Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2026 – 08:29 PM JST

PDB ID	:	9M56 / pdb_00009m56
Title	:	Bovine Heart Cytochrome c Oxidase in the Fully Reduced State
Authors	:	Muramoto, K.; Shinzawa-Itoh, K.
Deposited on	:	2025-03-05
Resolution	:	1.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

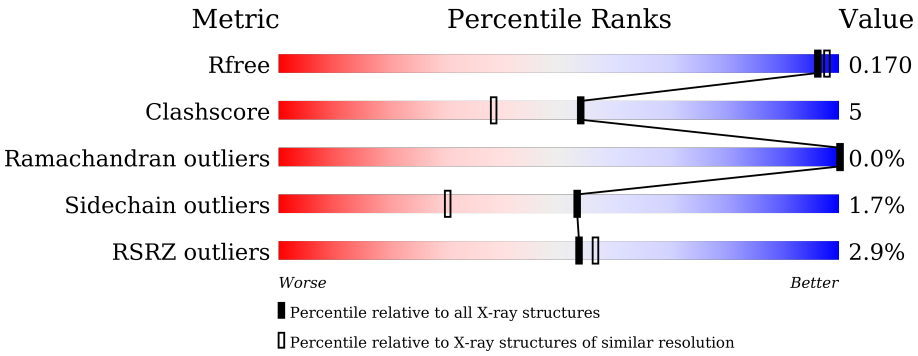
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	514	91% 8%
1	N	514	91% 8%
2	B	227	5% 83% 15%
2	O	227	4% 84% 14%
3	C	261	87% 12%
3	P	261	86% 11%

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Mol	Chain	Length	Quality of chain
4	D	147	91% 5%
4	Q	147	5% 88% 7%
5	E	109	90% 6%
5	R	109	89% 5% 6%
6	F	98	82% 8% 7%
6	S	98	84% 5% 7%
7	G	85	8% 73% 11% 15%
7	T	85	6% 75% 9% 15%
8	H	85	4% 80% 6% 12%
8	U	85	11% 81% 6% 12%
9	I	73	10% 89% 5%
9	V	73	12% 88% 8%
10	J	59	88% 5% 5%
10	W	59	7% 90% 5% 5%
11	K	56	5% 82% 12%
11	X	56	5% 86% 12%
12	L	47	4% 85% 9% 6%
12	Y	47	81% 13% 6%
13	M	46	80% 7% 13%
13	Z	46	76% 11% 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	LFA	P	311	-	-	-	X

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 33023 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

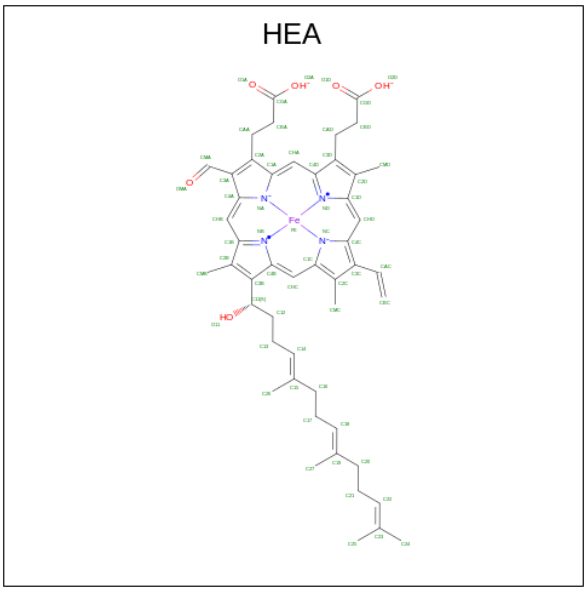
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

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



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

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

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

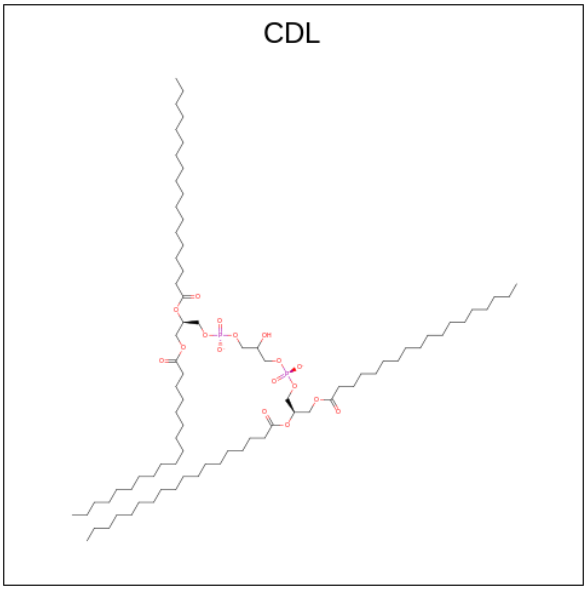
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

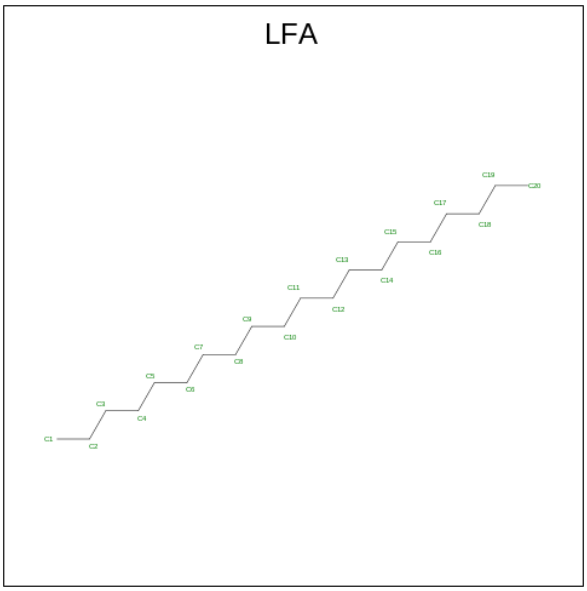
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

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



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

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



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

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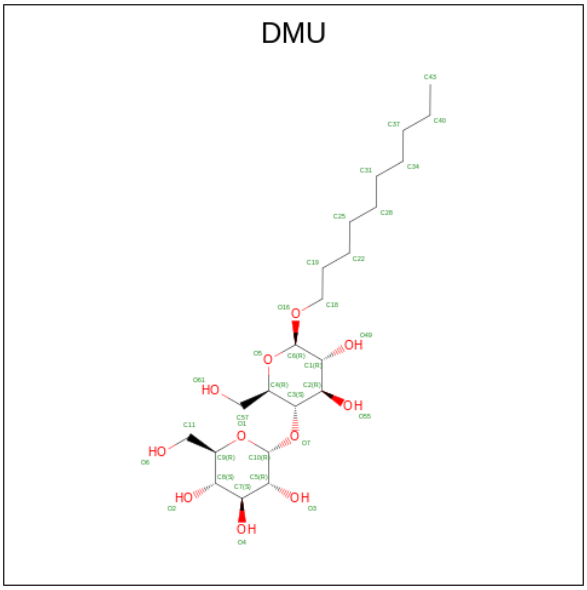
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	O	1	Total C 11 11	0	0
19	P	1	Total C 15 15	0	0
19	P	1	Total C 11 11	0	0
19	P	1	Total C 6 6	0	0
19	P	1	Total C 18 18	0	0
19	P	1	Total C 11 11	0	0
19	P	1	Total C 14 14	0	0
19	P	1	Total C 11 11	0	0
19	P	1	Total C 15 15	0	0
19	P	1	Total C 13 13	0	0
19	T	1	Total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

- Molecule 20 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

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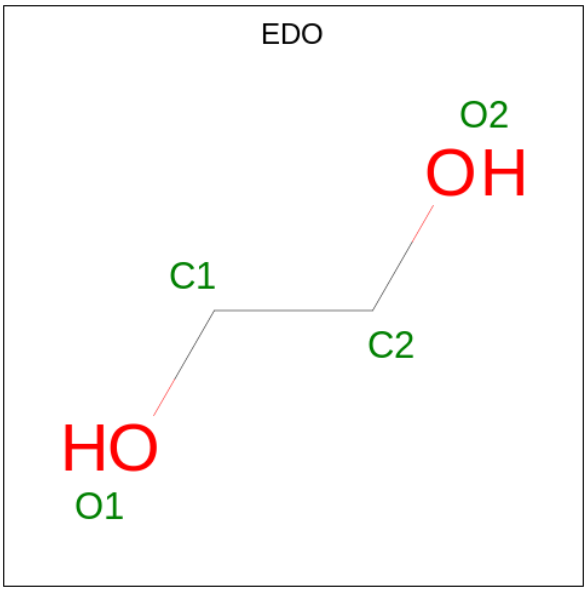
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	N	1	Total C 7 7	0	0
20	N	1	Total C O 33 22 11	0	0
20	N	1	Total C O 33 22 11	0	0
20	O	1	Total C O 22 16 6	0	0
20	O	1	Total C O 11 10 1	0	0
20	O	1	Total C O 11 10 1	0	0
20	O	1	Total C O 22 16 6	0	0
20	P	1	Total C O 11 10 1	0	0
20	P	1	Total C O 33 22 11	0	0
20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

- Molecule 21 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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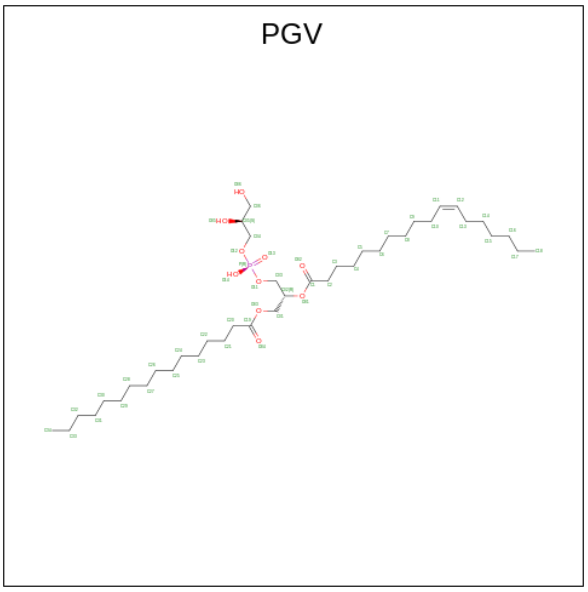
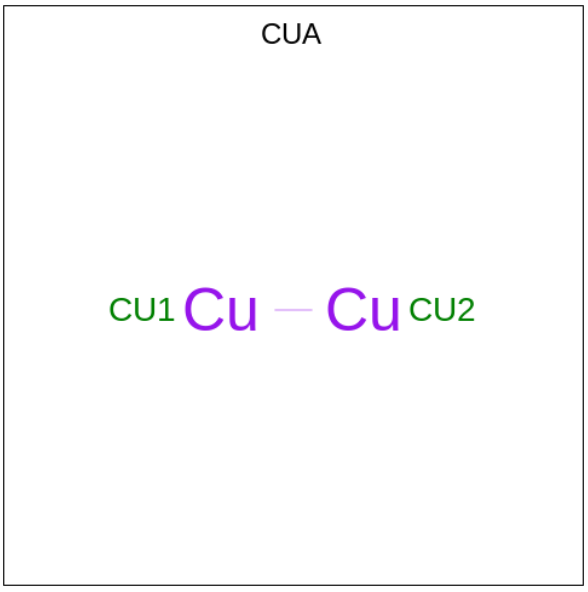
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	N	1	Total	C	O	0	0
			4	2	2		
21	O	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21	P	1	Total	C	O	0	0
			4	2	2		
21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

- Molecule 22 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



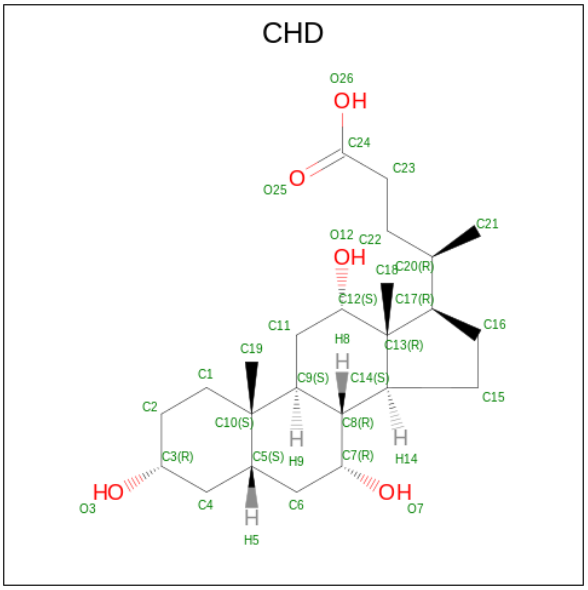
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	O	P	0	0
			51	40	10	1		
22	C	1	Total	C	O	P	0	0
			51	40	10	1		
22	N	1	Total	C	O	P	0	0
			51	40	10	1		
22	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 23 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



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

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



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

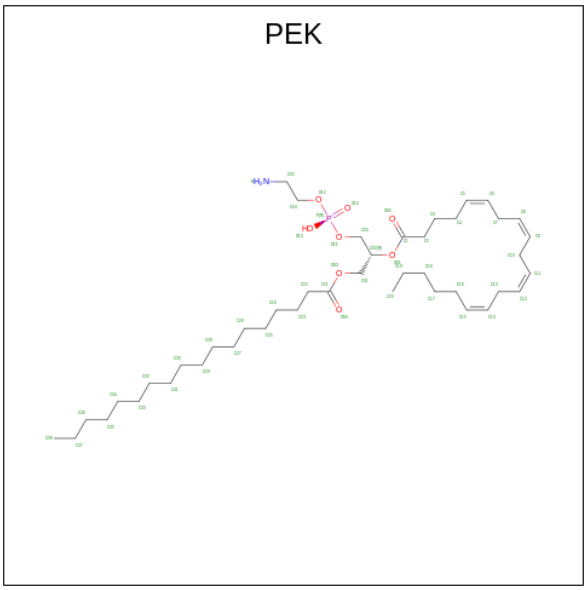
- Molecule 25 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

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

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

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

- Molecule 27 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$).



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

- Molecule 28 is water.

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

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

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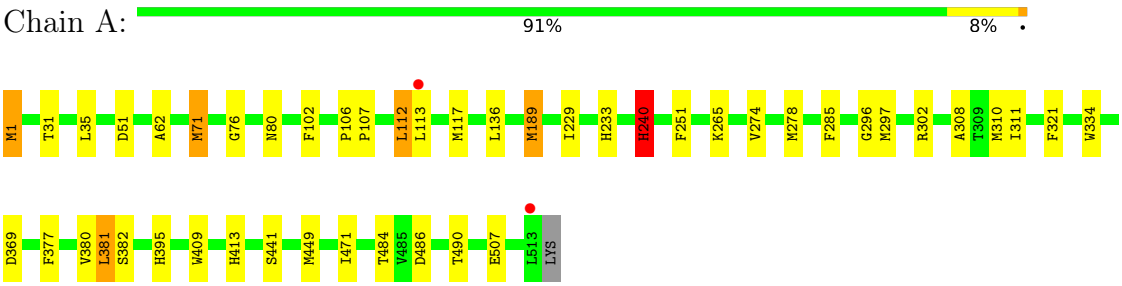
Continued from previous page...

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

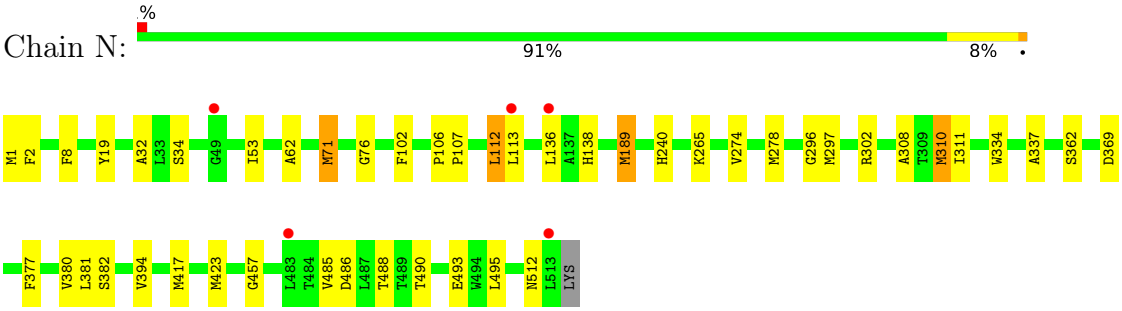
3 Residue-property plots (i)

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

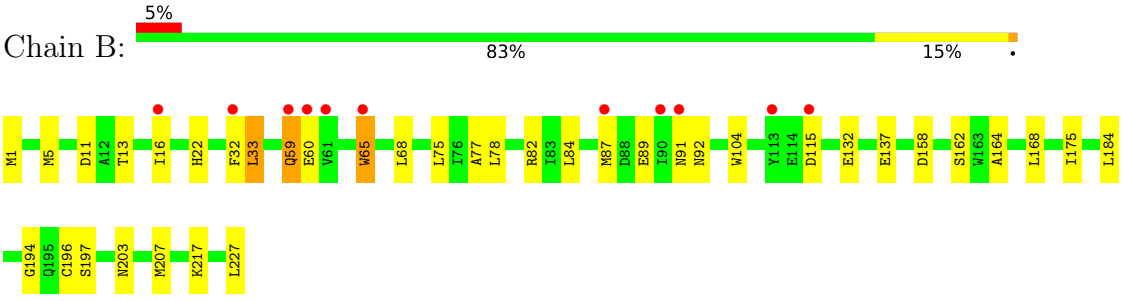
• Molecule 1: Cytochrome c oxidase subunit 1



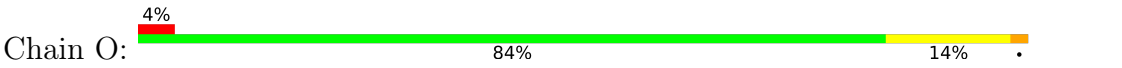
• Molecule 1: Cytochrome c oxidase subunit 1

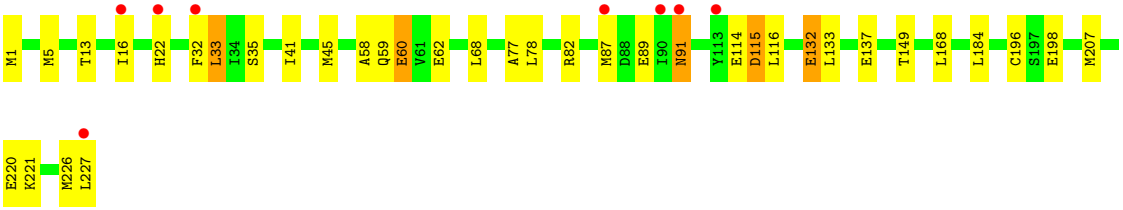


• Molecule 2: Cytochrome c oxidase subunit 2

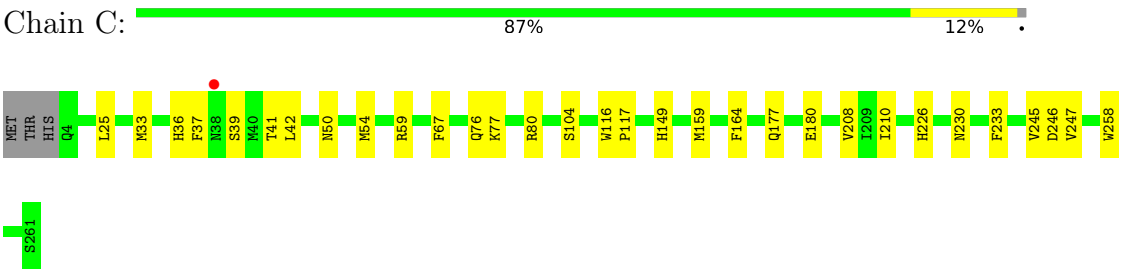


• Molecule 2: Cytochrome c oxidase subunit 2

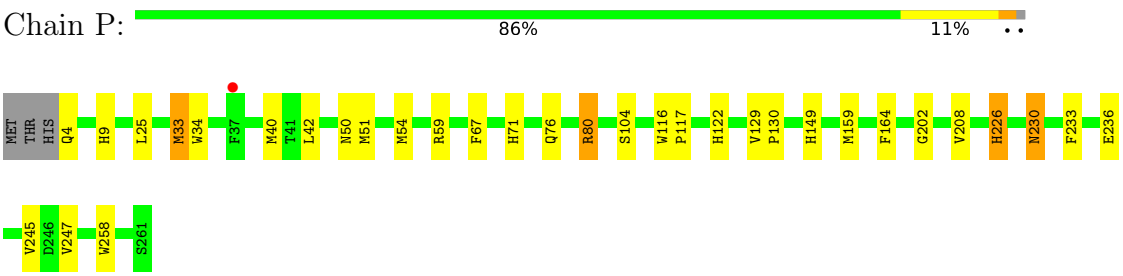




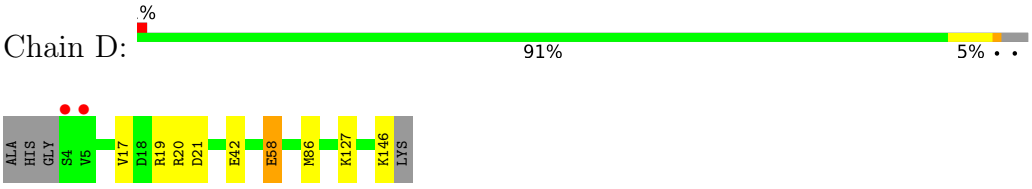
• Molecule 3: Cytochrome c oxidase subunit 3



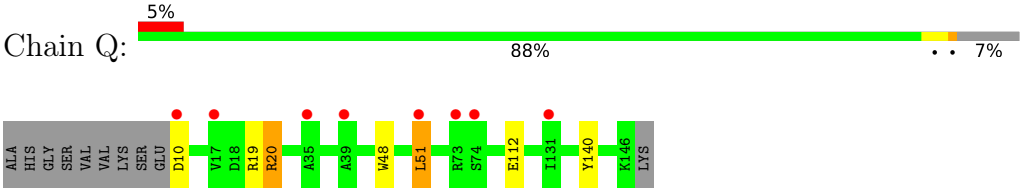
• Molecule 3: Cytochrome c oxidase subunit 3



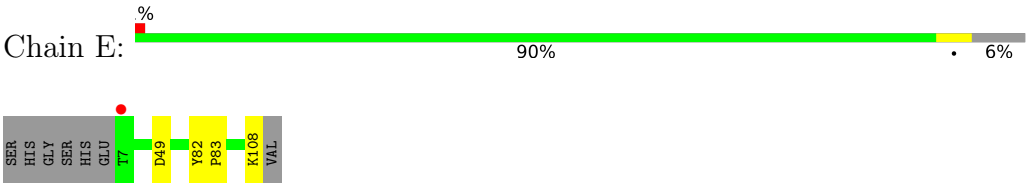
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



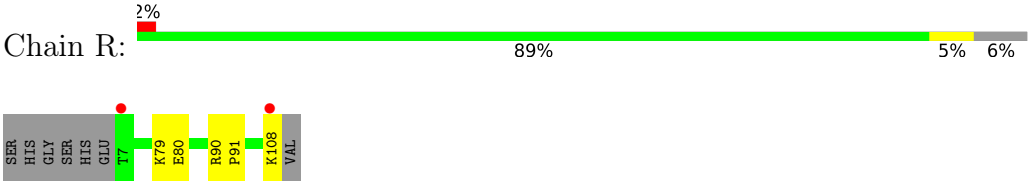
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



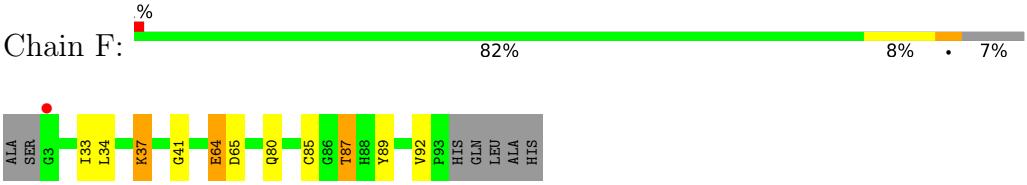
• Molecule 5: Cytochrome c oxidase subunit 5A



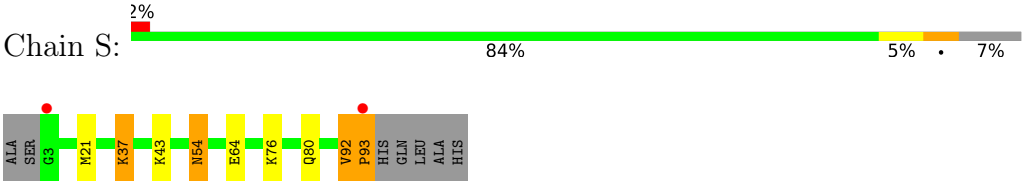
• Molecule 5: Cytochrome c oxidase subunit 5A



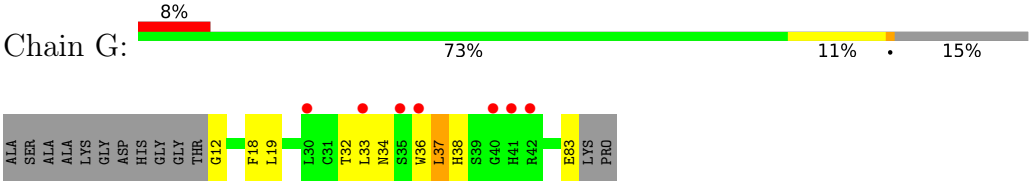
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



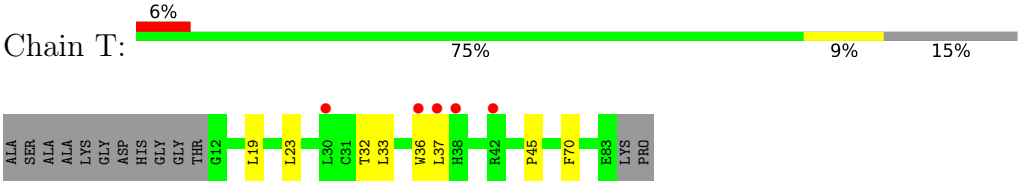
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



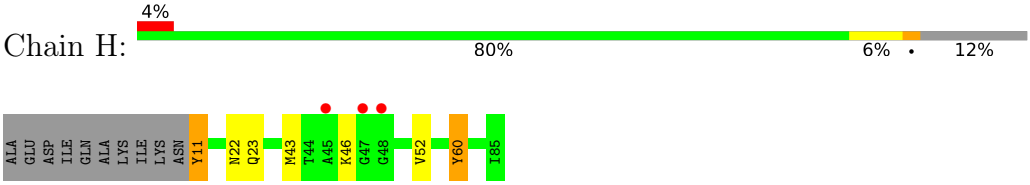
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



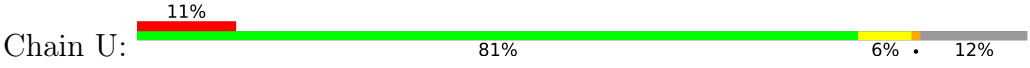
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

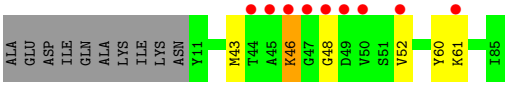


• Molecule 8: Cytochrome c oxidase subunit 6B1

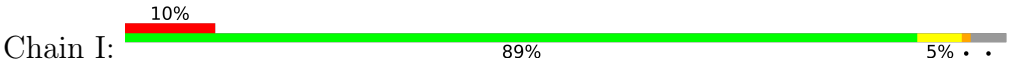


• Molecule 8: Cytochrome c oxidase subunit 6B1



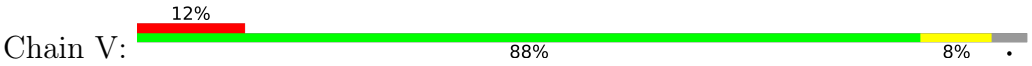


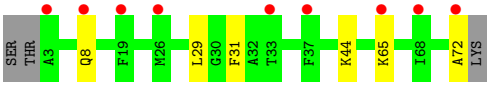
• Molecule 9: Cytochrome c oxidase subunit 6C



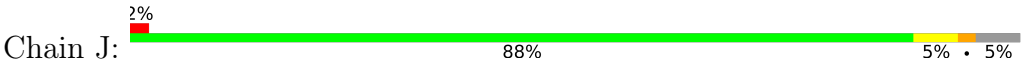


• Molecule 9: Cytochrome c oxidase subunit 6C



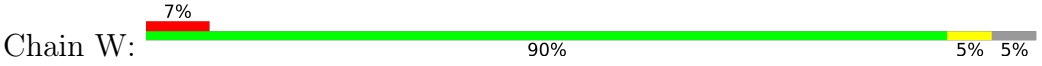


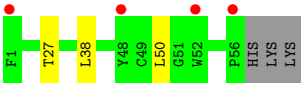
• Molecule 10: Cytochrome c oxidase subunit 7A1



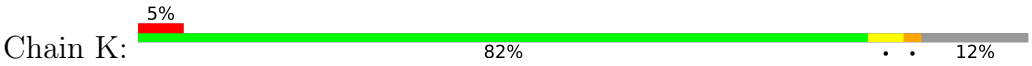


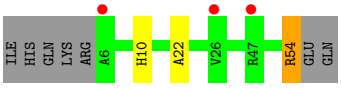
• Molecule 10: Cytochrome c oxidase subunit 7A1



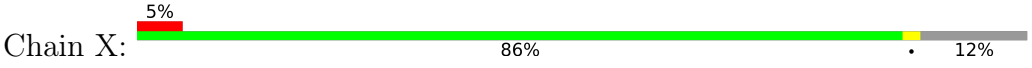


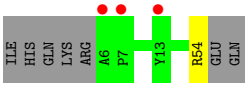
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial





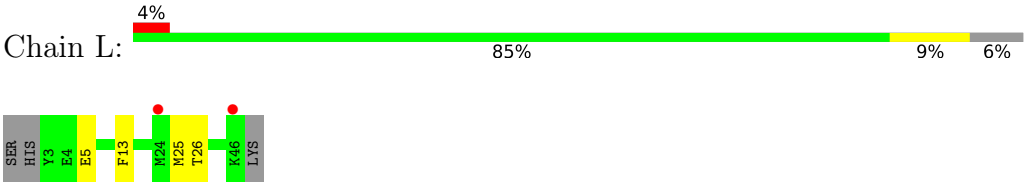
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial





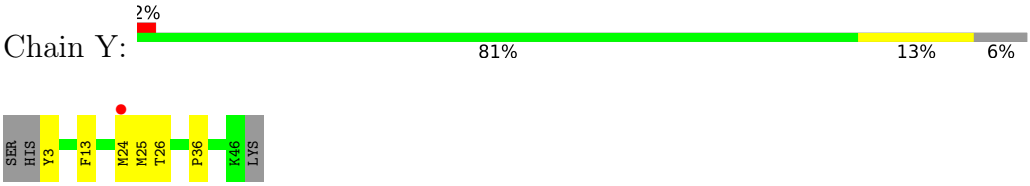
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:



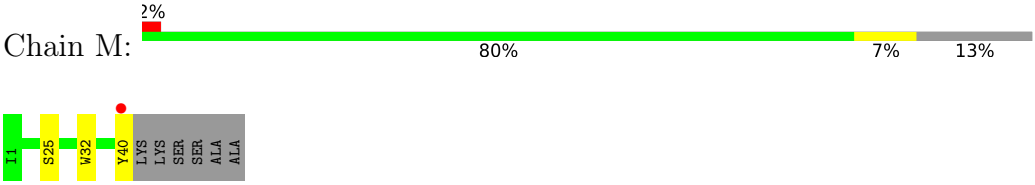
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



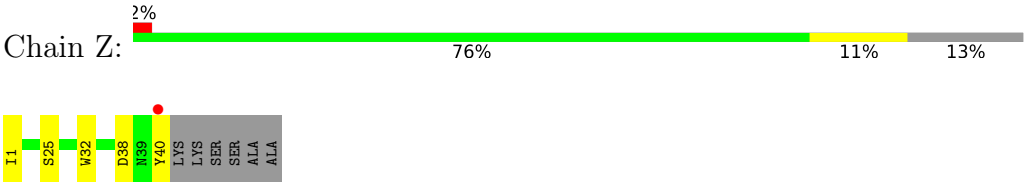
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:



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

Chain Z:



4 Data and refinement statistics (i)

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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

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

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

sidechain that are expected to be planar.

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

All (35) bond length outliers are listed below:

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

All (56) bond angle outliers are listed below:

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

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

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4102	40	0
1	N	4130	0	4102	44	0
2	B	1870	0	1870	27	0
2	O	1870	0	1870	29	0
3	C	2171	0	2080	31	0
3	P	2172	0	2081	25	0
4	D	1192	0	1178	7	0
4	Q	1148	0	1131	4	0
5	E	825	0	823	1	0
5	R	825	0	823	3	0

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	B	171	0	0	4	0
28	C	103	0	0	6	0
28	D	148	0	0	2	0
28	E	114	0	0	0	0
28	F	111	0	0	1	0
28	G	49	0	0	1	0
28	H	63	0	0	4	0
28	I	39	0	0	2	0
28	J	21	0	0	0	0
28	K	22	0	0	0	0
28	L	29	0	0	1	0
28	M	21	0	0	0	0
28	N	234	0	0	9	0
28	O	143	0	0	2	0
28	P	100	0	0	3	0
28	Q	81	0	0	2	0
28	R	96	0	0	1	0
28	S	97	0	0	1	0
28	T	37	0	0	0	0
28	U	48	0	0	0	0
28	V	25	0	0	0	0
28	W	16	0	0	0	0
28	X	18	0	0	0	0
28	Y	27	0	0	1	0
28	Z	18	0	0	0	0
All	All	33023	0	31505	308	0

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

All (308) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:C:309:LFA:H12	28:C:481:HOH:O	1.35	1.21
1:A:112:LEU:HG	28:A:2018:HOH:O	1.34	1.20
1:A:31:THR:O	1:A:35:LEU:HD23	1.45	1.16
1:N:112:LEU:HG	28:N:3015:HOH:O	1.47	1.13
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.29	1.10
2:B:16[A]:ILE:HG21	2:B:87[A]:MET:HE3	1.42	1.01
1:A:112:LEU:O	1:A:112:LEU:HD23	1.68	0.94
3:P:4:GLN:N	28:P:403:HOH:O	2.00	0.94

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

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:23:LEU:HB2	19:T:101:LFA:H92	2.03	0.40
1:A:377:PHE:O	1:A:381:LEU:HB3	2.21	0.40
10:J:31:LEU:HD12	10:J:31:LEU:HA	1.94	0.40
1:N:19:TYR:CD1	1:N:76:GLY:HA3	2.56	0.40
3:P:202:GLY:HA3	27:T:102:PEK:H21	2.03	0.40
12:Y:13:PHE:HB3	18:Y:101:CDL:H512	2.02	0.40
1:A:449:MET:SD	2:B:5:MET:HG2	2.62	0.40
8:H:60:TYR:CD1	8:H:60:TYR:C	3.00	0.40
1:N:334:TRP:HB2	20:Q:201:DMU:C57	2.52	0.40
1:N:334:TRP:HB2	20:Q:201:DMU:H29	2.03	0.40
2:O:5:MET:HE2	2:O:5:MET:HB3	1.90	0.40
19:T:101:LFA:H92	19:T:101:LFA:H121	1.94	0.40
8:U:43:MET:HE2	8:U:43:MET:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	526/514 (102%)	511 (97%)	15 (3%)	0	100	100
1	N	526/514 (102%)	515 (98%)	11 (2%)	0	100	100
2	B	230/227 (101%)	225 (98%)	4 (2%)	1 (0%)	30	14
2	O	230/227 (101%)	224 (97%)	6 (3%)	0	100	100
3	C	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
3	P	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	136/147 (92%)	133 (98%)	3 (2%)	0	100	100
5	E	100/109 (92%)	100 (100%)	0	0	100	100
5	R	100/109 (92%)	100 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	91/98 (93%)	91 (100%)	0	0	100	100
6	S	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
7	G	71/85 (84%)	67 (94%)	4 (6%)	0	100	100
7	T	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
8	H	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
8	U	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
9	I	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
9	V	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
10	J	54/59 (92%)	54 (100%)	0	0	100	100
10	W	54/59 (92%)	54 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
12	Y	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
13	M	38/46 (83%)	38 (100%)	0	0	100	100
13	Z	38/46 (83%)	38 (100%)	0	0	100	100
All	All	3488/3614 (96%)	3421 (98%)	66 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	92	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/426 (103%)	438 (100%)	2 (0%)	81	70
1	N	440/426 (103%)	438 (100%)	2 (0%)	81	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	215/210 (102%)	208 (97%)	7 (3%)	33 12
2	O	215/210 (102%)	208 (97%)	7 (3%)	33 12
3	C	232/226 (103%)	230 (99%)	2 (1%)	70 55
3	P	232/226 (103%)	228 (98%)	4 (2%)	53 30
4	D	128/129 (99%)	128 (100%)	0	100 100
4	Q	122/129 (95%)	120 (98%)	2 (2%)	55 33
5	E	89/95 (94%)	89 (100%)	0	100 100
5	R	89/95 (94%)	88 (99%)	1 (1%)	65 46
6	F	78/81 (96%)	74 (95%)	4 (5%)	21 5
6	S	78/81 (96%)	74 (95%)	4 (5%)	21 5
7	G	63/69 (91%)	61 (97%)	2 (3%)	34 12
7	T	63/69 (91%)	60 (95%)	3 (5%)	23 6
8	H	67/75 (89%)	65 (97%)	2 (3%)	36 13
8	U	67/75 (89%)	64 (96%)	3 (4%)	24 7
9	I	55/58 (95%)	54 (98%)	1 (2%)	51 28
9	V	55/58 (95%)	52 (94%)	3 (6%)	19 4
10	J	47/50 (94%)	46 (98%)	1 (2%)	47 23
10	W	47/50 (94%)	46 (98%)	1 (2%)	47 23
11	K	39/46 (85%)	38 (97%)	1 (3%)	40 17
11	X	39/46 (85%)	39 (100%)	0	100 100
12	L	37/40 (92%)	37 (100%)	0	100 100
12	Y	37/40 (92%)	37 (100%)	0	100 100
13	M	34/38 (90%)	34 (100%)	0	100 100
13	Z	34/38 (90%)	33 (97%)	1 (3%)	37 14
All	All	3042/3086 (99%)	2989 (98%)	53 (2%)	53 30

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

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

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Mol	Chain	Res	Type
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
3	C	159	MET
3	C	230	ASN
6	F	37	LYS
6	F	80	GLN
6	F	87[A]	THR
6	F	87[B]	THR
7	G	33	LEU
7	G	37	LEU
8	H	46	LYS
8	H	60	TYR
9	I	36	LYS
10	J	7	GLU
11	K	54	ARG
1	N	112	LEU
1	N	369	ASP
2	O	33	LEU
2	O	60	GLU
2	O	68	LEU
2	O	78	LEU
2	O	91	ASN
2	O	115	ASP
2	O	221	LYS
3	P	33[A]	MET
3	P	33[B]	MET
3	P	159	MET
3	P	230	ASN
4	Q	10	ASP
4	Q	51	LEU
5	R	79	LYS
6	S	37	LYS
6	S	43	LYS
6	S	54	ASN
6	S	80	GLN
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
8	U	46	LYS
8	U	60	TYR

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

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

Mol	Chain	Res	Type
1	A	170	ASN
1	A	422	ASN
2	B	52	HIS
2	B	59	GLN
2	B	203	ASN
3	C	50	ASN
3	C	56	GLN
3	C	76	GLN
4	D	119	GLN
5	E	94	ASN
6	F	54	ASN
7	G	38	HIS
8	H	22	ASN
8	H	37	HIS
10	J	29	ASN
11	K	35	GLN
1	N	170	ASN
1	N	422	ASN
2	O	91	ASN
2	O	92	ASN
3	P	50	ASN
4	Q	109	HIS
4	Q	119	GLN
5	R	94	ASN
6	S	54	ASN
8	U	22	ASN
10	W	29	ASN
11	X	35	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	N	1	1	8,9,10	0.68	0	7,9,11	1.12	1 (14%)
1	FME	A	1	1	8,9,10	0.50	0	7,9,11	0.98	1 (14%)
2	FME	O	1	2	8,9,10	0.66	0	7,9,11	0.99	0
2	FME	B	1	2	8,9,10	1.30	1 (12%)	7,9,11	1.31	1 (14%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-3.22	1.64	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CG-CB-CA	-2.94	104.78	112.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	1	FME	O-C-CA	-2.18	119.08	124.78
1	A	1	FME	C-CA-N	2.01	113.36	109.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	DMU	M	102	-	7,7,34	0.33	0	6,6,45	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	EDO	R	203	-	3,3,3	0.22	0	2,2,2	0.31	0
21	EDO	S	103	-	3,3,3	0.19	0	2,2,2	0.20	0
22	PGV	N	614	-	50,50,50	0.72	1 (2%)	53,56,56	1.19	2 (3%)
20	DMU	G	104	-	22,22,34	0.81	1 (4%)	27,27,45	0.99	2 (7%)
20	DMU	A	609	-	34,34,34	1.18	4 (11%)	45,45,45	1.33	7 (15%)
19	LFA	A	607	-	13,13,19	0.38	0	12,12,18	0.19	0
20	DMU	C	316	-	6,6,34	0.28	0	5,5,45	0.45	0
23	CUA	B	301	2	0,1,1	-	-	-		
18	CDL	L	101	-	93,93,99	0.42	0	99,105,111	0.54	1 (1%)
21	EDO	E	203	-	3,3,3	0.11	0	2,2,2	0.13	0
19	LFA	C	324	-	14,14,19	0.22	0	13,13,18	0.13	0
20	DMU	P	320	-	34,34,34	0.87	2 (5%)	45,45,45	1.17	4 (8%)
21	EDO	E	201	-	3,3,3	0.18	0	2,2,2	0.11	0
19	LFA	T	101	-	13,13,19	0.65	0	12,12,18	0.49	0
14	HEA	N	601	1	66,67,67	1.64	17 (25%)	78,103,103	2.32	23 (29%)
20	DMU	N	615	19	34,34,34	0.91	1 (2%)	45,45,45	1.38	5 (11%)
21	EDO	E	202	-	3,3,3	0.24	0	2,2,2	0.13	0
24	CHD	G	102	-	32,32,32	0.71	0	51,51,51	0.75	0
27	PEK	T	102	-	52,52,52	0.76	2 (3%)	55,57,57	1.08	3 (5%)
20	DMU	C	317	-	22,22,34	0.68	1 (4%)	27,27,45	1.43	3 (11%)
20	DMU	O	306	-	10,10,34	0.34	0	9,9,45	0.55	0
19	LFA	C	313	-	14,14,19	0.19	0	13,13,18	0.41	0
21	EDO	T	105	-	3,3,3	0.37	0	2,2,2	0.24	0
19	LFA	P	313	-	10,10,19	0.27	0	9,9,18	0.27	0
21	EDO	A	611	-	3,3,3	0.19	0	2,2,2	0.29	0
19	LFA	P	309	-	5,5,19	0.20	0	4,4,18	0.09	0
20	DMU	B	303	-	10,10,34	0.29	0	9,9,45	0.56	0
21	EDO	N	609	-	3,3,3	0.52	0	2,2,2	0.44	0
18	CDL	V	101	-	63,63,99	0.43	0	69,75,111	0.87	3 (4%)
20	DMU	P	307	-	10,10,34	0.27	0	9,9,45	0.68	0
20	DMU	C	323	-	34,34,34	0.81	1 (2%)	45,45,45	1.14	4 (8%)
20	DMU	A	614	-	10,10,34	0.34	0	9,9,45	0.53	0
19	LFA	C	310	-	10,10,19	0.18	0	9,9,18	0.07	0
20	DMU	C	319	-	34,34,34	0.69	0	45,45,45	1.34	7 (15%)
21	EDO	F	104	-	3,3,3	0.10	0	2,2,2	0.29	0
21	EDO	P	321	-	3,3,3	0.18	0	2,2,2	0.12	0
20	DMU	P	317	-	6,6,34	0.28	0	5,5,45	0.47	0
23	CUA	O	304	2	0,1,1	-	-	-		
20	DMU	O	305	-	10,10,34	0.13	0	9,9,45	0.63	0
18	CDL	A	606	-	63,63,99	0.44	0	69,75,111	0.93	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	EDO	C	322	-	3,3,3	0.87	0	2,2,2	0.83	0
14	HEA	A	602	1	66,67,67	1.83	22 (33%)	78,103,103	2.38	31 (39%)
21	EDO	P	322	-	3,3,3	0.38	0	2,2,2	0.20	0
22	PGV	P	304	-	50,50,50	0.70	0	53,56,56	1.03	4 (7%)
20	DMU	M	101	-	34,34,34	1.06	2 (5%)	45,45,45	0.96	2 (4%)
18	CDL	Y	101	-	93,93,99	0.38	0	99,105,111	0.49	0
20	DMU	C	306	-	10,10,34	0.40	0	9,9,45	0.56	0
19	LFA	N	606	-	13,13,19	0.30	0	12,12,18	0.49	0
27	PEK	G	101	-	52,52,52	0.64	1 (1%)	55,57,57	0.66	1 (1%)
20	DMU	P	316	-	34,34,34	0.94	2 (5%)	45,45,45	1.67	8 (17%)
19	LFA	C	312	-	10,10,19	0.21	0	9,9,18	0.23	0
20	DMU	O	307	-	22,22,34	0.71	1 (4%)	27,27,45	1.22	4 (14%)
19	LFA	C	307	-	10,10,19	0.23	0	9,9,18	0.24	0
20	DMU	N	607	-	6,6,34	0.40	0	5,5,45	0.32	0
20	DMU	D	201	-	34,34,34	1.54	7 (20%)	45,45,45	1.44	4 (8%)
20	DMU	Q	201	-	34,34,34	1.29	7 (20%)	45,45,45	1.65	9 (20%)
20	DMU	B	304	-	22,22,34	0.90	0	27,27,45	1.06	1 (3%)
19	LFA	C	308	-	5,5,19	0.20	0	4,4,18	0.14	0
22	PGV	A	613	-	50,50,50	0.66	0	53,56,56	1.05	2 (3%)
19	LFA	O	301	-	16,16,19	0.17	0	15,15,18	0.17	0
21	EDO	N	611	-	3,3,3	0.64	0	2,2,2	0.39	0
20	DMU	Z	101	-	34,34,34	1.10	2 (5%)	45,45,45	1.12	3 (6%)
19	LFA	C	311	-	13,13,19	0.23	0	12,12,18	0.10	0
19	LFA	P	308	-	10,10,19	0.24	0	9,9,18	0.19	0
24	CHD	B	306	-	32,32,32	0.77	1 (3%)	51,51,51	0.76	0
20	DMU	O	303	-	22,22,34	0.68	1 (4%)	27,27,45	1.54	4 (14%)
20	DMU	Y	102	-	22,22,34	0.63	0	27,27,45	1.19	2 (7%)
21	EDO	A	610	-	3,3,3	0.63	0	2,2,2	0.57	0
21	EDO	R	202	-	3,3,3	0.28	0	2,2,2	0.36	0
20	DMU	G	103	-	10,10,34	0.34	0	9,9,45	0.56	0
21	EDO	S	102	-	3,3,3	0.38	0	2,2,2	0.45	0
19	LFA	O	302	-	10,10,19	0.25	0	9,9,18	0.14	0
21	EDO	C	321	-	3,3,3	0.33	0	2,2,2	0.17	0
18	CDL	C	304	-	86,86,99	0.53	0	92,98,111	1.17	9 (9%)
21	EDO	C	320	-	3,3,3	0.15	0	2,2,2	0.08	0
20	DMU	J	101	-	10,10,34	0.18	0	9,9,45	0.60	0
20	DMU	L	102	-	22,22,34	0.62	0	27,27,45	1.07	1 (3%)
20	DMU	W	101	-	10,10,34	0.21	0	9,9,45	0.58	0
19	LFA	P	301	-	14,14,19	0.13	0	13,13,18	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	EDO	O	308	-	3,3,3	0.11	0	2,2,2	0.43	0
19	LFA	P	310	20	17,17,19	0.20	0	16,16,18	0.13	0
24	CHD	C	305	-	32,32,32	0.61	0	51,51,51	1.41	7 (13%)
21	EDO	G	105	-	3,3,3	0.52	0	2,2,2	0.30	0
19	LFA	G	106	-	13,13,19	0.50	0	12,12,18	0.39	0
20	DMU	P	319	-	34,34,34	0.85	2 (5%)	45,45,45	1.16	3 (6%)
19	LFA	T	103	-	10,10,19	0.21	0	9,9,18	0.23	0
19	LFA	B	307	-	16,16,19	0.26	0	15,15,18	0.17	0
21	EDO	F	101	-	3,3,3	0.33	0	2,2,2	0.10	0
21	EDO	B	305	-	3,3,3	0.11	0	2,2,2	0.29	0
18	CDL	P	305	-	86,86,99	0.56	0	92,98,111	0.88	8 (8%)
20	DMU	B	302	-	10,10,34	0.21	0	9,9,45	0.66	0
24	CHD	C	301	-	32,32,32	1.10	3 (9%)	51,51,51	0.83	2 (3%)
20	DMU	P	324	-	34,34,34	0.64	0	45,45,45	1.40	4 (8%)
19	LFA	C	314	-	12,12,19	0.20	0	11,11,18	0.12	0
24	CHD	P	306	-	32,32,32	0.67	0	51,51,51	1.37	8 (15%)
21	EDO	F	103	-	3,3,3	0.49	0	2,2,2	0.13	0
19	LFA	P	311	-	10,10,19	0.15	0	9,9,18	0.10	0
20	DMU	C	315	-	34,34,34	0.86	1 (2%)	45,45,45	1.35	5 (11%)
20	DMU	A	608	-	6,6,34	0.49	0	5,5,45	0.32	0
20	DMU	B	308	-	22,22,34	0.50	0	27,27,45	1.33	3 (11%)
19	LFA	P	314	-	14,14,19	0.37	0	13,13,18	0.26	0
19	LFA	C	309	20	17,17,19	0.23	0	16,16,18	0.19	0
20	DMU	N	608	-	34,34,34	1.35	4 (11%)	45,45,45	1.26	5 (11%)
21	EDO	P	323	-	3,3,3	0.42	0	2,2,2	0.75	0
19	LFA	P	315	-	12,12,19	0.18	0	11,11,18	0.21	0
24	CHD	P	302	-	32,32,32	0.96	2 (6%)	51,51,51	0.78	1 (1%)
20	DMU	T	104	-	22,22,34	0.69	0	27,27,45	1.42	3 (11%)
21	EDO	N	612	-	3,3,3	0.27	0	2,2,2	0.24	0
22	PGV	C	303	-	50,50,50	0.63	0	53,56,56	1.07	4 (7%)
20	DMU	H	101	19	34,34,34	1.13	5 (14%)	45,45,45	1.44	8 (17%)
19	LFA	P	312	-	13,13,19	0.14	0	12,12,18	0.10	0
21	EDO	N	613	-	3,3,3	0.65	0	2,2,2	0.05	0
20	DMU	C	318	-	34,34,34	0.93	3 (8%)	45,45,45	1.21	3 (6%)
21	EDO	A	612	-	3,3,3	0.56	0	2,2,2	0.33	0
21	EDO	R	201	-	3,3,3	0.15	0	2,2,2	0.15	0
21	EDO	N	610	-	3,3,3	0.15	0	2,2,2	0.39	0
14	HEA	A	601	1	66,67,67	1.71	13 (19%)	78,103,103	2.24	22 (28%)
20	DMU	P	318	-	22,22,34	0.87	1 (4%)	27,27,45	1.40	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	DMU	Z	102	-	7,7,34	0.25	0	6,6,45	0.65	0
14	HEA	N	602	1	66,67,67	1.85	19 (28%)	78,103,103	2.64	30 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	M	102	-	-	3/5/5/59	-
21	EDO	R	203	-	-	0/1/1/1	-
21	EDO	S	103	-	-	0/1/1/1	-
22	PGV	N	614	-	-	9/55/55/55	-
20	DMU	G	104	-	-	5/13/33/59	0/1/1/2
20	DMU	A	609	-	-	6/19/59/59	0/2/2/2
19	LFA	A	607	-	-	4/11/11/17	-
20	DMU	C	316	-	-	3/4/4/59	-
18	CDL	L	101	-	-	47/104/104/110	-
21	EDO	E	203	-	-	0/1/1/1	-
19	LFA	C	324	-	-	8/12/12/17	-
20	DMU	P	320	-	-	8/19/59/59	0/2/2/2
21	EDO	E	201	-	-	0/1/1/1	-
19	LFA	T	101	-	-	5/11/11/17	-
14	HEA	N	601	1	-	4/36/76/76	-
20	DMU	N	615	19	-	8/19/59/59	0/2/2/2
21	EDO	E	202	-	-	0/1/1/1	-
24	CHD	G	102	-	-	2/9/74/74	0/4/4/4
27	PEK	T	102	-	-	19/56/56/56	-
20	DMU	C	317	-	-	8/13/33/59	0/1/1/2
20	DMU	O	306	-	-	4/8/8/59	-
19	LFA	C	313	-	-	3/12/12/17	-
21	EDO	T	105	-	-	0/1/1/1	-
19	LFA	P	313	-	-	5/8/8/17	-
21	EDO	A	611	-	-	1/1/1/1	-
19	LFA	P	309	-	-	1/3/3/17	-
20	DMU	B	303	-	-	5/8/8/59	-
21	EDO	N	609	-	-	0/1/1/1	-
18	CDL	V	101	-	-	45/74/74/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	P	307	-	-	4/8/8/59	-
20	DMU	C	323	-	-	5/19/59/59	0/2/2/2
20	DMU	A	614	-	-	3/8/8/59	-
19	LFA	C	310	-	-	6/8/8/17	-
20	DMU	C	319	-	-	11/19/59/59	0/2/2/2
21	EDO	F	104	-	-	0/1/1/1	-
21	EDO	P	321	-	-	1/1/1/1	-
20	DMU	P	317	-	-	2/4/4/59	-
20	DMU	O	305	-	-	5/8/8/59	-
18	CDL	A	606	-	-	34/74/74/110	-
21	EDO	C	322	-	-	1/1/1/1	-
14	HEA	A	602	1	-	6/36/76/76	-
21	EDO	P	322	-	-	0/1/1/1	-
22	PGV	P	304	-	-	9/55/55/55	-
20	DMU	M	101	-	-	5/19/59/59	0/2/2/2
18	CDL	Y	101	-	-	52/104/104/110	-
20	DMU	C	306	-	-	2/8/8/59	-
19	LFA	N	606	-	-	4/11/11/17	-
27	PEK	G	101	-	-	13/56/56/56	-
20	DMU	P	316	-	-	7/19/59/59	0/2/2/2
19	LFA	C	312	-	-	3/8/8/17	-
20	DMU	O	307	-	-	5/13/33/59	0/1/1/2
19	LFA	C	307	-	-	6/8/8/17	-
20	DMU	N	607	-	-	1/4/4/59	-
20	DMU	D	201	-	-	8/19/59/59	0/2/2/2
20	DMU	Q	201	-	-	8/19/59/59	0/2/2/2
20	DMU	B	304	-	-	8/13/33/59	0/1/1/2
19	LFA	C	308	-	-	1/3/3/17	-
22	PGV	A	613	-	-	12/55/55/55	-
19	LFA	O	301	-	-	7/14/14/17	-
21	EDO	N	611	-	-	0/1/1/1	-
20	DMU	Z	101	-	-	8/19/59/59	0/2/2/2
19	LFA	C	311	-	-	5/11/11/17	-
19	LFA	P	308	-	-	4/8/8/17	-
24	CHD	B	306	-	-	2/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	O	303	-	-	4/13/33/59	0/1/1/2
20	DMU	Y	102	-	-	10/13/33/59	0/1/1/2
21	EDO	A	610	-	-	0/1/1/1	-
21	EDO	R	202	-	-	0/1/1/1	-
20	DMU	G	103	-	-	4/8/8/59	-
21	EDO	S	102	-	-	0/1/1/1	-
19	LFA	O	302	-	-	4/8/8/17	-
21	EDO	C	321	-	-	0/1/1/1	-
18	CDL	C	304	-	-	45/97/97/110	-
21	EDO	C	320	-	-	0/1/1/1	-
20	DMU	J	101	-	-	4/8/8/59	-
20	DMU	L	102	-	-	10/13/33/59	0/1/1/2
20	DMU	W	101	-	-	4/8/8/59	-
19	LFA	P	301	-	-	7/12/12/17	-
21	EDO	O	308	-	-	0/1/1/1	-
19	LFA	P	310	20	-	10/15/15/17	-
24	CHD	C	305	-	-	8/9/74/74	0/4/4/4
21	EDO	G	105	-	-	0/1/1/1	-
19	LFA	G	106	-	-	5/11/11/17	-
20	DMU	P	319	-	-	14/19/59/59	0/2/2/2
19	LFA	T	103	-	-	4/8/8/17	-
19	LFA	B	307	-	-	9/14/14/17	-
21	EDO	F	101	-	-	0/1/1/1	-
21	EDO	B	305	-	-	0/1/1/1	-
18	CDL	P	305	-	-	53/97/97/110	-
20	DMU	B	302	-	-	3/8/8/59	-
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
20	DMU	P	324	-	-	7/19/59/59	0/2/2/2
19	LFA	C	314	-	-	3/10/10/17	-
24	CHD	P	306	-	-	8/9/74/74	0/4/4/4
21	EDO	F	103	-	-	0/1/1/1	-
19	LFA	P	311	-	-	6/8/8/17	-
20	DMU	C	315	-	-	11/19/59/59	0/2/2/2
20	DMU	A	608	-	-	3/4/4/59	-
20	DMU	B	308	-	-	9/13/33/59	0/1/1/2
19	LFA	P	314	-	-	5/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LFA	C	309	20	-	11/15/15/17	-
20	DMU	N	608	-	-	6/19/59/59	0/2/2/2
21	EDO	P	323	-	-	0/1/1/1	-
19	LFA	P	315	-	-	5/10/10/17	-
24	CHD	P	302	-	-	2/9/74/74	0/4/4/4
20	DMU	T	104	-	-	7/13/33/59	0/1/1/2
21	EDO	N	612	-	-	1/1/1/1	-
22	PGV	C	303	-	-	14/55/55/55	-
20	DMU	H	101	19	-	9/19/59/59	0/2/2/2
19	LFA	P	312	-	-	7/11/11/17	-
21	EDO	N	613	-	-	0/1/1/1	-
20	DMU	C	318	-	-	11/19/59/59	0/2/2/2
21	EDO	A	612	-	-	0/1/1/1	-
21	EDO	R	201	-	-	1/1/1/1	-
21	EDO	N	610	-	-	0/1/1/1	-
14	HEA	A	601	1	-	4/36/76/76	-
20	DMU	P	318	-	-	8/13/33/59	0/1/1/2
20	DMU	Z	102	-	-	2/5/5/59	-
14	HEA	N	602	1	-	4/36/76/76	-

