,19	0.49	0	15,15,18	0.27	0
20	DMU	O	306	-	10,10,34	0.14	0	9,9,45	0.55	0
26	CDL	N	606	-	63,63,99	0.74	0	69,75,111	1.23	5 (7%)
19	LFA	A	607	-	13,13,19	0.42	0	12,12,18	0.25	0
20	DMU	M	102	-	7,7,34	0.35	0	6,6,45	0.40	0
20	DMU	O	307	-	10,10,34	0.26	0	9,9,45	0.61	0
21	EDO	C	323	-	3,3,3	0.78	0	2,2,2	0.74	0
20	DMU	Z	102	-	22,22,34	0.63	0	27,27,45	1.02	1 (3%)
21	EDO	B	305	-	3,3,3	0.17	0	2,2,2	0.31	0
14	HEA	A	602	1	67,67,67	2.20	24 (35%)	81,103,103	2.26	29 (35%)
20	DMU	M	101	-	34,34,34	1.43	4 (11%)	45,45,45	1.02	2 (4%)
20	DMU	Z	103	-	7,7,34	0.37	0	6,6,45	0.68	0
20	DMU	A	615	-	10,10,34	0.46	0	9,9,45	0.57	0
21	EDO	R	202	-	3,3,3	0.18	0	2,2,2	0.06	0
26	CDL	C	304	-	86,86,99	0.83	3 (3%)	92,98,111	1.32	11 (11%)
19	LFA	C	315	-	12,12,19	0.22	0	11,11,18	0.15	0
19	LFA	N	608	-	13,13,19	0.34	0	12,12,18	0.30	0
21	EDO	O	309	-	3,3,3	0.27	0	2,2,2	0.11	0
19	LFA	C	309	-	17,17,19	0.35	0	16,16,18	0.19	0
22	PGV	C	303	-	50,50,50	0.85	3 (6%)	53,56,56	0.95	2 (3%)
21	EDO	N	613	-	3,3,3	0.37	0	2,2,2	0.32	0
21	EDO	P	320	-	3,3,3	0.47	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	DMU	P	318	-	34,34,34	1.10	3 (8%)	45,45,45	1.35	3 (6%)
19	LFA	C	310	-	14,14,19	0.30	0	13,13,18	0.11	0
19	LFA	T	101	-	13,13,19	0.76	0	12,12,18	0.45	0
22	PGV	P	303	-	50,50,50	0.96	3 (6%)	53,56,56	1.05	3 (5%)
19	LFA	P	309	-	17,17,19	0.32	0	16,16,18	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LFA	P	311	-	-	3/8/8/17	-
21	EDO	N	615	-	-	0/1/1/1	-
26	CDL	L	101	-	-	49/104/104/110	-
26	CDL	Y	101	-	-	46/104/104/110	-
21	EDO	A	610	-	-	0/1/1/1	-
20	DMU	N	610	-	-	5/19/59/59	0/2/2/2
21	EDO	A	612	-	-	0/1/1/1	-
20	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
21	EDO	C	322	-	-	0/1/1/1	-
21	EDO	N	614	-	-	0/1/1/1	-
20	DMU	B	303	-	-	5/8/8/59	-
20	DMU	P	316	-	-	8/13/33/59	0/1/1/2
21	EDO	R	203	-	-	1/1/1/1	-
21	EDO	T	106	-	-	0/1/1/1	-
20	DMU	C	317	-	-	3/4/4/59	-
24	CHD	P	301	-	-	2/9/74/74	0/4/4/4
20	DMU	C	324	-	-	7/13/33/59	0/1/1/2
14	HEA	N	602	1	-	7/36/76/76	-
21	EDO	F	102	-	-	0/1/1/1	-
24	CHD	C	305	-	-	7/9/74/74	0/4/4/4
21	EDO	A	611	-	-	1/1/1/1	-
20	DMU	P	306	-	-	4/8/8/59	-
20	DMU	C	320	-	-	10/19/59/59	0/2/2/2
24	CHD	B	306	-	-	2/9/74/74	0/4/4/4
19	LFA	P	308	-	-	0/3/3/17	-
19	LFA	P	312	-	-	7/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHD	O	301	-	-	2/9/74/74	0/4/4/4
19	LFA	P	313	-	-	2/10/10/17	-
21	EDO	G	103	-	-	0/1/1/1	-
20	DMU	C	319	-	-	12/19/59/59	0/2/2/2
21	EDO	P	319	-	-	1/1/1/1	-
20	DMU	L	102	-	-	9/13/33/59	0/1/1/2
21	EDO	C	321	-	-	1/1/1/1	-
21	EDO	P	321	-	-	1/1/1/1	-
28	PEK	T	102	-	-	20/56/56/56	-
20	DMU	D	201	-	-	9/19/59/59	0/2/2/2
20	DMU	G	102	-	-	2/8/8/59	-
19	LFA	C	326	-	-	8/12/12/17	-
22	PGV	N	616	-	-	10/55/55/55	-
20	DMU	C	316	-	-	12/19/59/59	0/2/2/2
20	DMU	U	101	-	-	7/19/59/59	0/2/2/2
19	LFA	C	314	-	-	5/12/12/17	-
21	EDO	N	611	-	-	0/1/1/1	-
20	DMU	O	304	-	-	6/13/33/59	0/1/1/2
20	DMU	C	318	-	-	9/13/33/59	0/1/1/2
21	EDO	R	201	-	-	1/1/1/1	-
22	PGV	A	614	-	-	7/55/55/55	-
20	DMU	N	609	-	-	1/4/4/59	-
19	LFA	C	312	-	-	6/11/11/17	-
19	LFA	P	307	-	-	2/8/8/17	-
21	EDO	E	202	-	-	0/1/1/1	-
19	LFA	T	103	-	-	5/11/11/17	-
20	DMU	P	322	-	-	4/19/59/59	0/2/2/2
21	EDO	E	201	-	-	0/1/1/1	-
19	LFA	O	302	-	-	5/14/14/17	-
21	EDO	A	613	-	-	0/1/1/1	-
20	DMU	P	315	-	-	2/4/4/59	-
20	DMU	B	308	-	-	9/13/33/59	0/1/1/2
14	HEA	N	601	1	-	2/36/76/76	-
21	EDO	S	103	-	-	0/1/1/1	-
19	LFA	C	308	-	-	0/3/3/17	-
28	PEK	G	101	-	-	14/56/56/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	P	314	-	-	8/19/59/59	0/2/2/2
19	LFA	O	303	-	-	3/8/8/17	-
19	LFA	C	313	-	-	4/8/8/17	-
20	DMU	B	302	-	-	5/8/8/59	-
21	EDO	D	202	-	-	0/1/1/1	-
20	DMU	P	317	-	-	14/19/59/59	0/2/2/2
20	DMU	W	101	-	-	2/8/8/59	-
24	CHD	P	305	-	-	7/9/74/74	0/4/4/4
19	LFA	C	307	-	-	5/8/8/17	-
20	DMU	B	304	-	-	6/13/33/59	0/1/1/2
20	DMU	J	101	-	-	3/8/8/59	-
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
26	CDL	I	101	-	-	36/74/74/110	-
20	DMU	T	105	-	-	10/13/33/59	0/1/1/2
26	CDL	P	304	-	-	57/97/97/110	-
20	DMU	C	306	-	-	2/8/8/59	-
21	EDO	S	102	-	-	0/1/1/1	-
19	LFA	G	104	-	-	7/11/11/17	-
19	LFA	C	311	-	-	7/8/8/17	-
20	DMU	A	608	-	-	2/4/4/59	-
21	EDO	N	612	-	-	0/1/1/1	-
20	DMU	H	101	-	-	6/19/59/59	0/2/2/2
20	DMU	C	325	-	-	4/19/59/59	0/2/2/2
21	EDO	F	103	-	-	1/1/1/1	-
19	LFA	P	310	-	-	5/8/8/17	-
20	DMU	Q	201	-	-	7/19/59/59	0/2/2/2
20	DMU	O	308	-	-	3/13/33/59	0/1/1/2
20	DMU	A	609	-	-	6/19/59/59	0/2/2/2
19	LFA	T	104	-	-	4/8/8/17	-
14	HEA	A	601	1	-	4/36/76/76	-
19	LFA	B	307	-	-	7/14/14/17	-
20	DMU	O	306	-	-	6/8/8/59	-
26	CDL	N	606	-	-	45/74/74/110	-
19	LFA	A	607	-	-	3/11/11/17	-
20	DMU	M	102	-	-	3/5/5/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	O	307	-	-	5/8/8/59	-
21	EDO	C	323	-	-	1/1/1/1	-
20	DMU	Z	102	-	-	11/13/33/59	0/1/1/2
21	EDO	B	305	-	-	0/1/1/1	-
14	HEA	A	602	1	-	6/36/76/76	-
20	DMU	M	101	-	-	5/19/59/59	0/2/2/2
20	DMU	Z	103	-	-	3/5/5/59	-
20	DMU	A	615	-	-	5/8/8/59	-
21	EDO	R	202	-	-	0/1/1/1	-
26	CDL	C	304	-	-	49/97/97/110	-
19	LFA	C	315	-	-	3/10/10/17	-
19	LFA	N	608	-	-	4/11/11/17	-
21	EDO	O	309	-	-	0/1/1/1	-
19	LFA	C	309	-	-	10/15/15/17	-
22	PGV	C	303	-	-	13/55/55/55	-
21	EDO	N	613	-	-	1/1/1/1	-
21	EDO	P	320	-	-	0/1/1/1	-
20	DMU	P	318	-	-	11/19/59/59	0/2/2/2
19	LFA	C	310	-	-	8/12/12/17	-
19	LFA	T	101	-	-	6/11/11/17	-
22	PGV	P	303	-	-	10/55/55/55	-
19	LFA	P	309	-	-	10/15/15/17	-

All (190) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	C1D-ND	-5.86	1.30	1.40
14	A	602	HEA	C1D-ND	-5.69	1.30	1.40
14	N	602	HEA	CHB-C4A	5.30	1.48	1.38
14	A	601	HEA	C1D-ND	-5.03	1.31	1.40
14	A	602	HEA	C4D-ND	-4.94	1.29	1.38
20	N	610	DMU	O16-C6	-4.79	1.32	1.40
14	A	601	HEA	C3A-C2A	4.76	1.48	1.37
14	N	601	HEA	C3B-C2B	4.69	1.45	1.34
14	A	602	HEA	FE-ND	4.63	2.09	1.94
14	N	602	HEA	C4D-ND	-4.57	1.29	1.38
14	N	602	HEA	C3A-C2A	4.49	1.47	1.37
14	A	601	HEA	CHD-C1D	4.39	1.47	1.38
14	A	602	HEA	FE-NB	4.36	2.08	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	CHB-C4A	4.22	1.46	1.38
14	N	602	HEA	C1B-NB	-4.20	1.30	1.38
14	A	602	HEA	C1B-NB	-4.15	1.30	1.38
14	N	601	HEA	CHC-C4B	4.05	1.46	1.38
14	N	602	HEA	C4B-NB	-4.05	1.33	1.40
14	N	601	HEA	FE-NC	3.91	2.08	1.95
20	A	609	DMU	O16-C6	-3.89	1.33	1.40
20	M	101	DMU	C7-C5	-3.89	1.42	1.52
26	P	304	CDL	C31-CA7	-3.84	1.39	1.50
14	N	601	HEA	CHA-C1A	3.84	1.45	1.38
14	A	601	HEA	C11-C3B	-3.79	1.46	1.51
24	P	301	CHD	C22-C23	-3.72	1.41	1.52
14	A	601	HEA	C3B-C2B	3.71	1.43	1.34
14	N	601	HEA	C4C-NC	-3.71	1.32	1.39
14	A	601	HEA	C1A-NA	3.67	1.46	1.39
20	M	101	DMU	O3-C5	-3.65	1.33	1.43
20	D	201	DMU	O3-C5	-3.64	1.33	1.43
22	N	616	PGV	O03-C19	3.61	1.43	1.33
14	N	602	HEA	FE-ND	3.59	2.06	1.94
14	A	602	HEA	C3A-C2A	3.59	1.45	1.37
20	D	201	DMU	O16-C6	-3.58	1.34	1.40
14	N	602	HEA	C3B-C2B	3.57	1.42	1.34
14	N	602	HEA	FE-NC	3.56	2.06	1.95
14	A	602	HEA	C18-C19	3.49	1.41	1.33
20	B	304	DMU	O16-C6	3.47	1.46	1.40
14	A	602	HEA	CHC-C1C	3.44	1.47	1.39
22	A	614	PGV	O03-C19	3.42	1.43	1.33
14	A	601	HEA	CHA-C1A	3.35	1.44	1.38
14	A	601	HEA	C4C-NC	-3.30	1.33	1.39
14	N	601	HEA	C11-C3B	-3.27	1.47	1.51
22	A	614	PGV	O01-C1	3.17	1.43	1.34
14	N	601	HEA	CHB-C4A	3.15	1.44	1.38
14	A	601	HEA	FE-NC	3.11	2.05	1.95
20	A	609	DMU	O7-C10	3.11	1.50	1.41
22	P	303	PGV	O03-C01	-3.11	1.38	1.45
14	A	601	HEA	C1B-NB	-3.11	1.32	1.38
14	N	602	HEA	FE-NB	3.09	2.04	1.94
20	A	609	DMU	O3-C5	-3.05	1.35	1.43
22	P	303	PGV	O03-C19	3.04	1.42	1.33
14	N	601	HEA	C1D-ND	-3.04	1.35	1.40
14	N	601	HEA	C1B-NB	-3.04	1.32	1.38
20	P	317	DMU	C7-C5	-3.03	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	C3B-C2B	3.03	1.41	1.34
20	P	317	DMU	O5-C6	-3.00	1.34	1.41
14	A	602	HEA	CHD-C1D	2.98	1.44	1.38
14	A	601	HEA	C3D-C2D	2.97	1.43	1.36
14	N	601	HEA	C3A-C2A	2.97	1.43	1.37
14	N	602	HEA	C3D-C2D	2.97	1.43	1.36
26	C	304	CDL	OA7-CA5	2.95	1.31	1.22
14	A	602	HEA	CHA-C1A	2.94	1.44	1.38
28	G	101	PEK	C23-C22	-2.94	1.41	1.52
14	A	602	HEA	C4D-C3D	2.89	1.49	1.45
14	N	601	HEA	C4D-ND	-2.86	1.33	1.38
14	A	602	HEA	C4B-NB	-2.86	1.35	1.40
14	A	601	HEA	FE-ND	2.84	2.03	1.94
14	A	602	HEA	FE-NC	2.82	2.04	1.95
20	H	101	DMU	C7-C5	-2.81	1.45	1.52
14	N	601	HEA	C4B-C3B	2.79	1.49	1.44
20	N	610	DMU	O55-C2	-2.77	1.36	1.43
14	A	602	HEA	CBD-CAD	-2.77	1.42	1.51
24	C	301	CHD	C22-C23	-2.77	1.44	1.52
20	U	101	DMU	O1-C10	2.76	1.48	1.41
20	P	317	DMU	O3-C5	2.76	1.49	1.43
14	A	602	HEA	C3A-C4A	2.75	1.50	1.46
26	C	304	CDL	PA1-OA3	2.74	1.60	1.50
14	A	601	HEA	CHB-C4A	2.74	1.43	1.38
14	A	601	HEA	CHC-C4B	2.73	1.44	1.38
14	N	601	HEA	C4B-NB	-2.73	1.35	1.40
20	C	319	DMU	O5-C6	-2.72	1.34	1.41
14	N	602	HEA	CHB-C1B	2.71	1.45	1.39
20	H	101	DMU	O5-C6	-2.71	1.34	1.41
20	B	304	DMU	O16-C18	2.70	1.50	1.43
14	A	601	HEA	C26-C15	-2.70	1.44	1.50
20	Q	201	DMU	O55-C2	2.70	1.49	1.43
14	N	601	HEA	CHD-C1D	2.69	1.43	1.38
14	N	601	HEA	C16-C17	-2.68	1.44	1.53
20	P	318	DMU	C10-C5	-2.68	1.44	1.52
20	D	201	DMU	O5-C6	-2.67	1.35	1.41
20	P	318	DMU	O4-C7	2.67	1.49	1.43
14	N	601	HEA	C26-C15	-2.66	1.44	1.50
14	N	601	HEA	C3D-C2D	2.63	1.42	1.36
20	U	101	DMU	C7-C5	-2.61	1.45	1.52
14	N	601	HEA	FE-ND	2.60	2.02	1.94
20	O	304	DMU	C3-C4	-2.60	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	318	DMU	C3-C2	-2.59	1.45	1.52
14	N	602	HEA	C1A-NA	2.58	1.44	1.39
14	N	602	HEA	C4A-NA	2.58	1.44	1.39
20	O	308	DMU	C6-C1	-2.57	1.45	1.52
20	C	316	DMU	O3-C5	-2.56	1.36	1.43
20	P	318	DMU	C7-C5	-2.55	1.45	1.52
20	P	314	DMU	O1-C10	2.55	1.48	1.41
14	N	601	HEA	CHC-C1C	2.54	1.45	1.39
28	T	102	PEK	C2-C1	2.53	1.58	1.50
20	Q	201	DMU	C10-C5	-2.53	1.45	1.52
20	Z	101	DMU	O3-C5	-2.51	1.36	1.43
20	N	610	DMU	C10-C5	-2.50	1.45	1.52
14	A	601	HEA	CHC-C1C	2.50	1.45	1.39
26	P	304	CDL	OA7-CA5	2.49	1.29	1.22
14	A	602	HEA	C1C-NC	-2.48	1.34	1.39
14	A	601	HEA	CMD-C2D	-2.47	1.45	1.50
20	Q	201	DMU	O5-C6	-2.47	1.35	1.41
22	N	616	PGV	C01-C02	2.46	1.58	1.50
20	N	610	DMU	C7-C5	-2.46	1.45	1.52
20	D	201	DMU	C10-C5	-2.46	1.45	1.52
22	C	303	PGV	O01-C02	-2.46	1.40	1.46
14	A	601	HEA	C16-C17	-2.46	1.45	1.53
14	A	601	HEA	FE-NB	2.45	2.02	1.94
26	C	304	CDL	C11-CA5	2.45	1.57	1.50
20	N	610	DMU	O16-C18	-2.45	1.36	1.43
20	M	101	DMU	C6-C1	-2.45	1.45	1.52
14	A	601	HEA	C4B-NB	-2.41	1.36	1.40
14	N	601	HEA	C4A-NA	2.41	1.44	1.39
20	A	609	DMU	C7-C5	-2.40	1.46	1.52
14	N	602	HEA	C1C-NC	-2.39	1.35	1.39
14	A	601	HEA	C4B-C3B	2.39	1.48	1.44
20	Q	201	DMU	C7-C5	-2.38	1.46	1.52
20	C	318	DMU	O16-C6	2.38	1.44	1.40
14	A	602	HEA	C3D-C2D	2.38	1.41	1.36
14	N	602	HEA	C11-C3B	-2.37	1.48	1.51
20	C	320	DMU	O4-C7	2.37	1.48	1.43
20	P	316	DMU	C3-C4	-2.37	1.48	1.53
14	A	602	HEA	C1C-C2C	2.36	1.48	1.43
22	C	303	PGV	O03-C19	2.36	1.40	1.33
20	D	201	DMU	O2-C8	2.35	1.48	1.43
20	C	319	DMU	O16-C6	-2.35	1.36	1.40
20	Q	201	DMU	O1-C9	2.33	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	T	102	PEK	C23-C22	-2.33	1.43	1.52
24	C	305	CHD	C10-C5	2.32	1.59	1.55
14	A	601	HEA	CMC-C2C	-2.32	1.46	1.50
20	C	316	DMU	C7-C5	-2.30	1.46	1.52
20	C	324	DMU	C6-C1	-2.30	1.45	1.52
14	A	601	HEA	C14-C15	2.29	1.38	1.33
20	D	201	DMU	C2-C1	2.29	1.58	1.52
20	C	325	DMU	C7-C5	-2.28	1.46	1.52
14	N	602	HEA	CHC-C1C	2.27	1.44	1.39
20	P	316	DMU	O16-C6	2.27	1.44	1.40
14	A	602	HEA	CMA-C3A	2.27	1.50	1.45
20	A	609	DMU	O7-C3	2.26	1.49	1.43
14	N	602	HEA	CMD-C2D	-2.26	1.46	1.50
22	N	616	PGV	O01-C1	2.25	1.40	1.34
14	A	602	HEA	CHC-C4B	2.23	1.43	1.38
14	N	602	HEA	CHD-C4C	2.23	1.44	1.39
14	N	602	HEA	C4C-NC	-2.22	1.35	1.39
20	H	101	DMU	O1-C10	2.21	1.47	1.41
20	N	610	DMU	C6-C1	-2.21	1.46	1.52
20	Q	201	DMU	O1-C10	2.19	1.47	1.41
20	U	101	DMU	O7-C10	2.19	1.47	1.41
20	M	101	DMU	O5-C6	-2.19	1.36	1.41
20	N	610	DMU	O1-C10	2.19	1.47	1.41
20	H	101	DMU	O7-C10	2.18	1.47	1.41
20	Z	101	DMU	C6-C1	-2.18	1.46	1.52
20	H	101	DMU	O16-C6	-2.17	1.36	1.40
14	N	601	HEA	FE-NB	2.17	2.01	1.94
20	Q	201	DMU	O3-C5	-2.17	1.37	1.43
20	C	319	DMU	C7-C5	-2.16	1.46	1.52
14	A	601	HEA	C4A-NA	2.16	1.43	1.39
20	C	316	DMU	C6-C1	-2.15	1.46	1.52
14	A	601	HEA	O1D-CGD	2.14	1.29	1.22
14	N	602	HEA	C1B-C2B	2.14	1.48	1.44
20	Z	101	DMU	C7-C5	-2.12	1.46	1.52
20	N	610	DMU	C11-C9	2.11	1.58	1.51
22	P	303	PGV	O01-C02	-2.11	1.41	1.46
14	N	602	HEA	CHC-C4B	2.10	1.42	1.38
14	A	602	HEA	CHB-C1B	2.10	1.44	1.39
22	C	303	PGV	O01-C1	2.10	1.40	1.34
20	P	322	DMU	C8-C9	-2.09	1.48	1.53
20	P	314	DMU	O3-C5	-2.09	1.37	1.43
14	A	602	HEA	CHD-C4C	2.08	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	301	CHD	O26-C24	-2.08	1.23	1.30
26	L	101	CDL	C71-CB7	2.07	1.56	1.50
26	L	101	CDL	C51-CB5	-2.07	1.44	1.50
20	P	322	DMU	C2-C1	-2.05	1.47	1.52
20	N	610	DMU	O5-C6	-2.05	1.36	1.41
14	N	601	HEA	C12-C11	2.04	1.56	1.53
14	A	601	HEA	CAD-C3D	-2.03	1.46	1.51
20	D	201	DMU	O49-C1	-2.02	1.38	1.43
14	N	602	HEA	C3C-C4C	2.00	1.48	1.42

All (333) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601	HEA	C2B-C1B-NB	7.75	118.87	109.90
14	N	602	HEA	C3D-C4D-ND	7.20	117.31	110.35
14	A	601	HEA	C3D-C4D-ND	7.17	117.28	110.35
14	N	601	HEA	C3D-C4D-ND	7.11	117.22	110.35
14	N	601	HEA	C3C-C4C-NC	6.78	115.51	109.80
14	A	601	HEA	C3C-C4C-NC	6.67	115.42	109.80
14	N	602	HEA	C3C-C4C-NC	6.36	115.16	109.80
20	T	105	DMU	O16-C6-C1	6.35	117.91	108.27
14	N	601	HEA	C13-C12-C11	-6.02	104.78	114.39
14	A	601	HEA	C2B-C1B-NB	6.00	116.83	109.90
14	A	601	HEA	C13-C12-C11	-5.79	105.14	114.39
26	P	304	CDL	OA6-CA5-C11	-5.67	99.22	111.48
20	H	101	DMU	O16-C6-C1	5.66	116.88	108.27
14	N	602	HEA	CHA-C4D-C3D	-5.63	116.56	124.77
14	N	601	HEA	C3C-C2C-C1C	-5.57	100.61	107.17
26	N	606	CDL	OA6-CA4-CA3	5.56	128.28	108.34
14	A	602	HEA	C3C-C4C-NC	5.53	114.46	109.80
24	P	305	CHD	C16-C17-C20	5.31	120.22	112.18
20	Q	201	DMU	O16-C6-C1	5.30	116.33	108.27
14	A	601	HEA	C2D-C1D-ND	5.29	115.92	109.84
26	C	304	CDL	OA6-CA5-C11	-5.24	100.15	111.48
24	C	305	CHD	C16-C17-C20	5.20	120.05	112.18
20	P	314	DMU	O16-C6-C1	5.19	116.15	108.27
14	N	601	HEA	C3B-C4B-NB	5.15	115.76	109.84
14	A	602	HEA	CHA-C4D-C3D	-5.13	117.29	124.77
20	P	318	DMU	O16-C6-C1	5.11	116.04	108.27
14	N	601	HEA	C27-C19-C20	5.11	124.09	115.23
14	A	602	HEA	C2B-C1B-NB	5.08	115.78	109.90
20	C	316	DMU	O16-C6-C1	5.07	115.97	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	U	101	DMU	O16-C6-C1	4.99	115.85	108.27
14	N	602	HEA	C2A-C1A-NA	4.95	115.10	110.32
14	A	601	HEA	CHA-C4D-C3D	-4.91	117.61	124.77
20	C	316	DMU	C6-O5-C4	4.85	123.19	113.72
14	N	601	HEA	C2A-C1A-NA	4.83	114.98	110.32
20	P	317	DMU	O16-C6-C1	4.79	115.55	108.27
14	N	601	HEA	C1B-C2B-C3B	-4.78	101.26	106.80
14	A	601	HEA	C3C-C2C-C1C	-4.76	101.56	107.17
20	P	322	DMU	C10-C5-C7	4.75	120.01	110.01
14	N	602	HEA	C3C-C2C-C1C	-4.72	101.60	107.17
20	O	304	DMU	O5-C6-C1	4.71	120.05	110.37
14	N	602	HEA	C4D-C3D-C2D	-4.71	100.04	106.89
14	N	602	HEA	C2B-C1B-NB	4.67	115.30	109.90
14	N	601	HEA	C2C-C1C-NC	4.66	117.61	110.14
24	P	305	CHD	O7-C7-C6	-4.60	98.41	109.86
14	N	602	HEA	C2C-C1C-NC	4.60	117.52	110.14
20	Z	101	DMU	O16-C6-C1	4.59	115.25	108.27
20	B	308	DMU	O16-C6-C1	4.57	115.22	108.27
26	C	304	CDL	OA4-PA1-OA5	-4.53	87.01	107.57
14	A	601	HEA	C3B-C4B-NB	4.51	115.03	109.84
20	D	201	DMU	O16-C6-C1	4.51	115.12	108.27
14	A	602	HEA	C13-C12-C11	-4.50	107.21	114.39
26	I	101	CDL	CA4-OA6-CA5	4.48	128.52	117.80
20	P	322	DMU	O16-C6-C1	4.47	115.06	108.27
14	N	602	HEA	C3B-C4B-NB	4.39	114.89	109.84
14	N	602	HEA	CHB-C4A-NA	-4.37	119.69	124.45
14	N	602	HEA	CHA-C1A-NA	-4.36	119.70	124.45
26	P	304	CDL	OA2-PA1-OA3	4.34	126.14	108.94
14	N	601	HEA	C2D-C1D-ND	4.34	114.82	109.84
22	N	616	PGV	O03-C19-C20	4.33	125.05	111.83
20	U	101	DMU	C10-C5-C7	4.33	119.12	110.01
20	P	322	DMU	C10-O1-C9	-4.30	105.33	113.72
20	C	319	DMU	O16-C6-C1	4.22	114.68	108.27
24	C	305	CHD	C6-C7-C8	4.17	116.05	111.50
26	I	101	CDL	OA2-PA1-OA3	-4.17	92.43	108.94
14	N	602	HEA	CHB-C1B-C2B	-4.16	118.46	125.03
20	C	320	DMU	O16-C6-C1	4.16	114.59	108.27
14	A	601	HEA	C4D-C3D-C2D	-4.16	100.84	106.89
14	A	602	HEA	C1B-C2B-C3B	-4.12	102.02	106.80
20	C	320	DMU	C10-C5-C7	4.09	118.62	110.01
20	C	325	DMU	O16-C6-C1	4.09	114.49	108.27
26	P	304	CDL	OA4-PA1-OA5	-4.09	89.04	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	319	DMU	C10-C5-C7	4.07	118.57	110.01
14	A	602	HEA	C2A-C1A-NA	4.07	114.25	110.32
14	A	601	HEA	CHB-C4A-NA	-4.06	120.03	124.45
26	C	304	CDL	OA5-PA1-OA3	4.05	124.99	108.94
20	U	101	DMU	O3-C5-C10	4.02	119.65	110.08
26	P	304	CDL	OA4-PA1-OA3	4.00	131.06	112.44
24	C	305	CHD	C14-C13-C12	3.99	111.06	107.42
14	N	601	HEA	CHB-C1B-C2B	-3.98	118.74	125.03
20	M	101	DMU	O16-C6-C1	3.93	114.25	108.27
14	A	602	HEA	CHA-C1A-NA	-3.92	120.18	124.45
14	N	602	HEA	C1B-C2B-C3B	-3.92	102.26	106.80
24	C	305	CHD	C17-C13-C14	-3.89	96.21	100.11
14	N	602	HEA	C3A-C2A-C1A	-3.86	103.39	107.05
14	A	602	HEA	C3D-C4D-ND	3.85	114.07	110.35
14	A	602	HEA	C2D-C1D-ND	3.83	114.24	109.84
14	A	602	HEA	C1D-C2D-C3D	-3.81	102.97	106.98
26	C	304	CDL	OA4-PA1-OA3	3.78	130.02	112.44
14	A	602	HEA	C3B-C4B-NB	3.74	114.14	109.84
26	P	304	CDL	OA4-PA1-OA2	-3.66	90.97	107.57
28	T	102	PEK	O01-C1-O02	-3.64	115.18	123.70
20	B	304	DMU	O16-C6-C1	3.62	113.77	108.27
14	A	601	HEA	C2C-C1C-NC	3.59	115.89	110.14
24	P	305	CHD	C17-C13-C14	-3.58	96.52	100.11
24	C	305	CHD	C22-C23-C24	-3.58	102.95	112.49
24	P	305	CHD	C22-C23-C24	-3.56	103.00	112.49
14	A	601	HEA	C1B-C2B-C3B	-3.48	102.76	106.80
20	C	324	DMU	O16-C6-C1	3.47	113.54	108.27
14	N	601	HEA	C4D-C3D-C2D	-3.43	101.89	106.89
26	N	606	CDL	OA6-CA4-CA6	-3.42	96.07	108.34
20	P	316	DMU	O5-C6-C1	3.40	117.36	110.37
20	L	102	DMU	O5-C6-O16	3.39	118.05	110.04
22	A	614	PGV	O03-C19-O04	-3.38	115.17	123.63
14	A	602	HEA	C4A-C3A-C2A	-3.38	103.88	106.81
14	N	601	HEA	CHA-C4D-C3D	-3.38	119.85	124.77
20	Q	201	DMU	C6-O5-C4	-3.37	107.15	113.72
14	N	601	HEA	O11-C11-C3B	-3.36	105.10	111.26
14	A	602	HEA	C4D-C3D-C2D	-3.35	102.01	106.89
20	C	316	DMU	O5-C6-O16	-3.32	102.19	110.04
14	N	601	HEA	C4B-NB-C1B	-3.32	101.27	105.21
14	N	602	HEA	C2D-C1D-ND	3.32	113.65	109.84
26	C	304	CDL	OB5-PB2-OB3	3.27	121.89	108.94
14	A	602	HEA	CAA-C2A-C1A	3.26	131.48	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	610	DMU	C10-O1-C9	3.26	120.08	113.72
26	Y	101	CDL	OB5-PB2-OB3	-3.24	96.08	108.94
14	N	602	HEA	CAD-C3D-C4D	3.23	130.32	124.70
14	A	601	HEA	C26-C15-C16	3.22	120.82	115.23
14	A	602	HEA	CHB-C1B-C2B	-3.21	119.96	125.03
20	O	304	DMU	O16-C6-C1	3.21	113.14	108.27
26	N	606	CDL	CA4-OA6-CA5	3.20	125.46	117.80
20	D	201	DMU	C10-C5-C7	3.20	116.75	110.01
20	D	201	DMU	O1-C9-C8	3.20	115.47	109.70
28	T	102	PEK	C2-C3-C4	3.19	120.32	113.35
14	N	602	HEA	C13-C12-C11	-3.18	109.31	114.39
20	H	101	DMU	O3-C5-C10	3.18	117.64	110.08
26	P	304	CDL	CA4-OA6-CA5	-3.16	110.22	117.80
20	P	322	DMU	O7-C10-O1	-3.14	102.42	110.69
26	I	101	CDL	OA5-PA1-OA3	3.14	121.40	108.94
20	P	314	DMU	C10-C5-C7	3.14	116.62	110.01
14	N	602	HEA	C4A-NA-C1A	-3.14	100.70	105.82
26	P	304	CDL	OB4-PB2-OB3	3.13	127.03	112.44
14	A	602	HEA	C4A-NA-C1A	-3.12	100.74	105.82
26	N	606	CDL	OA5-PA1-OA3	3.11	121.25	108.94
14	N	601	HEA	C26-C15-C16	3.10	120.61	115.23
20	P	318	DMU	C8-C7-C5	-3.09	105.40	110.83
22	A	614	PGV	O03-C19-C20	3.09	121.26	111.83
20	P	317	DMU	C10-C5-C7	3.08	116.50	110.01
20	Q	201	DMU	C11-C9-C8	-3.07	105.47	113.02
14	A	601	HEA	C1D-ND-C4D	-3.06	101.58	105.21
20	Z	102	DMU	O5-C6-O16	3.06	117.27	110.04
14	A	601	HEA	C2A-C1A-NA	3.05	113.27	110.32
14	A	602	HEA	C3C-C2C-C1C	-3.05	103.58	107.17
14	A	601	HEA	O11-C11-C12	3.04	117.19	109.14
26	I	101	CDL	OB5-PB2-OB3	-3.04	96.90	108.94
26	C	304	CDL	OA7-CA5-C11	3.04	135.66	123.78
20	P	314	DMU	C6-O5-C4	3.03	119.64	113.72
20	P	318	DMU	C10-C5-C7	3.03	116.39	110.01
20	O	308	DMU	O5-C6-O16	3.03	117.20	110.04
20	C	316	DMU	O5-C6-C1	3.02	116.58	110.37
20	B	308	DMU	C3-C2-C1	-3.00	105.57	110.83
20	O	308	DMU	O16-C6-C1	-2.97	103.76	108.27
20	P	314	DMU	O5-C6-C1	2.96	116.45	110.37
26	P	304	CDL	OA8-CA6-CA4	-2.95	99.89	108.40
14	N	602	HEA	C4C-C3C-C2C	-2.94	103.64	107.30
14	N	602	HEA	CHC-C1C-C2C	-2.94	118.90	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	I	101	CDL	OA6-CA4-CA6	2.94	118.88	108.34
20	C	316	DMU	C10-C5-C7	2.93	116.18	110.01
20	C	318	DMU	C3-C2-C1	-2.92	105.70	110.83
22	P	303	PGV	C27-C26-C25	-2.92	99.63	114.37
14	N	601	HEA	C1D-C2D-C3D	-2.87	103.97	106.98
14	N	602	HEA	CAA-C2A-C1A	2.87	130.68	124.85
14	N	602	HEA	CHD-C1D-C2D	-2.84	118.87	126.95
14	A	602	HEA	C27-C19-C20	2.83	120.14	115.23
20	Q	201	DMU	C2-C3-C4	-2.83	104.67	110.93
14	A	601	HEA	CHB-C1B-C2B	-2.81	120.59	125.03
20	P	317	DMU	C8-C7-C5	-2.80	105.92	110.83
26	P	304	CDL	OA7-CA5-C11	2.79	134.70	123.78
20	Q	201	DMU	O1-C9-C8	2.77	114.69	109.70
20	A	609	DMU	O3-C5-C7	2.77	116.90	110.38
20	B	308	DMU	O5-C6-C1	2.77	116.05	110.37
24	P	305	CHD	C6-C7-C8	2.76	114.52	111.50
20	M	101	DMU	C10-C5-C7	2.76	115.82	110.01
20	H	101	DMU	O7-C3-C2	2.75	114.22	107.23
20	O	308	DMU	O5-C6-C1	2.75	116.02	110.37
14	N	601	HEA	C4B-C3B-C2B	-2.75	102.82	107.44
28	T	102	PEK	O02-C1-C2	2.75	134.53	123.78
20	D	201	DMU	C2-C3-C4	-2.74	104.86	110.93
14	A	601	HEA	C1D-C2D-C3D	-2.74	104.10	106.98
26	L	101	CDL	OA5-PA1-OA3	2.73	119.76	108.94
14	N	601	HEA	C3A-C2A-C1A	-2.72	104.47	107.05
26	P	304	CDL	OA6-CA4-CA3	2.72	118.11	108.34
24	P	305	CHD	O7-C7-C8	2.72	115.75	109.52
20	C	325	DMU	C10-C5-C7	2.71	115.71	110.01
14	A	602	HEA	CHD-C1D-C2D	-2.70	119.27	126.95
14	A	601	HEA	CMC-C2C-C3C	2.70	132.90	126.55
14	N	602	HEA	CHC-C4B-C3B	-2.70	118.99	125.80
22	N	616	PGV	O03-C19-O04	-2.69	116.90	123.63
14	N	602	HEA	C27-C19-C20	2.69	119.89	115.23
14	A	602	HEA	C4C-C3C-C2C	-2.68	103.97	107.30
20	O	304	DMU	C6-C1-C2	2.68	115.64	110.01
20	T	105	DMU	C18-O16-C6	-2.68	109.11	113.68
14	A	601	HEA	C4B-C3B-C2B	-2.67	102.95	107.44
14	N	601	HEA	C1D-ND-C4D	-2.66	102.06	105.21
14	A	602	HEA	C2C-C1C-NC	2.65	114.39	110.14
26	Y	101	CDL	OB4-PB2-OB2	2.64	119.52	107.57
26	Y	101	CDL	OA4-PA1-OA5	-2.64	95.62	107.57
14	N	602	HEA	CAD-CBD-CGD	-2.63	106.69	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	304	CDL	CA6-CA4-CA3	2.63	117.91	111.78
20	Z	101	DMU	C10-C5-C7	2.62	115.53	110.01
14	N	602	HEA	C4B-C3B-C2B	-2.62	103.04	107.44
24	P	301	CHD	C18-C13-C12	-2.61	106.45	109.06
14	N	602	HEA	C20-C19-C18	-2.61	115.31	121.17
14	N	602	HEA	C1D-C2D-C3D	-2.60	104.25	106.98
26	I	101	CDL	OA6-CA4-CA3	2.59	117.64	108.34
20	P	317	DMU	C10-O1-C9	-2.57	108.69	113.72
14	A	601	HEA	CAD-C3D-C4D	2.57	129.17	124.70
26	C	304	CDL	CB6-CB4-CB3	2.57	117.77	111.78
14	N	601	HEA	C4C-NC-C1C	-2.57	101.64	105.82
14	A	601	HEA	CHD-C1D-C2D	-2.56	119.67	126.95
14	N	601	HEA	O11-C11-C12	2.56	115.93	109.14
20	N	610	DMU	O5-C6-C1	2.55	115.62	110.37
14	A	602	HEA	CHC-C1C-C2C	-2.55	120.03	127.43
20	P	322	DMU	O5-C6-C1	2.54	115.59	110.37
14	N	601	HEA	C26-C15-C14	-2.53	117.12	123.63
26	I	101	CDL	OB6-CB4-CB6	2.53	117.43	108.34
20	B	308	DMU	C6-O5-C4	2.53	118.66	113.72
14	A	601	HEA	C4C-C3C-C2C	-2.52	104.16	107.30
14	A	602	HEA	CHB-C4A-NA	-2.52	121.71	124.45
26	P	304	CDL	O1-C1-CA2	2.52	118.40	109.70
26	C	304	CDL	O1-C1-CB2	2.52	118.40	109.70
22	N	616	PGV	O01-C1-O02	-2.52	117.82	123.70
14	N	601	HEA	C17-C18-C19	-2.51	121.87	127.62
20	H	101	DMU	C18-O16-C6	-2.51	109.39	113.68
14	N	601	HEA	CHC-C4B-C3B	-2.51	119.48	125.80
24	O	301	CHD	C6-C5-C4	-2.50	108.37	111.23
20	C	318	DMU	O5-C6-C1	2.50	115.50	110.37
24	C	305	CHD	C17-C13-C12	-2.47	115.44	117.67
20	P	316	DMU	C18-O16-C6	-2.45	109.49	113.68
26	C	304	CDL	OB4-PB2-OB3	2.45	123.85	112.44
20	C	325	DMU	O5-C6-C1	2.45	115.41	110.37
20	H	101	DMU	O5-C6-C1	2.44	115.38	110.37
20	T	105	DMU	C57-C4-C3	-2.43	107.04	113.02
14	A	601	HEA	C4B-NB-C1B	-2.43	102.33	105.21
14	A	602	HEA	C26-C15-C16	2.42	119.44	115.23
24	P	301	CHD	C11-C12-C13	-2.42	108.81	111.26
14	A	601	HEA	C3A-C2A-C1A	-2.42	104.76	107.05
22	C	303	PGV	O03-C19-O04	-2.41	117.59	123.63
20	N	610	DMU	C7-C8-C9	2.41	114.60	110.23
14	N	602	HEA	CMD-C2D-C1D	2.40	128.79	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	I	101	CDL	OA6-CA5-OA7	2.40	129.32	123.70
20	P	322	DMU	O6-C11-C9	-2.39	103.18	111.33
20	P	317	DMU	O7-C3-C2	2.39	113.31	107.23
20	D	201	DMU	O7-C3-C2	2.39	113.31	107.23
20	H	101	DMU	C10-C5-C7	2.39	115.04	110.01
26	L	101	CDL	OA6-CA5-C11	2.39	116.65	111.48
20	B	304	DMU	C6-O5-C4	2.38	118.37	113.72
26	N	606	CDL	OA2-PA1-OA3	-2.38	99.50	108.94
20	C	320	DMU	O5-C6-C1	2.38	115.26	110.37
24	P	305	CHD	C14-C13-C12	2.38	109.59	107.42
26	L	101	CDL	OB6-CB4-CB6	-2.37	99.84	108.34
22	A	614	PGV	C15-C14-C13	-2.37	102.47	113.86
20	C	319	DMU	C10-O1-C9	-2.36	109.11	113.72
14	N	602	HEA	O11-C11-C12	2.35	115.38	109.14
14	N	601	HEA	C4A-NA-C1A	-2.35	101.99	105.82
20	P	322	DMU	O49-C1-C2	-2.34	104.85	110.38
20	C	318	DMU	C18-O16-C6	-2.34	109.68	113.68
20	O	304	DMU	C2-C3-C4	-2.34	105.99	110.23
20	C	324	DMU	O5-C4-C57	2.34	112.23	106.44
26	Y	101	CDL	OB6-CB5-C51	2.33	116.53	111.48
14	N	602	HEA	CMC-C2C-C1C	2.33	128.96	125.42
14	N	602	HEA	C4C-NC-C1C	-2.32	102.04	105.82
20	T	105	DMU	C2-C3-C4	2.31	114.42	110.23
20	P	322	DMU	O1-C9-C8	-2.30	105.55	109.70
20	B	304	DMU	C3-C2-C1	-2.28	106.82	110.83
26	P	304	CDL	OB6-CB4-CB3	2.28	116.52	108.34
24	P	305	CHD	C11-C12-C13	-2.28	108.95	111.26
20	Z	101	DMU	O1-C9-C11	2.27	112.08	106.44
20	C	318	DMU	C2-C3-C4	-2.26	106.14	110.23
20	P	322	DMU	C7-C8-C9	-2.26	106.14	110.23
24	P	301	CHD	C18-C13-C14	2.26	114.74	111.20
14	N	601	HEA	CAD-C3D-C2D	2.26	132.09	127.87
20	A	609	DMU	O7-C10-C5	2.26	113.64	108.09
20	Q	201	DMU	O61-C57-C4	-2.25	103.68	111.33
24	C	305	CHD	C4-C5-C10	2.25	115.05	112.66
14	N	601	HEA	C27-C19-C18	-2.24	117.86	123.63
22	N	616	PGV	C23-C22-C21	-2.24	103.04	114.37
14	N	601	HEA	CHA-C1A-NA	-2.24	122.01	124.45
22	P	303	PGV	C03-C02-C01	-2.23	106.57	111.78
20	U	101	DMU	C10-O7-C3	-2.23	112.69	117.98
14	N	601	HEA	C4C-C3C-C2C	-2.23	104.53	107.30
20	A	609	DMU	C10-O7-C3	-2.22	112.72	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	CHD-C1D-ND	2.22	127.11	124.37
14	A	602	HEA	CAD-C3D-C2D	2.22	132.02	127.87
20	P	314	DMU	O5-C6-O16	-2.21	104.82	110.04
14	N	601	HEA	O2D-CGD-CBD	2.20	120.96	114.00
28	T	102	PEK	O01-C02-C03	-2.20	100.45	108.34
26	P	304	CDL	CB4-OB6-CB5	2.19	123.03	117.80
24	O	301	CHD	O7-C7-C6	2.18	115.27	109.86
26	I	101	CDL	OA4-PA1-OA3	2.16	122.52	112.44
20	U	101	DMU	O5-C6-O16	2.15	115.13	110.04
26	C	304	CDL	OA4-PA1-OA2	-2.15	97.82	107.57
20	B	308	DMU	C57-C4-C3	-2.15	107.74	113.02
20	Z	101	DMU	O3-C5-C7	2.15	115.44	110.38
14	A	601	HEA	C4A-NA-C1A	-2.15	102.32	105.82
14	A	602	HEA	O1A-CGA-CBA	-2.14	116.30	123.09
24	B	306	CHD	C14-C13-C12	-2.14	105.46	107.42
14	A	602	HEA	CHC-C4B-C3B	-2.14	120.40	125.80
26	Y	101	CDL	OA4-PA1-OA3	2.14	122.40	112.44
20	C	320	DMU	O3-C5-C10	2.14	115.17	110.08
14	N	601	HEA	CMD-C2D-C1D	2.14	128.38	125.03
28	G	101	PEK	C14-C13-C12	2.14	122.54	112.02
20	Z	101	DMU	C10-O1-C9	-2.13	109.56	113.72
14	N	601	HEA	CHD-C1D-ND	-2.13	121.73	124.37
14	N	601	HEA	CHB-C4A-NA	-2.13	122.14	124.45
24	B	306	CHD	C5-C6-C7	-2.13	111.87	114.40
26	Y	101	CDL	OB4-PB2-OB3	2.12	122.31	112.44
26	L	101	CDL	OB5-PB2-OB3	-2.11	100.56	108.94
26	L	101	CDL	OB4-PB2-OB3	2.11	122.27	112.44
14	A	602	HEA	CHA-C4D-ND	2.11	126.69	124.42
20	C	320	DMU	C11-C9-C8	-2.11	107.85	113.02
20	C	316	DMU	C18-O16-C6	-2.11	110.08	113.68
28	G	101	PEK	O03-C21-C22	-2.10	105.42	111.83
20	O	308	DMU	C3-C2-C1	-2.10	107.14	110.83
26	C	304	CDL	OA8-CA6-CA4	-2.10	102.34	108.40
14	N	601	HEA	OMA-CMA-C3A	-2.10	120.89	125.62
24	P	305	CHD	O25-C24-C23	-2.10	116.44	123.09
24	P	305	CHD	C16-C17-C13	-2.09	101.52	103.54
20	A	609	DMU	C11-C9-C8	-2.08	107.91	113.02
14	N	601	HEA	CMC-C2C-C1C	2.08	128.58	125.42
20	A	609	DMU	O5-C6-C1	2.07	114.63	110.37
14	A	601	HEA	O11-C11-C3B	-2.07	107.46	111.26
14	A	601	HEA	CAD-CBD-CGD	-2.06	108.19	113.67
26	I	101	CDL	OB4-PB2-OB3	2.06	122.01	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	101	CDL	OB4-PB2-OB2	2.05	116.88	107.57
22	P	303	PGV	O14-P-O13	2.04	121.93	112.44
24	C	301	CHD	C22-C20-C17	-2.04	106.11	110.33
20	P	314	DMU	O1-C9-C11	2.04	111.48	106.44
22	C	303	PGV	O03-C19-C20	2.03	118.02	111.83
20	Q	201	DMU	O3-C5-C10	2.03	114.90	110.08
26	L	101	CDL	OB6-CB5-C51	2.02	115.85	111.48
20	A	609	DMU	O7-C3-C4	2.01	114.75	109.48
14	A	602	HEA	C4B-NB-C1B	-2.01	102.83	105.21
26	L	101	CDL	OB2-PB2-OB3	-2.01	100.98	108.94

There are no chirality outliers.

