



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2025 – 02:51 PM JST

PDB ID : 9IKH / pdb_00009ikh
Title : Bovine Heart Cytochrome c Oxidase in the Nitrous Oxide-bound Fully Oxidized 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 Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

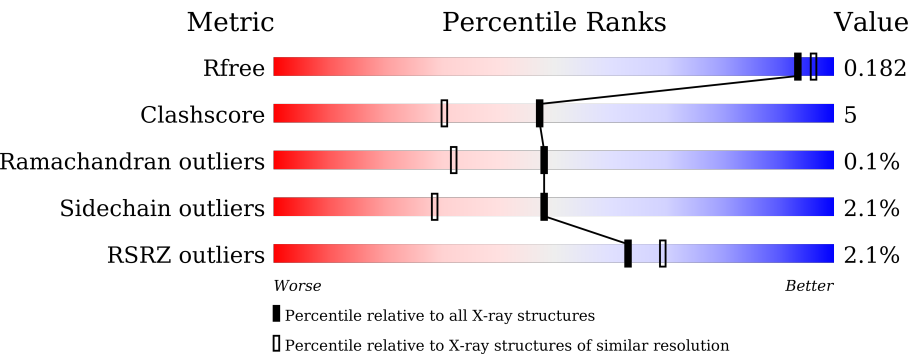
1 Overall quality at a glance i

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}	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (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	<div><div></div><div>90%9%</div><div></div></div>
1	N	514	<div><div>%</div><div>90%9%</div><div></div></div>
2	B	227	<div><div>5%</div><div>81%16%</div><div></div></div>
2	O	227	<div><div>3%</div><div>83%15%</div><div></div></div>
3	C	261	<div><div></div><div>89%10%</div><div></div></div>
3	P	261	<div><div></div><div>85%13%</div><div></div></div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	LFA	C	308	-	-	-	X
20	LFA	P	311	-	-	-	X
21	DMU	N	610	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 33055 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

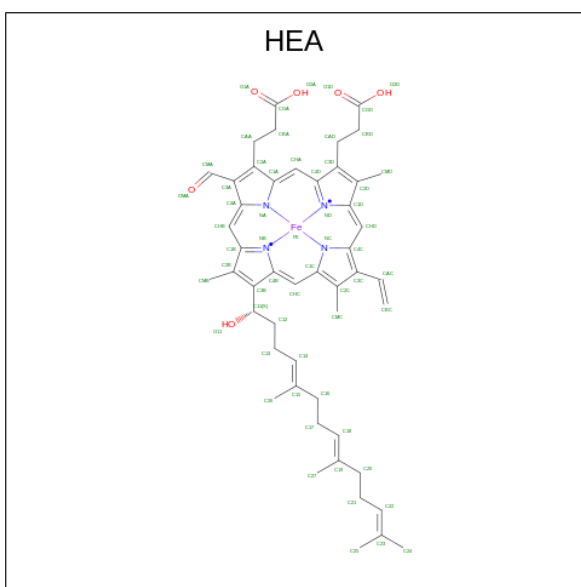
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

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



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

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

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

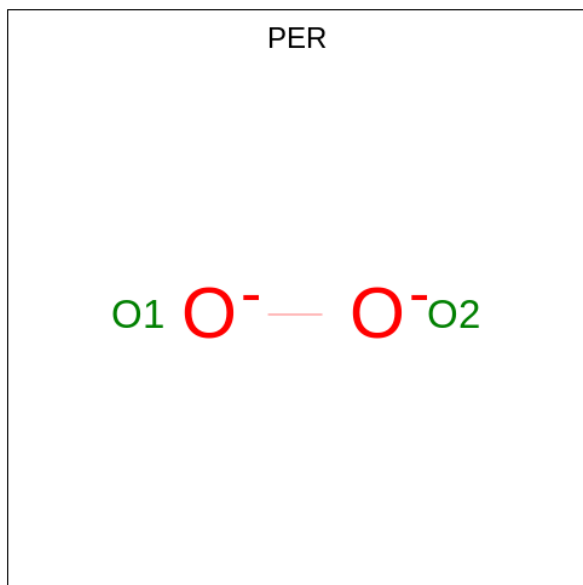
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

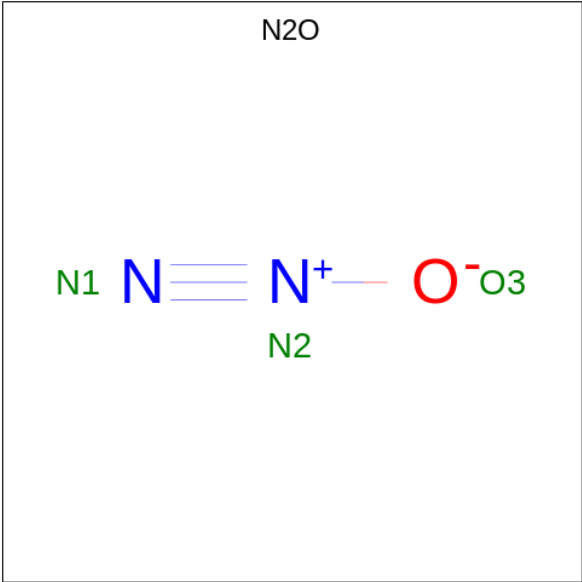
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total 1	Na 1	0	0
17	N	1	Total 1	Na 1	0	0

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



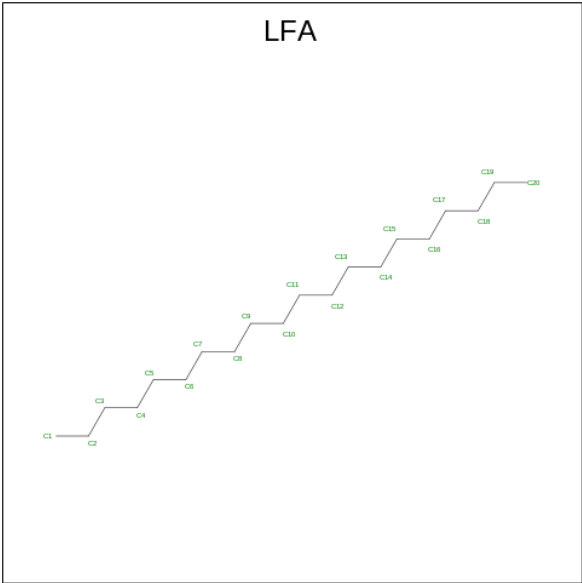
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total 2	O 2	0	0
18	N	1	Total 2	O 2	0	0

- Molecule 19 is NITROUS OXIDE (CCD ID: N2O) (formula: N₂O) (labeled as "Ligand of Interest" by depositor).



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

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	C	0	0
			14	14		
20	A	1	Total	C	0	0
			14	14		

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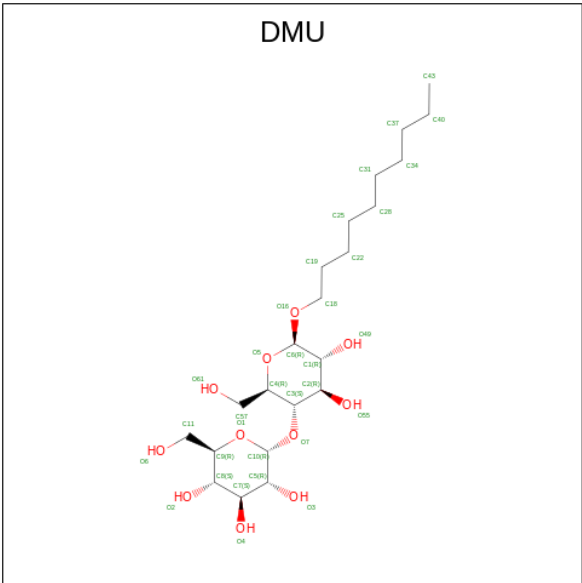
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	B	1	Total C 17 17	0	0
20	C	1	Total C 11 11	0	0
20	C	1	Total C 6 6	0	0
20	C	1	Total C 18 18	0	0
20	C	1	Total C 11 11	0	0
20	C	1	Total C 14 14	0	0
20	C	1	Total C 11 11	0	0
20	C	1	Total C 15 15	0	0
20	C	1	Total C 13 13	0	0
20	C	1	Total C 15 15	0	0
20	G	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	P	1	Total C 13 13	0	0
20	T	1	Total C 14 14	0	0
20	T	1	Total C 11 11	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 7 7	0	0
21	A	1	Total C O 33 22 11	0	0
21	A	1	Total C O 11 10 1	0	0
21	B	1	Total C O 11 10 1	0	0
21	B	1	Total C O 11 10 1	0	0
21	B	1	Total C O 22 16 6	0	0
21	B	1	Total C O 22 16 6	0	0
21	C	1	Total C O 11 10 1	0	0

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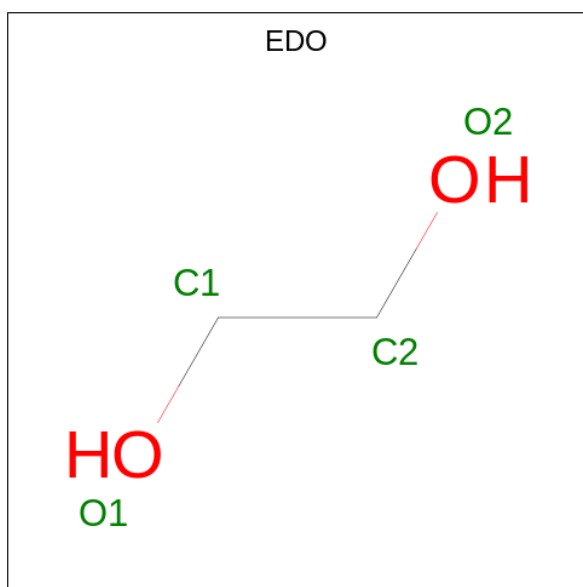
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	C	1	Total C O 33 22 11	0	0
21	C	1	Total C 7 7	0	0
21	C	1	Total C O 22 16 6	0	0
21	C	1	Total C O 33 22 11	0	0
21	C	1	Total C O 33 22 11	0	0
21	C	1	Total C O 22 16 6	0	0
21	C	1	Total C O 33 22 11	0	0
21	D	1	Total C O 33 22 11	0	0
21	H	1	Total C O 33 22 11	0	0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

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

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



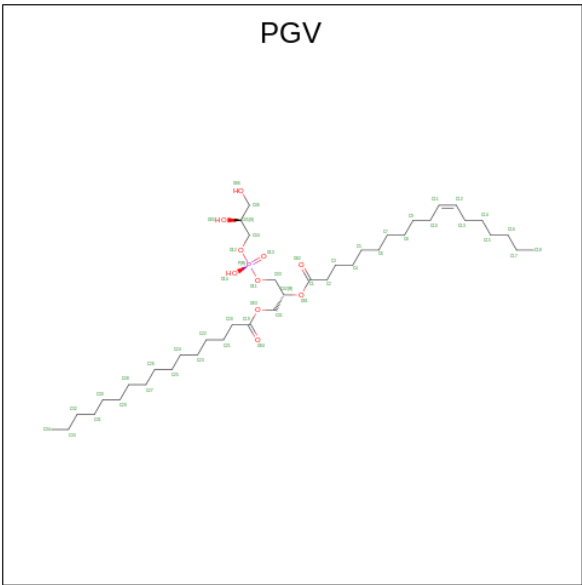
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			4	2	2		
22	A	1	Total	C	O	0	0
			4	2	2		
22	A	1	Total	C	O	0	0
			4	2	2		
22	A	1	Total	C	O	0	0
			4	2	2		
22	B	1	Total	C	O	0	0
			4	2	2		
22	C	1	Total	C	O	0	0
			4	2	2		
22	C	1	Total	C	O	0	0
			4	2	2		
22	C	1	Total	C	O	0	0
			4	2	2		
22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

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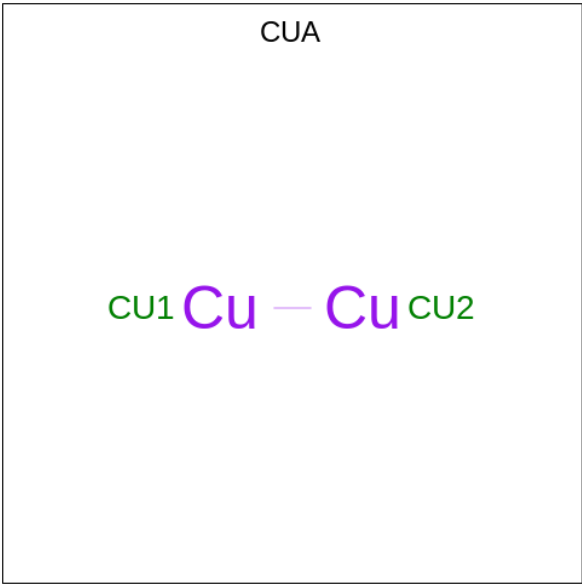
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	O	1	Total 4	C 2	O 2	0	0
22	P	1	Total 4	C 2	O 2	0	0
22	P	1	Total 4	C 2	O 2	0	0
22	P	1	Total 4	C 2	O 2	0	0
22	R	1	Total 4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

- Molecule 23 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



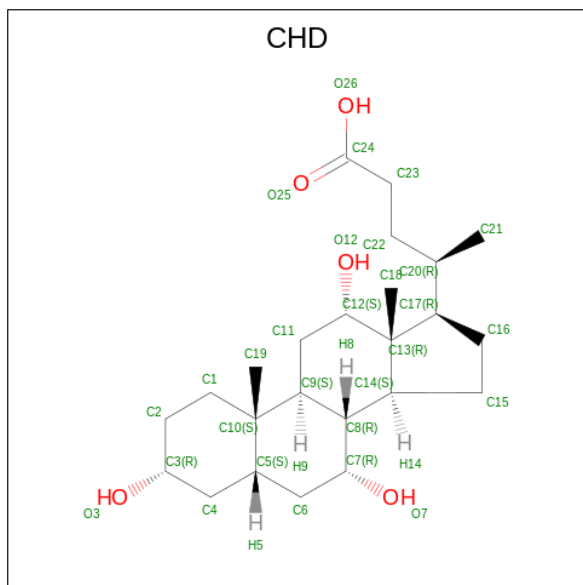
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	O	P	0	0
			51	40	10	1		
23	C	1	Total	C	O	P	0	0
			51	40	10	1		
23	N	1	Total	C	O	P	0	0
			51	40	10	1		
23	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 24 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 25 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).

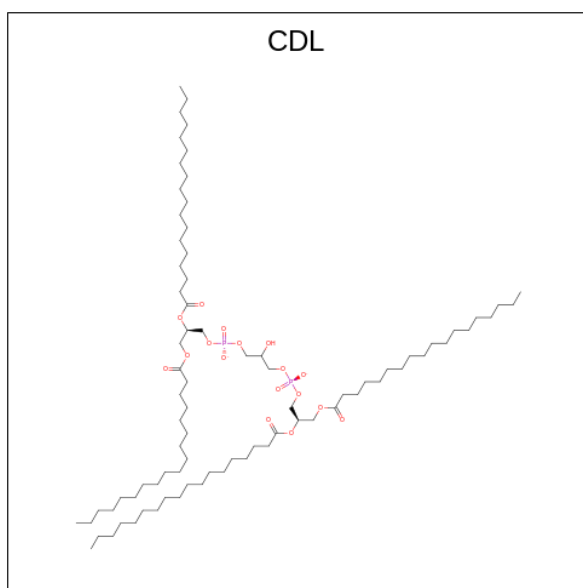


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B	1	Total C O 29 24 5	0	0
25	C	1	Total C O 29 24 5	0	0
25	C	1	Total C O 29 24 5	0	0
25	O	1	Total C O 29 24 5	0	0
25	P	1	Total C O 29 24 5	0	0
25	P	1	Total C O 29 24 5	0	0

- Molecule 26 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

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

- Molecule 27 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

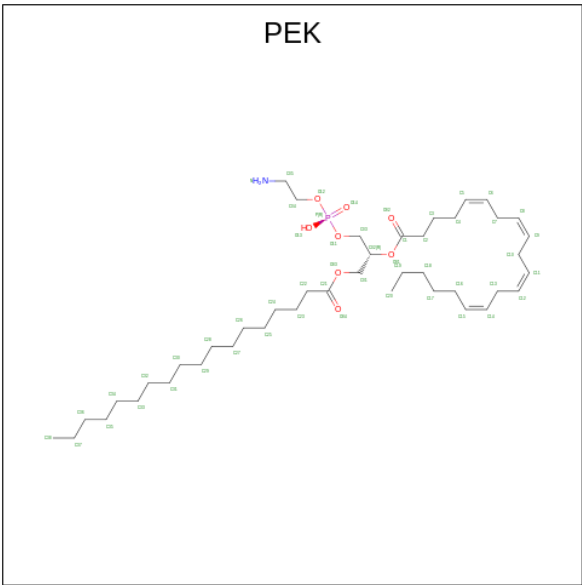


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	C	1	Total	C	O	P	0	0
			87	68	17	2		
27	I	1	Total	C	O	P	0	0
			64	45	17	2		
27	L	1	Total	C	O	P	0	0
			94	75	17	2		
27	P	1	Total	C	O	P	0	0
			87	68	17	2		
27	V	1	Total	C	O	P	0	0
			64	45	17	2		
27	Y	1	Total	C	O	P	0	0
			94	75	17	2		

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

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

- Molecule 29 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$).



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	233	Total	O	0	11
			244	244		
30	B	178	Total	O	0	2
			180	180		
30	C	101	Total	O	0	1
			102	102		
30	D	137	Total	O	0	9
			146	146		
30	E	109	Total	O	0	7
			116	116		
30	F	102	Total	O	0	7
			109	109		
30	G	44	Total	O	0	1
			45	45		
30	H	61	Total	O	0	0
			61	61		
30	I	39	Total	O	0	0
			39	39		
30	J	21	Total	O	0	0
			21	21		

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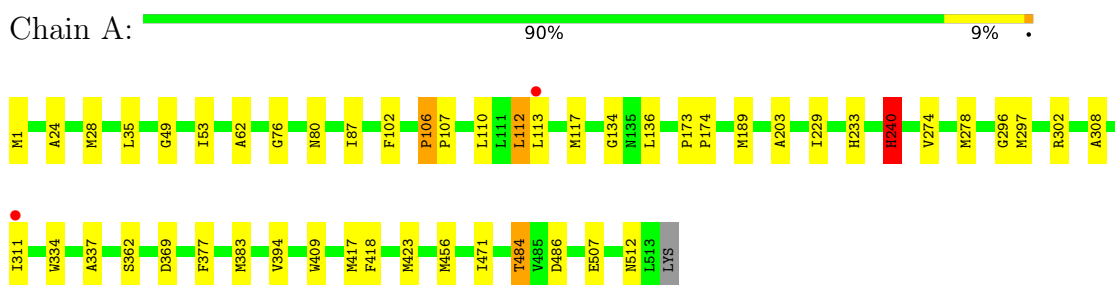
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	21	Total 21	O 21	0	0
30	L	26	Total 28	O 28	0	2
30	M	22	Total 22	O 22	0	0
30	N	222	Total 232	O 232	0	10
30	O	151	Total 152	O 152	0	1
30	P	103	Total 104	O 104	0	1
30	Q	77	Total 81	O 81	0	4
30	R	90	Total 98	O 98	0	8
30	S	90	Total 96	O 96	0	6
30	T	37	Total 38	O 38	0	1
30	U	48	Total 48	O 48	0	0
30	V	23	Total 23	O 23	0	0
30	W	15	Total 15	O 15	0	0
30	X	17	Total 17	O 17	0	0
30	Y	23	Total 25	O 25	0	2
30	Z	17	Total 17	O 17	0	0

3 Residue-property plots [i](#)

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

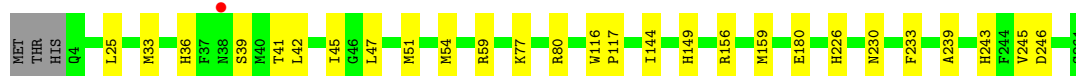
• Molecule 1: Cytochrome c oxidase subunit 1





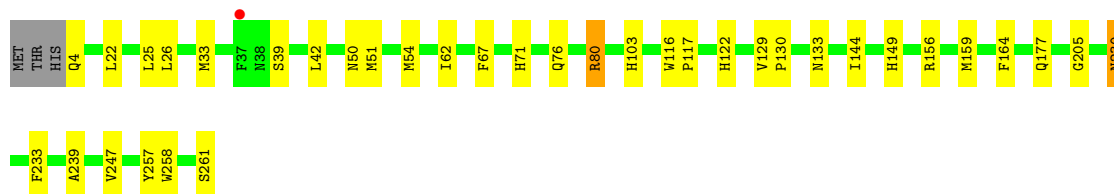
- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 89% 10% .



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 85% 13% ..



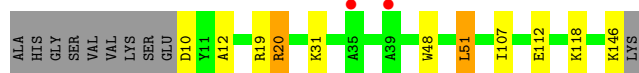
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 91% 5% ..



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

Chain Q: 86% 6% 7%



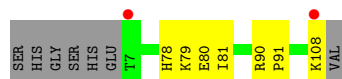
- Molecule 5: Cytochrome c oxidase subunit 5A

Chain E: 88% 6% 6%

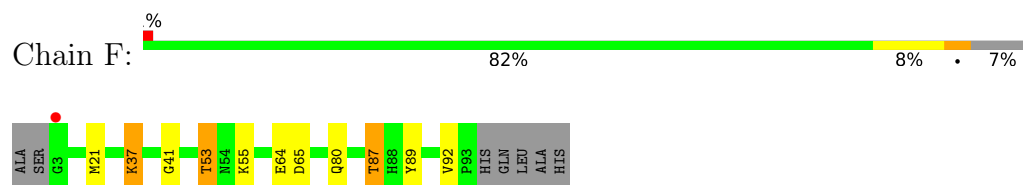


- Molecule 5: Cytochrome c oxidase subunit 5A

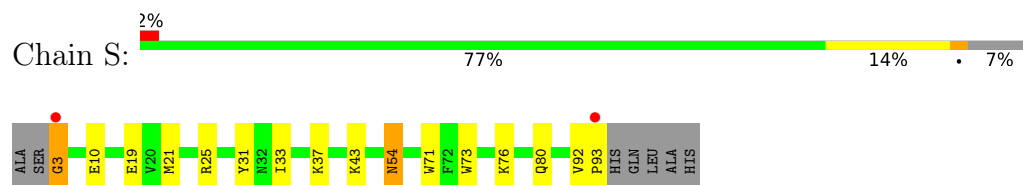
Chain R: 87% 6% 6%



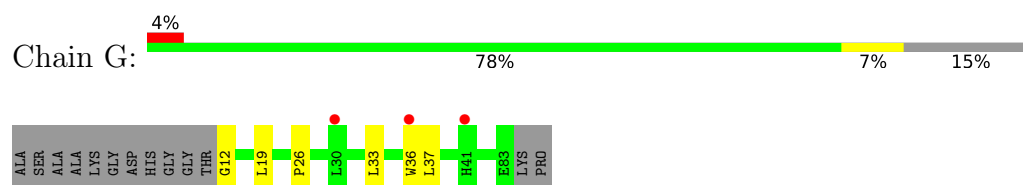
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



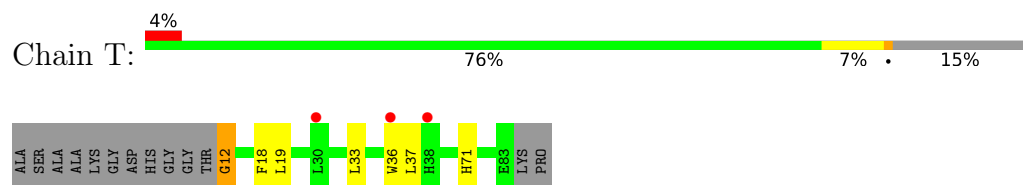
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



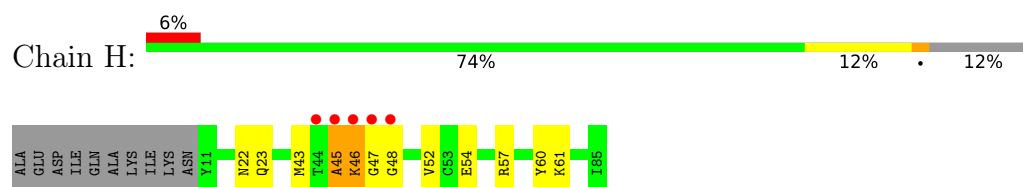
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



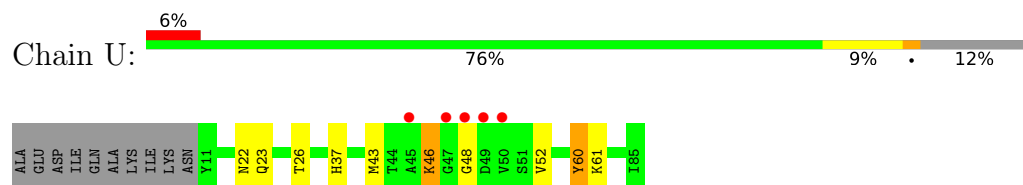
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



- Molecule 8: Cytochrome c oxidase subunit 6B1



- Molecule 8: Cytochrome c oxidase subunit 6B1

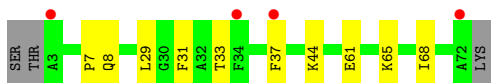
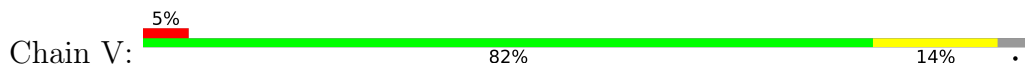


- Molecule 9: Cytochrome c oxidase subunit 6C

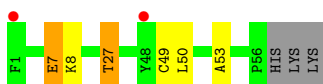
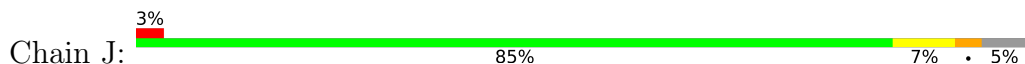




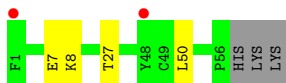
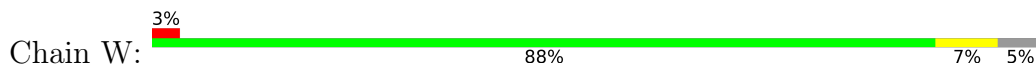
- Molecule 9: Cytochrome c oxidase subunit 6C



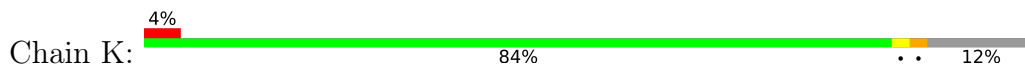
- Molecule 10: Cytochrome c oxidase subunit 7A1



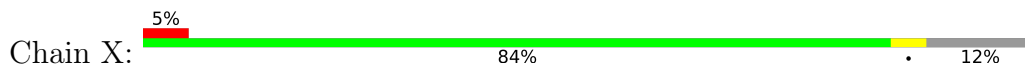
- Molecule 10: Cytochrome c oxidase subunit 7A1



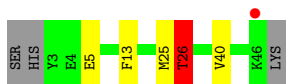
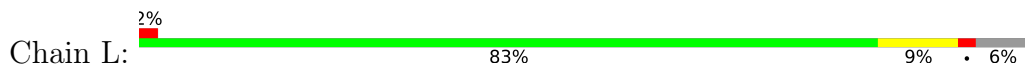
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



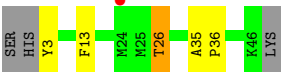
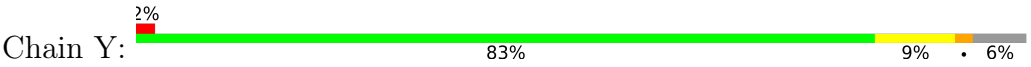
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



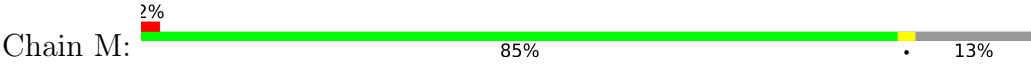
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.10Å 204.30Å 177.80Å 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	1.98 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.138 , 0.174 0.153 , 0.182	Depositor DCC
R_{free} test set	32888 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for l,k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33055	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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: CUA, HEA, CHD, UNX, LFA, MG, FME, EDO, CDL, CU, PER, PGV, PEK, N2O, DMU, NA, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.13	5/4259 (0.1%)	1.21	8/5816 (0.1%)
1	N	1.11	4/4259 (0.1%)	1.21	9/5816 (0.2%)
2	B	1.18	3/1908 (0.2%)	1.34	16/2598 (0.6%)
2	O	1.14	3/1908 (0.2%)	1.28	4/2598 (0.2%)
3	C	1.08	1/2258 (0.0%)	1.18	3/3084 (0.1%)
3	P	1.11	2/2258 (0.1%)	1.19	5/3084 (0.2%)
4	D	1.13	2/1226 (0.2%)	1.26	2/1657 (0.1%)
4	Q	1.09	0/1182	1.34	5/1598 (0.3%)
5	E	1.10	0/843	1.25	2/1145 (0.2%)
5	R	1.11	0/843	1.34	3/1145 (0.3%)
6	F	1.09	0/724	1.29	1/983 (0.1%)
6	S	1.24	1/724 (0.1%)	1.25	3/983 (0.3%)
7	G	1.14	1/633 (0.2%)	1.22	0/864
7	T	1.20	2/633 (0.3%)	1.28	0/864
8	H	1.07	0/648	1.37	0/877
8	U	1.12	1/648 (0.2%)	1.36	0/877
9	I	1.16	1/588 (0.2%)	1.47	1/781 (0.1%)
9	V	1.12	0/588	1.42	1/781 (0.1%)
10	J	1.10	0/451	1.27	2/610 (0.3%)
10	W	1.14	0/451	1.28	0/610
11	K	1.16	1/398 (0.3%)	1.43	1/546 (0.2%)
11	X	1.14	0/398	1.35	0/546
12	L	1.13	1/372 (0.3%)	1.29	3/500 (0.6%)
12	Y	1.12	1/372 (0.3%)	1.20	0/500
13	M	1.10	0/321	1.17	0/440
13	Z	1.07	0/321	1.44	2/440 (0.5%)
All	All	1.12	29/29214 (0.1%)	1.26	71/39743 (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	2
1	N	0	2
6	S	0	1
All	All	0	5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	GLY	C-O	11.37	1.36	1.23
1	N	49	GLY	C-O	9.27	1.34	1.23
7	T	12	GLY	N-CA	-8.07	1.32	1.45
4	D	58	GLU	CD-OE1	7.92	1.40	1.25
3	P	71	HIS	CE1-NE2	7.50	1.40	1.32
6	S	3	GLY	C-O	7.23	1.38	1.23
9	I	72	ALA	C-O	6.44	1.36	1.23
1	N	256	HIS	CE1-NE2	6.36	1.39	1.32
1	N	174	PRO	C-O	-6.02	1.16	1.24
2	O	198	GLU	C-O	5.86	1.30	1.23
2	B	113	TYR	C-O	-5.78	1.16	1.24
3	P	103	HIS	CE1-NE2	5.77	1.38	1.32
8	U	26	THR	C-O	5.77	1.30	1.24
1	A	134	GLY	C-O	5.72	1.30	1.23
3	C	36	HIS	CE1-NE2	5.64	1.38	1.32
2	O	60	GLU	CD-OE1	5.54	1.35	1.25
12	Y	3	TYR	N-CA	5.51	1.56	1.46
2	B	115	ASP	CG-OD2	5.48	1.35	1.25
7	T	71	HIS	CE1-NE2	5.43	1.38	1.32
4	D	21	ASP	CG-OD2	5.43	1.35	1.25
2	O	60	GLU	CD-OE2	5.37	1.35	1.25
1	A	174	PRO	C-O	-5.36	1.17	1.24
1	A	233	HIS	CE1-NE2	5.34	1.37	1.32
1	A	203	ALA	C-O	5.31	1.30	1.24
12	L	5	GLU	CD-OE2	-5.22	1.15	1.25
1	N	383	MET	C-O	-5.20	1.17	1.24
7	G	12	GLY	N-CA	-5.12	1.37	1.45
11	K	10	HIS	CE1-NE2	5.06	1.37	1.32
2	B	198	GLU	C-O	5.02	1.29	1.23

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	65	TRP	CA-CB-CG	10.57	133.69	113.60
1	A	240	HIS	CA-CB-CG	-10.40	103.40	113.80
9	I	72	ALA	CA-C-O	-10.39	103.13	120.80
1	N	240	HIS	CA-CB-CG	-10.39	103.41	113.80
2	B	65	TRP	CB-CG-CD1	-8.91	113.53	126.90
2	B	65	TRP	CB-CG-CD2	8.60	138.84	126.80
2	B	183	THR	CA-CB-OG1	-7.87	97.80	109.60
11	K	54	ARG	CA-C-O	-7.83	107.49	120.80
3	P	80	ARG	CG-CD-NE	-7.67	95.14	112.00
3	C	80	ARG	CG-CD-NE	-7.63	95.21	112.00
4	D	146	LYS	CA-C-O	-7.62	107.85	120.80
5	E	108	LYS	CA-C-O	-7.56	107.95	120.80
2	B	115	ASP	CB-CA-C	7.50	124.27	111.68
4	D	58	GLU	CB-CG-CD	6.99	124.48	112.60
2	B	59	GLN	CB-CG-CD	6.97	124.44	112.60
3	P	230	ASN	CA-CB-CG	-6.86	105.74	112.60
2	B	89	GLU	CA-C-N	6.77	129.64	120.63
2	B	89	GLU	C-N-CA	6.77	129.64	120.63
12	L	26	THR	CA-CB-OG1	-6.53	99.80	109.60
3	P	233	PHE	CA-CB-CG	-6.40	107.40	113.80
1	A	484	THR	CA-CB-OG1	-6.35	100.08	109.60
3	P	76	GLN	CG-CD-NE2	-6.30	106.95	116.40
5	R	80	GLU	CB-CG-CD	6.23	123.19	112.60
1	A	102	PHE	CA-CB-CG	-6.16	107.64	113.80
2	B	158	ASP	CA-CB-CG	6.13	118.73	112.60
3	P	122	HIS	CB-CA-C	6.12	117.02	110.65
3	C	233	PHE	CA-CB-CG	-6.07	107.73	113.80
1	N	102	PHE	CA-CB-CG	-6.06	107.74	113.80
12	L	25	MET	CA-C-N	6.06	128.72	120.54
12	L	25	MET	C-N-CA	6.06	128.72	120.54
4	Q	146	LYS	CA-C-O	-5.98	110.64	120.80
2	B	82	ARG	CG-CD-NE	-5.84	99.14	112.00
2	B	184	LEU	N-CA-CB	-5.84	100.69	110.80
1	N	377	PHE	CA-CB-CG	5.84	119.64	113.80
6	F	53	THR	CA-CB-OG1	-5.82	100.87	109.60
2	O	92	ASN	CB-CA-C	5.76	116.20	110.33
1	N	71	MET	CG-SD-CE	-5.66	88.44	100.90
13	Z	38	ASP	CA-C-N	5.66	127.86	120.28
13	Z	38	ASP	C-N-CA	5.66	127.86	120.28
1	N	513	LEU	CA-C-O	-5.60	111.28	120.80
1	N	512	ASN	CB-CA-C	5.55	120.05	110.45
5	R	78	HIS	CA-C-N	5.53	128.46	120.38
5	R	78	HIS	C-N-CA	5.53	128.46	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	PHE	CA-CB-CG	5.53	119.33	113.80
2	B	149	THR	CA-CB-OG1	-5.46	101.41	109.60
2	O	201	GLY	CA-C-N	5.45	127.85	120.38
2	O	201	GLY	C-N-CA	5.45	127.85	120.38
6	S	3	GLY	O-C-N	5.42	131.66	123.00
10	J	7	GLU	CB-CA-C	5.40	120.04	110.85
2	B	64	ILE	N-CA-C	-5.39	105.25	110.42
6	S	3	GLY	CA-C-N	5.35	131.90	121.41
6	S	3	GLY	C-N-CA	5.35	131.90	121.41
1	A	486	ASP	CA-CB-CG	5.35	117.95	112.60
4	Q	20	ARG	CG-CD-NE	-5.31	100.33	112.00
9	V	33	THR	CA-CB-OG1	-5.30	101.65	109.60
1	A	512	ASN	CB-CA-C	5.28	119.59	110.45
4	Q	20	ARG	NE-CZ-NH2	-5.28	114.45	119.20
1	A	507	GLU	CB-CA-C	5.21	115.79	109.85
1	N	96	ARG	CB-CA-C	5.20	120.21	110.70
1	N	83	VAL	N-CA-CB	5.18	114.49	110.45
2	B	139	ASP	CA-CB-CG	5.15	117.75	112.60
2	B	59	GLN	N-CA-CB	5.14	117.77	110.16
1	A	106	PRO	CB-CA-C	5.14	117.19	110.92
4	Q	10	ASP	CA-CB-CG	5.13	117.73	112.60
2	O	13	THR	CB-CA-C	5.10	118.12	109.55
3	C	45	ILE	N-CA-C	-5.08	105.59	110.72
4	Q	20	ARG	NE-CZ-NH1	5.07	126.57	121.50
2	B	65	TRP	CB-CA-C	-5.07	99.63	110.32
5	E	80	GLU	CB-CG-CD	5.05	121.19	112.60
10	J	27	THR	CA-CB-OG1	-5.03	102.05	109.60
1	N	240	HIS	N-CA-CB	5.03	116.35	110.42

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	383	MET	Mainchain
1	N	240	HIS	Sidechain
1	N	296	GLY	Mainchain
6	S	92	VAL	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4102	48	0
1	N	4130	0	4102	49	0
2	B	1870	0	1870	30	0
2	O	1870	0	1870	39	0
3	C	2171	0	2080	25	0
3	P	2172	0	2081	31	0
4	D	1192	0	1178	5	0
4	Q	1148	0	1131	7	0
5	E	825	0	823	2	0
5	R	825	0	823	4	0
6	F	709	0	691	8	0
6	S	709	0	691	9	0
7	G	606	0	577	3	0
7	T	606	0	577	4	0
8	H	628	0	580	15	0
8	U	628	0	580	12	0
9	I	575	0	584	5	0
9	V	575	0	584	4	0
10	J	441	0	439	7	0
10	W	441	0	439	3	0
11	K	384	0	366	0	0
11	X	384	0	366	2	0
12	L	360	0	360	4	0
12	Y	360	0	360	8	0
13	M	311	0	321	1	0
13	Z	311	0	321	3	0
14	A	129	0	88	6	0
14	N	129	0	88	3	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	1	0
19	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	3	0	0	0	0
20	A	28	0	54	9	0
20	B	17	0	33	2	0
20	C	114	0	205	4	0
20	G	14	0	27	4	0
20	N	14	0	27	6	0
20	O	28	0	54	5	0
20	P	100	0	173	7	0
20	T	25	0	48	0	0
21	A	51	0	75	2	0
21	B	66	0	104	1	0
21	C	194	0	262	6	0
21	D	33	0	41	3	0
21	H	33	0	28	1	0
21	J	11	0	21	0	0
21	L	22	0	31	2	0
21	M	41	0	56	0	0
21	N	51	0	75	0	0
21	O	66	0	104	1	0
21	P	194	0	262	2	0
21	Q	33	0	41	1	0
21	U	33	0	23	1	0
21	W	11	0	21	0	0
21	Z	63	0	87	3	0
22	A	16	0	24	1	0
22	B	4	0	6	0	0
22	C	12	0	17	0	0
22	E	12	0	18	0	0
22	F	8	0	12	0	0
22	G	4	0	6	0	0
22	N	20	0	30	1	0
22	O	4	0	6	0	0
22	P	12	0	17	0	0
22	R	12	0	18	0	0
22	S	8	0	12	0	0
22	T	4	0	6	0	0
23	A	51	0	76	0	0
23	C	51	0	76	1	0
23	N	51	0	76	0	0
23	P	51	0	76	0	0
24	B	2	0	0	0	0
24	O	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B	29	0	39	0	0
25	C	58	0	78	2	0
25	O	29	0	39	1	0
25	P	58	0	78	4	0
26	C	1	0	0	1	0
26	P	1	0	0	0	0
27	C	87	0	124	15	0
27	I	64	0	72	0	0
27	L	94	0	141	6	0
27	P	87	0	124	13	0
27	V	64	0	72	2	0
27	Y	94	0	141	8	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	G	53	0	77	0	0
29	T	53	0	77	3	0
30	A	244	0	0	9	0
30	B	180	0	0	4	0
30	C	102	0	0	3	0
30	D	146	0	0	1	0
30	E	116	0	0	0	0
30	F	109	0	0	1	0
30	G	45	0	0	0	0
30	H	61	0	0	1	0
30	I	39	0	0	1	0
30	J	21	0	0	0	0
30	K	21	0	0	0	0
30	L	28	0	0	1	0
30	M	22	0	0	1	0
30	N	232	0	0	7	0
30	O	152	0	0	2	0
30	P	104	0	0	8	0
30	Q	81	0	0	2	0
30	R	98	0	0	1	0
30	S	96	0	0	0	0
30	T	38	0	0	1	0
30	U	48	0	0	4	0
30	V	23	0	0	0	0
30	W	15	0	0	0	0
30	X	17	0	0	0	0
30	Y	25	0	0	2	0
30	Z	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	33055	0	31462	338	0

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

All (338) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:607:PER:O2	18:N:607:PER:O1	1.60	1.16
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.22	1.12
1:A:112:LEU:HG	30:A:2018:HOH:O	1.48	1.12
18:A:606:PER:O2	18:A:606:PER:O1	1.64	1.12
8:H:46:LYS:HE2	8:H:46:LYS:O	1.54	1.05
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:HE3	1.43	0.99
27:C:304:CDL:HA62	27:C:304:CDL:H121	1.45	0.99
3:P:4:GLN:N	30:P:402:HOH:O	1.96	0.96
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.01	0.95
8:H:52:VAL:HG12	8:U:46:LYS:CG	1.97	0.94
1:A:136[B]:LEU:HD11	30:A:2027:HOH:O	1.68	0.93
1:A:113[B]:LEU:HD11	1:A:117[B]:MET:SD	2.10	0.91
6:S:76:LYS:HE2	6:S:93:PRO:HG2	1.54	0.89
1:N:112:LEU:HG	30:N:915:HOH:O	1.72	0.89
3:C:245:VAL:C	3:C:246[B]:ASP:CA	2.46	0.88
8:H:43:MET:HE1	8:U:52:VAL:HG11	1.55	0.88
3:P:149:HIS:NE2	20:P:312:LFA:H11	1.89	0.87
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.15	0.85
8:H:52:VAL:CG1	8:U:46:LYS:HG2	2.07	0.84
1:N:112:LEU:HD23	1:N:112:LEU:C	2.04	0.83
27:C:304:CDL:HB22	10:J:8:LYS:HE3	1.61	0.82
27:C:304:CDL:H121	27:C:304:CDL:CA6	2.10	0.82
1:A:112:LEU:C	1:A:112:LEU:HD23	2.04	0.81
1:A:297[B]:MET:SD	1:A:302:ARG:HG2	2.19	0.81
3:C:33[A]:MET:HE3	3:C:39:SER:OG	1.79	0.81
27:C:304:CDL:HB61	27:C:304:CDL:HB21	1.61	0.81
8:H:46:LYS:O	8:H:46:LYS:CE	2.27	0.81
20:G:103:LFA:H11	20:N:609:LFA:H12	1.63	0.81
1:A:484:THR:HG22	30:A:2022:HOH:O	1.81	0.80
27:P:305:CDL:H121	27:P:305:CDL:HA62	1.64	0.78
20:A:608:LFA:H12	20:A:609:LFA:H11	1.65	0.78
26:C:302:UNX:UNK	30:C:493:HOH:O	1.65	0.77
1:N:274:VAL:HG12	1:N:278[A]:MET:HE2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:297[B]:MET:SD	1:N:302:ARG:CG	2.73	0.76
3:C:180[A]:GLU:OE2	30:C:403:HOH:O	2.03	0.75
3:P:33[B]:MET:CE	3:P:42:LEU:HD12	2.16	0.75
21:A:611:DMU:O6	30:A:1805:HOH:O	2.04	0.75
1:A:112:LEU:CG	30:A:2018:HOH:O	2.17	0.75
7:G:19:LEU:HD23	20:G:103:LFA:H61	1.70	0.74
3:P:33[B]:MET:HE3	3:P:42:LEU:HD12	1.70	0.74
4:D:42:GLU:OE2	30:D:301:HOH:O	2.07	0.73
2:B:53:THR:O	30:B:402:HOH:O	2.06	0.73
12:L:26:THR:HG21	21:L:102:DMU:H26	1.71	0.73
1:A:278[A]:MET:CE	20:A:609:LFA:H51	2.19	0.73
3:C:33[A]:MET:CE	3:C:42:LEU:H	2.02	0.73
8:H:43:MET:CE	8:U:52:VAL:HG11	2.20	0.72
1:A:278[A]:MET:HE1	20:A:609:LFA:H51	1.71	0.72
27:L:101:CDL:OB9	27:L:101:CDL:H122	1.89	0.72
2:B:16[A]:ILE:HD11	2:B:86:MET:HG2	1.70	0.72
8:H:52:VAL:HG21	8:U:43:MET:HE1	1.72	0.71
2:B:16[B]:ILE:HG23	30:B:537:HOH:O	1.90	0.70
2:B:22[B]:HIS:CE1	9:I:44:LYS:CE	2.75	0.70
1:N:136[B]:LEU:HD11	30:N:921:HOH:O	1.91	0.69
1:A:274:VAL:HG12	1:A:278[A]:MET:HE2	1.74	0.68
27:C:304:CDL:HB21	27:C:304:CDL:CB3	2.23	0.68
8:H:22:ASN:ND2	21:H:101:DMU:O3	2.27	0.68
6:F:37:LYS:HG2	30:F:296:HOH:O	1.93	0.67
4:Q:112:GLU:OE2	30:Q:301:HOH:O	2.11	0.67
2:B:16[A]:ILE:CG2	2:B:87[A]:MET:HE3	2.22	0.67
3:C:180[B]:GLU:HG2	30:C:423:HOH:O	1.94	0.67
2:B:220:GLU:OE1	30:B:403:HOH:O	2.12	0.66
1:N:278[B]:MET:HE1	20:N:609:LFA:H52	1.77	0.66
1:N:2:PHE:CE2	27:Y:101:CDL:H712	2.31	0.66
27:L:101:CDL:O1	30:L:221[B]:HOH:O	2.13	0.66
3:P:33[B]:MET:CE	21:P:324:DMU:H12	2.26	0.66
27:C:304:CDL:HB61	27:C:304:CDL:CB2	2.26	0.65
6:F:87[A]:THR:HG22	6:F:89:TYR:CE1	2.31	0.65
25:C:305:CHD:H162	25:C:305:CHD:H231	1.78	0.65
30:A:1871:HOH:O	3:C:77:LYS:HE3	1.97	0.65
2:B:33:LEU:HD13	9:I:31:PHE:CD2	2.33	0.65
1:A:297[B]:MET:SD	1:A:302:ARG:CG	2.86	0.64
2:O:84:LEU:HA	2:O:87[A]:MET:HE2	1.78	0.64
12:Y:26:THR:CG2	21:Z:102:DMU:H26	2.28	0.64
29:T:101:PEK:H32	29:T:101:PEK:H71	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:101:CDL:O1	30:Y:219[B]:HOH:O	2.14	0.64
20:G:103:LFA:H51	1:N:278[A]:MET:HE1	1.80	0.63
13:M:40:TYR:C	30:M:203:HOH:O	2.42	0.62
3:C:51[B]:MET:HE2	27:C:304:CDL:H861	1.79	0.62
27:C:304:CDL:HB21	27:C:304:CDL:HB32	1.82	0.62
3:C:33[A]:MET:HE1	3:C:41:THR:HB	1.82	0.61
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:HG2	1.83	0.61
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.81	0.61
3:C:33[B]:MET:CE	21:C:324:DMU:H12	2.30	0.60
27:Y:101:CDL:H711	27:Y:101:CDL:H342	1.83	0.60
12:Y:26:THR:OG1	30:Y:201:HOH:O	2.16	0.60
2:B:13:THR:HB	2:B:168:LEU:HD23	1.84	0.60
3:C:33[A]:MET:HE1	3:C:42:LEU:H	1.65	0.59
7:T:12:GLY:HA3	30:T:232:HOH:O	2.02	0.59
2:O:67:ILE:HD11	20:O:302:LFA:H42	1.85	0.59
27:L:101:CDL:H362	27:L:101:CDL:H711	1.84	0.59
30:P:411:HOH:O	6:S:3:GLY:HA3	2.03	0.58
1:A:113[B]:LEU:CD1	1:A:117[B]:MET:SD	2.90	0.58
2:O:60:GLU:CD	2:O:60:GLU:H	2.12	0.58
12:Y:26:THR:HG21	21:Z:102:DMU:H26	1.85	0.58
1:A:28:MET:CE	14:A:601[A]:HEA:H271	2.34	0.58
1:N:423[B]:MET:HE2	1:N:457:GLY:HA2	1.85	0.58
1:N:297[B]:MET:SD	1:N:302:ARG:HG3	2.44	0.58
9:I:36:LYS:HE3	9:I:36:LYS:HA	1.86	0.58
2:O:16[A]:ILE:HD12	2:O:87[A]:MET:CG	2.34	0.57
3:P:205:GLY:HA3	29:T:101:PEK:H182	1.86	0.57
5:R:90:ARG:NH1	30:R:303:HOH:O	2.24	0.57
30:N:848:HOH:O	4:Q:20:ARG:HG2	2.04	0.57
1:A:278[B]:MET:SD	20:A:608:LFA:H51	2.44	0.57
21:D:201:DMU:H36	21:D:201:DMU:O55	2.05	0.57
3:P:156:ARG:HE	25:P:306:CHD:C24	2.17	0.57
2:O:59:GLN:NE2	20:O:303:LFA:H31	2.19	0.57
1:N:112:LEU:CG	30:N:915:HOH:O	2.38	0.57
20:A:609:LFA:H61	7:T:19:LEU:HD23	1.87	0.56
2:B:67:ILE:HD11	20:B:307:LFA:H61	1.87	0.56
7:G:19:LEU:CD2	20:G:103:LFA:H61	2.35	0.56
12:L:26:THR:CG2	21:L:102:DMU:H26	2.36	0.56
3:C:33[B]:MET:HE1	21:C:324:DMU:H12	1.86	0.56
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.37	0.55
1:N:365:ILE:HD11	30:N:710:HOH:O	2.07	0.55
2:O:1:FME:HE1	2:O:133:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:92:ASN:ND2	30:O:403:HOH:O	2.29	0.55
13:Z:36:HIS:HD2	13:Z:39:ASN:ND2	2.04	0.55
2:B:67:ILE:CD1	20:B:307:LFA:H61	2.37	0.55
1:N:297[B]:MET:CG	1:N:302:ARG:HG3	2.37	0.55
20:P:310:LFA:C3	30:U:207:HOH:O	2.55	0.55
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:CE	2.27	0.54
30:Q:341:HOH:O	5:R:108:LYS:HD3	2.06	0.54
27:P:305:CDL:OB4	27:P:305:CDL:CA5	2.56	0.54
1:N:488:THR:HB	1:N:495:LEU:HD13	1.89	0.54
1:A:136[B]:LEU:CD1	30:A:2027:HOH:O	2.42	0.54
27:P:305:CDL:H1	27:P:305:CDL:OA3	2.07	0.54
3:P:133:ASN:ND2	30:P:403:HOH:O	2.18	0.54
6:S:54:ASN:HD22	6:S:54:ASN:C	2.16	0.54
3:C:33[B]:MET:HE3	3:C:42:LEU:HD12	1.90	0.54
27:C:304:CDL:CB2	10:J:8:LYS:HE3	2.36	0.53
3:P:33[B]:MET:HE1	21:P:324:DMU:H12	1.89	0.53
1:N:362[A]:SER:HA	2:O:87[A]:MET:HE1	1.90	0.53
3:C:149:HIS:NE2	20:C:312:LFA:H21	2.24	0.53
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.39	0.53
2:O:91:ASN:C	2:O:91:ASN:HD22	2.17	0.53
3:P:116:TRP:HA	3:P:117:PRO:C	2.33	0.53
2:B:227:LEU:HD21	30:B:536:HOH:O	2.08	0.53
2:O:58:ALA:O	2:O:62:GLU:HG3	2.09	0.52
3:P:51[B]:MET:HE3	27:P:305:CDL:H873	1.90	0.52
27:C:304:CDL:HB21	27:C:304:CDL:CB6	2.38	0.52
2:O:22[B]:HIS:ND1	2:O:22[B]:HIS:O	2.42	0.52
3:P:258:TRP:CE2	20:P:308:LFA:H32	2.45	0.52
3:C:33[A]:MET:HE2	3:C:42:LEU:H	1.72	0.51
3:C:226:HIS:HE1	27:C:304:CDL:H111	1.75	0.51
3:P:51[B]:MET:CE	27:P:305:CDL:H873	2.40	0.51
22:A:613:EDO:H12	2:B:58:ALA:HB3	1.92	0.51
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.10	0.51
1:N:87:ILE:O	1:N:173:PRO:HD3	2.10	0.51
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.92	0.51
6:S:19:GLU:OE1	6:S:31:TYR:OH	2.15	0.51
2:O:1:FME:CE	2:O:133:LEU:HD13	2.40	0.51
2:O:121:TYR:O	2:O:138:VAL:HA	2.10	0.51
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.93	0.51
2:O:114:GLU:HG3	2:O:227:LEU:HD21	1.93	0.50
27:C:304:CDL:H752	10:J:27:THR:HG21	1.94	0.50
1:A:110:LEU:HD21	21:C:324:DMU:H24	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.41	0.50
8:U:46:LYS:HE2	8:U:46:LYS:O	2.12	0.50
1:A:240:HIS:CD2	1:A:240:HIS:C	2.90	0.50
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.47	0.50
3:P:33[A]:MET:HG2	3:P:39:SER:O	2.12	0.50
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.93	0.49
8:H:46:LYS:HE2	8:H:46:LYS:C	2.35	0.49
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.93	0.49
1:N:423[B]:MET:HA	27:V:101:CDL:H782	1.94	0.49
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.95	0.49
1:N:112:LEU:HD23	1:N:113[A]:LEU:N	2.27	0.49
1:N:297[B]:MET:HG2	1:N:302:ARG:HG3	1.95	0.49
1:A:112:LEU:C	1:A:112:LEU:CD2	2.79	0.49
1:N:278[B]:MET:SD	20:N:609:LFA:C5	3.00	0.49
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.93	0.49
1:A:87:ILE:O	1:A:173:PRO:HD3	2.12	0.49
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.95	0.49
27:Y:101:CDL:C41	27:Y:101:CDL:H801	2.42	0.49
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.48	0.48
1:A:334:TRP:HB2	21:D:201:DMU:C57	2.43	0.48
1:A:423[B]:MET:HE2	1:A:456:MET:HB2	1.94	0.48
1:A:1:FME:HE2	1:A:1:FME:HA	1.94	0.48
1:N:423[A]:MET:HA	27:V:101:CDL:H782	1.95	0.48
2:B:58:ALA:O	2:B:62:GLU:HG3	2.13	0.48
1:N:240:HIS:C	1:N:240:HIS:CD2	2.91	0.48
12:Y:26:THR:HG22	21:Z:102:DMU:H26	1.94	0.48
21:C:324:DMU:H11	10:J:49:CYS:HB3	1.95	0.48
1:N:2:PHE:HE2	27:Y:101:CDL:H712	1.76	0.48
25:O:301:CHD:H212	25:O:301:CHD:H12	1.94	0.48
2:O:33:LEU:HD13	9:V:31:PHE:CD2	2.49	0.48
27:P:305:CDL:HB61	27:P:305:CDL:HB22	1.94	0.48
2:O:22[B]:HIS:CD2	9:V:44:LYS:HE2	2.48	0.48
25:P:306:CHD:H232	25:P:306:CHD:H162	1.96	0.48
1:A:24:ALA:HB2	14:A:601[B]:HEA:H253	1.96	0.47
2:B:1:FME:HE1	2:B:133:LEU:HD22	1.94	0.47
1:A:297[B]:MET:HG2	1:A:302:ARG:HG3	1.96	0.47
1:N:417[B]:MET:CE	30:N:879:HOH:O	2.62	0.47
21:C:324:DMU:H10	10:J:53:ALA:HB2	1.95	0.47
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.14	0.47
1:A:278[B]:MET:HE1	20:A:608:LFA:H52	1.96	0.47
4:D:82:VAL:HG12	4:D:86:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.97	0.47
1:N:278[B]:MET:SD	20:N:609:LFA:H51	2.55	0.47
21:Q:201:DMU:O55	21:Q:201:DMU:H36	2.14	0.47
2:O:13:THR:HB	2:O:168:LEU:HD23	1.96	0.47
1:A:112:LEU:HD23	1:A:112:LEU:O	2.14	0.47
1:N:24:ALA:HB2	14:N:602[B]:HEA:H253	1.96	0.47
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.97	0.47
3:P:33[B]:MET:HB2	3:P:33[B]:MET:HE2	1.49	0.47
2:B:61:VAL:HG22	2:B:65:TRP:CZ3	2.50	0.47
27:L:101:CDL:OB9	27:L:101:CDL:C12	2.59	0.47
29:T:101:PEK:H32	29:T:101:PEK:C7	2.44	0.47
30:P:448[B]:HOH:O	10:W:27:THR:HG22	2.13	0.47
3:P:51[B]:MET:HE3	27:P:305:CDL:C86	2.45	0.47
1:A:189:MET:HE3	20:A:608:LFA:H31	1.96	0.46
1:A:297[B]:MET:CG	1:A:302:ARG:HG3	2.45	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.14	0.46
21:C:324:DMU:H20	10:J:50:LEU:HB2	1.97	0.46
1:N:310:MET:HE1	2:O:77:ALA:HB2	1.97	0.46
3:P:258:TRP:CD2	20:P:308:LFA:H32	2.51	0.46
4:Q:118:LYS:HE3	11:X:51:LYS:HE3	1.96	0.46
1:N:112:LEU:HD23	1:N:113[B]:LEU:N	2.28	0.46
2:O:164:ALA:O	2:O:194:GLY:HA3	2.15	0.46
3:P:257:TYR:O	3:P:261:SER:HB3	2.16	0.46
2:B:56:MET:HB3	21:B:304:DMU:H7	1.97	0.46
1:N:278[B]:MET:CE	20:N:609:LFA:H52	2.43	0.46
1:N:362[A]:SER:OG	2:O:87[A]:MET:CE	2.64	0.46
8:H:54:GLU:OE2	8:H:57:ARG:NH2	2.38	0.46
1:A:334:TRP:CE3	21:A:610:DMU:H19	2.50	0.46
6:S:21[B]:MET:HE2	6:S:21[B]:MET:HB2	1.80	0.46
1:N:136[B]:LEU:CD1	30:N:921:HOH:O	2.55	0.45
1:A:28:MET:HE2	14:A:601[A]:HEA:C27	2.46	0.45
1:N:494:TRP:O	22:N:616:EDO:H22	2.17	0.45
1:A:28:MET:CE	14:A:601[A]:HEA:C27	2.94	0.45
27:L:101:CDL:H362	27:L:101:CDL:C73	2.47	0.45
27:Y:101:CDL:H711	27:Y:101:CDL:C34	2.46	0.45
2:O:16[A]:ILE:HG21	2:O:87[A]:MET:HG2	1.99	0.45
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.98	0.45
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.99	0.45
12:L:13:PHE:HB3	27:L:101:CDL:H512	1.98	0.45
3:C:144[A]:ILE:HD13	3:C:239:ALA:HA	1.98	0.45
2:O:1:FME:HE1	2:O:133:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.98	0.44
1:N:278[B]:MET:SD	20:N:609:LFA:H52	2.56	0.44
20:A:609:LFA:C6	7:T:19:LEU:HD23	2.48	0.44
2:O:59:GLN:HE22	20:O:303:LFA:C3	2.30	0.44
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.52	0.44
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.52	0.44
1:N:76:GLY:O	1:N:80:ASN:HB2	2.18	0.44
8:H:45:ALA:C	8:H:47:GLY:H	2.26	0.44
1:A:308:ALA:O	1:A:311[B]:ILE:HG12	2.18	0.44
3:C:54[A]:MET:HE1	23:C:303:PGV:H141	2.00	0.44
6:F:64:GLU:O	6:F:65:ASP:HB2	2.17	0.44
1:N:489:THR:HA	6:S:71:TRP:O	2.18	0.44
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.99	0.44
14:N:603:HEA:HBC1	14:N:603:HEA:HMC3	1.99	0.43
1:A:106:PRO:HB2	1:A:107:PRO:HD3	2.00	0.43
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.17	0.43
1:A:76:GLY:O	1:A:80:ASN:HB2	2.19	0.43
3:C:33[A]:MET:HG2	3:C:39:SER:O	2.19	0.43
2:O:59:GLN:NE2	20:O:303:LFA:C3	2.82	0.43
2:B:91:ASN:HD22	2:B:92:ASN:N	2.17	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.18	0.43
3:P:144[A]:ILE:HD13	3:P:239:ALA:HA	2.01	0.43
8:H:45:ALA:O	8:H:47:GLY:N	2.52	0.43
8:U:22:ASN:ND2	21:U:101:DMU:O3	2.51	0.43
2:O:32[B]:PHE:CD2	9:V:31:PHE:CZ	3.06	0.43
3:P:67:PHE:CE2	27:P:305:CDL:O1	2.63	0.43
3:C:149:HIS:NE2	20:C:312:LFA:H11	2.34	0.43
27:C:304:CDL:HB22	10:J:8:LYS:CE	2.40	0.43
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.01	0.43
2:O:16[B]:ILE:HG12	30:O:516:HOH:O	2.18	0.43
3:P:4:GLN:CA	30:P:402:HOH:O	2.54	0.43
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.19	0.43
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.53	0.43
1:N:379:TYR:O	1:N:383:MET:HB2	2.19	0.43
1:A:28:MET:HE2	14:A:601[A]:HEA:H271	2.01	0.42
3:C:59:ARG:HG3	27:C:304:CDL:HA4	2.01	0.42
3:C:156:ARG:HE	25:C:305:CHD:C24	2.31	0.42
6:F:53:THR:HG23	6:F:55:LYS:H	1.83	0.42
1:A:409:TRP:HB3	1:A:471:ILE:HG12	2.00	0.42
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	3.07	0.42
2:B:86:MET:HE2	2:B:86:MET:HB2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:60:GLU:CD	2:O:60:GLU:N	2.76	0.42
20:P:313:LFA:H22	20:P:314:LFA:H71	2.00	0.42
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	2.02	0.42
27:Y:101:CDL:OA5	27:Y:101:CDL:OA8	2.38	0.42
3:C:243:HIS:HB2	20:C:313:LFA:H12	2.01	0.42
1:N:325:ALA:HB2	21:O:308:DMU:H19	2.01	0.42
25:P:306:CHD:H162	25:P:306:CHD:C23	2.50	0.42
3:P:22:LEU:O	3:P:26:LEU:HG	2.20	0.42
5:R:81:ILE:HA	9:V:7:PRO:HG2	2.01	0.42
2:O:91:ASN:C	2:O:91:ASN:ND2	2.78	0.42
30:P:503:HOH:O	6:S:33:ILE:HD13	2.19	0.42
7:G:26:PRO:HB3	20:O:302:LFA:H92	2.00	0.41
1:N:362[A]:SER:OG	2:O:87[A]:MET:HE2	2.20	0.41
27:P:305:CDL:CA2	30:P:475:HOH:O	2.68	0.41
27:P:305:CDL:C75	10:W:27:THR:HG21	2.50	0.41
12:Y:13:PHE:HB3	27:Y:101:CDL:H512	2.02	0.41
27:C:304:CDL:CA6	27:C:304:CDL:C12	2.90	0.41
3:P:51[A]:MET:SD	3:P:54[A]:MET:CE	3.09	0.41
1:A:112:LEU:CD1	30:A:2018:HOH:O	2.62	0.41
20:A:609:LFA:H52	7:T:18:PHE:CG	2.56	0.41
2:B:91:ASN:HD22	2:B:91:ASN:C	2.29	0.41
6:F:92:VAL:HG23	6:F:92:VAL:O	2.20	0.41
8:H:54:GLU:OE1	8:H:54:GLU:HA	2.21	0.41
14:N:603:HEA:HBC1	14:N:603:HEA:CMC	2.50	0.41
20:P:310:LFA:H32	30:U:207:HOH:O	2.17	0.41
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	2.03	0.41
1:N:486:ASP:OD2	4:Q:19:ARG:NE	2.53	0.41
3:P:50:ASN:ND2	3:P:54[A]:MET:HE2	2.35	0.41
3:P:62:ILE:HD12	27:P:305:CDL:H312	2.03	0.41
3:P:80:ARG:HD3	30:P:416:HOH:O	2.20	0.41
3:P:129:VAL:N	3:P:130:PRO:CD	2.82	0.41
8:U:37:HIS:CE1	30:U:212:HOH:O	2.74	0.41
8:U:37:HIS:HE1	30:U:212:HOH:O	2.03	0.41
14:A:602:HEA:HBC1	14:A:602:HEA:HMC3	2.03	0.41
3:P:177:GLN:OE1	3:P:177:GLN:HA	2.20	0.41
6:F:21[B]:MET:HB3	6:F:21[B]:MET:HE3	1.83	0.41
2:O:116:LEU:HD13	2:O:226:MET:CG	2.51	0.41
3:P:164:PHE:CD1	25:P:306:CHD:H192	2.56	0.41
4:Q:107:ILE:HD13	11:X:39:GLU:HB2	2.03	0.41
1:A:418:PHE:CD1	21:D:201:DMU:H24	2.55	0.40
8:U:60:TYR:CD1	8:U:60:TYR:C	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:116:TRP:HA	3:C:117:PRO:C	2.45	0.40
4:D:60:TYR:OH	5:E:69:GLU:OE1	2.38	0.40
4:D:127:LYS:HD2	30:I:237:HOH:O	2.21	0.40
2:O:5:MET:HE2	2:O:5:MET:HB3	1.90	0.40
1:A:362[B]:SER:O	2:B:87[B]:MET:HE1	2.21	0.40
1:N:379:TYR:CZ	1:N:383:MET:HE1	2.57	0.40
27:P:305:CDL:O1	10:W:8:LYS:HD2	2.21	0.40
1:A:35:LEU:HD21	30:A:1976:HOH:O	2.21	0.40
2:B:1:FME:HE1	2:B:133:LEU:CD2	2.51	0.40
20:C:309:LFA:C5	30:H:242:HOH:O	2.70	0.40
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.02	0.40
3:P:247:VAL:HG11	20:P:313:LFA:H71	2.03	0.40
27:P:305:CDL:H121	27:P:305:CDL:CA6	2.43	0.40
6:S:10:GLU:OE2	6:S:25:ARG:NH1	2.49	0.40
2:O:1:FME:HE1	2:O:133:LEU:CD2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	526/514 (102%)	511 (97%)	15 (3%)	0	100	100
1	N	526/514 (102%)	512 (97%)	14 (3%)	0	100	100
2	B	230/227 (101%)	224 (97%)	6 (3%)	0	100	100
2	O	230/227 (101%)	223 (97%)	7 (3%)	0	100	100
3	C	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
3	P	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	136/147 (92%)	132 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	100/109 (92%)	100 (100%)	0	0	100	100
5	R	100/109 (92%)	100 (100%)	0	0	100	100
6	F	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
6	S	91/98 (93%)	89 (98%)	2 (2%)	0	100	100
7	G	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
7	T	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
8	H	73/85 (86%)	69 (94%)	2 (3%)	2 (3%)	4	0
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%)	37 (97%)	0	1 (3%)	4	0
All	All	3488/3614 (96%)	3410 (98%)	74 (2%)	4 (0%)	48	32

