wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2025 – 02:36 PM JST

PDB ID	:	9IKH / pdb_00009ikh
Title	:	Bovine Heart Cytochrome c Oxidase in the Nitrous Oxide-bound Fully Oxidized State
Authors	:	Muramoto, K.; Ide, T.; Shinzawa-Itoh, K.
Deposited on	:	2024-06-27
Resolution	:	1.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

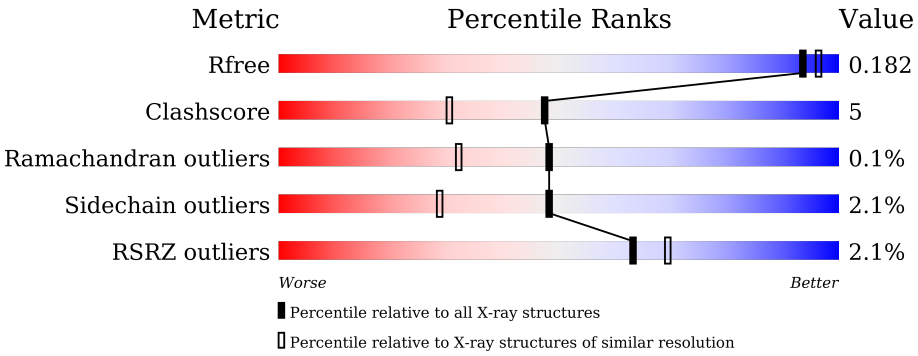
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	90% 9%
1	N	514	% 90% 9%
2	B	227	5% 81% 16%
2	O	227	3% 83% 15%
3	C	261	89% 10%
3	P	261	85% 13%

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Mol	Chain	Length	Quality of chain
4	D	147	91% 5%
4	Q	147	86% 6% 7%
5	E	109	88% 6% 6%
5	R	109	87% 6% 6%
6	F	98	82% 8% 7%
6	S	98	77% 14% 7%
7	G	85	78% 7% 15%
7	T	85	76% 7% 15%
8	H	85	74% 12% 12%
8	U	85	76% 9% 12%
9	I	73	90%
9	V	73	82% 14%
10	J	59	85% 7% 5%
10	W	59	88% 7% 5%
11	K	56	84% 12%
11	X	56	84% 12%
12	L	47	83% 9% 6%
12	Y	47	83% 9% 6%
13	M	46	85% 13%
13	Z	46	74% 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
20	LFA	C	308	-	-	-	X
20	LFA	P	311	-	-	-	X
21	DMU	N	610	-	-	-	X

2 Entry composition (i)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

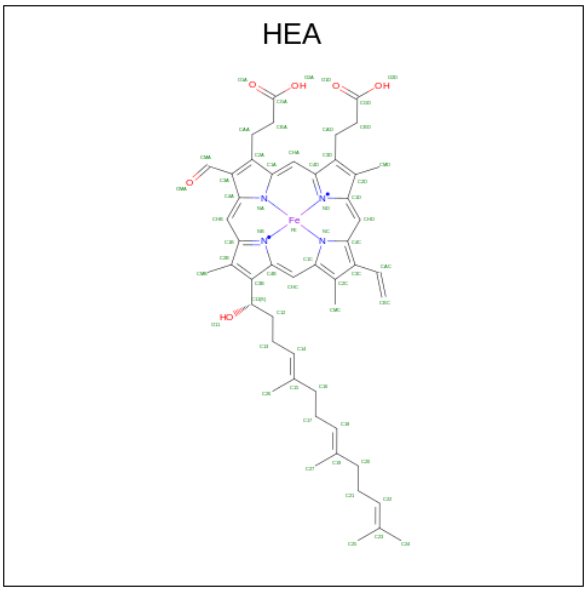
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

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



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

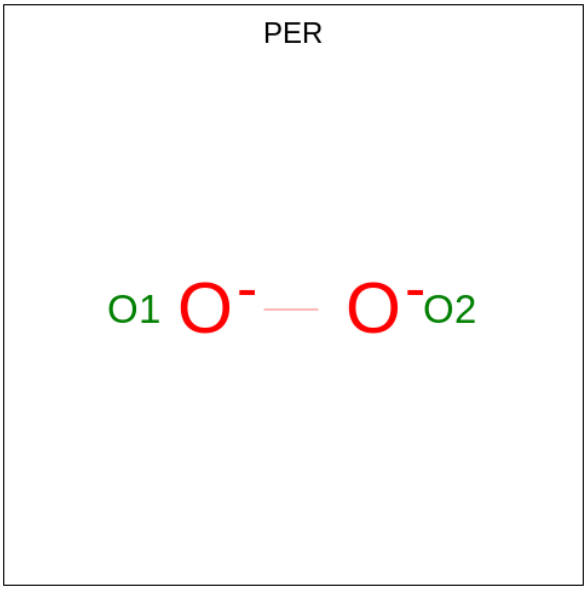
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

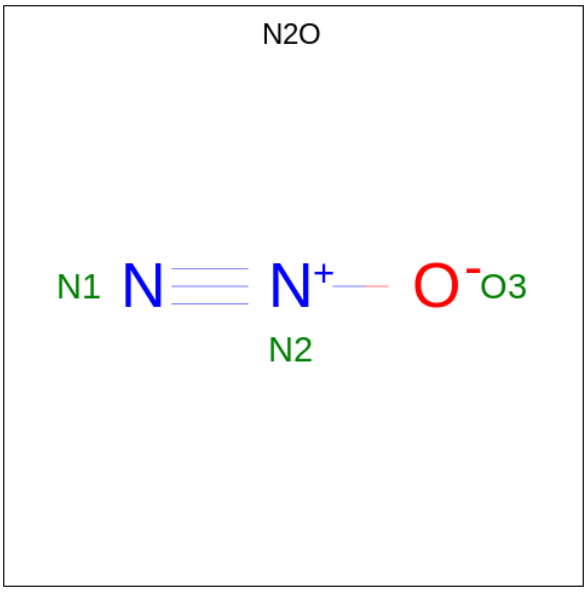
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is PEROXIDE ION (CCD ID: PER) (formula: O_2).



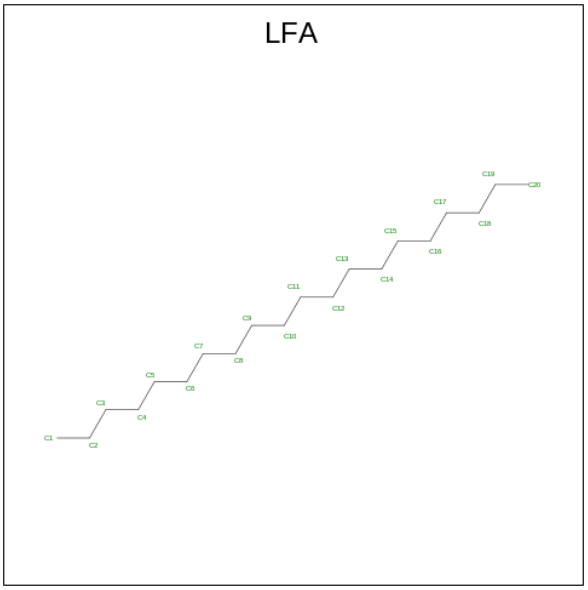
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total O 2 2	0	0
18	N	1	Total O 2 2	0	0

- Molecule 19 is NITROUS OXIDE (CCD ID: N2O) (formula: N_2O) (labeled as "Ligand of Interest" by depositor).



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

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



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

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

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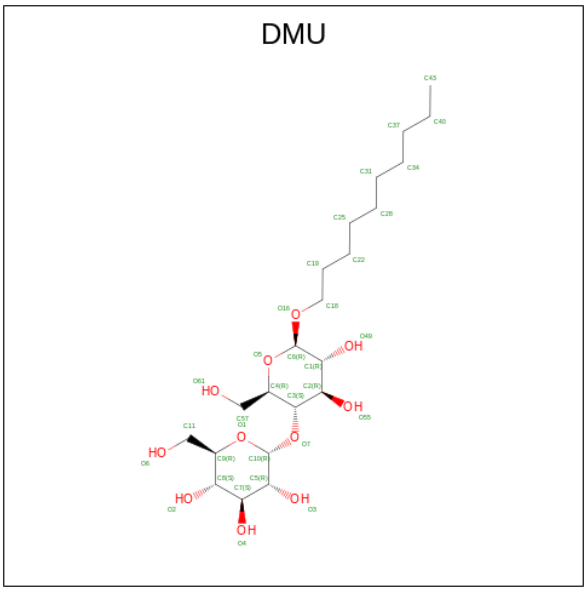
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	P	1	Total C 13 13	0	0
20	T	1	Total C 14 14	0	0
20	T	1	Total C 11 11	0	0

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



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

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

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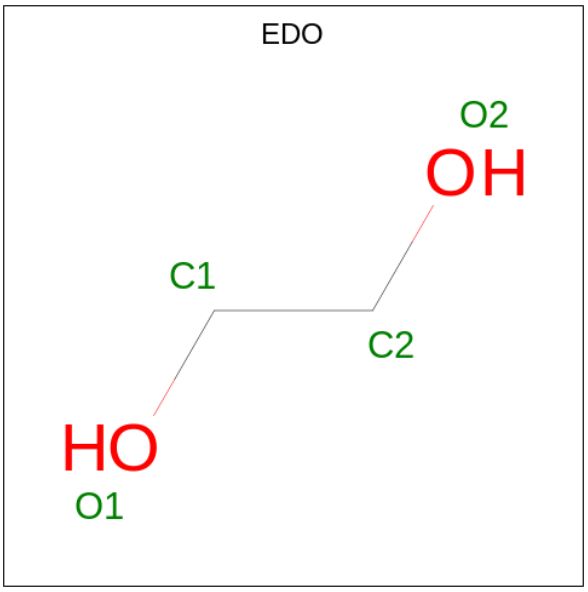
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	P	1	Total C O 33 22 11	0	0
21	P	1	Total C 7 7	0	0
21	P	1	Total C O 22 16 6	0	0
21	P	1	Total C O 33 22 11	0	0
21	P	1	Total C O 33 22 11	0	0
21	P	1	Total C O 22 16 6	0	0
21	P	1	Total C O 33 22 11	0	0
21	Q	1	Total C O 33 22 11	0	0
21	U	1	Total C O 33 22 11	0	0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

- Molecule 22 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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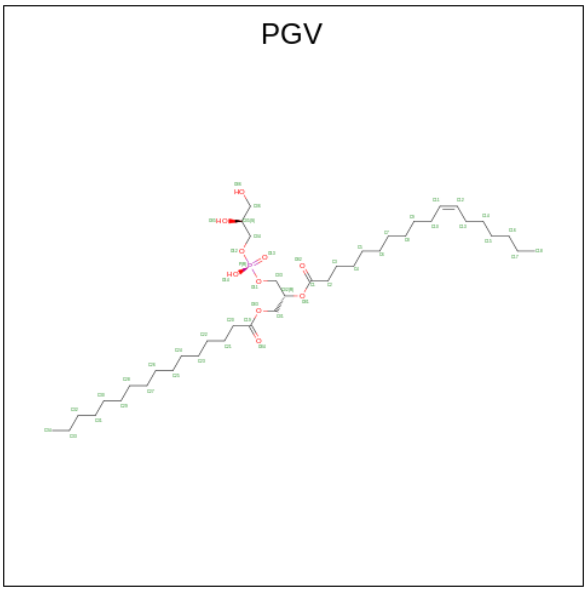
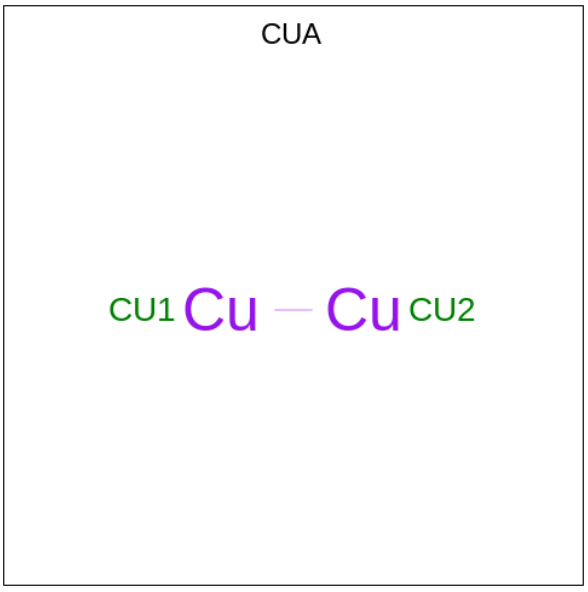
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	N	1	Total C O 4 2 2	0	0
22	N	1	Total C O 4 2 2	0	0
22	N	1	Total C O 4 2 2	0	0
22	N	1	Total C O 4 2 2	0	0
22	N	1	Total C O 4 2 2	0	0
22	O	1	Total C O 4 2 2	0	0
22	P	1	Total C O 4 2 2	0	0
22	P	1	Total C O 4 2 2	0	0
22	P	1	Total C O 4 2 2	0	0
22	R	1	Total C O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

- Molecule 23 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



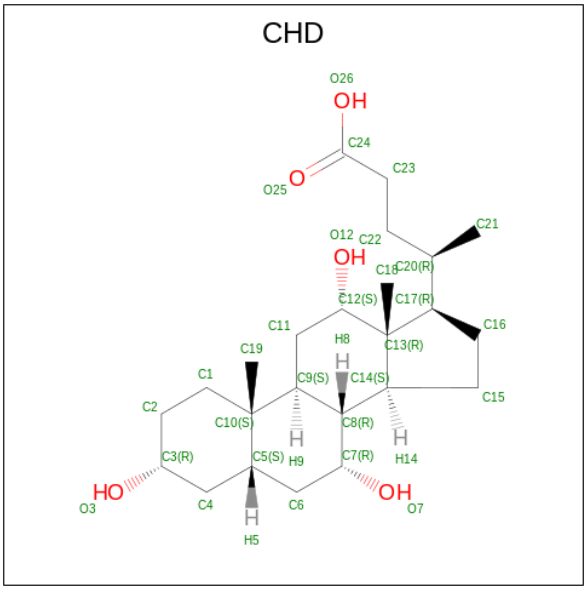
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	O	P	0	0
			51	40	10	1		
23	C	1	Total	C	O	P	0	0
			51	40	10	1		
23	N	1	Total	C	O	P	0	0
			51	40	10	1		
23	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 24 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



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

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

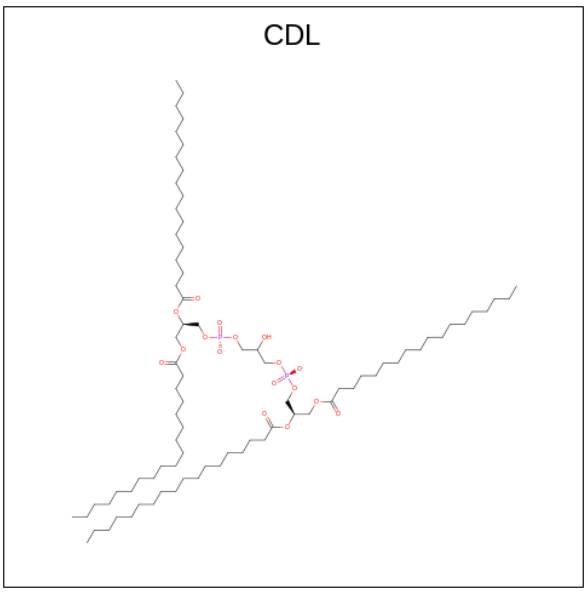


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B	1	Total C O 29 24 5	0	0
25	C	1	Total C O 29 24 5	0	0
25	C	1	Total C O 29 24 5	0	0
25	O	1	Total C O 29 24 5	0	0
25	P	1	Total C O 29 24 5	0	0
25	P	1	Total C O 29 24 5	0	0

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

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

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

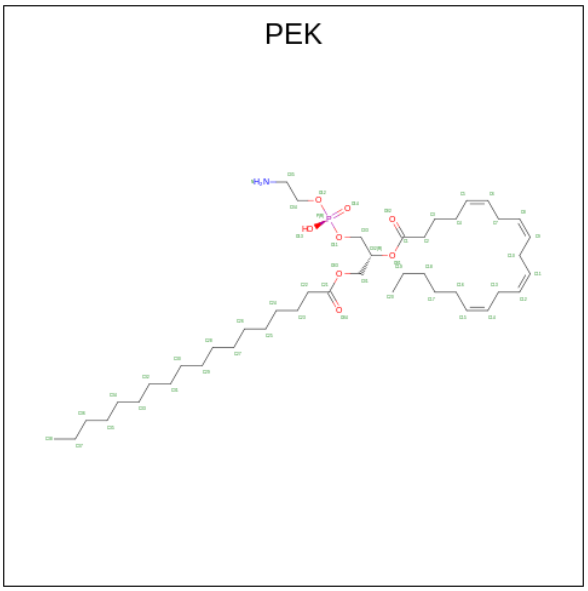


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O P 87 68 17 2	0	0
27	I	1	Total C O P 64 45 17 2	0	0
27	L	1	Total C O P 94 75 17 2	0	0
27	P	1	Total C O P 87 68 17 2	0	0
27	V	1	Total C O P 64 45 17 2	0	0
27	Y	1	Total C O P 94 75 17 2	0	0

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

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

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



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

- Molecule 30 is water.

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

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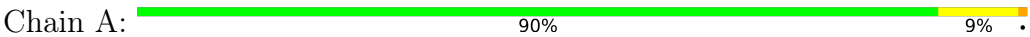
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	K	21	Total O 21 21	0	0
30	L	26	Total O 28 28	0	2
30	M	22	Total O 22 22	0	0
30	N	222	Total O 232 232	0	10
30	O	151	Total O 152 152	0	1
30	P	103	Total O 104 104	0	1
30	Q	77	Total O 81 81	0	4
30	R	90	Total O 98 98	0	8
30	S	90	Total O 96 96	0	6
30	T	37	Total O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

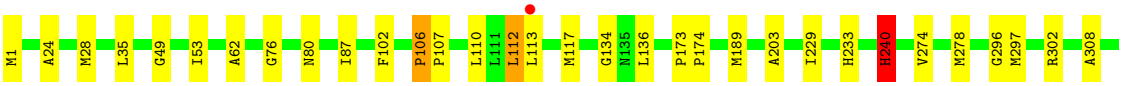
3 Residue-property plots (i)

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

• Molecule 1: Cytochrome c oxidase subunit 1

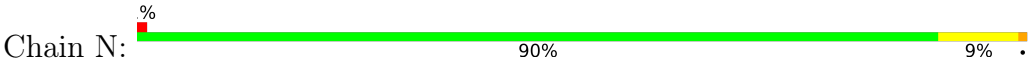
Chain A:

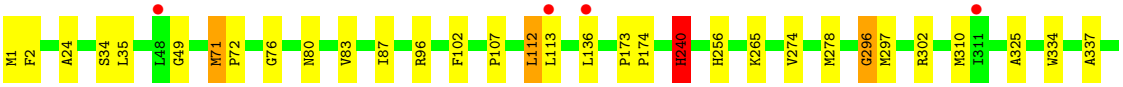




• Molecule 1: Cytochrome c oxidase subunit 1

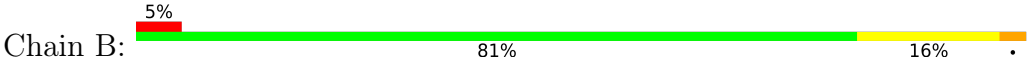
Chain N:

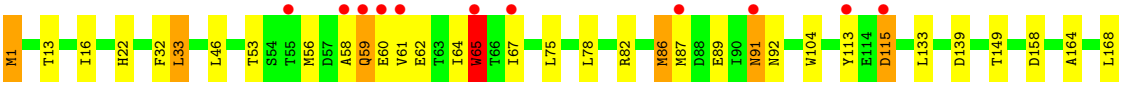




• Molecule 2: Cytochrome c oxidase subunit 2

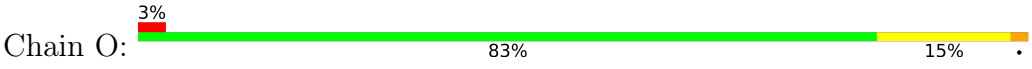
Chain B:

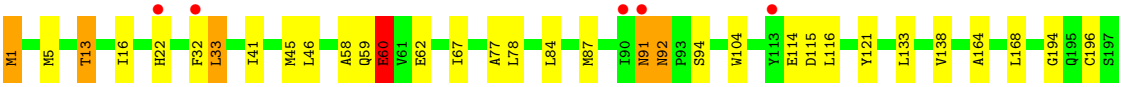


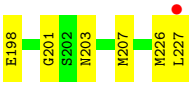


• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:

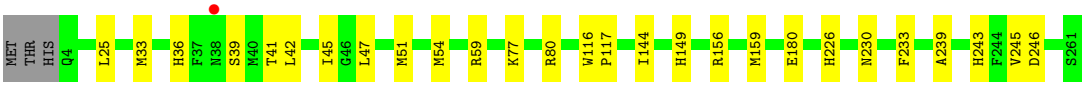






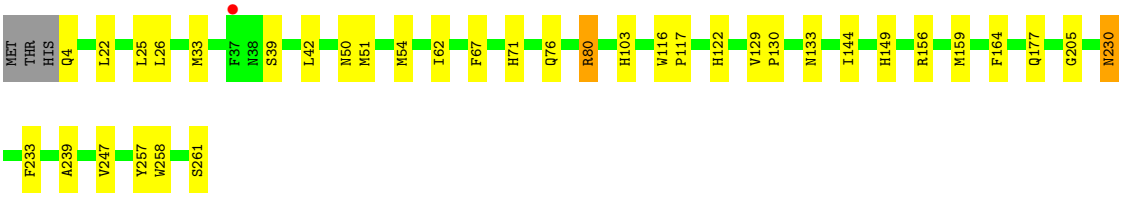
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:



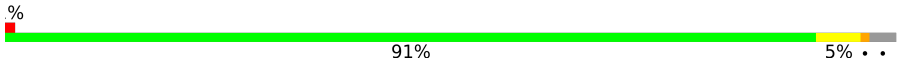
• Molecule 3: Cytochrome c oxidase subunit 3

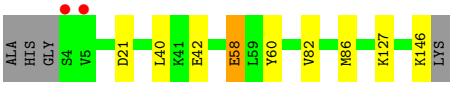
Chain P:



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

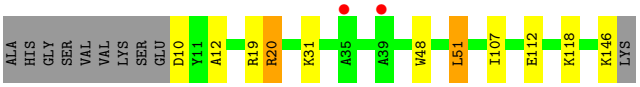
Chain D:





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

Chain Q:

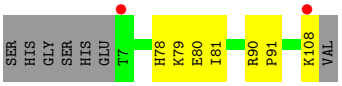


• Molecule 5: Cytochrome c oxidase subunit 5A

Chain E:

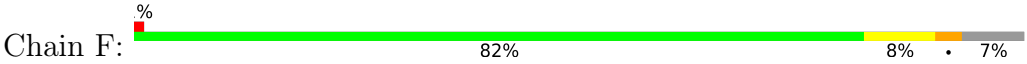
• Molecule 5: Cytochrome c oxidase subunit 5A

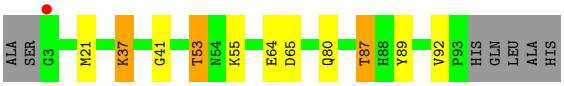
Chain R:



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

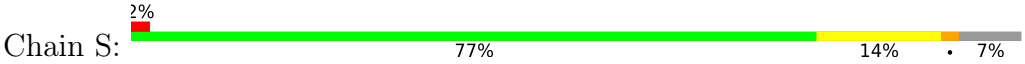
Chain F:

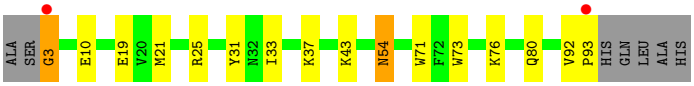




• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

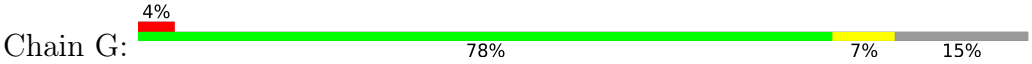
Chain S:

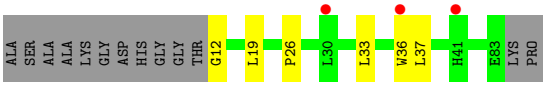




• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

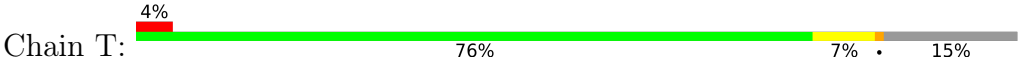
Chain G:

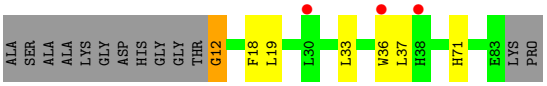




• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

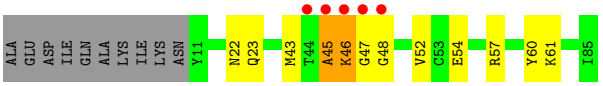
Chain T:





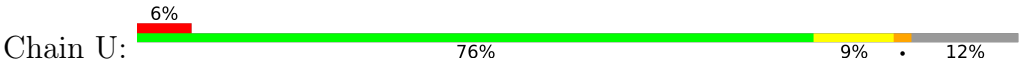
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



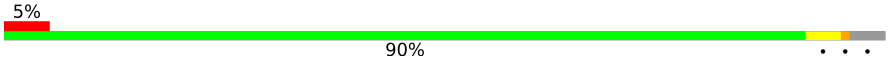
• Molecule 8: Cytochrome c oxidase subunit 6B1

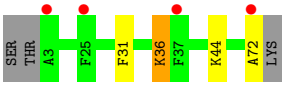
Chain U:



• Molecule 9: Cytochrome c oxidase subunit 6C

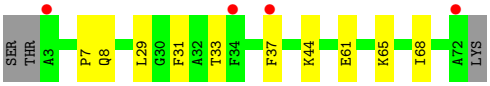
Chain I:





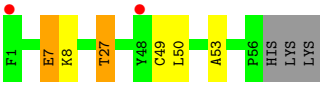
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



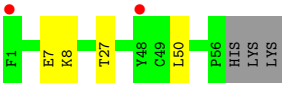
• Molecule 10: Cytochrome c oxidase subunit 7A1

Chain J:



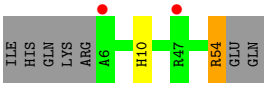
• Molecule 10: Cytochrome c oxidase subunit 7A1

Chain W:



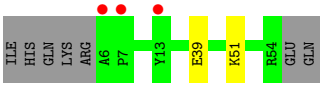
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



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

Chain X:

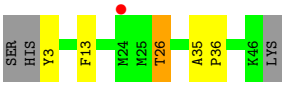


• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:

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

Chain Y:

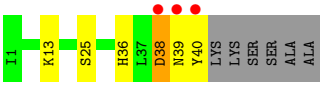


• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

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	182.10Å 204.30Å 177.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.75 40.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.75) 100.0 (40.00-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.138 , 0.174 0.153 , 0.182	Depositor DCC
R_{free} test set	32888 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 57.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33055	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: CUA, HEA, CHD, UNX, LFA, MG, FME, EDO, CDL, CU, PER, PGV, PEK, N2O, DMU, NA, ZN

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

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

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

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	2
6	S	0	1
All	All	0	5

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	GLY	C-O	11.37	1.36	1.23
1	N	49	GLY	C-O	9.27	1.34	1.23
7	T	12	GLY	N-CA	-8.07	1.32	1.45
4	D	58	GLU	CD-OE1	7.92	1.40	1.25
3	P	71	HIS	CE1-NE2	7.50	1.40	1.32

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	65	TRP	CA-CB-CG	10.57	133.69	113.60
1	A	240	HIS	CA-CB-CG	-10.40	103.40	113.80
9	I	72	ALA	CA-C-O	-10.39	103.13	120.80
1	N	240	HIS	CA-CB-CG	-10.39	103.41	113.80
2	B	65	TRP	CB-CG-CD1	-8.91	113.53	126.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4102	48	0
1	N	4130	0	4102	49	0
2	B	1870	0	1870	30	0
2	O	1870	0	1870	39	0
3	C	2171	0	2080	25	0
3	P	2172	0	2081	31	0
4	D	1192	0	1178	5	0
4	Q	1148	0	1131	7	0
5	E	825	0	823	2	0
5	R	825	0	823	4	0
6	F	709	0	691	8	0
6	S	709	0	691	9	0
7	G	606	0	577	3	0
7	T	606	0	577	4	0
8	H	628	0	580	15	0
8	U	628	0	580	12	0
9	I	575	0	584	5	0
9	V	575	0	584	4	0
10	J	441	0	439	7	0
10	W	441	0	439	3	0
11	K	384	0	366	0	0
11	X	384	0	366	2	0
12	L	360	0	360	4	0
12	Y	360	0	360	8	0
13	M	311	0	321	1	0
13	Z	311	0	321	3	0
14	A	129	0	88	6	0
14	N	129	0	88	3	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	1	0
19	A	3	0	0	0	0
19	N	3	0	0	0	0
20	A	28	0	54	9	0
20	B	17	0	33	2	0
20	C	114	0	205	4	0
20	G	14	0	27	4	0
20	N	14	0	27	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	O	28	0	54	5	0
20	P	100	0	173	7	0
20	T	25	0	48	0	0
21	A	51	0	75	2	0
21	B	66	0	104	1	0
21	C	194	0	262	6	0
21	D	33	0	41	3	0
21	H	33	0	28	1	0
21	J	11	0	21	0	0
21	L	22	0	31	2	0
21	M	41	0	56	0	0
21	N	51	0	75	0	0
21	O	66	0	104	1	0
21	P	194	0	262	2	0
21	Q	33	0	41	1	0
21	U	33	0	23	1	0
21	W	11	0	21	0	0
21	Z	63	0	87	3	0
22	A	16	0	24	1	0
22	B	4	0	6	0	0
22	C	12	0	17	0	0
22	E	12	0	18	0	0
22	F	8	0	12	0	0
22	G	4	0	6	0	0
22	N	20	0	30	1	0
22	O	4	0	6	0	0
22	P	12	0	17	0	0
22	R	12	0	18	0	0
22	S	8	0	12	0	0
22	T	4	0	6	0	0
23	A	51	0	76	0	0
23	C	51	0	76	1	0
23	N	51	0	76	0	0
23	P	51	0	76	0	0
24	B	2	0	0	0	0
24	O	2	0	0	0	0
25	B	29	0	39	0	0
25	C	58	0	78	2	0
25	O	29	0	39	1	0
25	P	58	0	78	4	0
26	C	1	0	0	1	0
26	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	C	87	0	124	15	0
27	I	64	0	72	0	0
27	L	94	0	141	6	0
27	P	87	0	124	13	0
27	V	64	0	72	2	0
27	Y	94	0	141	8	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	G	53	0	77	0	0
29	T	53	0	77	3	0
30	A	244	0	0	9	0
30	B	180	0	0	4	0
30	C	102	0	0	3	0
30	D	146	0	0	1	0
30	E	116	0	0	0	0
30	F	109	0	0	1	0
30	G	45	0	0	0	0
30	H	61	0	0	1	0
30	I	39	0	0	1	0
30	J	21	0	0	0	0
30	K	21	0	0	0	0
30	L	28	0	0	1	0
30	M	22	0	0	1	0
30	N	232	0	0	7	0
30	O	152	0	0	2	0
30	P	104	0	0	8	0
30	Q	81	0	0	2	0
30	R	98	0	0	1	0
30	S	96	0	0	0	0
30	T	38	0	0	1	0
30	U	48	0	0	4	0
30	V	23	0	0	0	0
30	W	15	0	0	0	0
30	X	17	0	0	0	0
30	Y	25	0	0	2	0
30	Z	17	0	0	0	0
All	All	33055	0	31462	338	0

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

The worst 5 of 338 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:607:PER:O2	18:N:607:PER:O1	1.60	1.16
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.22	1.12
1:A:112:LEU:HG	30:A:2018:HOH:O	1.48	1.12
18:A:606:PER:O2	18:A:606:PER:O1	1.64	1.12
8:H:46:LYS:HE2	8:H:46:LYS:O	1.54	1.05

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%)	512 (97%)	14 (3%)	0	100	100
2	B	230/227 (101%)	224 (97%)	6 (3%)	0	100	100
2	O	230/227 (101%)	223 (97%)	7 (3%)	0	100	100
3	C	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
3	P	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	136/147 (92%)	132 (97%)	4 (3%)	0	100	100
5	E	100/109 (92%)	100 (100%)	0	0	100	100
5	R	100/109 (92%)	100 (100%)	0	0	100	100
6	F	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
6	S	91/98 (93%)	89 (98%)	2 (2%)	0	100	100
7	G	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
7	T	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
8	H	73/85 (86%)	69 (94%)	2 (3%)	2 (3%)	4	0
8	U	73/85 (86%)	71 (97%)	1 (1%)	1 (1%)	9	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	I	68/73 (93%)	67 (98%)	1 (2%)	0	100 100
9	V	68/73 (93%)	67 (98%)	1 (2%)	0	100 100
10	J	54/59 (92%)	54 (100%)	0	0	100 100
10	W	54/59 (92%)	54 (100%)	0	0	100 100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100 100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100 100
12	L	42/47 (89%)	41 (98%)	1 (2%)	0	100 100
12	Y	42/47 (89%)	41 (98%)	1 (2%)	0	100 100
13	M	38/46 (83%)	38 (100%)	0	0	100 100
13	Z	38/46 (83%)	37 (97%)	0	1 (3%)	4 0
All	All	3488/3614 (96%)	3410 (98%)	74 (2%)	4 (0%)	48 32

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (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%)	86 82
1	N	440/426 (103%)	437 (99%)	3 (1%)	81 74
2	B	215/210 (102%)	206 (96%)	9 (4%)	25 8
2	O	215/210 (102%)	209 (97%)	6 (3%)	38 18
3	C	232/226 (103%)	230 (99%)	2 (1%)	75 65
3	P	232/226 (103%)	230 (99%)	2 (1%)	75 65

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

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	112	LEU
9	V	61	GLU
2	O	94	SER
9	V	37	PHE
10	W	50	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
5	R	94	ASN
13	Z	36	HIS
6	S	54	ASN
8	U	22	ASN
7	G	38	HIS

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	A	1	1	8,9,10	0.51	0	7,9,11	1.16	0
2	FME	O	1	2	8,9,10	0.86	1 (12%)	7,9,11	1.16	1 (14%)
1	FME	N	1	1	8,9,10	0.76	0	7,9,11	1.33	2 (28%)
2	FME	B	1	2	8,9,10	1.34	1 (12%)	7,9,11	1.36	2 (28%)

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

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

All (2) bond length outliers are listed below:

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

All (5) bond angle outliers are listed below:

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

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 8 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 137 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 127 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	EDO	S	103	-	3,3,3	0.21	0	2,2,2	0.13	0
14	HEA	N	602[B]	-	57,67,67	1.95	17 (29%)	61,103,103	2.42	21 (34%)
25	CHD	P	306	-	32,32,32	1.00	1 (3%)	51,51,51	1.04	1 (1%)
22	EDO	O	309	-	3,3,3	0.23	0	2,2,2	0.23	0
21	DMU	P	318	-	34,34,34	0.89	3 (8%)	45,45,45	1.16	3 (6%)
21	DMU	N	610	-	6,6,34	0.38	0	5,5,45	0.32	0
22	EDO	N	615	-	3,3,3	0.32	0	2,2,2	0.21	0
20	LFA	P	311	-	10,10,19	0.23	0	9,9,18	0.19	0
22	EDO	E	202	-	3,3,3	0.28	0	2,2,2	0.12	0
27	CDL	Y	101	-	93,93,99	0.48	0	99,105,111	0.72	4 (4%)
25	CHD	O	301	-	32,32,32	0.75	0	51,51,51	0.89	2 (3%)
20	LFA	C	314	-	12,12,19	0.27	0	11,11,18	0.22	0
21	DMU	O	307	-	10,10,34	0.45	0	9,9,45	0.52	0
20	LFA	B	307	-	16,16,19	0.39	0	15,15,18	0.19	0
25	CHD	C	301	-	32,32,32	0.91	3 (9%)	51,51,51	0.86	2 (3%)
22	EDO	E	203	-	3,3,3	0.19	0	2,2,2	0.05	0
22	EDO	F	103	-	3,3,3	0.31	0	2,2,2	0.39	0
22	EDO	A	612	-	3,3,3	0.36	0	2,2,2	0.28	0
22	EDO	F	102	-	3,3,3	0.34	0	2,2,2	0.41	0
20	LFA	P	314	-	12,12,19	0.31	0	11,11,18	0.36	0
20	LFA	P	308	-	10,10,19	0.31	0	9,9,18	0.28	0
21	DMU	D	201	-	34,34,34	1.35	6 (17%)	45,45,45	1.48	8 (17%)
20	LFA	C	309	-	17,17,19	0.23	0	16,16,18	0.13	0
20	LFA	C	312	-	10,10,19	0.32	0	9,9,18	0.30	0
14	HEA	A	601[B]	-	57,67,67	2.01	17 (29%)	61,103,103	2.46	26 (42%)
20	LFA	P	301	-	14,14,19	0.30	0	13,13,18	0.12	0
22	EDO	S	102	-	3,3,3	0.18	0	2,2,2	0.26	0
20	LFA	C	311	-	13,13,19	0.27	0	12,12,18	0.14	0
27	CDL	C	304	-	86,86,99	0.75	3 (3%)	92,98,111	1.36	11 (11%)
25	CHD	B	306	-	32,32,32	0.72	0	51,51,51	0.87	1 (1%)
27	CDL	L	101	-	93,93,99	0.53	0	99,105,111	0.99	8 (8%)
20	LFA	O	302	-	16,16,19	0.32	0	15,15,18	0.24	0
22	EDO	A	613	-	3,3,3	0.25	0	2,2,2	0.30	0
21	DMU	C	315	-	34,34,34	0.86	3 (8%)	45,45,45	1.64	9 (20%)
21	DMU	P	316	-	6,6,34	0.23	0	5,5,45	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	DMU	P	323	-	22,22,34	0.68	0	27,27,45	1.51	3 (11%)
21	DMU	P	324	-	34,34,34	0.73	0	45,45,45	1.51	6 (13%)
21	DMU	Z	103	-	7,7,34	0.33	0	6,6,45	0.45	0
22	EDO	T	104	-	3,3,3	0.37	0	2,2,2	0.07	0
22	EDO	N	614	-	3,3,3	0.36	0	2,2,2	0.15	0
21	DMU	A	611	-	34,34,34	1.30	6 (17%)	45,45,45	1.20	5 (11%)
22	EDO	N	613	-	3,3,3	0.16	0	2,2,2	0.39	0
21	DMU	C	318	-	34,34,34	0.95	3 (8%)	45,45,45	1.35	7 (15%)
21	DMU	O	306	-	10,10,34	0.18	0	9,9,45	0.61	0
21	DMU	A	617	-	10,10,34	0.31	0	9,9,45	0.55	0
22	EDO	A	615	-	3,3,3	0.35	0	2,2,2	0.39	0
18	PER	A	606	15,14	0,1,1	-	-	-		
22	EDO	P	321	-	3,3,3	0.25	0	2,2,2	0.14	0
25	CHD	P	302	-	32,32,32	0.94	2 (6%)	51,51,51	0.88	1 (1%)
21	DMU	U	101	-	34,34,34	0.86	1 (2%)	45,45,45	1.29	4 (8%)
22	EDO	C	321	-	3,3,3	0.28	0	2,2,2	0.05	0
21	DMU	P	317	-	22,22,34	0.78	1 (4%)	27,27,45	1.21	3 (11%)
20	LFA	P	313	-	14,14,19	0.40	0	13,13,18	0.21	0
21	DMU	W	101	-	10,10,34	0.31	0	9,9,45	0.57	0
21	DMU	C	319	-	34,34,34	0.95	3 (8%)	45,45,45	1.41	6 (13%)
20	LFA	C	310	-	10,10,19	0.17	0	9,9,18	0.17	0
21	DMU	C	324	-	34,34,34	0.82	0	45,45,45	1.17	2 (4%)
23	PGV	A	616	-	50,50,50	0.90	2 (4%)	53,56,56	1.12	2 (3%)
21	DMU	Q	201	-	34,34,34	1.51	8 (23%)	45,45,45	1.53	7 (15%)
19	N2O	N	608	-	0,2,2	-	-	0,1,1	-	-
21	DMU	N	611	-	34,34,34	1.50	6 (17%)	45,45,45	1.22	4 (8%)
21	DMU	P	319	-	34,34,34	1.08	3 (8%)	45,45,45	1.34	4 (8%)
20	LFA	P	312	-	10,10,19	0.23	0	9,9,18	0.33	0
27	CDL	V	101	-	63,63,99	0.65	0	69,75,111	1.29	5 (7%)
21	DMU	B	302	-	10,10,34	0.22	0	9,9,45	0.57	0
22	EDO	E	201	-	3,3,3	0.13	0	2,2,2	0.10	0
14	HEA	N	603	18,1	57,67,67	2.03	18 (31%)	61,103,103	2.49	22 (36%)
21	DMU	C	317	-	22,22,34	0.64	0	27,27,45	1.46	4 (14%)
21	DMU	Z	102	-	22,22,34	0.73	0	27,27,45	1.11	2 (7%)
24	CUA	B	301	2	0,1,1	-	-	-		
27	CDL	I	101	-	63,63,99	0.65	0	69,75,111	1.18	5 (7%)
21	DMU	N	601	-	10,10,34	0.27	0	9,9,45	0.55	0
20	LFA	O	303	-	10,10,19	0.28	0	9,9,18	0.17	0
20	LFA	C	308	-	5,5,19	0.18	0	4,4,18	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	PGV	N	617	-	50,50,50	0.82	3 (6%)	53,56,56	1.43	4 (7%)
21	DMU	P	315	-	34,34,34	0.85	1 (2%)	45,45,45	1.33	3 (6%)
22	EDO	N	616	-	3,3,3	0.50	0	2,2,2	0.24	0
22	EDO	B	305	-	3,3,3	0.20	0	2,2,2	0.21	0
22	EDO	A	614	-	3,3,3	0.54	0	2,2,2	0.38	0
29	PEK	T	101	-	52,52,52	0.66	2 (3%)	55,57,57	1.00	3 (5%)
21	DMU	C	306	-	10,10,34	0.44	0	9,9,45	0.60	0
21	DMU	J	101	-	10,10,34	0.21	0	9,9,45	0.71	0
22	EDO	C	320	-	3,3,3	0.16	0	2,2,2	0.26	0
21	DMU	O	308	-	22,22,34	0.74	1 (4%)	27,27,45	1.12	3 (11%)
20	LFA	A	608	-	13,13,19	0.45	0	12,12,18	0.22	0
14	HEA	A	602	18,1	57,67,67	1.79	13 (22%)	61,103,103	2.16	20 (32%)
23	PGV	C	303	-	50,50,50	0.77	0	53,56,56	1.06	3 (5%)
21	DMU	L	102	-	22,22,34	0.77	0	27,27,45	1.25	2 (7%)
14	HEA	N	602[A]	-	57,67,67	1.93	17 (29%)	61,103,103	2.48	21 (34%)
20	LFA	P	310	-	17,17,19	0.26	0	16,16,18	0.19	0
22	EDO	R	203	-	3,3,3	0.56	0	2,2,2	0.40	0
22	EDO	R	201	-	3,3,3	0.17	0	2,2,2	0.14	0
21	DMU	P	307	-	10,10,34	0.25	0	9,9,45	0.66	0
22	EDO	P	320	-	3,3,3	0.18	0	2,2,2	0.10	0
18	PER	N	607	15,14	0,1,1	-	-	-		
27	CDL	P	305	-	86,86,99	0.73	2 (2%)	92,98,111	1.00	6 (6%)
20	LFA	P	309	-	5,5,19	0.29	0	4,4,18	0.09	0
21	DMU	B	303	-	10,10,34	0.32	0	9,9,45	0.56	0
21	DMU	O	304	-	22,22,34	0.98	1 (4%)	27,27,45	1.30	4 (14%)
21	DMU	A	610	-	6,6,34	0.55	0	5,5,45	0.30	0
20	LFA	G	103	-	13,13,19	0.64	0	12,12,18	0.44	0
20	LFA	T	103	-	10,10,19	0.22	0	9,9,18	0.19	0
21	DMU	C	323	-	22,22,34	0.62	0	27,27,45	1.03	1 (3%)
21	DMU	B	304	-	22,22,34	0.89	1 (4%)	27,27,45	1.06	2 (7%)
20	LFA	T	102	-	13,13,19	0.22	0	12,12,18	0.21	0
21	DMU	C	316	-	6,6,34	0.25	0	5,5,45	0.62	0
19	N2O	A	607	-	0,2,2	-	-	0,1,1	-	-
20	LFA	C	313	-	14,14,19	0.42	0	13,13,18	0.48	0
21	DMU	M	101	-	34,34,34	1.07	2 (5%)	45,45,45	1.00	4 (8%)
22	EDO	P	322	-	3,3,3	0.66	0	2,2,2	1.20	0
20	LFA	N	609	-	13,13,19	0.33	0	12,12,18	0.38	0
21	DMU	B	308	-	22,22,34	0.59	0	27,27,45	1.34	2 (7%)
24	CUA	O	305	2	0,1,1	-	-	-		
22	EDO	C	322	-	3,3,3	0.74	0	2,2,2	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	DMU	Z	101	-	34,34,34	1.02	3 (8%)	45,45,45	1.06	6 (13%)
23	PGV	P	304	-	50,50,50	0.99	4 (8%)	53,56,56	1.03	3 (5%)
20	LFA	A	609	-	13,13,19	0.62	0	12,12,18	0.32	0
21	DMU	M	102	-	7,7,34	0.21	0	6,6,45	0.67	0
22	EDO	R	202	-	3,3,3	0.12	0	2,2,2	0.23	0
22	EDO	N	612	-	3,3,3	0.39	0	2,2,2	0.19	0
20	LFA	C	325	-	14,14,19	0.19	0	13,13,18	0.14	0
29	PEK	G	101	-	52,52,52	0.70	1 (1%)	55,57,57	0.72	2 (3%)
14	HEA	A	601[A]	-	57,67,67	2.02	17 (29%)	61,103,103	2.48	24 (39%)
25	CHD	C	305	-	32,32,32	0.78	0	51,51,51	1.58	9 (17%)
21	DMU	H	101	-	34,34,34	0.95	2 (5%)	45,45,45	1.10	4 (8%)
22	EDO	G	102	-	3,3,3	0.24	0	2,2,2	0.17	0
20	LFA	C	307	-	10,10,19	0.22	0	9,9,18	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	S	103	-	-	0/1/1/1	-
14	HEA	N	602[B]	-	-	4/32/76/76	-
25	CHD	P	306	-	-	5/9/74/74	0/4/4/4
22	EDO	O	309	-	-	0/1/1/1	-
21	DMU	P	318	-	-	15/19/59/59	0/2/2/2
21	DMU	N	610	-	-	4/4/4/59	-
22	EDO	N	615	-	-	0/1/1/1	-
20	LFA	P	311	-	-	5/8/8/17	-
22	EDO	E	202	-	-	0/1/1/1	-
27	CDL	Y	101	-	-	55/104/104/110	-
25	CHD	O	301	-	-	2/9/74/74	0/4/4/4
20	LFA	C	314	-	-	3/10/10/17	-
21	DMU	O	307	-	-	3/8/8/59	-
20	LFA	B	307	-	-	10/14/14/17	-
25	CHD	C	301	-	-	2/9/74/74	0/4/4/4
22	EDO	E	203	-	-	0/1/1/1	-
22	EDO	F	103	-	-	1/1/1/1	-
22	EDO	A	612	-	-	0/1/1/1	-
22	EDO	F	102	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LFA	P	314	-	-	2/10/10/17	-
20	LFA	P	308	-	-	6/8/8/17	-
21	DMU	D	201	-	-	9/19/59/59	0/2/2/2
20	LFA	C	309	-	-	8/15/15/17	-
14	HEA	A	601[B]	-	-	4/32/76/76	-
20	LFA	P	301	-	-	7/12/12/17	-
20	LFA	C	312	-	-	4/8/8/17	-
22	EDO	S	102	-	-	0/1/1/1	-
20	LFA	C	311	-	-	6/11/11/17	-
27	CDL	C	304	-	-	44/97/97/110	-
25	CHD	B	306	-	-	2/9/74/74	0/4/4/4
27	CDL	L	101	-	-	51/104/104/110	-
20	LFA	O	302	-	-	9/14/14/17	-
22	EDO	A	613	-	-	0/1/1/1	-
21	DMU	C	315	-	-	10/19/59/59	0/2/2/2
21	DMU	P	316	-	-	3/4/4/59	-
21	DMU	P	323	-	-	8/13/33/59	0/1/1/2
21	DMU	P	324	-	-	5/19/59/59	0/2/2/2
21	DMU	Z	103	-	-	3/5/5/59	-
22	EDO	T	104	-	-	0/1/1/1	-
22	EDO	N	614	-	-	0/1/1/1	-
21	DMU	A	611	-	-	7/19/59/59	0/2/2/2
22	EDO	N	613	-	-	0/1/1/1	-
21	DMU	C	318	-	-	15/19/59/59	0/2/2/2
21	DMU	A	617	-	-	5/8/8/59	-
21	DMU	O	306	-	-	5/8/8/59	-
22	EDO	A	615	-	-	1/1/1/1	-
22	EDO	P	321	-	-	0/1/1/1	-
25	CHD	P	302	-	-	2/9/74/74	0/4/4/4
21	DMU	U	101	-	-	5/19/59/59	0/2/2/2
22	EDO	C	321	-	-	0/1/1/1	-
21	DMU	P	317	-	-	7/13/33/59	0/1/1/2
21	DMU	W	101	-	-	5/8/8/59	-
20	LFA	P	313	-	-	6/12/12/17	-
21	DMU	C	319	-	-	10/19/59/59	0/2/2/2
20	LFA	C	310	-	-	7/8/8/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	DMU	C	324	-	-	5/19/59/59	0/2/2/2
23	PGV	A	616	-	-	8/55/55/55	-
21	DMU	Q	201	-	-	7/19/59/59	0/2/2/2
21	DMU	N	611	-	-	5/19/59/59	0/2/2/2
21	DMU	P	319	-	-	10/19/59/59	0/2/2/2
20	LFA	P	312	-	-	5/8/8/17	-
27	CDL	V	101	-	-	37/74/74/110	-
21	DMU	B	302	-	-	5/8/8/59	-
22	EDO	E	201	-	-	0/1/1/1	-
14	HEA	N	603	18,1	-	4/32/76/76	-
21	DMU	C	317	-	-	6/13/33/59	0/1/1/2
21	DMU	Z	102	-	-	10/13/33/59	0/1/1/2
27	CDL	I	101	-	-	37/74/74/110	-
21	DMU	N	601	-	-	5/8/8/59	-
20	LFA	O	303	-	-	2/8/8/17	-
20	LFA	C	308	-	-	1/3/3/17	-
23	PGV	N	617	-	-	4/55/55/55	-
21	DMU	P	315	-	-	9/19/59/59	0/2/2/2
22	EDO	N	616	-	-	0/1/1/1	-
22	EDO	B	305	-	-	0/1/1/1	-
22	EDO	A	614	-	-	0/1/1/1	-
29	PEK	T	101	-	-	17/56/56/56	-
21	DMU	C	306	-	-	3/8/8/59	-
21	DMU	J	101	-	-	5/8/8/59	-
22	EDO	C	320	-	-	1/1/1/1	-
21	DMU	O	308	-	-	2/13/33/59	0/1/1/2
20	LFA	A	608	-	-	4/11/11/17	-
14	HEA	A	602	18,1	-	4/32/76/76	-
23	PGV	C	303	-	-	12/55/55/55	-
21	DMU	L	102	-	-	10/13/33/59	0/1/1/2
14	HEA	N	602[A]	-	-	7/32/76/76	-
20	LFA	P	310	-	-	10/15/15/17	-
22	EDO	R	203	-	-	1/1/1/1	-
22	EDO	R	201	-	-	1/1/1/1	-
21	DMU	P	307	-	-	1/8/8/59	-
22	EDO	P	320	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CDL	P	305	-	-	51/97/97/110	-
20	LFA	P	309	-	-	0/3/3/17	-
21	DMU	B	303	-	-	6/8/8/59	-
21	DMU	O	304	-	-	7/13/33/59	0/1/1/2
21	DMU	A	610	-	-	3/4/4/59	-
20	LFA	G	103	-	-	7/11/11/17	-
20	LFA	T	103	-	-	3/8/8/17	-
21	DMU	C	323	-	-	8/13/33/59	0/1/1/2
21	DMU	B	304	-	-	6/13/33/59	0/1/1/2
20	LFA	T	102	-	-	5/11/11/17	-
21	DMU	C	316	-	-	3/4/4/59	-
20	LFA	C	313	-	-	1/12/12/17	-
21	DMU	M	101	-	-	4/19/59/59	0/2/2/2
22	EDO	P	322	-	-	0/1/1/1	-
20	LFA	N	609	-	-	2/11/11/17	-
21	DMU	B	308	-	-	9/13/33/59	0/1/1/2
22	EDO	C	322	-	-	0/1/1/1	-
21	DMU	Z	101	-	-	7/19/59/59	0/2/2/2
23	PGV	P	304	-	-	11/55/55/55	-
20	LFA	A	609	-	-	5/11/11/17	-
21	DMU	M	102	-	-	3/5/5/59	-
22	EDO	R	202	-	-	0/1/1/1	-
22	EDO	N	612	-	-	0/1/1/1	-
20	LFA	C	325	-	-	8/12/12/17	-
29	PEK	G	101	-	-	13/56/56/56	-
14	HEA	A	601[A]	-	-	5/32/76/76	-
25	CHD	C	305	-	-	7/9/74/74	0/4/4/4
21	DMU	H	101	-	-	3/19/59/59	0/2/2/2
22	EDO	G	102	-	-	0/1/1/1	-
20	LFA	C	307	-	-	6/8/8/17	-

The worst 5 of 176 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[A]	HEA	C1D-ND	-5.79	1.30	1.40
14	A	601[B]	HEA	C1D-ND	-5.79	1.30	1.40
14	N	603	HEA	C1D-ND	-5.25	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	611	DMU	O16-C6	-5.20	1.31	1.40
14	A	601[A]	HEA	C3A-C2A	4.87	1.47	1.40

The worst 5 of 314 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	603	HEA	C3D-C4D-ND	7.36	117.49	110.36
14	N	602[A]	HEA	C3D-C4D-ND	7.01	117.15	110.36
14	N	602[B]	HEA	C3D-C4D-ND	7.01	117.15	110.36
27	C	304	CDL	OA6-CA5-C11	-6.58	97.31	111.50
14	N	602[A]	HEA	C2B-C1B-NB	6.32	117.45	109.88

There are no chirality outliers.

5 of 787 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C18-C19-C20-C21
14	A	601[A]	HEA	C27-C19-C20-C21
21	B	304	DMU	C1-C6-O16-C18
21	B	304	DMU	O5-C6-O16-C18
21	B	308	DMU	O5-C6-O16-C18

There are no ring outliers.

46 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	602[B]	HEA	1	0
25	P	306	CHD	4	0
27	Y	101	CDL	8	0
25	O	301	CHD	1	0
20	B	307	LFA	2	0
20	P	314	LFA	1	0
20	P	308	LFA	2	0
21	D	201	DMU	3	0
20	C	309	LFA	1	0
20	C	312	LFA	2	0
14	A	601[B]	HEA	1	0
27	C	304	CDL	15	0
27	L	101	CDL	6	0
20	O	302	LFA	2	0
22	A	613	EDO	1	0

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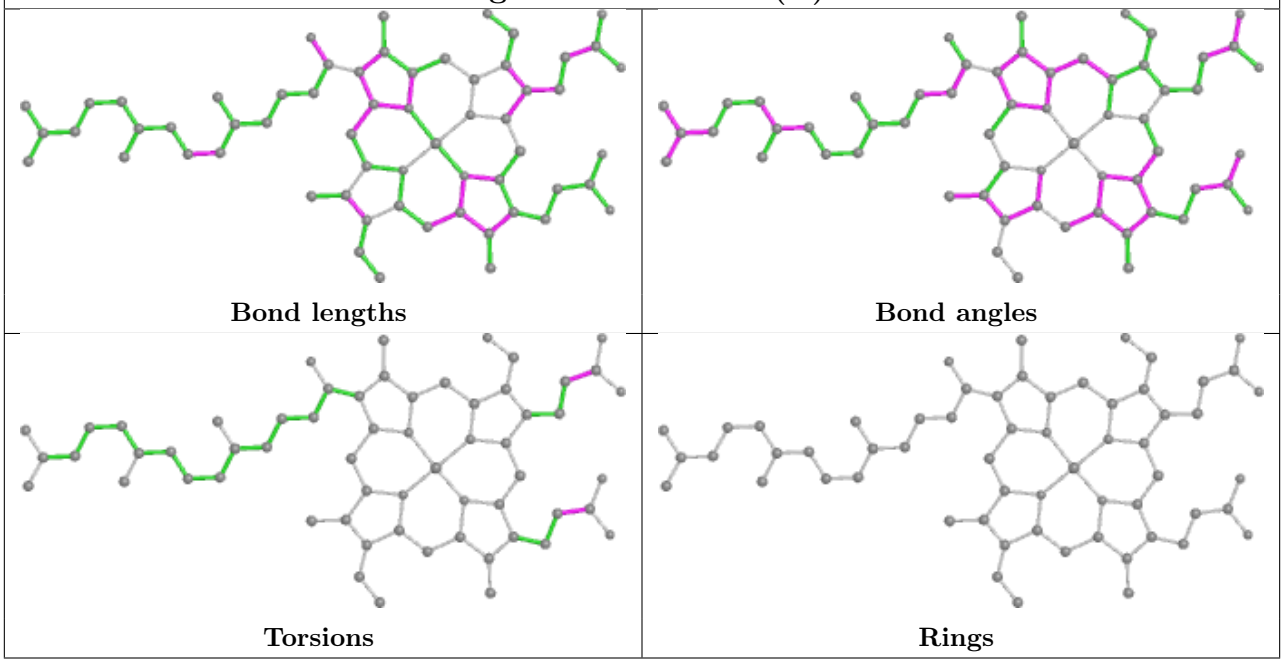
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	P	324	DMU	2	0
21	A	611	DMU	1	0
18	A	606	PER	1	0
21	U	101	DMU	1	0
20	P	313	LFA	2	0
21	C	324	DMU	6	0
21	Q	201	DMU	1	0
20	P	312	LFA	1	0
27	V	101	CDL	2	0
14	N	603	HEA	2	0
21	Z	102	DMU	3	0
20	O	303	LFA	3	0
22	N	616	EDO	1	0
29	T	101	PEK	3	0
21	O	308	DMU	1	0
20	A	608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

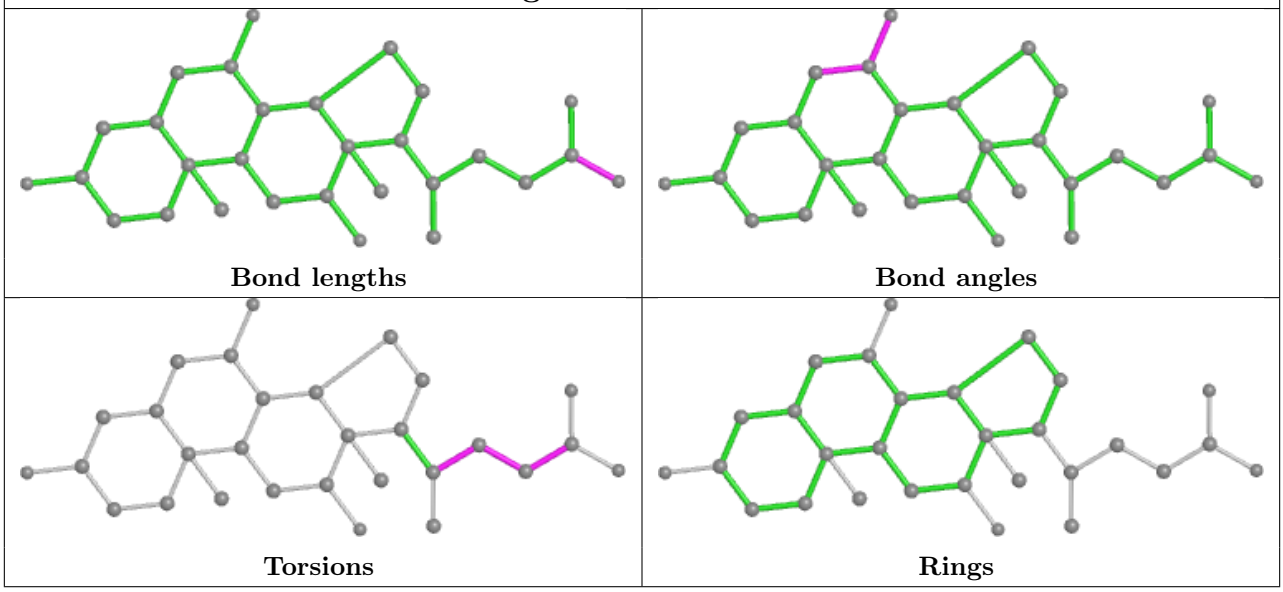
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

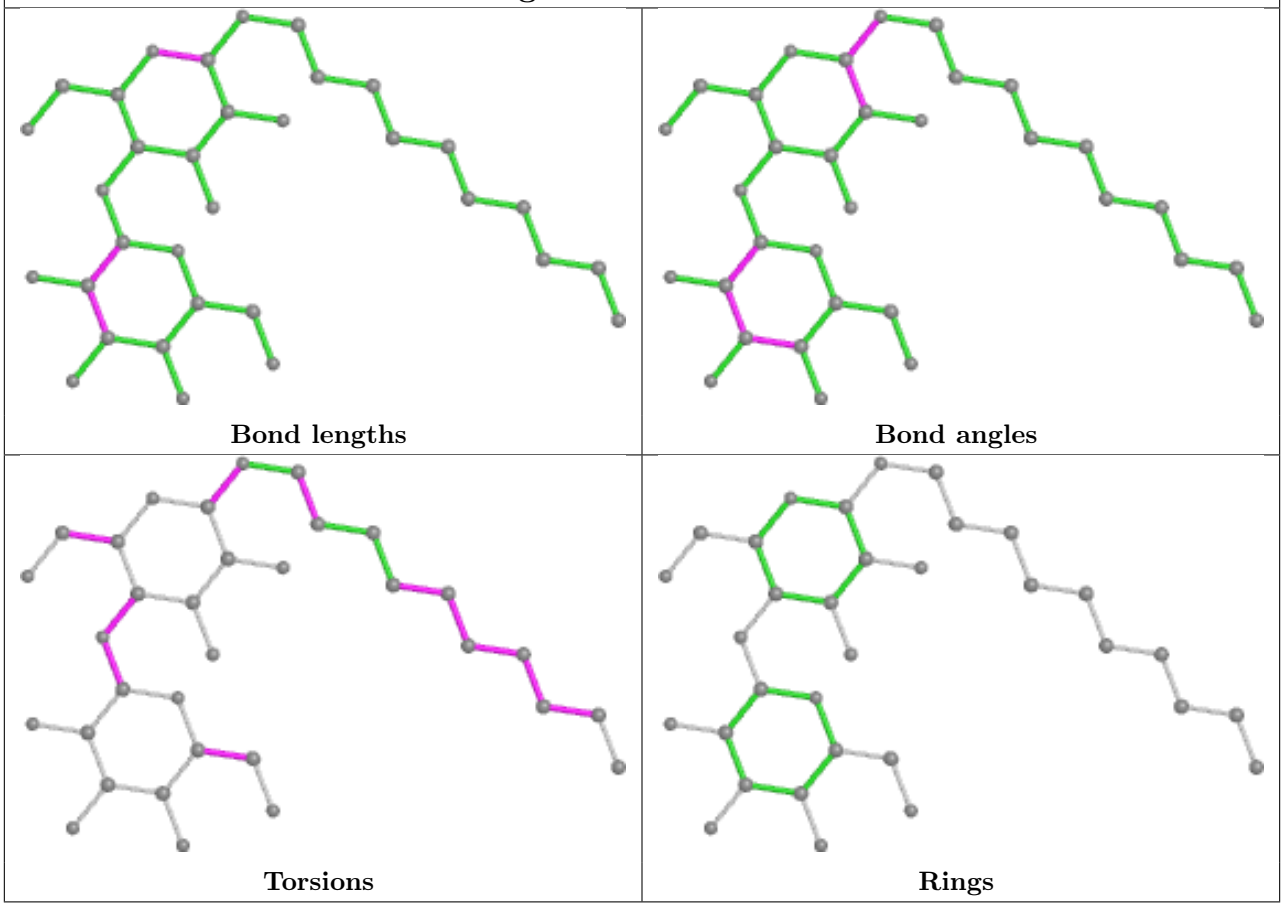
Ligand HEA N 602 (B)