All (792) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	B	304	DMU	C1-C6-O16-C18
20	B	304	DMU	C19-C18-O16-C6
20	B	308	DMU	O5-C6-O16-C18
20	B	308	DMU	C19-C18-O16-C6
20	C	318	DMU	C19-C18-O16-C6
20	D	201	DMU	C19-C18-O16-C6
20	O	304	DMU	C19-C18-O16-C6
20	O	308	DMU	C19-C18-O16-C6
20	P	316	DMU	C19-C18-O16-C6
20	Q	201	DMU	O5-C6-O16-C18
20	Z	102	DMU	C19-C18-O16-C6
24	C	305	CHD	C13-C17-C20-C21
24	C	305	CHD	C13-C17-C20-C22
24	P	305	CHD	C13-C17-C20-C21
24	P	305	CHD	C16-C17-C20-C22
26	C	304	CDL	O1-C1-CB2-OB2
26	C	304	CDL	C1-CA2-OA2-PA1
26	C	304	CDL	CA2-OA2-PA1-OA5
26	C	304	CDL	CA3-OA5-PA1-OA2
26	C	304	CDL	C11-CA5-OA6-CA4
26	C	304	CDL	CB3-OB5-PB2-OB4
26	C	304	CDL	OB7-CB5-OB6-CB4
26	C	304	CDL	C51-CB5-OB6-CB4
26	I	101	CDL	CA2-OA2-PA1-OA3
26	I	101	CDL	CA3-OA5-PA1-OA2
26	I	101	CDL	CB2-OB2-PB2-OB3
26	I	101	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
26	I	101	CDL	CB3-OB5-PB2-OB3
26	I	101	CDL	CB3-OB5-PB2-OB4
26	I	101	CDL	C51-CB5-OB6-CB4
26	L	101	CDL	CA2-OA2-PA1-OA3
26	L	101	CDL	CA2-OA2-PA1-OA4
26	L	101	CDL	CA2-OA2-PA1-OA5
26	L	101	CDL	OA7-CA5-OA6-CA4
26	L	101	CDL	CB2-OB2-PB2-OB5
26	L	101	CDL	C51-CB5-OB6-CB4
26	N	606	CDL	CA3-OA5-PA1-OA2
26	N	606	CDL	CA3-OA5-PA1-OA3
26	N	606	CDL	CB2-OB2-PB2-OB3
26	N	606	CDL	CB2-OB2-PB2-OB5
26	N	606	CDL	CB3-OB5-PB2-OB2
26	N	606	CDL	CB3-OB5-PB2-OB3
26	N	606	CDL	CB3-OB5-PB2-OB4
26	N	606	CDL	C51-CB5-OB6-CB4
26	P	304	CDL	C1-CA2-OA2-PA1
26	P	304	CDL	CA2-OA2-PA1-OA3
26	P	304	CDL	CA2-OA2-PA1-OA5
26	P	304	CDL	CA3-OA5-PA1-OA2
26	P	304	CDL	CB3-OB5-PB2-OB4
26	P	304	CDL	OB7-CB5-OB6-CB4
26	P	304	CDL	C51-CB5-OB6-CB4
26	Y	101	CDL	C11-CA5-OA6-CA4
26	Y	101	CDL	CB2-OB2-PB2-OB3
26	Y	101	CDL	CB2-OB2-PB2-OB5
26	Y	101	CDL	C51-CB5-OB6-CB4
28	G	101	PEK	C11-C12-C13-C14
28	G	101	PEK	C12-C13-C14-C15
28	T	102	PEK	C11-C12-C13-C14
28	T	102	PEK	C12-C13-C14-C15
24	C	305	CHD	C16-C17-C20-C21
24	P	305	CHD	C16-C17-C20-C21
24	P	305	CHD	C13-C17-C20-C22
20	Z	101	DMU	O6-C11-C9-O1
26	C	304	CDL	OA7-CA5-OA6-CA4
26	I	101	CDL	OB7-CB5-OB6-CB4
26	L	101	CDL	OB7-CB5-OB6-CB4
26	N	606	CDL	OB7-CB5-OB6-CB4
26	Y	101	CDL	OA7-CA5-OA6-CA4
26	Y	101	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
20	C	320	DMU	O5-C4-C57-O61
20	O	304	DMU	O5-C4-C57-O61
26	L	101	CDL	C11-CA5-OA6-CA4
24	C	305	CHD	C16-C17-C20-C22
20	L	102	DMU	C3-C4-C57-O61
20	C	318	DMU	O5-C4-C57-O61
14	A	602	HEA	C4D-C3D-CAD-CBD
20	H	101	DMU	C3-C4-C57-O61
26	P	304	CDL	O1-C1-CA2-OA2
26	P	304	CDL	O1-C1-CB2-OB2
26	C	304	CDL	C31-CA7-OA8-CA6
20	C	320	DMU	C3-C4-C57-O61
20	Z	101	DMU	O6-C11-C9-C8
20	C	320	DMU	O6-C11-C9-O1
20	C	318	DMU	C3-C4-C57-O61
19	C	326	LFA	C9-C10-C11-C12
20	O	304	DMU	C3-C4-C57-O61
26	I	101	CDL	C1-CA2-OA2-PA1
20	C	324	DMU	O5-C4-C57-O61
20	D	201	DMU	O6-C11-C9-O1
20	B	304	DMU	O5-C6-O16-C18
20	T	105	DMU	O5-C6-O16-C18
20	Z	102	DMU	O5-C6-O16-C18
22	C	303	PGV	C28-C29-C30-C31
26	Y	101	CDL	C31-CA7-OA8-CA6
20	C	316	DMU	O5-C4-C57-O61
20	C	316	DMU	O6-C11-C9-O1
20	L	102	DMU	O5-C4-C57-O61
20	A	609	DMU	O6-C11-C9-C8
20	H	101	DMU	O5-C4-C57-O61
20	P	318	DMU	O6-C11-C9-O1
20	P	318	DMU	O6-C11-C9-C8
26	Y	101	CDL	OA9-CA7-OA8-CA6
26	Y	101	CDL	CB2-C1-CA2-OA2
26	N	606	CDL	C31-CA7-OA8-CA6
26	P	304	CDL	C31-CA7-OA8-CA6
20	C	324	DMU	C3-C4-C57-O61
19	C	309	LFA	C11-C10-C9-C8
19	P	307	LFA	C7-C8-C9-C10
20	C	316	DMU	O6-C11-C9-C8
20	C	319	DMU	C3-C4-C57-O61
20	T	105	DMU	C1-C6-O16-C18

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Mol	Chain	Res	Type	Atoms
20	U	101	DMU	C1-C6-O16-C18
20	Z	102	DMU	C1-C6-O16-C18
26	L	101	CDL	CB7-C71-C72-C73
20	P	318	DMU	C2-C3-O7-C10
26	Y	101	CDL	O1-C1-CB2-OB2
26	C	304	CDL	OA9-CA7-OA8-CA6
20	P	316	DMU	O5-C4-C57-O61
20	P	317	DMU	C4-C3-O7-C10
26	C	304	CDL	CA7-C31-C32-C33
19	C	309	LFA	C12-C13-C14-C15
20	A	609	DMU	O6-C11-C9-O1
26	Y	101	CDL	OB6-CB4-CB6-OB8
20	C	320	DMU	O6-C11-C9-C8
20	N	610	DMU	O6-C11-C9-C8
20	Z	102	DMU	O16-C18-C19-C22
20	C	318	DMU	O16-C18-C19-C22
20	P	318	DMU	C4-C3-O7-C10
20	Q	201	DMU	O5-C4-C57-O61
20	D	201	DMU	O6-C11-C9-C8
26	N	606	CDL	CA5-C11-C12-C13
20	P	317	DMU	O6-C11-C9-O1
20	C	324	DMU	O16-C18-C19-C22
20	D	201	DMU	C4-C3-O7-C10
20	C	320	DMU	O16-C18-C19-C22
26	P	304	CDL	CB5-C51-C52-C53
20	C	319	DMU	O5-C4-C57-O61
20	Z	102	DMU	O5-C4-C57-O61
26	C	304	CDL	CB5-C51-C52-C53
26	Y	101	CDL	CA5-C11-C12-C13
26	P	304	CDL	OA9-CA7-OA8-CA6
20	U	101	DMU	O5-C6-O16-C18
20	P	317	DMU	O16-C18-C19-C22
26	C	304	CDL	O1-C1-CA2-OA2
26	L	101	CDL	O1-C1-CA2-OA2
26	N	606	CDL	O1-C1-CB2-OB2
26	Y	101	CDL	O1-C1-CA2-OA2
26	N	606	CDL	OA9-CA7-OA8-CA6
26	N	606	CDL	CA7-C31-C32-C33
20	L	102	DMU	O16-C18-C19-C22
28	T	102	PEK	C7-C8-C9-C10
26	I	101	CDL	CA5-C11-C12-C13
26	P	304	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
26	C	304	CDL	CB7-C71-C72-C73
26	L	101	CDL	CB2-C1-CA2-OA2
26	N	606	CDL	CA2-C1-CB2-OB2
26	C	304	CDL	C71-CB7-OB8-CB6
26	L	101	CDL	C72-C73-C74-C75
20	Q	201	DMU	C4-C3-O7-C10
26	I	101	CDL	OA7-CA5-OA6-CA4
20	C	319	DMU	C1-C6-O16-C18
20	C	320	DMU	C1-C6-O16-C18
20	P	317	DMU	C1-C6-O16-C18
28	T	102	PEK	C10-C11-C12-C13
20	P	318	DMU	C19-C22-C25-C28
20	B	308	DMU	O5-C4-C57-O61
20	H	101	DMU	C25-C28-C31-C34
26	N	606	CDL	C13-C14-C15-C16
20	C	319	DMU	O16-C18-C19-C22
19	P	309	LFA	C11-C10-C9-C8
26	L	101	CDL	C31-CA7-OA8-CA6
19	P	311	LFA	C1-C2-C3-C4
20	T	105	DMU	O5-C4-C57-O61
19	T	101	LFA	C9-C10-C11-C12
20	P	317	DMU	C2-C3-O7-C10
20	C	319	DMU	O6-C11-C9-O1
20	C	317	DMU	C28-C31-C34-C37
19	C	309	LFA	C3-C4-C5-C6
19	T	103	LFA	C10-C11-C12-C13
20	N	610	DMU	C31-C34-C37-C40
26	C	304	CDL	C22-C23-C24-C25
26	L	101	CDL	C34-C35-C36-C37
19	O	302	LFA	C13-C14-C15-C16
19	P	309	LFA	C5-C6-C7-C8
19	T	103	LFA	C3-C4-C5-C6
20	A	608	DMU	C28-C31-C34-C37
28	T	102	PEK	C26-C27-C28-C29
26	C	304	CDL	OB9-CB7-OB8-CB6
19	G	104	LFA	C11-C10-C9-C8
19	P	309	LFA	C3-C4-C5-C6
26	Y	101	CDL	C71-C72-C73-C74
20	C	319	DMU	C19-C18-O16-C6
26	I	101	CDL	C19-C20-C21-C22
26	P	304	CDL	C11-C12-C13-C14
20	B	303	DMU	C18-C19-C22-C25

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Mol	Chain	Res	Type	Atoms
20	H	101	DMU	C19-C22-C25-C28
28	G	101	PEK	C26-C27-C28-C29
28	G	101	PEK	C28-C29-C30-C31
19	C	309	LFA	C5-C6-C7-C8
26	N	606	CDL	C31-C32-C33-C34
28	T	102	PEK	C1-C2-C3-C4
19	C	310	LFA	C6-C7-C8-C9
19	C	326	LFA	C6-C7-C8-C9
20	A	615	DMU	C19-C22-C25-C28
20	P	318	DMU	C22-C25-C28-C31
20	Z	101	DMU	C28-C31-C34-C37
19	C	313	LFA	C1-C2-C3-C4
28	T	102	PEK	C17-C18-C19-C20
22	N	616	PGV	C14-C15-C16-C17
26	P	304	CDL	C56-C57-C58-C59
28	G	101	PEK	C34-C35-C36-C37
20	O	308	DMU	C34-C37-C40-C43
20	D	201	DMU	C2-C3-O7-C10
20	Z	101	DMU	C22-C25-C28-C31
22	C	303	PGV	C7-C8-C9-C10
26	L	101	CDL	C13-C14-C15-C16
26	C	304	CDL	C35-C36-C37-C38
20	C	324	DMU	C28-C31-C34-C37
28	G	101	PEK	C16-C17-C18-C19
20	P	322	DMU	C4-C3-O7-C10
19	C	312	LFA	C4-C5-C6-C7
19	P	310	LFA	C7-C8-C9-C10
20	C	324	DMU	C25-C28-C31-C34
26	C	304	CDL	C75-C76-C77-C78
26	Y	101	CDL	C80-C81-C82-C83
26	L	101	CDL	OA9-CA7-OA8-CA6
20	B	304	DMU	C31-C34-C37-C40
26	Y	101	CDL	C79-C80-C81-C82
26	L	101	CDL	C37-C38-C39-C40
19	B	307	LFA	C13-C14-C15-C16
20	M	102	DMU	C31-C34-C37-C40
26	I	101	CDL	C78-C79-C80-C81
26	Y	101	CDL	C63-C64-C65-C66
20	P	316	DMU	C3-C4-C57-O61
19	C	310	LFA	C10-C11-C12-C13
20	P	317	DMU	C28-C31-C34-C37
26	C	304	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
20	B	302	DMU	C18-C19-C22-C25
19	C	307	LFA	C4-C5-C6-C7
19	O	303	LFA	C5-C6-C7-C8
20	A	609	DMU	C31-C34-C37-C40
26	N	606	CDL	C17-C18-C19-C20
22	P	303	PGV	C24-C25-C26-C27
20	D	201	DMU	O16-C18-C19-C22
19	P	310	LFA	C6-C7-C8-C9
20	C	316	DMU	C28-C31-C34-C37
19	P	309	LFA	C4-C5-C6-C7
20	C	319	DMU	C31-C34-C37-C40
26	N	606	CDL	C73-C74-C75-C76
20	P	317	DMU	O5-C6-O16-C18
19	G	104	LFA	C5-C6-C7-C8
26	Y	101	CDL	C13-C14-C15-C16
20	C	316	DMU	C19-C22-C25-C28
20	C	320	DMU	C19-C22-C25-C28
22	C	303	PGV	C22-C23-C24-C25
19	C	326	LFA	C7-C8-C9-C10
19	P	309	LFA	C13-C14-C15-C16
19	P	310	LFA	C2-C3-C4-C5
20	O	306	DMU	C19-C22-C25-C28
26	L	101	CDL	C17-C18-C19-C20
26	I	101	CDL	C11-CA5-OA6-CA4
26	P	304	CDL	CB7-C71-C72-C73
20	Z	102	DMU	C18-C19-C22-C25
22	N	616	PGV	C29-C30-C31-C32
26	L	101	CDL	C36-C37-C38-C39
26	N	606	CDL	C74-C75-C76-C77
22	N	616	PGV	C12-C13-C14-C15
26	N	606	CDL	C76-C77-C78-C79
20	P	322	DMU	C2-C3-O7-C10
22	N	616	PGV	C27-C28-C29-C30
22	C	303	PGV	C30-C31-C32-C33
20	B	303	DMU	C19-C22-C25-C28
20	P	316	DMU	C31-C34-C37-C40
20	Z	102	DMU	C25-C28-C31-C34
20	O	307	DMU	C18-C19-C22-C25
20	P	306	DMU	O16-C18-C19-C22
20	P	314	DMU	C28-C31-C34-C37
26	L	101	CDL	C14-C15-C16-C17
19	C	312	LFA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
26	P	304	CDL	OA7-CA5-OA6-CA4
20	P	316	DMU	C18-C19-C22-C25
20	U	101	DMU	C18-C19-C22-C25
20	L	102	DMU	C31-C34-C37-C40
26	L	101	CDL	C58-C59-C60-C61
26	P	304	CDL	C75-C76-C77-C78
28	T	102	PEK	C22-C23-C24-C25
20	B	308	DMU	C18-C19-C22-C25
20	P	314	DMU	C18-C19-C22-C25
19	T	103	LFA	C4-C5-C6-C7
26	I	101	CDL	OA6-CA4-CA6-OA8
20	L	102	DMU	C25-C28-C31-C34
19	C	310	LFA	C9-C10-C11-C12
22	C	303	PGV	C24-C25-C26-C27
19	B	307	LFA	C4-C5-C6-C7
19	O	303	LFA	C2-C3-C4-C5
22	P	303	PGV	C11-C12-C13-C14
26	P	304	CDL	C73-C74-C75-C76
26	C	304	CDL	CA4-CA3-OA5-PA1
20	P	316	DMU	C22-C25-C28-C31
20	B	303	DMU	O16-C18-C19-C22
20	O	306	DMU	O16-C18-C19-C22
19	C	311	LFA	C5-C6-C7-C8
20	C	319	DMU	C19-C22-C25-C28
19	C	309	LFA	C11-C12-C13-C14
19	T	101	LFA	C5-C6-C7-C8
28	T	102	PEK	C4-C5-C6-C7
19	B	307	LFA	C7-C8-C9-C10
20	C	318	DMU	C22-C25-C28-C31
20	P	322	DMU	O16-C18-C19-C22
19	A	607	LFA	C6-C7-C8-C9
19	C	309	LFA	C1-C2-C3-C4
20	U	101	DMU	O5-C4-C57-O61
20	C	318	DMU	C31-C34-C37-C40
26	I	101	CDL	C71-C72-C73-C74
26	L	101	CDL	C21-C22-C23-C24
26	N	606	CDL	C77-C78-C79-C80
20	Z	102	DMU	C31-C34-C37-C40
26	I	101	CDL	C17-C18-C19-C20
26	L	101	CDL	C76-C77-C78-C79
26	N	606	CDL	C18-C19-C20-C21
26	N	606	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
22	A	614	PGV	C11-C10-C9-C8
22	P	303	PGV	C12-C13-C14-C15
20	Q	201	DMU	C2-C3-O7-C10
20	M	101	DMU	C22-C25-C28-C31
26	P	304	CDL	C35-C36-C37-C38
20	O	306	DMU	C18-C19-C22-C25
26	N	606	CDL	OA7-CA5-OA6-CA4
19	A	607	LFA	C9-C10-C11-C12
19	P	312	LFA	C9-C10-C11-C12
26	P	304	CDL	C52-C53-C54-C55
20	A	615	DMU	O16-C18-C19-C22
20	B	302	DMU	C19-C22-C25-C28
26	L	101	CDL	C80-C81-C82-C83
19	C	313	LFA	C5-C6-C7-C8
19	P	312	LFA	C4-C5-C6-C7
20	P	314	DMU	O6-C11-C9-O1
26	Y	101	CDL	C51-C52-C53-C54
26	C	304	CDL	CB3-CB4-CB6-OB8
26	N	606	CDL	CA3-CA4-CA6-OA8
26	P	304	CDL	CB3-CB4-CB6-OB8
28	G	101	PEK	C15-C16-C17-C18
28	T	102	PEK	C2-C3-C4-C5
20	C	317	DMU	C31-C34-C37-C40
26	I	101	CDL	C13-C14-C15-C16
20	B	302	DMU	O16-C18-C19-C22
20	G	102	DMU	O16-C18-C19-C22
20	O	307	DMU	O16-C18-C19-C22
20	W	101	DMU	O16-C18-C19-C22
20	L	102	DMU	C22-C25-C28-C31
26	P	304	CDL	C33-C34-C35-C36
26	P	304	CDL	C54-C55-C56-C57
20	P	315	DMU	C28-C31-C34-C37
19	N	608	LFA	C7-C8-C9-C10
20	A	609	DMU	C3-C4-C57-O61
20	M	101	DMU	O6-C11-C9-C8
19	B	307	LFA	C9-C10-C11-C12
20	N	610	DMU	O16-C18-C19-C22
22	P	303	PGV	C30-C31-C32-C33
20	Z	101	DMU	C25-C28-C31-C34
26	I	101	CDL	C16-C17-C18-C19
26	L	101	CDL	C74-C75-C76-C77
19	P	312	LFA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	Y	101	CDL	C21-C22-C23-C24
28	G	101	PEK	C25-C26-C27-C28
19	P	311	LFA	C3-C4-C5-C6
19	P	312	LFA	C6-C7-C8-C9
20	J	101	DMU	C25-C28-C31-C34
26	Y	101	CDL	C22-C23-C24-C25
26	L	101	CDL	OB5-CB3-CB4-OB6
19	C	309	LFA	C2-C3-C4-C5
26	Y	101	CDL	C84-C85-C86-C87
19	O	302	LFA	C11-C12-C13-C14
20	U	101	DMU	C19-C22-C25-C28
26	P	304	CDL	C57-C58-C59-C60
19	C	310	LFA	C1-C2-C3-C4
19	P	307	LFA	C11-C10-C9-C8
20	N	610	DMU	O6-C11-C9-O1
20	B	302	DMU	C31-C34-C37-C40
20	C	318	DMU	C19-C22-C25-C28
26	I	101	CDL	C75-C76-C77-C78
26	Y	101	CDL	C59-C60-C61-C62
26	N	606	CDL	OA6-CA4-CA6-OA8
20	A	608	DMU	C25-C28-C31-C34
20	C	319	DMU	C34-C37-C40-C43
26	P	304	CDL	C53-C54-C55-C56
20	L	102	DMU	C34-C37-C40-C43
22	A	614	PGV	C31-C32-C33-C34
22	N	616	PGV	C31-C32-C33-C34
26	Y	101	CDL	C64-C65-C66-C67
20	M	101	DMU	C25-C28-C31-C34
19	O	302	LFA	C14-C15-C16-C17
20	C	316	DMU	C34-C37-C40-C43
19	C	310	LFA	C4-C5-C6-C7
19	P	312	LFA	C2-C3-C4-C5
26	P	304	CDL	C71-C72-C73-C74
26	Y	101	CDL	C71-CB7-OB8-CB6
26	L	101	CDL	C84-C85-C86-C87
28	G	101	PEK	C17-C18-C19-C20
26	C	304	CDL	C12-C11-CA5-OA6
22	A	614	PGV	C14-C15-C16-C17
26	C	304	CDL	C58-C59-C60-C61
26	L	101	CDL	C75-C76-C77-C78
22	P	303	PGV	C7-C8-C9-C10
19	P	310	LFA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
19	B	307	LFA	C14-C15-C16-C17
19	T	104	LFA	C3-C4-C5-C6
20	P	322	DMU	C25-C28-C31-C34
26	C	304	CDL	C23-C24-C25-C26
20	L	102	DMU	C19-C18-O16-C6
20	P	318	DMU	C19-C18-O16-C6
26	Y	101	CDL	C19-C20-C21-C22
26	Y	101	CDL	C31-C32-C33-C34
22	P	303	PGV	C02-C03-O11-P
19	T	104	LFA	C4-C5-C6-C7
20	T	105	DMU	C34-C37-C40-C43
20	B	308	DMU	C34-C37-C40-C43
19	T	103	LFA	C5-C6-C7-C8
26	Y	101	CDL	C32-C33-C34-C35
19	C	311	LFA	C7-C8-C9-C10
20	C	318	DMU	C25-C28-C31-C34
22	C	303	PGV	C14-C15-C16-C17
26	N	606	CDL	C72-C73-C74-C75
20	C	317	DMU	C34-C37-C40-C43
19	C	326	LFA	C12-C13-C14-C15
20	G	102	DMU	C34-C37-C40-C43
20	Q	201	DMU	C3-C4-C57-O61
26	Y	101	CDL	OB9-CB7-OB8-CB6
26	C	304	CDL	C59-C60-C61-C62
26	C	304	CDL	C12-C13-C14-C15
26	Y	101	CDL	CB5-C51-C52-C53
20	D	201	DMU	C19-C22-C25-C28
26	P	304	CDL	C72-C73-C74-C75
20	W	101	DMU	C34-C37-C40-C43
20	C	320	DMU	C34-C37-C40-C43
20	P	317	DMU	C25-C28-C31-C34
26	L	101	CDL	C59-C60-C61-C62
20	C	316	DMU	C3-C4-C57-O61
20	O	307	DMU	C19-C22-C25-C28
20	C	320	DMU	C18-C19-C22-C25
26	L	101	CDL	CB5-C51-C52-C53
26	Y	101	CDL	C16-C17-C18-C19
26	C	304	CDL	CB2-C1-CA2-OA2
19	T	104	LFA	C6-C7-C8-C9
26	P	304	CDL	CA3-CA4-CA6-OA8
26	Y	101	CDL	CB3-CB4-CB6-OB8
26	C	304	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
26	I	101	CDL	C73-C74-C75-C76
20	M	101	DMU	O6-C11-C9-O1
26	N	606	CDL	OA5-CA3-CA4-OA6
19	B	307	LFA	C1-C2-C3-C4
19	C	310	LFA	C7-C8-C9-C10
26	L	101	CDL	C72-C71-CB7-OB8
22	C	303	PGV	C02-C03-O11-P
26	N	606	CDL	C1-CA2-OA2-PA1
20	B	304	DMU	C34-C37-C40-C43
19	P	311	LFA	C4-C5-C6-C7
28	G	101	PEK	C29-C30-C31-C32
19	C	311	LFA	C3-C4-C5-C6
26	Y	101	CDL	C61-C62-C63-C64
26	L	101	CDL	OB6-CB4-CB6-OB8
28	G	101	PEK	C9-C10-C11-C12
28	T	102	PEK	C11-C10-C9-C8
22	A	614	PGV	C29-C30-C31-C32
26	Y	101	CDL	C58-C59-C60-C61
20	C	325	DMU	O6-C11-C9-O1
19	C	307	LFA	C3-C4-C5-C6
20	A	615	DMU	C28-C31-C34-C37
20	B	308	DMU	C31-C34-C37-C40
20	H	101	DMU	C28-C31-C34-C37
28	T	102	PEK	C14-C15-C16-C17
26	I	101	CDL	C20-C21-C22-C23
19	A	607	LFA	C7-C8-C9-C10
26	C	304	CDL	C71-C72-C73-C74
22	N	616	PGV	C11-C10-C9-C8
20	C	325	DMU	O16-C18-C19-C22
19	C	312	LFA	C6-C7-C8-C9
26	N	606	CDL	C12-C13-C14-C15
26	L	101	CDL	C15-C16-C17-C18
19	C	309	LFA	C6-C7-C8-C9
19	C	311	LFA	C6-C7-C8-C9
19	N	608	LFA	C6-C7-C8-C9
20	M	102	DMU	C34-C37-C40-C43
28	T	102	PEK	C32-C33-C34-C35
20	C	318	DMU	C28-C31-C34-C37
19	G	104	LFA	C9-C10-C11-C12
20	O	306	DMU	C22-C25-C28-C31
20	P	316	DMU	C19-C22-C25-C28
26	I	101	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
26	P	304	CDL	C13-C14-C15-C16
19	G	104	LFA	C6-C7-C8-C9
26	P	304	CDL	OB5-CB3-CB4-CB6
26	N	606	CDL	C79-C80-C81-C82
19	C	309	LFA	C13-C14-C15-C16
20	O	306	DMU	C25-C28-C31-C34
19	C	326	LFA	C4-C5-C6-C7
22	C	303	PGV	C25-C26-C27-C28
26	P	304	CDL	C21-C22-C23-C24
26	Y	101	CDL	C57-C58-C59-C60
26	P	304	CDL	C22-C23-C24-C25
20	B	308	DMU	C25-C28-C31-C34
20	P	318	DMU	C25-C28-C31-C34
19	C	307	LFA	C6-C7-C8-C9
20	A	609	DMU	O5-C4-C57-O61
20	P	317	DMU	C34-C37-C40-C43
26	C	304	CDL	C52-C53-C54-C55
26	L	101	CDL	O1-C1-CB2-OB2
26	P	304	CDL	OB5-CB3-CB4-OB6
26	Y	101	CDL	OA5-CA3-CA4-OA6
26	L	101	CDL	C57-C58-C59-C60
26	L	101	CDL	CB3-CB4-CB6-OB8
19	T	103	LFA	C1-C2-C3-C4
19	C	313	LFA	C11-C10-C9-C8
26	P	304	CDL	OB6-CB4-CB6-OB8
19	P	309	LFA	C14-C15-C16-C17
26	C	304	CDL	C33-C34-C35-C36
19	C	312	LFA	C10-C11-C12-C13
19	P	309	LFA	C7-C8-C9-C10
20	B	303	DMU	C28-C31-C34-C37
24	C	305	CHD	C21-C20-C22-C23
19	G	104	LFA	C3-C4-C5-C6
19	C	315	LFA	C11-C10-C9-C8
19	T	101	LFA	C3-C4-C5-C6
20	P	315	DMU	C31-C34-C37-C40
20	P	317	DMU	C3-C4-C57-O61
20	Z	102	DMU	C19-C22-C25-C28
26	P	304	CDL	C71-CB7-OB8-CB6
20	O	307	DMU	C28-C31-C34-C37
19	P	310	LFA	C5-C6-C7-C8
14	A	602	HEA	C2D-C3D-CAD-CBD
20	T	105	DMU	C18-C19-C22-C25

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Mol	Chain	Res	Type	Atoms
26	N	606	CDL	C32-C33-C34-C35
19	C	310	LFA	C2-C3-C4-C5
22	C	303	PGV	C13-C14-C15-C16
20	C	316	DMU	C2-C3-O7-C10
26	N	606	CDL	OA5-CA3-CA4-CA6
26	Y	101	CDL	OA5-CA3-CA4-CA6
19	G	104	LFA	C1-C2-C3-C4
20	Z	101	DMU	C34-C37-C40-C43
20	P	314	DMU	C19-C22-C25-C28
26	L	101	CDL	C51-C52-C53-C54
20	P	317	DMU	O6-C11-C9-C8
19	P	309	LFA	C11-C12-C13-C14
20	U	101	DMU	C25-C28-C31-C34
20	C	316	DMU	C18-C19-C22-C25
20	P	306	DMU	C31-C34-C37-C40
19	T	101	LFA	C11-C12-C13-C14
19	C	326	LFA	C3-C4-C5-C6
20	C	316	DMU	C4-C3-O7-C10
19	C	311	LFA	C11-C10-C9-C8
26	I	101	CDL	C32-C33-C34-C35
28	T	102	PEK	C2-C1-O01-C02
20	C	319	DMU	C4-C3-O7-C10
26	L	101	CDL	C19-C20-C21-C22
26	N	606	CDL	C52-C51-CB5-OB7
26	C	304	CDL	OB6-CB4-CB6-OB8
26	Y	101	CDL	OA6-CA4-CA6-OA8
19	C	307	LFA	C11-C10-C9-C8
20	U	101	DMU	C22-C25-C28-C31
20	T	105	DMU	O16-C18-C19-C22
20	J	101	DMU	C31-C34-C37-C40
26	L	101	CDL	C22-C23-C24-C25
26	C	304	CDL	CA3-OA5-PA1-OA3
26	I	101	CDL	CA3-OA5-PA1-OA3
26	L	101	CDL	CA3-OA5-PA1-OA2
26	L	101	CDL	CA3-OA5-PA1-OA3
26	L	101	CDL	CA3-OA5-PA1-OA4
26	L	101	CDL	CB2-OB2-PB2-OB3
26	N	606	CDL	CA2-OA2-PA1-OA3
26	N	606	CDL	CB2-OB2-PB2-OB4
26	P	304	CDL	CA3-OA5-PA1-OA3
26	Y	101	CDL	CB2-OB2-PB2-OB4
19	C	315	LFA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
20	P	314	DMU	C31-C34-C37-C40
20	C	324	DMU	C18-C19-C22-C25
28	T	102	PEK	C30-C31-C32-C33
26	C	304	CDL	C79-C80-C81-C82
22	N	616	PGV	C23-C24-C25-C26
26	Y	101	CDL	C1-CA2-OA2-PA1
20	Z	102	DMU	C34-C37-C40-C43
20	M	101	DMU	C19-C22-C25-C28
26	Y	101	CDL	C73-C74-C75-C76
20	Z	103	DMU	C22-C25-C28-C31
19	C	312	LFA	C11-C10-C9-C8
26	C	304	CDL	C51-C52-C53-C54
22	P	303	PGV	C1-C2-C3-C4
19	C	311	LFA	C4-C5-C6-C7
26	Y	101	CDL	C14-C15-C16-C17
20	C	319	DMU	C2-C3-O7-C10
19	T	101	LFA	C6-C7-C8-C9
22	P	303	PGV	C22-C23-C24-C25
14	N	602	HEA	C4D-C3D-CAD-CBD
26	P	304	CDL	CA2-C1-CB2-OB2
20	P	306	DMU	C18-C19-C22-C25
26	P	304	CDL	C20-C21-C22-C23
20	Z	103	DMU	C31-C34-C37-C40
24	P	305	CHD	C21-C20-C22-C23
20	B	304	DMU	O16-C18-C19-C22
26	P	304	CDL	CA7-C31-C32-C33
14	N	602	HEA	C3B-C11-C12-C13
20	P	318	DMU	C28-C31-C34-C37
26	L	101	CDL	C73-C74-C75-C76
19	C	310	LFA	C11-C12-C13-C14
20	H	101	DMU	O6-C11-C9-O1
28	G	101	PEK	C22-C23-C24-C25
20	J	101	DMU	C28-C31-C34-C37
20	C	324	DMU	C19-C18-O16-C6
26	N	606	CDL	C52-C51-CB5-OB6
20	P	316	DMU	C28-C31-C34-C37
20	P	318	DMU	C31-C34-C37-C40
19	C	309	LFA	C14-C15-C16-C17
19	O	303	LFA	C1-C2-C3-C4
20	A	615	DMU	C34-C37-C40-C43
28	T	102	PEK	C15-C16-C17-C18
20	L	102	DMU	C1-C6-O16-C18

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Mol	Chain	Res	Type	Atoms
20	P	317	DMU	O5-C4-C57-O61
20	C	316	DMU	O1-C10-O7-C3
20	P	314	DMU	O5-C4-C57-O61
20	M	102	DMU	C22-C25-C28-C31
26	C	304	CDL	C16-C17-C18-C19
26	Y	101	CDL	C24-C25-C26-C27
20	B	308	DMU	O16-C18-C19-C22
26	I	101	CDL	C77-C78-C79-C80
14	N	602	HEA	CAD-CBD-CGD-O1D
26	P	304	CDL	C19-C20-C21-C22
26	P	304	CDL	C80-C81-C82-C83
22	C	303	PGV	C05-C04-O12-P
20	T	105	DMU	C22-C25-C28-C31
24	C	305	CHD	C22-C23-C24-O25
20	D	201	DMU	C28-C31-C34-C37
20	P	314	DMU	O1-C10-O7-C3
20	C	320	DMU	C28-C31-C34-C37
26	I	101	CDL	CA3-CA4-CA6-OA8
26	P	304	CDL	OB9-CB7-OB8-CB6
19	C	312	LFA	C5-C6-C7-C8
26	P	304	CDL	C17-C18-C19-C20
19	G	104	LFA	C7-C8-C9-C10
26	C	304	CDL	C72-C71-CB7-OB8
20	C	316	DMU	C5-C10-O7-C3
19	N	608	LFA	C10-C11-C12-C13
26	P	304	CDL	C23-C24-C25-C26
20	Q	201	DMU	O16-C18-C19-C22
19	P	309	LFA	C1-C2-C3-C4
24	B	306	CHD	C22-C23-C24-O26
24	P	305	CHD	C22-C23-C24-O26
26	N	606	CDL	CB4-CB3-OB5-PB2
26	Y	101	CDL	C76-C77-C78-C79
14	A	602	HEA	CAD-CBD-CGD-O1D
24	O	301	CHD	C22-C23-C24-O25
24	O	301	CHD	C22-C23-C24-O26
19	C	326	LFA	C5-C6-C7-C8
22	C	303	PGV	C29-C30-C31-C32
14	A	602	HEA	CAD-CBD-CGD-O2D
14	N	602	HEA	CAD-CBD-CGD-O2D
19	P	312	LFA	C7-C8-C9-C10
14	A	601	HEA	CAD-CBD-CGD-O1D
14	N	601	HEA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	N	602	HEA	CAA-CBA-CGA-O1A
26	C	304	CDL	C21-C22-C23-C24
28	G	101	PEK	C5-C6-C7-C8
20	C	306	DMU	C28-C31-C34-C37
26	P	304	CDL	C74-C75-C76-C77
22	P	303	PGV	C27-C28-C29-C30
22	C	303	PGV	C23-C24-C25-C26
19	C	311	LFA	C1-C2-C3-C4
14	A	602	HEA	CAA-CBA-CGA-O1A
20	B	308	DMU	C28-C31-C34-C37
24	P	305	CHD	C22-C23-C24-O25
26	I	101	CDL	O1-C1-CA2-OA2
26	C	304	CDL	C74-C75-C76-C77
20	Z	103	DMU	C25-C28-C31-C34
19	N	608	LFA	C9-C10-C11-C12
20	T	105	DMU	C25-C28-C31-C34
24	B	306	CHD	C22-C23-C24-O25
20	N	610	DMU	O5-C6-O16-C18
19	P	313	LFA	C6-C7-C8-C9
24	C	305	CHD	C22-C23-C24-O26
28	G	101	PEK	C23-C24-C25-C26
19	C	314	LFA	C6-C7-C8-C9
26	I	101	CDL	C15-C16-C17-C18
14	A	601	HEA	CAD-CBD-CGD-O2D
26	P	304	CDL	OA5-CA3-CA4-OA6
19	O	302	LFA	C7-C8-C9-C10
28	T	102	PEK	C25-C26-C27-C28
21	C	321	EDO	O1-C1-C2-O2
21	F	103	EDO	O1-C1-C2-O2
21	P	321	EDO	O1-C1-C2-O2
21	R	201	EDO	O1-C1-C2-O2
14	N	602	HEA	CAA-CBA-CGA-O2A
20	O	306	DMU	C31-C34-C37-C40
22	A	614	PGV	O03-C19-C20-C21
26	P	304	CDL	C12-C11-CA5-OA6
20	A	615	DMU	C25-C28-C31-C34
26	P	304	CDL	C12-C13-C14-C15
20	T	105	DMU	C28-C31-C34-C37
14	A	602	HEA	CAA-CBA-CGA-O2A
14	N	601	HEA	CAD-CBD-CGD-O2D
26	C	304	CDL	C13-C14-C15-C16
19	C	307	LFA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
20	C	319	DMU	O5-C6-O16-C18
22	P	303	PGV	C05-C04-O12-P
26	P	304	CDL	CA4-CA3-OA5-PA1
26	Y	101	CDL	C12-C13-C14-C15
19	T	101	LFA	C7-C8-C9-C10
20	C	325	DMU	C18-C19-C22-C25
19	C	315	LFA	C6-C7-C8-C9
22	C	303	PGV	C11-C12-C13-C14
20	O	304	DMU	C34-C37-C40-C43
22	N	616	PGV	O03-C19-C20-C21
24	C	301	CHD	C22-C23-C24-O26
20	Q	201	DMU	C25-C28-C31-C34
26	C	304	CDL	C11-C12-C13-C14
28	T	102	PEK	C13-C14-C15-C16
26	N	606	CDL	C16-C17-C18-C19
26	C	304	CDL	C72-C73-C74-C75
26	I	101	CDL	CB4-CB3-OB5-PB2
26	P	304	CDL	C14-C15-C16-C17
20	P	314	DMU	C5-C10-O7-C3
20	T	105	DMU	C31-C34-C37-C40
26	I	101	CDL	C31-CA7-OA8-CA6
19	C	314	LFA	C4-C5-C6-C7
20	P	306	DMU	C22-C25-C28-C31
24	C	301	CHD	C22-C23-C24-O25
21	A	611	EDO	O1-C1-C2-O2
21	C	323	EDO	O1-C1-C2-O2
21	N	613	EDO	O1-C1-C2-O2
21	P	319	EDO	O1-C1-C2-O2
21	R	203	EDO	O1-C1-C2-O2
26	N	606	CDL	C11-CA5-OA6-CA4
20	P	317	DMU	C19-C22-C25-C28
19	C	326	LFA	C10-C11-C12-C13
28	T	102	PEK	O02-C1-O01-C02
20	Z	102	DMU	C22-C25-C28-C31
20	O	304	DMU	C22-C25-C28-C31
19	B	307	LFA	C10-C11-C12-C13
22	N	616	PGV	C30-C31-C32-C33
22	N	616	PGV	C15-C16-C17-C18
26	C	304	CDL	C52-C51-CB5-OB6
26	I	101	CDL	C32-C31-CA7-OA8
20	D	201	DMU	C31-C34-C37-C40
20	O	304	DMU	C18-C19-C22-C25

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Mol	Chain	Res	Type	Atoms
19	C	313	LFA	C6-C7-C8-C9
26	I	101	CDL	C72-C71-CB7-OB8
26	N	606	CDL	C72-C71-CB7-OB8
20	N	609	DMU	C34-C37-C40-C43
19	C	314	LFA	C11-C10-C9-C8
26	P	304	CDL	C52-C51-CB5-OB6
20	C	325	DMU	C31-C34-C37-C40
26	C	304	CDL	C53-C54-C55-C56
20	P	317	DMU	C22-C25-C28-C31
20	B	302	DMU	C25-C28-C31-C34
19	C	314	LFA	C12-C13-C14-C15
19	T	104	LFA	C7-C8-C9-C10
14	N	602	HEA	C26-C15-C16-C17
19	P	313	LFA	C1-C2-C3-C4
22	A	614	PGV	C11-C12-C13-C14
26	L	101	CDL	C82-C83-C84-C85
24	P	301	CHD	C22-C23-C24-O25
26	C	304	CDL	C36-C37-C38-C39
26	L	101	CDL	C72-C71-CB7-OB9
26	N	606	CDL	CA3-CA4-OA6-CA5
24	P	301	CHD	C22-C23-C24-O26
26	P	304	CDL	C72-C71-CB7-OB8
26	P	304	CDL	C31-C32-C33-C34
20	O	307	DMU	C22-C25-C28-C31
26	C	304	CDL	C12-C11-CA5-OA7
26	Y	101	CDL	C74-C75-C76-C77
20	C	306	DMU	O16-C18-C19-C22
26	I	101	CDL	C72-C71-CB7-OB9
26	P	304	CDL	C52-C51-CB5-OB7
26	I	101	CDL	C79-C80-C81-C82
19	P	312	LFA	C11-C10-C9-C8
26	N	606	CDL	C20-C21-C22-C23
28	T	102	PEK	C3-C4-C5-C6
19	O	302	LFA	C11-C10-C9-C8
20	B	303	DMU	C22-C25-C28-C31
14	A	601	HEA	CAA-CBA-CGA-O2A
26	C	304	CDL	C52-C51-CB5-OB7
20	O	308	DMU	C1-C6-O16-C18
20	P	318	DMU	C1-C6-O16-C18
26	N	606	CDL	C72-C71-CB7-OB9
19	C	314	LFA	C7-C8-C9-C10
26	P	304	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
26	L	101	CDL	C32-C31-CA7-OA8
22	A	614	PGV	C28-C29-C30-C31
19	P	309	LFA	C12-C13-C14-C15
26	L	101	CDL	OB5-CB3-CB4-CB6
26	P	304	CDL	C55-C56-C57-C58
26	I	101	CDL	C32-C31-CA7-OA9
20	A	609	DMU	C4-C3-O7-C10
14	A	601	HEA	CAA-CBA-CGA-O1A
26	L	101	CDL	C64-C65-C66-C67

There are no ring outliers.

50 monomers are involved in 154 short contacts:

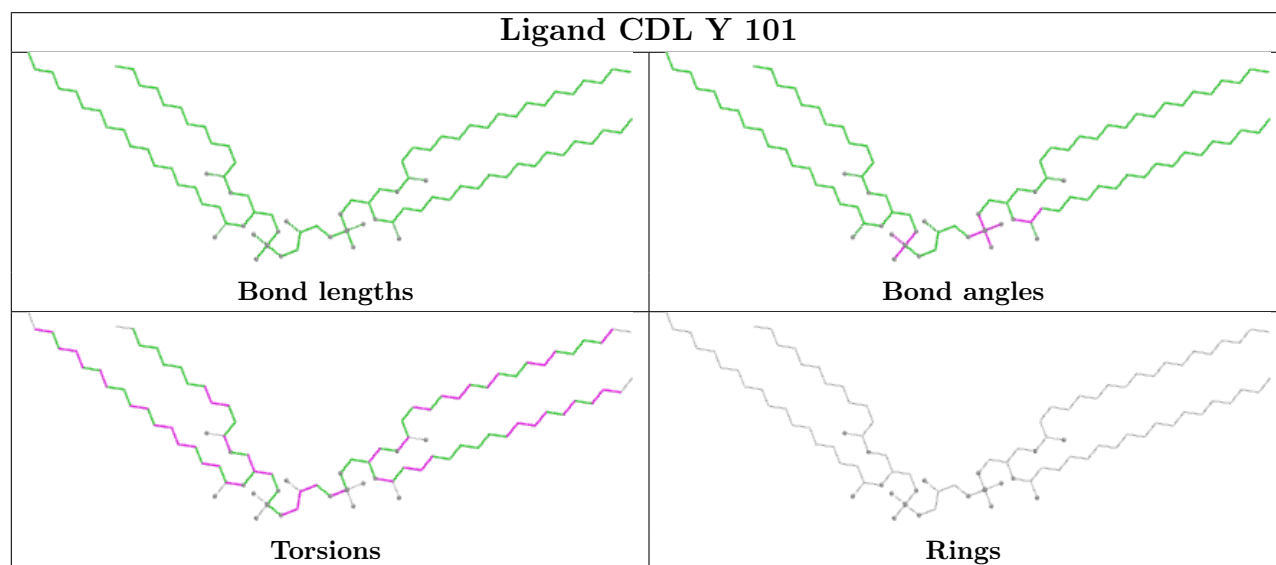
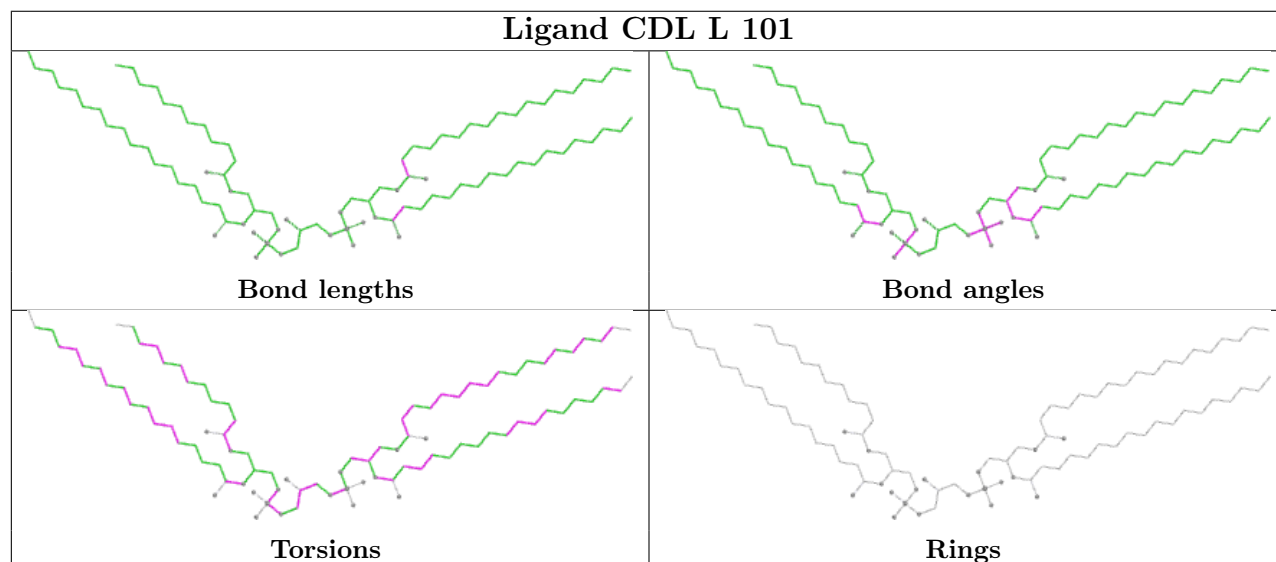
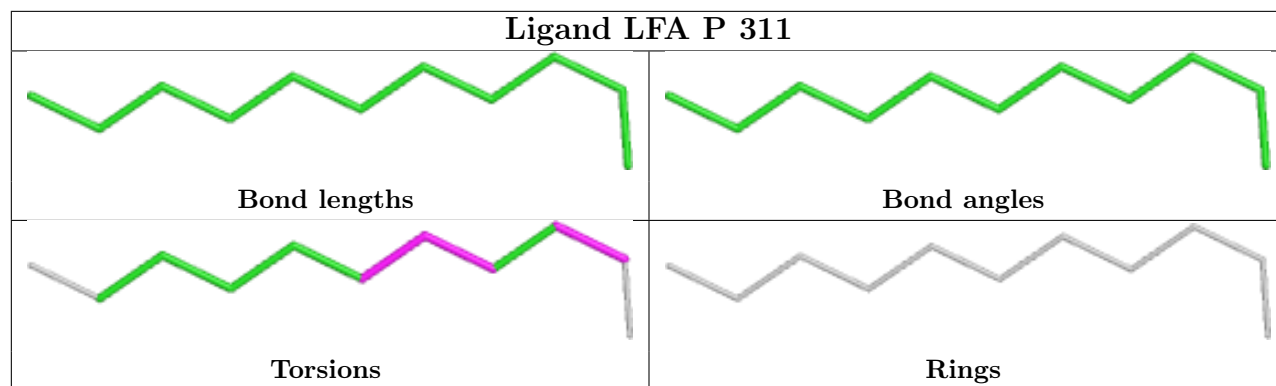
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19	P	311	LFA	1	0
21	N	615	EDO	1	0
26	L	101	CDL	4	0
26	Y	101	CDL	10	0
20	Z	101	DMU	1	0
24	P	301	CHD	2	0
20	C	324	DMU	1	0
14	N	602	HEA	2	0
24	C	305	CHD	2	0
21	A	611	EDO	1	0
20	C	320	DMU	1	0
19	P	312	LFA	2	0
24	O	301	CHD	1	0
28	T	102	PEK	4	0
20	D	201	DMU	2	0
22	N	616	PGV	2	0
19	C	314	LFA	3	0
20	O	304	DMU	1	0
19	P	307	LFA	1	0
20	P	322	DMU	2	0
19	O	302	LFA	3	0
14	N	601	HEA	2	0
19	O	303	LFA	1	0
19	C	313	LFA	1	0
24	P	305	CHD	3	0
19	C	307	LFA	3	0
26	I	101	CDL	3	0
20	T	105	DMU	1	0