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/426 (103%)	438 (100%)	2 (0%)	86	82
1	N	440/426 (103%)	437 (99%)	3 (1%)	81	74
2	B	215/210 (102%)	206 (96%)	9 (4%)	25	8
2	O	215/210 (102%)	209 (97%)	6 (3%)	38	18
3	C	232/226 (103%)	230 (99%)	2 (1%)	75	65
3	P	232/226 (103%)	230 (99%)	2 (1%)	75	65
4	D	128/129 (99%)	128 (100%)	0	100	100
4	Q	122/129 (95%)	120 (98%)	2 (2%)	58	42
5	E	89/95 (94%)	88 (99%)	1 (1%)	70	58
5	R	89/95 (94%)	88 (99%)	1 (1%)	70	58
6	F	78/81 (96%)	74 (95%)	4 (5%)	20	5
6	S	78/81 (96%)	74 (95%)	4 (5%)	20	5
7	G	63/69 (91%)	60 (95%)	3 (5%)	21	6
7	T	63/69 (91%)	60 (95%)	3 (5%)	21	6
8	H	67/75 (89%)	64 (96%)	3 (4%)	23	7
8	U	67/75 (89%)	64 (96%)	3 (4%)	23	7
9	I	55/58 (95%)	54 (98%)	1 (2%)	54	37
9	V	55/58 (95%)	49 (89%)	6 (11%)	5	0
10	J	47/50 (94%)	46 (98%)	1 (2%)	48	29
10	W	47/50 (94%)	45 (96%)	2 (4%)	25	7
11	K	39/46 (85%)	38 (97%)	1 (3%)	41	21
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	37/40 (92%)	36 (97%)	1 (3%)	40	19
12	Y	37/40 (92%)	36 (97%)	1 (3%)	40	19
13	M	34/38 (90%)	34 (100%)	0	100	100
13	Z	34/38 (90%)	32 (94%)	2 (6%)	16	3
All	All	3042/3086 (99%)	2979 (98%)	63 (2%)	48	29

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	A	369	ASP
2	B	33	LEU

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Mol	Chain	Res	Type
2	B	59	GLN
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	86	MET
2	B	91	ASN
2	B	115	ASP
3	C	159	MET
3	C	230	ASN
5	E	70	VAL
6	F	37	LYS
6	F	80	GLN
6	F	87[A]	THR
6	F	87[B]	THR
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
8	H	46	LYS
8	H	60	TYR
8	H	61	LYS
9	I	36	LYS
10	J	7	GLU
11	K	54	ARG
12	L	26	THR
1	N	112	LEU
1	N	363	LEU
1	N	369	ASP
2	O	33	LEU
2	O	60	GLU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	115	ASP
3	P	159	MET
3	P	230	ASN
4	Q	31	LYS
4	Q	51	LEU
5	R	79	LYS
6	S	37	LYS
6	S	43	LYS
6	S	54	ASN

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Mol	Chain	Res	Type
6	S	80	GLN
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
8	U	46	LYS
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	29	LEU
9	V	37	PHE
9	V	61	GLU
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	40	TYR

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

Mol	Chain	Res	Type
1	A	55	ASN
1	A	80	ASN
1	A	98	ASN
1	A	422	ASN
1	A	503	HIS
2	B	203	ASN
3	C	50	ASN
4	D	119	GLN
4	D	143	ASN
5	E	94	ASN
6	F	54	ASN
7	G	34	ASN
7	G	38	HIS
8	H	22	ASN
8	H	37	HIS
10	J	29	ASN
11	K	35	GLN
1	N	43	GLN
1	N	170	ASN
1	N	422	ASN

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Mol	Chain	Res	Type
2	O	59	GLN
3	P	50	ASN
3	P	56	GLN
3	P	76	GLN
4	Q	32	ASN
4	Q	76	ASN
4	Q	109	HIS
4	Q	119	GLN
5	R	94	ASN
6	S	54	ASN
7	T	34	ASN
8	U	12	GLN
8	U	22	ASN
8	U	37	HIS
11	X	35	GLN
13	Z	36	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	$\# Z > 2$
1	FME	A	1	1	8,9,10	0.51	0	7,9,11	1.16	0
2	FME	O	1	2	8,9,10	0.86	1 (12%)	7,9,11	1.16	1 (14%)
1	FME	N	1	1	8,9,10	0.76	0	7,9,11	1.33	2 (28%)
2	FME	B	1	2	8,9,10	1.34	1 (12%)	7,9,11	1.36	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-3.17	1.64	1.81
2	O	1	FME	CG-SD	-2.15	1.69	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-2.56	105.84	112.95
1	N	1	FME	CA-N-CN	2.32	126.39	122.82
1	N	1	FME	O-C-CA	-2.10	119.26	124.78
2	B	1	FME	CA-N-CN	2.08	126.02	122.82
2	O	1	FME	O-C-CA	-2.04	119.42	124.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
2	O	1	FME	5	0
2	B	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 137 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 127 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	$\# Z > 2$
22	EDO	S	103	-	3,3,3	0.21	0	2,2,2	0.13	0
14	HEA	N	602[B]	-	57,67,67	1.95	17 (29%)	61,103,103	2.42	21 (34%)
25	CHD	P	306	-	32,32,32	1.00	1 (3%)	51,51,51	1.04	1 (1%)
22	EDO	O	309	-	3,3,3	0.23	0	2,2,2	0.23	0
21	DMU	P	318	-	34,34,34	0.89	3 (8%)	45,45,45	1.16	3 (6%)
21	DMU	N	610	-	6,6,34	0.38	0	5,5,45	0.32	0
22	EDO	N	615	-	3,3,3	0.32	0	2,2,2	0.21	0
20	LFA	P	311	-	10,10,19	0.23	0	9,9,18	0.19	0
22	EDO	E	202	-	3,3,3	0.28	0	2,2,2	0.12	0
27	CDL	Y	101	-	93,93,99	0.48	0	99,105,111	0.72	4 (4%)
25	CHD	O	301	-	32,32,32	0.75	0	51,51,51	0.89	2 (3%)
20	LFA	C	314	-	12,12,19	0.27	0	11,11,18	0.22	0
21	DMU	O	307	-	10,10,34	0.45	0	9,9,45	0.52	0
20	LFA	B	307	-	16,16,19	0.39	0	15,15,18	0.19	0
25	CHD	C	301	-	32,32,32	0.91	3 (9%)	51,51,51	0.86	2 (3%)
22	EDO	E	203	-	3,3,3	0.19	0	2,2,2	0.05	0
22	EDO	F	103	-	3,3,3	0.31	0	2,2,2	0.39	0
22	EDO	A	612	-	3,3,3	0.36	0	2,2,2	0.28	0
22	EDO	F	102	-	3,3,3	0.34	0	2,2,2	0.41	0
20	LFA	P	314	-	12,12,19	0.31	0	11,11,18	0.36	0
20	LFA	P	308	-	10,10,19	0.31	0	9,9,18	0.28	0
21	DMU	D	201	-	34,34,34	1.35	6 (17%)	45,45,45	1.48	8 (17%)
20	LFA	C	309	-	17,17,19	0.23	0	16,16,18	0.13	0
20	LFA	C	312	-	10,10,19	0.32	0	9,9,18	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	A	601[B]	-	57,67,67	2.01	17 (29%)	61,103,103	2.46	26 (42%)
20	LFA	P	301	-	14,14,19	0.30	0	13,13,18	0.12	0
22	EDO	S	102	-	3,3,3	0.18	0	2,2,2	0.26	0
20	LFA	C	311	-	13,13,19	0.27	0	12,12,18	0.14	0
27	CDL	C	304	-	86,86,99	0.75	3 (3%)	92,98,111	1.36	11 (11%)
25	CHD	B	306	-	32,32,32	0.72	0	51,51,51	0.87	1 (1%)
27	CDL	L	101	-	93,93,99	0.53	0	99,105,111	0.99	8 (8%)
20	LFA	O	302	-	16,16,19	0.32	0	15,15,18	0.24	0
22	EDO	A	613	-	3,3,3	0.25	0	2,2,2	0.30	0
21	DMU	C	315	-	34,34,34	0.86	3 (8%)	45,45,45	1.64	9 (20%)
21	DMU	P	316	-	6,6,34	0.23	0	5,5,45	0.48	0
21	DMU	P	323	-	22,22,34	0.68	0	27,27,45	1.51	3 (11%)
21	DMU	P	324	-	34,34,34	0.73	0	45,45,45	1.51	6 (13%)
21	DMU	Z	103	-	7,7,34	0.33	0	6,6,45	0.45	0
22	EDO	T	104	-	3,3,3	0.37	0	2,2,2	0.07	0
22	EDO	N	614	-	3,3,3	0.36	0	2,2,2	0.15	0
21	DMU	A	611	-	34,34,34	1.30	6 (17%)	45,45,45	1.20	5 (11%)
22	EDO	N	613	-	3,3,3	0.16	0	2,2,2	0.39	0
21	DMU	C	318	-	34,34,34	0.95	3 (8%)	45,45,45	1.35	7 (15%)
21	DMU	O	306	-	10,10,34	0.18	0	9,9,45	0.61	0
21	DMU	A	617	-	10,10,34	0.31	0	9,9,45	0.55	0
22	EDO	A	615	-	3,3,3	0.35	0	2,2,2	0.39	0
18	PER	A	606	15,14	0,1,1	-	-	-	-	-
22	EDO	P	321	-	3,3,3	0.25	0	2,2,2	0.14	0
25	CHD	P	302	-	32,32,32	0.94	2 (6%)	51,51,51	0.88	1 (1%)
21	DMU	U	101	-	34,34,34	0.86	1 (2%)	45,45,45	1.29	4 (8%)
22	EDO	C	321	-	3,3,3	0.28	0	2,2,2	0.05	0
21	DMU	P	317	-	22,22,34	0.78	1 (4%)	27,27,45	1.21	3 (11%)
20	LFA	P	313	-	14,14,19	0.40	0	13,13,18	0.21	0
21	DMU	W	101	-	10,10,34	0.31	0	9,9,45	0.57	0
21	DMU	C	319	-	34,34,34	0.95	3 (8%)	45,45,45	1.41	6 (13%)
20	LFA	C	310	-	10,10,19	0.17	0	9,9,18	0.17	0
21	DMU	C	324	-	34,34,34	0.82	0	45,45,45	1.17	2 (4%)
23	PGV	A	616	-	50,50,50	0.90	2 (4%)	53,56,56	1.12	2 (3%)
21	DMU	Q	201	-	34,34,34	1.51	8 (23%)	45,45,45	1.53	7 (15%)
19	N2O	N	608	-	0,2,2	-	-	0,1,1	-	-
21	DMU	N	611	-	34,34,34	1.50	6 (17%)	45,45,45	1.22	4 (8%)
21	DMU	P	319	-	34,34,34	1.08	3 (8%)	45,45,45	1.34	4 (8%)
20	LFA	P	312	-	10,10,19	0.23	0	9,9,18	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CDL	V	101	-	63,63,99	0.65	0	69,75,111	1.29	5 (7%)
21	DMU	B	302	-	10,10,34	0.22	0	9,9,45	0.57	0
22	EDO	E	201	-	3,3,3	0.13	0	2,2,2	0.10	0
14	HEA	N	603	18,1	57,67,67	2.03	18 (31%)	61,103,103	2.49	22 (36%)
21	DMU	C	317	-	22,22,34	0.64	0	27,27,45	1.46	4 (14%)
21	DMU	Z	102	-	22,22,34	0.73	0	27,27,45	1.11	2 (7%)
24	CUA	B	301	2	0,1,1	-	-	-	-	-
27	CDL	I	101	-	63,63,99	0.65	0	69,75,111	1.18	5 (7%)
21	DMU	N	601	-	10,10,34	0.27	0	9,9,45	0.55	0
20	LFA	O	303	-	10,10,19	0.28	0	9,9,18	0.17	0
20	LFA	C	308	-	5,5,19	0.18	0	4,4,18	0.11	0
23	PGV	N	617	-	50,50,50	0.82	3 (6%)	53,56,56	1.43	4 (7%)
21	DMU	P	315	-	34,34,34	0.85	1 (2%)	45,45,45	1.33	3 (6%)
22	EDO	N	616	-	3,3,3	0.50	0	2,2,2	0.24	0
22	EDO	B	305	-	3,3,3	0.20	0	2,2,2	0.21	0
22	EDO	A	614	-	3,3,3	0.54	0	2,2,2	0.38	0
29	PEK	T	101	-	52,52,52	0.66	2 (3%)	55,57,57	1.00	3 (5%)
21	DMU	C	306	-	10,10,34	0.44	0	9,9,45	0.60	0
21	DMU	J	101	-	10,10,34	0.21	0	9,9,45	0.71	0
22	EDO	C	320	-	3,3,3	0.16	0	2,2,2	0.26	0
21	DMU	O	308	-	22,22,34	0.74	1 (4%)	27,27,45	1.12	3 (11%)
20	LFA	A	608	-	13,13,19	0.45	0	12,12,18	0.22	0
14	HEA	A	602	18,1	57,67,67	1.79	13 (22%)	61,103,103	2.16	20 (32%)
23	PGV	C	303	-	50,50,50	0.77	0	53,56,56	1.06	3 (5%)
21	DMU	L	102	-	22,22,34	0.77	0	27,27,45	1.25	2 (7%)
14	HEA	N	602[A]	-	57,67,67	1.93	17 (29%)	61,103,103	2.48	21 (34%)
20	LFA	P	310	-	17,17,19	0.26	0	16,16,18	0.19	0
22	EDO	R	203	-	3,3,3	0.56	0	2,2,2	0.40	0
22	EDO	R	201	-	3,3,3	0.17	0	2,2,2	0.14	0
21	DMU	P	307	-	10,10,34	0.25	0	9,9,45	0.66	0
22	EDO	P	320	-	3,3,3	0.18	0	2,2,2	0.10	0
18	PER	N	607	15,14	0,1,1	-	-	-	-	-
27	CDL	P	305	-	86,86,99	0.73	2 (2%)	92,98,111	1.00	6 (6%)
20	LFA	P	309	-	5,5,19	0.29	0	4,4,18	0.09	0
21	DMU	B	303	-	10,10,34	0.32	0	9,9,45	0.56	0
21	DMU	O	304	-	22,22,34	0.98	1 (4%)	27,27,45	1.30	4 (14%)
21	DMU	A	610	-	6,6,34	0.55	0	5,5,45	0.30	0
20	LFA	G	103	-	13,13,19	0.64	0	12,12,18	0.44	0
20	LFA	T	103	-	10,10,19	0.22	0	9,9,18	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	DMU	C	323	-	22,22,34	0.62	0	27,27,45	1.03	1 (3%)
21	DMU	B	304	-	22,22,34	0.89	1 (4%)	27,27,45	1.06	2 (7%)
20	LFA	T	102	-	13,13,19	0.22	0	12,12,18	0.21	0
21	DMU	C	316	-	6,6,34	0.25	0	5,5,45	0.62	0
19	N2O	A	607	-	0,2,2	-	-	0,1,1	-	-
20	LFA	C	313	-	14,14,19	0.42	0	13,13,18	0.48	0
21	DMU	M	101	-	34,34,34	1.07	2 (5%)	45,45,45	1.00	4 (8%)
22	EDO	P	322	-	3,3,3	0.66	0	2,2,2	1.20	0
20	LFA	N	609	-	13,13,19	0.33	0	12,12,18	0.38	0
21	DMU	B	308	-	22,22,34	0.59	0	27,27,45	1.34	2 (7%)
24	CUA	O	305	2	0,1,1	-	-	-	-	-
22	EDO	C	322	-	3,3,3	0.74	0	2,2,2	0.84	0
21	DMU	Z	101	-	34,34,34	1.02	3 (8%)	45,45,45	1.06	6 (13%)
23	PGV	P	304	-	50,50,50	0.99	4 (8%)	53,56,56	1.03	3 (5%)
20	LFA	A	609	-	13,13,19	0.62	0	12,12,18	0.32	0
21	DMU	M	102	-	7,7,34	0.21	0	6,6,45	0.67	0
22	EDO	R	202	-	3,3,3	0.12	0	2,2,2	0.23	0
22	EDO	N	612	-	3,3,3	0.39	0	2,2,2	0.19	0
20	LFA	C	325	-	14,14,19	0.19	0	13,13,18	0.14	0
29	PEK	G	101	-	52,52,52	0.70	1 (1%)	55,57,57	0.72	2 (3%)
14	HEA	A	601[A]	-	57,67,67	2.02	17 (29%)	61,103,103	2.48	24 (39%)
25	CHD	C	305	-	32,32,32	0.78	0	51,51,51	1.58	9 (17%)
21	DMU	H	101	-	34,34,34	0.95	2 (5%)	45,45,45	1.10	4 (8%)
22	EDO	G	102	-	3,3,3	0.24	0	2,2,2	0.17	0
20	LFA	C	307	-	10,10,19	0.22	0	9,9,18	0.16	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
22	EDO	S	103	-	-	0/1/1/1	-
14	HEA	N	602[B]	-	-	4/32/76/76	-
25	CHD	P	306	-	-	5/9/74/74	0/4/4/4
22	EDO	O	309	-	-	0/1/1/1	-
21	DMU	P	318	-	-	15/19/59/59	0/2/2/2
21	DMU	N	610	-	-	4/4/4/59	-
22	EDO	N	615	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LFA	P	311	-	-	5/8/8/17	-
22	EDO	E	202	-	-	0/1/1/1	-
27	CDL	Y	101	-	-	55/104/104/110	-
25	CHD	O	301	-	-	2/9/74/74	0/4/4/4
20	LFA	C	314	-	-	3/10/10/17	-
21	DMU	O	307	-	-	3/8/8/59	-
20	LFA	B	307	-	-	10/14/14/17	-
25	CHD	C	301	-	-	2/9/74/74	0/4/4/4
22	EDO	E	203	-	-	0/1/1/1	-
22	EDO	F	103	-	-	1/1/1/1	-
22	EDO	A	612	-	-	0/1/1/1	-
22	EDO	F	102	-	-	0/1/1/1	-
20	LFA	P	314	-	-	2/10/10/17	-
20	LFA	P	308	-	-	6/8/8/17	-
21	DMU	D	201	-	-	9/19/59/59	0/2/2/2
20	LFA	C	309	-	-	8/15/15/17	-
14	HEA	A	601[B]	-	-	4/32/76/76	-
20	LFA	P	301	-	-	7/12/12/17	-
20	LFA	C	312	-	-	4/8/8/17	-
22	EDO	S	102	-	-	0/1/1/1	-
20	LFA	C	311	-	-	6/11/11/17	-
27	CDL	C	304	-	-	44/97/97/110	-
25	CHD	B	306	-	-	2/9/74/74	0/4/4/4
27	CDL	L	101	-	-	51/104/104/110	-
20	LFA	O	302	-	-	9/14/14/17	-
22	EDO	A	613	-	-	0/1/1/1	-
21	DMU	C	315	-	-	10/19/59/59	0/2/2/2
21	DMU	P	316	-	-	3/4/4/59	-
21	DMU	P	323	-	-	8/13/33/59	0/1/1/2
21	DMU	P	324	-	-	5/19/59/59	0/2/2/2
21	DMU	Z	103	-	-	3/5/5/59	-
22	EDO	T	104	-	-	0/1/1/1	-
22	EDO	N	614	-	-	0/1/1/1	-
21	DMU	A	611	-	-	7/19/59/59	0/2/2/2
22	EDO	N	613	-	-	0/1/1/1	-
21	DMU	C	318	-	-	15/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	DMU	A	617	-	-	5/8/8/59	-
21	DMU	O	306	-	-	5/8/8/59	-
22	EDO	A	615	-	-	1/1/1/1	-
22	EDO	P	321	-	-	0/1/1/1	-
25	CHD	P	302	-	-	2/9/74/74	0/4/4/4
21	DMU	U	101	-	-	5/19/59/59	0/2/2/2
22	EDO	C	321	-	-	0/1/1/1	-
21	DMU	P	317	-	-	7/13/33/59	0/1/1/2
21	DMU	W	101	-	-	5/8/8/59	-
20	LFA	P	313	-	-	6/12/12/17	-
21	DMU	C	319	-	-	10/19/59/59	0/2/2/2
20	LFA	C	310	-	-	7/8/8/17	-
21	DMU	C	324	-	-	5/19/59/59	0/2/2/2
23	PGV	A	616	-	-	8/55/55/55	-
21	DMU	Q	201	-	-	7/19/59/59	0/2/2/2
21	DMU	N	611	-	-	5/19/59/59	0/2/2/2
21	DMU	P	319	-	-	10/19/59/59	0/2/2/2
20	LFA	P	312	-	-	5/8/8/17	-
27	CDL	V	101	-	-	37/74/74/110	-
21	DMU	B	302	-	-	5/8/8/59	-
22	EDO	E	201	-	-	0/1/1/1	-
14	HEA	N	603	18,1	-	4/32/76/76	-
21	DMU	C	317	-	-	6/13/33/59	0/1/1/2
21	DMU	Z	102	-	-	10/13/33/59	0/1/1/2
27	CDL	I	101	-	-	37/74/74/110	-
21	DMU	N	601	-	-	5/8/8/59	-
20	LFA	O	303	-	-	2/8/8/17	-
20	LFA	C	308	-	-	1/3/3/17	-
23	PGV	N	617	-	-	4/55/55/55	-
21	DMU	P	315	-	-	9/19/59/59	0/2/2/2
22	EDO	N	616	-	-	0/1/1/1	-
22	EDO	B	305	-	-	0/1/1/1	-
22	EDO	A	614	-	-	0/1/1/1	-
29	PEK	T	101	-	-	17/56/56/56	-
21	DMU	C	306	-	-	3/8/8/59	-
21	DMU	J	101	-	-	5/8/8/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	C	320	-	-	1/1/1/1	-
21	DMU	O	308	-	-	2/13/33/59	0/1/1/2
20	LFA	A	608	-	-	4/11/11/17	-
14	HEA	A	602	18,1	-	4/32/76/76	-
23	PGV	C	303	-	-	12/55/55/55	-
21	DMU	L	102	-	-	10/13/33/59	0/1/1/2
14	HEA	N	602[A]	-	-	7/32/76/76	-
20	LFA	P	310	-	-	10/15/15/17	-
22	EDO	R	203	-	-	1/1/1/1	-
22	EDO	R	201	-	-	1/1/1/1	-
21	DMU	P	307	-	-	1/8/8/59	-
22	EDO	P	320	-	-	1/1/1/1	-
27	CDL	P	305	-	-	51/97/97/110	-
20	LFA	P	309	-	-	0/3/3/17	-
21	DMU	B	303	-	-	6/8/8/59	-
21	DMU	O	304	-	-	7/13/33/59	0/1/1/2
21	DMU	A	610	-	-	3/4/4/59	-
20	LFA	G	103	-	-	7/11/11/17	-
20	LFA	T	103	-	-	3/8/8/17	-
21	DMU	C	323	-	-	8/13/33/59	0/1/1/2
21	DMU	B	304	-	-	6/13/33/59	0/1/1/2
20	LFA	T	102	-	-	5/11/11/17	-
21	DMU	C	316	-	-	3/4/4/59	-
20	LFA	C	313	-	-	1/12/12/17	-
21	DMU	M	101	-	-	4/19/59/59	0/2/2/2
22	EDO	P	322	-	-	0/1/1/1	-
20	LFA	N	609	-	-	2/11/11/17	-
21	DMU	B	308	-	-	9/13/33/59	0/1/1/2
22	EDO	C	322	-	-	0/1/1/1	-
21	DMU	Z	101	-	-	7/19/59/59	0/2/2/2
23	PGV	P	304	-	-	11/55/55/55	-
20	LFA	A	609	-	-	5/11/11/17	-
21	DMU	M	102	-	-	3/5/5/59	-
22	EDO	R	202	-	-	0/1/1/1	-
22	EDO	N	612	-	-	0/1/1/1	-
20	LFA	C	325	-	-	8/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEK	G	101	-	-	13/56/56/56	-
14	HEA	A	601[A]	-	-	5/32/76/76	-
25	CHD	C	305	-	-	7/9/74/74	0/4/4/4
21	DMU	H	101	-	-	3/19/59/59	0/2/2/2
22	EDO	G	102	-	-	0/1/1/1	-
20	LFA	C	307	-	-	6/8/8/17	-

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[A]	HEA	C1D-ND	-5.79	1.30	1.40
14	A	601[B]	HEA	C1D-ND	-5.79	1.30	1.40
14	N	603	HEA	C1D-ND	-5.25	1.31	1.40
21	N	611	DMU	O16-C6	-5.20	1.31	1.40
14	A	601[A]	HEA	C3A-C2A	4.87	1.47	1.40
14	A	601[B]	HEA	C3A-C2A	4.87	1.47	1.40
14	N	603	HEA	C3A-C2A	4.68	1.46	1.40
14	N	602[A]	HEA	CHC-C4B	4.68	1.47	1.35
14	N	602[B]	HEA	CHC-C4B	4.68	1.47	1.35
14	A	602	HEA	C1D-ND	-4.35	1.32	1.40
14	A	602	HEA	C1B-NB	-4.33	1.29	1.38
14	A	601[A]	HEA	C3D-C2D	4.21	1.45	1.36
14	A	601[B]	HEA	C3D-C2D	4.21	1.45	1.36
14	N	603	HEA	C4B-NB	-4.20	1.33	1.40
14	N	603	HEA	C3B-C2B	4.16	1.44	1.34
14	N	602[A]	HEA	C3B-C2B	4.08	1.43	1.34
14	N	602[B]	HEA	C3B-C2B	4.08	1.43	1.34
14	N	602[A]	HEA	C1D-ND	-3.95	1.33	1.40
14	N	602[B]	HEA	C1D-ND	-3.95	1.33	1.40
14	N	602[A]	HEA	C1B-NB	-3.95	1.30	1.38
14	N	602[B]	HEA	C1B-NB	-3.95	1.30	1.38
14	N	603	HEA	C4D-ND	-3.88	1.30	1.38
14	A	601[A]	HEA	C16-C17	-3.84	1.40	1.53
14	A	601[B]	HEA	C16-C17	-3.84	1.40	1.53
14	N	603	HEA	CHD-C1D	3.83	1.44	1.35
14	A	602	HEA	CHD-C1D	3.79	1.44	1.35
14	A	602	HEA	C4D-ND	-3.77	1.31	1.38
14	N	602[A]	HEA	C3C-C2C	3.70	1.45	1.40
14	N	602[B]	HEA	C3C-C2C	3.70	1.45	1.40
14	N	603	HEA	C4B-C3B	3.62	1.50	1.44
14	N	602[A]	HEA	C3A-C2A	3.61	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602[B]	HEA	C3A-C2A	3.61	1.45	1.40
14	A	601[A]	HEA	CHD-C1D	3.59	1.44	1.35
14	A	601[B]	HEA	CHD-C1D	3.59	1.44	1.35
14	N	602[A]	HEA	C4B-C3B	3.54	1.50	1.44
14	N	602[B]	HEA	C4B-C3B	3.54	1.50	1.44
14	N	603	HEA	C1B-NB	-3.54	1.31	1.38
29	G	101	PEK	C23-C22	-3.53	1.39	1.52
23	A	616	PGV	O03-C19	3.50	1.43	1.33
14	N	602[A]	HEA	CHD-C1D	3.47	1.43	1.35
14	N	602[B]	HEA	CHD-C1D	3.47	1.43	1.35
14	A	602	HEA	C3B-C2B	3.45	1.42	1.34
14	A	601[A]	HEA	C1B-NB	-3.36	1.31	1.38
14	A	601[B]	HEA	C1B-NB	-3.36	1.31	1.38
14	A	601[A]	HEA	CHC-C4B	3.34	1.43	1.35
14	A	601[B]	HEA	CHC-C4B	3.34	1.43	1.35
25	P	302	CHD	C22-C23	-3.28	1.42	1.52
14	A	602	HEA	C4B-NB	-3.24	1.34	1.40
21	P	319	DMU	C7-C5	-3.23	1.44	1.52
14	N	603	HEA	C3D-C2D	3.19	1.43	1.36
21	Q	201	DMU	O55-C2	3.16	1.50	1.43
21	D	201	DMU	O5-C6	-3.15	1.33	1.41
14	A	602	HEA	CHC-C4B	3.11	1.42	1.35
14	A	601[A]	HEA	C3C-C2C	3.10	1.44	1.40
14	A	601[B]	HEA	C3C-C2C	3.10	1.44	1.40
27	P	305	CDL	C31-CA7	-3.06	1.41	1.50
21	Q	201	DMU	C10-C5	-3.03	1.43	1.52
23	P	304	PGV	O03-C19	3.02	1.42	1.33
25	P	306	CHD	O25-C24	3.02	1.32	1.22
21	P	319	DMU	O4-C7	2.97	1.50	1.43
21	C	318	DMU	O5-C6	-2.95	1.34	1.41
21	D	201	DMU	O16-C6	-2.94	1.35	1.40
14	A	601[A]	HEA	C3B-C2B	2.93	1.41	1.34
14	A	601[B]	HEA	C3B-C2B	2.93	1.41	1.34
21	A	611	DMU	O5-C6	-2.92	1.34	1.41
23	N	617	PGV	O03-C19	2.92	1.41	1.33
14	N	603	HEA	CMD-C2D	-2.91	1.44	1.50
14	A	601[A]	HEA	C4B-NB	-2.89	1.35	1.40
14	A	601[B]	HEA	C4B-NB	-2.89	1.35	1.40
21	Q	201	DMU	O3-C5	-2.87	1.36	1.43
14	N	602[A]	HEA	O11-C11	2.87	1.49	1.42
14	N	602[B]	HEA	O11-C11	2.87	1.49	1.42
14	N	603	HEA	C3C-C2C	2.86	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602[A]	HEA	C16-C17	-2.85	1.44	1.53
14	N	602[B]	HEA	C16-C17	-2.85	1.44	1.53
23	A	616	PGV	O01-C1	2.84	1.42	1.34
14	N	602[A]	HEA	C3D-C2D	2.84	1.42	1.36
14	N	602[B]	HEA	C3D-C2D	2.84	1.42	1.36
23	P	304	PGV	O03-C01	-2.83	1.38	1.45
21	D	201	DMU	O3-C5	-2.83	1.36	1.43
14	A	602	HEA	C2A-C1A	2.82	1.49	1.42
21	A	611	DMU	O3-C5	-2.82	1.36	1.43
21	H	101	DMU	C7-C5	-2.81	1.45	1.52
21	Z	101	DMU	O3-C5	-2.80	1.36	1.43
21	P	317	DMU	O16-C6	2.79	1.45	1.40
21	A	611	DMU	C7-C5	-2.79	1.45	1.52
21	Q	201	DMU	C7-C5	-2.77	1.45	1.52
21	U	101	DMU	C7-C5	-2.76	1.45	1.52
14	N	603	HEA	C1B-C2B	2.75	1.49	1.44
14	A	601[A]	HEA	CAA-C2A	-2.74	1.47	1.52
14	A	601[B]	HEA	CAA-C2A	-2.74	1.47	1.52
21	M	101	DMU	C7-C5	-2.74	1.45	1.52
27	C	304	CDL	C11-CA5	2.69	1.58	1.50
21	N	611	DMU	C6-C1	-2.66	1.44	1.52
14	A	602	HEA	CBD-CGD	2.65	1.56	1.50
21	M	101	DMU	O3-C5	-2.65	1.36	1.43
14	A	601[A]	HEA	C12-C11	-2.65	1.48	1.52
14	A	601[B]	HEA	C12-C11	-2.65	1.48	1.52
21	N	611	DMU	O55-C2	-2.64	1.36	1.43
21	P	319	DMU	C10-C5	-2.63	1.44	1.52
21	O	304	DMU	C3-C4	-2.62	1.47	1.53
14	A	602	HEA	C3A-C2A	2.61	1.44	1.40
25	C	301	CHD	C22-C23	-2.60	1.44	1.52
14	N	602[A]	HEA	C4B-NB	-2.55	1.35	1.40
14	N	602[B]	HEA	C4B-NB	-2.55	1.35	1.40
23	P	304	PGV	O01-C02	-2.55	1.40	1.46
25	C	301	CHD	O26-C24	-2.54	1.22	1.30
21	D	201	DMU	O61-C57	2.54	1.53	1.42
14	A	601[A]	HEA	O1D-CGD	2.53	1.30	1.22
14	A	601[B]	HEA	O1D-CGD	2.53	1.30	1.22
21	P	318	DMU	C7-C5	-2.53	1.45	1.52
21	B	304	DMU	O16-C6	2.51	1.44	1.40
21	A	611	DMU	O7-C10	2.51	1.48	1.41
21	Q	201	DMU	O5-C6	-2.50	1.35	1.41
21	C	318	DMU	C7-C5	-2.48	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	603	HEA	C2A-C1A	2.47	1.48	1.42
14	N	603	HEA	CMC-C2C	-2.45	1.46	1.51
14	N	602[A]	HEA	C1D-C2D	2.45	1.49	1.44
14	N	602[B]	HEA	C1D-C2D	2.45	1.49	1.44
21	A	611	DMU	O16-C6	-2.44	1.36	1.40
14	N	602[A]	HEA	C4D-ND	-2.44	1.33	1.38
14	N	602[B]	HEA	C4D-ND	-2.44	1.33	1.38
25	P	302	CHD	O26-C24	-2.43	1.22	1.30
23	N	617	PGV	O03-C01	2.43	1.50	1.45
21	N	611	DMU	C10-C5	-2.43	1.45	1.52
14	N	603	HEA	CHC-C4B	2.43	1.41	1.35
14	A	601[A]	HEA	C4B-C3B	2.43	1.48	1.44
14	A	601[B]	HEA	C4B-C3B	2.43	1.48	1.44
27	C	304	CDL	OA7-CA5	2.40	1.29	1.22
14	N	602[A]	HEA	C2A-C1A	2.38	1.47	1.42
14	N	602[B]	HEA	C2A-C1A	2.38	1.47	1.42
21	Z	101	DMU	O16-C6	-2.37	1.36	1.40
21	C	319	DMU	O49-C1	2.36	1.48	1.43
21	O	308	DMU	C6-C1	-2.32	1.45	1.52
21	A	611	DMU	C10-C5	-2.31	1.45	1.52
14	A	601[A]	HEA	CMD-C2D	-2.31	1.45	1.50
14	A	601[B]	HEA	CMD-C2D	-2.31	1.45	1.50
14	A	601[A]	HEA	CBD-CGD	2.31	1.55	1.50
14	A	601[B]	HEA	CBD-CGD	2.31	1.55	1.50
21	Z	101	DMU	O55-C2	2.31	1.48	1.43
21	C	319	DMU	O55-C2	-2.29	1.37	1.43
21	H	101	DMU	C10-C5	-2.29	1.45	1.52
21	C	315	DMU	C7-C5	-2.28	1.46	1.52
21	Q	201	DMU	O16-C6	-2.28	1.36	1.40
14	N	602[A]	HEA	CAA-C2A	-2.27	1.48	1.52
14	N	602[B]	HEA	CAA-C2A	-2.27	1.48	1.52
14	N	603	HEA	C1D-C2D	2.25	1.48	1.44
29	T	101	PEK	C2-C1	2.21	1.57	1.50
14	N	603	HEA	C18-C19	2.17	1.38	1.33
14	A	601[A]	HEA	C4D-ND	-2.16	1.34	1.38
14	A	601[B]	HEA	C4D-ND	-2.16	1.34	1.38
27	P	305	CDL	C12-C11	-2.15	1.44	1.52
21	C	318	DMU	O3-C5	2.15	1.48	1.43
21	Q	201	DMU	O61-C57	2.14	1.51	1.42
29	T	101	PEK	C23-C22	-2.13	1.44	1.52
27	C	304	CDL	PA1-OA3	2.12	1.58	1.50
14	N	602[A]	HEA	CBA-CGA	2.11	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602[B]	HEA	CBA-CGA	2.11	1.55	1.50
21	C	315	DMU	C6-C1	-2.11	1.46	1.52
14	N	603	HEA	C4D-C3D	2.10	1.48	1.45
21	P	318	DMU	O5-C6	-2.10	1.36	1.41
21	C	319	DMU	C8-C9	-2.10	1.48	1.53
14	A	602	HEA	C4D-C3D	2.09	1.48	1.45
23	P	304	PGV	O01-C1	2.08	1.40	1.34
14	A	602	HEA	C3D-C2D	2.07	1.41	1.36
21	N	611	DMU	C7-C5	-2.07	1.47	1.52
21	D	201	DMU	O1-C10	2.05	1.47	1.41
21	N	611	DMU	O5-C6	-2.05	1.36	1.41
21	C	315	DMU	O3-C5	-2.05	1.38	1.43
21	D	201	DMU	C10-C5	-2.04	1.46	1.52
14	A	602	HEA	FE-ND	2.03	2.06	1.96
21	P	318	DMU	C10-C5	-2.03	1.46	1.52
21	P	315	DMU	O3-C5	-2.02	1.38	1.43
23	N	617	PGV	O01-C1	2.02	1.40	1.34
25	C	301	CHD	O25-C24	2.02	1.28	1.22
21	Q	201	DMU	O1-C10	2.01	1.47	1.41

All (314) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	603	HEA	C3D-C4D-ND	7.36	117.49	110.36
14	N	602[A]	HEA	C3D-C4D-ND	7.01	117.15	110.36
14	N	602[B]	HEA	C3D-C4D-ND	7.01	117.15	110.36
27	C	304	CDL	OA6-CA5-C11	-6.58	97.31	111.50
14	N	602[A]	HEA	C2B-C1B-NB	6.32	117.45	109.88
14	N	602[B]	HEA	C2B-C1B-NB	6.32	117.45	109.88
14	A	601[A]	HEA	C3D-C4D-ND	6.11	116.27	110.36
14	A	601[B]	HEA	C3D-C4D-ND	6.11	116.27	110.36
27	V	101	CDL	OA6-CA4-CA3	6.08	130.41	108.40
14	A	601[A]	HEA	C3C-C4C-NC	5.37	116.16	109.21
14	A	601[B]	HEA	C3C-C4C-NC	5.37	116.16	109.21
14	A	601[A]	HEA	C2B-C1B-NB	5.36	116.30	109.88
14	A	601[B]	HEA	C2B-C1B-NB	5.36	116.30	109.88
21	P	315	DMU	O16-C6-C1	5.35	116.66	108.30
25	C	305	CHD	C16-C17-C20	5.31	120.36	112.15
21	C	315	DMU	C6-O5-C4	5.30	124.08	113.69
14	A	601[A]	HEA	C27-C19-C20	5.29	124.18	115.27
14	N	603	HEA	CHA-C4D-C3D	-5.21	117.18	124.84
14	N	602[A]	HEA	C27-C19-C20	5.20	124.02	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	323	DMU	O16-C6-C1	5.18	116.39	108.30
23	N	617	PGV	O03-C19-O04	-5.15	110.58	123.59
23	N	617	PGV	O03-C19-C20	5.14	128.03	111.91
21	B	308	DMU	O16-C6-C1	5.04	116.17	108.30
14	A	601[A]	HEA	C2D-C1D-ND	5.03	115.80	109.84
14	A	601[B]	HEA	C2D-C1D-ND	5.03	115.80	109.84
21	P	324	DMU	C10-C5-C7	5.00	120.40	110.00
14	A	602	HEA	C3B-C4B-NB	4.94	115.69	109.84
14	N	603	HEA	C3B-C4B-NB	4.94	115.69	109.84
21	Q	201	DMU	O16-C6-C1	4.89	115.94	108.30
21	P	319	DMU	O16-C6-C1	4.87	115.91	108.30
14	A	601[A]	HEA	CHA-C4D-C3D	-4.75	117.86	124.84
14	A	601[B]	HEA	CHA-C4D-C3D	-4.75	117.86	124.84
14	N	603	HEA	C4D-C3D-C2D	-4.67	100.09	106.90
14	N	603	HEA	CAD-C3D-C4D	4.62	132.73	124.66
21	C	315	DMU	O16-C6-C1	4.62	115.51	108.30
14	N	603	HEA	C2B-C1B-NB	4.60	115.39	109.88
14	A	602	HEA	C2B-C1B-NB	4.54	115.32	109.88
14	N	602[A]	HEA	C2D-C1D-ND	4.53	115.21	109.84
14	N	602[B]	HEA	C2D-C1D-ND	4.53	115.21	109.84
21	D	201	DMU	O16-C6-C1	4.51	115.34	108.30
14	N	603	HEA	CAD-CBD-CGD	-4.48	103.96	113.60
14	A	601[A]	HEA	C3B-C4B-NB	4.48	115.15	109.84
14	A	601[B]	HEA	C3B-C4B-NB	4.48	115.15	109.84
27	I	101	CDL	OA6-CA4-CA6	4.46	124.54	108.40
14	N	602[A]	HEA	CHB-C1B-C2B	-4.44	118.05	124.98
14	N	602[B]	HEA	CHB-C1B-C2B	-4.44	118.05	124.98
14	A	602	HEA	CHA-C4D-C3D	-4.43	118.32	124.84
21	C	324	DMU	O16-C6-C1	4.40	115.17	108.30
27	I	101	CDL	CA4-OA6-CA5	4.40	128.62	117.79
27	V	101	CDL	OA6-CA4-CA6	-4.35	92.64	108.40
14	A	601[A]	HEA	C4D-C3D-C2D	-4.29	100.65	106.90
14	A	601[B]	HEA	C4D-C3D-C2D	-4.29	100.65	106.90
14	N	603	HEA	CHB-C1B-C2B	-4.27	118.30	124.98
14	A	602	HEA	C3D-C4D-ND	4.26	114.49	110.36
14	N	603	HEA	C3C-C4C-NC	4.26	114.72	109.21
14	N	602[A]	HEA	C13-C12-C11	-4.19	108.05	114.35
14	N	602[B]	HEA	C13-C12-C11	-4.19	108.05	114.35
27	C	304	CDL	OA4-PA1-OA5	-4.18	88.35	107.75
27	I	101	CDL	OA5-PA1-OA3	4.16	125.33	109.07
21	C	318	DMU	O16-C6-C1	4.15	114.78	108.30
21	C	319	DMU	O16-C6-C1	4.12	114.73	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	317	DMU	C2-C3-C4	-4.01	103.08	110.24
21	U	101	DMU	C10-C5-C7	4.01	118.35	110.00
21	L	102	DMU	O5-C6-O16	4.01	119.46	109.97
14	N	602[A]	HEA	C3C-C4C-NC	3.99	114.36	109.21
14	N	602[B]	HEA	C3C-C4C-NC	3.99	114.36	109.21
14	N	603	HEA	CBA-CAA-C2A	-3.98	105.90	112.60
21	C	317	DMU	O5-C6-C1	3.97	118.75	110.35
14	A	601[B]	HEA	C27-C19-C20	3.93	121.88	115.27
14	A	602	HEA	CAD-CBD-CGD	-3.91	105.19	113.60
23	A	616	PGV	O03-C19-O04	-3.91	113.72	123.59
21	U	101	DMU	O16-C6-C1	3.88	114.36	108.30
27	C	304	CDL	OA7-CA5-C11	3.82	138.63	123.73
21	P	317	DMU	O5-C6-C1	3.81	118.41	110.35
14	N	602[A]	HEA	C3B-C4B-NB	3.80	114.35	109.84
14	N	602[B]	HEA	C3B-C4B-NB	3.80	114.35	109.84
14	N	603	HEA	C2D-C1D-ND	3.79	114.33	109.84
14	A	602	HEA	C3C-C4C-NC	3.78	114.10	109.21
21	P	318	DMU	O16-C6-C1	3.75	114.16	108.30
14	A	601[A]	HEA	CHB-C1B-C2B	-3.74	119.14	124.98
14	A	601[B]	HEA	CHB-C1B-C2B	-3.74	119.14	124.98
29	T	101	PEK	C2-C3-C4	3.67	119.77	113.23
23	C	303	PGV	C27-C26-C25	-3.65	95.87	114.42
14	N	602[A]	HEA	CMC-C2C-C3C	3.63	131.47	124.68
14	N	602[B]	HEA	CMC-C2C-C3C	3.63	131.47	124.68
14	N	602[A]	HEA	C4D-C3D-C2D	-3.62	101.62	106.90
14	N	602[B]	HEA	C4D-C3D-C2D	-3.62	101.62	106.90
14	A	602	HEA	C13-C12-C11	-3.60	108.94	114.35
14	A	601[A]	HEA	C13-C12-C11	-3.58	108.97	114.35
14	A	601[B]	HEA	C13-C12-C11	-3.58	108.97	114.35
27	C	304	CDL	OA5-PA1-OA3	3.57	123.03	109.07
14	A	602	HEA	C4D-C3D-C2D	-3.57	101.69	106.90
27	V	101	CDL	OA4-PA1-OA5	3.54	124.19	107.75
14	N	602[A]	HEA	CHA-C4D-C3D	-3.53	119.64	124.84
14	N	602[B]	HEA	CHA-C4D-C3D	-3.53	119.64	124.84
21	N	611	DMU	C10-O1-C9	3.53	120.62	113.69
25	C	305	CHD	C22-C23-C24	-3.53	103.14	112.51
14	A	601[A]	HEA	CMC-C2C-C3C	3.53	131.28	124.68
14	A	601[B]	HEA	CMC-C2C-C3C	3.53	131.28	124.68
21	O	304	DMU	O5-C6-C1	3.50	117.77	110.35
21	M	101	DMU	O16-C6-C1	3.49	113.76	108.30
27	L	101	CDL	OB4-PB2-OB2	3.48	123.91	107.75
21	P	324	DMU	C10-O1-C9	-3.47	106.87	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	603	HEA	C4B-C3B-C2B	-3.47	101.48	107.41
21	C	323	DMU	O16-C6-C1	3.46	113.71	108.30
14	N	603	HEA	C27-C19-C20	3.45	121.07	115.27
27	P	305	CDL	OA4-PA1-OA3	3.44	129.24	112.24
21	D	201	DMU	O1-C9-C8	3.41	115.89	109.69
21	P	324	DMU	O16-C6-C1	3.40	113.61	108.30
14	A	601[A]	HEA	CHC-C4B-NB	-3.39	120.19	124.38
14	A	601[B]	HEA	CHC-C4B-NB	-3.39	120.19	124.38
27	L	101	CDL	OB5-PB2-OB3	-3.38	95.85	109.07
21	C	318	DMU	C10-O1-C9	-3.38	107.05	113.69
21	H	101	DMU	O16-C6-C1	3.38	113.58	108.30
21	U	101	DMU	O3-C5-C10	3.37	118.23	110.05
21	C	315	DMU	O5-C6-C1	3.37	117.47	110.35
14	N	602[A]	HEA	C1B-C2B-C3B	-3.36	102.79	106.80
14	N	602[B]	HEA	C1B-C2B-C3B	-3.36	102.79	106.80
25	C	305	CHD	C6-C7-C8	3.33	115.03	111.48
14	A	602	HEA	C2D-C1D-ND	3.32	113.77	109.84
23	A	616	PGV	O03-C19-C20	3.31	122.30	111.91
23	C	303	PGV	O03-C19-O04	-3.26	115.36	123.59
27	C	304	CDL	OA4-PA1-OA3	3.25	128.32	112.24
21	P	318	DMU	C10-C5-C7	3.23	116.72	110.00
25	C	305	CHD	C14-C13-C12	3.22	110.40	107.40
27	L	101	CDL	OA2-PA1-OA3	-3.21	96.53	109.07
14	A	602	HEA	C4B-C3B-C2B	-3.20	101.95	107.41
21	P	319	DMU	C8-C7-C5	-3.16	105.31	110.82
21	C	319	DMU	O3-C5-C10	3.15	117.71	110.05
21	P	323	DMU	C18-O16-C6	-3.13	108.66	113.84
29	T	101	PEK	O01-C1-O02	-3.13	116.15	123.70
27	C	304	CDL	OA4-PA1-OA2	-3.11	93.30	107.75
21	C	319	DMU	C10-C5-C7	3.10	116.45	110.00
14	N	602[A]	HEA	C1D-C2D-C3D	-3.10	103.70	106.96
14	N	602[B]	HEA	C1D-C2D-C3D	-3.10	103.70	106.96
21	C	318	DMU	C10-C5-C7	3.06	116.36	110.00
27	V	101	CDL	CA4-OA6-CA5	3.05	125.31	117.79
14	A	601[A]	HEA	C1D-C2D-C3D	-3.05	103.75	106.96
14	A	601[B]	HEA	C1D-C2D-C3D	-3.05	103.75	106.96
23	P	304	PGV	C27-C26-C25	-3.04	98.97	114.42
27	Y	101	CDL	OB5-PB2-OB3	-3.04	97.19	109.07
27	C	304	CDL	OB5-PB2-OB3	3.02	120.87	109.07
21	P	315	DMU	C10-C5-C7	3.01	116.27	110.00
27	P	305	CDL	OA4-PA1-OA5	-3.01	93.76	107.75
21	D	201	DMU	C10-C5-C7	3.00	116.25	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602[A]	HEA	C4B-C3B-C2B	-3.00	102.28	107.41
14	N	602[B]	HEA	C4B-C3B-C2B	-3.00	102.28	107.41
14	N	603	HEA	C1B-C2B-C3B	-2.99	103.23	106.80
21	O	304	DMU	O16-C6-C1	2.98	112.95	108.30
27	L	101	CDL	OA4-PA1-OA2	2.96	121.50	107.75
14	A	601[A]	HEA	CAD-C3D-C4D	2.95	129.82	124.66
14	A	601[B]	HEA	CAD-C3D-C4D	2.95	129.82	124.66
14	A	602	HEA	CMB-C2B-C1B	2.92	129.49	125.04
14	N	603	HEA	C20-C19-C18	-2.92	115.21	121.12
14	A	602	HEA	C1B-C2B-C3B	-2.90	103.33	106.80
14	A	601[A]	HEA	C4B-C3B-C2B	-2.89	102.47	107.41
14	A	601[B]	HEA	C4B-C3B-C2B	-2.89	102.47	107.41
27	P	305	CDL	OB4-PB2-OB3	2.88	126.46	112.24
14	N	602[A]	HEA	C20-C19-C18	-2.87	115.30	121.12
25	C	305	CHD	C17-C13-C14	-2.86	97.21	100.09
14	N	602[A]	HEA	C4A-CHB-C1B	2.85	126.32	122.56
14	N	602[B]	HEA	C4A-CHB-C1B	2.85	126.32	122.56
14	N	603	HEA	CMD-C2D-C1D	2.85	129.38	125.04
14	A	602	HEA	CHB-C1B-C2B	-2.82	120.57	124.98
21	D	201	DMU	C2-C3-C4	-2.81	104.49	110.93
14	A	602	HEA	CMD-C2D-C1D	2.79	129.29	125.04
21	Q	201	DMU	C6-O5-C4	-2.79	108.22	113.69
14	N	602[A]	HEA	C1D-ND-C4D	-2.77	102.21	105.07
14	N	602[B]	HEA	C1D-ND-C4D	-2.77	102.21	105.07
21	A	611	DMU	C10-O7-C3	-2.77	111.11	117.96
27	C	304	CDL	OB6-CB5-C51	2.76	117.45	111.50
27	L	101	CDL	OA6-CA5-C11	2.76	117.44	111.50
14	N	603	HEA	C1D-C2D-C3D	-2.75	104.06	106.96
14	A	602	HEA	CMC-C2C-C3C	2.75	129.83	124.68
21	Z	101	DMU	O16-C6-C1	2.75	112.59	108.30
29	T	101	PEK	O02-C1-C2	2.72	134.35	123.73
21	C	315	DMU	O5-C4-C3	2.72	115.48	109.75
21	C	319	DMU	O3-C5-C7	2.71	116.61	110.35
21	Z	102	DMU	O5-C6-O16	2.70	116.37	109.97
21	C	315	DMU	C18-O16-C6	-2.69	109.38	113.84
21	Q	201	DMU	C10-O1-C9	2.68	118.96	113.69
21	O	304	DMU	C6-C1-C2	2.68	115.58	110.00
21	P	319	DMU	C10-O7-C3	-2.68	111.33	117.96
14	N	603	HEA	CHD-C1D-C2D	-2.68	119.32	126.72
21	H	101	DMU	C10-C5-C7	2.68	115.57	110.00
23	N	617	PGV	O01-C1-O02	-2.67	117.24	123.70
14	A	601[A]	HEA	C1B-C2B-C3B	-2.65	103.64	106.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601[B]	HEA	C1B-C2B-C3B	-2.65	103.64	106.80
21	N	611	DMU	C10-C5-C7	2.64	115.48	110.00
25	C	301	CHD	C22-C20-C17	-2.61	104.89	110.28
21	A	611	DMU	C18-O16-C6	2.61	118.17	113.84
21	B	304	DMU	O5-C6-C1	2.60	115.85	110.35
27	C	304	CDL	CA6-CA4-CA3	2.59	117.91	111.79
14	A	602	HEA	C20-C19-C18	-2.59	115.88	121.12
27	Y	101	CDL	OB4-PB2-OB2	2.58	119.73	107.75
14	A	601[A]	HEA	C4B-NB-C1B	-2.58	102.41	105.07
14	A	601[B]	HEA	C4B-NB-C1B	-2.58	102.41	105.07
14	N	603	HEA	C4D-CHA-C1A	2.56	125.94	122.56
27	L	101	CDL	OB4-PB2-OB3	2.56	124.91	112.24
25	P	306	CHD	O7-C7-C6	-2.56	103.60	109.94
21	N	611	DMU	C7-C8-C9	2.55	114.80	110.24
14	A	601[A]	HEA	C4A-CHB-C1B	2.55	125.92	122.56
14	A	601[B]	HEA	C4A-CHB-C1B	2.55	125.92	122.56
21	C	315	DMU	O5-C6-O16	-2.55	103.94	109.97
21	C	318	DMU	C1-C2-C3	2.54	115.49	109.68
14	A	602	HEA	OMA-CMA-C3A	-2.54	119.37	124.91
21	Q	201	DMU	C11-C9-C8	-2.53	107.07	113.00
21	Z	102	DMU	O5-C4-C57	2.53	112.71	106.44
21	D	201	DMU	C7-C8-C9	2.52	114.74	110.24
21	P	324	DMU	O5-C6-O16	2.52	115.94	109.97
21	U	101	DMU	C10-O7-C3	-2.52	111.73	117.96
21	Q	201	DMU	C2-C3-C4	-2.50	105.19	110.93
21	C	315	DMU	C10-C5-C7	2.49	115.19	110.00
27	P	305	CDL	OA4-PA1-OA2	-2.46	96.31	107.75
27	L	101	CDL	OB2-PB2-OB3	-2.45	99.48	109.07
21	M	101	DMU	C18-O16-C6	-2.45	109.78	113.84
14	A	601[A]	HEA	CHD-C1D-C2D	-2.45	119.95	126.72
14	A	601[B]	HEA	CHD-C1D-C2D	-2.45	119.95	126.72
25	C	305	CHD	C5-C6-C7	2.42	117.14	114.46
21	D	201	DMU	C11-C9-C8	-2.42	107.34	113.00
21	C	319	DMU	O5-C6-C1	2.41	115.46	110.35
14	A	601[B]	HEA	C21-C22-C23	-2.41	119.52	127.75
25	C	301	CHD	C18-C13-C12	2.41	111.52	109.07
21	H	101	DMU	O3-C5-C10	2.41	115.89	110.05
25	O	301	CHD	O7-C7-C6	2.40	115.89	109.94
25	C	305	CHD	C16-C17-C13	-2.39	101.21	103.55
14	N	603	HEA	C13-C12-C11	-2.39	110.75	114.35
14	N	602[B]	HEA	C25-C23-C22	-2.38	115.75	122.65
21	C	318	DMU	O3-C5-C10	2.38	115.83	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601[B]	HEA	C20-C19-C18	-2.38	116.30	121.12
21	C	319	DMU	O1-C9-C11	2.37	112.33	106.44
21	P	317	DMU	C18-O16-C6	-2.36	109.92	113.84
21	P	324	DMU	O7-C10-O1	-2.35	104.10	110.67
21	Q	201	DMU	C18-O16-C6	2.35	117.73	113.84
23	C	303	PGV	O01-C1-O02	-2.34	118.04	123.70
23	P	304	PGV	C22-C21-C20	-2.33	104.81	113.19
14	A	601[A]	HEA	CMD-C2D-C1D	2.32	128.58	125.04
14	A	601[B]	HEA	CMD-C2D-C1D	2.32	128.58	125.04
25	C	305	CHD	C4-C5-C10	2.32	115.12	112.66
14	N	602[B]	HEA	C25-C23-C24	2.31	119.71	114.60
21	H	101	DMU	O5-C6-C1	2.31	115.23	110.35
21	A	611	DMU	O3-C5-C7	2.31	115.68	110.35
21	C	324	DMU	C10-C5-C7	2.31	114.80	110.00
21	C	315	DMU	C10-O1-C9	2.30	118.21	113.69
23	N	617	PGV	C15-C14-C13	-2.29	103.79	113.79
21	O	308	DMU	O5-C6-O16	2.29	115.39	109.97
21	A	611	DMU	C10-C5-C7	2.27	114.72	110.00
14	A	602	HEA	C4A-CHB-C1B	2.27	125.55	122.56
21	C	317	DMU	C18-O16-C6	-2.27	110.08	113.84
14	A	601[A]	HEA	C20-C19-C18	-2.26	116.55	121.12
21	Q	201	DMU	O1-C9-C8	2.26	113.80	109.69
21	O	308	DMU	O5-C6-C1	2.25	115.12	110.35
21	P	324	DMU	C18-O16-C6	2.25	117.57	113.84
14	N	602[B]	HEA	C20-C19-C18	-2.24	116.57	121.12
21	Z	101	DMU	C10-O1-C9	-2.22	109.32	113.69
27	Y	101	CDL	OB4-PB2-OB3	2.21	123.17	112.24
21	Z	101	DMU	O3-C5-C7	2.21	115.46	110.35
23	P	304	PGV	O03-C19-O04	-2.21	118.01	123.59
25	B	306	CHD	C1-C2-C3	2.19	113.27	110.47
21	Z	101	DMU	O1-C9-C11	2.18	111.86	106.44
14	A	602	HEA	CHA-C4D-ND	2.18	126.79	124.43
14	N	602[A]	HEA	C21-C22-C23	-2.17	120.32	127.75
21	C	318	DMU	C6-C1-C2	2.17	114.52	110.00
14	N	602[A]	HEA	CHD-C1D-C2D	-2.17	120.71	126.72
14	N	602[B]	HEA	CHD-C1D-C2D	-2.17	120.71	126.72
27	Y	101	CDL	OA2-PA1-OA3	-2.17	100.59	109.07
27	I	101	CDL	OA2-PA1-OA3	-2.16	100.65	109.07
14	A	601[A]	HEA	CAD-CBD-CGD	-2.15	108.97	113.60
14	A	601[B]	HEA	CAD-CBD-CGD	-2.15	108.97	113.60
27	P	305	CDL	OA6-CA5-C11	-2.15	106.87	111.50
21	O	304	DMU	C2-C3-C4	-2.15	106.41	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	315	DMU	O3-C5-C10	2.14	115.25	110.05
27	V	101	CDL	OA8-CA6-CA4	2.14	114.67	108.43
14	A	601[A]	HEA	O2D-CGD-CBD	2.14	120.90	114.03
14	A	601[B]	HEA	O2D-CGD-CBD	2.14	120.90	114.03
14	A	601[B]	HEA	C25-C23-C24	2.14	119.33	114.60
27	C	304	CDL	O1-C1-CB2	2.14	117.05	109.56
21	P	317	DMU	C2-C3-C4	-2.14	106.43	110.24
25	O	301	CHD	C13-C17-C20	-2.13	116.95	119.50
21	O	308	DMU	C57-C4-C3	-2.13	108.01	113.00
14	N	602[A]	HEA	O2D-CGD-CBD	2.12	120.85	114.03
14	N	602[B]	HEA	O2D-CGD-CBD	2.12	120.85	114.03
21	L	102	DMU	C57-C4-C3	-2.12	108.03	113.00
27	L	101	CDL	OB6-CB5-C51	2.12	116.07	111.50
21	B	308	DMU	O5-C6-C1	2.12	114.84	110.35
21	M	101	DMU	O5-C6-C1	2.11	114.82	110.35
29	G	101	PEK	O03-C21-C22	-2.11	105.28	111.91
21	P	315	DMU	C57-C4-C3	-2.11	107.18	113.33
21	N	611	DMU	O5-C6-C1	2.11	114.81	110.35
21	P	323	DMU	C57-C4-C3	-2.11	108.06	113.00
21	D	201	DMU	O3-C5-C7	2.11	115.22	110.35
21	B	304	DMU	C3-C2-C1	-2.09	107.17	110.82
27	P	305	CDL	O1-C1-CA2	2.09	116.88	109.56
21	P	318	DMU	C8-C7-C5	-2.08	107.19	110.82
21	C	317	DMU	C3-C2-C1	-2.07	107.20	110.82
14	A	602	HEA	O11-C11-C12	2.07	115.21	109.42
21	Z	101	DMU	O5-C6-C1	2.07	114.73	110.35
25	P	302	CHD	C18-C13-C14	2.07	114.45	111.21
27	C	304	CDL	OB4-PB2-OB3	2.07	122.46	112.24
21	A	611	DMU	O16-C6-C1	2.07	111.53	108.30
21	M	101	DMU	C10-C5-C7	2.07	114.30	110.00
21	D	201	DMU	O4-C7-C8	-2.07	105.57	110.35
21	P	319	DMU	O4-C7-C8	2.06	115.11	110.35
14	N	603	HEA	CHC-C4B-C3B	-2.03	120.56	125.80
14	N	602[A]	HEA	O2A-CGA-CBA	2.03	120.56	114.03
14	N	602[B]	HEA	O2A-CGA-CBA	2.03	120.56	114.03
21	Z	101	DMU	C10-C5-C7	2.02	114.20	110.00
25	C	305	CHD	C17-C13-C12	-2.02	115.83	117.67
14	N	603	HEA	C21-C20-C19	2.01	119.60	112.98
21	C	318	DMU	C8-C7-C5	-2.01	107.31	110.82
29	G	101	PEK	O04-C21-C22	2.01	131.57	123.73
14	A	601[A]	HEA	C26-C15-C16	2.01	118.65	115.27
14	A	601[B]	HEA	C26-C15-C16	2.01	118.65	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	I	101	CDL	OA6-CA5-C11	2.00	115.81	111.50

There are no chirality outliers.