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	CHB-C4A	5.28	1.48	1.38
14	A	601	HEA	C3A-C2A	4.56	1.46	1.36
20	D	201	DMU	O49-C1	-4.04	1.33	1.43
14	N	602	HEA	C3D-C2D	4.01	1.45	1.36
14	A	601	HEA	C4B-NB	-4.00	1.33	1.40
14	N	601	HEA	C1D-ND	-4.00	1.33	1.40
20	N	608	DMU	O16-C6	-3.95	1.33	1.40
20	Z	101	DMU	O3-C5	-3.94	1.33	1.43
14	A	602	HEA	C3B-C2B	3.87	1.43	1.34
14	N	602	HEA	C1A-C2A	3.86	1.52	1.45
14	N	601	HEA	C3A-C2A	3.79	1.44	1.36
14	A	601	HEA	C3D-C2D	3.71	1.44	1.36
14	A	602	HEA	CHD-C1D	3.63	1.45	1.38
14	N	602	HEA	C3B-C2B	3.61	1.42	1.34
20	A	609	DMU	O7-C10	3.54	1.51	1.41
14	A	602	HEA	CBD-CAD	-3.51	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	C3A-C2A	3.49	1.44	1.36
14	N	601	HEA	C4D-ND	-3.44	1.31	1.38
27	G	101	PEK	C23-C22	-3.43	1.39	1.52
24	C	301	CHD	O26-C24	-3.38	1.19	1.30
14	A	602	HEA	C1D-ND	-3.32	1.34	1.40
14	N	602	HEA	C1C-NC	-3.31	1.33	1.39
20	H	101	DMU	O5-C6	-3.30	1.33	1.41
24	P	302	CHD	O26-C24	-3.29	1.19	1.30
14	A	602	HEA	C3D-C2D	3.28	1.43	1.36
20	P	318	DMU	O16-C6	3.26	1.45	1.40
14	A	601	HEA	C1D-ND	-3.25	1.34	1.40
14	N	602	HEA	FE-NC	3.22	2.06	1.95
14	A	602	HEA	CHB-C4A	3.18	1.44	1.38
14	N	601	HEA	CHB-C4A	3.17	1.44	1.38
14	A	601	HEA	C1B-NB	-3.13	1.32	1.38
14	N	602	HEA	C3A-C2A	3.13	1.43	1.36
14	A	602	HEA	C1C-NC	-3.13	1.33	1.39
14	N	601	HEA	C16-C17	-3.10	1.43	1.53
14	N	602	HEA	C3C-C4C	3.09	1.50	1.42
14	N	602	HEA	C1D-ND	-3.09	1.35	1.40
14	A	601	HEA	CHB-C4A	3.06	1.44	1.38
14	A	602	HEA	C3C-C4C	3.04	1.49	1.42
14	A	602	HEA	FE-NC	3.04	2.05	1.95
14	A	602	HEA	C4D-ND	-3.03	1.32	1.38
14	N	602	HEA	CMA-C3A	2.98	1.51	1.45
14	A	601	HEA	C12-C11	-2.98	1.47	1.52
20	P	319	DMU	O3-C5	2.97	1.50	1.43
20	P	320	DMU	C7-C5	-2.97	1.44	1.52
14	N	602	HEA	CHC-C4B	2.96	1.44	1.38
20	N	608	DMU	C7-C5	-2.95	1.44	1.52
20	D	201	DMU	O3-C5	-2.93	1.36	1.43
24	P	302	CHD	C22-C23	-2.88	1.43	1.52
24	C	301	CHD	C22-C23	-2.86	1.43	1.52
14	A	601	HEA	CHA-C1A	2.85	1.43	1.38
20	N	608	DMU	C10-C5	-2.85	1.44	1.52
27	T	102	PEK	C2-C1	2.84	1.59	1.50
20	D	201	DMU	O55-C2	2.84	1.49	1.43
14	N	601	HEA	FE-NC	2.84	2.04	1.95
27	T	102	PEK	C23-C22	-2.83	1.41	1.52
14	A	602	HEA	CHA-C1A	2.82	1.43	1.38
20	M	101	DMU	O3-C5	-2.79	1.36	1.43
20	Q	201	DMU	C10-C5	-2.79	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	601	HEA	C4C-NC	-2.77	1.34	1.39
24	C	301	CHD	O25-C24	2.77	1.31	1.22
14	A	601	HEA	C16-C17	-2.75	1.44	1.53
20	D	201	DMU	O5-C6	-2.74	1.34	1.41
20	D	201	DMU	O61-C57	2.74	1.54	1.42
20	H	101	DMU	O16-C6	-2.73	1.35	1.40
14	N	601	HEA	C3B-C2B	2.72	1.40	1.34
14	A	602	HEA	C4C-NC	-2.68	1.34	1.39
14	A	602	HEA	C1B-NB	-2.66	1.33	1.38
20	P	316	DMU	O1-C10	2.66	1.48	1.41
14	N	601	HEA	FE-ND	2.65	2.03	1.94
20	Q	201	DMU	O16-C6	-2.61	1.35	1.40
14	N	602	HEA	CHD-C1D	2.59	1.43	1.38
14	N	602	HEA	C1C-C2C	2.58	1.49	1.43
20	C	318	DMU	C7-C5	-2.58	1.45	1.52
14	A	602	HEA	FE-NB	2.56	2.02	1.94
14	N	601	HEA	C1B-NB	-2.55	1.33	1.38
14	A	602	HEA	FE-ND	2.54	2.02	1.94
20	N	615	DMU	C7-C5	-2.54	1.45	1.52
14	A	601	HEA	FE-ND	2.54	2.02	1.94
14	A	602	HEA	C1C-C2C	2.53	1.49	1.43
14	N	602	HEA	C4D-ND	-2.52	1.33	1.38
20	D	201	DMU	C10-C5	-2.48	1.45	1.52
20	P	320	DMU	C10-C5	-2.47	1.45	1.52
20	C	318	DMU	O5-C6	-2.45	1.35	1.41
20	A	609	DMU	O7-C3	2.43	1.50	1.43
14	N	602	HEA	FE-ND	2.42	2.02	1.94
14	N	602	HEA	C4C-NC	-2.42	1.35	1.39
20	A	609	DMU	O3-C5	-2.41	1.37	1.43
20	C	315	DMU	O5-C6	-2.40	1.35	1.41
20	N	608	DMU	O1-C10	2.39	1.47	1.41
14	A	602	HEA	CHC-C1C	2.36	1.44	1.39
20	Z	101	DMU	C10-C5	-2.35	1.45	1.52
14	N	602	HEA	C1B-NB	-2.33	1.34	1.38
14	A	602	HEA	O1A-CGA	2.33	1.29	1.22
14	A	602	HEA	CHC-C4B	2.32	1.43	1.38
20	C	318	DMU	O3-C5	2.30	1.48	1.43
14	N	601	HEA	C4B-NB	-2.30	1.36	1.40
20	H	101	DMU	C10-C5	-2.28	1.45	1.52
14	N	602	HEA	CBD-CAD	-2.27	1.44	1.52
20	O	307	DMU	C6-C1	-2.27	1.46	1.52
14	A	601	HEA	CHD-C1D	2.27	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	P	316	DMU	O5-C6	-2.26	1.36	1.41
14	N	601	HEA	CHC-C4B	2.25	1.43	1.38
20	P	319	DMU	C7-C5	-2.24	1.46	1.52
20	Q	201	DMU	O3-C5	-2.22	1.37	1.43
20	A	609	DMU	O16-C6	-2.22	1.36	1.40
14	A	601	HEA	FE-NB	2.19	2.01	1.94
20	Q	201	DMU	O55-C2	2.19	1.48	1.43
14	A	602	HEA	CMA-C3A	2.18	1.49	1.45
14	N	601	HEA	C12-C13	2.18	1.60	1.53
14	N	601	HEA	O11-C11	2.17	1.47	1.42
14	N	601	HEA	C3D-C2D	2.15	1.41	1.36
14	A	601	HEA	C3B-C2B	2.14	1.39	1.34
20	C	317	DMU	O16-C6	2.13	1.43	1.40
20	H	101	DMU	C7-C5	-2.13	1.46	1.52
14	N	601	HEA	C3C-C4C	2.12	1.47	1.42
20	D	201	DMU	C7-C5	-2.12	1.46	1.52
20	Q	201	DMU	O49-C1	-2.11	1.38	1.43
20	H	101	DMU	O2-C8	2.11	1.47	1.43
14	N	602	HEA	CHA-C1A	2.11	1.42	1.38
14	A	602	HEA	C1A-C2A	2.08	1.48	1.45
20	O	303	DMU	C3-C4	-2.07	1.48	1.53
22	N	614	PGV	O01-C1	2.06	1.40	1.34
20	M	101	DMU	C6-C1	-2.05	1.46	1.52
20	G	104	DMU	C6-C1	-2.05	1.46	1.52
14	N	601	HEA	C26-C15	-2.02	1.45	1.50
24	B	306	CHD	O26-C24	-2.02	1.24	1.30
20	Q	201	DMU	O1-C10	2.01	1.47	1.41
20	C	323	DMU	C10-C5	-2.01	1.46	1.52
20	Q	201	DMU	C7-C5	-2.00	1.47	1.52

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	601	HEA	C3C-C4C-NC	8.83	115.68	110.25
14	A	601	HEA	C3D-C4D-ND	8.27	118.37	110.36
14	N	602	HEA	C3C-C4C-NC	7.84	115.07	110.25
20	P	316	DMU	O16-C6-C1	7.14	119.45	108.30
14	N	602	HEA	C3D-C4D-ND	6.93	117.07	110.36
14	A	601	HEA	C3C-C4C-NC	6.77	114.42	110.25
14	A	602	HEA	C2B-C1B-NB	6.57	117.75	109.88
14	N	601	HEA	C13-C12-C11	-6.37	104.77	114.35
14	A	601	HEA	C13-C12-C11	-6.30	104.88	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	602	HEA	C3D-C4D-ND	6.20	116.36	110.36
14	N	602	HEA	C2B-C1B-NB	6.19	117.30	109.88
20	Q	201	DMU	O16-C6-C1	6.09	117.81	108.30
20	D	201	DMU	O16-C6-C1	5.95	117.59	108.30
14	A	602	HEA	C3C-C4C-NC	5.76	113.79	110.25
14	N	602	HEA	CHB-C1B-C2B	-5.68	116.11	124.98
14	A	601	HEA	CHA-C4D-C3D	-5.34	116.99	124.84
20	C	315	DMU	O16-C6-C1	5.33	116.62	108.30
14	N	601	HEA	C3D-C4D-ND	5.26	115.45	110.36
14	N	601	HEA	C2B-C1B-NB	5.19	116.09	109.88
20	H	101	DMU	O16-C6-C1	5.17	116.38	108.30
20	P	324	DMU	C10-C5-C7	5.12	120.66	110.00
20	O	303	DMU	O5-C6-C1	5.05	121.03	110.35
14	N	602	HEA	C2D-C1D-ND	4.97	115.73	109.84
14	A	602	HEA	C2D-C1D-ND	4.96	115.72	109.84
14	N	602	HEA	C3B-C4B-NB	4.95	115.70	109.84
27	T	102	PEK	O01-C1-O02	-4.94	111.76	123.70
24	P	306	CHD	C17-C13-C14	-4.73	95.32	100.09
20	T	104	DMU	O16-C6-C1	4.69	115.63	108.30
20	P	318	DMU	O5-C6-C1	4.65	120.19	110.35
18	A	606	CDL	CA4-OA6-CA5	4.56	129.02	117.79
20	P	320	DMU	O16-C6-C1	4.54	115.38	108.30
20	Z	101	DMU	O16-C6-C1	4.52	115.36	108.30
20	C	317	DMU	O5-C6-C1	4.52	119.92	110.35
14	N	602	HEA	CHA-C4D-C3D	-4.50	118.23	124.84
14	A	602	HEA	CHA-C4D-C3D	-4.39	118.38	124.84
14	N	602	HEA	C4B-NB-C1B	-4.38	100.55	105.07
14	N	602	HEA	C2C-C1C-NC	4.35	116.70	110.08
14	N	601	HEA	C4D-C3D-C2D	-4.29	100.65	106.90
14	A	602	HEA	C3B-C4B-NB	4.27	114.90	109.84
20	P	324	DMU	O16-C6-C1	4.27	114.97	108.30
14	A	602	HEA	CMD-C2D-C1D	4.27	131.54	125.04
14	N	602	HEA	CAD-C3D-C4D	4.25	132.08	124.66
24	C	305	CHD	C5-C6-C7	4.21	119.10	114.46
18	C	304	CDL	OA6-CA5-C11	-4.17	102.52	111.50
18	C	304	CDL	OA4-PA1-OA5	-4.16	88.43	107.75
14	A	601	HEA	C4D-C3D-C2D	-4.13	100.89	106.90
20	N	615	DMU	O16-C6-C1	4.11	114.71	108.30
14	A	602	HEA	C4B-NB-C1B	-4.09	100.84	105.07
14	N	602	HEA	CMD-C2D-C1D	4.05	131.21	125.04
14	N	602	HEA	C3A-C2A-C1A	-4.03	103.23	107.08
18	C	304	CDL	OA5-PA1-OA3	4.01	124.75	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	601	HEA	C2C-C1C-NC	3.97	116.12	110.08
20	C	323	DMU	O16-C6-C1	3.97	114.50	108.30
20	C	318	DMU	O16-C6-C1	3.93	114.44	108.30
22	N	614	PGV	O03-C19-O04	-3.93	113.68	123.59
14	N	601	HEA	CHB-C1B-C2B	-3.91	118.87	124.98
20	N	615	DMU	C10-C5-C7	3.85	118.01	110.00
14	N	602	HEA	C3C-C2C-C1C	-3.82	102.55	107.16
14	N	601	HEA	C2A-C1A-NA	3.80	114.02	110.32
20	N	608	DMU	C10-O1-C9	3.79	121.12	113.69
22	A	613	PGV	O03-C19-O04	-3.78	114.04	123.59
14	A	601	HEA	C2C-C1C-NC	3.78	115.83	110.08
14	N	601	HEA	C3C-C2C-C1C	-3.75	102.64	107.16
14	A	601	HEA	C3C-C2C-C1C	-3.74	102.64	107.16
24	C	305	CHD	C6-C7-C8	3.68	115.41	111.48
14	N	602	HEA	C1D-C2D-C3D	-3.66	103.11	106.96
18	A	606	CDL	OA6-CA4-CA6	3.66	121.65	108.40
14	A	602	HEA	C3C-C2C-C1C	-3.63	102.78	107.16
14	A	602	HEA	C2C-C1C-NC	3.62	115.59	110.08
14	N	601	HEA	C4C-NC-C1C	-3.61	101.81	105.35
18	V	101	CDL	OA6-CA5-C11	3.61	119.28	111.50
22	C	303	PGV	O03-C19-O04	-3.58	114.56	123.59
14	N	602	HEA	C4C-NC-C1C	-3.58	101.85	105.35
20	C	317	DMU	C18-O16-C6	-3.55	107.95	113.84
20	C	318	DMU	C10-C5-C7	3.53	117.35	110.00
20	B	308	DMU	O16-C6-C1	3.50	113.77	108.30
14	A	601	HEA	C3B-C4B-NB	3.50	113.98	109.84
20	C	319	DMU	O16-C6-C1	3.48	113.74	108.30
20	L	102	DMU	O5-C6-O16	3.47	118.18	109.97
14	A	602	HEA	C4D-C3D-C2D	-3.46	101.85	106.90
20	A	609	DMU	O3-C5-C7	3.46	118.34	110.35
24	C	305	CHD	C17-C13-C14	-3.45	96.61	100.09
14	A	601	HEA	CAD-C3D-C4D	3.44	130.67	124.66
14	N	601	HEA	C3B-C4B-NB	3.42	113.89	109.84
27	T	102	PEK	O02-C1-C2	3.40	137.01	123.73
20	P	319	DMU	O16-C6-C1	3.40	113.61	108.30
24	P	306	CHD	C16-C17-C20	3.40	117.41	112.15
20	Y	102	DMU	O5-C6-O16	3.39	118.01	109.97
18	C	304	CDL	OA4-PA1-OA3	3.38	128.96	112.24
20	B	308	DMU	O5-C6-C1	3.37	117.49	110.35
14	N	602	HEA	C4D-C3D-C2D	-3.37	101.98	106.90
20	T	104	DMU	C18-O16-C6	-3.37	108.25	113.84
14	A	602	HEA	CMB-C2B-C1B	3.34	130.12	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	P	316	DMU	C10-C5-C7	3.26	116.78	110.00
24	C	305	CHD	C14-C13-C12	3.25	110.43	107.40
14	A	601	HEA	C26-C15-C16	3.24	120.72	115.27
24	C	305	CHD	C16-C17-C20	3.24	117.16	112.15
14	N	602	HEA	C4A-CHB-C1B	-3.23	119.09	126.06
18	V	101	CDL	OA6-CA4-CA3	3.21	120.03	108.40
14	N	601	HEA	C26-C15-C16	3.20	120.65	115.27
20	P	320	DMU	C10-C5-C7	3.19	116.64	110.00
27	T	102	PEK	C2-C3-C4	3.18	118.89	113.23
22	P	304	PGV	C27-C26-C25	-3.17	98.32	114.42
18	C	304	CDL	OA7-CA5-C11	3.17	136.10	123.73
20	C	319	DMU	C10-C5-C7	3.17	116.59	110.00
20	M	101	DMU	O16-C6-C1	3.16	113.24	108.30
14	A	602	HEA	CHB-C1B-C2B	-3.14	120.07	124.98
20	P	319	DMU	C10-C5-C7	3.14	116.53	110.00
20	O	303	DMU	O16-C6-C1	3.14	113.20	108.30
14	N	601	HEA	CHA-C4D-C3D	-3.13	120.24	124.84
14	A	602	HEA	C1B-C2B-C3B	-3.12	103.07	106.80
14	A	602	HEA	C1D-C2D-C3D	-3.09	103.71	106.96
14	N	602	HEA	CAD-CBD-CGD	-3.08	106.98	113.60
14	N	601	HEA	C3A-C2A-C1A	-3.05	104.16	107.08
20	Q	201	DMU	C10-O1-C9	3.04	119.66	113.69
20	Q	201	DMU	C6-O5-C4	-3.03	107.73	113.69
14	N	602	HEA	CHC-C1C-C2C	-3.02	118.69	127.24
14	N	602	HEA	C1D-ND-C4D	-3.00	101.98	105.07
20	H	101	DMU	C18-O16-C6	-2.99	108.88	113.84
20	Q	201	DMU	O1-C9-C8	2.95	115.05	109.69
20	H	101	DMU	C7-C8-C9	-2.95	104.98	110.24
20	A	609	DMU	O1-C10-C5	-2.94	104.13	110.35
14	A	602	HEA	CHC-C1C-C2C	-2.93	118.97	127.24
20	Q	201	DMU	C11-C9-C8	-2.93	106.15	113.00
14	A	601	HEA	C4C-NC-C1C	-2.89	102.51	105.35
18	P	305	CDL	OA4-PA1-OA2	-2.86	94.48	107.75
14	A	601	HEA	CHB-C1B-C2B	-2.86	120.52	124.98
20	P	316	DMU	O1-C9-C11	2.84	113.50	106.44
20	P	316	DMU	O5-C6-O16	-2.83	103.28	109.97
14	A	601	HEA	C2D-C1D-ND	2.82	113.19	109.84
20	N	615	DMU	C18-O16-C6	-2.80	109.20	113.84
14	A	601	HEA	C1D-ND-C4D	-2.79	102.19	105.07
20	D	201	DMU	C10-O1-C9	2.77	119.13	113.69
20	P	318	DMU	C18-O16-C6	-2.77	109.25	113.84
14	A	601	HEA	C3A-C2A-C1A	-2.77	104.43	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	304	PGV	C22-C21-C20	-2.76	103.27	113.19
14	A	602	HEA	O1D-CGD-CBD	-2.75	114.24	123.08
24	P	306	CHD	C14-C13-C12	2.75	109.96	107.40
14	N	602	HEA	CMB-C2B-C1B	2.74	129.22	125.04
14	A	601	HEA	CHC-C1C-C2C	-2.74	119.51	127.24
18	V	101	CDL	OA6-CA4-CA6	-2.73	98.50	108.40
20	C	317	DMU	C6-C1-C2	2.73	115.68	110.00
20	A	609	DMU	O5-C6-O16	2.73	116.43	109.97
20	N	615	DMU	O3-C5-C10	2.72	116.64	110.05
14	N	602	HEA	C1B-C2B-C3B	-2.70	103.58	106.80
20	H	101	DMU	O5-C6-C1	2.69	116.03	110.35
20	M	101	DMU	O3-C5-C7	2.69	116.56	110.35
18	P	305	CDL	OA5-PA1-OA3	2.67	119.50	109.07
14	A	602	HEA	C1D-ND-C4D	-2.66	102.32	105.07
20	P	318	DMU	C6-C1-C2	2.66	115.53	110.00
14	N	602	HEA	C4B-C3B-C2B	-2.66	102.87	107.41
20	G	104	DMU	O16-C6-C1	2.65	112.45	108.30
20	N	615	DMU	C10-O7-C3	-2.65	111.42	117.96
18	C	304	CDL	OA4-PA1-OA2	-2.64	95.49	107.75
14	A	602	HEA	C3A-C2A-C1A	-2.64	104.56	107.08
20	B	304	DMU	O5-C6-C1	2.63	115.91	110.35
20	B	308	DMU	C6-O5-C4	2.60	118.80	113.69
20	C	315	DMU	C6-O5-C4	2.60	118.79	113.69
20	P	324	DMU	C10-O1-C9	-2.59	108.61	113.69
14	N	601	HEA	C4B-NB-C1B	-2.58	102.41	105.07
20	H	101	DMU	C10-C5-C7	2.58	115.37	110.00
20	C	315	DMU	C10-C5-C7	2.58	115.36	110.00
20	P	316	DMU	O7-C3-C2	2.57	114.13	107.28
20	C	319	DMU	O3-C5-C10	2.57	116.30	110.05
14	A	601	HEA	C2B-C1B-NB	2.57	112.96	109.88
20	D	201	DMU	C10-C5-C7	2.57	115.35	110.00
14	N	601	HEA	C1B-C2B-C3B	-2.57	103.73	106.80
20	Y	102	DMU	O5-C6-C1	2.56	115.77	110.35
14	N	602	HEA	C21-C20-C19	2.56	121.39	112.98
18	C	304	CDL	OB6-CB5-C51	2.55	117.00	111.50
22	C	303	PGV	C24-C23-C22	2.54	127.31	114.42
20	O	303	DMU	C6-C1-C2	2.53	115.27	110.00
20	P	316	DMU	C57-C4-C3	-2.52	105.98	113.33
14	A	602	HEA	C4A-C3A-C2A	-2.52	104.68	106.75
20	N	608	DMU	C7-C8-C9	2.52	114.74	110.24
20	O	307	DMU	O5-C6-C1	2.51	115.67	110.35
20	P	319	DMU	O3-C5-C10	2.50	116.13	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	319	DMU	O5-C6-C1	2.50	115.64	110.35
18	C	304	CDL	O1-C1-CB2	2.48	118.25	109.56
20	C	315	DMU	O3-C5-C10	2.47	116.04	110.05
14	A	602	HEA	CAD-CBD-CGD	-2.46	108.30	113.60
20	P	320	DMU	O5-C6-C1	2.41	115.45	110.35
14	N	602	HEA	O1D-CGD-CBD	-2.40	115.37	123.08
20	N	608	DMU	O5-C6-C1	2.39	115.42	110.35
22	C	303	PGV	C25-C24-C23	2.39	126.54	114.42
14	A	602	HEA	C4B-C3B-C2B	-2.39	103.33	107.41
20	H	101	DMU	C2-C3-C4	-2.38	105.48	110.93
14	N	601	HEA	O11-C11-C12	2.37	116.03	109.42
14	A	601	HEA	C13-C14-C15	-2.37	121.97	127.66
20	N	608	DMU	O5-C6-O16	2.35	115.54	109.97
20	H	101	DMU	O3-C5-C10	2.34	115.72	110.05
18	C	304	CDL	OB5-PB2-OB3	2.34	118.19	109.07
20	O	307	DMU	O5-C6-O16	2.33	115.50	109.97
20	Q	201	DMU	C57-C4-C3	2.32	120.09	113.33
20	Q	201	DMU	C2-C3-C4	-2.32	105.61	110.93
14	A	601	HEA	CMC-C2C-C1C	2.32	128.90	125.37
22	A	613	PGV	C25-C24-C23	2.31	126.17	114.42
14	A	602	HEA	CBD-CAD-C3D	2.30	119.03	112.63
18	P	305	CDL	O1-C1-CB2	2.30	117.63	109.56
20	Q	201	DMU	O3-C5-C7	2.29	115.65	110.35
27	G	101	PEK	O13-P-O14	2.29	123.56	112.24
20	O	307	DMU	C57-C4-C3	-2.29	107.64	113.00
18	L	101	CDL	OB4-PB2-OB2	2.28	118.35	107.75
20	O	303	DMU	C57-C4-C3	-2.28	107.67	113.00
24	C	301	CHD	C18-C13-C12	2.27	111.38	109.07
14	A	602	HEA	CHD-C1D-C2D	-2.27	120.42	126.73
24	P	302	CHD	C22-C20-C17	-2.27	105.61	110.28
14	N	601	HEA	C26-C15-C14	-2.26	117.88	123.68
22	P	304	PGV	O03-C19-O04	-2.26	117.90	123.59
20	Z	101	DMU	C10-C5-C7	2.25	114.68	110.00
20	H	101	DMU	O7-C3-C2	2.25	113.26	107.28
20	C	323	DMU	O3-C5-C7	2.24	115.53	110.35
14	N	601	HEA	C25-C23-C24	2.24	119.55	114.60
20	P	320	DMU	C10-O7-C3	-2.22	112.48	117.96
24	P	306	CHD	C16-C17-C13	-2.21	101.38	103.55
20	D	201	DMU	C2-C3-C4	-2.21	105.86	110.93
14	N	602	HEA	CBD-CAD-C3D	2.21	118.76	112.63
14	A	601	HEA	C2A-C1A-NA	2.21	112.47	110.32
14	N	602	HEA	CHC-C4B-C3B	-2.20	120.14	125.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	P	306	CHD	C6-C7-C8	2.19	113.82	111.48
14	A	602	HEA	C4C-NC-C1C	-2.19	103.20	105.35
20	P	316	DMU	O3-C5-C10	2.19	115.36	110.05
14	A	601	HEA	C4B-C3B-C2B	-2.18	103.69	107.41
18	P	305	CDL	OA8-CA6-CA4	-2.18	102.09	108.43
20	O	307	DMU	C18-O16-C6	-2.17	110.23	113.84
20	A	609	DMU	O3-C5-C10	2.16	115.31	110.05
14	N	602	HEA	C2A-C1A-NA	2.16	112.43	110.32
20	N	608	DMU	O1-C9-C8	2.16	113.62	109.69
20	T	104	DMU	C57-C4-C3	-2.16	107.96	113.00
22	N	614	PGV	O03-C01-C02	2.15	114.70	108.43
24	P	306	CHD	C18-C13-C14	2.15	114.58	111.21
20	A	609	DMU	C10-C5-C7	2.14	114.45	110.00
14	A	602	HEA	CAD-C3D-C4D	2.14	128.39	124.66
18	P	305	CDL	OA4-PA1-OA5	-2.13	97.83	107.75
18	P	305	CDL	OA2-PA1-OA3	2.13	117.38	109.07
20	Z	101	DMU	O3-C5-C7	2.12	115.26	110.35
20	C	323	DMU	C10-C5-C7	2.12	114.41	110.00
18	P	305	CDL	OB5-PB2-OB3	2.12	117.33	109.07
14	N	602	HEA	C27-C19-C20	2.11	118.82	115.27
20	Q	201	DMU	C10-C5-C7	2.11	114.39	110.00
20	A	609	DMU	O7-C3-C4	2.10	115.19	109.45
14	N	601	HEA	C4B-C3B-C2B	-2.10	103.83	107.41
14	A	602	HEA	CHA-C1A-C2A	-2.09	121.54	124.94
24	C	305	CHD	C9-C8-C7	2.09	114.38	111.88
20	G	104	DMU	C18-O16-C6	-2.09	110.37	113.84
24	C	301	CHD	C22-C20-C17	-2.09	105.98	110.28
18	A	606	CDL	OA5-PA1-OA3	2.08	117.21	109.07
24	P	306	CHD	C18-C13-C12	-2.08	106.95	109.07
20	P	316	DMU	C6-O5-C4	2.08	117.76	113.69
18	P	305	CDL	OA4-PA1-OA3	2.07	122.49	112.24
20	C	315	DMU	O5-C6-O16	-2.07	105.07	109.97
20	C	319	DMU	O5-C6-O16	2.07	114.88	109.97
14	A	602	HEA	CHB-C1B-NB	-2.07	122.17	124.42
24	C	305	CHD	O25-C24-C23	-2.06	116.46	123.08
20	A	609	DMU	O7-C10-C5	2.06	113.44	108.10
24	P	306	CHD	C14-C8-C7	-2.06	109.07	111.81
14	N	601	HEA	C2D-C1D-ND	2.06	112.28	109.84
14	A	602	HEA	C26-C15-C16	2.06	118.73	115.27
14	A	602	HEA	C16-C15-C14	-2.06	116.96	121.12
20	P	324	DMU	O7-C10-O1	-2.05	104.94	110.67
22	P	304	PGV	O14-P-O13	2.05	122.35	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	318	DMU	C10-O1-C9	-2.04	109.68	113.69
14	N	601	HEA	CHC-C1C-C2C	-2.03	121.49	127.24
14	A	601	HEA	C1B-C2B-C3B	-2.03	104.37	106.80
20	C	319	DMU	C11-C9-C8	-2.03	108.24	113.00
20	C	319	DMU	O3-C5-C7	2.03	115.04	110.35
14	N	602	HEA	CBA-CAA-C2A	-2.02	107.01	112.63
18	A	606	CDL	OA2-PA1-OA3	-2.02	101.17	109.07
14	A	602	HEA	CAA-C2A-C1A	2.02	128.71	124.89
14	N	601	HEA	CAD-C3D-C2D	2.02	131.64	127.88
20	C	323	DMU	O5-C6-O16	2.01	114.74	109.97
22	C	303	PGV	O04-C19-C20	2.01	131.57	123.73

There are no chirality outliers.

All (795) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
18	V	101	CDL	CB3-OB5-PB2-OB2
18	V	101	CDL	CB3-OB5-PB2-OB3
18	V	101	CDL	CB3-OB5-PB2-OB4
18	V	101	CDL	OB7-CB5-OB6-CB4
18	Y	101	CDL	CA2-OA2-PA1-OA3
18	Y	101	CDL	C11-CA5-OA6-CA4
18	Y	101	CDL	CB2-OB2-PB2-OB3
18	Y	101	CDL	OB6-CB4-CB6-OB8
18	Y	101	CDL	C51-CB5-OB6-CB4
20	B	304	DMU	C1-C6-O16-C18
20	B	304	DMU	O5-C6-O16-C18
20	B	308	DMU	O5-C6-O16-C18
20	B	308	DMU	C19-C18-O16-C6
20	C	318	DMU	C1-C6-O16-C18
20	C	318	DMU	C19-C18-O16-C6
20	D	201	DMU	C19-C18-O16-C6
20	L	102	DMU	C19-C18-O16-C6
20	N	615	DMU	C1-C6-O16-C18
20	O	307	DMU	C19-C18-O16-C6
20	Q	201	DMU	O5-C6-O16-C18
20	T	104	DMU	C1-C6-O16-C18
20	Y	102	DMU	C1-C6-O16-C18
24	C	305	CHD	C13-C17-C20-C21
24	C	305	CHD	C13-C17-C20-C22
24	C	305	CHD	C16-C17-C20-C22
24	P	306	CHD	C13-C17-C20-C21
24	P	306	CHD	C13-C17-C20-C22
24	P	306	CHD	C16-C17-C20-C21
27	G	101	PEK	C11-C12-C13-C14
27	T	102	PEK	C11-C10-C9-C8
27	T	102	PEK	C12-C13-C14-C15
18	Y	101	CDL	OA9-CA7-OA8-CA6
24	C	305	CHD	C16-C17-C20-C21
20	O	303	DMU	O5-C4-C57-O61
18	A	606	CDL	OB7-CB5-OB6-CB4
18	L	101	CDL	OA7-CA5-OA6-CA4
18	L	101	CDL	OB7-CB5-OB6-CB4
18	P	305	CDL	OA7-CA5-OA6-CA4
18	V	101	CDL	OA7-CA5-OA6-CA4
18	Y	101	CDL	OA7-CA5-OA6-CA4
18	Y	101	CDL	OB7-CB5-OB6-CB4
18	V	101	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
18	C	304	CDL	C11-CA5-OA6-CA4
18	P	305	CDL	C11-CA5-OA6-CA4
18	P	305	CDL	C51-CB5-OB6-CB4
18	V	101	CDL	C51-CB5-OB6-CB4
20	C	319	DMU	O5-C4-C57-O61
20	T	104	DMU	O5-C4-C57-O61
20	L	102	DMU	C3-C4-C57-O61
24	P	306	CHD	C16-C17-C20-C22
18	Y	101	CDL	C31-CA7-OA8-CA6
20	P	320	DMU	O6-C11-C9-O1
19	C	324	LFA	C9-C10-C11-C12
19	P	308	LFA	C7-C8-C9-C10
20	C	317	DMU	O5-C4-C57-O61
20	C	318	DMU	O6-C11-C9-O1
20	C	319	DMU	O6-C11-C9-O1
18	P	305	CDL	O1-C1-CB2-OB2
18	Y	101	CDL	O1-C1-CB2-OB2
18	C	304	CDL	C31-CA7-OA8-CA6
20	P	318	DMU	O5-C4-C57-O61
20	C	319	DMU	C3-C4-C57-O61
19	C	309	LFA	C11-C10-C9-C8
22	A	613	PGV	C26-C27-C28-C29
19	P	311	LFA	C5-C6-C7-C8
19	T	101	LFA	C9-C10-C11-C12
20	B	308	DMU	O5-C4-C57-O61
20	A	609	DMU	O6-C11-C9-C8
20	O	303	DMU	C3-C4-C57-O61
20	T	104	DMU	C3-C4-C57-O61
20	C	315	DMU	O6-C11-C9-O1
20	L	102	DMU	O5-C4-C57-O61
18	C	304	CDL	OA7-CA5-OA6-CA4
20	P	320	DMU	O6-C11-C9-C8
19	P	301	LFA	C2-C3-C4-C5
18	V	101	CDL	OA9-CA7-OA8-CA6
20	A	609	DMU	O6-C11-C9-O1
22	C	303	PGV	C28-C29-C30-C31
20	N	608	DMU	O6-C11-C9-C8
20	N	608	DMU	O5-C6-O16-C18
19	C	309	LFA	C12-C13-C14-C15
20	P	318	DMU	C3-C4-C57-O61
19	P	301	LFA	C7-C8-C9-C10
18	C	304	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
18	Y	101	CDL	CB2-C1-CA2-OA2
18	A	606	CDL	OA7-CA5-OA6-CA4
20	C	319	DMU	O6-C11-C9-C8
18	C	304	CDL	OA9-CA7-OA8-CA6
18	C	304	CDL	C71-CB7-OB8-CB6
18	C	304	CDL	CB5-C51-C52-C53
22	N	614	PGV	C26-C27-C28-C29
19	B	307	LFA	C9-C10-C11-C12
22	A	613	PGV	C23-C24-C25-C26
18	L	101	CDL	O1-C1-CA2-OA2
18	P	305	CDL	O1-C1-CA2-OA2
18	Y	101	CDL	O1-C1-CA2-OA2
18	P	305	CDL	CB5-C51-C52-C53
18	L	101	CDL	CB7-C71-C72-C73
18	P	305	CDL	C31-CA7-OA8-CA6
20	N	615	DMU	O5-C4-C57-O61
18	A	606	CDL	CA5-C11-C12-C13
18	C	304	CDL	CA7-C31-C32-C33
20	P	319	DMU	O6-C11-C9-O1
18	C	304	CDL	CB7-C71-C72-C73
18	V	101	CDL	CA5-C11-C12-C13
20	C	318	DMU	O16-C18-C19-C22
20	L	102	DMU	O16-C18-C19-C22
20	D	201	DMU	O6-C11-C9-O1
20	H	101	DMU	O5-C4-C57-O61
20	C	317	DMU	C3-C4-C57-O61
20	Y	102	DMU	O16-C18-C19-C22
18	V	101	CDL	CA7-C31-C32-C33
18	Y	101	CDL	CA5-C11-C12-C13
20	B	308	DMU	C3-C4-C57-O61
20	P	319	DMU	O16-C18-C19-C22
18	C	304	CDL	OB9-CB7-OB8-CB6
20	C	317	DMU	O16-C18-C19-C22
20	C	318	DMU	O5-C6-O16-C18
20	N	615	DMU	O5-C6-O16-C18
20	T	104	DMU	O5-C6-O16-C18
20	G	104	DMU	O16-C18-C19-C22
18	C	304	CDL	O1-C1-CA2-OA2
18	V	101	CDL	O1-C1-CB2-OB2
20	C	318	DMU	O6-C11-C9-C8
27	T	102	PEK	C7-C8-C9-C10
20	P	319	DMU	C3-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
19	P	310	LFA	C11-C10-C9-C8
18	A	606	CDL	CA3-OA5-PA1-OA2
18	A	606	CDL	CB3-OB5-PB2-OB2
18	L	101	CDL	CB2-OB2-PB2-OB5
18	P	305	CDL	CA2-OA2-PA1-OA5
18	P	305	CDL	CA3-OA5-PA1-OA2
18	V	101	CDL	CA3-OA5-PA1-OA2
18	V	101	CDL	CB2-OB2-PB2-OB5
20	P	319	DMU	O5-C4-C57-O61
18	V	101	CDL	CA2-C1-CB2-OB2
19	C	312	LFA	C1-C2-C3-C4
18	L	101	CDL	C31-CA7-OA8-CA6
20	N	608	DMU	O16-C18-C19-C22
19	G	106	LFA	C11-C10-C9-C8
18	A	606	CDL	C11-CA5-OA6-CA4
18	A	606	CDL	C17-C18-C19-C20
18	C	304	CDL	C35-C36-C37-C38
18	P	305	CDL	C11-C12-C13-C14
18	Y	101	CDL	C79-C80-C81-C82
19	B	307	LFA	C13-C14-C15-C16
19	P	310	LFA	C5-C6-C7-C8
20	P	319	DMU	C28-C31-C34-C37
18	P	305	CDL	C56-C57-C58-C59
19	P	311	LFA	C7-C8-C9-C10
19	P	312	LFA	C10-C11-C12-C13
18	A	606	CDL	C75-C76-C77-C78
19	P	312	LFA	C3-C4-C5-C6
19	T	101	LFA	C5-C6-C7-C8
20	B	303	DMU	C19-C22-C25-C28
22	N	614	PGV	C14-C15-C16-C17
19	B	307	LFA	C4-C5-C6-C7
19	B	307	LFA	C7-C8-C9-C10
22	C	303	PGV	C7-C8-C9-C10
18	A	606	CDL	C78-C79-C80-C81
18	Y	101	CDL	C13-C14-C15-C16
19	P	310	LFA	C13-C14-C15-C16
20	G	104	DMU	C28-C31-C34-C37
27	T	102	PEK	C22-C23-C24-C25
20	N	608	DMU	O6-C11-C9-O1
20	P	319	DMU	C1-C6-O16-C18
18	L	101	CDL	C37-C38-C39-C40
18	V	101	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
18	V	101	CDL	C77-C78-C79-C80
18	Y	101	CDL	C16-C17-C18-C19
20	B	304	DMU	C31-C34-C37-C40
20	P	316	DMU	C28-C31-C34-C37
27	G	101	PEK	C16-C17-C18-C19
19	P	313	LFA	C1-C2-C3-C4
20	P	320	DMU	C4-C3-O7-C10
22	P	304	PGV	C24-C25-C26-C27
18	C	304	CDL	C22-C23-C24-C25
18	C	304	CDL	C51-C52-C53-C54
20	C	315	DMU	C19-C22-C25-C28
20	C	315	DMU	C28-C31-C34-C37
18	Y	101	CDL	C63-C64-C65-C66
19	O	301	LFA	C5-C6-C7-C8
20	L	102	DMU	C31-C34-C37-C40
27	T	102	PEK	C26-C27-C28-C29
19	O	301	LFA	C13-C14-C15-C16
19	P	313	LFA	C4-C5-C6-C7
22	P	304	PGV	C12-C13-C14-C15
27	T	102	PEK	C1-C2-C3-C4
18	L	101	CDL	C14-C15-C16-C17
18	V	101	CDL	C17-C18-C19-C20
18	V	101	CDL	C76-C77-C78-C79
19	C	309	LFA	C5-C6-C7-C8
19	G	106	LFA	C5-C6-C7-C8
20	C	318	DMU	C31-C34-C37-C40
20	G	104	DMU	C25-C28-C31-C34
20	P	318	DMU	C31-C34-C37-C40
22	C	303	PGV	C14-C15-C16-C17
27	G	101	PEK	C26-C27-C28-C29
18	P	305	CDL	OA9-CA7-OA8-CA6
20	C	315	DMU	O6-C11-C9-C8
20	Y	102	DMU	O5-C6-O16-C18
19	C	312	LFA	C5-C6-C7-C8
19	O	302	LFA	C5-C6-C7-C8
19	P	301	LFA	C9-C10-C11-C12
20	C	317	DMU	C22-C25-C28-C31
20	L	102	DMU	C25-C28-C31-C34
20	Z	101	DMU	C22-C25-C28-C31
20	P	318	DMU	C18-C19-C22-C25
18	Y	101	CDL	C61-C62-C63-C64
18	Y	101	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
19	P	310	LFA	C4-C5-C6-C7
20	C	316	DMU	C28-C31-C34-C37
22	A	613	PGV	C29-C30-C31-C32
18	V	101	CDL	C78-C79-C80-C81
19	P	301	LFA	C6-C7-C8-C9
19	P	314	LFA	C2-C3-C4-C5
27	G	101	PEK	C34-C35-C36-C37
20	B	304	DMU	C19-C18-O16-C6
20	G	104	DMU	C19-C18-O16-C6
20	H	101	DMU	C19-C18-O16-C6
20	P	320	DMU	C19-C18-O16-C6
20	Y	102	DMU	C19-C18-O16-C6
18	C	304	CDL	C33-C34-C35-C36
19	C	310	LFA	C5-C6-C7-C8
20	B	303	DMU	C18-C19-C22-C25
27	T	102	PEK	C13-C14-C15-C16
19	C	311	LFA	C4-C5-C6-C7
19	P	312	LFA	C5-C6-C7-C8
20	P	317	DMU	C31-C34-C37-C40
22	C	303	PGV	C13-C14-C15-C16
19	N	606	LFA	C10-C11-C12-C13
19	P	301	LFA	C4-C5-C6-C7
19	A	607	LFA	C9-C10-C11-C12
20	L	102	DMU	C22-C25-C28-C31
22	C	303	PGV	C25-C26-C27-C28
18	C	304	CDL	C71-C72-C73-C74
18	L	101	CDL	C17-C18-C19-C20
18	P	305	CDL	C52-C53-C54-C55
20	J	101	DMU	C25-C28-C31-C34
27	G	101	PEK	C15-C16-C17-C18
27	T	102	PEK	C2-C3-C4-C5
19	C	324	LFA	C6-C7-C8-C9
18	C	304	CDL	C75-C76-C77-C78
20	D	201	DMU	O16-C18-C19-C22
18	L	101	CDL	OA9-CA7-OA8-CA6
20	M	101	DMU	C22-C25-C28-C31
20	P	318	DMU	C28-C31-C34-C37
20	C	317	DMU	C19-C22-C25-C28
27	G	101	PEK	C28-C29-C30-C31
18	Y	101	CDL	C51-C52-C53-C54
19	C	311	LFA	C11-C10-C9-C8
22	P	304	PGV	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
18	Y	101	CDL	C76-C77-C78-C79
20	A	608	DMU	C28-C31-C34-C37
22	C	303	PGV	C22-C23-C24-C25
27	T	102	PEK	C17-C18-C19-C20
18	L	101	CDL	C13-C14-C15-C16
18	L	101	CDL	C72-C73-C74-C75
20	A	609	DMU	C31-C34-C37-C40
20	C	317	DMU	C31-C34-C37-C40
24	C	305	CHD	C21-C20-C22-C23
20	O	307	DMU	C34-C37-C40-C43
20	P	320	DMU	C2-C3-O7-C10
18	C	304	CDL	C23-C24-C25-C26
22	P	304	PGV	C30-C31-C32-C33
20	P	324	DMU	O16-C18-C19-C22
18	L	101	CDL	C34-C35-C36-C37
22	C	303	PGV	C24-C25-C26-C27
22	P	304	PGV	C7-C8-C9-C10
24	P	306	CHD	C21-C20-C22-C23
19	C	324	LFA	C7-C8-C9-C10
19	P	313	LFA	C3-C4-C5-C6
20	O	306	DMU	C18-C19-C22-C25
18	Y	101	CDL	C21-C22-C23-C24
19	C	309	LFA	C3-C4-C5-C6
20	P	320	DMU	C22-C25-C28-C31
19	C	309	LFA	C1-C2-C3-C4
19	P	310	LFA	C3-C4-C5-C6
20	B	304	DMU	O16-C18-C19-C22
20	N	608	DMU	C31-C34-C37-C40
19	C	307	LFA	C3-C4-C5-C6
20	A	614	DMU	C19-C22-C25-C28
22	N	614	PGV	C30-C31-C32-C33
20	C	316	DMU	C31-C34-C37-C40
22	N	614	PGV	C29-C30-C31-C32
22	A	613	PGV	C12-C13-C14-C15
22	N	614	PGV	C12-C13-C14-C15
18	V	101	CDL	C72-C73-C74-C75
19	C	307	LFA	C4-C5-C6-C7
19	C	308	LFA	C2-C3-C4-C5
20	M	101	DMU	C25-C28-C31-C34
20	W	101	DMU	C25-C28-C31-C34
20	B	303	DMU	C28-C31-C34-C37
20	O	306	DMU	C19-C22-C25-C28

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Mol	Chain	Res	Type	Atoms
18	Y	101	CDL	CA2-OA2-PA1-OA5
18	Y	101	CDL	CB3-OB5-PB2-OB2
20	C	319	DMU	C22-C25-C28-C31
27	G	101	PEK	C25-C26-C27-C28
18	V	101	CDL	C1-CA2-OA2-PA1
19	O	301	LFA	C11-C12-C13-C14
20	P	316	DMU	C18-C19-C22-C25
18	A	606	CDL	C19-C20-C21-C22
20	B	308	DMU	O16-C18-C19-C22
20	P	307	DMU	O16-C18-C19-C22
18	Y	101	CDL	C57-C58-C59-C60
20	C	319	DMU	C19-C22-C25-C28
18	P	305	CDL	C53-C54-C55-C56
18	V	101	CDL	C31-C32-C33-C34
19	P	314	LFA	C6-C7-C8-C9
20	P	320	DMU	C25-C28-C31-C34
20	Y	102	DMU	C19-C22-C25-C28
18	L	101	CDL	CB5-C51-C52-C53
19	C	310	LFA	C6-C7-C8-C9
19	T	103	LFA	C4-C5-C6-C7
20	Y	102	DMU	C18-C19-C22-C25
18	P	305	CDL	CA2-C1-CB2-OB2
18	C	304	CDL	C13-C14-C15-C16
18	Y	101	CDL	C73-C74-C75-C76
20	P	316	DMU	C19-C22-C25-C28
18	L	101	CDL	C80-C81-C82-C83
19	C	324	LFA	C3-C4-C5-C6
18	L	101	CDL	CB3-CB4-CB6-OB8
18	L	101	CDL	C84-C85-C86-C87
18	Y	101	CDL	CB3-CB4-CB6-OB8
18	Y	101	CDL	C84-C85-C86-C87
19	P	308	LFA	C3-C4-C5-C6
20	B	308	DMU	C34-C37-C40-C43
20	C	315	DMU	C18-C19-C22-C25
18	A	606	CDL	C16-C17-C18-C19
19	C	310	LFA	C11-C10-C9-C8
19	C	324	LFA	C4-C5-C6-C7
19	C	324	LFA	C12-C13-C14-C15
20	L	102	DMU	C34-C37-C40-C43
20	O	305	DMU	C25-C28-C31-C34
20	B	302	DMU	O16-C18-C19-C22
20	B	303	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
20	G	103	DMU	O16-C18-C19-C22
20	W	101	DMU	O16-C18-C19-C22
18	P	305	CDL	C54-C55-C56-C57
19	O	301	LFA	C14-C15-C16-C17
19	P	308	LFA	C11-C10-C9-C8
19	P	310	LFA	C14-C15-C16-C17
20	C	316	DMU	C34-C37-C40-C43
18	Y	101	CDL	C64-C65-C66-C67
19	B	307	LFA	C14-C15-C16-C17
19	C	311	LFA	C10-C11-C12-C13
19	C	312	LFA	C11-C10-C9-C8
19	P	312	LFA	C4-C5-C6-C7
20	C	318	DMU	C34-C37-C40-C43
20	H	101	DMU	C19-C22-C25-C28
20	P	319	DMU	C25-C28-C31-C34
20	C	323	DMU	O16-C18-C19-C22
22	C	303	PGV	C30-C31-C32-C33
18	Y	101	CDL	C58-C59-C60-C61
20	B	302	DMU	C18-C19-C22-C25
18	A	606	CDL	C20-C21-C22-C23
18	P	305	CDL	C73-C74-C75-C76
22	A	613	PGV	C30-C31-C32-C33
18	L	101	CDL	C74-C75-C76-C77
19	P	311	LFA	C11-C10-C9-C8
20	G	103	DMU	C34-C37-C40-C43
20	C	315	DMU	O5-C4-C57-O61
20	A	608	DMU	C25-C28-C31-C34
20	P	319	DMU	C34-C37-C40-C43
19	N	606	LFA	C6-C7-C8-C9
18	P	305	CDL	C20-C21-C22-C23
18	P	305	CDL	C75-C76-C77-C78
19	O	301	LFA	C11-C10-C9-C8
19	P	315	LFA	C6-C7-C8-C9
20	M	102	DMU	C34-C37-C40-C43
20	P	316	DMU	O6-C11-C9-O1
20	Y	102	DMU	O5-C4-C57-O61
18	Y	101	CDL	C32-C33-C34-C35
20	Z	101	DMU	O6-C11-C9-C8
18	P	305	CDL	C57-C58-C59-C60
18	Y	101	CDL	C22-C23-C24-C25
19	C	310	LFA	C7-C8-C9-C10
20	Z	101	DMU	C25-C28-C31-C34

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Mol	Chain	Res	Type	Atoms
18	C	304	CDL	CA4-CA3-OA5-PA1
18	P	305	CDL	C35-C36-C37-C38
20	C	315	DMU	C34-C37-C40-C43
20	Y	102	DMU	C25-C28-C31-C34
20	Z	101	DMU	C34-C37-C40-C43
18	P	305	CDL	C71-CB7-OB8-CB6
18	V	101	CDL	C18-C19-C20-C21
18	Y	101	CDL	C80-C81-C82-C83
20	P	316	DMU	O5-C4-C57-O61
20	L	102	DMU	C1-C6-O16-C18
19	C	309	LFA	C15-C16-C17-C18
18	L	101	CDL	C72-C71-CB7-OB8
18	A	606	CDL	OA6-CA4-CA6-OA8
18	L	101	CDL	OB6-CB4-CB6-OB8
18	V	101	CDL	OA6-CA4-CA6-OA8
19	C	313	LFA	C4-C5-C6-C7
20	O	303	DMU	C22-C25-C28-C31
18	Y	101	CDL	CA7-C31-C32-C33
20	O	305	DMU	O16-C18-C19-C22
20	C	319	DMU	C18-C19-C22-C25
18	P	305	CDL	C33-C34-C35-C36
20	N	615	DMU	C18-C19-C22-C25
18	Y	101	CDL	C59-C60-C61-C62
19	B	307	LFA	C1-C2-C3-C4
19	B	307	LFA	C11-C12-C13-C14
19	C	310	LFA	C1-C2-C3-C4
22	N	614	PGV	C31-C32-C33-C34
20	B	308	DMU	C31-C34-C37-C40
20	W	101	DMU	C34-C37-C40-C43
19	P	314	LFA	C9-C10-C11-C12
20	T	104	DMU	C25-C28-C31-C34
27	T	102	PEK	C4-C5-C6-C7
20	Z	101	DMU	O6-C11-C9-O1
20	A	614	DMU	O16-C18-C19-C22
20	O	306	DMU	O16-C18-C19-C22
19	A	607	LFA	C6-C7-C8-C9
19	C	314	LFA	C1-C2-C3-C4
19	O	302	LFA	C2-C3-C4-C5
20	P	319	DMU	C4-C3-O7-C10
20	P	324	DMU	C25-C28-C31-C34
27	G	101	PEK	C17-C18-C19-C20
18	C	304	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
20	P	324	DMU	C4-C3-O7-C10
18	L	101	CDL	C58-C59-C60-C61
20	B	303	DMU	C22-C25-C28-C31
20	C	317	DMU	C19-C18-O16-C6
20	O	303	DMU	C19-C18-O16-C6
20	P	318	DMU	C19-C18-O16-C6
20	P	319	DMU	C2-C3-O7-C10
20	P	324	DMU	C2-C3-O7-C10
22	A	613	PGV	C28-C29-C30-C31
22	A	613	PGV	C11-C10-C9-C8
22	N	614	PGV	C11-C10-C9-C8
18	L	101	CDL	C57-C58-C59-C60
19	O	302	LFA	C1-C2-C3-C4
20	C	318	DMU	C2-C3-O7-C10
18	P	305	CDL	CB3-CB4-CB6-OB8
18	V	101	CDL	CA3-CA4-CA6-OA8
19	C	310	LFA	C3-C4-C5-C6
19	P	301	LFA	C11-C12-C13-C14
20	D	201	DMU	C4-C3-O7-C10
20	P	317	DMU	C28-C31-C34-C37
19	C	324	LFA	C10-C11-C12-C13
18	A	606	CDL	C71-C72-C73-C74
18	A	606	CDL	C77-C78-C79-C80
19	P	314	LFA	C11-C10-C9-C8
27	G	101	PEK	C9-C10-C11-C12
27	T	102	PEK	C11-C12-C13-C14
20	B	304	DMU	C34-C37-C40-C43
27	G	101	PEK	C29-C30-C31-C32
20	O	305	DMU	C18-C19-C22-C25
20	P	319	DMU	O1-C10-O7-C3
18	P	305	CDL	OA5-CA3-CA4-OA6
18	P	305	CDL	OB9-CB7-OB8-CB6
18	L	101	CDL	C19-C20-C21-C22
19	P	311	LFA	C6-C7-C8-C9
18	P	305	CDL	CA7-C31-C32-C33
20	C	318	DMU	C4-C3-O7-C10
18	C	304	CDL	OB6-CB4-CB6-OB8
18	A	606	CDL	C12-C13-C14-C15
20	P	324	DMU	O1-C10-O7-C3
18	Y	101	CDL	CA2-C1-CB2-OB2
18	Y	101	CDL	C19-C20-C21-C22
18	L	101	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
20	C	315	DMU	C4-C3-O7-C10
18	A	606	CDL	CA7-C31-C32-C33
20	M	102	DMU	C31-C34-C37-C40
19	C	324	LFA	C5-C6-C7-C8
19	P	311	LFA	C2-C3-C4-C5
22	P	304	PGV	C14-C15-C16-C17
18	A	606	CDL	C13-C14-C15-C16
19	N	606	LFA	C7-C8-C9-C10
22	A	613	PGV	C15-C16-C17-C18
22	A	613	PGV	C31-C32-C33-C34
19	P	310	LFA	C1-C2-C3-C4
19	P	314	LFA	C5-C6-C7-C8
20	Z	102	DMU	C22-C25-C28-C31
19	C	307	LFA	C6-C7-C8-C9
18	L	101	CDL	C21-C22-C23-C24
19	P	310	LFA	C11-C12-C13-C14
18	P	305	CDL	C21-C22-C23-C24
18	P	305	CDL	OA5-CA3-CA4-CA6
20	C	319	DMU	C28-C31-C34-C37
19	P	301	LFA	C1-C2-C3-C4
20	H	101	DMU	C25-C28-C31-C34
20	O	305	DMU	C22-C25-C28-C31
20	Q	201	DMU	C4-C3-O7-C10
18	P	305	CDL	C71-C72-C73-C74
18	Y	101	CDL	C38-C39-C40-C41
20	B	308	DMU	C25-C28-C31-C34
18	A	606	CDL	C71-CB7-OB8-CB6
18	L	101	CDL	C59-C60-C61-C62
20	C	319	DMU	O16-C18-C19-C22
19	P	310	LFA	C7-C8-C9-C10
20	C	318	DMU	C19-C22-C25-C28
20	H	101	DMU	C28-C31-C34-C37
20	M	101	DMU	O16-C18-C19-C22
20	O	305	DMU	C19-C22-C25-C28
22	P	304	PGV	C11-C12-C13-C14
18	C	304	CDL	C73-C74-C75-C76
20	G	103	DMU	C19-C22-C25-C28
20	D	201	DMU	O5-C6-O16-C18
18	P	305	CDL	CA3-CA4-CA6-OA8
18	L	101	CDL	C76-C77-C78-C79
27	G	101	PEK	C13-C14-C15-C16
18	C	304	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
19	T	103	LFA	C6-C7-C8-C9
20	P	316	DMU	C34-C37-C40-C43
18	C	304	CDL	C20-C21-C22-C23
19	T	103	LFA	C7-C8-C9-C10
20	C	306	DMU	O16-C18-C19-C22
19	O	301	LFA	C1-C2-C3-C4
19	B	307	LFA	C11-C10-C9-C8
18	A	606	CDL	OB9-CB7-OB8-CB6
20	D	201	DMU	C2-C3-O7-C10
20	C	315	DMU	C2-C3-O7-C10
18	A	606	CDL	C15-C16-C17-C18
19	C	311	LFA	C5-C6-C7-C8
20	H	101	DMU	C22-C25-C28-C31
19	C	314	LFA	C6-C7-C8-C9
20	H	101	DMU	O6-C11-C9-O1
18	P	305	CDL	CA4-CA3-OA5-PA1
22	C	303	PGV	C02-C03-O11-P
22	P	304	PGV	C02-C03-O11-P
20	P	324	DMU	C5-C10-O7-C3
18	C	304	CDL	C77-C78-C79-C80
18	C	304	CDL	CA3-OA5-PA1-OA3
18	V	101	CDL	CA3-OA5-PA1-OA3
18	V	101	CDL	CB2-OB2-PB2-OB4
18	Y	101	CDL	CA2-OA2-PA1-OA4
18	Y	101	CDL	CB2-OB2-PB2-OB4
19	C	307	LFA	C11-C10-C9-C8
20	N	615	DMU	C22-C25-C28-C31
27	T	102	PEK	C10-C11-C12-C13
18	P	305	CDL	C23-C24-C25-C26
20	M	102	DMU	C22-C25-C28-C31
18	L	101	CDL	C22-C23-C24-C25
19	P	313	LFA	C11-C10-C9-C8
20	Y	102	DMU	C22-C25-C28-C31
20	Q	201	DMU	C25-C28-C31-C34
18	C	304	CDL	C79-C80-C81-C82
18	P	305	CDL	C13-C14-C15-C16
18	V	101	CDL	OA5-CA3-CA4-OA6
20	D	201	DMU	C19-C22-C25-C28
20	T	104	DMU	C34-C37-C40-C43
20	C	319	DMU	C34-C37-C40-C43
27	T	102	PEK	C2-C1-O01-C02
18	P	305	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
20	H	101	DMU	C3-C4-C57-O61
20	N	615	DMU	C3-C4-C57-O61
18	C	304	CDL	CB3-CB4-CB6-OB8
18	Y	101	CDL	CA3-CA4-CA6-OA8
19	P	311	LFA	C4-C5-C6-C7
20	J	101	DMU	C34-C37-C40-C43
20	N	615	DMU	C19-C22-C25-C28
18	P	305	CDL	OB6-CB4-CB6-OB8
18	Y	101	CDL	OA6-CA4-CA6-OA8
19	C	314	LFA	C11-C10-C9-C8
20	P	318	DMU	C22-C25-C28-C31
19	P	309	LFA	C1-C2-C3-C4
19	P	312	LFA	C1-C2-C3-C4
20	C	317	DMU	C25-C28-C31-C34
24	P	306	CHD	C17-C20-C22-C23
19	G	106	LFA	C9-C10-C11-C12
20	J	101	DMU	C31-C34-C37-C40
20	P	319	DMU	O6-C11-C9-C8
20	P	320	DMU	C19-C22-C25-C28
20	Y	102	DMU	C31-C34-C37-C40
27	G	101	PEK	C27-C28-C29-C30
18	V	101	CDL	C16-C17-C18-C19
27	T	102	PEK	O02-C1-O01-C02
19	C	309	LFA	C2-C3-C4-C5
19	G	106	LFA	C6-C7-C8-C9
19	T	103	LFA	C3-C4-C5-C6
20	Q	201	DMU	O6-C11-C9-C8
19	G	106	LFA	C1-C2-C3-C4
20	J	101	DMU	C18-C19-C22-C25
18	P	305	CDL	C74-C75-C76-C77
21	P	321	EDO	O1-C1-C2-O2
20	P	318	DMU	C19-C22-C25-C28
22	C	303	PGV	C21-C22-C23-C24
18	P	305	CDL	C80-C81-C82-C83
18	C	304	CDL	C59-C60-C61-C62
18	V	101	CDL	C12-C13-C14-C15
20	B	302	DMU	C31-C34-C37-C40
18	Y	101	CDL	C55-C56-C57-C58
20	Q	201	DMU	C2-C3-O7-C10
14	A	602	HEA	C4D-C3D-CAD-CBD
19	B	307	LFA	C6-C7-C8-C9
20	C	306	DMU	C28-C31-C34-C37