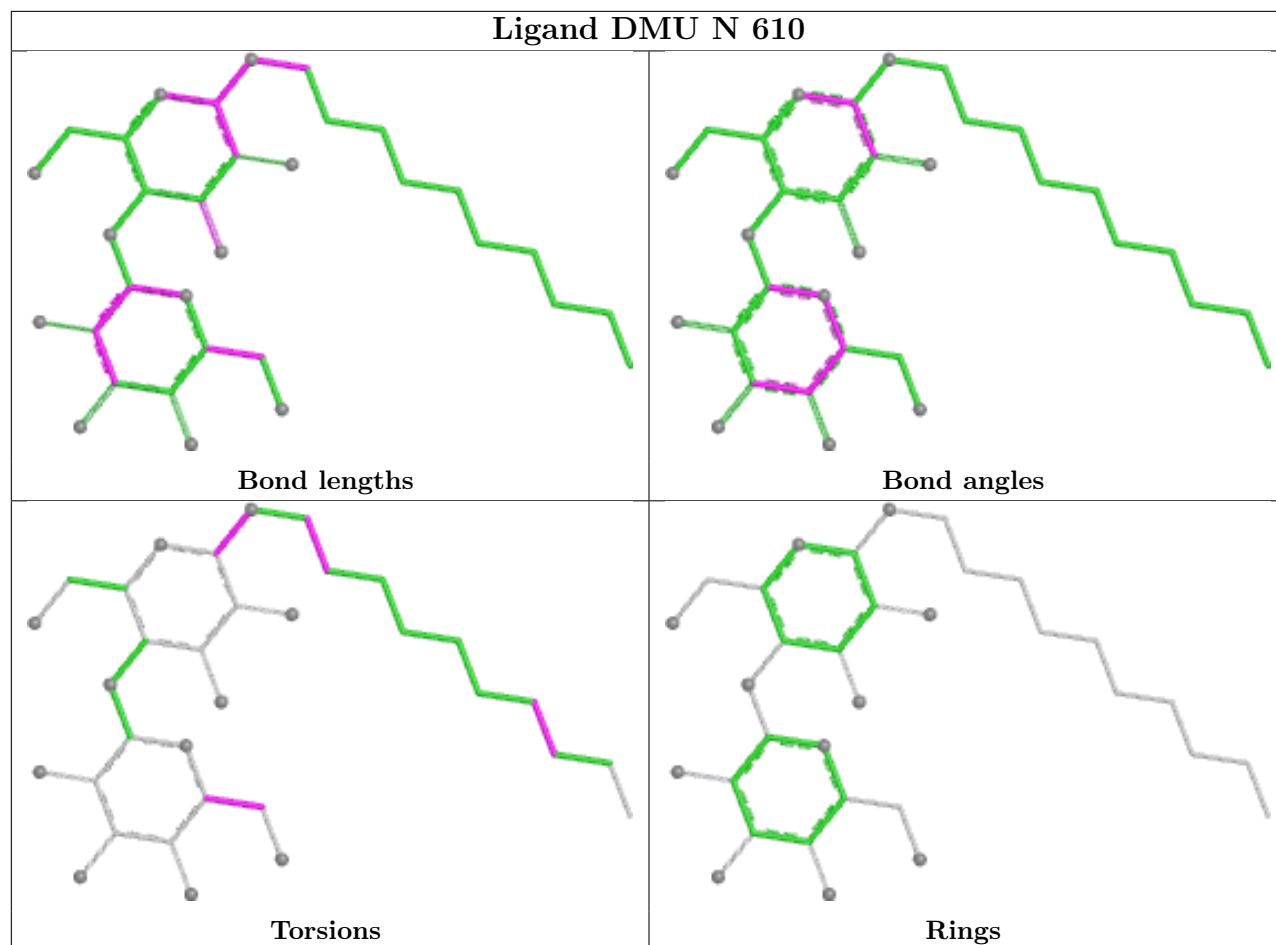
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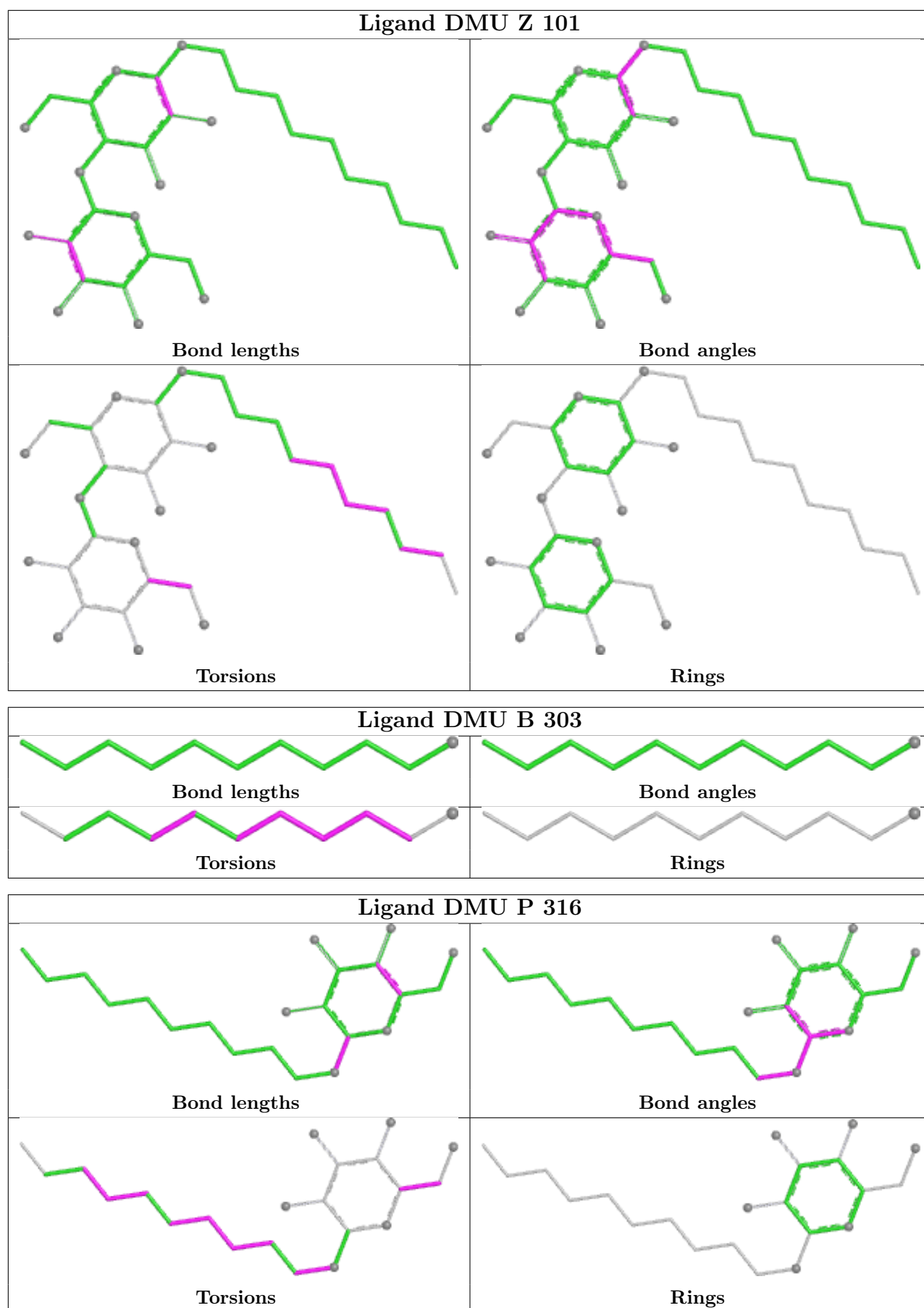
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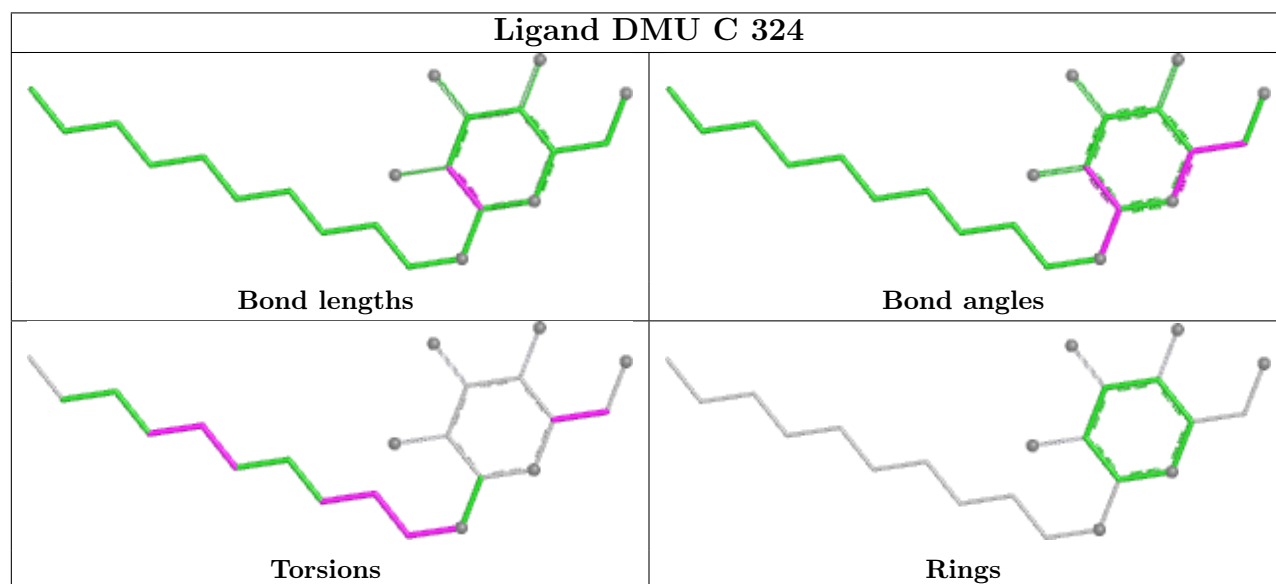
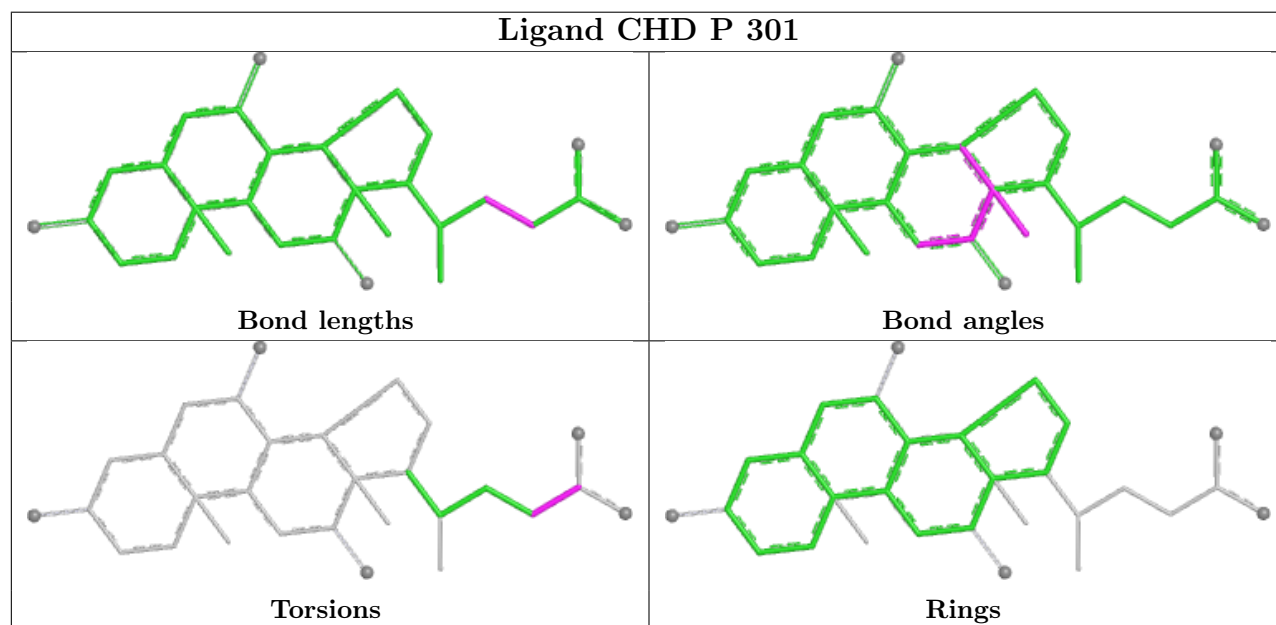
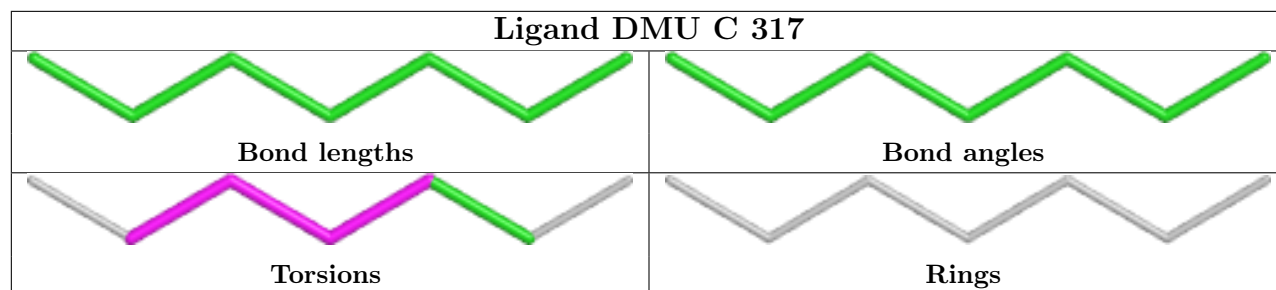
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	P	304	CDL	16	0
19	G	104	LFA	5	0
20	A	608	DMU	1	0
20	H	101	DMU	1	0
20	C	325	DMU	3	0
20	Q	201	DMU	3	0
20	A	609	DMU	1	0
14	A	601	HEA	4	0
19	B	307	LFA	4	0
26	N	606	CDL	6	0
19	A	607	LFA	7	0
20	Z	102	DMU	3	0
14	A	602	HEA	2	0
20	A	615	DMU	1	0
26	C	304	CDL	24	0
19	C	315	LFA	1	0
19	N	608	LFA	5	0
19	C	309	LFA	2	0
22	C	303	PGV	2	0
19	T	101	LFA	6	0
22	P	303	PGV	1	0
19	P	309	LFA	2	0

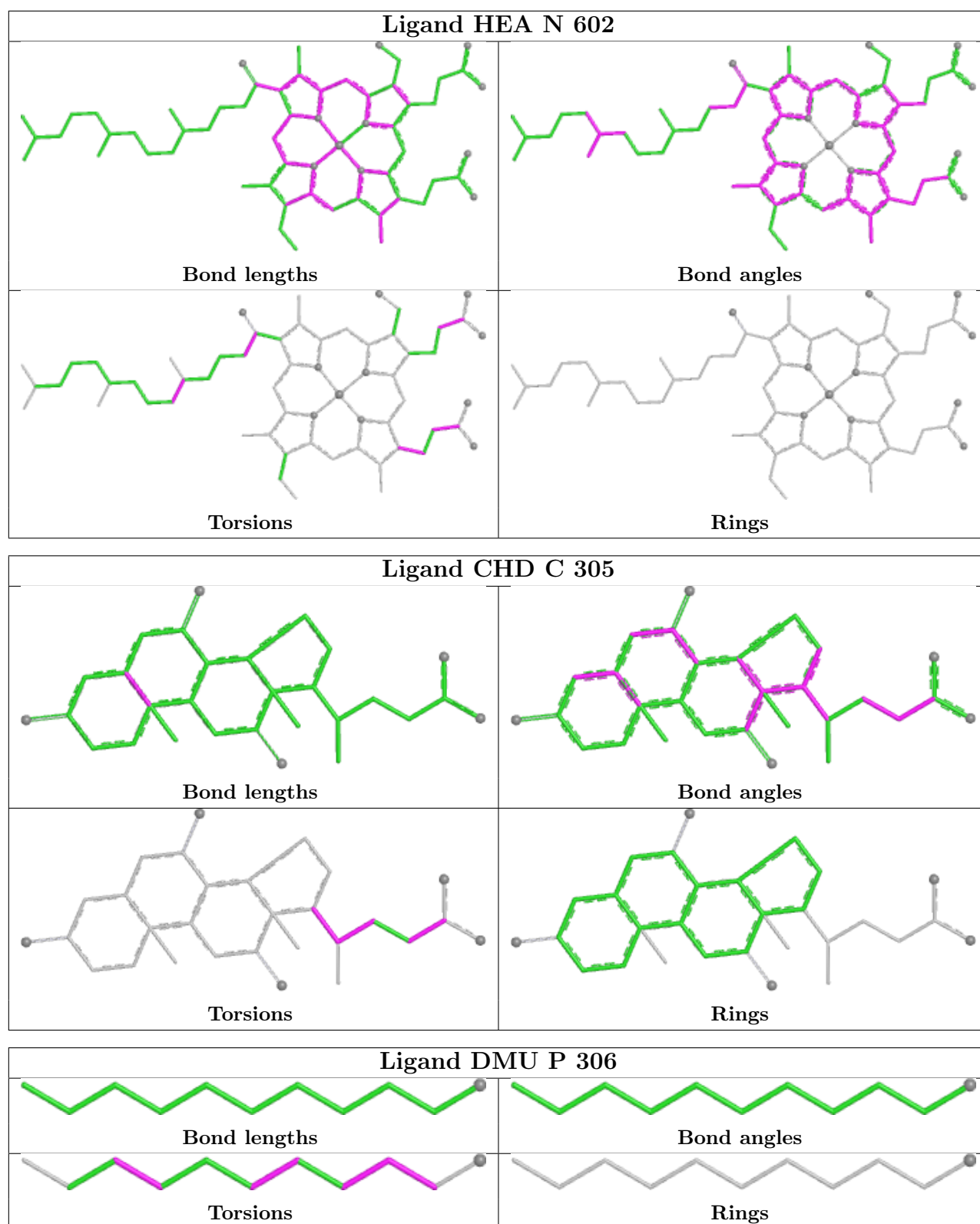
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

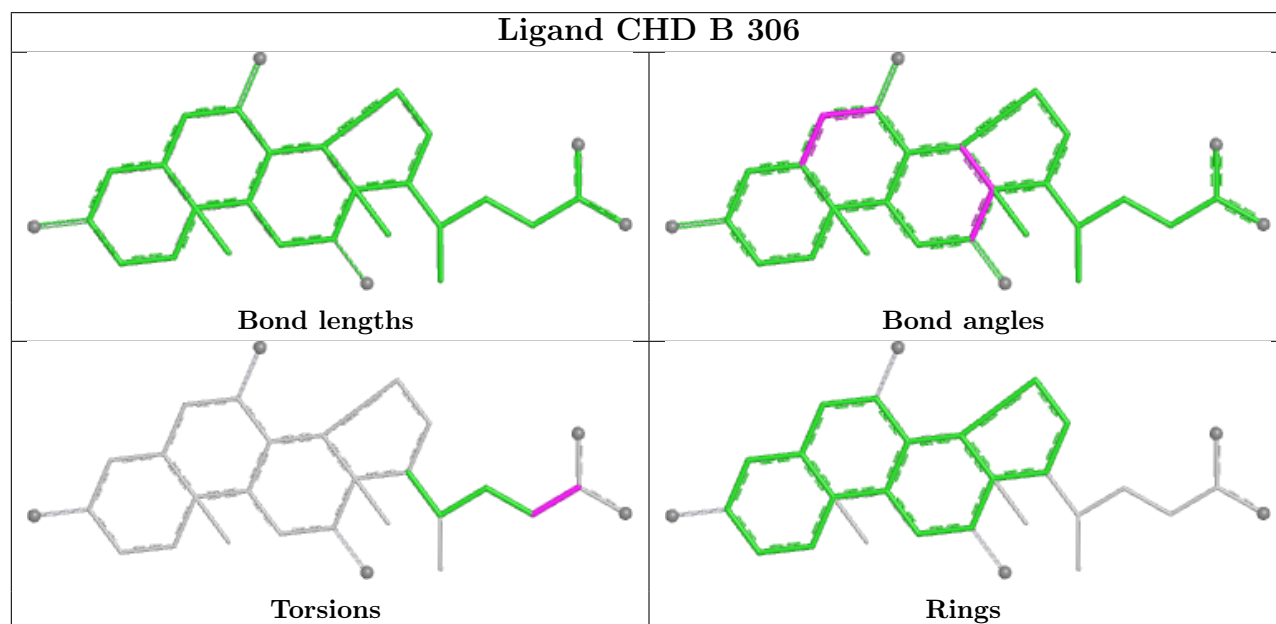
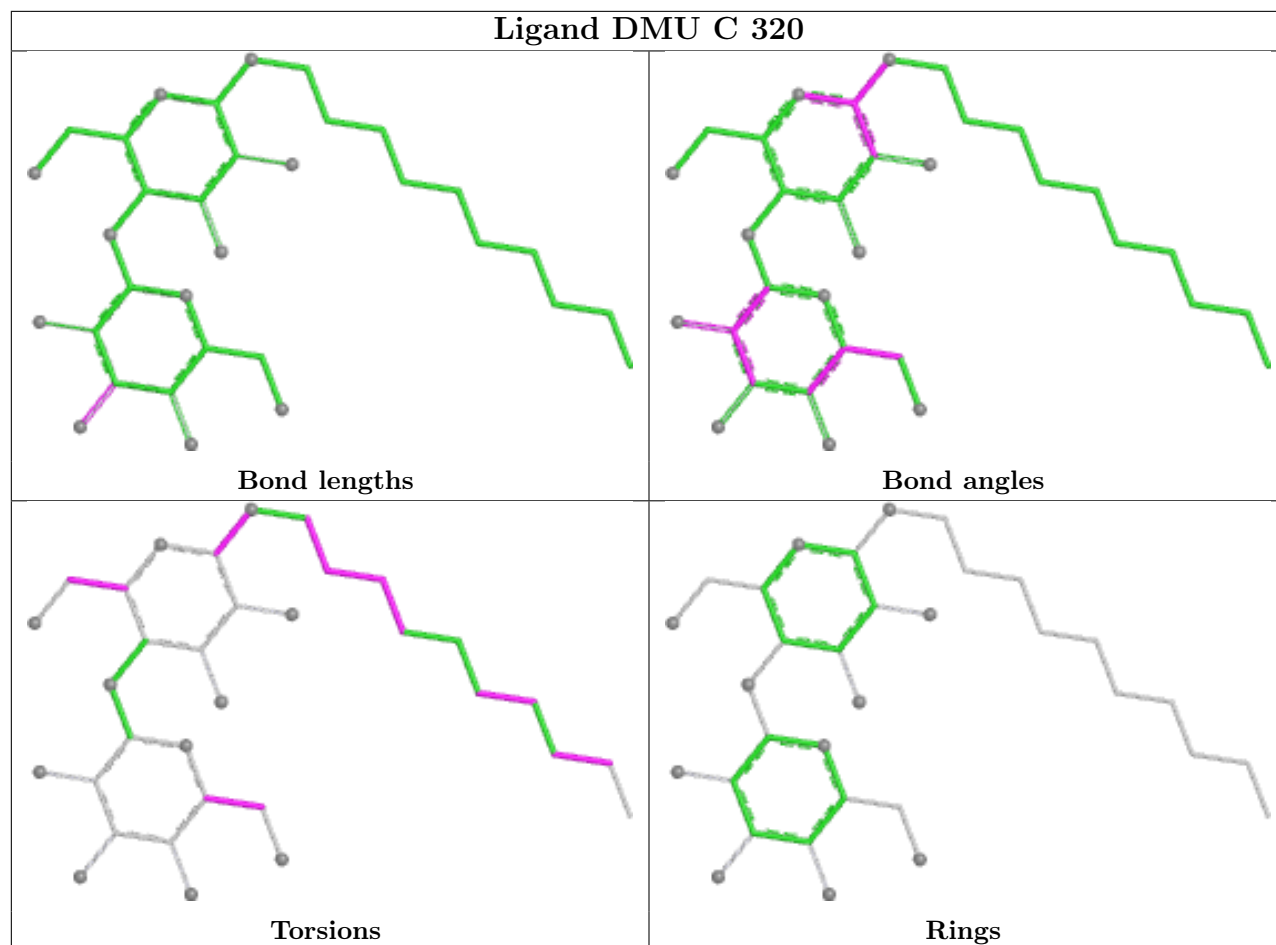


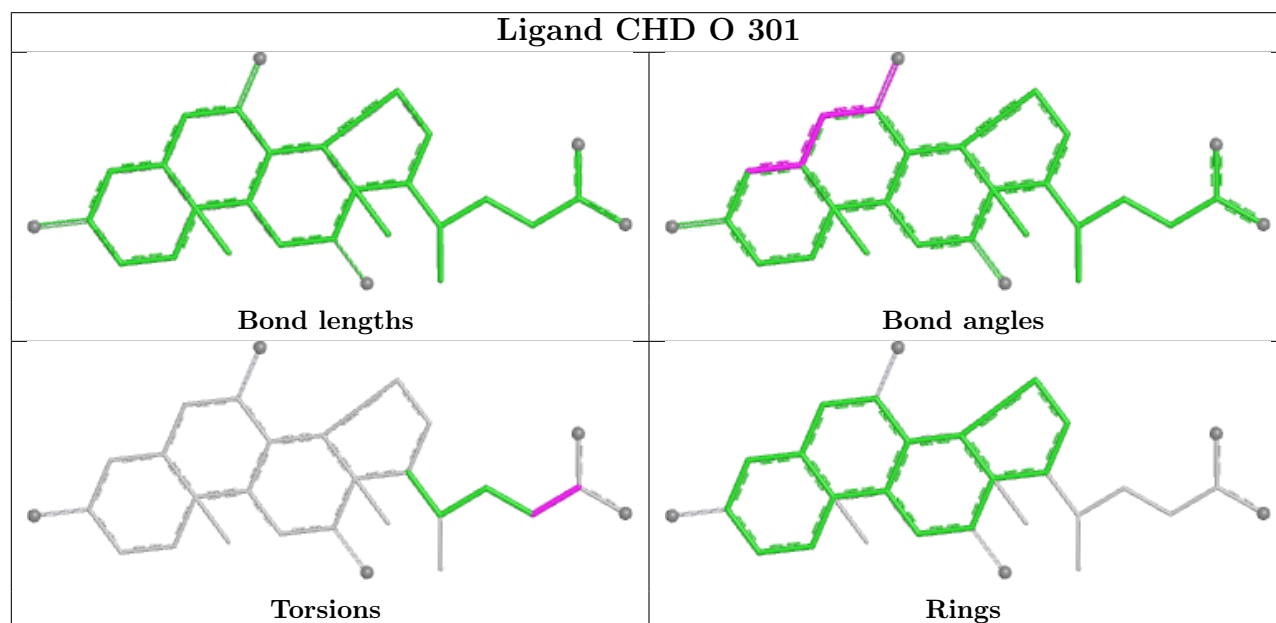
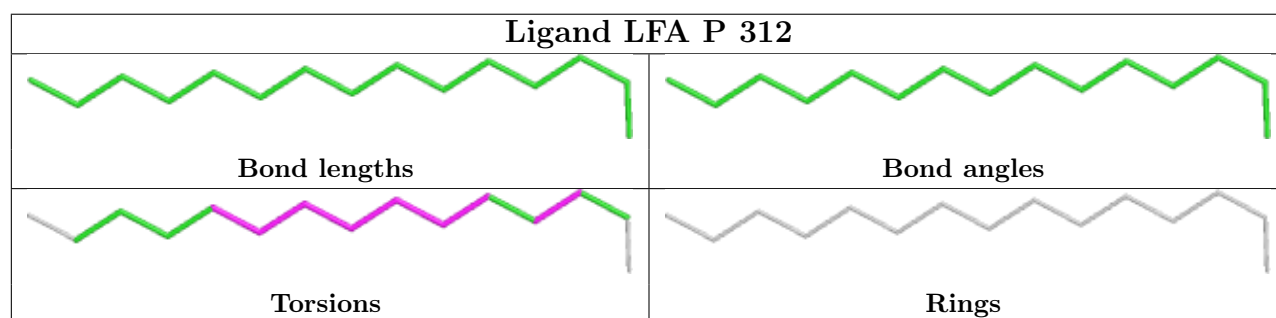
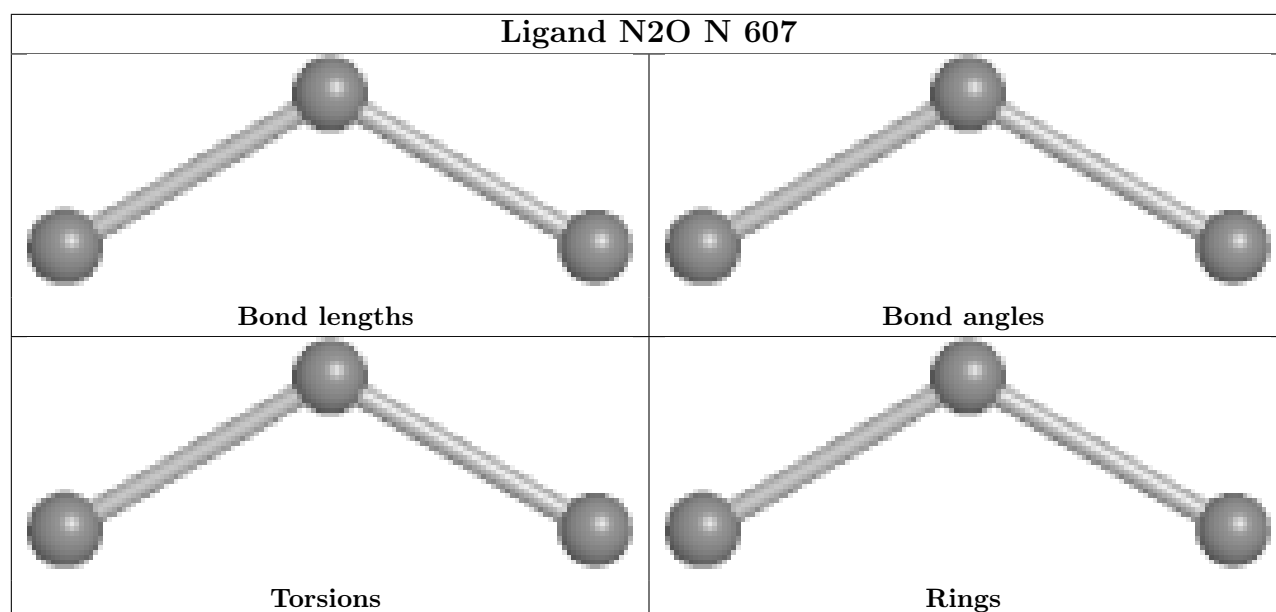


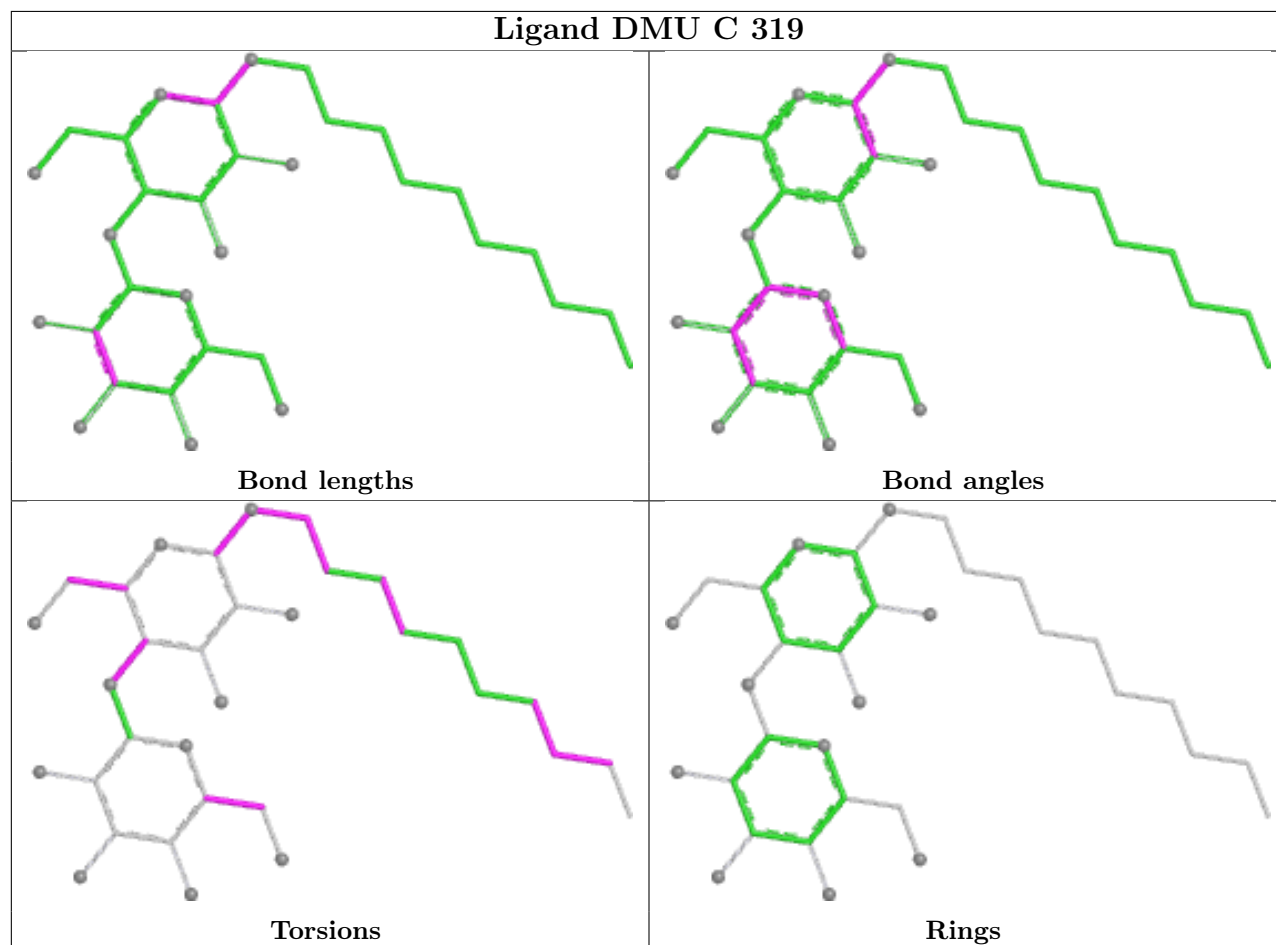
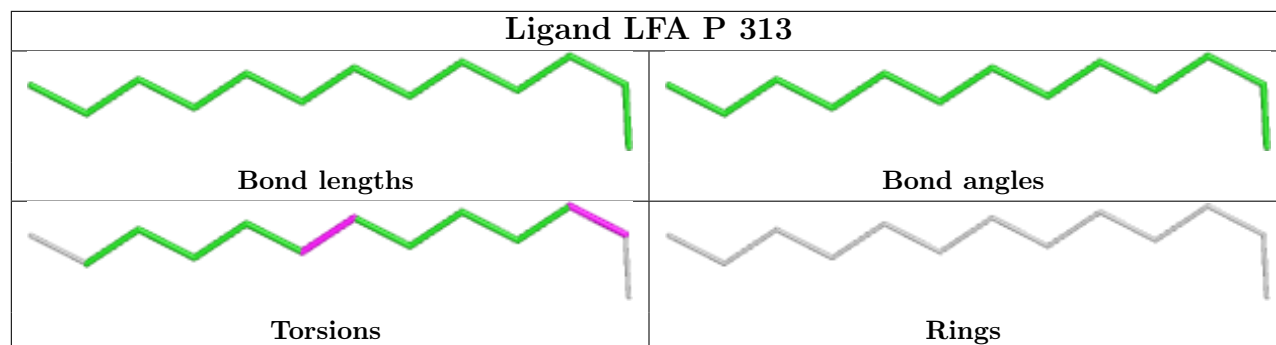


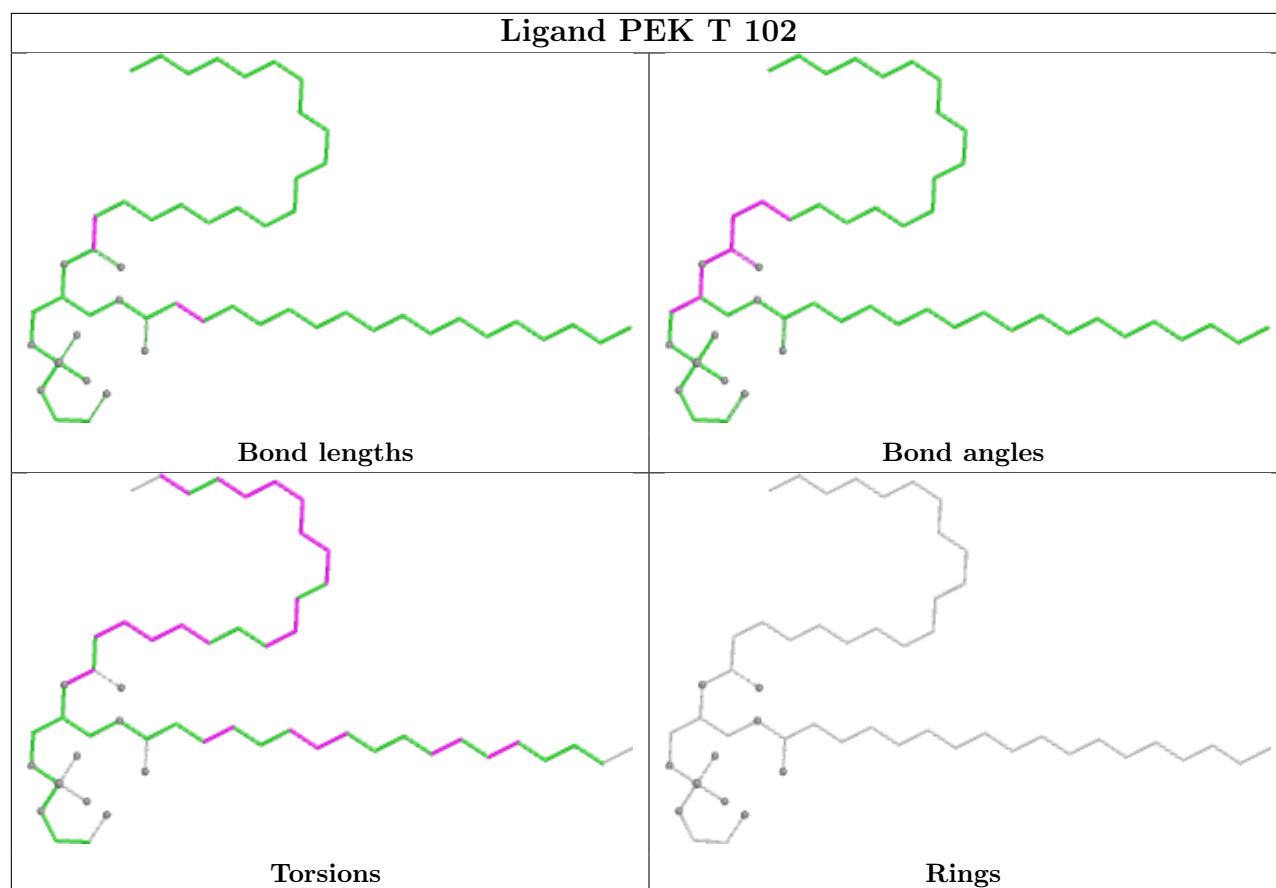
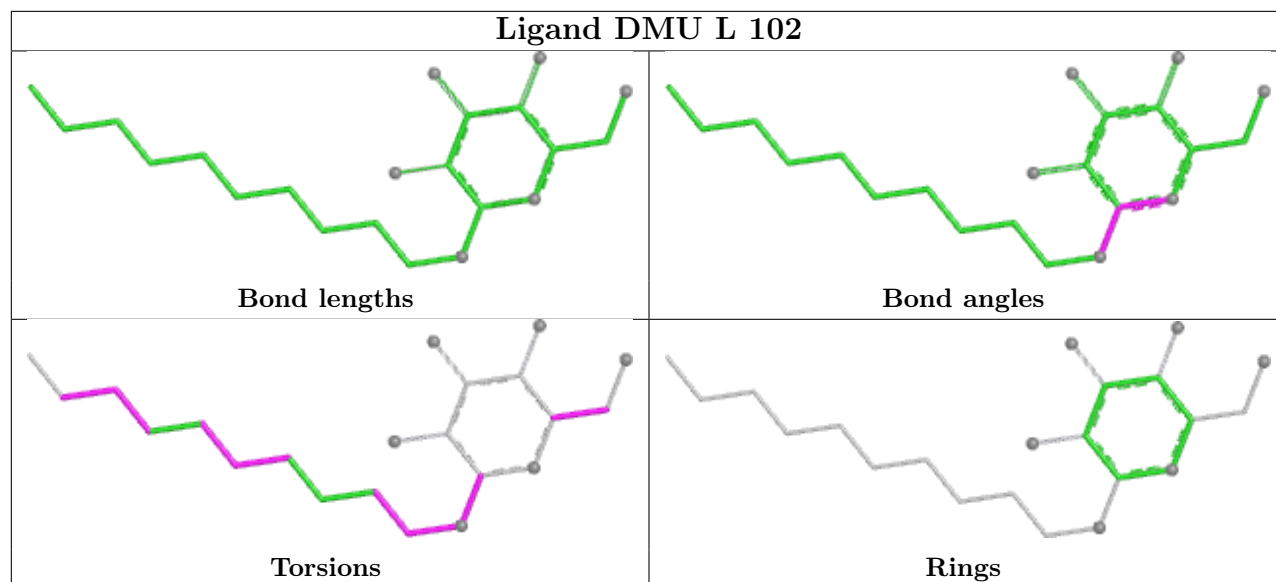


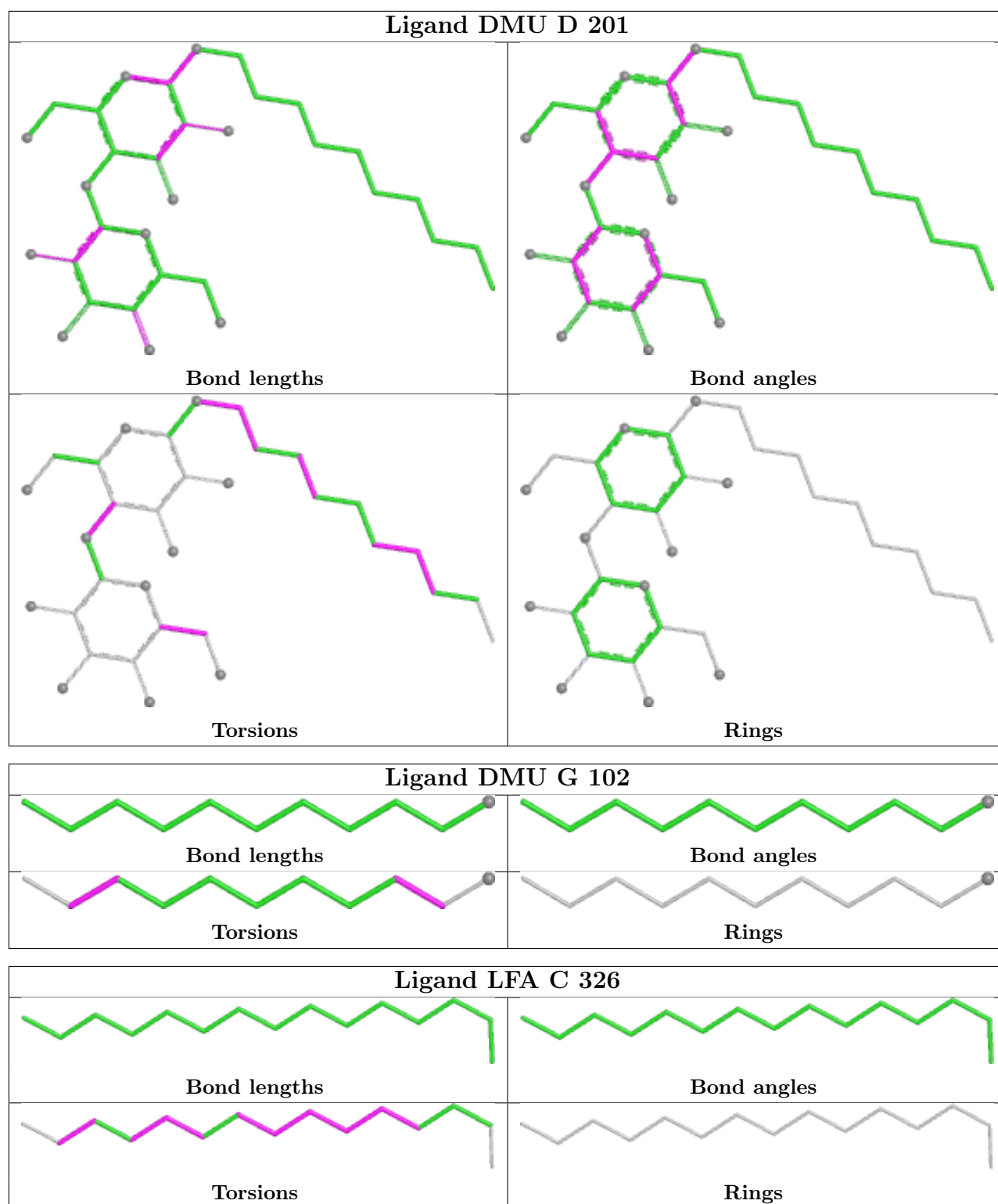


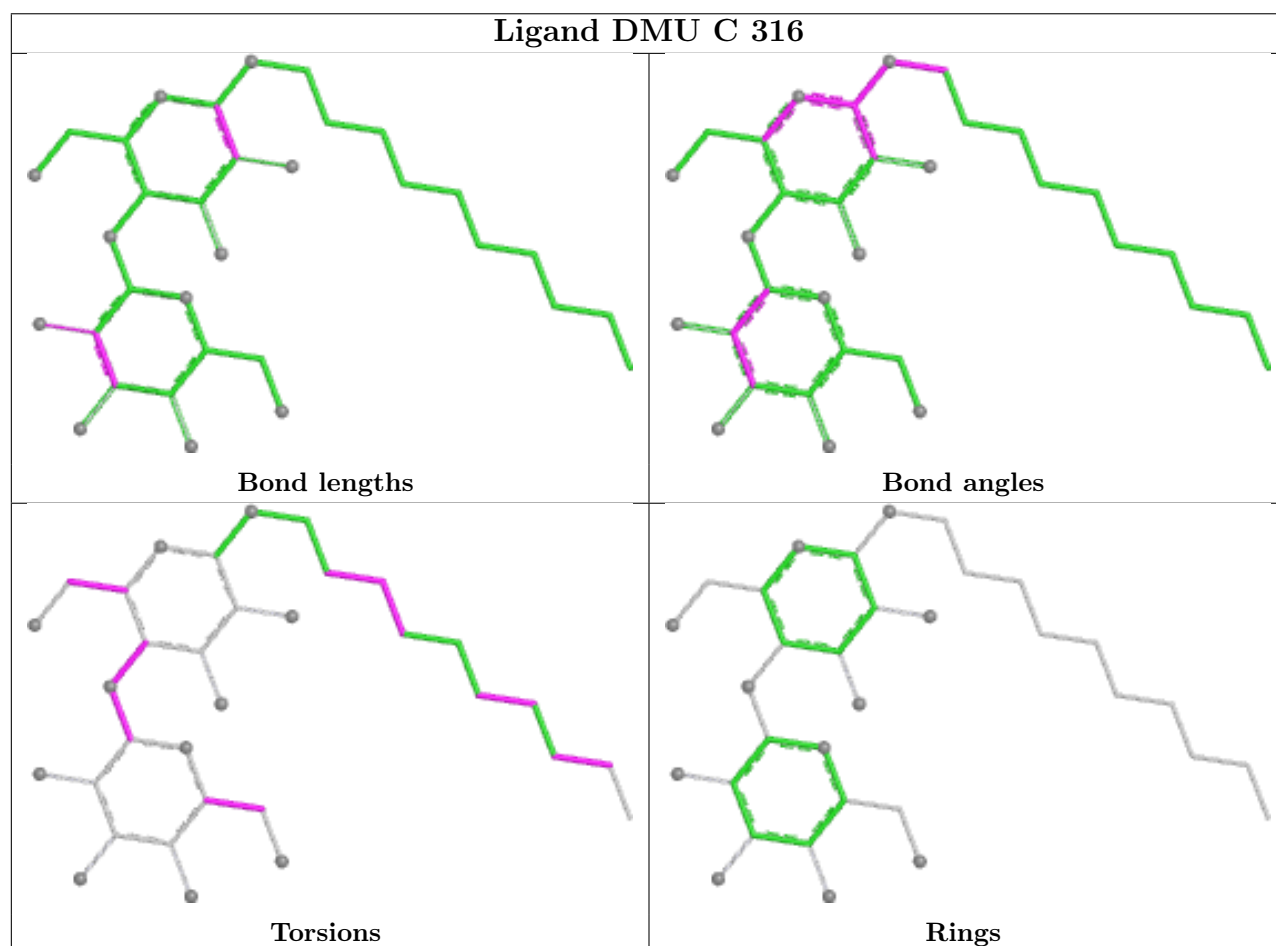
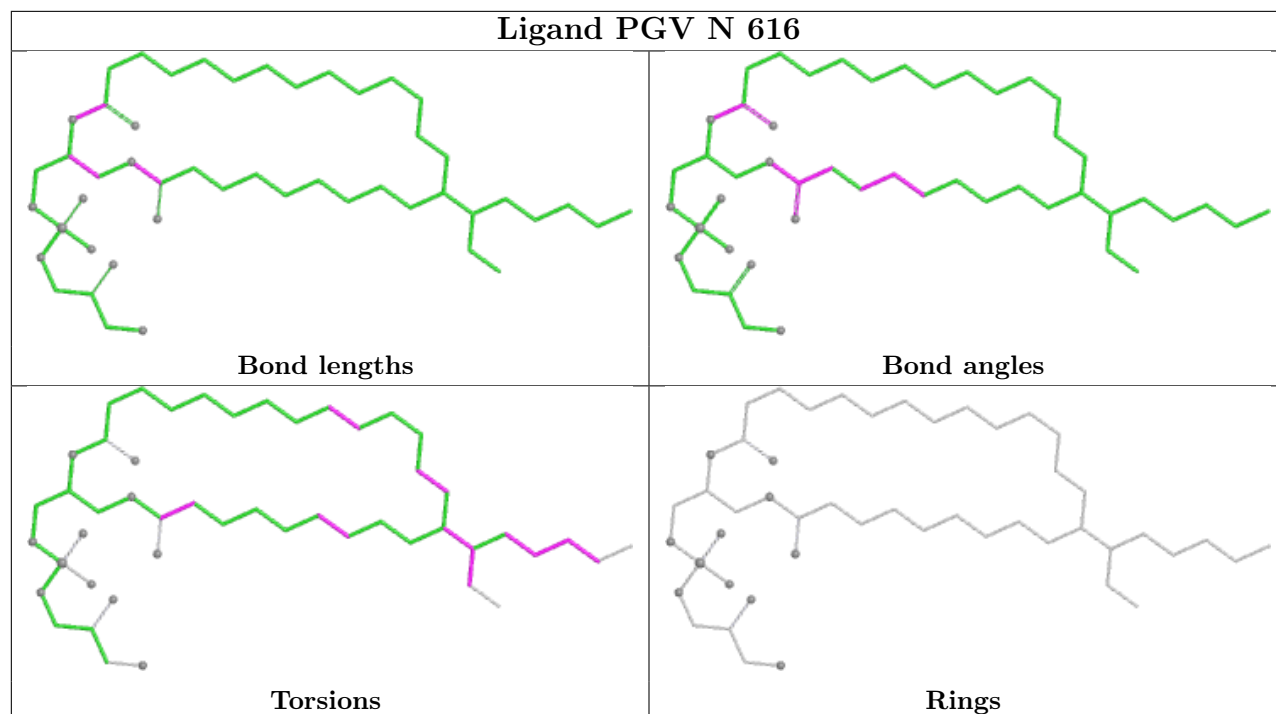