All (787) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C18-C19-C20-C21
14	A	601[A]	HEA	C27-C19-C20-C21
21	B	304	DMU	C1-C6-O16-C18
21	B	304	DMU	O5-C6-O16-C18
21	B	308	DMU	O5-C6-O16-C18
21	B	308	DMU	C19-C18-O16-C6
21	C	318	DMU	C1-C6-O16-C18
21	C	318	DMU	O5-C6-O16-C18
21	C	318	DMU	C19-C18-O16-C6
21	C	323	DMU	C19-C18-O16-C6
21	D	201	DMU	C19-C18-O16-C6
21	L	102	DMU	C19-C18-O16-C6
21	O	304	DMU	C19-C18-O16-C6
21	O	308	DMU	C19-C18-O16-C6
21	P	323	DMU	C1-C6-O16-C18
21	P	323	DMU	O5-C6-O16-C18
21	Q	201	DMU	C19-C18-O16-C6
21	U	101	DMU	C1-C6-O16-C18
21	Z	102	DMU	O5-C6-O16-C18
21	Z	102	DMU	C19-C18-O16-C6
25	C	305	CHD	C13-C17-C20-C21
25	C	305	CHD	C16-C17-C20-C22
27	C	304	CDL	O1-C1-CB2-OB2
27	C	304	CDL	C1-CA2-OA2-PA1
27	C	304	CDL	CA3-OA5-PA1-OA2
27	C	304	CDL	C11-CA5-OA6-CA4
27	C	304	CDL	CB3-OB5-PB2-OB4
27	C	304	CDL	OB7-CB5-OB6-CB4
27	C	304	CDL	C51-CB5-OB6-CB4
27	I	101	CDL	CA3-OA5-PA1-OA2
27	I	101	CDL	OA6-CA4-CA6-OA8
27	I	101	CDL	CB2-OB2-PB2-OB3
27	I	101	CDL	CB3-OB5-PB2-OB3
27	I	101	CDL	CB3-OB5-PB2-OB4
27	I	101	CDL	C51-CB5-OB6-CB4
27	L	101	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
27	L	101	CDL	CA2-OA2-PA1-OA3
27	L	101	CDL	CA2-OA2-PA1-OA4
27	L	101	CDL	CA3-OA5-PA1-OA3
27	L	101	CDL	C11-CA5-OA6-CA4
27	L	101	CDL	CB2-OB2-PB2-OB3
27	L	101	CDL	OB6-CB4-CB6-OB8
27	P	305	CDL	C1-CA2-OA2-PA1
27	P	305	CDL	CB3-OB5-PB2-OB4
27	P	305	CDL	OB7-CB5-OB6-CB4
27	P	305	CDL	C51-CB5-OB6-CB4
27	V	101	CDL	CA3-OA5-PA1-OA4
27	V	101	CDL	CB2-OB2-PB2-OB3
27	V	101	CDL	CB3-OB5-PB2-OB2
27	V	101	CDL	CB3-OB5-PB2-OB3
27	V	101	CDL	CB3-OB5-PB2-OB4
27	V	101	CDL	C51-CB5-OB6-CB4
27	Y	101	CDL	CA3-OA5-PA1-OA3
27	Y	101	CDL	C11-CA5-OA6-CA4
27	Y	101	CDL	CB2-OB2-PB2-OB4
27	Y	101	CDL	CB2-OB2-PB2-OB5
27	Y	101	CDL	C51-CB5-OB6-CB4
29	T	101	PEK	C11-C12-C13-C14
29	T	101	PEK	C12-C13-C14-C15
25	C	305	CHD	C16-C17-C20-C21
25	C	305	CHD	C13-C17-C20-C22
27	C	304	CDL	OA7-CA5-OA6-CA4
27	I	101	CDL	OA7-CA5-OA6-CA4
27	L	101	CDL	OA7-CA5-OA6-CA4
27	V	101	CDL	OB7-CB5-OB6-CB4
27	Y	101	CDL	OA7-CA5-OA6-CA4
27	Y	101	CDL	OB7-CB5-OB6-CB4
27	L	101	CDL	C31-CA7-OA8-CA6
21	C	318	DMU	O5-C4-C57-O61
21	C	323	DMU	O5-C4-C57-O61
27	Y	101	CDL	C31-CA7-OA8-CA6
27	I	101	CDL	OB7-CB5-OB6-CB4
21	L	102	DMU	C3-C4-C57-O61
21	O	304	DMU	O5-C4-C57-O61
21	P	318	DMU	O5-C4-C57-O61
21	U	101	DMU	O5-C4-C57-O61
27	P	305	CDL	O1-C1-CB2-OB2
27	Y	101	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
21	A	611	DMU	O6-C11-C9-O1
21	C	319	DMU	O5-C4-C57-O61
21	C	319	DMU	O6-C11-C9-O1
21	P	323	DMU	O5-C4-C57-O61
27	P	305	CDL	C11-CA5-OA6-CA4
20	G	103	LFA	C9-C10-C11-C12
21	A	611	DMU	O6-C11-C9-C8
20	P	301	LFA	C2-C3-C4-C5
20	P	311	LFA	C5-C6-C7-C8
20	C	309	LFA	C12-C13-C14-C15
21	P	319	DMU	C2-C3-O7-C10
21	C	318	DMU	O6-C11-C9-O1
21	D	201	DMU	O6-C11-C9-O1
21	D	201	DMU	O6-C11-C9-C8
20	P	310	LFA	C11-C10-C9-C8
21	P	319	DMU	O6-C11-C9-O1
27	I	101	CDL	C1-CA2-OA2-PA1
27	L	101	CDL	OA9-CA7-OA8-CA6
27	L	101	CDL	C72-C73-C74-C75
21	C	315	DMU	O5-C4-C57-O61
14	N	602[A]	HEA	C27-C19-C20-C21
21	C	318	DMU	C3-C4-C57-O61
21	C	323	DMU	C3-C4-C57-O61
14	N	602[A]	HEA	C18-C19-C20-C21
21	L	102	DMU	O5-C4-C57-O61
21	C	319	DMU	O6-C11-C9-C8
21	O	304	DMU	C3-C4-C57-O61
21	Q	201	DMU	O5-C6-O16-C18
14	A	601[A]	HEA	C15-C16-C17-C18
14	N	602[A]	HEA	C15-C16-C17-C18
27	C	304	CDL	C71-CB7-OB8-CB6
21	B	308	DMU	O5-C4-C57-O61
21	P	323	DMU	C3-C4-C57-O61
25	P	306	CHD	C17-C20-C22-C23
21	C	315	DMU	C3-C4-C57-O61
27	P	305	CDL	CA2-C1-CB2-OB2
27	Y	101	CDL	CB2-C1-CA2-OA2
27	C	304	CDL	C31-CA7-OA8-CA6
27	P	305	CDL	C31-CA7-OA8-CA6
27	V	101	CDL	C31-CA7-OA8-CA6
27	Y	101	CDL	C72-C73-C74-C75
21	P	318	DMU	C3-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
27	L	101	CDL	C31-C32-C33-C34
21	C	319	DMU	C3-C4-C57-O61
21	P	319	DMU	O6-C11-C9-C8
27	C	304	CDL	O1-C1-CA2-OA2
27	L	101	CDL	O1-C1-CA2-OA2
25	P	306	CHD	C21-C20-C22-C23
27	C	304	CDL	CB5-C51-C52-C53
21	Z	102	DMU	C1-C6-O16-C18
20	O	302	LFA	C5-C6-C7-C8
21	P	315	DMU	O5-C4-C57-O61
27	L	101	CDL	C51-CB5-OB6-CB4
23	P	304	PGV	C28-C29-C30-C31
21	N	611	DMU	O6-C11-C9-C8
27	P	305	CDL	CB5-C51-C52-C53
21	P	315	DMU	C31-C34-C37-C40
27	C	304	CDL	CB7-C71-C72-C73
27	P	305	CDL	CB7-C71-C72-C73
27	V	101	CDL	CA7-C31-C32-C33
20	P	310	LFA	C12-C13-C14-C15
23	C	303	PGV	C28-C29-C30-C31
20	O	302	LFA	C7-C8-C9-C10
21	L	102	DMU	O16-C18-C19-C22
27	V	101	CDL	OA9-CA7-OA8-CA6
21	N	611	DMU	O5-C6-O16-C18
27	C	304	CDL	CA7-C31-C32-C33
27	I	101	CDL	CA5-C11-C12-C13
27	L	101	CDL	CA5-C11-C12-C13
20	P	312	LFA	C1-C2-C3-C4
21	C	319	DMU	O16-C18-C19-C22
21	Z	101	DMU	O16-C18-C19-C22
21	A	611	DMU	O5-C4-C57-O61
27	V	101	CDL	O1-C1-CB2-OB2
27	Y	101	CDL	O1-C1-CA2-OA2
27	Y	101	CDL	C31-C32-C33-C34
27	C	304	CDL	OB9-CB7-OB8-CB6
21	U	101	DMU	C3-C4-C57-O61
21	Z	101	DMU	O6-C11-C9-C8
21	C	317	DMU	O16-C18-C19-C22
29	T	101	PEK	C7-C8-C9-C10
27	C	304	CDL	OA9-CA7-OA8-CA6
20	C	325	LFA	C9-C10-C11-C12
21	D	201	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
27	C	304	CDL	CB2-OB2-PB2-OB5
27	I	101	CDL	CB3-OB5-PB2-OB2
27	L	101	CDL	CA2-OA2-PA1-OA5
27	L	101	CDL	CA3-OA5-PA1-OA2
27	L	101	CDL	CB2-OB2-PB2-OB5
27	P	305	CDL	CA3-OA5-PA1-OA2
27	P	305	CDL	CB3-OB5-PB2-OB2
27	V	101	CDL	CA3-OA5-PA1-OA2
27	V	101	CDL	CB2-OB2-PB2-OB5
27	Y	101	CDL	CA3-OA5-PA1-OA2
21	Z	101	DMU	O6-C11-C9-O1
21	A	611	DMU	C3-C4-C57-O61
21	C	323	DMU	O16-C18-C19-C22
27	L	101	CDL	C19-C20-C21-C22
27	C	304	CDL	CB2-C1-CA2-OA2
27	L	101	CDL	OB7-CB5-OB6-CB4
27	P	305	CDL	OA7-CA5-OA6-CA4
21	C	318	DMU	O16-C18-C19-C22
20	C	309	LFA	C11-C10-C9-C8
21	C	315	DMU	O6-C11-C9-O1
20	P	311	LFA	C2-C3-C4-C5
21	A	617	DMU	C19-C22-C25-C28
27	V	101	CDL	C31-C32-C33-C34
27	I	101	CDL	C11-CA5-OA6-CA4
20	A	608	LFA	C6-C7-C8-C9
21	J	101	DMU	C25-C28-C31-C34
27	L	101	CDL	C34-C35-C36-C37
27	V	101	CDL	C73-C74-C75-C76
27	V	101	CDL	C76-C77-C78-C79
27	Y	101	CDL	C63-C64-C65-C66
20	C	307	LFA	C3-C4-C5-C6
20	O	302	LFA	C13-C14-C15-C16
20	P	301	LFA	C6-C7-C8-C9
21	W	101	DMU	C25-C28-C31-C34
21	Z	101	DMU	C22-C25-C28-C31
27	C	304	CDL	C51-C52-C53-C54
20	O	302	LFA	C11-C12-C13-C14
21	B	308	DMU	O16-C18-C19-C22
21	C	315	DMU	C19-C22-C25-C28
27	V	101	CDL	C74-C75-C76-C77
20	C	309	LFA	C3-C4-C5-C6
21	C	316	DMU	C28-C31-C34-C37

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Mol	Chain	Res	Type	Atoms
21	C	318	DMU	C31-C34-C37-C40
21	N	601	DMU	C19-C22-C25-C28
27	C	304	CDL	C22-C23-C24-C25
27	I	101	CDL	O1-C1-CA2-OA2
27	P	305	CDL	O1-C1-CA2-OA2
21	C	324	DMU	O16-C18-C19-C22
21	Z	102	DMU	O16-C18-C19-C22
27	C	304	CDL	C35-C36-C37-C38
21	O	304	DMU	C1-C6-O16-C18
21	P	318	DMU	C1-C6-O16-C18
21	Z	102	DMU	C25-C28-C31-C34
27	P	305	CDL	C53-C54-C55-C56
27	Y	101	CDL	C76-C77-C78-C79
27	P	305	CDL	OA9-CA7-OA8-CA6
20	B	307	LFA	C10-C11-C12-C13
20	T	102	LFA	C3-C4-C5-C6
21	B	302	DMU	C19-C22-C25-C28
21	P	318	DMU	C25-C28-C31-C34
23	C	303	PGV	C7-C8-C9-C10
23	P	304	PGV	C30-C31-C32-C33
20	P	310	LFA	C4-C5-C6-C7
20	T	102	LFA	C10-C11-C12-C13
21	C	316	DMU	C31-C34-C37-C40
21	O	306	DMU	C19-C22-C25-C28
21	Z	103	DMU	C31-C34-C37-C40
29	G	101	PEK	C34-C35-C36-C37
21	Z	102	DMU	C31-C34-C37-C40
23	C	303	PGV	C30-C31-C32-C33
21	P	318	DMU	O6-C11-C9-O1
20	B	307	LFA	C4-C5-C6-C7
21	M	101	DMU	C19-C22-C25-C28
27	C	304	CDL	C57-C58-C59-C60
27	I	101	CDL	C71-C72-C73-C74
29	T	101	PEK	C1-C2-C3-C4
20	B	307	LFA	C13-C14-C15-C16
20	C	307	LFA	C7-C8-C9-C10
21	C	315	DMU	C28-C31-C34-C37
21	C	317	DMU	C31-C34-C37-C40
21	N	611	DMU	C31-C34-C37-C40
21	P	319	DMU	C22-C25-C28-C31
23	A	616	PGV	C29-C30-C31-C32
23	C	303	PGV	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	L	101	CDL	C21-C22-C23-C24
27	L	101	CDL	C58-C59-C60-C61
27	L	101	CDL	C59-C60-C61-C62
27	P	305	CDL	C13-C14-C15-C16
27	V	101	CDL	C12-C13-C14-C15
27	V	101	CDL	C18-C19-C20-C21
29	G	101	PEK	C26-C27-C28-C29
29	G	101	PEK	C28-C29-C30-C31
21	U	101	DMU	O5-C6-O16-C18
21	C	317	DMU	C19-C22-C25-C28
20	C	309	LFA	C5-C6-C7-C8
20	C	325	LFA	C4-C5-C6-C7
20	P	311	LFA	C6-C7-C8-C9
21	M	101	DMU	C22-C25-C28-C31
21	N	601	DMU	C25-C28-C31-C34
27	P	305	CDL	C74-C75-C76-C77
27	P	305	CDL	C75-C76-C77-C78
27	Y	101	CDL	C22-C23-C24-C25
29	G	101	PEK	C16-C17-C18-C19
20	C	307	LFA	C4-C5-C6-C7
21	Z	101	DMU	C25-C28-C31-C34
23	N	617	PGV	C29-C30-C31-C32
27	Y	101	CDL	C19-C20-C21-C22
27	Y	101	CDL	C79-C80-C81-C82
20	A	609	LFA	C11-C10-C9-C8
20	C	312	LFA	C1-C2-C3-C4
20	P	310	LFA	C5-C6-C7-C8
21	A	617	DMU	C25-C28-C31-C34
21	B	303	DMU	C19-C22-C25-C28
21	L	102	DMU	C25-C28-C31-C34
21	P	317	DMU	C19-C18-O16-C6
20	P	301	LFA	C11-C12-C13-C14
21	P	318	DMU	O16-C18-C19-C22
21	Z	102	DMU	O5-C4-C57-O61
27	I	101	CDL	CA3-CA4-CA6-OA8
27	P	305	CDL	CB3-CB4-CB6-OB8
20	O	303	LFA	C2-C3-C4-C5
23	P	304	PGV	C14-C15-C16-C17
21	O	306	DMU	C22-C25-C28-C31
20	T	102	LFA	C4-C5-C6-C7
21	Q	201	DMU	O5-C4-C57-O61
21	B	302	DMU	C18-C19-C22-C25

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Mol	Chain	Res	Type	Atoms
21	B	303	DMU	C18-C19-C22-C25
20	G	103	LFA	C3-C4-C5-C6
21	L	102	DMU	C31-C34-C37-C40
21	M	102	DMU	C25-C28-C31-C34
21	P	317	DMU	C31-C34-C37-C40
27	L	101	CDL	C12-C13-C14-C15
27	L	101	CDL	C51-C52-C53-C54
29	G	101	PEK	C15-C16-C17-C18
21	P	317	DMU	C18-C19-C22-C25
27	L	101	CDL	C37-C38-C39-C40
27	P	305	CDL	C57-C58-C59-C60
21	B	303	DMU	C28-C31-C34-C37
23	P	304	PGV	C24-C25-C26-C27
29	T	101	PEK	C26-C27-C28-C29
21	J	101	DMU	C31-C34-C37-C40
27	C	304	CDL	C75-C76-C77-C78
27	I	101	CDL	C12-C13-C14-C15
21	A	617	DMU	C18-C19-C22-C25
21	C	306	DMU	C18-C19-C22-C25
21	P	315	DMU	C3-C4-C57-O61
20	B	307	LFA	C12-C13-C14-C15
21	A	611	DMU	C31-C34-C37-C40
21	P	319	DMU	C4-C3-O7-C10
23	C	303	PGV	C24-C25-C26-C27
27	C	304	CDL	C71-C72-C73-C74
27	I	101	CDL	C16-C17-C18-C19
27	Y	101	CDL	CA5-C11-C12-C13
22	C	320	EDO	O1-C1-C2-O2
22	R	201	EDO	O1-C1-C2-O2
20	C	325	LFA	C10-C11-C12-C13
20	A	609	LFA	C5-C6-C7-C8
20	G	103	LFA	C11-C10-C9-C8
20	P	301	LFA	C10-C11-C12-C13
21	Z	102	DMU	C18-C19-C22-C25
27	L	101	CDL	C74-C75-C76-C77
23	N	617	PGV	C11-C10-C9-C8
23	P	304	PGV	C12-C13-C14-C15
27	V	101	CDL	OA7-CA5-OA6-CA4
20	C	310	LFA	C3-C4-C5-C6
21	C	323	DMU	C19-C22-C25-C28
25	P	306	CHD	C20-C22-C23-C24
21	D	201	DMU	C19-C22-C25-C28

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Mol	Chain	Res	Type	Atoms
27	Y	101	CDL	C80-C81-C82-C83
21	B	308	DMU	C18-C19-C22-C25
20	C	310	LFA	C5-C6-C7-C8
21	B	304	DMU	C31-C34-C37-C40
21	H	101	DMU	C19-C22-C25-C28
20	C	309	LFA	C11-C12-C13-C14
21	C	323	DMU	C18-C19-C22-C25
27	C	304	CDL	C23-C24-C25-C26
21	P	318	DMU	C31-C34-C37-C40
27	L	101	CDL	C17-C18-C19-C20
27	Y	101	CDL	C59-C60-C61-C62
27	I	101	CDL	C19-C20-C21-C22
27	P	305	CDL	C35-C36-C37-C38
20	B	307	LFA	C11-C12-C13-C14
21	L	102	DMU	C22-C25-C28-C31
21	D	201	DMU	C4-C3-O7-C10
21	C	319	DMU	C1-C6-O16-C18
21	P	319	DMU	C1-C6-O16-C18
21	P	324	DMU	O16-C18-C19-C22
20	T	103	LFA	C3-C4-C5-C6
27	V	101	CDL	C78-C79-C80-C81
29	G	101	PEK	C25-C26-C27-C28
14	A	601[B]	HEA	C27-C19-C20-C21
14	A	601[B]	HEA	C18-C19-C20-C21
27	I	101	CDL	C78-C79-C80-C81
27	P	305	CDL	C73-C74-C75-C76
21	N	611	DMU	O16-C18-C19-C22
21	P	315	DMU	O1-C10-O7-C3
20	O	302	LFA	C4-C5-C6-C7
21	N	601	DMU	C28-C31-C34-C37
20	C	311	LFA	C5-C6-C7-C8
23	P	304	PGV	C7-C8-C9-C10
20	P	311	LFA	C7-C8-C9-C10
20	P	312	LFA	C3-C4-C5-C6
27	I	101	CDL	C18-C19-C20-C21
27	I	101	CDL	CB2-OB2-PB2-OB5
20	C	311	LFA	C11-C10-C9-C8
20	P	313	LFA	C9-C10-C11-C12
27	L	101	CDL	C80-C81-C82-C83
21	Q	201	DMU	C4-C3-O7-C10
27	I	101	CDL	C73-C74-C75-C76
27	P	305	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
21	O	307	DMU	C18-C19-C22-C25
27	L	101	CDL	C75-C76-C77-C78
27	Y	101	CDL	C16-C17-C18-C19
21	B	308	DMU	C3-C4-C57-O61
27	P	305	CDL	C22-C23-C24-C25
20	P	313	LFA	C5-C6-C7-C8
27	L	101	CDL	C71-C72-C73-C74
27	Y	101	CDL	C32-C33-C34-C35
27	L	101	CDL	C76-C77-C78-C79
27	V	101	CDL	CA2-C1-CB2-OB2
20	C	311	LFA	C4-C5-C6-C7
20	T	103	LFA	C6-C7-C8-C9
27	I	101	CDL	C17-C18-C19-C20
23	P	304	PGV	C11-C12-C13-C14
29	T	101	PEK	C14-C15-C16-C17
20	P	301	LFA	C9-C10-C11-C12
20	P	310	LFA	C13-C14-C15-C16
20	P	313	LFA	C6-C7-C8-C9
23	C	303	PGV	C22-C23-C24-C25
27	Y	101	CDL	OB9-CB7-OB8-CB6
21	C	323	DMU	C22-C25-C28-C31
27	P	305	CDL	CA3-CA4-CA6-OA8
27	V	101	CDL	CA3-CA4-CA6-OA8
21	P	316	DMU	C28-C31-C34-C37
21	P	324	DMU	C25-C28-C31-C34
27	Y	101	CDL	C13-C14-C15-C16
21	C	306	DMU	O16-C18-C19-C22
21	W	101	DMU	O16-C18-C19-C22
21	C	316	DMU	C34-C37-C40-C43
27	P	305	CDL	C20-C21-C22-C23
20	P	314	LFA	C6-C7-C8-C9
21	C	318	DMU	C34-C37-C40-C43
21	P	317	DMU	C22-C25-C28-C31
27	Y	101	CDL	C64-C65-C66-C67
20	G	103	LFA	C5-C6-C7-C8
21	B	308	DMU	C34-C37-C40-C43
20	B	307	LFA	C1-C2-C3-C4
21	C	317	DMU	C25-C28-C31-C34
21	N	601	DMU	C34-C37-C40-C43
27	Y	101	CDL	C84-C85-C86-C87
29	G	101	PEK	C17-C18-C19-C20
27	P	305	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
21	A	610	DMU	C28-C31-C34-C37
29	T	101	PEK	C2-C3-C4-C5
20	P	311	LFA	C11-C10-C9-C8
27	L	101	CDL	C84-C85-C86-C87
21	J	101	DMU	C18-C19-C22-C25
21	A	610	DMU	C34-C37-C40-C43
21	P	318	DMU	C22-C25-C28-C31
21	Z	101	DMU	C34-C37-C40-C43
27	L	101	CDL	C36-C37-C38-C39
20	O	303	LFA	C5-C6-C7-C8
21	C	315	DMU	C34-C37-C40-C43
27	V	101	CDL	C17-C18-C19-C20
27	V	101	CDL	C32-C33-C34-C35
21	C	319	DMU	C34-C37-C40-C43
27	C	304	CDL	C33-C34-C35-C36
21	P	315	DMU	O6-C11-C9-O1
21	B	303	DMU	O16-C18-C19-C22
21	N	601	DMU	O16-C18-C19-C22
21	O	306	DMU	O16-C18-C19-C22
21	P	307	DMU	O16-C18-C19-C22
20	C	325	LFA	C12-C13-C14-C15
21	C	315	DMU	C25-C28-C31-C34
21	O	306	DMU	C25-C28-C31-C34
21	W	101	DMU	C34-C37-C40-C43
27	Y	101	CDL	C73-C74-C75-C76
21	J	101	DMU	C34-C37-C40-C43
21	O	307	DMU	C19-C22-C25-C28
27	Y	101	CDL	C71-CB7-OB8-CB6
21	Z	102	DMU	C19-C22-C25-C28
22	P	320	EDO	O1-C1-C2-O2
20	A	609	LFA	C9-C10-C11-C12
20	N	609	LFA	C6-C7-C8-C9
20	O	302	LFA	C14-C15-C16-C17
21	A	610	DMU	C25-C28-C31-C34
27	Y	101	CDL	C51-C52-C53-C54
23	A	616	PGV	C11-C10-C9-C8
21	C	319	DMU	C25-C28-C31-C34
21	L	102	DMU	C34-C37-C40-C43
27	V	101	CDL	OA6-CA4-CA6-OA8
20	C	310	LFA	C11-C10-C9-C8
21	N	610	DMU	C25-C28-C31-C34
27	V	101	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
27	P	305	CDL	OB9-CB7-OB8-CB6
21	P	316	DMU	C31-C34-C37-C40
21	B	303	DMU	C25-C28-C31-C34
27	L	101	CDL	C15-C16-C17-C18
20	C	314	LFA	C1-C2-C3-C4
27	V	101	CDL	C77-C78-C79-C80
20	C	312	LFA	C11-C10-C9-C8
27	C	304	CDL	C11-C12-C13-C14
27	I	101	CDL	C15-C16-C17-C18
20	C	310	LFA	C4-C5-C6-C7
27	P	305	CDL	C19-C20-C21-C22
29	T	101	PEK	C32-C33-C34-C35
29	T	101	PEK	C4-C5-C6-C7
20	A	608	LFA	C7-C8-C9-C10
27	Y	101	CDL	C12-C13-C14-C15
20	C	310	LFA	C7-C8-C9-C10
21	M	102	DMU	C22-C25-C28-C31
21	B	308	DMU	C31-C34-C37-C40
21	B	302	DMU	O16-C18-C19-C22
25	C	305	CHD	C21-C20-C22-C23
23	C	303	PGV	C13-C14-C15-C16
27	P	305	CDL	CA7-C31-C32-C33
21	C	318	DMU	C2-C3-O7-C10
21	P	323	DMU	C22-C25-C28-C31
21	W	101	DMU	C31-C34-C37-C40
20	C	309	LFA	C2-C3-C4-C5
21	D	201	DMU	C2-C3-O7-C10
21	N	610	DMU	C34-C37-C40-C43
20	A	609	LFA	C6-C7-C8-C9
21	B	304	DMU	O16-C18-C19-C22
29	T	101	PEK	C17-C18-C19-C20
20	C	307	LFA	C5-C6-C7-C8
21	P	317	DMU	C19-C22-C25-C28
23	N	617	PGV	C31-C32-C33-C34
27	C	304	CDL	CA4-CA3-OA5-PA1
21	B	304	DMU	C19-C18-O16-C6
21	C	317	DMU	C19-C18-O16-C6
23	P	304	PGV	C15-C16-C17-C18
27	P	305	CDL	C72-C73-C74-C75
21	P	323	DMU	C18-C19-C22-C25
21	A	617	DMU	O16-C18-C19-C22
20	B	307	LFA	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	C	304	CDL	CB3-CB4-CB6-OB8
27	L	101	CDL	CB3-CB4-CB6-OB8
27	C	304	CDL	C18-C19-C20-C21
21	A	617	DMU	C28-C31-C34-C37
21	Z	103	DMU	C22-C25-C28-C31
27	P	305	CDL	C12-C11-CA5-OA6
20	P	308	LFA	C1-C2-C3-C4
27	P	305	CDL	C33-C34-C35-C36
20	P	312	LFA	C4-C5-C6-C7
23	A	616	PGV	C14-C15-C16-C17
29	T	101	PEK	C11-C10-C9-C8
21	O	304	DMU	C22-C25-C28-C31
21	O	308	DMU	O16-C18-C19-C22
21	P	318	DMU	C34-C37-C40-C43
21	C	318	DMU	O6-C11-C9-C8
27	C	304	CDL	C12-C11-CA5-OA6
21	B	304	DMU	C34-C37-C40-C43
21	P	315	DMU	C19-C22-C25-C28
27	P	305	CDL	C52-C53-C54-C55
21	P	317	DMU	C28-C31-C34-C37
27	C	304	CDL	C52-C53-C54-C55
27	Y	101	CDL	OB6-CB4-CB6-OB8
20	O	302	LFA	C12-C13-C14-C15
23	C	303	PGV	C29-C30-C31-C32
29	T	101	PEK	C10-C11-C12-C13
27	I	101	CDL	CA2-C1-CB2-OB2
20	A	608	LFA	C9-C10-C11-C12
21	C	318	DMU	C4-C3-O7-C10
27	L	101	CDL	C22-C23-C24-C25
27	Y	101	CDL	C58-C59-C60-C61
23	C	303	PGV	C02-C03-O11-P
23	P	304	PGV	C02-C03-O11-P
27	P	305	CDL	CA4-CA3-OA5-PA1
27	V	101	CDL	C1-CA2-OA2-PA1
21	P	318	DMU	O1-C10-O7-C3
20	C	307	LFA	C6-C7-C8-C9
20	N	609	LFA	C7-C8-C9-C10
20	O	302	LFA	C6-C7-C8-C9
21	C	319	DMU	C19-C22-C25-C28
21	M	101	DMU	C25-C28-C31-C34
21	Q	201	DMU	C2-C3-O7-C10
27	P	305	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
27	Y	101	CDL	C77-C78-C79-C80
20	P	310	LFA	C3-C4-C5-C6
27	C	304	CDL	C20-C21-C22-C23
27	Y	101	CDL	C61-C62-C63-C64
20	C	307	LFA	C11-C10-C9-C8
23	A	616	PGV	C31-C32-C33-C34
20	C	309	LFA	C13-C14-C15-C16
20	C	325	LFA	C7-C8-C9-C10
21	W	101	DMU	C28-C31-C34-C37
21	Q	201	DMU	C25-C28-C31-C34
21	N	611	DMU	O6-C11-C9-O1
29	G	101	PEK	C29-C30-C31-C32
27	I	101	CDL	C32-C33-C34-C35
21	P	318	DMU	O5-C6-O16-C18
27	Y	101	CDL	C1-CA2-OA2-PA1
27	P	305	CDL	OB5-CB3-CB4-OB6
27	Y	101	CDL	OA5-CA3-CA4-OA6
20	P	313	LFA	C4-C5-C6-C7
21	P	324	DMU	C4-C3-O7-C10
20	C	325	LFA	C6-C7-C8-C9
27	L	101	CDL	OA6-CA4-CA6-OA8
27	P	305	CDL	OB6-CB4-CB6-OB8
21	P	319	DMU	C25-C28-C31-C34
20	C	310	LFA	C1-C2-C3-C4
20	G	103	LFA	C6-C7-C8-C9
20	P	313	LFA	C2-C3-C4-C5
20	C	312	LFA	C5-C6-C7-C8
21	P	324	DMU	C2-C3-O7-C10
20	C	325	LFA	C1-C2-C3-C4
20	A	609	LFA	C2-C3-C4-C5
20	P	301	LFA	C1-C2-C3-C4
20	P	308	LFA	C11-C10-C9-C8
27	C	304	CDL	C36-C37-C38-C39
27	C	304	CDL	C84-C85-C86-C87
27	I	101	CDL	C75-C76-C77-C78
27	C	304	CDL	CA3-OA5-PA1-OA3
27	I	101	CDL	CA3-OA5-PA1-OA3
27	I	101	CDL	CB2-OB2-PB2-OB4
27	P	305	CDL	CA3-OA5-PA1-OA3
27	P	305	CDL	CB3-OB5-PB2-OB3
27	V	101	CDL	CA3-OA5-PA1-OA3
27	V	101	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
27	Y	101	CDL	CA3-OA5-PA1-OA4
21	L	102	DMU	C19-C22-C25-C28
27	P	305	CDL	OB5-CB3-CB4-CB6
27	Y	101	CDL	OA5-CA3-CA4-CA6
20	P	308	LFA	C4-C5-C6-C7
23	A	616	PGV	C26-C27-C28-C29
21	B	308	DMU	C25-C28-C31-C34
27	V	101	CDL	C11-CA5-OA6-CA4
29	T	101	PEK	C15-C16-C17-C18
27	Y	101	CDL	C53-C54-C55-C56
27	L	101	CDL	C56-C57-C58-C59
27	Y	101	CDL	C37-C38-C39-C40
21	C	318	DMU	C19-C22-C25-C28
27	C	304	CDL	OB6-CB4-CB6-OB8
21	M	102	DMU	C31-C34-C37-C40
27	C	304	CDL	C79-C80-C81-C82
21	B	303	DMU	C22-C25-C28-C31
20	C	314	LFA	C6-C7-C8-C9
29	G	101	PEK	C32-C33-C34-C35
27	L	101	CDL	C14-C15-C16-C17
20	C	313	LFA	C4-C5-C6-C7
27	L	101	CDL	C18-C19-C20-C21
27	L	101	CDL	C77-C78-C79-C80
20	P	308	LFA	C2-C3-C4-C5
20	P	308	LFA	C3-C4-C5-C6
21	O	306	DMU	C31-C34-C37-C40
27	I	101	CDL	CA6-CA4-OA6-CA5
21	C	324	DMU	C18-C19-C22-C25
21	O	307	DMU	O16-C18-C19-C22
21	D	201	DMU	C22-C25-C28-C31
27	V	101	CDL	CB4-CB3-OB5-PB2
27	L	101	CDL	C16-C17-C18-C19
27	P	305	CDL	C11-C12-C13-C14
20	C	309	LFA	C14-C15-C16-C17
20	P	312	LFA	C11-C10-C9-C8
22	R	203	EDO	O1-C1-C2-O2
21	P	323	DMU	C25-C28-C31-C34
23	C	303	PGV	C25-C26-C27-C28
27	Y	101	CDL	C24-C25-C26-C27
20	T	103	LFA	C7-C8-C9-C10
21	C	306	DMU	C31-C34-C37-C40
20	B	307	LFA	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
21	C	318	DMU	O1-C10-O7-C3
20	A	608	LFA	C2-C3-C4-C5
21	C	315	DMU	C2-C3-O7-C10
20	P	310	LFA	C10-C11-C12-C13
21	C	315	DMU	C4-C3-O7-C10
21	P	315	DMU	C18-C19-C22-C25
27	Y	101	CDL	C74-C75-C76-C77
20	C	311	LFA	C10-C11-C12-C13
21	P	317	DMU	O5-C4-C57-O61
27	C	304	CDL	C77-C78-C79-C80
27	Y	101	CDL	C20-C21-C22-C23
29	G	101	PEK	C27-C28-C29-C30
14	A	602	HEA	CAA-CBA-CGA-O1A
20	P	310	LFA	C6-C7-C8-C9
20	B	307	LFA	C9-C10-C11-C12
27	I	101	CDL	O1-C1-CB2-OB2
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
14	A	601[B]	HEA	CAD-CBD-CGD-O1D
23	N	617	PGV	O03-C19-C20-C21
27	Y	101	CDL	C57-C58-C59-C60
21	P	323	DMU	C34-C37-C40-C43
21	C	319	DMU	C18-C19-C22-C25
20	P	310	LFA	C2-C3-C4-C5
25	C	305	CHD	C22-C23-C24-O25
25	O	301	CHD	C22-C23-C24-O25
21	P	318	DMU	C4-C3-O7-C10
21	P	319	DMU	C31-C34-C37-C40
27	L	101	CDL	C13-C14-C15-C16
20	G	103	LFA	C1-C2-C3-C4
21	C	324	DMU	C28-C31-C34-C37
20	O	302	LFA	C3-C4-C5-C6
21	N	610	DMU	C28-C31-C34-C37
25	C	305	CHD	C22-C23-C24-O26
27	I	101	CDL	C31-C32-C33-C34
25	B	306	CHD	C22-C23-C24-O26
21	Z	102	DMU	C34-C37-C40-C43
27	C	304	CDL	C21-C22-C23-C24
27	L	101	CDL	C24-C25-C26-C27
25	P	306	CHD	C22-C23-C24-O25
21	C	318	DMU	C5-C10-O7-C3
14	N	603	HEA	CAA-CBA-CGA-O1A
25	B	306	CHD	C22-C23-C24-O25

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Mol	Chain	Res	Type	Atoms
25	O	301	CHD	C22-C23-C24-O26
21	Z	103	DMU	C34-C37-C40-C43
27	I	101	CDL	C52-C51-CB5-OB6
29	G	101	PEK	C9-C10-C11-C12
20	C	308	LFA	C3-C4-C5-C6
20	T	102	LFA	C2-C3-C4-C5
21	N	610	DMU	C31-C34-C37-C40
21	H	101	DMU	O6-C11-C9-O1
29	G	101	PEK	C4-C5-C6-C7
14	A	602	HEA	CAD-CBD-CGD-O1D
20	T	102	LFA	C5-C6-C7-C8
21	L	102	DMU	C18-C19-C22-C25
14	A	602	HEA	CAA-CBA-CGA-O2A
27	Y	101	CDL	C52-C53-C54-C55
21	P	315	DMU	C5-C10-O7-C3
21	P	318	DMU	C2-C3-O7-C10
14	N	603	HEA	CAA-CBA-CGA-O2A
29	T	101	PEK	C22-C23-C24-C25
20	C	311	LFA	C6-C7-C8-C9
20	P	313	LFA	C11-C10-C9-C8
21	H	101	DMU	C25-C28-C31-C34
25	P	306	CHD	C22-C23-C24-O26
20	P	308	LFA	C5-C6-C7-C8
27	C	304	CDL	C73-C74-C75-C76
27	L	101	CDL	CA3-CA4-CA6-OA8
22	F	103	EDO	O1-C1-C2-O2
27	V	101	CDL	OA5-CA3-CA4-OA6
23	A	616	PGV	O03-C19-C20-C21
21	B	302	DMU	C31-C34-C37-C40
14	N	602[A]	HEA	CAD-CBD-CGD-O1D
14	N	602[B]	HEA	CAD-CBD-CGD-O1D
27	P	305	CDL	C23-C24-C25-C26
14	A	602	HEA	CAD-CBD-CGD-O2D
21	O	304	DMU	C34-C37-C40-C43
14	N	603	HEA	CAD-CBD-CGD-O1D
25	C	301	CHD	C22-C23-C24-O26
25	P	302	CHD	C22-C23-C24-O26
20	P	314	LFA	C5-C6-C7-C8
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
14	A	601[B]	HEA	CAD-CBD-CGD-O2D
27	L	101	CDL	C53-C54-C55-C56
27	Y	101	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
20	C	325	LFA	C5-C6-C7-C8
27	P	305	CDL	C17-C18-C19-C20
27	C	304	CDL	C52-C51-CB5-OB6
27	Y	101	CDL	CB3-CB4-CB6-OB8
27	L	101	CDL	C78-C79-C80-C81
27	Y	101	CDL	OB5-CB3-CB4-OB6
27	P	305	CDL	C52-C51-CB5-OB6
25	P	302	CHD	C22-C23-C24-O25
20	P	301	LFA	C5-C6-C7-C8
21	P	316	DMU	C25-C28-C31-C34
21	P	319	DMU	C28-C31-C34-C37
14	N	603	HEA	CAD-CBD-CGD-O2D
20	C	312	LFA	C4-C5-C6-C7
27	Y	101	CDL	C60-C61-C62-C63
25	C	301	CHD	C22-C23-C24-O25
21	U	101	DMU	C25-C28-C31-C34
23	A	616	PGV	C23-C24-C25-C26
27	Y	101	CDL	OB5-CB3-CB4-CB6
21	Q	201	DMU	C28-C31-C34-C37
27	C	304	CDL	C59-C60-C61-C62
27	V	101	CDL	C71-CB7-OB8-CB6
27	Y	101	CDL	C72-C71-CB7-OB8
14	N	602[A]	HEA	CAA-CBA-CGA-O1A
14	N	602[B]	HEA	CAA-CBA-CGA-O1A
23	P	304	PGV	C05-C04-O12-P
21	D	201	DMU	O5-C6-O16-C18
27	P	305	CDL	C59-C60-C61-C62
27	V	101	CDL	C52-C51-CB5-OB6
20	C	311	LFA	C1-C2-C3-C4
23	A	616	PGV	C15-C16-C17-C18
21	C	324	DMU	O1-C10-O7-C3
27	C	304	CDL	C52-C51-CB5-OB7
21	C	323	DMU	C28-C31-C34-C37
21	C	317	DMU	C28-C31-C34-C37
27	Y	101	CDL	C56-C57-C58-C59
20	C	314	LFA	C5-C6-C7-C8
21	A	611	DMU	C2-C3-O7-C10
27	V	101	CDL	C72-C71-CB7-OB8
27	P	305	CDL	C52-C51-CB5-OB7
21	B	302	DMU	C34-C37-C40-C43
21	P	315	DMU	C28-C31-C34-C37
20	G	103	LFA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
21	P	318	DMU	C28-C31-C34-C37
29	T	101	PEK	C2-C1-O01-C02
27	I	101	CDL	C52-C51-CB5-OB7
21	J	101	DMU	C28-C31-C34-C37
21	P	318	DMU	C5-C10-O7-C3
20	C	310	LFA	C6-C7-C8-C9
23	C	303	PGV	C05-C04-O12-P
20	B	307	LFA	C5-C6-C7-C8
21	O	304	DMU	O16-C18-C19-C22
14	N	602[A]	HEA	CAD-CBD-CGD-O2D
14	N	602[B]	HEA	CAD-CBD-CGD-O2D
27	I	101	CDL	C20-C21-C22-C23
27	I	101	CDL	CA2-OA2-PA1-OA3
21	A	611	DMU	C4-C3-O7-C10
29	G	101	PEK	O12-C04-C05-N
22	A	615	EDO	O1-C1-C2-O2
23	C	303	PGV	C21-C22-C23-C24
27	L	101	CDL	C60-C61-C62-C63
27	P	305	CDL	C58-C59-C60-C61
27	P	305	CDL	C51-C52-C53-C54
29	T	101	PEK	C30-C31-C32-C33
27	I	101	CDL	C13-C14-C15-C16
27	Y	101	CDL	C14-C15-C16-C17
21	M	101	DMU	O6-C11-C9-C8
20	P	310	LFA	C11-C12-C13-C14
29	T	101	PEK	O01-C1-C2-C3
21	Z	101	DMU	C28-C31-C34-C37
14	N	602[A]	HEA	CAA-CBA-CGA-O2A
14	N	602[B]	HEA	CAA-CBA-CGA-O2A
21	P	319	DMU	C19-C18-O16-C6
21	P	324	DMU	C19-C18-O16-C6
27	L	101	CDL	C72-C71-CB7-OB8
21	C	315	DMU	O6-C11-C9-C8
20	P	312	LFA	C5-C6-C7-C8
23	P	304	PGV	C27-C28-C29-C30
27	P	305	CDL	C54-C55-C56-C57
21	C	324	DMU	C5-C10-O7-C3

There are no ring outliers.

46 monomers are involved in 127 short contacts:

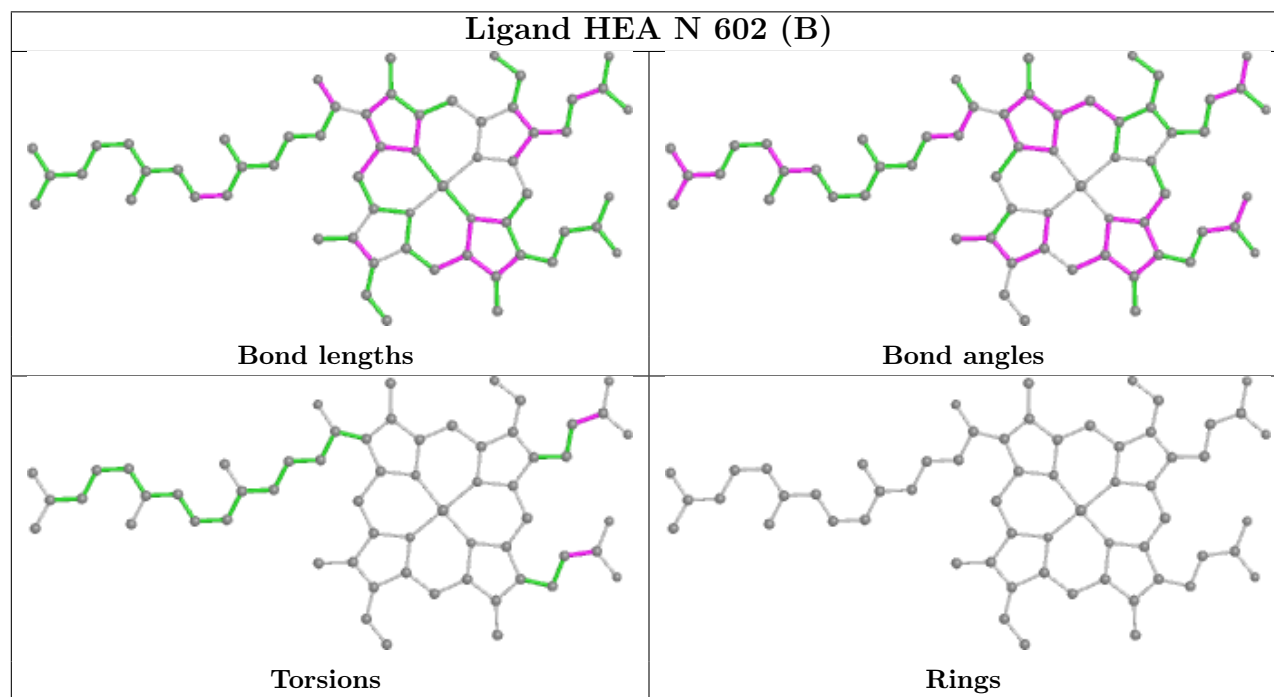
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	602[B]	HEA	1	0
25	P	306	CHD	4	0
27	Y	101	CDL	8	0
25	O	301	CHD	1	0
20	B	307	LFA	2	0
20	P	314	LFA	1	0
20	P	308	LFA	2	0
21	D	201	DMU	3	0
20	C	309	LFA	1	0
20	C	312	LFA	2	0
14	A	601[B]	HEA	1	0
27	C	304	CDL	15	0
27	L	101	CDL	6	0
20	O	302	LFA	2	0
22	A	613	EDO	1	0
21	P	324	DMU	2	0
21	A	611	DMU	1	0
18	A	606	PER	1	0
21	U	101	DMU	1	0
20	P	313	LFA	2	0
21	C	324	DMU	6	0
21	Q	201	DMU	1	0
20	P	312	LFA	1	0
27	V	101	CDL	2	0
14	N	603	HEA	2	0
21	Z	102	DMU	3	0
20	O	303	LFA	3	0
22	N	616	EDO	1	0
29	T	101	PEK	3	0
21	O	308	DMU	1	0
20	A	608	LFA	4	0
14	A	602	HEA	1	0
23	C	303	PGV	1	0
21	L	102	DMU	2	0
20	P	310	LFA	2	0
18	N	607	PER	1	0
27	P	305	CDL	13	0
21	A	610	DMU	1	0
20	G	103	LFA	4	0
21	B	304	DMU	1	0
20	C	313	LFA	1	0
20	N	609	LFA	6	0
20	A	609	LFA	6	0