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Mol	Chain	Res	Type	Atoms
20	Z	101	DMU	O16-C18-C19-C22
14	N	602	HEA	CAA-CBA-CGA-O1A
18	L	101	CDL	C36-C37-C38-C39
18	V	101	CDL	C19-C20-C21-C22
18	L	101	CDL	C15-C16-C17-C18
20	Z	102	DMU	C31-C34-C37-C40
19	C	313	LFA	C9-C10-C11-C12
14	N	601	HEA	CAD-CBD-CGD-O1D
20	P	319	DMU	O5-C6-O16-C18
18	V	101	CDL	C74-C75-C76-C77
19	C	313	LFA	C2-C3-C4-C5
27	T	102	PEK	C29-C30-C31-C32
14	A	601	HEA	CAD-CBD-CGD-O1D
18	L	101	CDL	OB5-CB3-CB4-OB6
20	N	615	DMU	C25-C28-C31-C34
18	Y	101	CDL	OB9-CB7-OB8-CB6
20	P	307	DMU	C18-C19-C22-C25
14	A	602	HEA	CAA-CBA-CGA-O1A
18	P	305	CDL	C12-C11-CA5-OA6
21	A	611	EDO	O1-C1-C2-O2
27	T	102	PEK	C30-C31-C32-C33
18	Y	101	CDL	C12-C13-C14-C15
22	N	614	PGV	C23-C24-C25-C26
20	A	614	DMU	C25-C28-C31-C34
18	C	304	CDL	CA2-C1-CB2-OB2
18	P	305	CDL	C17-C18-C19-C20
24	B	306	CHD	C22-C23-C24-O25
24	B	306	CHD	C22-C23-C24-O26
24	G	102	CHD	C22-C23-C24-O25
18	L	101	CDL	C72-C71-CB7-OB9
19	P	308	LFA	C2-C3-C4-C5
27	T	102	PEK	C32-C33-C34-C35
24	C	305	CHD	C22-C23-C24-O25
24	P	306	CHD	C22-C23-C24-O25
19	C	307	LFA	C7-C8-C9-C10
18	A	606	CDL	CA6-CA4-OA6-CA5
20	P	307	DMU	C31-C34-C37-C40
24	C	305	CHD	C22-C23-C24-O26
24	G	102	CHD	C22-C23-C24-O26
20	B	304	DMU	C3-C4-C57-O61
18	Y	101	CDL	CB2-OB2-PB2-OB5
20	G	103	DMU	C31-C34-C37-C40

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Mol	Chain	Res	Type	Atoms
20	O	306	DMU	C25-C28-C31-C34
14	A	602	HEA	CAD-CBD-CGD-O1D
14	N	602	HEA	CAA-CBA-CGA-O2A
19	P	310	LFA	C12-C13-C14-C15
22	C	303	PGV	C05-C04-O12-P
20	Z	101	DMU	C19-C22-C25-C28
14	A	601	HEA	CAD-CBD-CGD-O2D
18	C	304	CDL	C52-C53-C54-C55
19	A	607	LFA	C7-C8-C9-C10
20	C	323	DMU	O1-C10-O7-C3
18	L	101	CDL	C77-C78-C79-C80
20	A	609	DMU	C2-C3-O7-C10
20	G	104	DMU	C22-C25-C28-C31
20	Q	201	DMU	O5-C4-C57-O61
14	A	602	HEA	CAA-CBA-CGA-O2A
14	N	602	HEA	CAD-CBD-CGD-O1D
20	N	608	DMU	C19-C22-C25-C28
27	G	101	PEK	C10-C11-C12-C13
24	P	306	CHD	C22-C23-C24-O26
20	P	324	DMU	C28-C31-C34-C37
14	A	602	HEA	CAD-CBD-CGD-O2D
20	B	304	DMU	C18-C19-C22-C25
20	A	609	DMU	C3-C4-C57-O61
21	R	201	EDO	O1-C1-C2-O2
20	A	609	DMU	C4-C3-O7-C10
20	O	307	DMU	C22-C25-C28-C31
18	C	304	CDL	C72-C71-CB7-OB8
22	A	613	PGV	O03-C19-C20-C21
20	P	307	DMU	C22-C25-C28-C31
18	L	101	CDL	C78-C79-C80-C81
18	V	101	CDL	C13-C14-C15-C16
20	H	101	DMU	C18-C19-C22-C25
20	O	307	DMU	C18-C19-C22-C25
20	A	608	DMU	C31-C34-C37-C40
14	N	602	HEA	CAD-CBD-CGD-O2D
20	M	101	DMU	C34-C37-C40-C43
22	N	614	PGV	O03-C19-C20-C21
18	V	101	CDL	C20-C21-C22-C23
20	C	315	DMU	O1-C10-O7-C3
18	V	101	CDL	C15-C16-C17-C18
19	P	313	LFA	C6-C7-C8-C9
19	P	315	LFA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
19	P	312	LFA	C7-C8-C9-C10
19	O	302	LFA	C6-C7-C8-C9
18	V	101	CDL	C52-C51-CB5-OB6
20	O	307	DMU	C1-C6-O16-C18
24	C	305	CHD	C17-C20-C22-C23
19	P	315	LFA	C5-C6-C7-C8
24	P	302	CHD	C22-C23-C24-O26
20	P	319	DMU	C5-C10-O7-C3
18	P	305	CDL	C77-C78-C79-C80
19	A	607	LFA	C2-C3-C4-C5
18	A	606	CDL	C32-C31-CA7-OA8
18	V	101	CDL	C72-C71-CB7-OB8
18	V	101	CDL	C52-C51-CB5-OB7
19	T	101	LFA	C11-C10-C9-C8
18	P	305	CDL	C52-C51-CB5-OB6
19	T	101	LFA	C6-C7-C8-C9
19	C	309	LFA	C7-C8-C9-C10
18	L	101	CDL	C73-C74-C75-C76
19	O	301	LFA	C6-C7-C8-C9
14	N	601	HEA	CAD-CBD-CGD-O2D
18	A	606	CDL	C72-C71-CB7-OB8
18	P	305	CDL	C72-C71-CB7-OB8
22	A	613	PGV	C14-C15-C16-C17
24	P	302	CHD	C22-C23-C24-O25
18	C	304	CDL	C55-C56-C57-C58
19	N	606	LFA	C2-C3-C4-C5
20	C	323	DMU	C31-C34-C37-C40
18	C	304	CDL	C52-C51-CB5-OB6
27	T	102	PEK	C15-C16-C17-C18
20	C	315	DMU	C5-C10-O7-C3
18	P	305	CDL	C1-CB2-OB2-PB2
14	A	602	HEA	C2D-C3D-CAD-CBD
18	Y	101	CDL	OA5-CA3-CA4-OA6
18	P	305	CDL	C72-C73-C74-C75
20	Z	101	DMU	C28-C31-C34-C37
19	P	315	LFA	C3-C4-C5-C6
21	N	612	EDO	O1-C1-C2-O2
22	C	303	PGV	C9-C10-C11-C12
18	Y	101	CDL	OA5-CA3-CA4-CA6
20	M	101	DMU	C19-C22-C25-C28
24	C	301	CHD	C22-C23-C24-O25
20	T	104	DMU	C28-C31-C34-C37

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Mol	Chain	Res	Type	Atoms
18	C	304	CDL	C12-C11-CA5-OA7
22	C	303	PGV	C23-C24-C25-C26
18	P	305	CDL	C14-C15-C16-C17
20	D	201	DMU	O6-C11-C9-C8
20	B	308	DMU	C18-C19-C22-C25
18	V	101	CDL	CB4-CB3-OB5-PB2
20	W	101	DMU	C22-C25-C28-C31
18	A	606	CDL	C32-C31-CA7-OA9
18	L	101	CDL	C56-C57-C58-C59
24	C	301	CHD	C22-C23-C24-O26
18	P	305	CDL	C55-C56-C57-C58
18	V	101	CDL	C72-C71-CB7-OB9
19	C	311	LFA	C3-C4-C5-C6
19	P	312	LFA	C11-C10-C9-C8
20	N	607	DMU	C31-C34-C37-C40
18	A	606	CDL	CA2-C1-CB2-OB2
22	A	613	PGV	C13-C14-C15-C16
18	A	606	CDL	C72-C71-CB7-OB9
18	A	606	CDL	C18-C19-C20-C21
18	Y	101	CDL	C71-CB7-OB8-CB6
18	P	305	CDL	C52-C51-CB5-OB7
19	C	309	LFA	C13-C14-C15-C16
18	L	101	CDL	C32-C31-CA7-OA8
18	Y	101	CDL	C83-C84-C85-C86
19	T	101	LFA	C10-C11-C12-C13
20	C	323	DMU	C5-C10-O7-C3
18	C	304	CDL	C1-CB2-OB2-PB2
18	P	305	CDL	C72-C71-CB7-OB9
20	C	319	DMU	C31-C34-C37-C40
14	N	601	HEA	CAA-CBA-CGA-O2A
18	A	606	CDL	CA2-OA2-PA1-OA3
18	L	101	CDL	CA3-OA5-PA1-OA3
18	Y	101	CDL	CB3-OB5-PB2-OB3
20	L	102	DMU	O5-C6-O16-C18
19	C	309	LFA	C6-C7-C8-C9
21	C	322	EDO	O1-C1-C2-O2
19	C	309	LFA	C11-C12-C13-C14
22	C	303	PGV	C29-C30-C31-C32
14	A	601	HEA	CAA-CBA-CGA-O1A
27	T	102	PEK	O01-C1-C2-C3
18	Y	101	CDL	C60-C61-C62-C63
18	C	304	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
20	C	323	DMU	C18-C19-C22-C25
18	V	101	CDL	C71-CB7-OB8-CB6
19	C	307	LFA	C2-C3-C4-C5
14	A	601	HEA	CAA-CBA-CGA-O2A
22	P	304	PGV	C1-C2-C3-C4
14	N	601	HEA	CAA-CBA-CGA-O1A
20	Q	201	DMU	O1-C10-O7-C3
20	Q	201	DMU	C19-C18-O16-C6
19	P	315	LFA	C1-C2-C3-C4
18	C	304	CDL	C36-C37-C38-C39
18	L	101	CDL	C32-C31-CA7-OA9
20	P	316	DMU	C3-C4-C57-O61
18	V	101	CDL	C32-C33-C34-C35

There are no ring outliers.

41 monomers are involved in 116 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	609	DMU	1	0
19	A	607	LFA	6	0
18	L	101	CDL	2	0
19	T	101	LFA	7	0
14	N	601	HEA	3	0
24	G	102	CHD	1	0
27	T	102	PEK	5	0
19	C	313	LFA	3	0
19	P	313	LFA	2	0
18	V	101	CDL	1	0
20	C	323	DMU	1	0
20	C	319	DMU	1	0
14	A	602	HEA	1	0
18	Y	101	CDL	8	0
19	N	606	LFA	5	0
19	C	312	LFA	2	0
19	C	307	LFA	2	0
20	D	201	DMU	2	0
20	Q	201	DMU	3	0
19	P	308	LFA	2	0
20	O	303	DMU	1	0
20	Y	102	DMU	2	0
18	C	304	CDL	16	0
20	L	102	DMU	1	0

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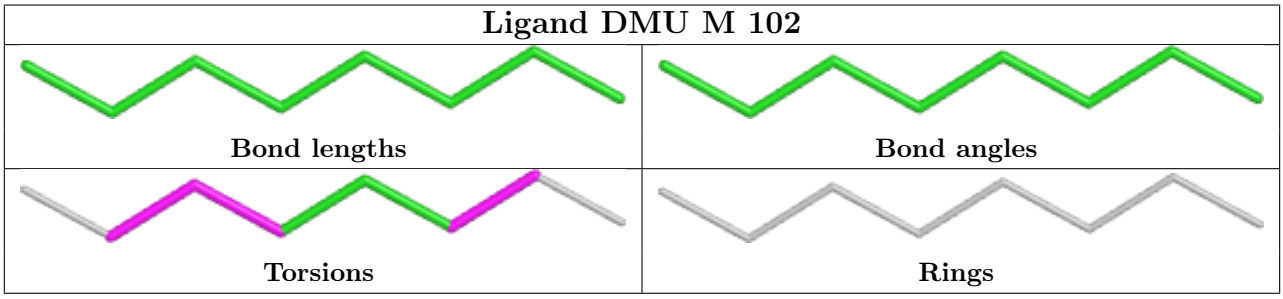
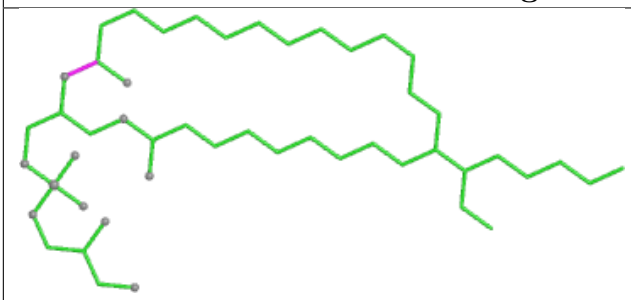
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	P	310	LFA	2	0
24	C	305	CHD	2	0
19	G	106	LFA	7	0
20	P	319	DMU	1	0
18	P	305	CDL	12	0
24	C	301	CHD	1	0
20	P	324	DMU	2	0
19	C	314	LFA	1	0
24	P	306	CHD	2	0
20	A	608	DMU	1	0
19	P	314	LFA	1	0
19	C	309	LFA	3	0
24	P	302	CHD	1	0
22	C	303	PGV	3	0
20	H	101	DMU	1	0
14	A	601	HEA	2	0
14	N	602	HEA	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

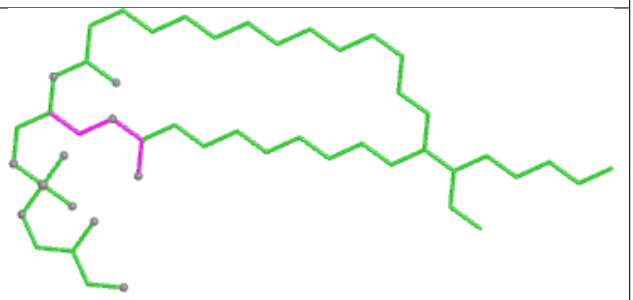
Ligand DMU M 102



Ligand PGV N 614



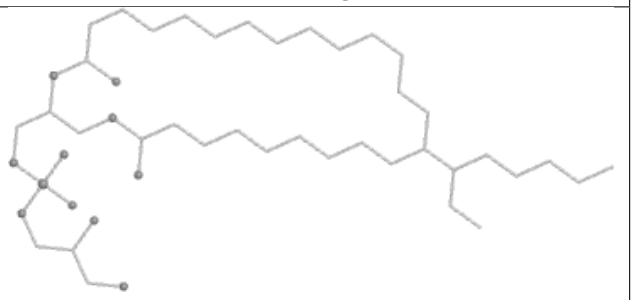
Bond lengths



Bond angles

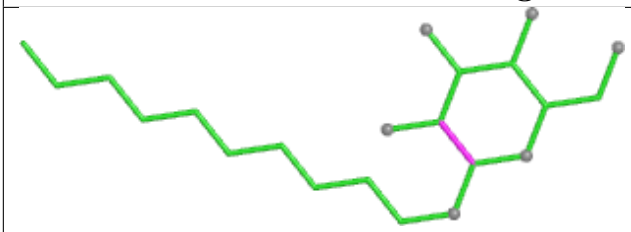


Torsions

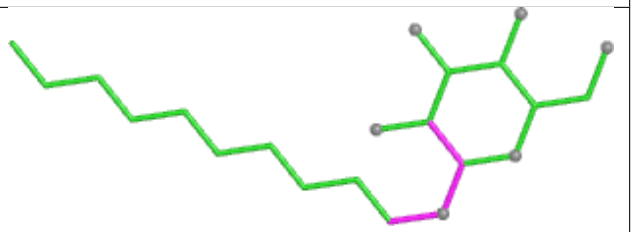


Rings

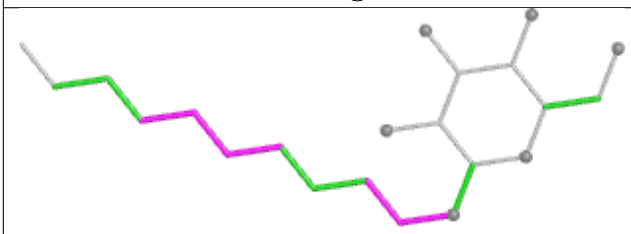
Ligand DMU G 104



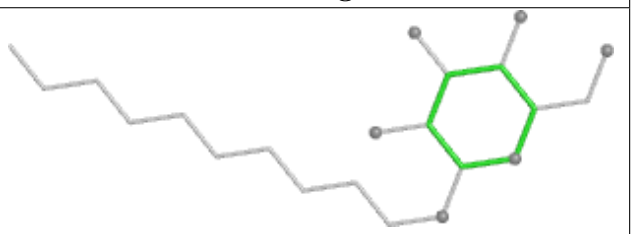
Bond lengths



Bond angles

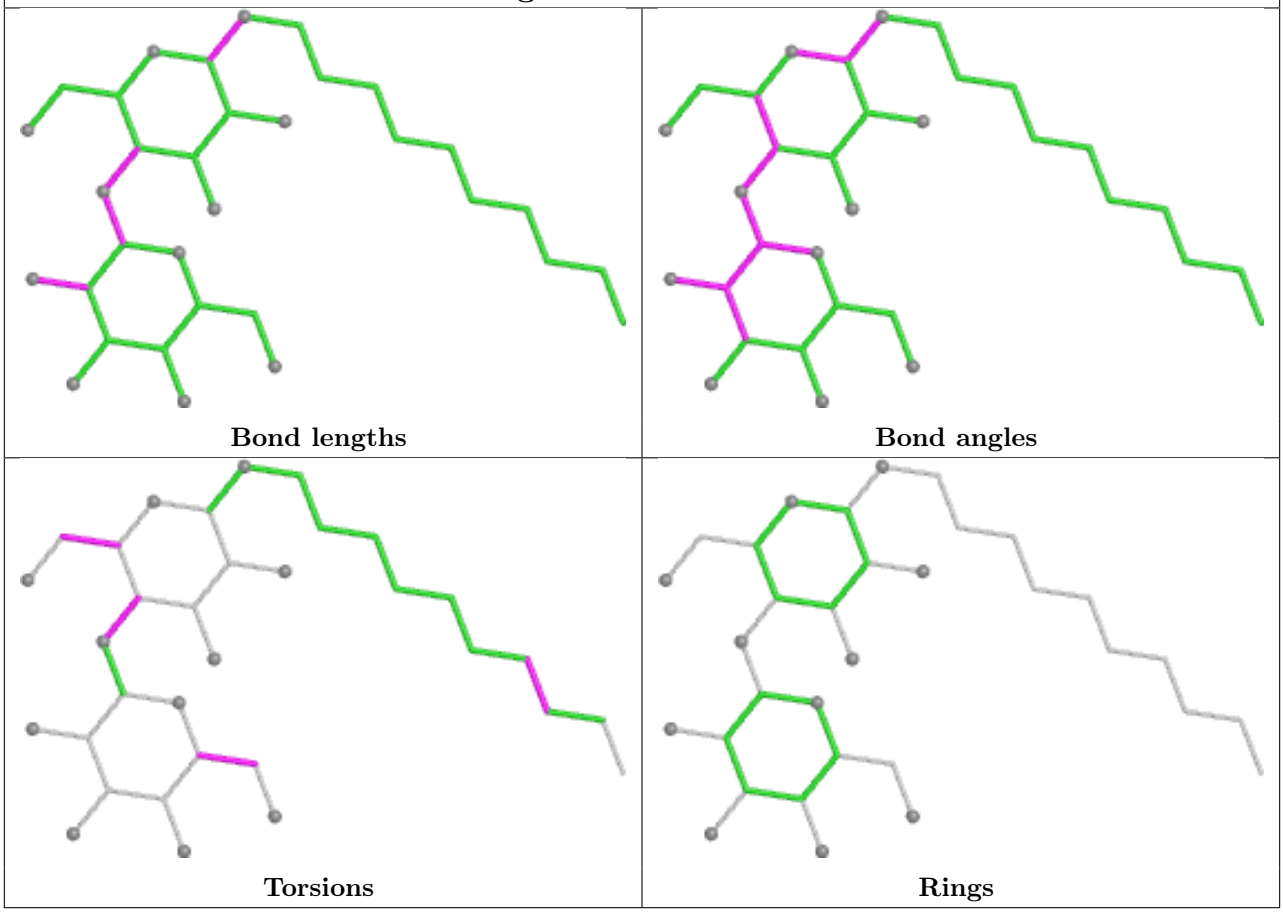


Torsions

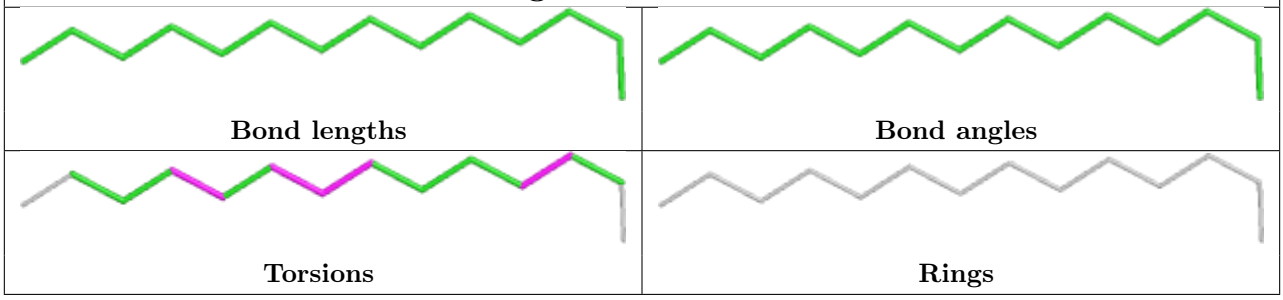


Rings

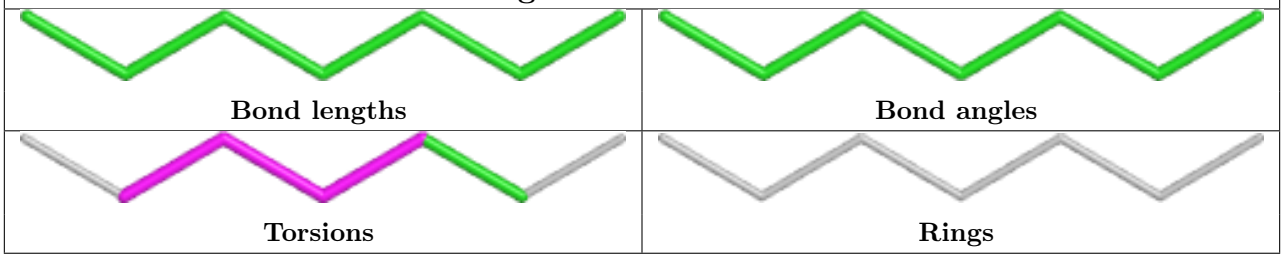
Ligand DMU A 609



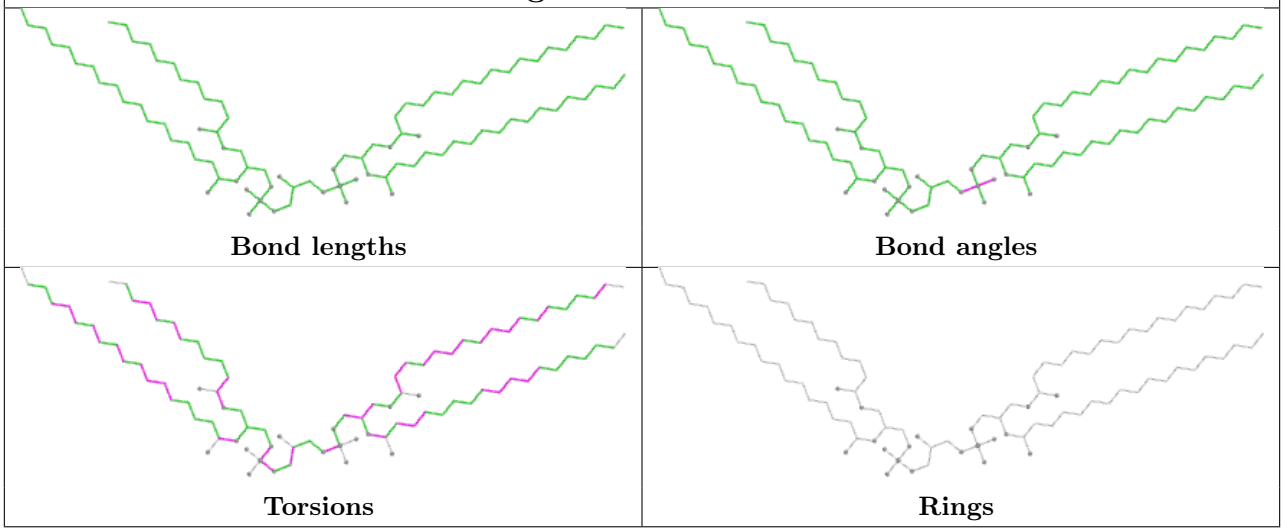
Ligand LFA A 607



Ligand DMU C 316



Ligand CDL L 101



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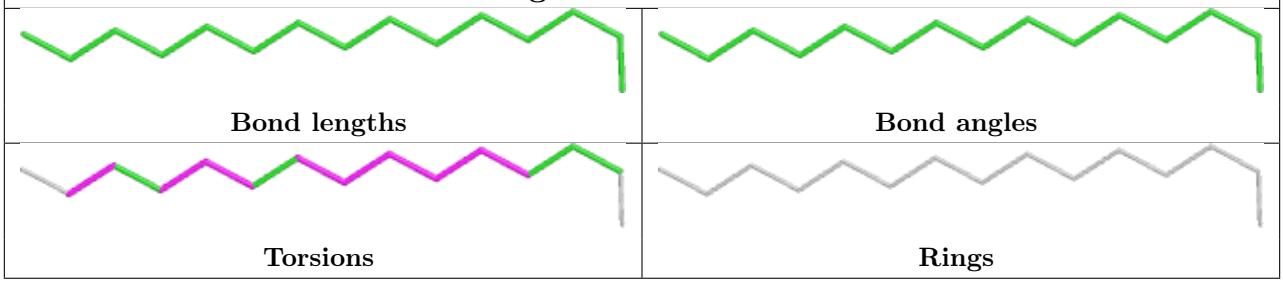
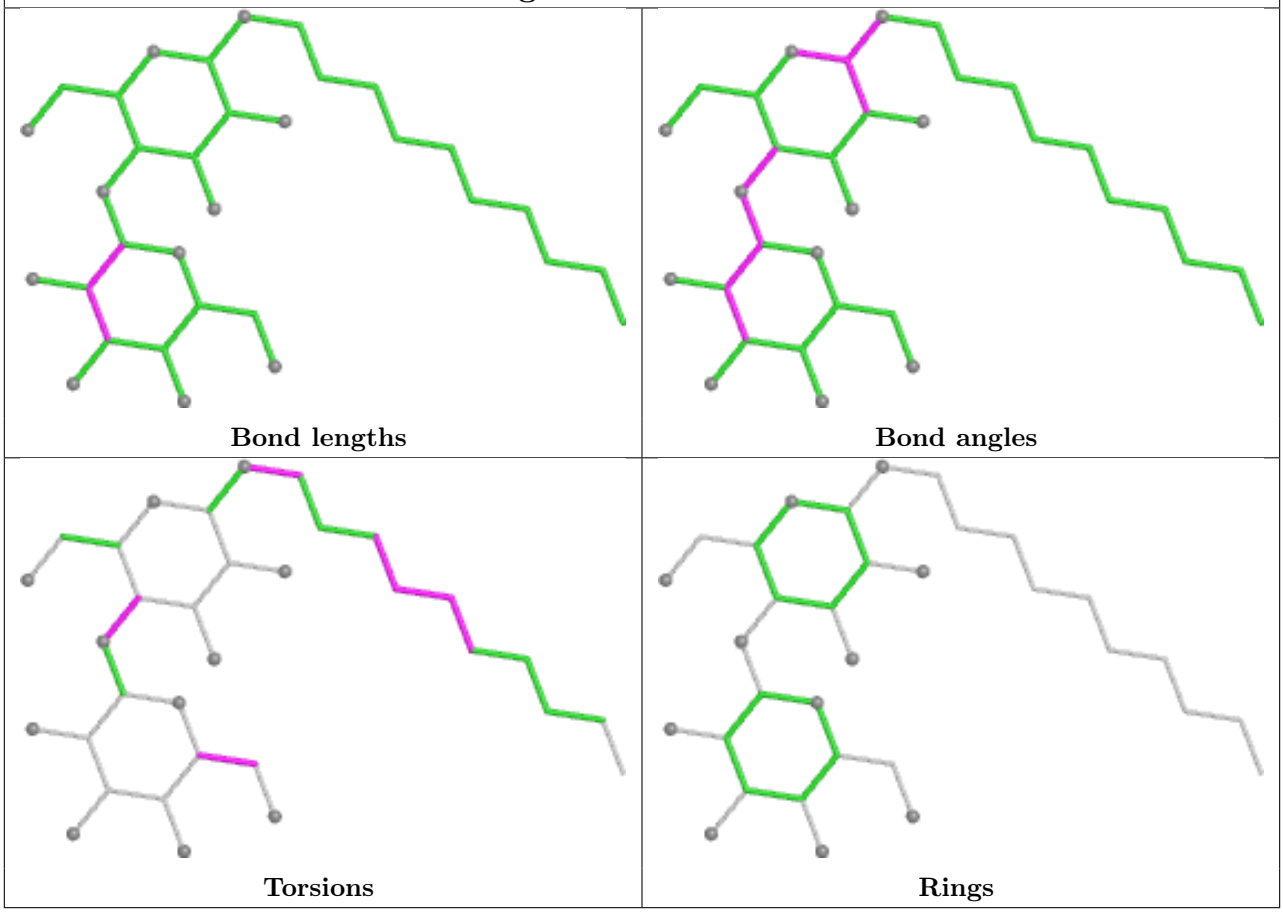
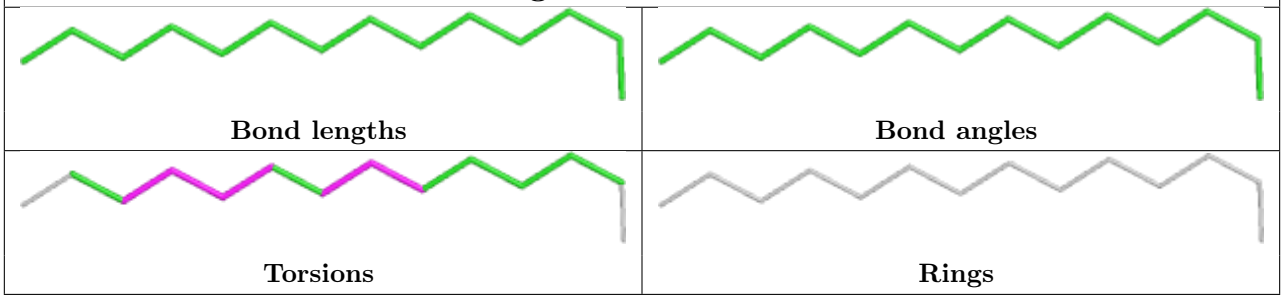


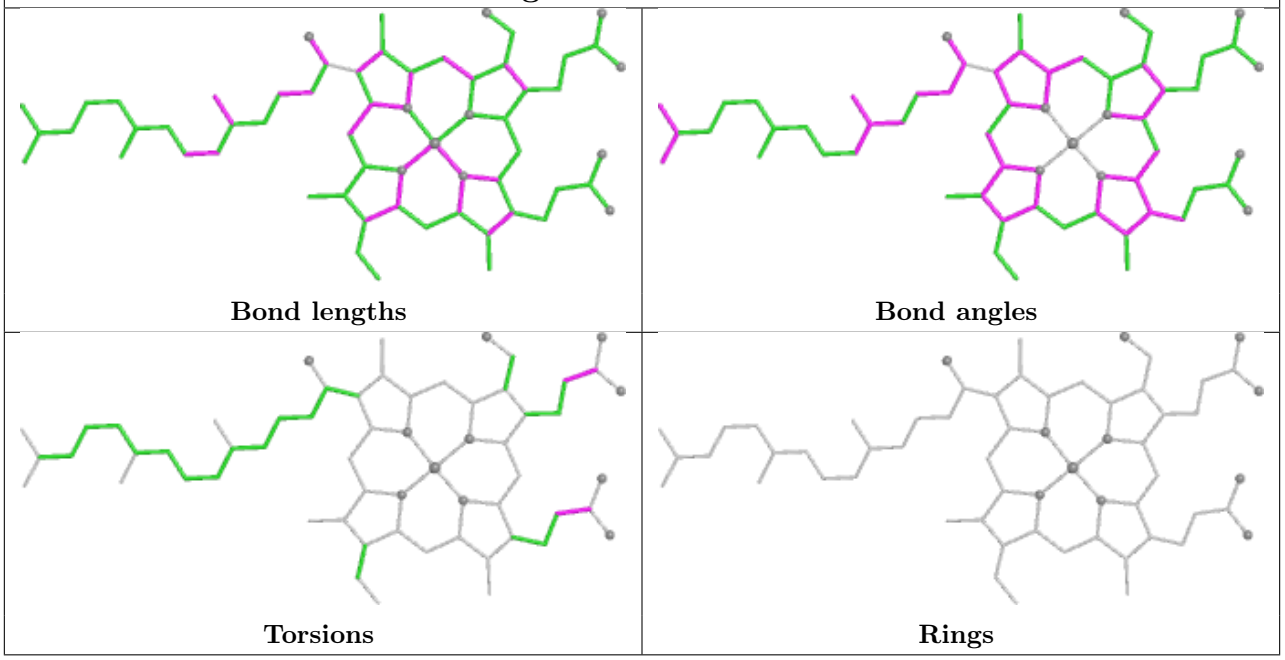
Ligand DMU P 320



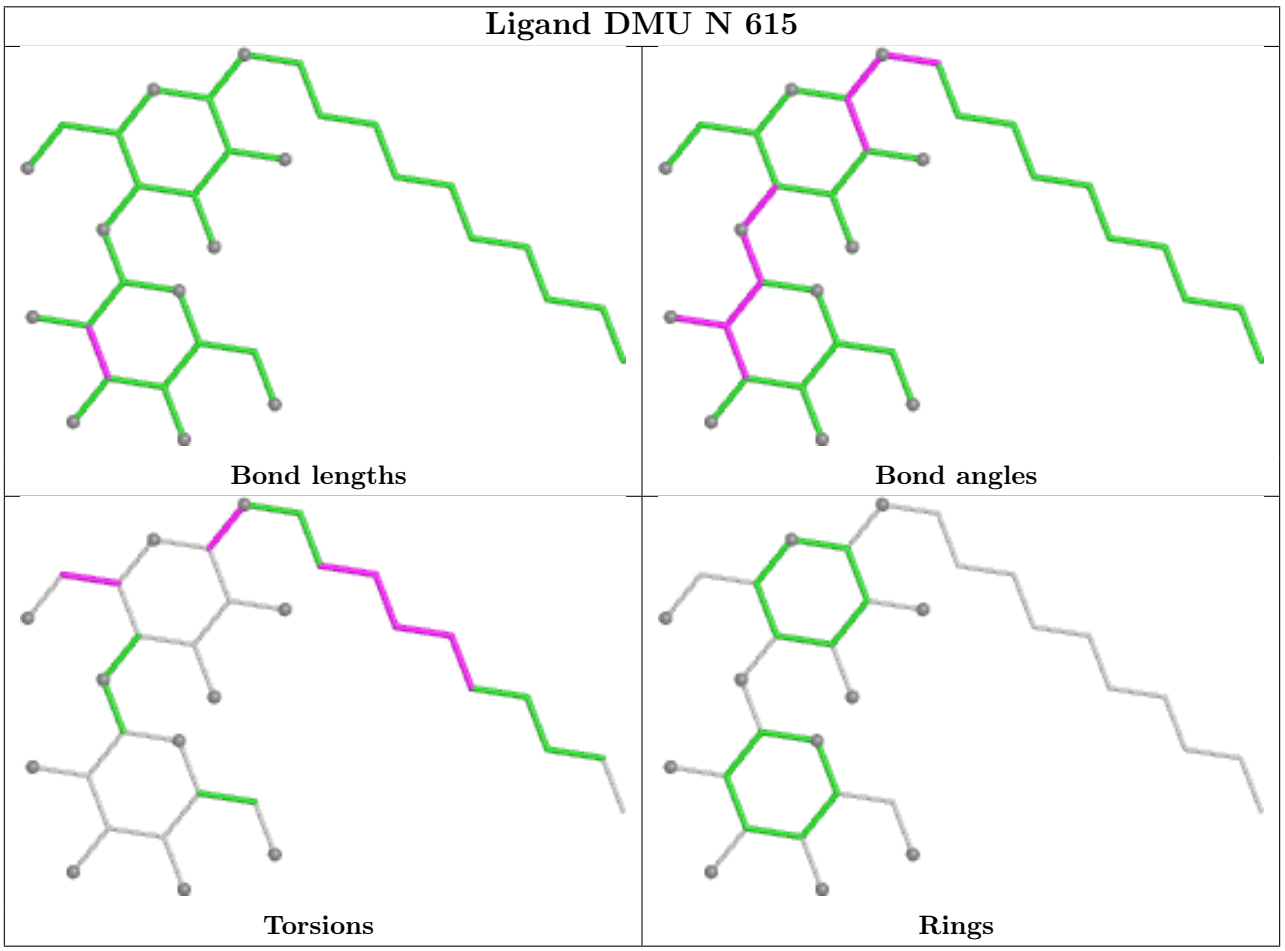
Ligand LFA T 101



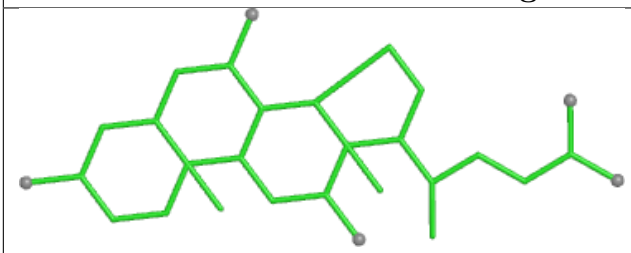
Ligand HEA N 601



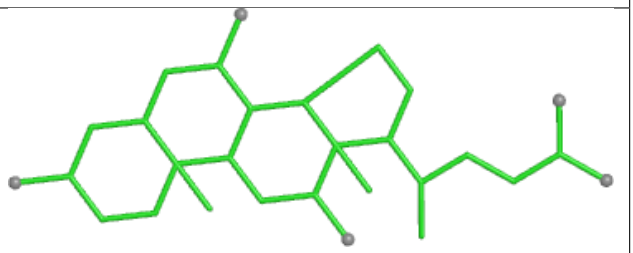
Ligand DMU N 615



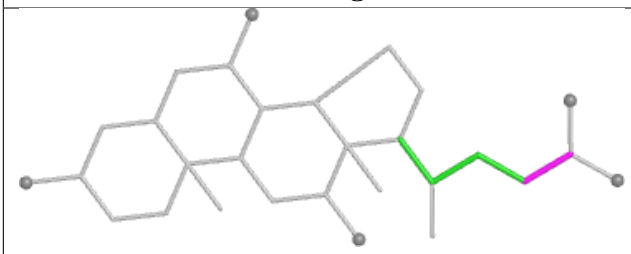
Ligand CHD G 102



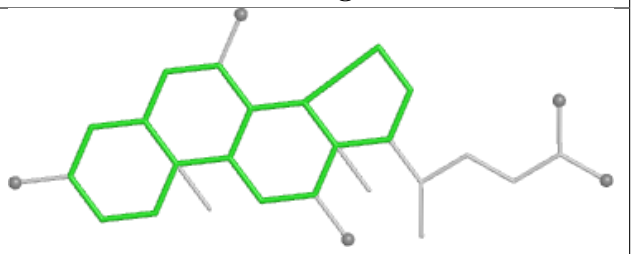
Bond lengths



Bond angles

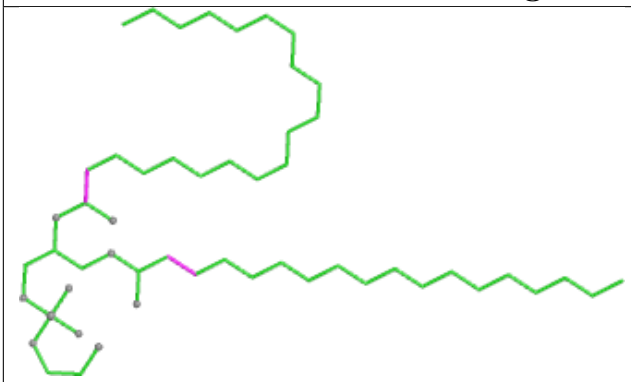


Torsions



Rings

Ligand PEK T 102



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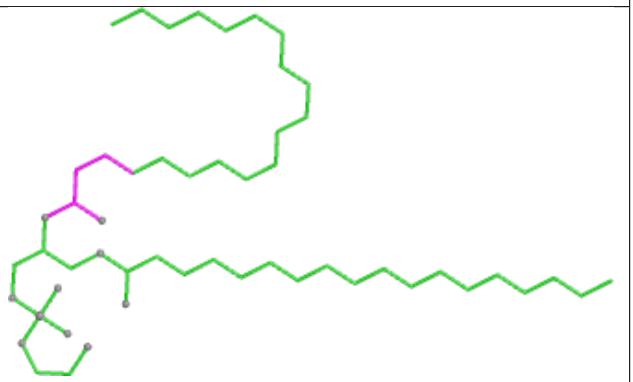
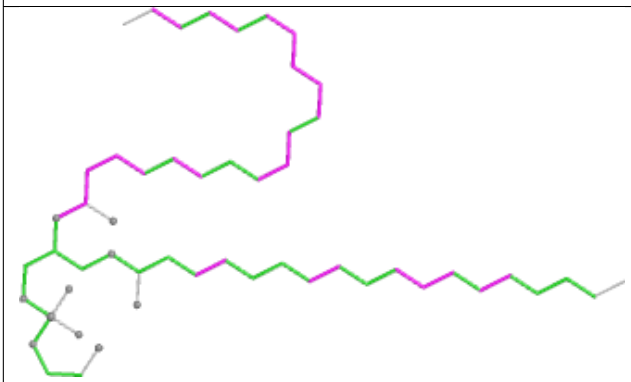


Bond angles



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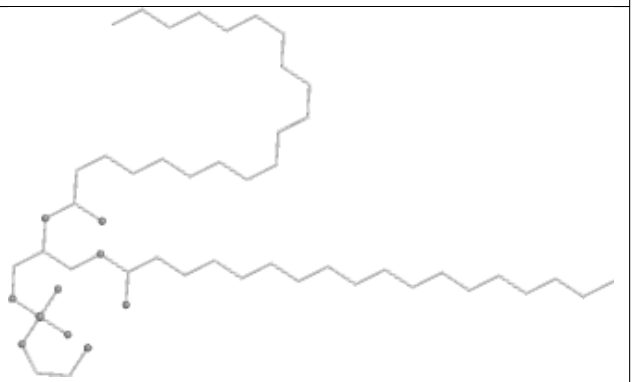
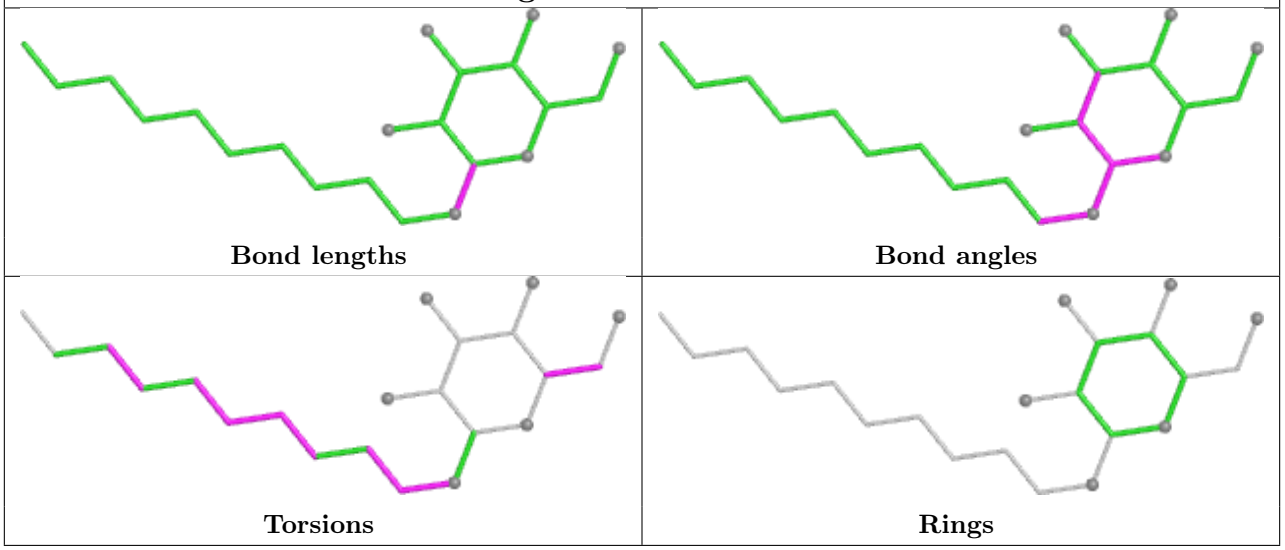
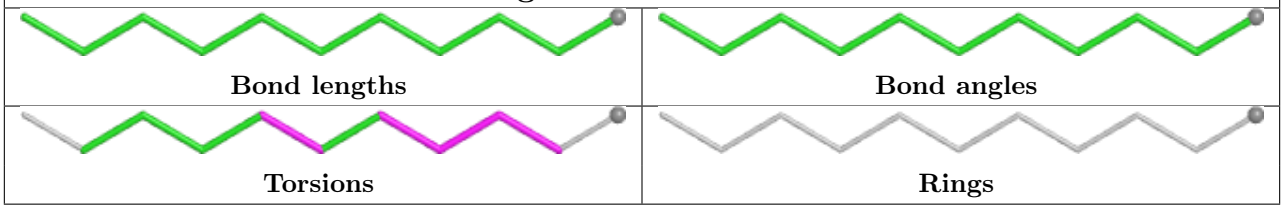


Rings

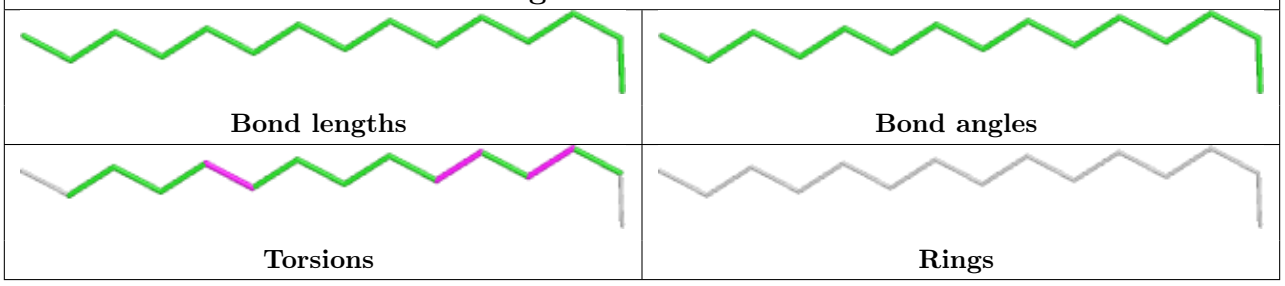
Ligand DMU C 317



Ligand DMU O 306



Ligand LFA C 313



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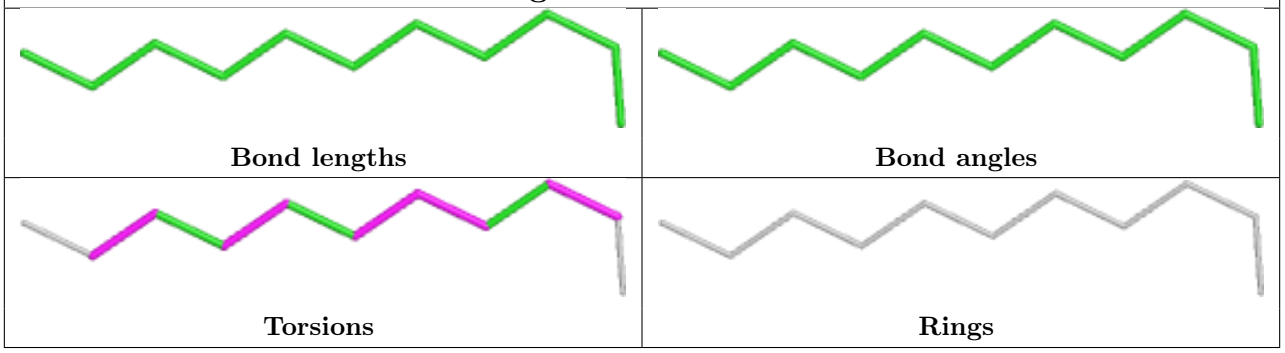

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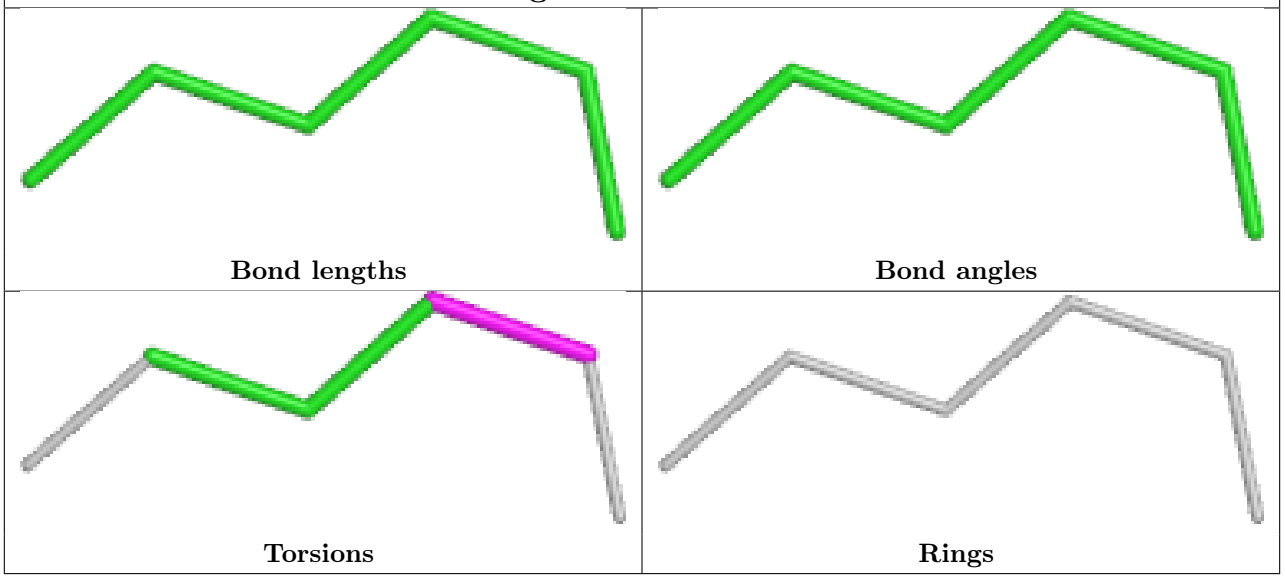
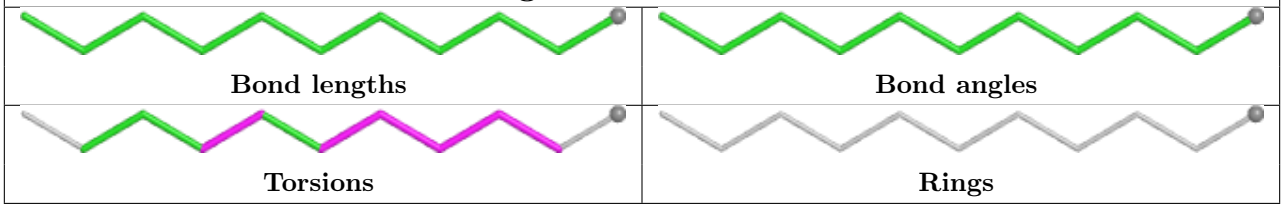
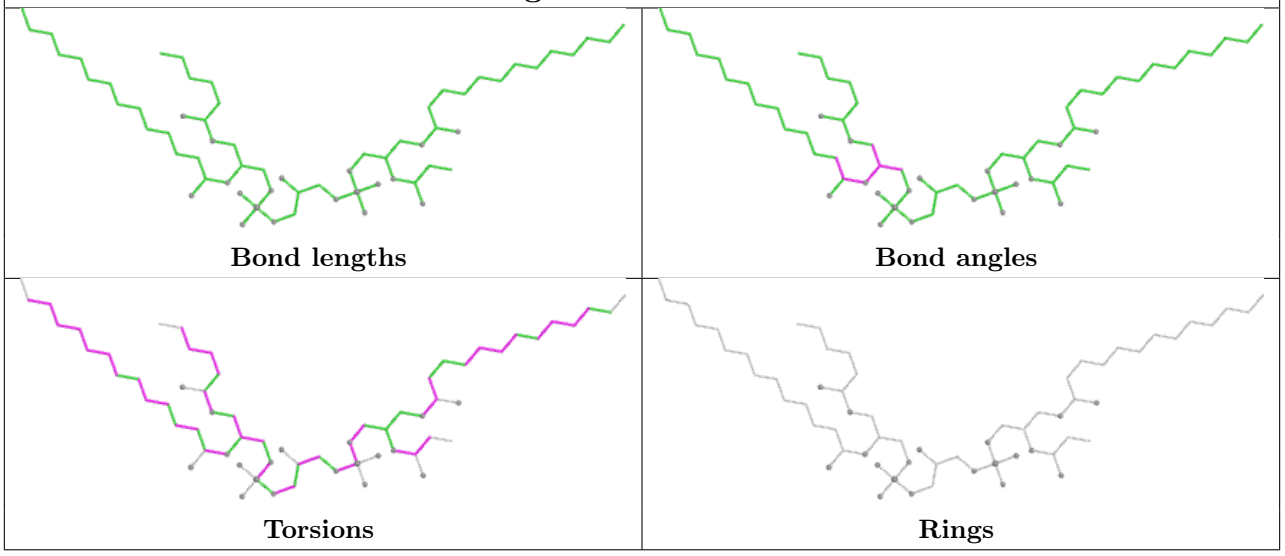