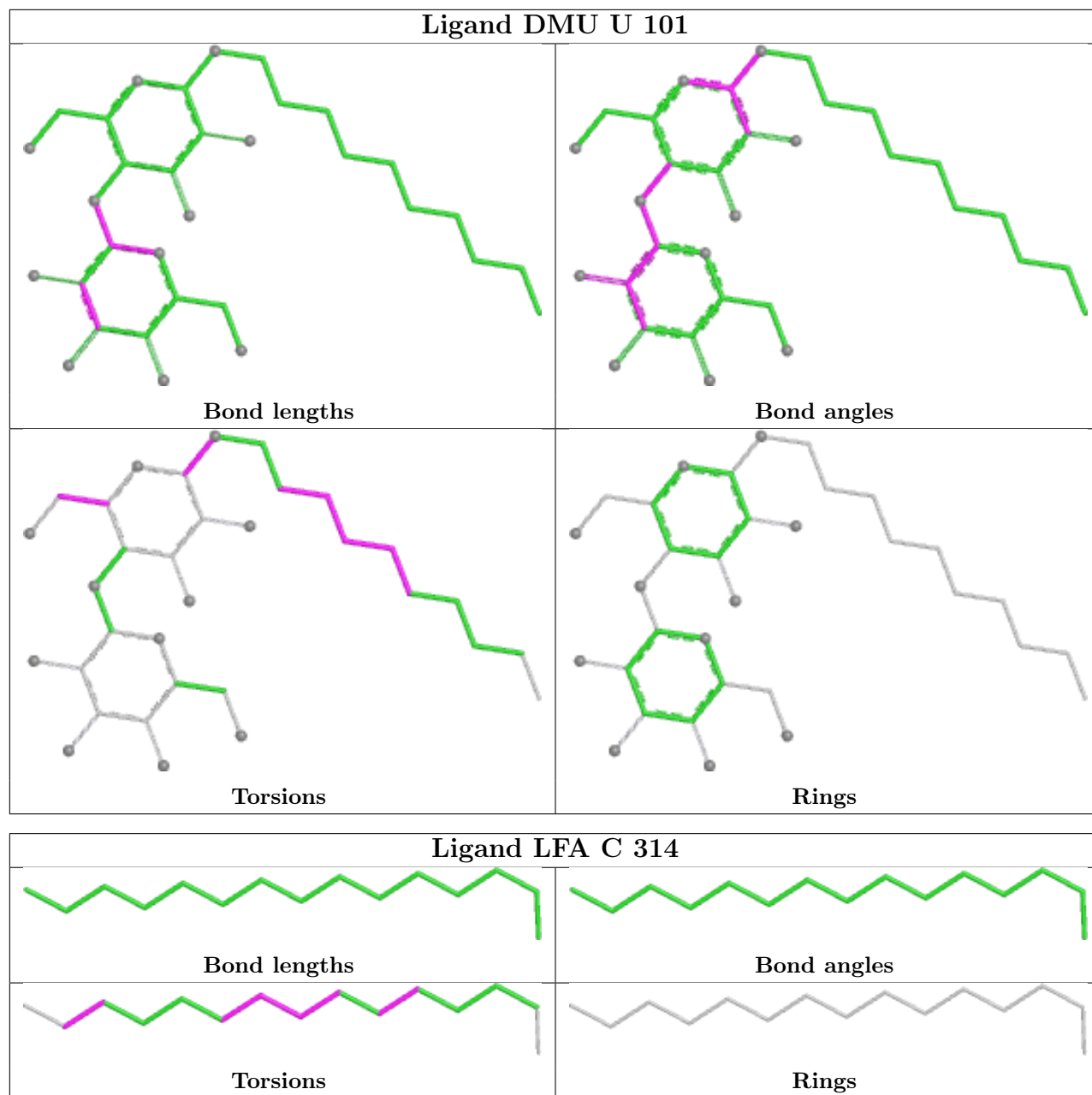


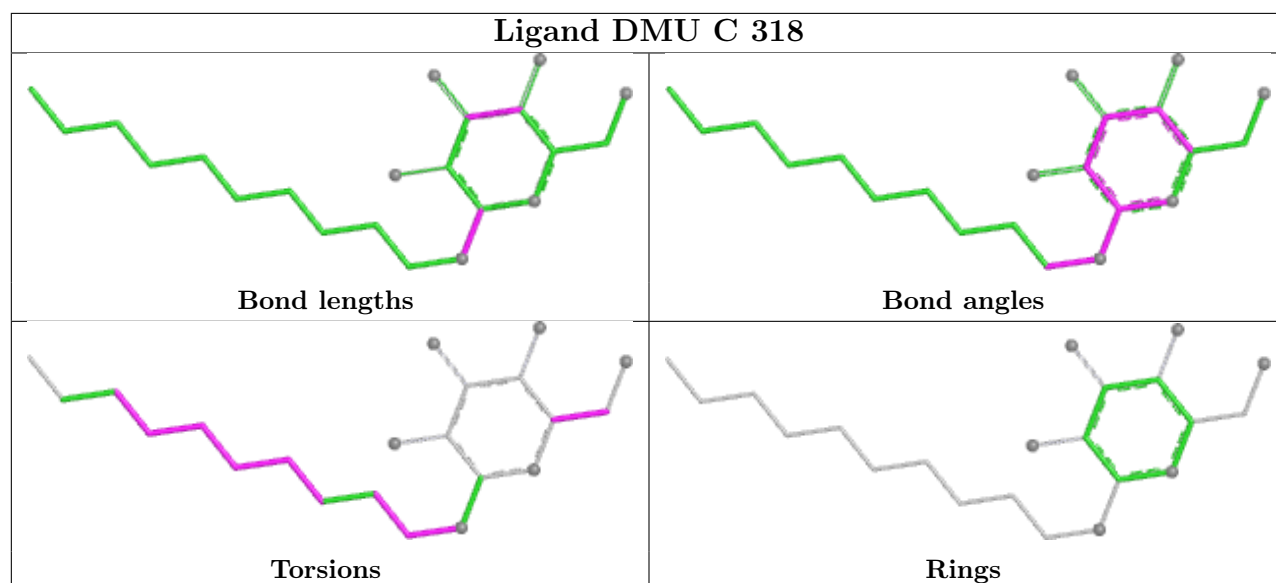
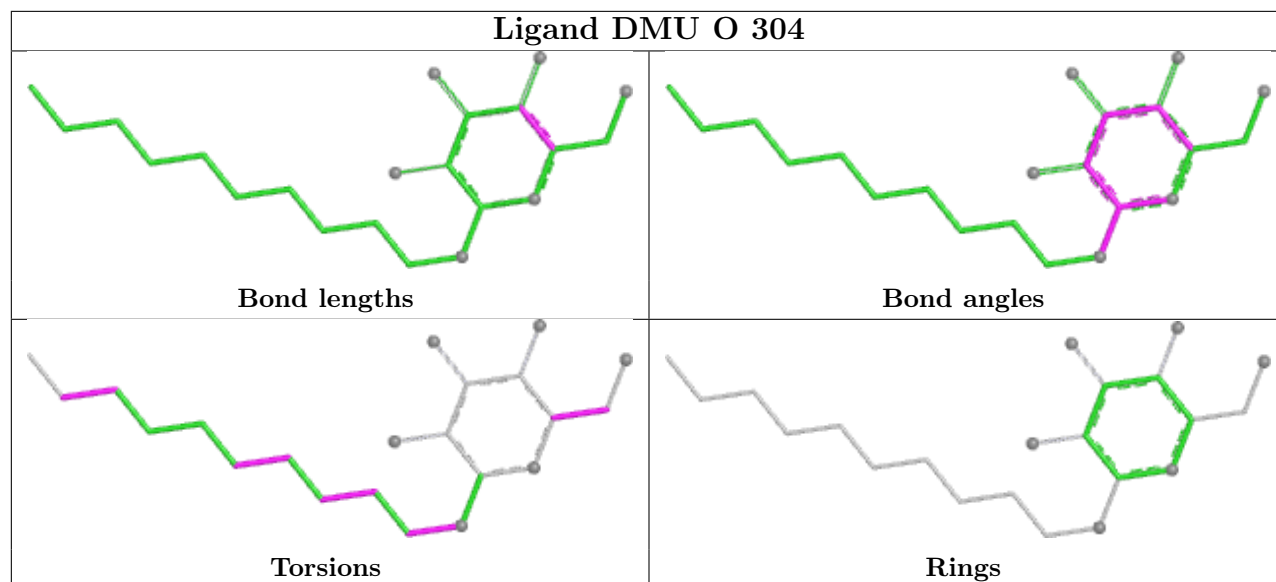


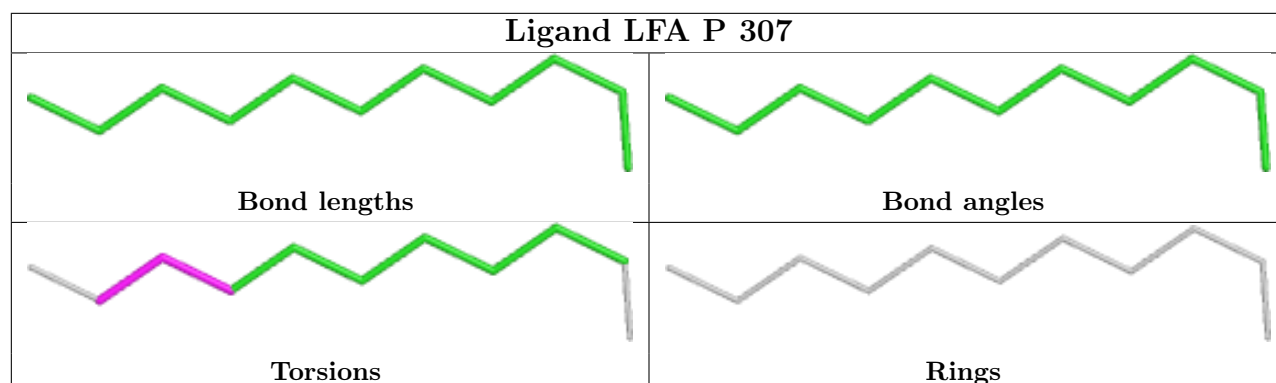
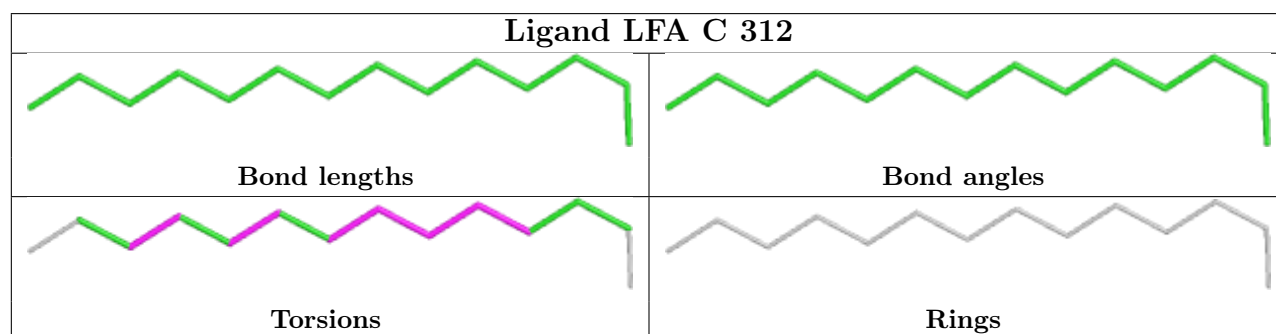
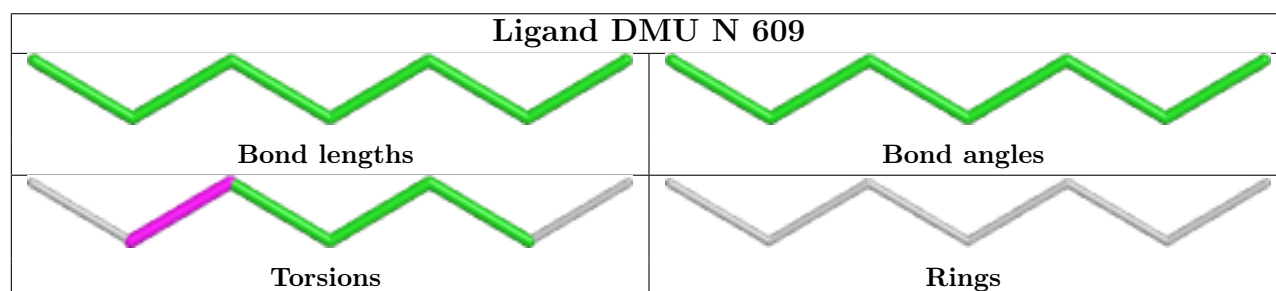
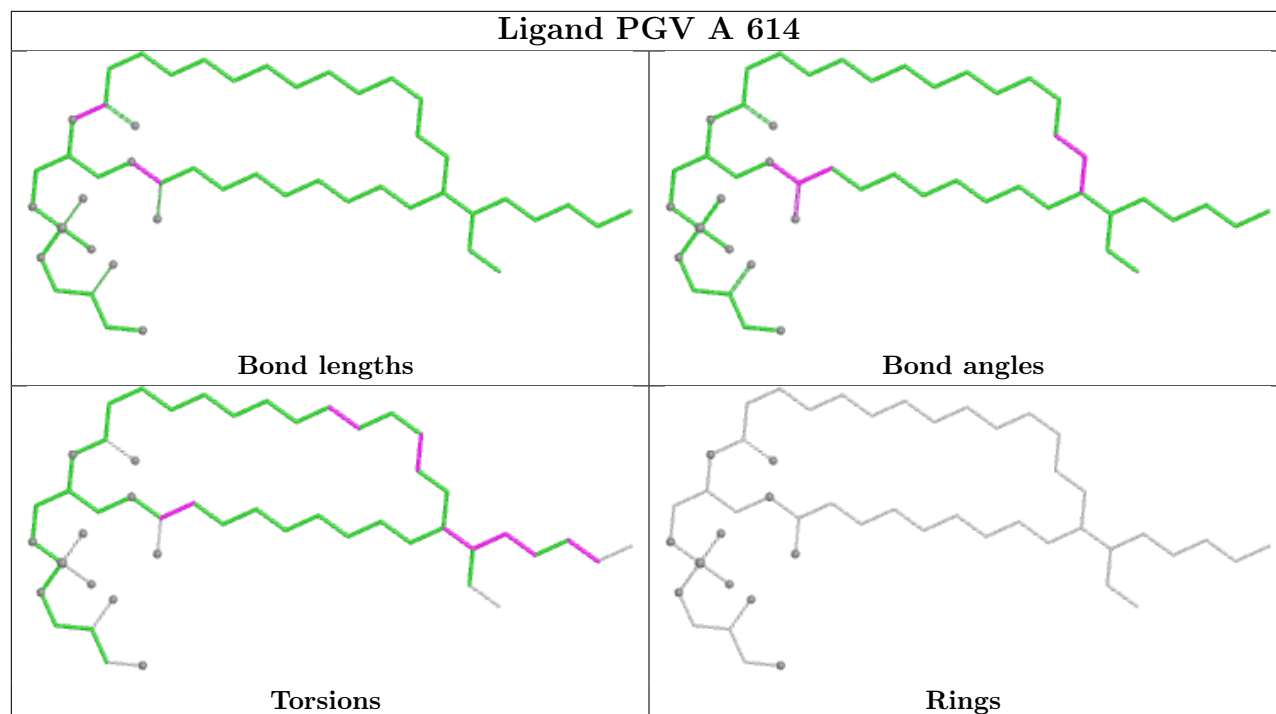


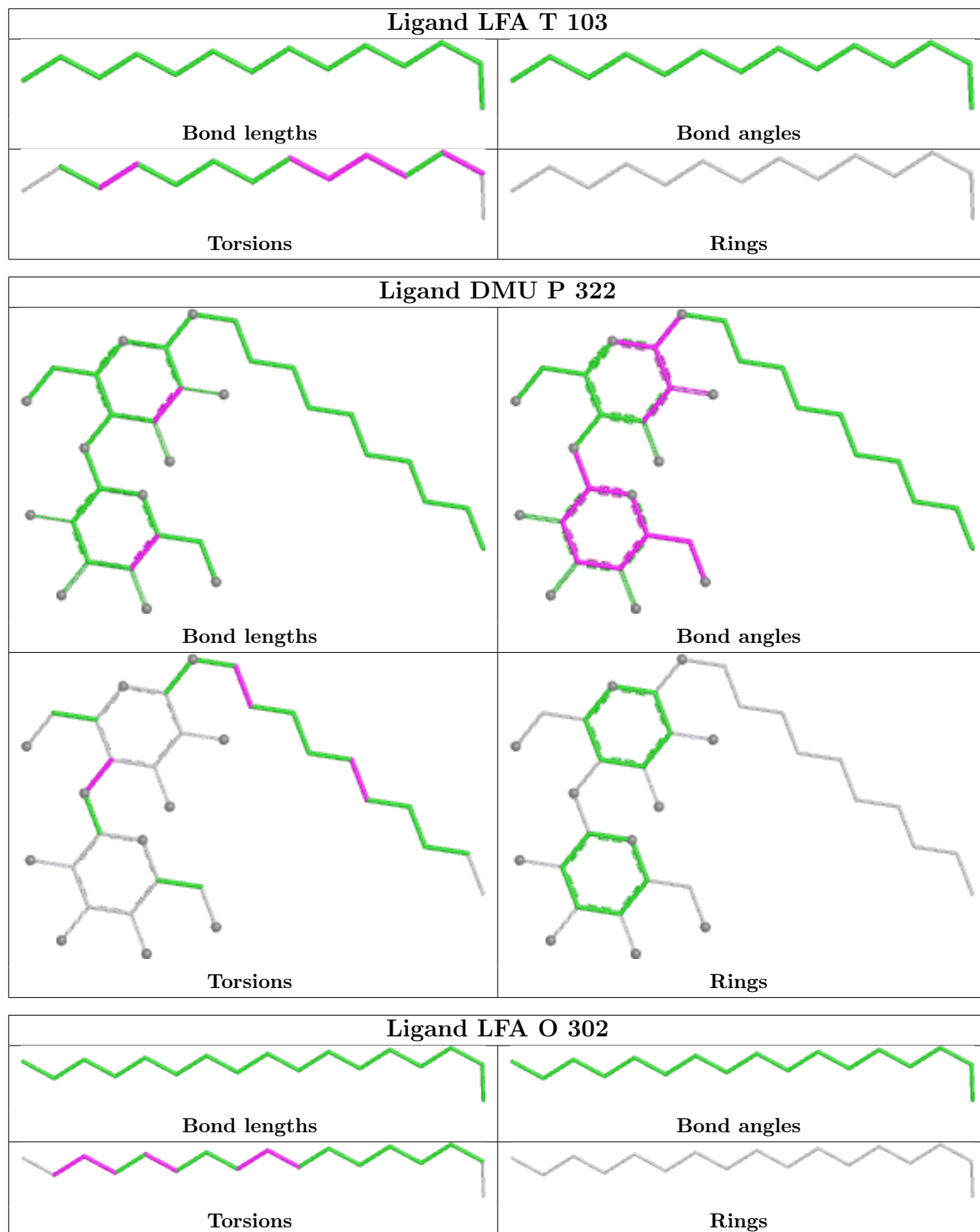


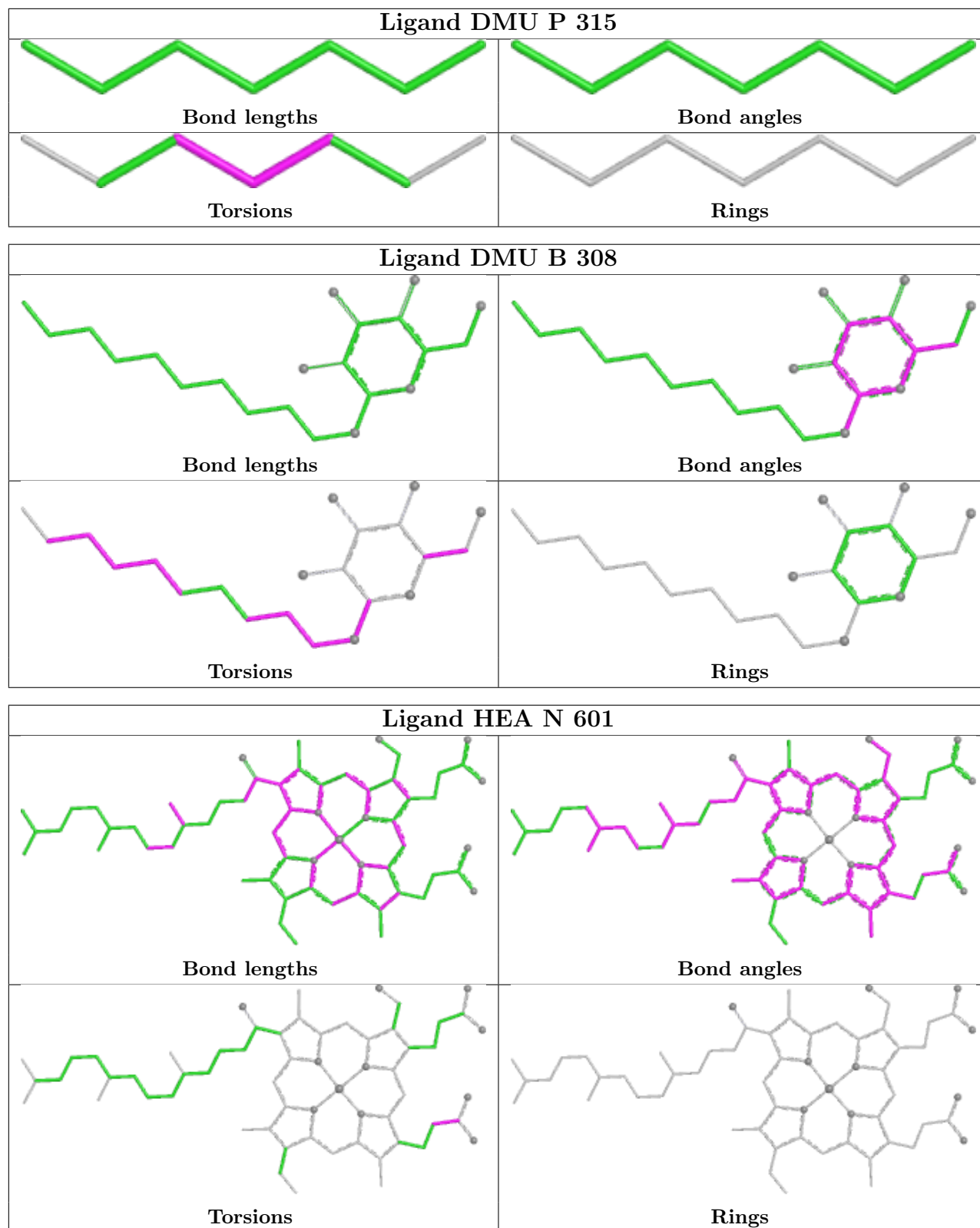


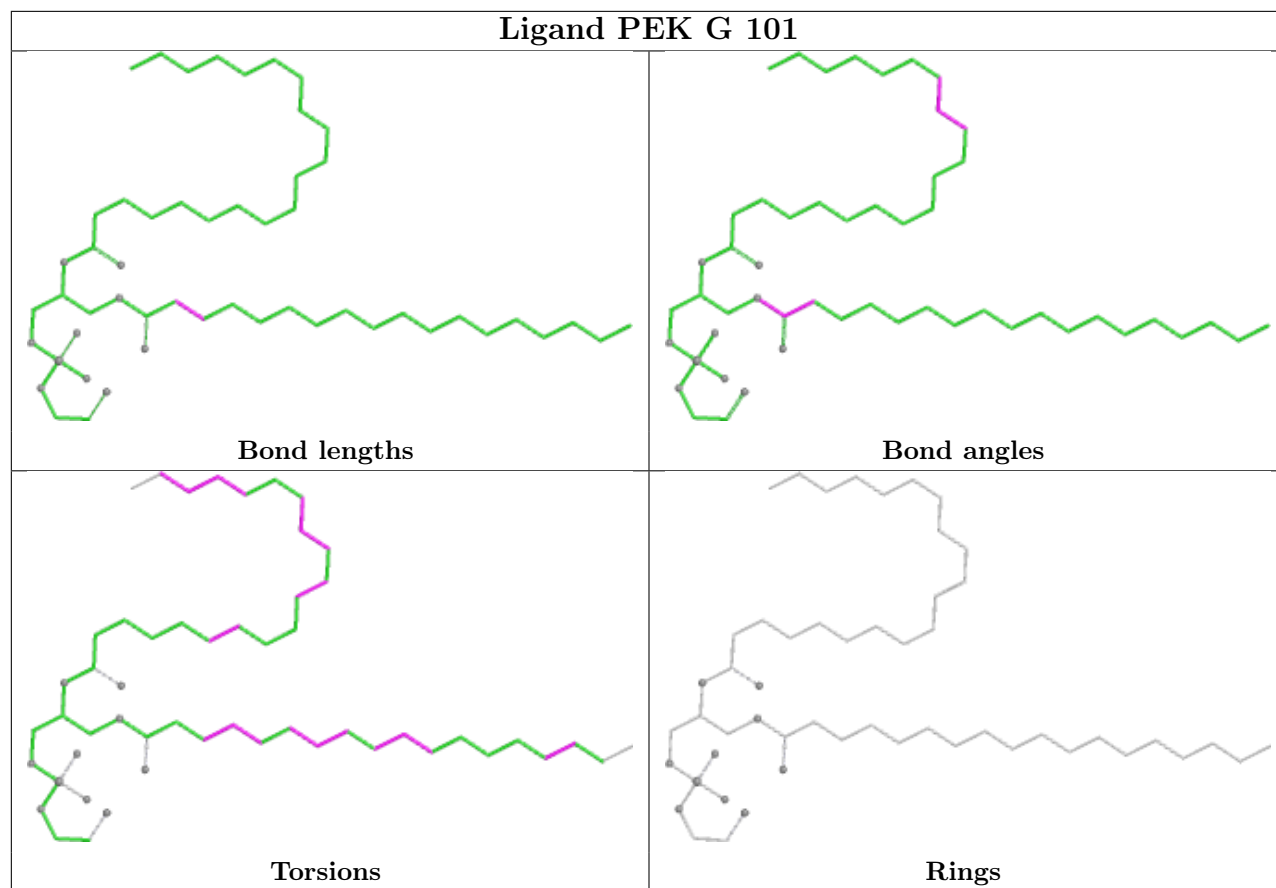


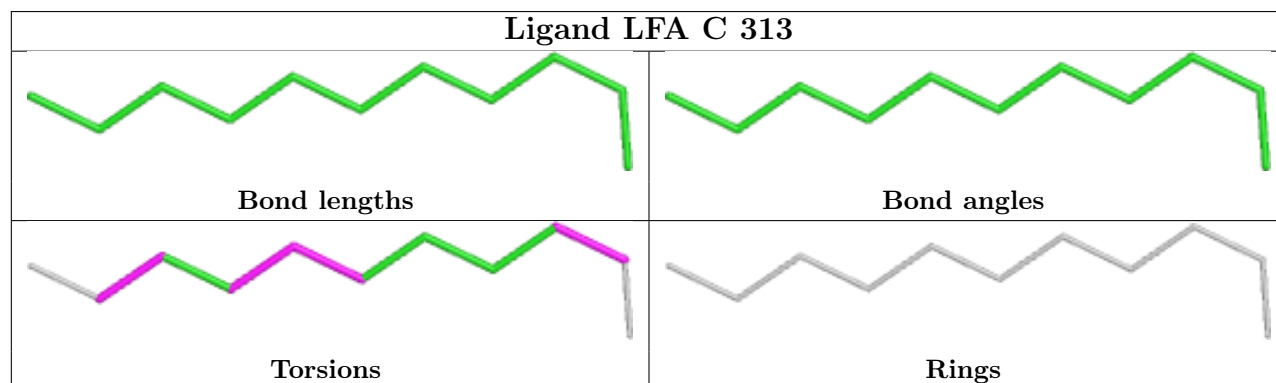
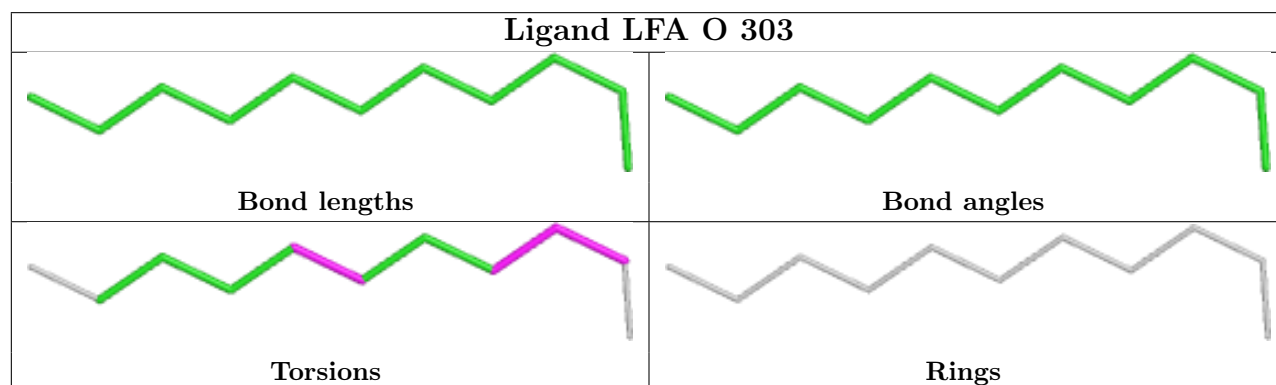
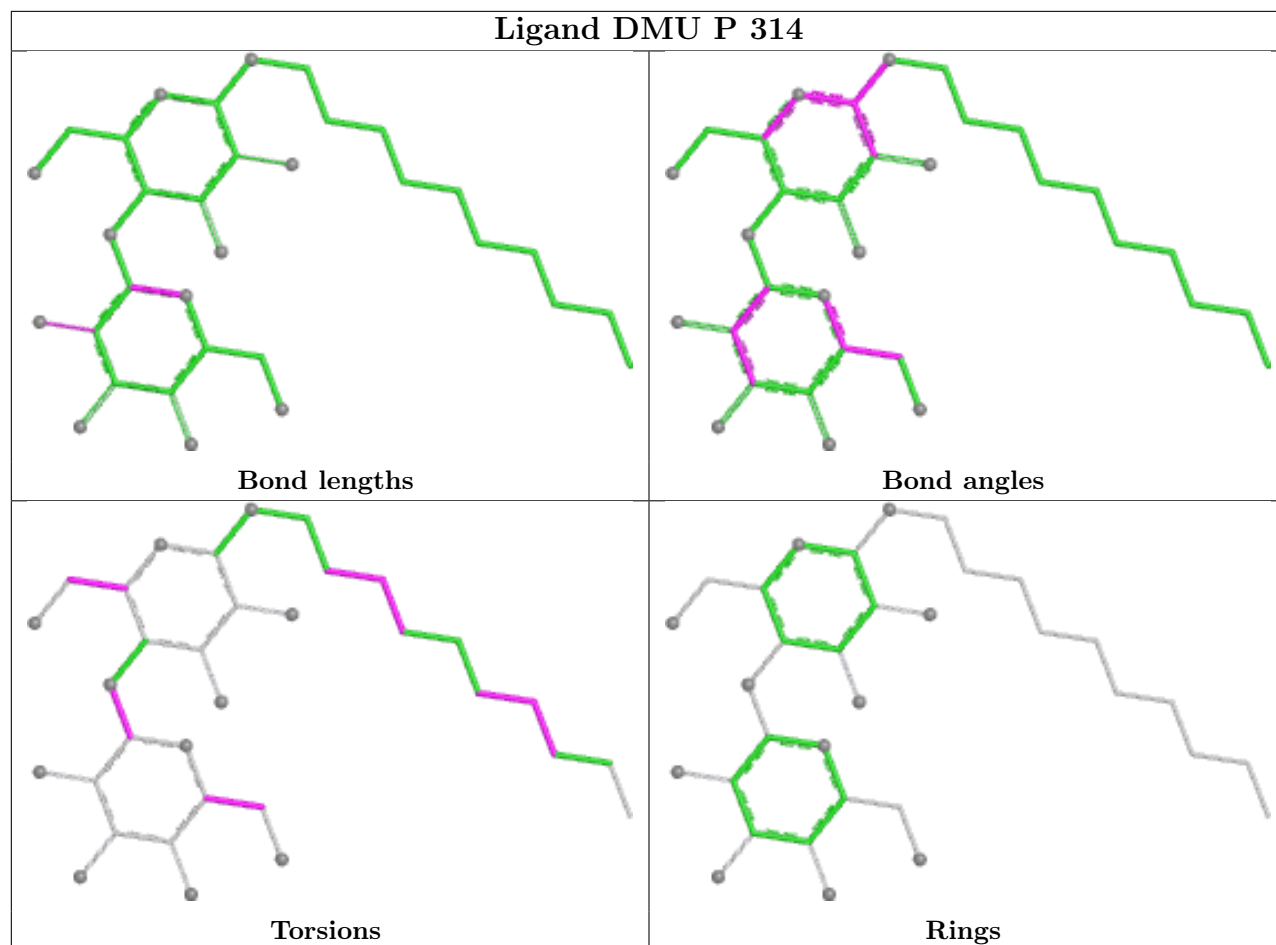


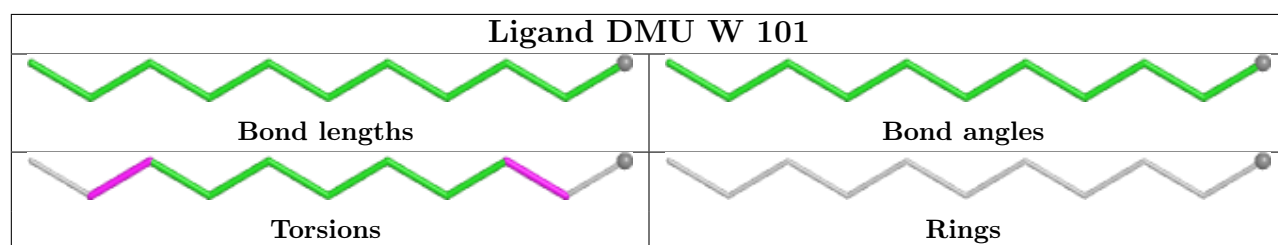
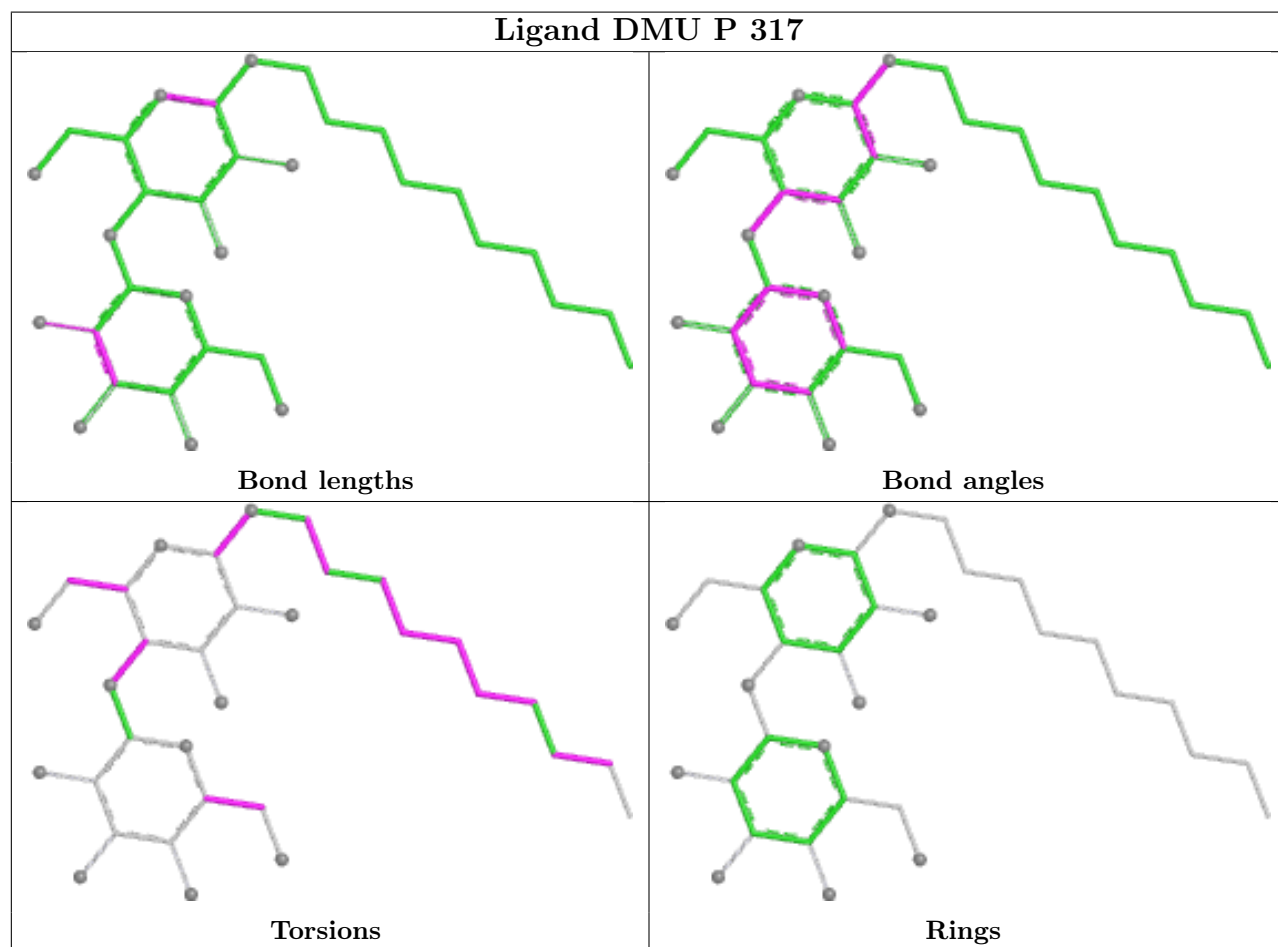
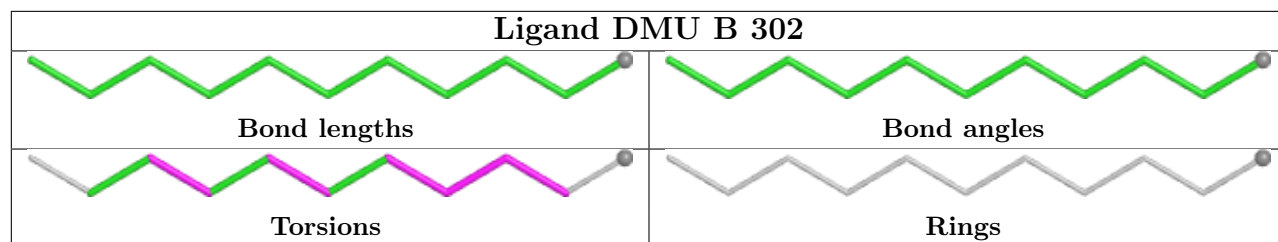


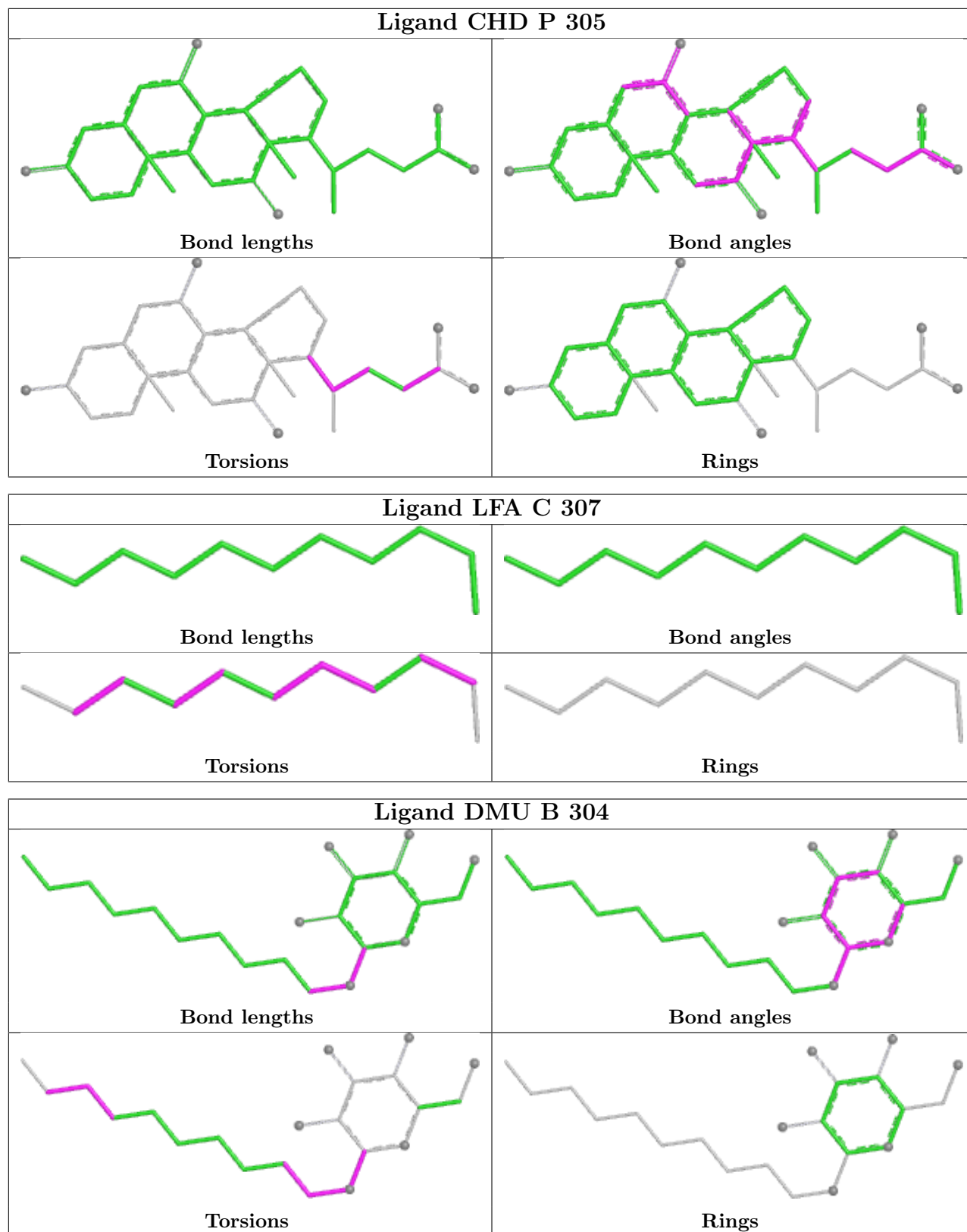


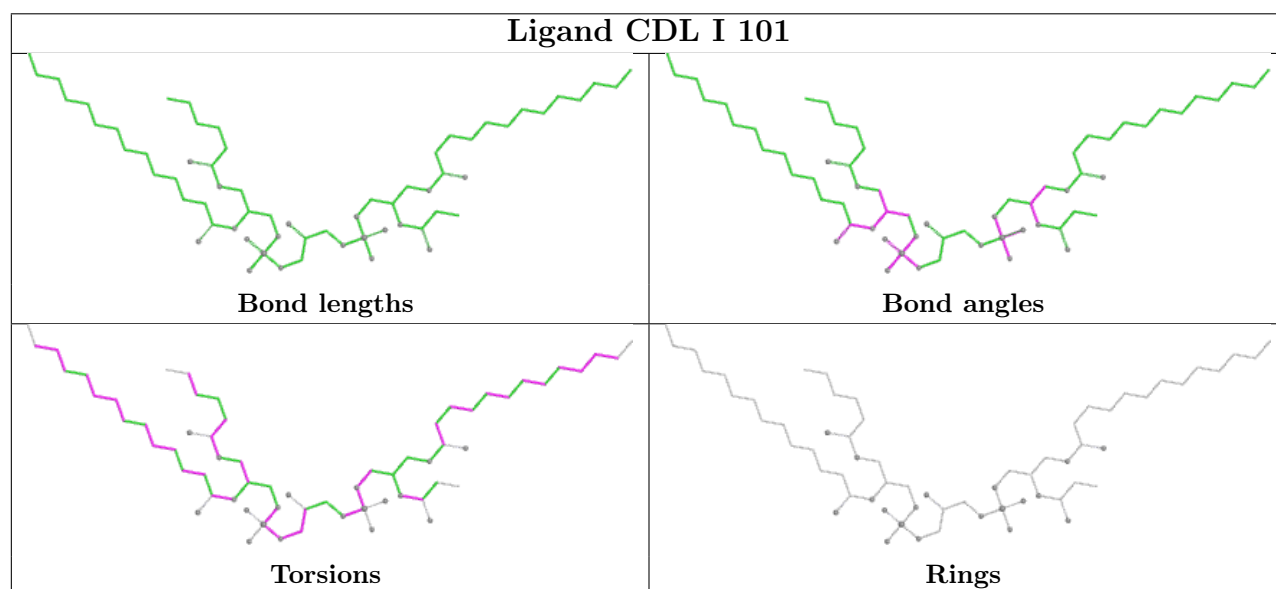
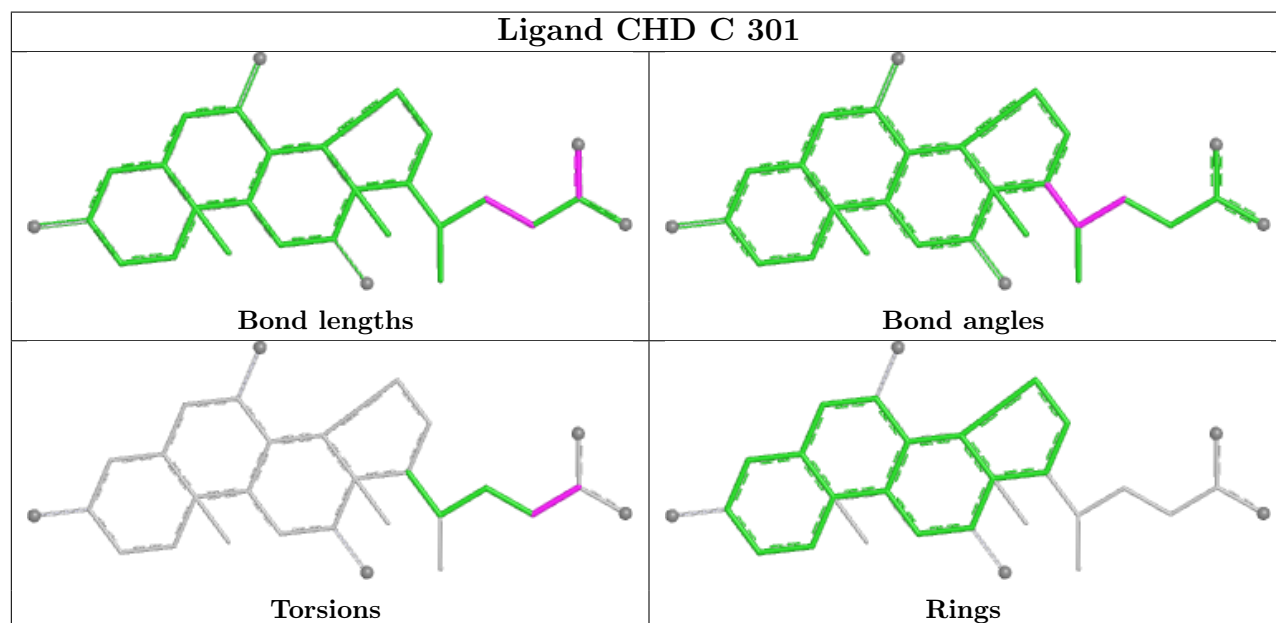
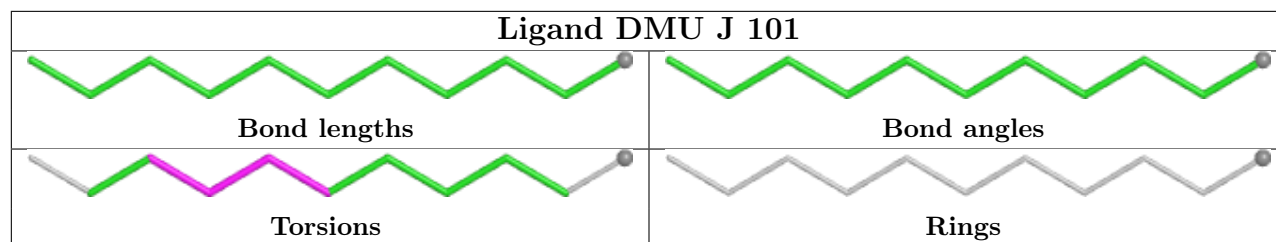