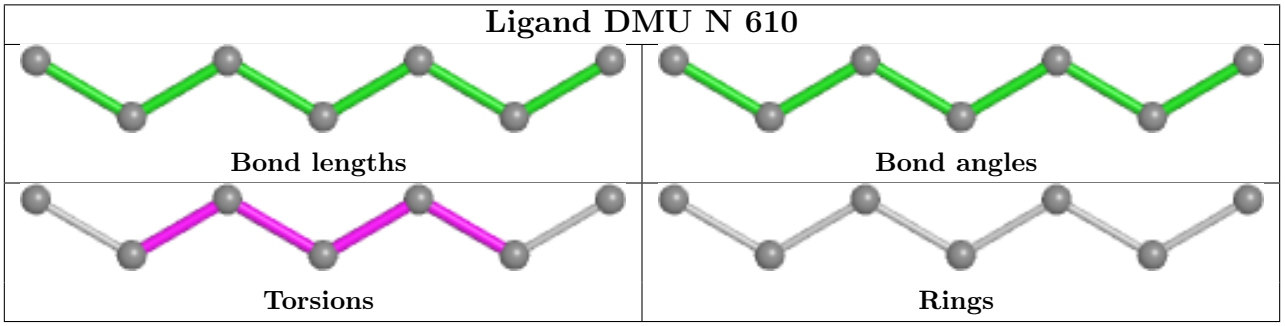
Ligand CHD P 306



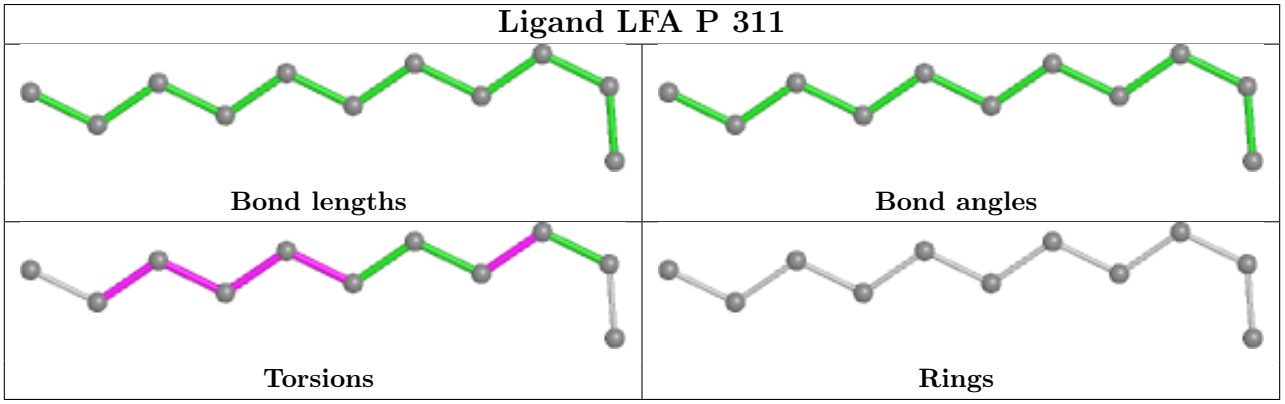
Ligand DMU P 318



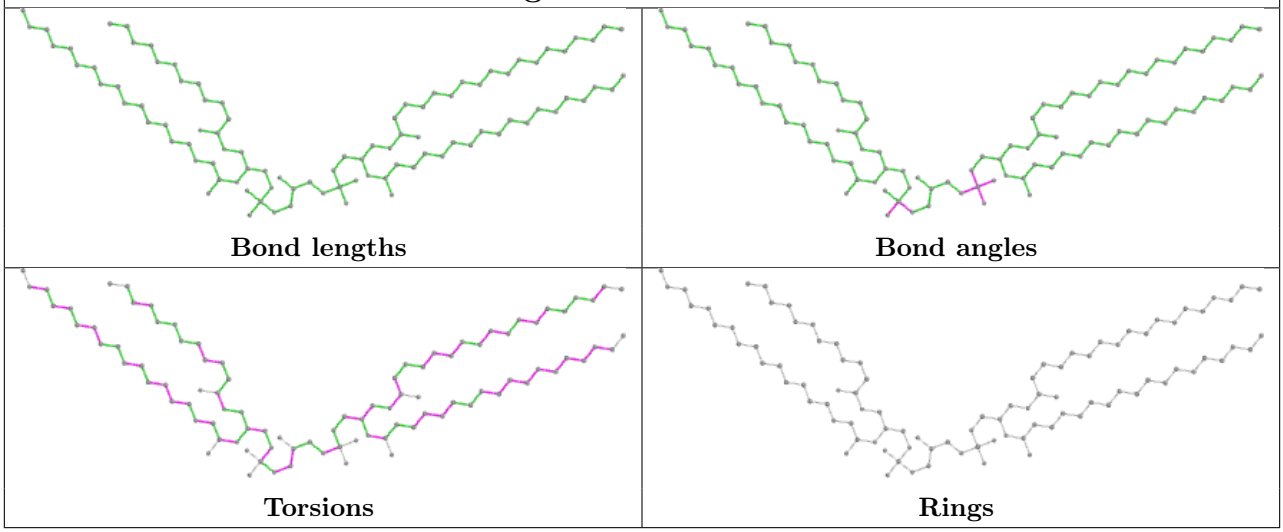
Ligand DMU N 610



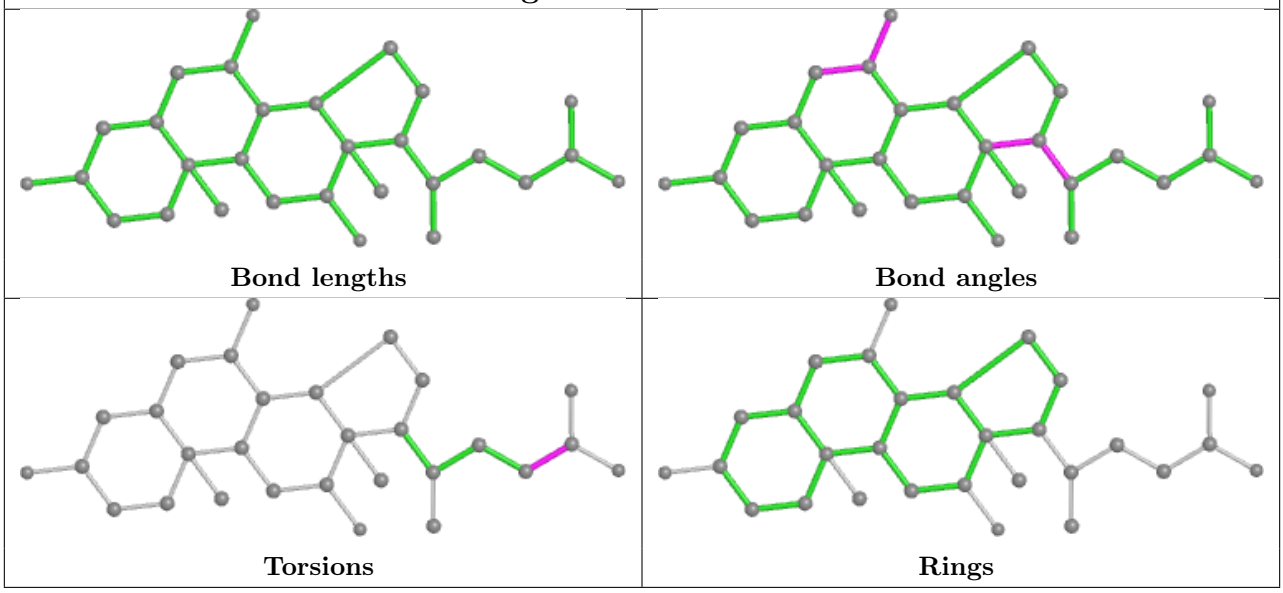
Ligand LFA P 311



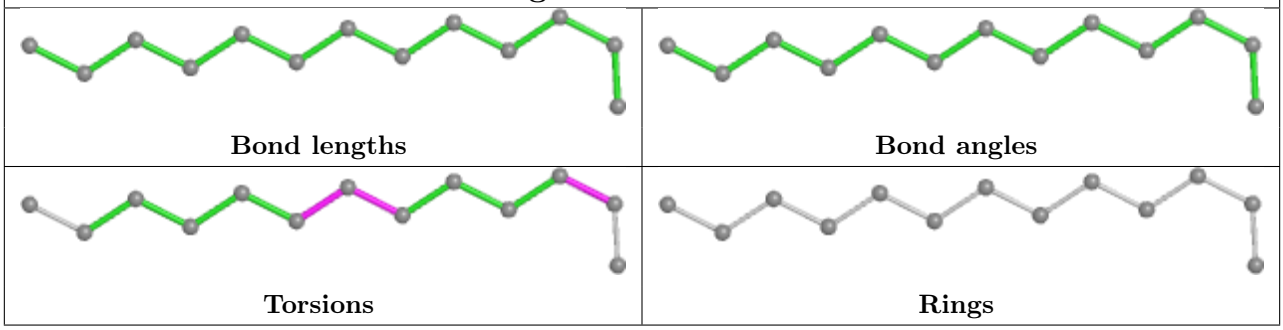
Ligand CDL Y 101



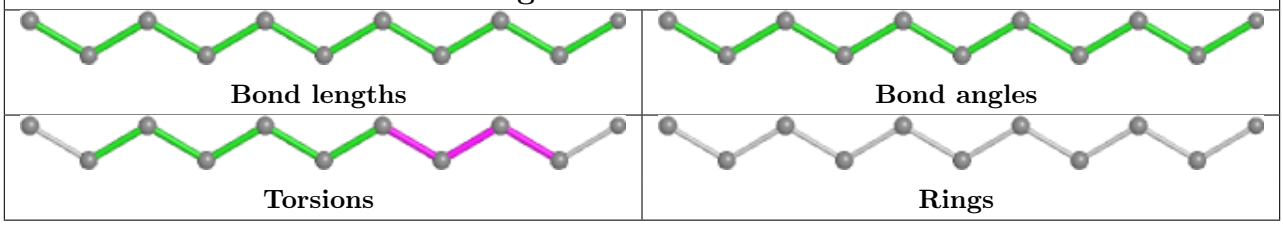
Ligand CHD O 301



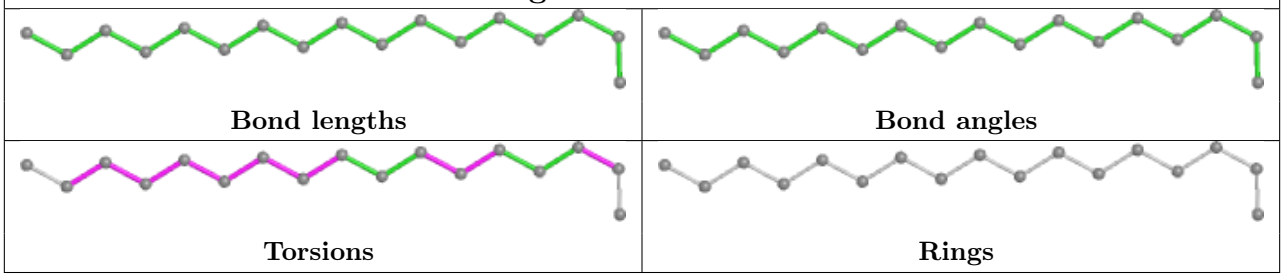
Ligand LFA C 314



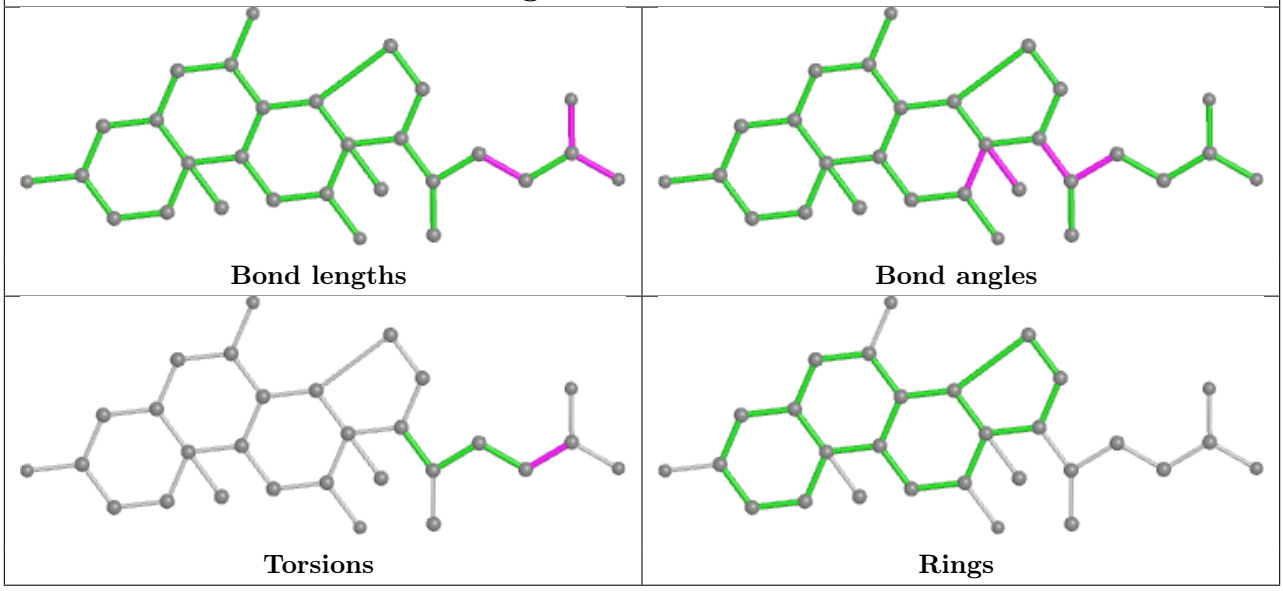
Ligand DMU O 307



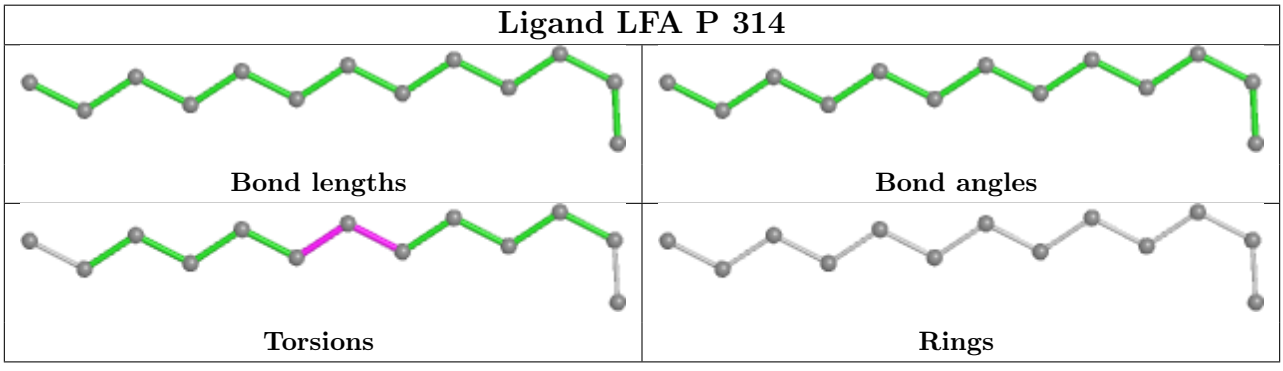
Ligand LFA B 307



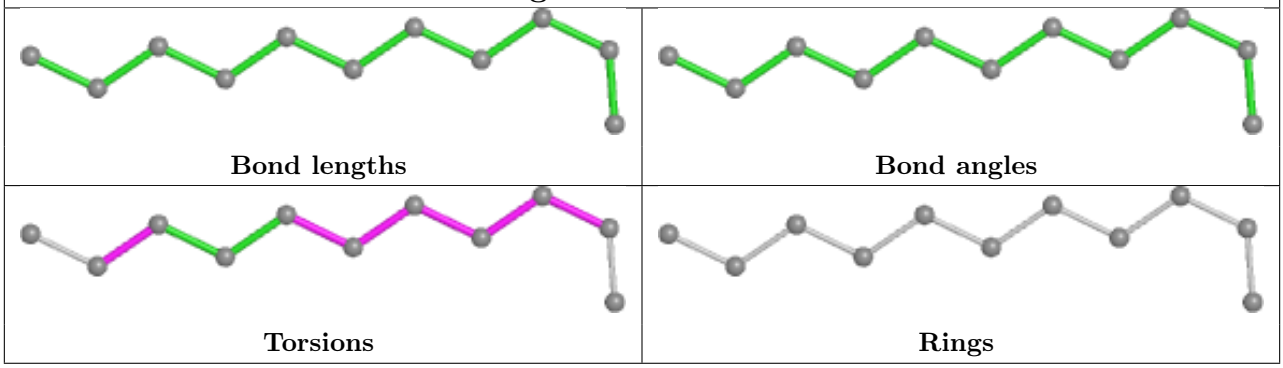
Ligand CHD C 301



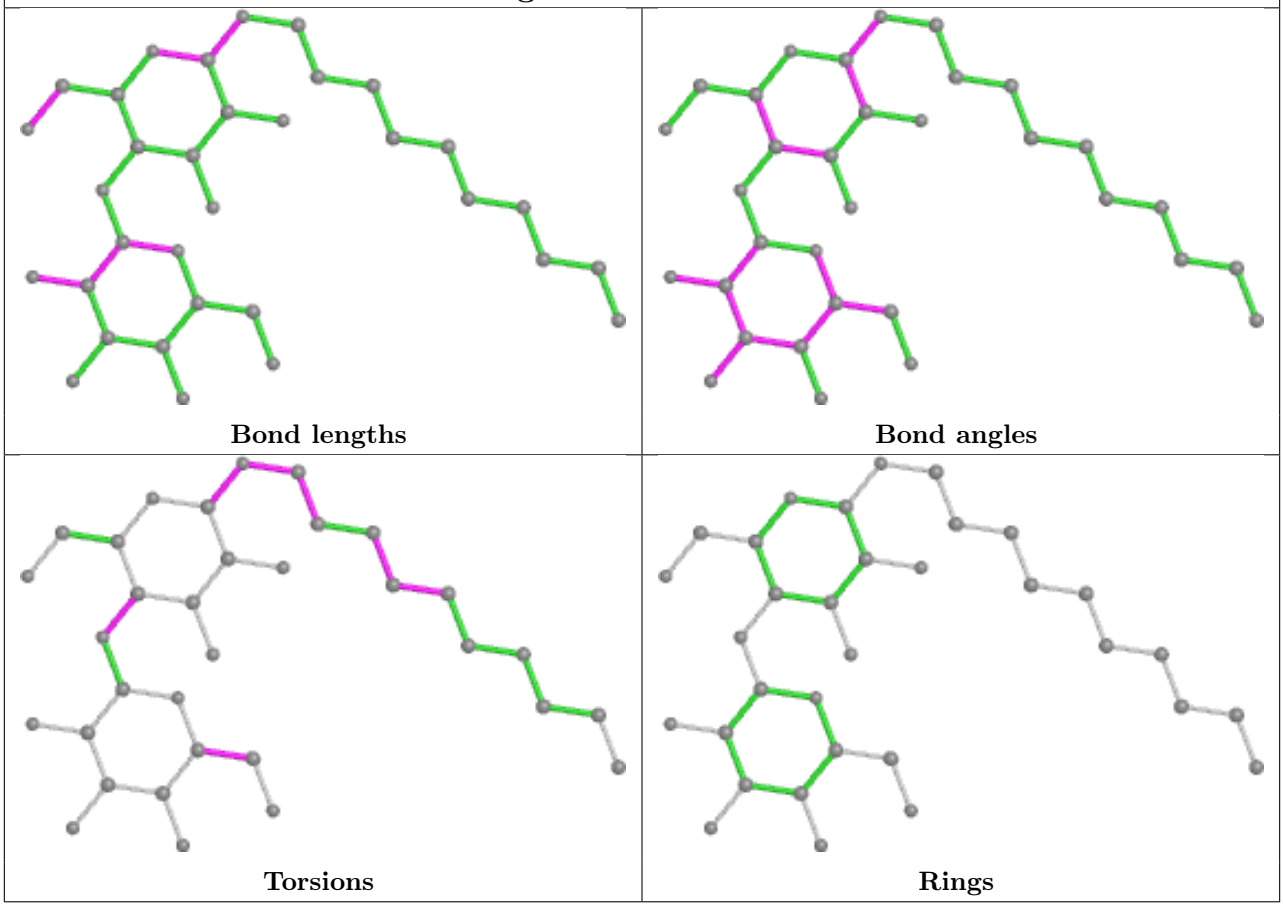
Ligand LFA P 314



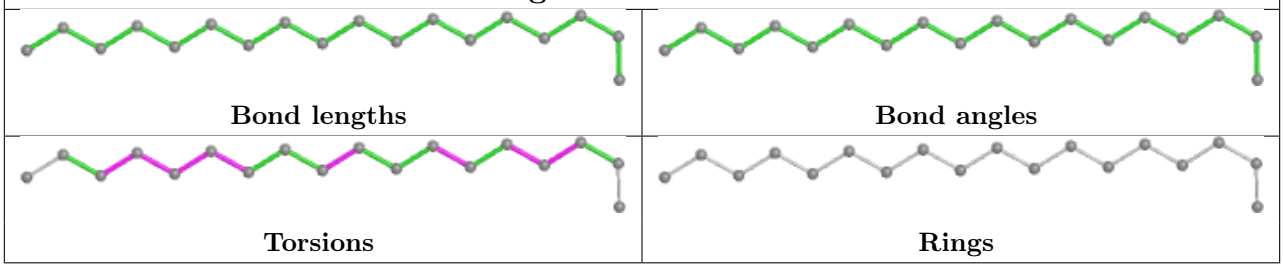
Ligand LFA P 308



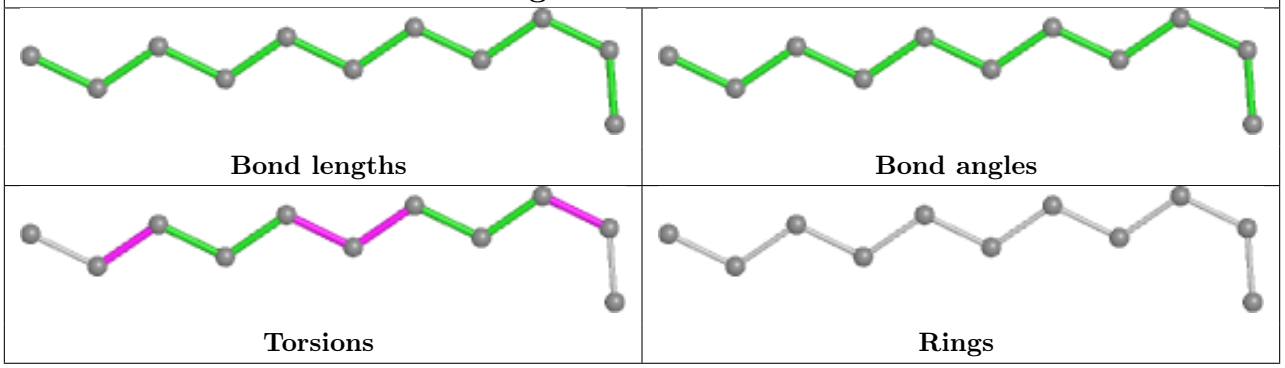
Ligand DMU D 201



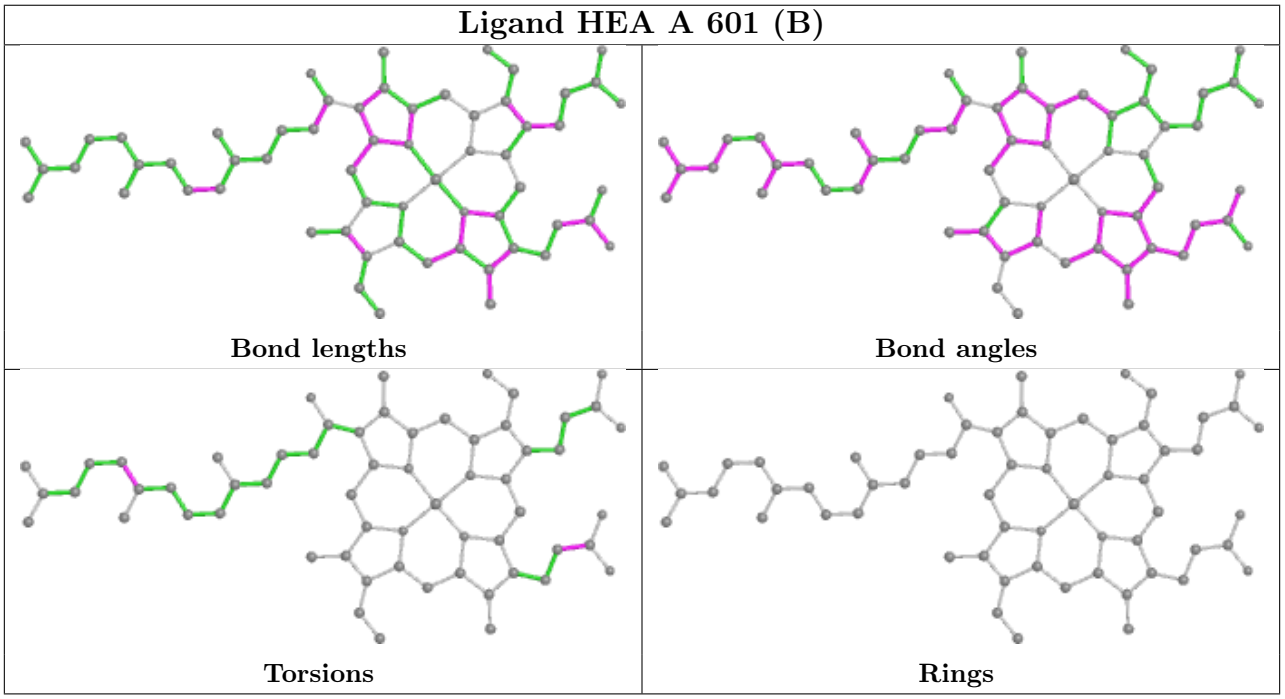
Ligand LFA C 309



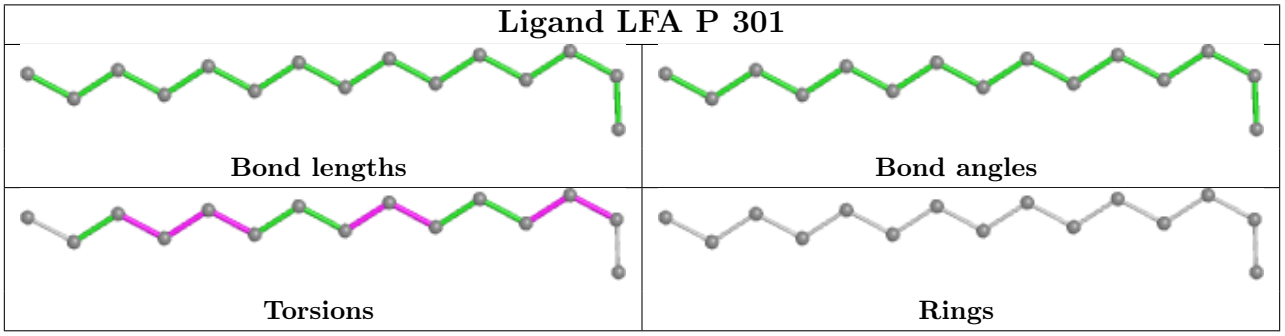
Ligand LFA C 312



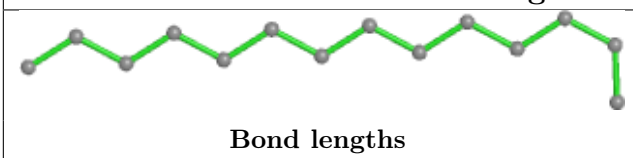
Ligand HEA A 601 (B)