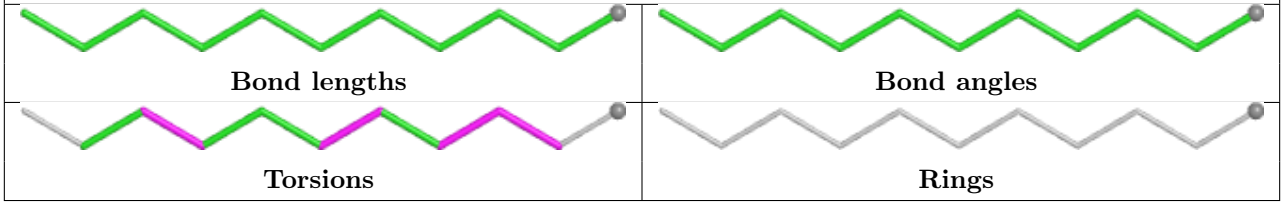
Ligand DMU B 303



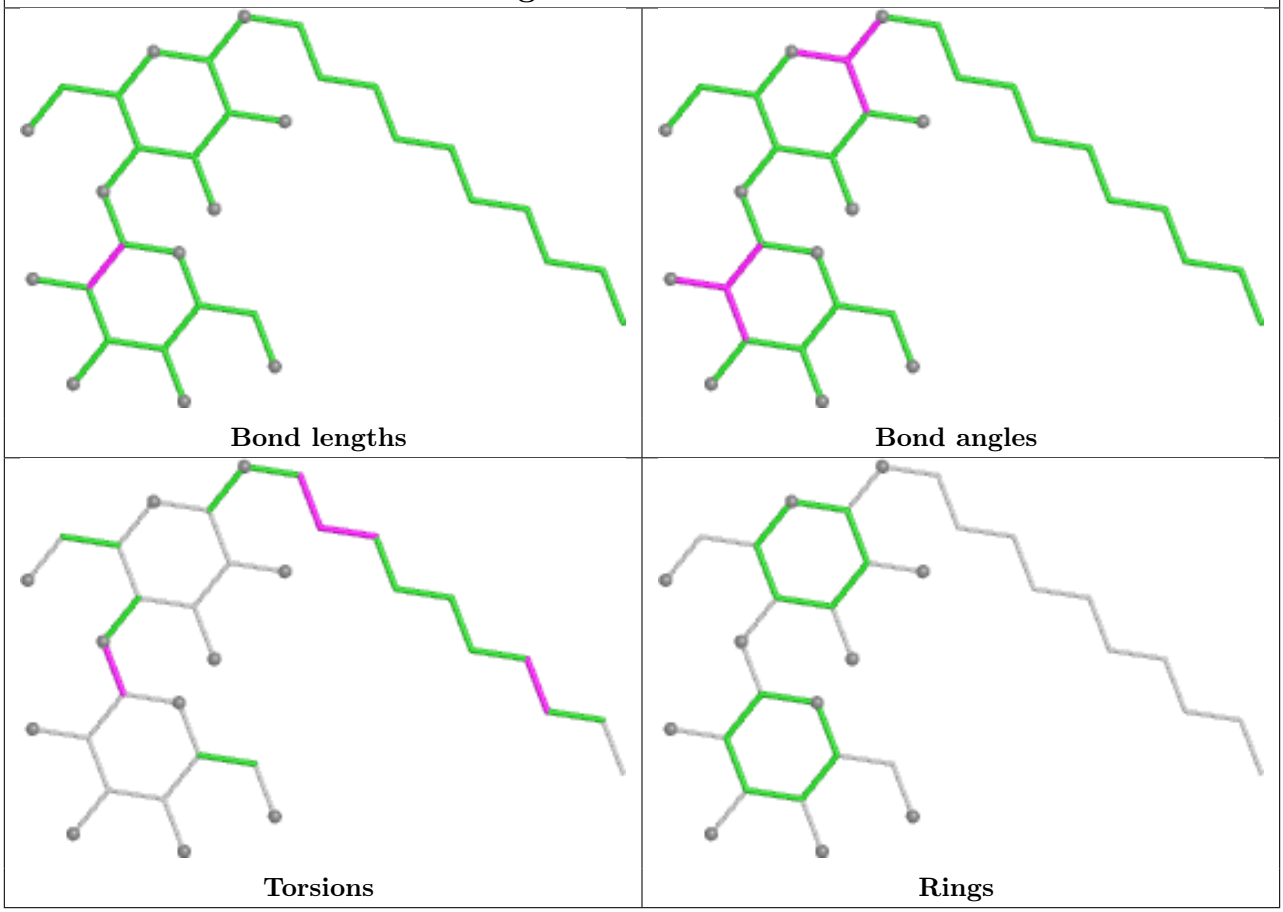
Ligand CDL V 101



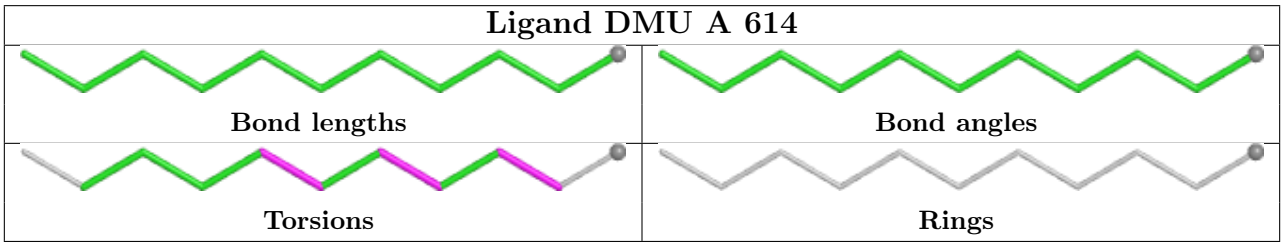
Ligand DMU P 307



Ligand DMU C 323



Ligand DMU A 614



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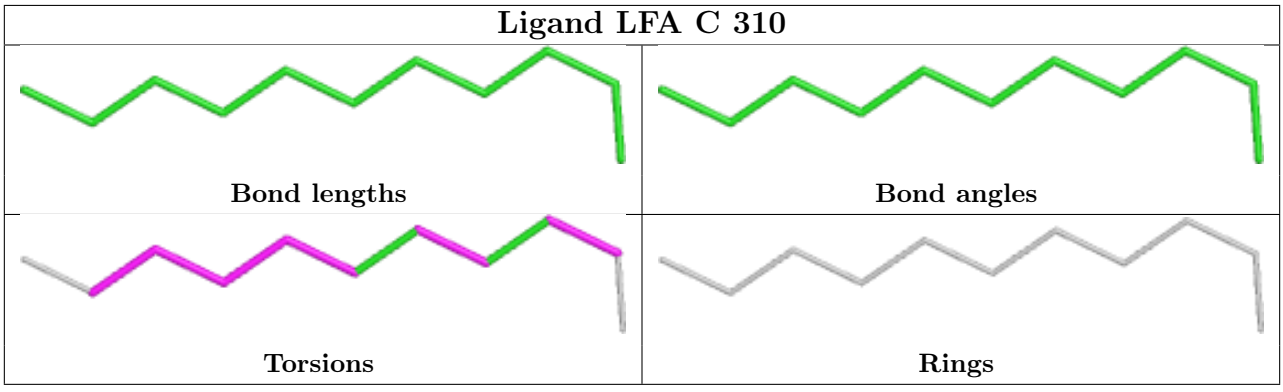
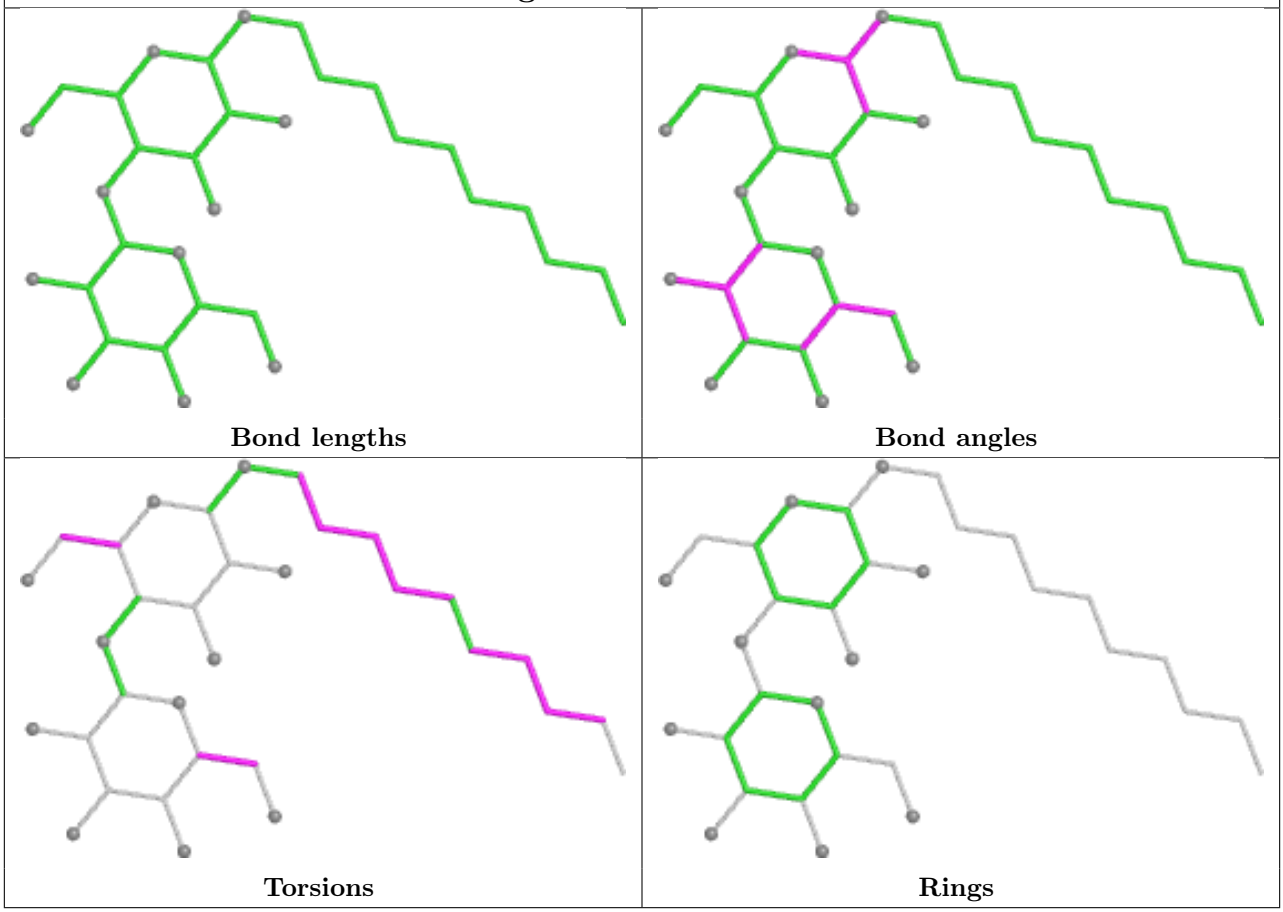
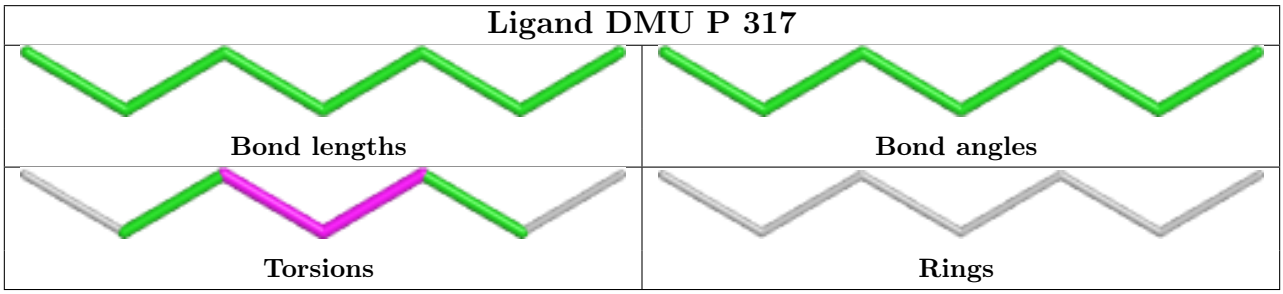


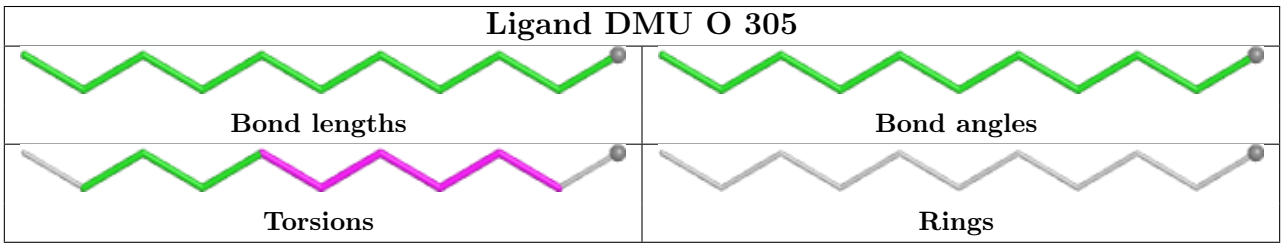
Ligand DMU C 319



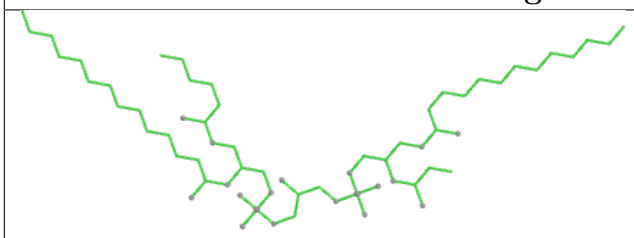
Ligand DMU P 317



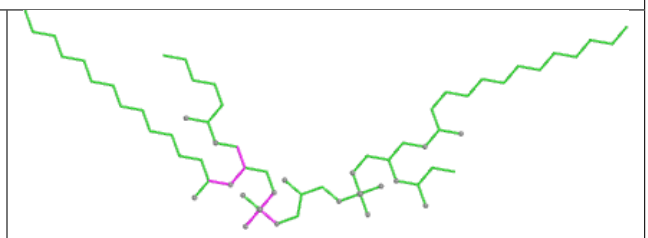
Ligand DMU O 305



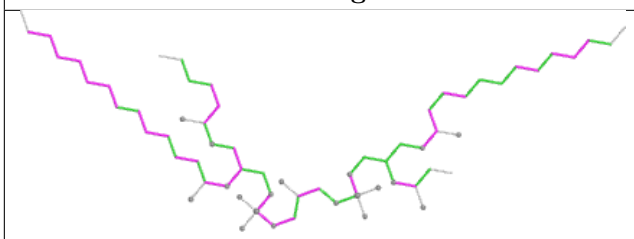
Ligand CDL A 606



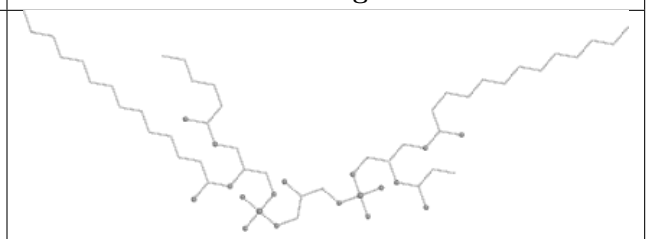
Bond lengths



Bond angles

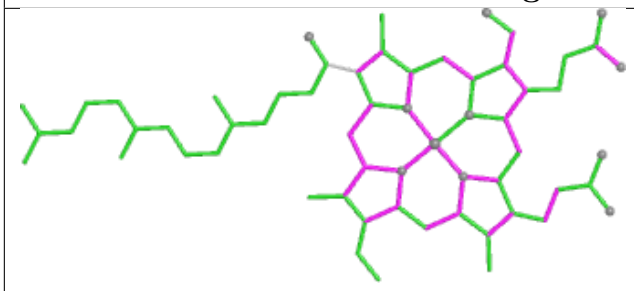


Torsions

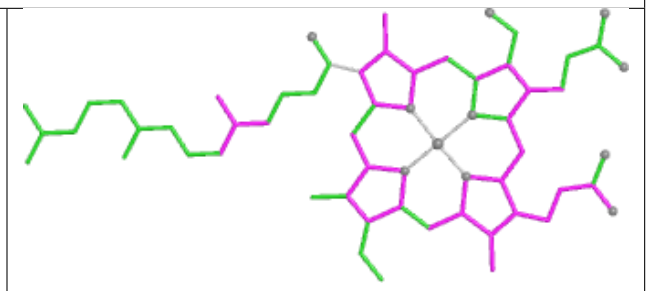


Rings

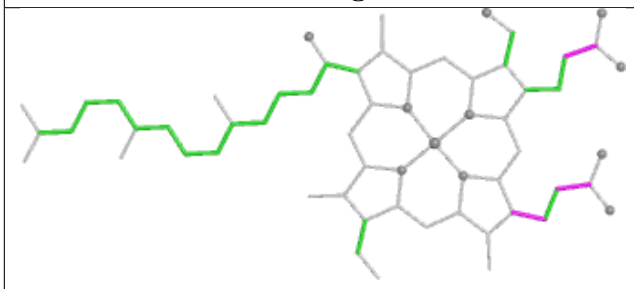
Ligand HEA A 602



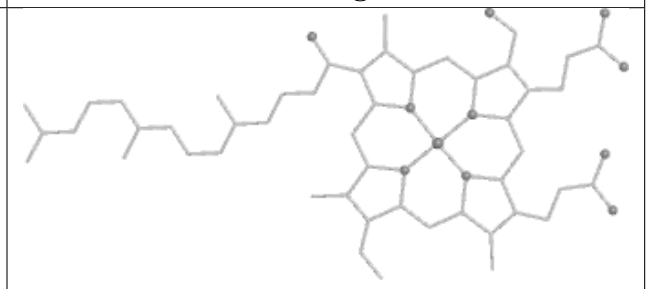
Bond lengths



Bond angles

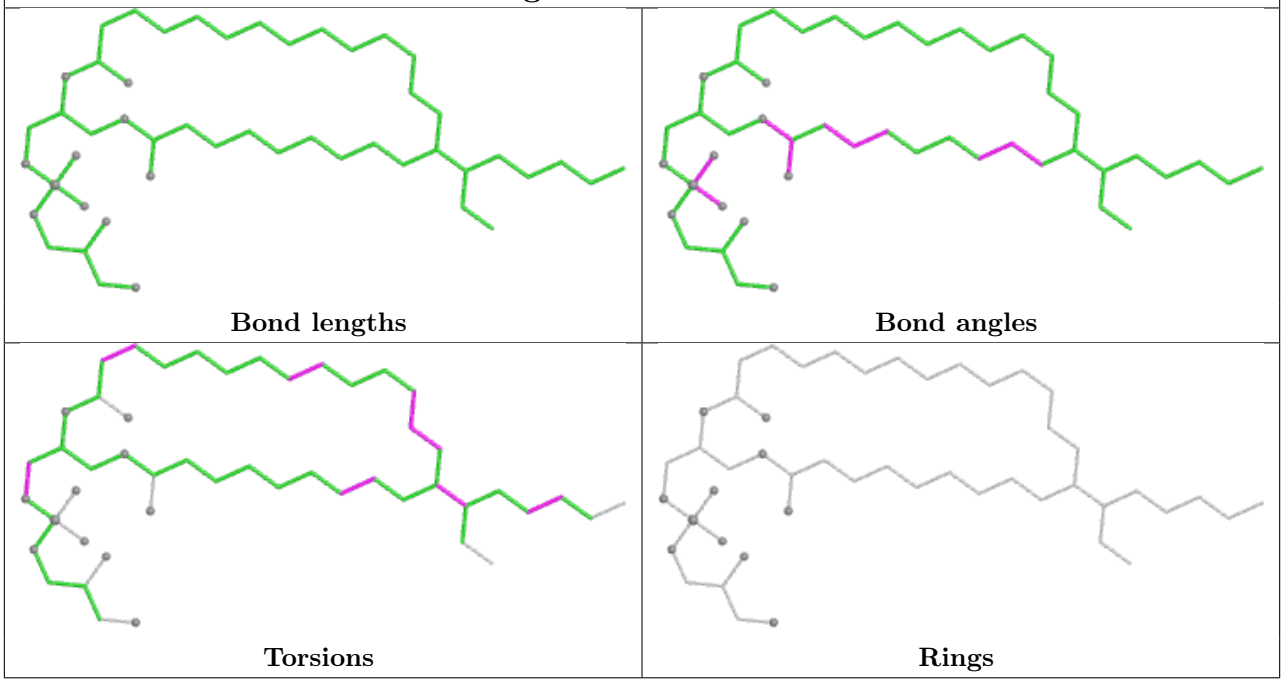


Torsions

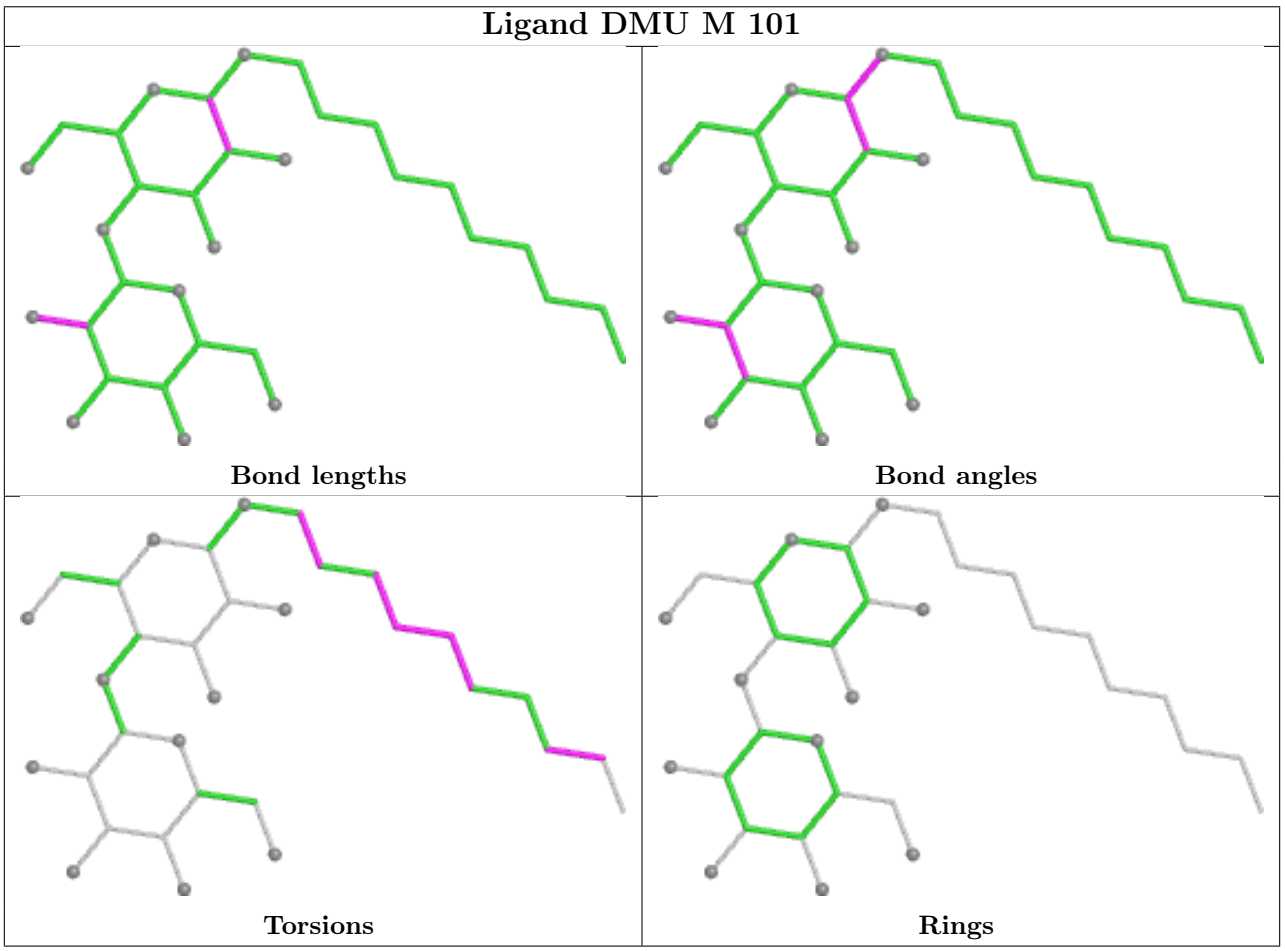


Rings

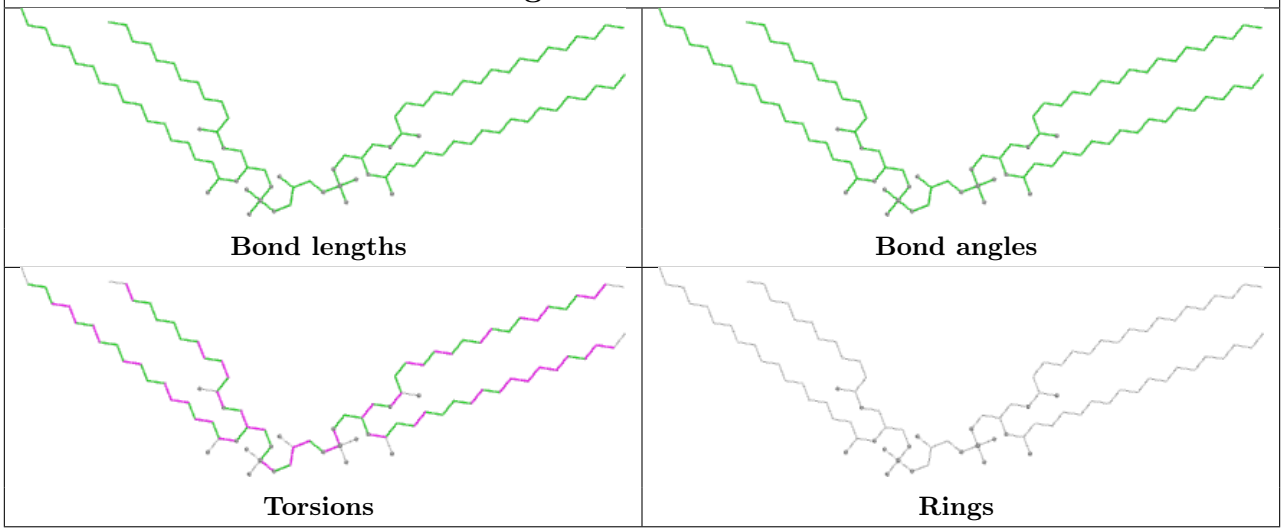
Ligand PGV P 304



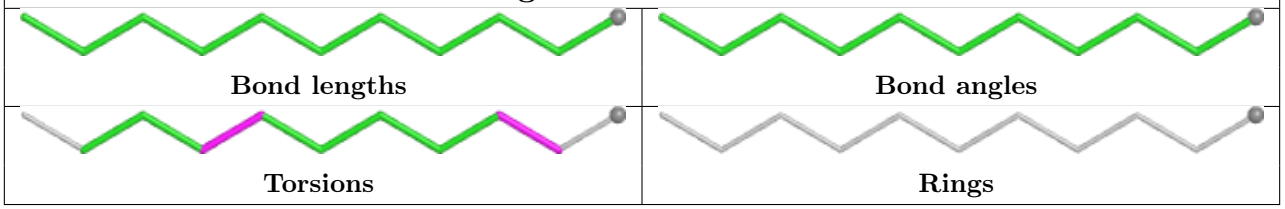
Ligand DMU M 101



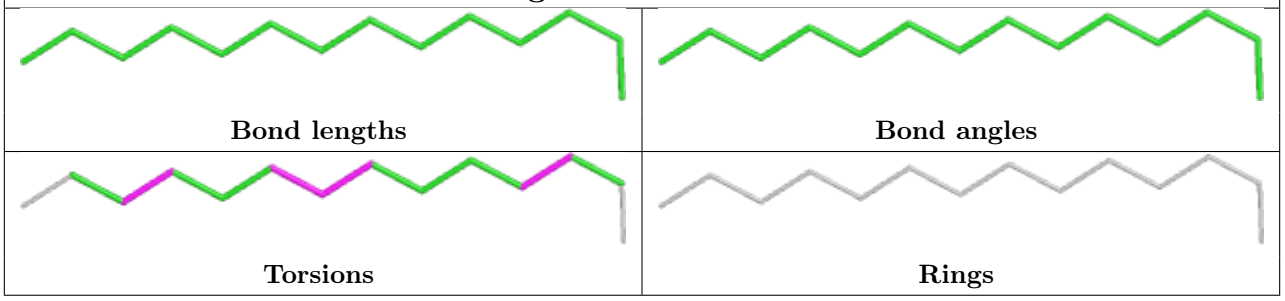
Ligand CDL Y 101



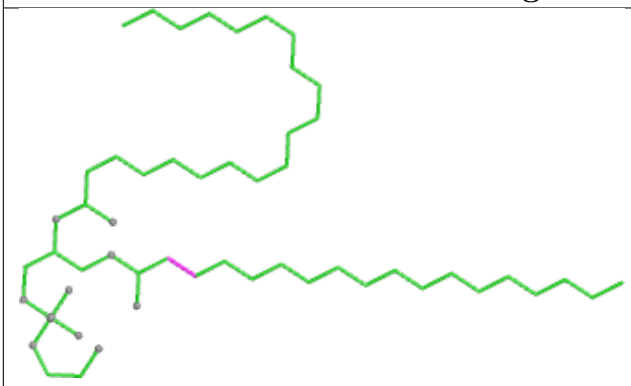
Ligand DMU C 306



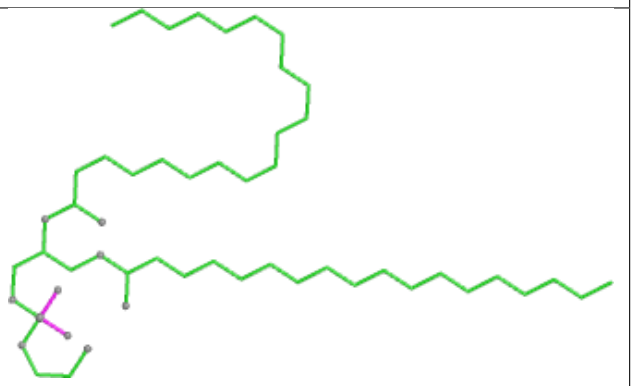
Ligand LFA N 606



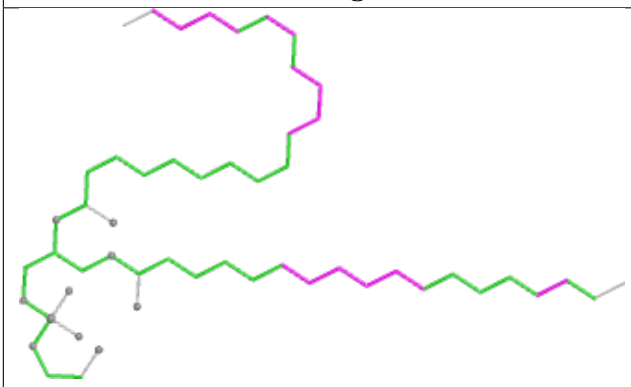
Ligand PEK G 101



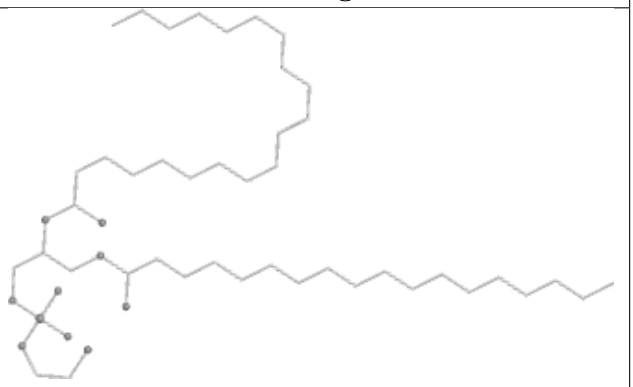
Bond lengths



Bond angles

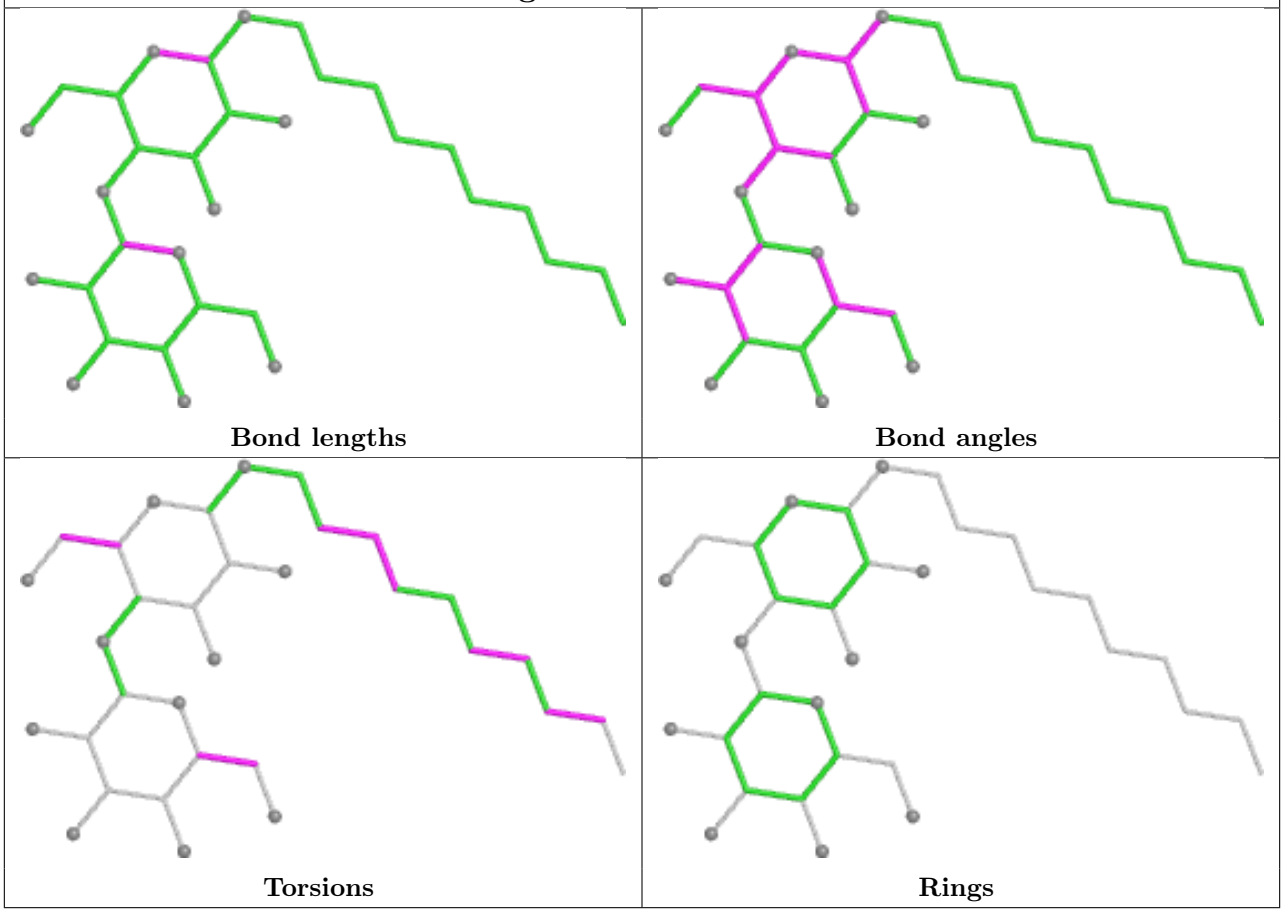


Torsions

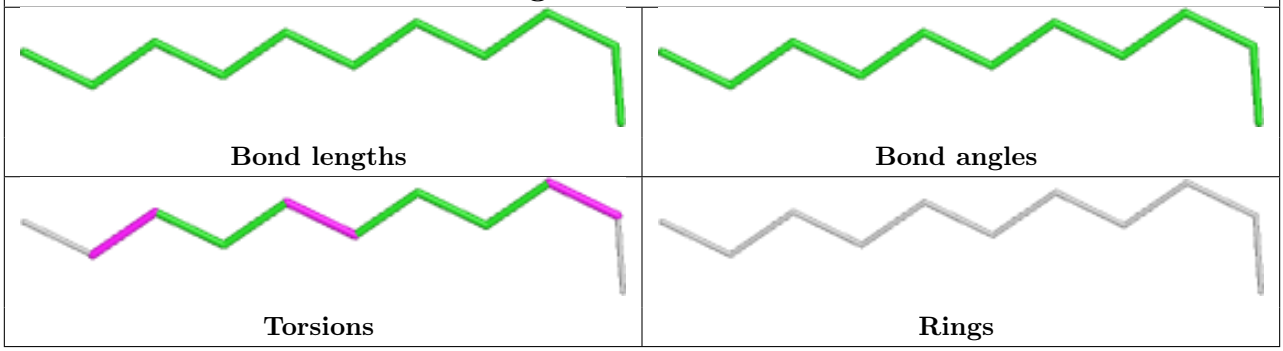


Rings

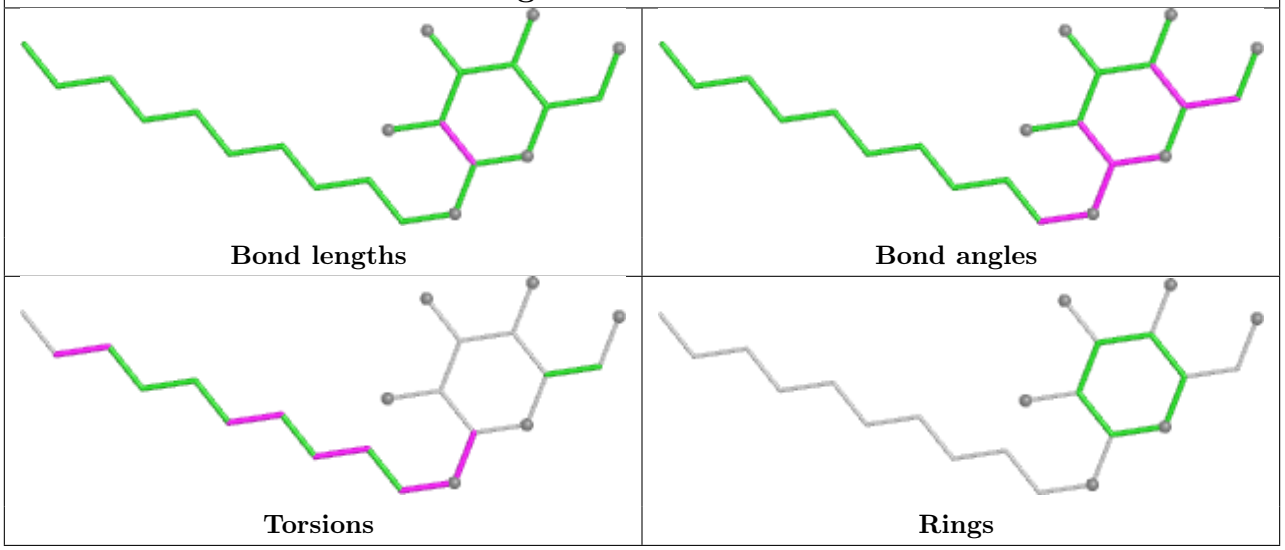
Ligand DMU P 316



Ligand LFA C 312



Ligand DMU O 307



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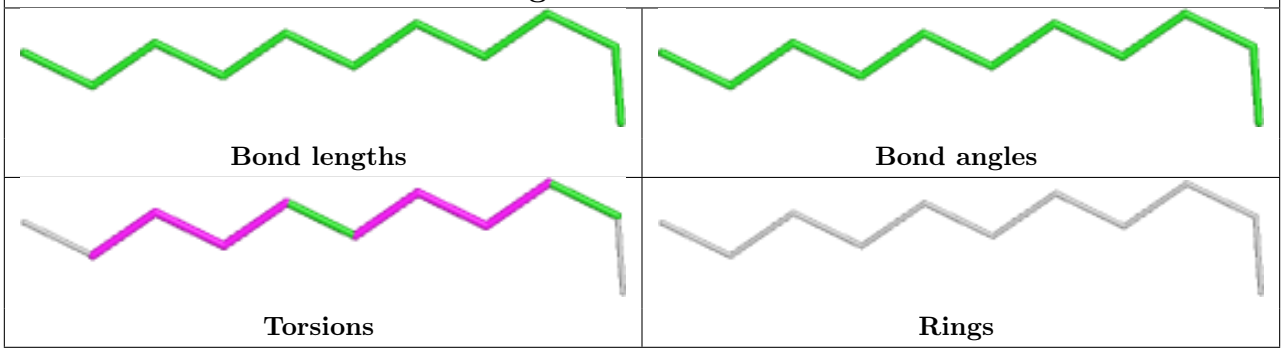
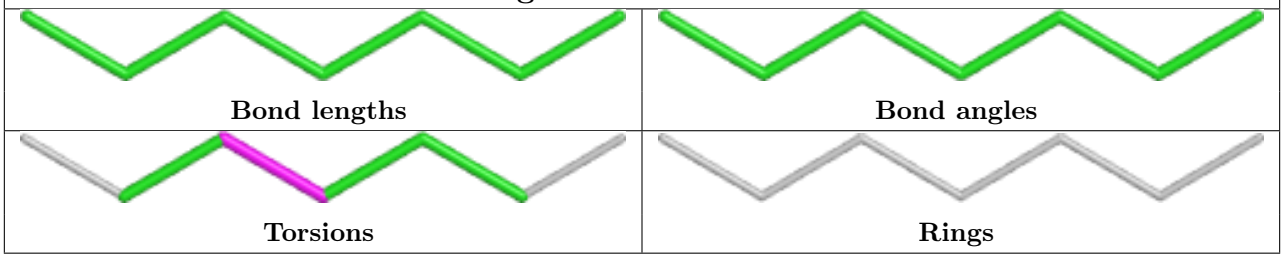
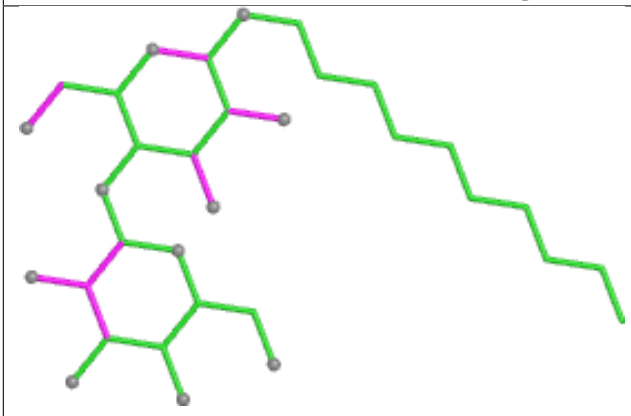