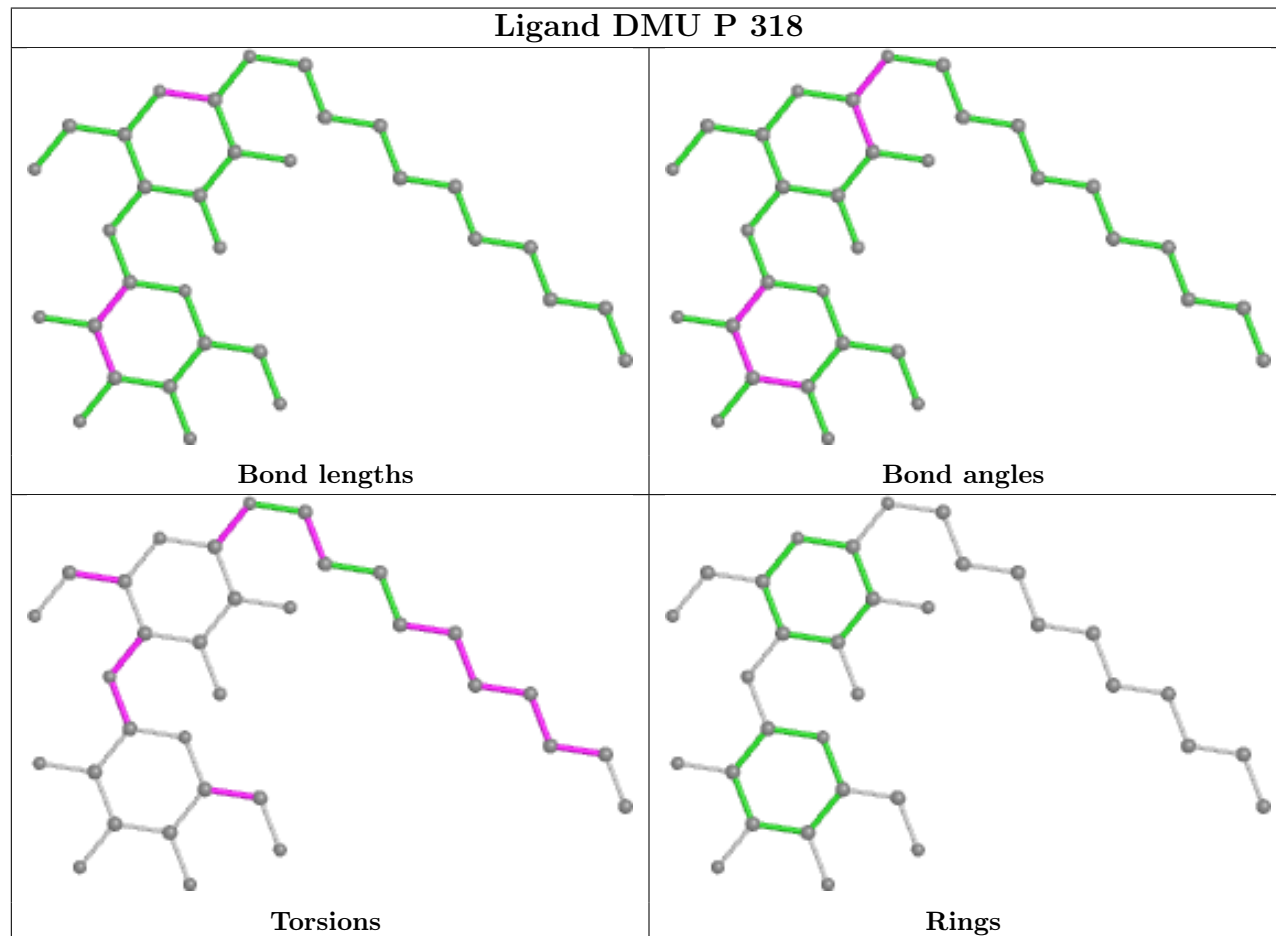
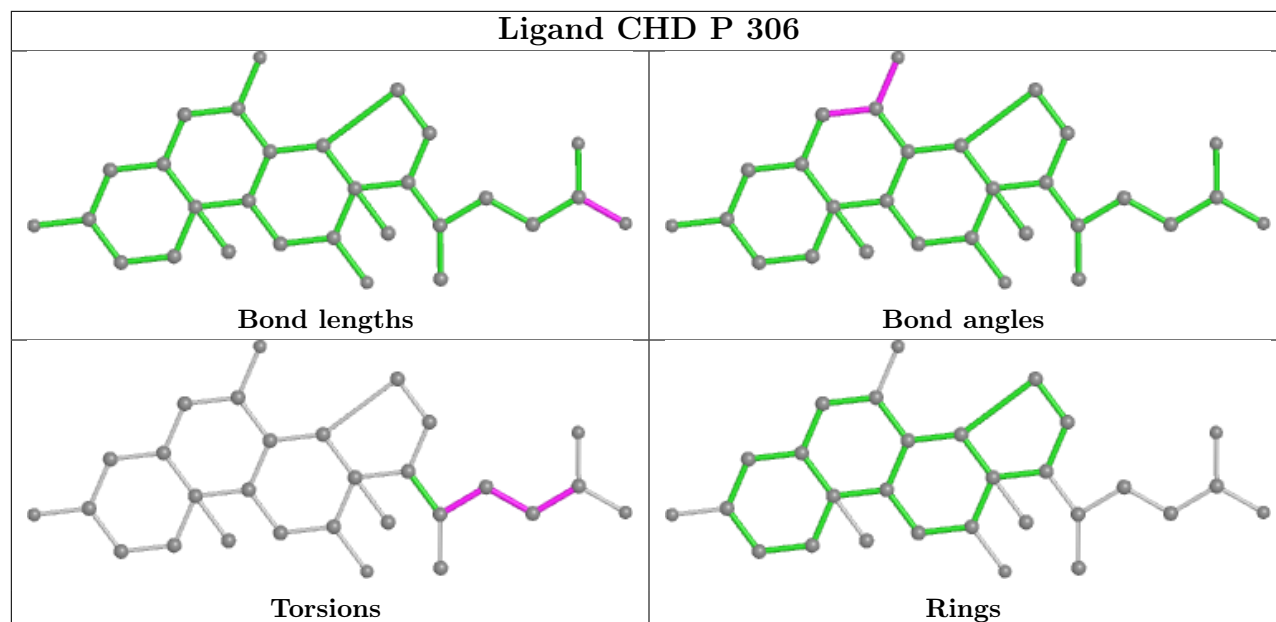
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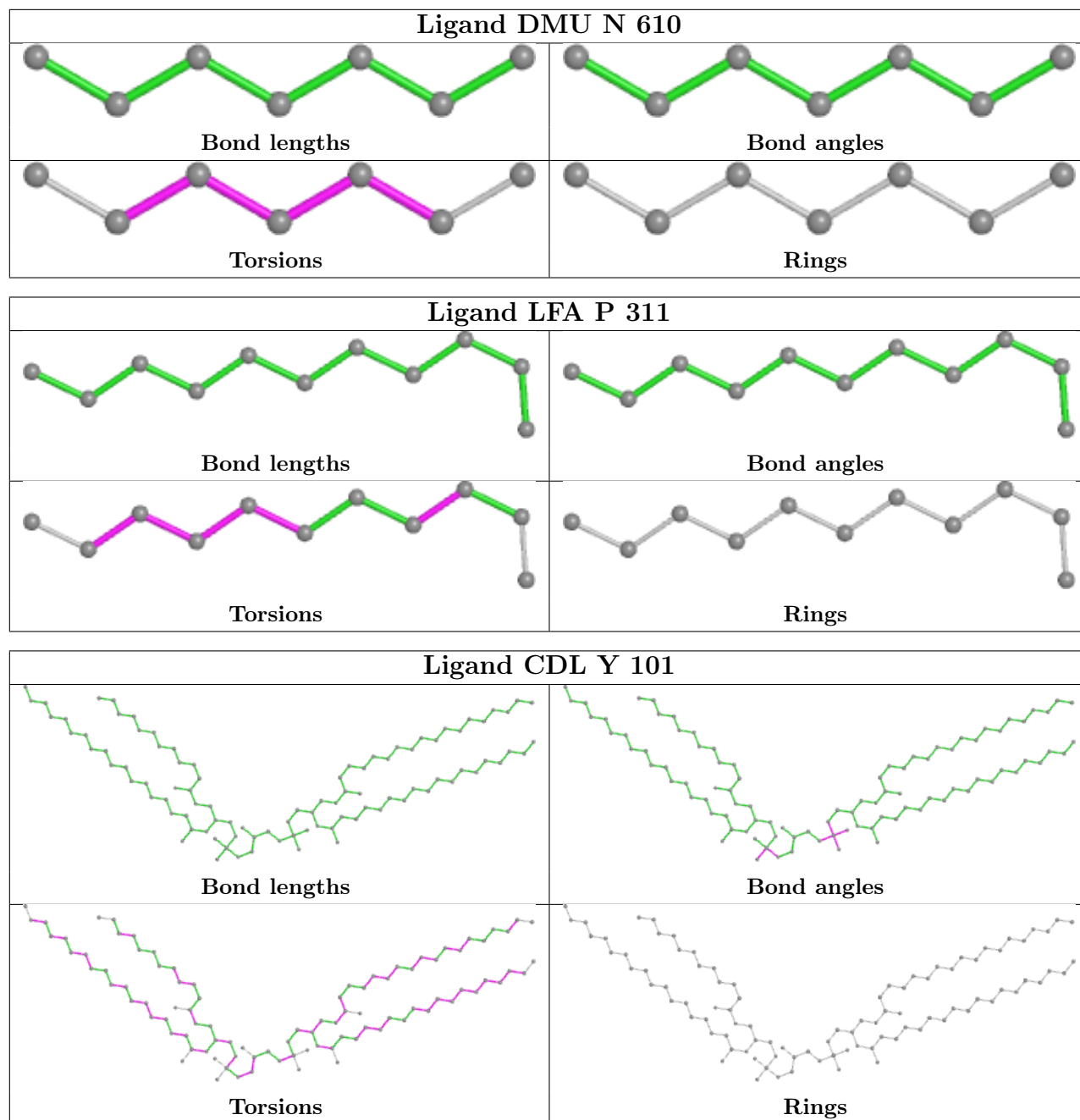
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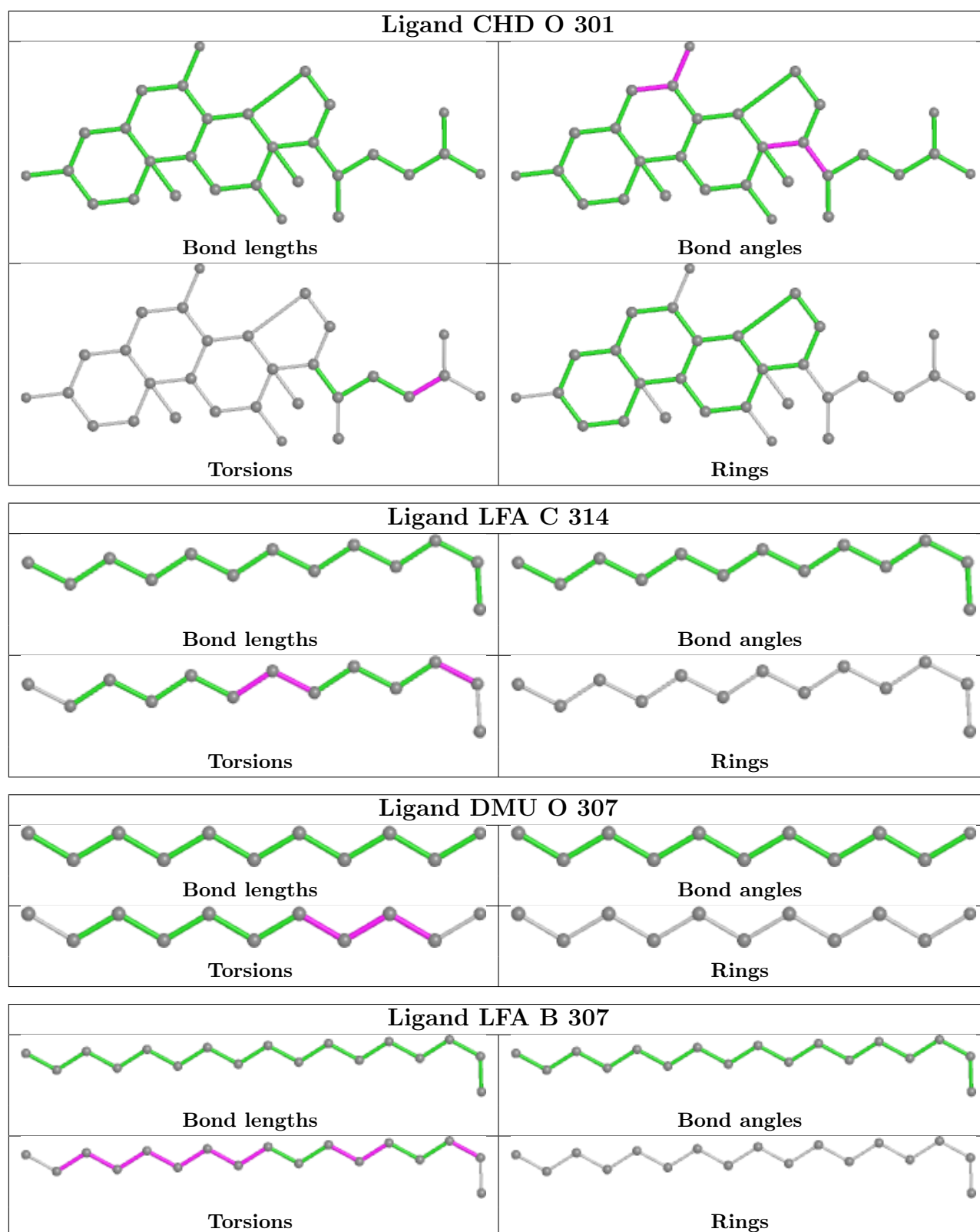
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601[A]	HEA	4	0
25	C	305	CHD	2	0
21	H	101	DMU	1	0

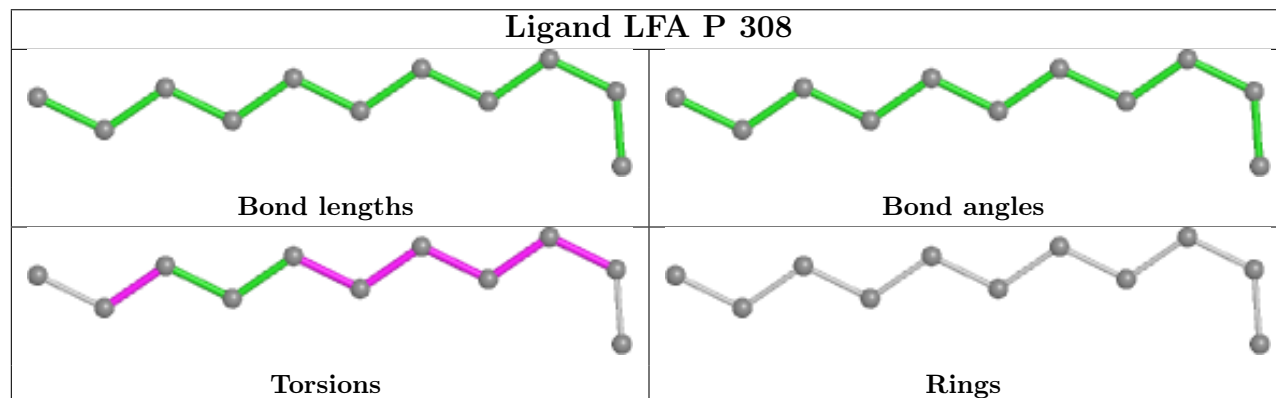
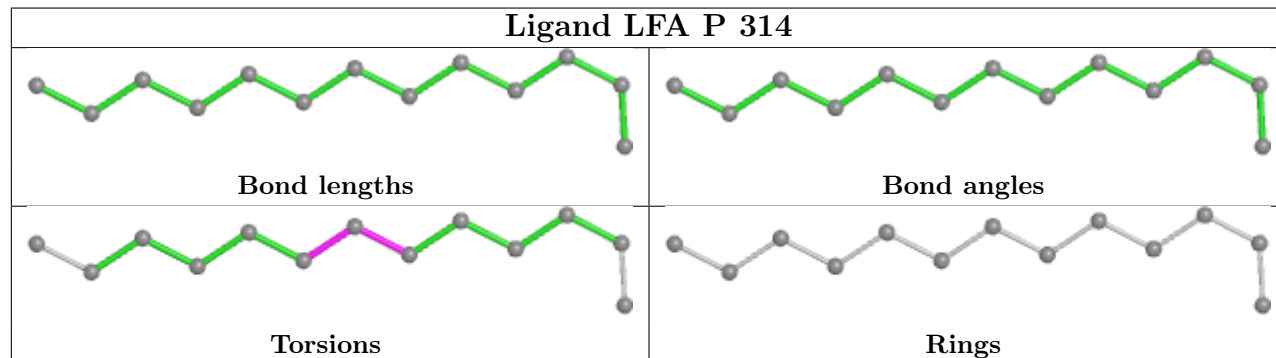
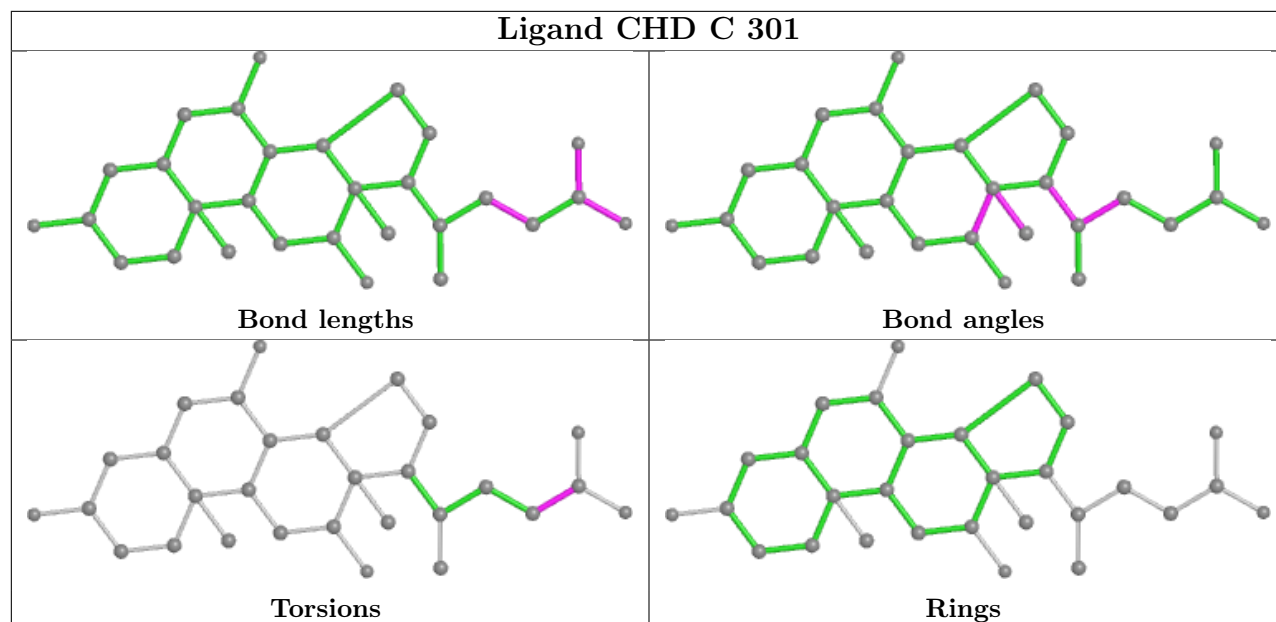
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

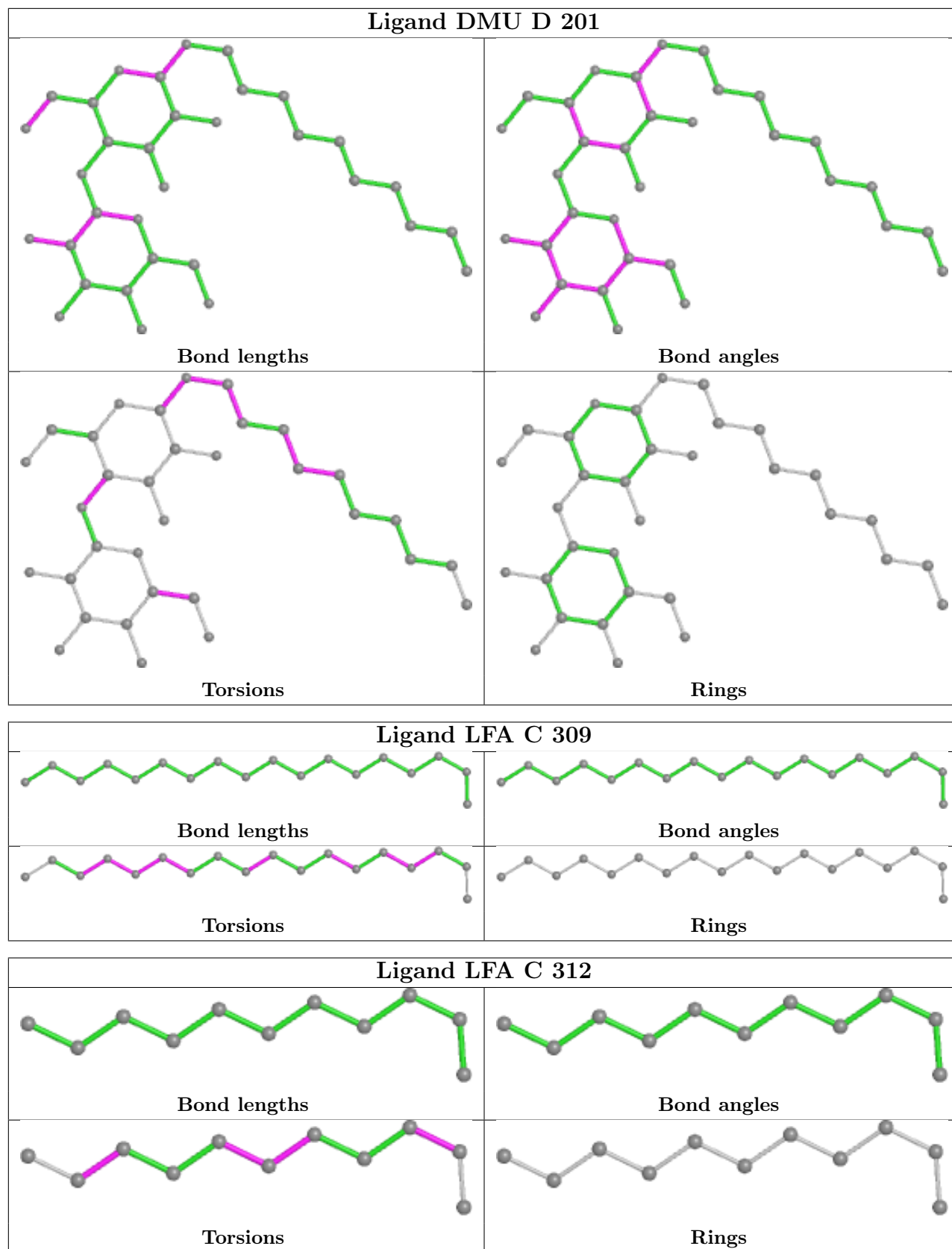


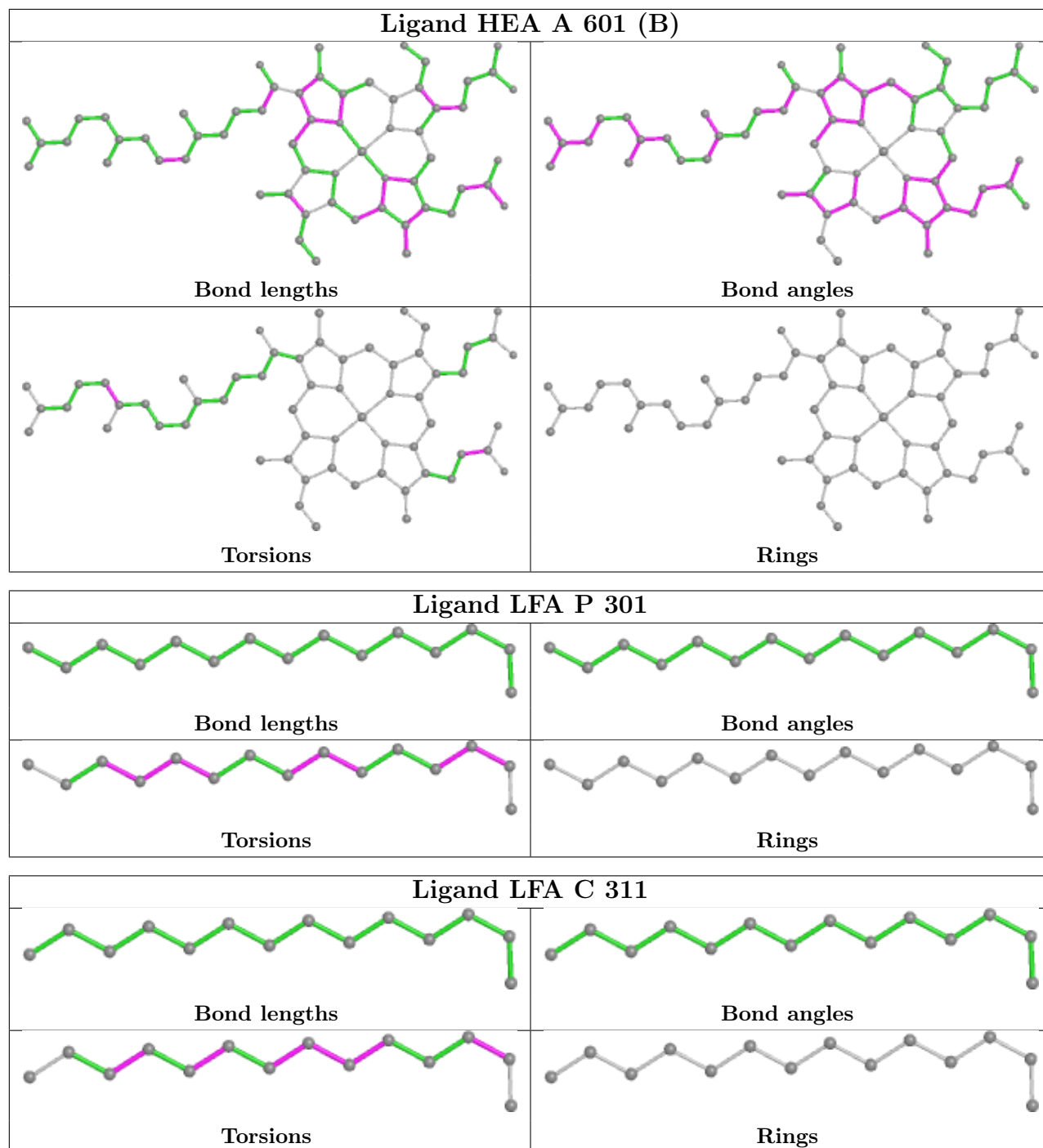


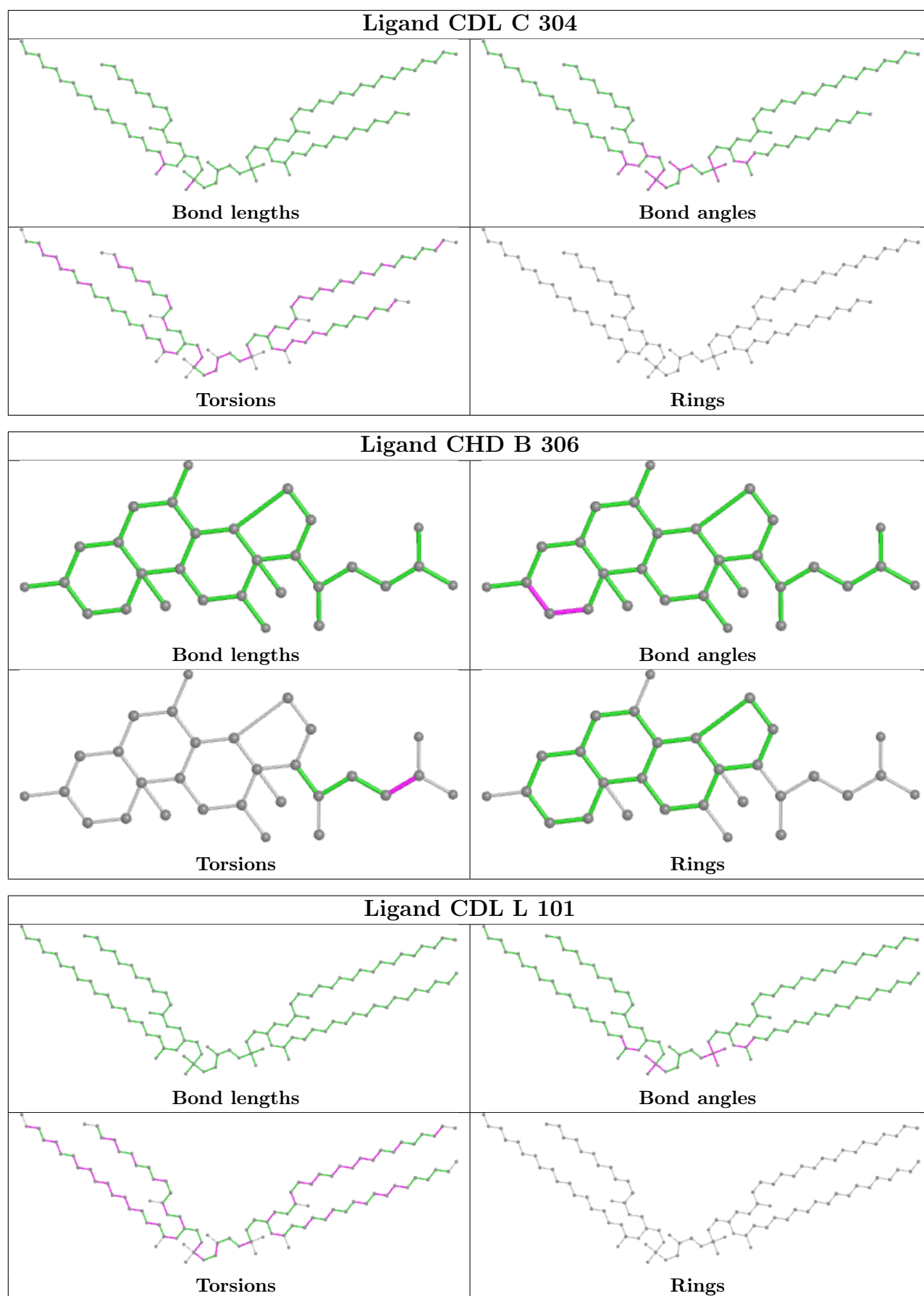


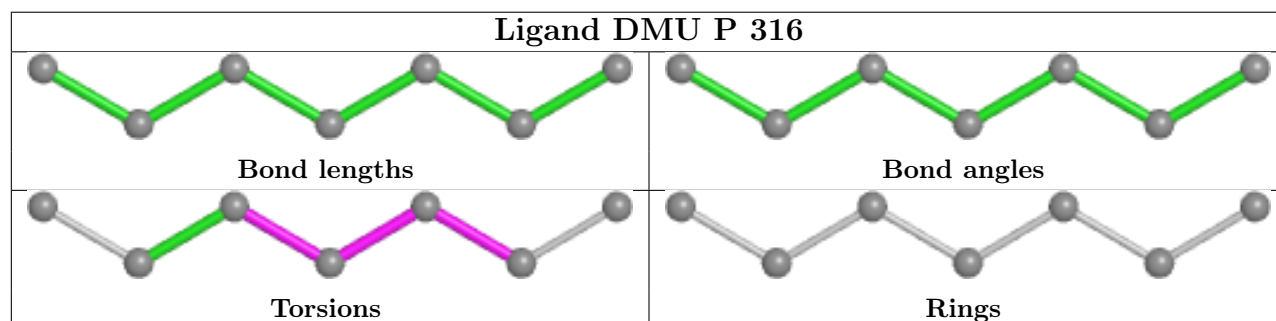
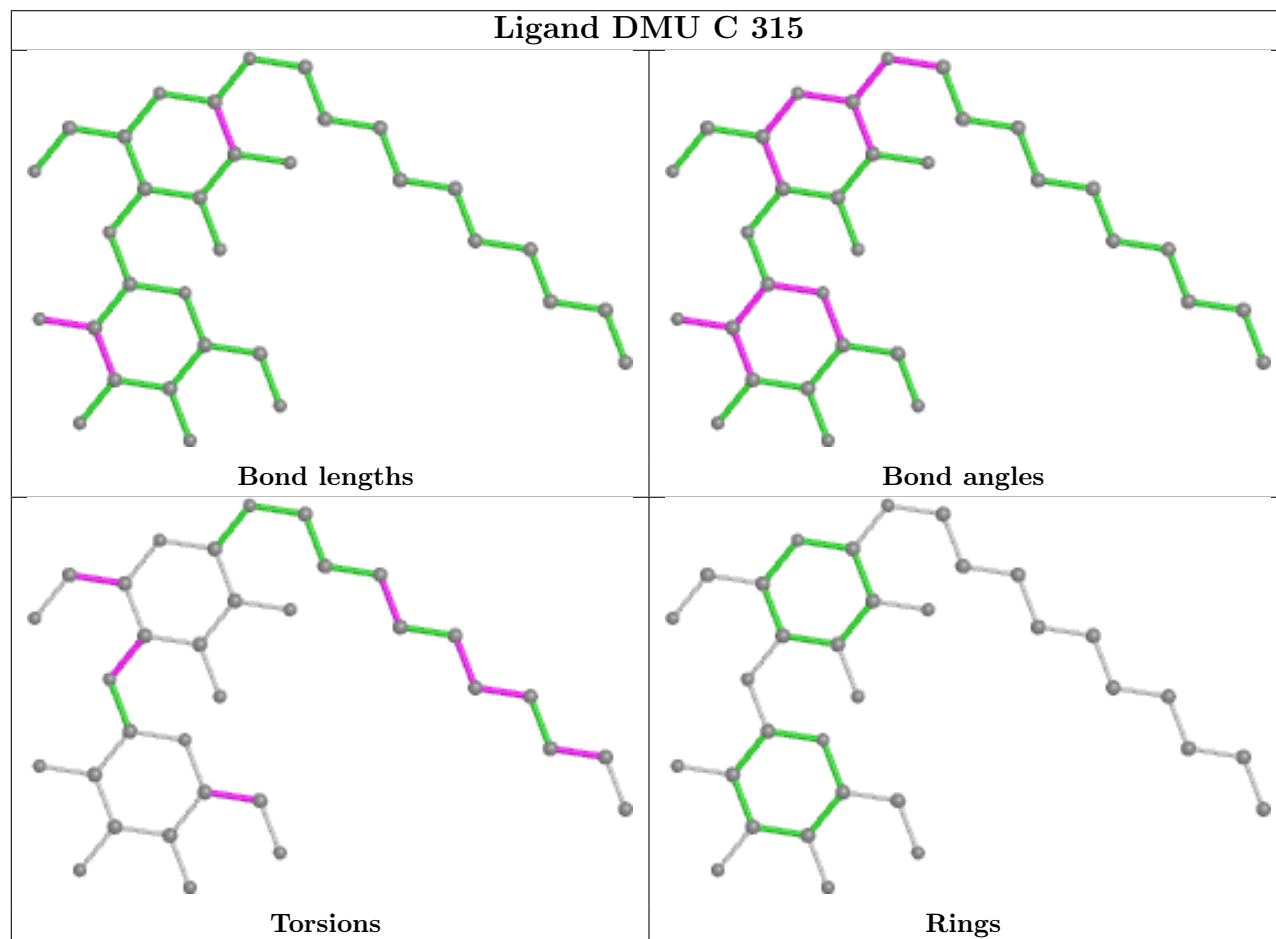
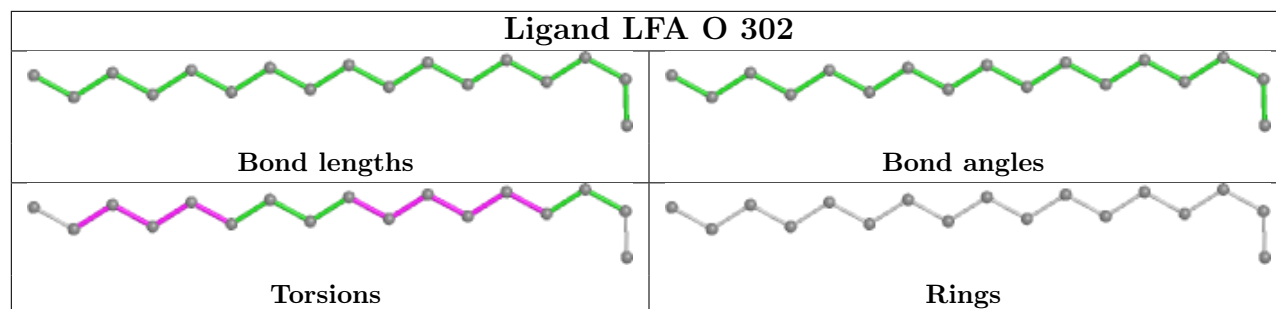


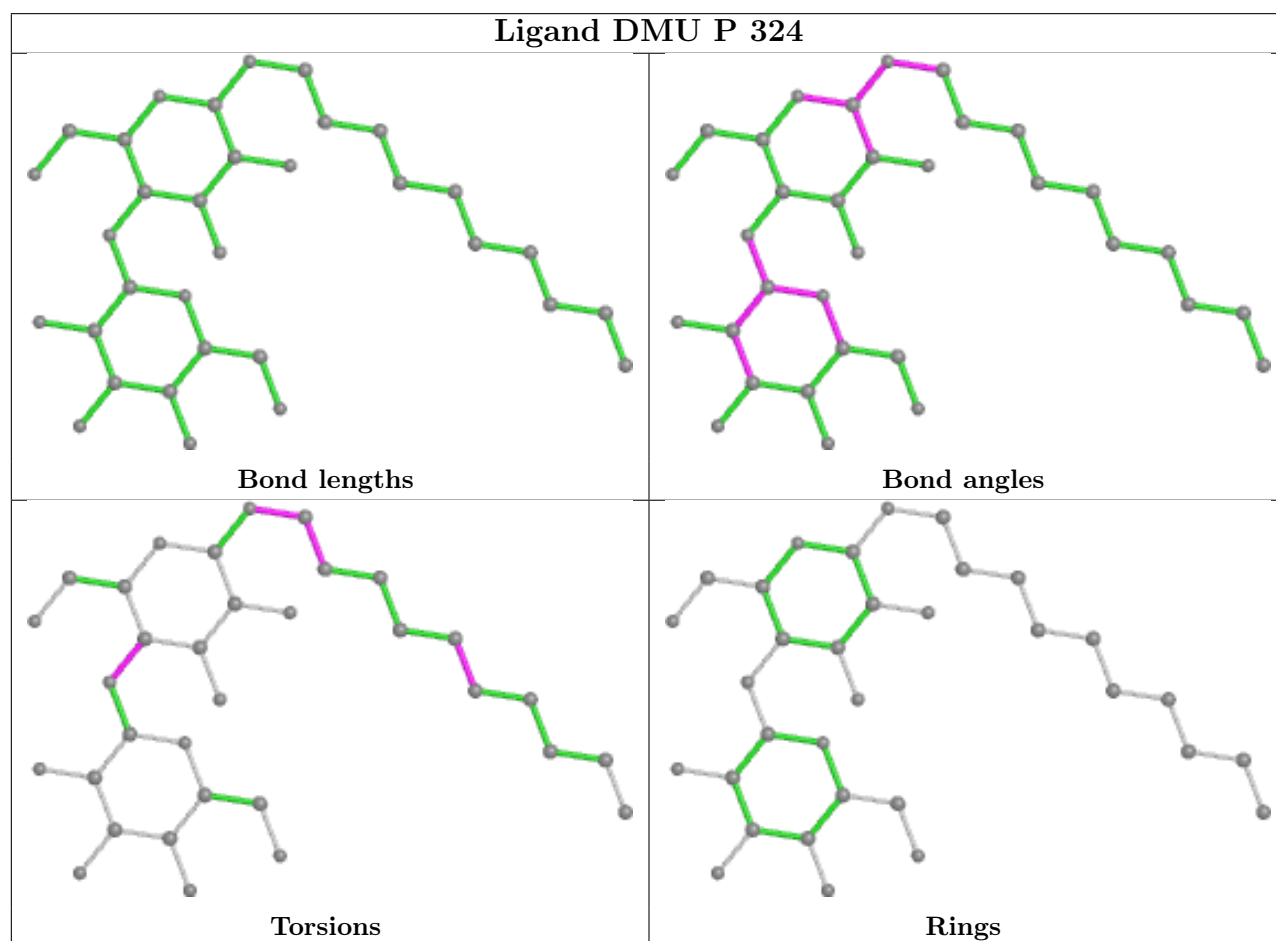
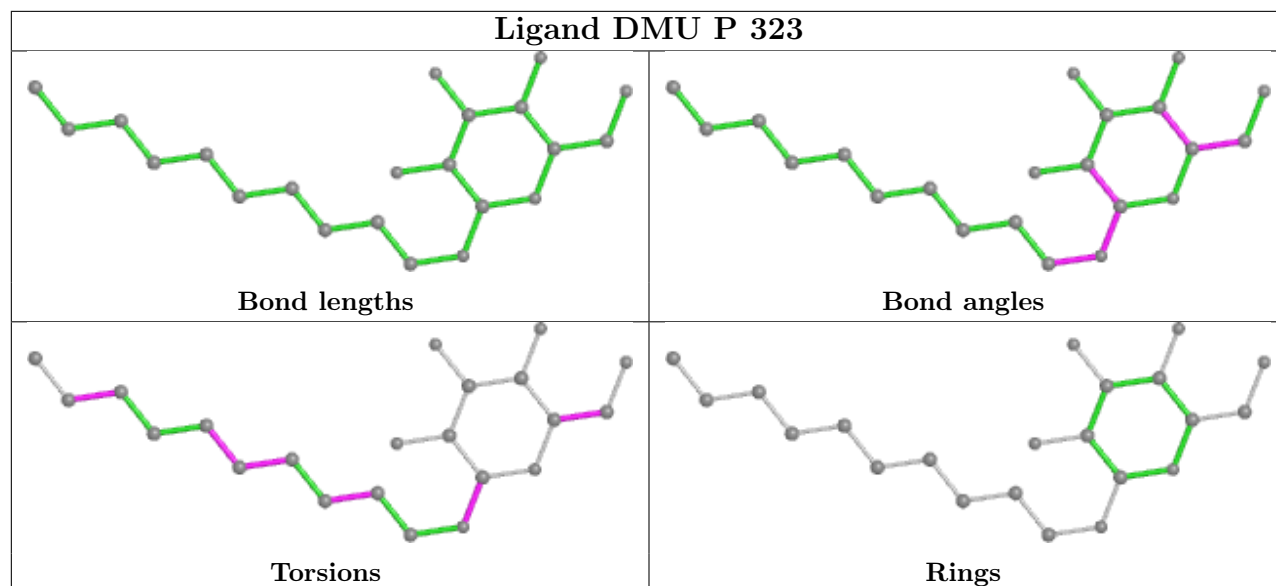


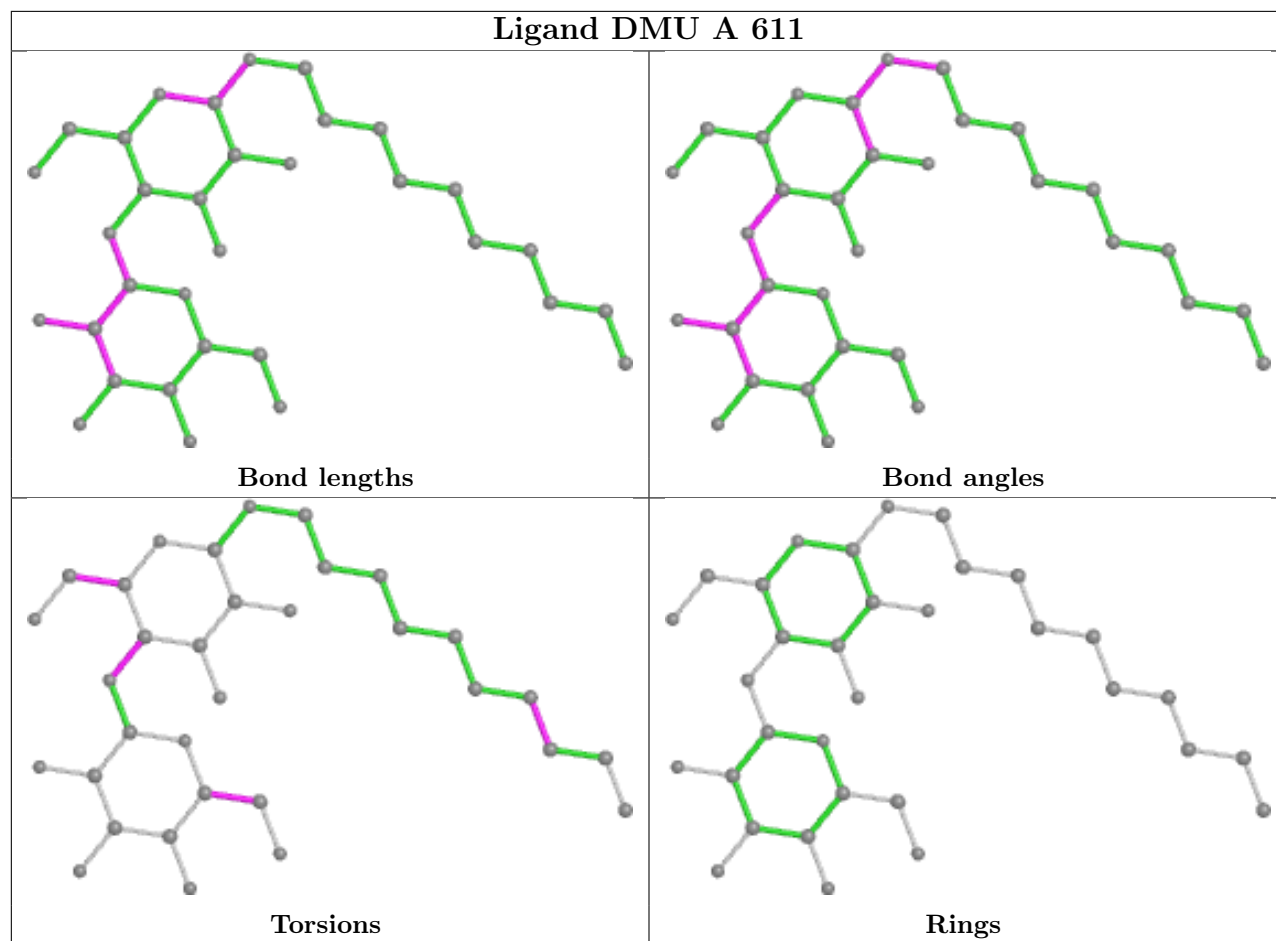
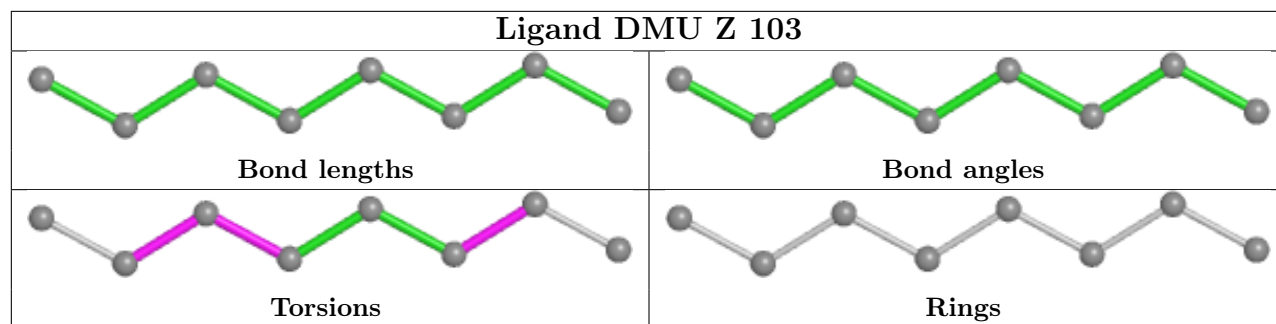


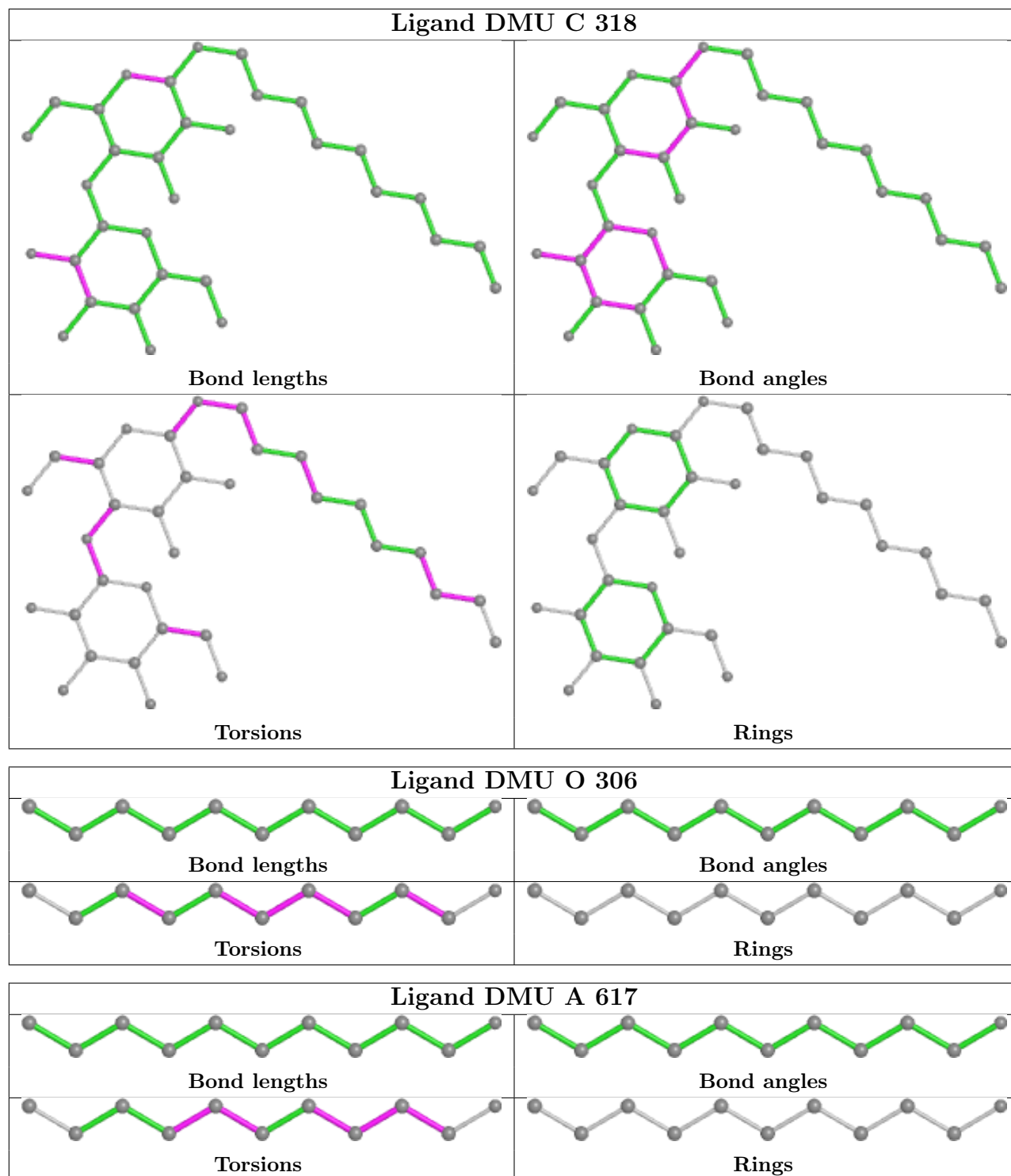


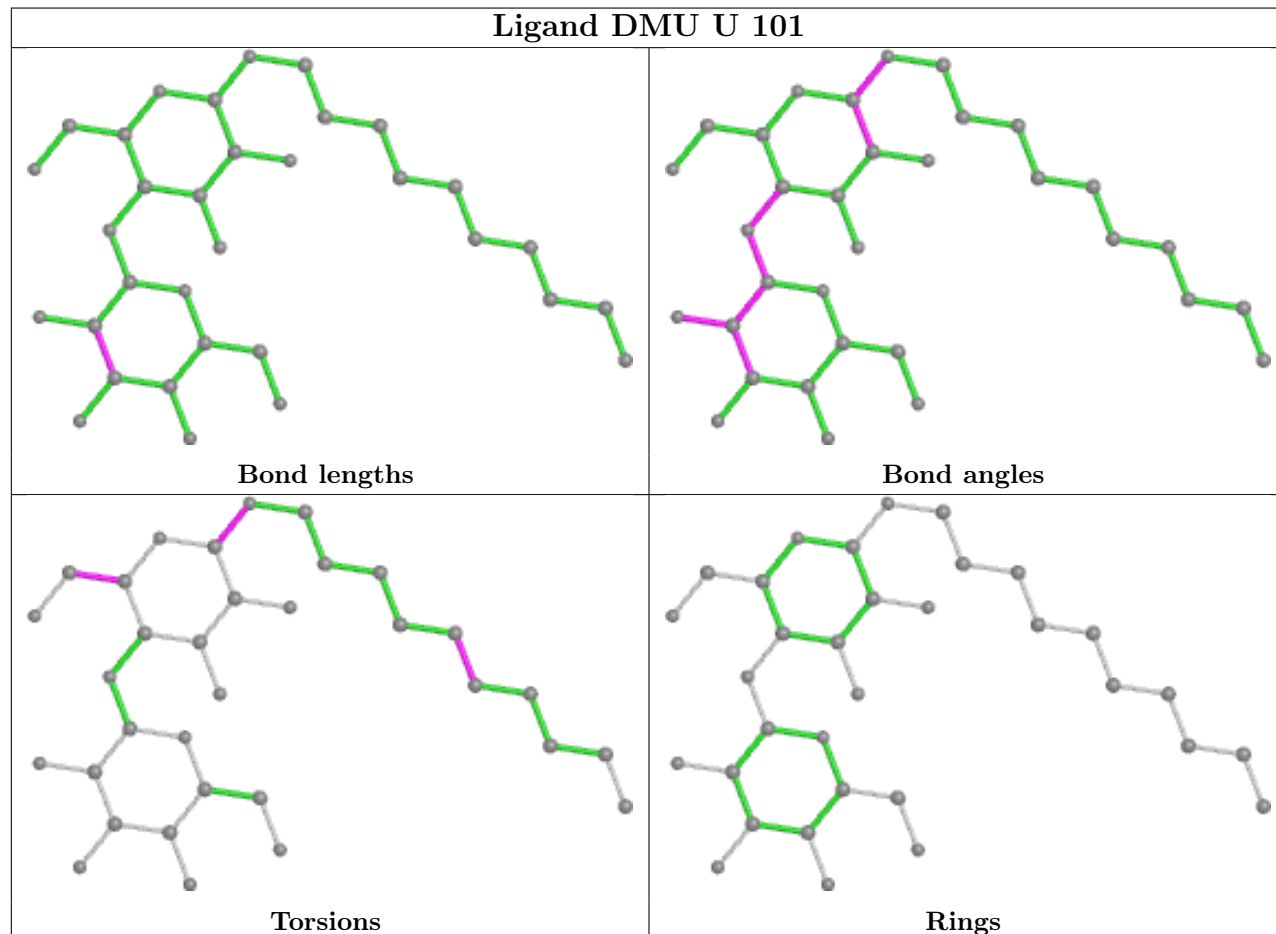
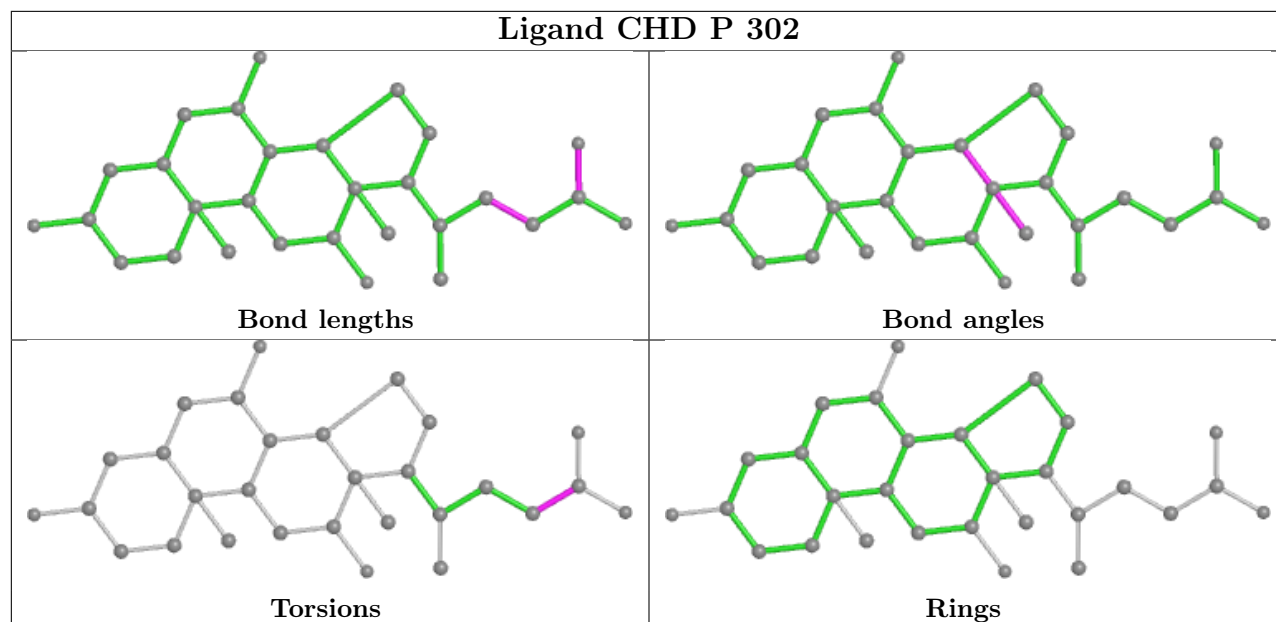