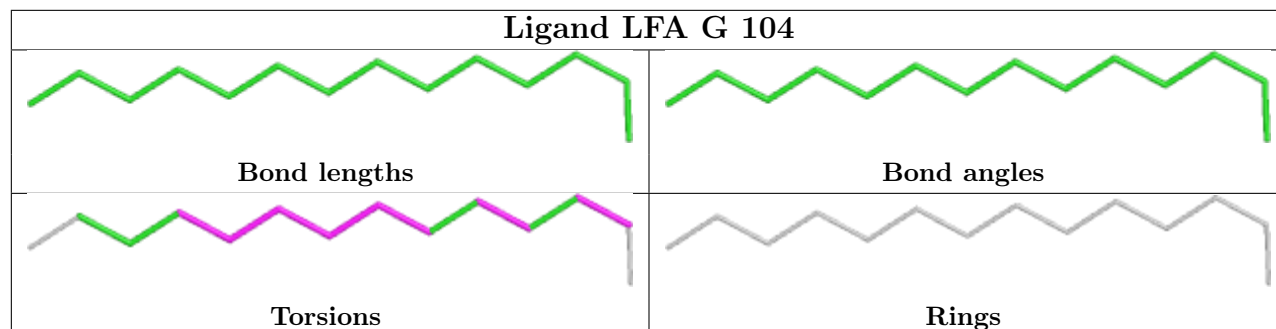
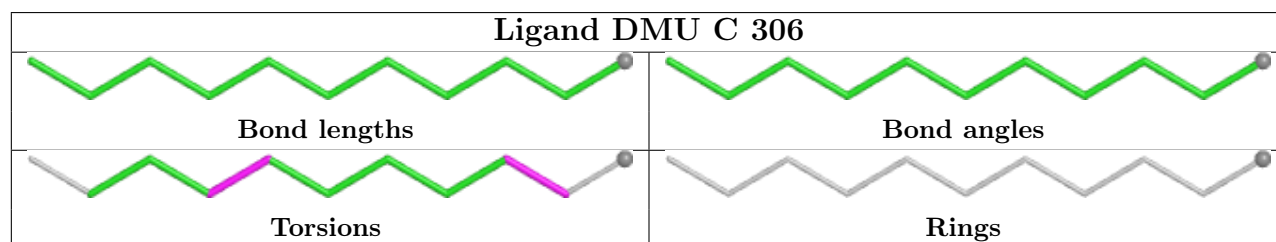
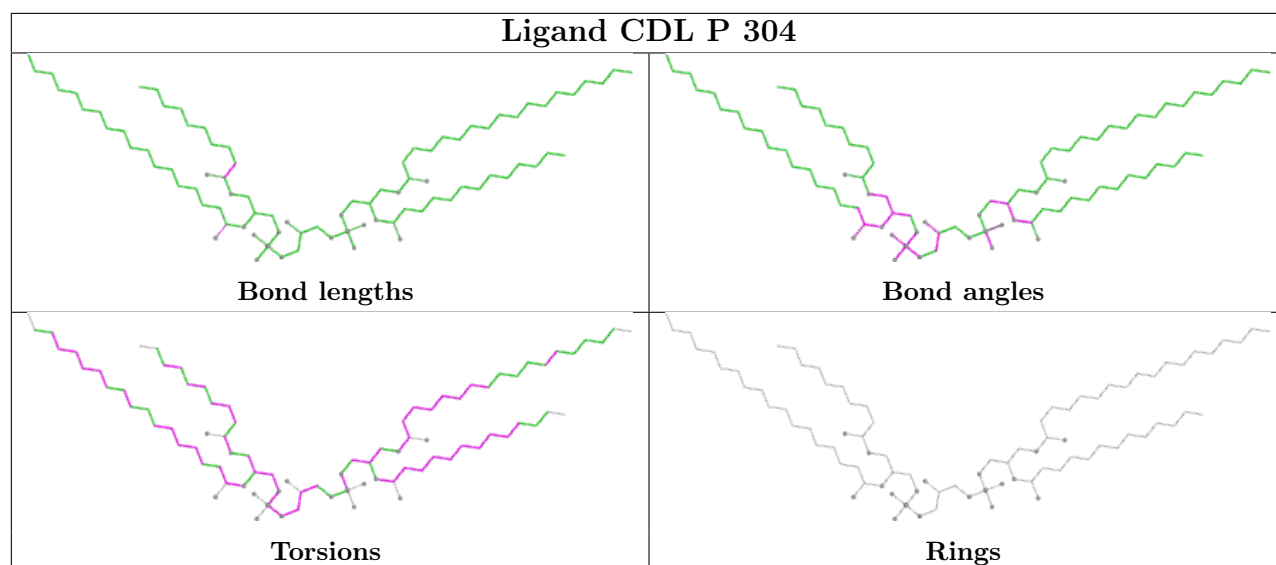
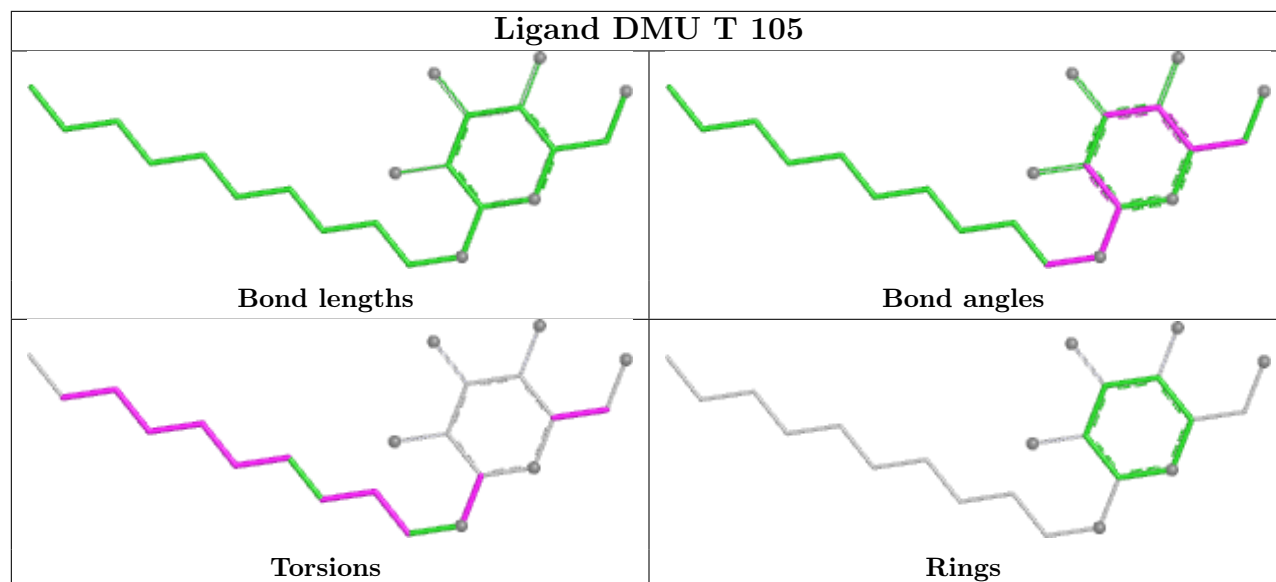


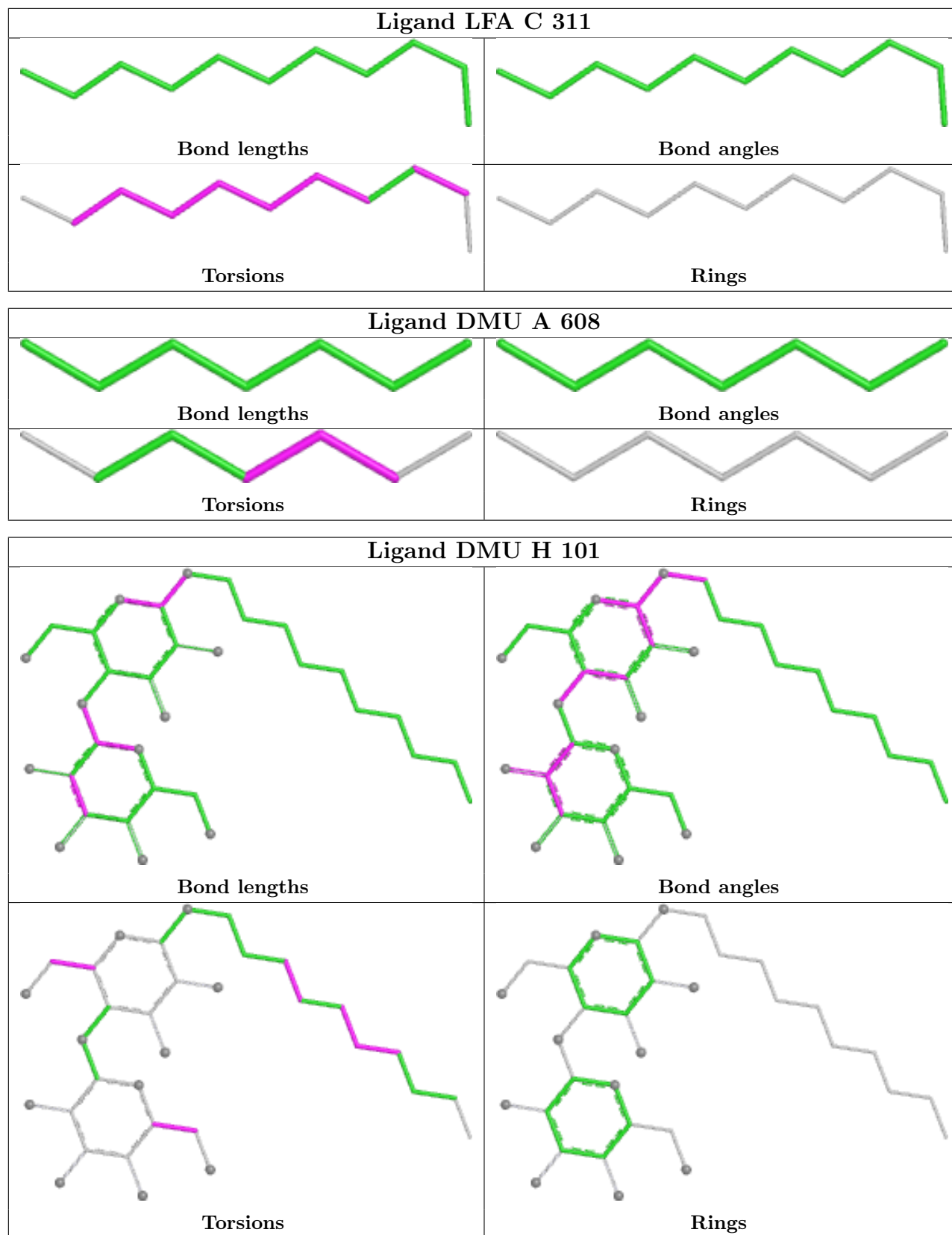


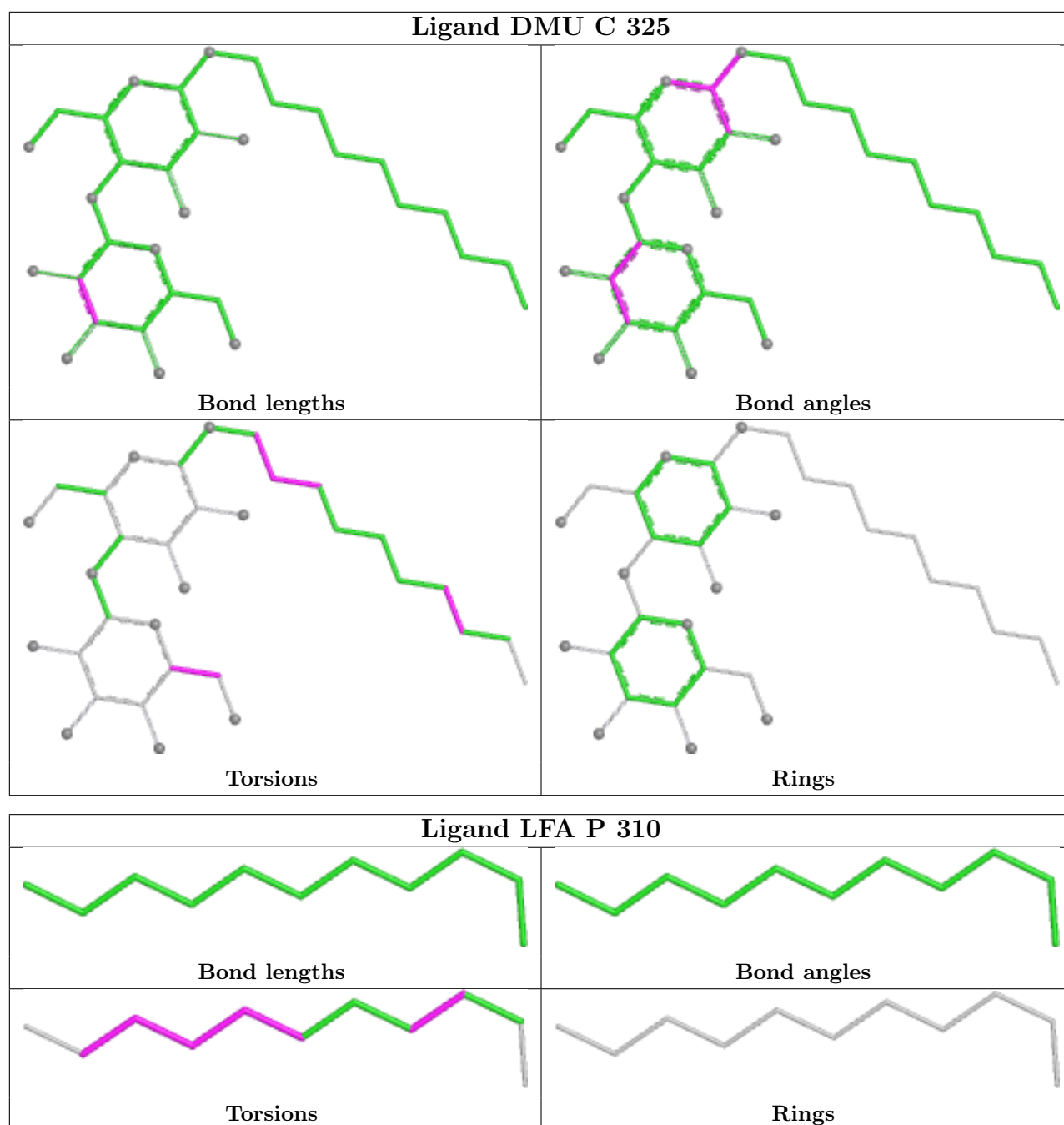


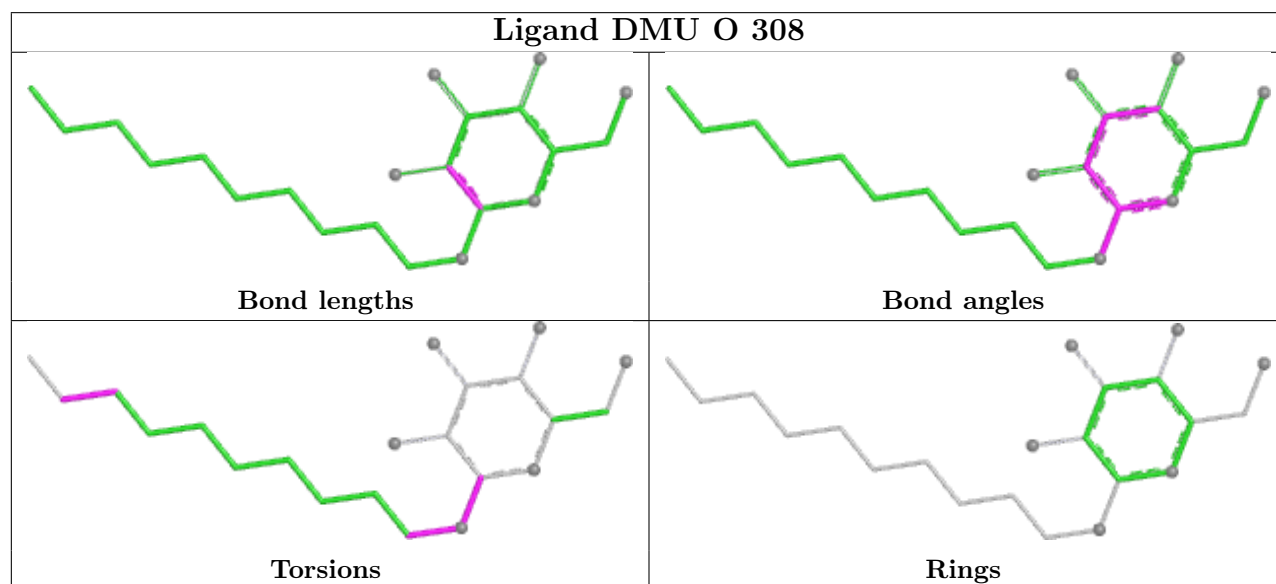
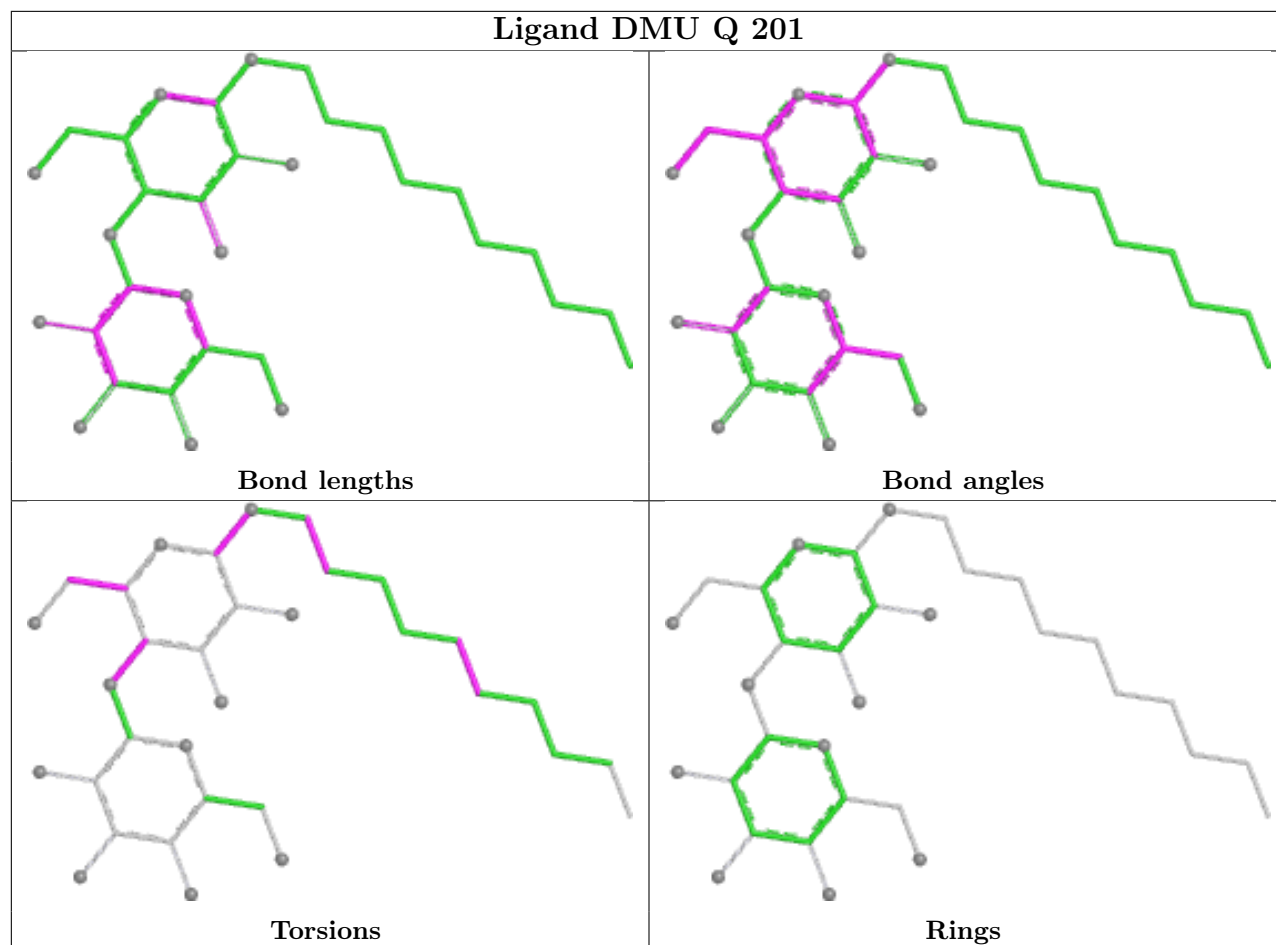


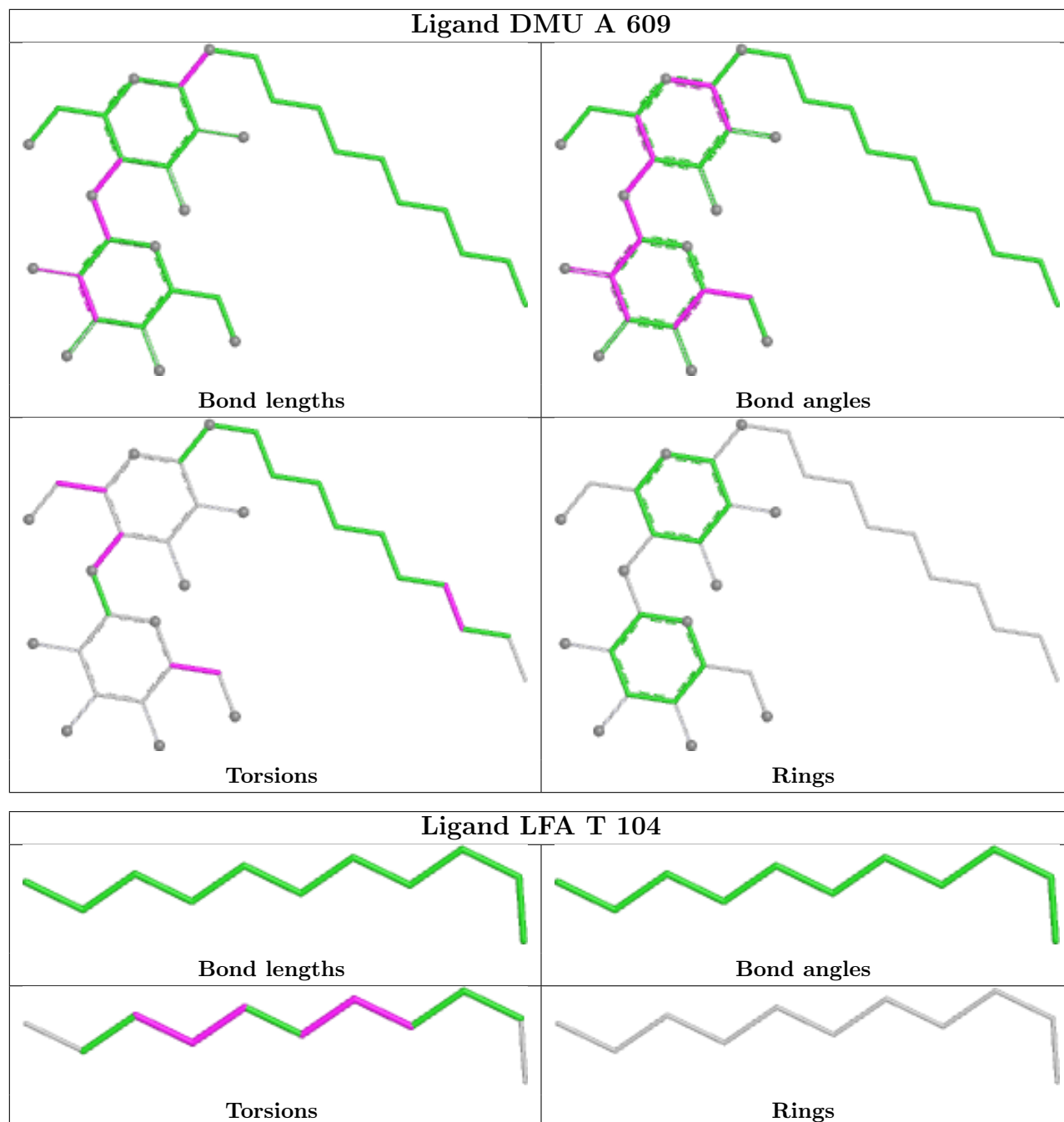


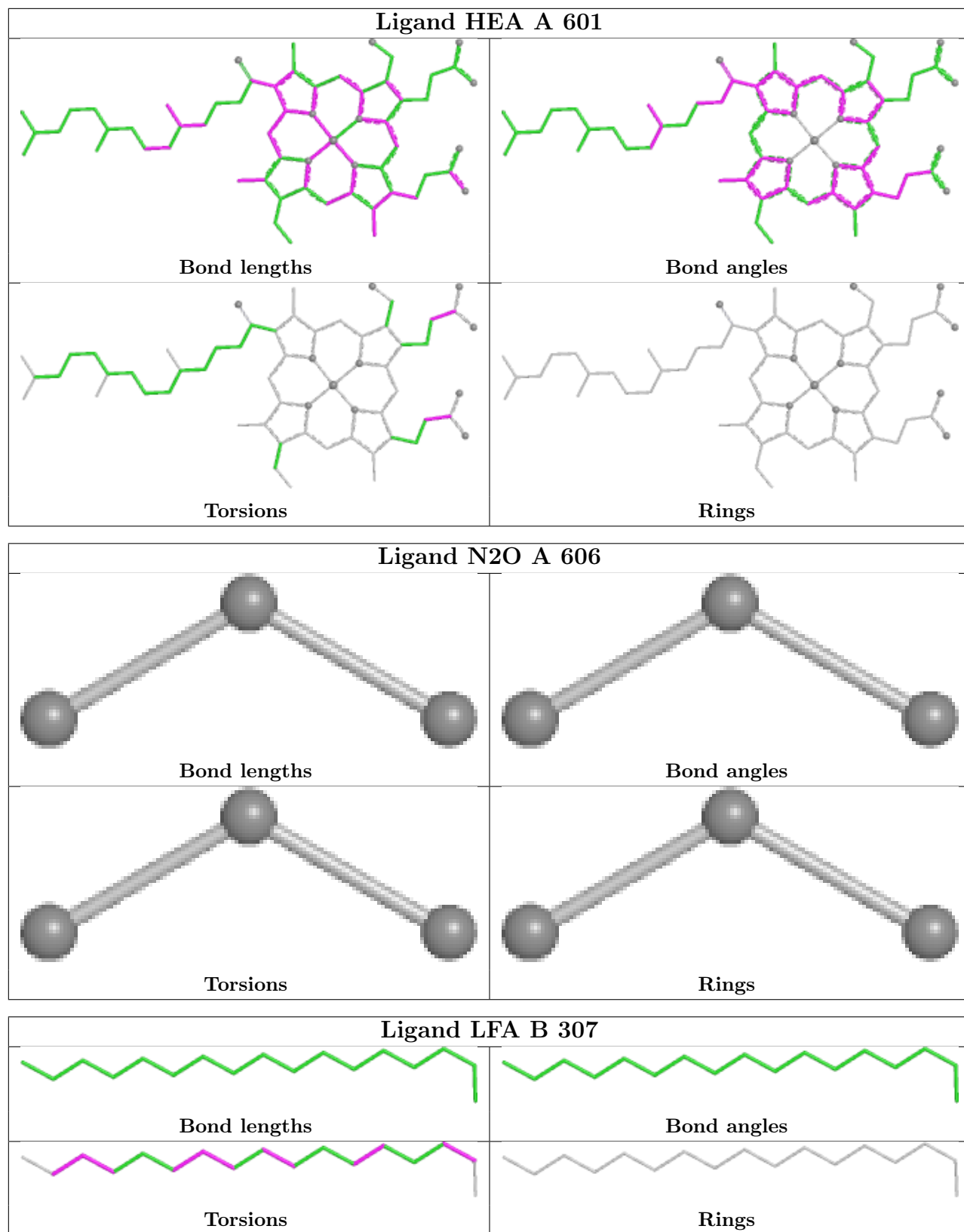


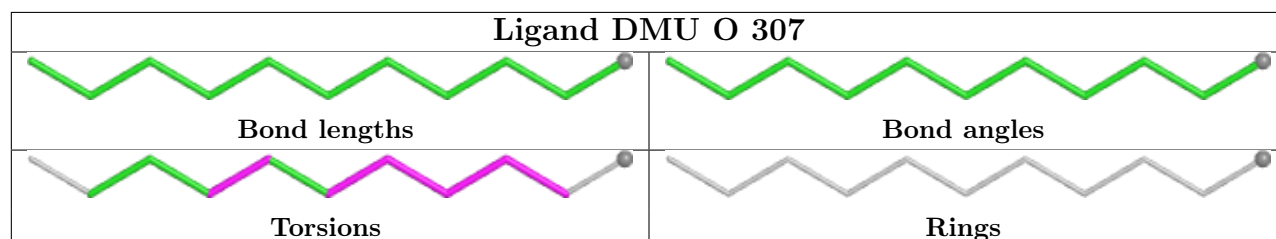
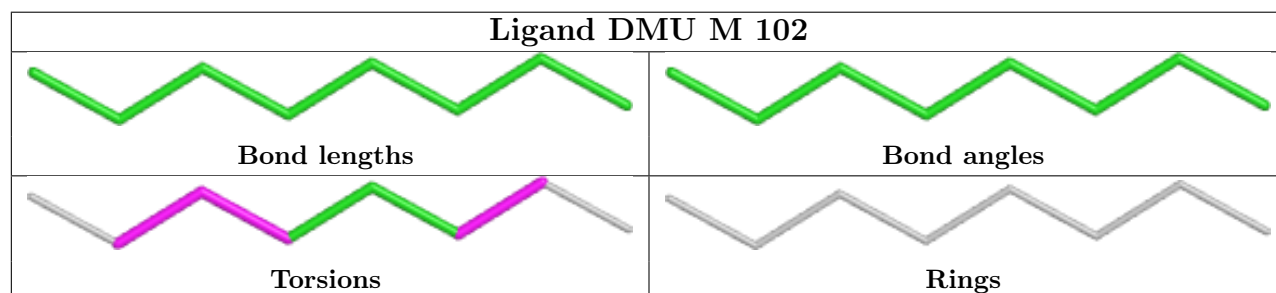
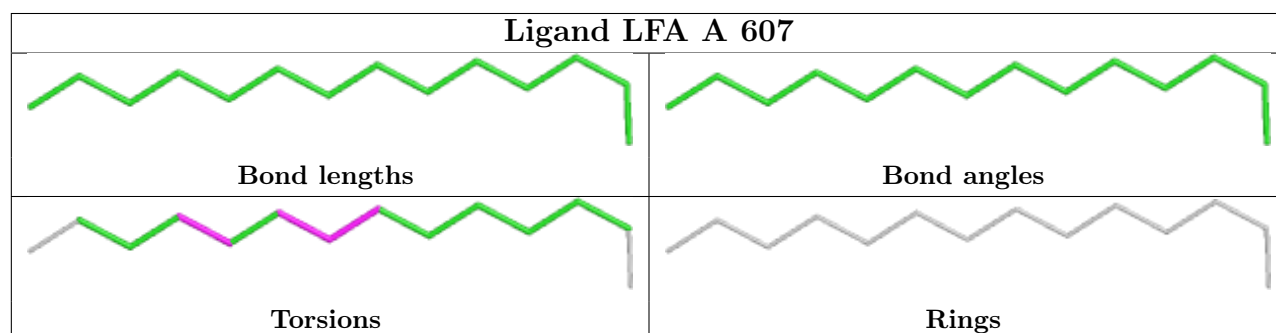
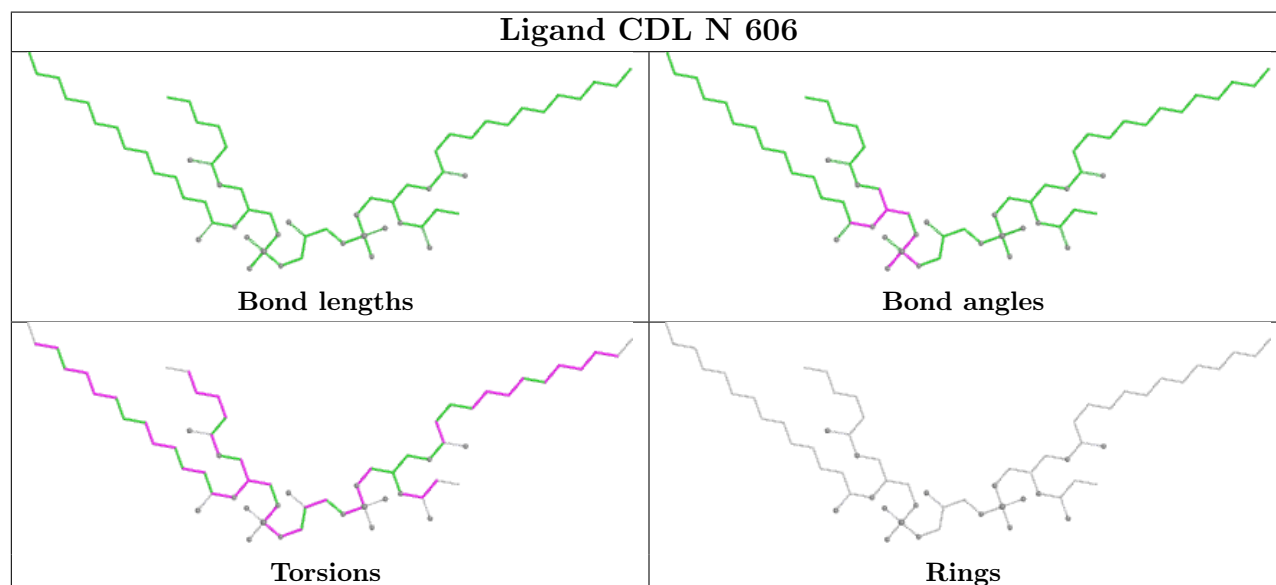
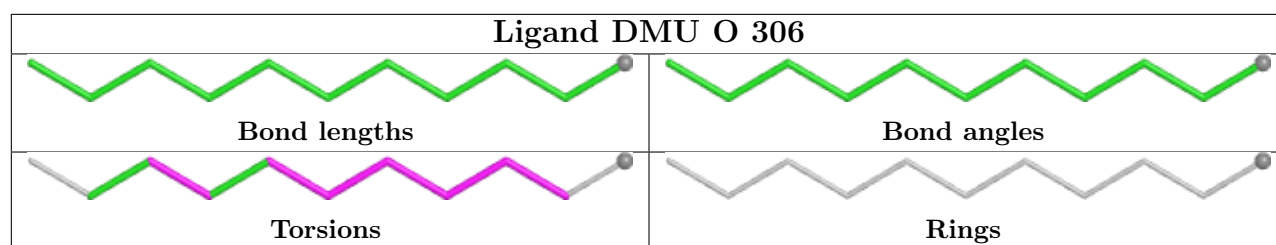


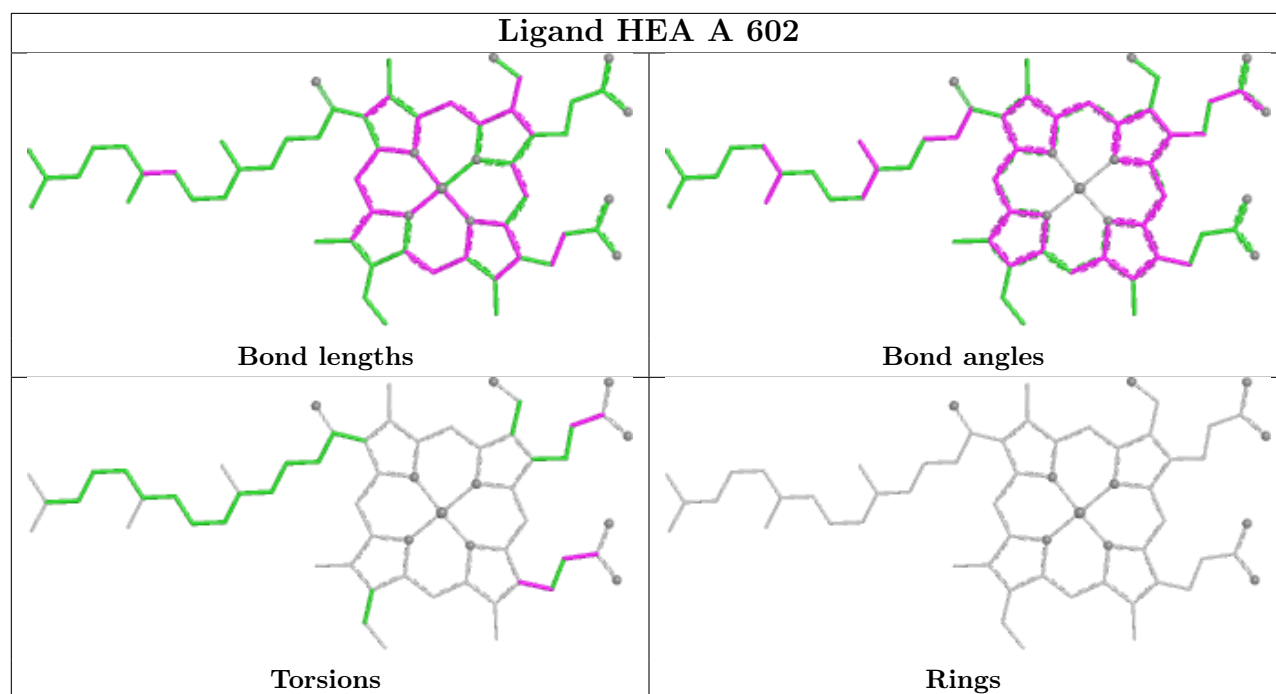
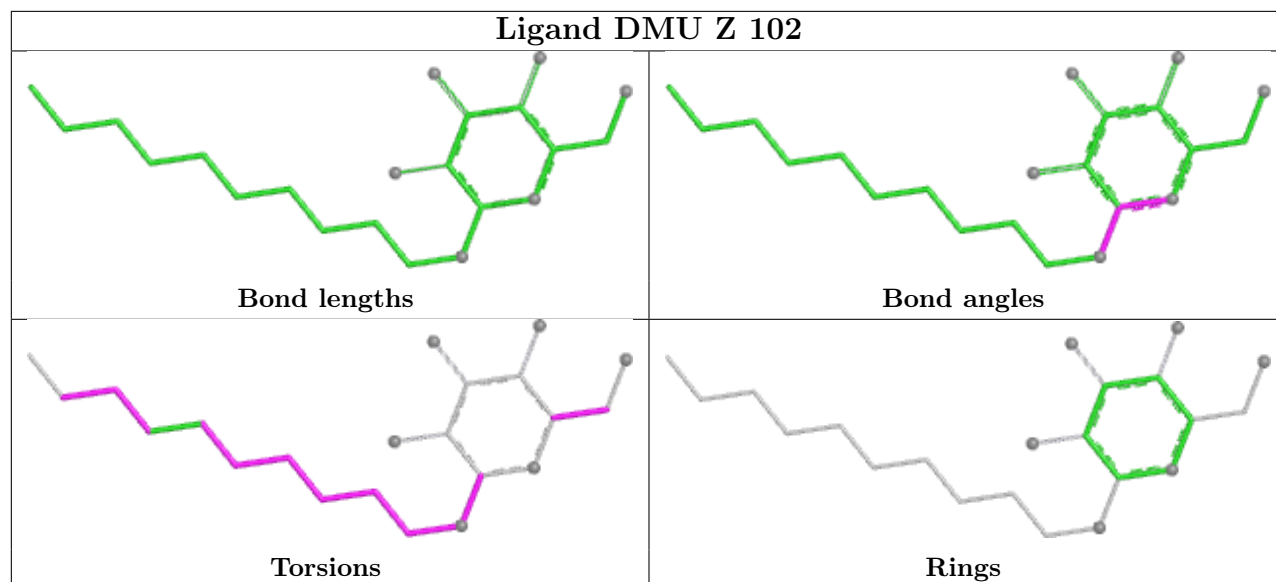


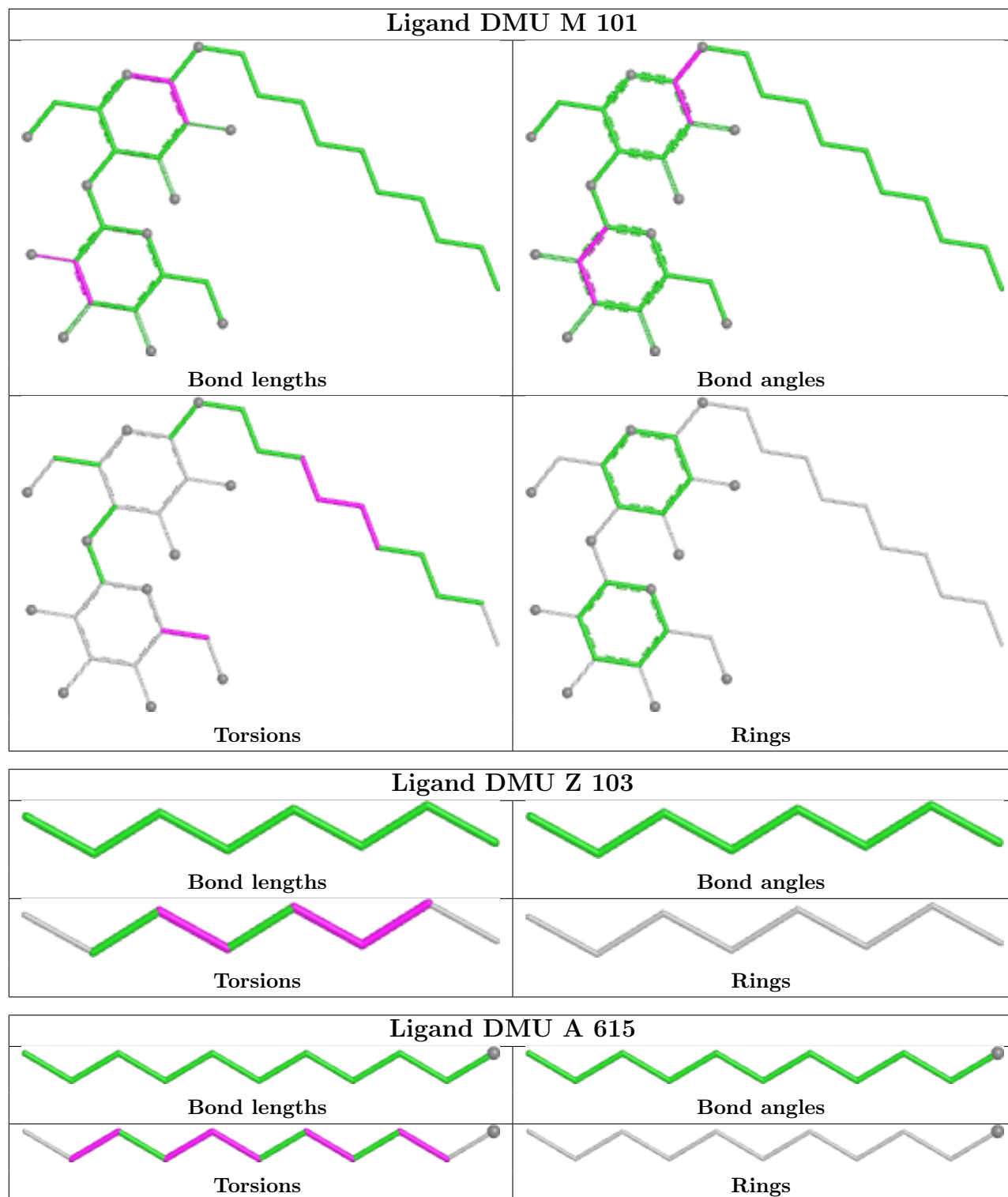


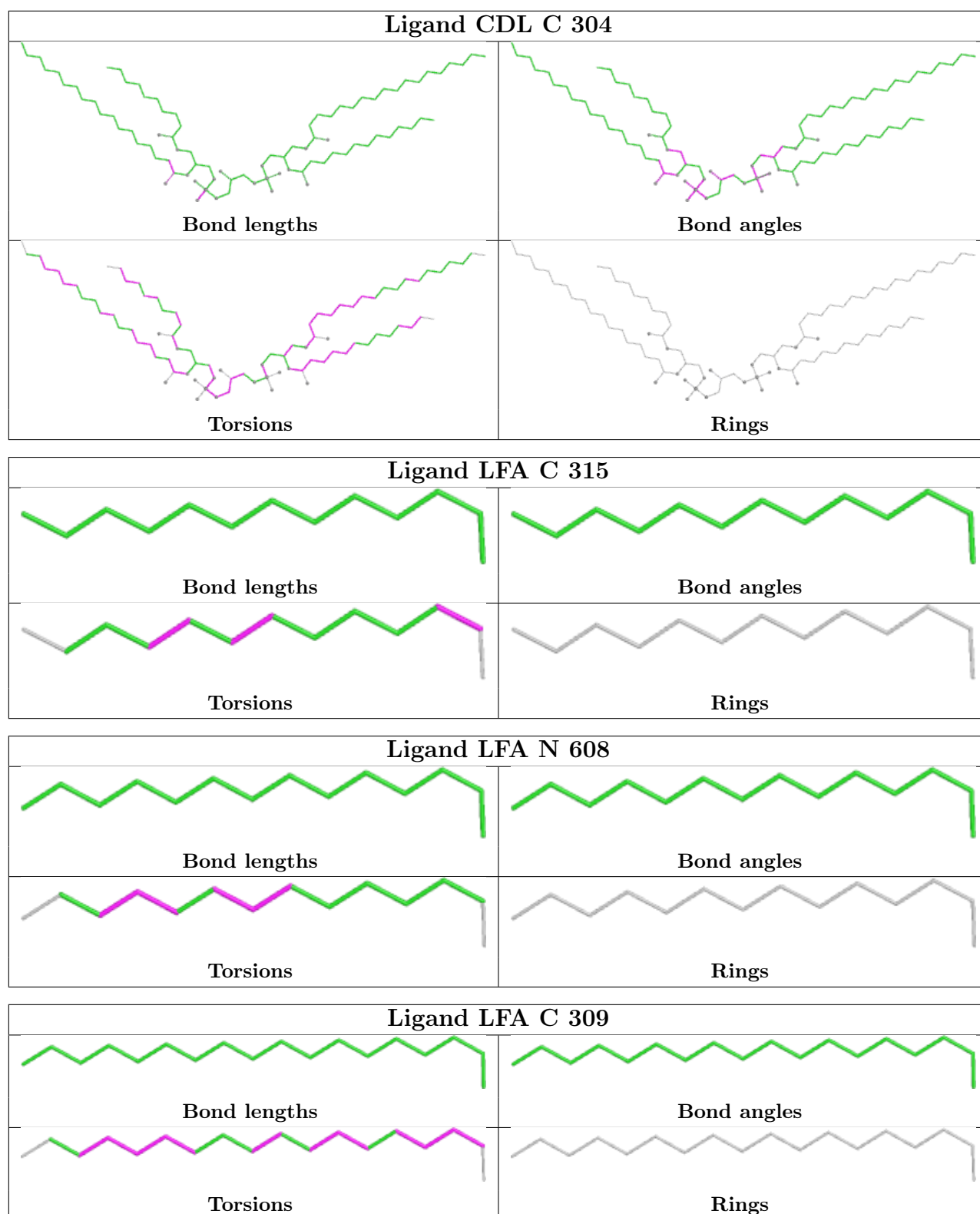


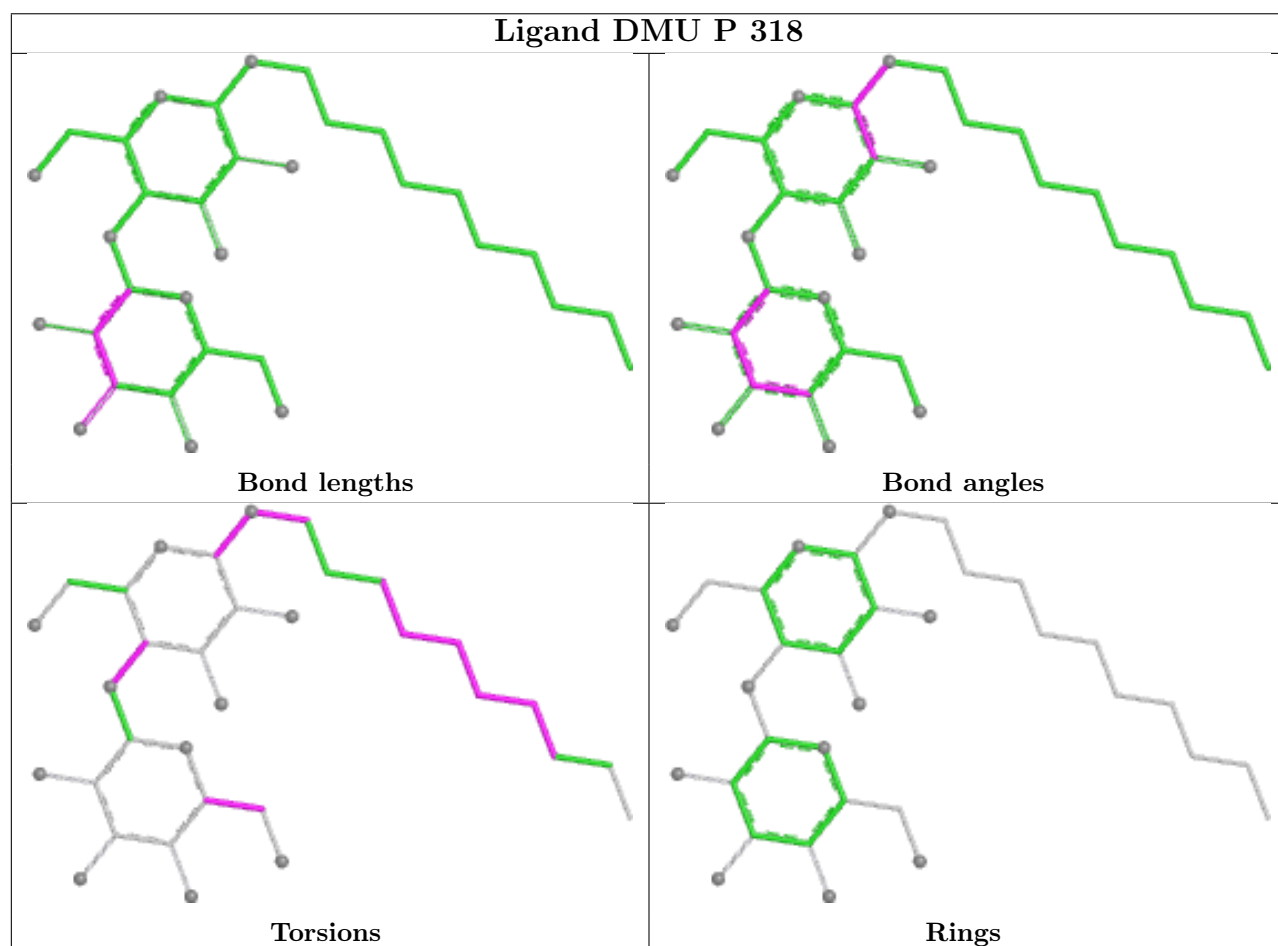
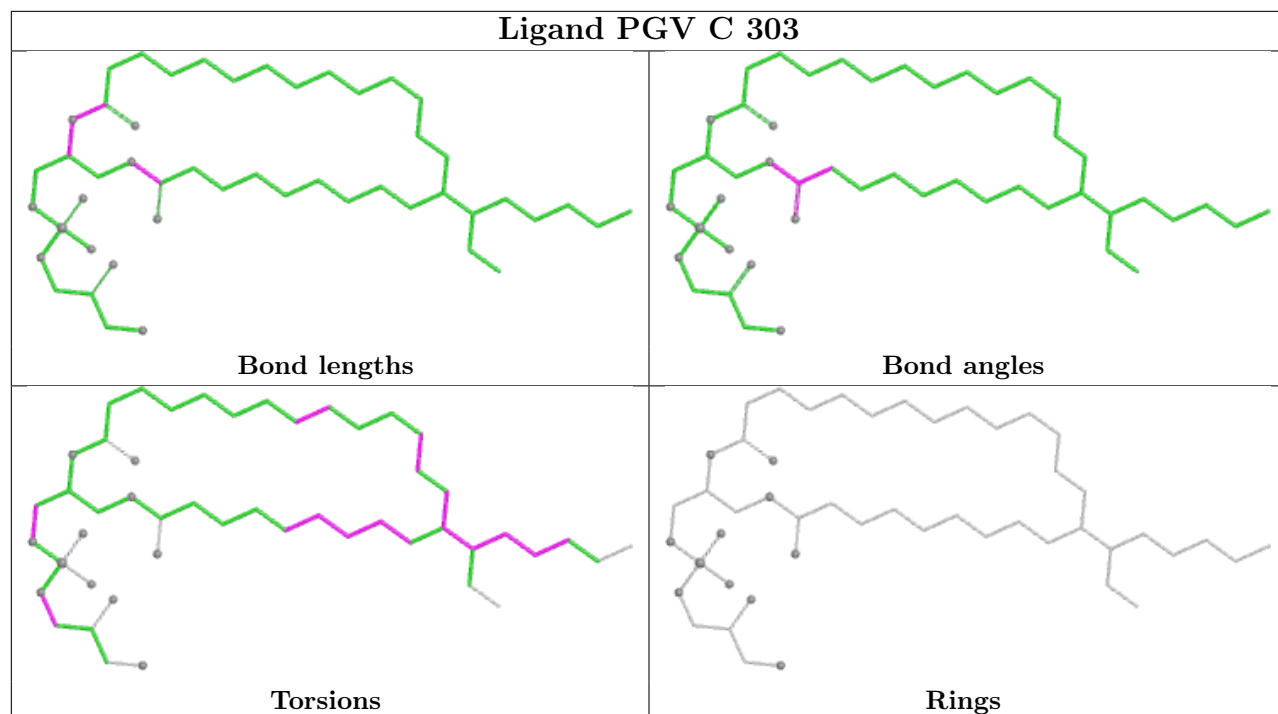