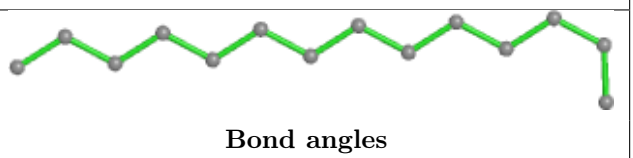
Ligand LFA P 301



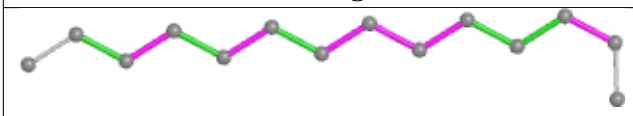
Ligand LFA C 311



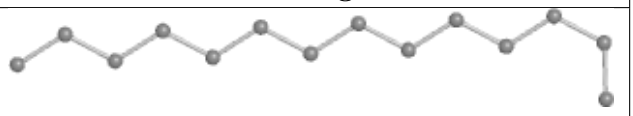
Bond lengths



Bond angles

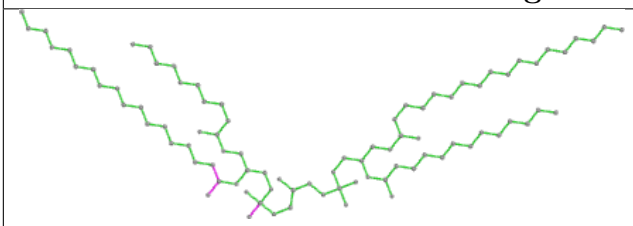


Torsions

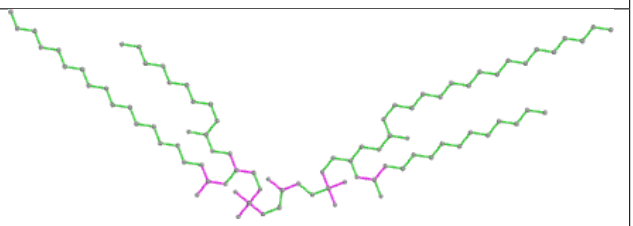


Rings

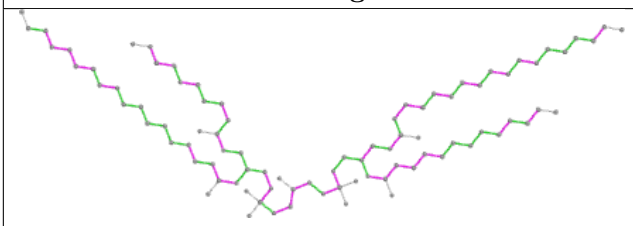
Ligand CDL C 304



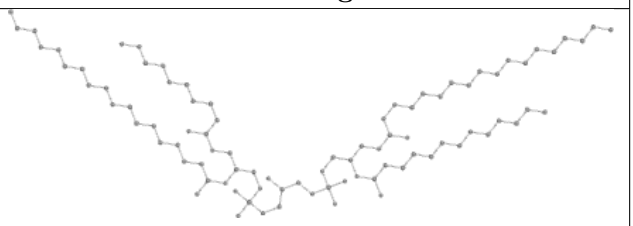
Bond lengths



Bond angles

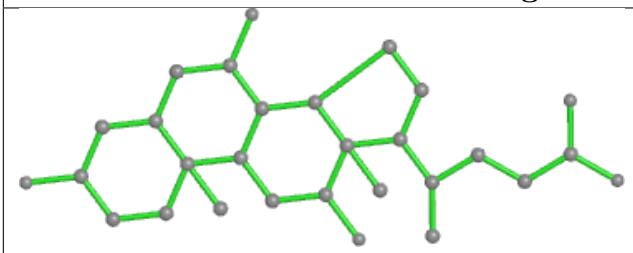


Torsions

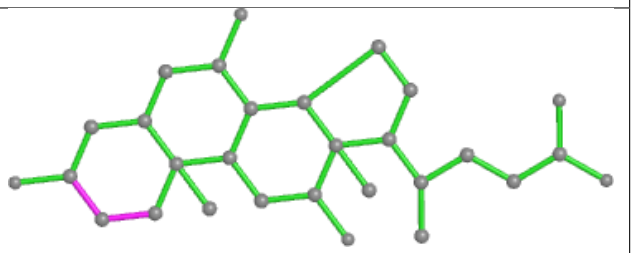


Rings

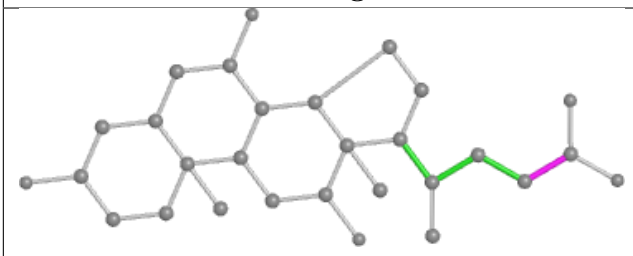
Ligand CHD B 306



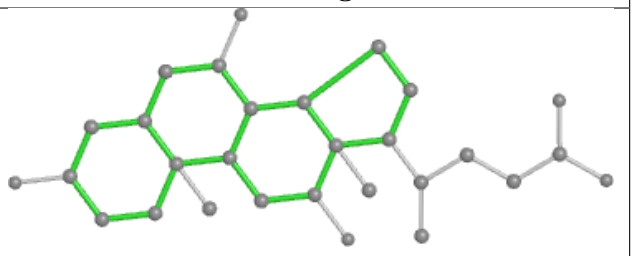
Bond lengths



Bond angles

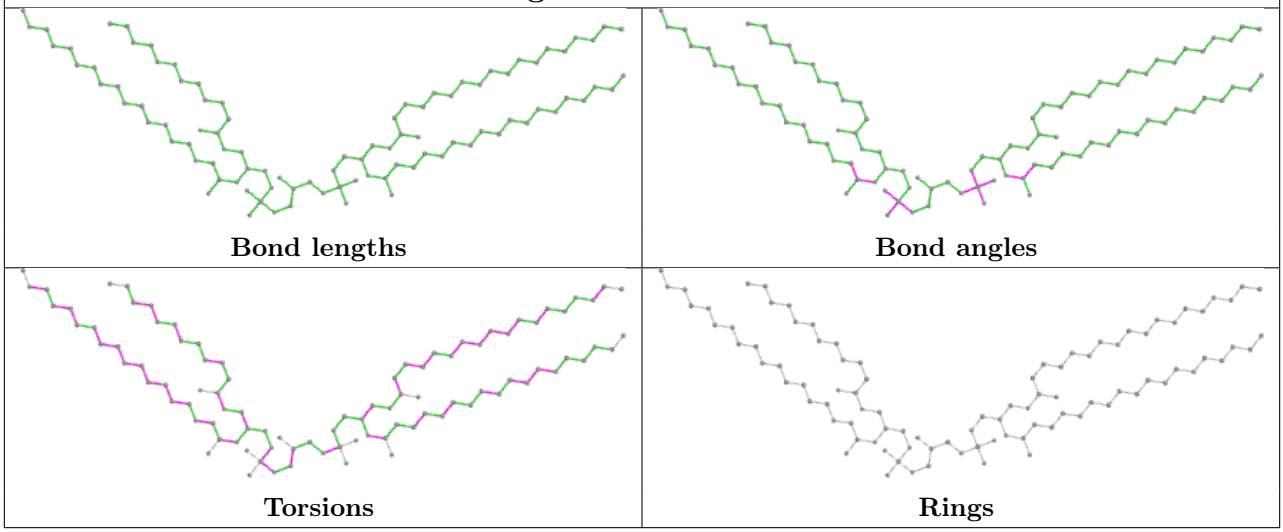


Torsions

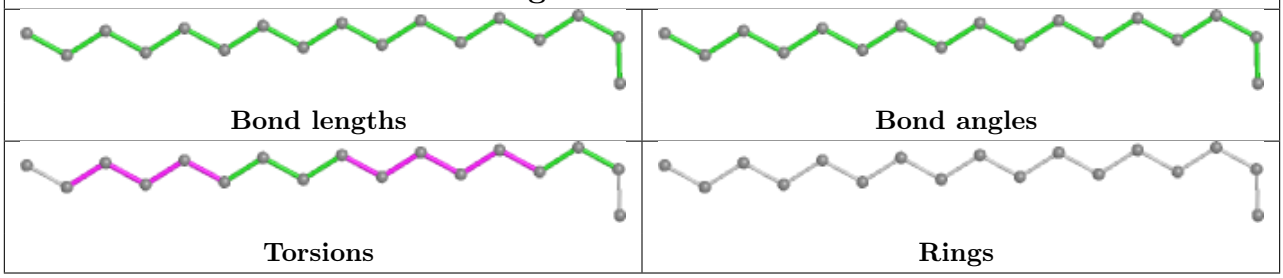


Rings

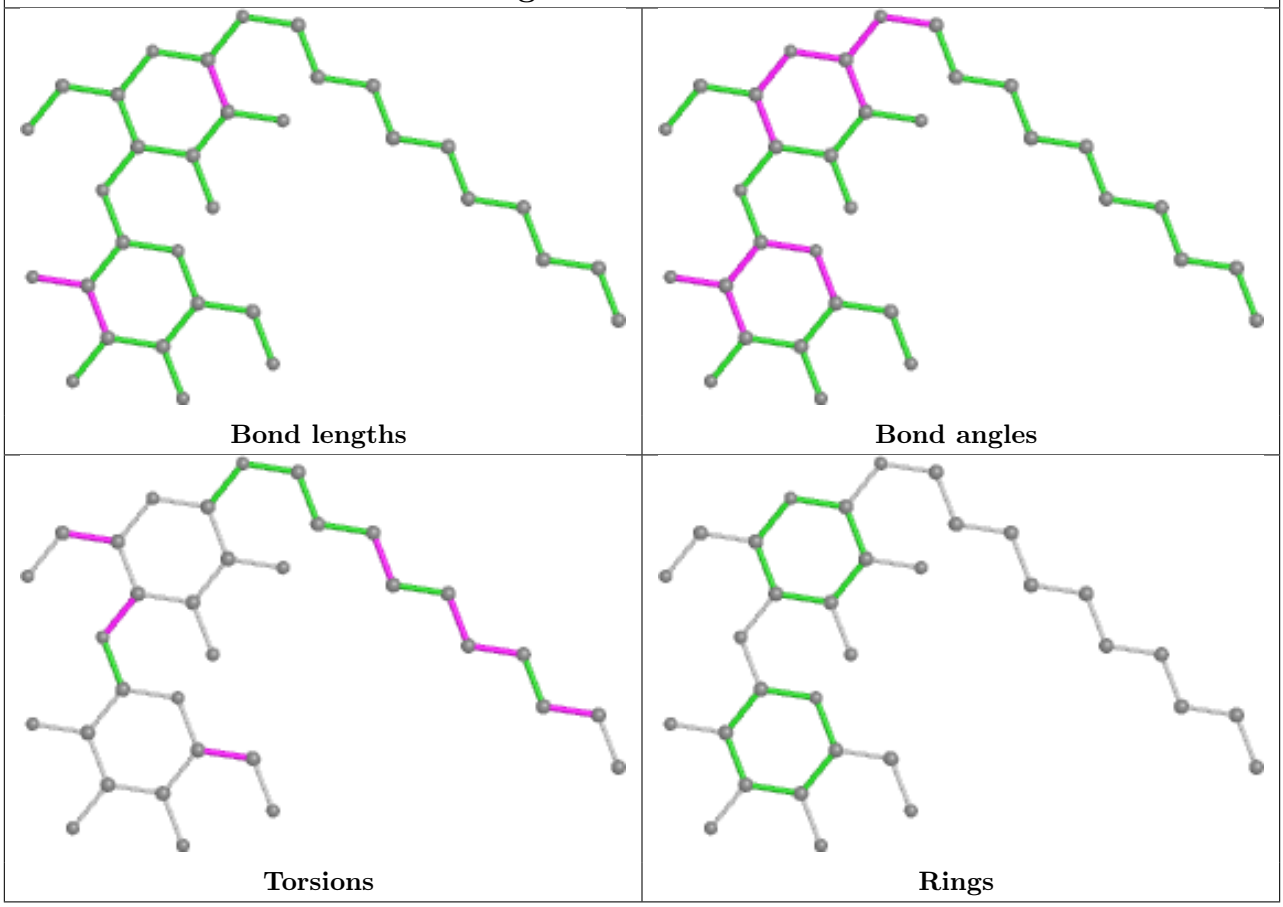
Ligand CDL L 101



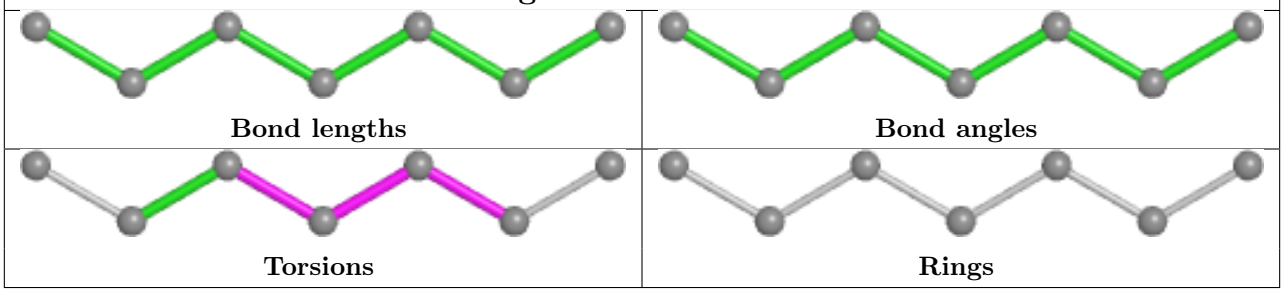
Ligand LFA O 302



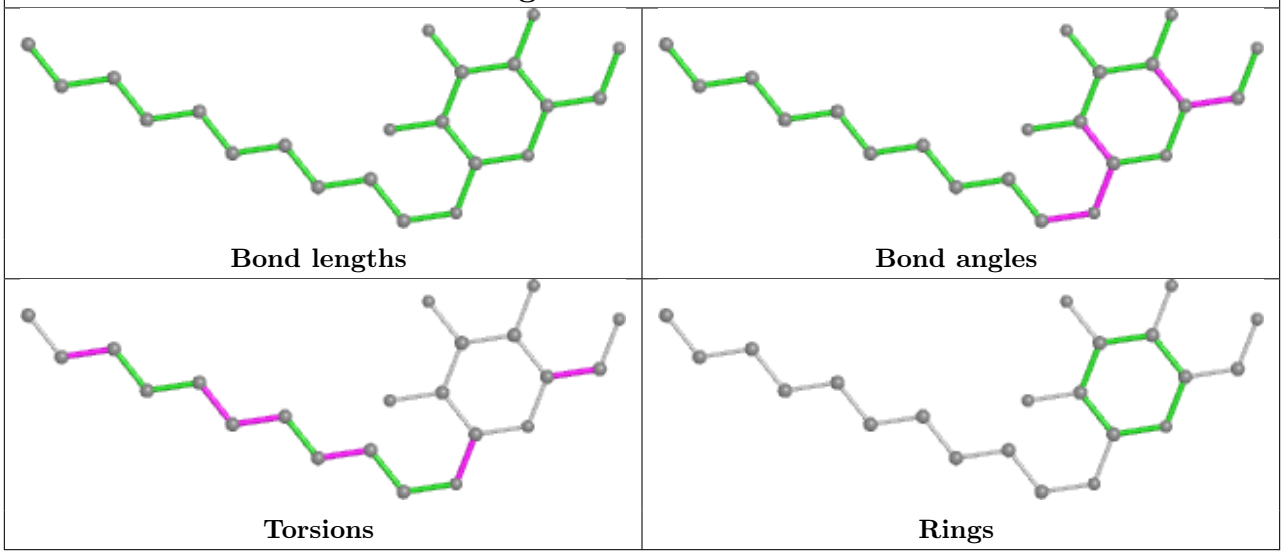
Ligand DMU C 315



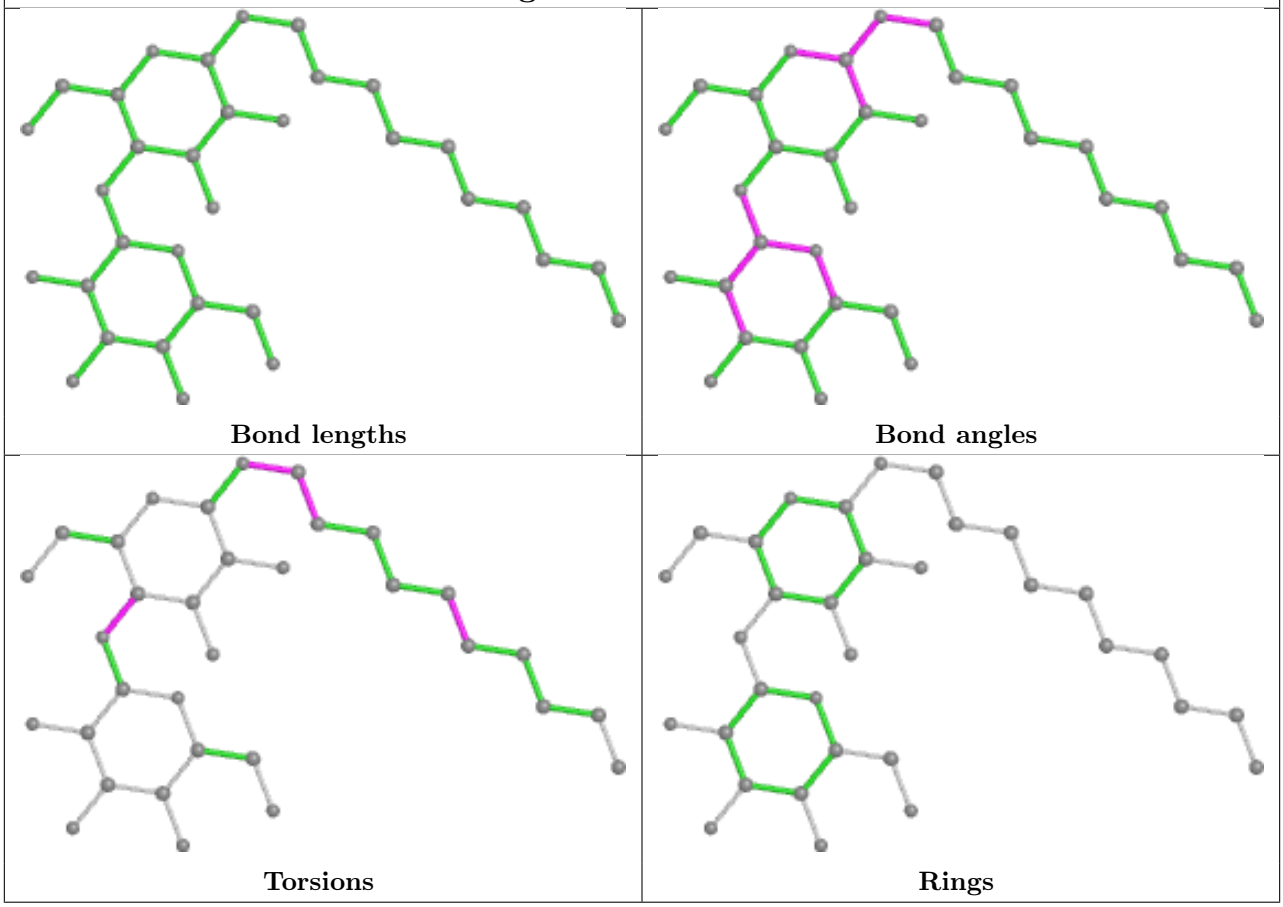
Ligand DMU P 316



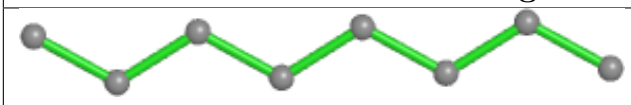
Ligand DMU P 323



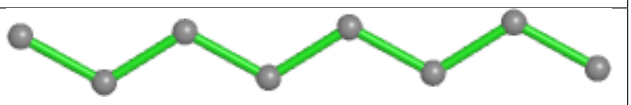
Ligand DMU P 324



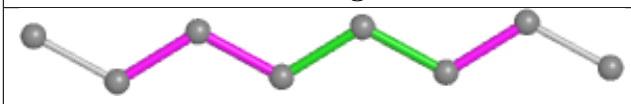
Ligand DMU Z 103



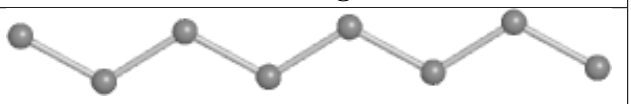
Bond lengths



Bond angles

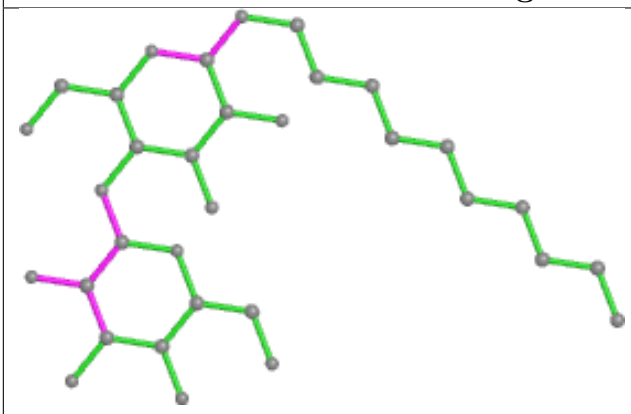


Torsions

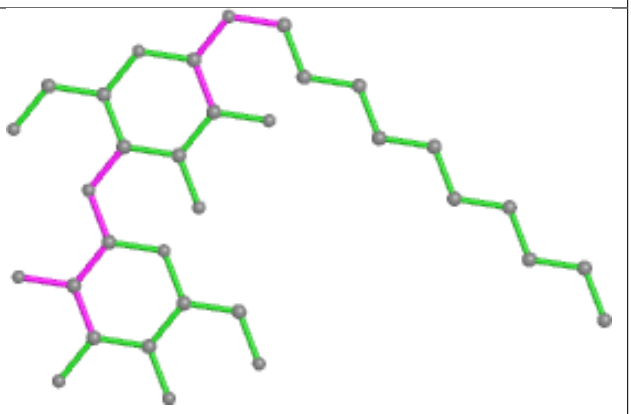


Rings

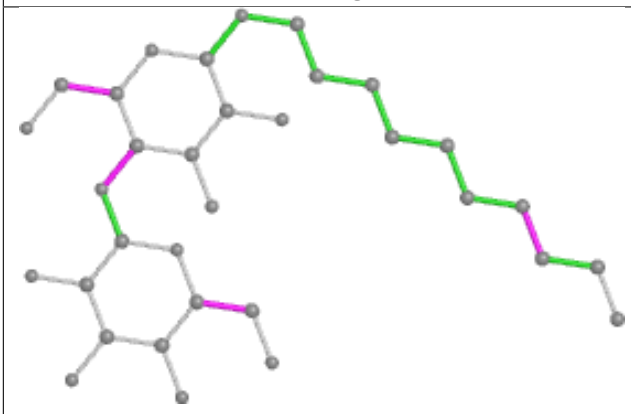
Ligand DMU A 611



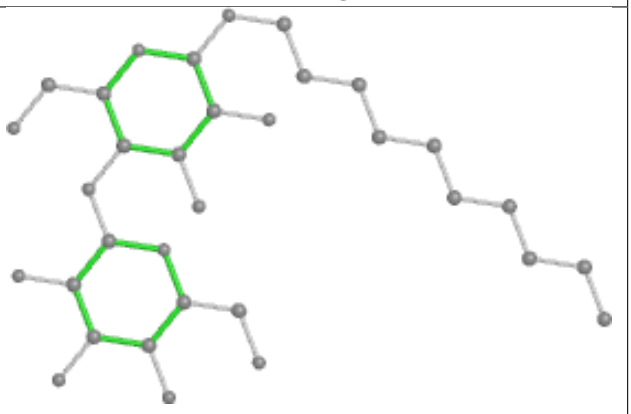
Bond lengths



Bond angles

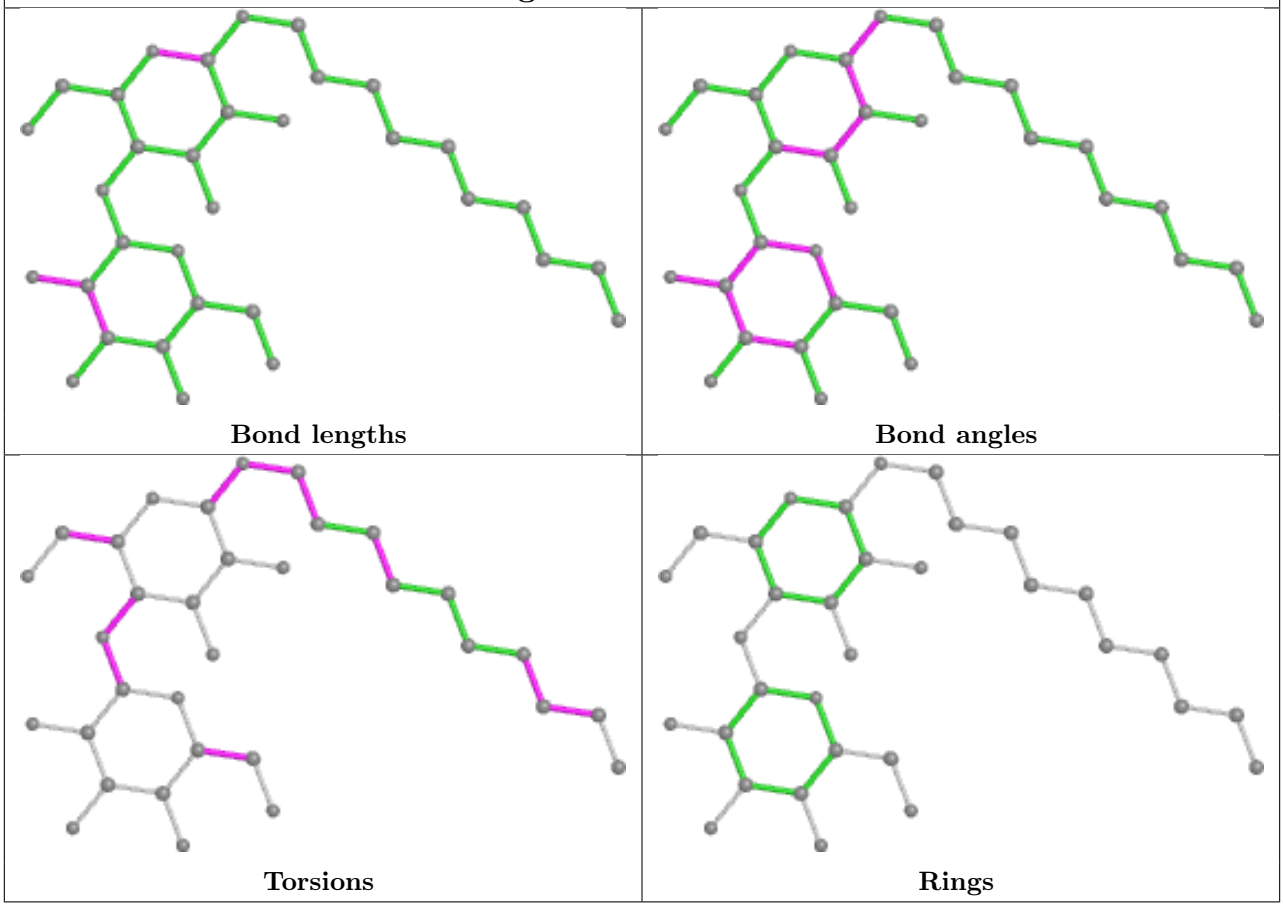


Torsions

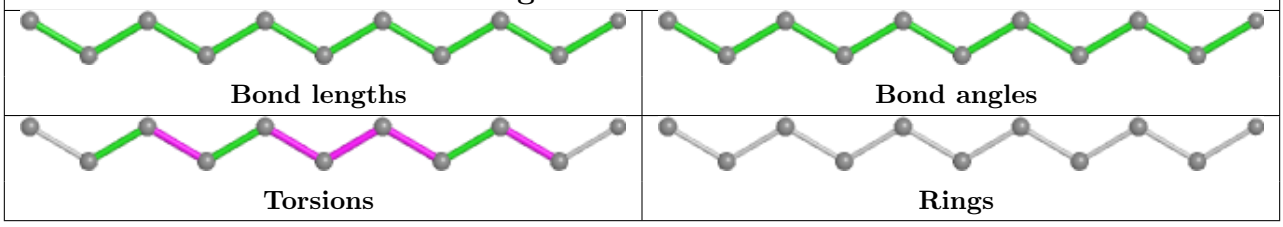


Rings

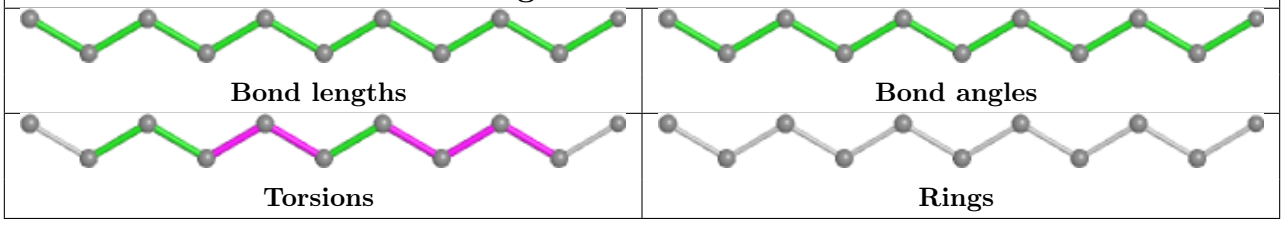
Ligand DMU C 318



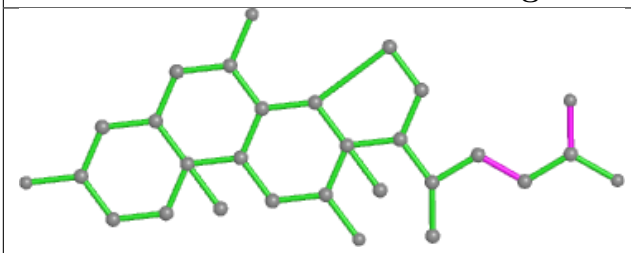
Ligand DMU O 306



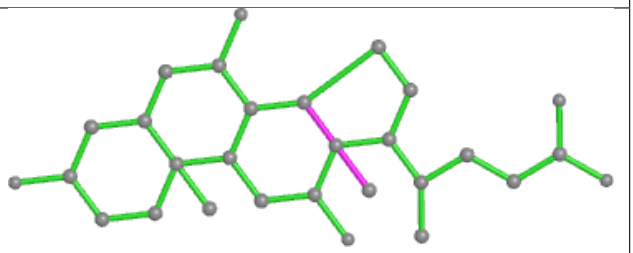
Ligand DMU A 617



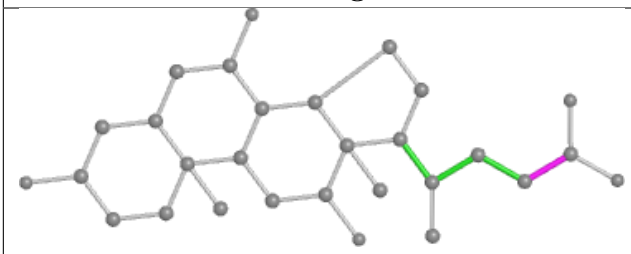
Ligand CHD P 302



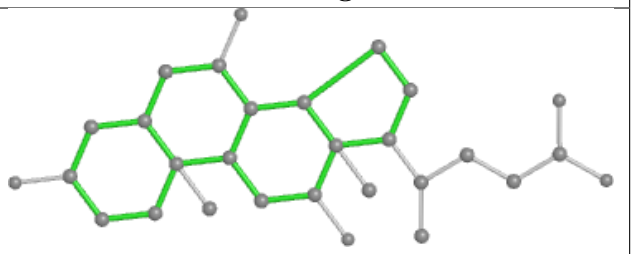
Bond lengths



Bond angles

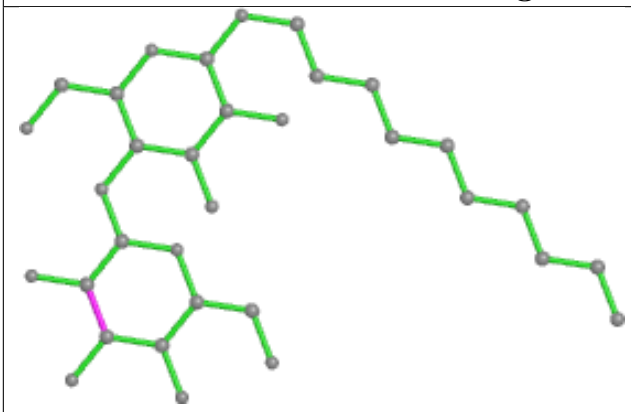


Torsions

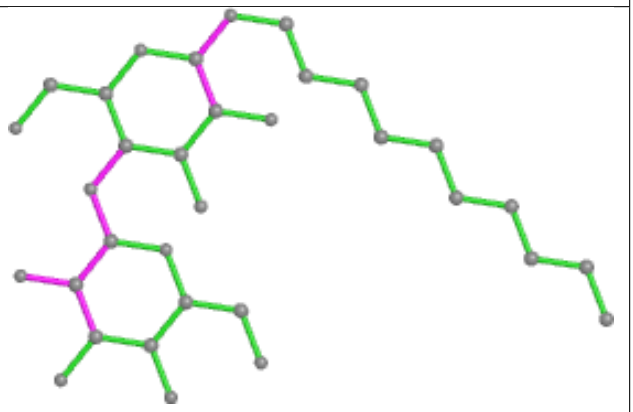


Rings

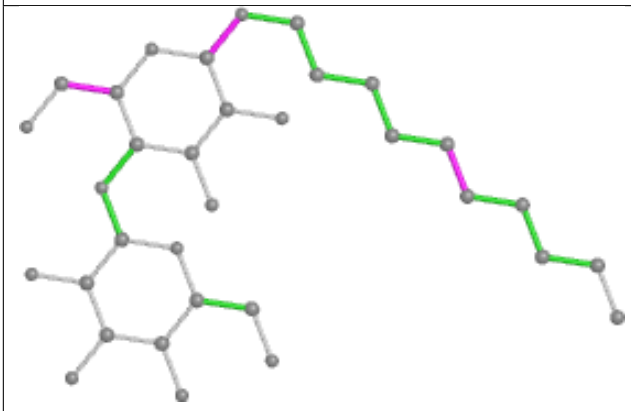
Ligand DMU U 101



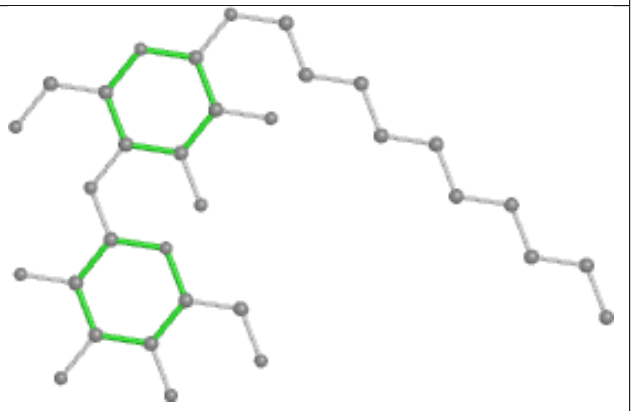
Bond lengths



Bond angles

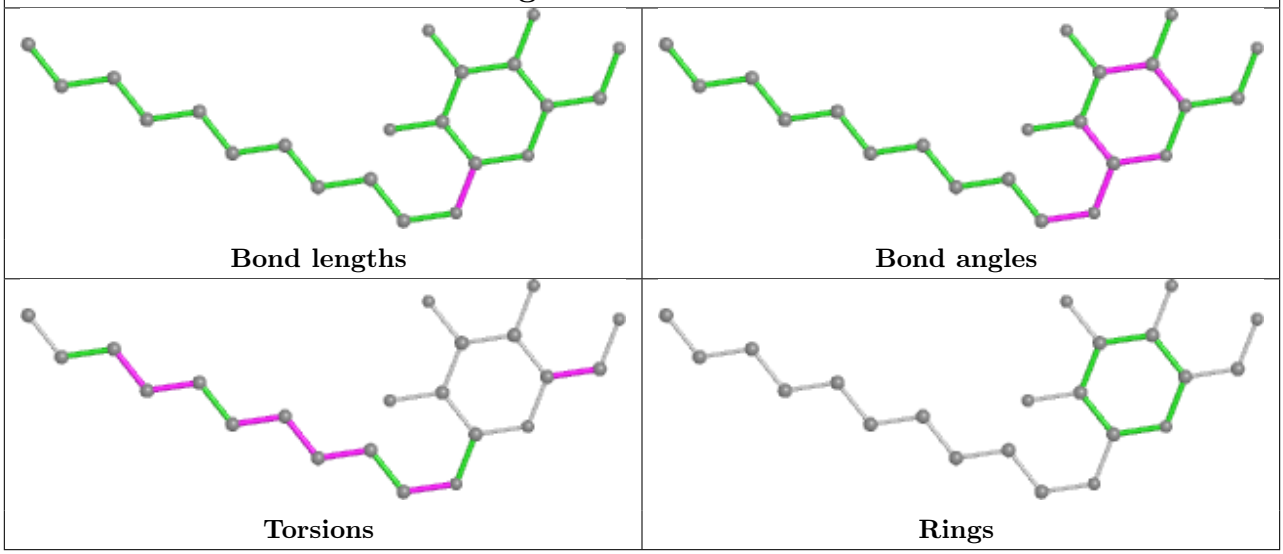


Torsions

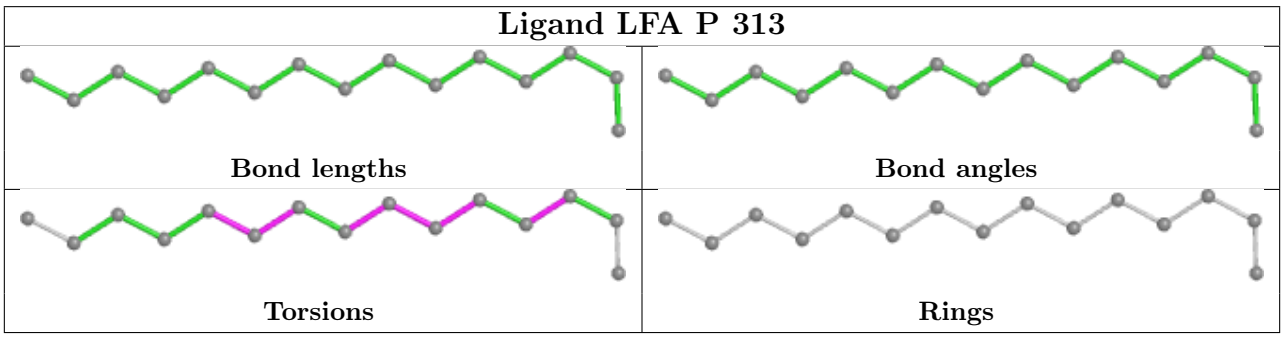


Rings

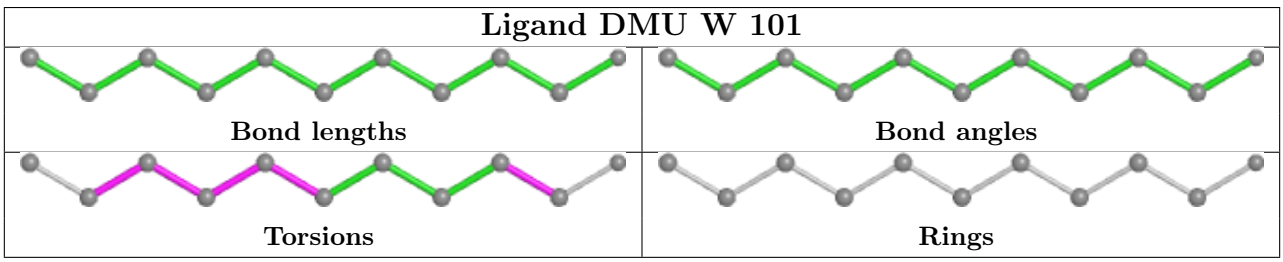
Ligand DMU P 317



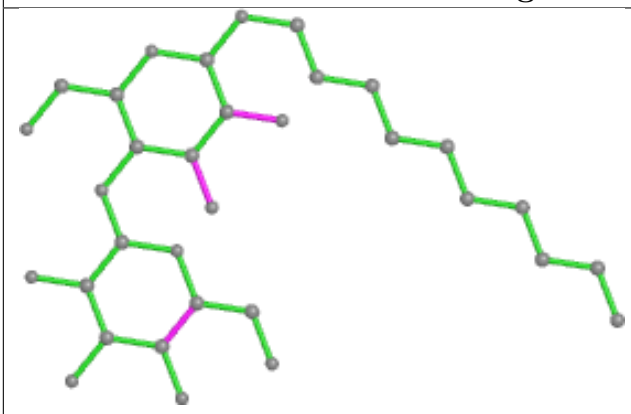
Ligand LFA P 313



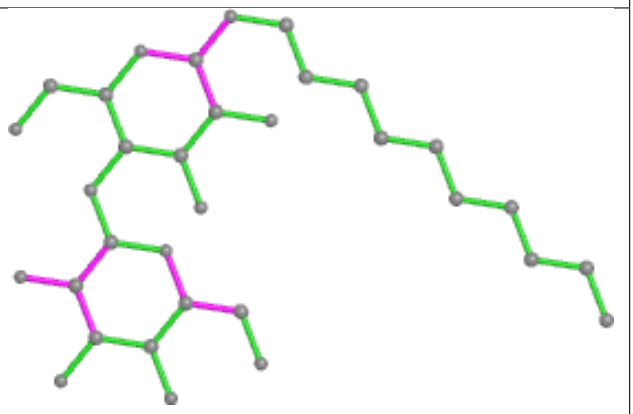
Ligand DMU W 101



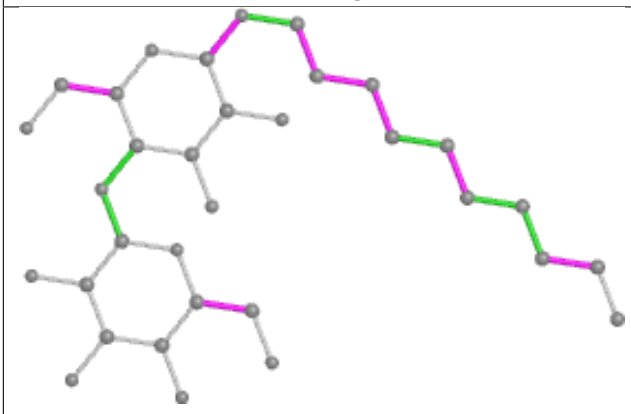
Ligand DMU C 319



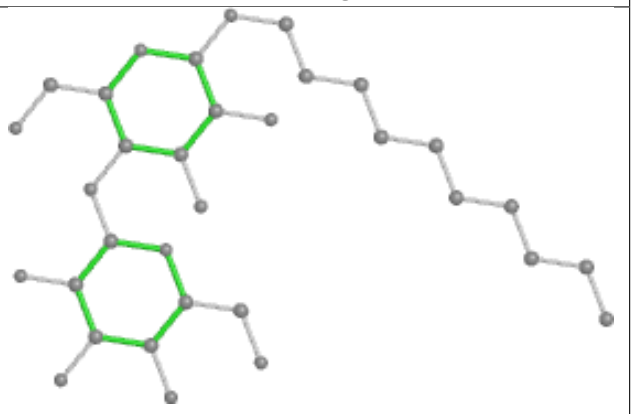
Bond lengths



Bond angles

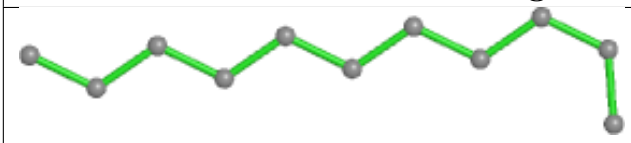


Torsions

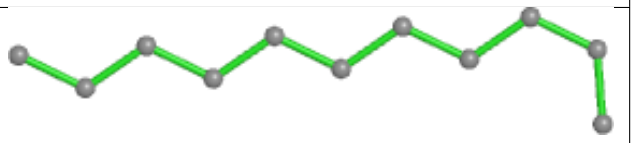


Rings

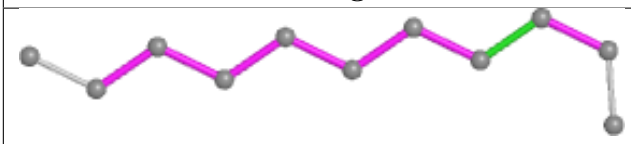