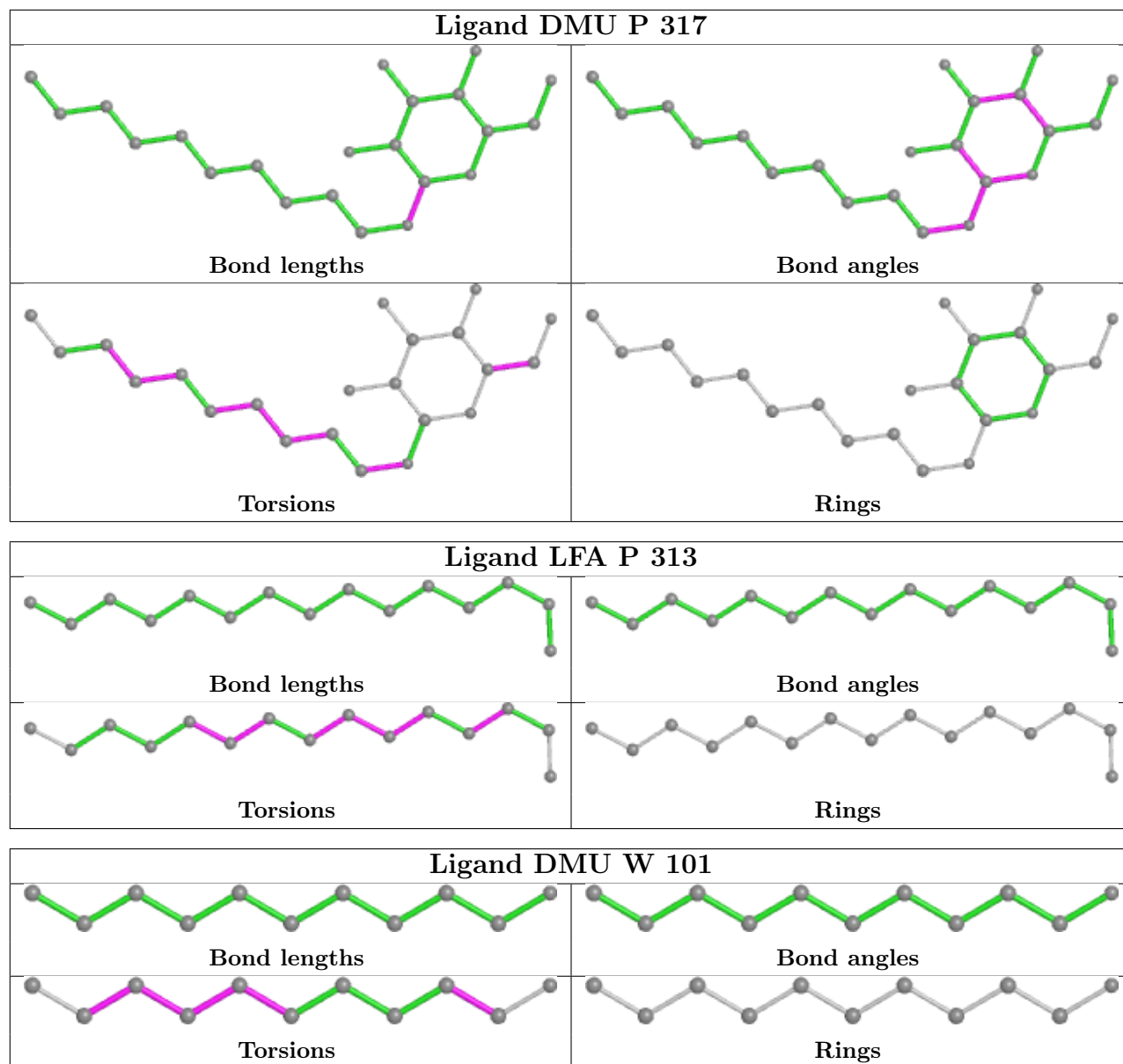


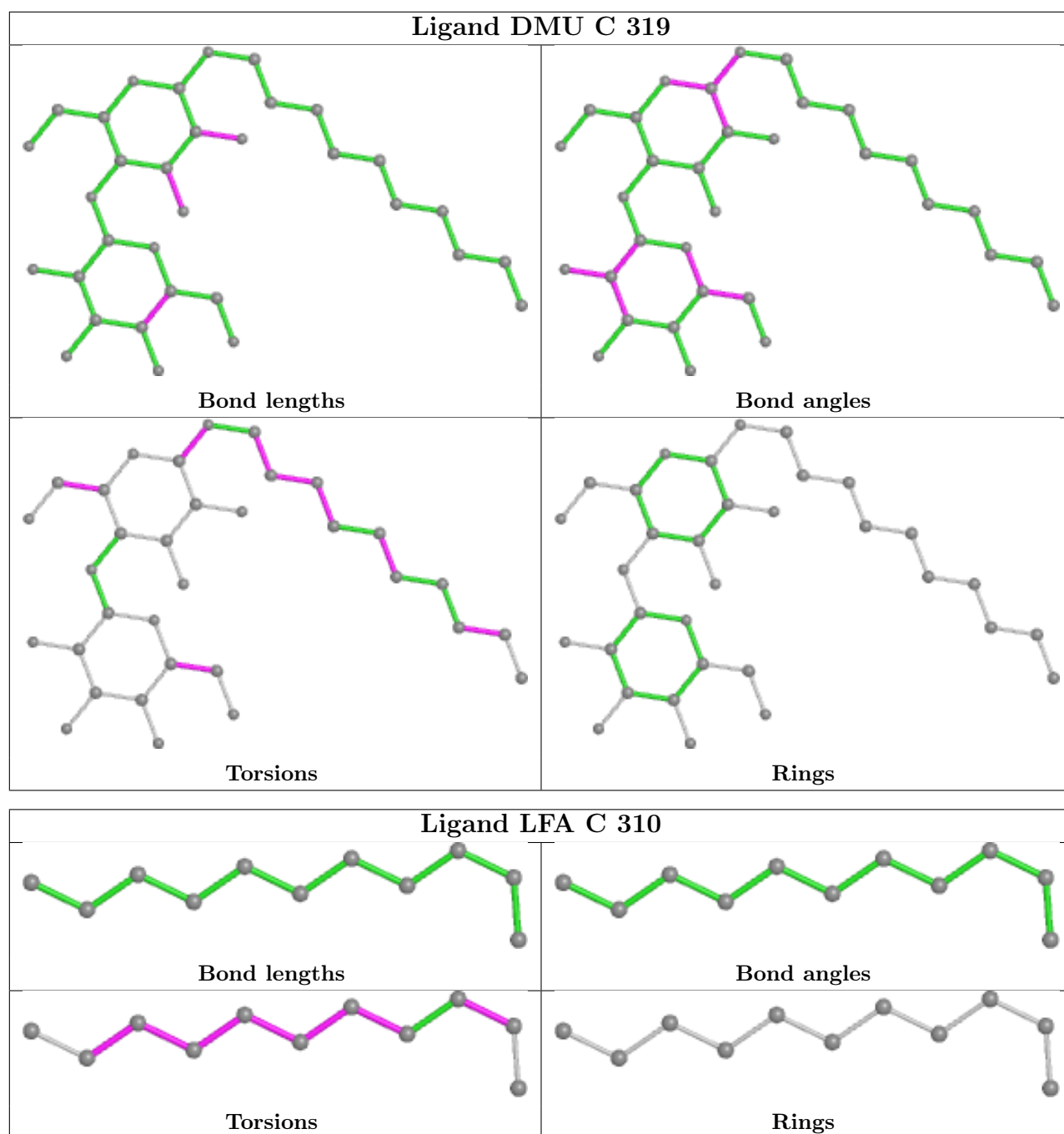




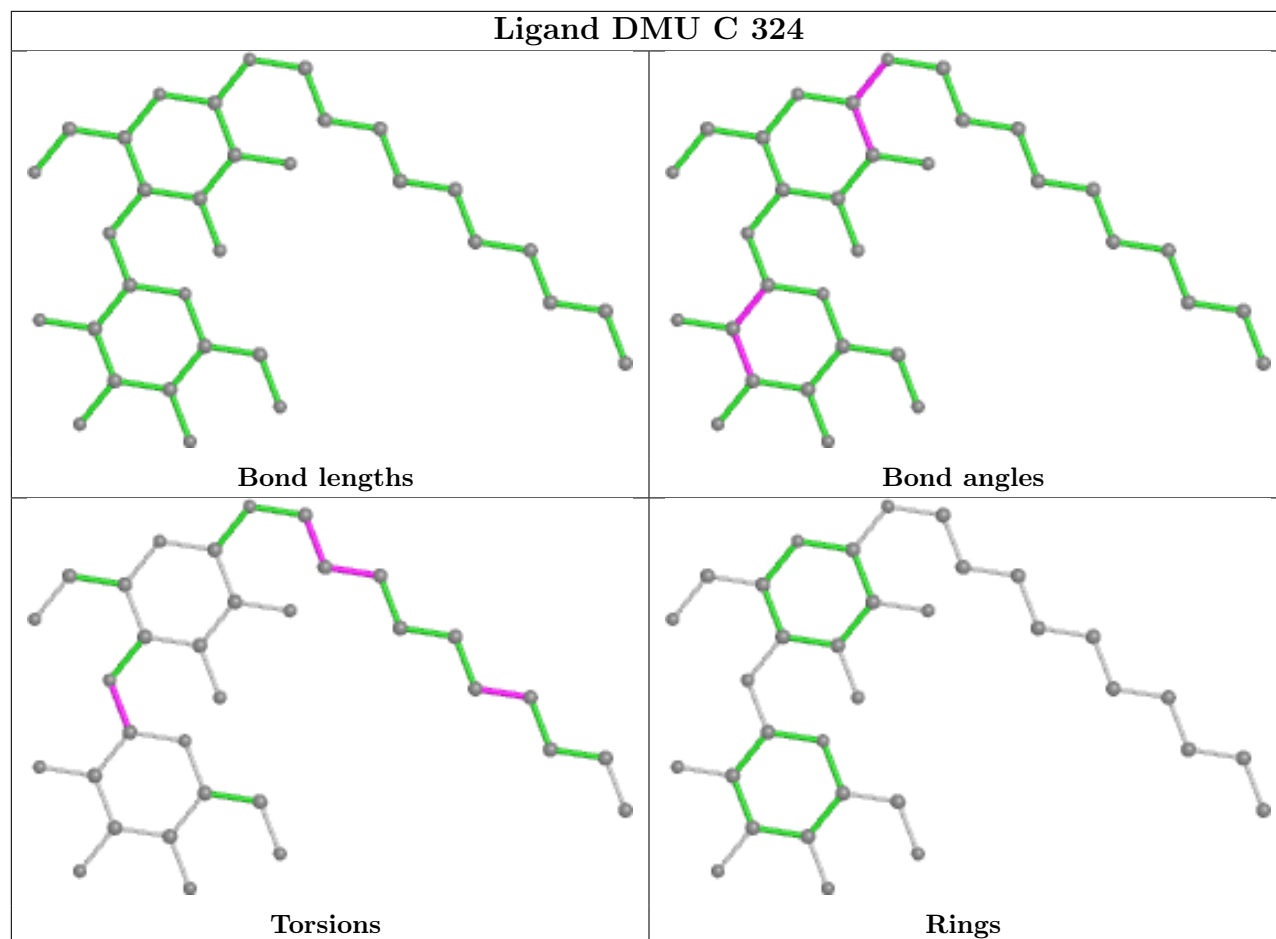




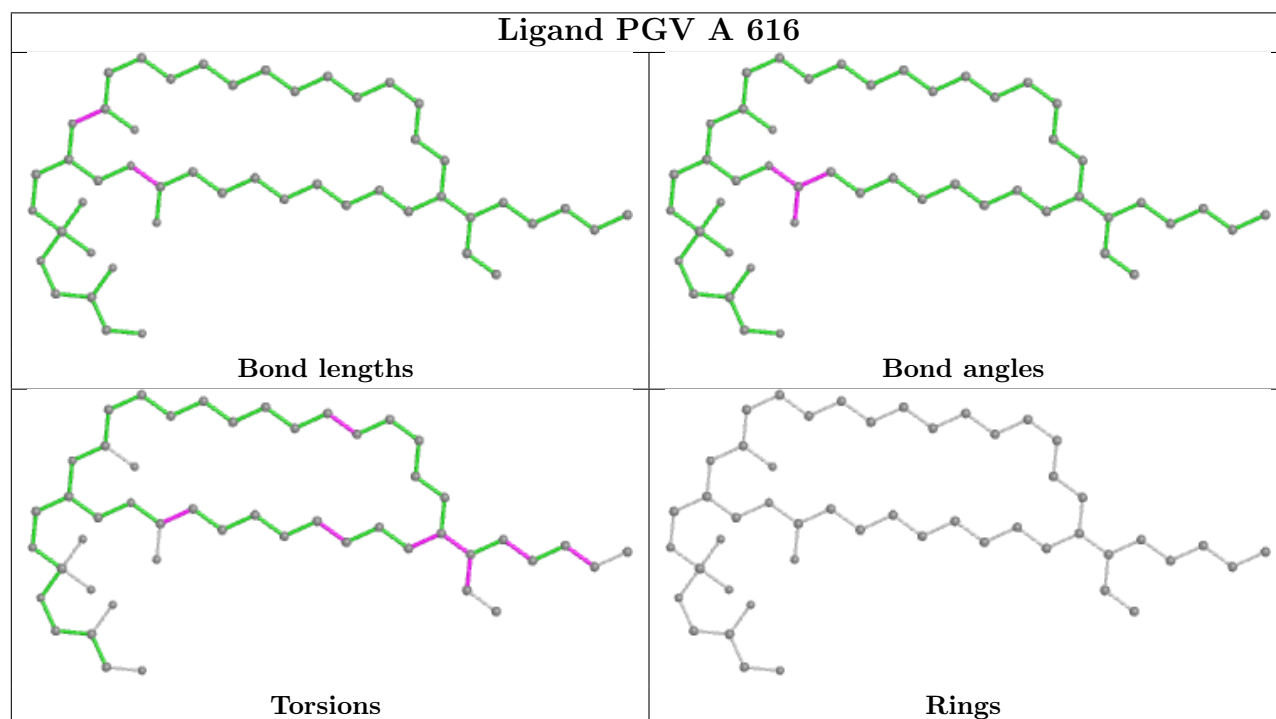


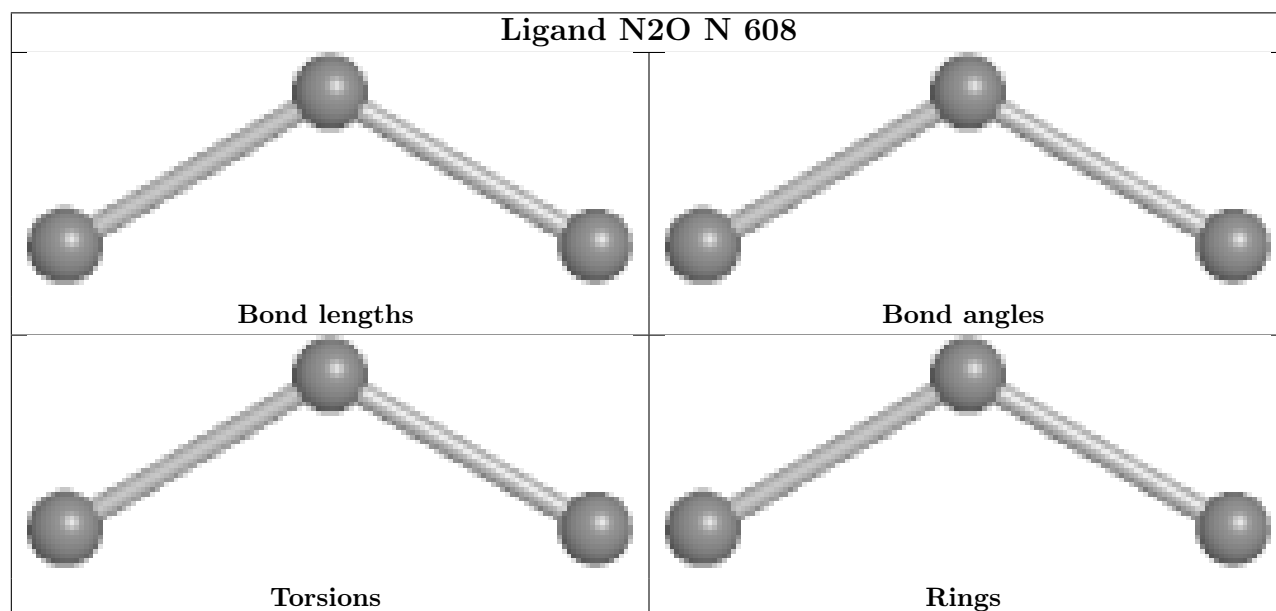
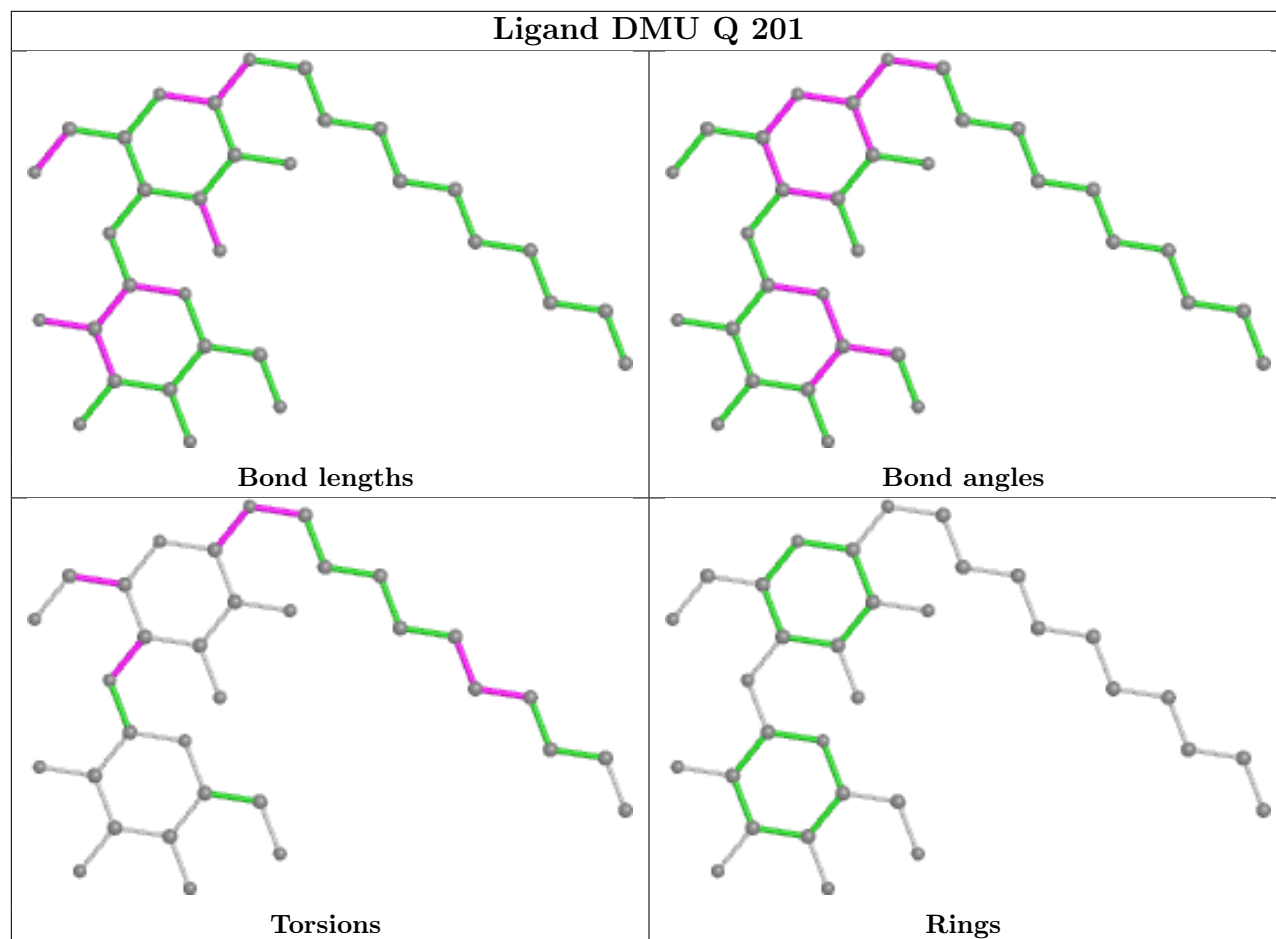


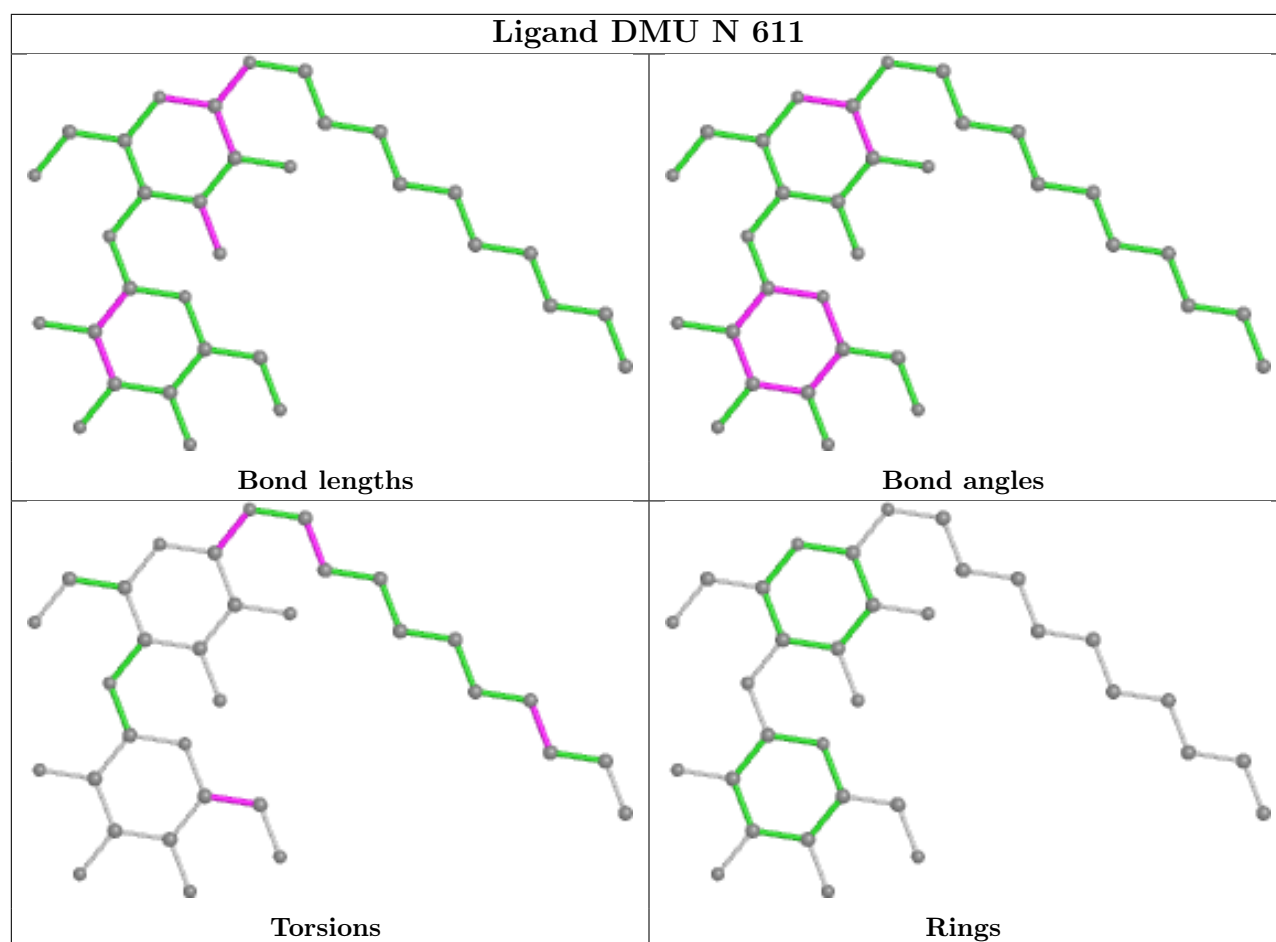
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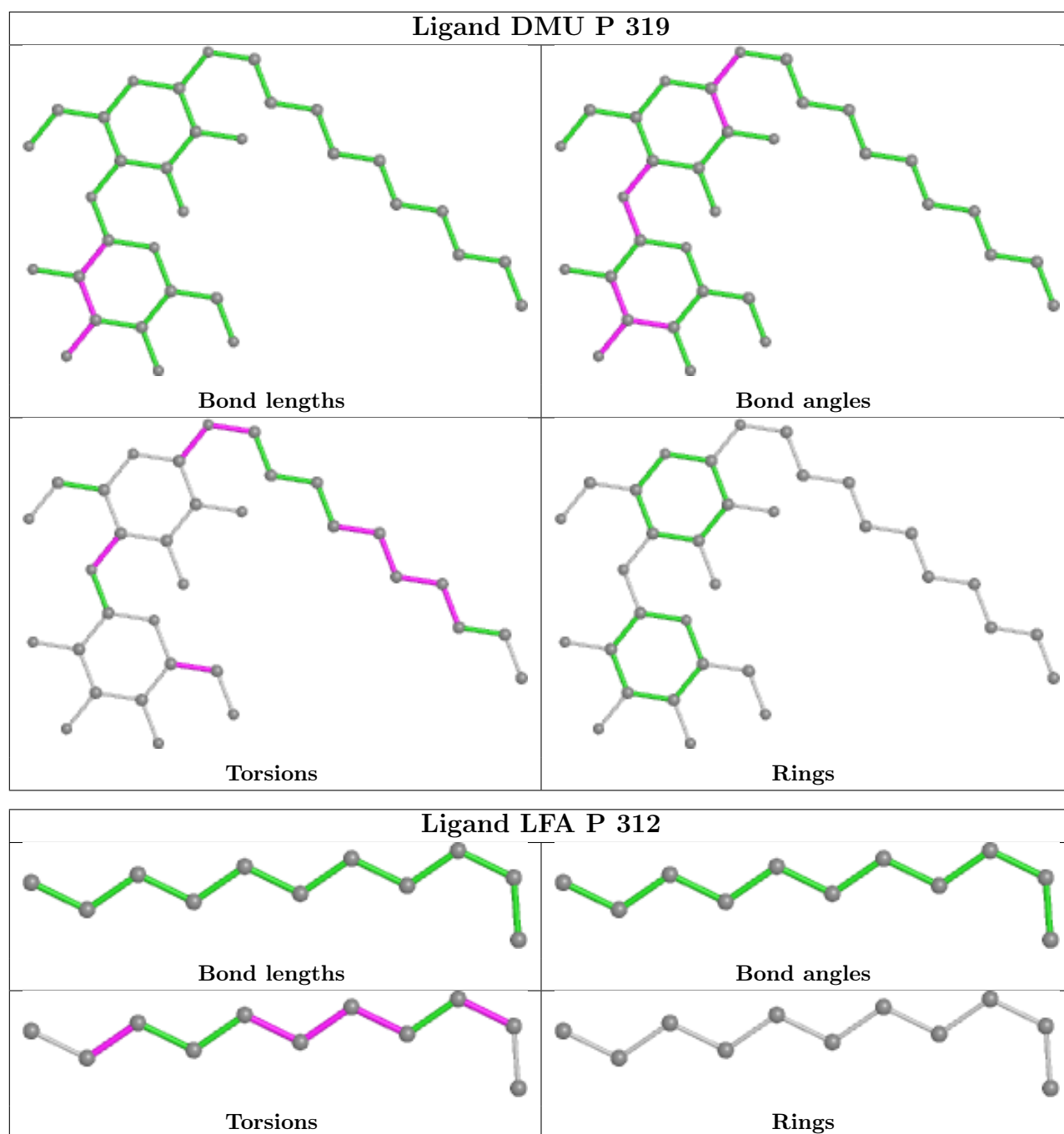


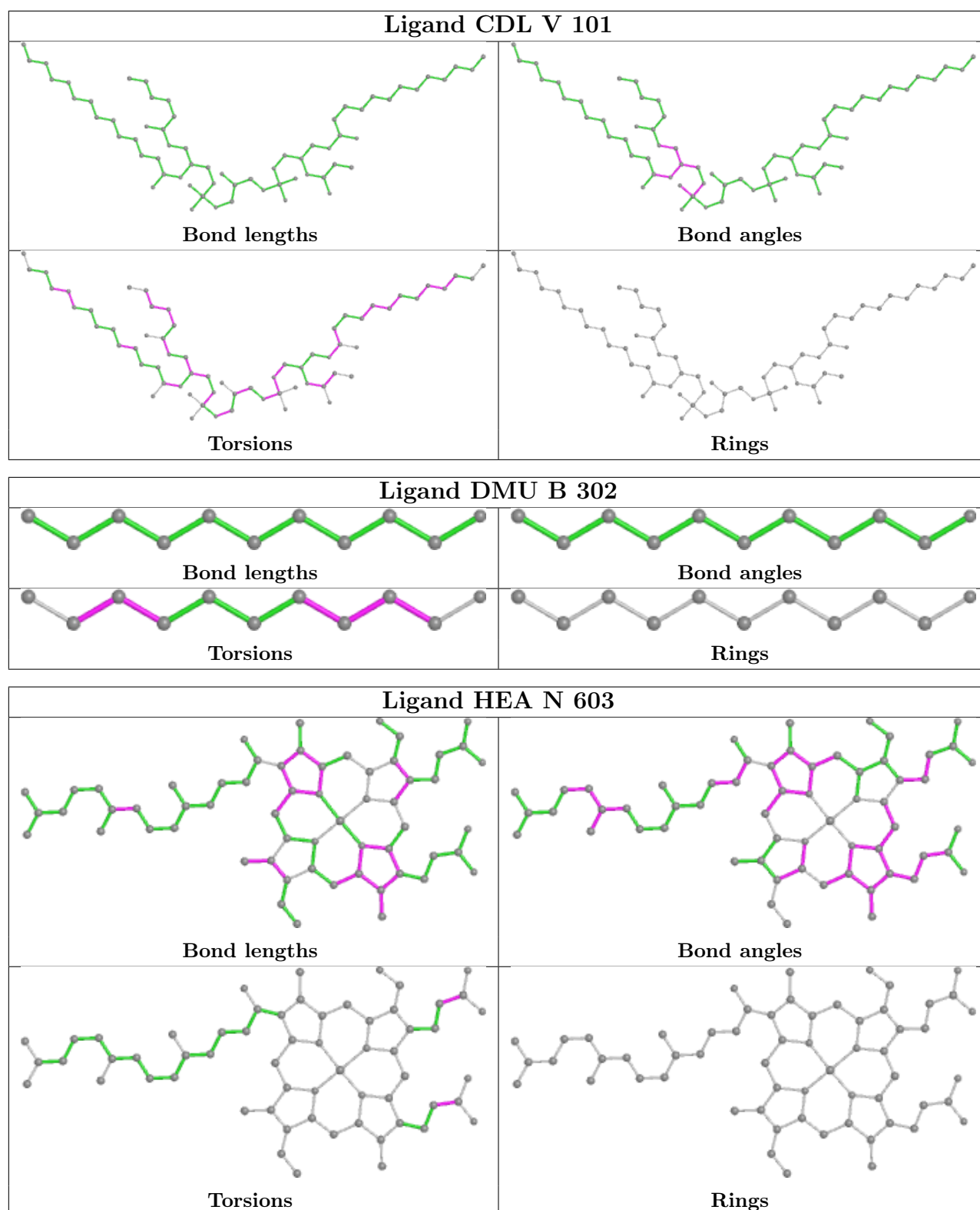
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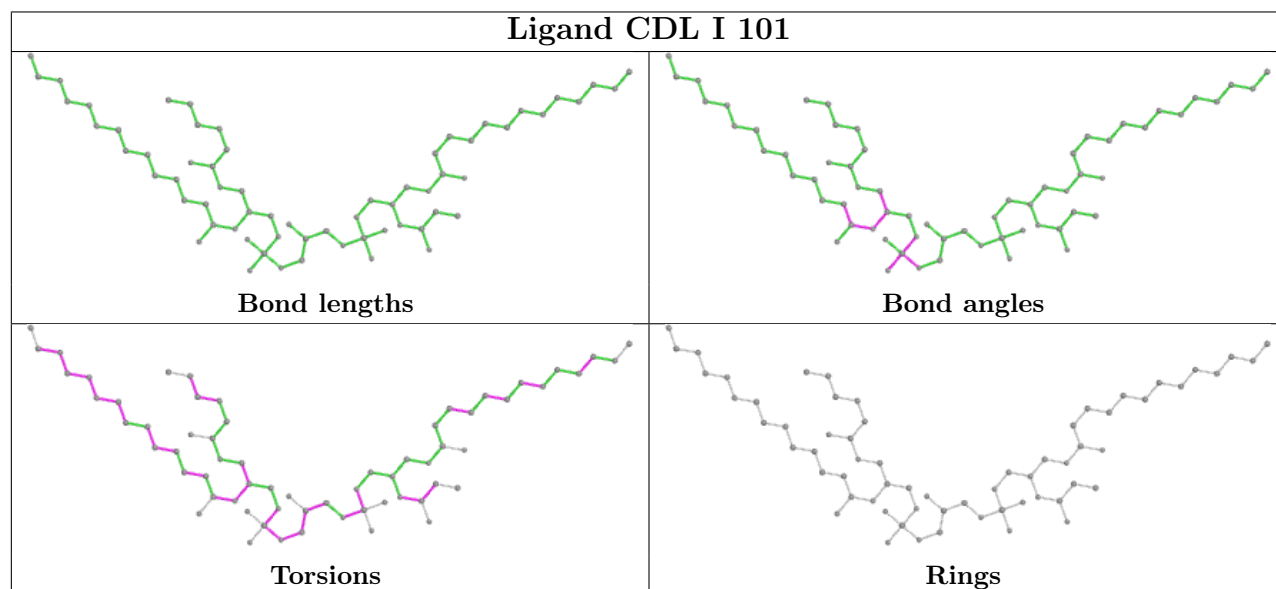
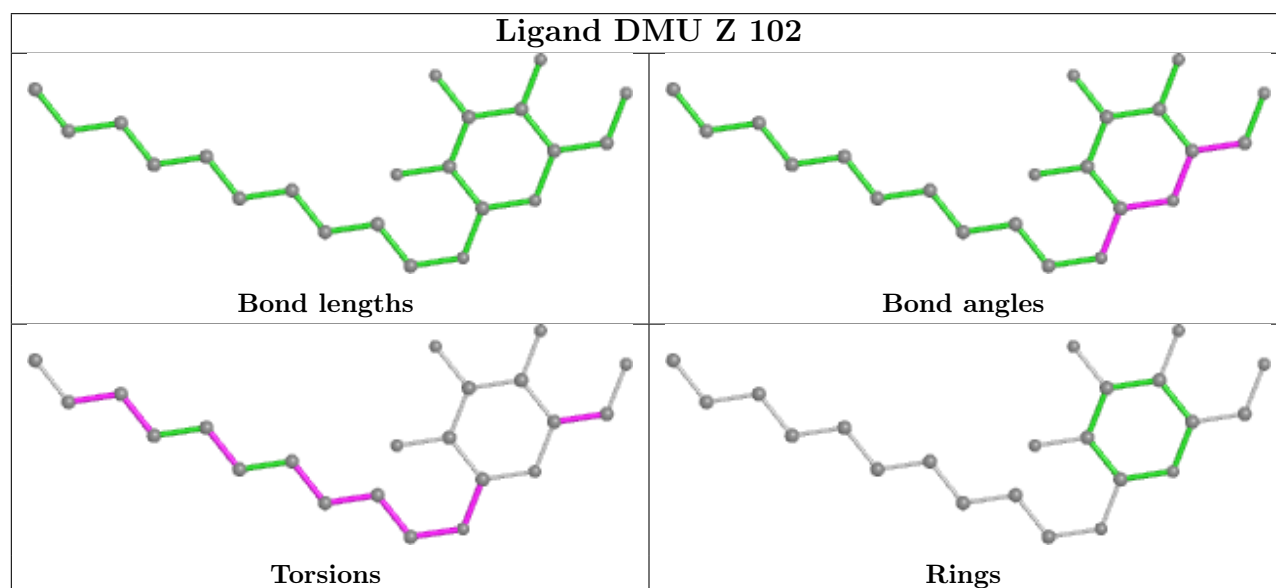
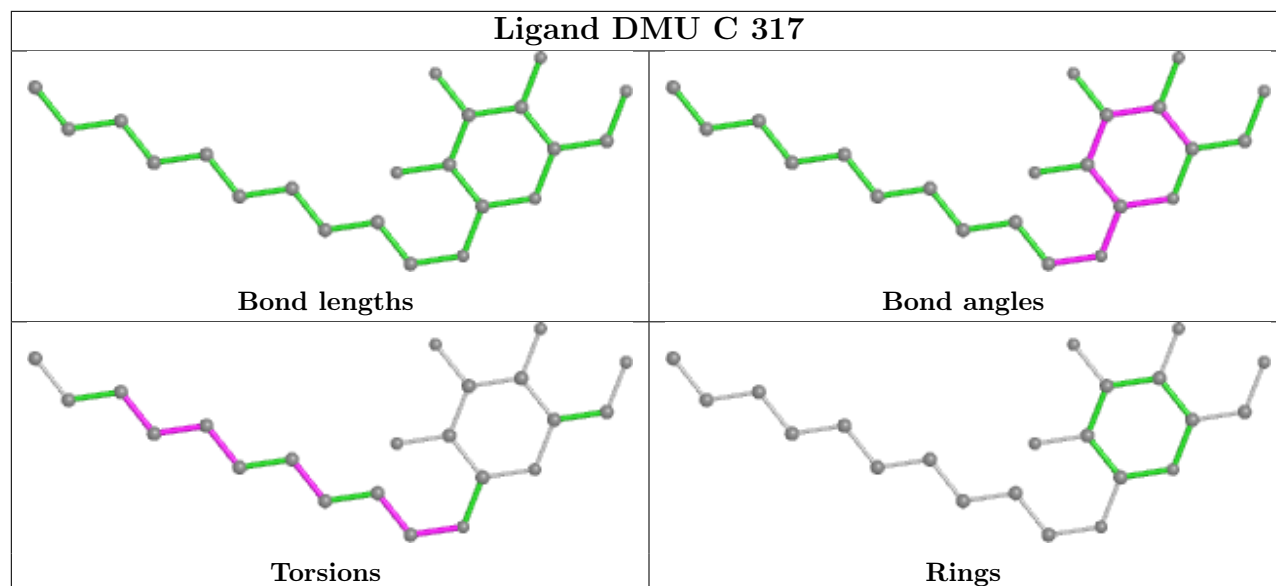


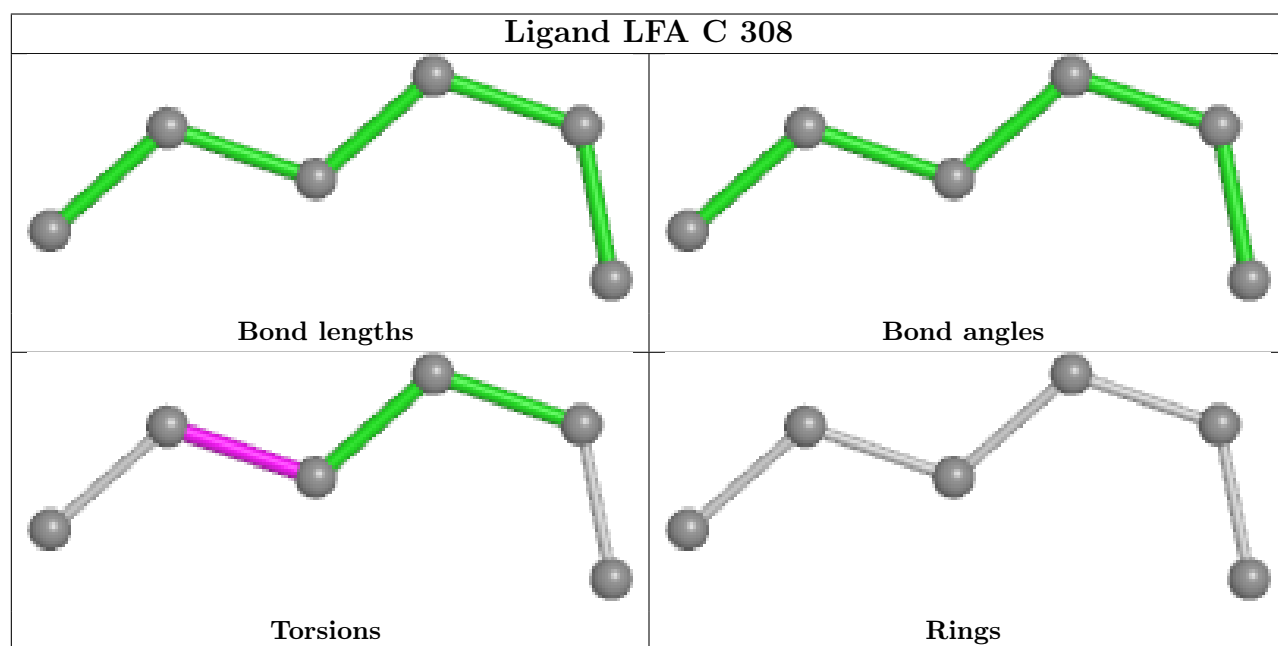
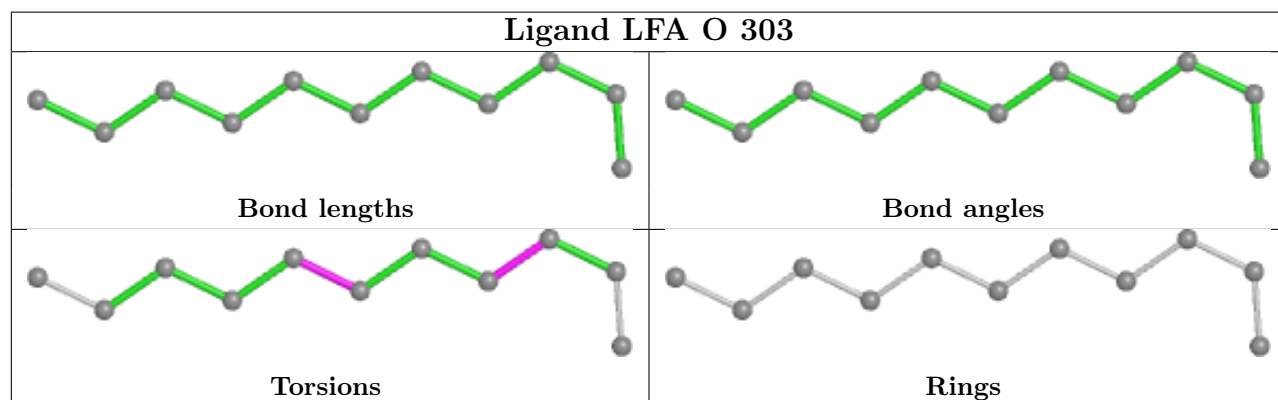
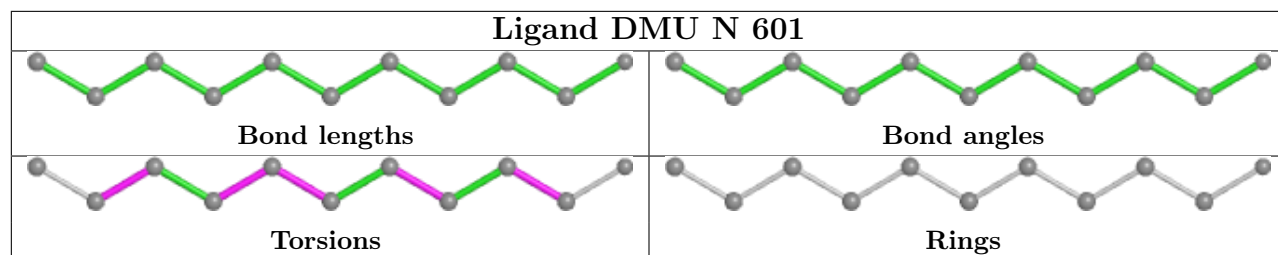


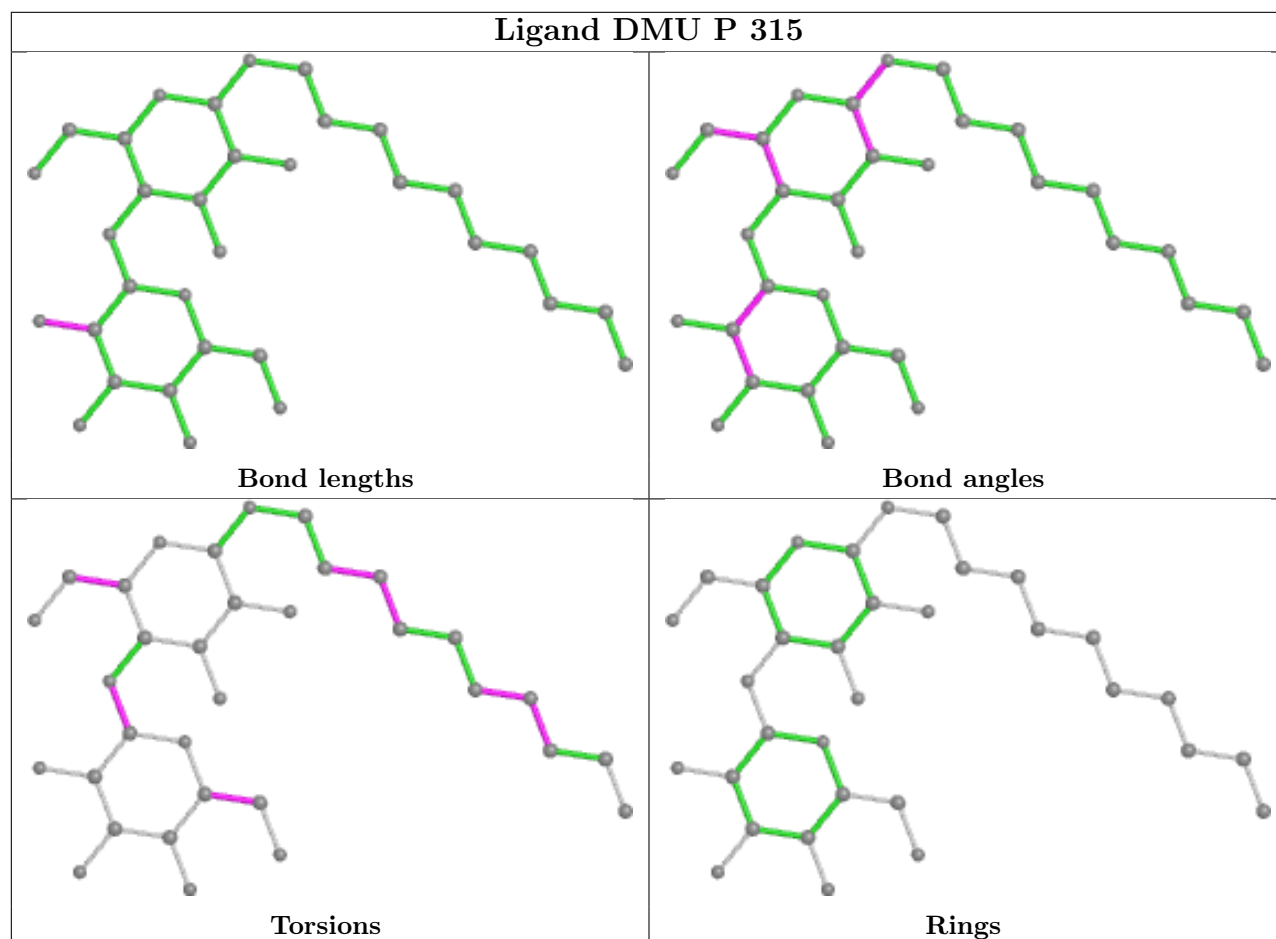
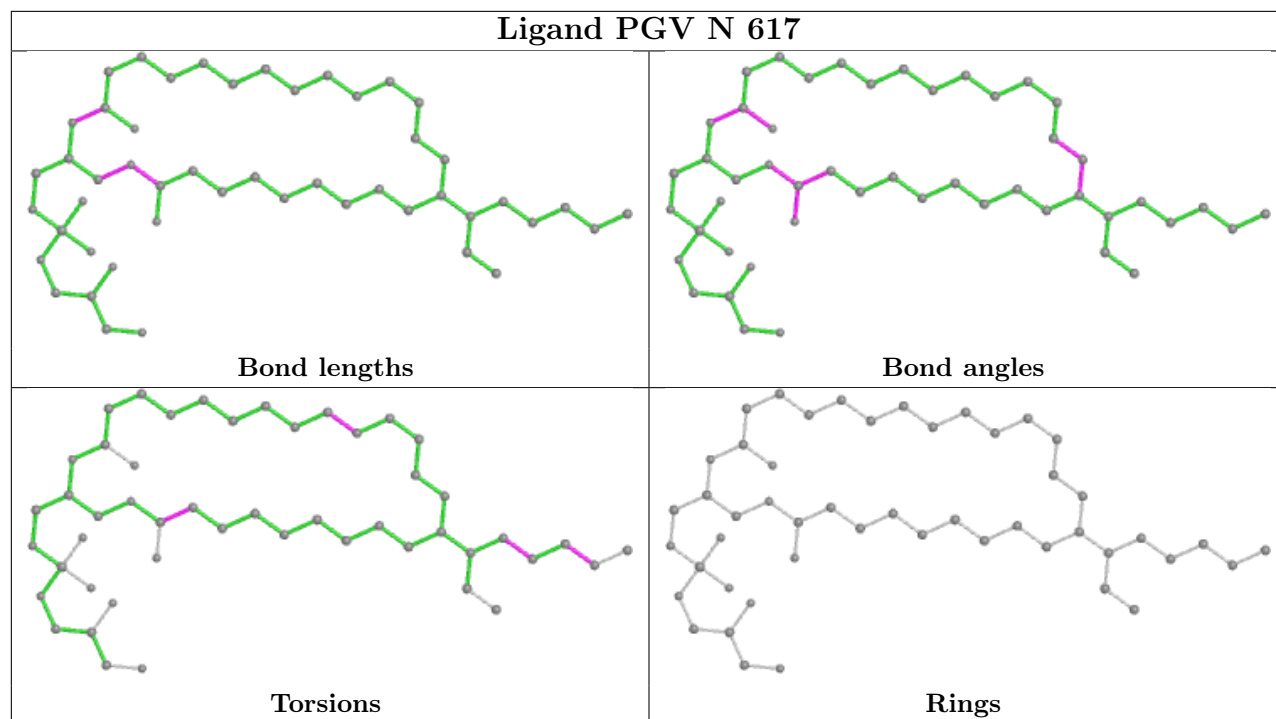


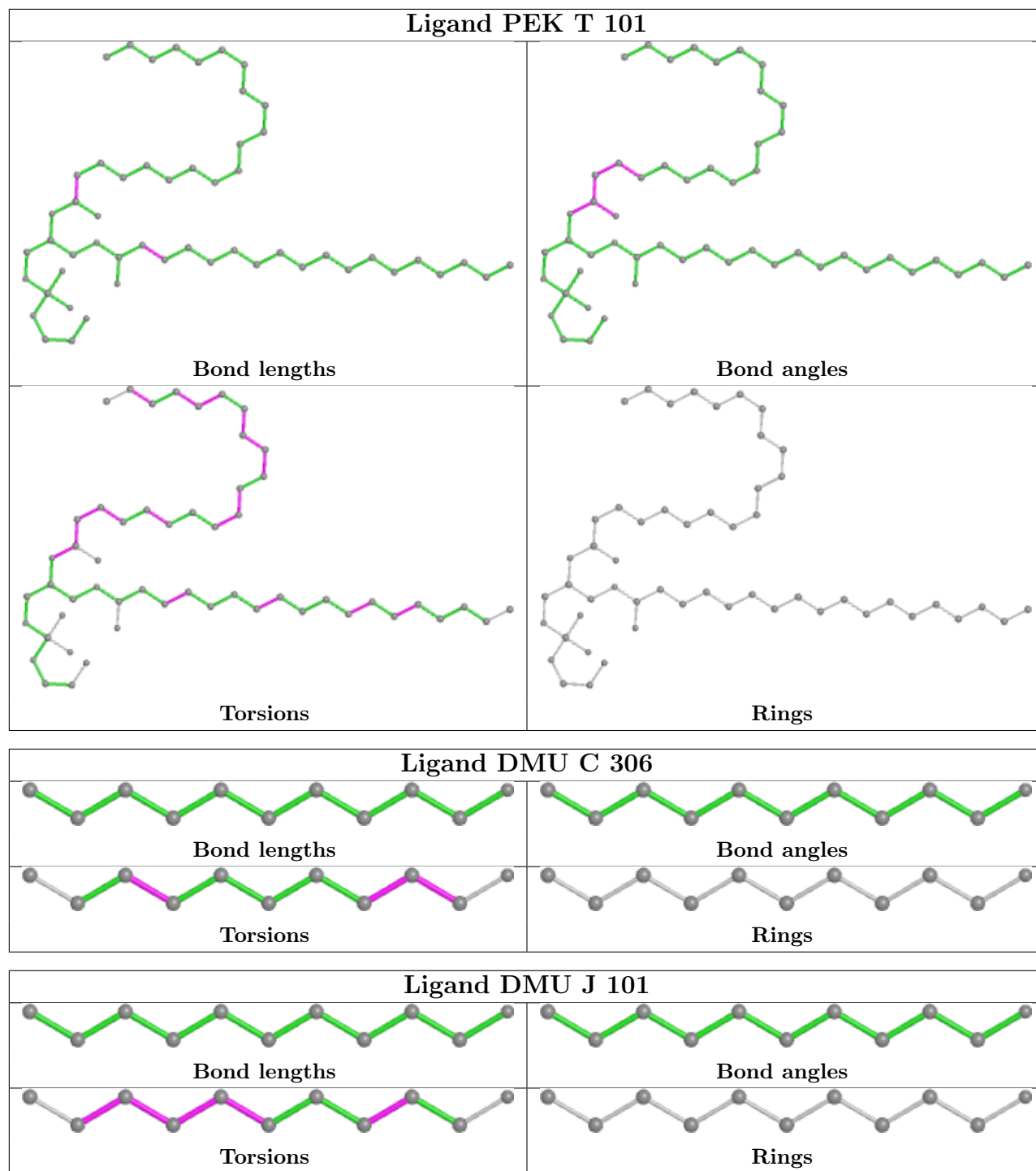


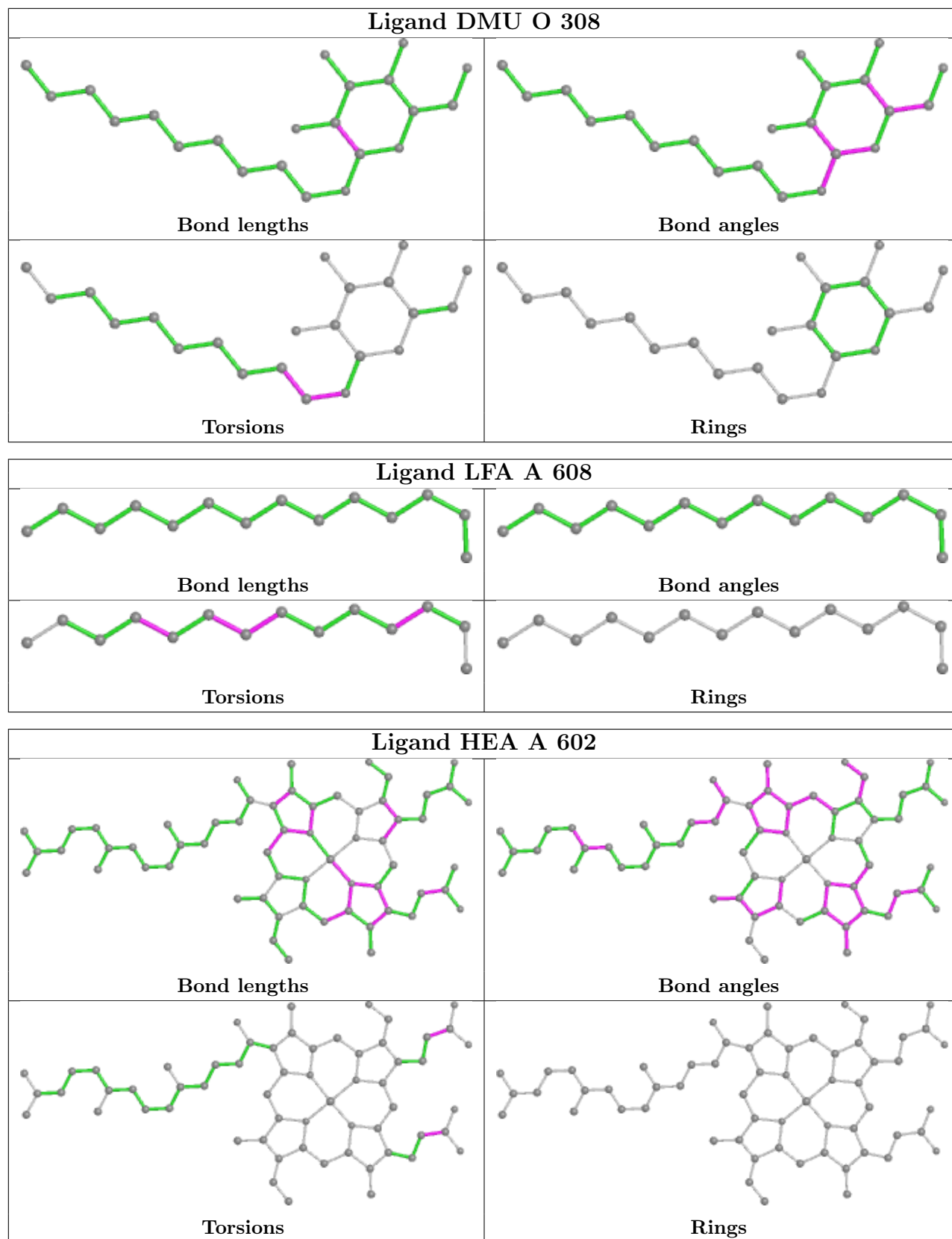


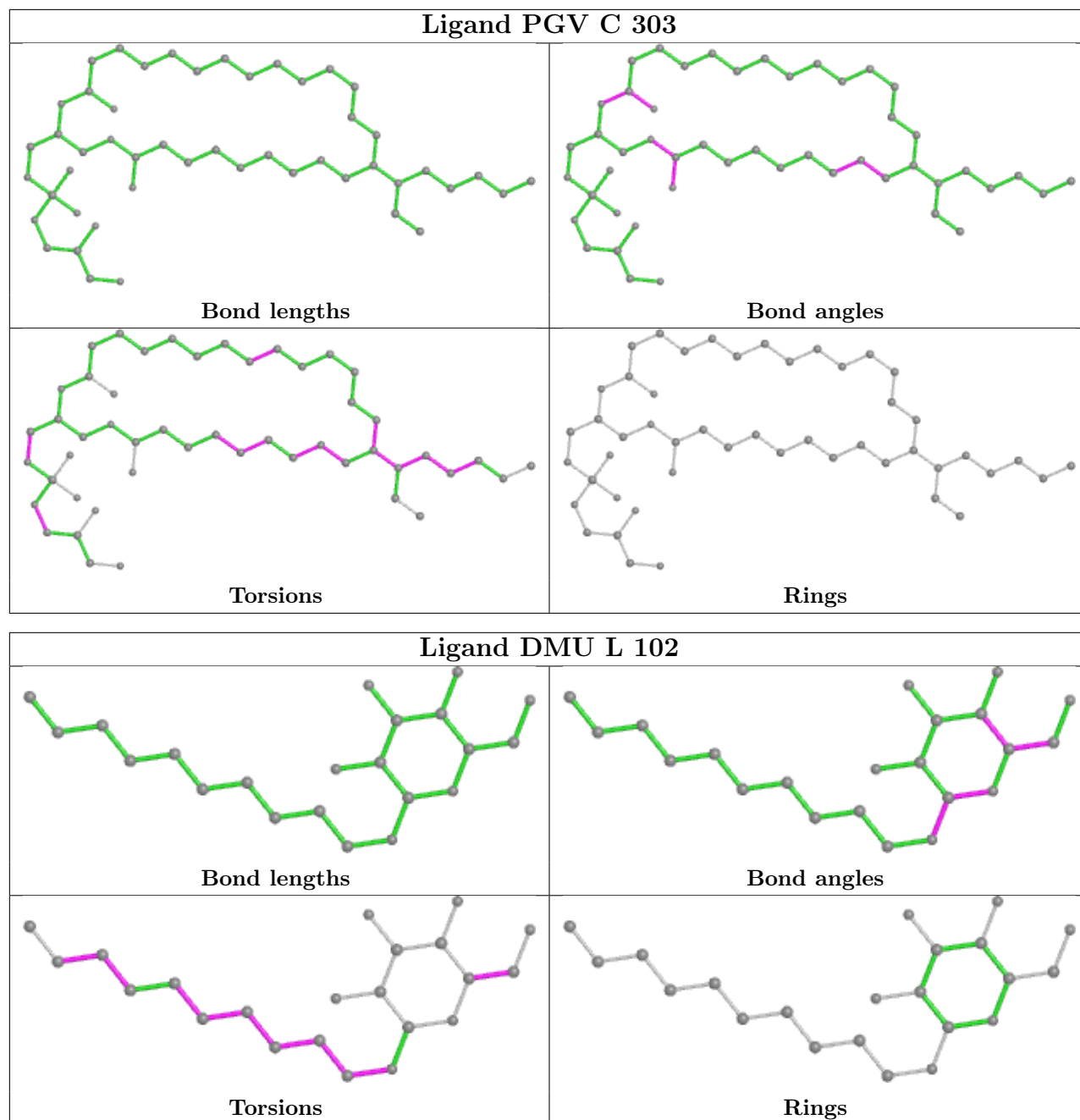


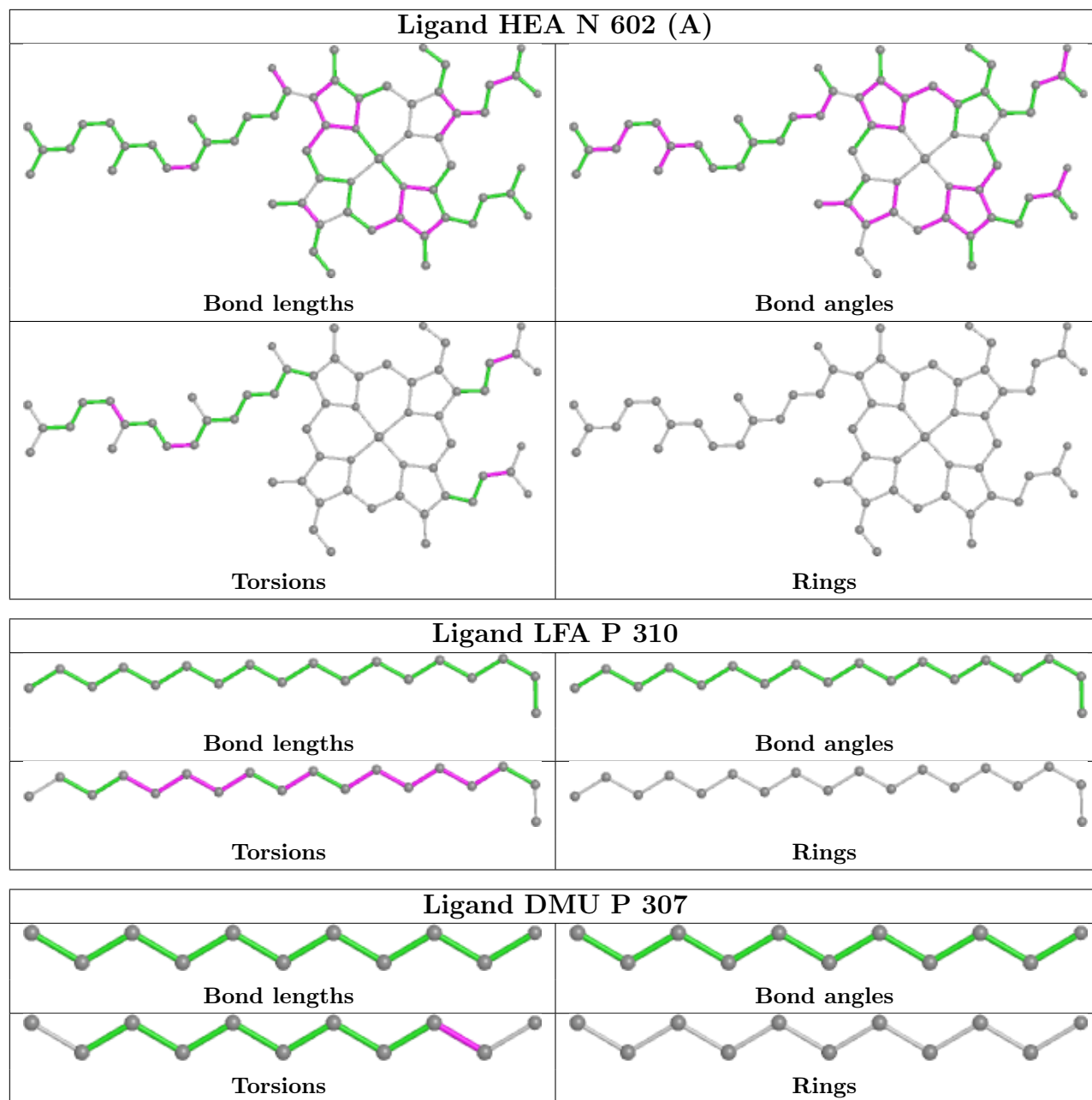


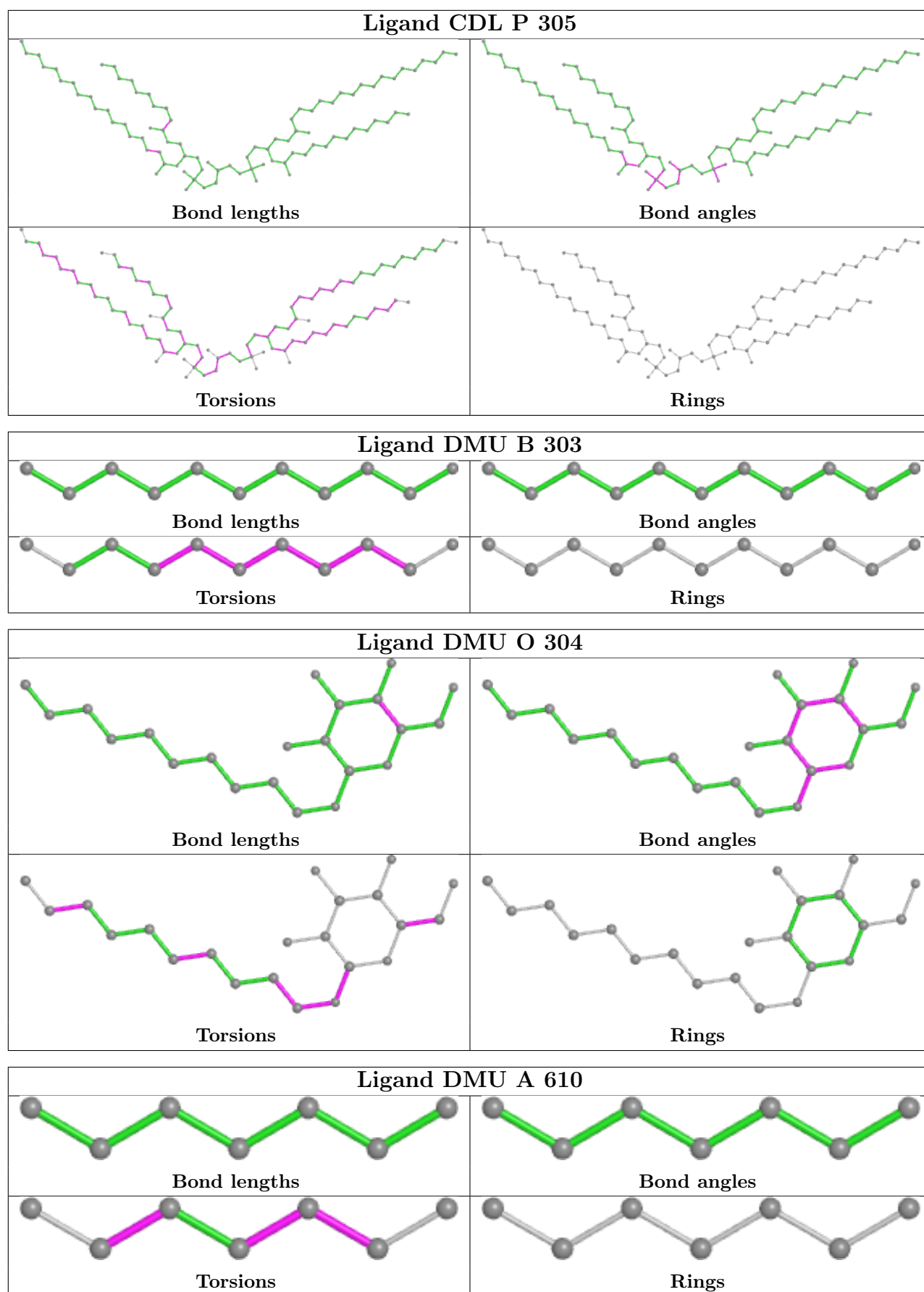


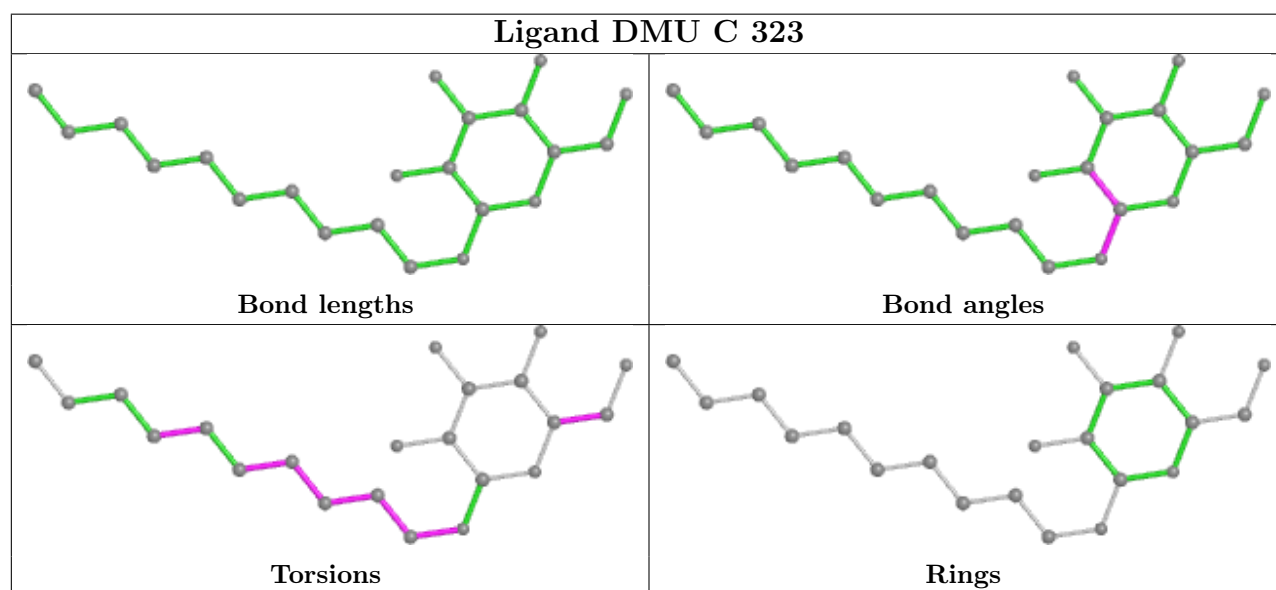
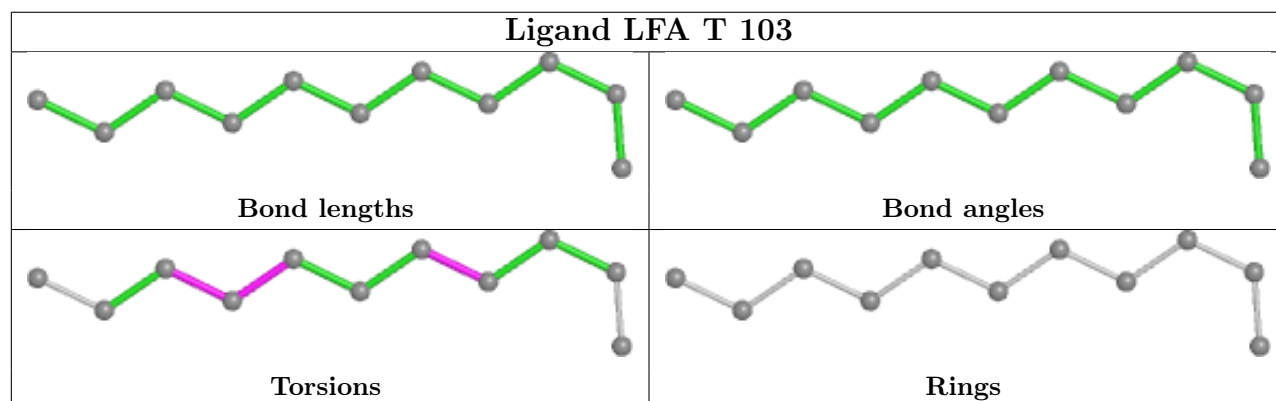
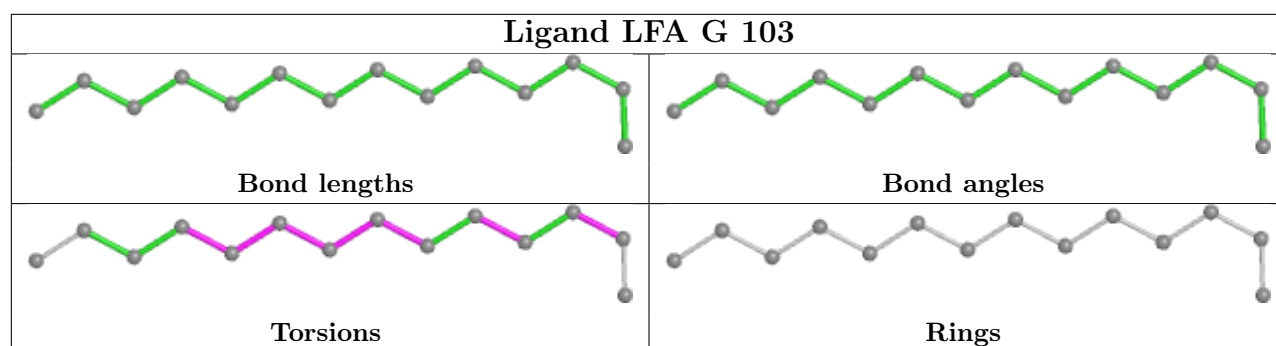