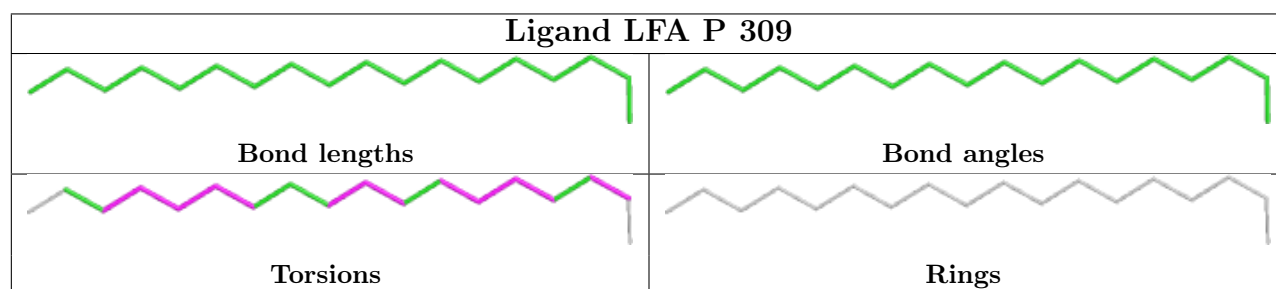
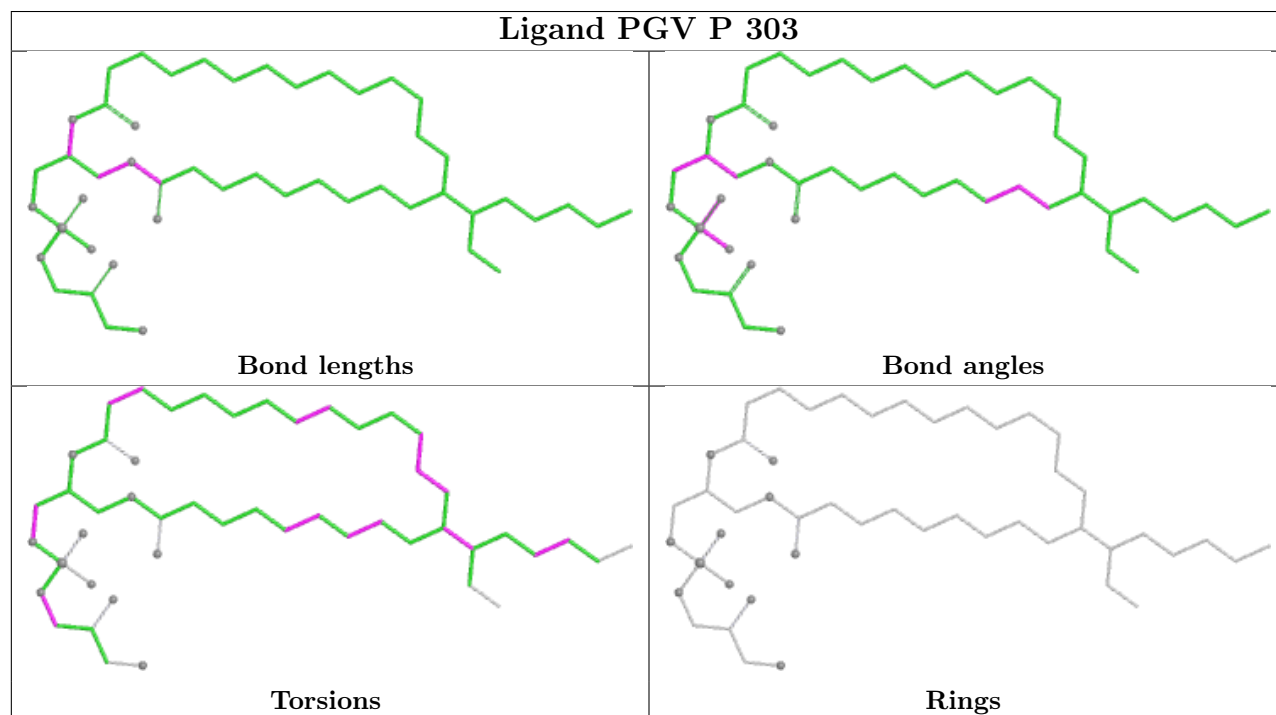
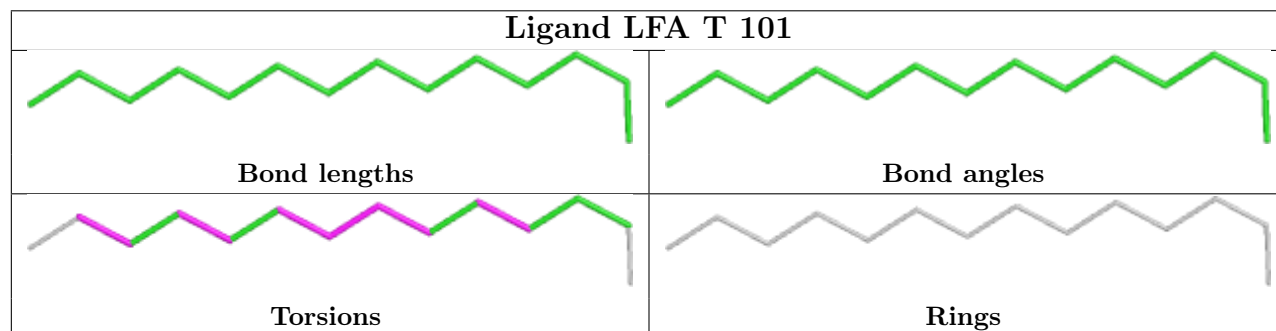
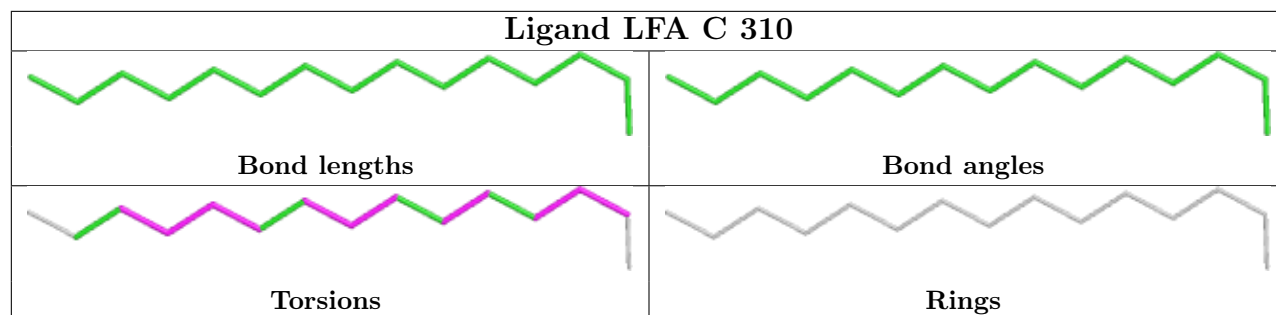












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.03	4 (0%) 82 86	16, 34, 40, 50	15 (2%)
1	N	512/514 (99%)	0.03	3 (0%) 85 89	17, 36, 43, 54	15 (2%)
2	B	226/227 (99%)	0.32	12 (5%) 32 36	21, 41, 53, 64	5 (2%)
2	O	226/227 (99%)	0.31	7 (3%) 51 58	22, 44, 62, 73	5 (2%)
3	C	258/261 (98%)	0.02	2 (0%) 82 86	16, 37, 44, 53	9 (3%)
3	P	258/261 (98%)	-0.02	2 (0%) 82 86	16, 37, 45, 57	9 (3%)
4	D	143/147 (97%)	0.17	3 (2%) 63 70	20, 42, 52, 64	1 (0%)
4	Q	137/147 (93%)	0.48	8 (5%) 29 33	23, 51, 67, 74	1 (0%)
5	E	102/109 (93%)	0.06	0 100 100	37, 43, 51, 60	0
5	R	102/109 (93%)	0.12	2 (1%) 65 71	38, 48, 59, 68	0
6	F	91/98 (92%)	0.09	1 (1%) 78 83	20, 41, 53, 65	2 (2%)
6	S	91/98 (92%)	0.21	2 (2%) 62 69	19, 40, 53, 59	2 (2%)
7	G	72/85 (84%)	0.46	4 (5%) 30 34	21, 42, 65, 72	1 (1%)
7	T	72/85 (84%)	0.50	2 (2%) 55 61	22, 44, 66, 78	1 (1%)
8	H	75/85 (88%)	0.45	4 (5%) 32 36	38, 45, 70, 79	0
8	U	75/85 (88%)	0.63	6 (8%) 18 22	42, 48, 75, 87	0
9	I	70/73 (95%)	0.70	9 (12%) 7 8	38, 49, 60, 69	0
9	V	70/73 (95%)	0.55	4 (5%) 29 33	38, 55, 65, 76	0
10	J	56/59 (94%)	0.32	2 (3%) 46 52	37, 45, 57, 64	0
10	W	56/59 (94%)	0.32	2 (3%) 46 52	38, 45, 58, 64	0
11	K	49/56 (87%)	0.47	3 (6%) 27 31	41, 46, 57, 64	0
11	X	49/56 (87%)	0.84	3 (6%) 27 31	46, 53, 66, 74	0
12	L	44/47 (93%)	0.03	0 100 100	35, 38, 46, 51	0
12	Y	44/47 (93%)	0.22	0 100 100	38, 43, 52, 56	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	40/46 (86%)	0.29	1 (2%) 58 64	37, 40, 51, 57	0
13	Z	40/46 (86%)	0.48	1 (2%) 58 64	43, 47, 62, 64	0
All	All	3470/3614 (96%)	0.19	87 (2%) 58 64	16, 40, 58, 87	66 (1%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	U	48	GLY	7.0
7	T	36	TRP	6.9
11	X	6	ALA	5.4
2	O	113	TYR	5.4
2	O	90	ILE	5.2
6	F	3	GLY	5.1
6	S	3	GLY	4.9
1	N	113[A]	LEU	4.9
8	U	47	GLY	4.5
10	J	1	PHE	4.4
8	H	45	ALA	4.4
2	B	59	GLN	4.2
2	B	91	ASN	4.2
2	B	87[A]	MET	4.0
8	H	48	GLY	4.0
9	V	72	ALA	4.0
7	G	36	TRP	4.0
6	S	93	PRO	4.0
2	B	90	ILE	3.8
1	A	113[A]	LEU	3.6
4	D	4	SER	3.5
8	U	45	ALA	3.5
9	I	3	ALA	3.5
3	C	38	ASN	3.5
4	D	5	VAL	3.5
9	I	37	PHE	3.4
9	V	37	PHE	3.3
11	K	6	ALA	3.3
2	B	65	TRP	3.2
13	M	32	TRP	3.2
9	I	72	ALA	3.2
7	G	41	HIS	3.1
2	O	32[A]	PHE	3.1
2	O	91	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
11	K	26	VAL	3.0
1	N	136[A]	LEU	3.0
2	B	60	GLU	3.0
9	I	25	PHE	3.0
9	V	3	ALA	3.0
2	B	32[A]	PHE	3.0
4	Q	35	ALA	2.9
8	U	49	ASP	2.9
2	O	22[A]	HIS	2.9
9	I	21	ILE	2.9
9	I	29	LEU	2.8
8	U	46	LYS	2.8
10	W	1	PHE	2.8
2	B	16[A]	ILE	2.8
1	A	311[A]	ILE	2.8
7	T	38	HIS	2.8
8	H	47	GLY	2.8
11	X	13	TYR	2.7
11	X	7	PRO	2.6
3	P	37	PHE	2.6
3	P	44[A]	MET	2.6
5	R	7	THR	2.6
2	O	227	LEU	2.5
4	Q	73	ARG	2.5
9	I	33	THR	2.5
8	H	46	LYS	2.5
1	A	297[A]	MET	2.5
8	U	44	THR	2.5
2	B	113	TYR	2.5
4	Q	93	ALA	2.5
10	W	48	TYR	2.4
7	G	33	LEU	2.4
4	Q	39	ALA	2.4
7	G	37	LEU	2.3
5	R	108	LYS	2.3
13	Z	32	TRP	2.3
2	O	87[A]	MET	2.3
4	Q	117	ALA	2.3
4	Q	131	ILE	2.3
2	B	61	VAL	2.3
11	K	47	ARG	2.3
4	Q	72	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
9	V	34	PHE	2.2
3	C	258	TRP	2.2
4	Q	87	PHE	2.2
4	D	102	TYR	2.2
2	B	67	ILE	2.2
1	N	48	LEU	2.1
9	I	19	PHE	2.1
10	J	56	PRO	2.1
9	I	34	PHE	2.1
1	A	298[A]	ASP	2.1
2	B	92	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	FME	A	1	10/11	0.91	0.14	41,47,64,69	0
1	FME	N	1	10/11	0.92	0.14	44,49,65,75	0
2	FME	B	1	10/11	0.97	0.08	38,41,48,68	0
2	FME	O	1	10/11	0.97	0.10	43,46,54,63	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	DMU	C	318	22/33	0.68	0.29	39,46,54,64	22
20	DMU	P	316	22/33	0.68	0.33	36,50,58,64	22
19	LFA	P	310	11/20	0.74	0.40	42,50,57,64	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	LFA	C	312	14/20	0.75	0.39	38,49,56,56	14
20	DMU	A	608	7/33	0.76	0.35	40,44,47,47	7
21	EDO	P	321	4/4	0.78	0.37	35,36,37,42	4
19	LFA	P	311	11/20	0.79	0.30	38,43,51,51	11
20	DMU	C	319	33/33	0.79	0.32	36,48,58,66	33
20	DMU	C	316	33/33	0.80	0.33	40,46,56,57	33
24	CHD	C	305	29/29	0.80	0.17	54,62,74,90	0
24	CHD	P	305	29/29	0.80	0.17	54,62,74,103	0
26	CDL	N	606	64/100	0.80	0.19	48,66,80,96	0
19	LFA	P	308	6/20	0.81	0.35	38,41,43,44	6
26	CDL	I	101	64/100	0.81	0.19	41,63,73,83	0
19	LFA	C	326	15/20	0.81	0.38	40,47,55,57	15
19	LFA	C	308	6/20	0.82	0.42	40,45,46,48	6
19	LFA	T	101	14/20	0.82	0.26	36,41,49,51	14
19	LFA	G	104	14/20	0.82	0.27	34,42,51,51	14
20	DMU	O	304	22/33	0.83	0.27	46,59,68,69	22
20	DMU	P	314	33/33	0.83	0.28	39,48,56,66	33
19	LFA	O	303	11/20	0.83	0.33	43,50,58,59	11
20	DMU	P	317	33/33	0.83	0.29	39,50,56,61	33
20	DMU	Q	201	33/33	0.83	0.23	40,50,59,62	33
20	DMU	Z	102	22/33	0.83	0.38	46,57,63,72	22
19	LFA	C	313	11/20	0.83	0.28	37,41,51,54	11
19	LFA	C	315	13/20	0.83	0.26	41,46,54,59	13
20	DMU	C	320	33/33	0.83	0.23	40,55,60,62	33
26	CDL	C	304	87/100	0.83	0.20	43,61,77,82	0
20	DMU	G	102	11/33	0.83	0.38	43,51,56,58	11
20	DMU	M	102	8/33	0.83	0.26	39,43,45,51	8
26	CDL	P	304	87/100	0.83	0.20	42,63,83,88	0
26	CDL	Y	101	94/100	0.83	0.18	46,63,81,92	0
19	LFA	P	307	11/20	0.84	0.33	41,45,48,51	11
19	LFA	P	313	13/20	0.84	0.27	39,45,53,58	13
21	EDO	A	611	4/4	0.84	0.31	35,41,42,45	4
21	EDO	D	202	4/4	0.84	0.36	40,40,42,43	4
20	DMU	C	324	22/33	0.84	0.28	41,51,59,60	22
20	DMU	P	318	33/33	0.84	0.24	47,57,67,74	33
19	LFA	C	314	15/20	0.85	0.23	38,42,53,54	15
21	EDO	C	323	4/4	0.85	0.32	35,38,38,42	4
20	DMU	C	317	7/33	0.85	0.26	41,43,47,49	7
21	EDO	N	612	4/4	0.85	0.29	39,40,42,44	4
19	LFA	C	307	11/20	0.85	0.30	42,46,51,51	11
21	EDO	R	203	4/4	0.85	0.28	39,40,45,50	4
19	LFA	T	103	14/20	0.85	0.31	41,50,54,58	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	LFA	T	104	11/20	0.85	0.30	45,47,61,63	11
19	LFA	C	311	11/20	0.85	0.28	42,52,56,57	11
20	DMU	B	308	22/33	0.85	0.30	48,64,72,73	22
20	DMU	Z	101	33/33	0.85	0.14	48,58,70,73	0
20	DMU	H	101	33/33	0.85	0.25	36,45,51,60	33
21	EDO	A	610	4/4	0.85	0.24	31,33,34,34	4
20	DMU	N	609	7/33	0.86	0.34	47,48,50,53	7
20	DMU	N	610	33/33	0.86	0.21	38,52,65,67	33
19	LFA	P	309	18/20	0.86	0.24	36,44,48,48	18
21	EDO	C	321	4/4	0.86	0.29	46,47,48,57	4
20	DMU	A	615	11/33	0.86	0.35	43,51,57,57	11
20	DMU	U	101	33/33	0.86	0.26	36,46,57,65	33
20	DMU	W	101	11/33	0.86	0.32	50,56,61,66	11
20	DMU	P	315	7/33	0.86	0.29	44,46,53,61	7
20	DMU	T	105	22/33	0.87	0.24	44,50,56,65	22
19	LFA	C	309	18/20	0.87	0.23	35,41,47,49	18
26	CDL	L	101	94/100	0.87	0.16	40,59,75,80	0
19	LFA	O	302	17/20	0.87	0.28	43,54,60,68	17
19	LFA	C	310	15/20	0.87	0.32	38,50,54,54	15
20	DMU	C	325	33/33	0.87	0.16	39,47,63,68	33
20	DMU	A	609	33/33	0.88	0.19	33,44,52,57	33
20	DMU	P	322	33/33	0.88	0.16	38,52,69,74	33
19	LFA	P	312	15/20	0.89	0.17	36,41,46,51	15
19	LFA	B	307	17/20	0.89	0.28	42,53,63,63	17
20	DMU	L	102	22/33	0.89	0.30	40,48,54,59	22
20	DMU	B	302	11/33	0.89	0.27	39,43,51,58	11
20	DMU	B	304	22/33	0.89	0.20	36,52,58,70	22
20	DMU	M	101	33/33	0.90	0.11	46,52,64,74	0
21	EDO	E	202	4/4	0.90	0.24	36,37,41,44	4
20	DMU	J	101	11/33	0.90	0.29	48,52,55,68	11
21	EDO	N	613	4/4	0.90	0.18	31,31,32,33	4
20	DMU	O	306	11/33	0.90	0.27	38,41,49,53	11
20	DMU	O	308	22/33	0.90	0.20	33,47,51,52	22
20	DMU	D	201	33/33	0.90	0.16	29,42,50,55	33
20	DMU	P	306	11/33	0.91	0.27	40,46,49,56	11
21	EDO	P	319	4/4	0.91	0.22	46,48,55,63	4
21	EDO	N	611	4/4	0.91	0.16	30,31,32,34	4
20	DMU	B	303	11/33	0.91	0.22	38,45,55,56	11
21	EDO	C	322	4/4	0.92	0.24	35,37,38,39	4
21	EDO	R	202	4/4	0.92	0.20	34,35,39,42	4
19	LFA	A	607	14/20	0.92	0.21	34,40,57,57	14
20	DMU	C	306	11/33	0.92	0.22	43,49,53,57	11

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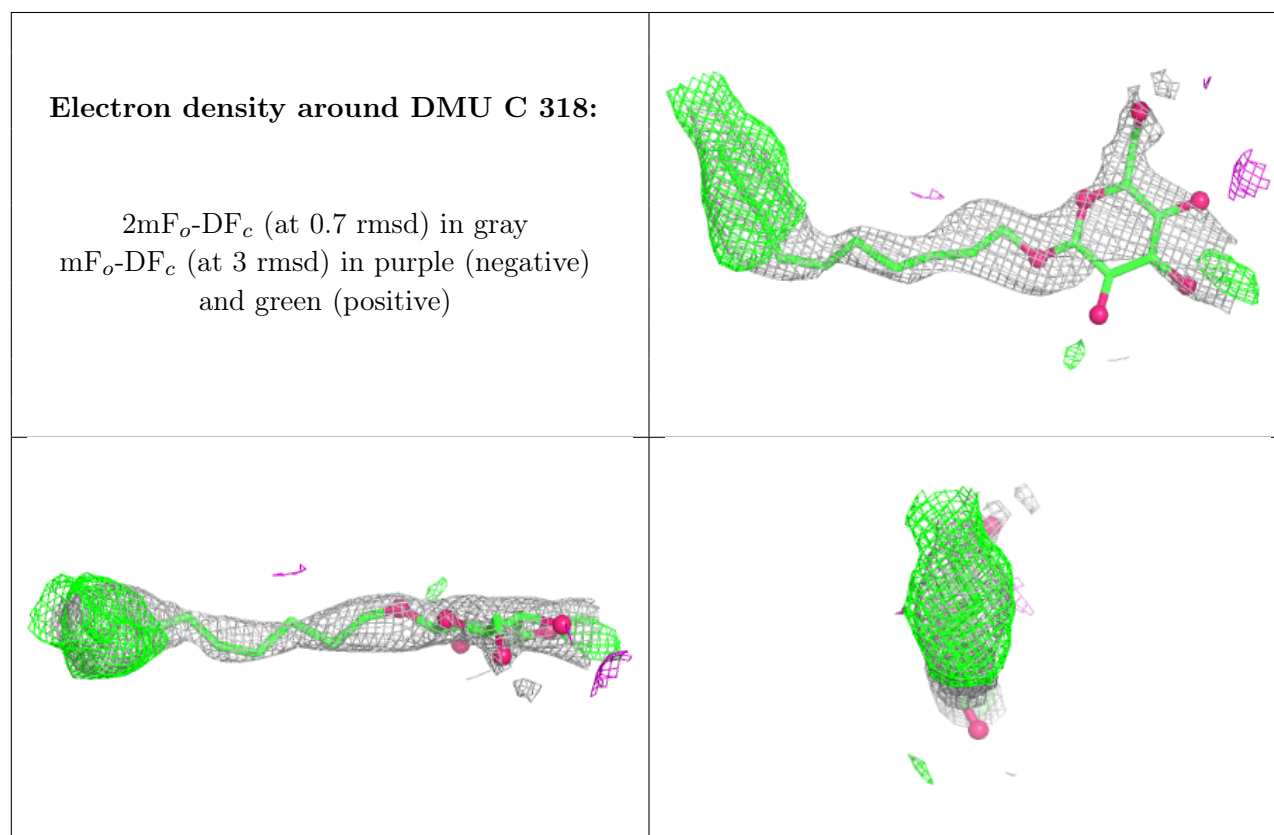
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	DMU	Z	103	8/33	0.92	0.20	42,45,47,49	8
25	UNX	P	302	1/1	0.92	0.28	44,44,44,44	0
21	EDO	A	613	4/4	0.93	0.19	39,40,41,45	4
21	EDO	N	615	4/4	0.93	0.22	32,32,32,34	4
21	EDO	A	612	4/4	0.93	0.20	30,30,30,31	4
21	EDO	N	614	4/4	0.94	0.19	34,34,35,39	4
21	EDO	G	103	4/4	0.94	0.16	38,38,39,41	4
19	LFA	N	608	14/20	0.94	0.17	34,40,52,53	14
21	EDO	E	201	4/4	0.94	0.21	34,34,34,37	4
20	DMU	O	307	11/33	0.94	0.21	38,44,50,56	11
28	PEK	T	102	53/53	0.94	0.12	38,48,67,69	0
21	EDO	F	103	4/4	0.95	0.11	31,34,35,36	4
21	EDO	R	201	4/4	0.95	0.25	54,59,60,62	4
21	EDO	F	102	4/4	0.95	0.12	27,27,31,32	4
21	EDO	P	320	4/4	0.95	0.23	33,35,36,38	4
28	PEK	G	101	53/53	0.95	0.11	36,46,68,76	0
21	EDO	T	106	4/4	0.95	0.12	40,40,40,43	4
25	UNX	C	302	1/1	0.96	0.15	45,45,45,45	0
24	CHD	C	301	29/29	0.96	0.07	34,37,39,42	0
22	PGV	N	616	51/51	0.97	0.08	33,38,55,62	0
22	PGV	P	303	51/51	0.97	0.08	33,39,63,67	0
24	CHD	B	306	29/29	0.97	0.07	35,39,41,47	0
21	EDO	S	103	4/4	0.97	0.09	31,37,37,38	4
21	EDO	O	309	4/4	0.97	0.12	35,37,37,40	4
24	CHD	O	301	29/29	0.97	0.07	35,39,41,47	0
24	CHD	P	301	29/29	0.97	0.07	34,38,41,44	0
22	PGV	A	614	51/51	0.97	0.09	32,38,55,59	0
22	PGV	C	303	51/51	0.97	0.09	33,40,64,68	0
14	HEA	N	602	60/60	0.98	0.06	32,34,38,43	0
21	EDO	B	305	4/4	0.98	0.08	32,33,35,36	4
17	NA	A	605	1/1	0.98	0.07	36,36,36,36	0
18	N2O	A	606	3/3	0.98	0.10	33,33,35,38	0
18	N2O	N	607	3/3	0.98	0.13	36,36,41,41	0
21	EDO	S	102	4/4	0.98	0.07	26,28,29,29	4
14	HEA	A	602	60/60	0.98	0.06	29,32,37,42	0
14	HEA	A	601	60/60	0.99	0.06	28,32,41,47	0
15	CU	A	603	1/1	0.99	0.02	31,31,31,31	0
16	MG	A	604	1/1	0.99	0.04	31,31,31,31	0
23	CUA	B	301	2/2	0.99	0.03	33,33,33,34	0
23	CUA	O	305	2/2	0.99	0.03	37,37,37,38	0
27	ZN	F	101	1/1	0.99	0.02	37,37,37,37	0
27	ZN	S	101	1/1	0.99	0.03	37,37,37,37	0

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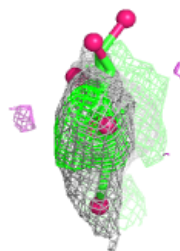
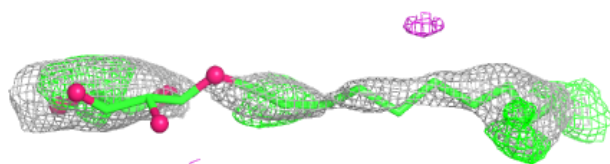
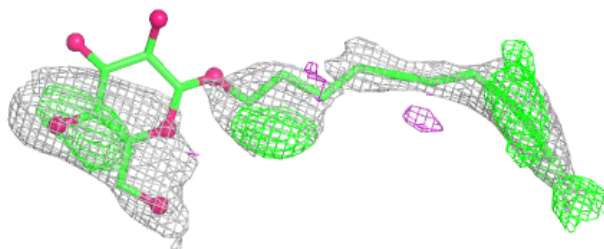
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	HEA	N	601	60/60	0.99	0.06	31,35,44,52	0
17	NA	N	605	1/1	0.99	0.04	41,41,41,41	0
16	MG	N	604	1/1	1.00	0.04	36,36,36,36	0
15	CU	N	603	1/1	1.00	0.02	33,33,33,33	0

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

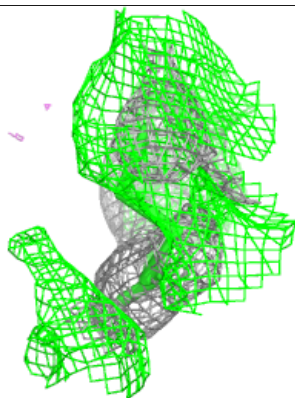
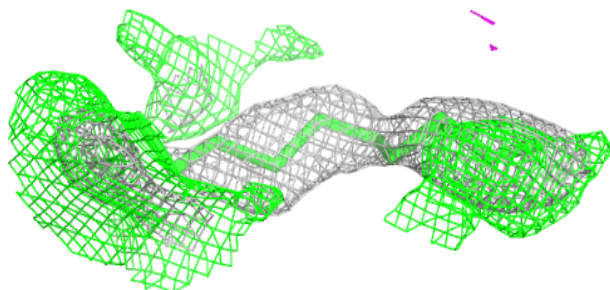
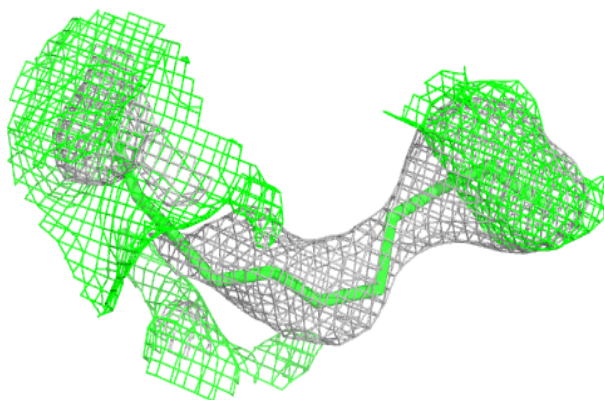


Electron density around DMU P 316:

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

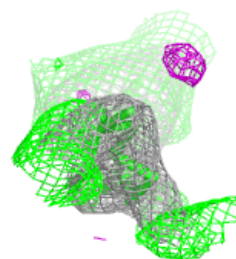
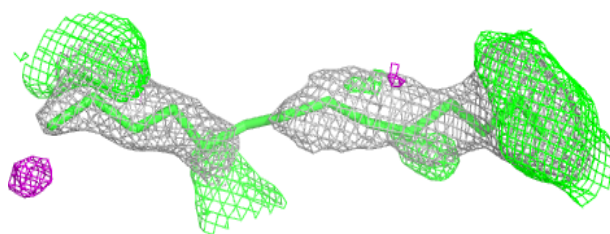
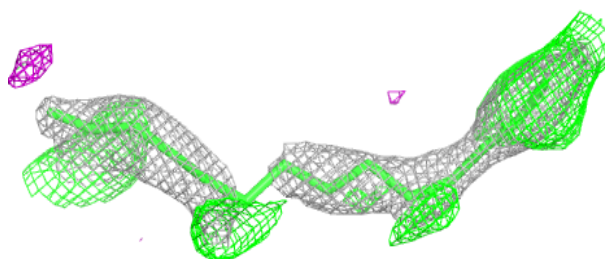
**Electron density around LFA P 310:**

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

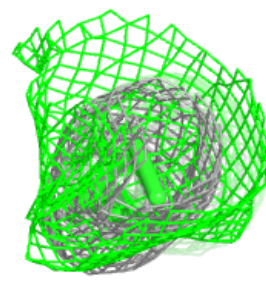
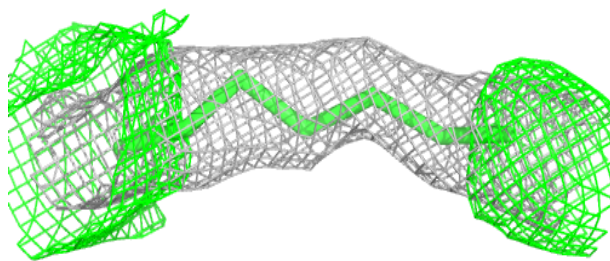
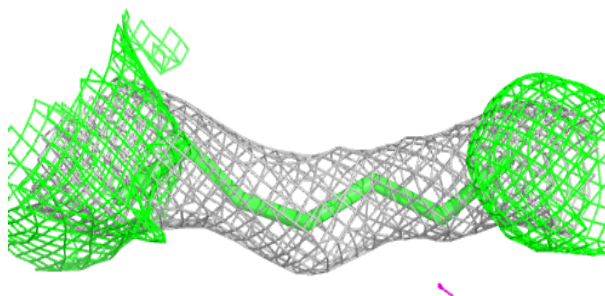


Electron density around LFA C 312:

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

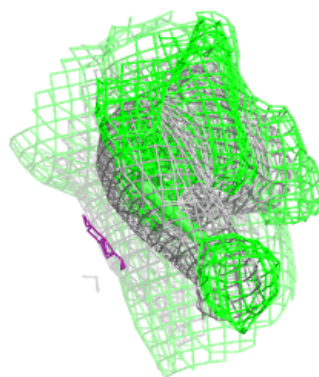
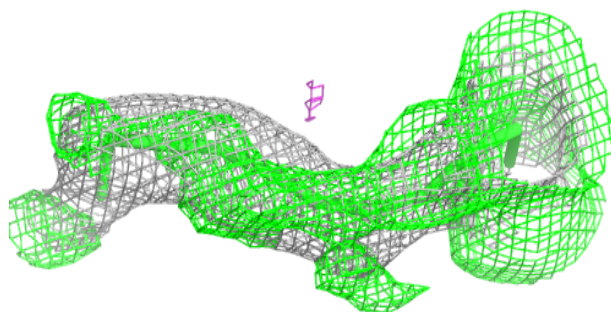
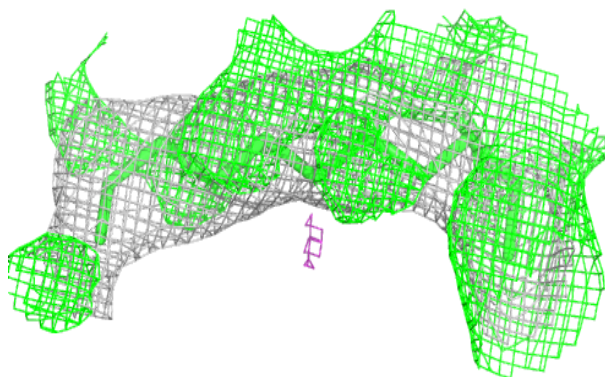
**Electron density around DMU A 608:**

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

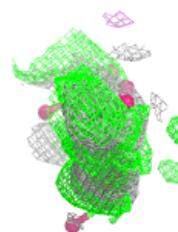
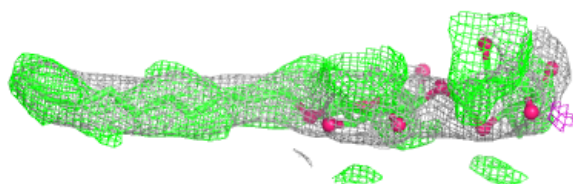
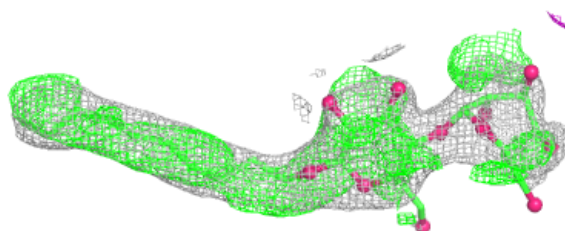


Electron density around LFA P 311:

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

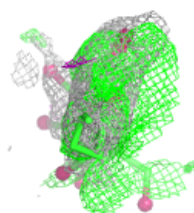
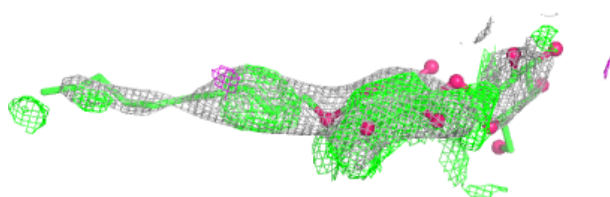
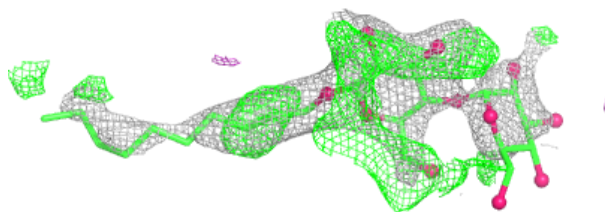
**Electron density around DMU C 319:**

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

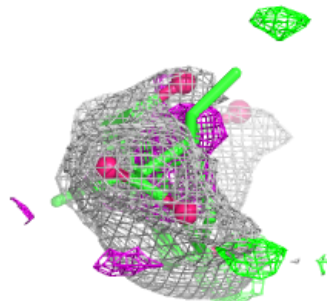
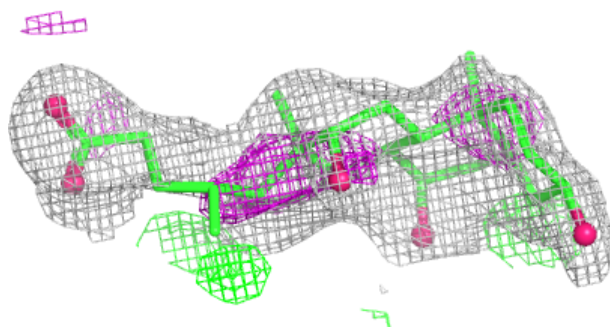
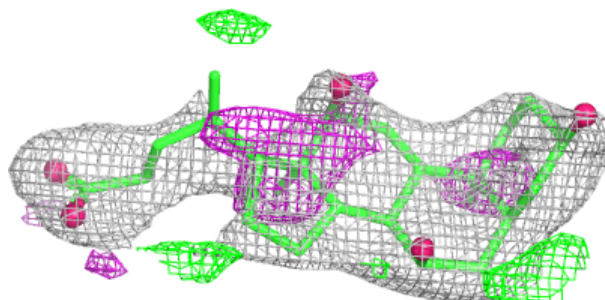


Electron density around DMU C 316:

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

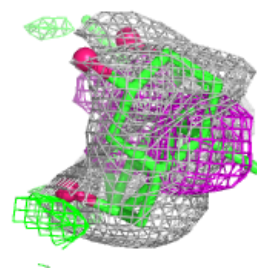
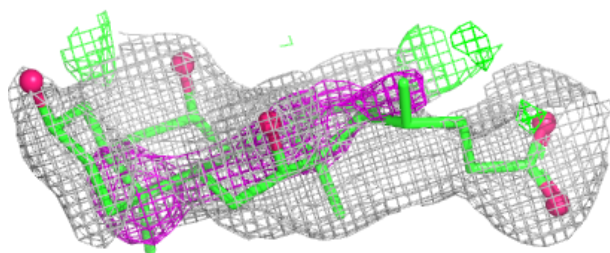
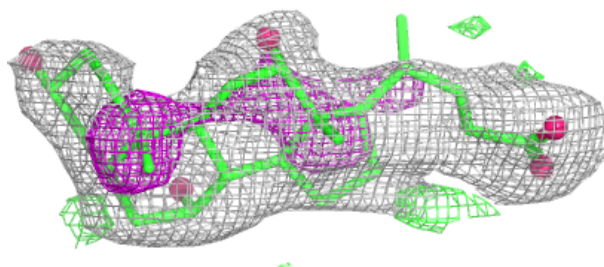
**Electron density around CHD C 305:**

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

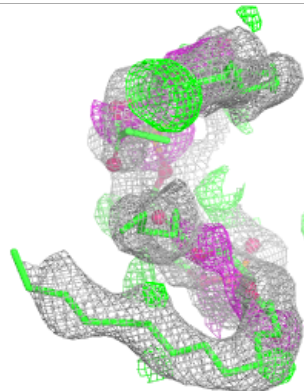
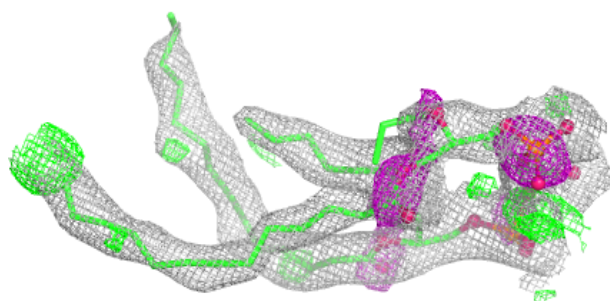
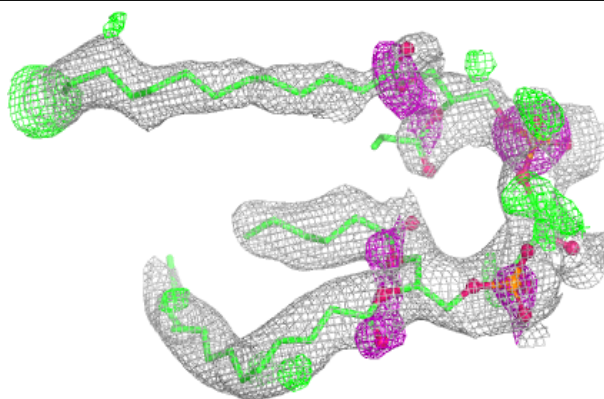


Electron density around CHD P 305:

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

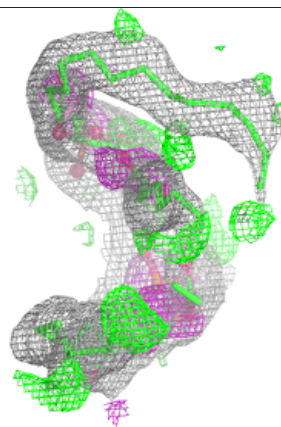
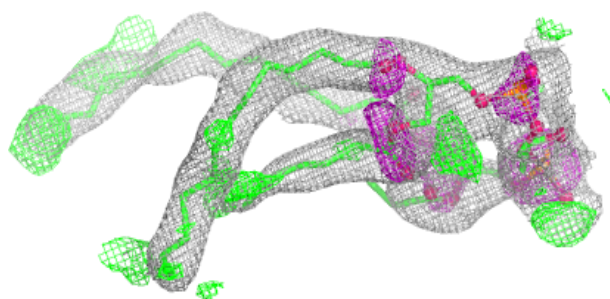
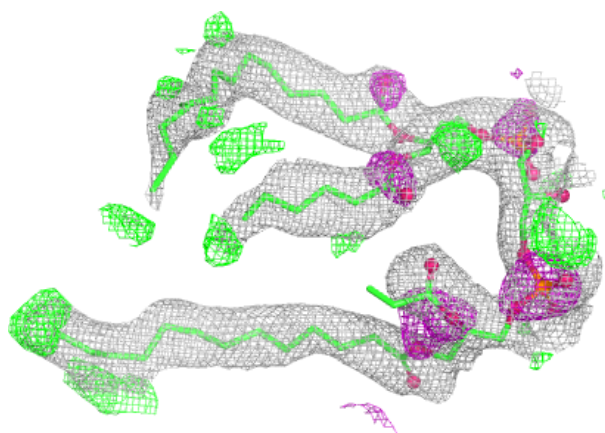
**Electron density around CDL N 606:**

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

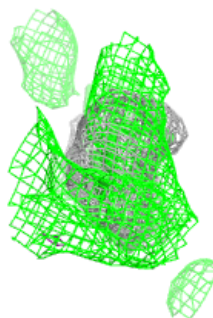
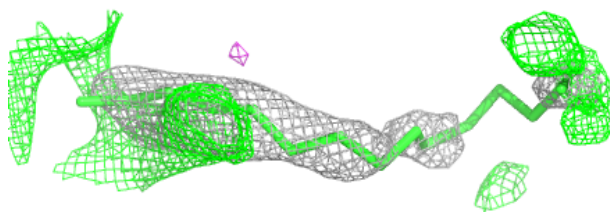
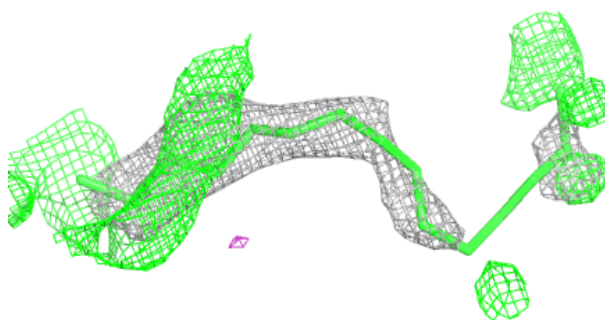


Electron density around CDL I 101:

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

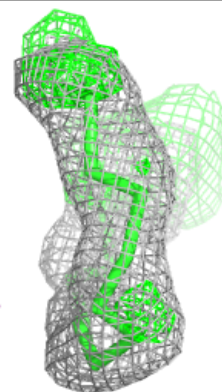
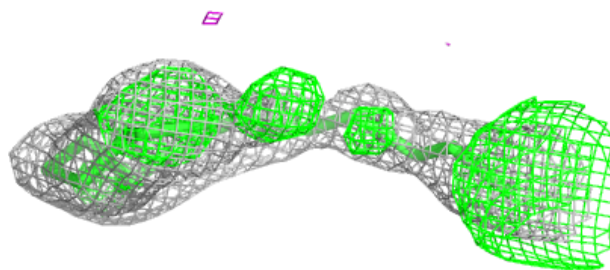
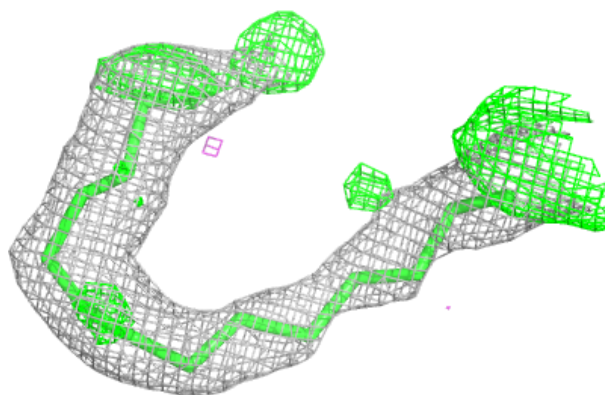
**Electron density around LFA C 326:**