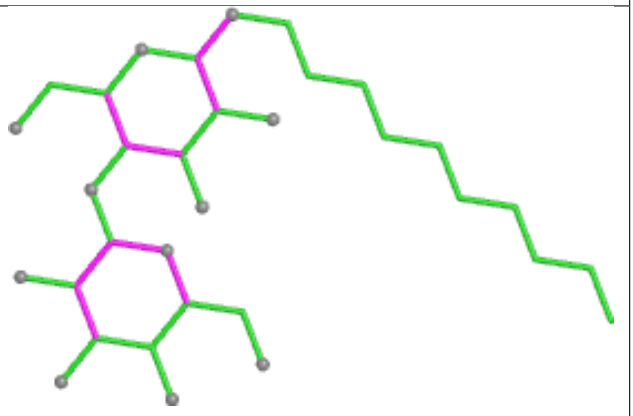
Ligand DMU N 607



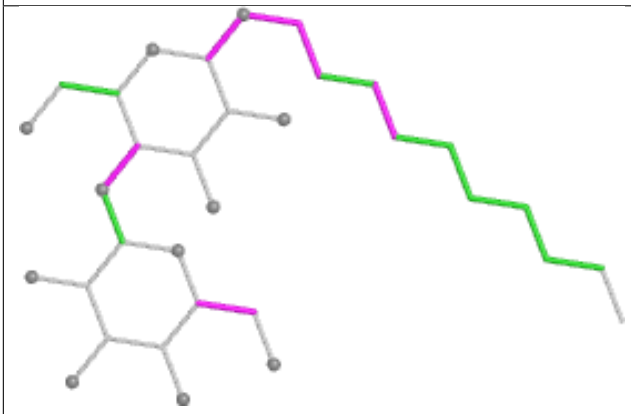
Ligand DMU D 201



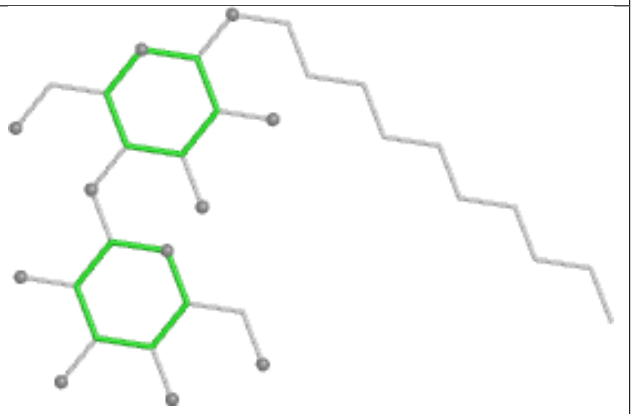
Bond lengths



Bond angles

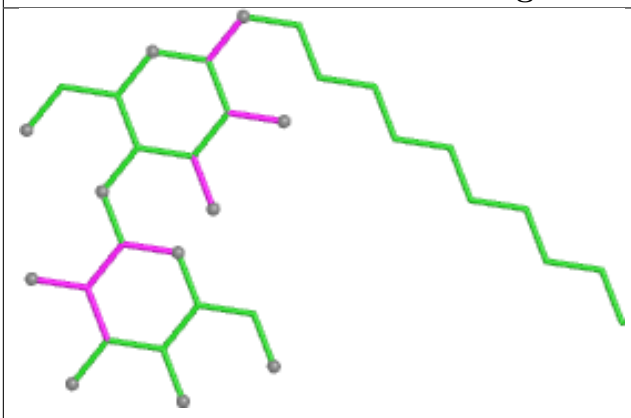


Torsions



Rings

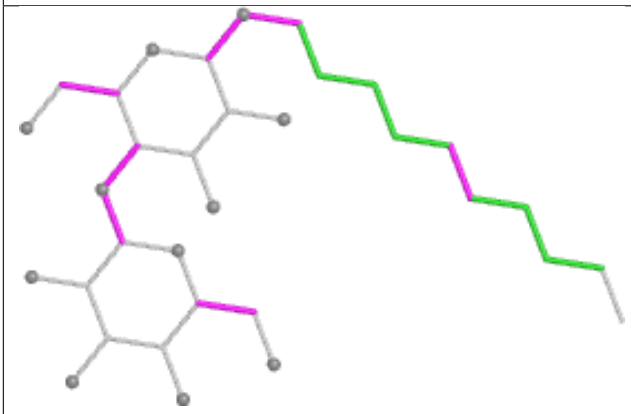
Ligand DMU Q 201



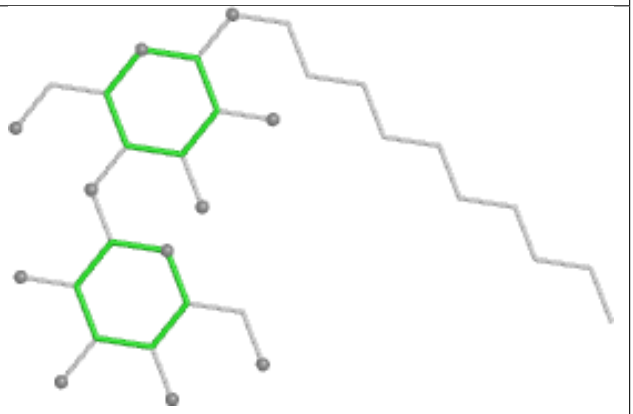
Bond lengths



Bond angles

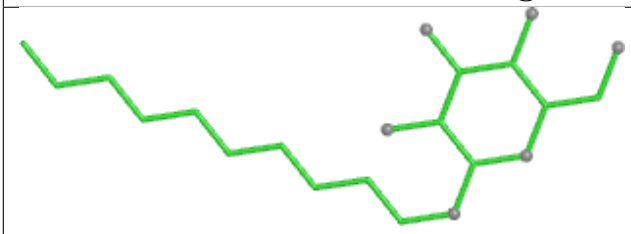


Torsions

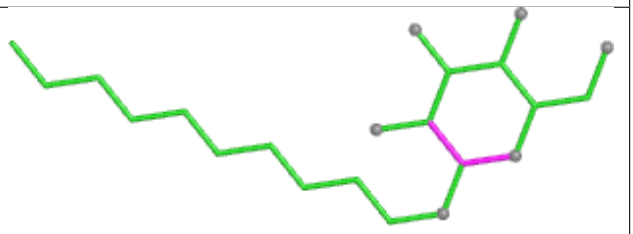


Rings

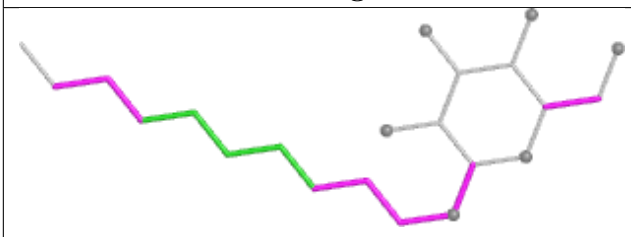
Ligand DMU B 304



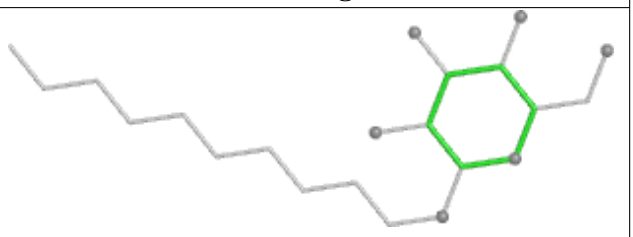
Bond lengths



Bond angles

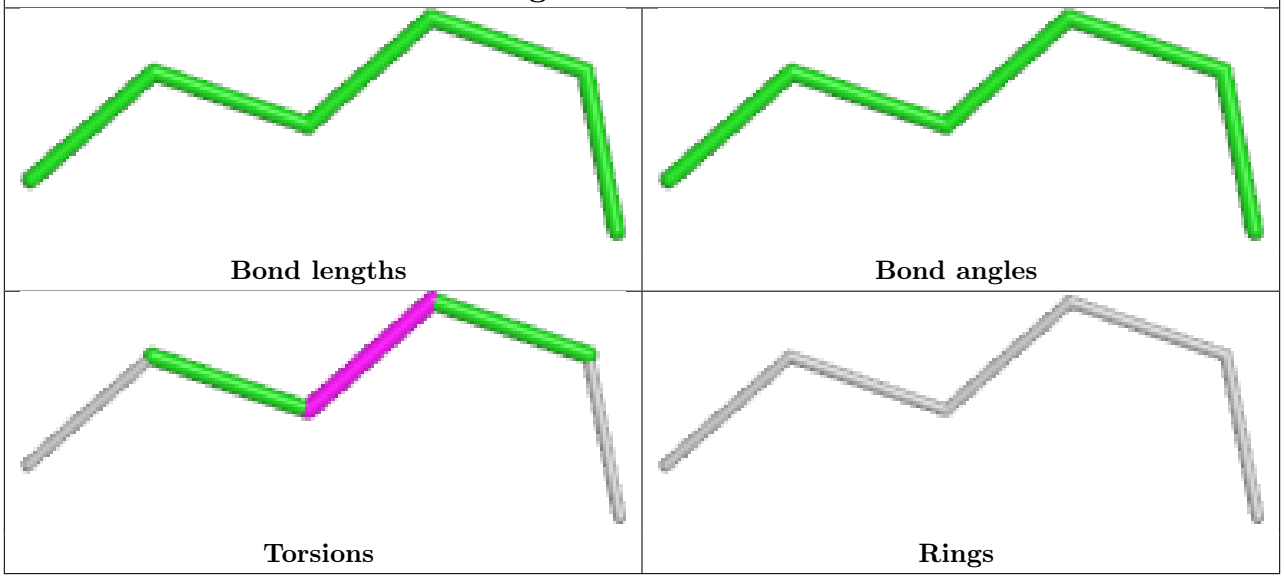


Torsions

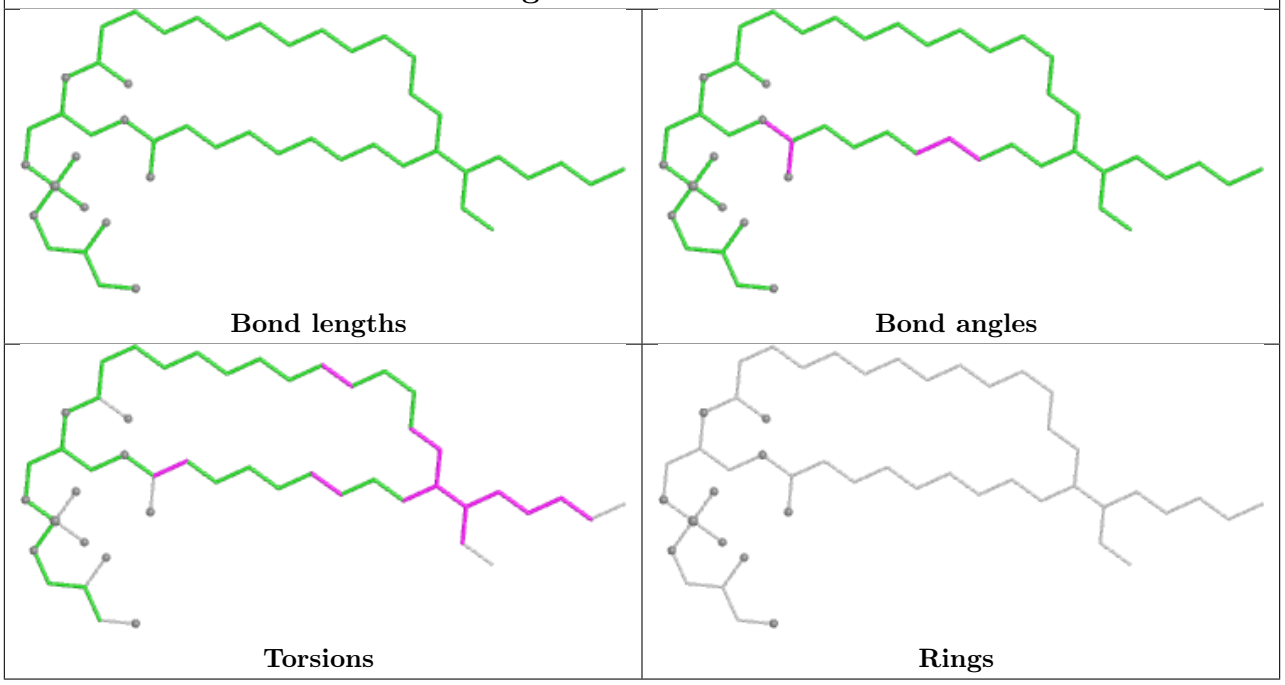


Rings

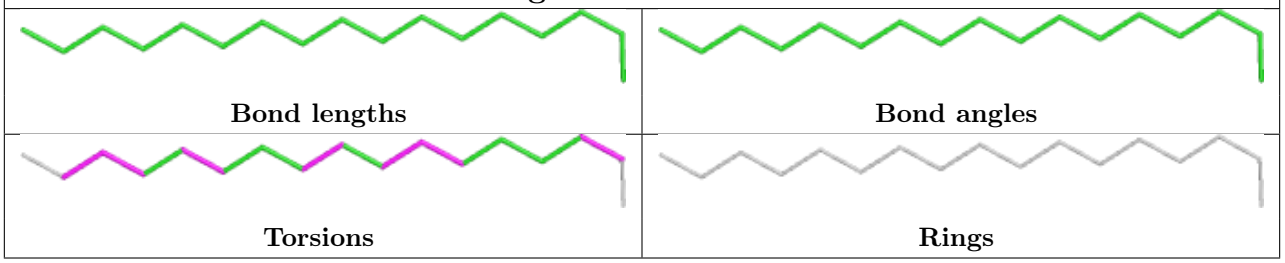
Ligand LFA C 308



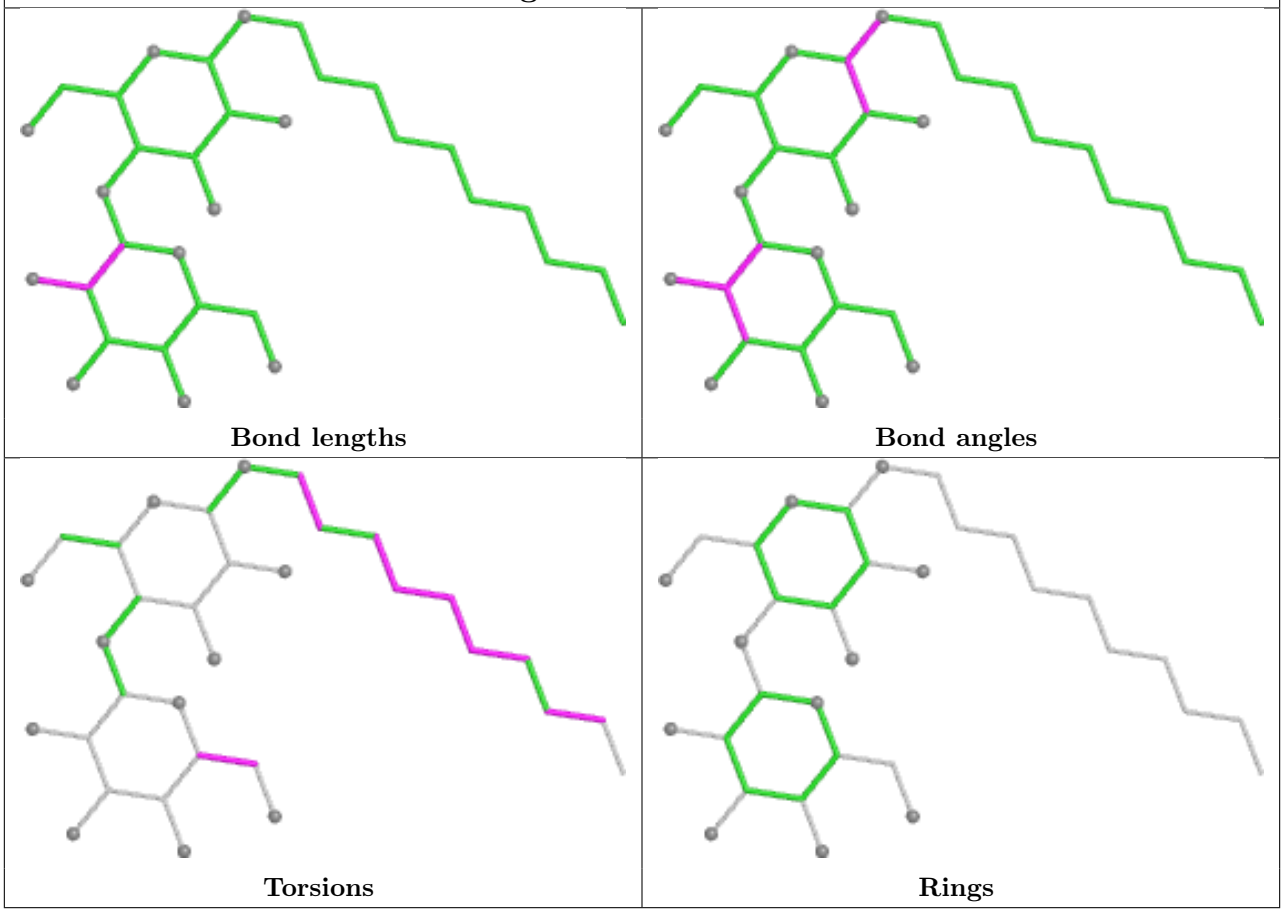
Ligand PGV A 613



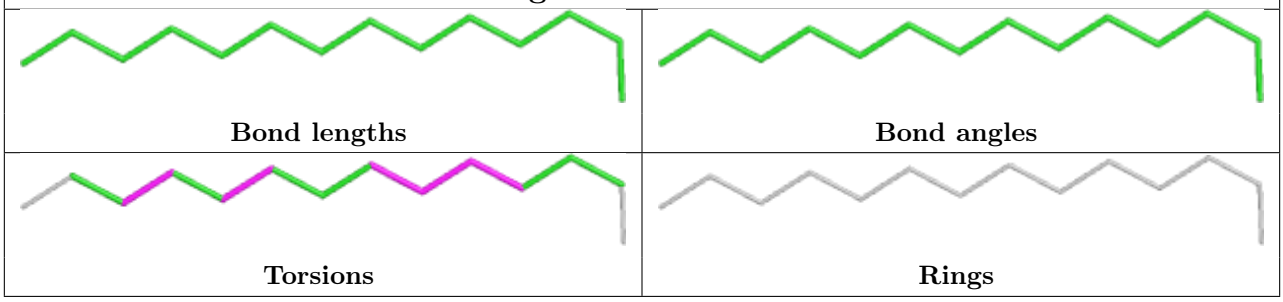
Ligand LFA O 301



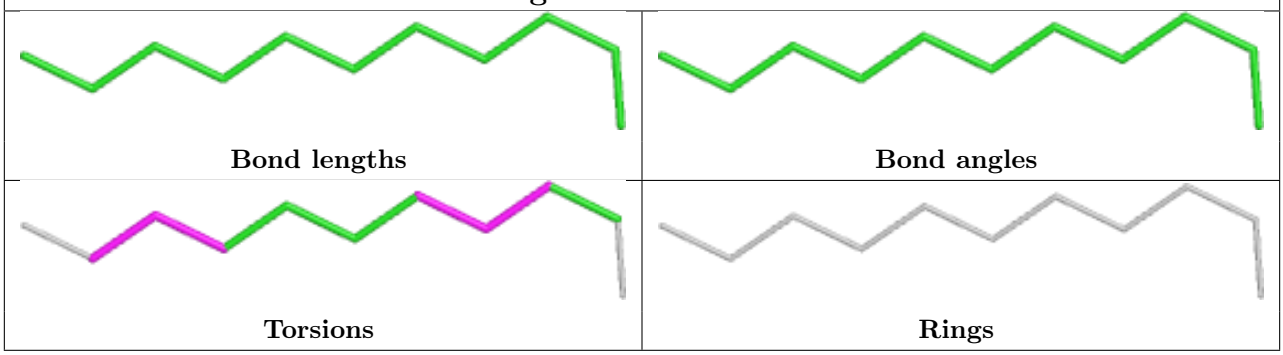
Ligand DMU Z 101



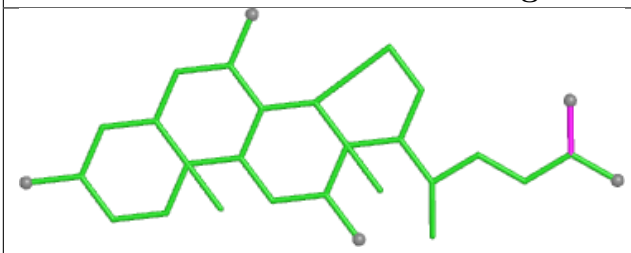
Ligand LFA C 311



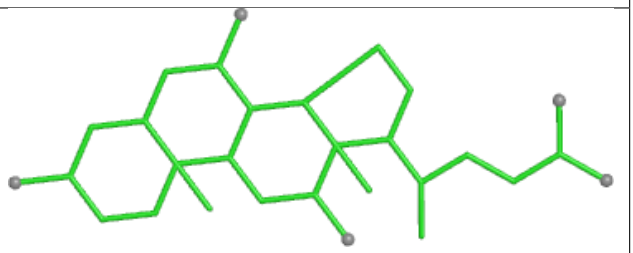
Ligand LFA P 308



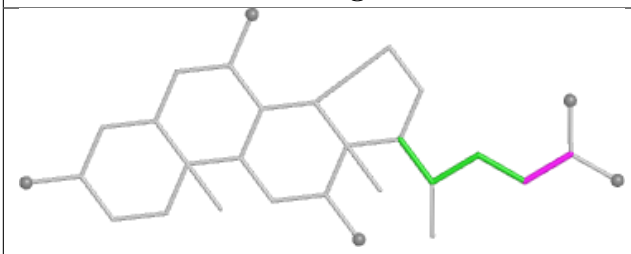
Ligand CHD B 306



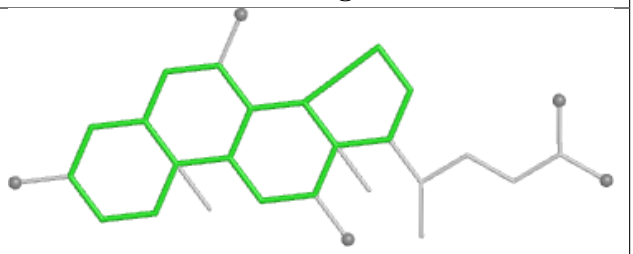
Bond lengths



Bond angles

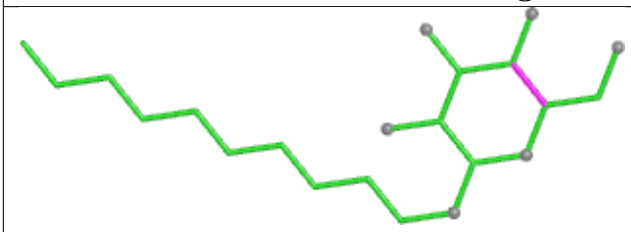


Torsions



Rings

Ligand DMU O 303



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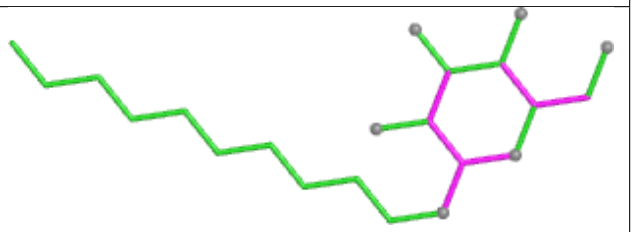
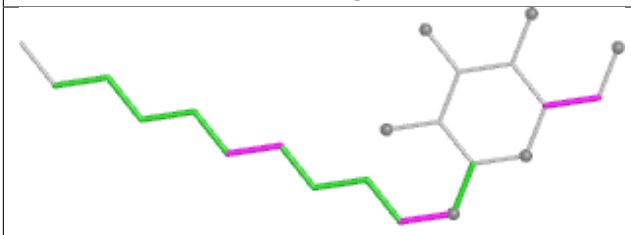
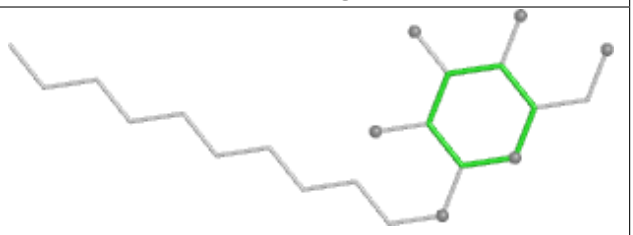


Bond angles

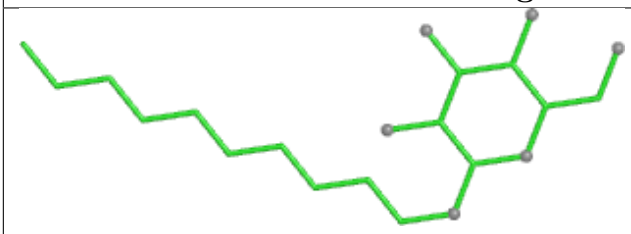


Torsions

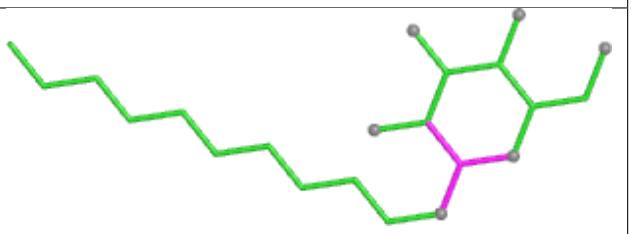


Rings

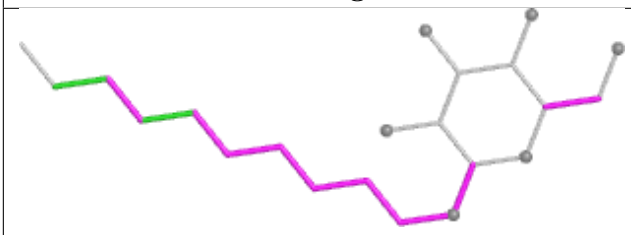
Ligand DMU Y 102



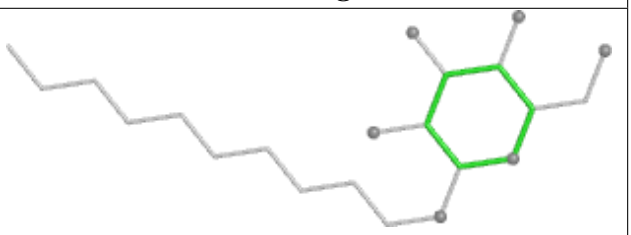
Bond lengths



Bond angles

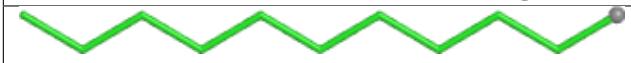


Torsions



Rings

Ligand DMU G 103



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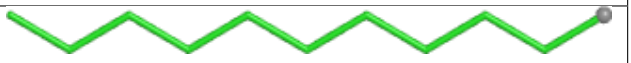


Bond angles

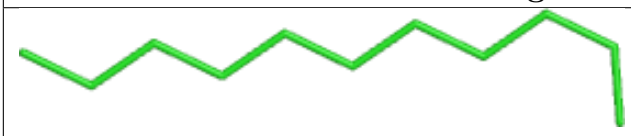


Torsions

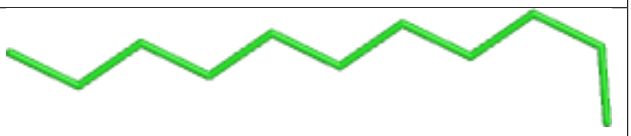


Rings

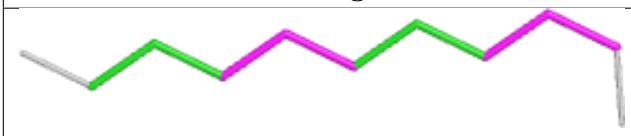
Ligand LFA O 302



Bond lengths



Bond angles



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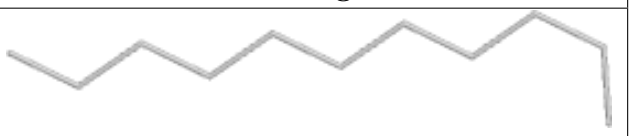
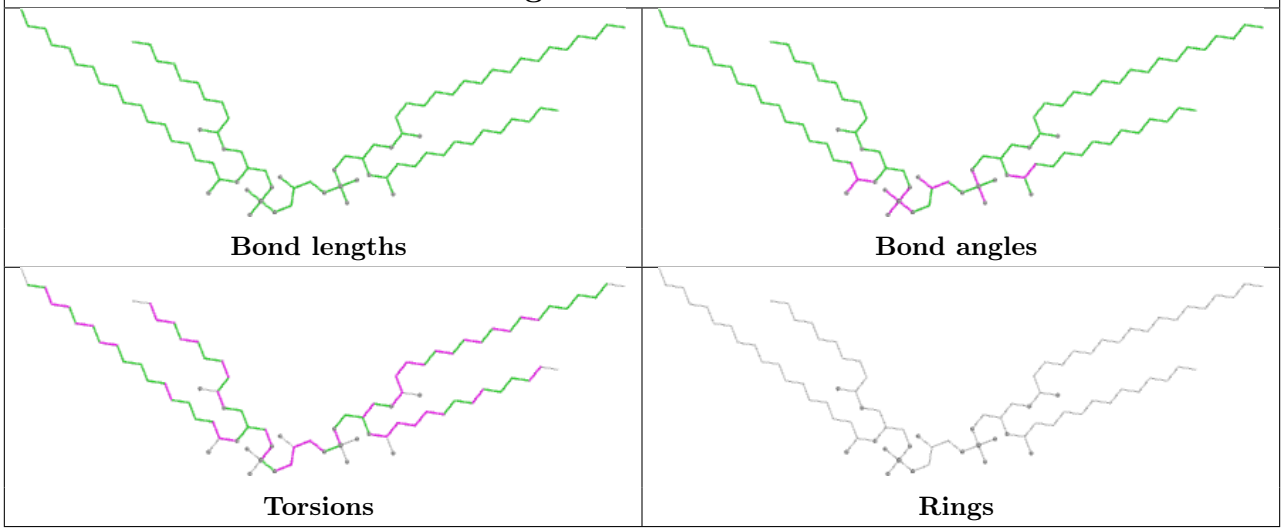
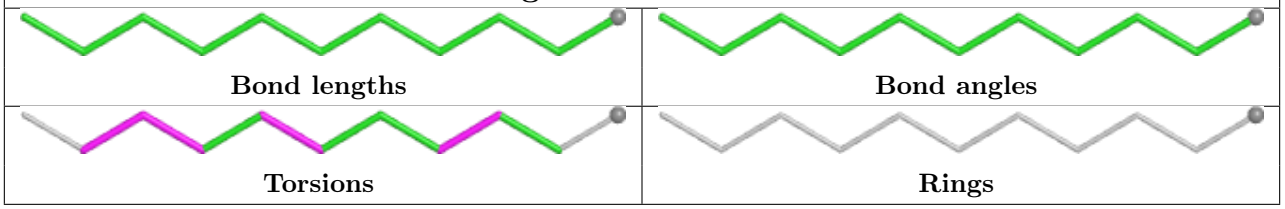


Rings

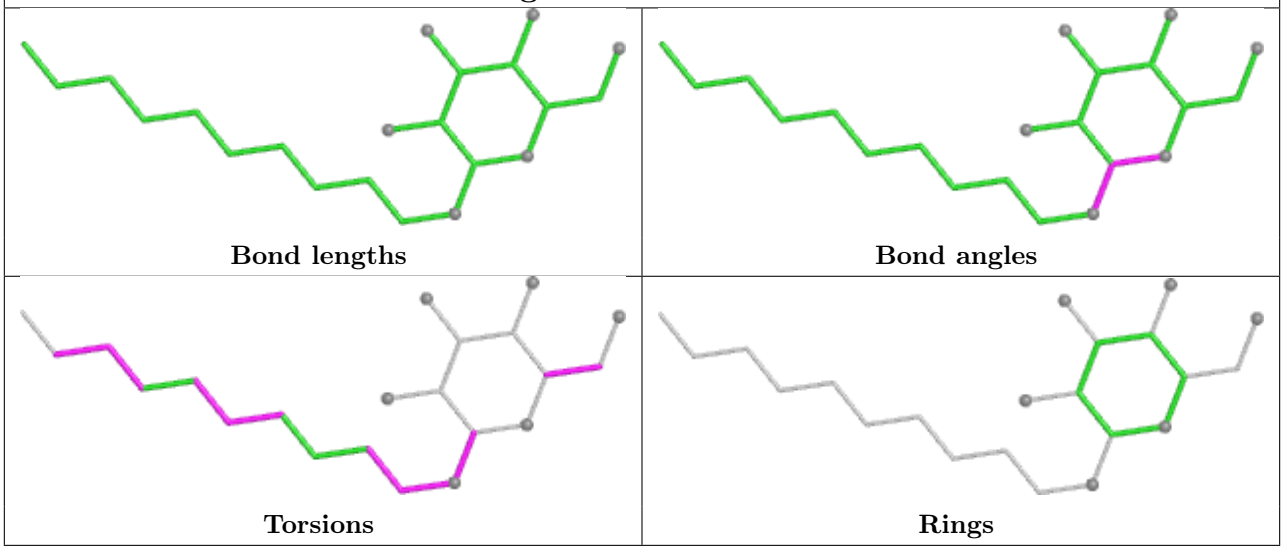
Ligand CDL C 304



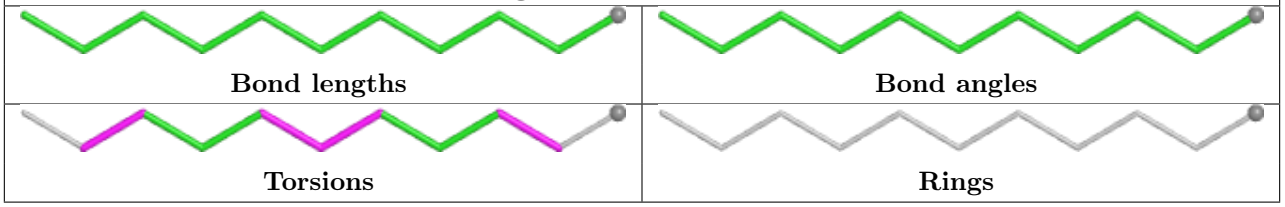
Ligand DMU J 101



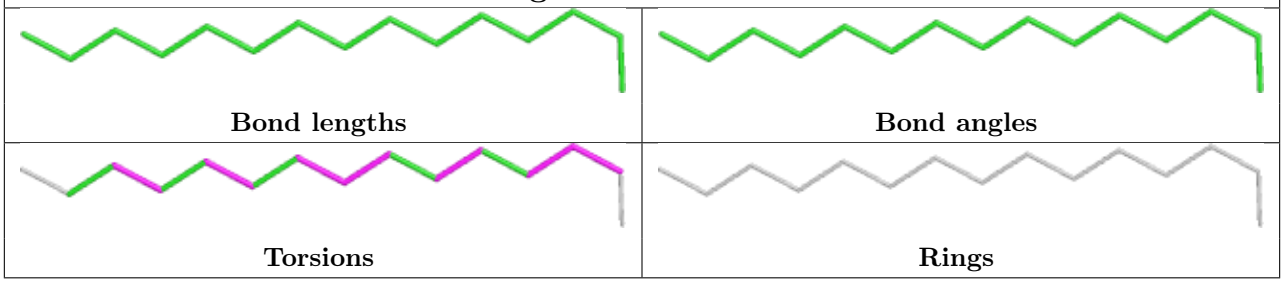
Ligand DMU L 102



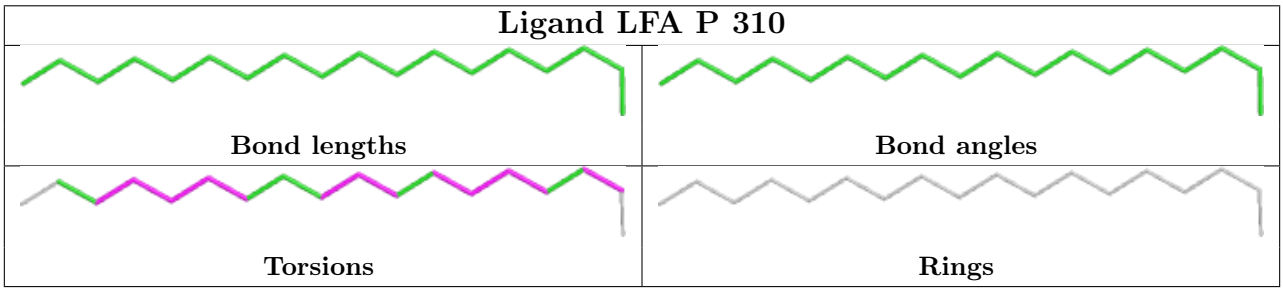
Ligand DMU W 101



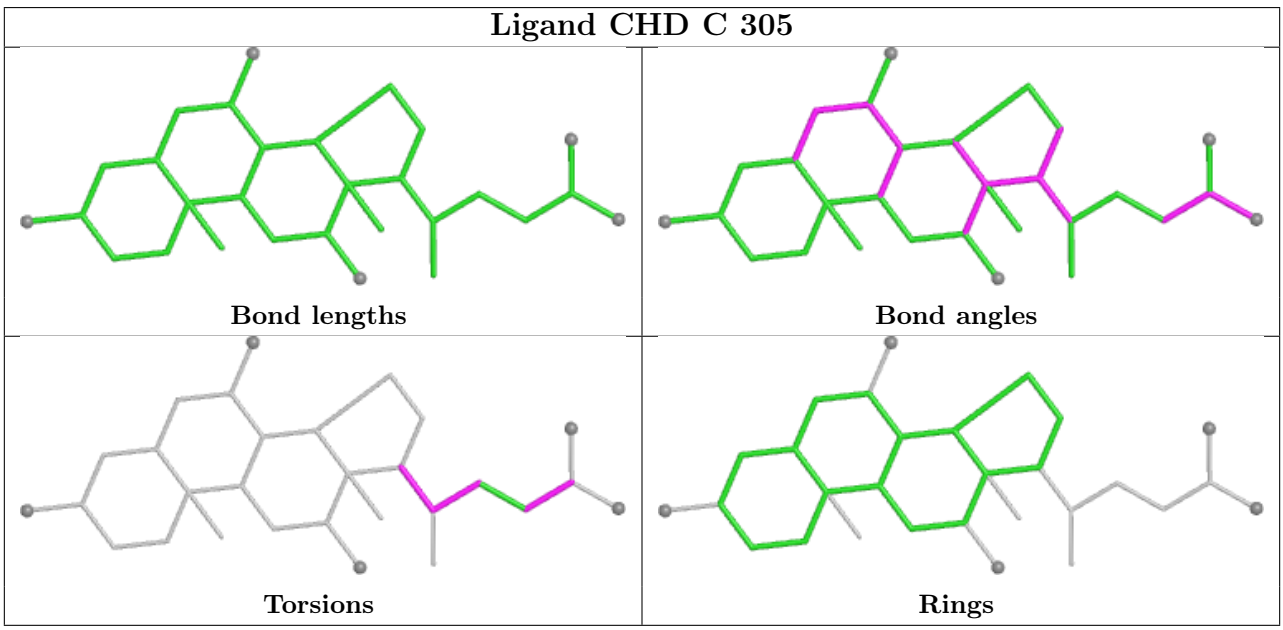
Ligand LFA P 301



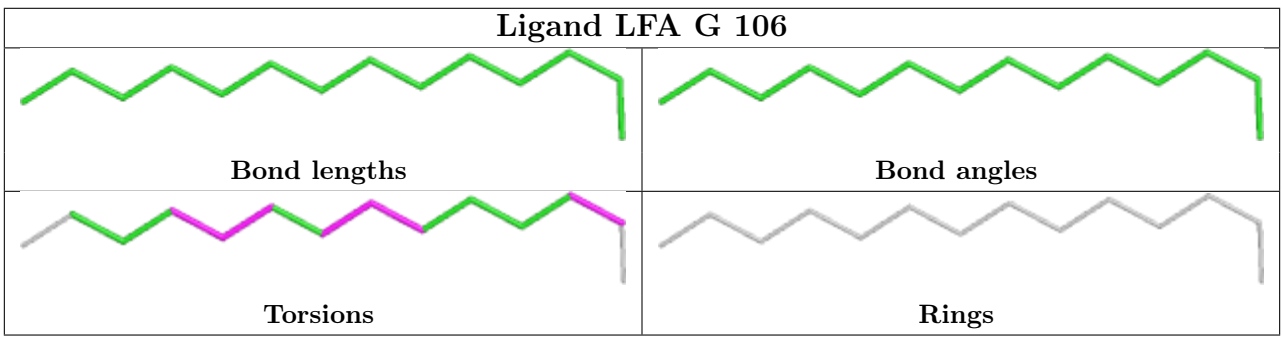
Ligand LFA P 310



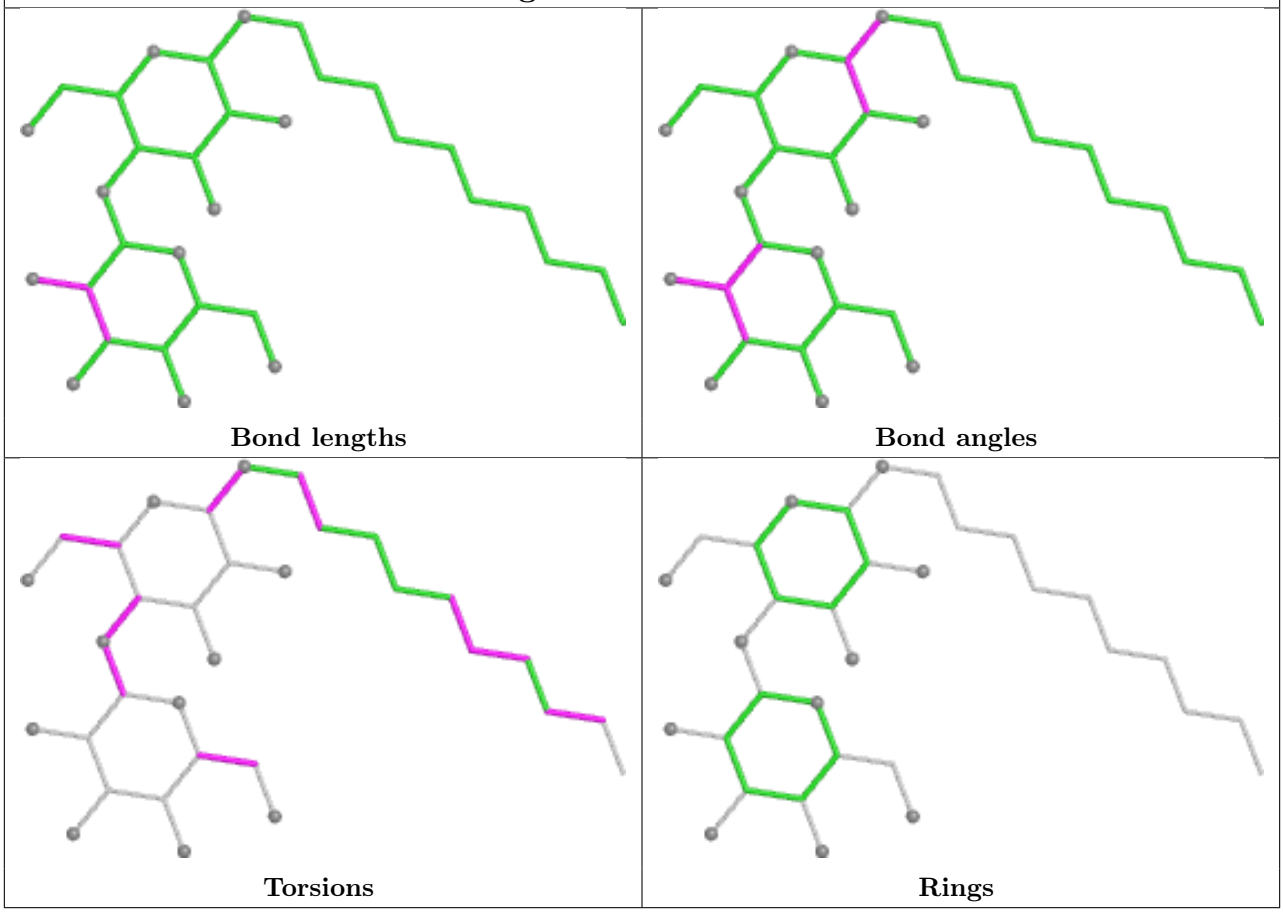
Ligand CHD C 305



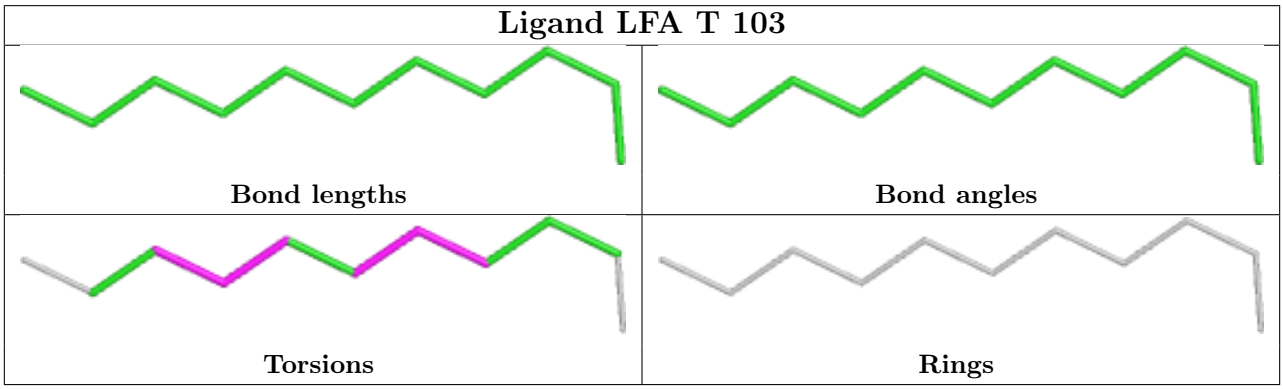
Ligand LFA G 106



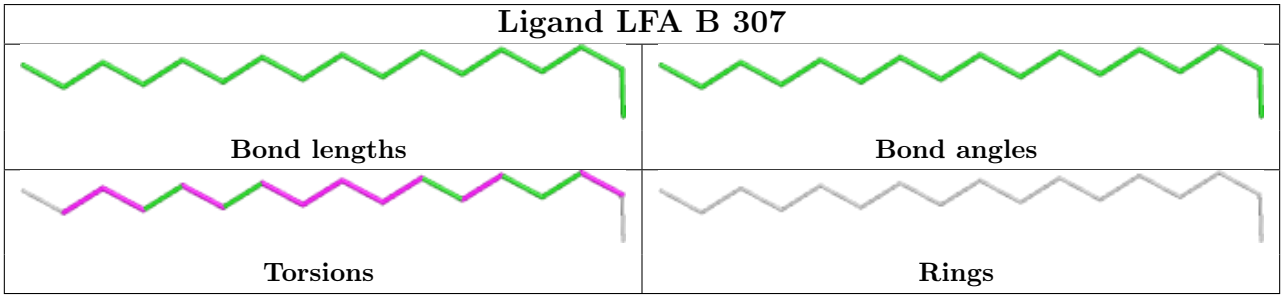
Ligand DMU P 319



Ligand LFA T 103



Ligand LFA B 307



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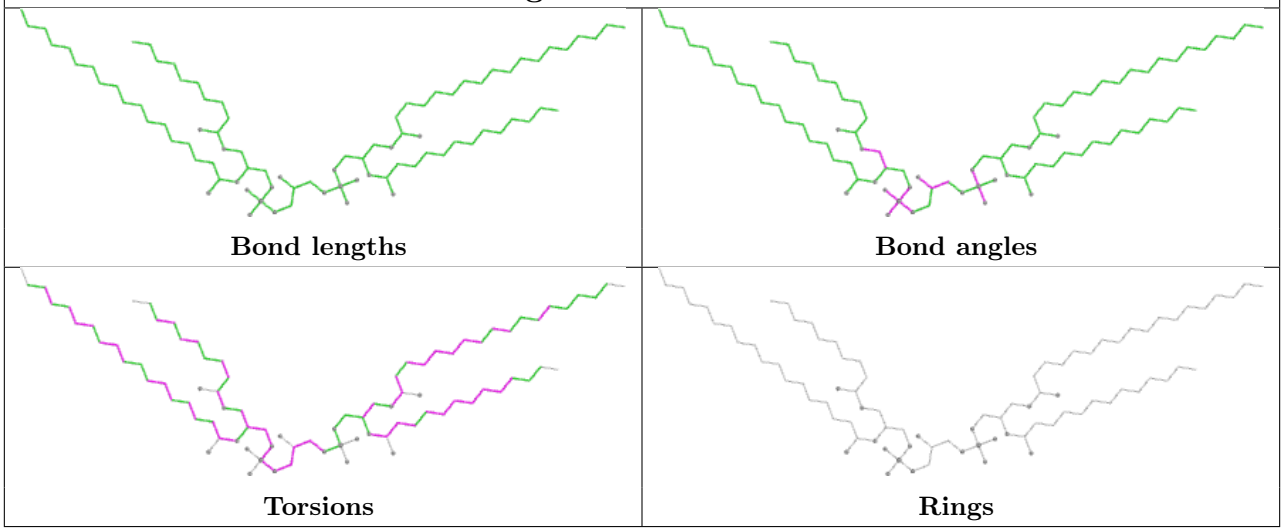

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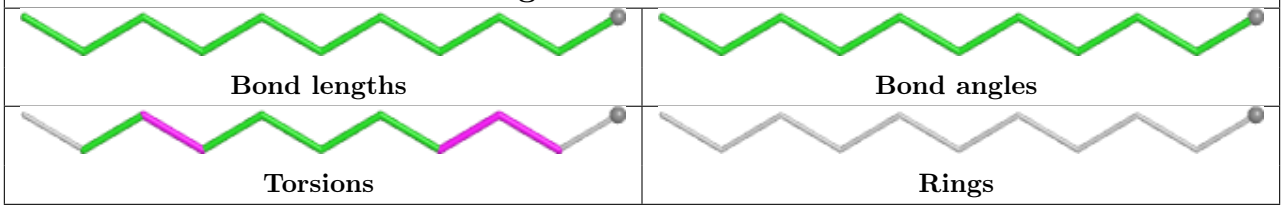
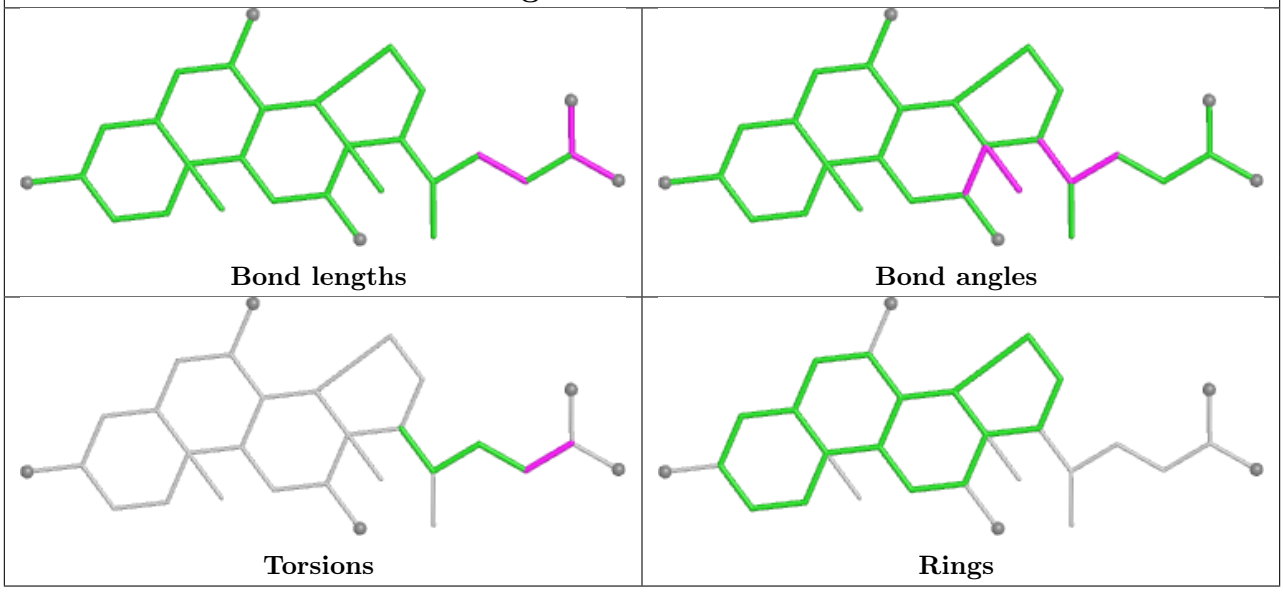
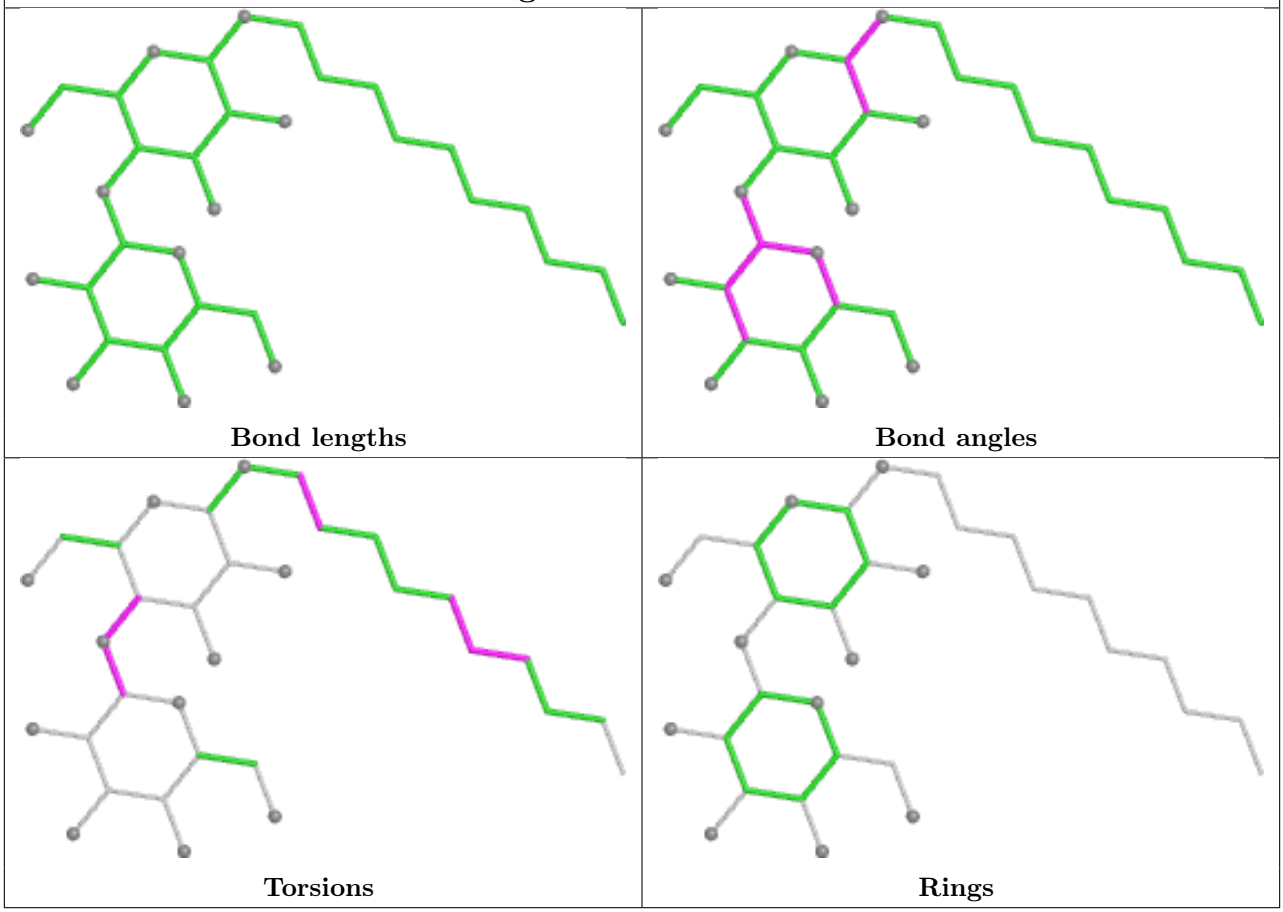


Ligand CHD C 301



Ligand DMU P 324



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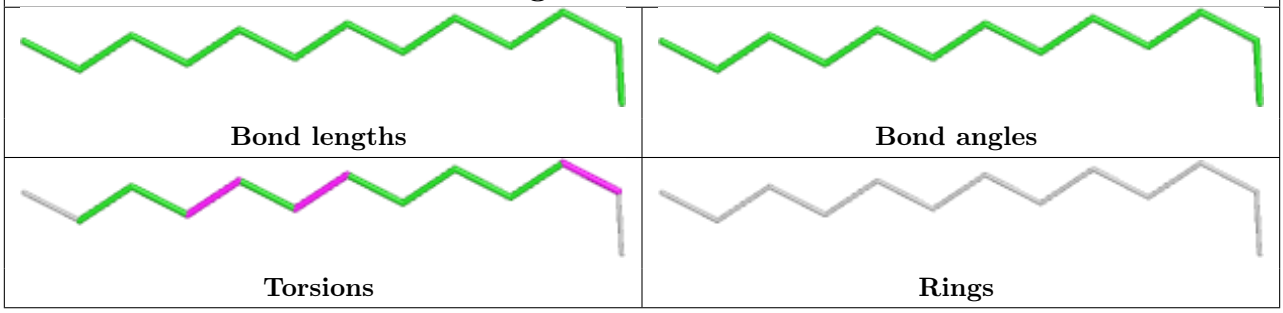
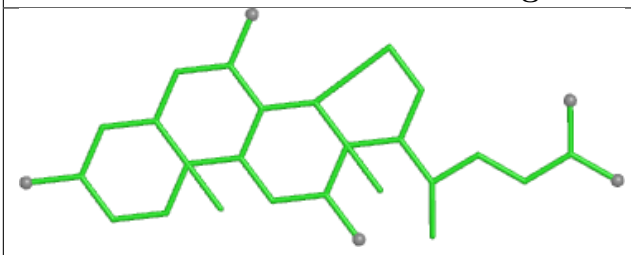
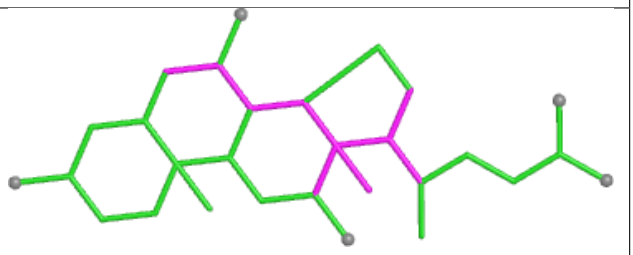