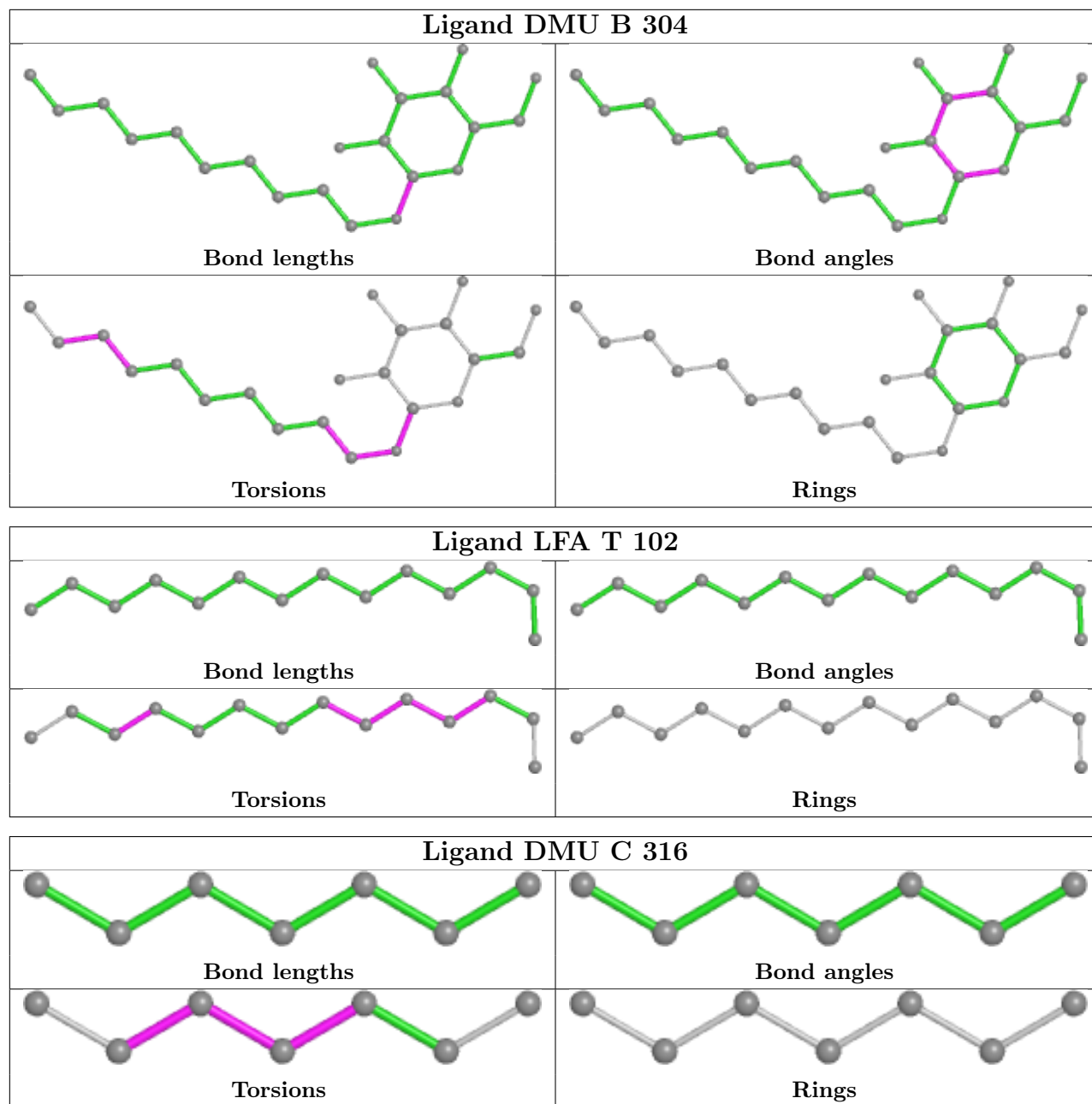


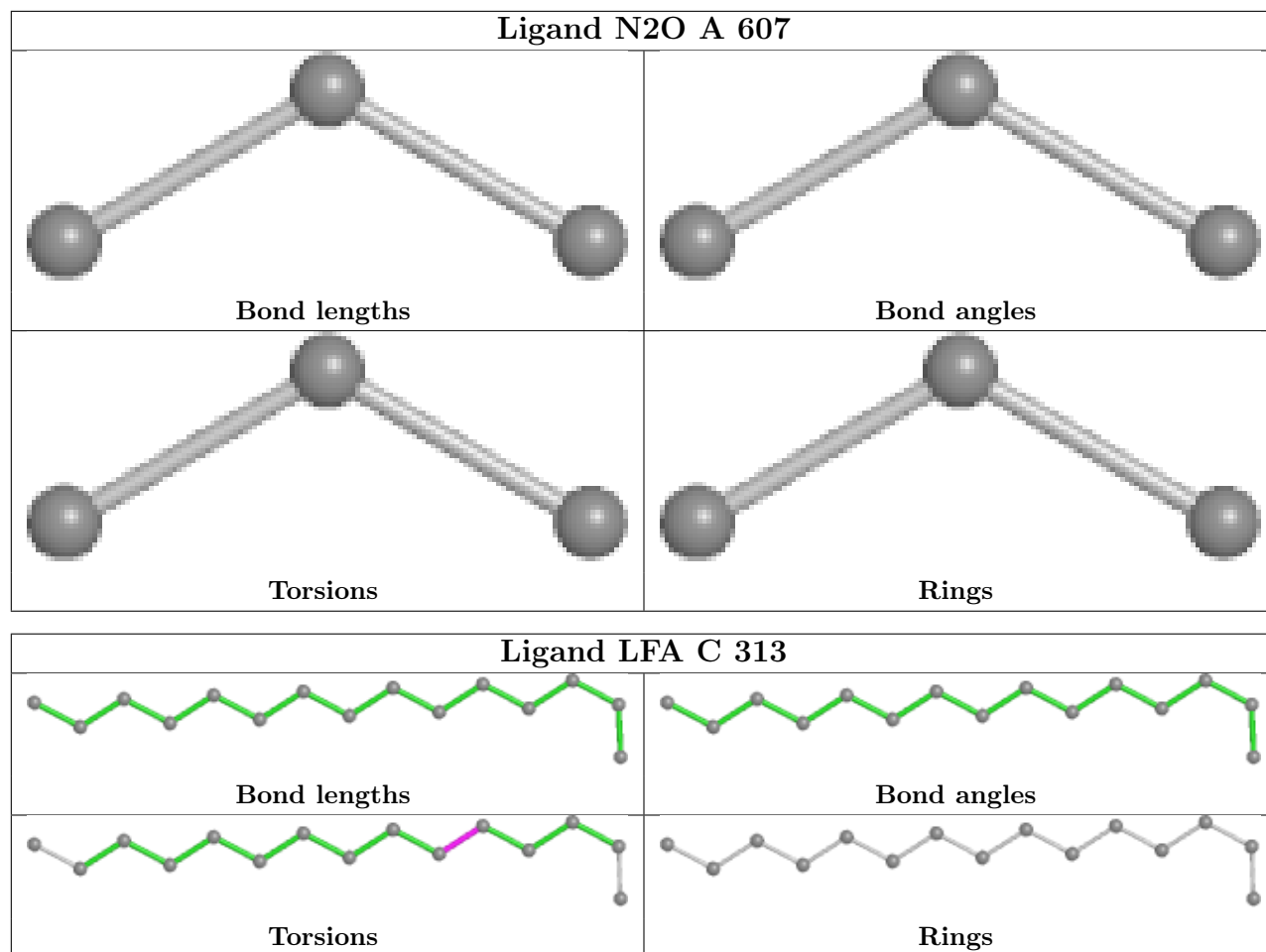


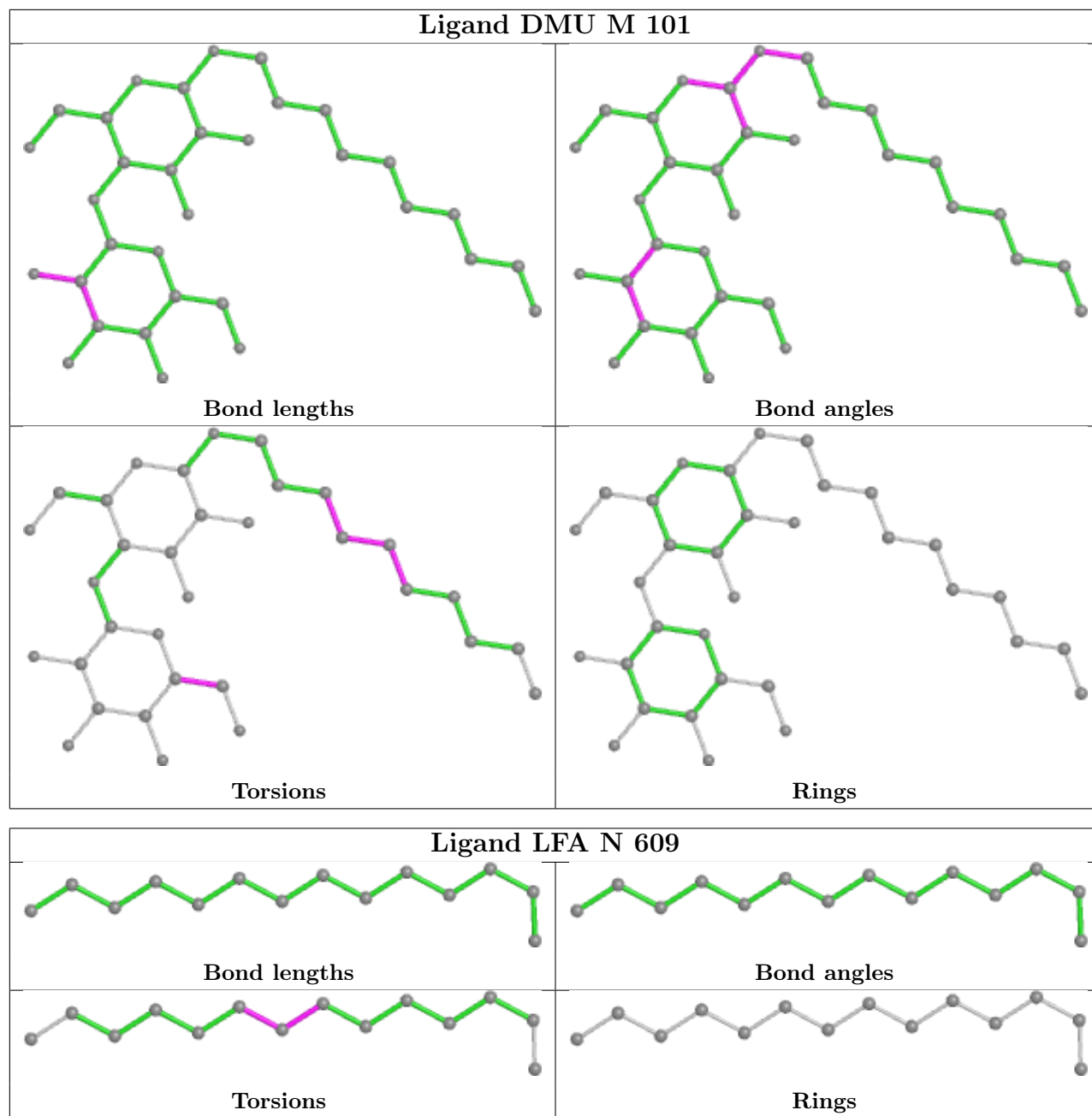


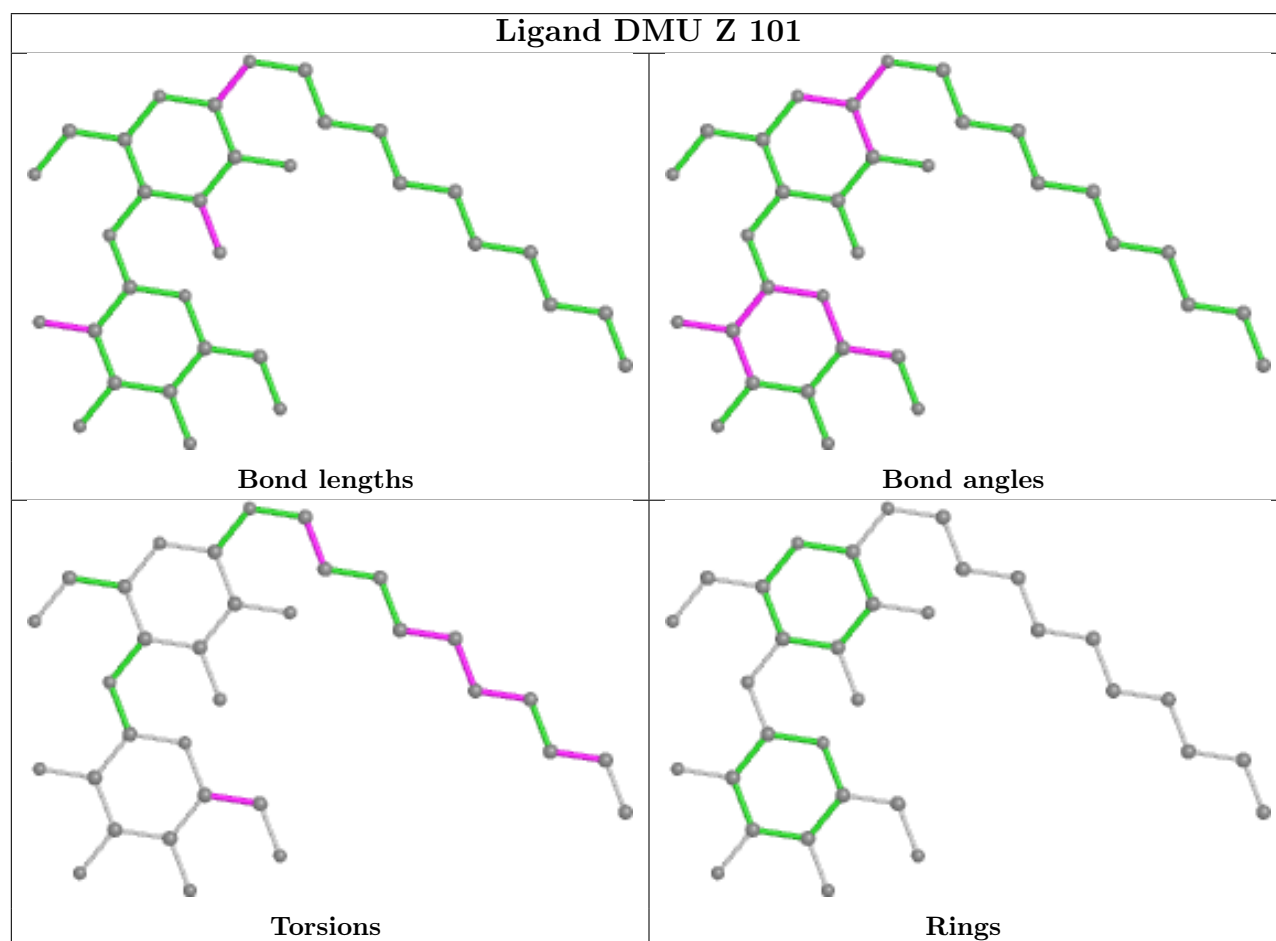
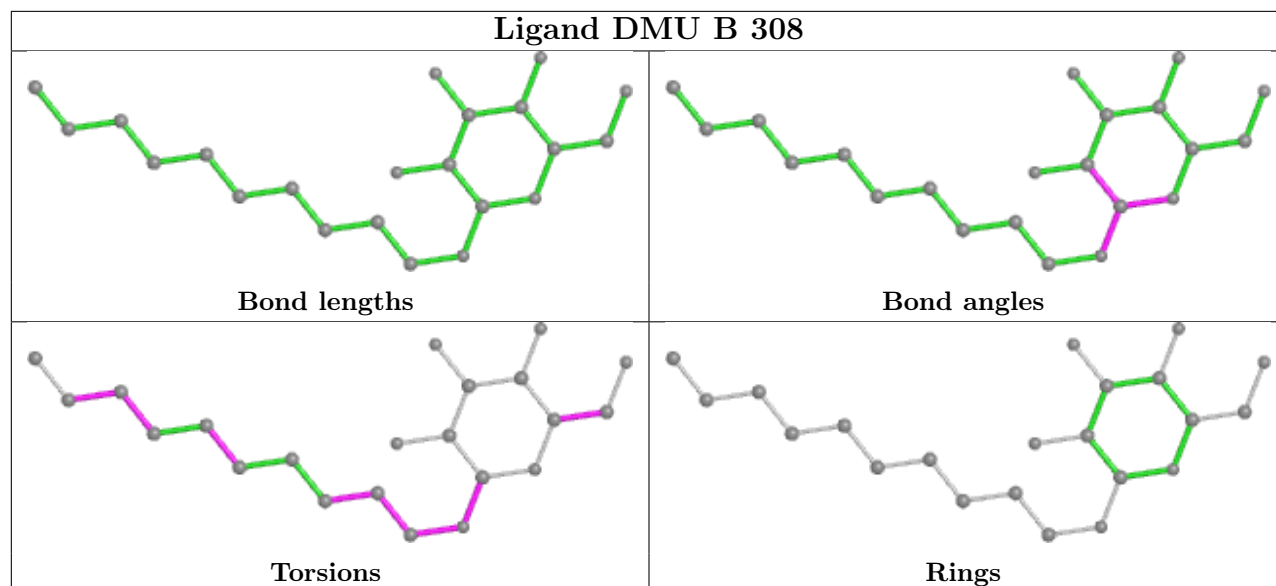


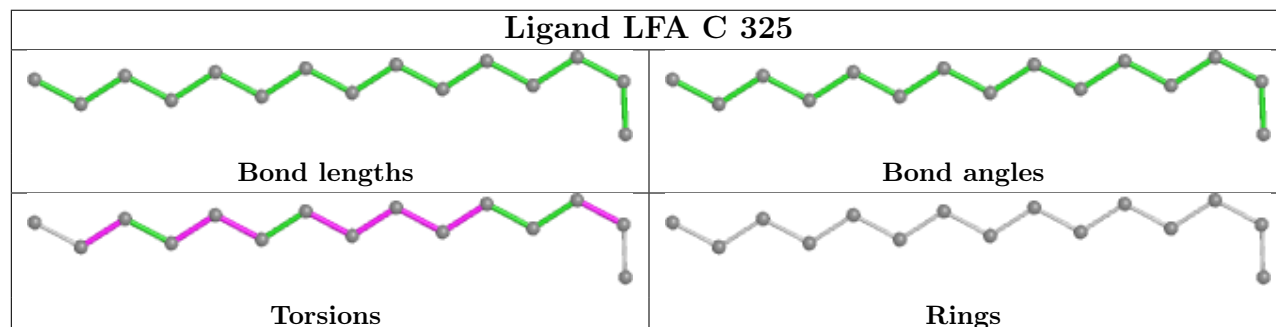
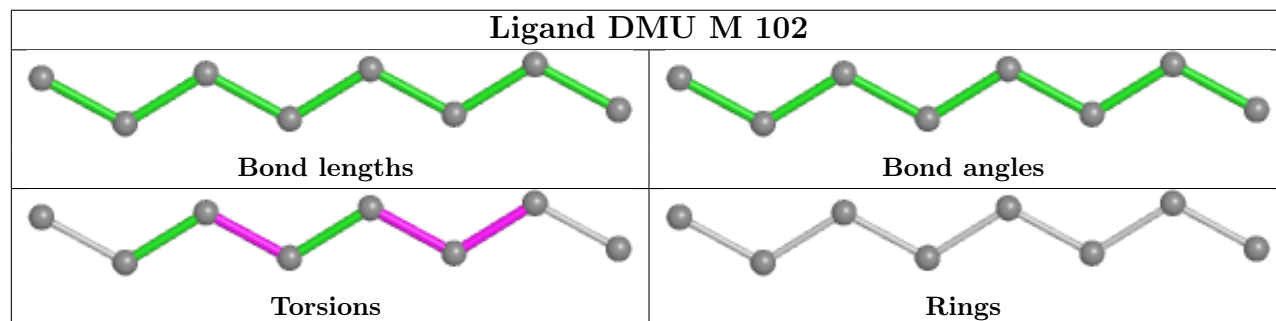
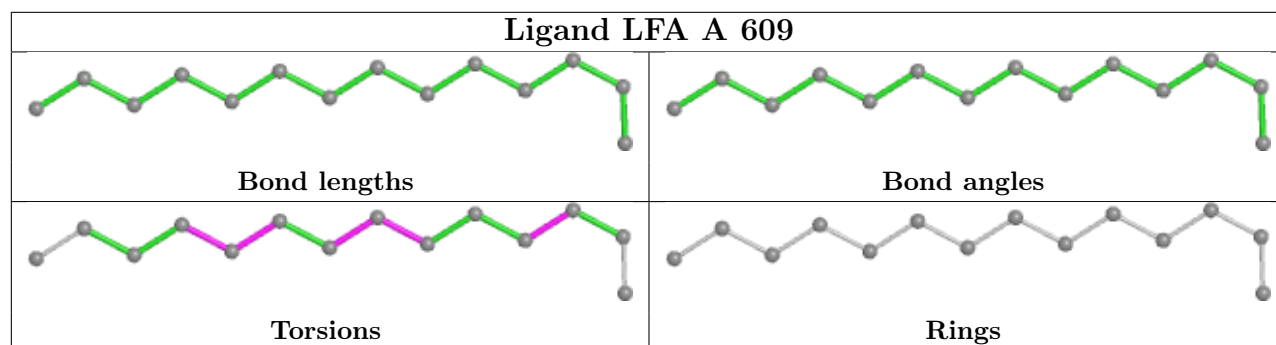
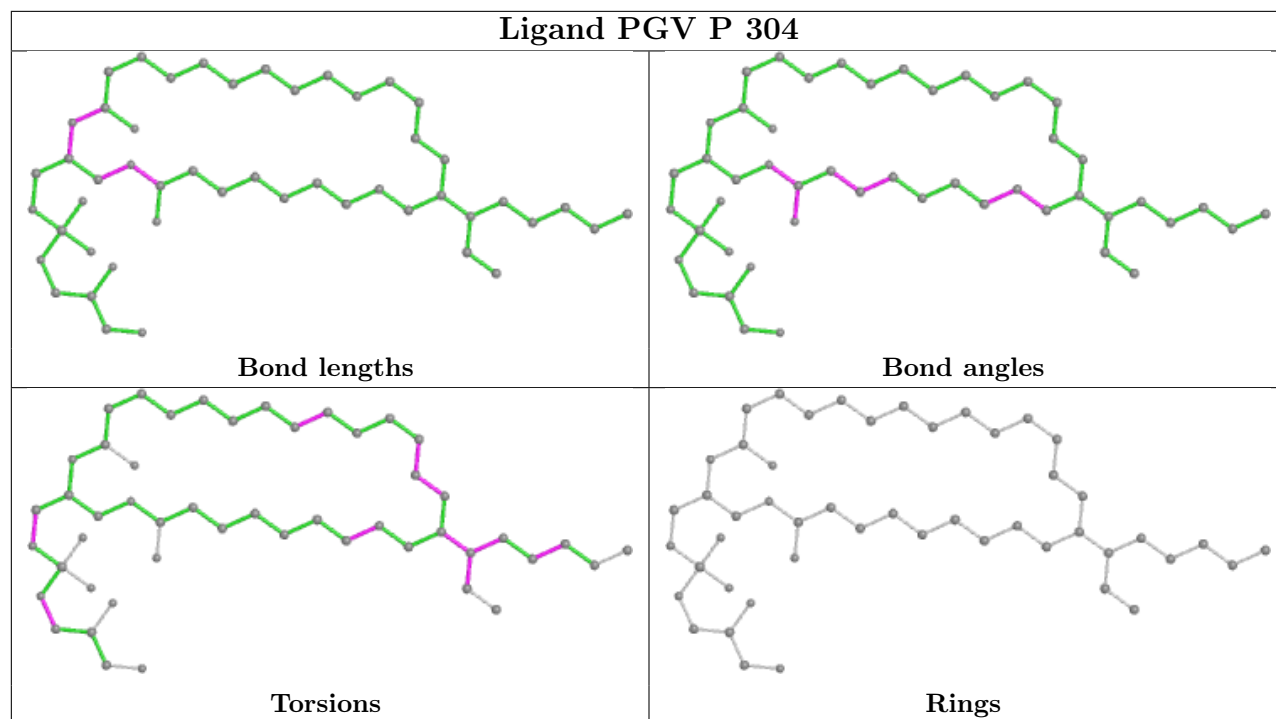


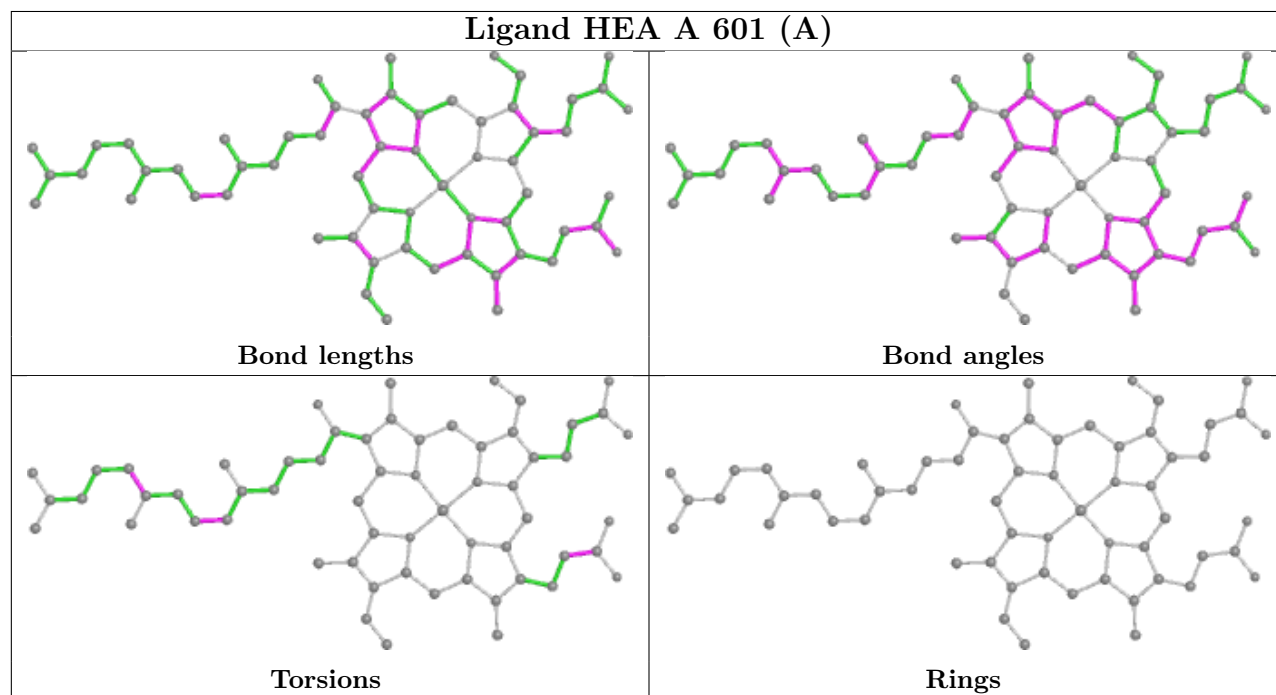
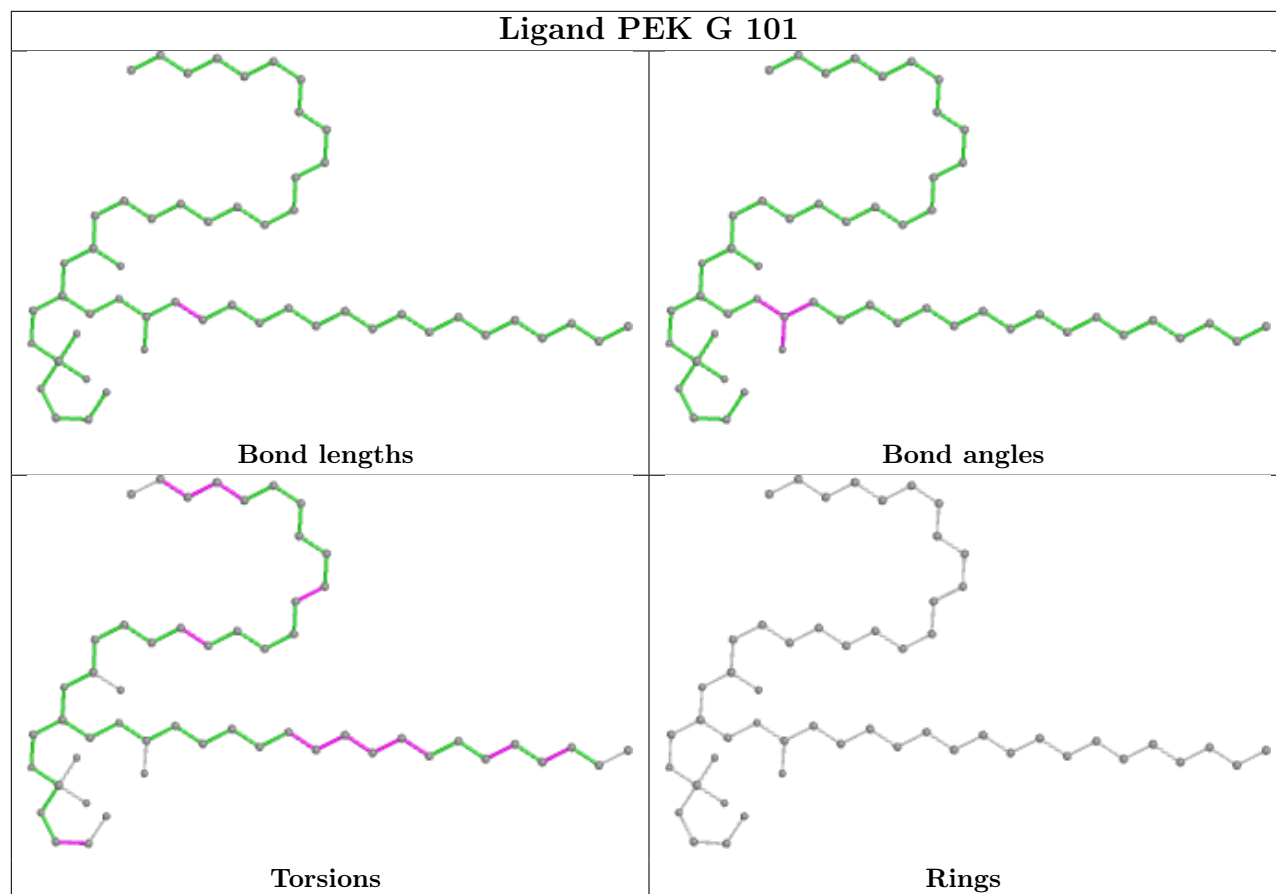


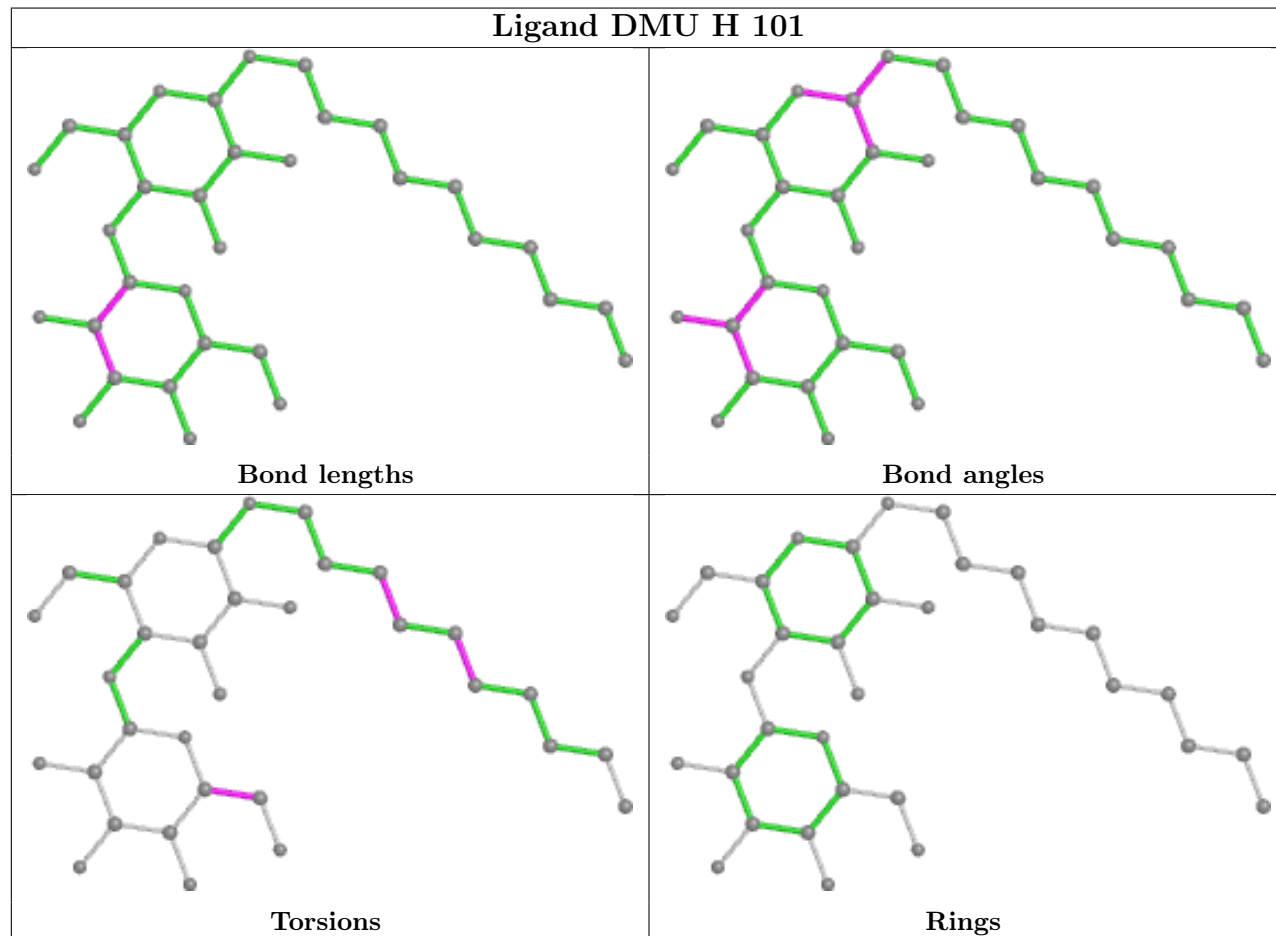
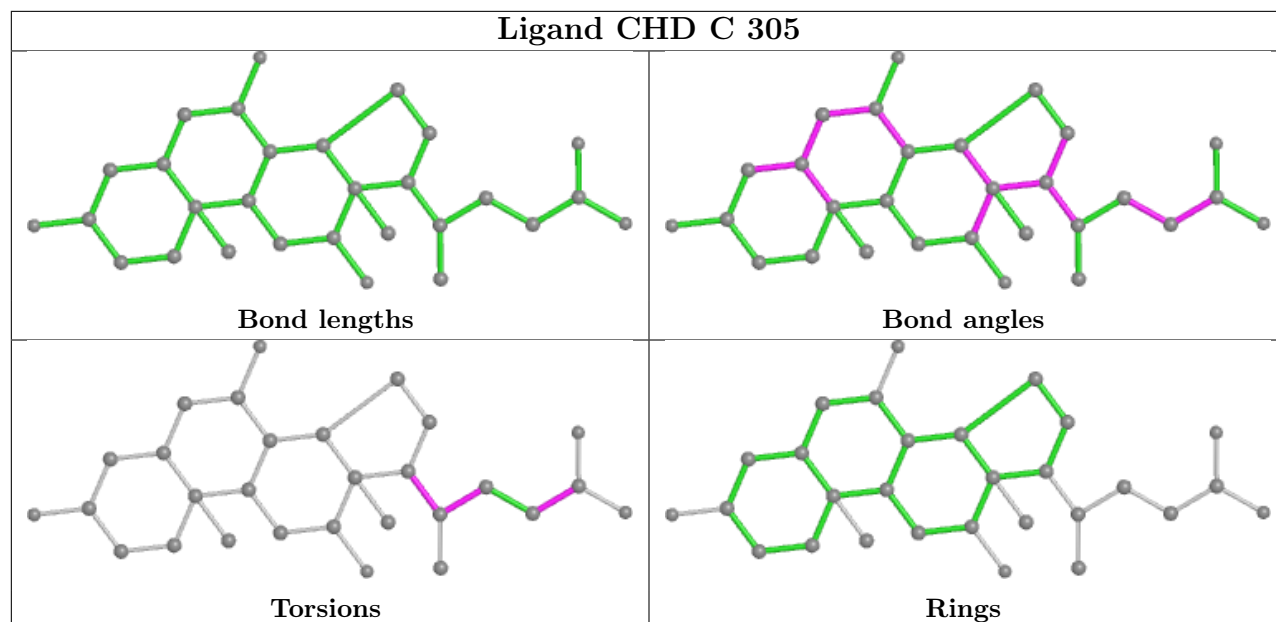


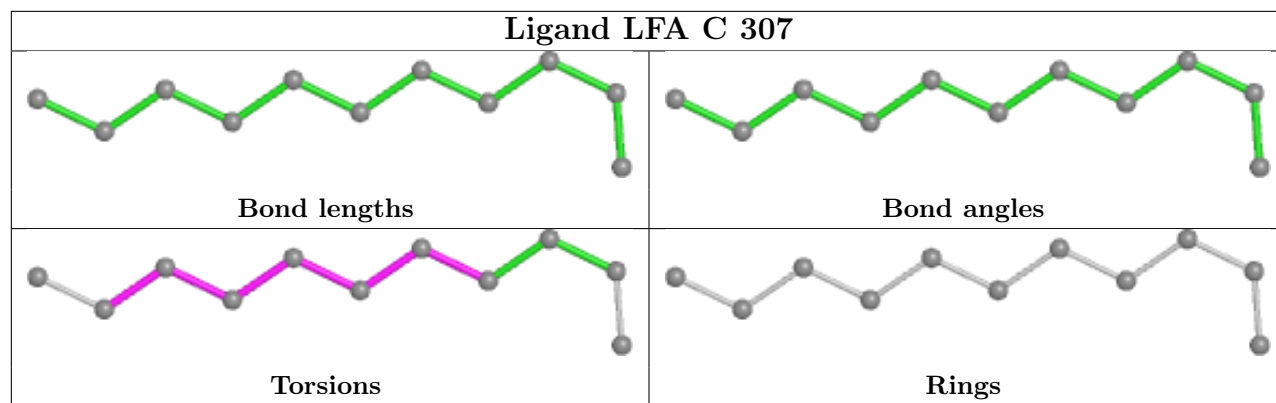












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	512/514 (99%)	-0.34	2 (0%) 89 92	15, 32, 38, 53	15 (2%)
1	N	512/514 (99%)	-0.27	4 (0%) 82 86	16, 35, 42, 54	15 (2%)
2	B	226/227 (99%)	0.11	11 (4%) 36 39	19, 38, 54, 71	5 (2%)
2	O	226/227 (99%)	0.13	6 (2%) 56 62	21, 43, 63, 77	5 (2%)
3	C	258/261 (98%)	-0.25	1 (0%) 89 92	15, 35, 44, 56	9 (3%)
3	P	258/261 (98%)	-0.24	1 (0%) 89 92	15, 36, 44, 63	9 (3%)
4	D	143/147 (97%)	-0.10	2 (1%) 73 79	18, 40, 51, 64	1 (0%)
4	Q	137/147 (93%)	0.28	2 (1%) 71 77	23, 51, 70, 79	1 (0%)
5	E	102/109 (93%)	-0.23	0 100 100	34, 40, 53, 65	0
5	R	102/109 (93%)	-0.15	2 (1%) 64 71	37, 48, 60, 71	0
6	F	91/98 (92%)	-0.10	1 (1%) 77 83	19, 40, 56, 64	2 (2%)
6	S	91/98 (92%)	-0.02	2 (2%) 62 68	19, 39, 57, 60	2 (2%)
7	G	72/85 (84%)	0.21	3 (4%) 41 47	20, 41, 72, 87	1 (1%)
7	T	72/85 (84%)	0.21	3 (4%) 41 47	22, 44, 73, 91	1 (1%)
8	H	75/85 (88%)	0.33	5 (6%) 25 28	36, 43, 73, 85	0
8	U	75/85 (88%)	0.35	5 (6%) 25 28	40, 47, 81, 100	0
9	I	70/73 (95%)	0.29	4 (5%) 30 34	36, 47, 64, 80	0
9	V	70/73 (95%)	0.38	4 (5%) 30 34	37, 54, 68, 88	0
10	J	56/59 (94%)	0.06	2 (3%) 46 53	36, 44, 60, 74	0
10	W	56/59 (94%)	0.13	2 (3%) 46 53	37, 47, 65, 74	0
11	K	49/56 (87%)	0.14	2 (4%) 42 48	39, 45, 57, 67	0
11	X	49/56 (87%)	0.63	3 (6%) 28 32	45, 53, 69, 84	0
12	L	44/47 (93%)	-0.14	1 (2%) 61 67	33, 37, 47, 59	0
12	Y	44/47 (93%)	0.06	1 (2%) 61 67	37, 42, 55, 62	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	40/46 (86%)	-0.05	1 (2%) 58 65	35, 38, 57, 64	0
13	Z	40/46 (86%)	0.32	3 (7%) 22 24	42, 47, 68, 76	0
All	All	3470/3614 (96%)	-0.06	73 (2%) 63 69	15, 38, 60, 100	66 (1%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	36	TRP	6.5
9	V	72	ALA	5.5
8	H	45	ALA	5.4
6	S	3	GLY	4.8
2	O	113	TYR	4.8
6	F	3	GLY	4.7
7	G	36	TRP	4.7
8	U	48	GLY	4.6
1	N	136[A]	LEU	4.5
2	B	67	ILE	4.5
11	X	6	ALA	4.1
2	B	59	GLN	4.0
8	H	48	GLY	3.9
1	N	113[A]	LEU	3.7
2	O	32[A]	PHE	3.5
8	U	45	ALA	3.5
6	S	93	PRO	3.5
9	V	3	ALA	3.4
9	V	37	PHE	3.4
4	D	4	SER	3.4
2	O	90	ILE	3.4
2	B	61	VAL	3.3
1	A	311[A]	ILE	3.3
8	H	46	LYS	3.3
10	J	1	PHE	3.3
7	G	30	LEU	3.2
9	I	3	ALA	3.1
1	N	311[A]	ILE	3.1
1	A	113[A]	LEU	3.0
4	Q	35	ALA	3.0
4	D	5	VAL	2.9
9	I	37	PHE	2.9
2	O	91	ASN	2.8
10	W	48	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
3	P	37	PHE	2.8
8	U	49	ASP	2.8
11	K	6	ALA	2.8
11	K	47	ARG	2.7
2	B	91	ASN	2.6
13	M	40	TYR	2.6
2	B	55	THR	2.6
7	G	41	HIS	2.5
7	T	38	HIS	2.5
2	B	58	ALA	2.5
8	U	47	GLY	2.4
8	H	47	GLY	2.4
8	H	44	THR	2.4
2	B	65	TRP	2.4
13	Z	38	ASP	2.4
3	C	38	ASN	2.4
11	X	7	PRO	2.4
4	Q	39	ALA	2.3
5	R	7	THR	2.3
10	W	1	PHE	2.3
2	B	115	ASP	2.3
12	Y	24	MET	2.3
8	U	50	VAL	2.3
10	J	48	TYR	2.3
13	Z	40	TYR	2.3
2	O	227	LEU	2.2
13	Z	39	ASN	2.2
9	I	72	ALA	2.2
2	B	60	GLU	2.2
7	T	30	LEU	2.2
5	R	108	LYS	2.1
9	I	25	PHE	2.1
2	O	22[A]	HIS	2.1
1	N	48	LEU	2.1
11	X	13	TYR	2.1
9	V	34	PHE	2.1
2	B	87[A]	MET	2.1
12	L	46	LYS	2.0
2	B	113	TYR	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	0.92	0.14	42,47,73,81	0
1	FME	N	1	10/11	0.94	0.13	43,49,72,85	0
2	FME	B	1	10/11	0.97	0.10	36,38,46,80	0
2	FME	O	1	10/11	0.98	0.08	42,44,53,68	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
21	DMU	C	317	22/33	0.68	0.31	39,55,63,76	22
22	EDO	P	322	4/4	0.71	0.35	31,34,36,39	4
21	DMU	P	317	22/33	0.73	0.30	34,52,64,65	22
20	LFA	P	311	11/20	0.73	0.43	43,51,60,66	11
22	EDO	C	322	4/4	0.74	0.35	33,36,36,40	4
21	DMU	A	610	7/33	0.74	0.40	45,48,51,56	7
21	DMU	N	610	7/33	0.78	0.44	50,55,59,60	7
20	LFA	C	308	6/20	0.79	0.41	38,42,48,48	6
20	LFA	C	313	15/20	0.81	0.27	42,46,56,59	15
20	LFA	C	314	13/20	0.81	0.31	46,50,63,65	13
20	LFA	C	311	14/20	0.81	0.36	37,54,60,61	14
25	CHD	C	305	29/29	0.81	0.17	56,67,79,96	0
21	DMU	C	315	33/33	0.82	0.33	37,50,58,60	33
20	LFA	O	303	11/20	0.82	0.32	43,52,59,60	11
22	EDO	A	613	4/4	0.82	0.33	34,40,43,48	4
25	CHD	P	306	29/29	0.82	0.17	58,68,79,91	0
21	DMU	C	318	33/33	0.83	0.30	37,53,65,77	33
22	EDO	E	201	4/4	0.83	0.37	35,38,41,43	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	LFA	C	312	11/20	0.83	0.28	39,44,55,59	11
20	LFA	C	325	15/20	0.83	0.38	44,48,57,60	15
20	LFA	P	312	11/20	0.83	0.30	34,46,55,60	11
21	DMU	C	319	33/33	0.84	0.24	40,58,67,74	33
22	EDO	R	203	4/4	0.84	0.32	37,40,48,51	4
20	LFA	O	302	17/20	0.84	0.32	40,55,69,72	17
20	LFA	G	103	14/20	0.84	0.28	36,44,57,58	14
21	DMU	C	316	7/33	0.85	0.31	41,46,56,62	7
22	EDO	N	613	4/4	0.85	0.25	36,42,42,45	4
21	DMU	P	319	33/33	0.85	0.21	47,65,78,81	33
20	LFA	A	609	14/20	0.86	0.26	37,46,53,55	14
21	DMU	M	102	8/33	0.86	0.23	40,44,47,51	8
20	LFA	P	301	15/20	0.86	0.30	40,50,56,59	15
21	DMU	O	304	22/33	0.86	0.29	48,62,73,79	22
20	LFA	P	314	13/20	0.86	0.26	40,47,60,73	13
21	DMU	P	318	33/33	0.86	0.27	44,53,62,80	33
20	LFA	P	308	11/20	0.86	0.31	42,49,55,56	11
22	EDO	A	612	4/4	0.86	0.20	29,30,31,33	4
27	CDL	P	305	87/100	0.86	0.19	44,72,100,133	0
20	LFA	T	102	14/20	0.87	0.34	41,54,64,67	14
20	LFA	T	103	11/20	0.87	0.30	48,53,62,63	11
21	DMU	P	323	22/33	0.87	0.22	42,53,58,69	22
21	DMU	Q	201	33/33	0.87	0.21	39,50,59,69	33
20	LFA	B	307	17/20	0.87	0.29	39,51,68,71	17
21	DMU	C	323	22/33	0.87	0.29	41,54,62,63	22
21	DMU	C	324	33/33	0.87	0.17	39,50,67,77	33
21	DMU	H	101	33/33	0.87	0.24	33,45,58,68	33
21	DMU	A	617	11/33	0.87	0.30	43,50,56,60	11
21	DMU	B	308	22/33	0.87	0.29	53,67,76,80	22
21	DMU	N	611	33/33	0.87	0.21	38,51,70,72	33
20	LFA	C	310	11/20	0.87	0.30	47,57,63,67	11
21	DMU	P	315	33/33	0.87	0.27	41,50,61,62	33
27	CDL	C	304	87/100	0.87	0.18	43,67,96,103	0
27	CDL	I	101	64/100	0.87	0.17	45,69,91,95	0
20	LFA	P	309	6/20	0.87	0.33	39,41,46,47	6
27	CDL	V	101	64/100	0.87	0.16	50,73,93,108	0
27	CDL	Y	101	94/100	0.87	0.17	47,72,106,134	0
20	LFA	A	608	14/20	0.88	0.24	35,42,63,67	14
20	LFA	P	313	15/20	0.88	0.20	38,44,50,51	15
20	LFA	C	309	18/20	0.88	0.21	37,43,49,50	18
20	LFA	P	310	18/20	0.88	0.25	37,49,55,59	18
20	LFA	C	307	11/20	0.88	0.26	44,44,49,49	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	DMU	P	324	33/33	0.88	0.17	41,53,78,87	33
21	DMU	O	306	11/33	0.88	0.28	41,43,51,57	11
21	DMU	U	101	33/33	0.89	0.24	33,46,60,61	33
21	DMU	N	601	11/33	0.89	0.31	43,55,62,68	11
21	DMU	B	302	11/33	0.89	0.26	42,45,53,55	11
22	EDO	C	320	4/4	0.89	0.28	43,51,54,66	4
21	DMU	A	611	33/33	0.90	0.18	32,43,53,59	33
22	EDO	R	202	4/4	0.90	0.20	34,35,39,40	4
27	CDL	L	101	94/100	0.90	0.15	41,68,94,113	0
21	DMU	Z	102	22/33	0.90	0.33	50,54,62,64	22
21	DMU	B	303	11/33	0.90	0.26	43,50,62,64	11
21	DMU	P	316	7/33	0.90	0.25	44,50,58,59	7
22	EDO	P	320	4/4	0.91	0.24	51,53,64,77	4
21	DMU	D	201	33/33	0.91	0.16	28,44,55,61	33
21	DMU	J	101	11/33	0.91	0.28	51,58,65,72	11
21	DMU	W	101	11/33	0.92	0.25	53,60,70,70	11
21	DMU	P	307	11/33	0.92	0.24	40,47,51,60	11
21	DMU	B	304	22/33	0.92	0.19	40,61,66,84	22
20	LFA	N	609	14/20	0.92	0.20	36,43,56,58	14
22	EDO	A	615	4/4	0.92	0.20	41,43,45,47	4
21	DMU	L	102	22/33	0.92	0.26	44,50,54,61	22
21	DMU	O	308	22/33	0.92	0.17	36,46,53,58	22
22	EDO	P	321	4/4	0.93	0.26	35,35,38,40	4
22	EDO	F	102	4/4	0.93	0.16	24,24,29,33	4
22	EDO	G	102	4/4	0.93	0.15	34,35,35,37	4
22	EDO	N	612	4/4	0.93	0.15	30,33,33,33	4
21	DMU	C	306	11/33	0.93	0.22	47,48,55,59	11
22	EDO	C	321	4/4	0.93	0.21	34,35,36,37	4
21	DMU	Z	103	8/33	0.94	0.18	44,46,50,51	8
22	EDO	N	614	4/4	0.94	0.19	30,30,31,32	4
22	EDO	N	616	4/4	0.94	0.19	30,31,31,36	4
22	EDO	E	202	4/4	0.94	0.24	33,34,34,37	4
22	EDO	E	203	4/4	0.94	0.25	33,36,38,41	4
21	DMU	Z	101	33/33	0.94	0.09	51,55,66,72	0
21	DMU	O	307	11/33	0.94	0.21	40,45,53,58	11
22	EDO	A	614	4/4	0.94	0.19	27,28,28,28	4
25	CHD	C	301	29/29	0.95	0.08	33,37,39,43	0
26	UNX	P	303	1/1	0.95	0.35	41,41,41,41	0
25	CHD	P	302	29/29	0.96	0.07	33,38,41,44	0
21	DMU	M	101	33/33	0.96	0.07	43,48,61,67	0
26	UNX	C	302	1/1	0.96	0.22	39,39,39,39	0
22	EDO	R	201	4/4	0.96	0.22	51,52,55,58	4

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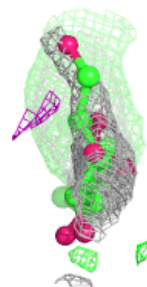
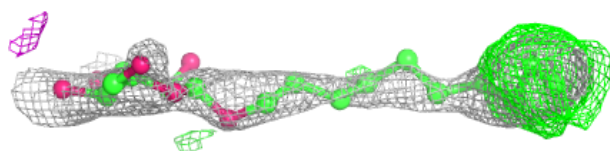
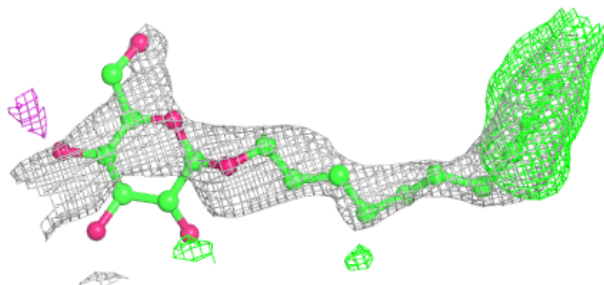
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	EDO	O	309	4/4	0.96	0.12	34,35,35,39	4
29	PEK	G	101	53/53	0.96	0.11	34,49,75,96	0
29	PEK	T	101	53/53	0.96	0.11	37,51,82,93	0
19	N2O	N	608	3/3	0.97	0.19	39,39,42,45	0
25	CHD	O	301	29/29	0.97	0.06	32,36,39,44	0
22	EDO	F	103	4/4	0.97	0.10	30,31,33,36	4
22	EDO	T	104	4/4	0.97	0.08	36,37,39,40	4
23	PGV	N	617	51/51	0.97	0.09	32,43,63,68	0
25	CHD	B	306	29/29	0.97	0.07	33,36,40,47	0
22	EDO	N	615	4/4	0.97	0.15	33,35,36,37	4
18	PER	N	607	2/2	0.98	0.09	32,32,32,35	0
23	PGV	P	304	51/51	0.98	0.08	31,40,76,88	0
22	EDO	S	102	4/4	0.98	0.06	25,26,26,30	4
22	EDO	B	305	4/4	0.98	0.09	27,28,29,31	4
23	PGV	A	616	51/51	0.98	0.08	30,39,66,71	0
23	PGV	C	303	51/51	0.98	0.08	31,40,75,82	0
14	HEA	A	601[A]	60/60	0.99	0.05	26,29,40,43	9
19	N2O	A	607	3/3	0.99	0.15	33,33,35,44	0
14	HEA	A	601[B]	60/60	0.99	0.05	26,29,41,43	9
14	HEA	A	602	60/60	0.99	0.05	27,30,36,40	0
14	HEA	N	602[A]	60/60	0.99	0.05	29,33,42,47	9
14	HEA	N	602[B]	60/60	0.99	0.05	29,33,41,44	9
14	HEA	N	603	60/60	0.99	0.06	29,32,38,43	0
17	NA	A	605	1/1	0.99	0.05	33,33,33,33	0
22	EDO	S	103	4/4	0.99	0.07	28,32,35,36	4
18	PER	A	606	2/2	0.99	0.05	28,28,28,34	0
16	MG	N	605	1/1	1.00	0.02	33,33,33,33	0
15	CU	A	603	1/1	1.00	0.01	29,29,29,29	0
17	NA	N	606	1/1	1.00	0.04	40,40,40,40	0
24	CUA	B	301	2/2	1.00	0.02	31,31,31,31	0
24	CUA	O	305	2/2	1.00	0.02	36,36,36,36	0
28	ZN	F	101	1/1	1.00	0.01	35,35,35,35	0
28	ZN	S	101	1/1	1.00	0.01	36,36,36,36	0
15	CU	N	604	1/1	1.00	0.01	31,31,31,31	0
16	MG	A	604	1/1	1.00	0.03	30,30,30,30	0