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

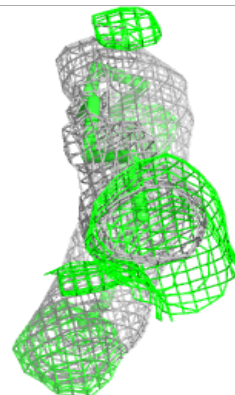
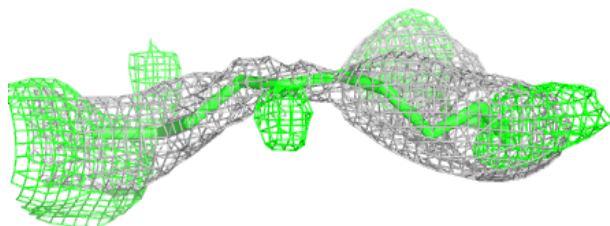
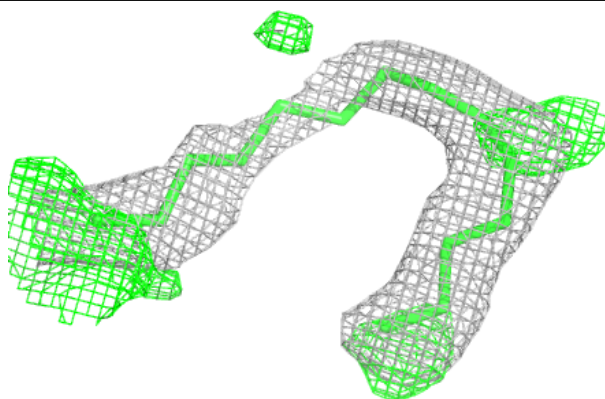


Electron density around LFA T 101:

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

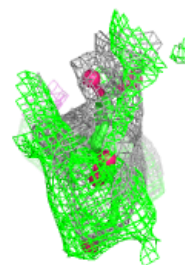
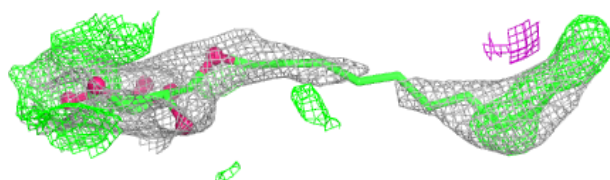
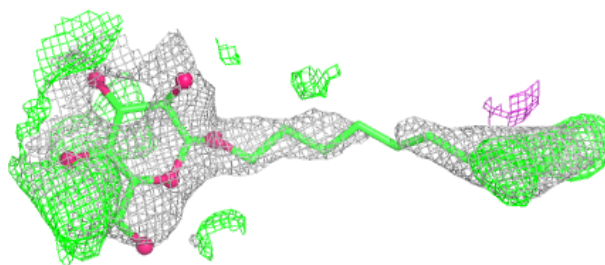
**Electron density around LFA G 104:**

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

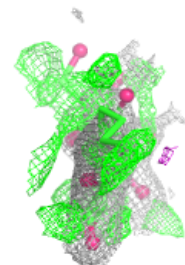
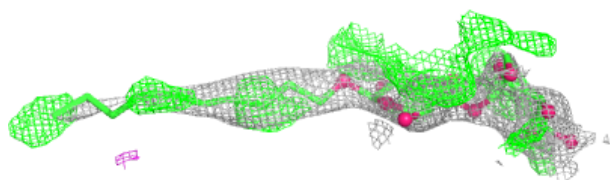
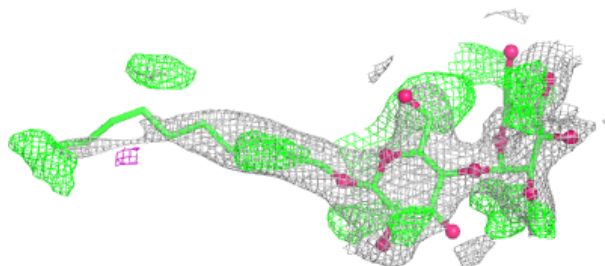


Electron density around DMU O 304:

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

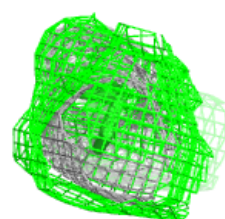
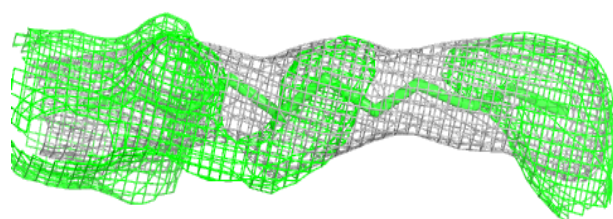
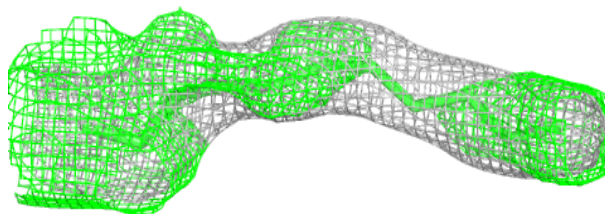
**Electron density around DMU P 314:**

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

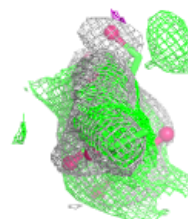
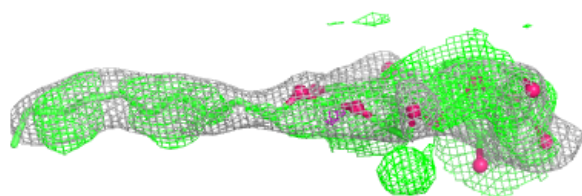
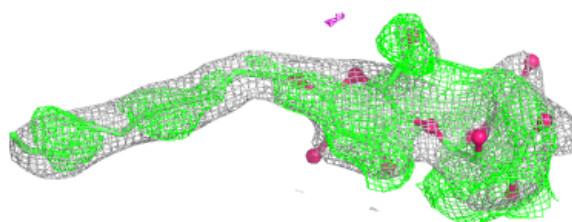


Electron density around LFA O 303:

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

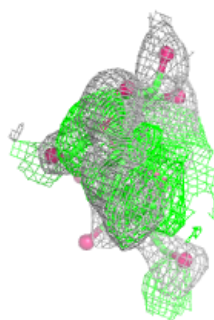
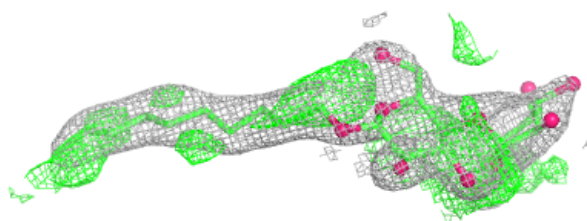
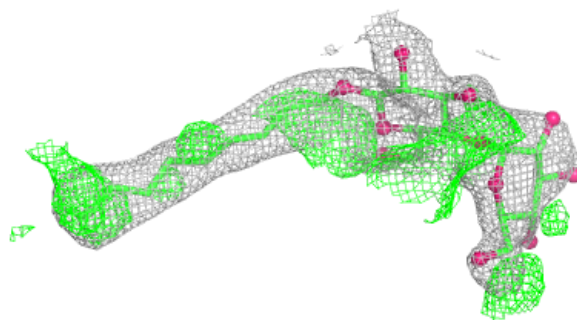
**Electron density around DMU P 317:**

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

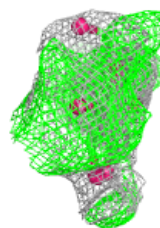
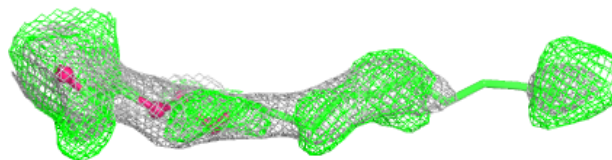
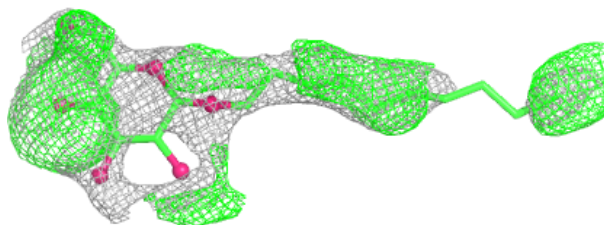


Electron density around DMU Q 201:

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

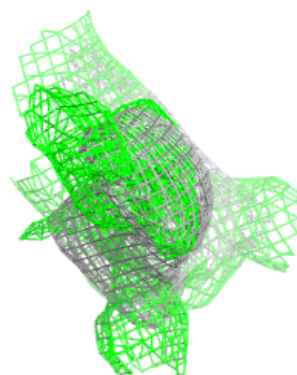
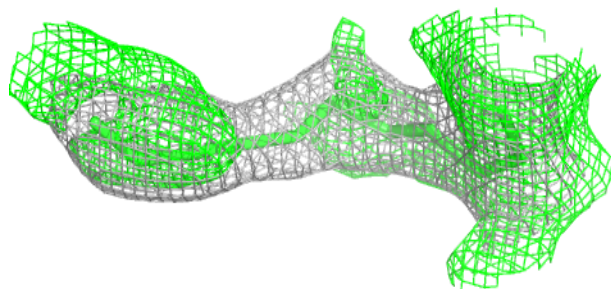
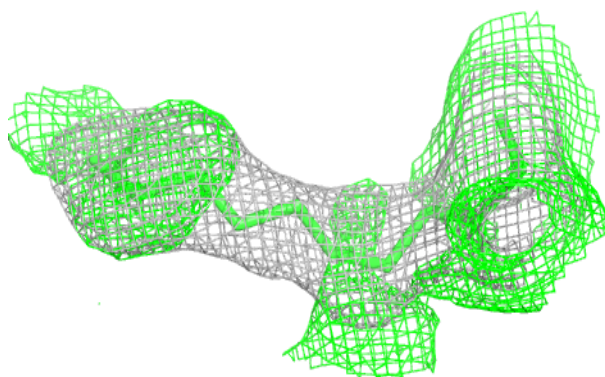
**Electron density around DMU Z 102:**

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

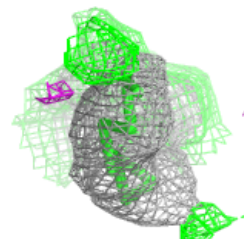
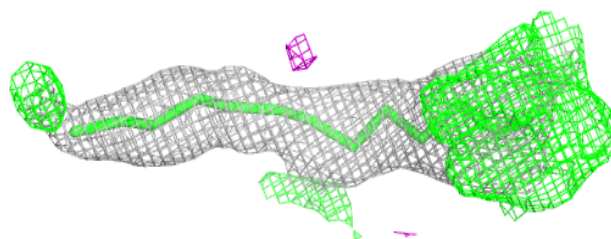
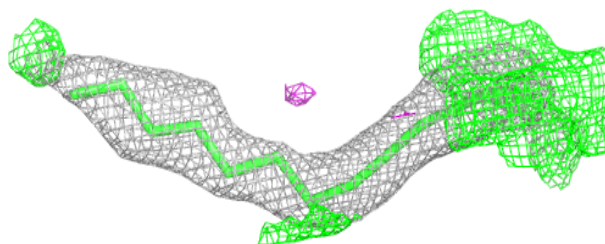


Electron density around LFA C 313:

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

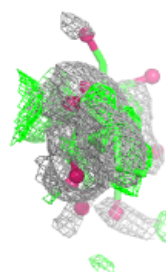
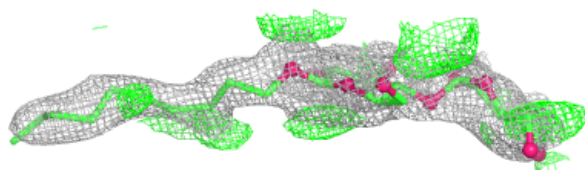
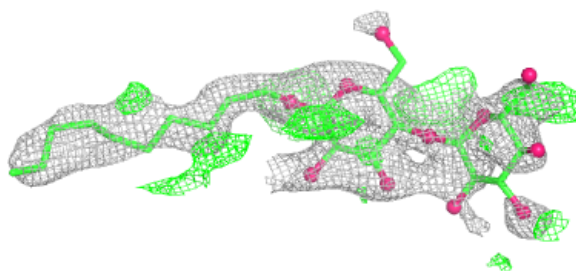
**Electron density around LFA C 315:**

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

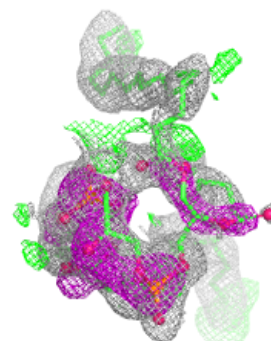
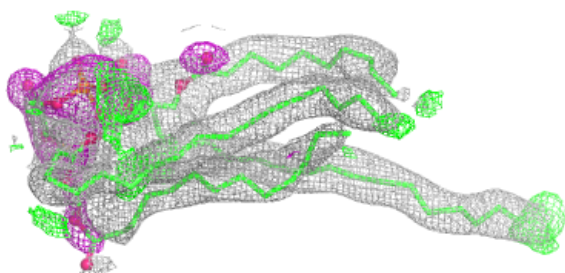
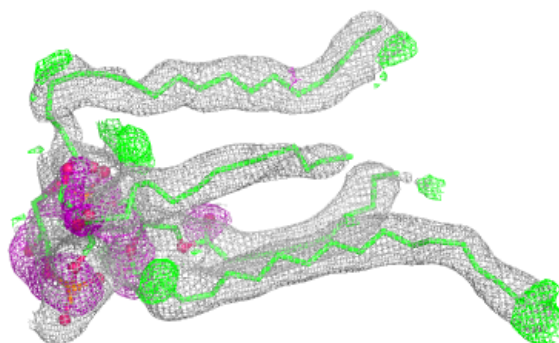


Electron density around DMU C 320:

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

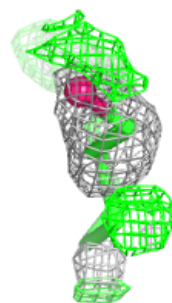
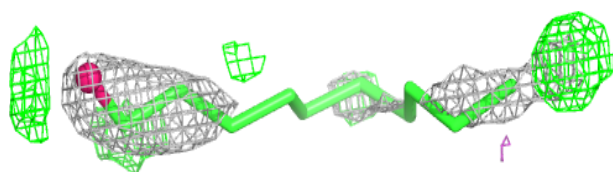
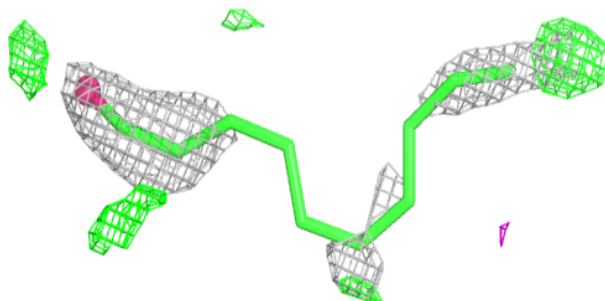
**Electron density around CDL C 304:**

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

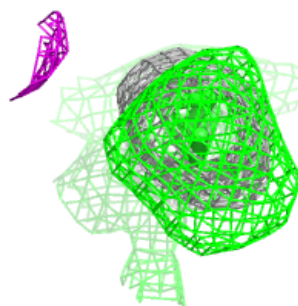
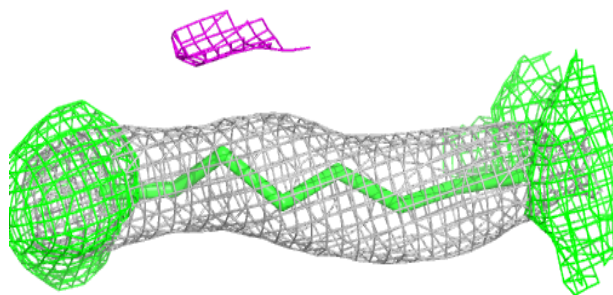
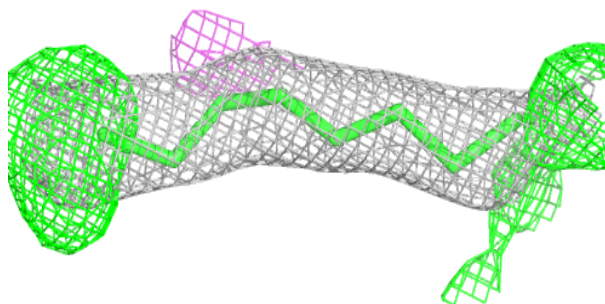


Electron density around DMU G 102:

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

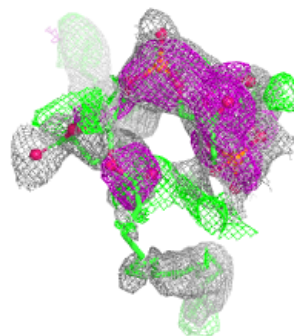
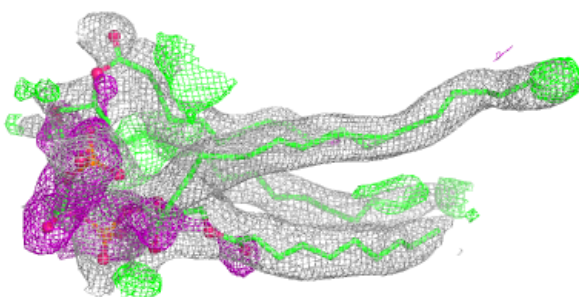
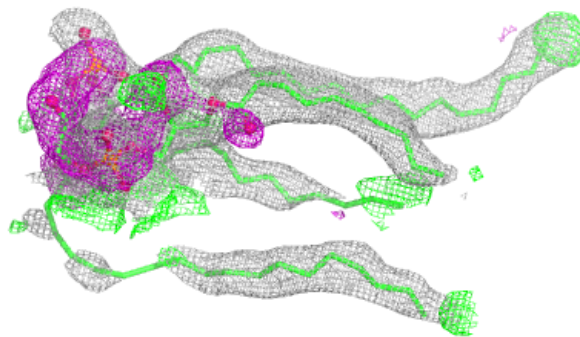
**Electron density around DMU M 102:**

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



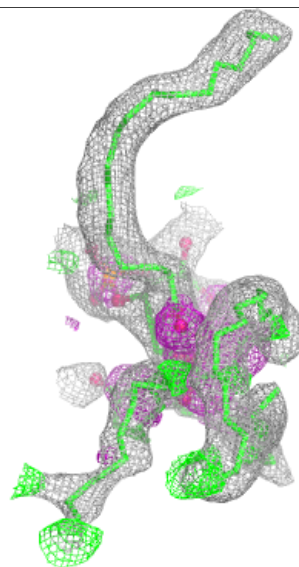
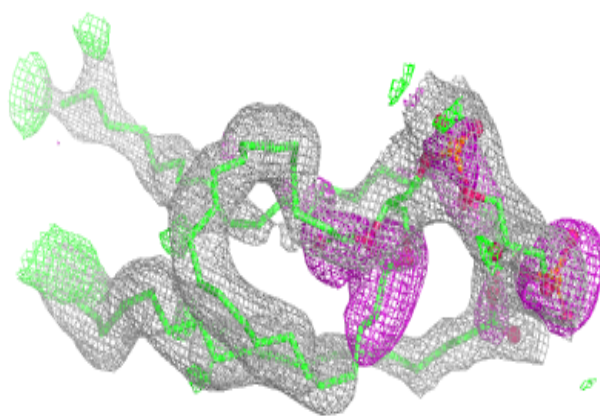
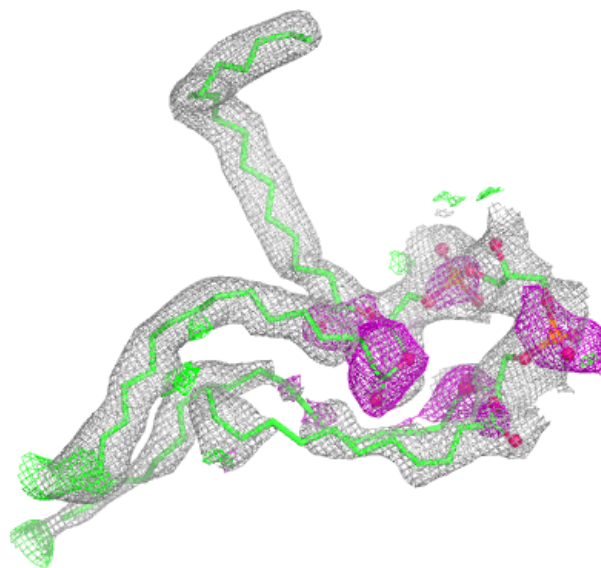
Electron density around CDL P 304:

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



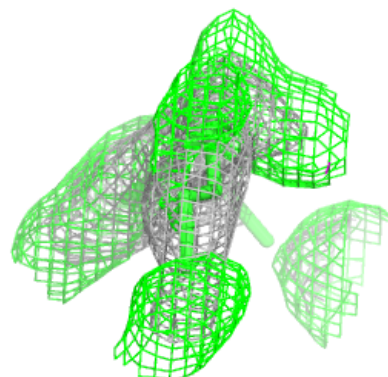
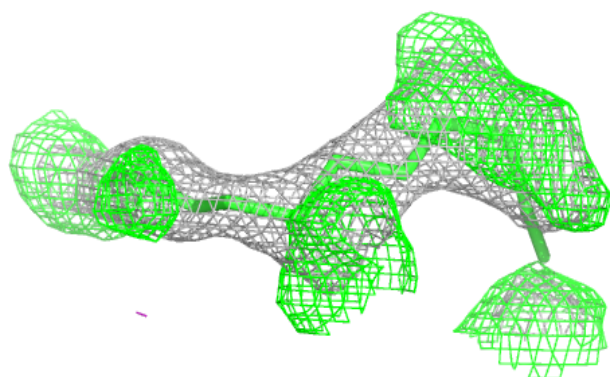
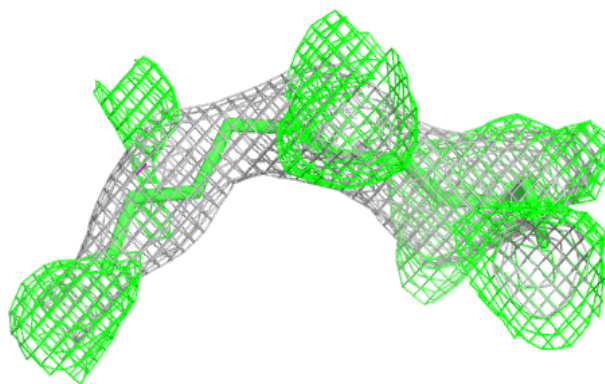
Electron density around CDL Y 101:

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

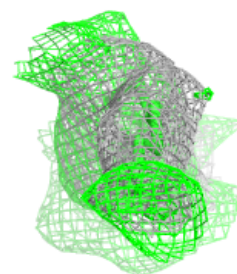
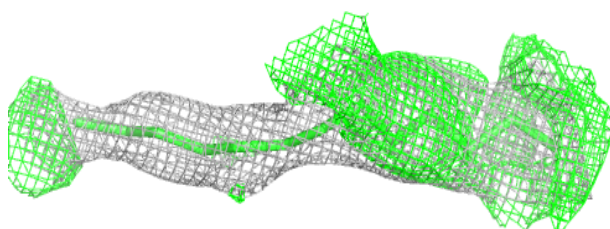
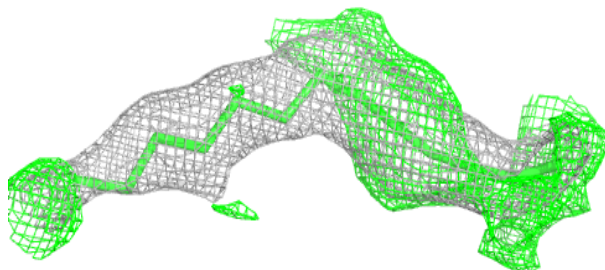


Electron density around LFA P 307:

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

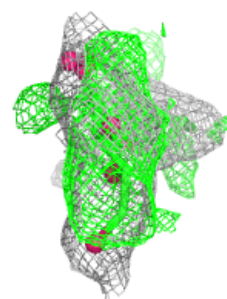
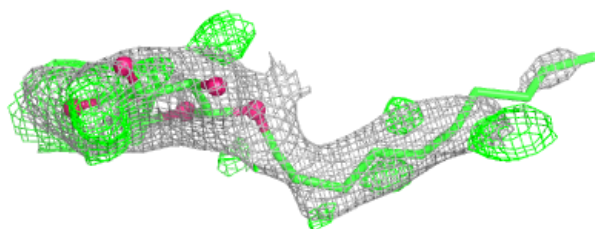
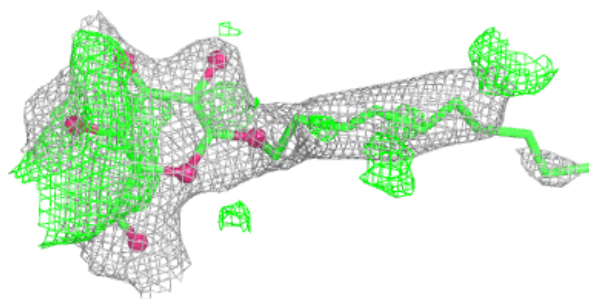
**Electron density around LFA P 313:**

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

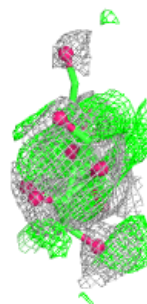
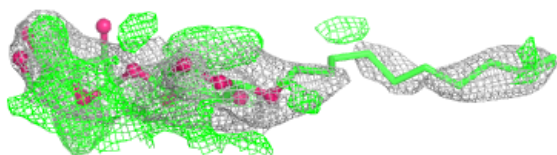
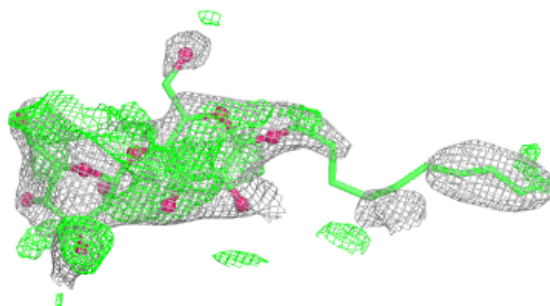


Electron density around DMU C 324:

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

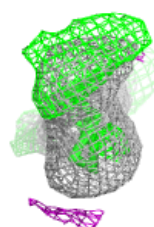
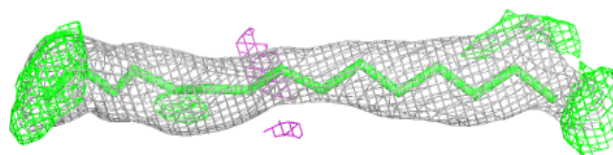
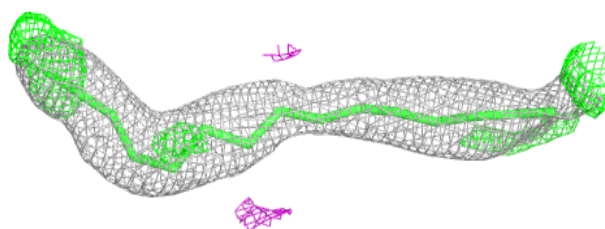
**Electron density around DMU P 318:**

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

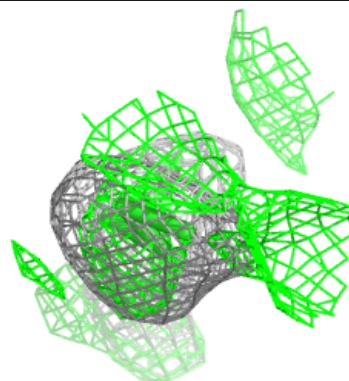
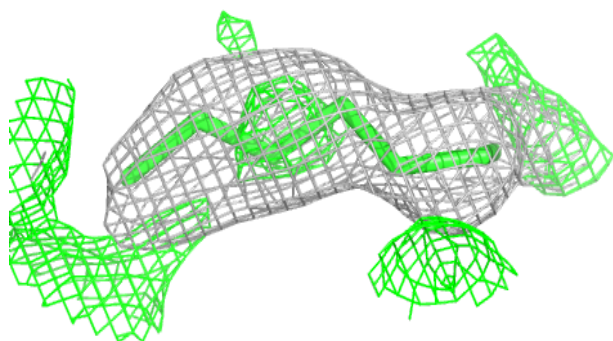
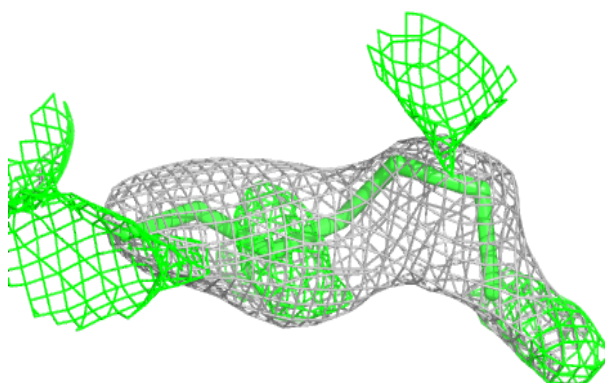


Electron density around LFA C 314:

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

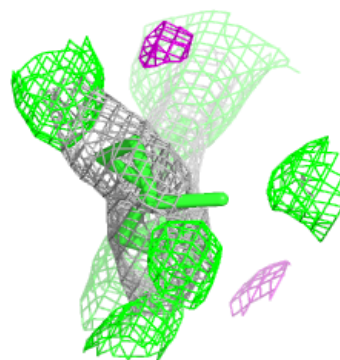
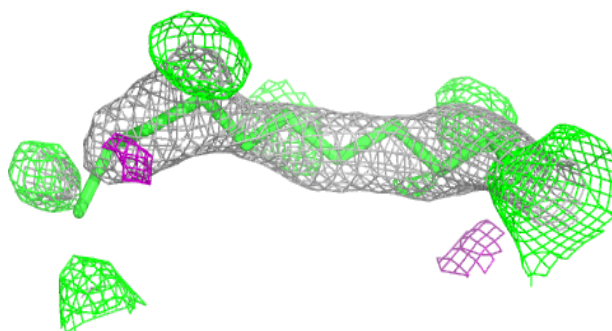
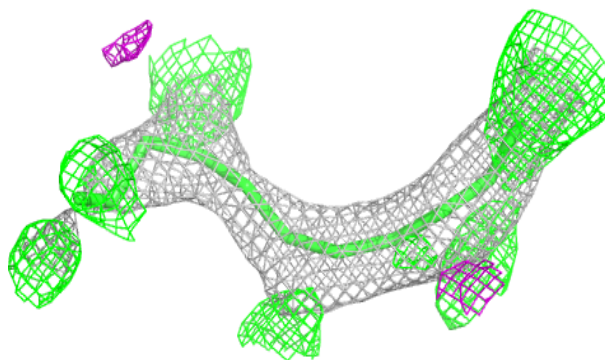
**Electron density around DMU C 317:**

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

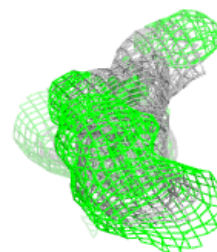
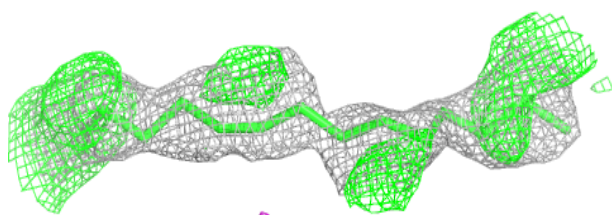
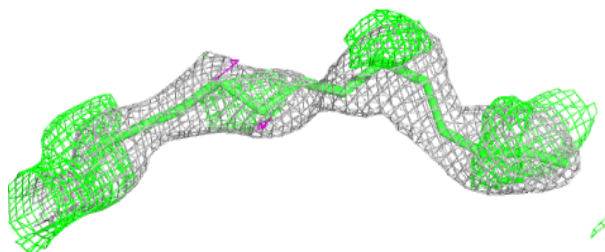


Electron density around LFA C 307:

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

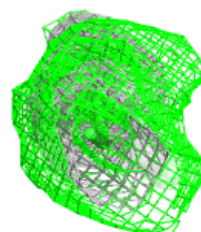
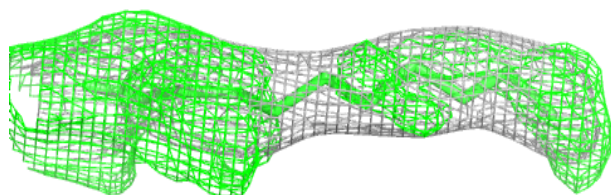
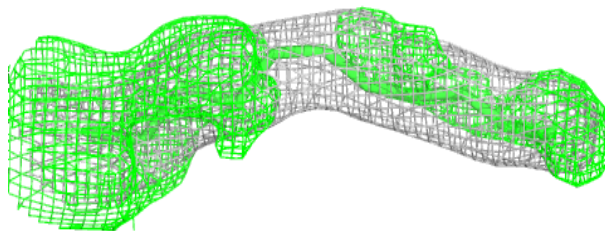
**Electron density around LFA T 103:**

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

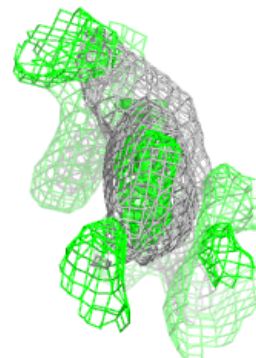
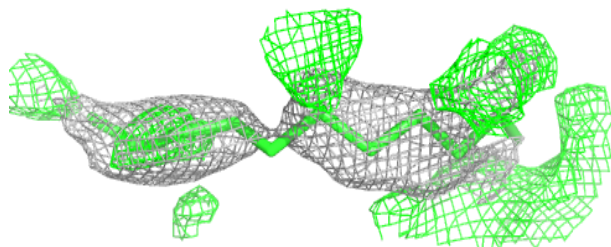
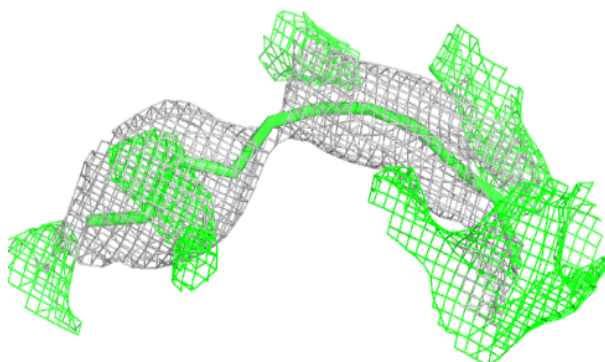


Electron density around LFA T 104:

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

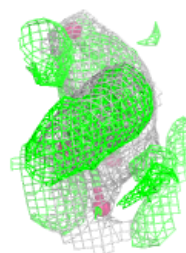
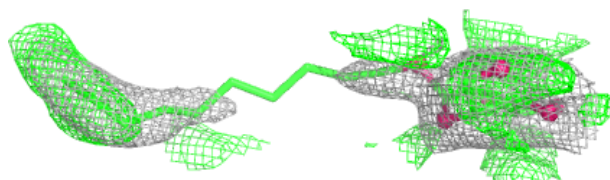
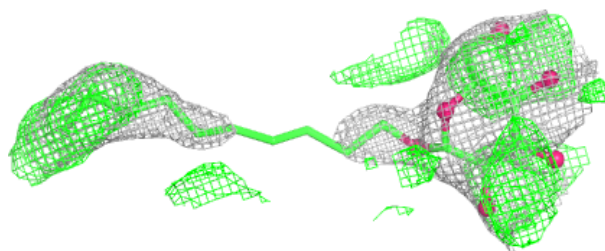
**Electron density around LFA C 311:**

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

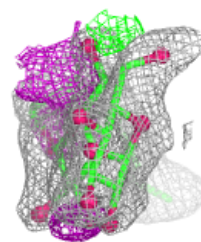
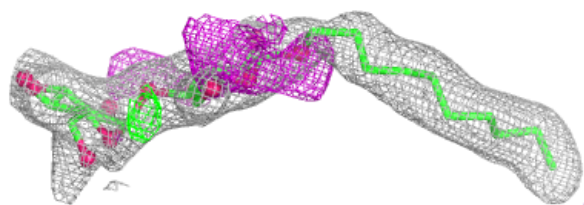
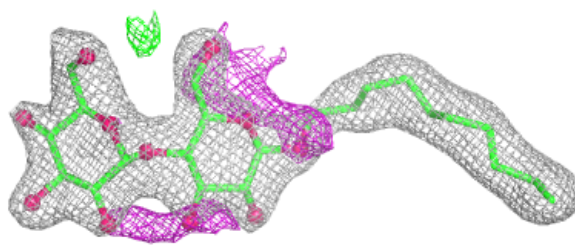


Electron density around DMU B 308:

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

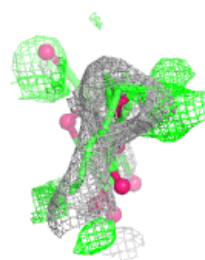
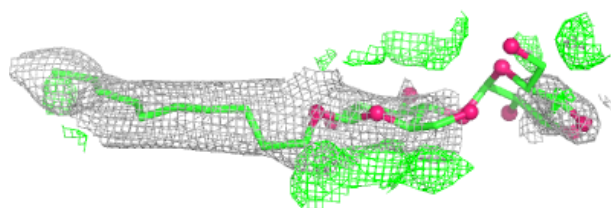
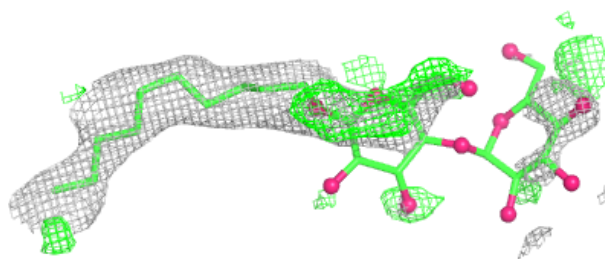
**Electron density around DMU Z 101:**

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

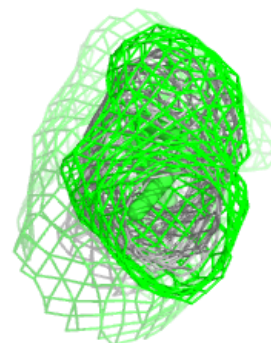
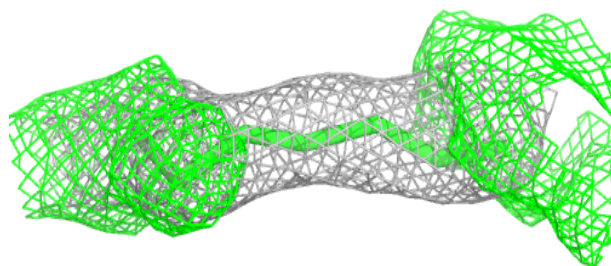
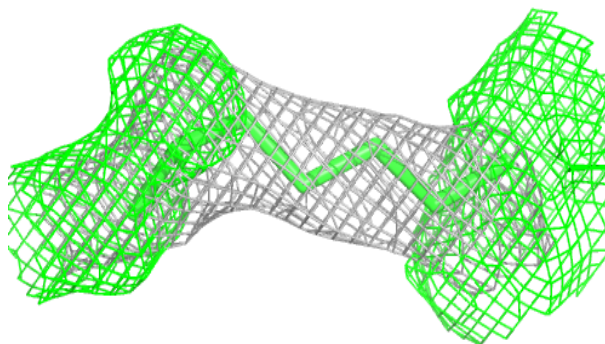


Electron density around DMU H 101:

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

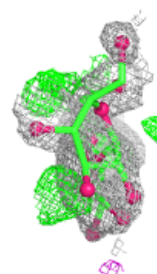
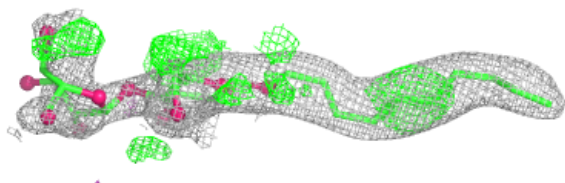
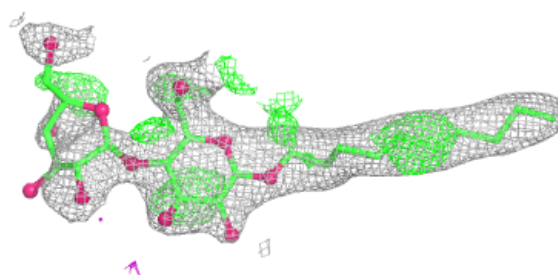
**Electron density around DMU N 609:**

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

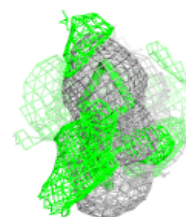
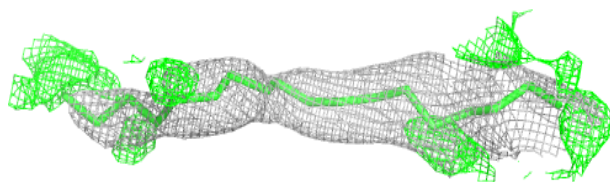
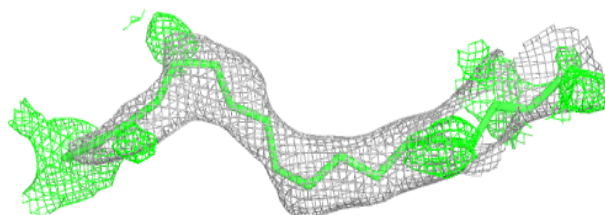


Electron density around DMU N 610:

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

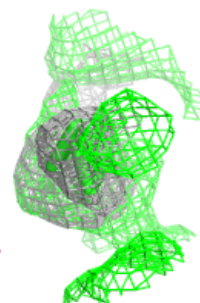
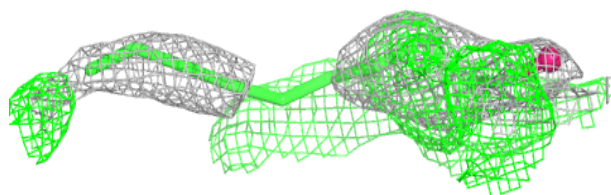
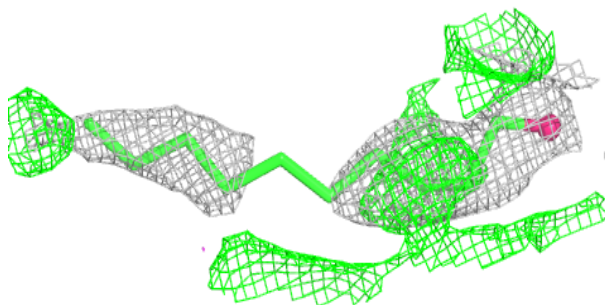
**Electron density around LFA P 309:**

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

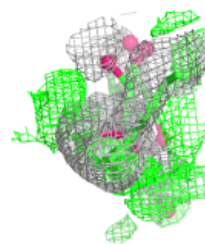
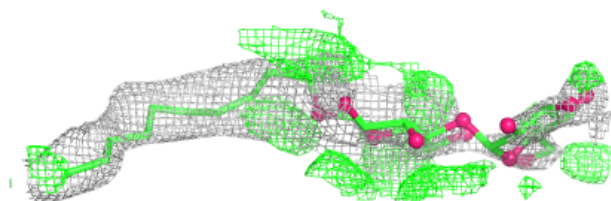
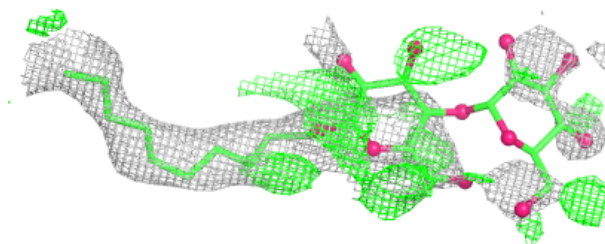


Electron density around DMU A 615:

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

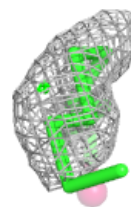
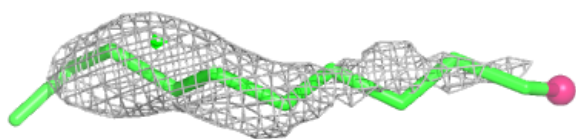
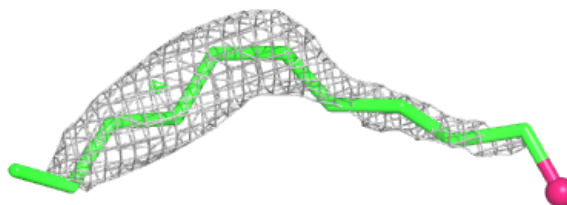
**Electron density around DMU U 101:**

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

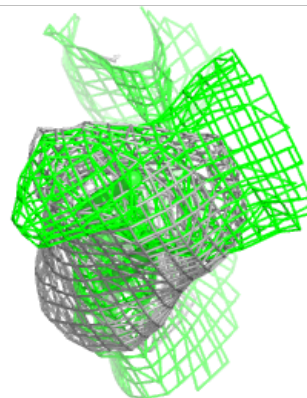
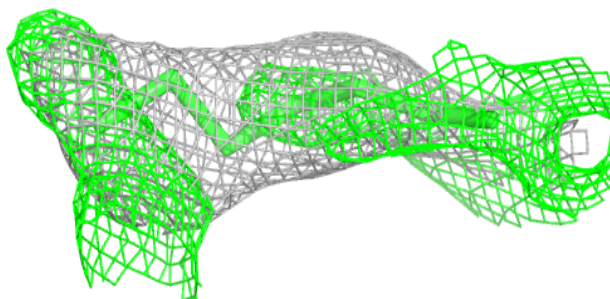
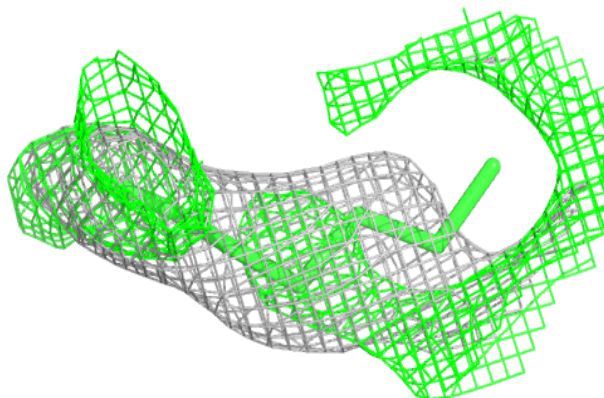


Electron density around DMU W 101:

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

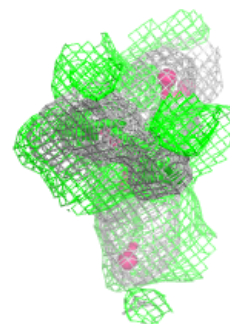
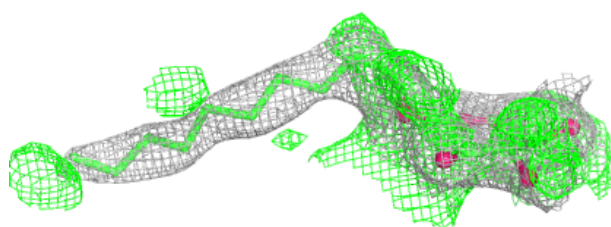
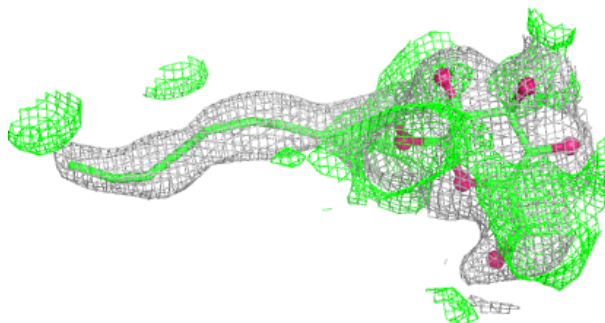
**Electron density around DMU P 315:**

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

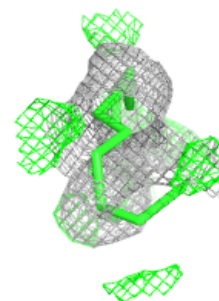
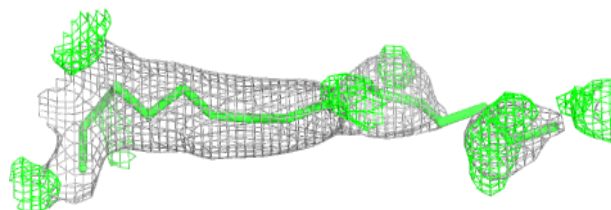
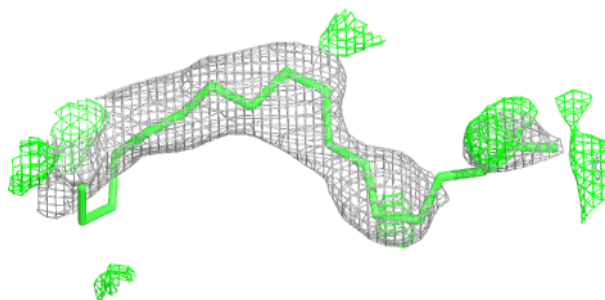


Electron density around DMU T 105:

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

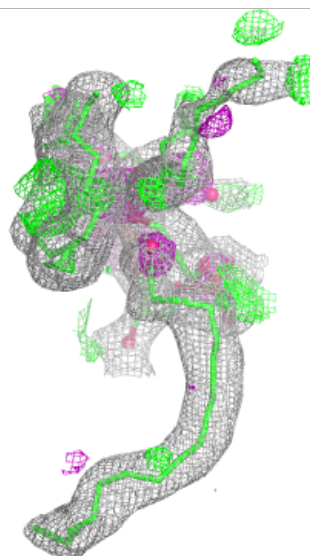
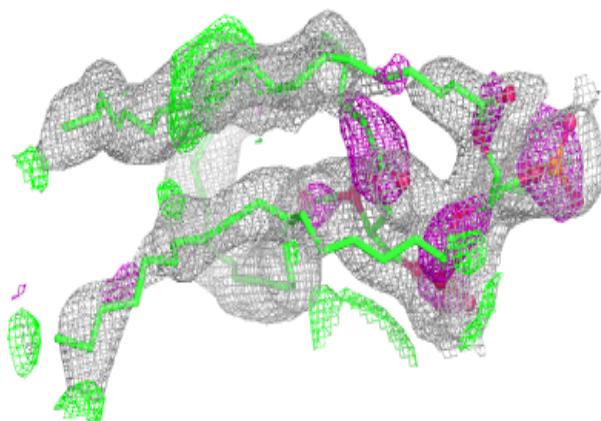
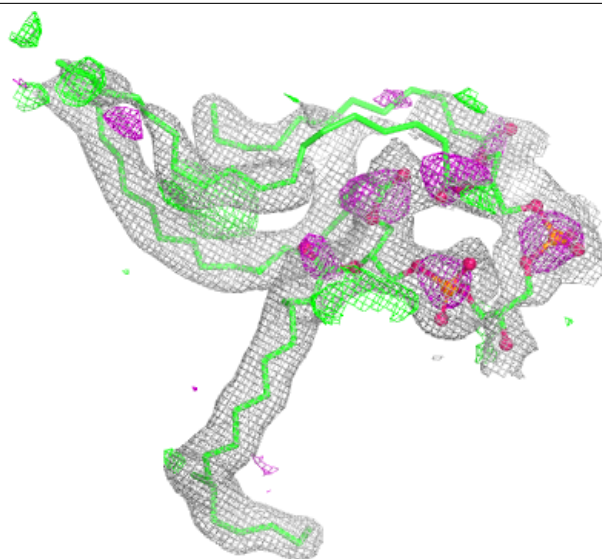
**Electron density around LFA C 309:**