Ligand LFA C 310



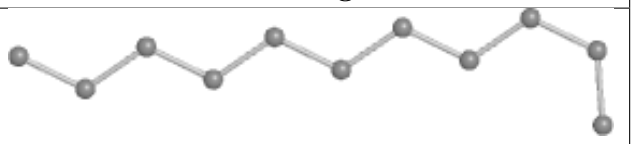
Bond lengths



Bond angles

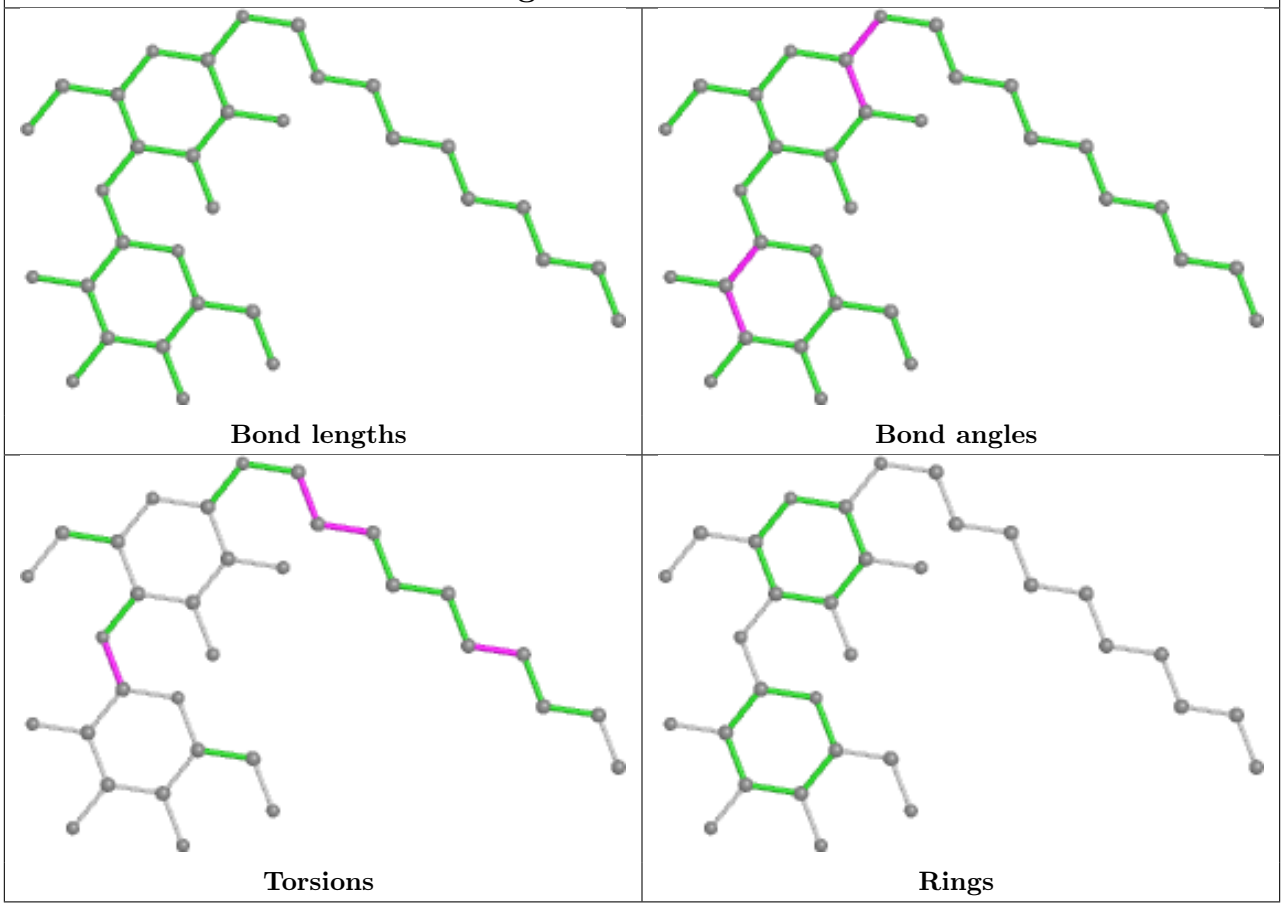


Torsions

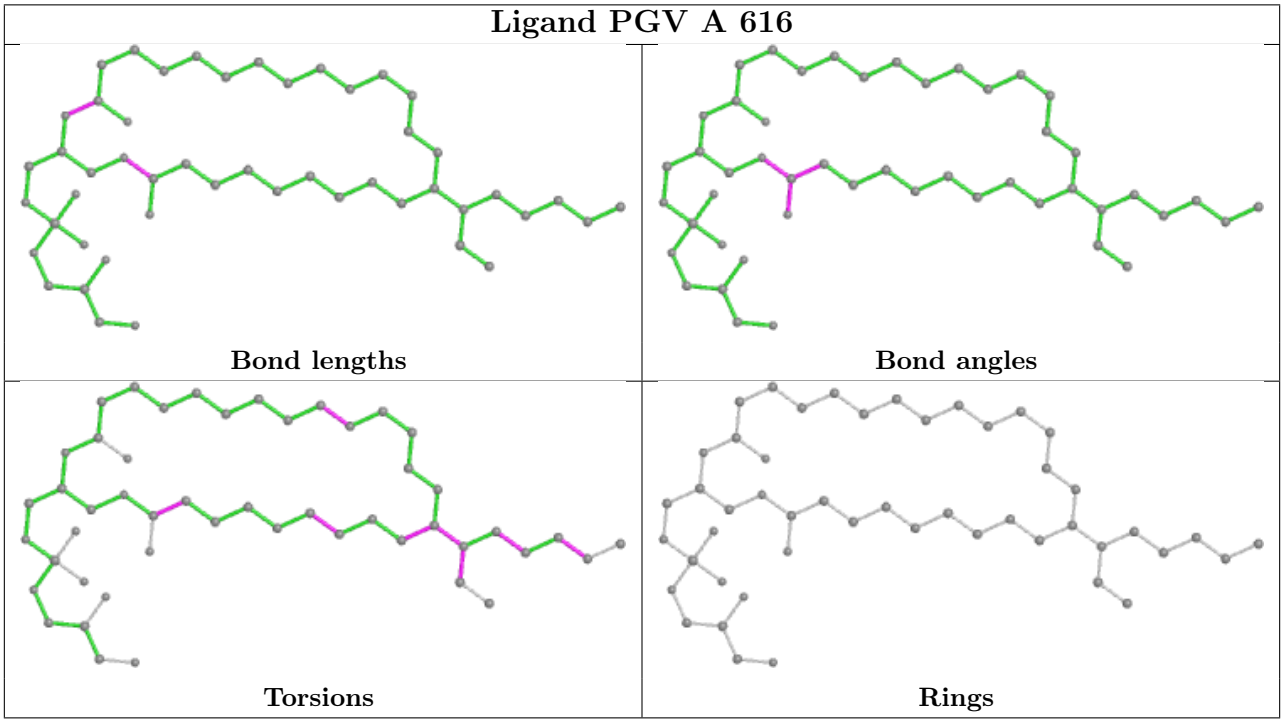


Rings

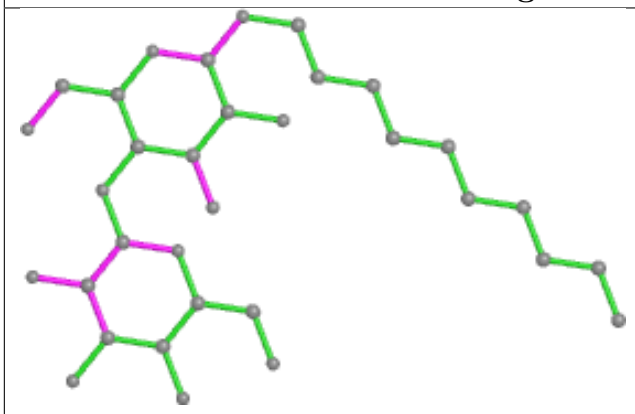
Ligand DMU C 324



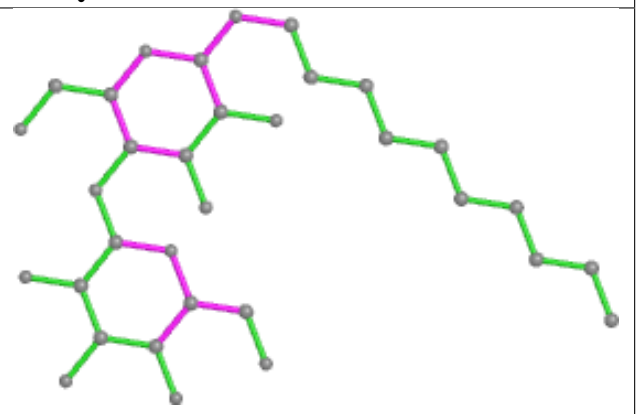
Ligand PGV A 616



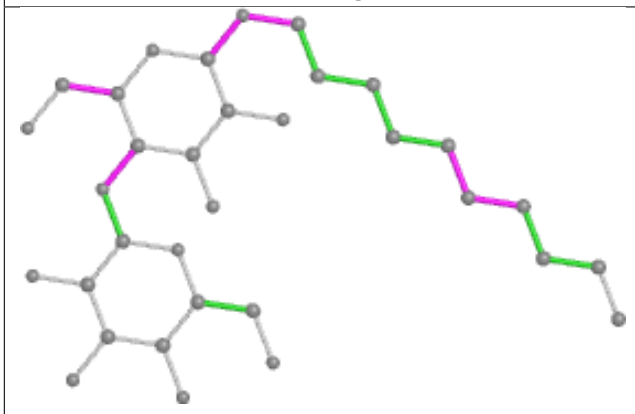
Ligand DMU Q 201



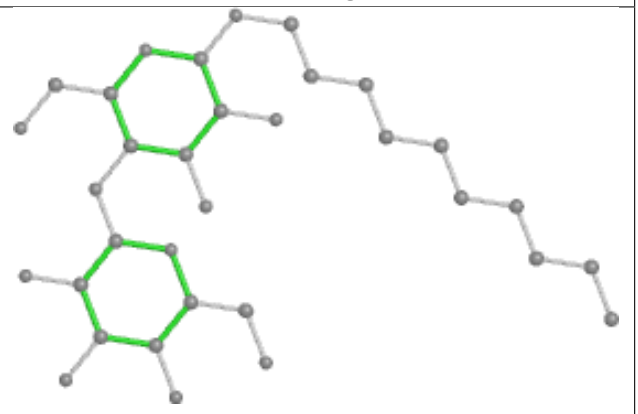
Bond lengths



Bond angles

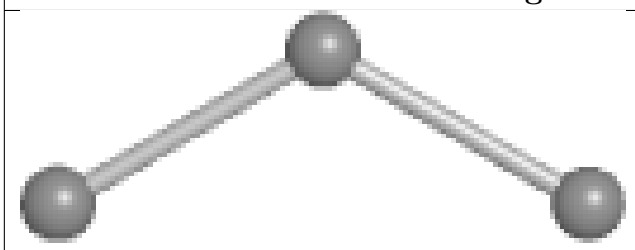


Torsions

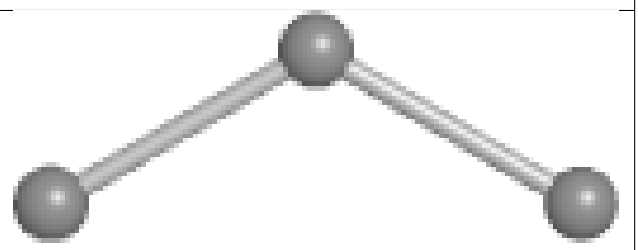


Rings

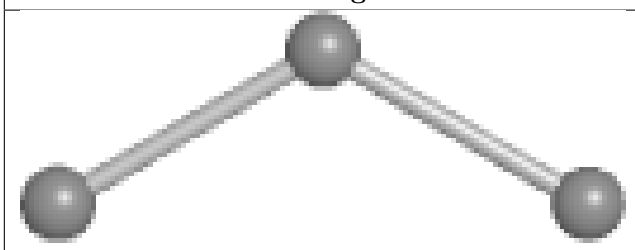
Ligand N2O N 608



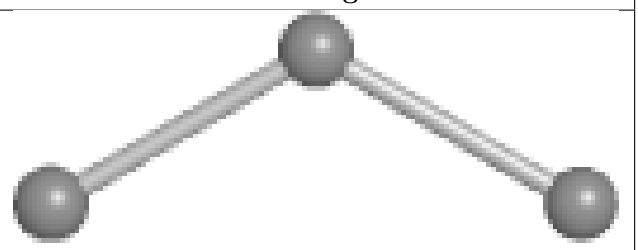
Bond lengths



Bond angles

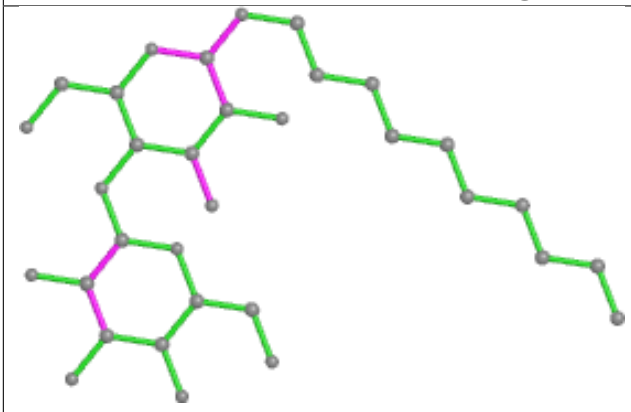


Torsions

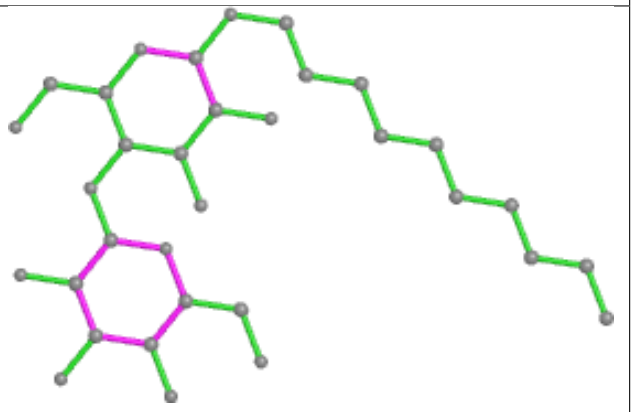


Rings

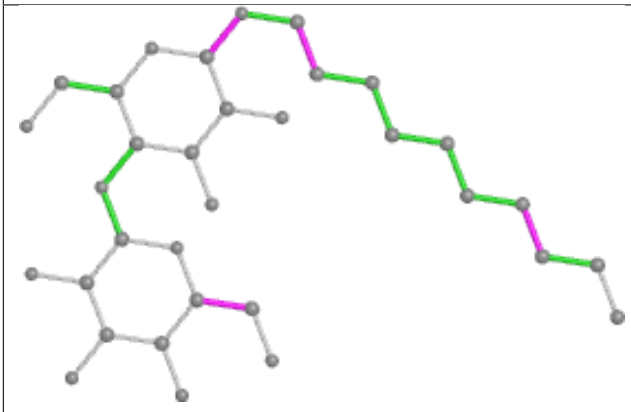
Ligand DMU N 611



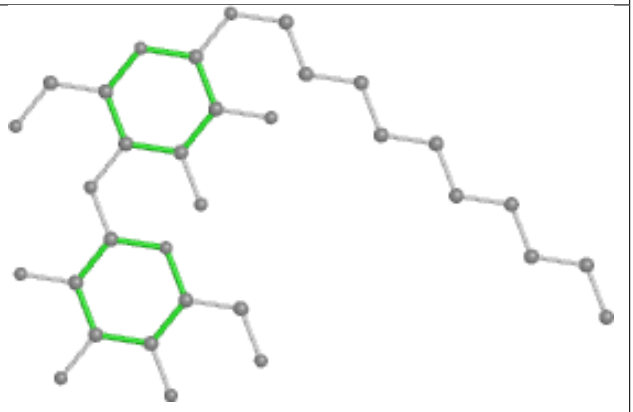
Bond lengths



Bond angles

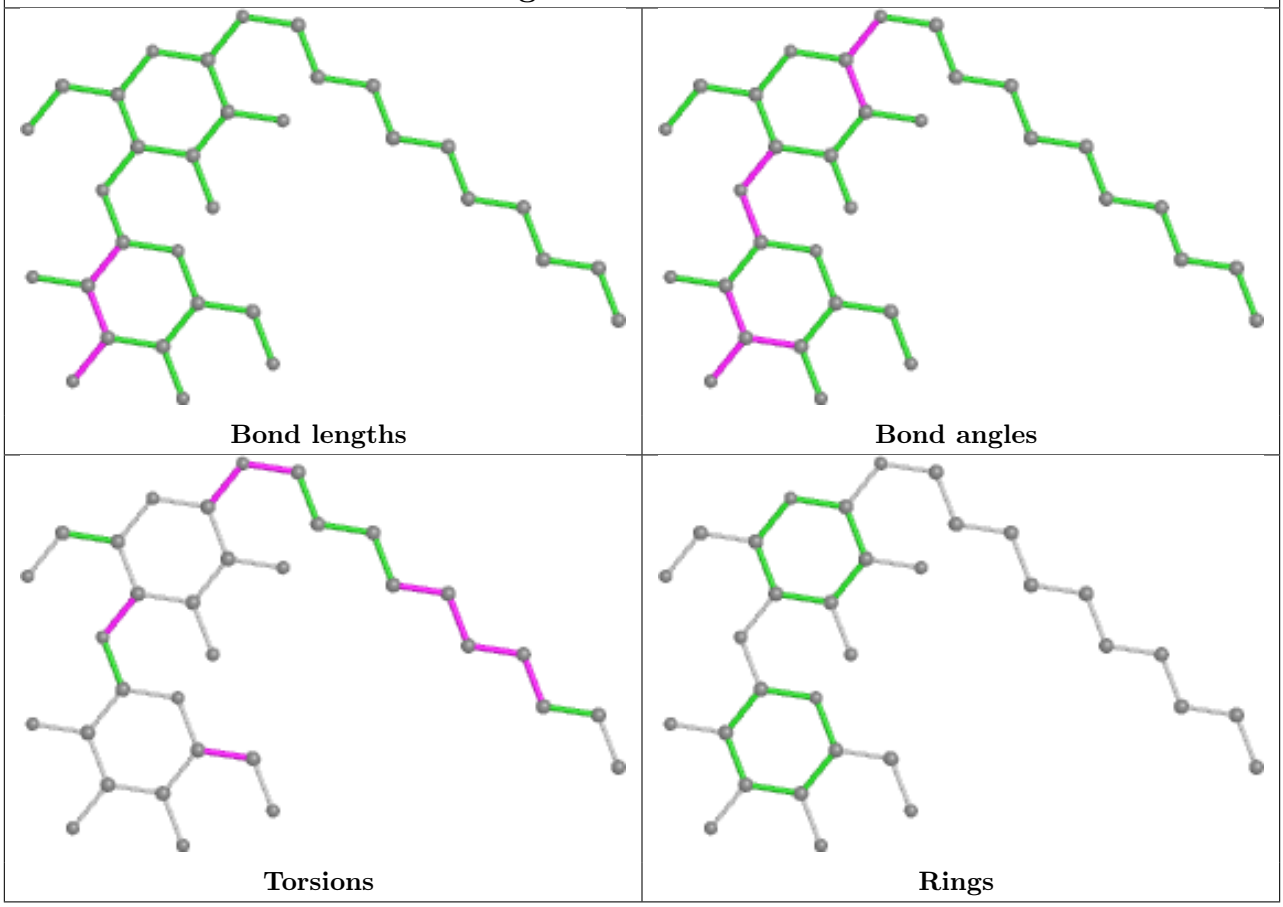


Torsions

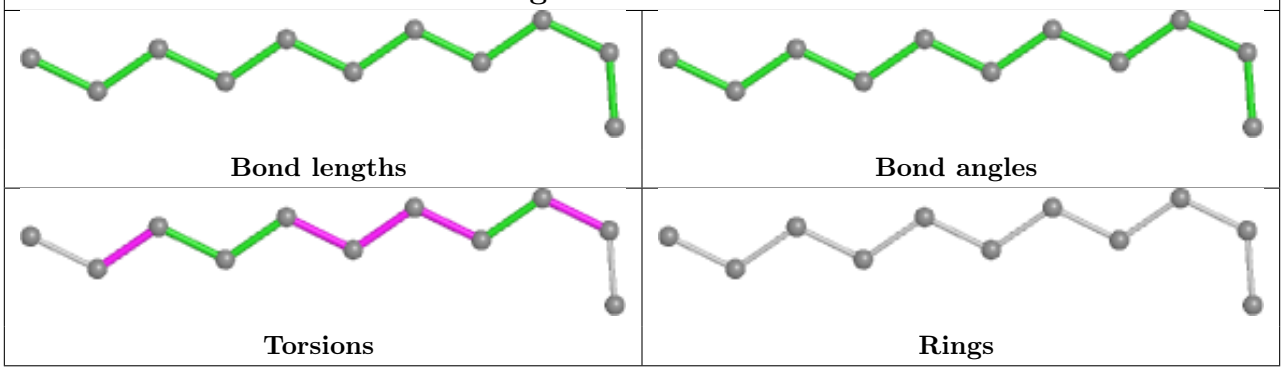


Rings

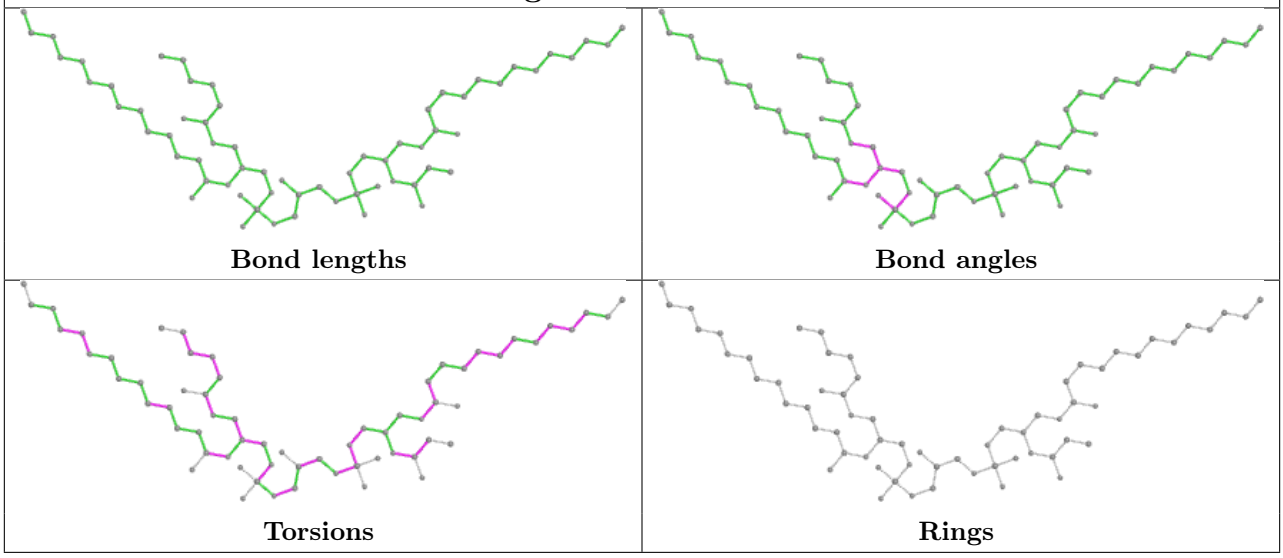
Ligand DMU P 319



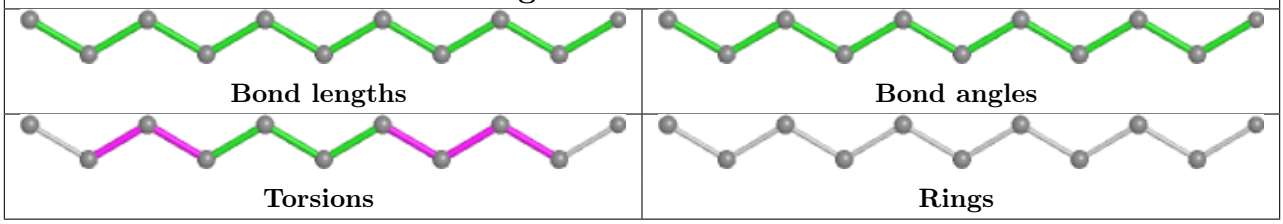
Ligand LFA P 312



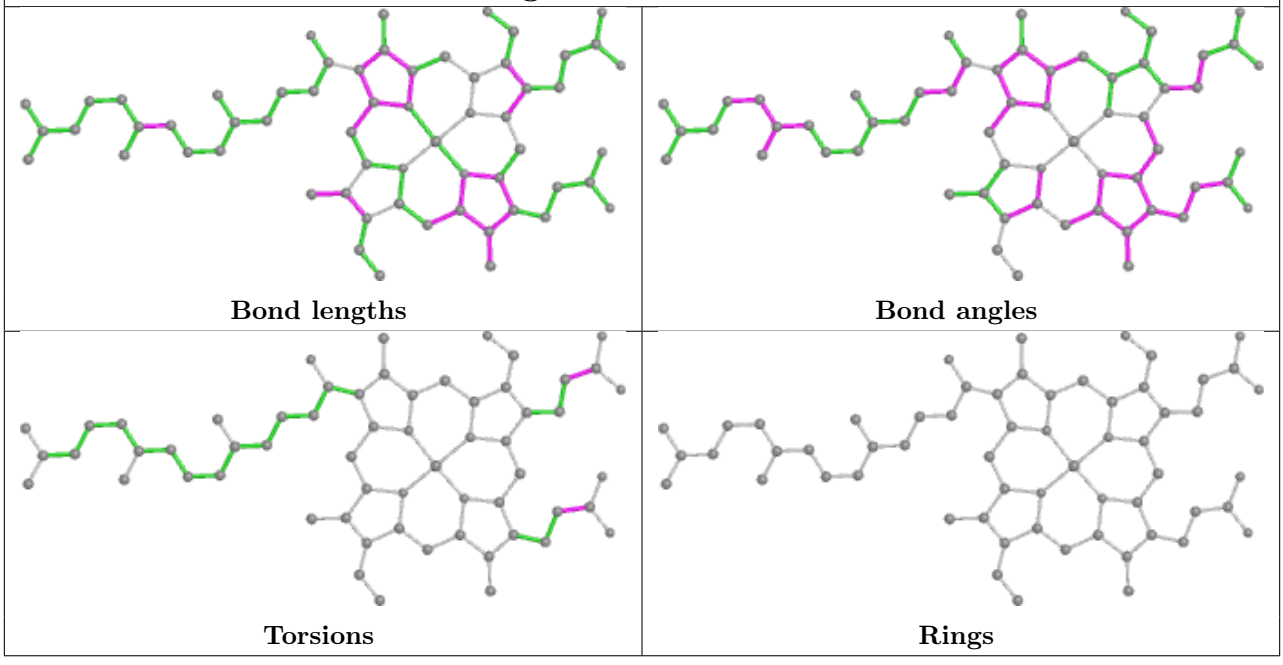
Ligand CDL V 101



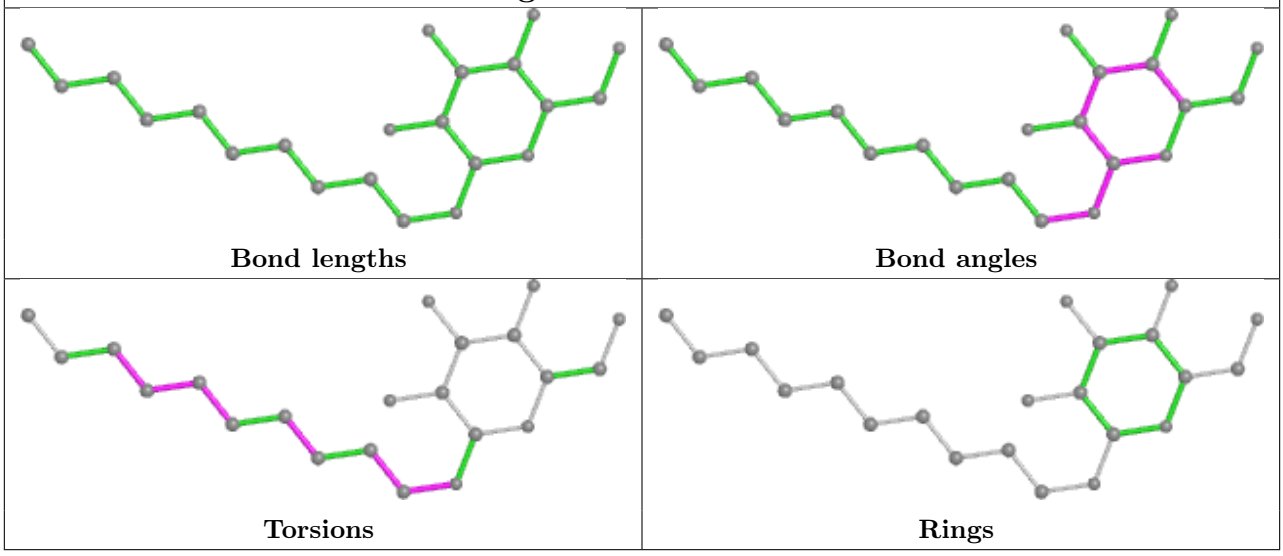
Ligand DMU B 302



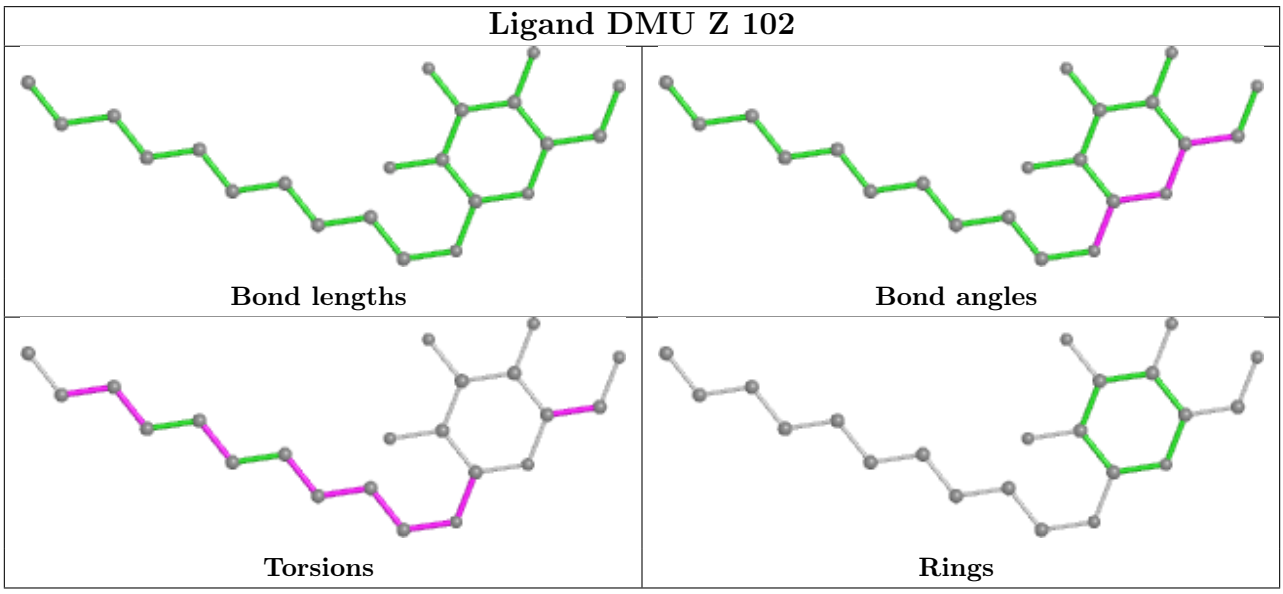
Ligand HEA N 603



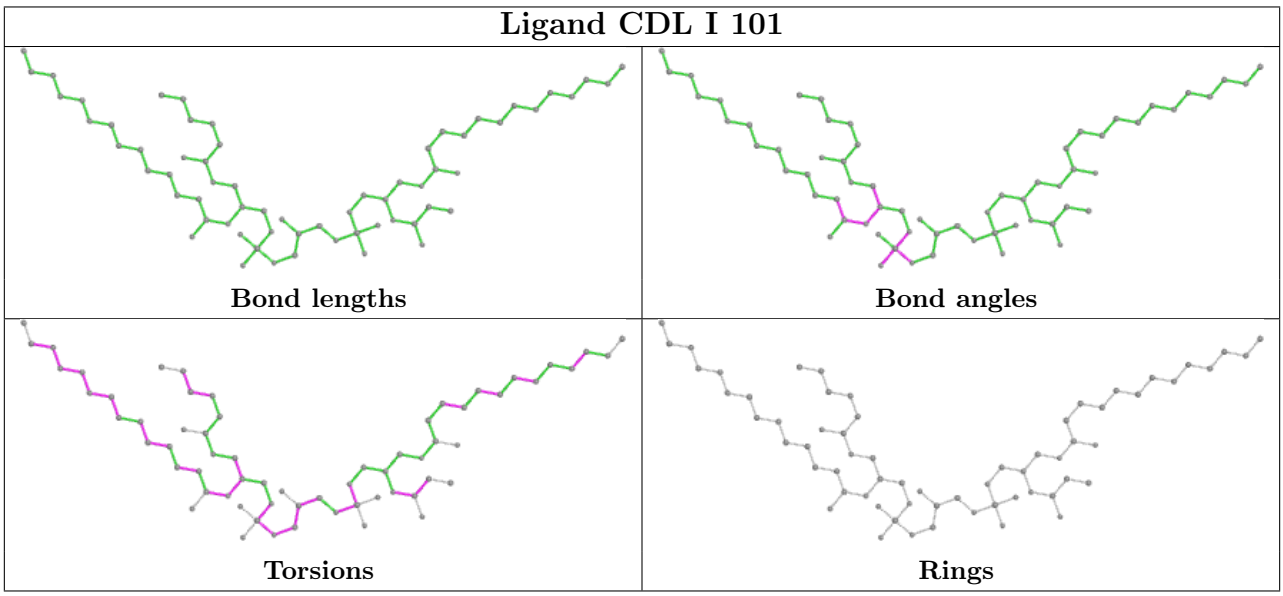
Ligand DMU C 317



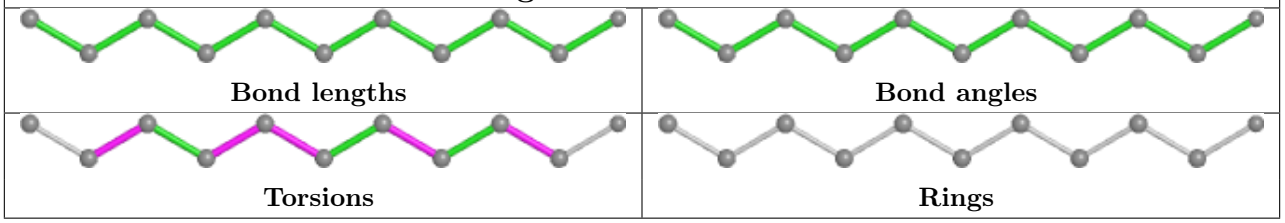
Ligand DMU Z 102



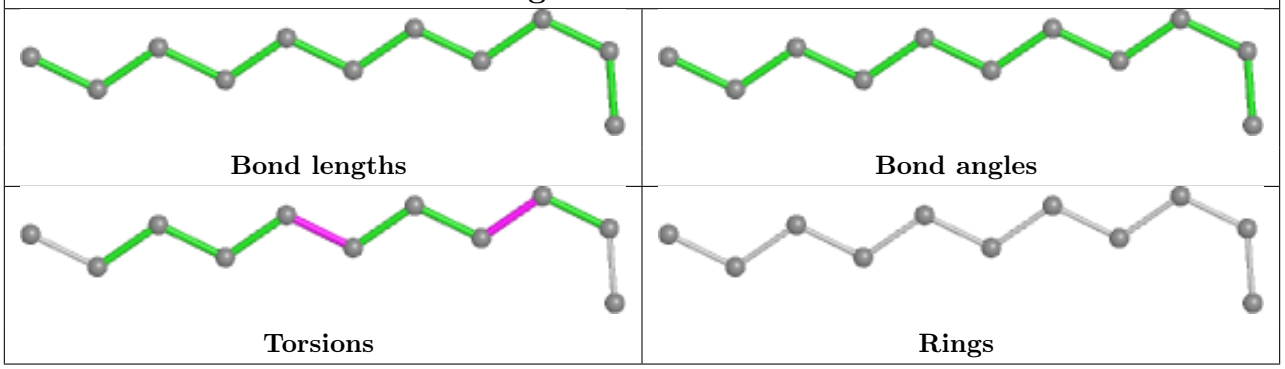
Ligand CDL I 101



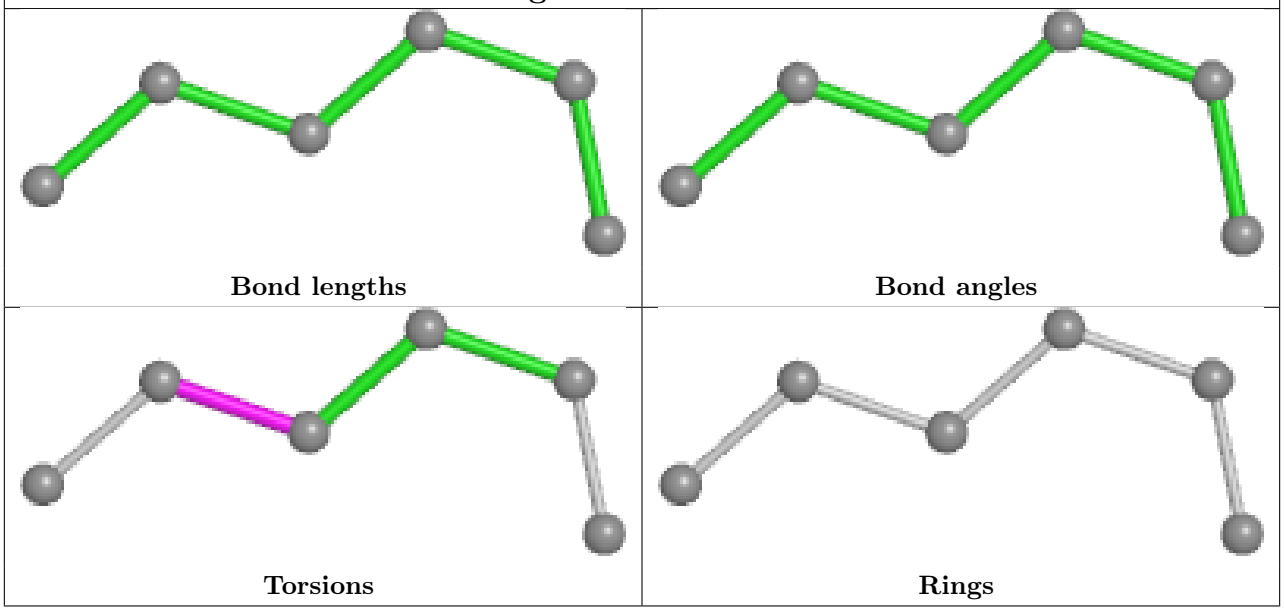
Ligand DMU N 601



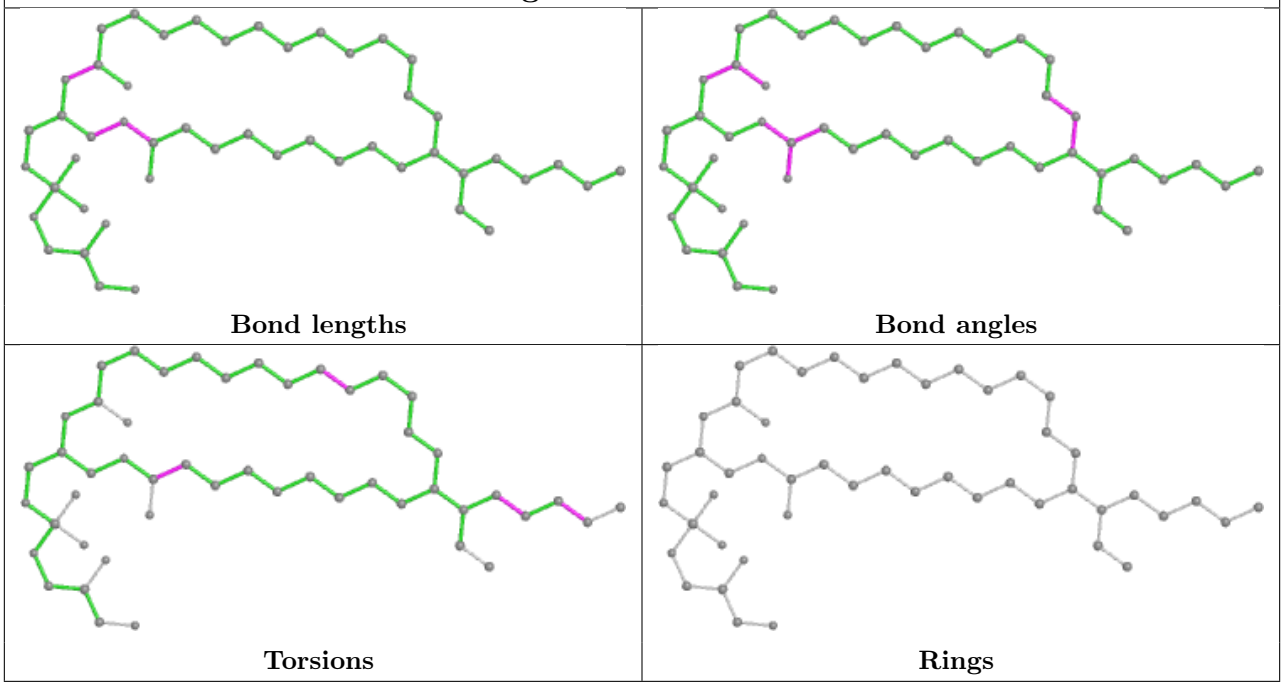
Ligand LFA O 303



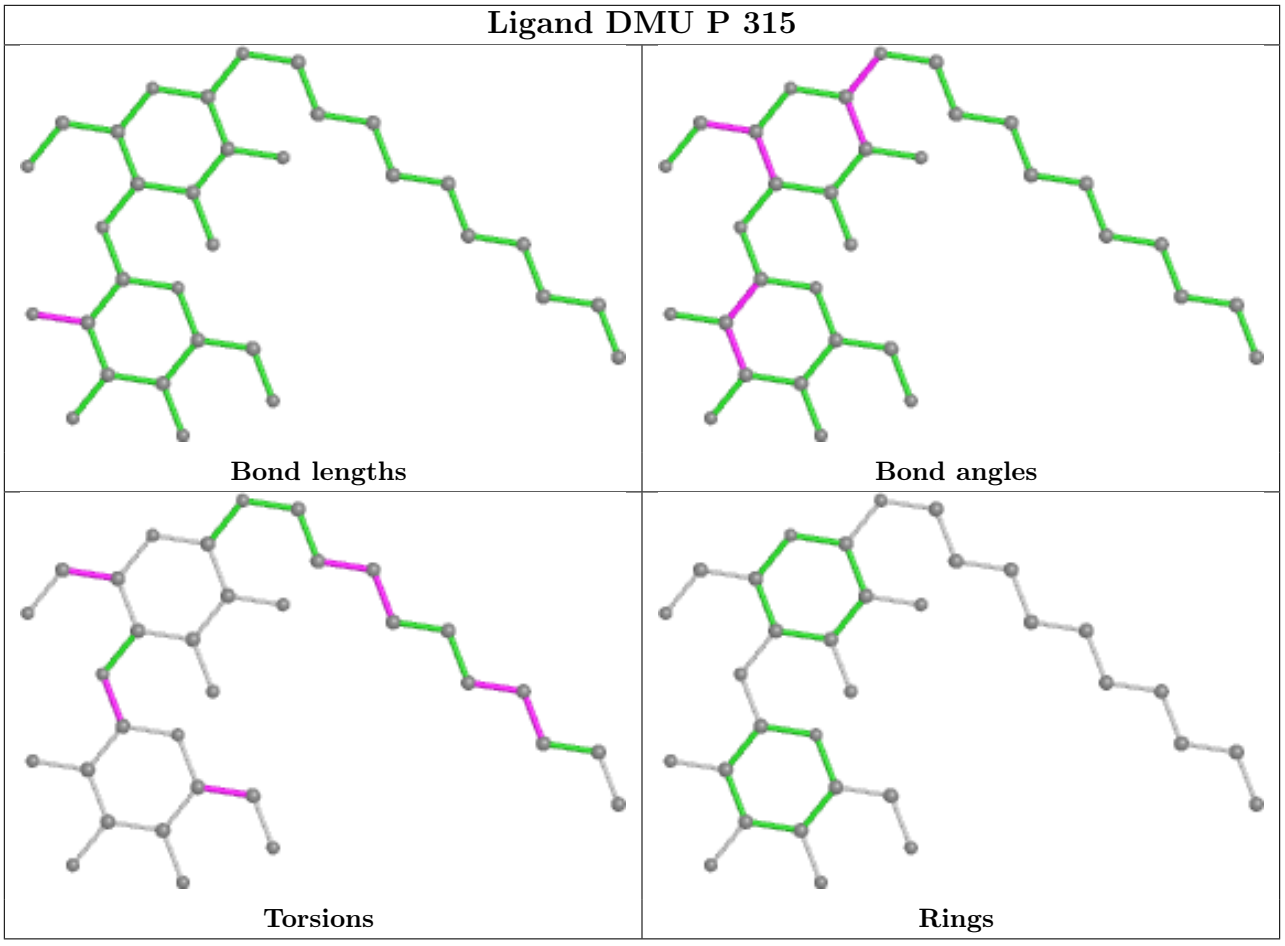
Ligand LFA C 308



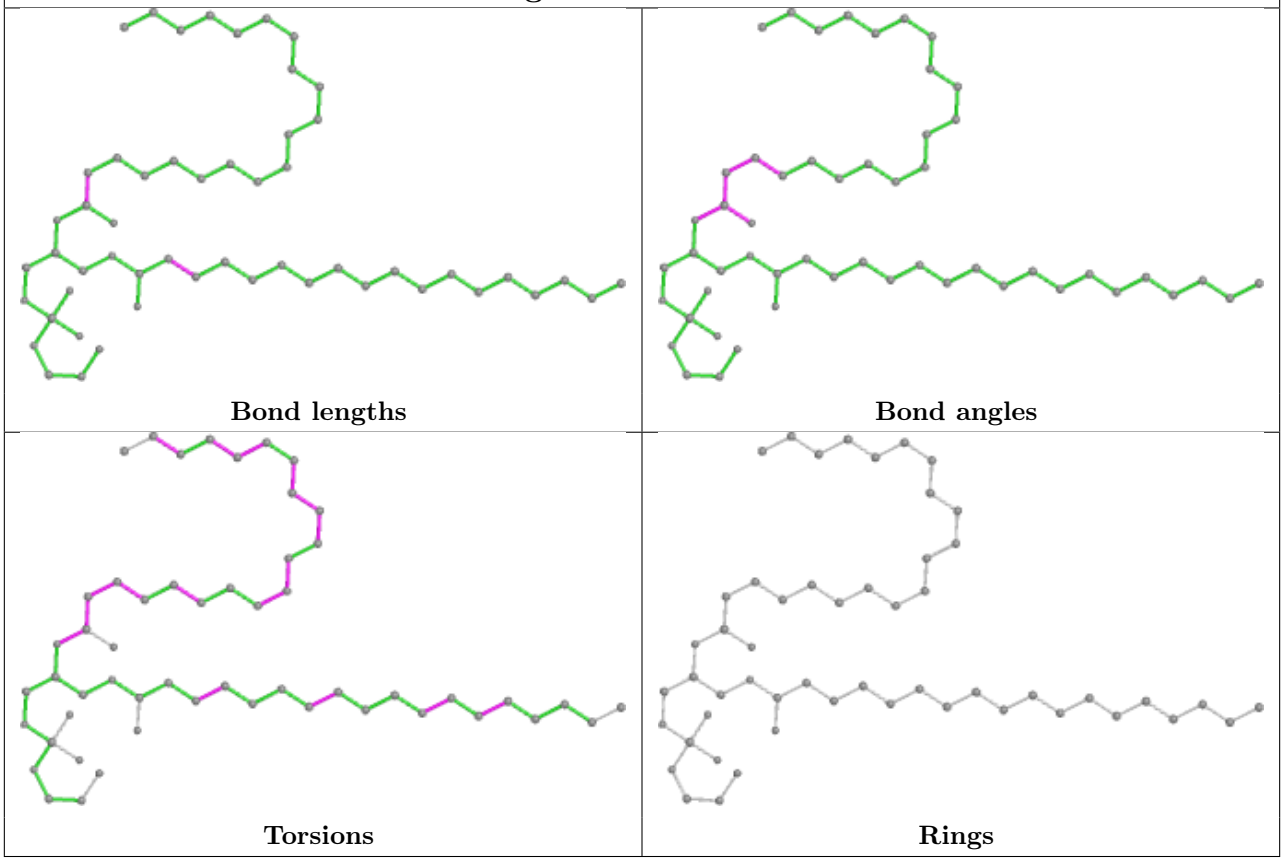
Ligand PGV N 617



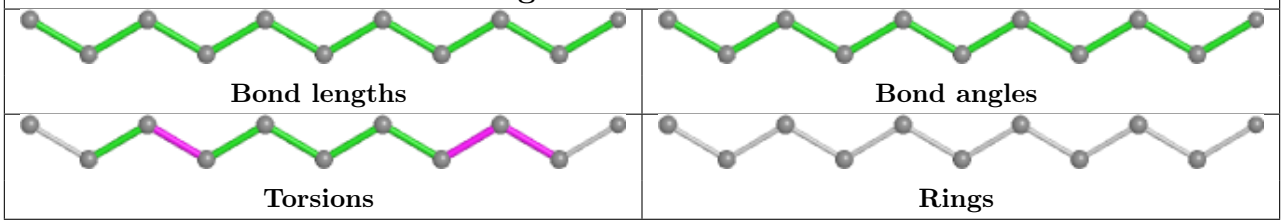
Ligand DMU P 315



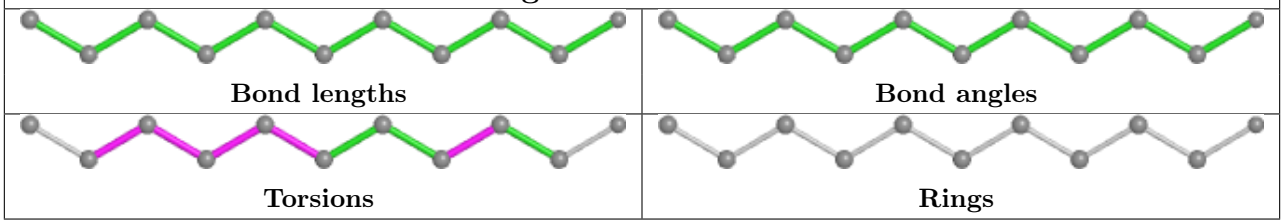
Ligand PEK T 101



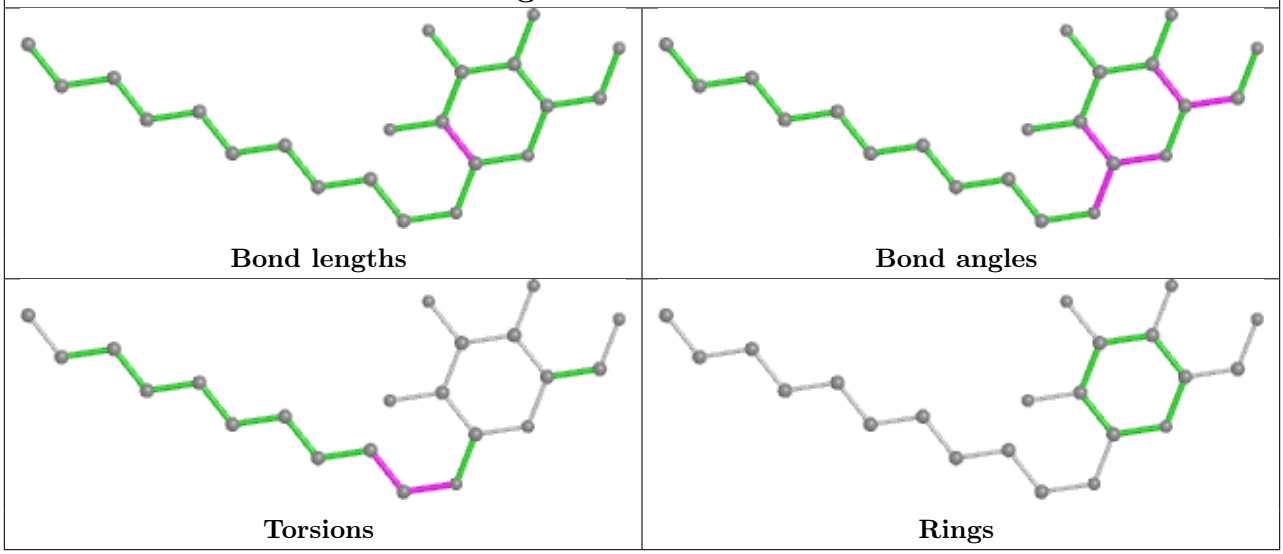
Ligand DMU C 306



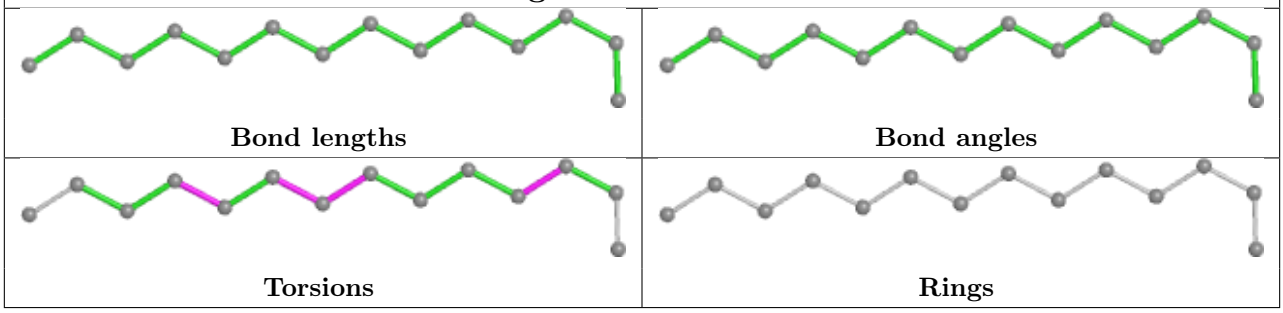
Ligand DMU J 101



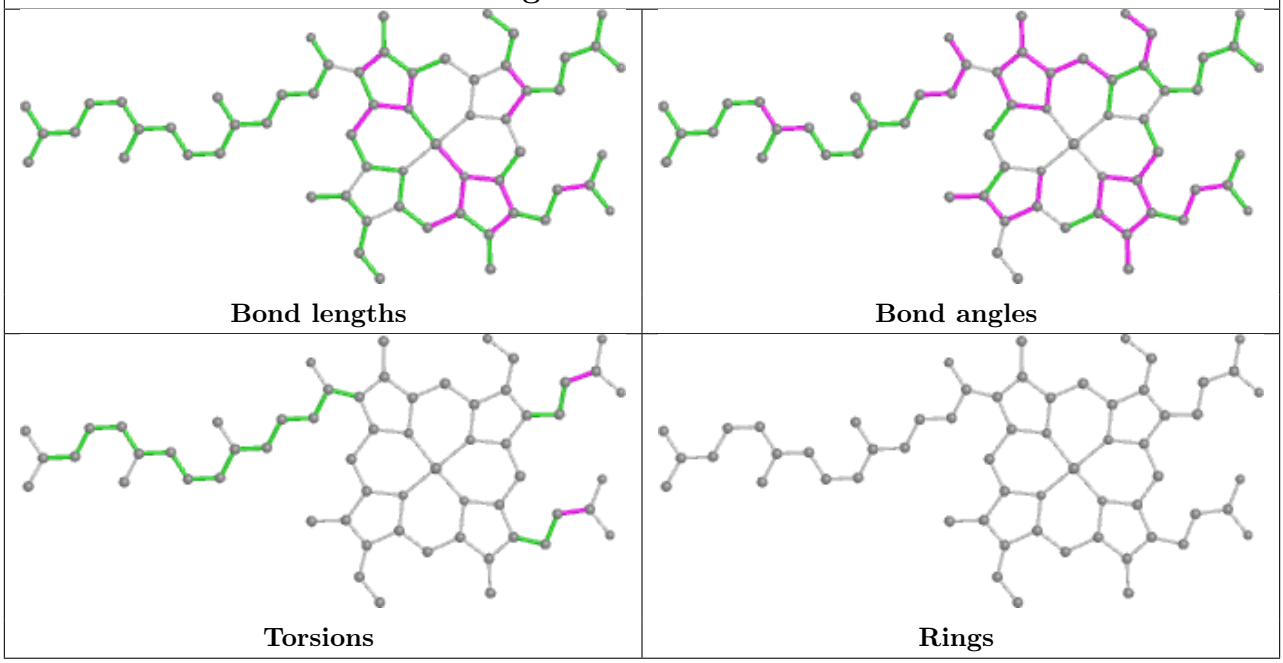
Ligand DMU O 308



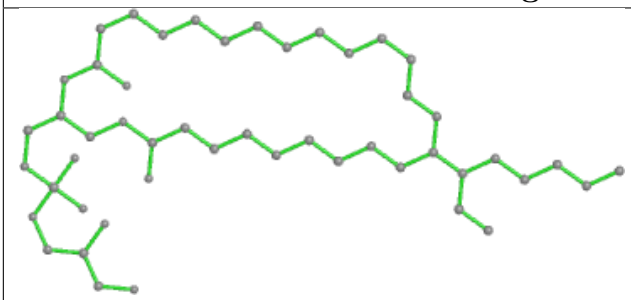
Ligand LFA A 608



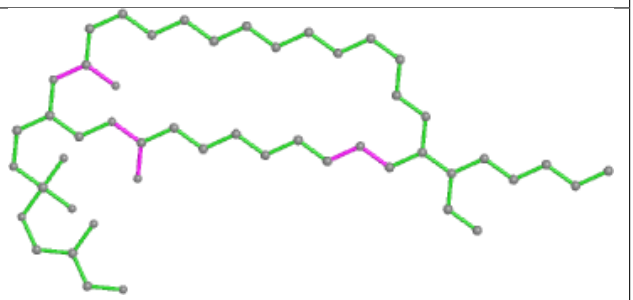
Ligand HEA A 602



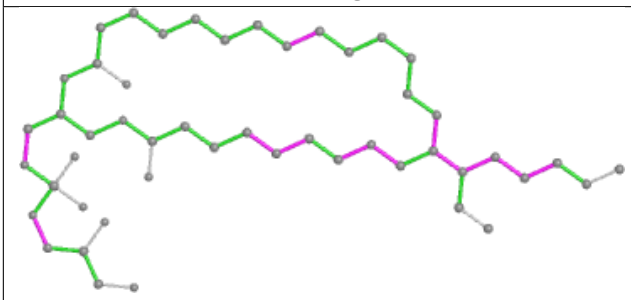
Ligand PGV C 303



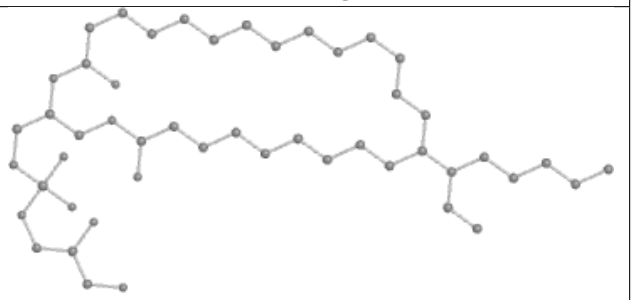
Bond lengths



Bond angles

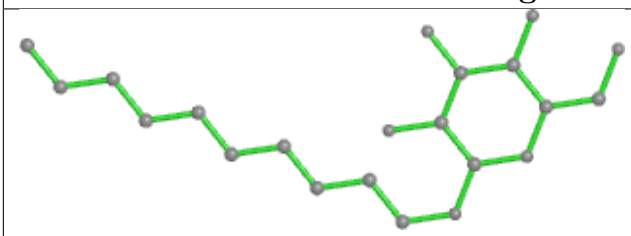


Torsions

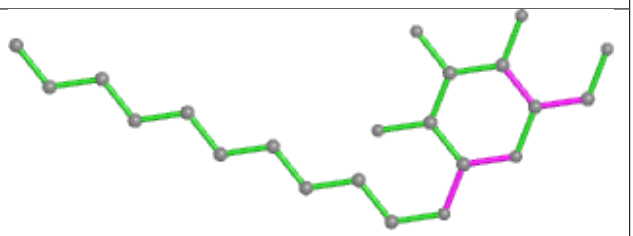


Rings

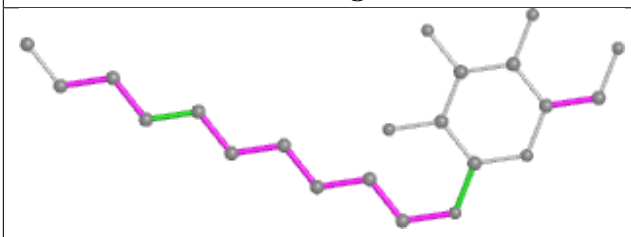
Ligand DMU L 102



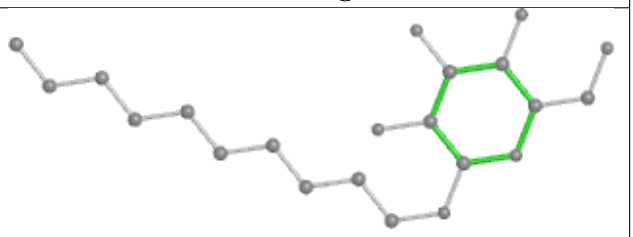
Bond lengths



Bond angles

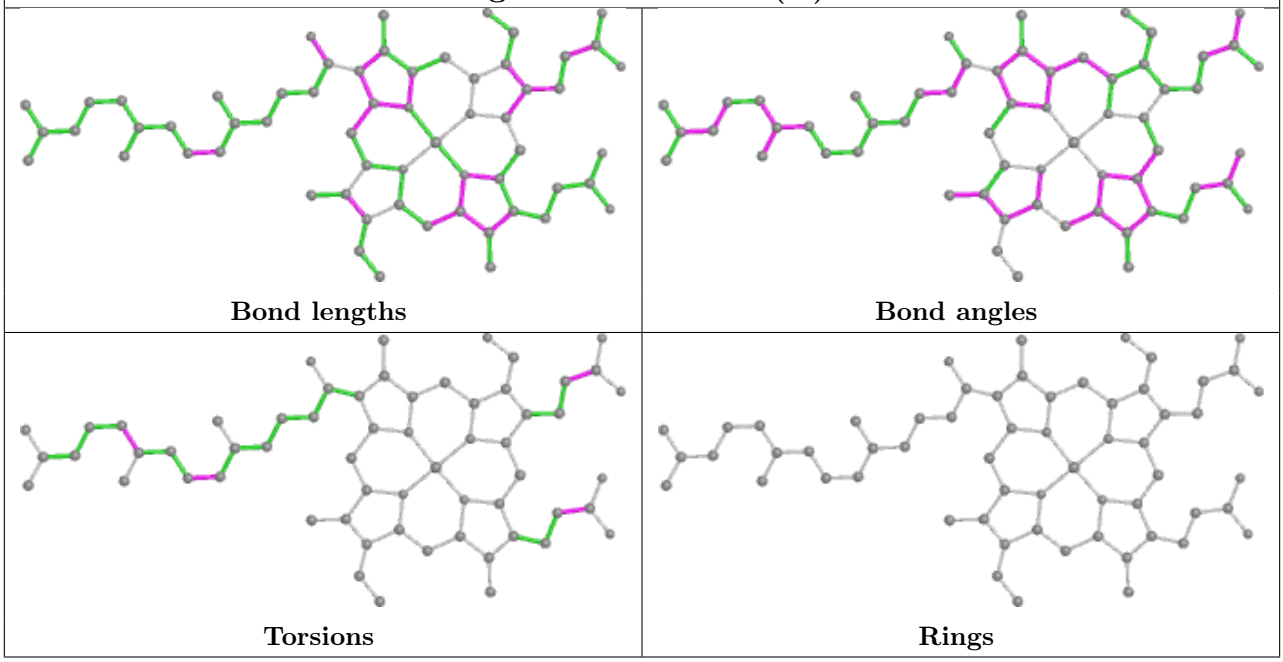


Torsions

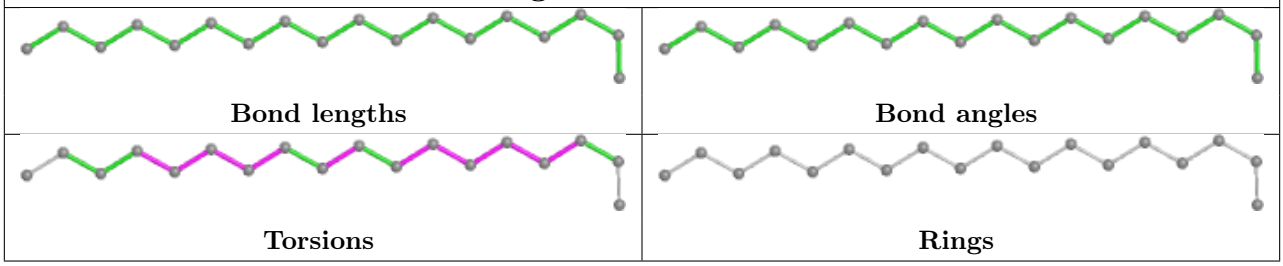


Rings

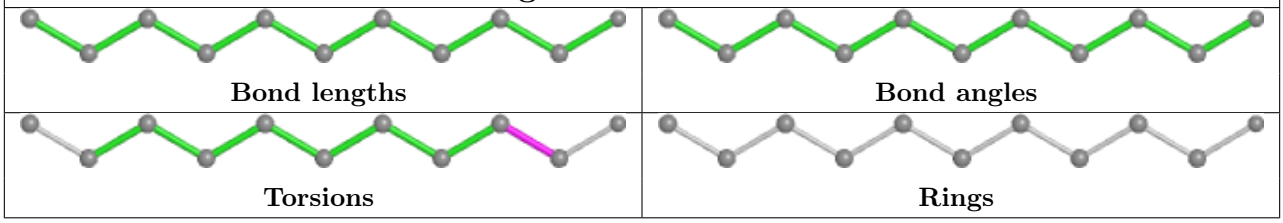
Ligand HEA N 602 (A)