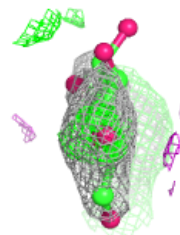
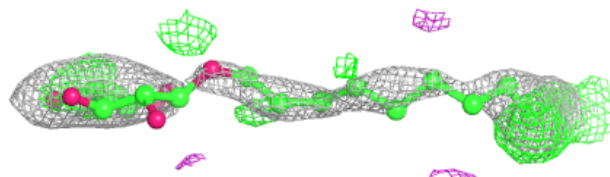
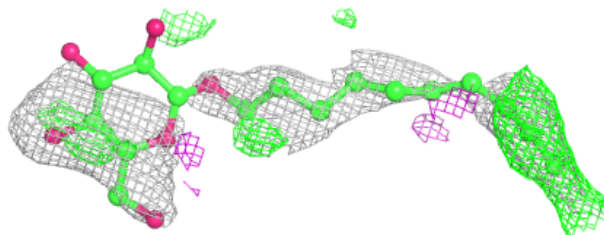
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU C 317:

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

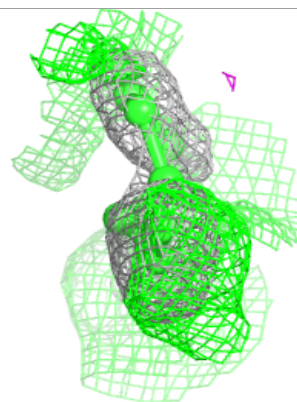
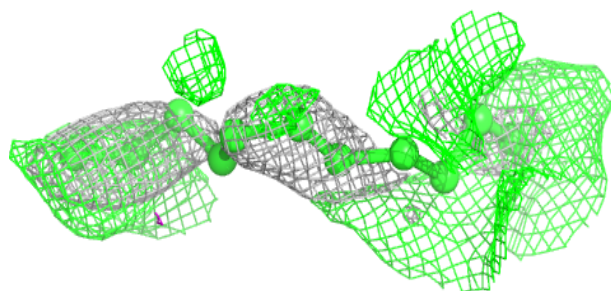
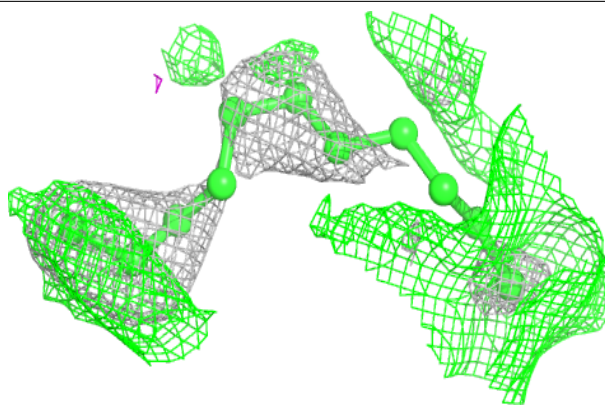
**Electron density around DMU P 317:**

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

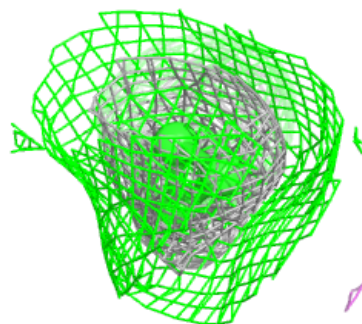
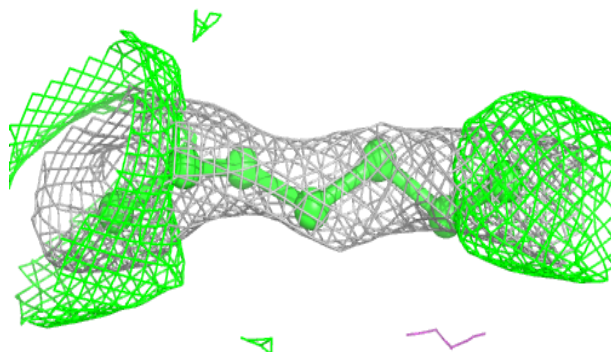
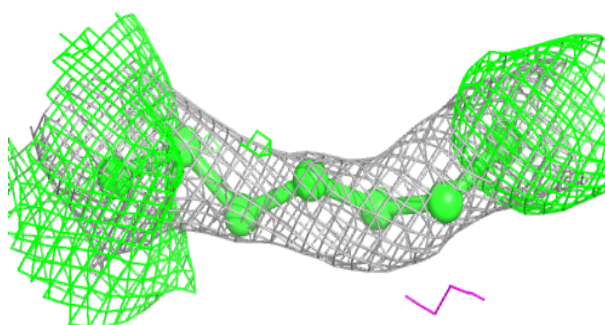


Electron density around LFA P 311:

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

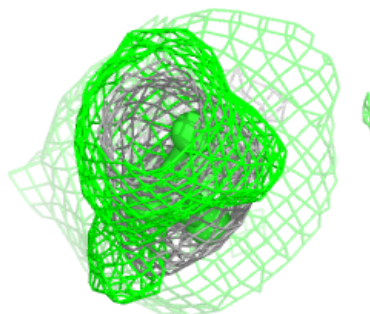
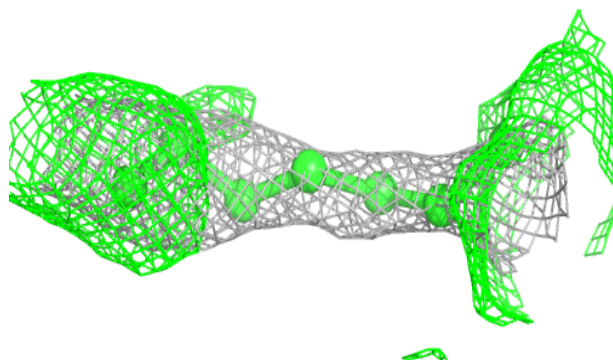
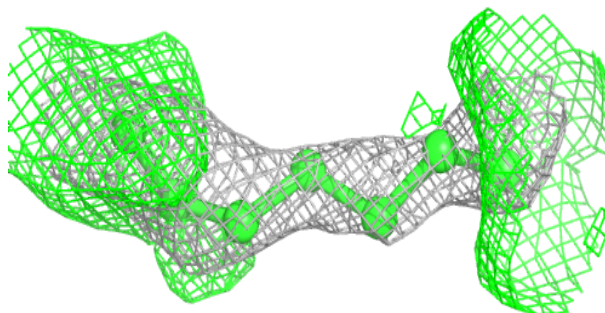
**Electron density around DMU A 610:**

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

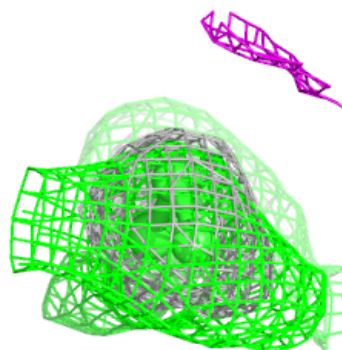
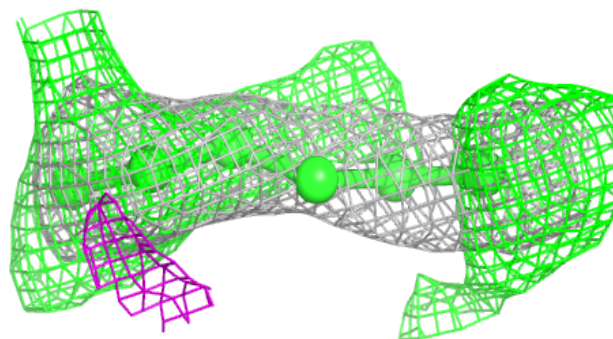
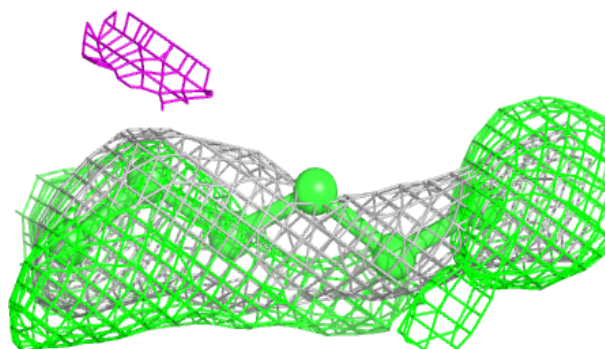


Electron density around DMU N 610:

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

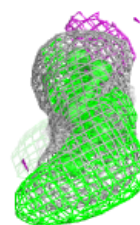
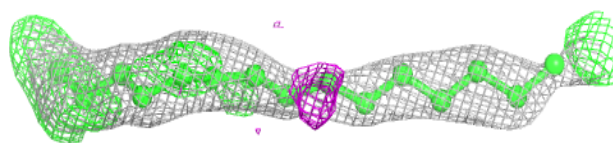
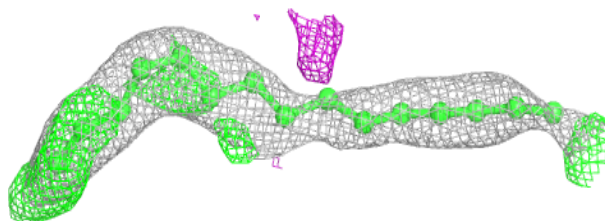
**Electron density around LFA C 308:**

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

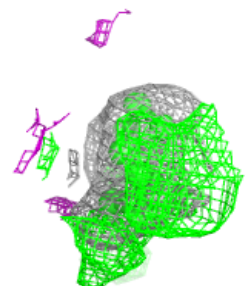
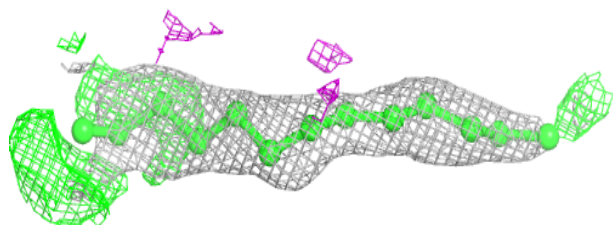
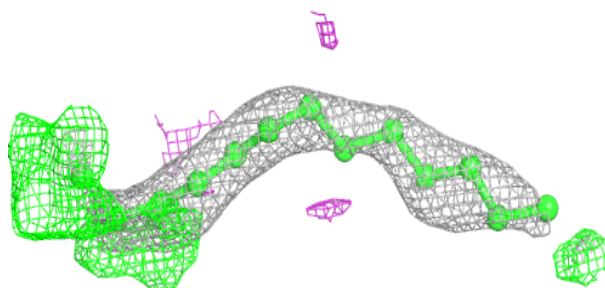


Electron density around LFA C 313:

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

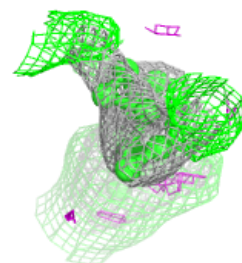
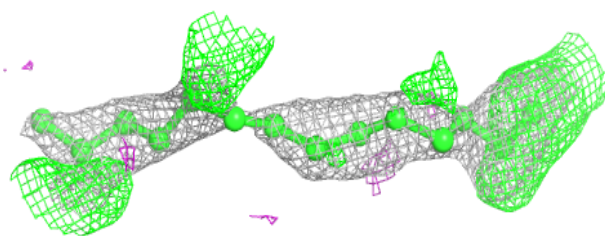
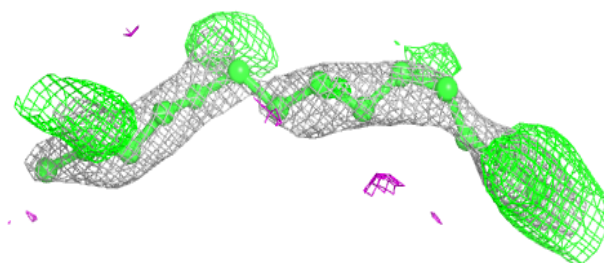
**Electron density around LFA C 314:**

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

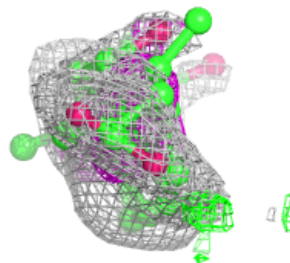
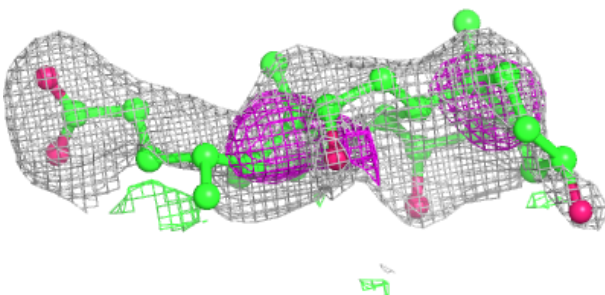
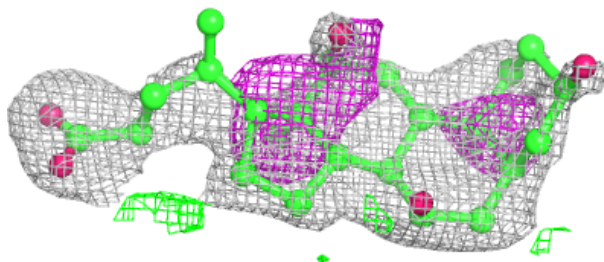


Electron density around LFA C 311:

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

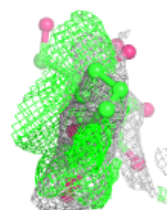
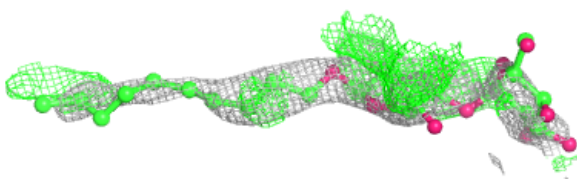
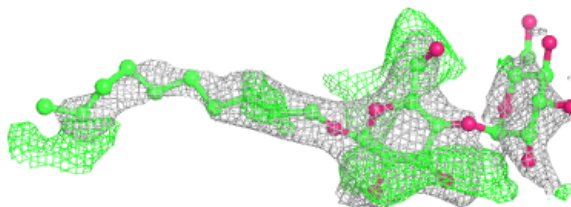
**Electron density around CHD C 305:**

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

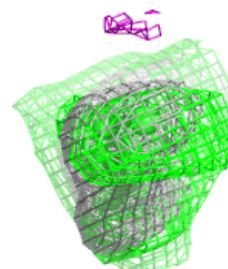
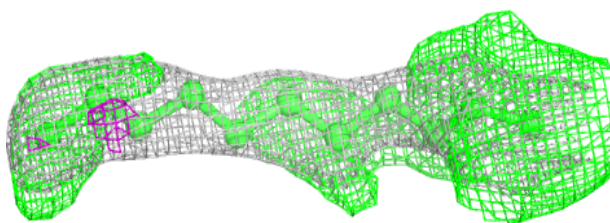
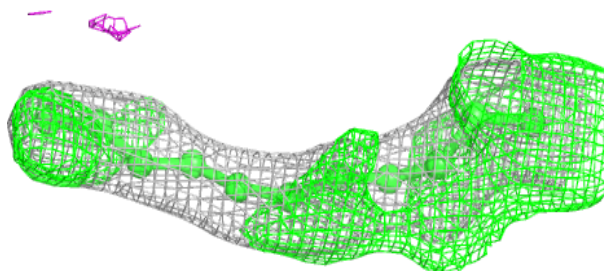


Electron density around DMU C 315:

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

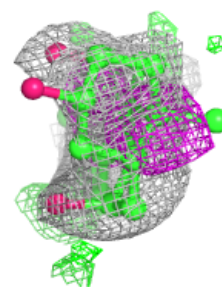
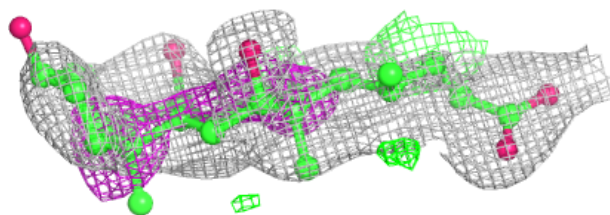
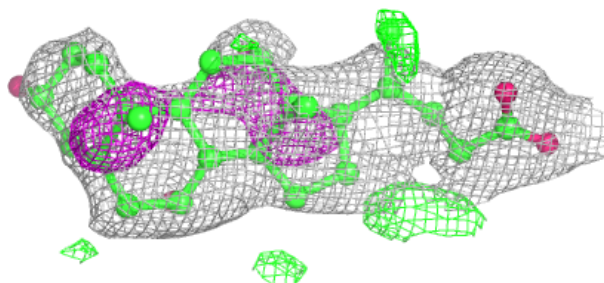
**Electron density around LFA O 303:**

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

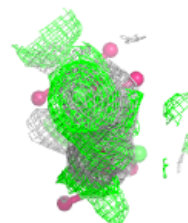
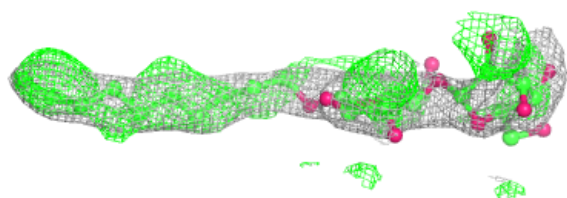
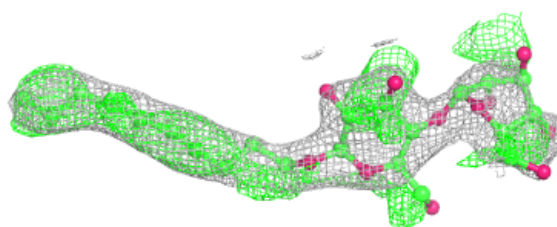


Electron density around CHD P 306:

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

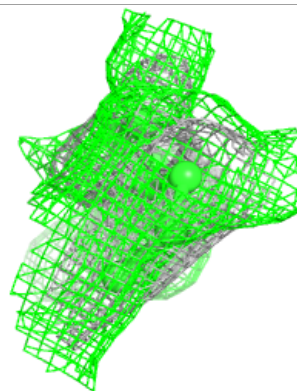
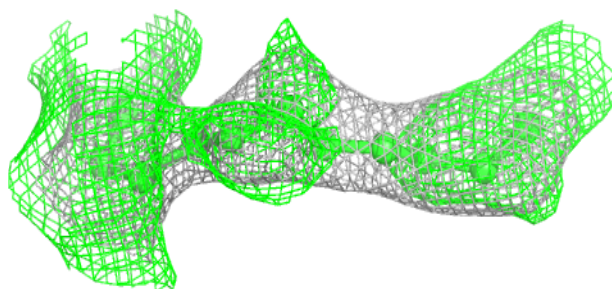
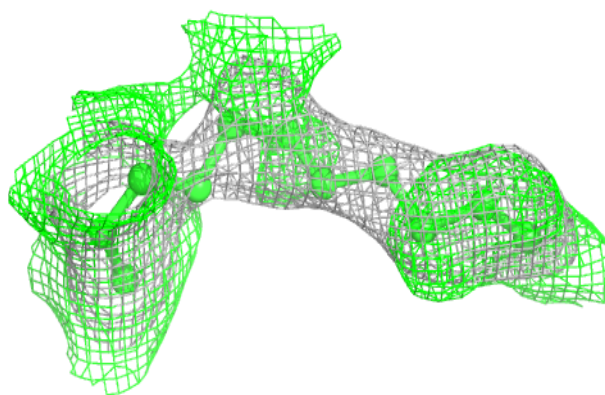
**Electron density around DMU C 318:**

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

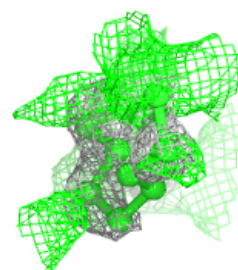
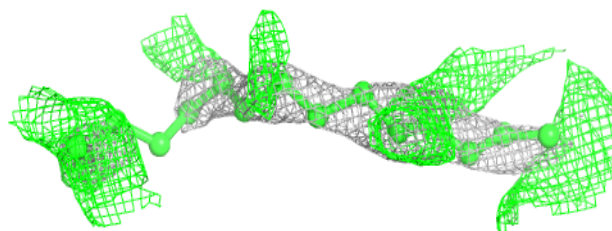
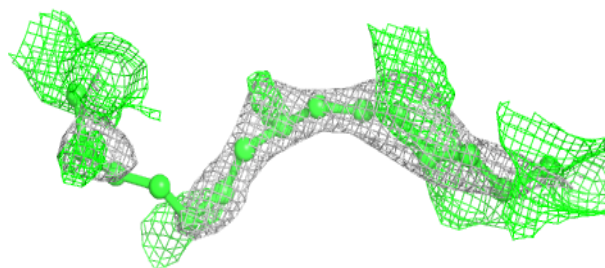


Electron density around LFA C 312:

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

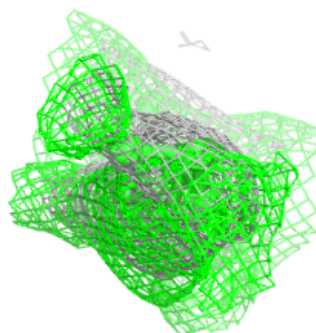
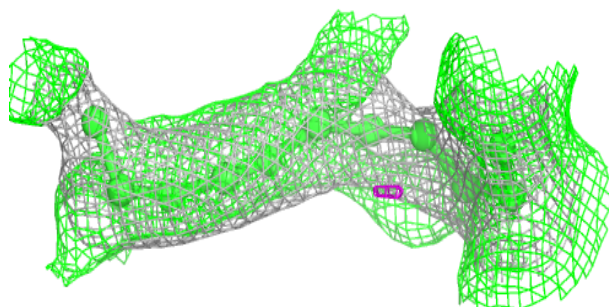
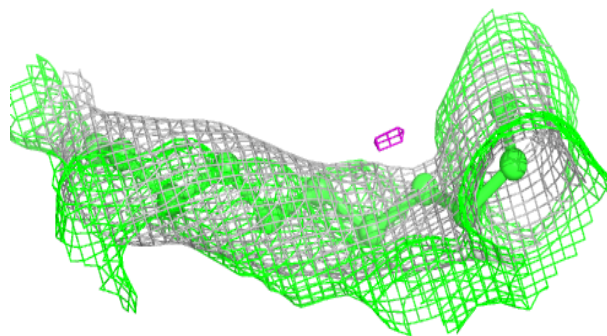
**Electron density around LFA C 325:**

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

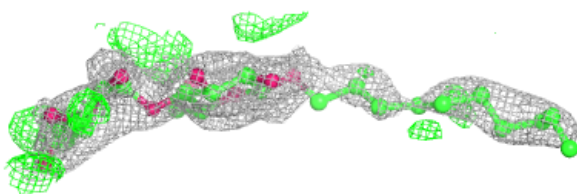
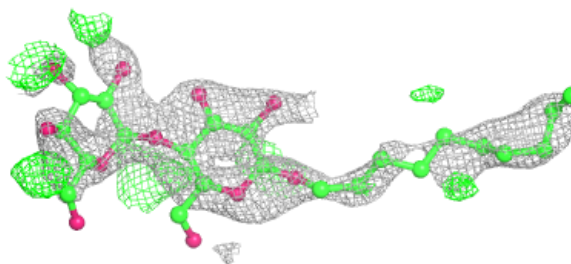


Electron density around LFA P 312:

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

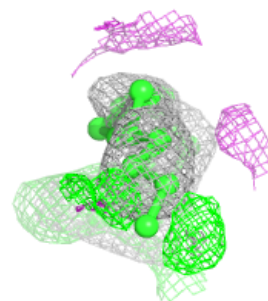
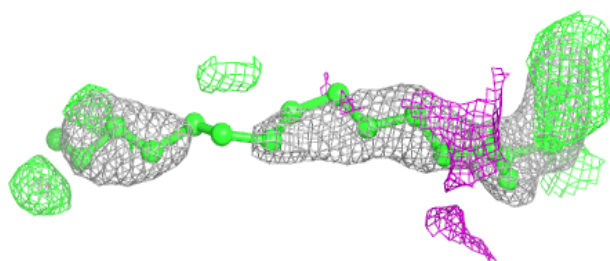
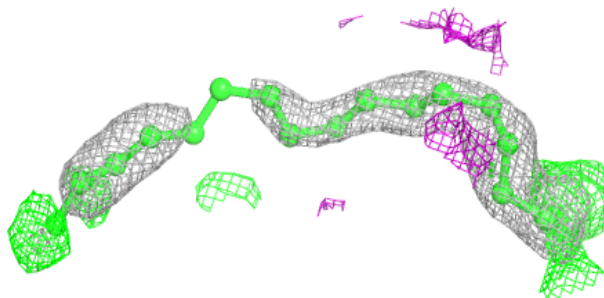
**Electron density around DMU C 319:**

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

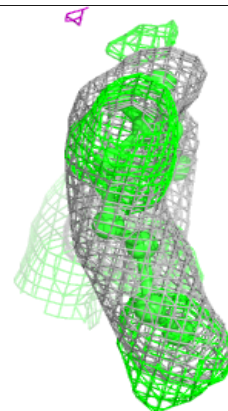
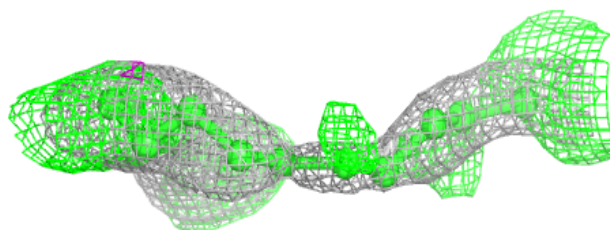
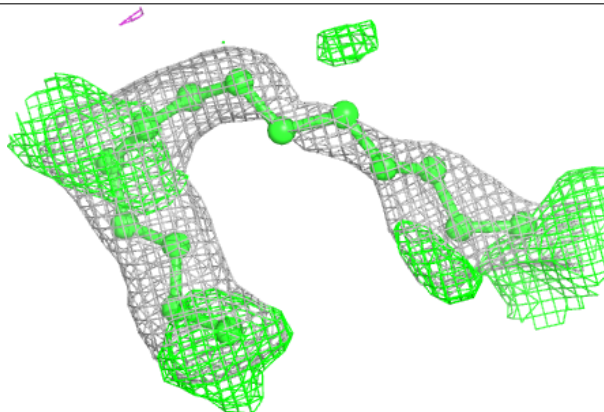


Electron density around LFA O 302:

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

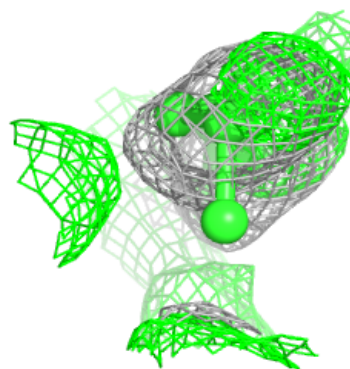
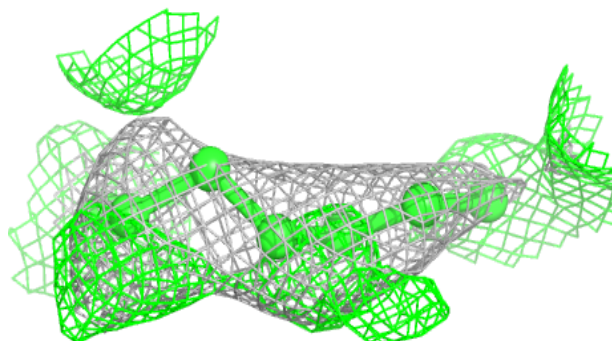
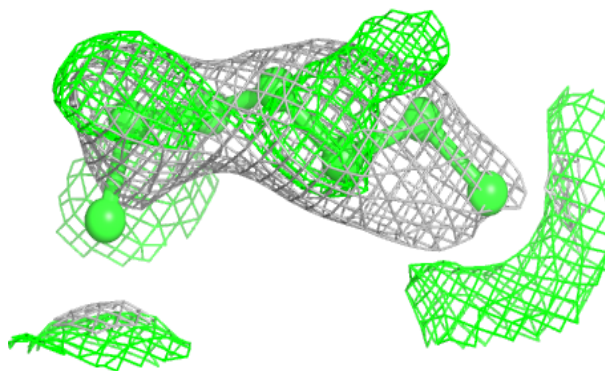
**Electron density around LFA G 103:**

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

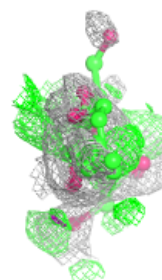
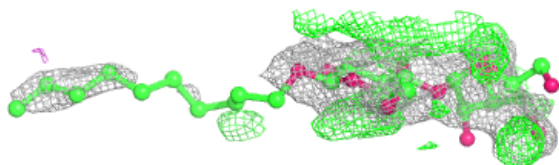
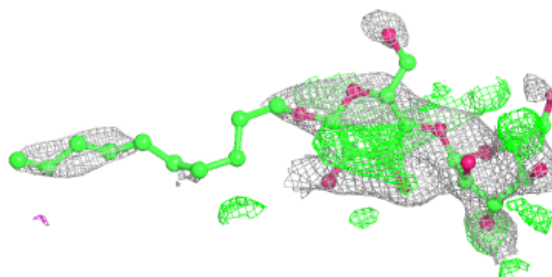


Electron density around DMU C 316:

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

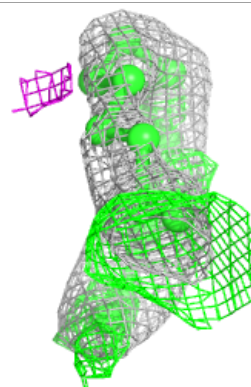
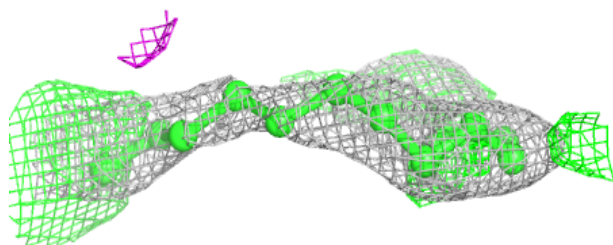
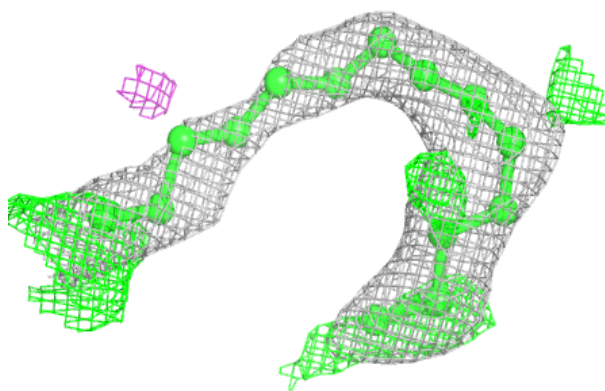
**Electron density around DMU P 319:**

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

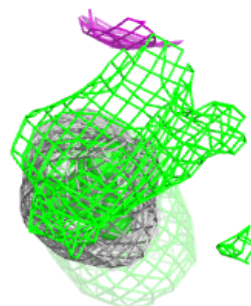
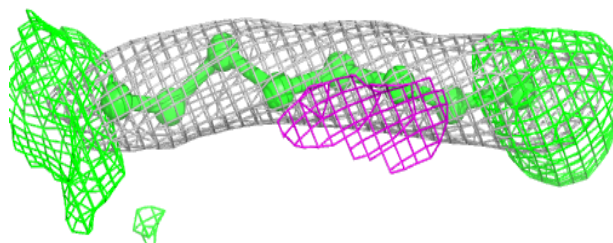
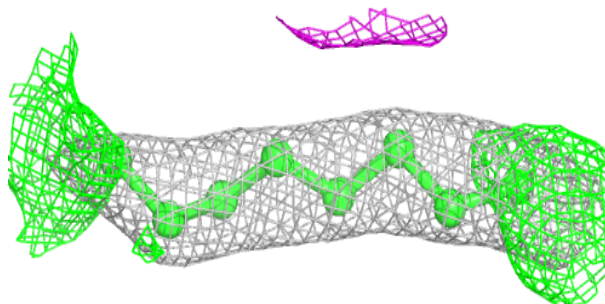


Electron density around LFA A 609:

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

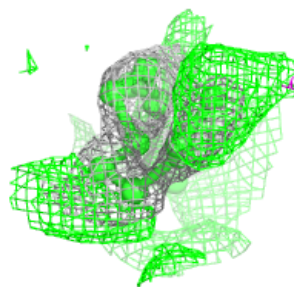
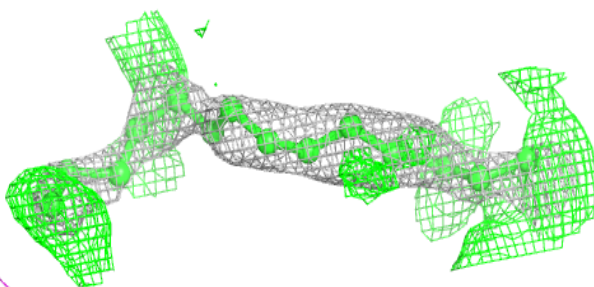
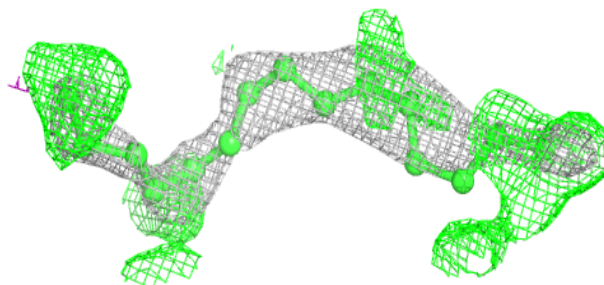
**Electron density around DMU M 102:**

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

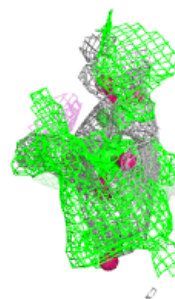
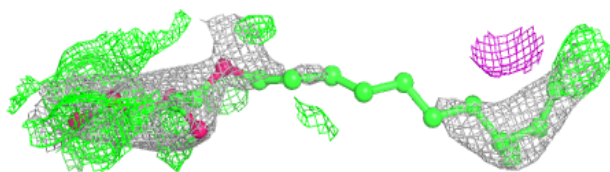
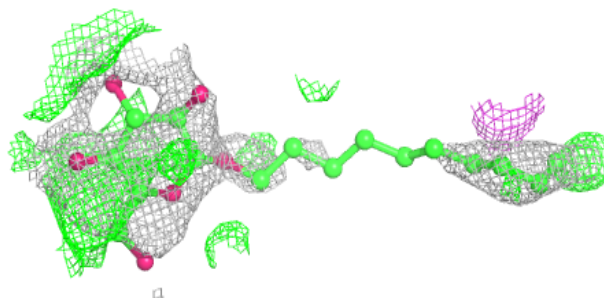


Electron density around LFA P 301:

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

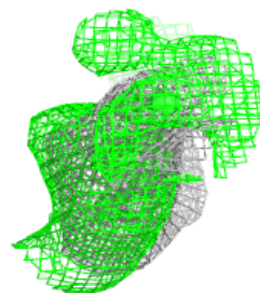
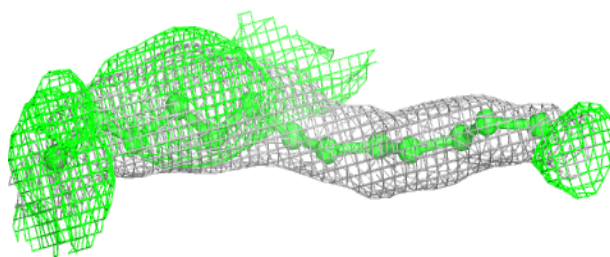
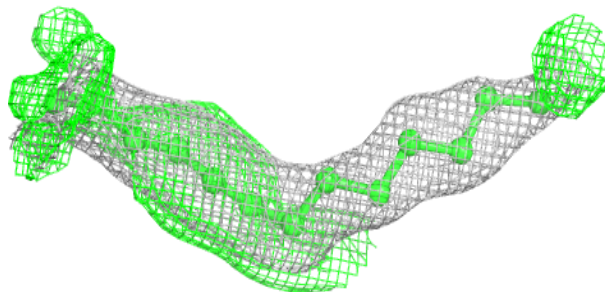
**Electron density around DMU O 304:**

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

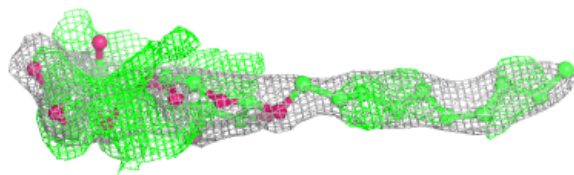
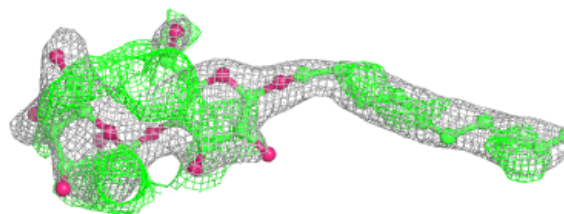


Electron density around LFA P 314:

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

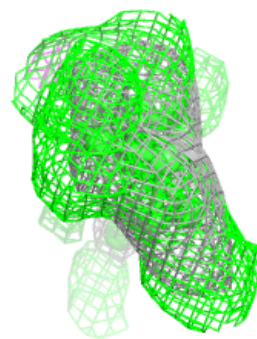
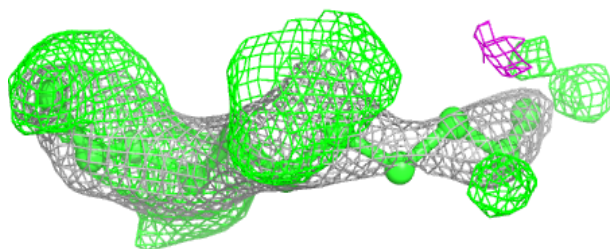
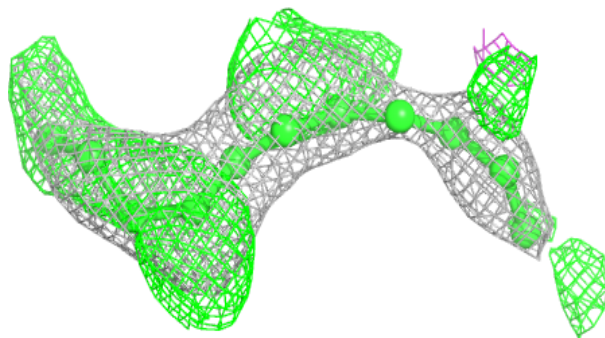
**Electron density around DMU P 318:**

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

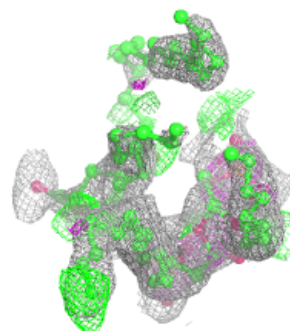
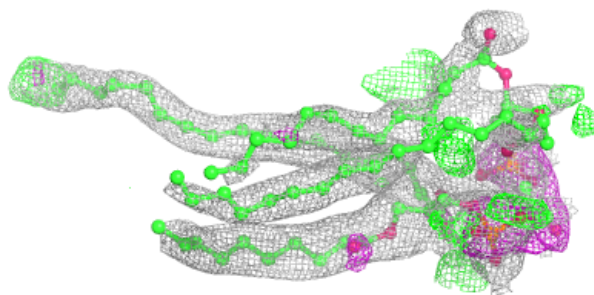
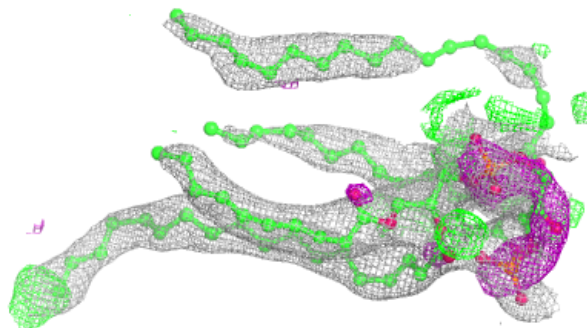


Electron density around LFA P 308:

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

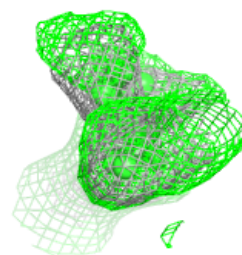
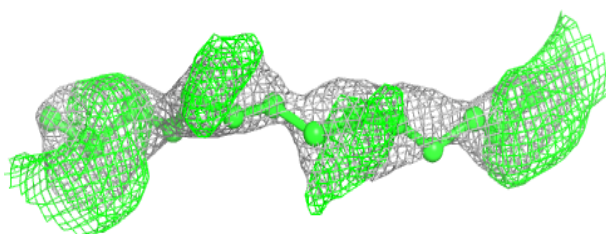
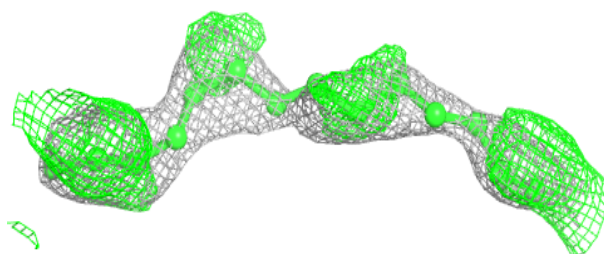
**Electron density around CDL P 305:**

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

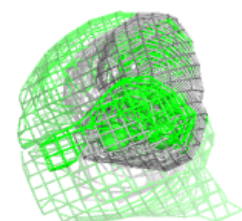
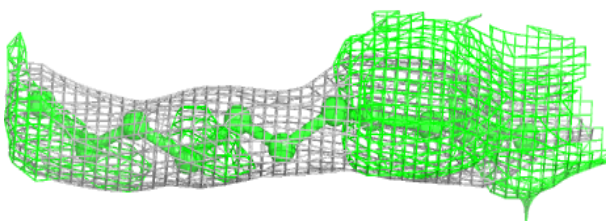
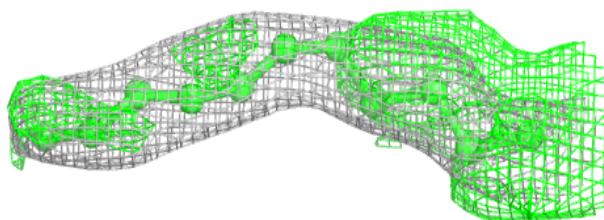


Electron density around LFA T 102:

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

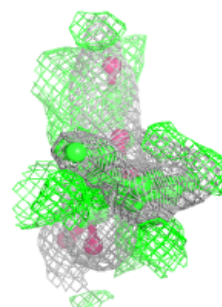
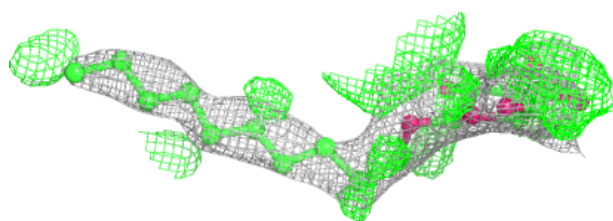
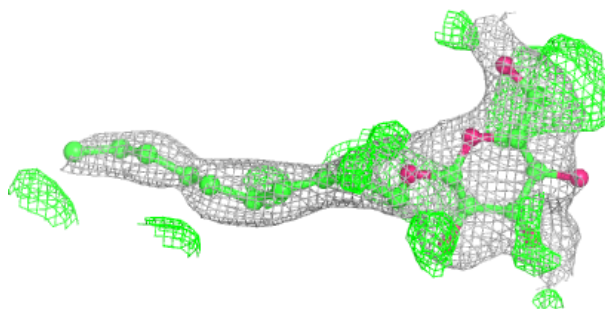
**Electron density around LFA T 103:**

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

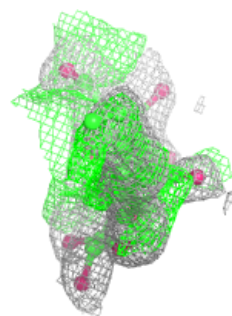
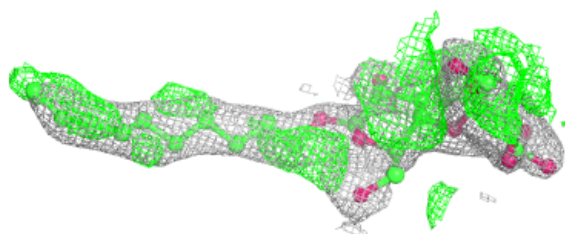
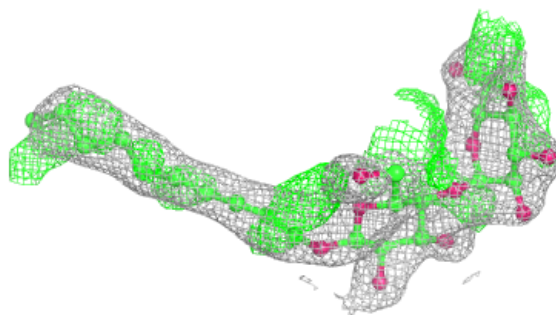


Electron density around DMU P 323:

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

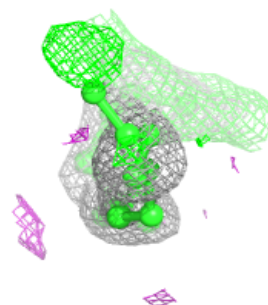
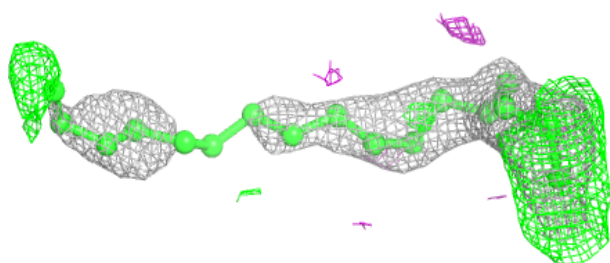
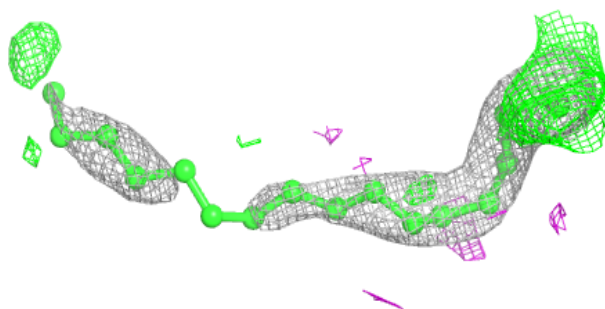
**Electron density around DMU Q 201:**

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

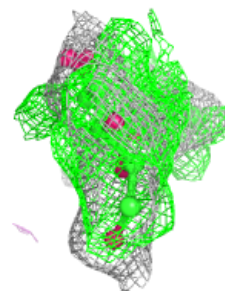
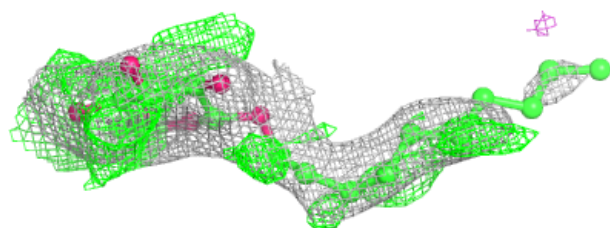
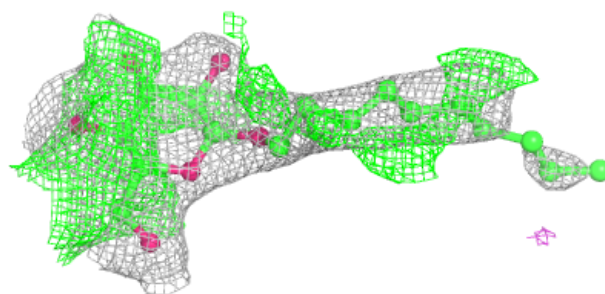


Electron density around LFA B 307:

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

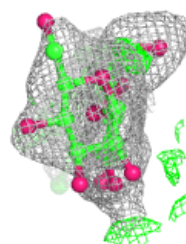
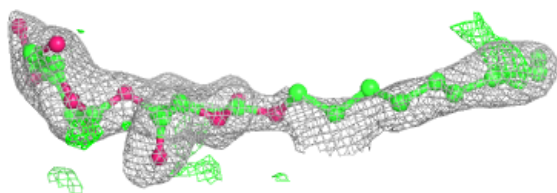
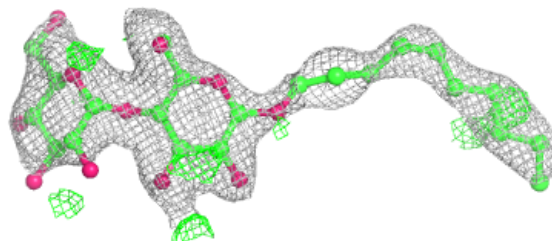
**Electron density around DMU C 323:**

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

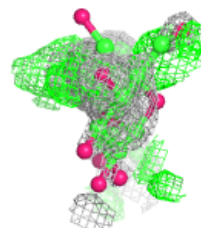
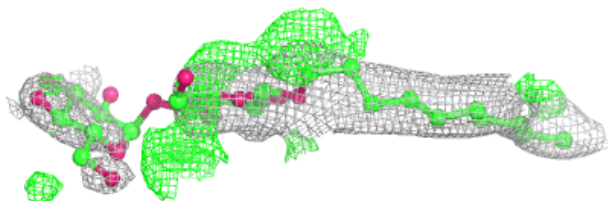
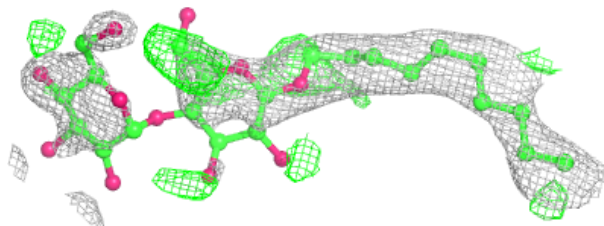


Electron density around DMU C 324:

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

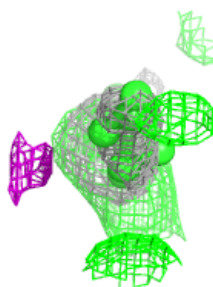
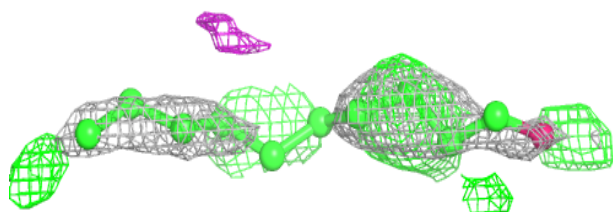
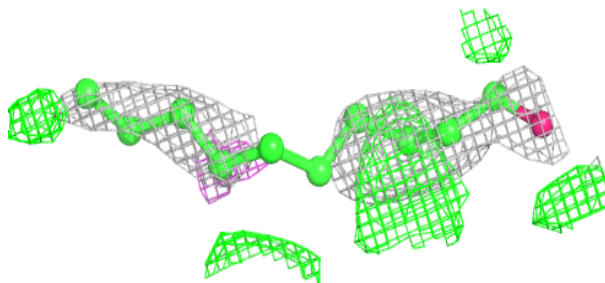
**Electron density around DMU H 101:**

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

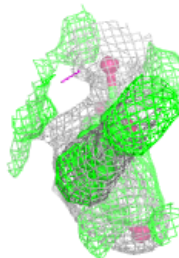
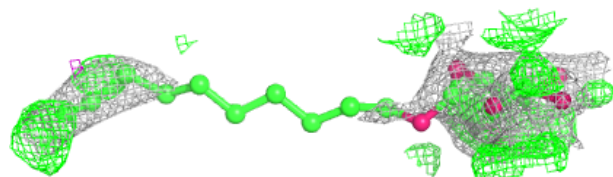
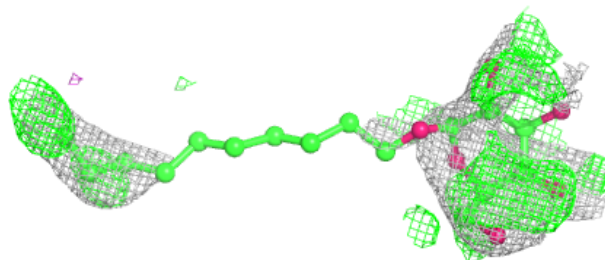


Electron density around DMU A 617:

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

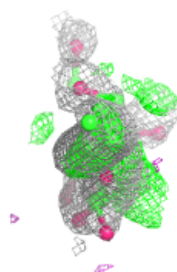
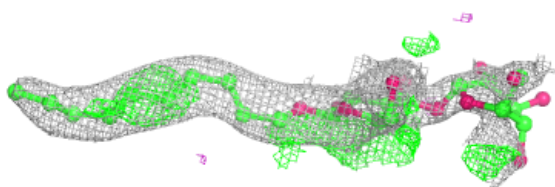
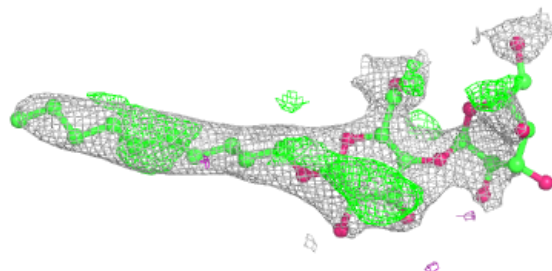
**Electron density around DMU B 308:**

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

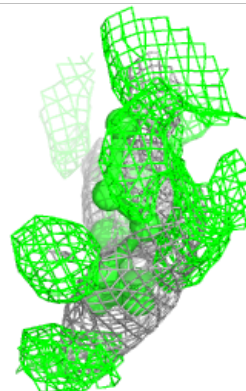
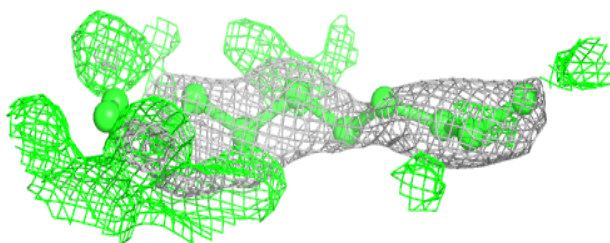
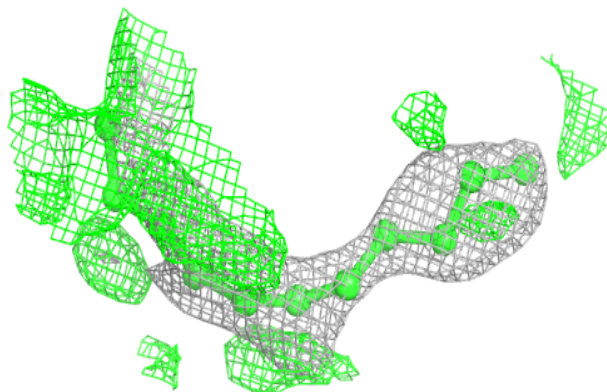


Electron density around DMU N 611:

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

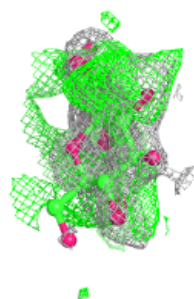
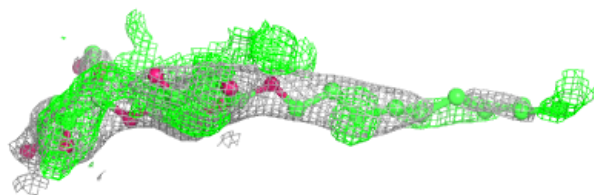
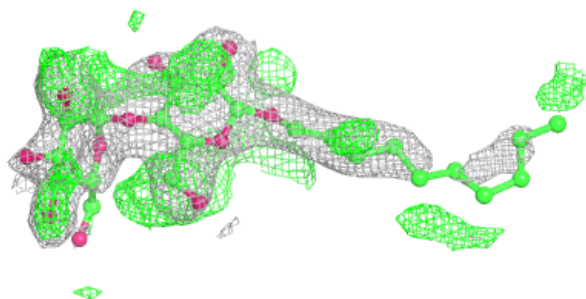
**Electron density around LFA C 310:**

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

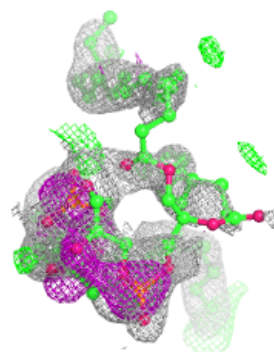
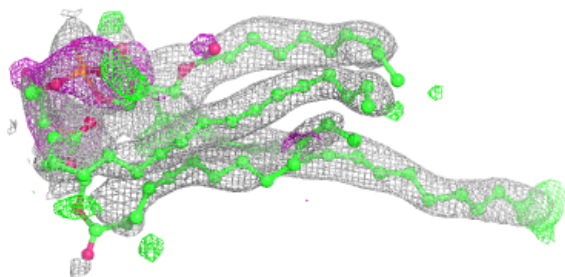
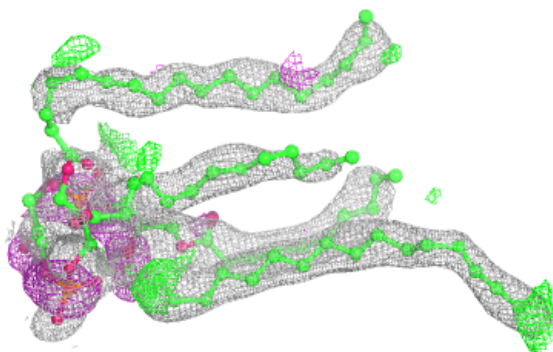


Electron density around DMU P 315:

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

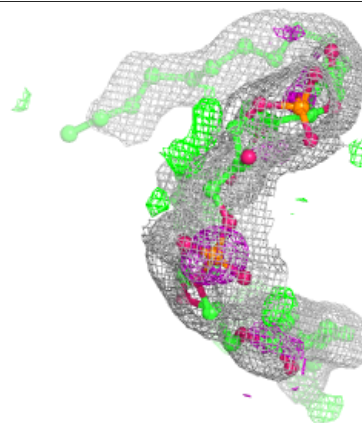
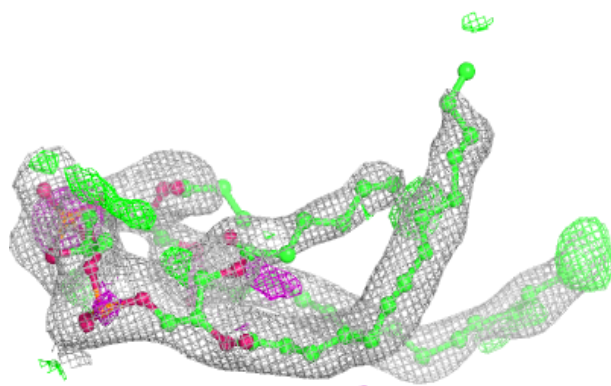
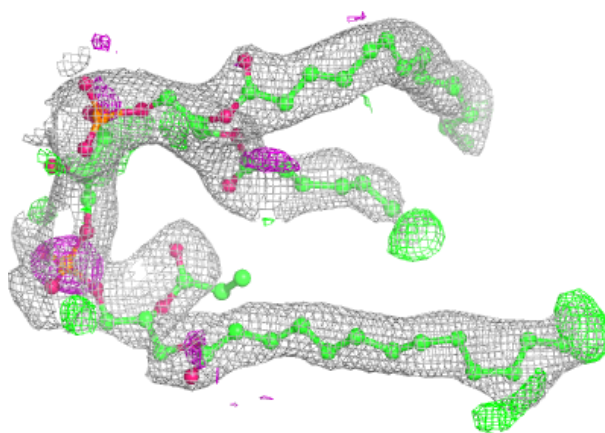
**Electron density around CDL C 304:**

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

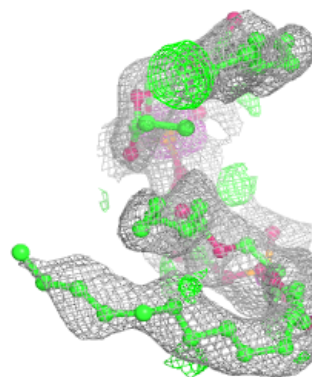
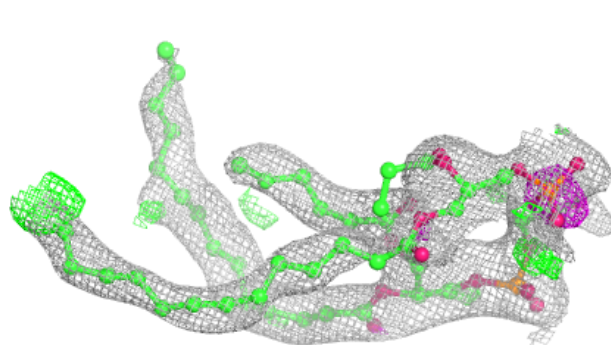
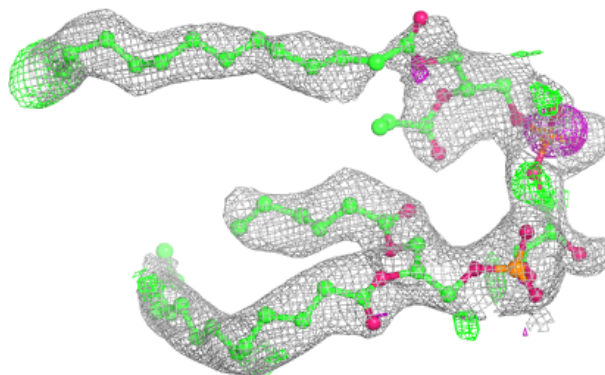