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



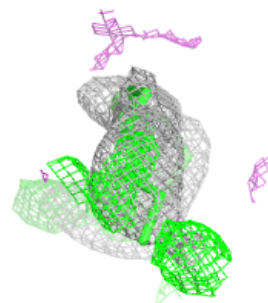
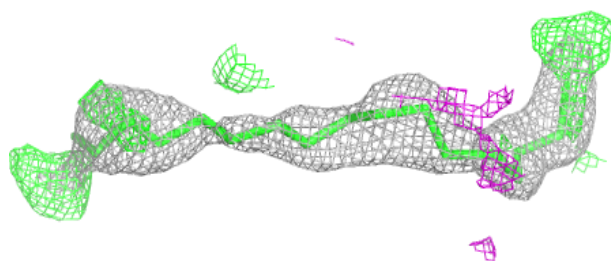
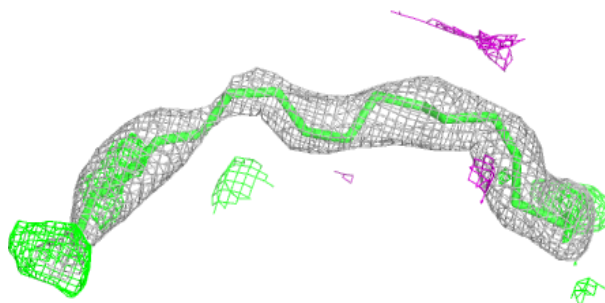
Electron density around CDL L 101:

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

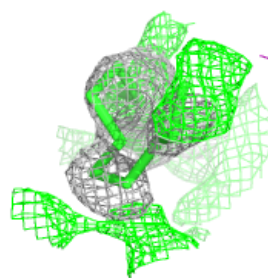
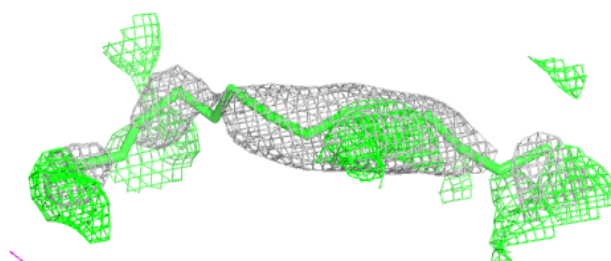
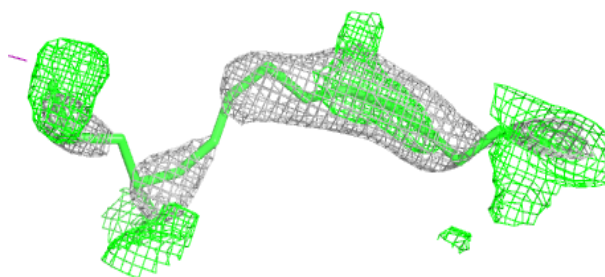


Electron density around LFA O 302:

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

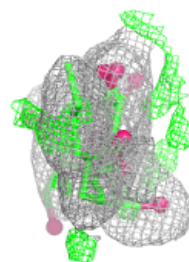
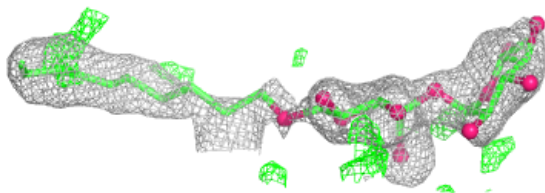
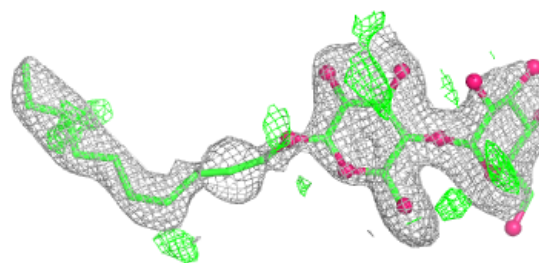
**Electron density around LFA C 310:**

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

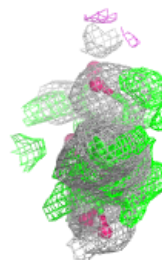
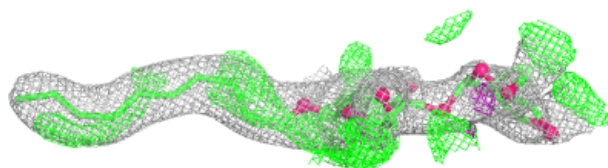
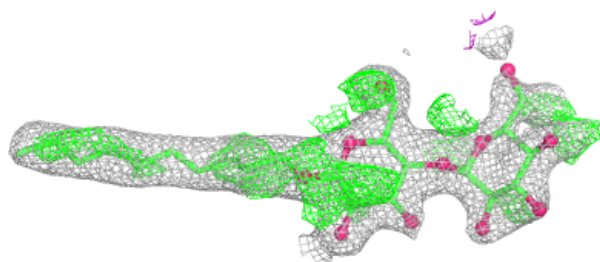


Electron density around DMU C 325:

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

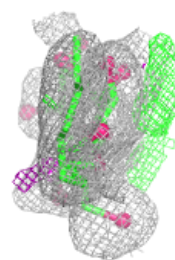
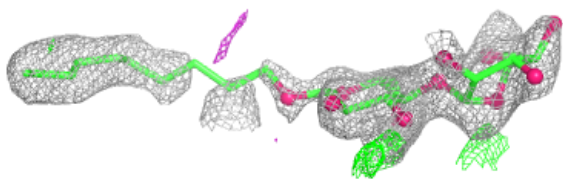
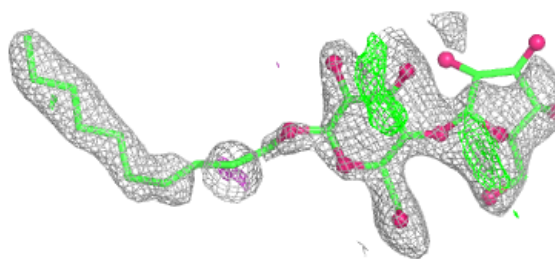
**Electron density around DMU A 609:**

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

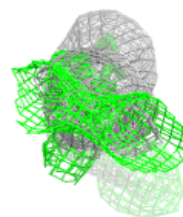
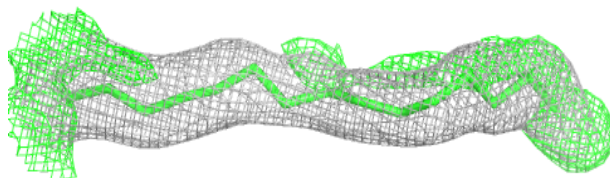
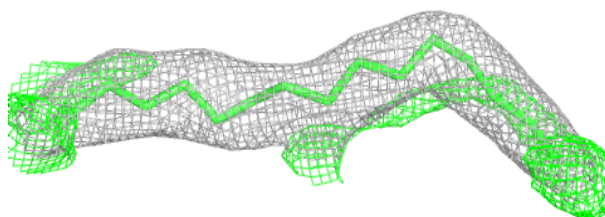


Electron density around DMU P 322:

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

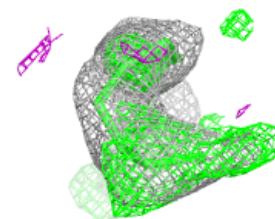
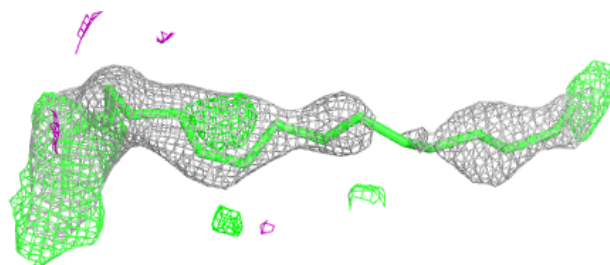
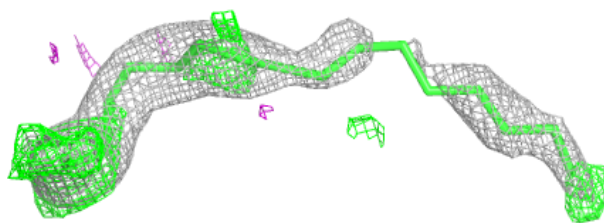
**Electron density around LFA P 312:**

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

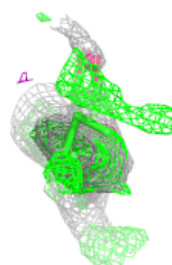
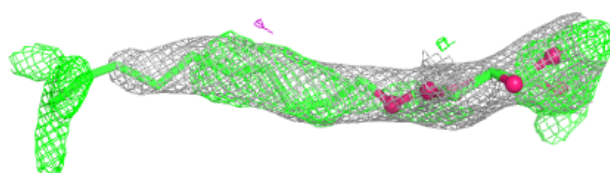
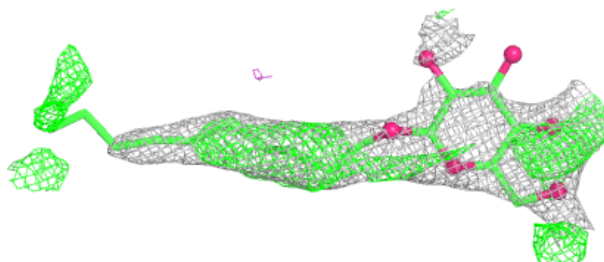


Electron density around LFA B 307:

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

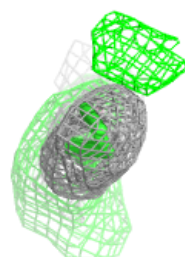
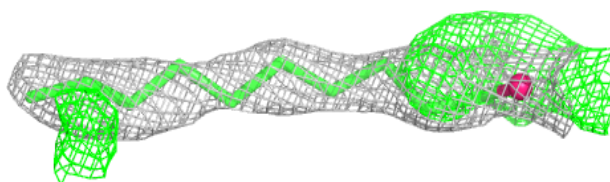
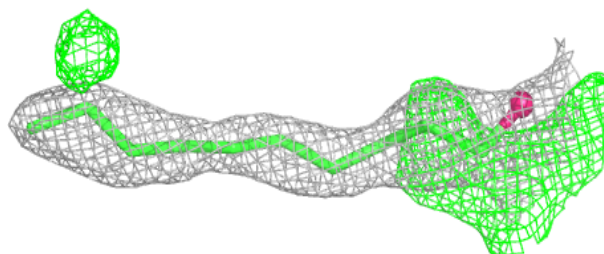
**Electron density around DMU L 102:**

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

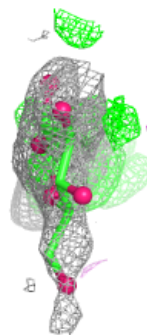
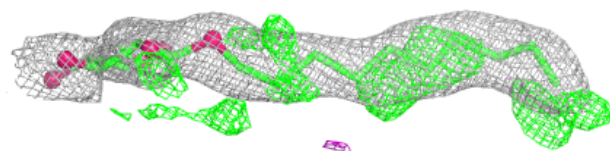
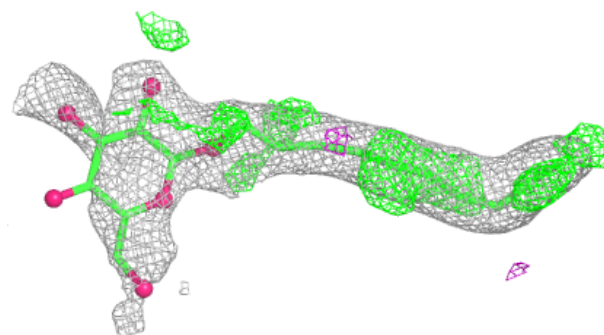


Electron density around DMU B 302:

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

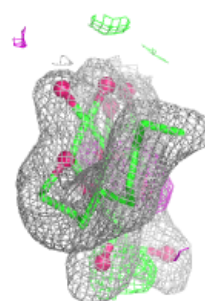
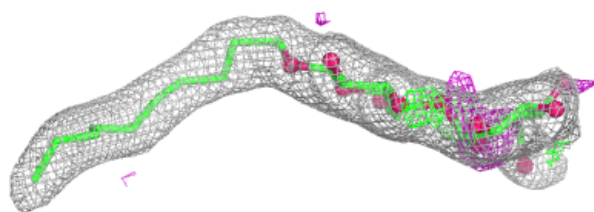
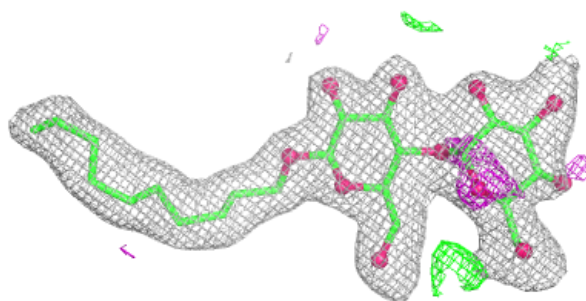
**Electron density around DMU B 304:**

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

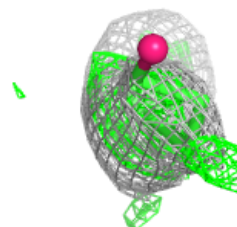
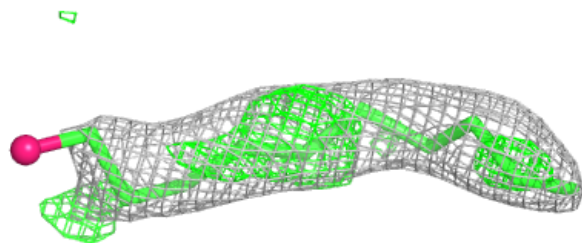
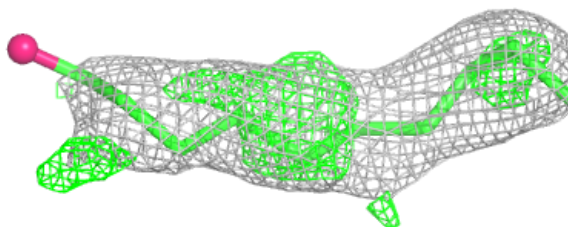


Electron density around DMU M 101:

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

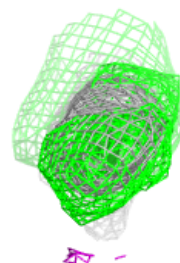
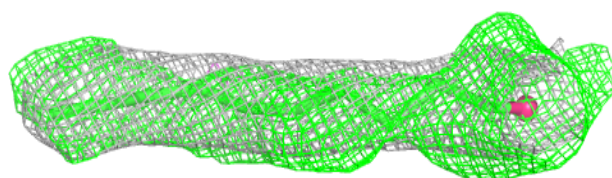
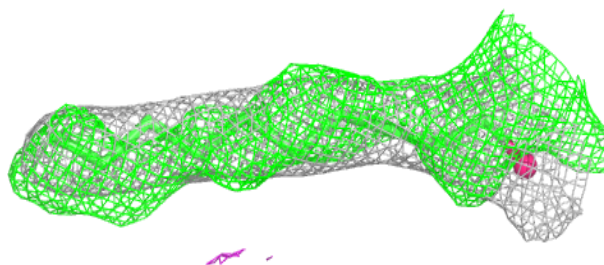
**Electron density around DMU J 101:**

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

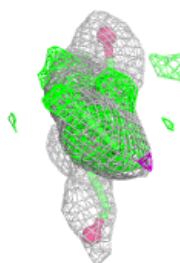
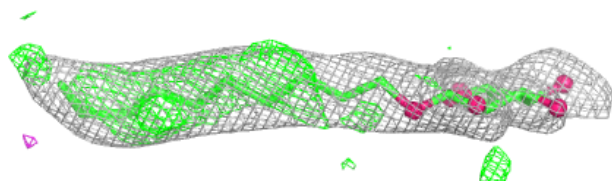
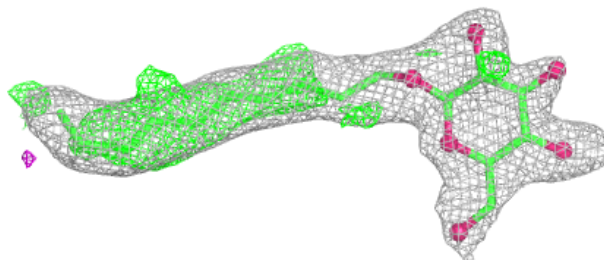


Electron density around DMU O 306:

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

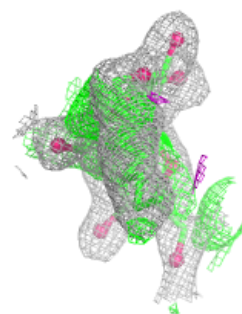
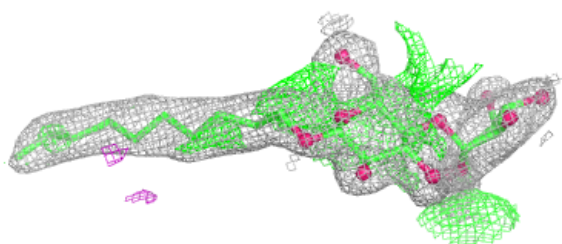
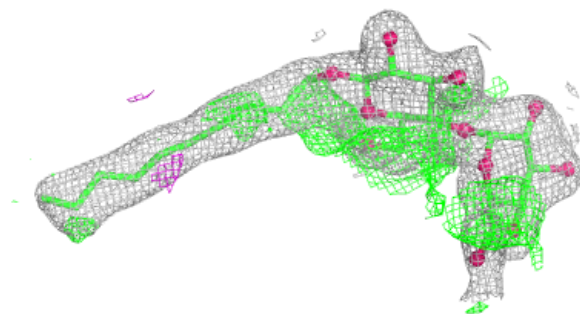
**Electron density around DMU O 308:**

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

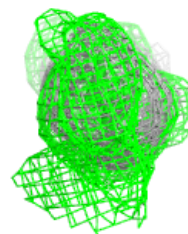
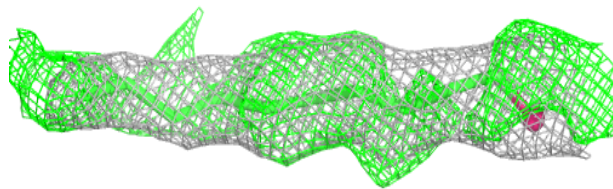
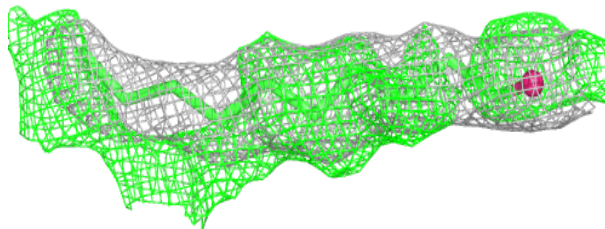


Electron density around DMU D 201:

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

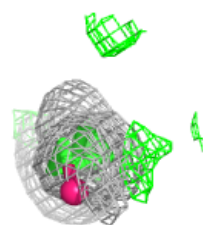
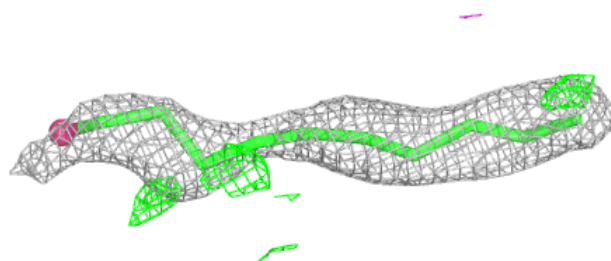
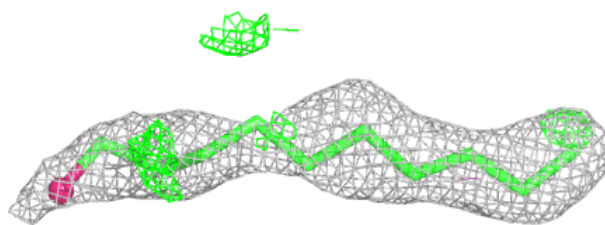
**Electron density around DMU P 306:**

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

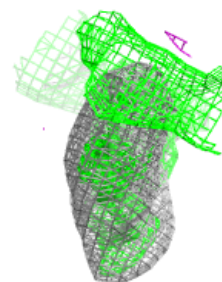
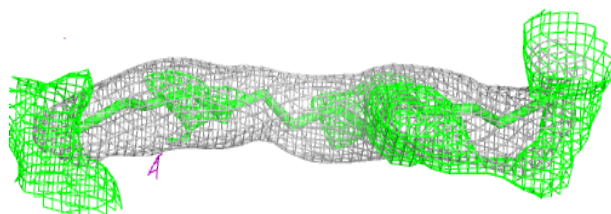
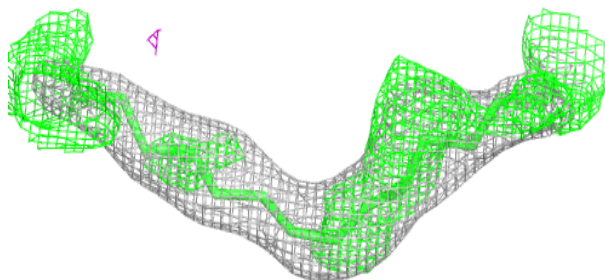


Electron density around DMU B 303:

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

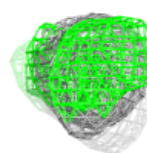
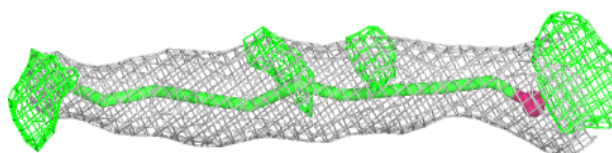
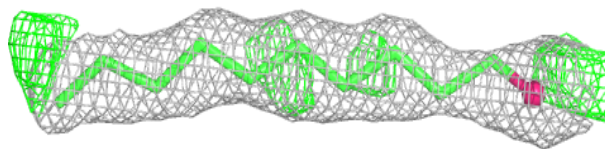
**Electron density around LFA A 607:**

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

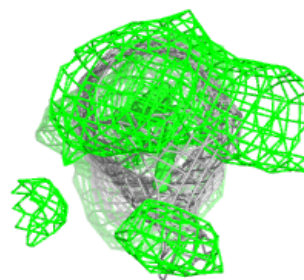
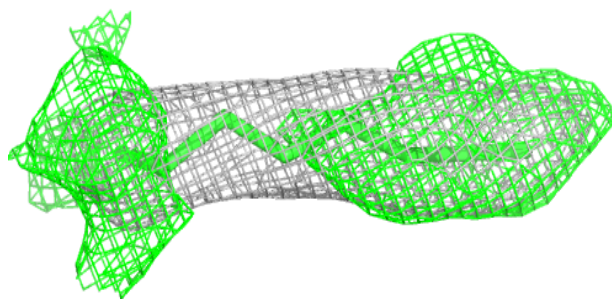
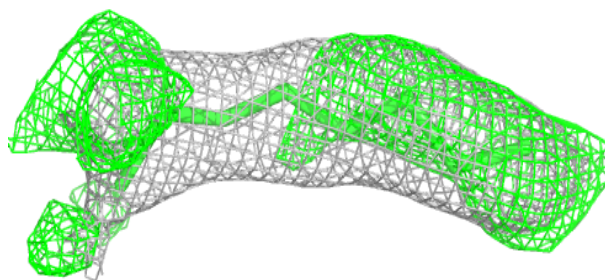


Electron density around DMU C 306:

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

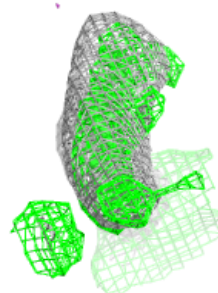
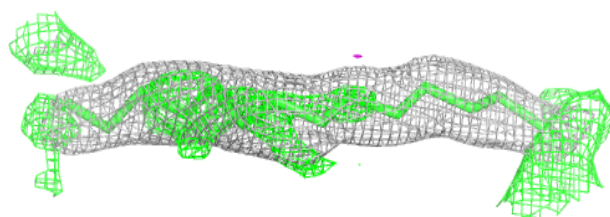
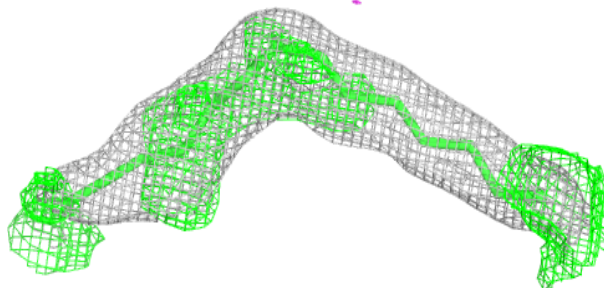
**Electron density around DMU Z 103:**

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

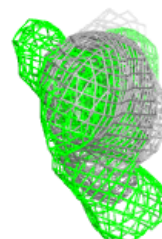
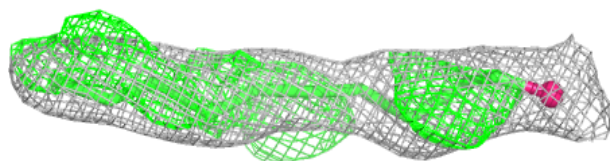
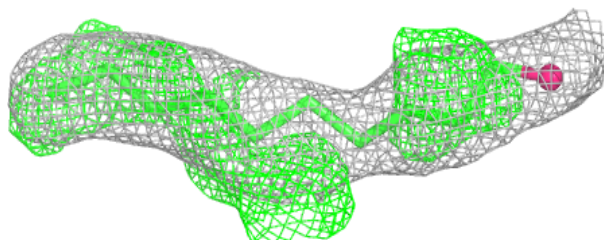


Electron density around LFA N 608:

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

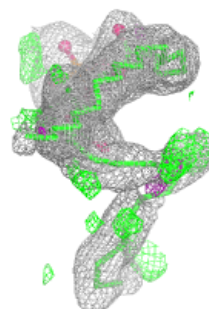
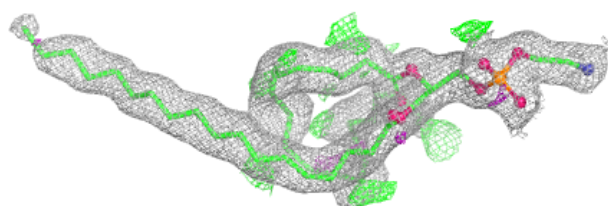
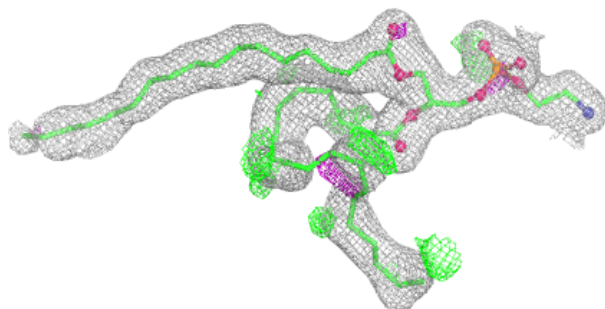
**Electron density around DMU O 307:**

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

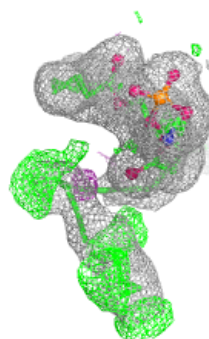
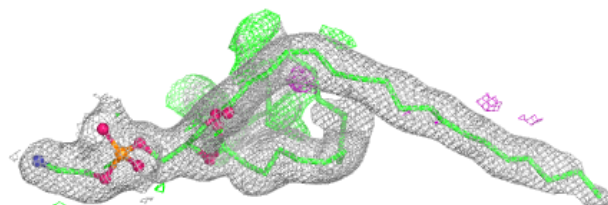
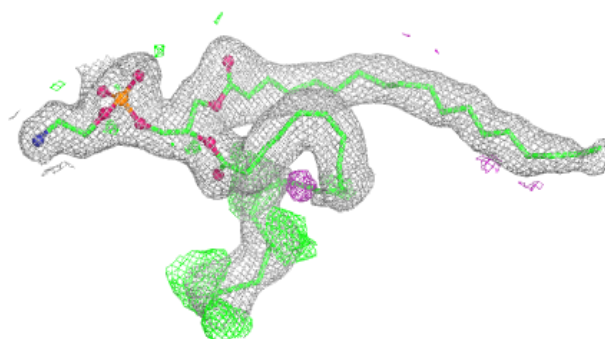


Electron density around PEK T 102:

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

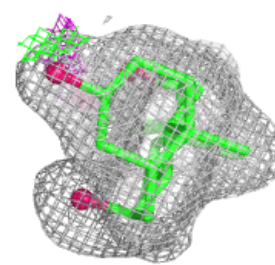
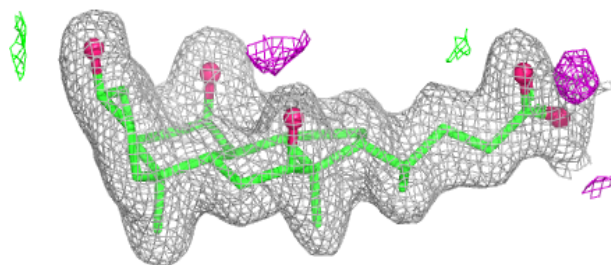
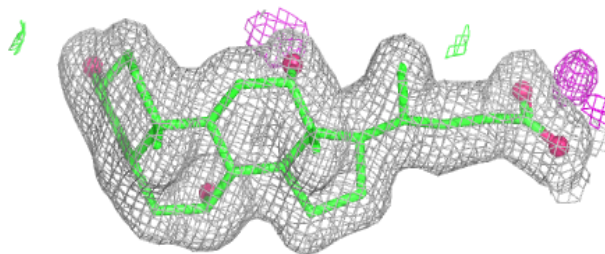
**Electron density around PEK G 101:**

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

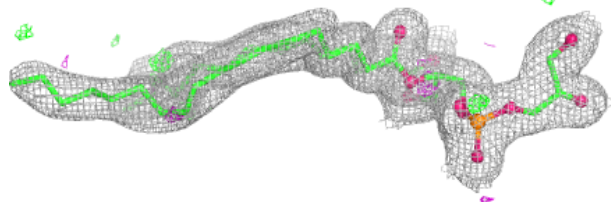
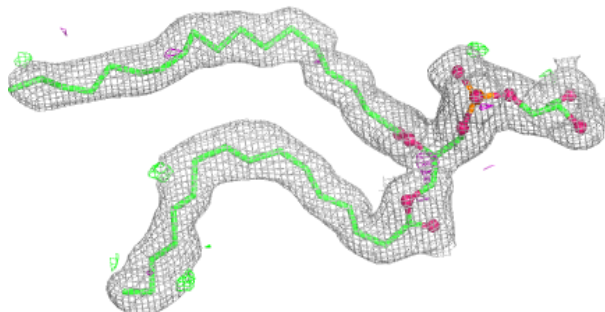


Electron density around CHD C 301:

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

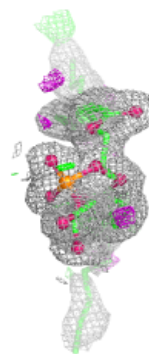
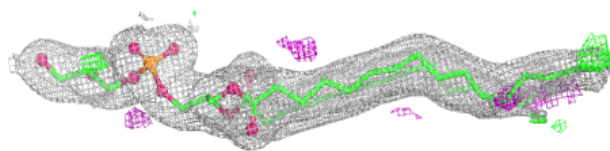
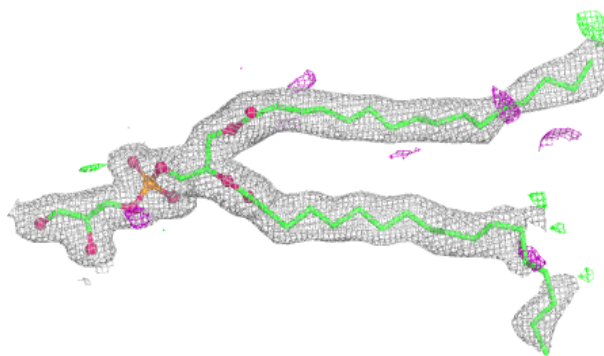
**Electron density around PGV N 616:**

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

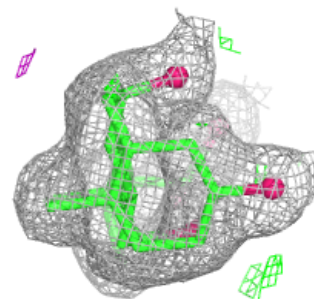
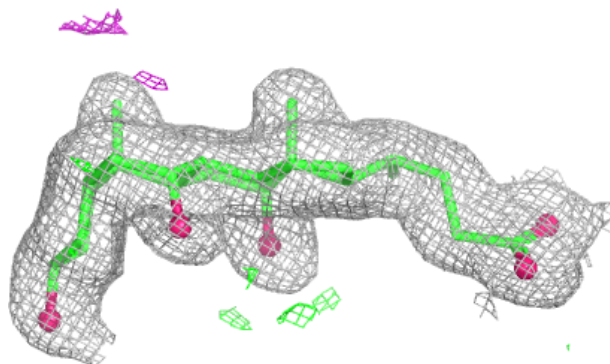
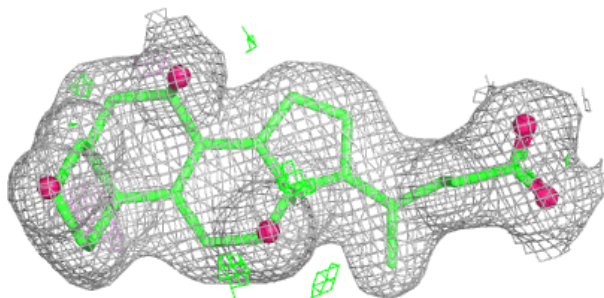


Electron density around PGV P 303:

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

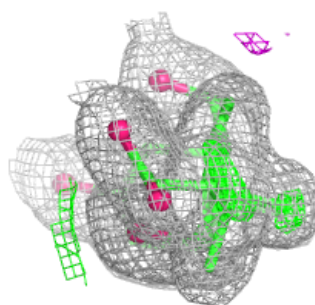
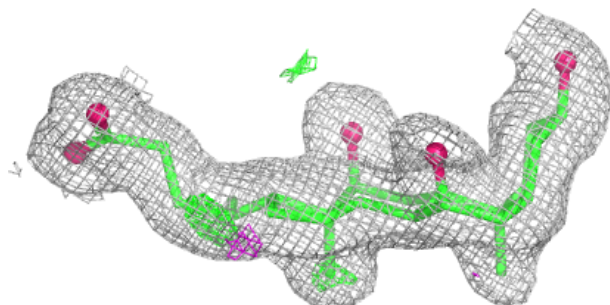
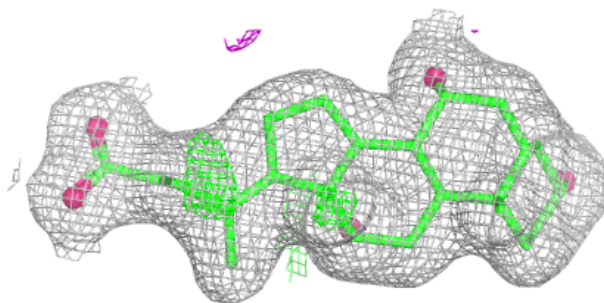
**Electron density around CHD B 306:**

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

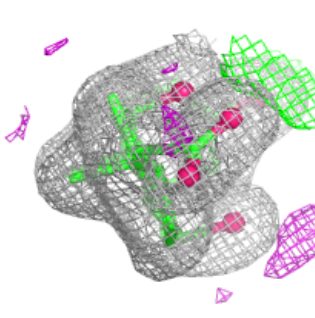
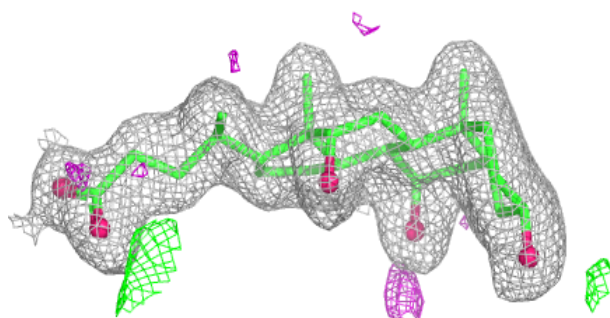
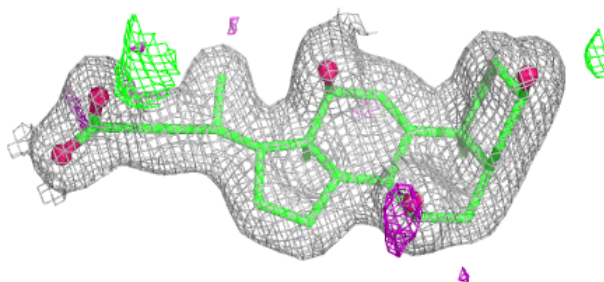


Electron density around CHD O 301:

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

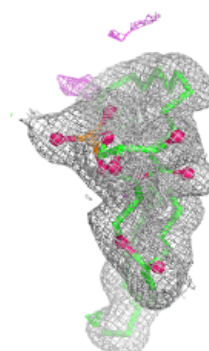
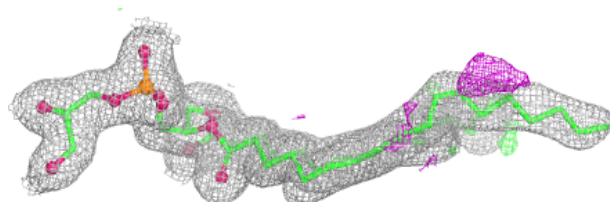
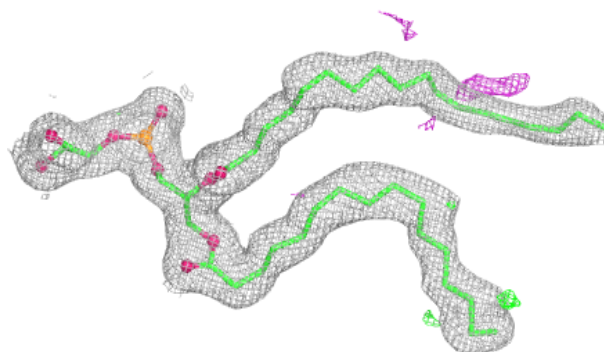
**Electron density around CHD P 301:**

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

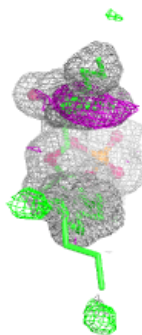
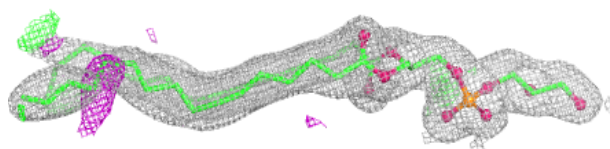
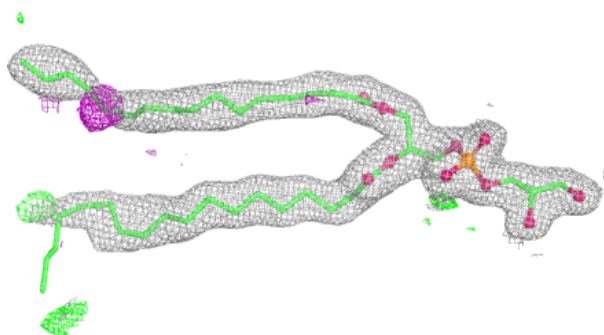


Electron density around PGV A 614:

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

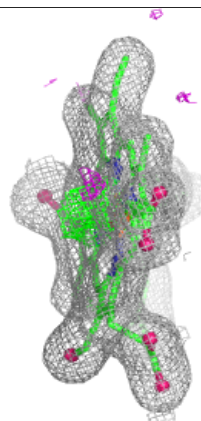
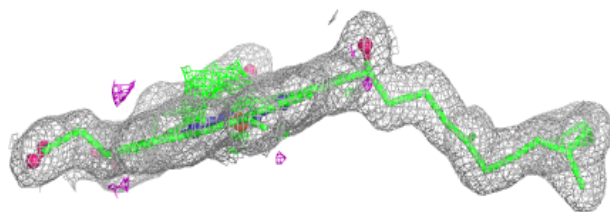
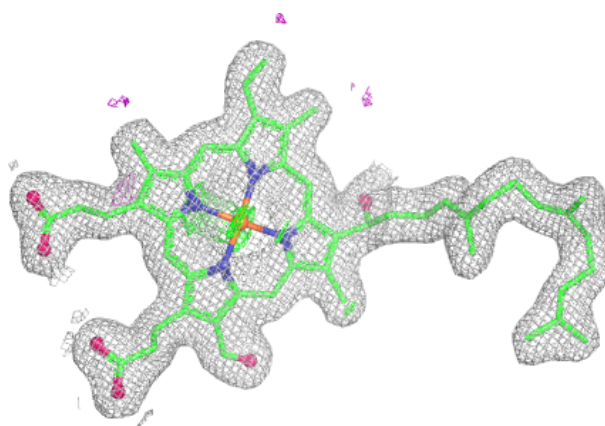
**Electron density around PGV C 303:**

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



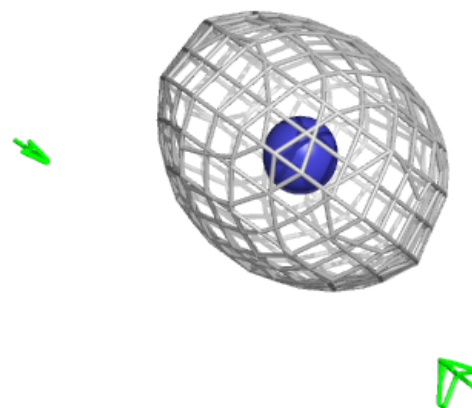
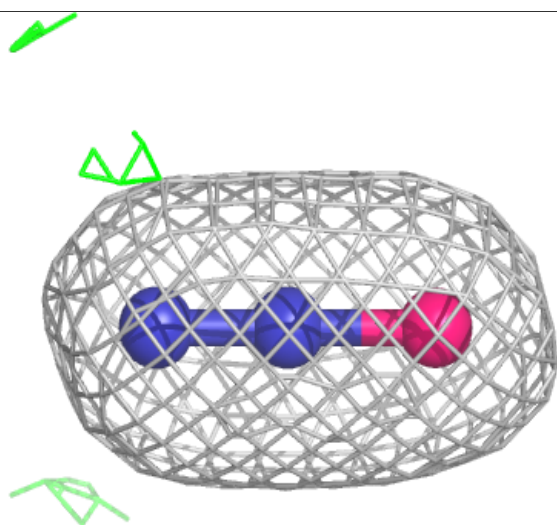
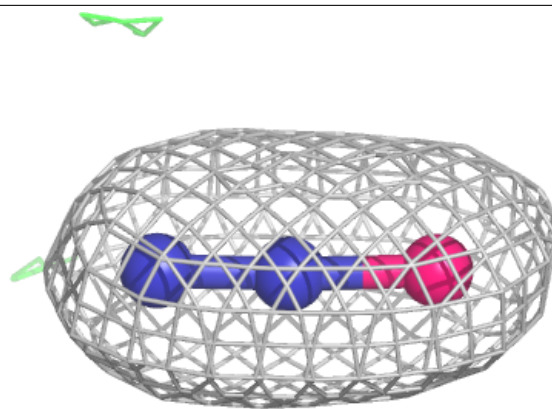
Electron density around HEA N 602:

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



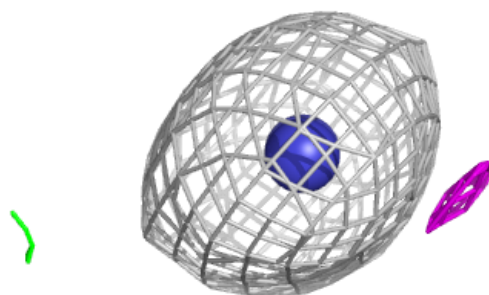
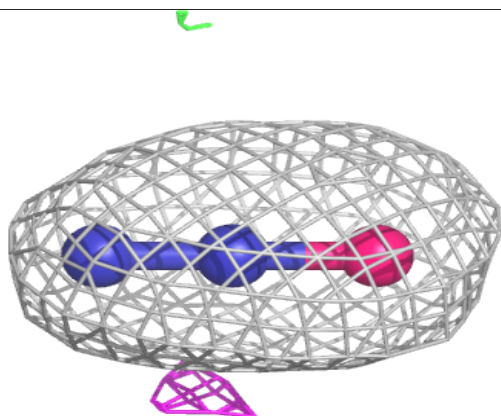
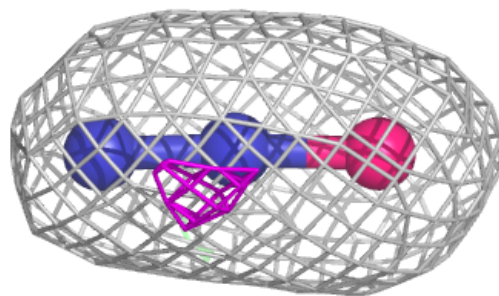
Electron density around N2O A 606:

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

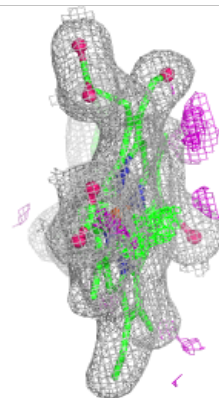
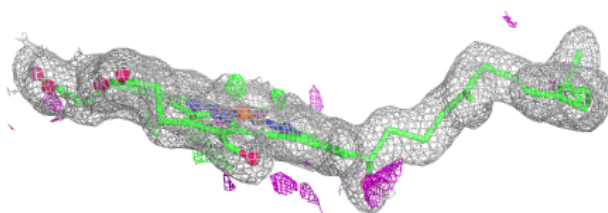
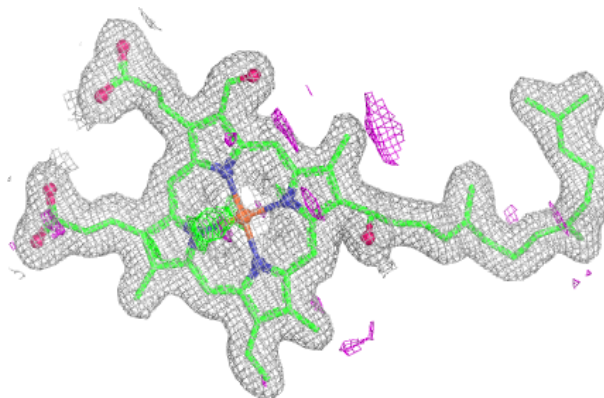


Electron density around N2O N 607:

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

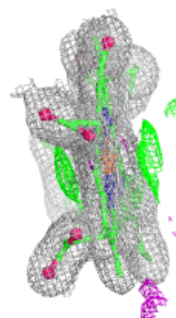
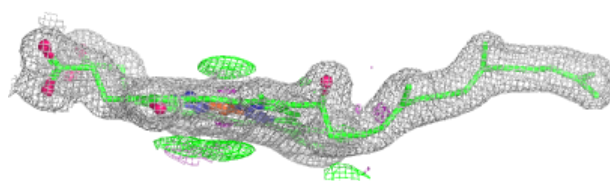
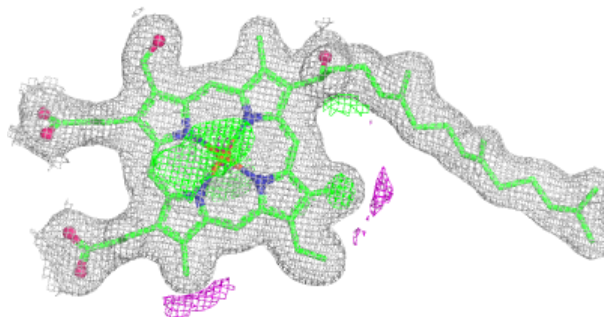
**Electron density around HEA A 602:**

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

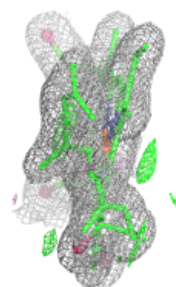
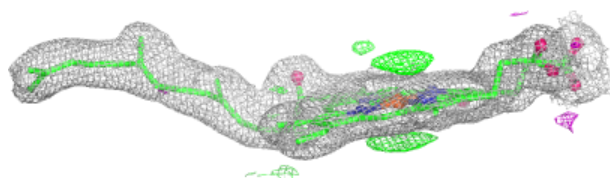
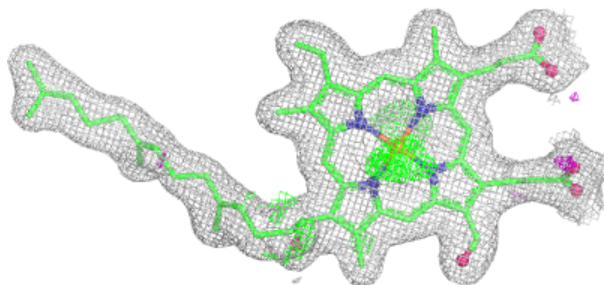


Electron density around HEA A 601:

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

**Electron density around HEA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.