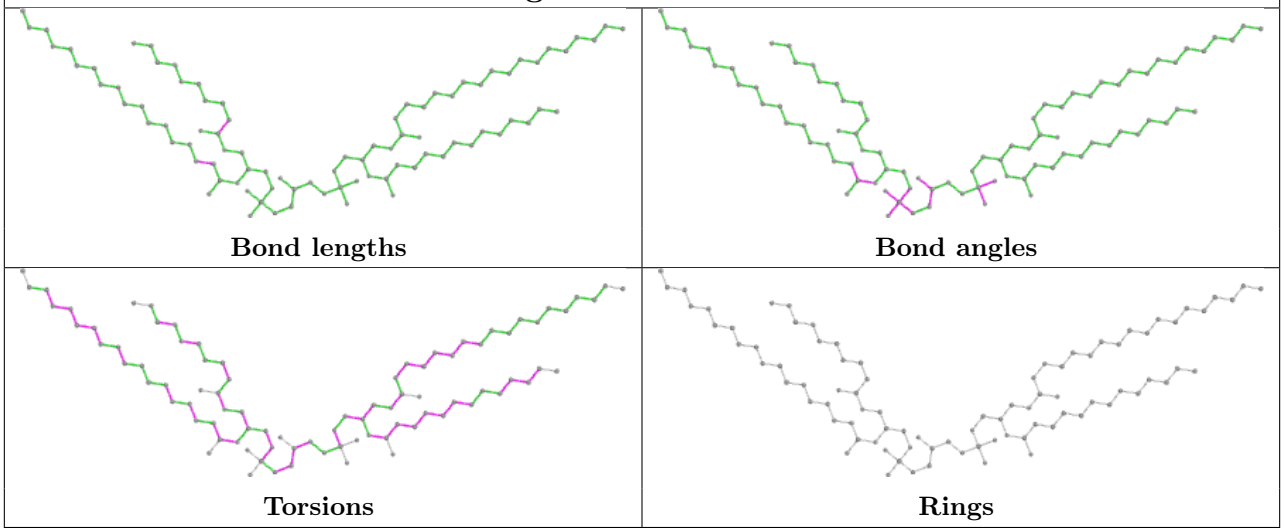
Ligand LFA P 310



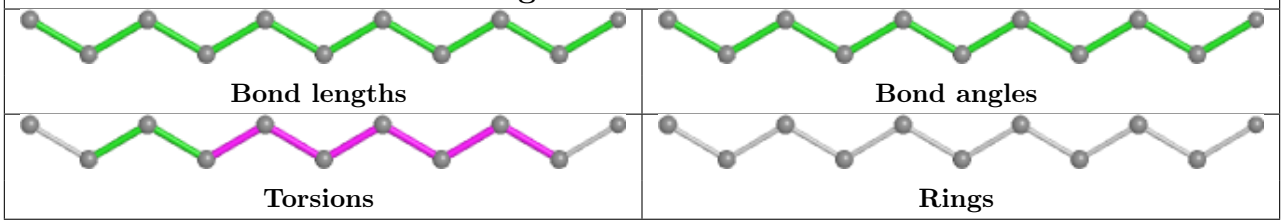
Ligand DMU P 307



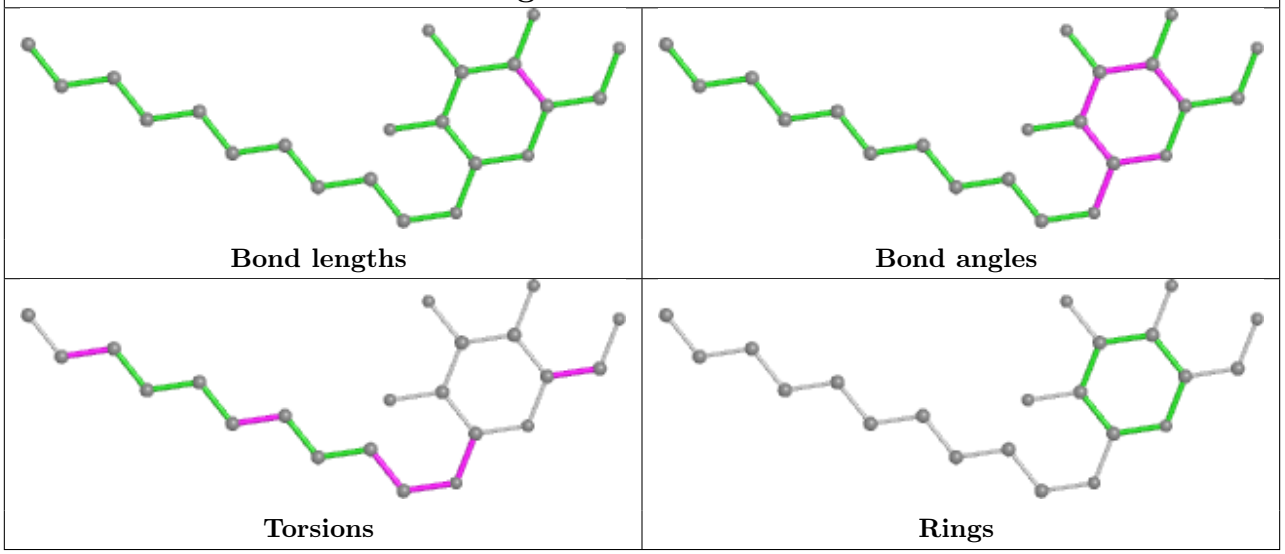
Ligand CDL P 305



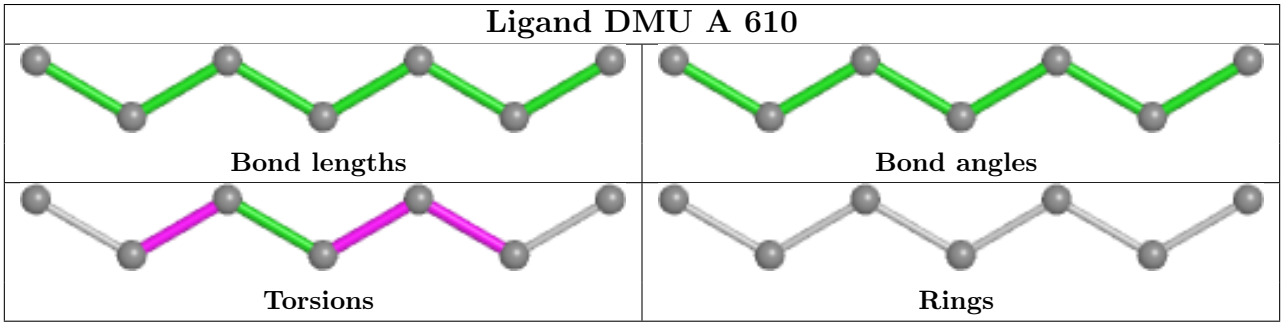
Ligand DMU B 303



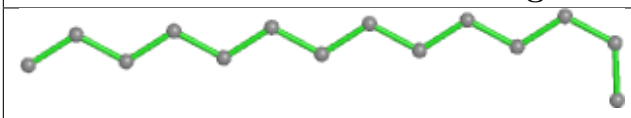
Ligand DMU O 304



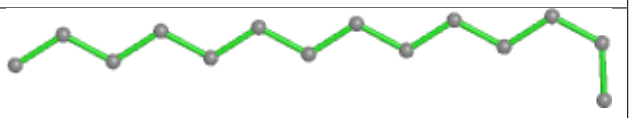
Ligand DMU A 610



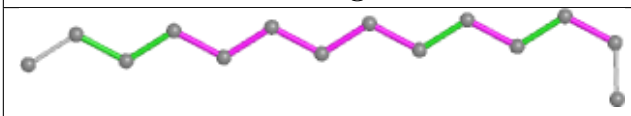
Ligand LFA G 103



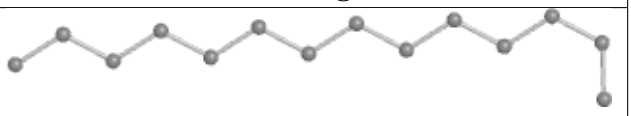
Bond lengths



Bond angles

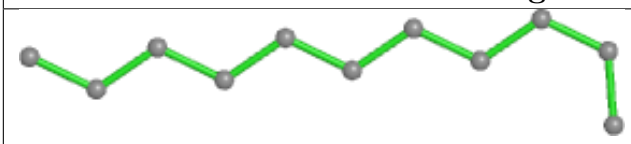


Torsions

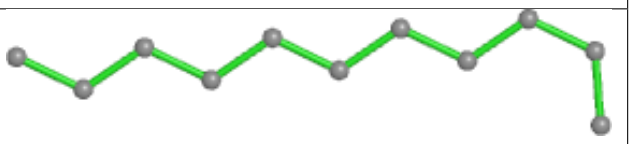


Rings

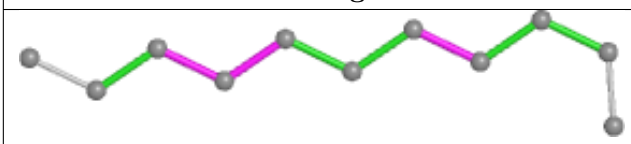
Ligand LFA T 103



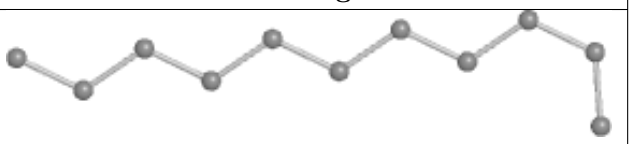
Bond lengths



Bond angles

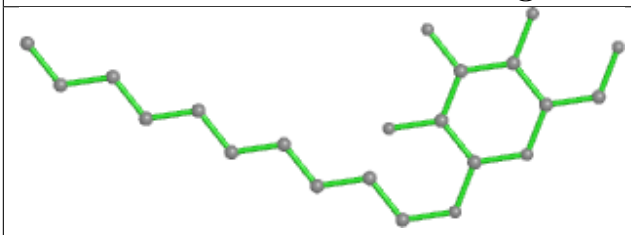


Torsions

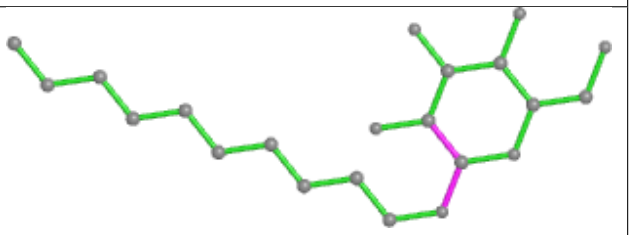


Rings

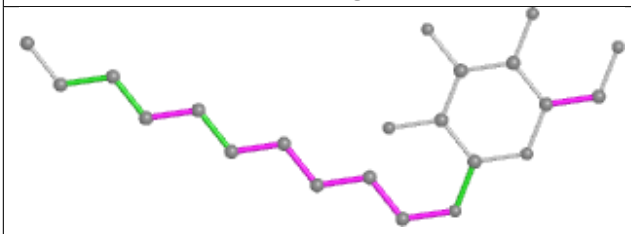
Ligand DMU C 323



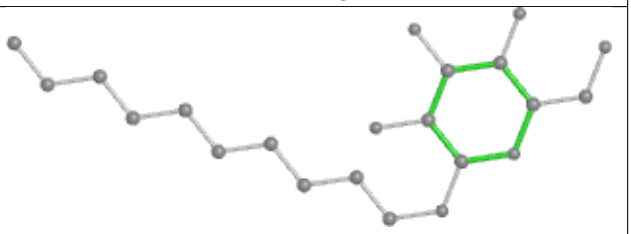
Bond lengths



Bond angles

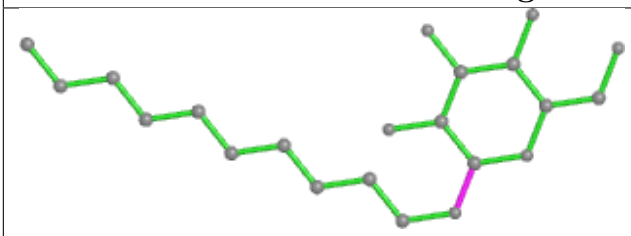


Torsions

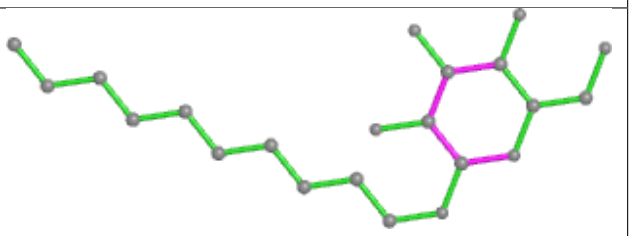


Rings

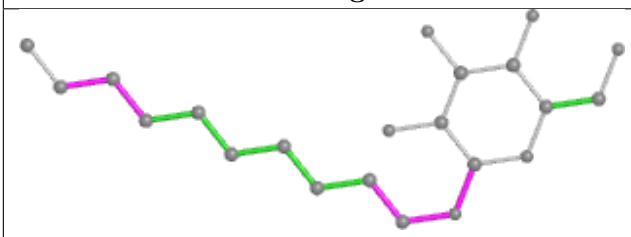
Ligand DMU B 304



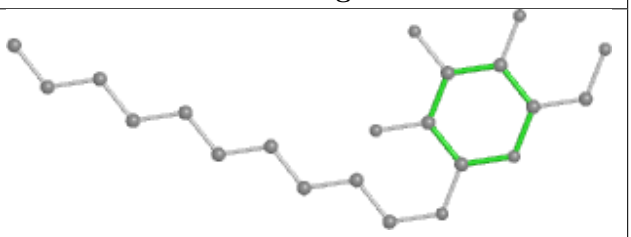
Bond lengths



Bond angles

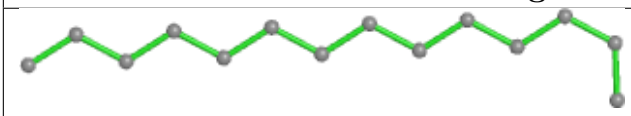


Torsions

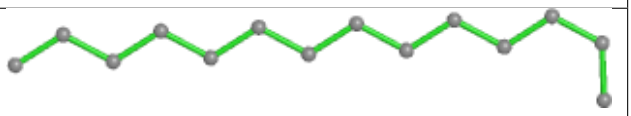


Rings

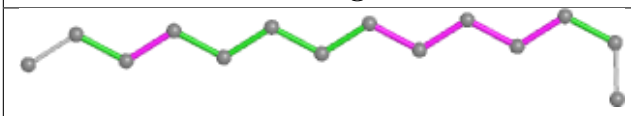
Ligand LFA T 102



Bond lengths



Bond angles



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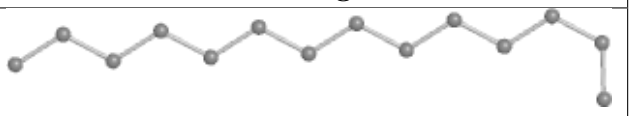
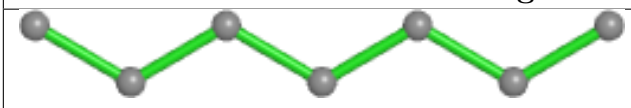
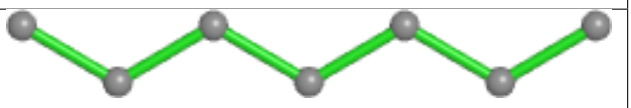


Rings

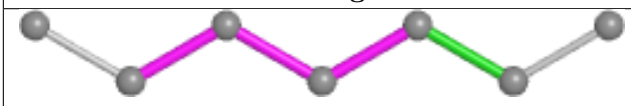
Ligand DMU C 316



Bond lengths



Bond angles



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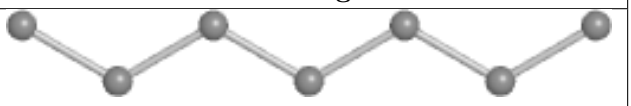
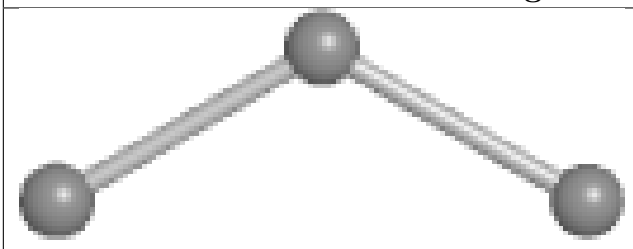
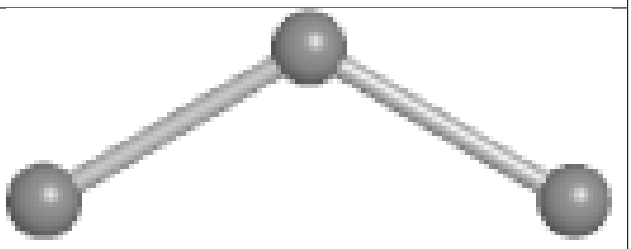


Rings

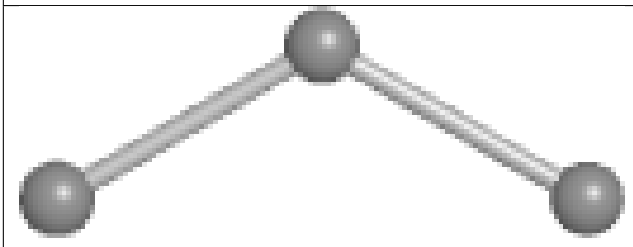
Ligand N2O A 607



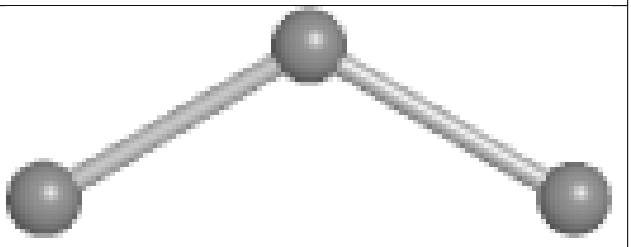
Bond lengths



Bond angles

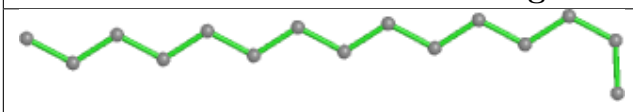


Torsions

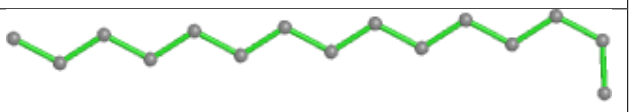


Rings

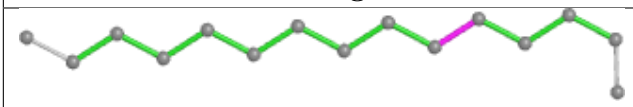
Ligand LFA C 313



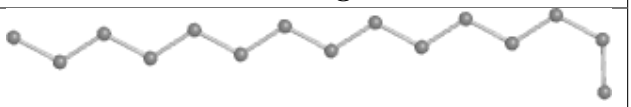
Bond lengths



Bond angles

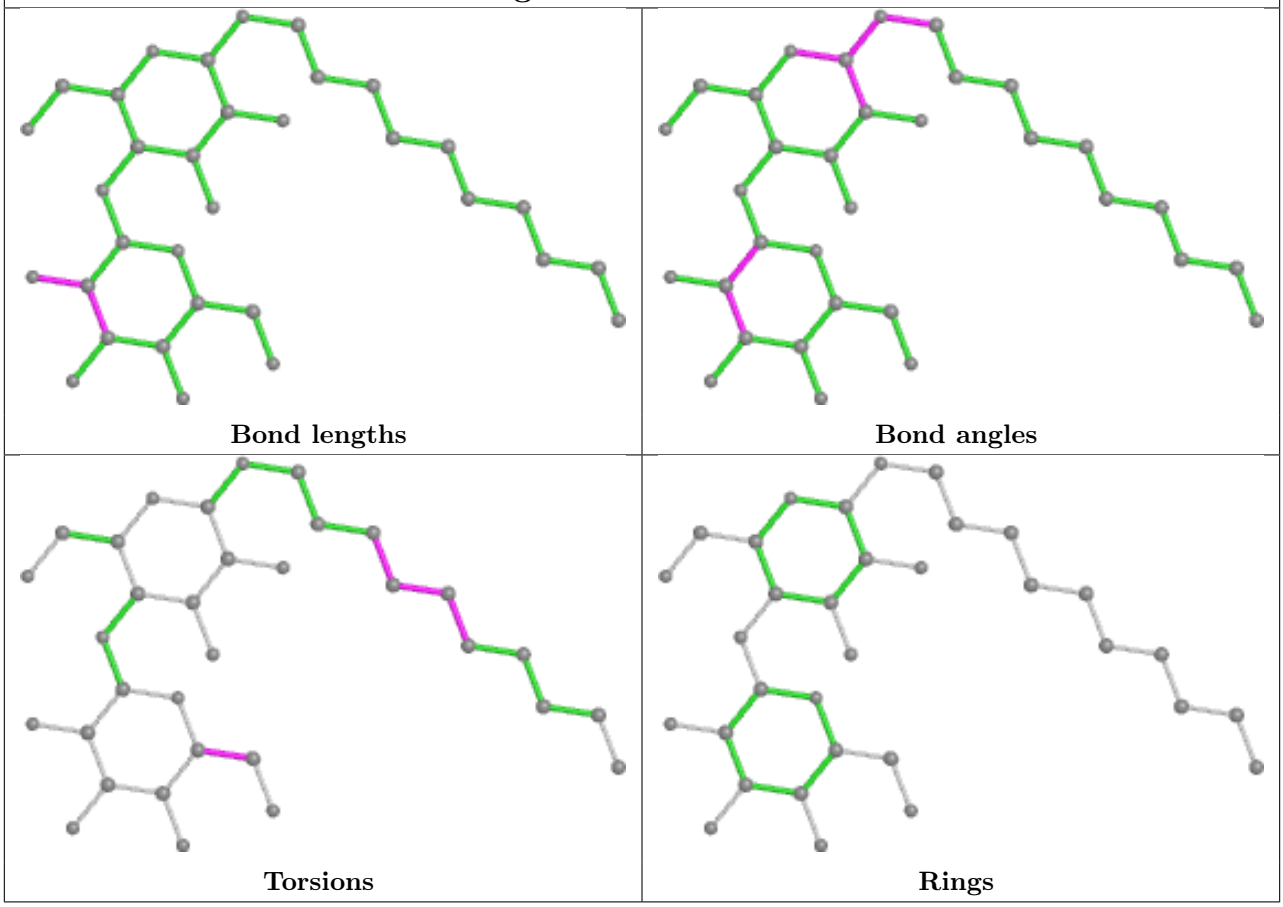


Torsions

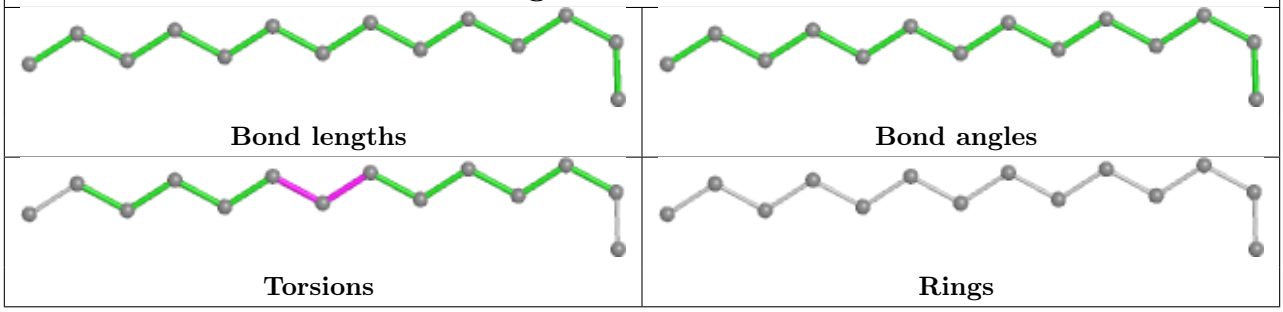


Rings

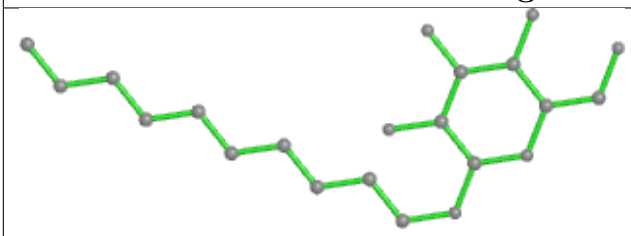
Ligand DMU M 101



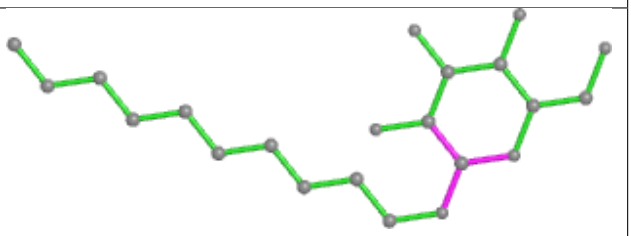
Ligand LFA N 609



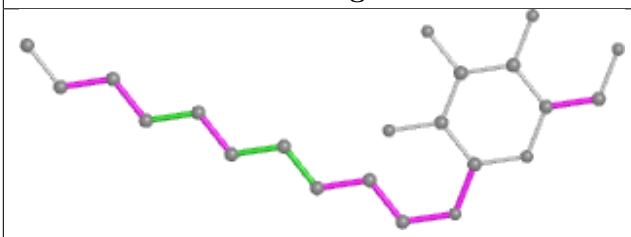
Ligand DMU B 308



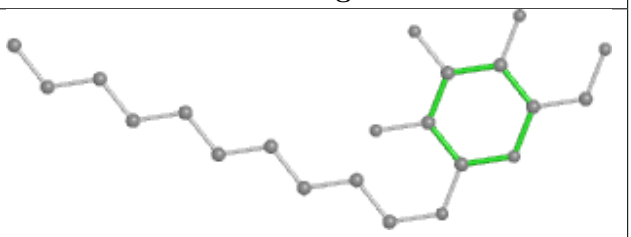
Bond lengths



Bond angles

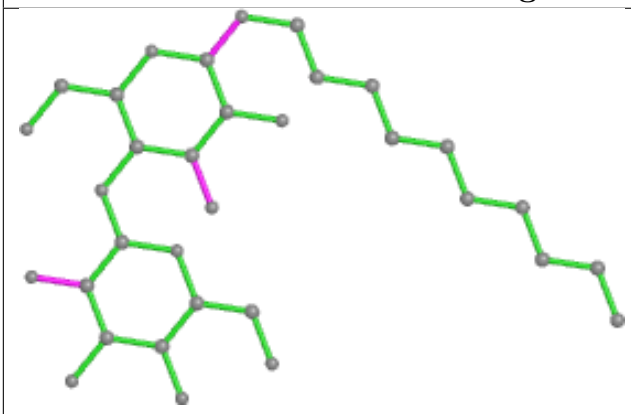


Torsions

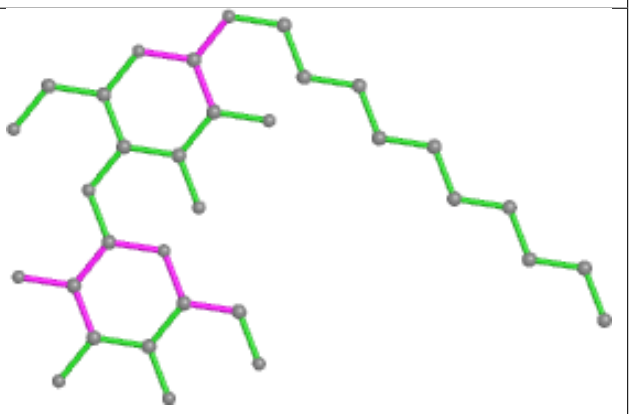


Rings

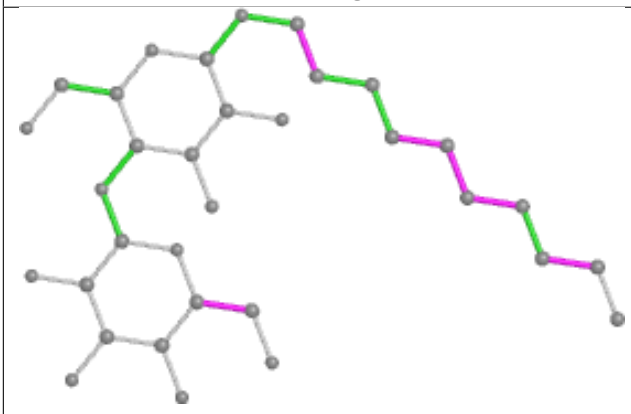
Ligand DMU Z 101



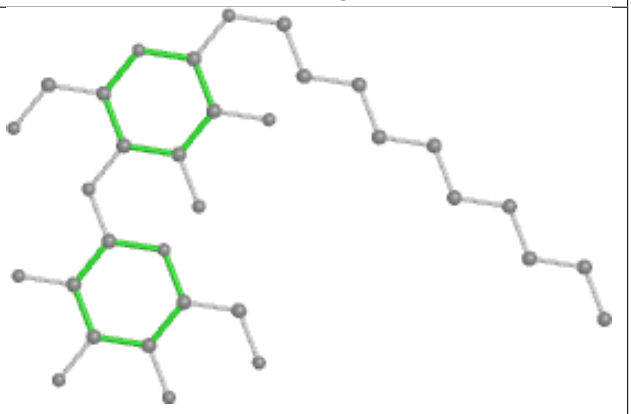
Bond lengths



Bond angles

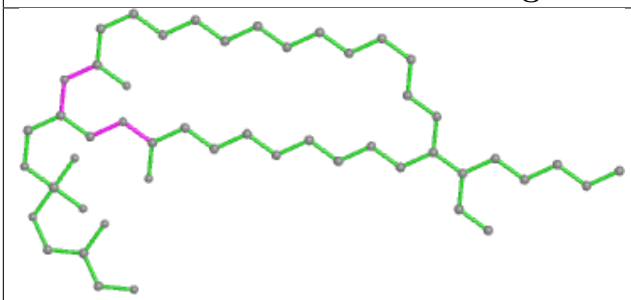


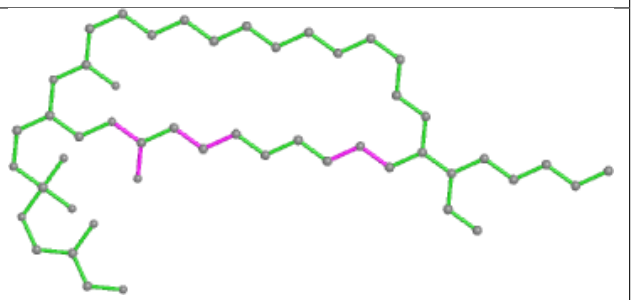
Torsions

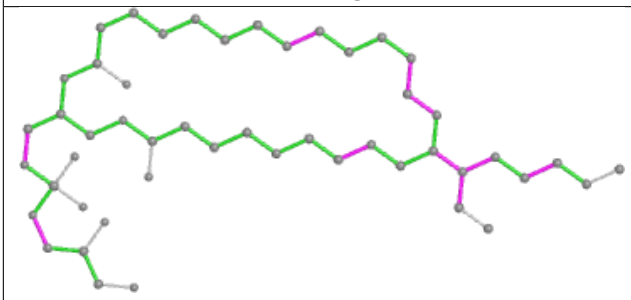


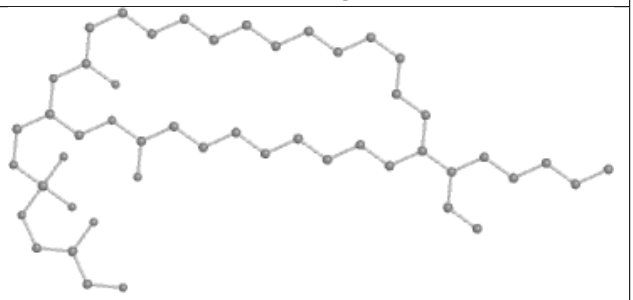
Rings

Ligand PGV P 304

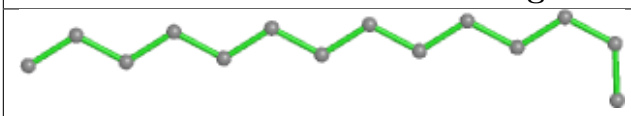

Bond lengths

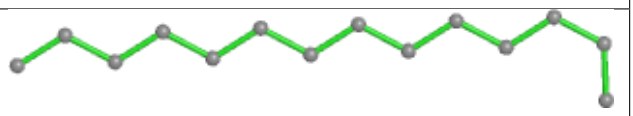

Bond angles

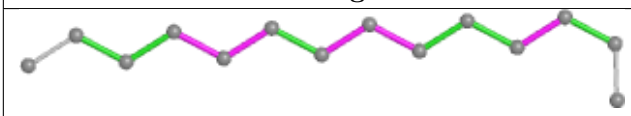

Torsions

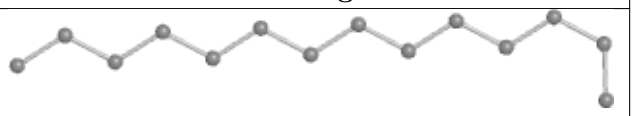

Rings

Ligand LFA A 609

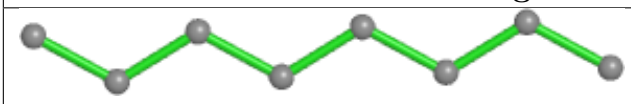

Bond lengths


Bond angles


Torsions


Rings

Ligand DMU M 102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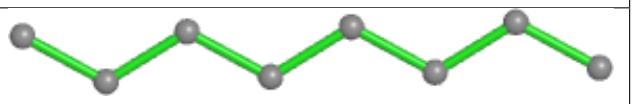
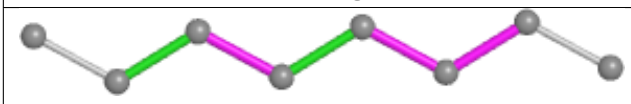
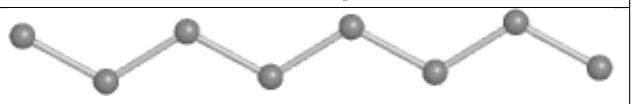
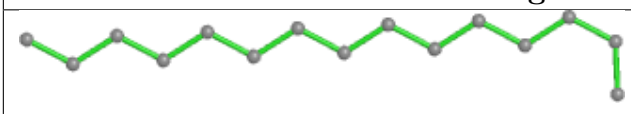
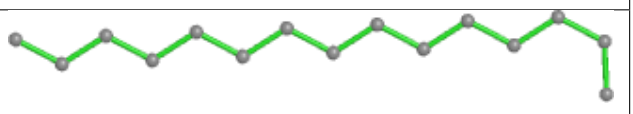