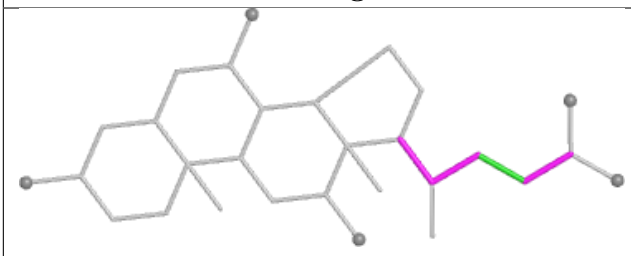
Ligand CHD P 306



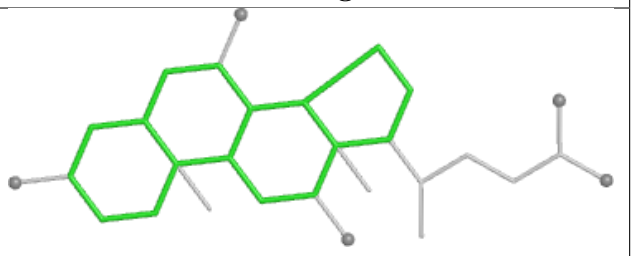
Bond lengths



Bond angles

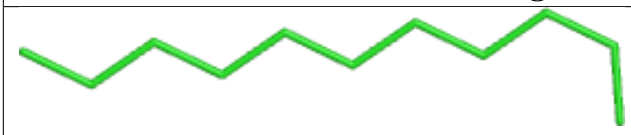


Torsions

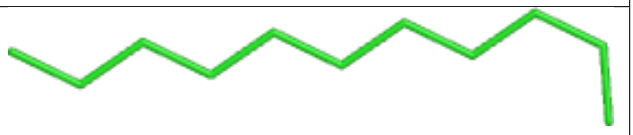


Rings

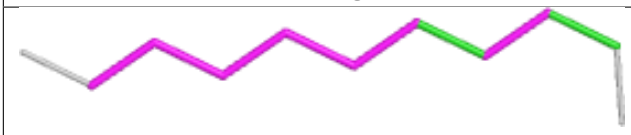
Ligand LFA P 311



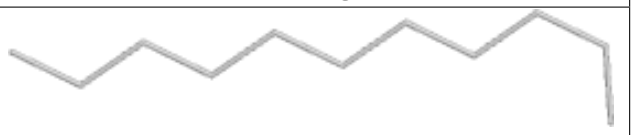
Bond lengths



Bond angles

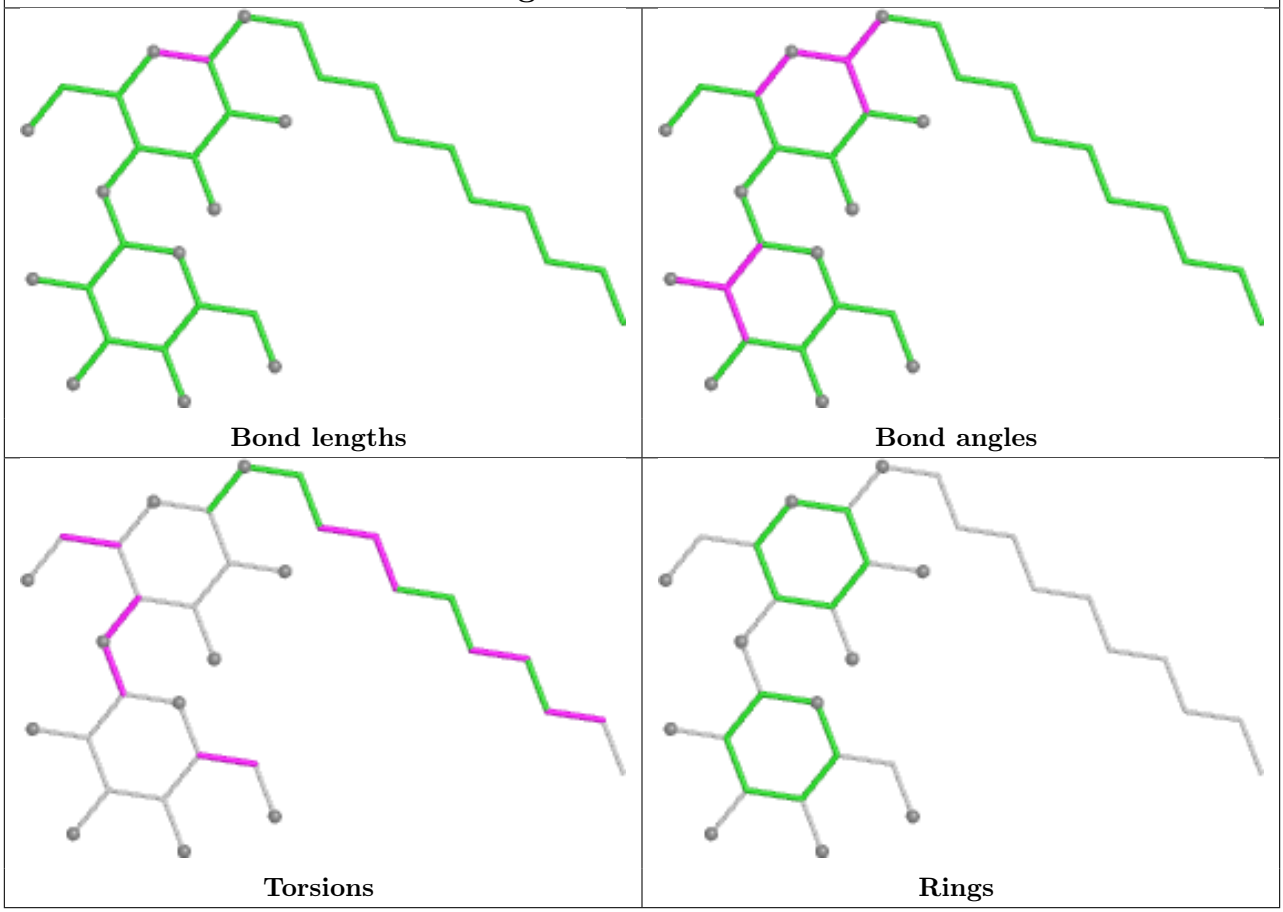


Torsions

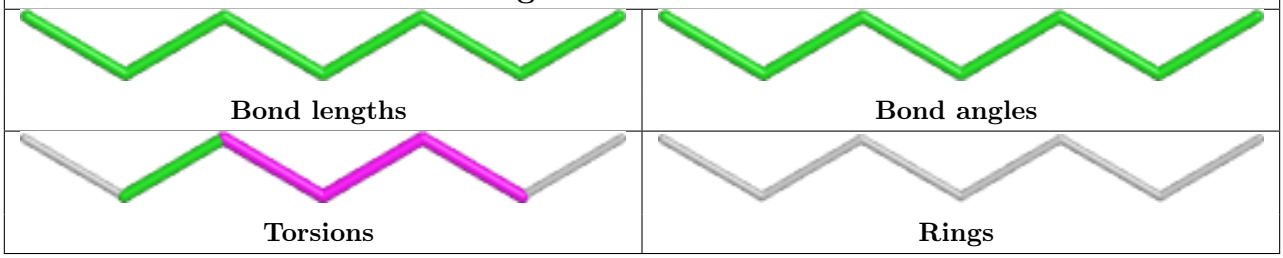


Rings

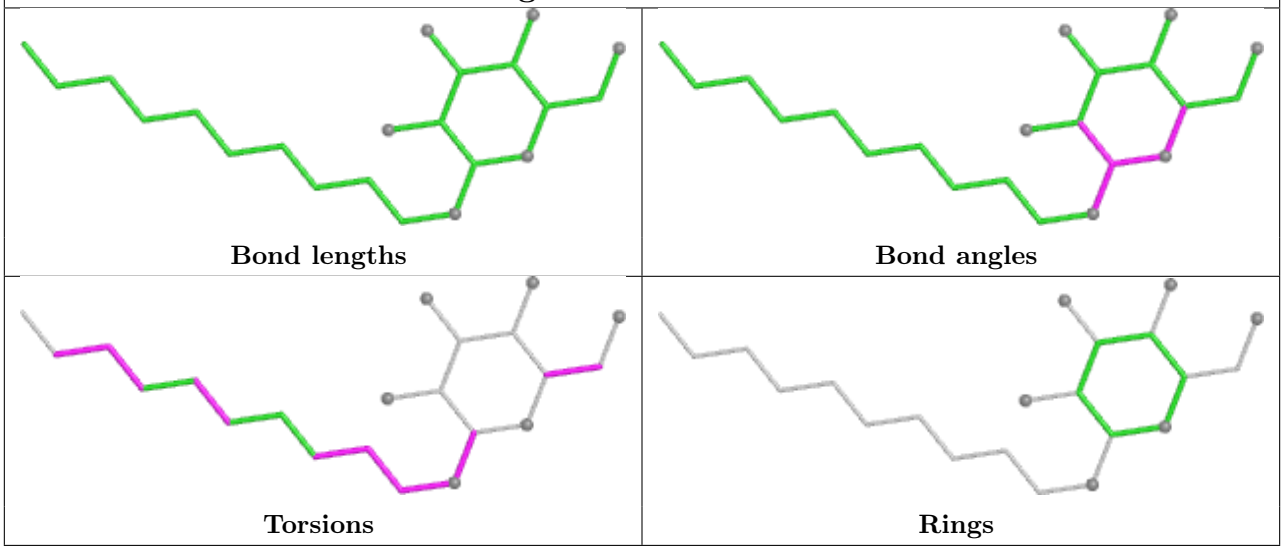
Ligand DMU C 315



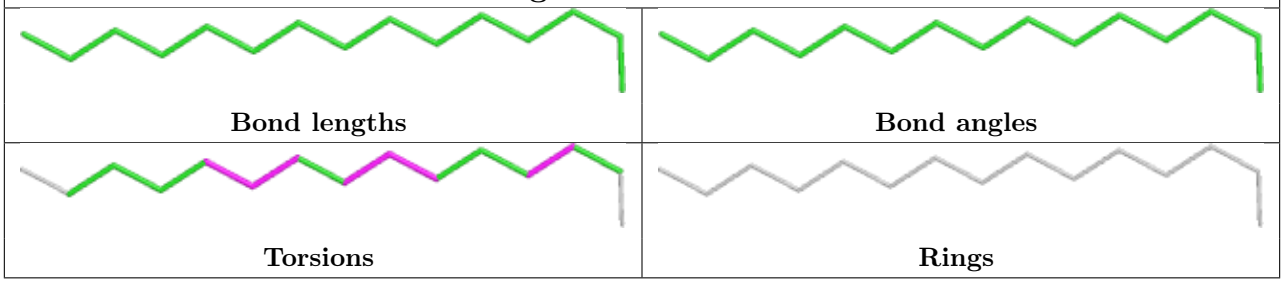
Ligand DMU A 608



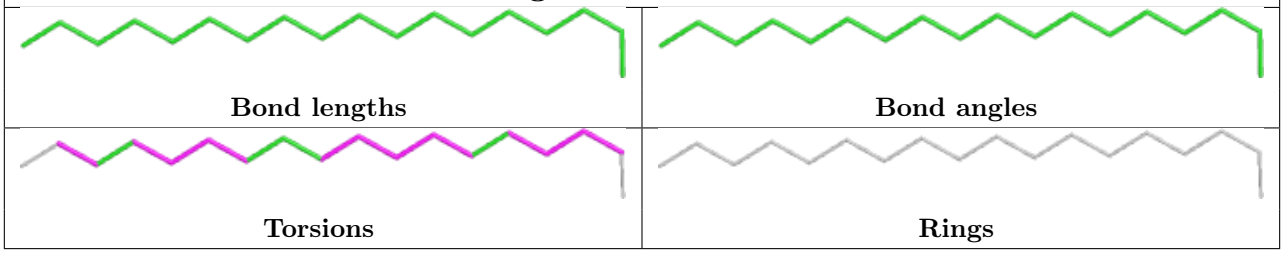
Ligand DMU B 308



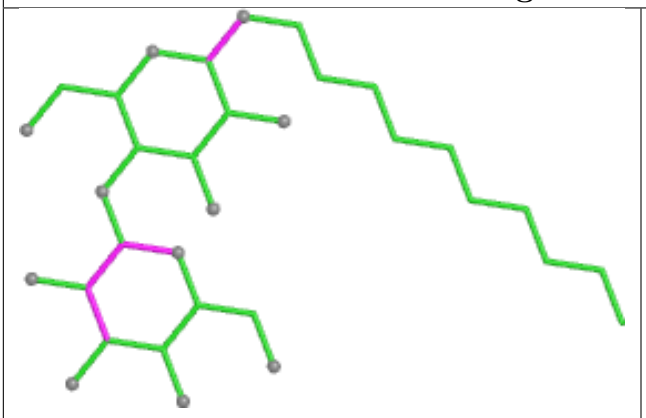
Ligand LFA P 314



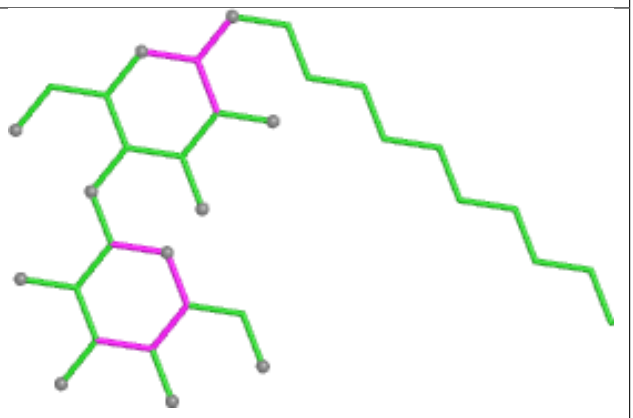
Ligand LFA C 309



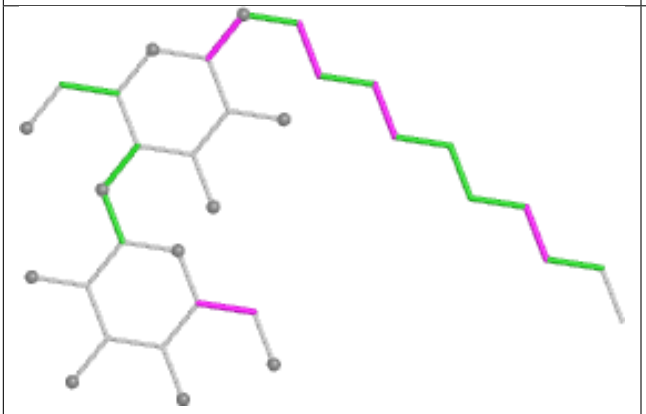
Ligand DMU N 608



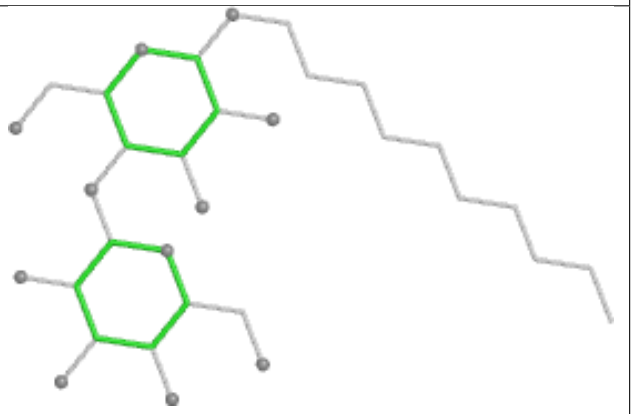
Bond lengths



Bond angles

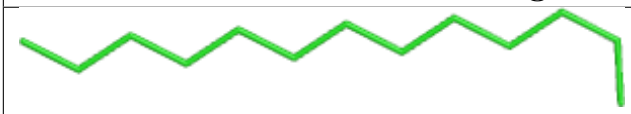


Torsions

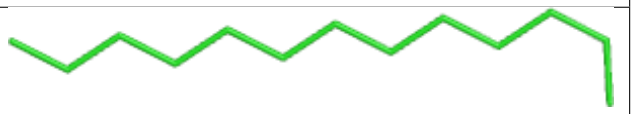


Rings

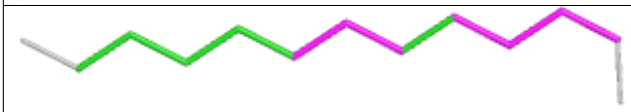
Ligand LFA P 315



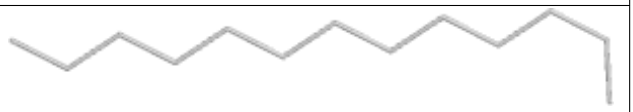
Bond lengths



Bond angles

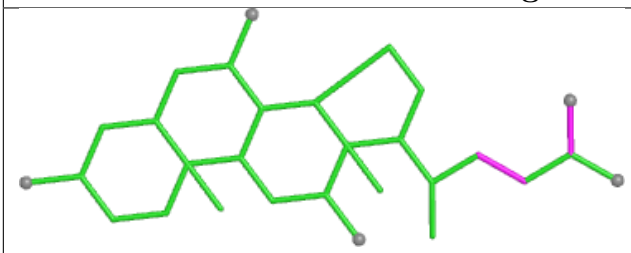


Torsions

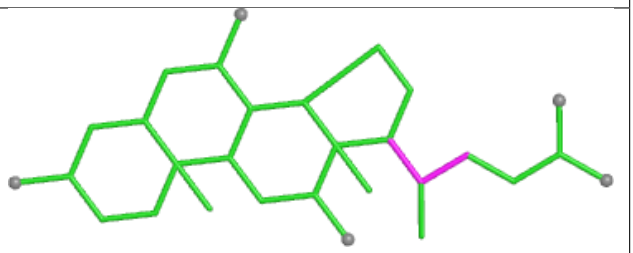


Rings

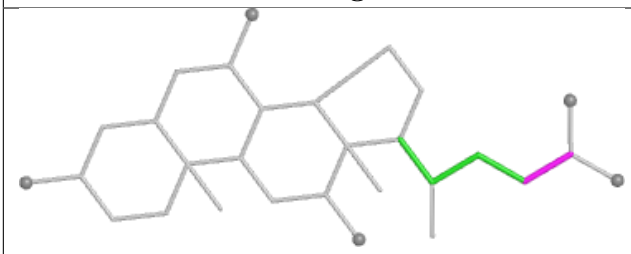
Ligand CHD P 302



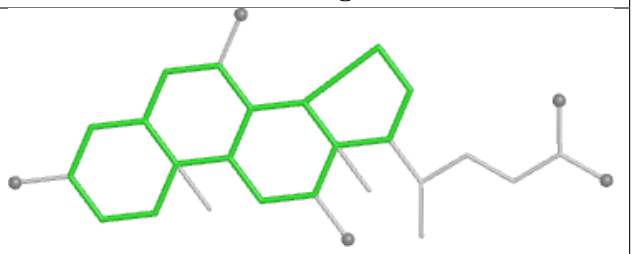
Bond lengths



Bond angles

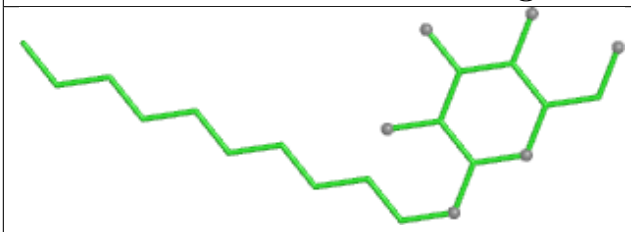


Torsions

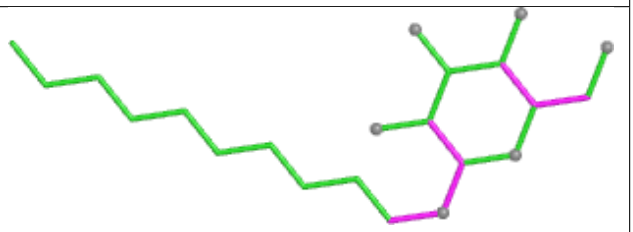


Rings

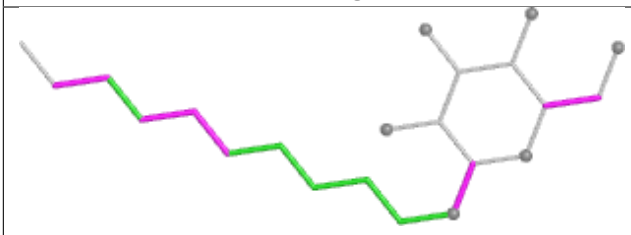
Ligand DMU T 104



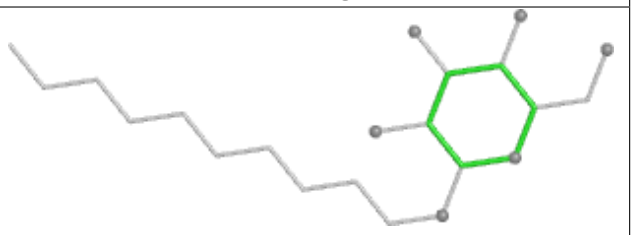
Bond lengths



Bond angles

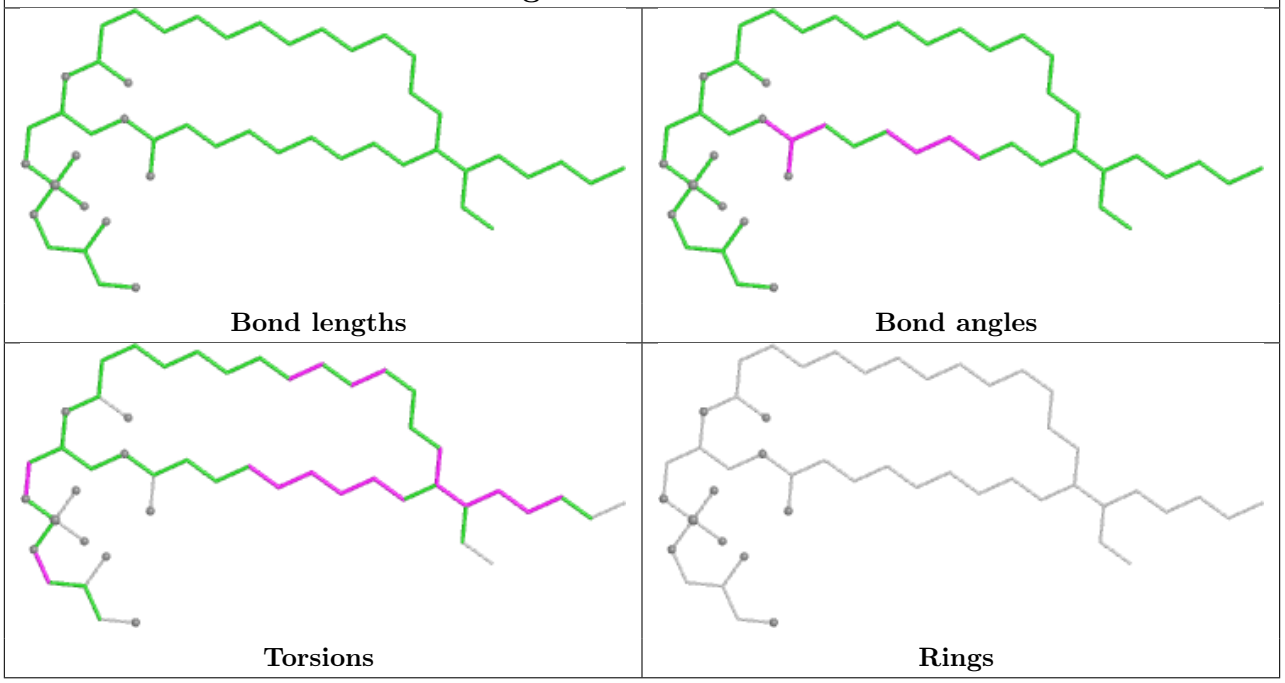


Torsions

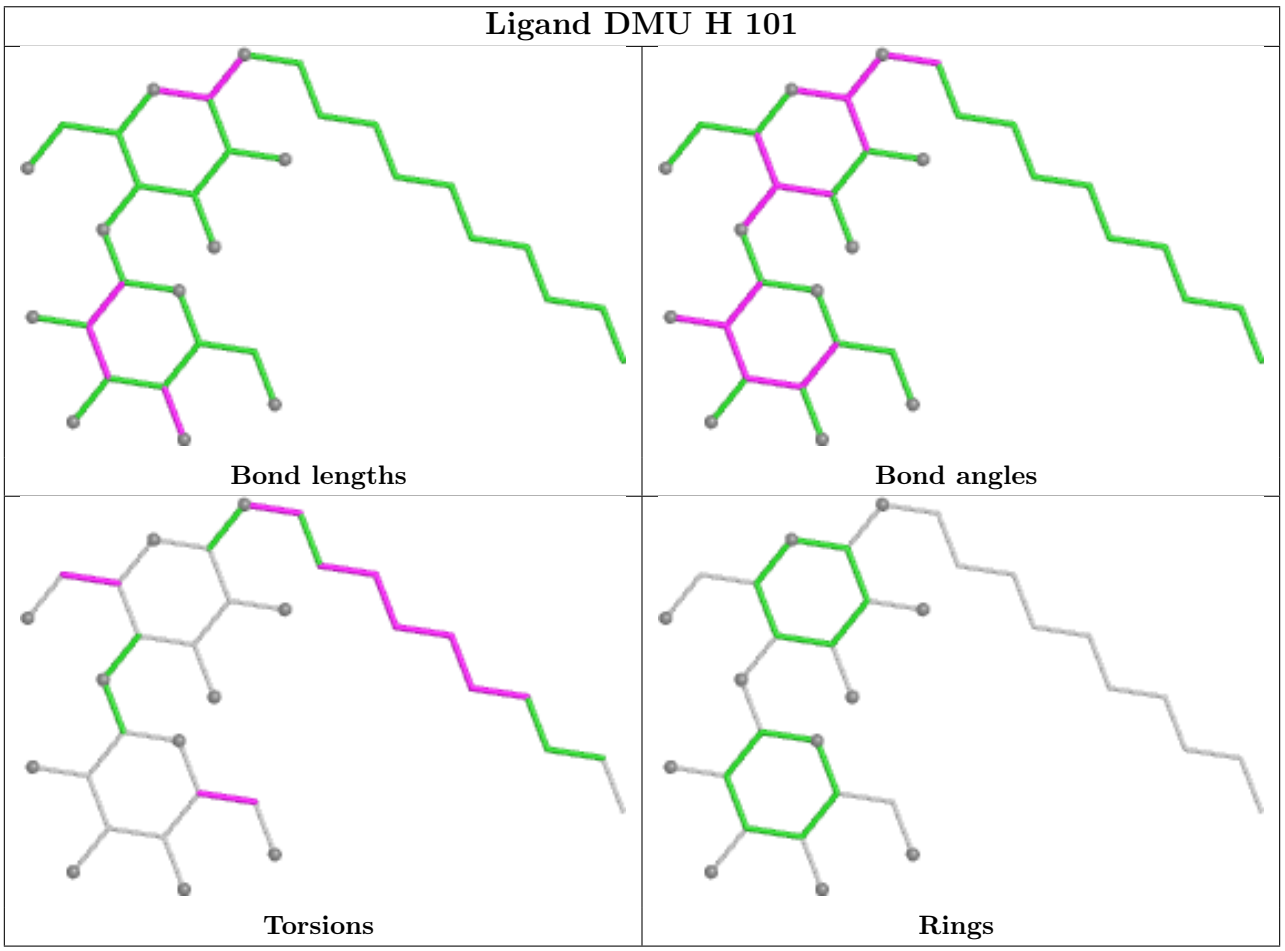


Rings

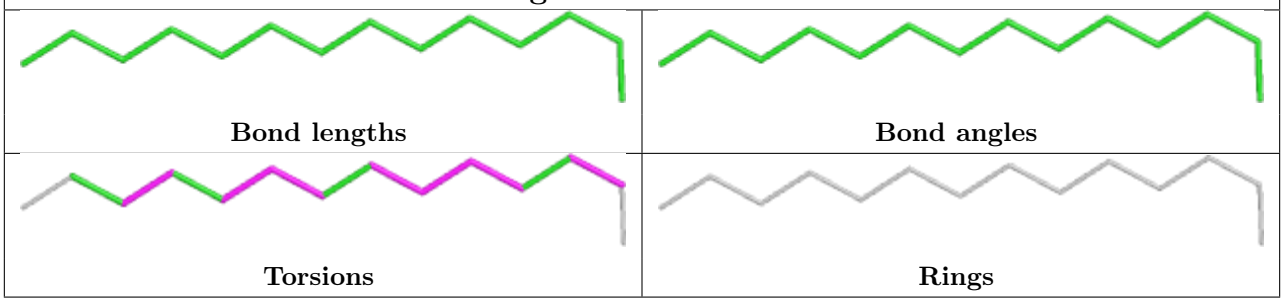
Ligand PGV C 303



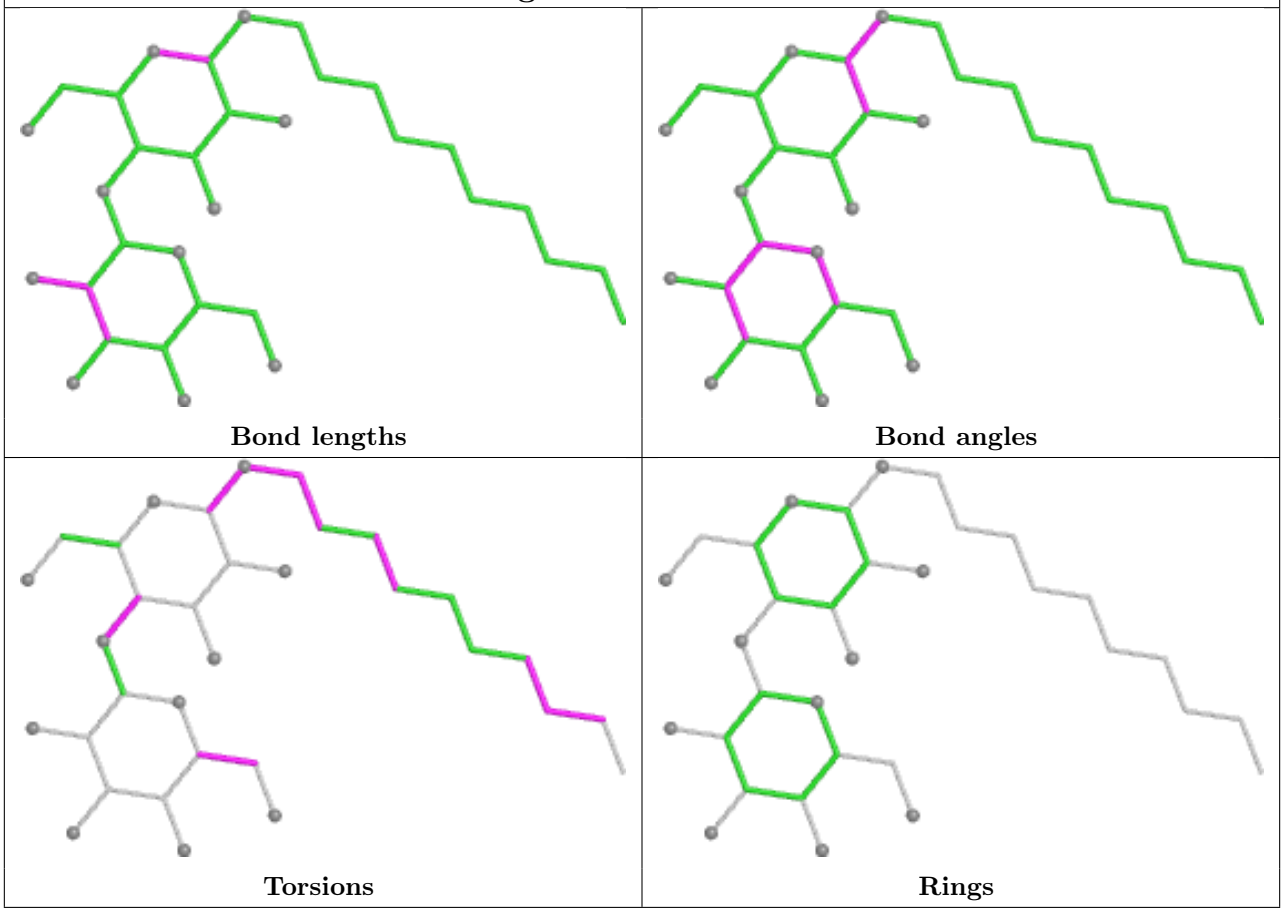
Ligand DMU H 101



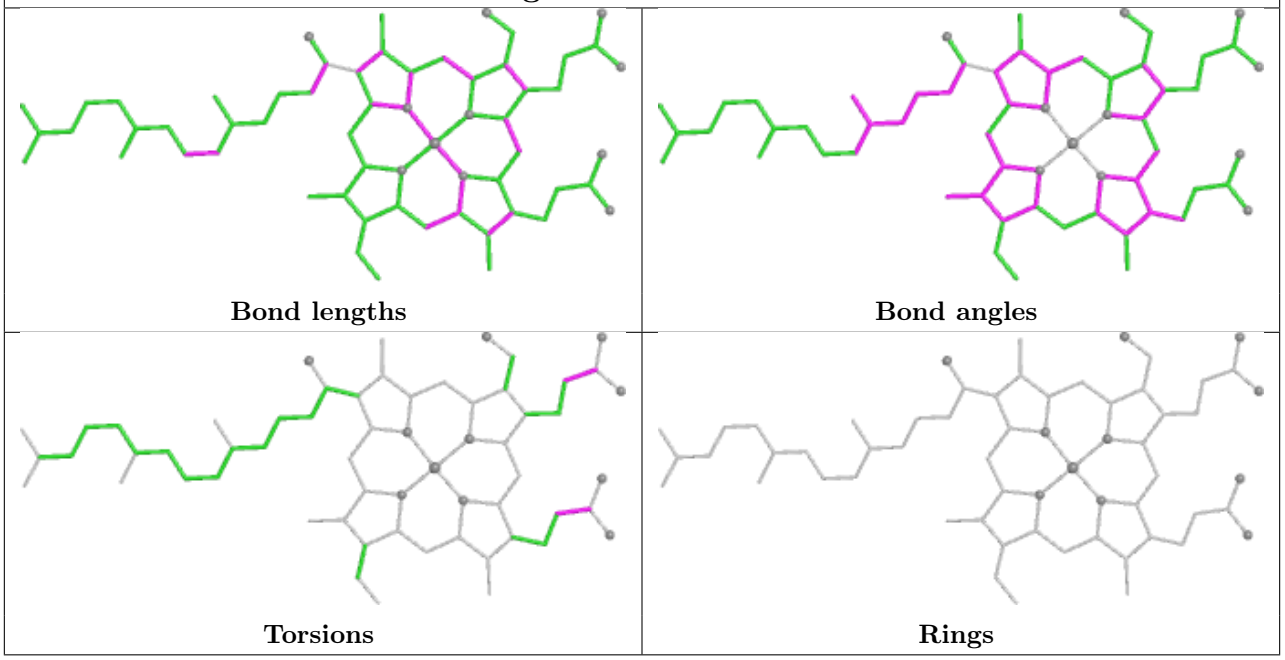
Ligand LFA P 312



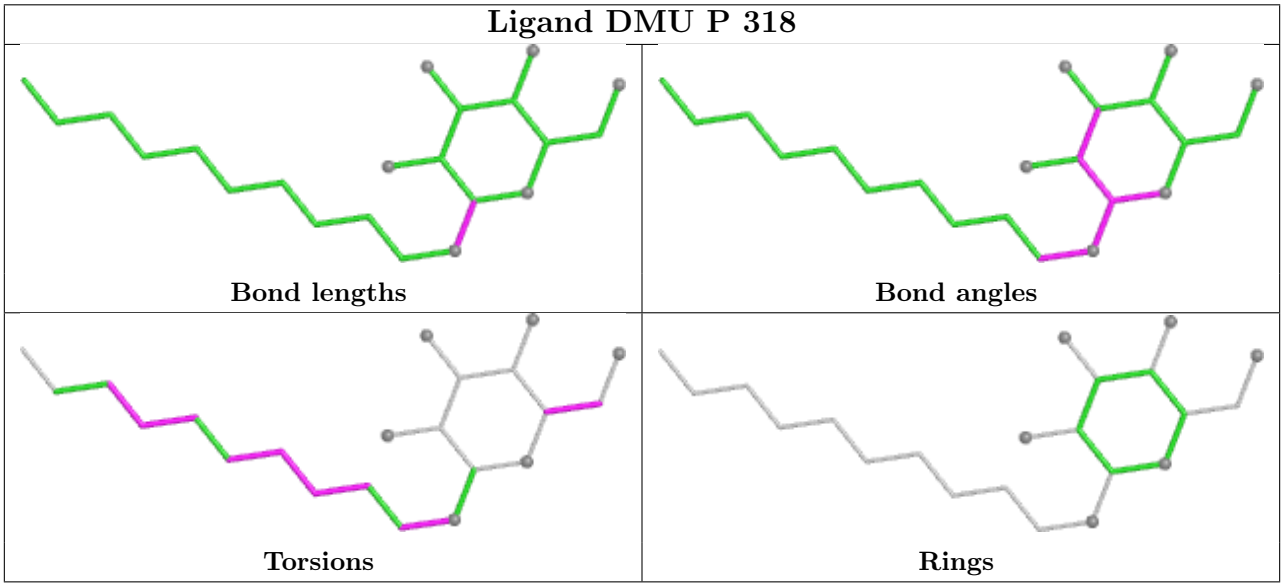
Ligand DMU C 318



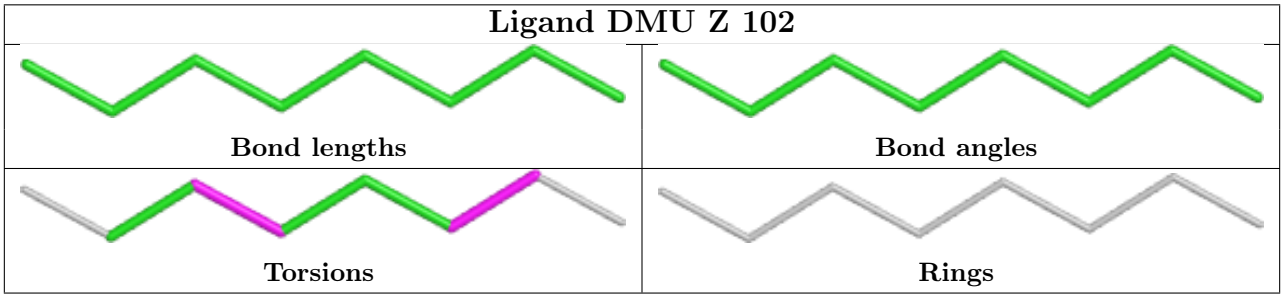
Ligand HEA A 601



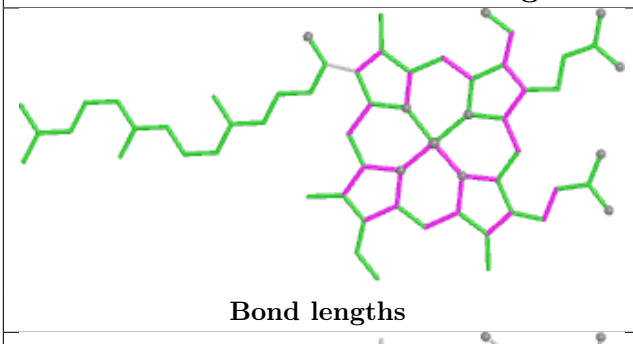
Ligand DMU P 318



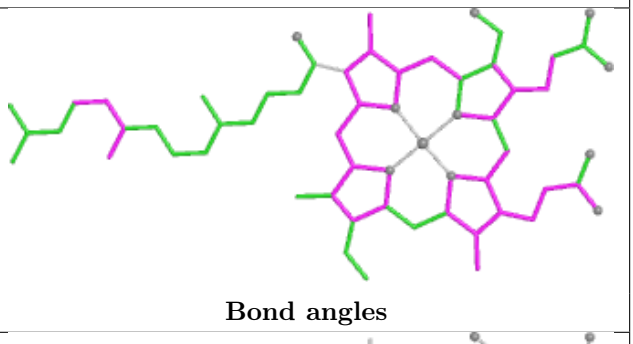
Ligand DMU Z 102



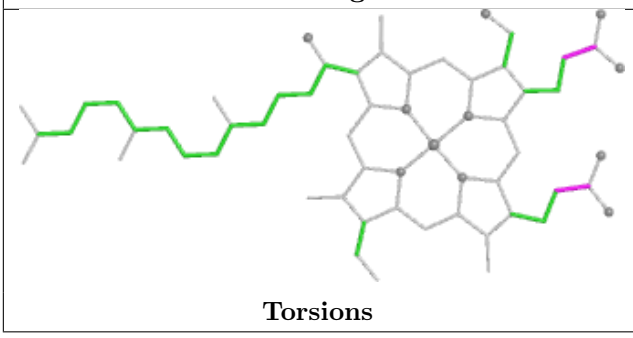
Ligand HEA N 602



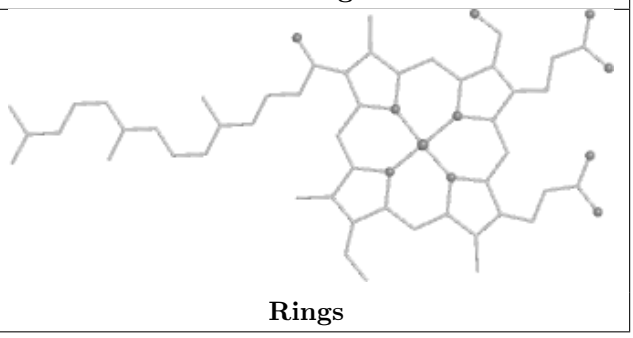
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	512/514 (99%)	-0.17	2 (0%)	88	91	16, 33, 41, 58	15 (2%)
1	N	512/514 (99%)	-0.07	5 (0%)	79	83	16, 35, 44, 62	15 (2%)
2	B	226/227 (99%)	0.25	11 (4%)	35	36	22, 39, 60, 89	5 (2%)
2	O	226/227 (99%)	0.25	8 (3%)	47	49	23, 44, 66, 96	5 (2%)
3	C	258/261 (98%)	-0.06	1 (0%)	88	91	17, 36, 46, 64	9 (3%)
3	P	258/261 (98%)	-0.06	1 (0%)	88	91	16, 36, 47, 68	9 (3%)
4	D	143/147 (97%)	0.12	2 (1%)	73	78	20, 42, 57, 73	1 (0%)
4	Q	137/147 (93%)	0.46	8 (5%)	29	29	24, 52, 79, 90	1 (0%)
5	E	102/109 (93%)	0.03	1 (0%)	79	83	35, 42, 56, 75	0
5	R	102/109 (93%)	0.19	2 (1%)	65	69	37, 50, 67, 85	0
6	F	91/98 (92%)	0.11	1 (1%)	78	82	20, 42, 65, 73	2 (2%)
6	S	91/98 (92%)	0.20	2 (2%)	62	66	19, 40, 63, 71	2 (2%)
7	G	72/85 (84%)	0.42	7 (9%)	13	13	21, 42, 82, 102	1 (1%)
7	T	72/85 (84%)	0.51	5 (6%)	23	23	22, 44, 75, 105	1 (1%)
8	H	75/85 (88%)	0.41	3 (4%)	42	44	36, 45, 90, 130	0
8	U	75/85 (88%)	0.53	9 (12%)	9	8	40, 47, 89, 124	0
9	I	70/73 (95%)	0.62	7 (10%)	12	12	39, 51, 77, 96	0
9	V	70/73 (95%)	0.72	9 (12%)	7	7	39, 58, 78, 102	0
10	J	56/59 (94%)	0.41	1 (1%)	67	71	37, 46, 73, 87	0
10	W	56/59 (94%)	0.55	4 (7%)	22	22	37, 48, 72, 89	0
11	K	49/56 (87%)	0.49	3 (6%)	27	27	39, 47, 64, 85	0
11	X	49/56 (87%)	0.86	3 (6%)	27	27	45, 55, 73, 103	0
12	L	44/47 (93%)	0.08	2 (4%)	38	40	33, 38, 51, 59	0
12	Y	44/47 (93%)	0.20	1 (2%)	61	64	38, 44, 59, 62	0

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

All (100) RSRZ outliers are listed below:

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

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

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Mol	Chain	Res	Type	RSRZ
2	O	16[A]	ILE	2.2
7	T	38	HIS	2.2
11	K	26	VAL	2.2
4	Q	74	SER	2.2
5	R	108	LYS	2.2
1	N	483	LEU	2.2
2	B	115	ASP	2.2
4	Q	39	ALA	2.2
2	O	22[A]	HIS	2.2
4	Q	131	ILE	2.2
12	Y	24	MET	2.1
1	N	49	GLY	2.1
4	Q	51	LEU	2.1
7	G	30	LEU	2.1
9	V	68	ILE	2.1
4	Q	73	ARG	2.1
4	Q	17[A]	VAL	2.1
8	U	50	VAL	2.1
12	L	46	LYS	2.1
1	N	136[A]	LEU	2.1
8	U	52	VAL	2.1
10	W	52	TRP	2.1
9	V	65	LYS	2.1
9	V	26	MET	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	FME	A	1	10/11	0.93	0.14	42,51,82,101	0
1	FME	N	1	10/11	0.95	0.13	45,50,81,99	0
2	FME	B	1	10/11	0.97	0.09	36,37,48,77	0
2	FME	O	1	10/11	0.97	0.09	40,43,52,76	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	DMU	C	317	22/33	0.70	0.33	44,64,74,80	22
20	DMU	P	318	22/33	0.72	0.36	44,66,86,96	22
19	LFA	P	311	11/20	0.73	0.41	58,67,71,74	11
24	CHD	P	306	29/29	0.73	0.22	66,86,116,130	0
21	EDO	P	323	4/4	0.75	0.36	33,33,41,44	4
20	DMU	A	608	7/33	0.76	0.38	53,55,64,71	7
19	LFA	P	308	11/20	0.79	0.35	38,49,63,65	11
24	CHD	C	305	29/29	0.80	0.18	65,90,115,123	0
20	DMU	B	308	22/33	0.81	0.31	54,73,83,91	22
20	DMU	O	303	22/33	0.81	0.29	46,66,85,98	22
20	DMU	P	320	33/33	0.82	0.28	52,76,88,96	33
19	LFA	C	311	14/20	0.82	0.37	39,64,70,72	14
19	LFA	P	313	11/20	0.82	0.33	41,59,68,72	11
20	DMU	C	315	33/33	0.82	0.34	45,58,70,77	33
20	DMU	N	607	7/33	0.83	0.39	53,69,72,72	7
19	LFA	C	310	11/20	0.83	0.38	56,75,96,97	11
19	LFA	C	308	6/20	0.83	0.40	43,53,62,62	6
19	LFA	P	312	14/20	0.83	0.35	43,68,78,83	14
21	EDO	C	322	4/4	0.83	0.29	35,37,41,44	4
21	EDO	E	201	4/4	0.83	0.34	44,45,47,53	4
19	LFA	C	324	15/20	0.83	0.39	56,60,67,72	15
20	DMU	C	318	33/33	0.83	0.32	44,56,67,100	33
20	DMU	M	102	8/33	0.83	0.29	48,56,61,65	8
20	DMU	N	608	33/33	0.84	0.25	45,60,79,85	33
20	DMU	G	103	11/33	0.84	0.33	48,58,62,71	11
20	DMU	P	317	7/33	0.84	0.29	54,58,67,73	7
19	LFA	P	301	15/20	0.84	0.33	52,61,67,68	15
19	LFA	C	312	11/20	0.84	0.33	46,58,73,76	11
20	DMU	P	319	33/33	0.85	0.32	49,60,88,103	33
19	LFA	P	309	6/20	0.85	0.33	41,51,53,55	6
19	LFA	P	315	13/20	0.85	0.29	50,59,79,80	13
19	LFA	T	103	11/20	0.85	0.33	55,62,77,80	11
20	DMU	P	316	33/33	0.85	0.28	47,58,75,77	33
19	LFA	C	314	13/20	0.85	0.28	53,61,75,80	13
19	LFA	O	302	11/20	0.85	0.31	47,59,69,71	11
21	EDO	C	320	4/4	0.86	0.37	56,56,63,82	4
18	CDL	V	101	64/100	0.86	0.19	56,94,138,149	0

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

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

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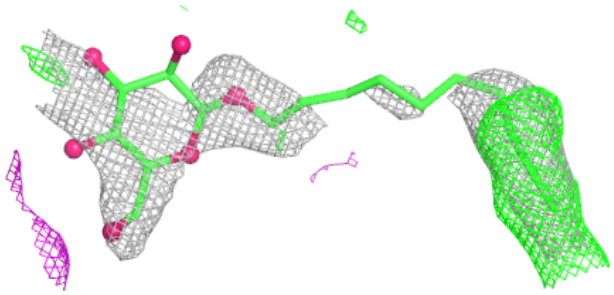
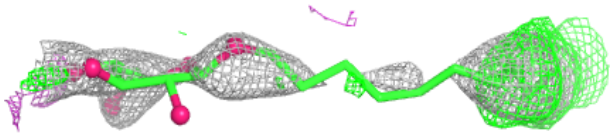
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	HEA	A	602	60/60	0.99	0.05	27,31,37,43	0
14	HEA	N	601	60/60	0.99	0.06	30,33,47,51	0
14	HEA	N	602	60/60	0.99	0.05	30,32,38,43	0
16	MG	A	604	1/1	1.00	0.03	32,32,32,32	0
15	CU	A	603	1/1	1.00	0.02	30,30,30,30	0
15	CU	N	603	1/1	1.00	0.01	32,32,32,32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

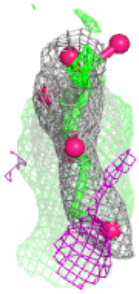
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU 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)

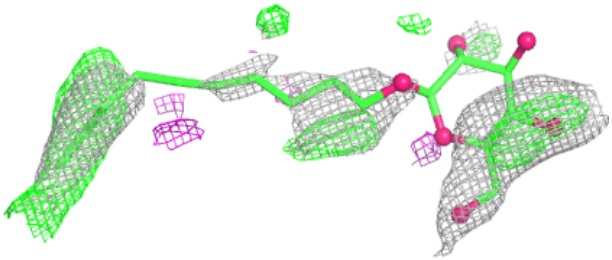


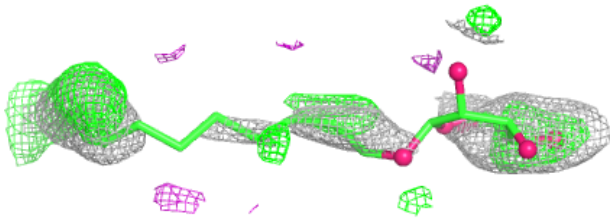


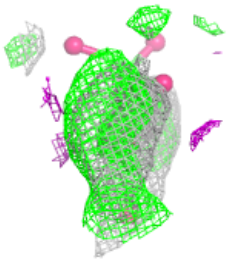


Electron density around DMU P 318:

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

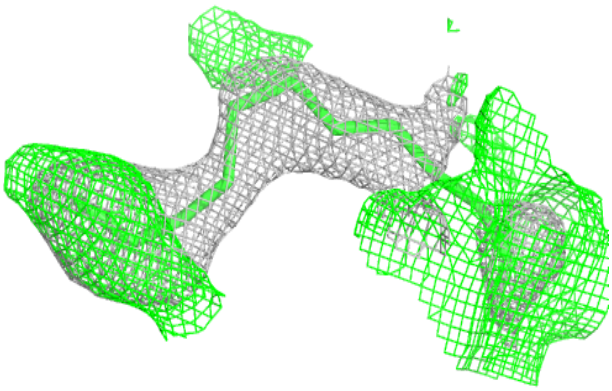


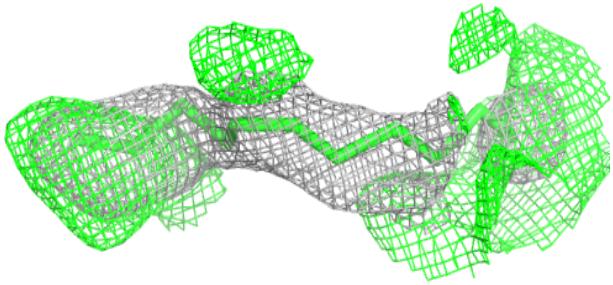


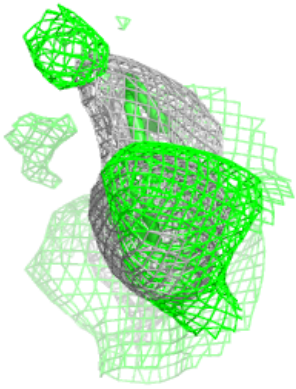


Electron density around LFA P 311:

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

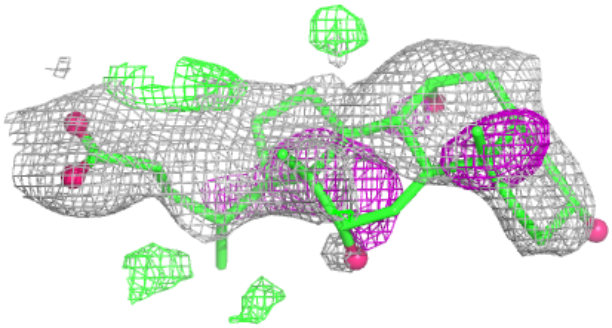


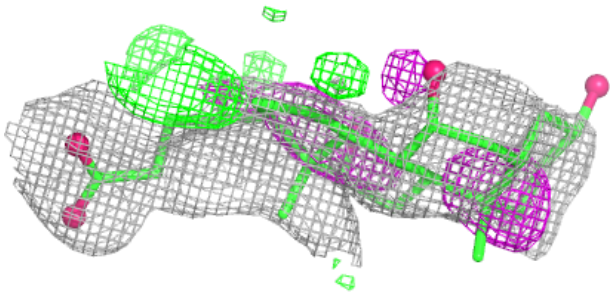


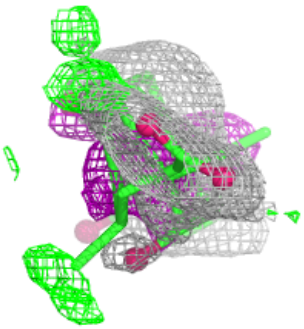


Electron density around CHD P 306:

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

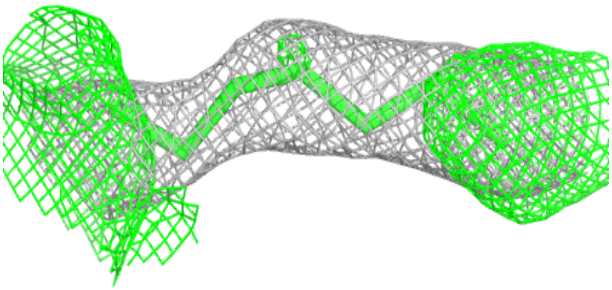


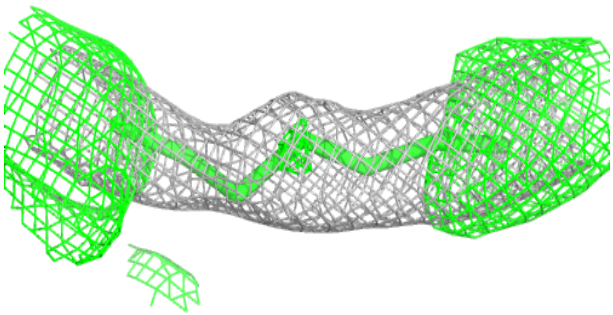


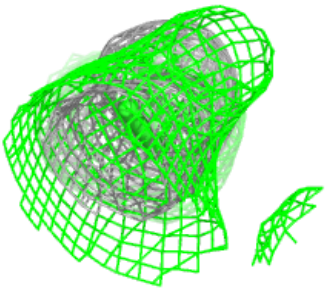


Electron density around DMU A 608:

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

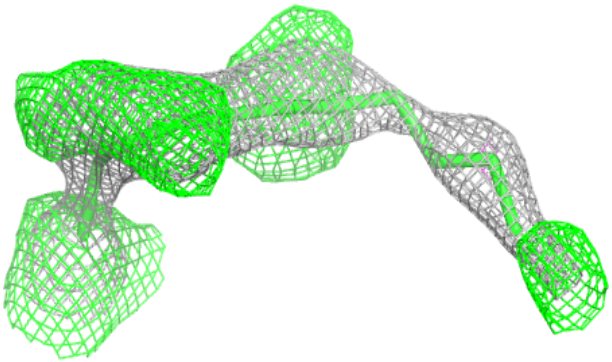


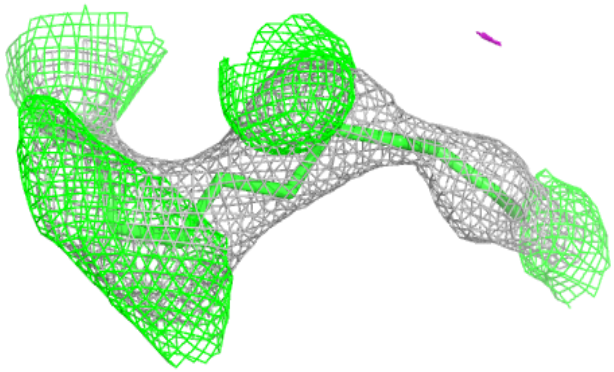


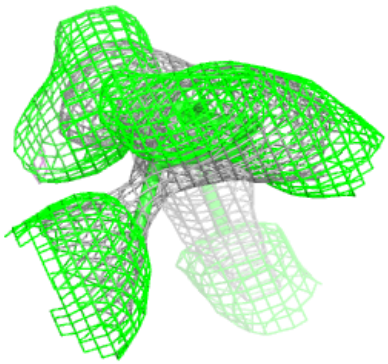


Electron density around LFA P 308:

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

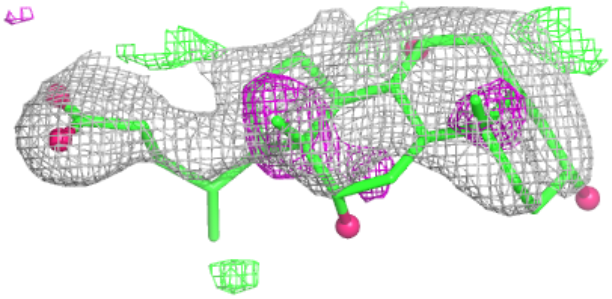


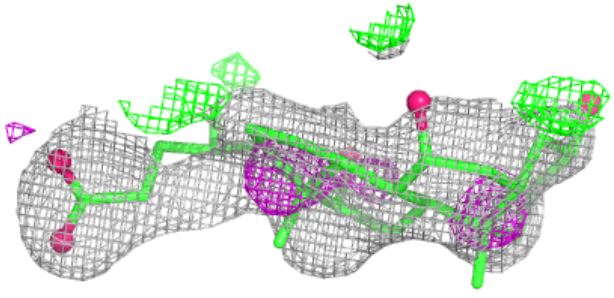


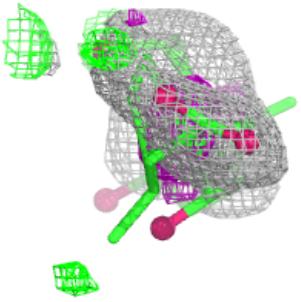


Electron density around CHD C 305:

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

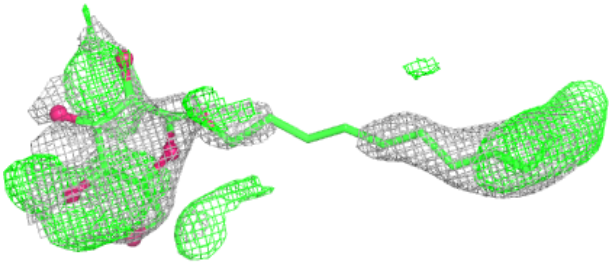


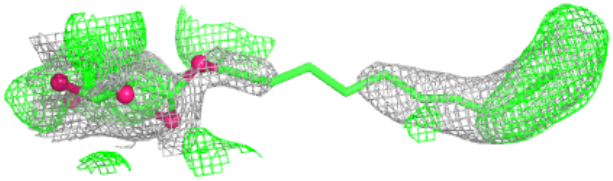


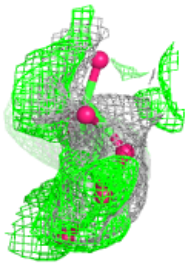


Electron density around DMU B 308:

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

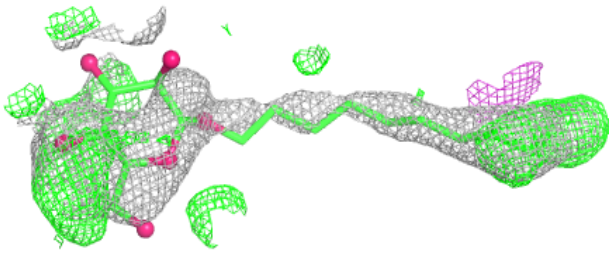


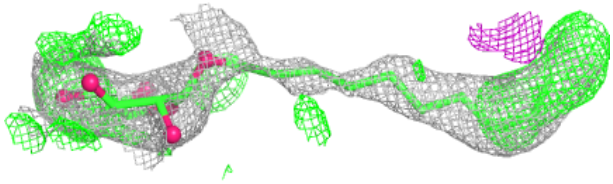


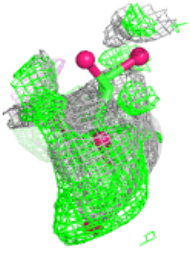


Electron density around DMU O 303:

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

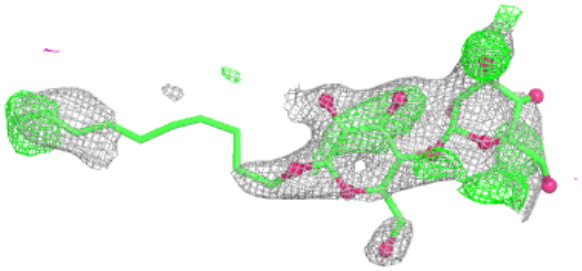


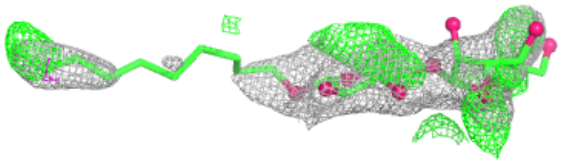


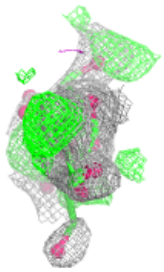


Electron density around DMU P 320:

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

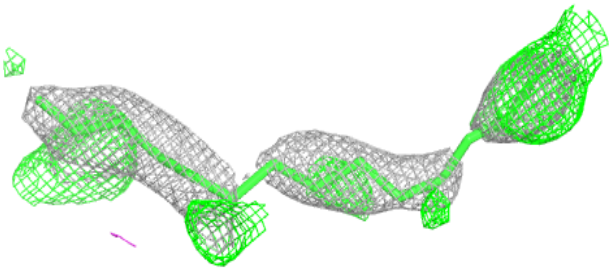


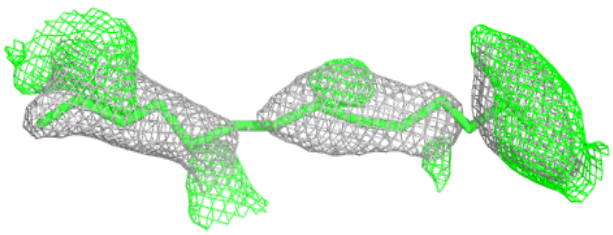


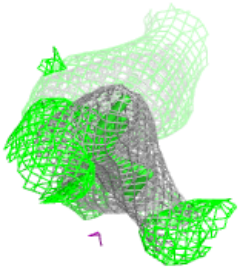


Electron density around LFA C 311:

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

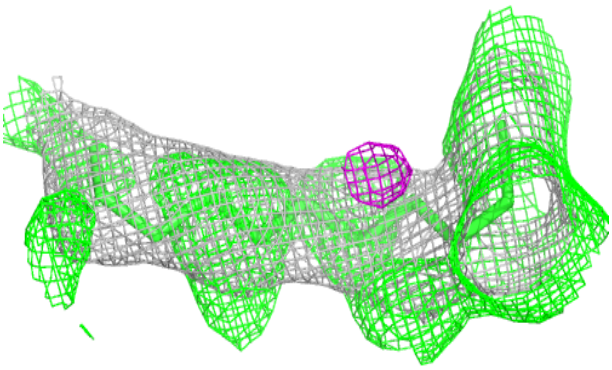


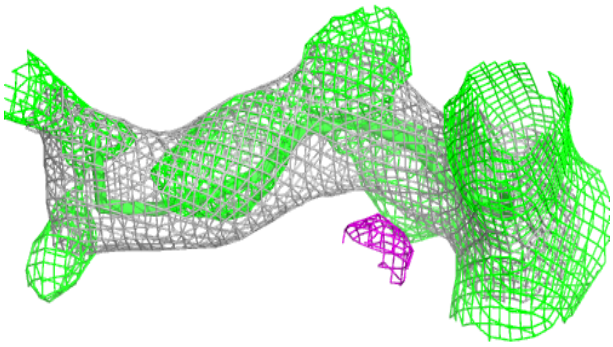


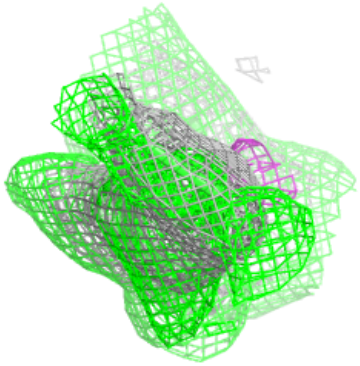


Electron density around LFA P 313:

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

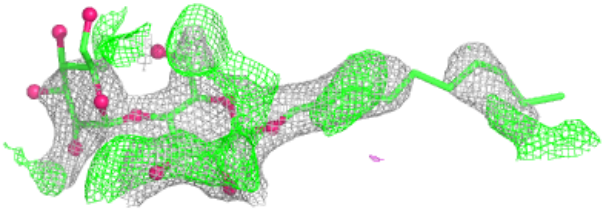


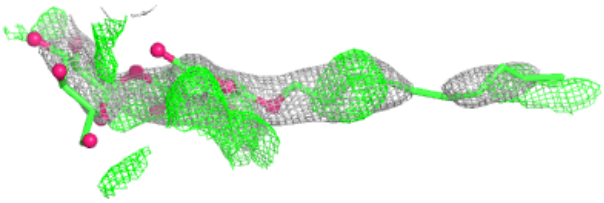


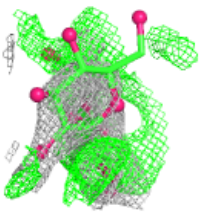


Electron density around DMU C 315:

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

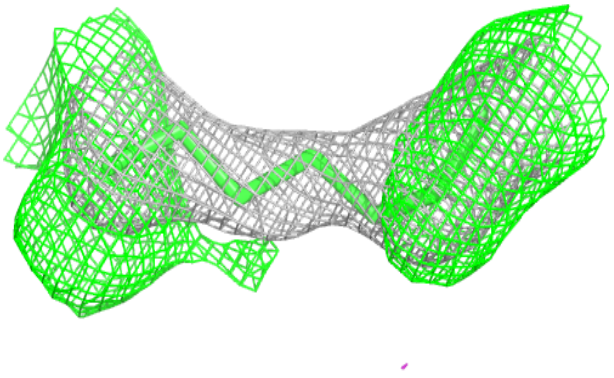


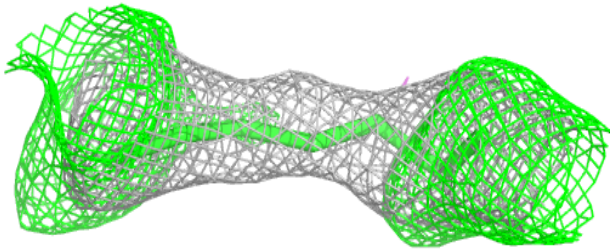


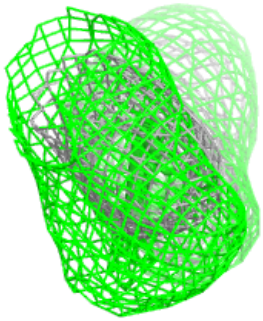


Electron density around DMU N 607:

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

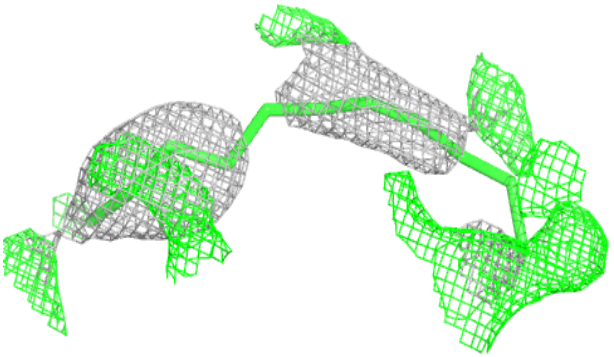


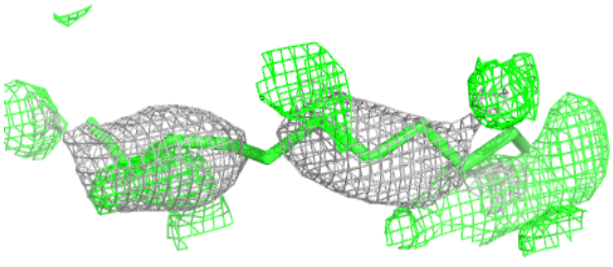


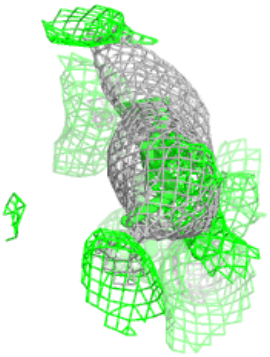


Electron density around LFA C 310:

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

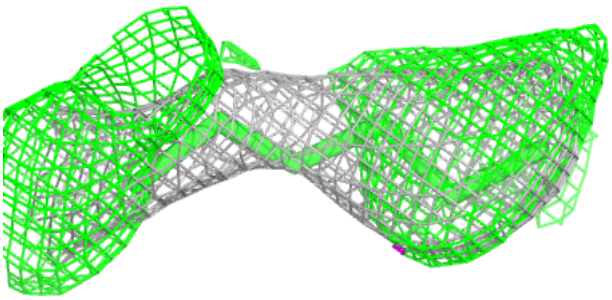


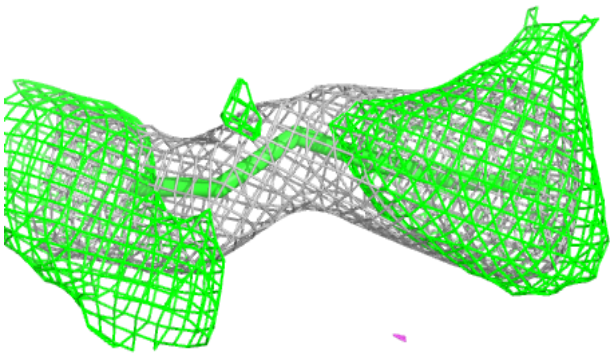


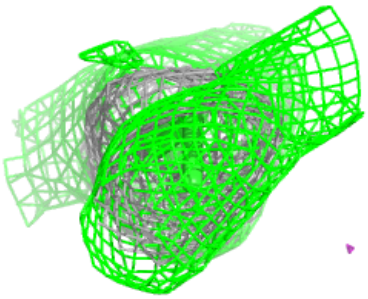


Electron density around LFA C 308:

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

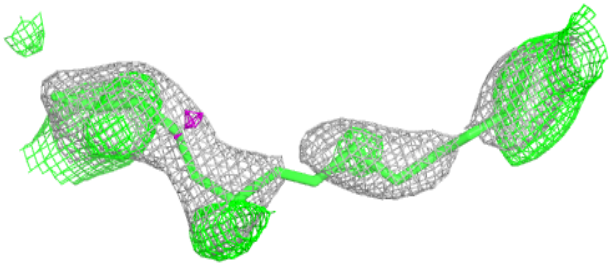


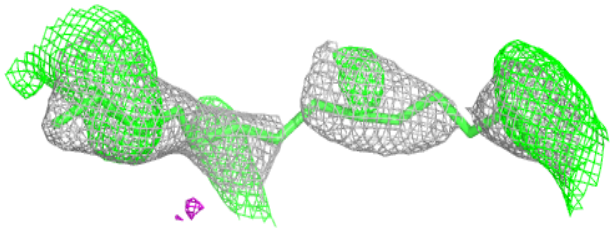


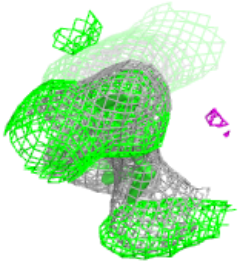


Electron density around LFA P 312:

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

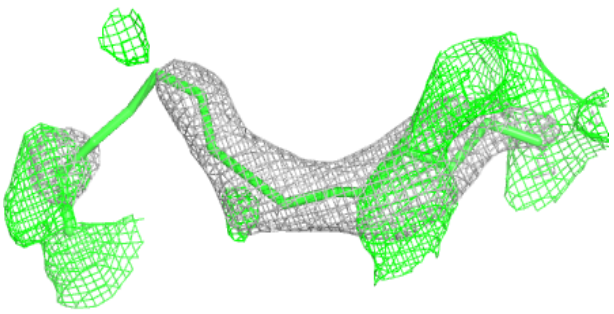


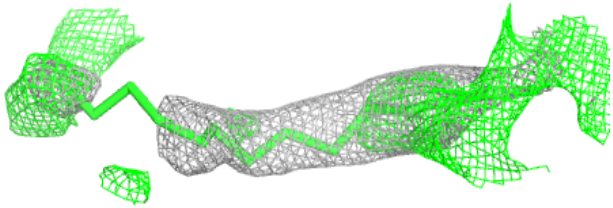


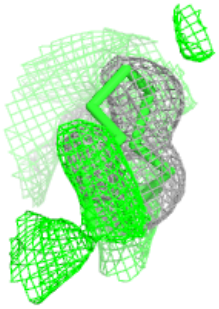


Electron density around LFA C 324:

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

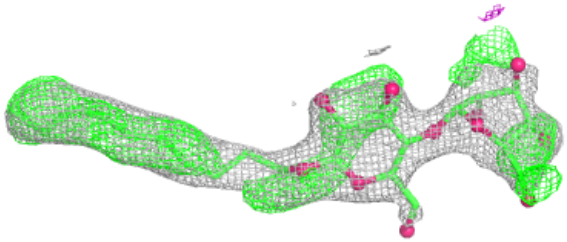


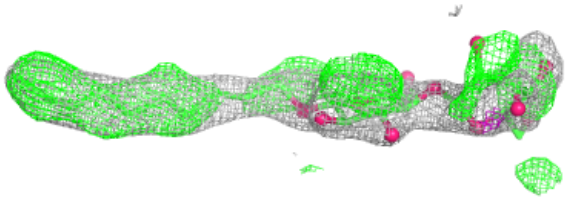


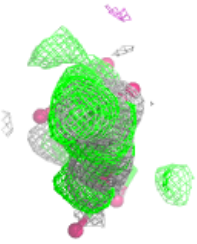


Electron density around DMU C 318:

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

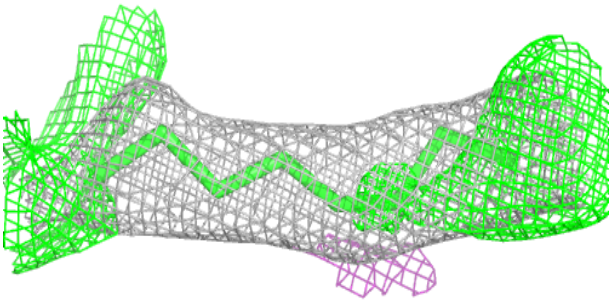


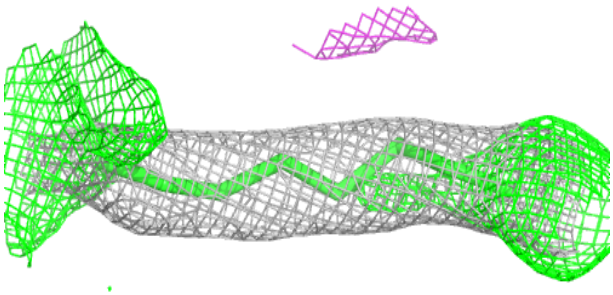


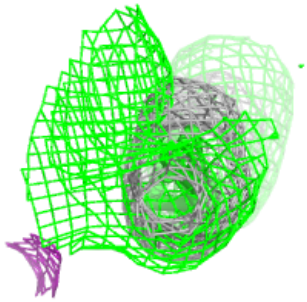


Electron density around DMU M 102:

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

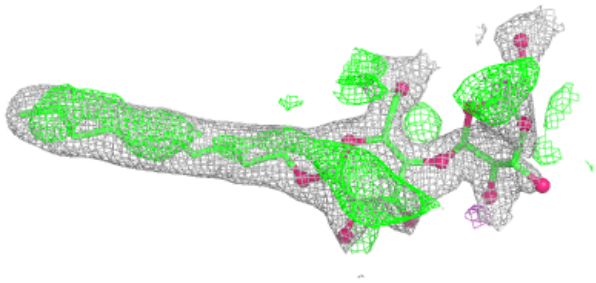


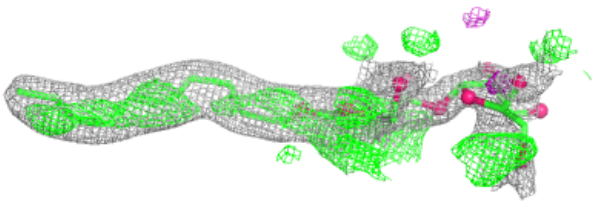


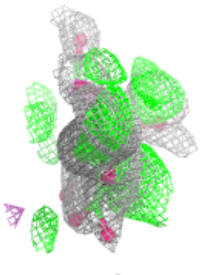


Electron density around DMU N 608:

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

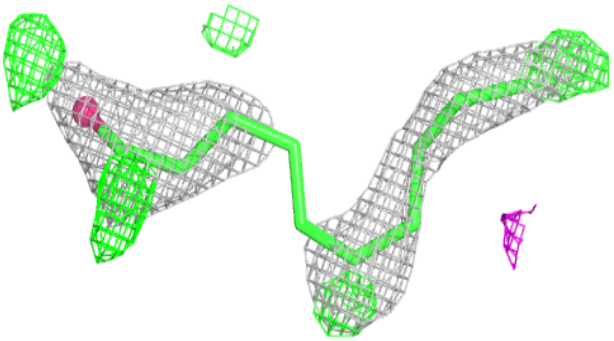


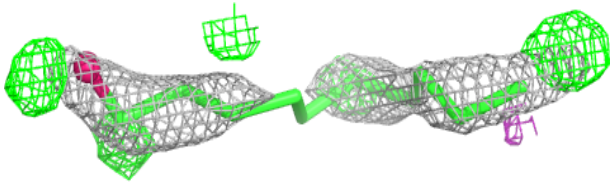


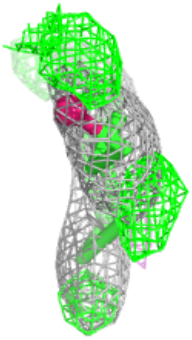


Electron density around DMU G 103:

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

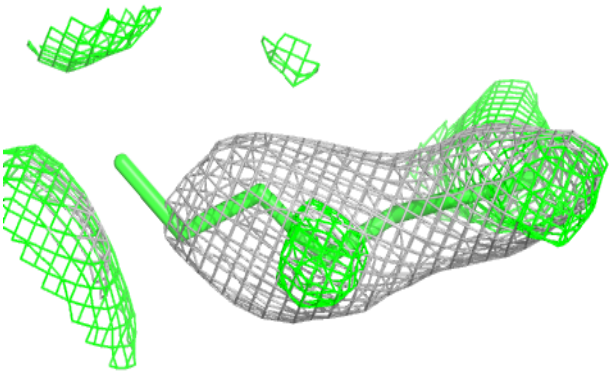


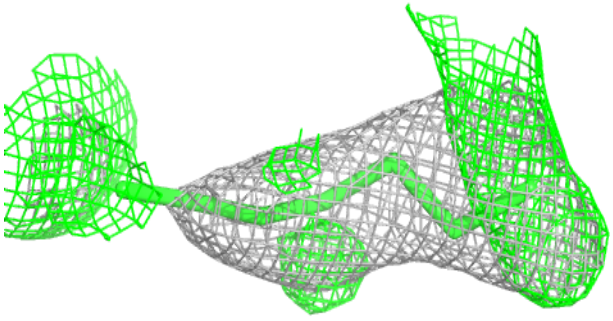


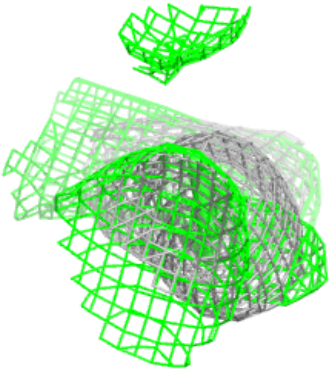


Electron density around DMU P 317:

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

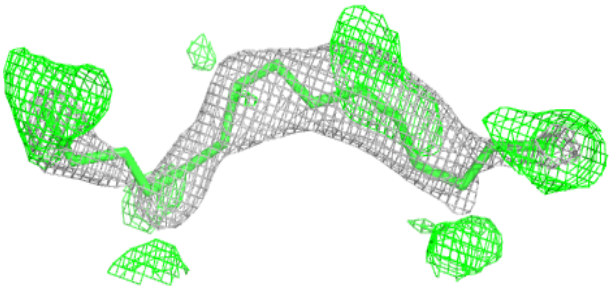


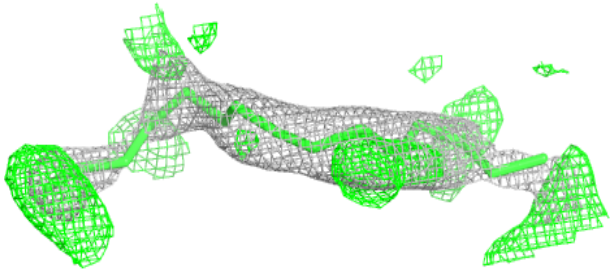


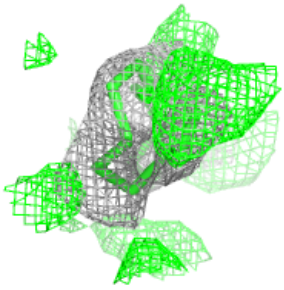


Electron density around LFA P 301:

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

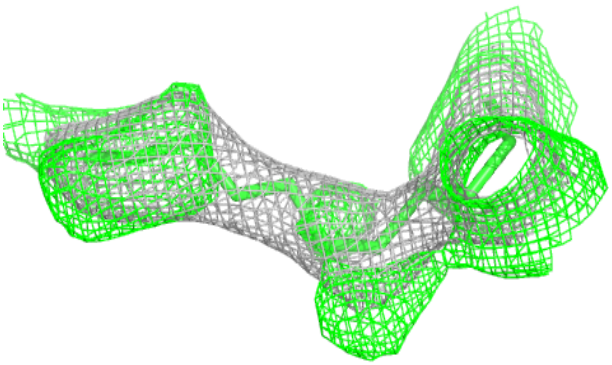


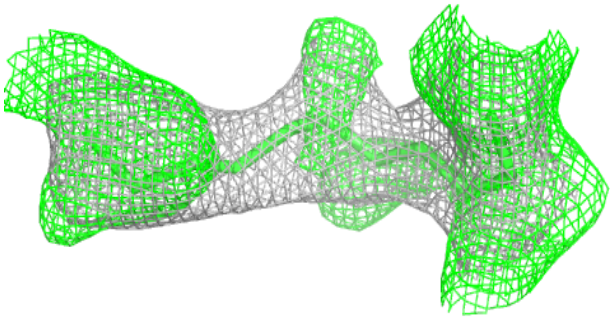


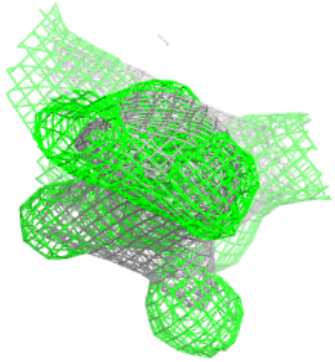


Electron density around LFA C 312:

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

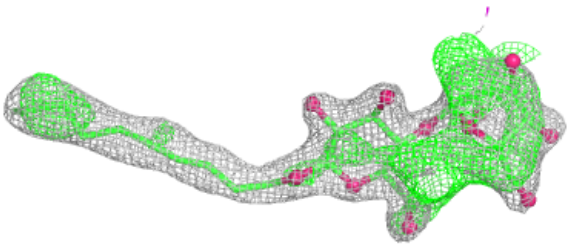


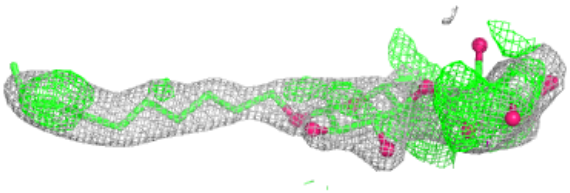


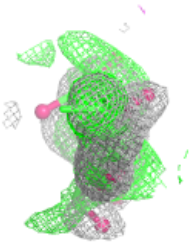


Electron density around DMU P 319:

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

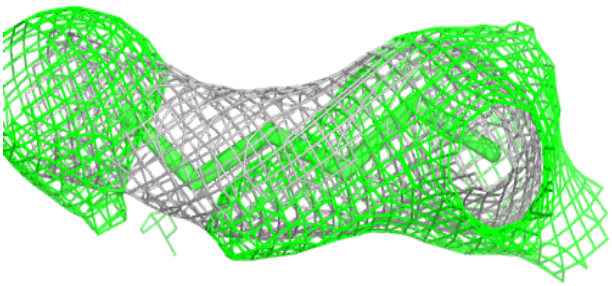


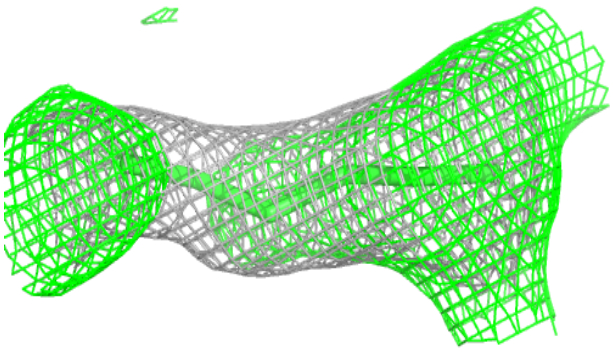


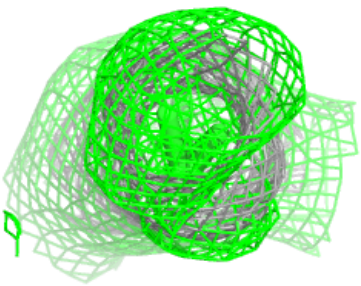


Electron density around LFA P 309:

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

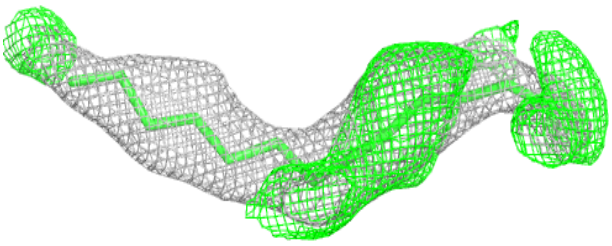


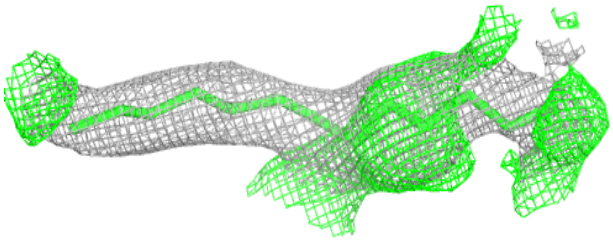


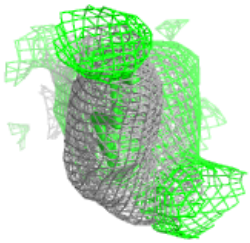


Electron density around LFA P 315:

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

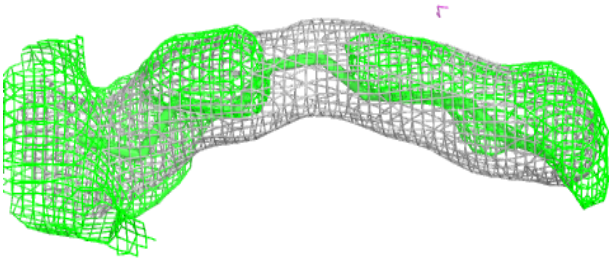


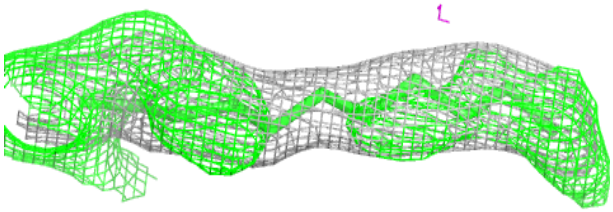


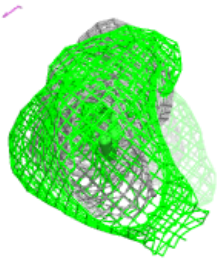


Electron density around LFA T 103:

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

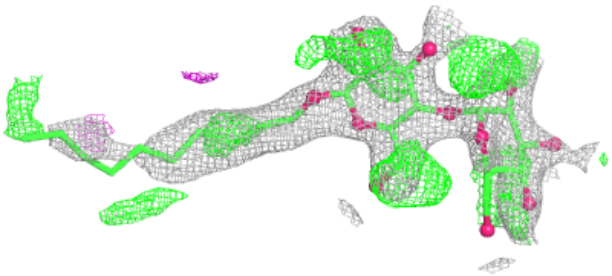


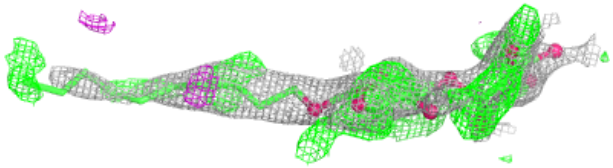


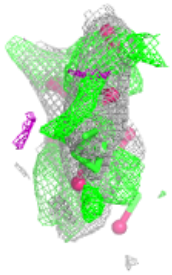


Electron density around DMU P 316:

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

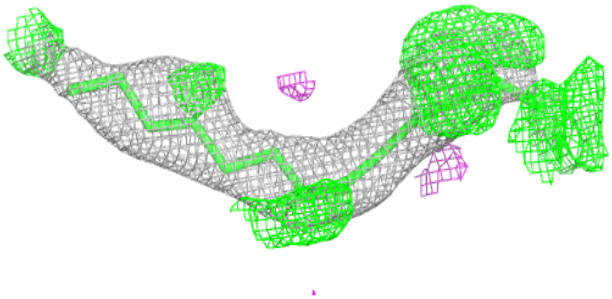


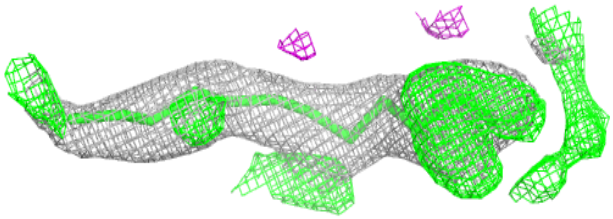


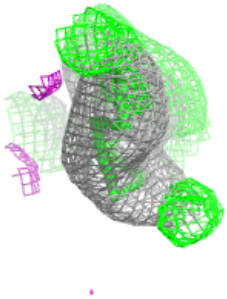


Electron density around LFA C 314:

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

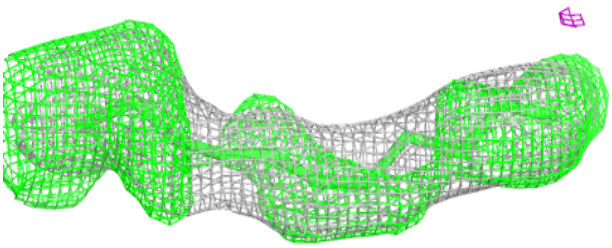


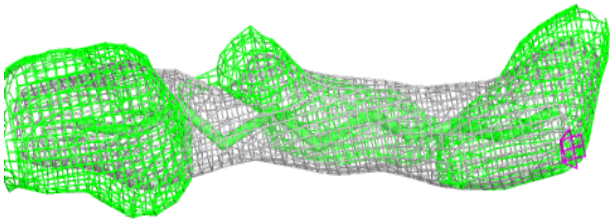


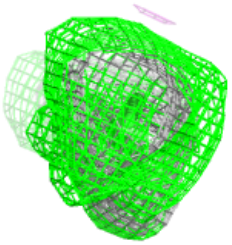


Electron density around LFA O 302:

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

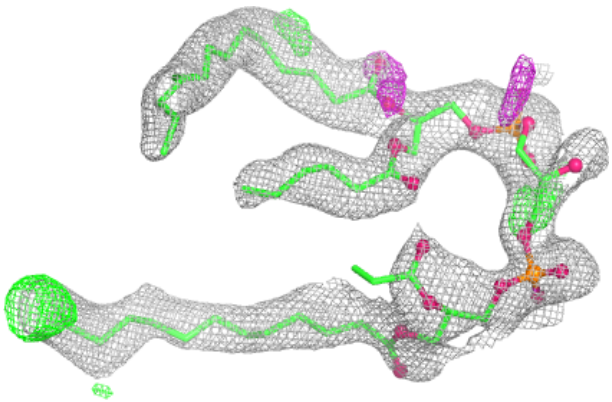


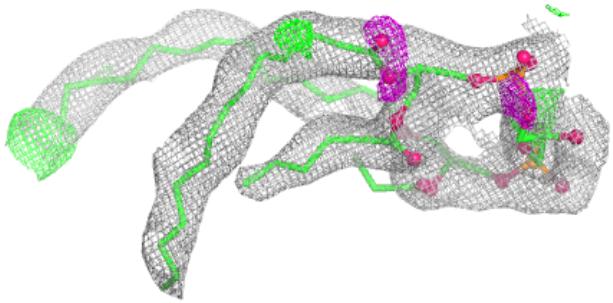


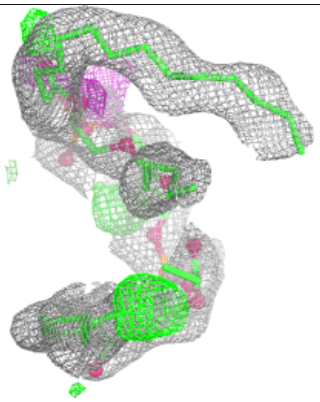


Electron density around CDL V 101:

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

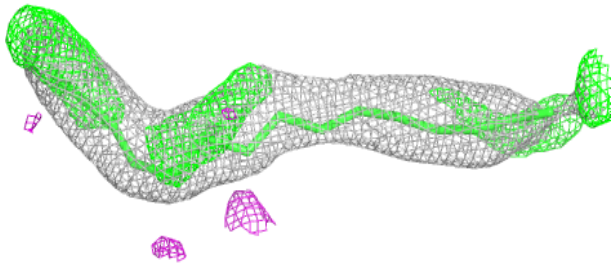


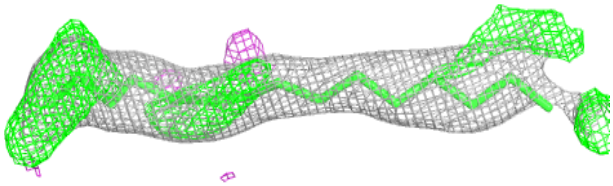


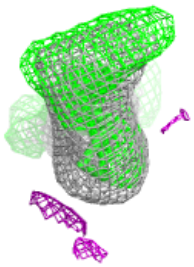


Electron density around LFA C 313:

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

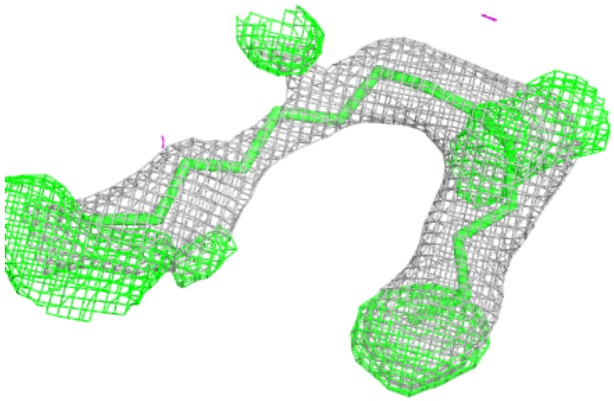


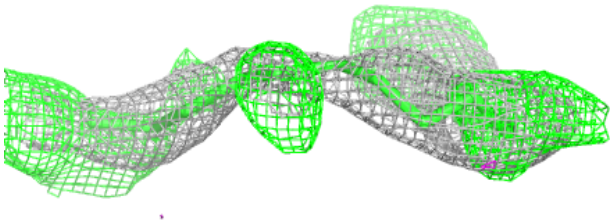


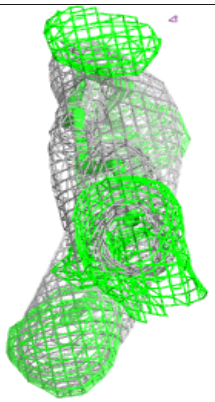


Electron density around LFA G 106:

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

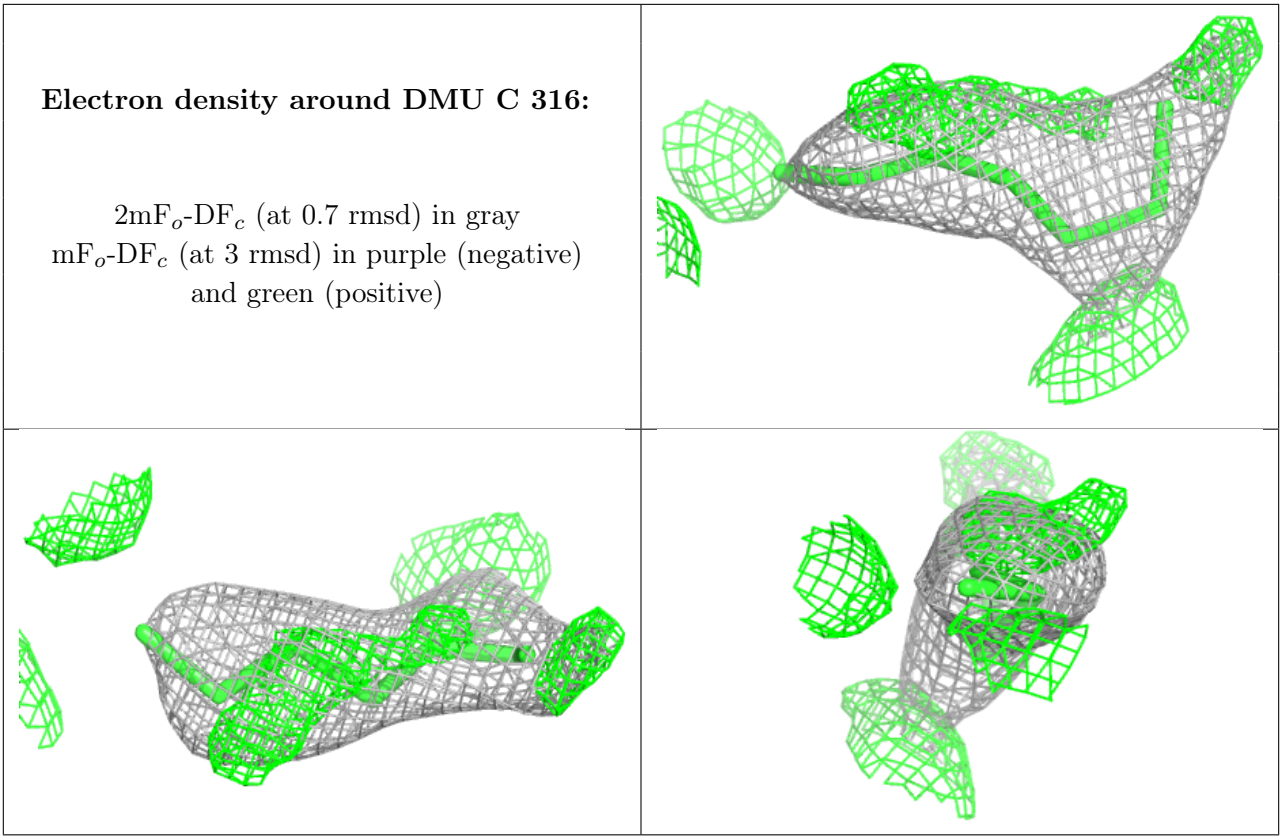






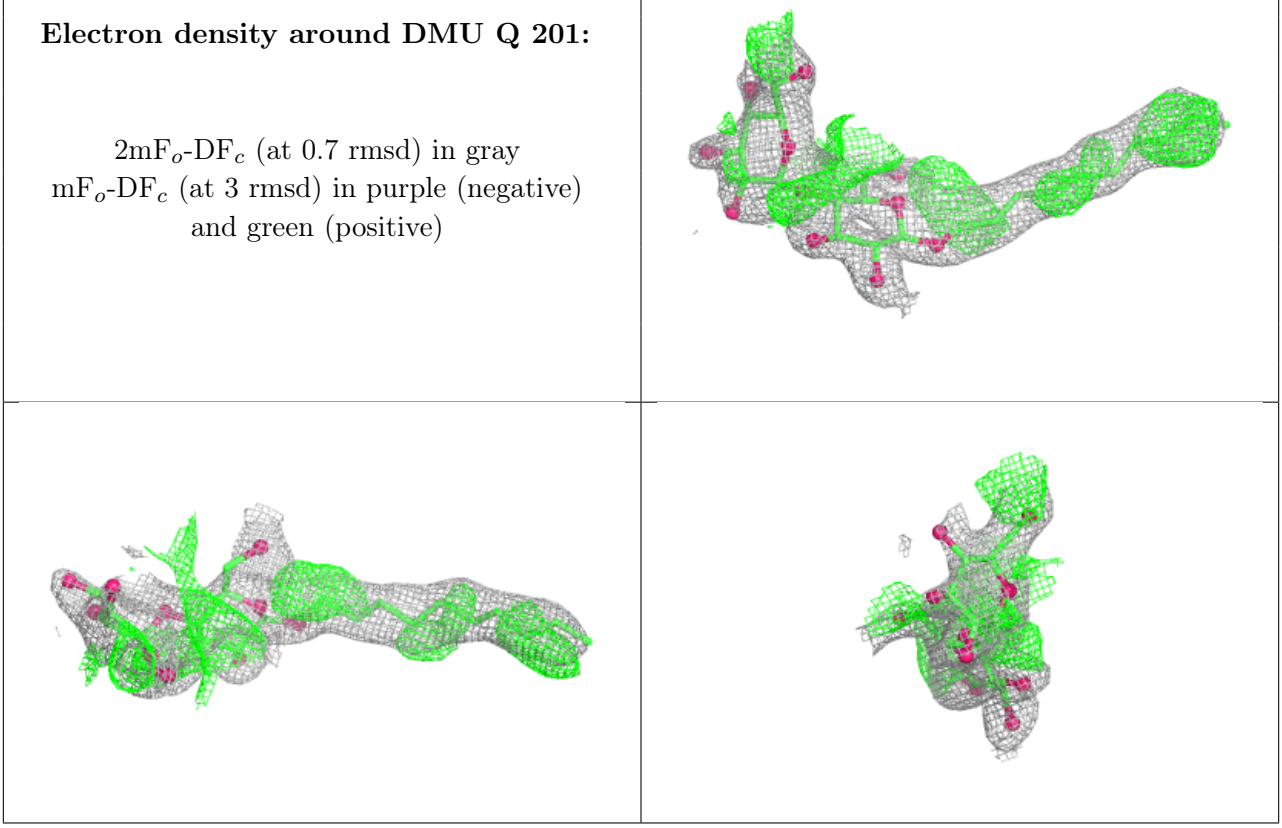
Electron density around DMU C 316:

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



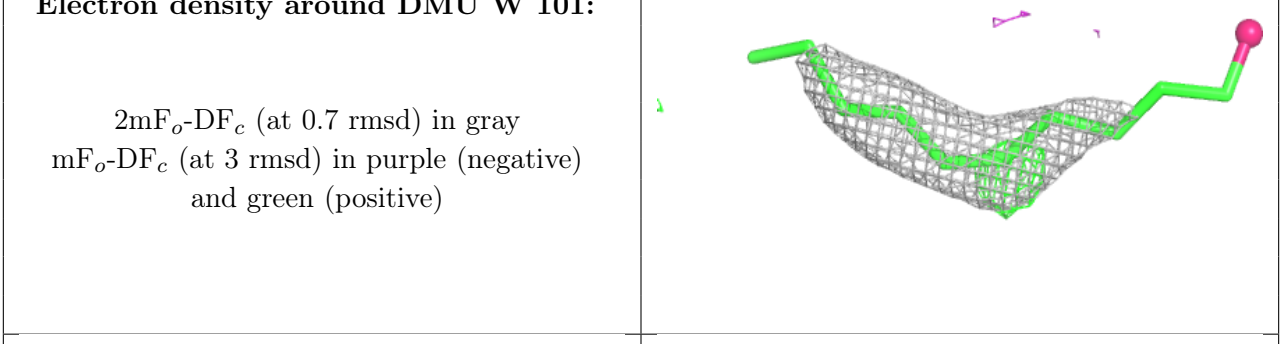
Electron density around DMU Q 201:

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



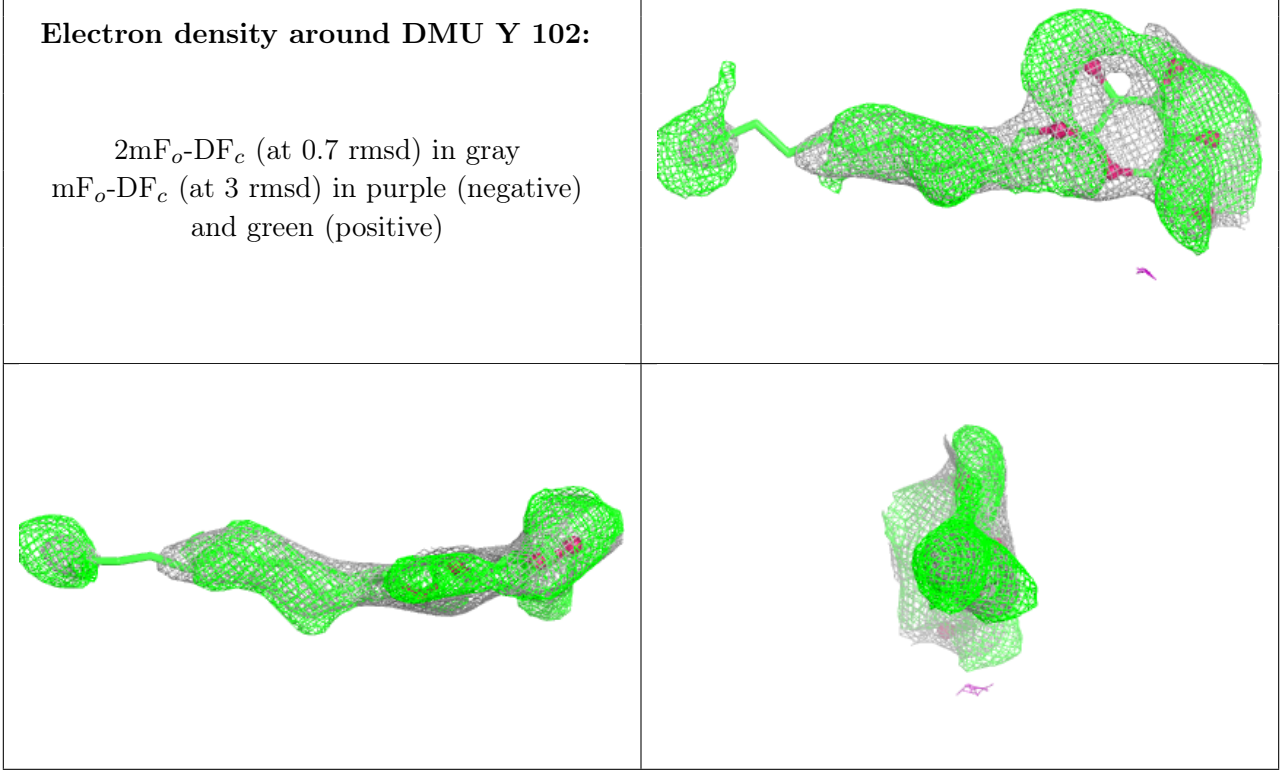
Electron density around DMU W 101:

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



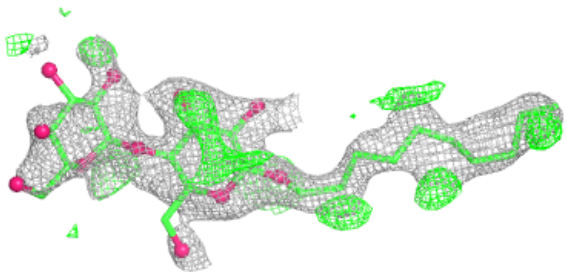
Electron density around DMU Y 102:

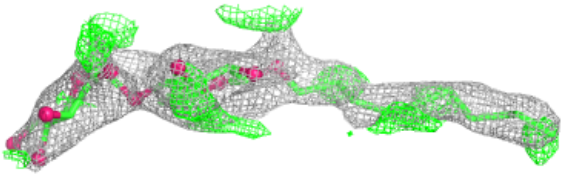
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

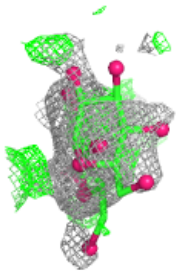


Electron density around DMU C 319:

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

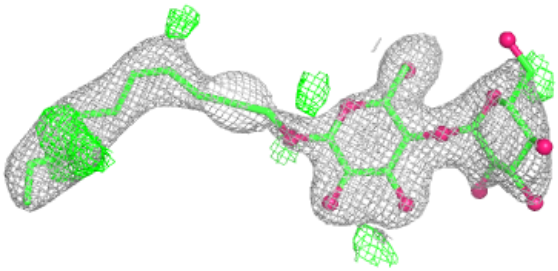


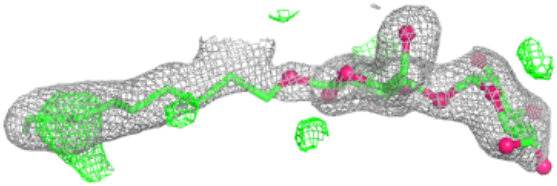


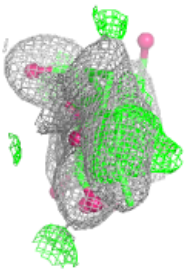


Electron density around DMU C 323:

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

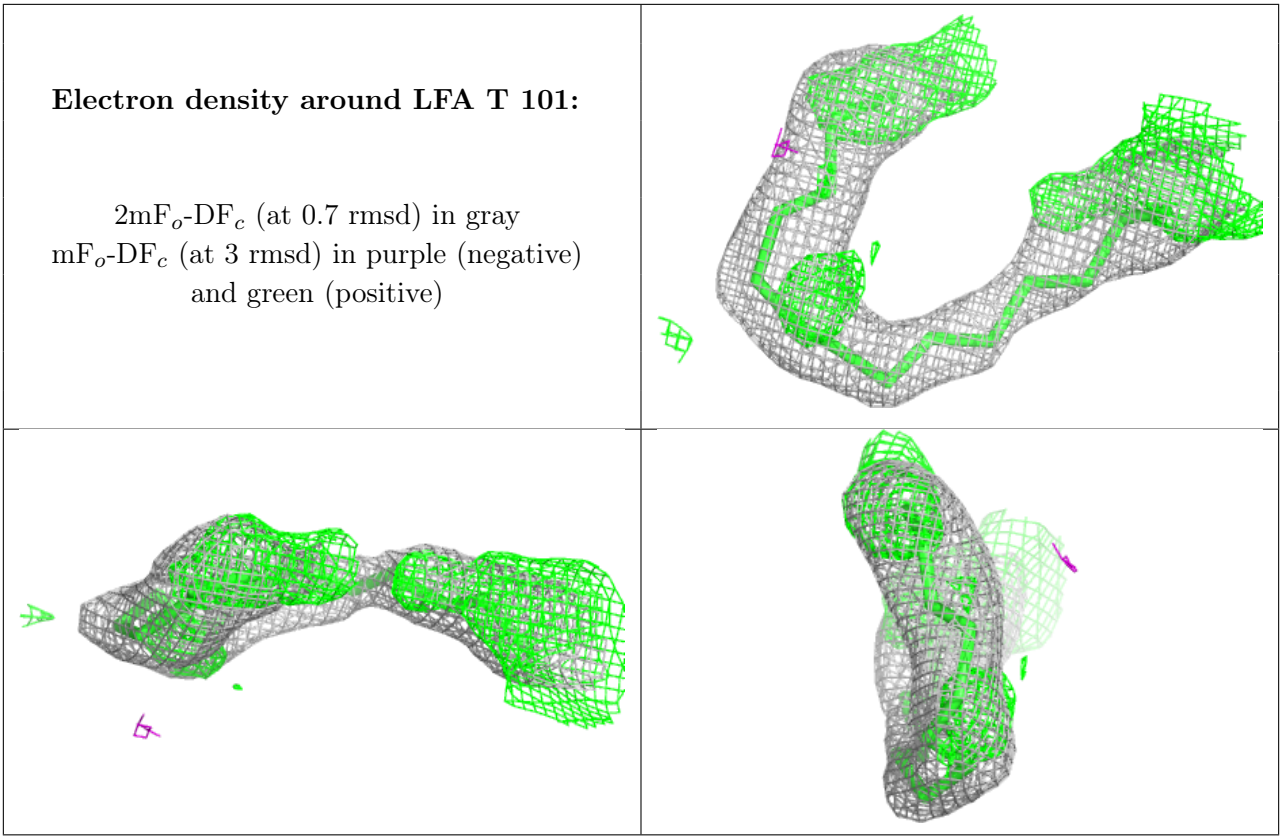






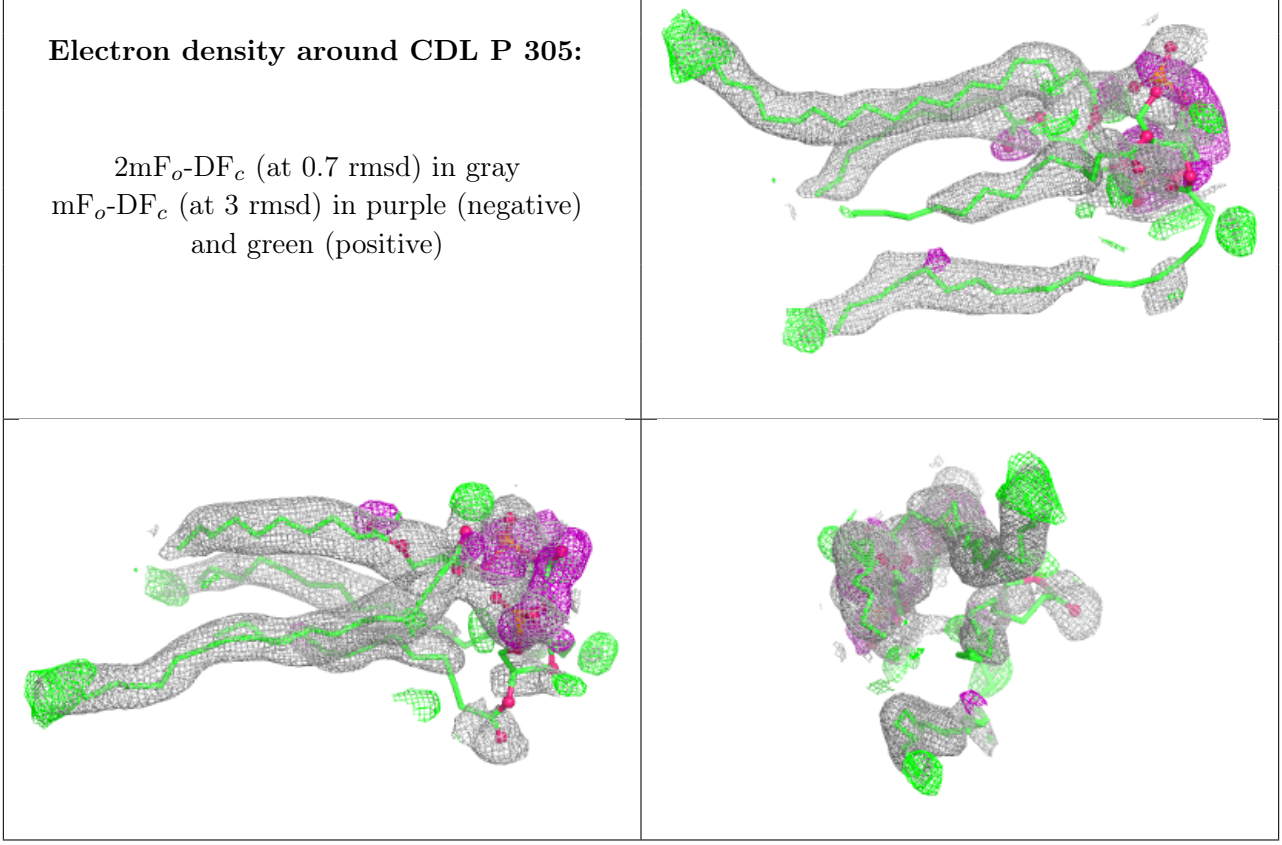
Electron density around LFA T 101:

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



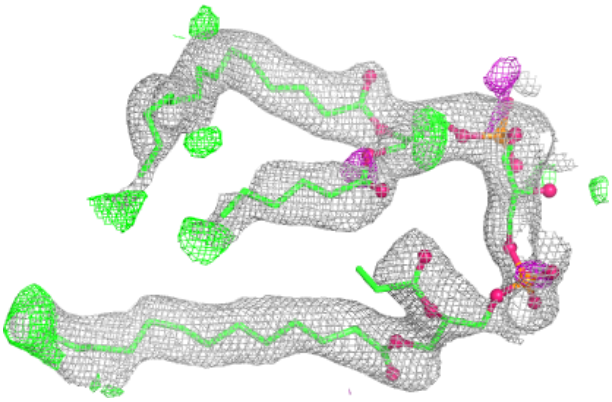
Electron density around CDL P 305:

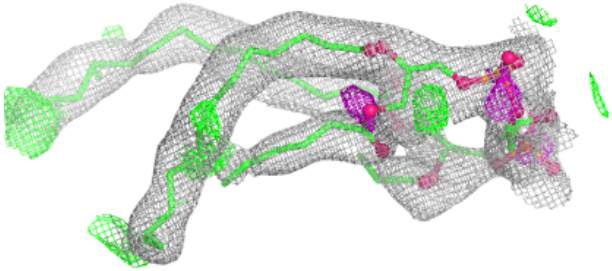
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

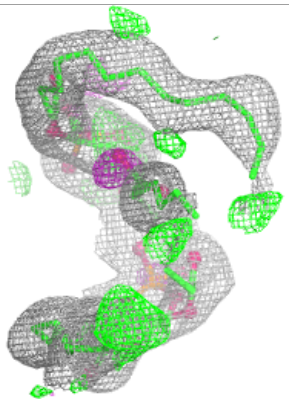


Electron density around CDL A 606:

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

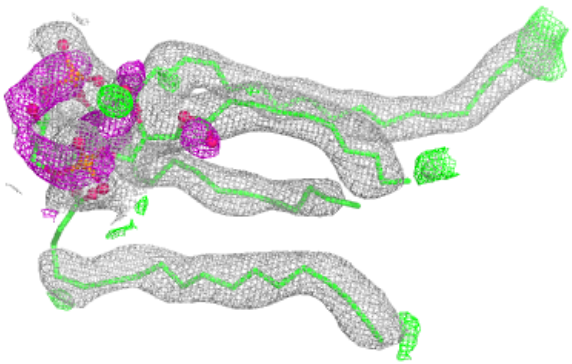


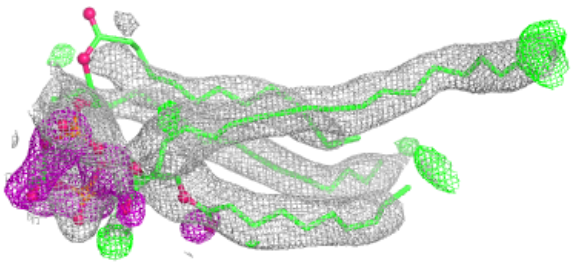


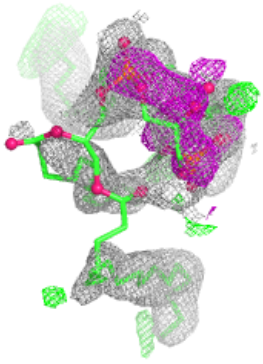


Electron density around CDL C 304:

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

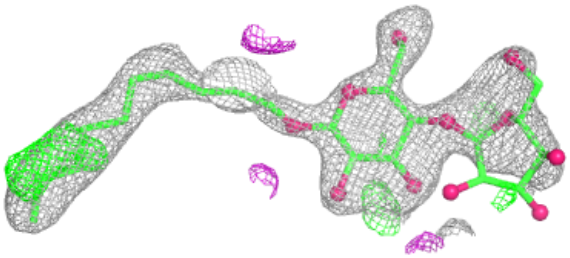


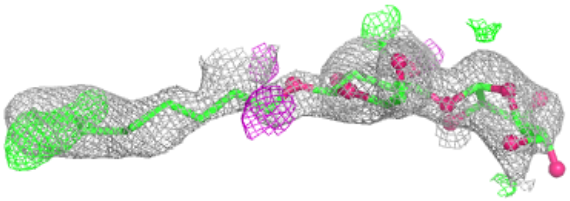


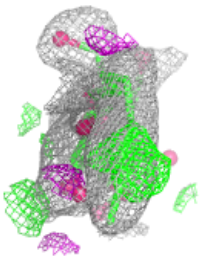


Electron density around DMU P 324:

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

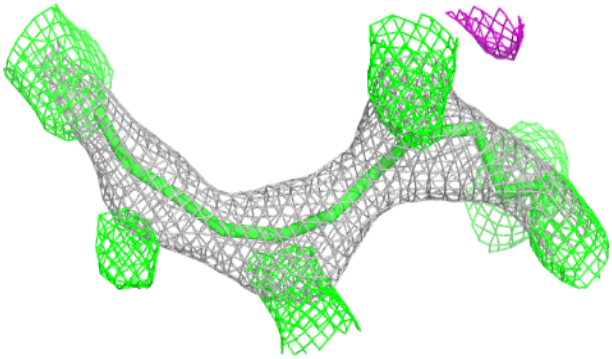


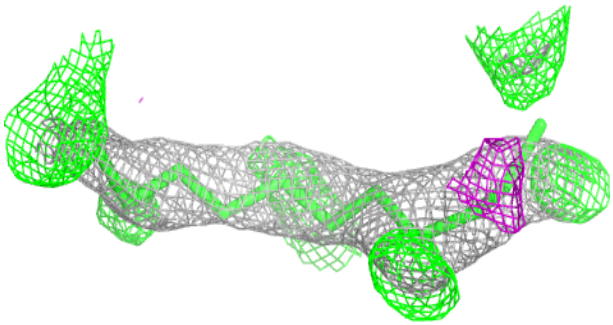


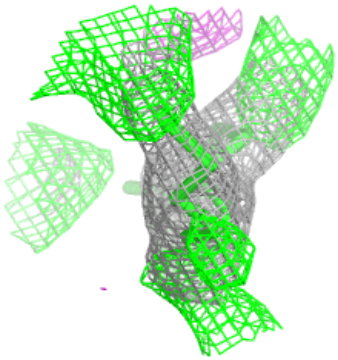


Electron density around LFA C 307:

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

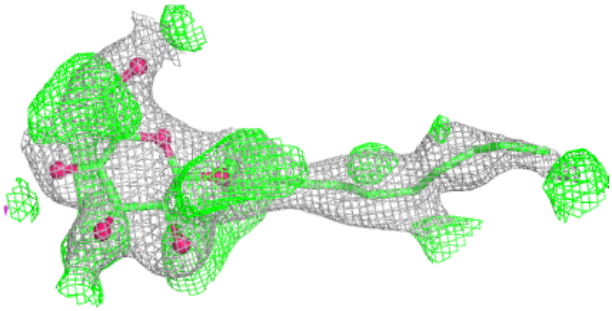


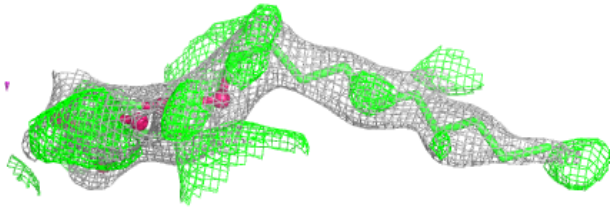


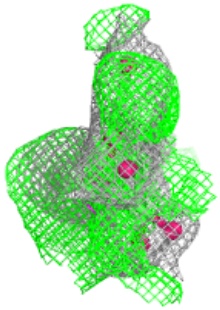


Electron density around DMU T 104:

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

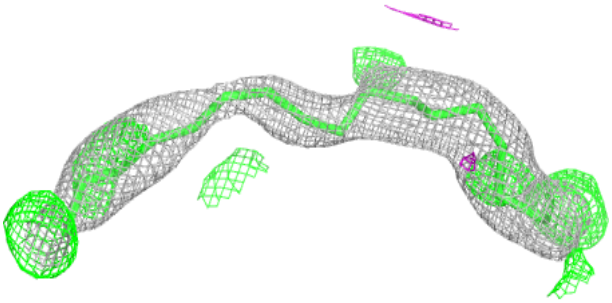


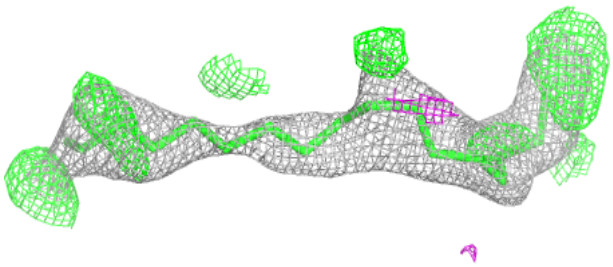


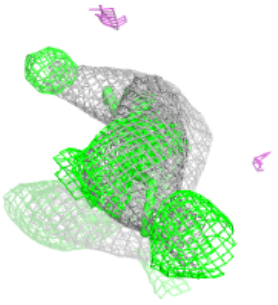


Electron density around LFA O 301:

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

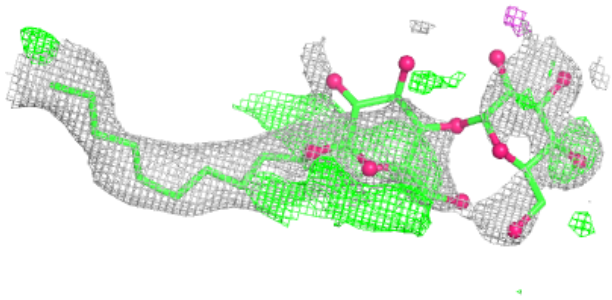


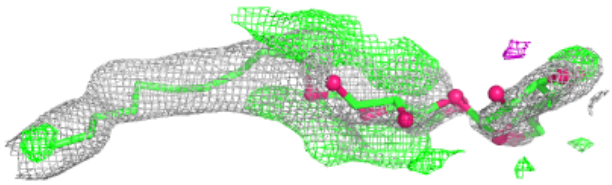


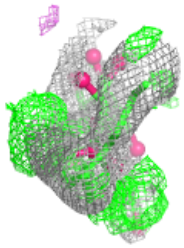


Electron density around DMU N 615:

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

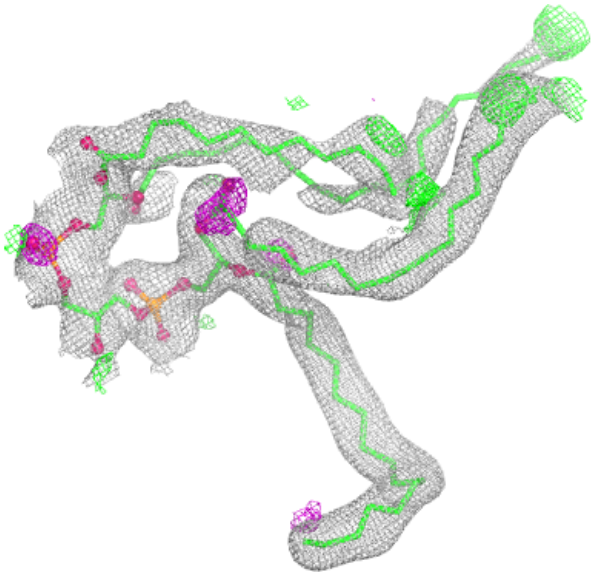


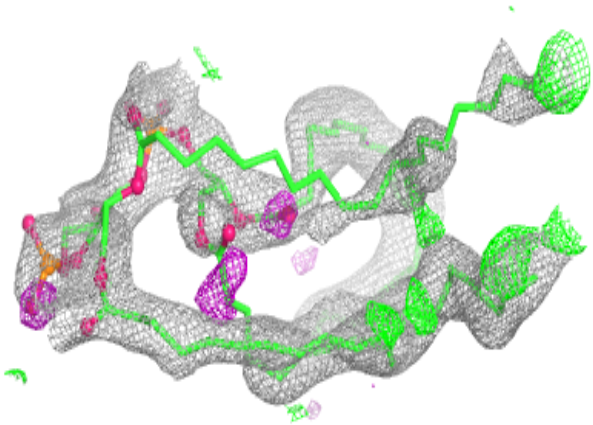


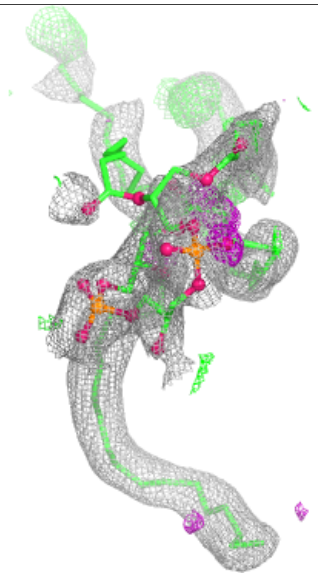


Electron density around CDL Y 101:

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

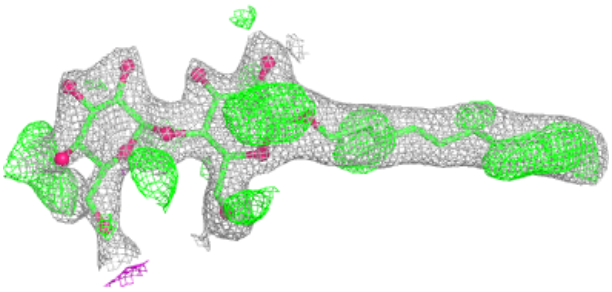


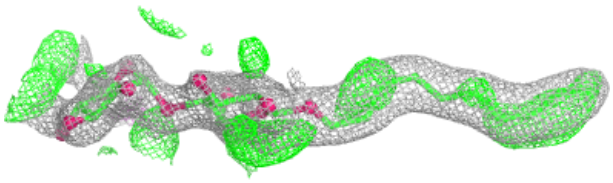


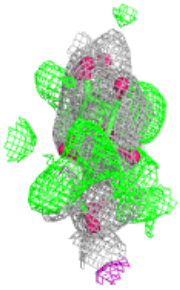


Electron density around DMU A 609:

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

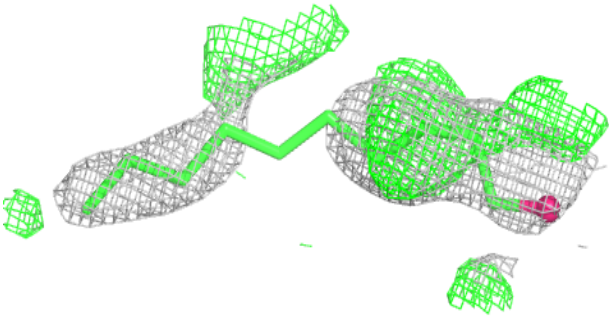


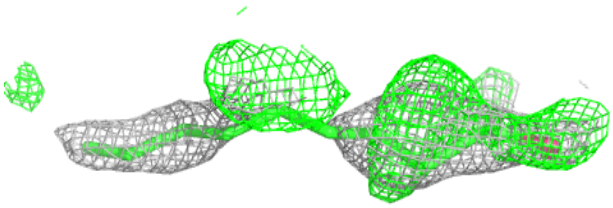


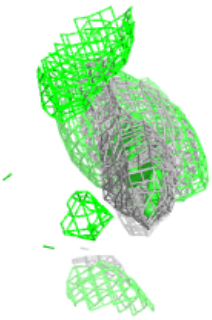


Electron density around DMU A 614:

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

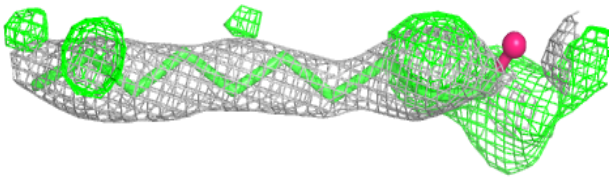


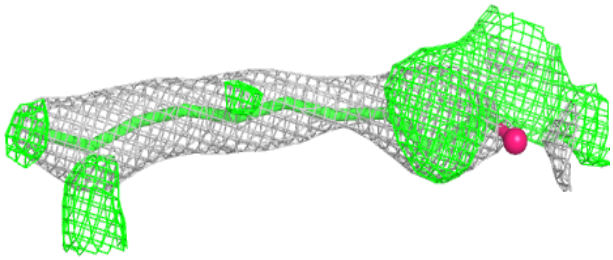


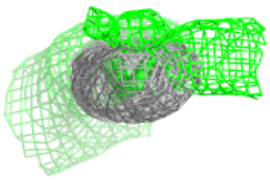


Electron density around DMU B 302:

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

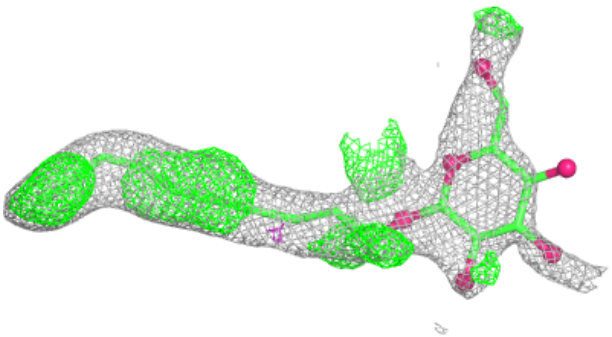


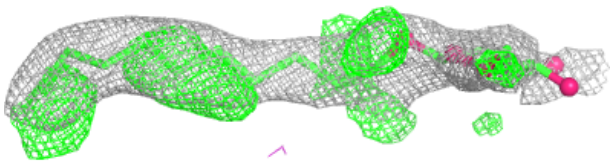


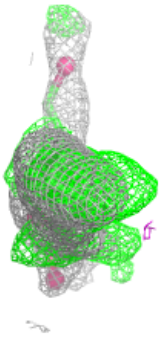


Electron density around DMU B 304:

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

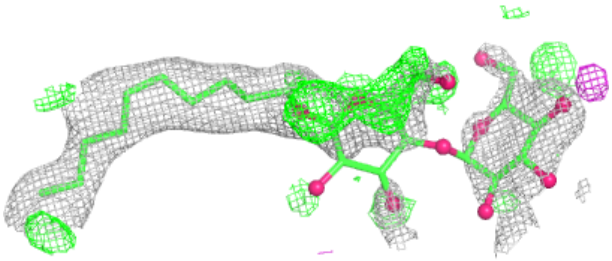


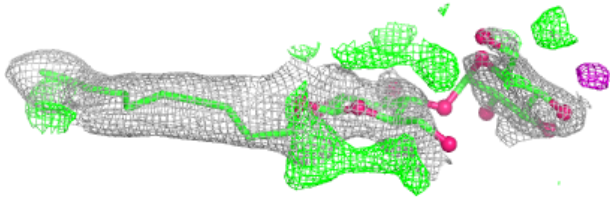


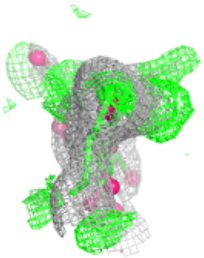


Electron density around DMU H 101:

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

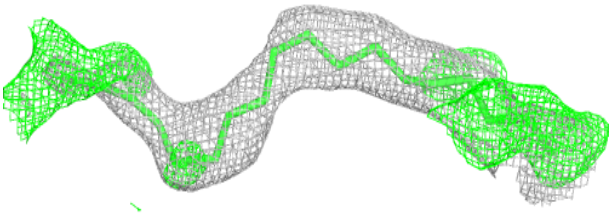


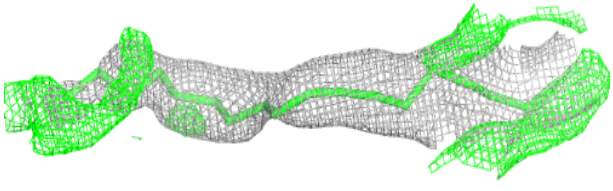


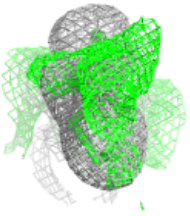


Electron density around LFA P 310:

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

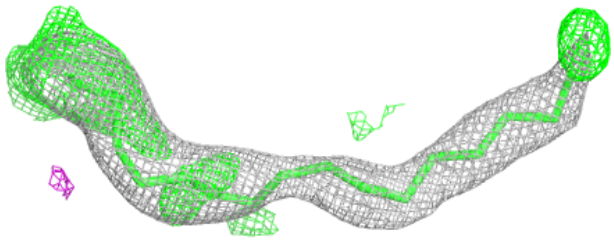


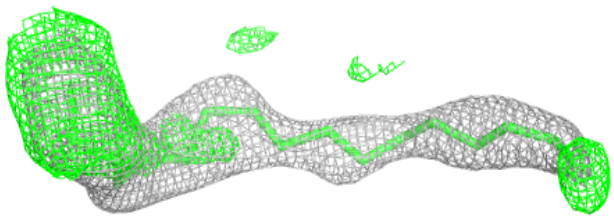


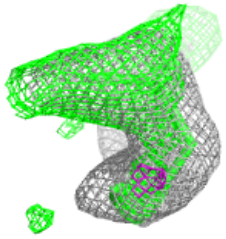


Electron density around LFA B 307:

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

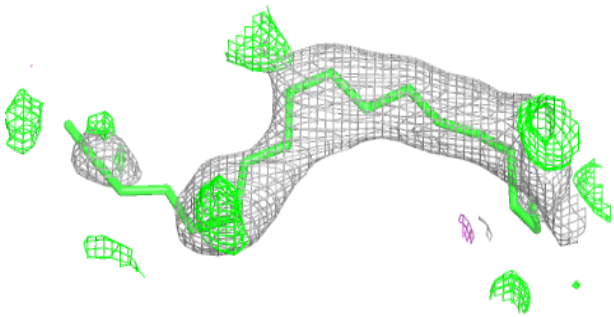


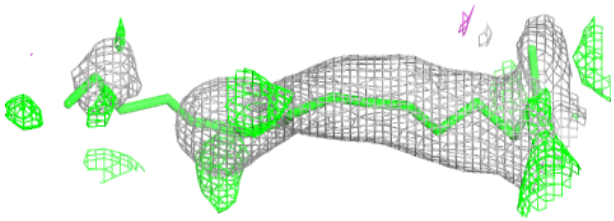


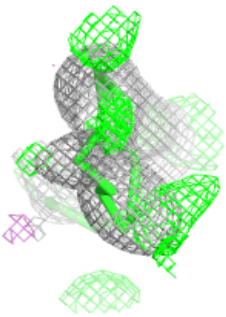


Electron density around LFA C 309:

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

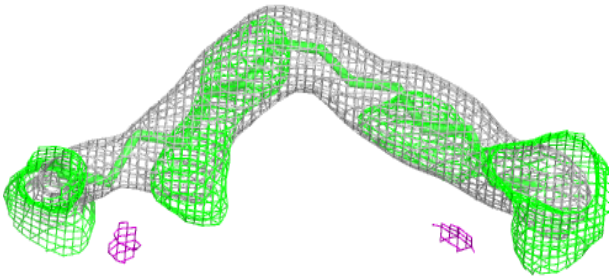


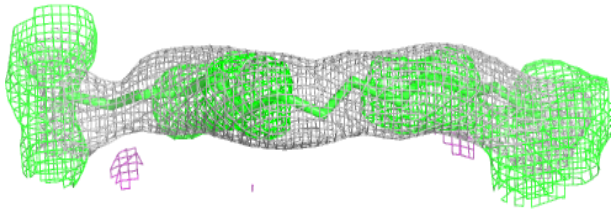


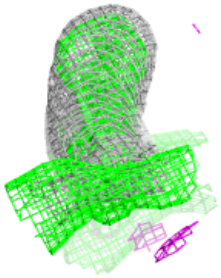


Electron density around LFA A 607:

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

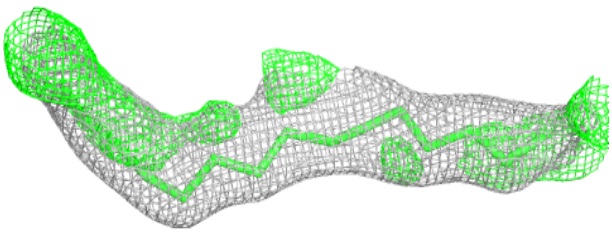


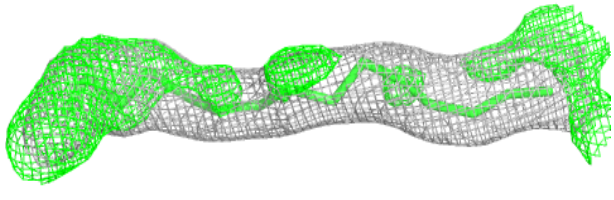


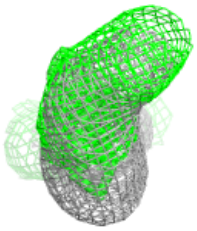


Electron density around LFA P 314:

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

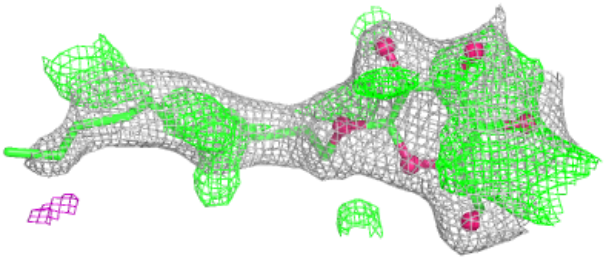


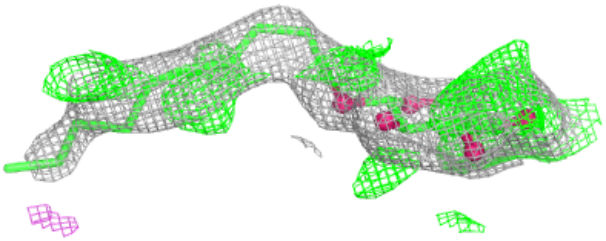


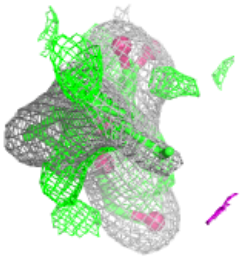


Electron density around DMU G 104:

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

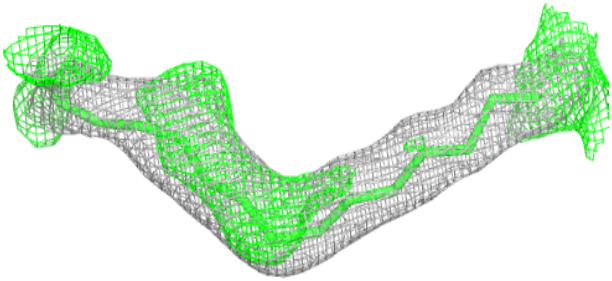


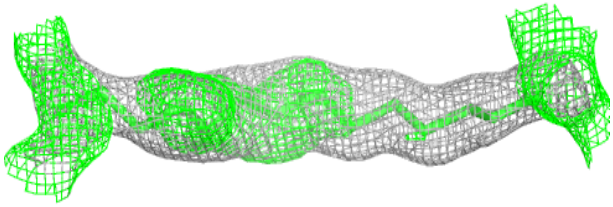


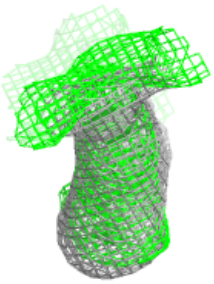


Electron density around LFA N 606:

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

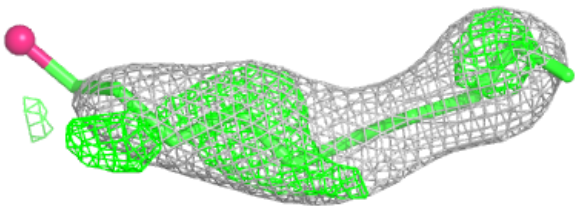


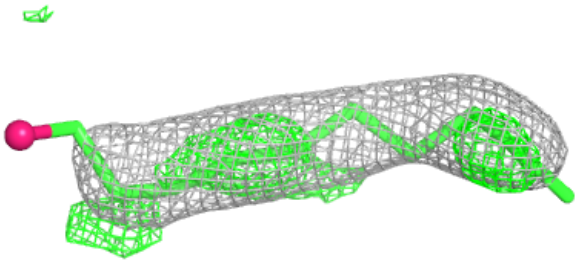


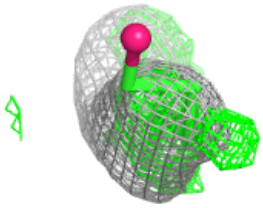


Electron density around DMU J 101:

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

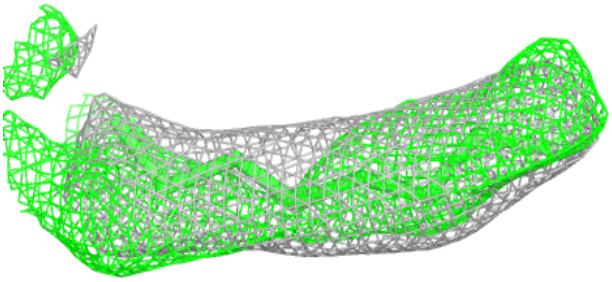


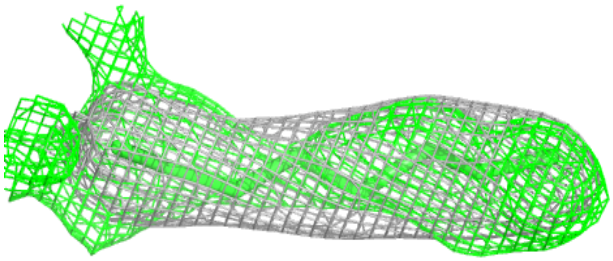


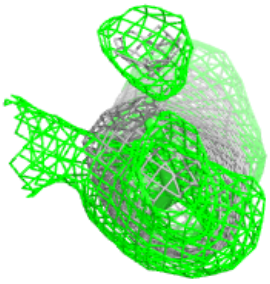


Electron density around DMU Z 102:

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

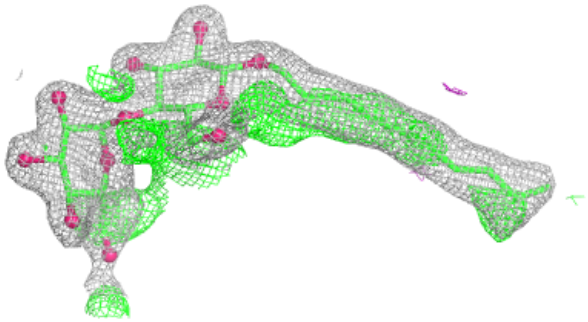


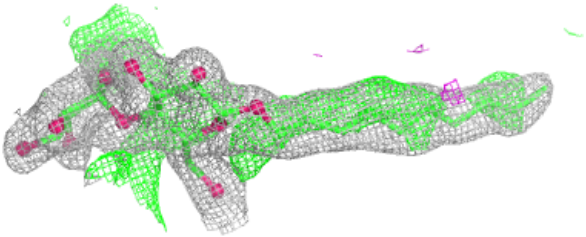


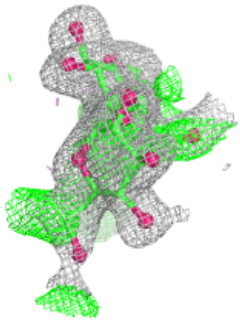


Electron density around DMU D 201:

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

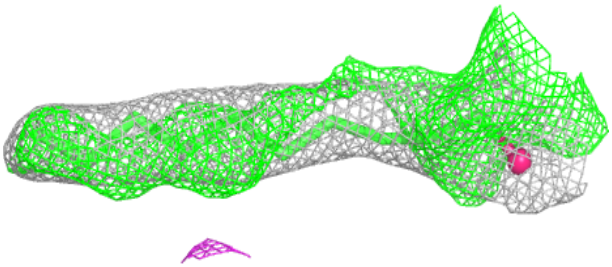


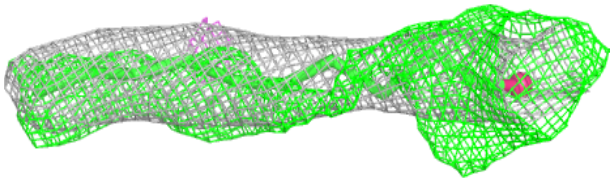


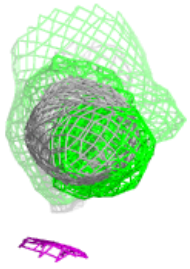


Electron density around DMU O 305:

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

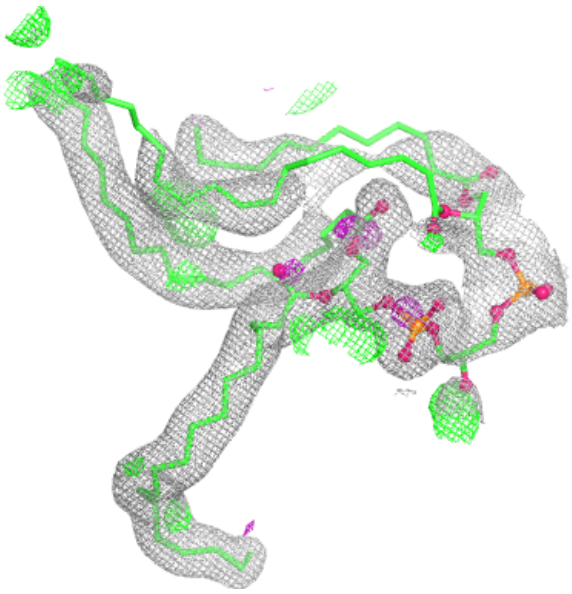


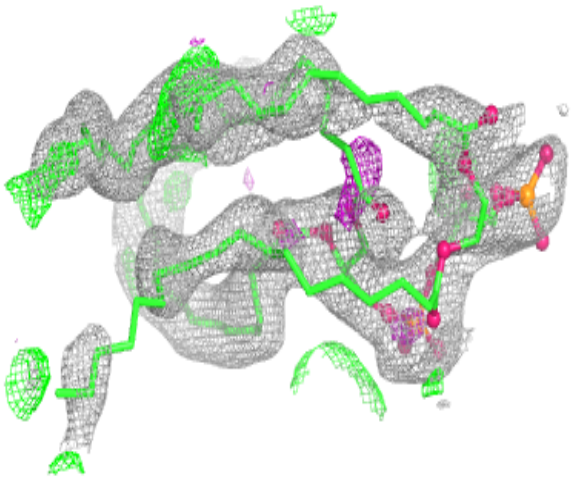


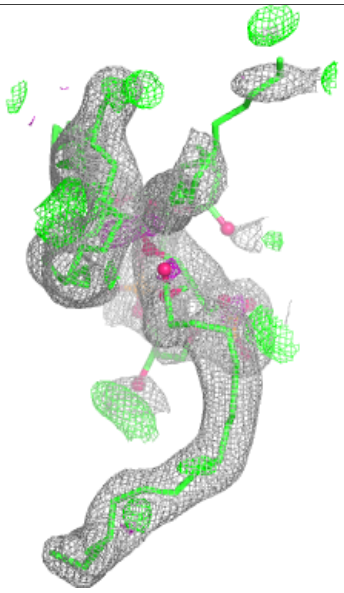


Electron density around CDL L 101:

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

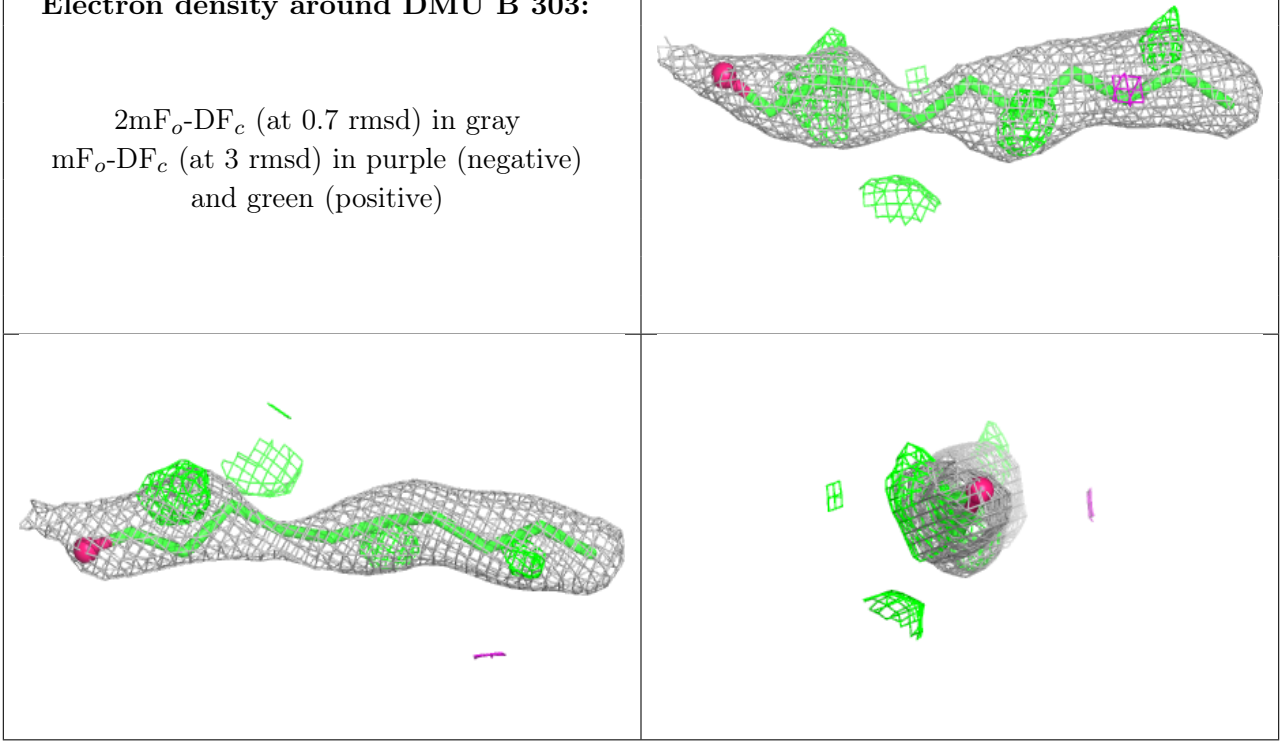






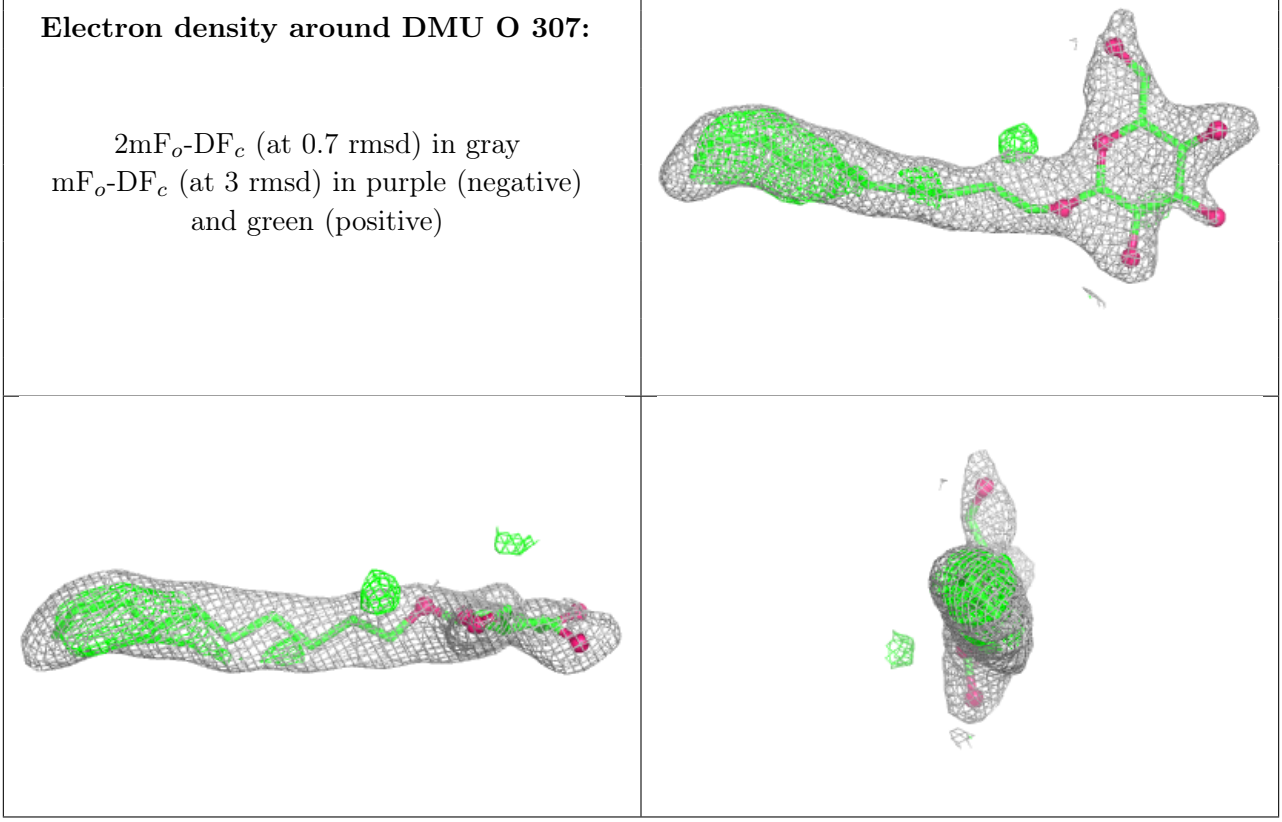
Electron density around DMU B 303:

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



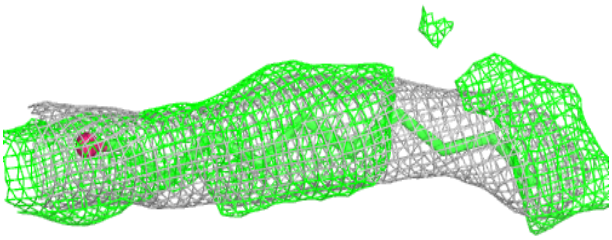
Electron density around DMU O 307:

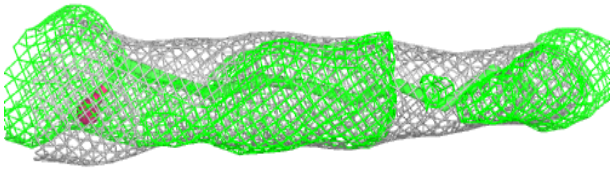
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

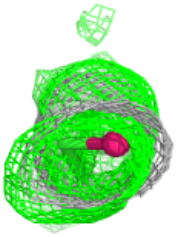


Electron density around DMU P 307:

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

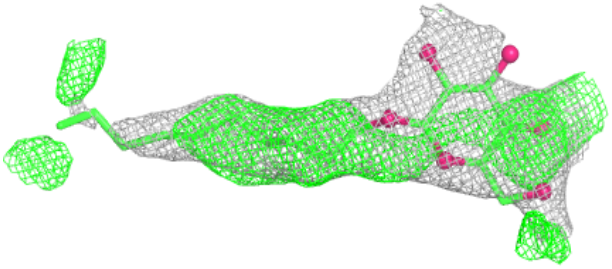


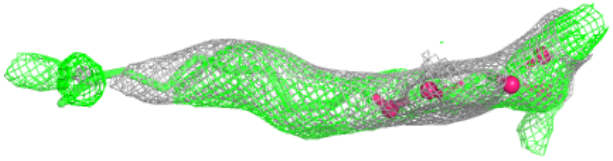


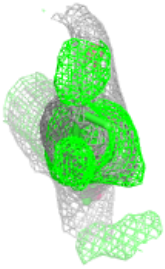


Electron density around DMU L 102:

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

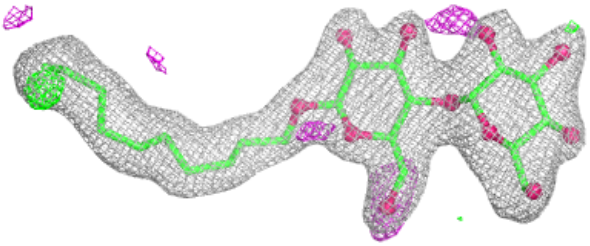


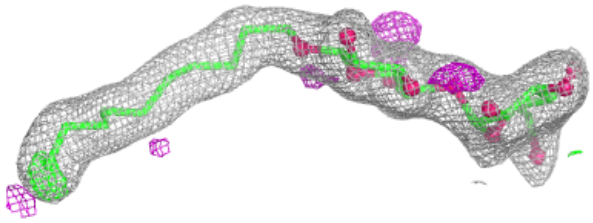


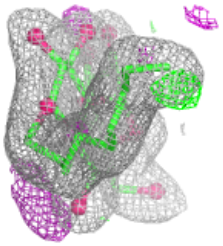


Electron density around DMU Z 101:

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

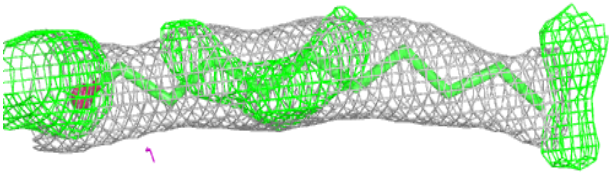


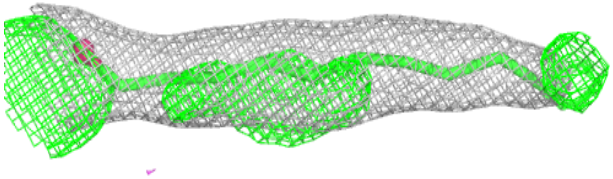


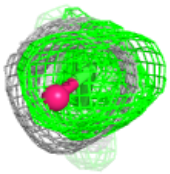


Electron density around DMU C 306:

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

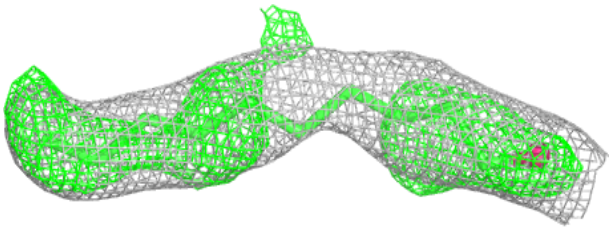


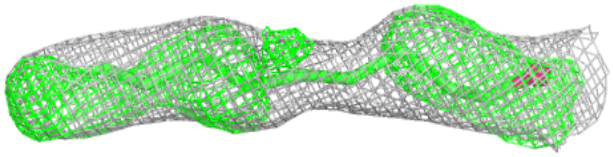


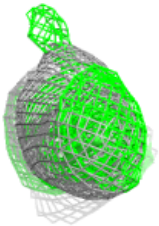


Electron density around DMU O 306:

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

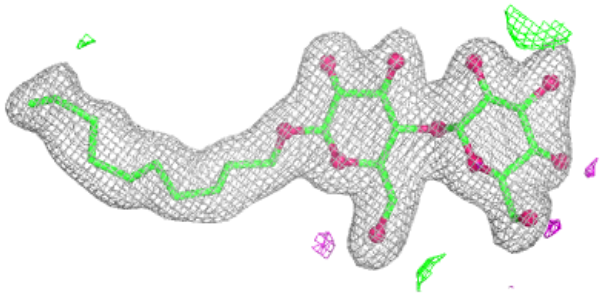


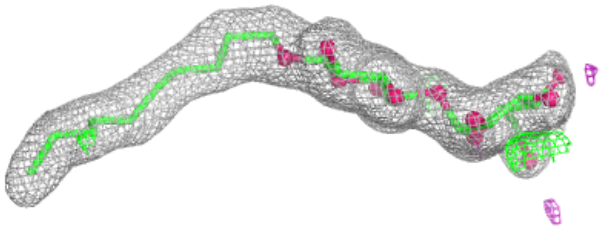


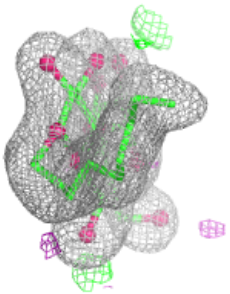


Electron density around DMU M 101:

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

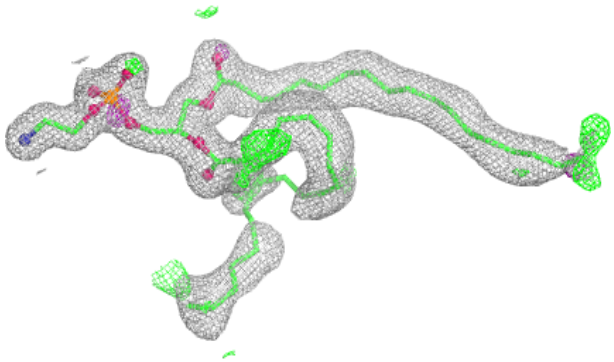


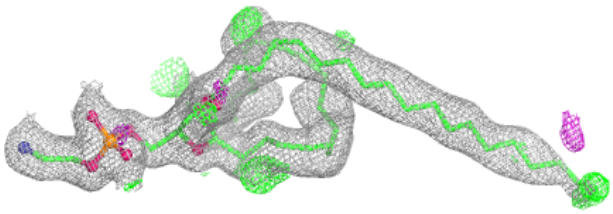


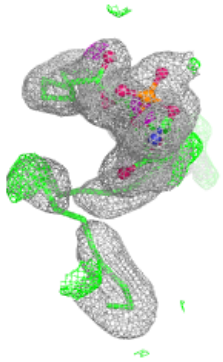


Electron density around PEK T 102:

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

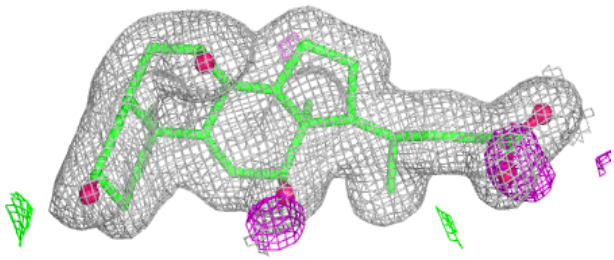


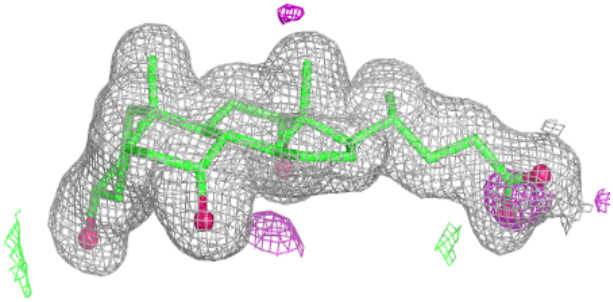


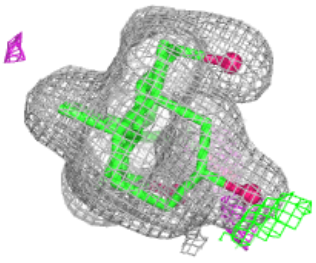


Electron density around CHD C 301:

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

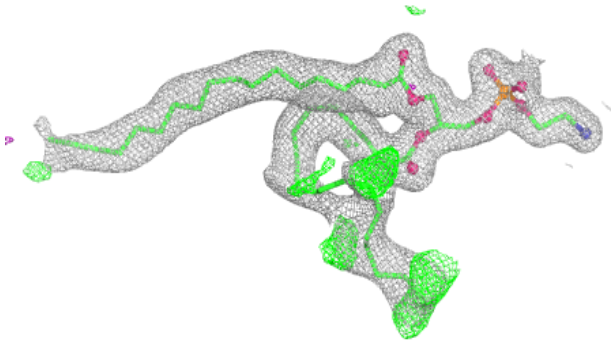


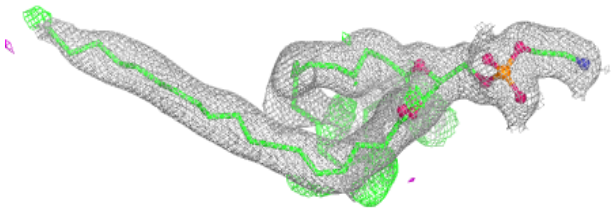


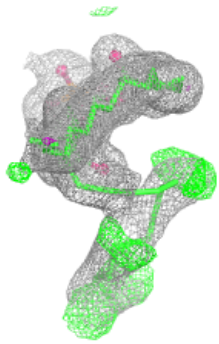


Electron density around PEK G 101:

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

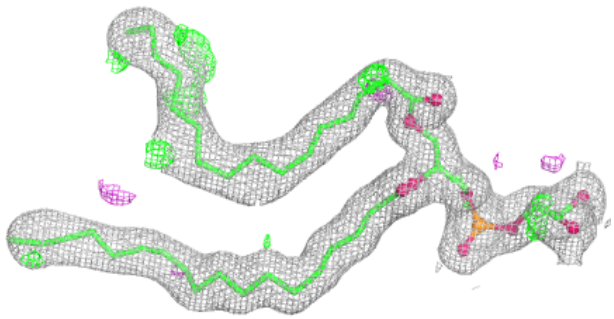


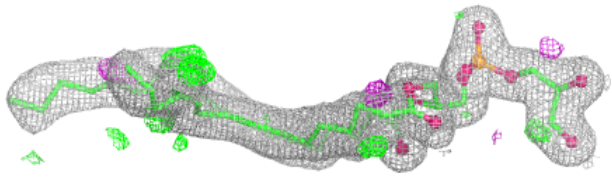


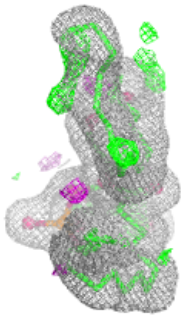


Electron density around PGV N 614:

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

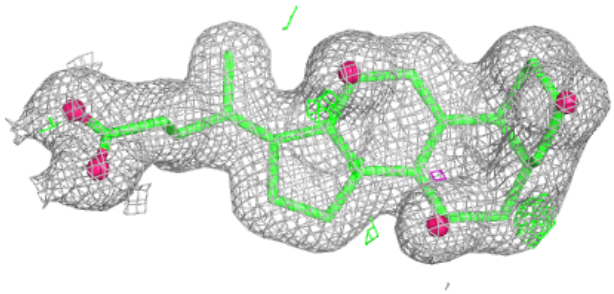


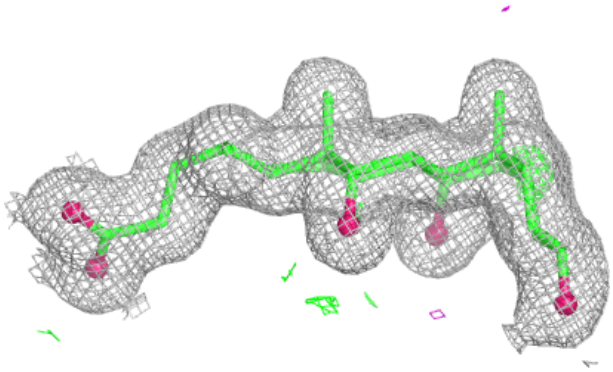


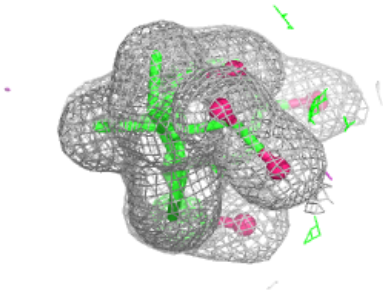


Electron density around CHD B 306:

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

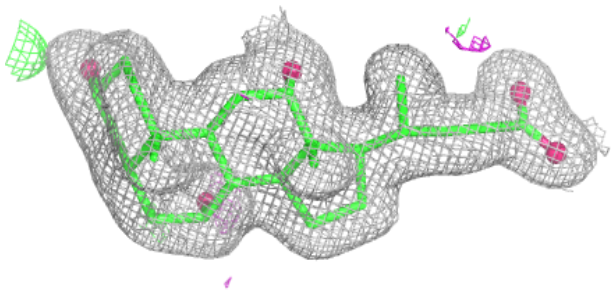


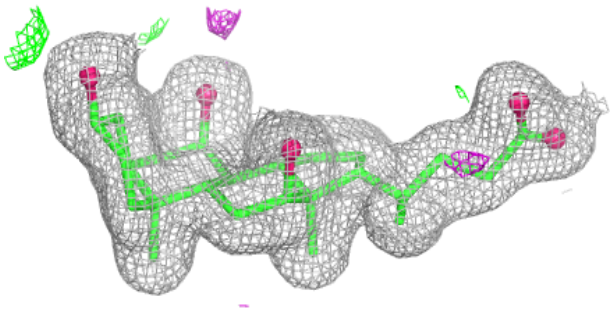


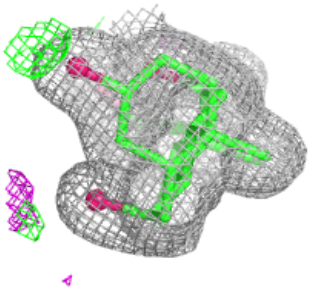


Electron density around CHD P 302:

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

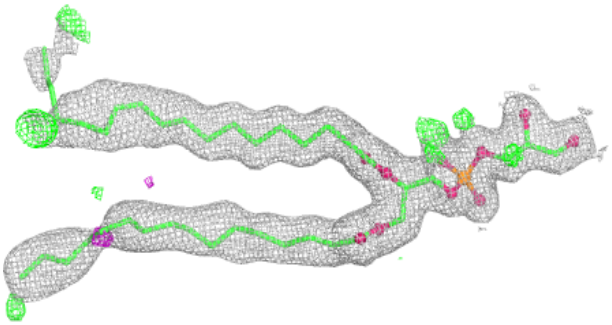




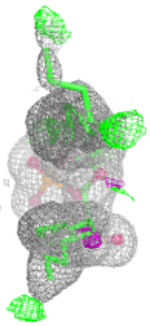


Electron density around PGV C 303:

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

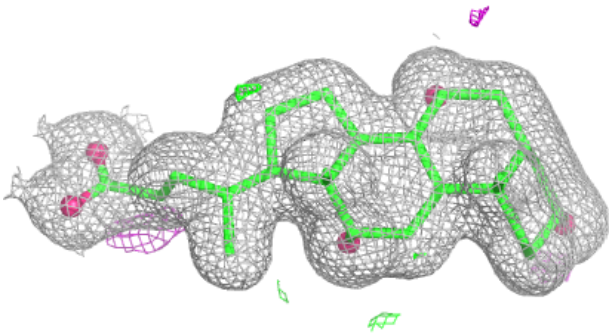


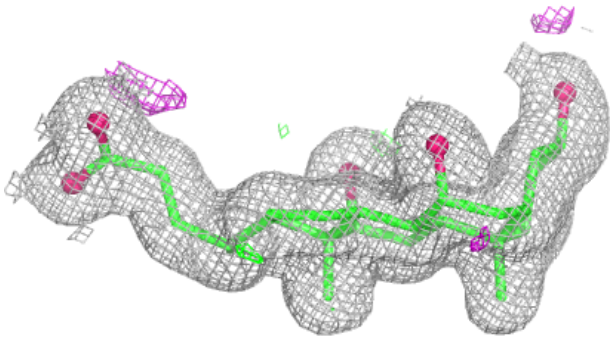


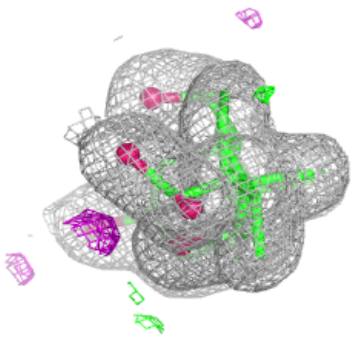


Electron density around CHD G 102:

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

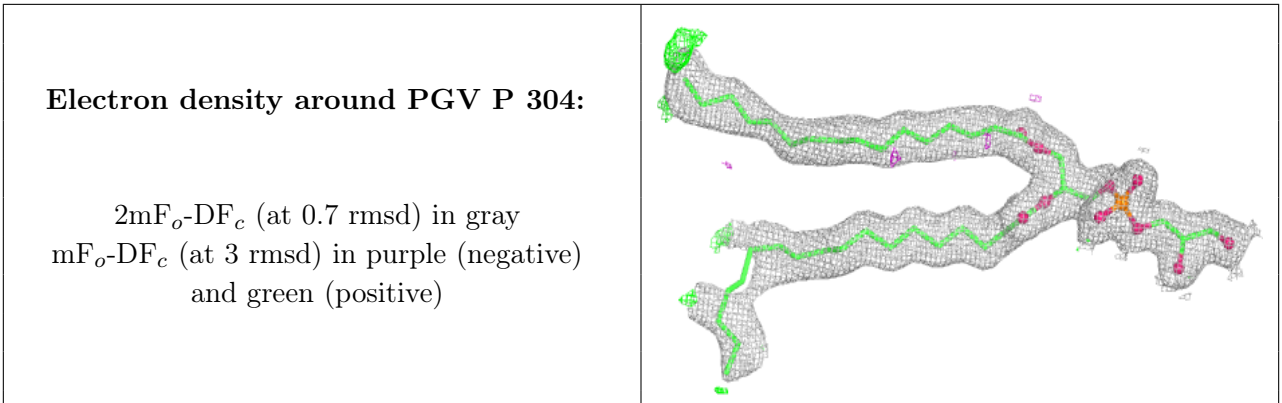


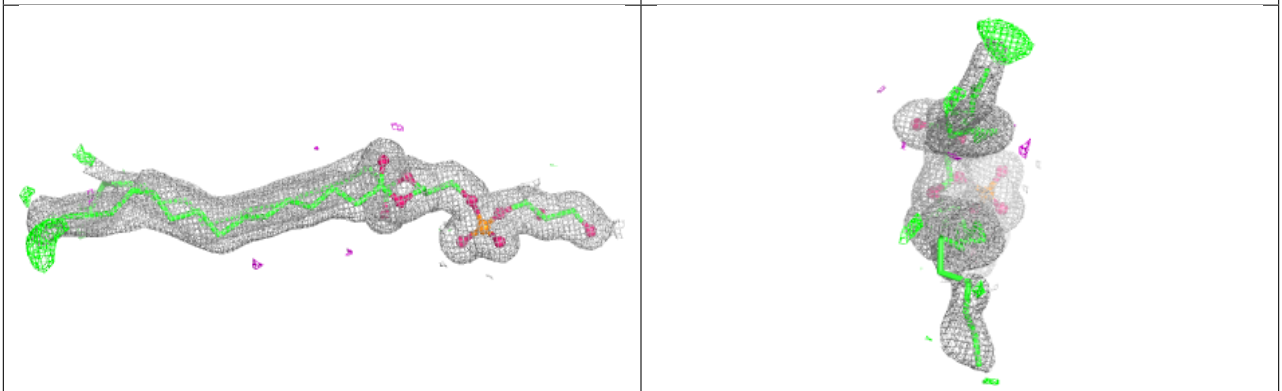




Electron density around PGV P 304:

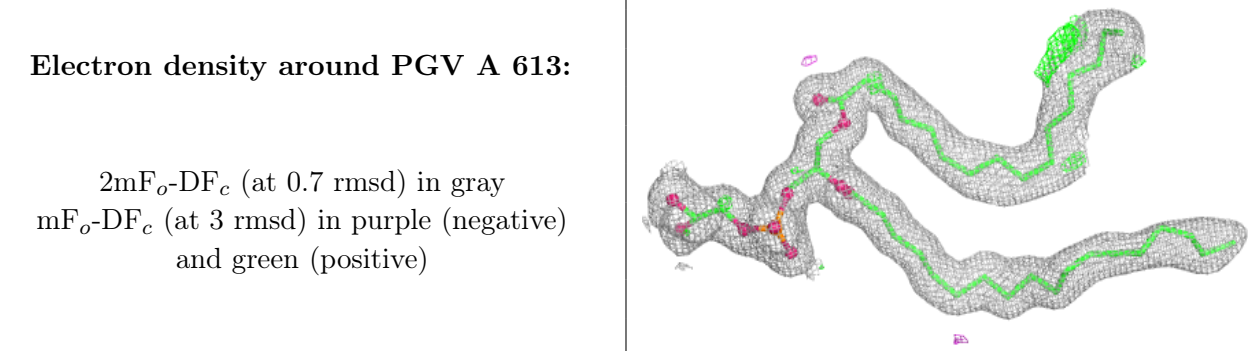
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

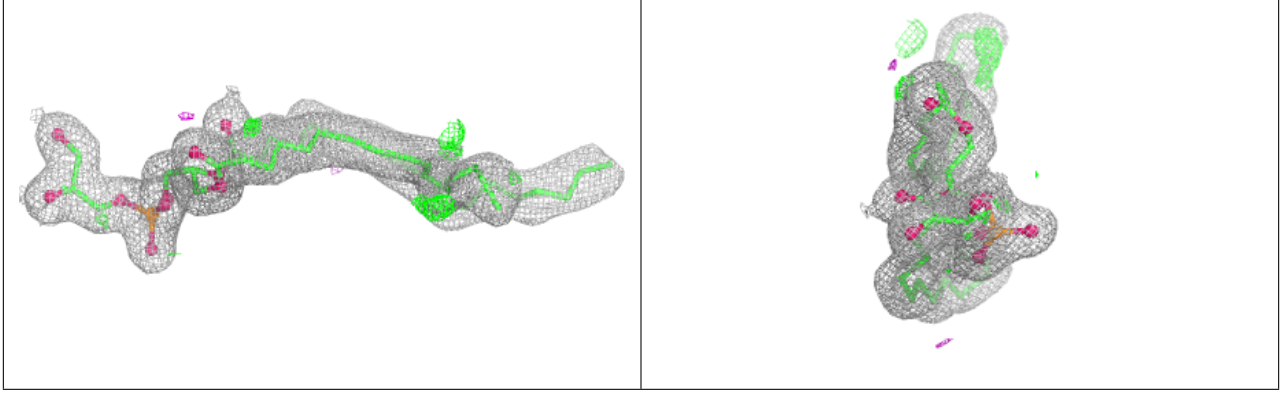




Electron density around PGV A 613:

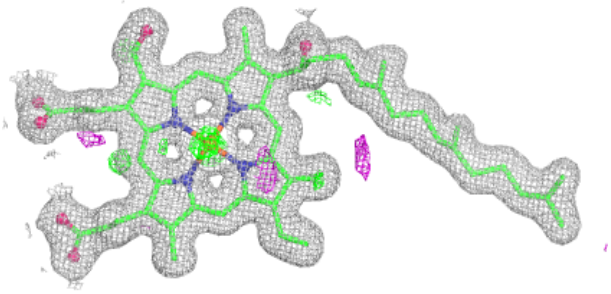
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

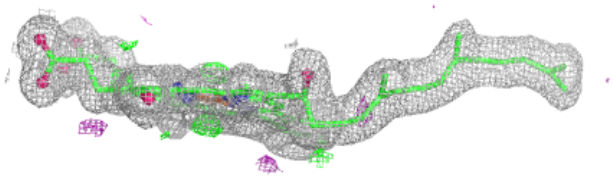


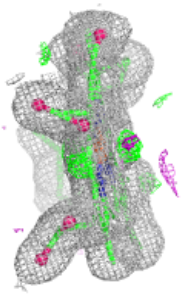


Electron density around HEA A 601:

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

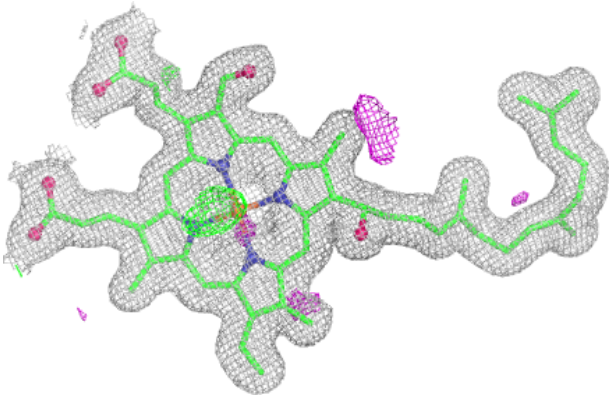


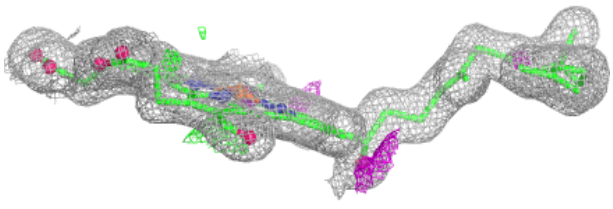


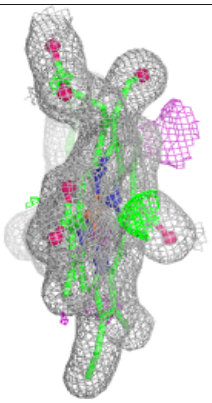


Electron density around HEA A 602:

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

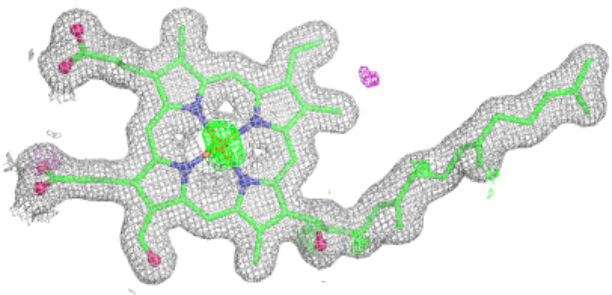


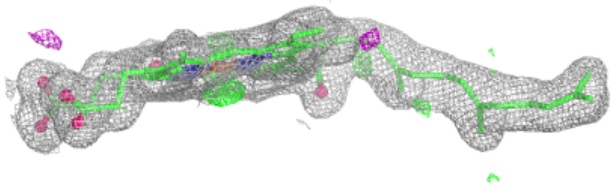


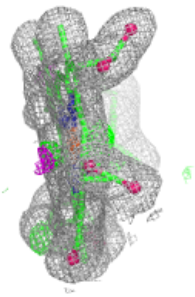


Electron density around HEA N 601:

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

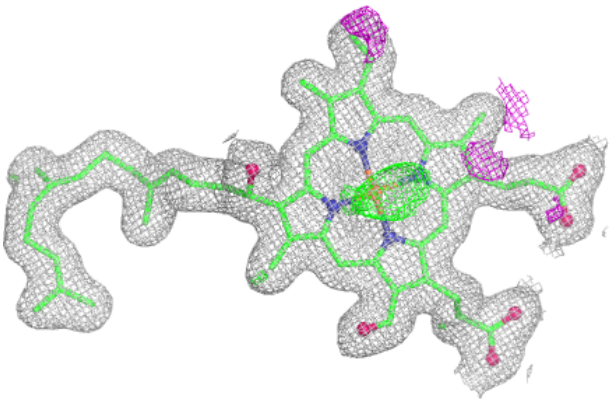


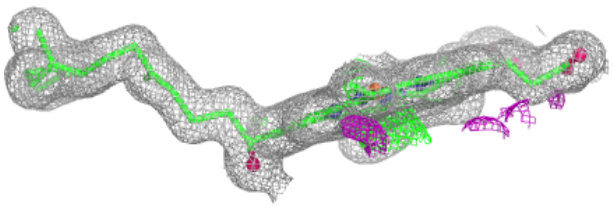


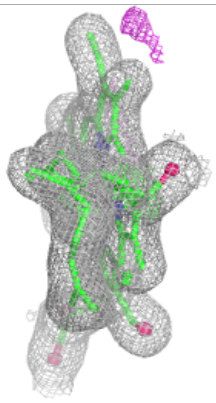


Electron density around HEA N 602:

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







6.5 Other polymers (i)

There are no such residues in this entry.