Electron density around CDL I 101:

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

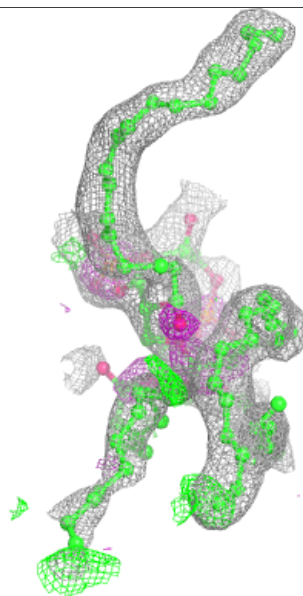
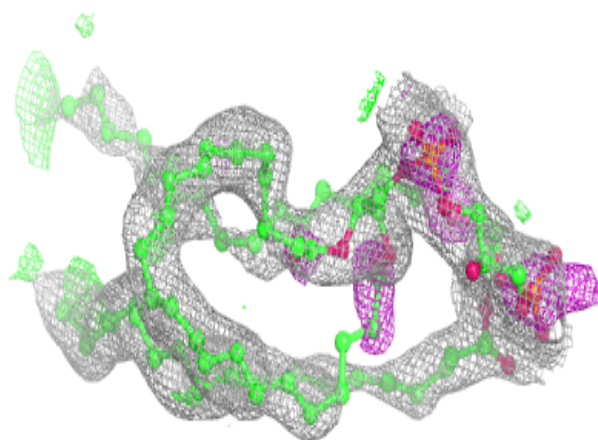
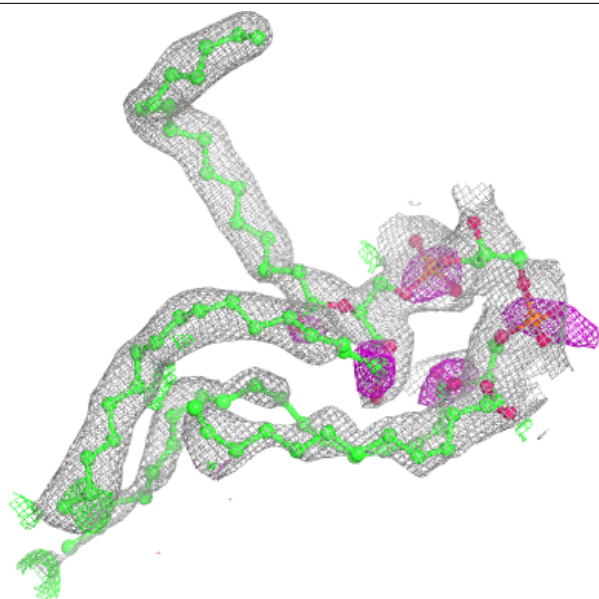
**Electron density around CDL V 101:**

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



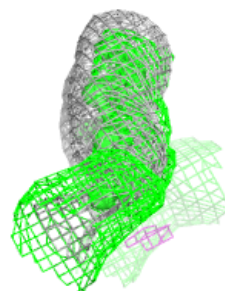
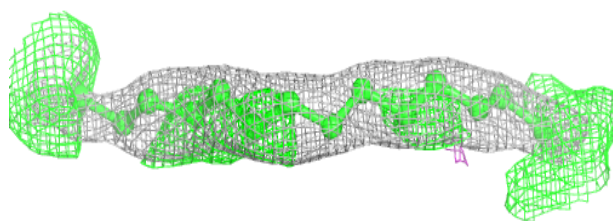
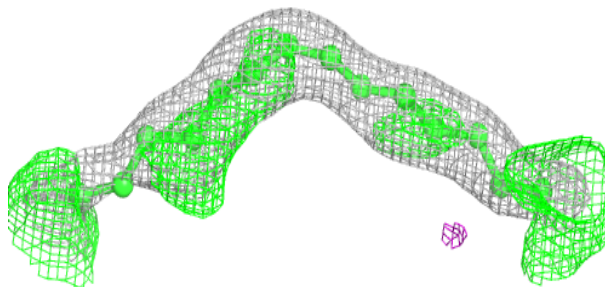
Electron density around CDL Y 101:

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

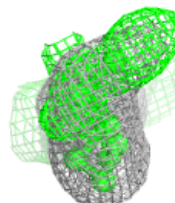
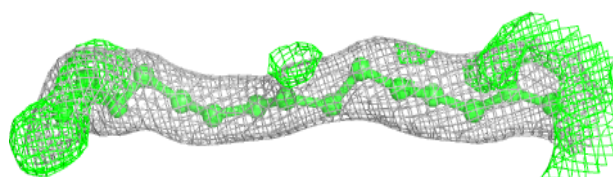
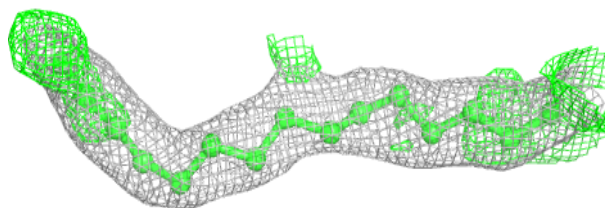


Electron density around LFA A 608:

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

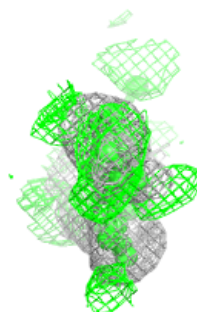
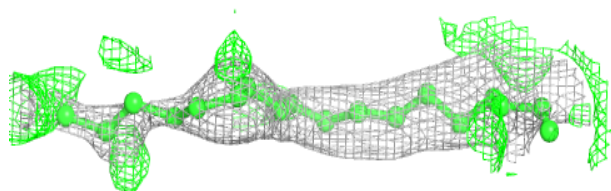
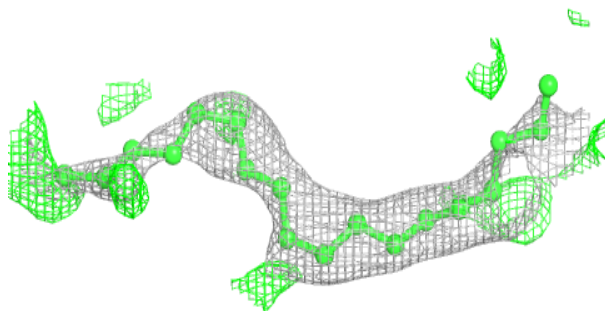
**Electron density around LFA P 313:**

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

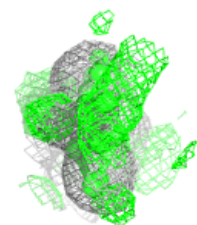
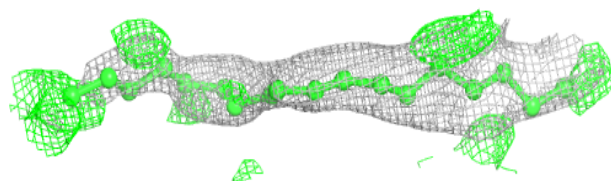
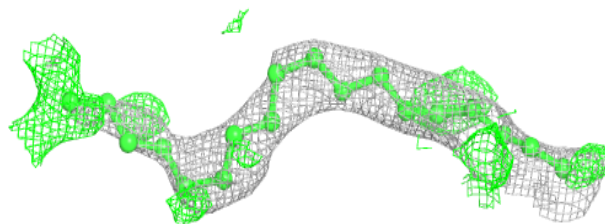


Electron density around LFA C 309:

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

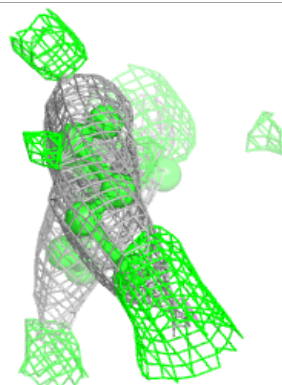
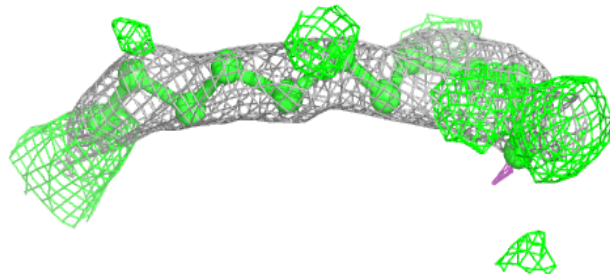
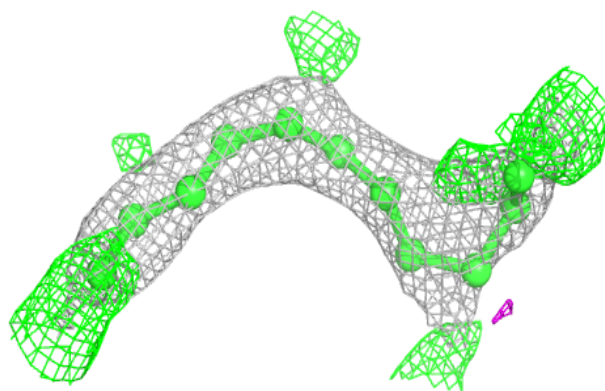
**Electron density around LFA P 310:**

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

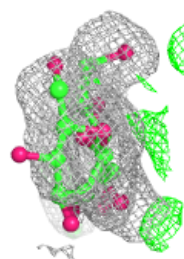
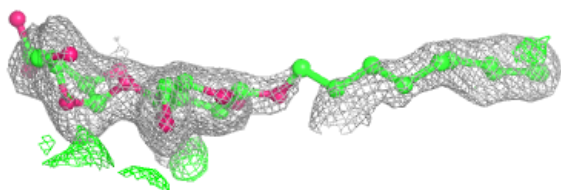
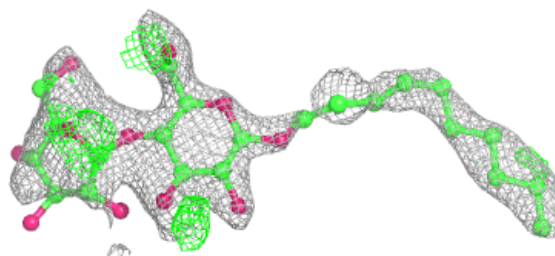


Electron density around LFA C 307:

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

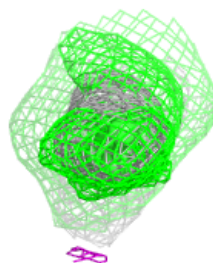
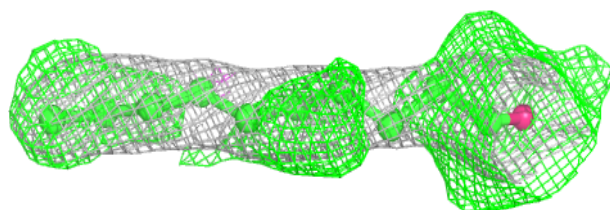
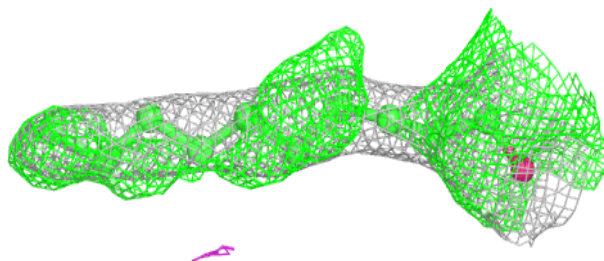
**Electron density around DMU P 324:**

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

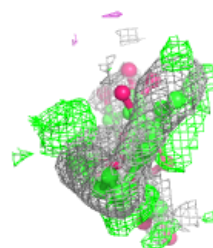
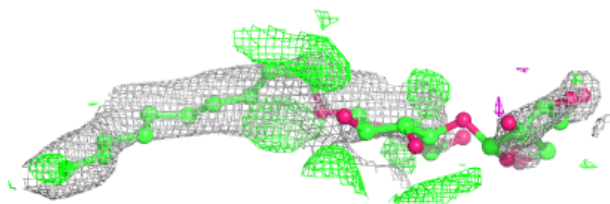
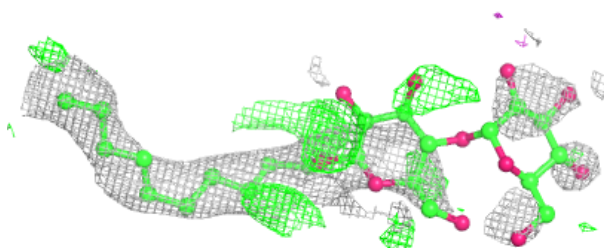


Electron density around DMU O 306:

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

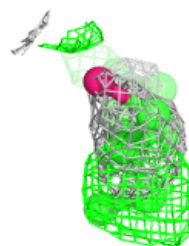
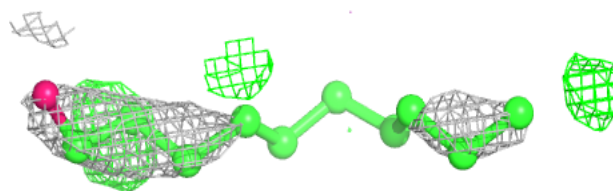
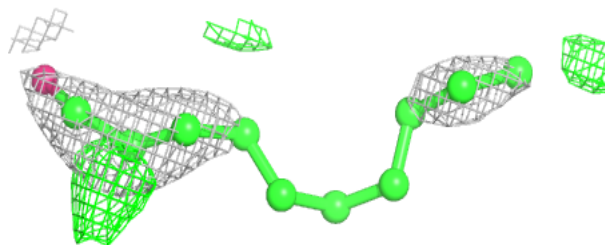
**Electron density around DMU U 101:**

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

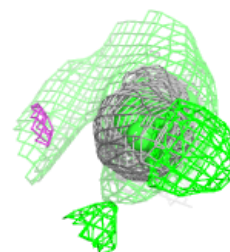
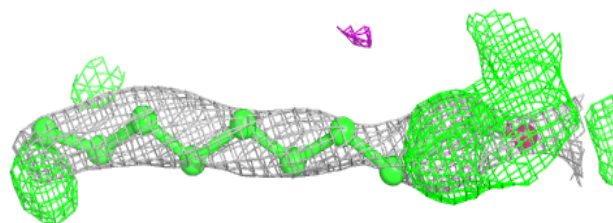
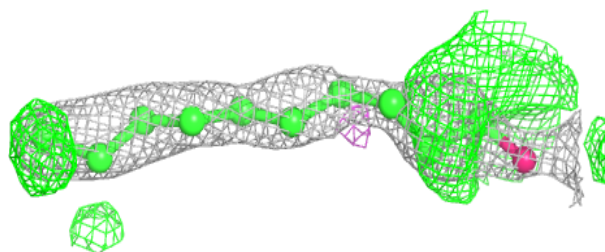


Electron density around DMU N 601:

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

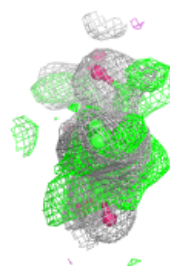
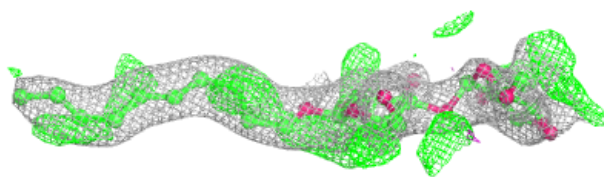
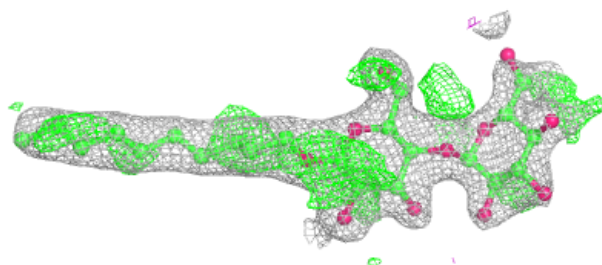
**Electron density around DMU B 302:**

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



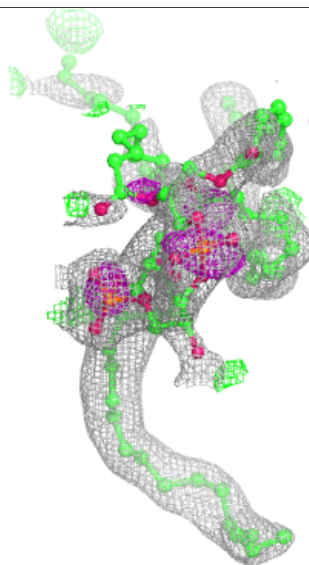
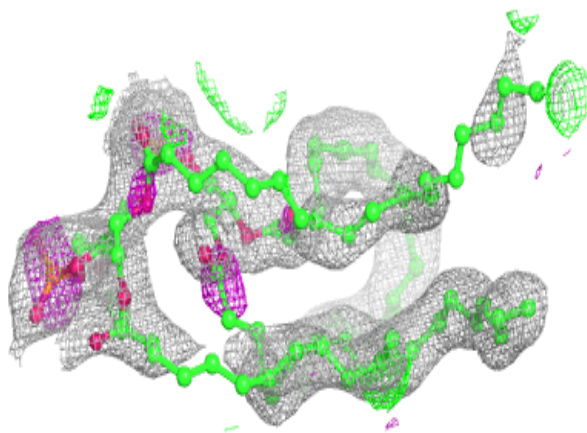
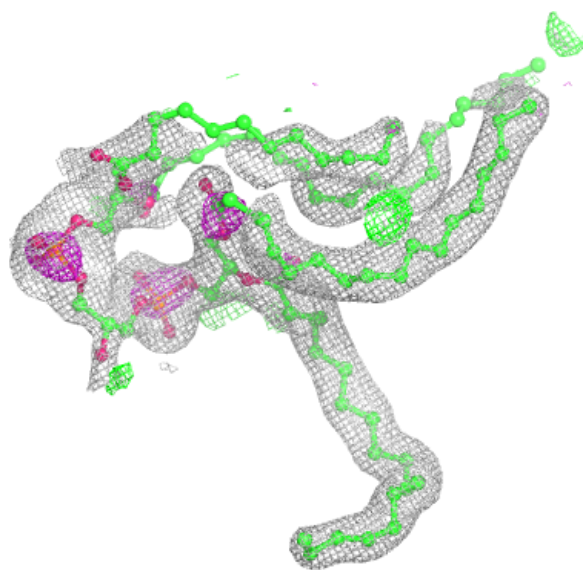
Electron density around DMU A 611:

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



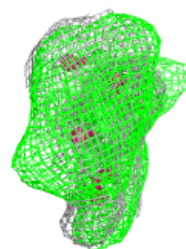
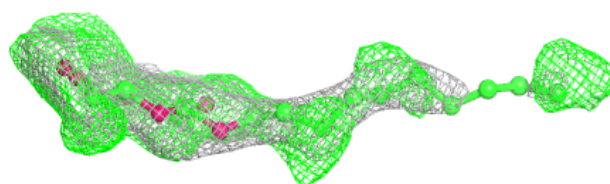
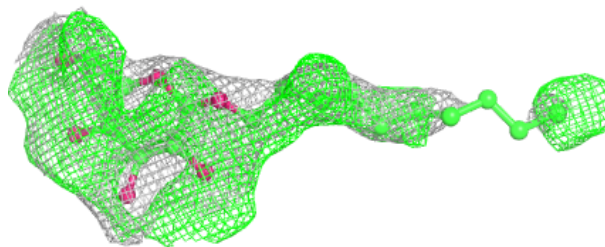
Electron density around CDL L 101:

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

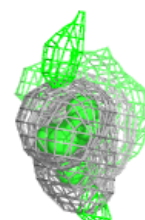
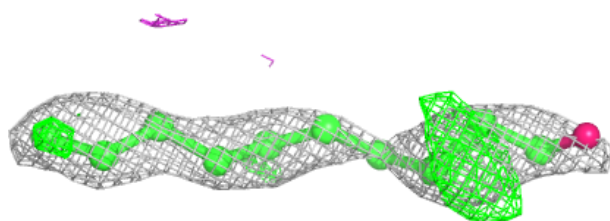
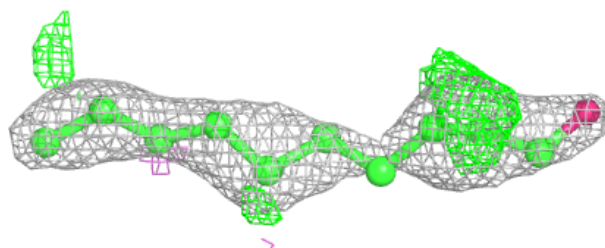


Electron density around DMU Z 102:

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

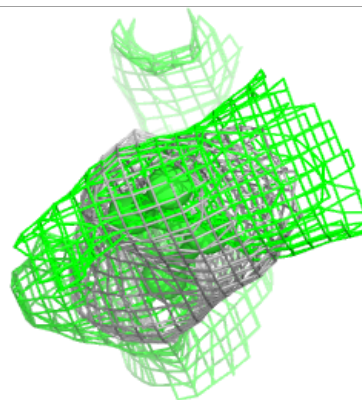
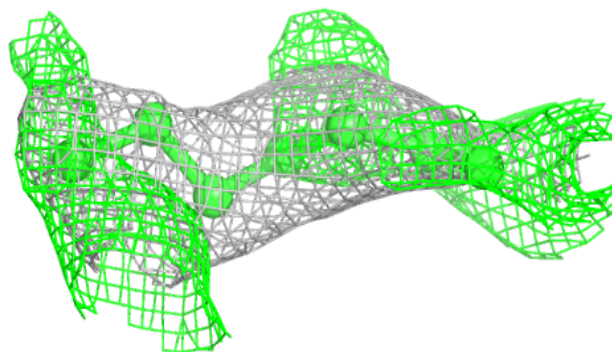
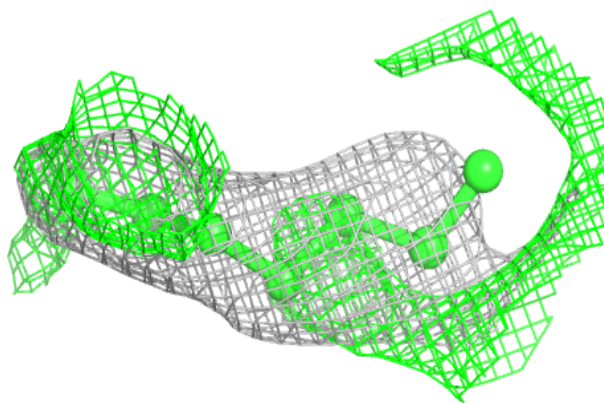
**Electron density around DMU B 303:**

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

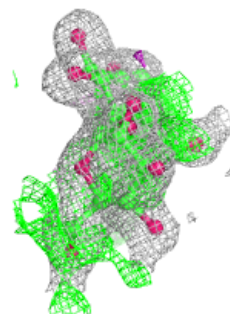
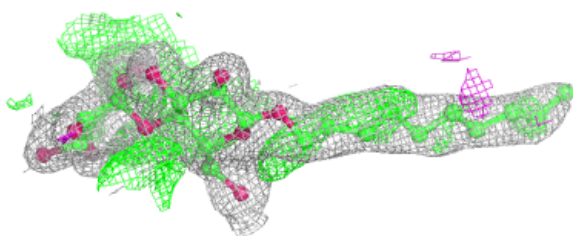
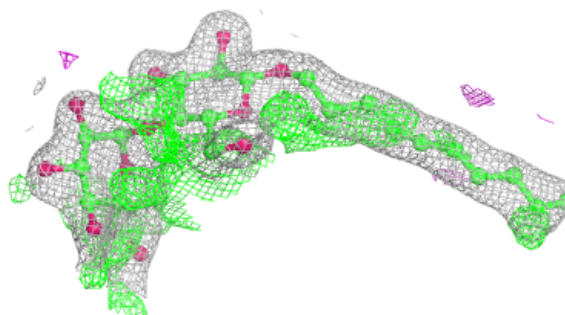


Electron density around DMU P 316:

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

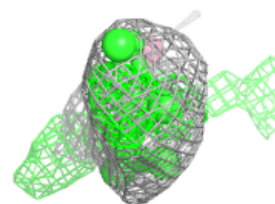
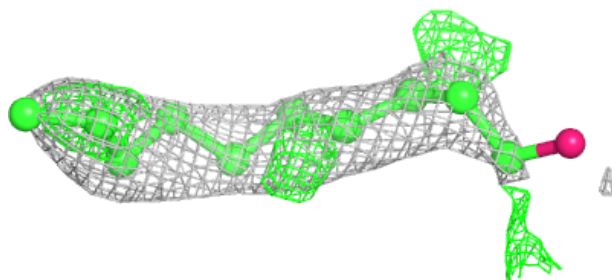
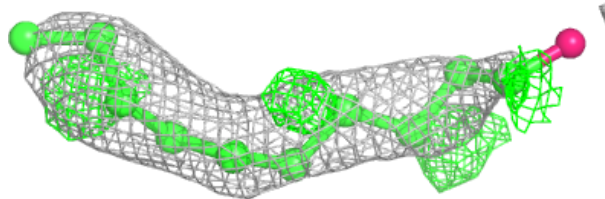
**Electron density around DMU D 201:**

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

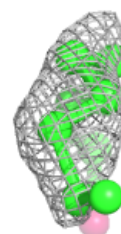
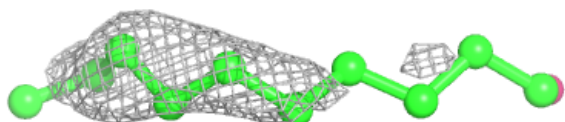
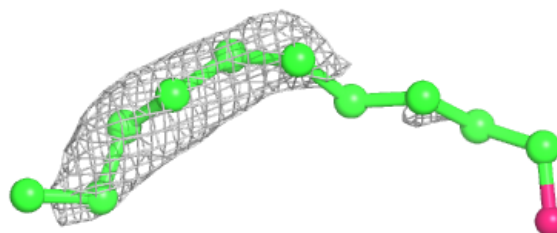


Electron density around DMU J 101:

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

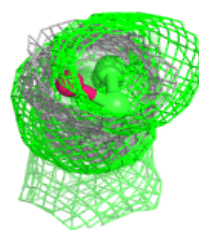
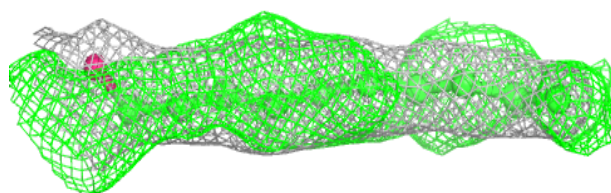
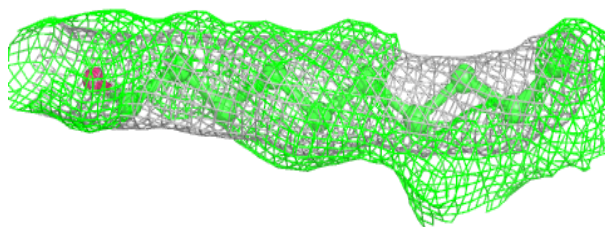
**Electron density around DMU W 101:**

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

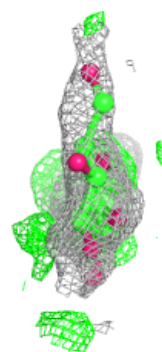
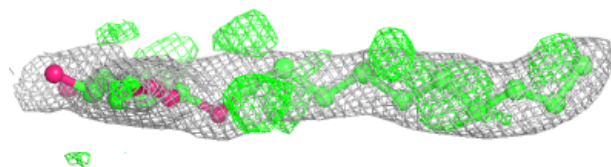
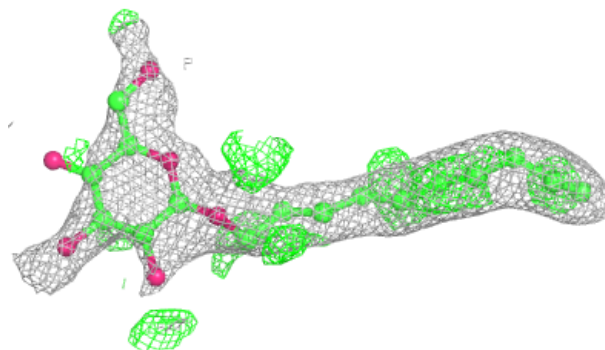


Electron density around DMU P 307:

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

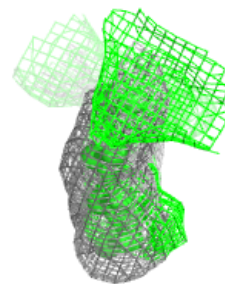
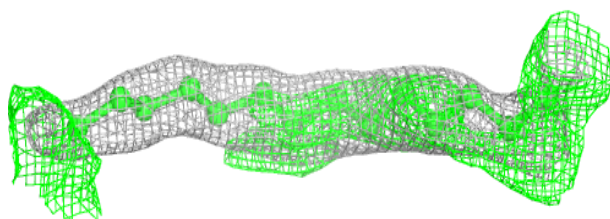
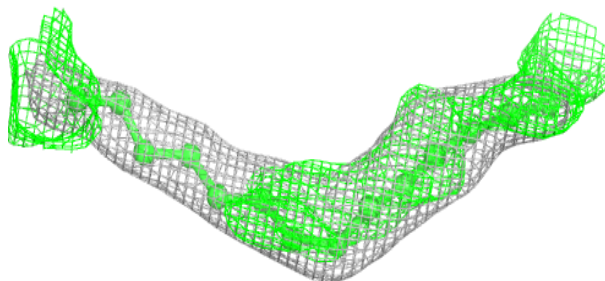
**Electron density around DMU B 304:**

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

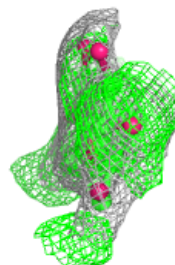
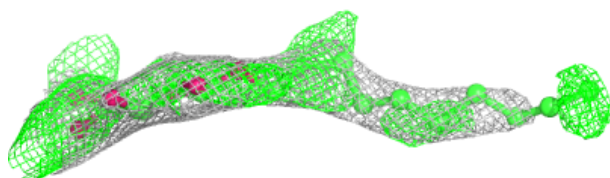
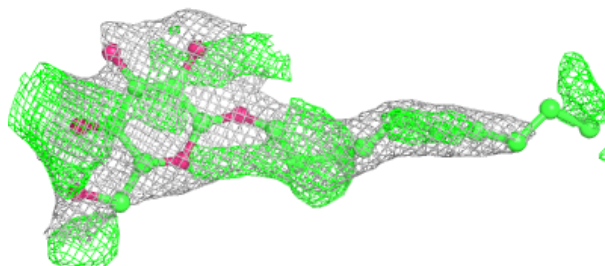


Electron density around LFA N 609:

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

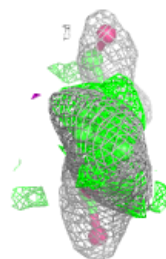
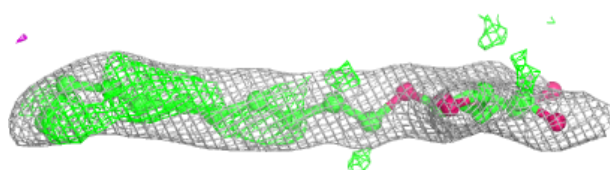
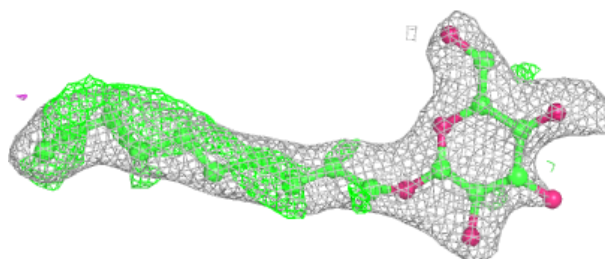
**Electron density around DMU L 102:**

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

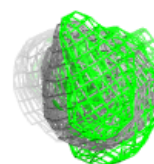
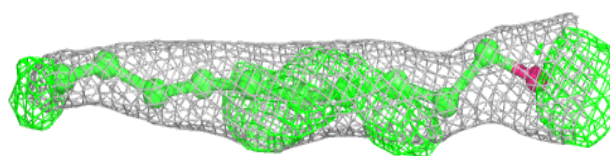
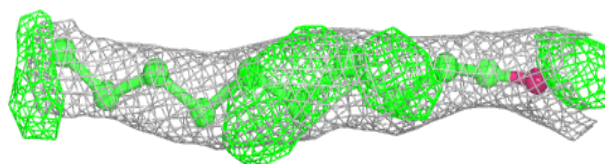


Electron density around DMU O 308:

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

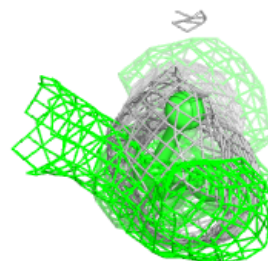
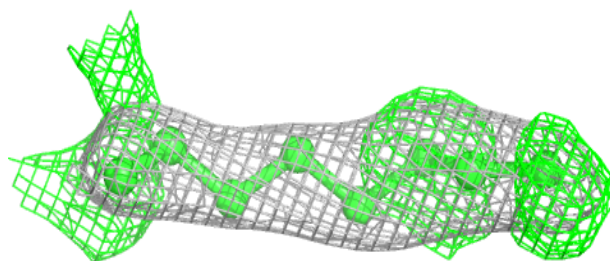
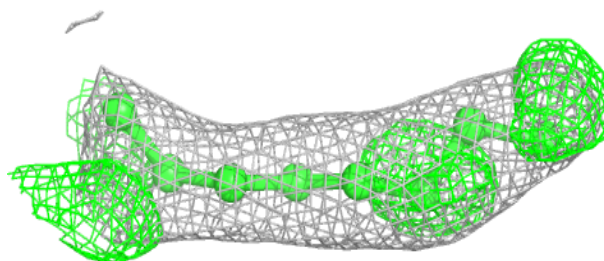
**Electron density around DMU C 306:**

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

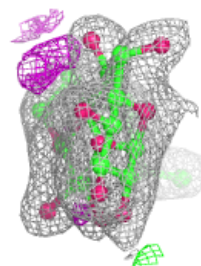
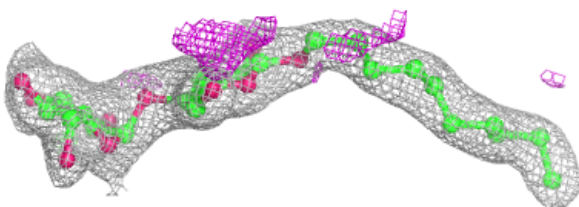
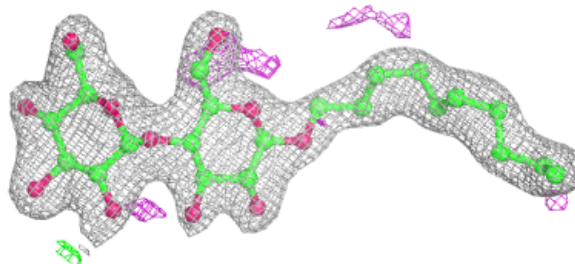


Electron density around DMU Z 103:

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

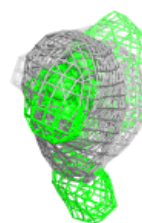
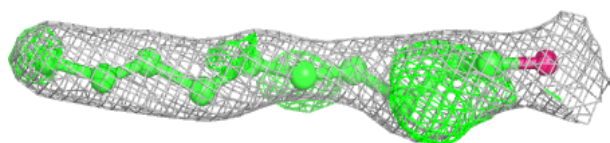
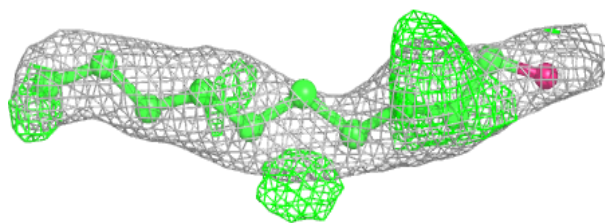
**Electron density around DMU Z 101:**

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

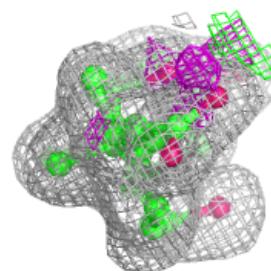
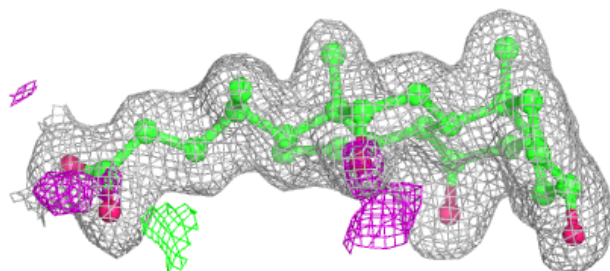
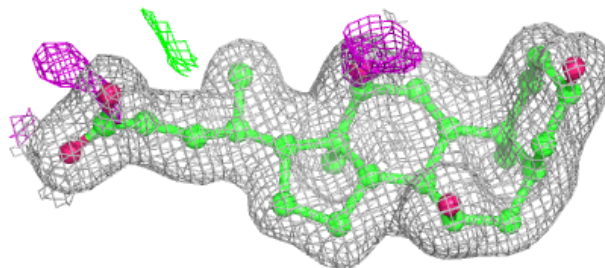


Electron density around DMU O 307:

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

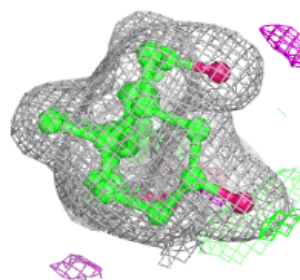
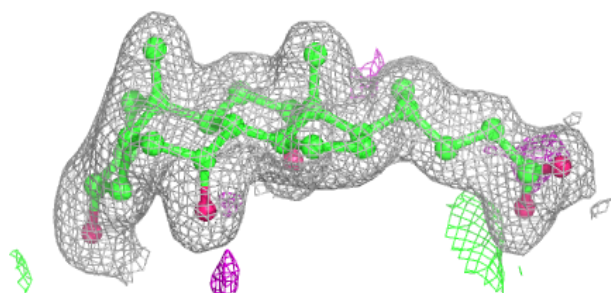
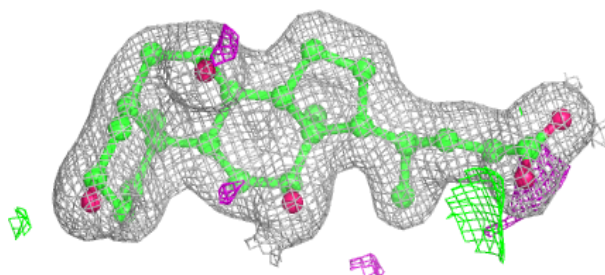
**Electron density around CHD C 301:**

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

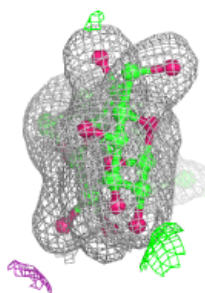
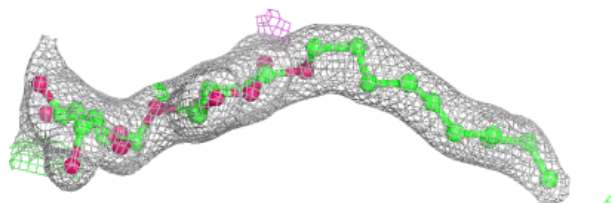
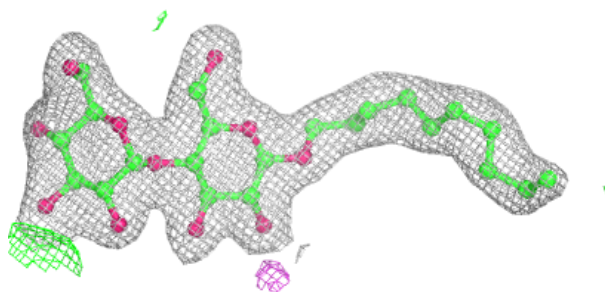


Electron density around CHD P 302:

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

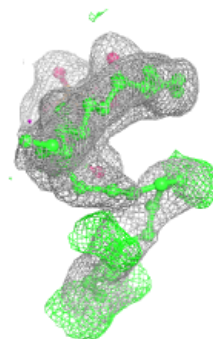
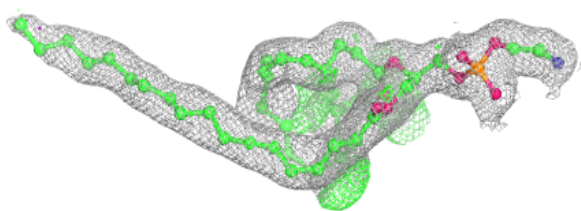
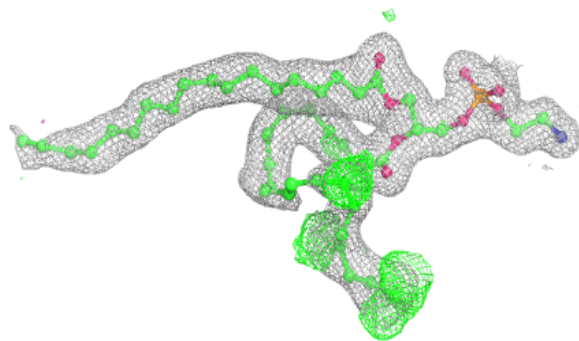
**Electron density around DMU M 101:**

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

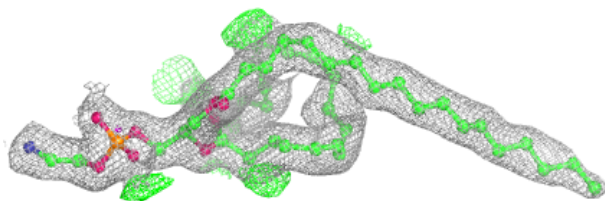
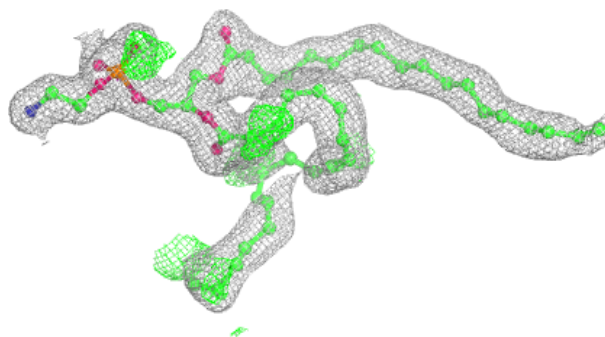


Electron density around PEK G 101:

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

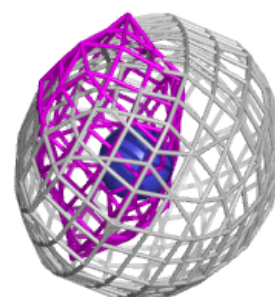
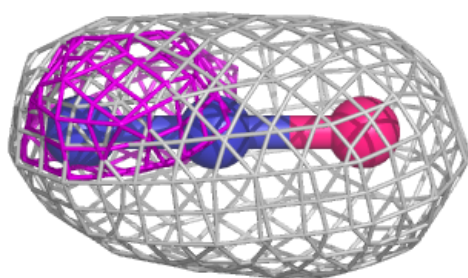
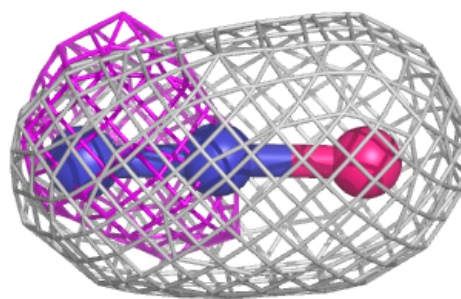
**Electron density around PEK T 101:**

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

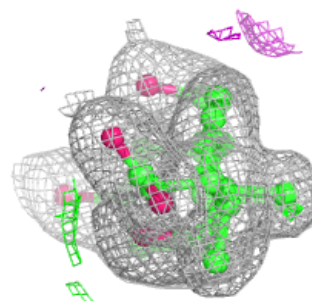
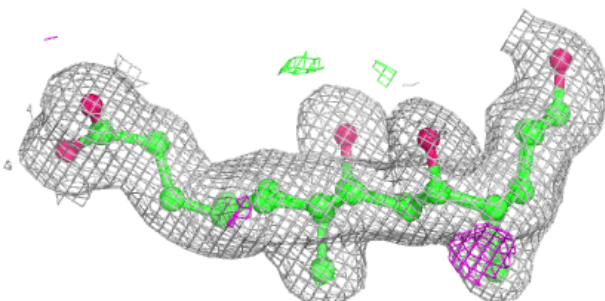
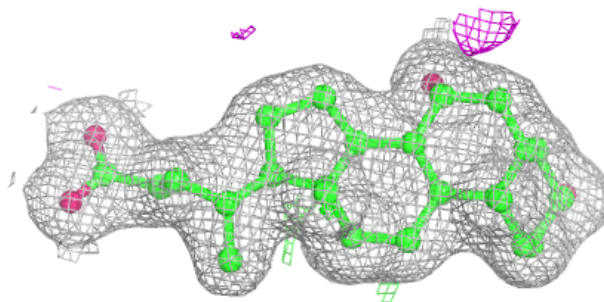


Electron density around N2O N 608:

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

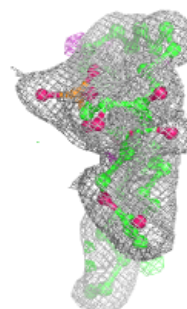
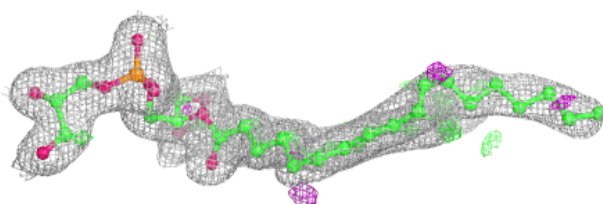
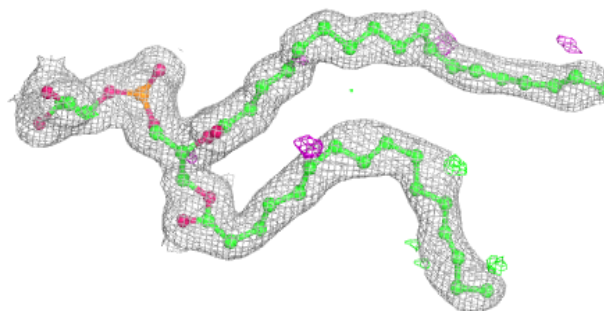
**Electron density around CHD O 301:**

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

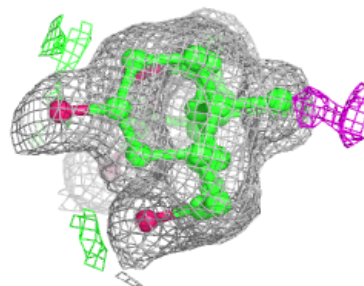
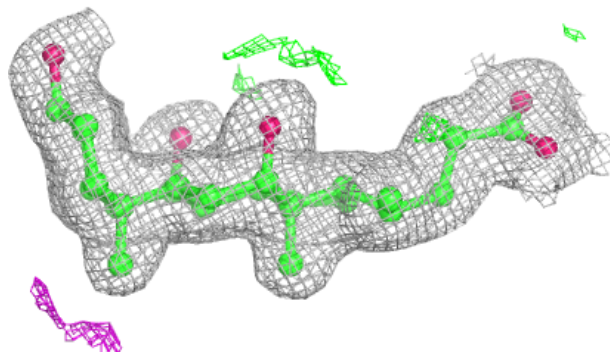
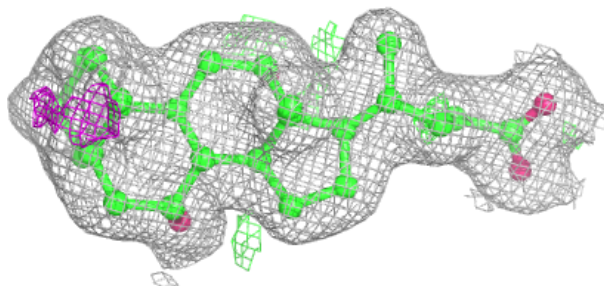


Electron density around PGV N 617:

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

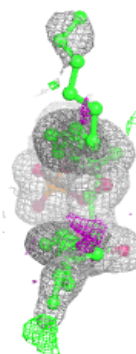
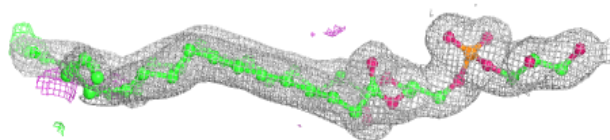
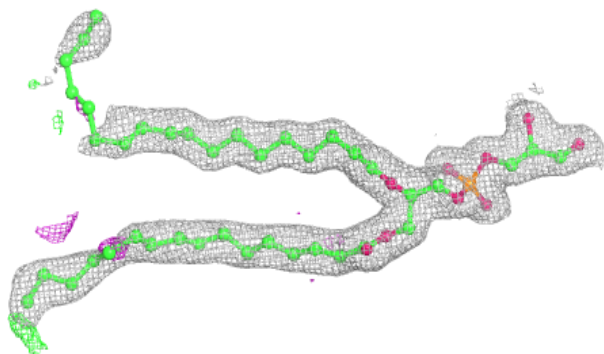
**Electron density around CHD B 306:**

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

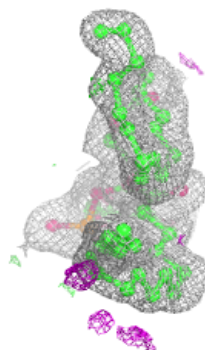
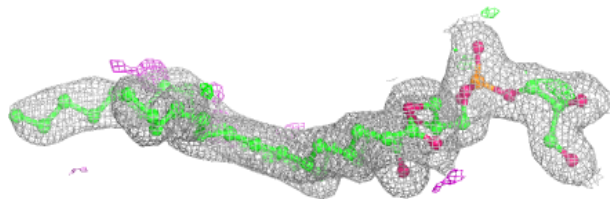
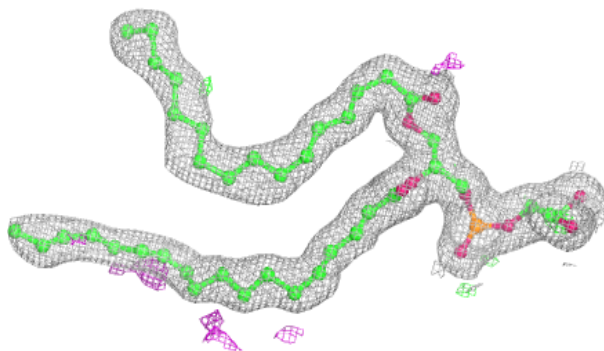


Electron density around PGV P 304:

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

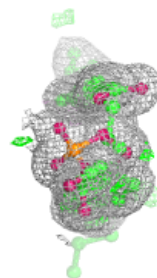
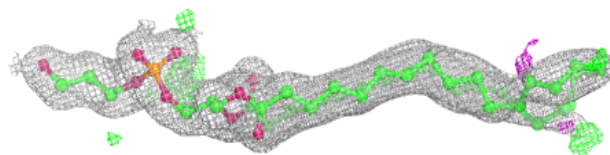
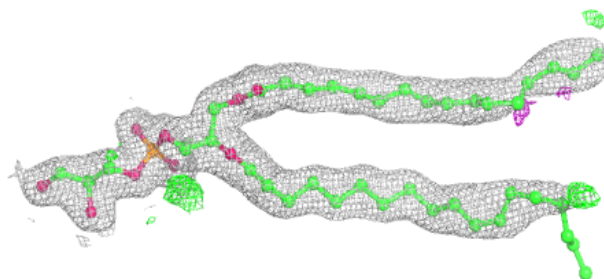
**Electron density around PGV A 616:**

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

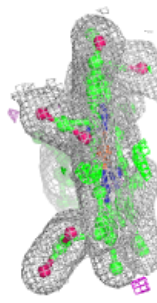
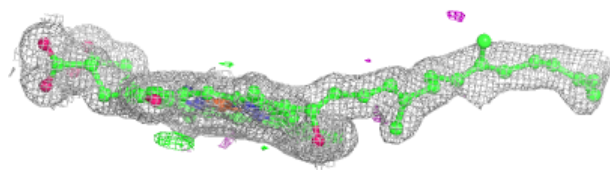
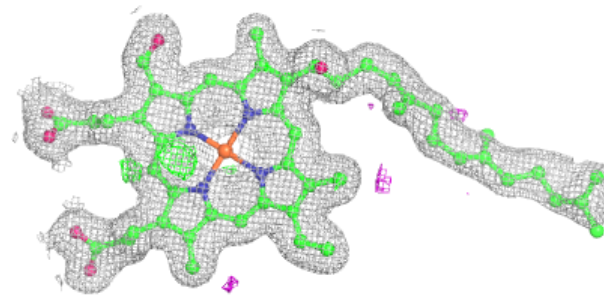


Electron density around PGV C 303:

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

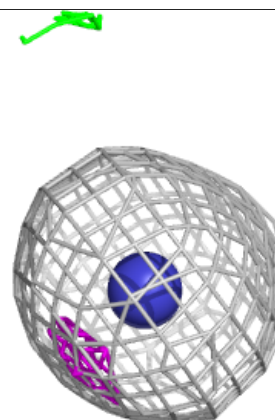
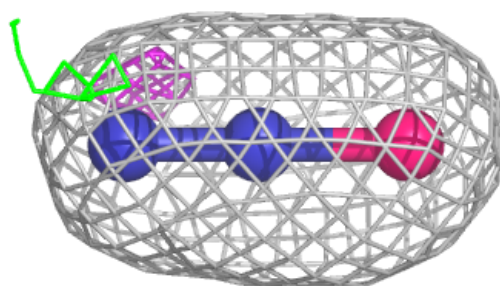
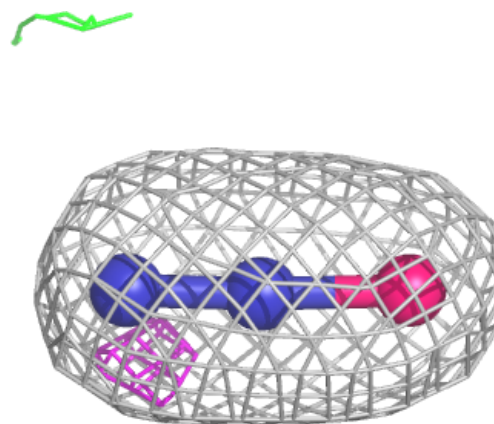
**Electron density around HEA A 601 (A):**

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

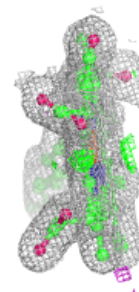
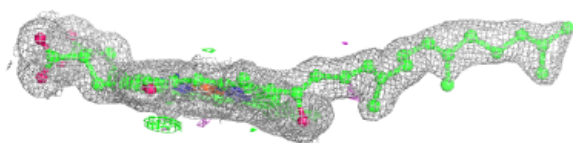
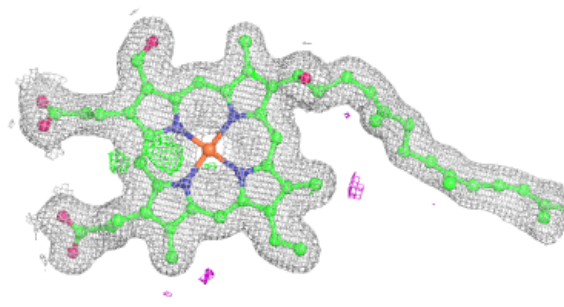


Electron density around N2O A 607:

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

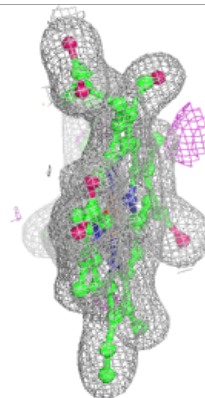
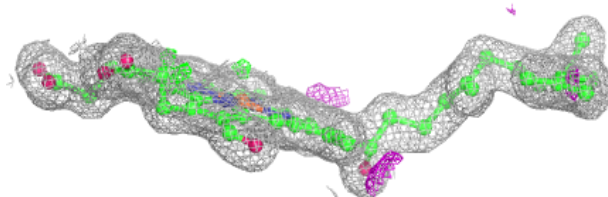
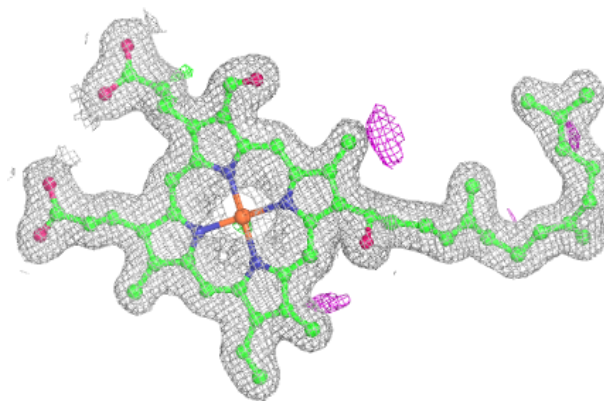
**Electron density around HEA A 601 (B):**

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

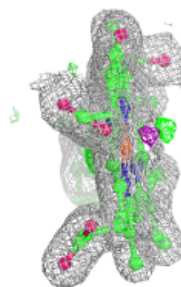
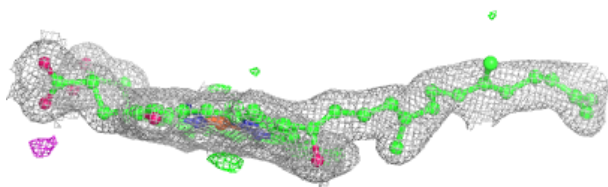
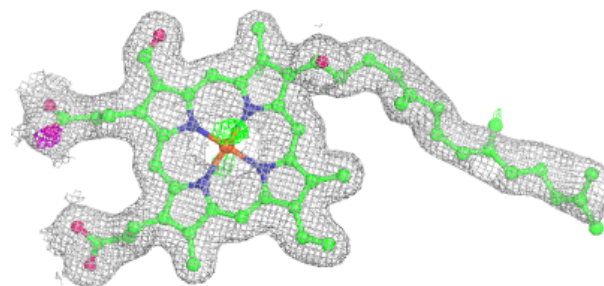


Electron density around HEA A 602:

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

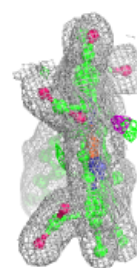
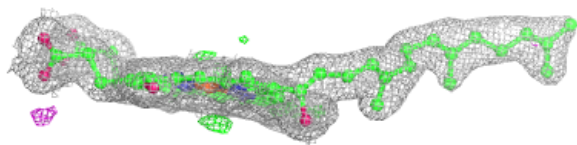
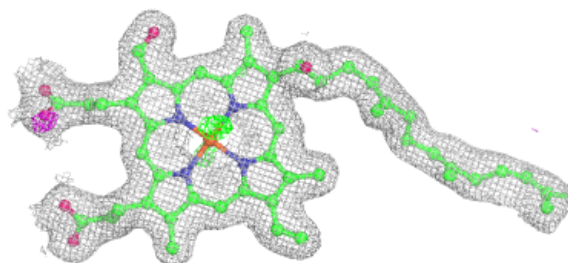
**Electron density around HEA N 602 (A):**

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

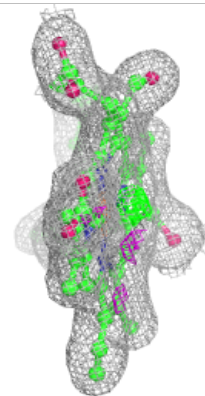
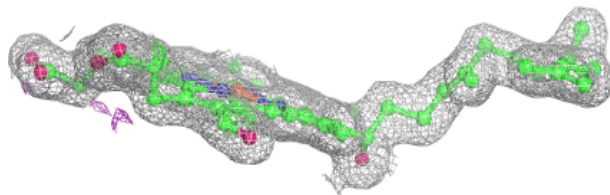
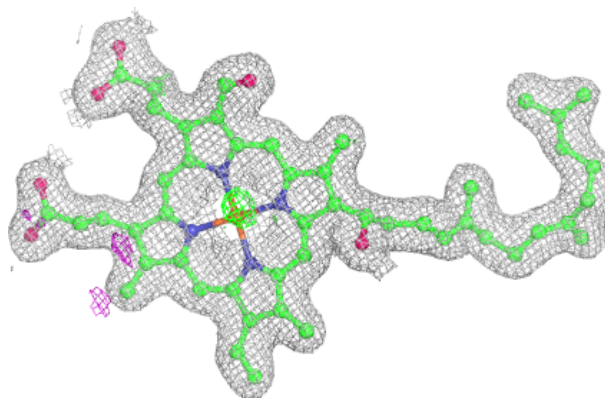


Electron density around HEA N 602 (B):

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

**Electron density around HEA N 603:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.