Bond angles

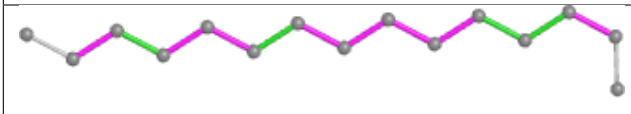

Torsions

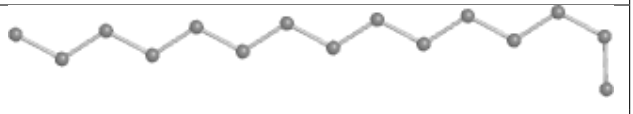

Rings

Ligand LFA C 325

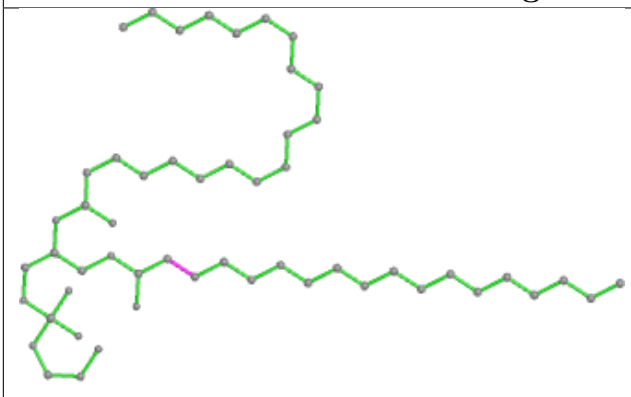

Bond lengths


Bond angles

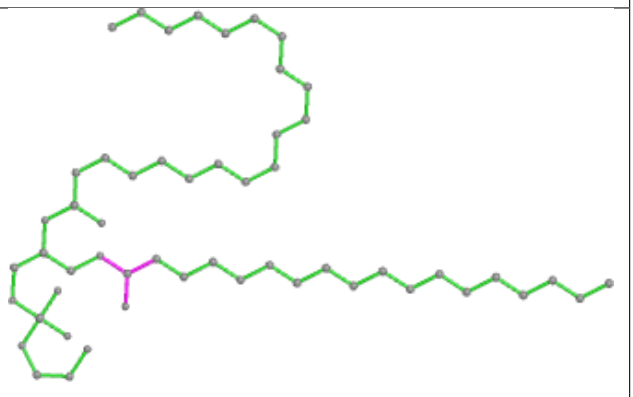

Torsions


Rings

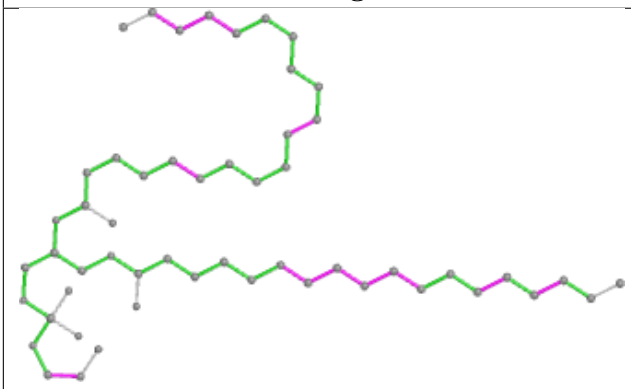
Ligand PEK G 101



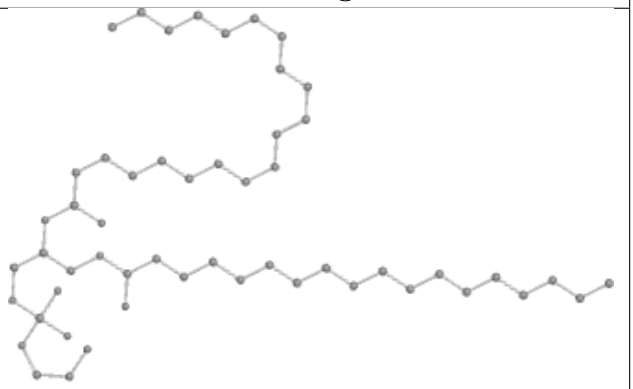
Bond lengths



Bond angles

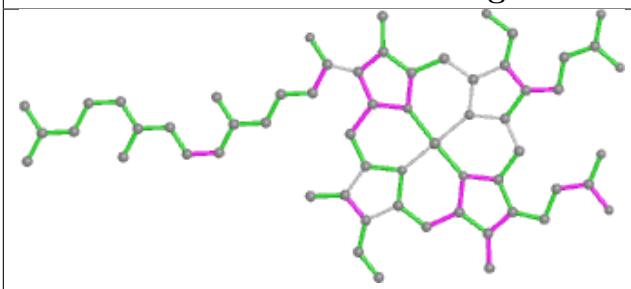


Torsions

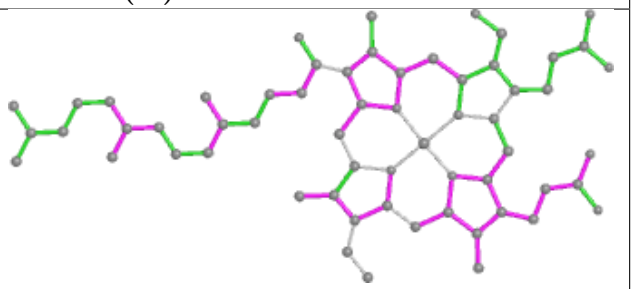


Rings

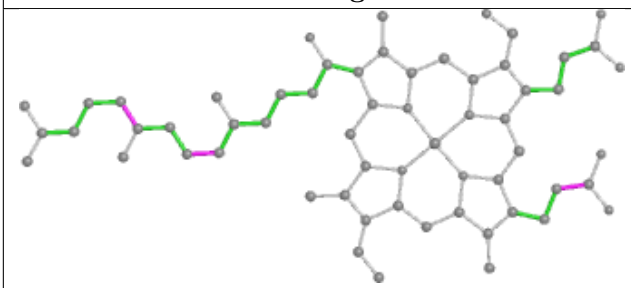
Ligand HEA A 601 (A)



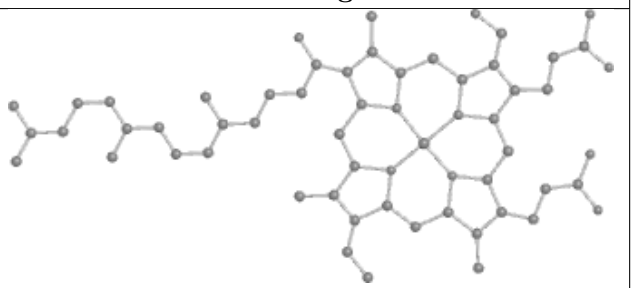
Bond lengths



Bond angles

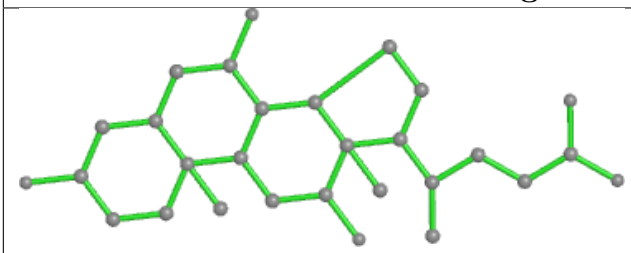


Torsions

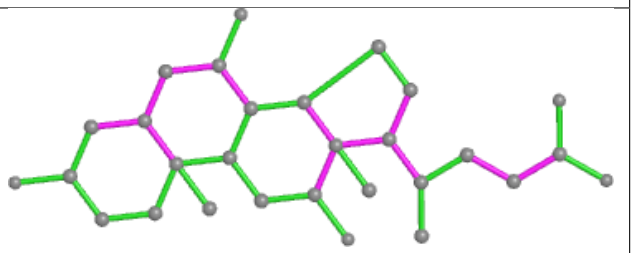


Rings

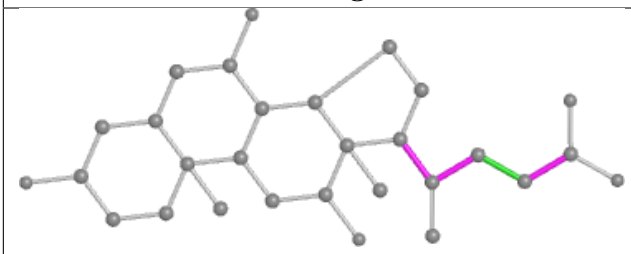
Ligand CHD C 305



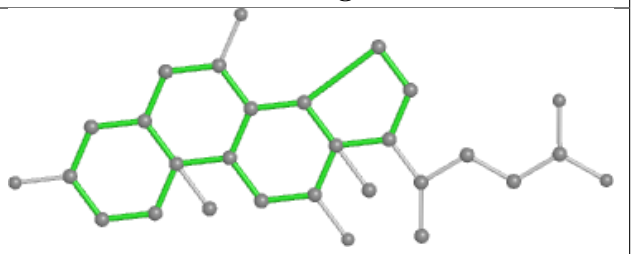
Bond lengths



Bond angles

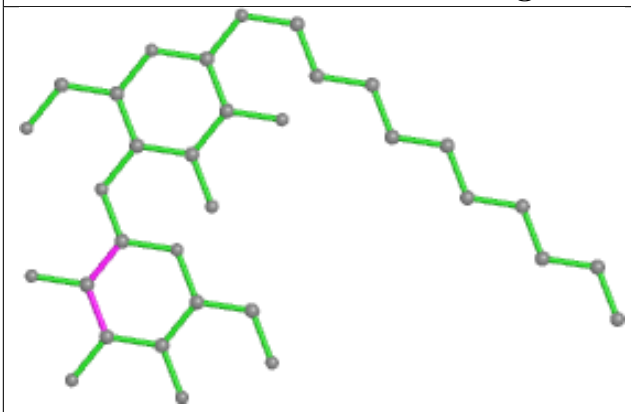


Torsions

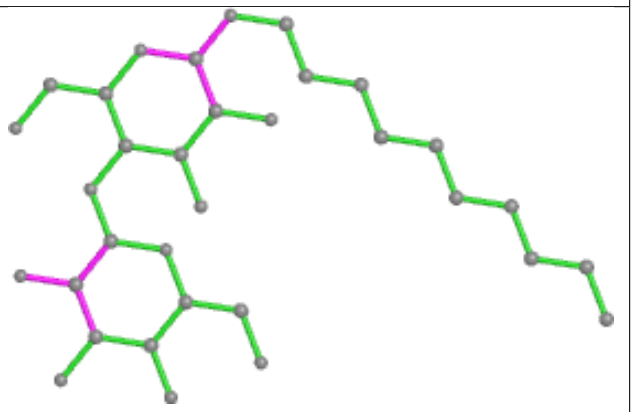


Rings

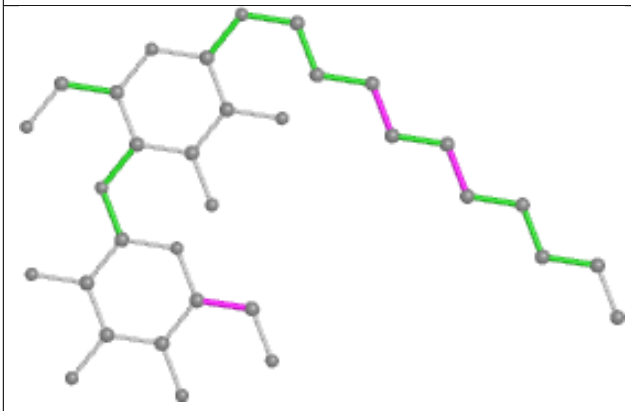
Ligand DMU H 101



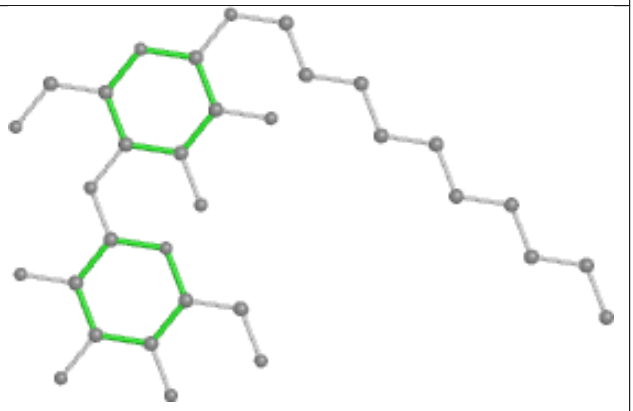
Bond lengths



Bond angles

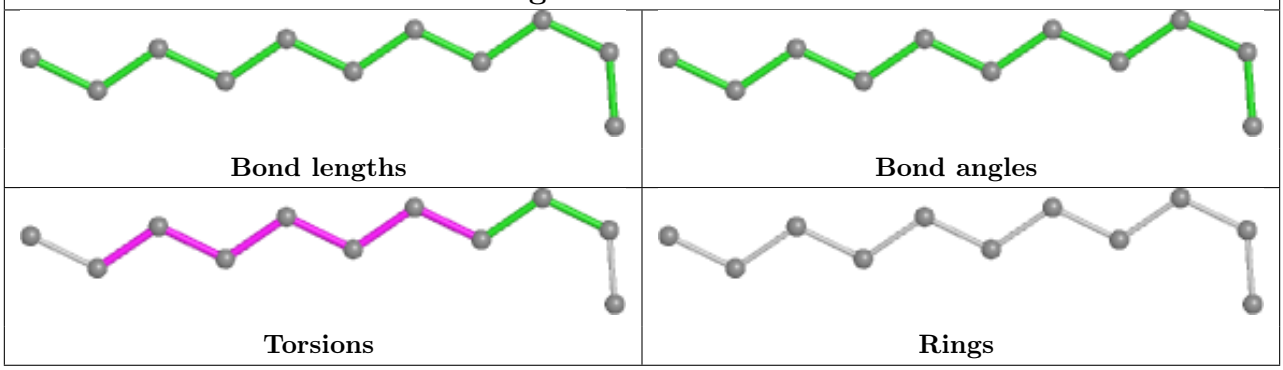


Torsions



Rings

Ligand LFA C 307



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

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

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

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	36	TRP	6.5
9	V	72	ALA	5.5
8	H	45	ALA	5.4
6	S	3	GLY	4.8
2	O	113	TYR	4.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	FME	A	1	10/11	0.92	0.14	42,47,73,81	0
1	FME	N	1	10/11	0.94	0.13	43,49,72,85	0
2	FME	B	1	10/11	0.97	0.10	36,38,46,80	0
2	FME	O	1	10/11	0.98	0.08	42,44,53,68	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	DMU	C	317	22/33	0.68	0.31	39,55,63,76	22

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	EDO	P	322	4/4	0.71	0.35	31,34,36,39	4
21	DMU	P	317	22/33	0.73	0.30	34,52,64,65	22
20	LFA	P	311	11/20	0.73	0.43	43,51,60,66	11
22	EDO	C	322	4/4	0.74	0.35	33,36,36,40	4
21	DMU	A	610	7/33	0.74	0.40	45,48,51,56	7
21	DMU	N	610	7/33	0.78	0.44	50,55,59,60	7
20	LFA	C	308	6/20	0.79	0.41	38,42,48,48	6
20	LFA	C	313	15/20	0.81	0.27	42,46,56,59	15
20	LFA	C	314	13/20	0.81	0.31	46,50,63,65	13
20	LFA	C	311	14/20	0.81	0.36	37,54,60,61	14
25	CHD	C	305	29/29	0.81	0.17	56,67,79,96	0
21	DMU	C	315	33/33	0.82	0.33	37,50,58,60	33
20	LFA	O	303	11/20	0.82	0.32	43,52,59,60	11
22	EDO	A	613	4/4	0.82	0.33	34,40,43,48	4
25	CHD	P	306	29/29	0.82	0.17	58,68,79,91	0
21	DMU	C	318	33/33	0.83	0.30	37,53,65,77	33
22	EDO	E	201	4/4	0.83	0.37	35,38,41,43	4
20	LFA	C	312	11/20	0.83	0.28	39,44,55,59	11
20	LFA	C	325	15/20	0.83	0.38	44,48,57,60	15
20	LFA	P	312	11/20	0.83	0.30	34,46,55,60	11
21	DMU	C	319	33/33	0.84	0.24	40,58,67,74	33
22	EDO	R	203	4/4	0.84	0.32	37,40,48,51	4
20	LFA	O	302	17/20	0.84	0.32	40,55,69,72	17
20	LFA	G	103	14/20	0.84	0.28	36,44,57,58	14
21	DMU	C	316	7/33	0.85	0.31	41,46,56,62	7
22	EDO	N	613	4/4	0.85	0.25	36,42,42,45	4
21	DMU	P	319	33/33	0.85	0.21	47,65,78,81	33
20	LFA	A	609	14/20	0.86	0.26	37,46,53,55	14
21	DMU	M	102	8/33	0.86	0.23	40,44,47,51	8
20	LFA	P	301	15/20	0.86	0.30	40,50,56,59	15
21	DMU	O	304	22/33	0.86	0.29	48,62,73,79	22
20	LFA	P	314	13/20	0.86	0.26	40,47,60,73	13
21	DMU	P	318	33/33	0.86	0.27	44,53,62,80	33
20	LFA	P	308	11/20	0.86	0.31	42,49,55,56	11
22	EDO	A	612	4/4	0.86	0.20	29,30,31,33	4
27	CDL	P	305	87/100	0.86	0.19	44,72,100,133	0
20	LFA	T	102	14/20	0.87	0.34	41,54,64,67	14
20	LFA	T	103	11/20	0.87	0.30	48,53,62,63	11
21	DMU	P	323	22/33	0.87	0.22	42,53,58,69	22
21	DMU	Q	201	33/33	0.87	0.21	39,50,59,69	33
20	LFA	B	307	17/20	0.87	0.29	39,51,68,71	17
21	DMU	C	323	22/33	0.87	0.29	41,54,62,63	22

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	DMU	C	324	33/33	0.87	0.17	39,50,67,77	33
21	DMU	H	101	33/33	0.87	0.24	33,45,58,68	33
21	DMU	A	617	11/33	0.87	0.30	43,50,56,60	11
21	DMU	B	308	22/33	0.87	0.29	53,67,76,80	22
21	DMU	N	611	33/33	0.87	0.21	38,51,70,72	33
20	LFA	C	310	11/20	0.87	0.30	47,57,63,67	11
21	DMU	P	315	33/33	0.87	0.27	41,50,61,62	33
27	CDL	C	304	87/100	0.87	0.18	43,67,96,103	0
27	CDL	I	101	64/100	0.87	0.17	45,69,91,95	0
20	LFA	P	309	6/20	0.87	0.33	39,41,46,47	6
27	CDL	V	101	64/100	0.87	0.16	50,73,93,108	0
27	CDL	Y	101	94/100	0.87	0.17	47,72,106,134	0
20	LFA	A	608	14/20	0.88	0.24	35,42,63,67	14
20	LFA	P	313	15/20	0.88	0.20	38,44,50,51	15
20	LFA	C	309	18/20	0.88	0.21	37,43,49,50	18
20	LFA	P	310	18/20	0.88	0.25	37,49,55,59	18
20	LFA	C	307	11/20	0.88	0.26	44,44,49,49	11
21	DMU	P	324	33/33	0.88	0.17	41,53,78,87	33
21	DMU	O	306	11/33	0.88	0.28	41,43,51,57	11
21	DMU	U	101	33/33	0.89	0.24	33,46,60,61	33
21	DMU	N	601	11/33	0.89	0.31	43,55,62,68	11
21	DMU	B	302	11/33	0.89	0.26	42,45,53,55	11
22	EDO	C	320	4/4	0.89	0.28	43,51,54,66	4
21	DMU	A	611	33/33	0.90	0.18	32,43,53,59	33
22	EDO	R	202	4/4	0.90	0.20	34,35,39,40	4
27	CDL	L	101	94/100	0.90	0.15	41,68,94,113	0
21	DMU	Z	102	22/33	0.90	0.33	50,54,62,64	22
21	DMU	B	303	11/33	0.90	0.26	43,50,62,64	11
21	DMU	P	316	7/33	0.90	0.25	44,50,58,59	7
22	EDO	P	320	4/4	0.91	0.24	51,53,64,77	4
21	DMU	D	201	33/33	0.91	0.16	28,44,55,61	33
21	DMU	J	101	11/33	0.91	0.28	51,58,65,72	11
21	DMU	W	101	11/33	0.92	0.25	53,60,70,70	11
21	DMU	P	307	11/33	0.92	0.24	40,47,51,60	11
21	DMU	B	304	22/33	0.92	0.19	40,61,66,84	22
20	LFA	N	609	14/20	0.92	0.20	36,43,56,58	14
22	EDO	A	615	4/4	0.92	0.20	41,43,45,47	4
21	DMU	L	102	22/33	0.92	0.26	44,50,54,61	22
21	DMU	O	308	22/33	0.92	0.17	36,46,53,58	22
22	EDO	P	321	4/4	0.93	0.26	35,35,38,40	4
22	EDO	F	102	4/4	0.93	0.16	24,24,29,33	4
22	EDO	G	102	4/4	0.93	0.15	34,35,35,37	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	EDO	N	612	4/4	0.93	0.15	30,33,33,33	4
21	DMU	C	306	11/33	0.93	0.22	47,48,55,59	11
22	EDO	C	321	4/4	0.93	0.21	34,35,36,37	4
21	DMU	Z	103	8/33	0.94	0.18	44,46,50,51	8
22	EDO	N	614	4/4	0.94	0.19	30,30,31,32	4
22	EDO	N	616	4/4	0.94	0.19	30,31,31,36	4
22	EDO	E	202	4/4	0.94	0.24	33,34,34,37	4
22	EDO	E	203	4/4	0.94	0.25	33,36,38,41	4
21	DMU	Z	101	33/33	0.94	0.09	51,55,66,72	0
21	DMU	O	307	11/33	0.94	0.21	40,45,53,58	11
22	EDO	A	614	4/4	0.94	0.19	27,28,28,28	4
25	CHD	C	301	29/29	0.95	0.08	33,37,39,43	0
26	UNX	P	303	1/1	0.95	0.35	41,41,41,41	0
25	CHD	P	302	29/29	0.96	0.07	33,38,41,44	0
21	DMU	M	101	33/33	0.96	0.07	43,48,61,67	0
26	UNX	C	302	1/1	0.96	0.22	39,39,39,39	0
22	EDO	R	201	4/4	0.96	0.22	51,52,55,58	4
22	EDO	O	309	4/4	0.96	0.12	34,35,35,39	4
29	PEK	G	101	53/53	0.96	0.11	34,49,75,96	0
29	PEK	T	101	53/53	0.96	0.11	37,51,82,93	0
19	N2O	N	608	3/3	0.97	0.19	39,39,42,45	0
25	CHD	O	301	29/29	0.97	0.06	32,36,39,44	0
22	EDO	F	103	4/4	0.97	0.10	30,31,33,36	4
22	EDO	T	104	4/4	0.97	0.08	36,37,39,40	4
23	PGV	N	617	51/51	0.97	0.09	32,43,63,68	0
25	CHD	B	306	29/29	0.97	0.07	33,36,40,47	0
22	EDO	N	615	4/4	0.97	0.15	33,35,36,37	4
18	PER	N	607	2/2	0.98	0.09	32,32,32,35	0
23	PGV	P	304	51/51	0.98	0.08	31,40,76,88	0
22	EDO	S	102	4/4	0.98	0.06	25,26,26,30	4
22	EDO	B	305	4/4	0.98	0.09	27,28,29,31	4
23	PGV	A	616	51/51	0.98	0.08	30,39,66,71	0
23	PGV	C	303	51/51	0.98	0.08	31,40,75,82	0
14	HEA	A	601[A]	60/60	0.99	0.05	26,29,40,43	9
19	N2O	A	607	3/3	0.99	0.15	33,33,35,44	0
14	HEA	A	601[B]	60/60	0.99	0.05	26,29,41,43	9
14	HEA	A	602	60/60	0.99	0.05	27,30,36,40	0
14	HEA	N	602[A]	60/60	0.99	0.05	29,33,42,47	9
14	HEA	N	602[B]	60/60	0.99	0.05	29,33,41,44	9
14	HEA	N	603	60/60	0.99	0.06	29,32,38,43	0
17	NA	A	605	1/1	0.99	0.05	33,33,33,33	0
22	EDO	S	103	4/4	0.99	0.07	28,32,35,36	4

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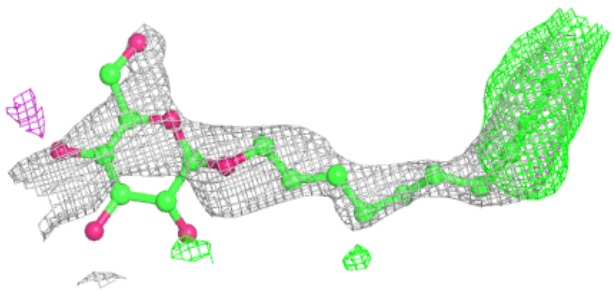
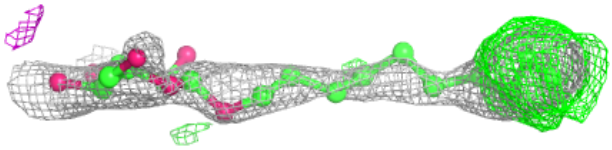
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	PER	A	606	2/2	0.99	0.05	28,28,28,34	0
16	MG	N	605	1/1	1.00	0.02	33,33,33,33	0
15	CU	A	603	1/1	1.00	0.01	29,29,29,29	0
17	NA	N	606	1/1	1.00	0.04	40,40,40,40	0
24	CUA	B	301	2/2	1.00	0.02	31,31,31,31	0
24	CUA	O	305	2/2	1.00	0.02	36,36,36,36	0
28	ZN	F	101	1/1	1.00	0.01	35,35,35,35	0
28	ZN	S	101	1/1	1.00	0.01	36,36,36,36	0
15	CU	N	604	1/1	1.00	0.01	31,31,31,31	0
16	MG	A	604	1/1	1.00	0.03	30,30,30,30	0

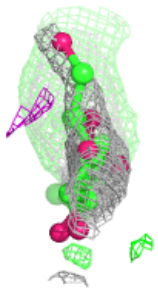
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU C 317:

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

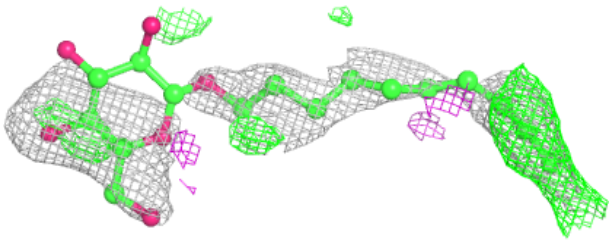


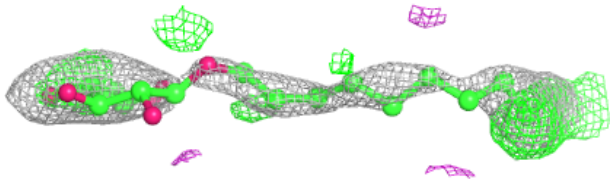


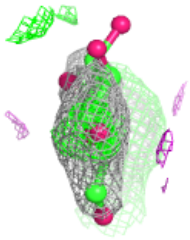


Electron density around DMU P 317:

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

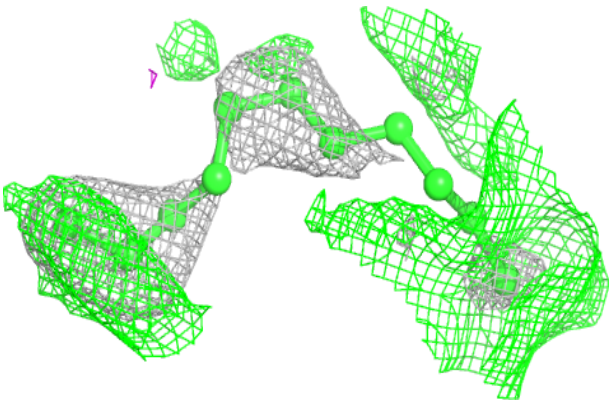


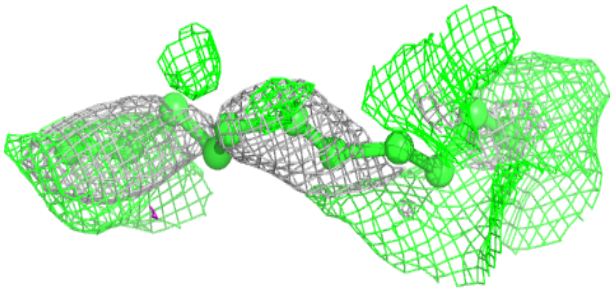


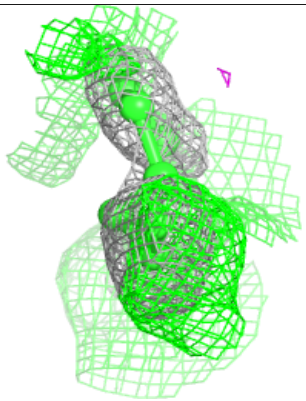


Electron density around LFA P 311:

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

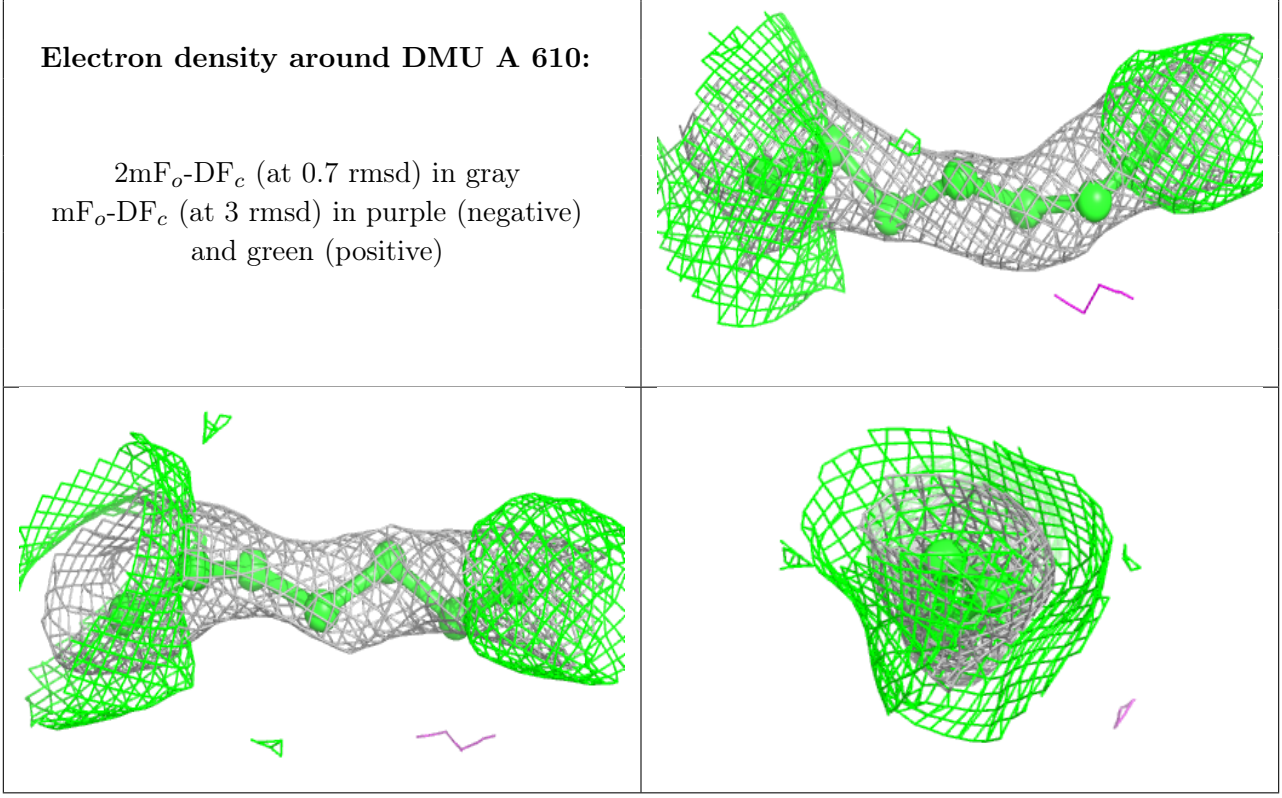






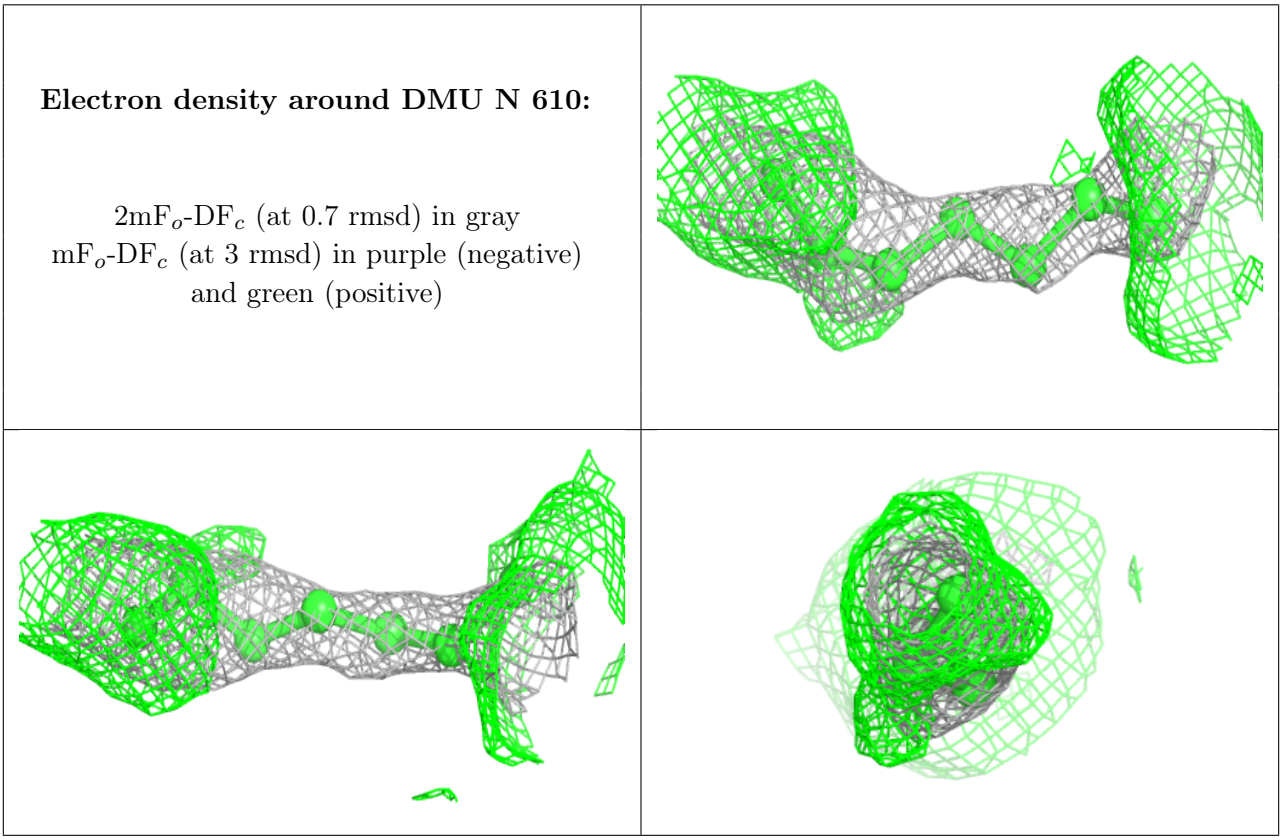
Electron density around DMU A 610:

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



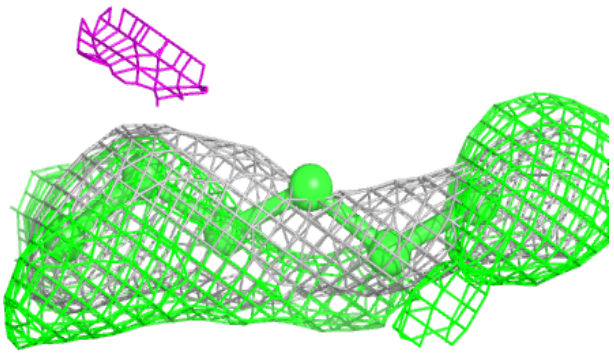
Electron density around DMU N 610:

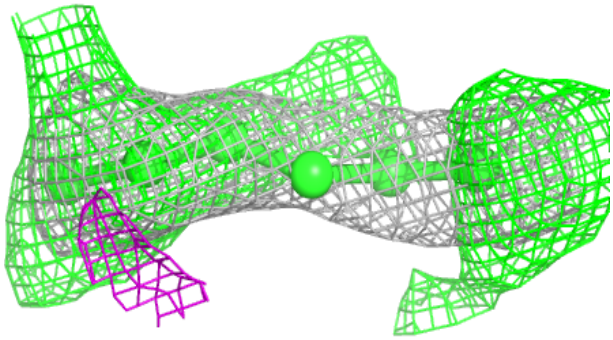
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

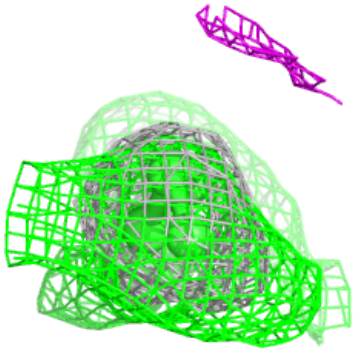


Electron density around LFA C 308:

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

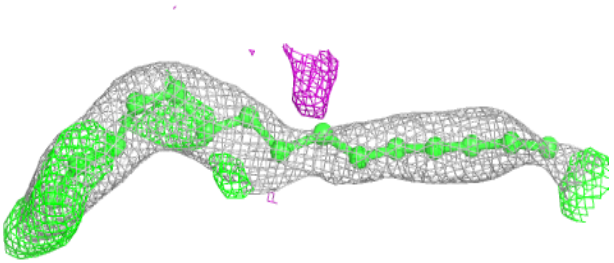


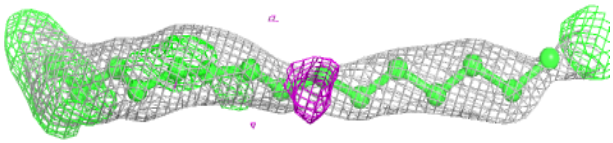


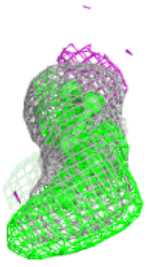


Electron density around LFA C 313:

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

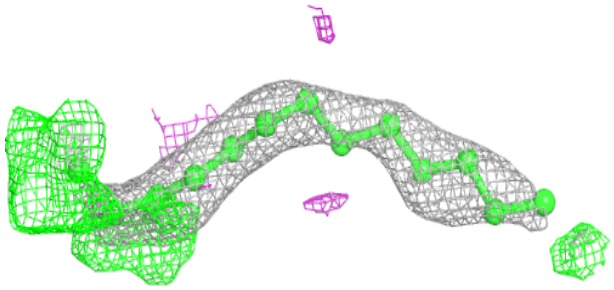


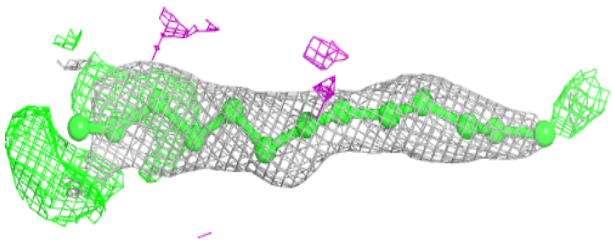


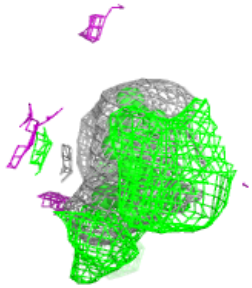


Electron density around LFA C 314:

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

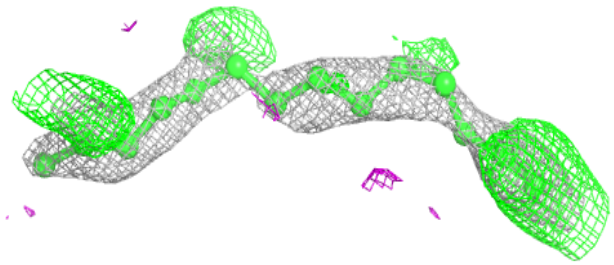


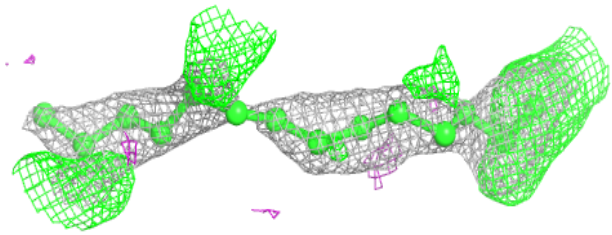


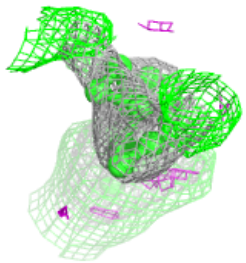


Electron density around LFA C 311:

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

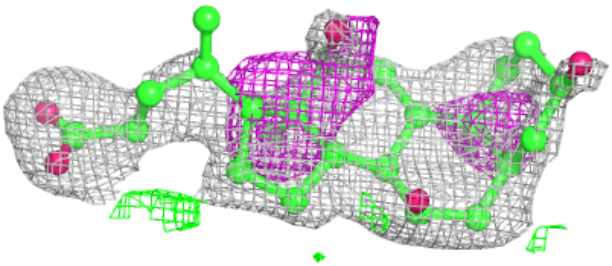


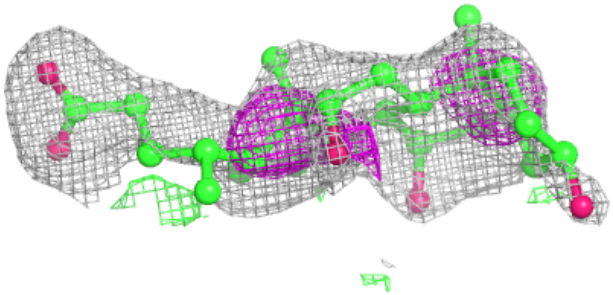


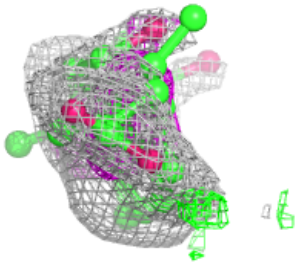


Electron density around CHD C 305:

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

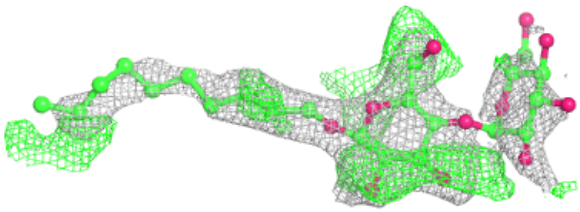


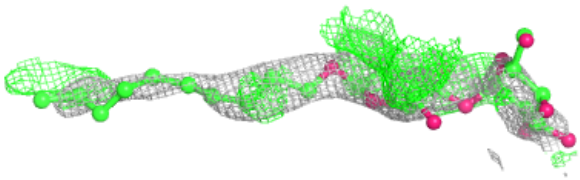


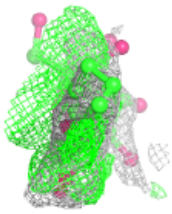


Electron density around DMU C 315:

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

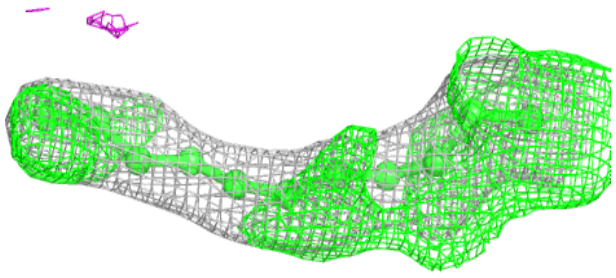


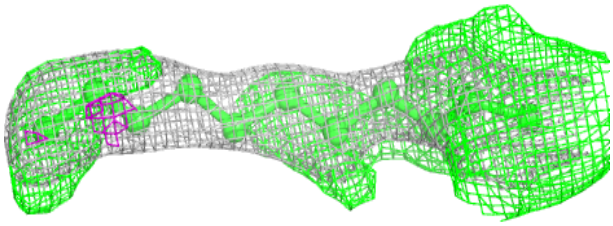


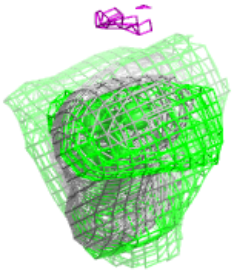


Electron density around LFA O 303:

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

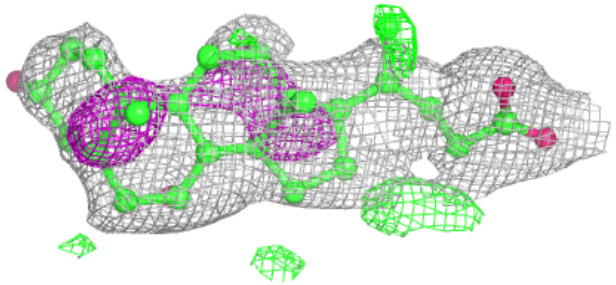


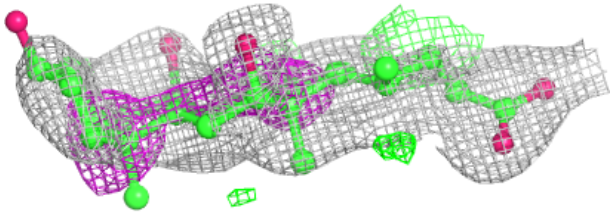


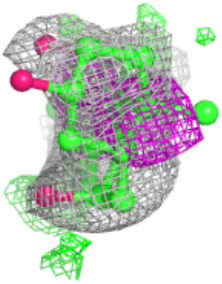


Electron density around CHD P 306:

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

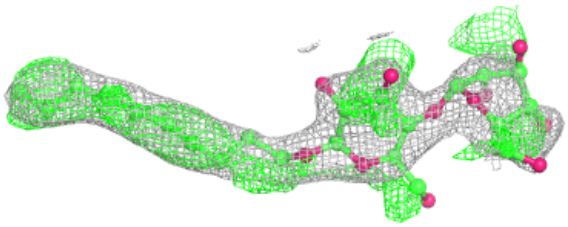


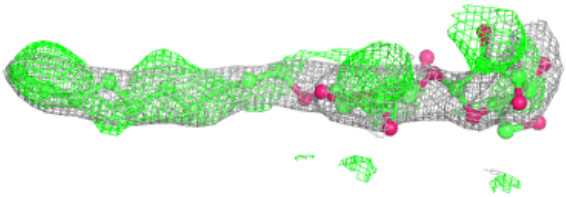


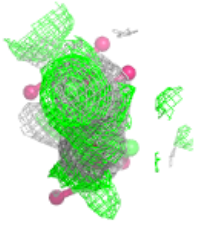


Electron density around DMU C 318:

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

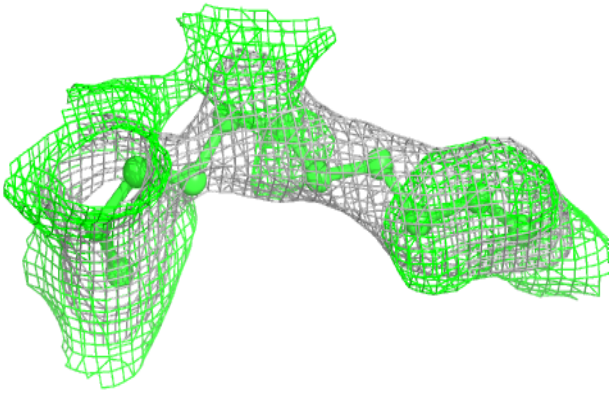


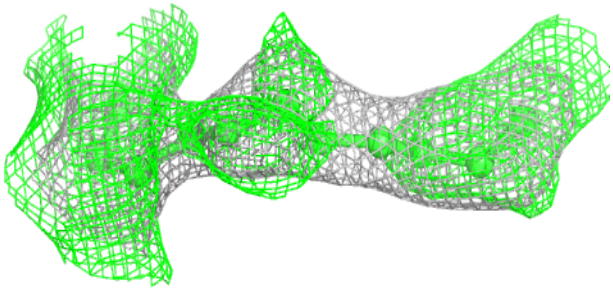


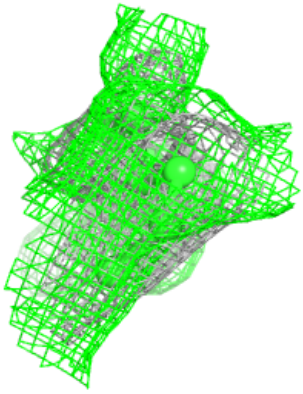


Electron density around LFA C 312:

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

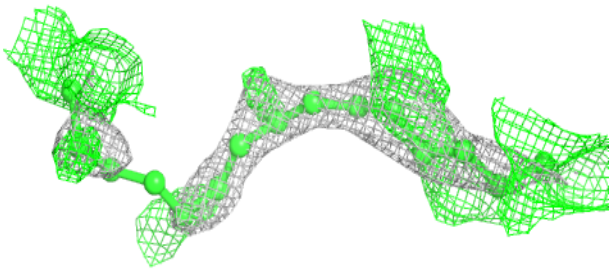


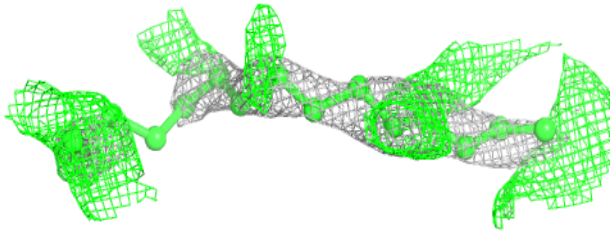


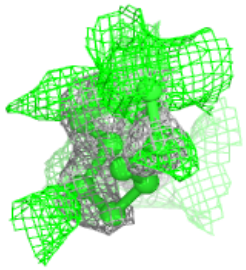


Electron density around LFA C 325:

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

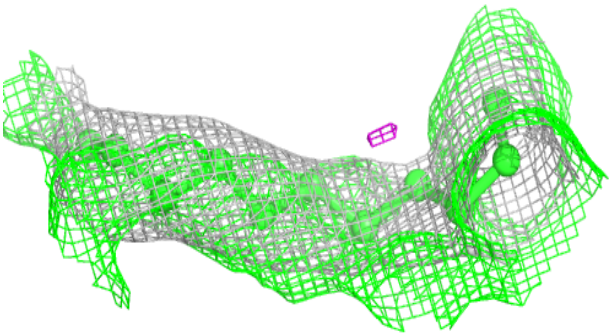


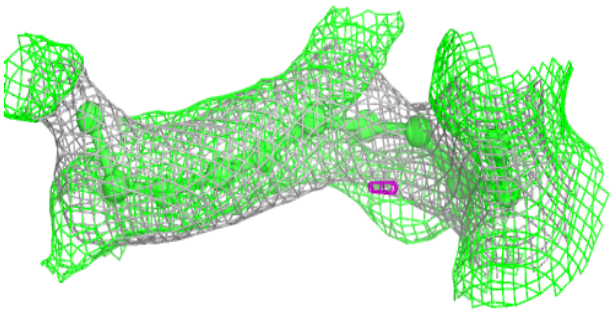


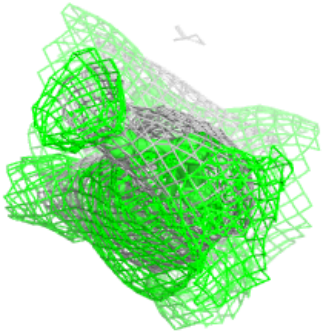


Electron density around LFA P 312:

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

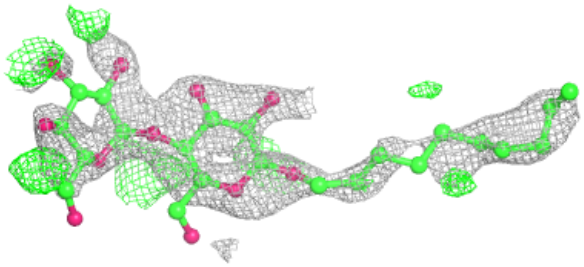


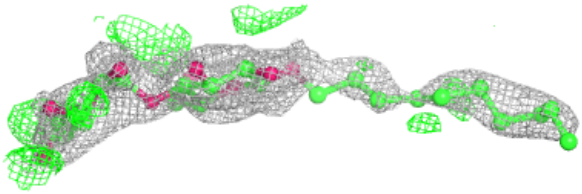


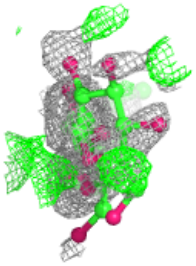


Electron density around DMU C 319:

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

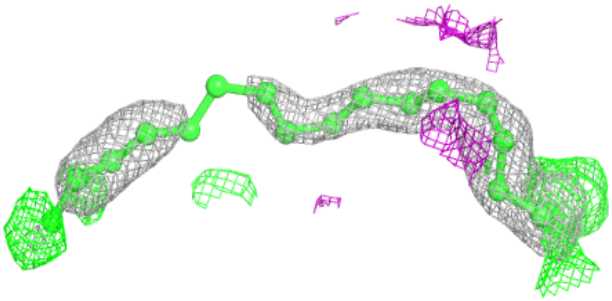


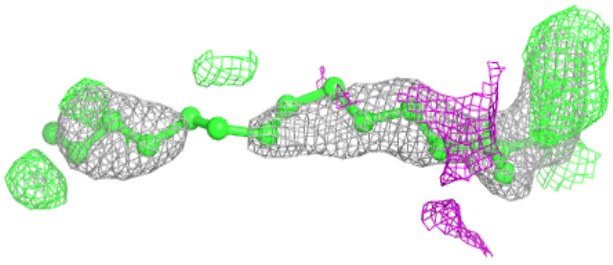


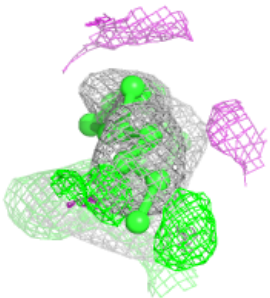


Electron density around LFA O 302:

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

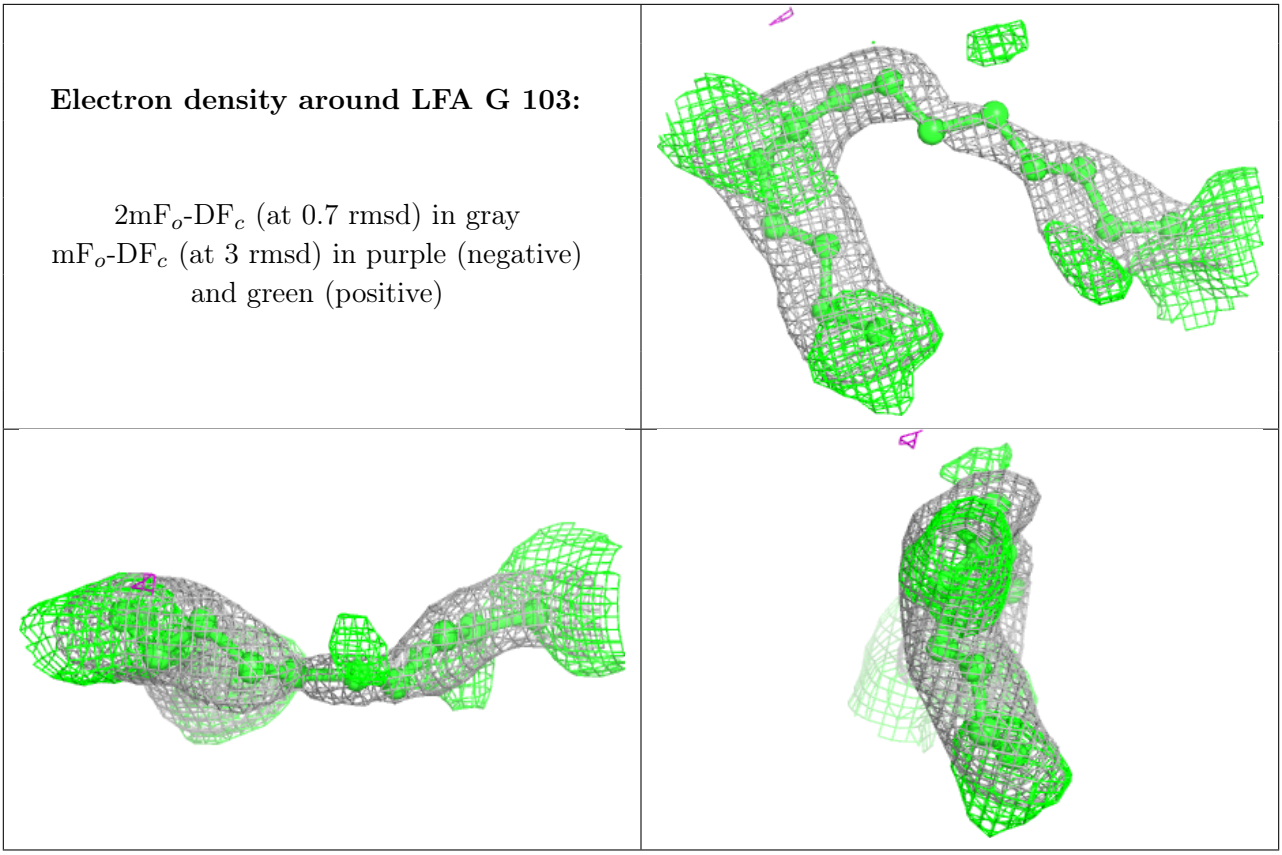






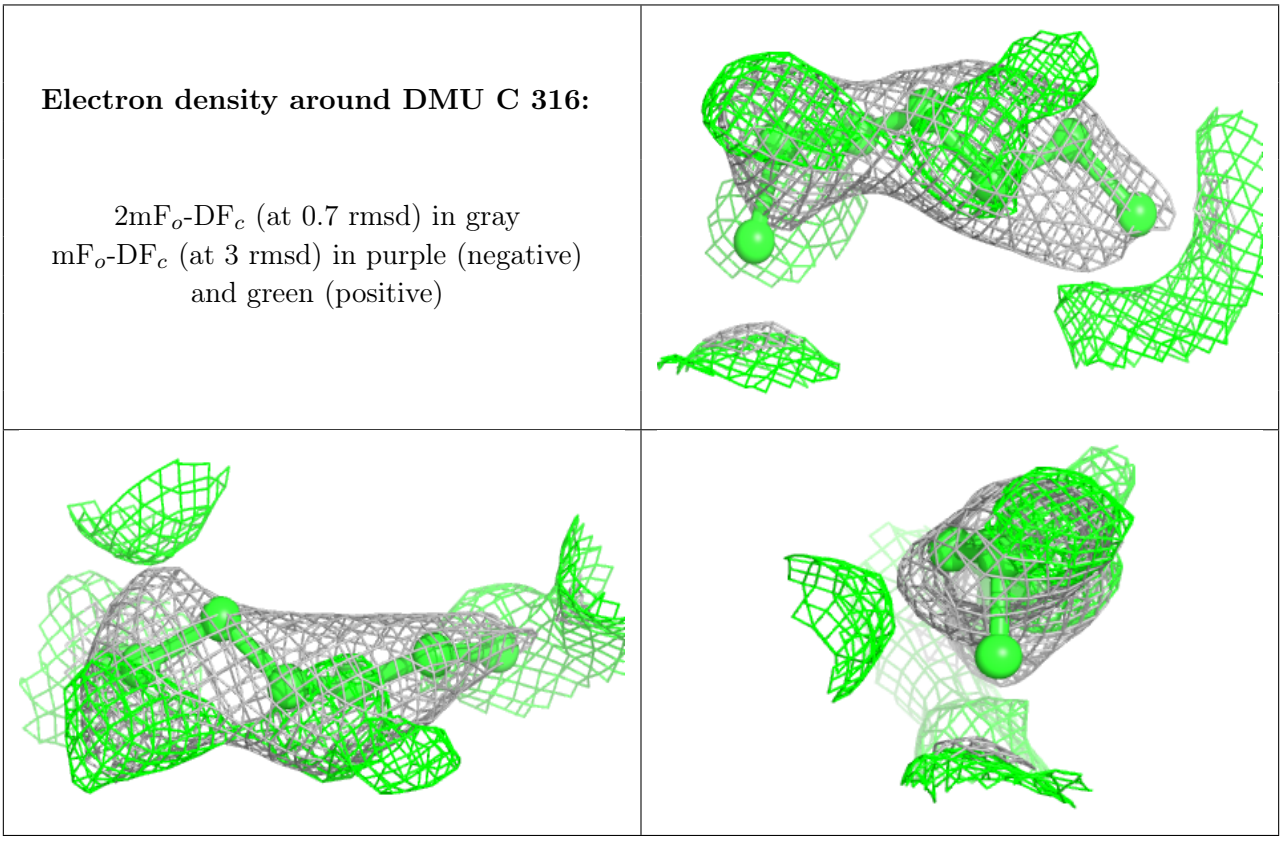
Electron density around LFA G 103:

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



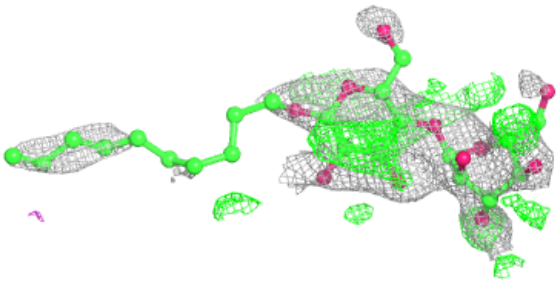
Electron density around DMU C 316:

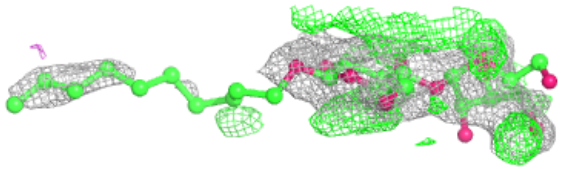
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

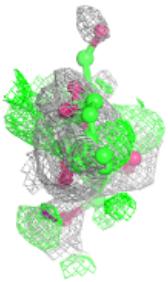


Electron density around DMU P 319:

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

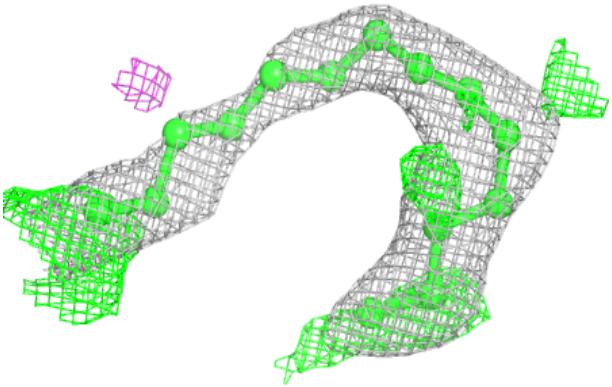


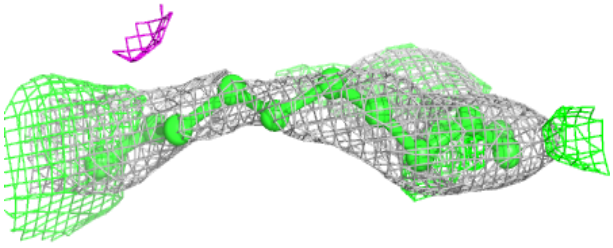


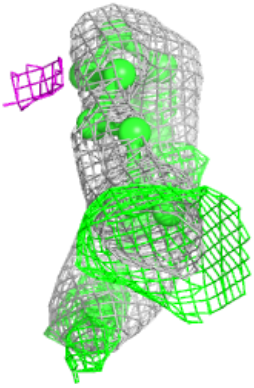


Electron density around LFA A 609:

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

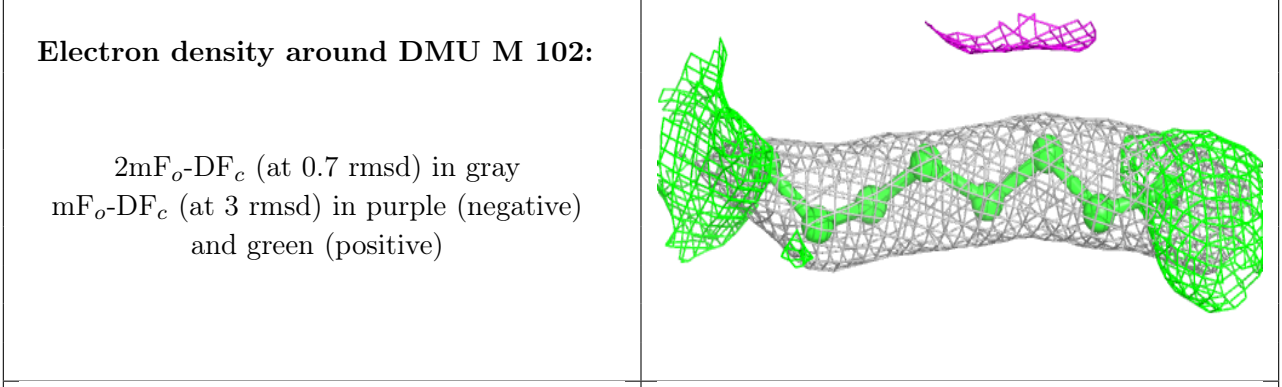






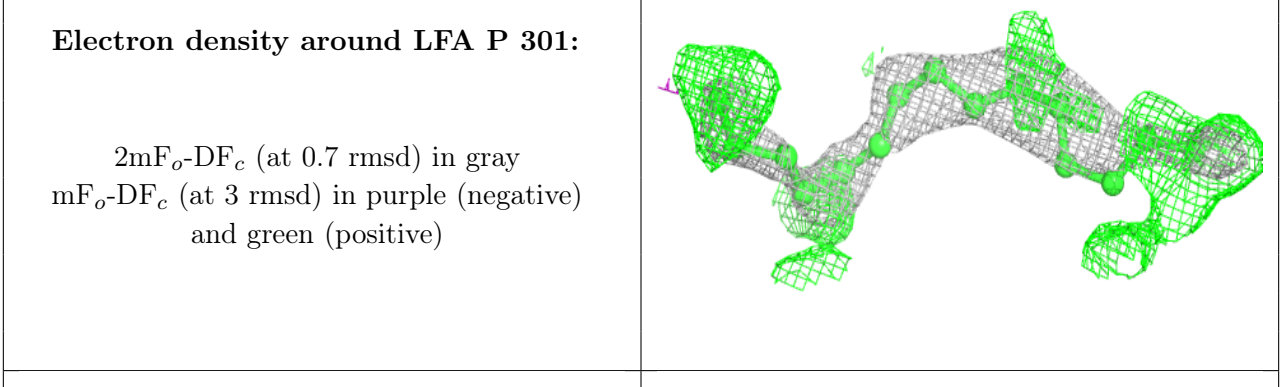
Electron density around DMU M 102:

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



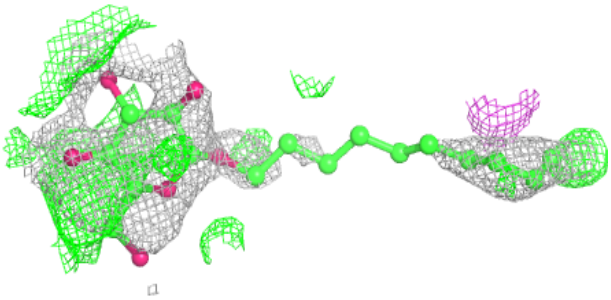
Electron density around LFA P 301:

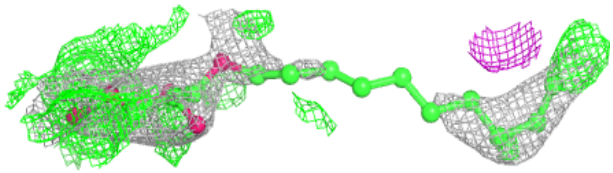
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

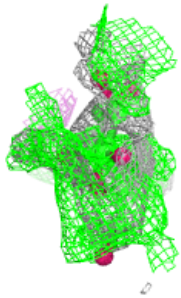


Electron density around DMU O 304:

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

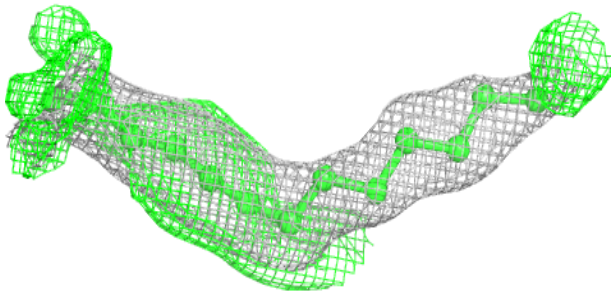


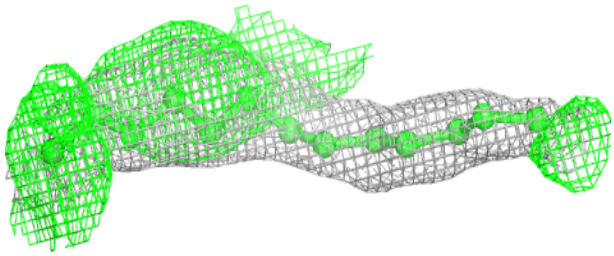


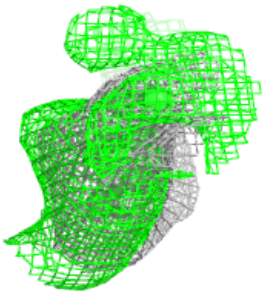


Electron density around LFA P 314:

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

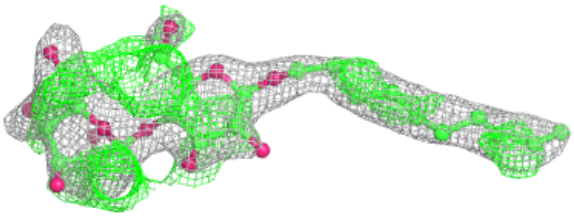


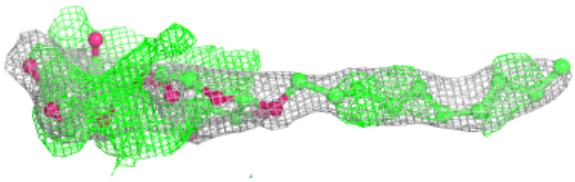


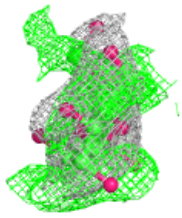


Electron density around DMU P 318:

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

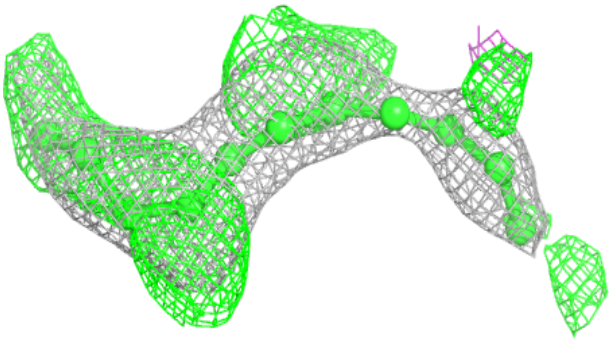


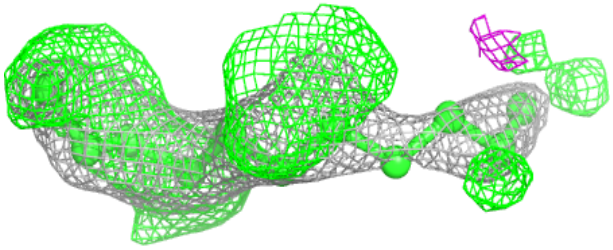


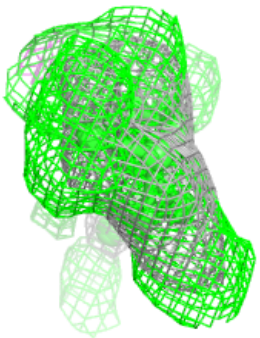


Electron density around LFA P 308:

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

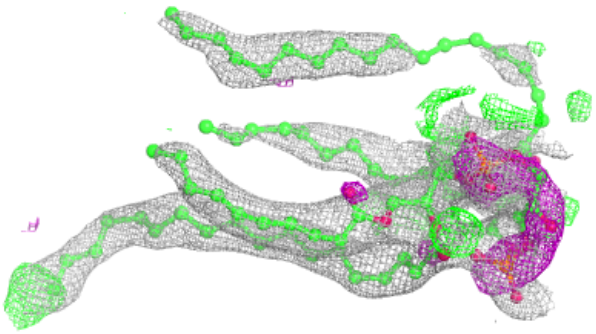


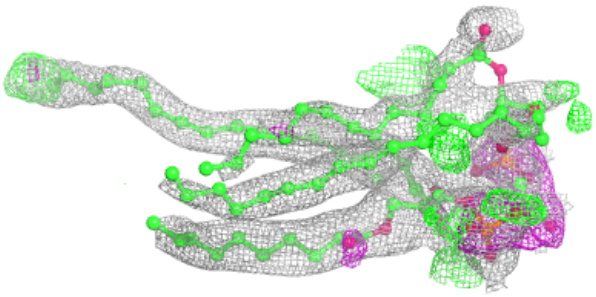


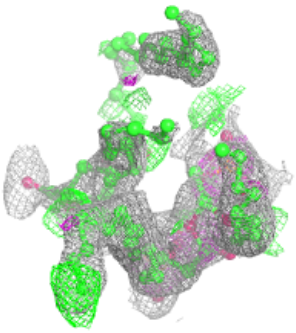


Electron density around CDL P 305:

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

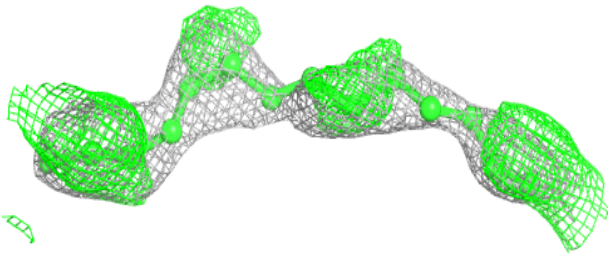


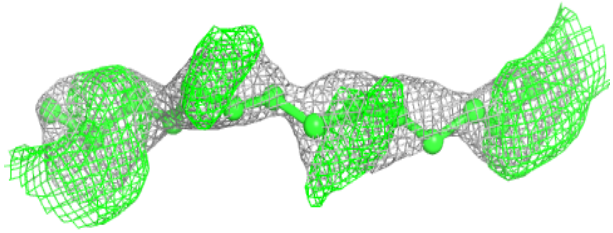


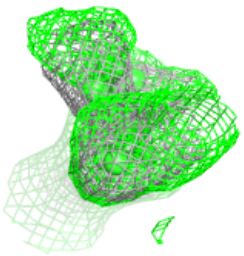


Electron density around LFA T 102:

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

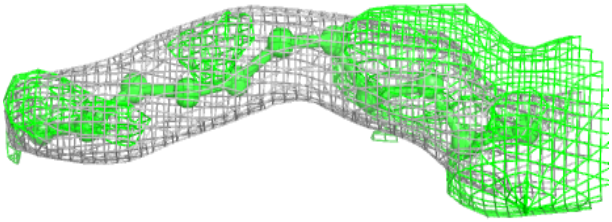


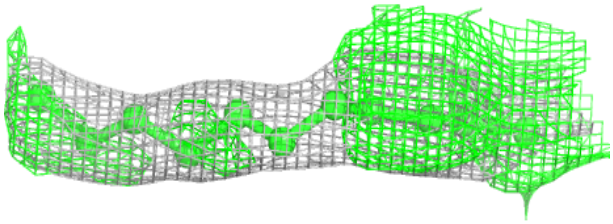


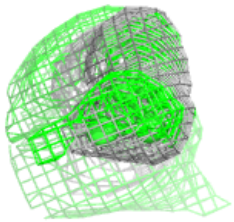


Electron density around LFA T 103:

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

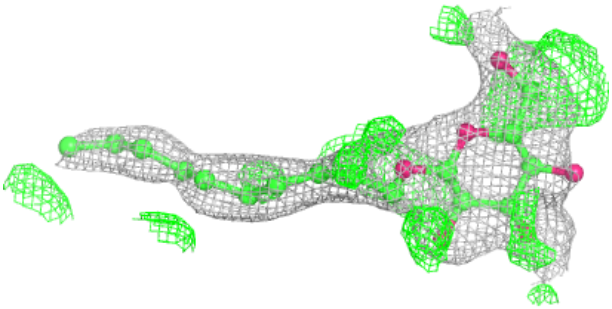


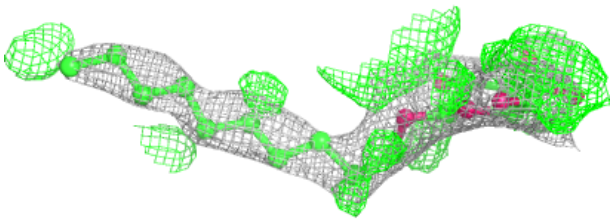


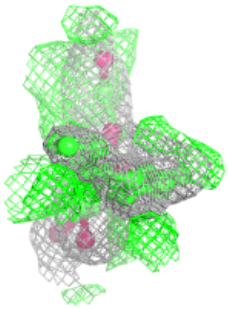


Electron density around DMU P 323:

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

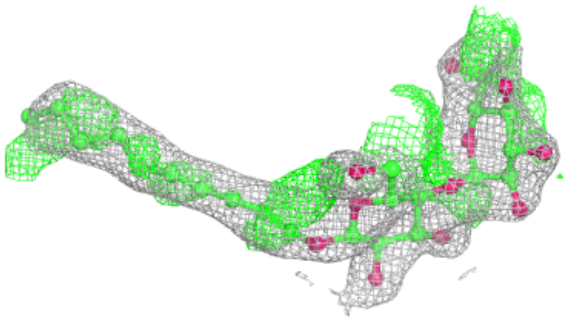


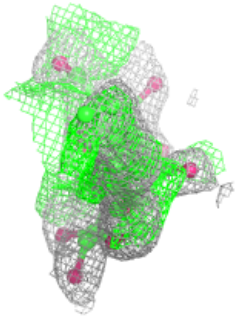




Electron density around DMU Q 201:

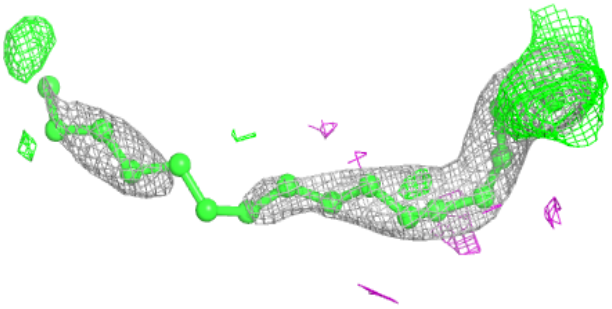
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

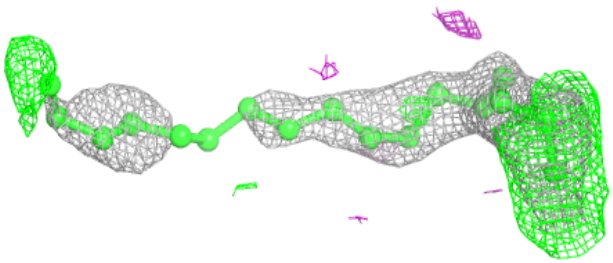


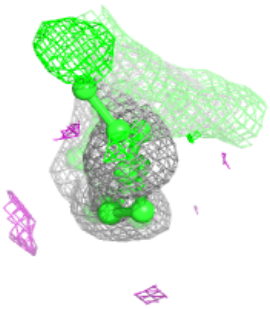


Electron density around LFA B 307:

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

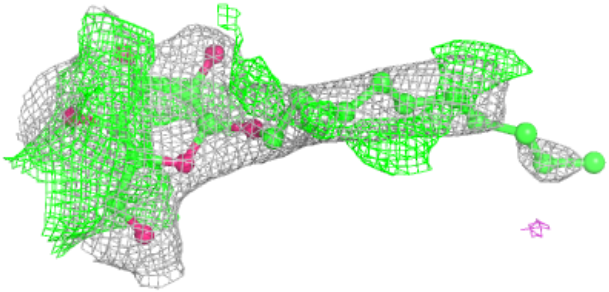


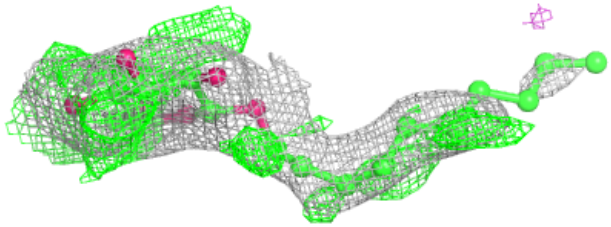


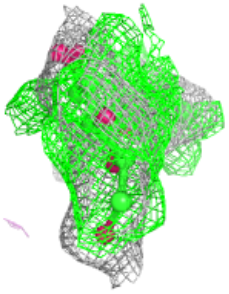


Electron density around DMU C 323:

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

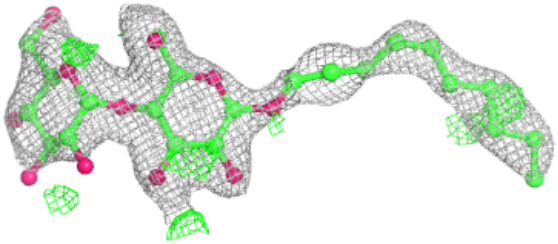


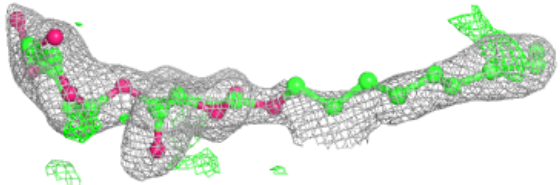


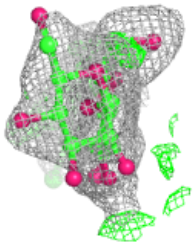


Electron density around DMU C 324:

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

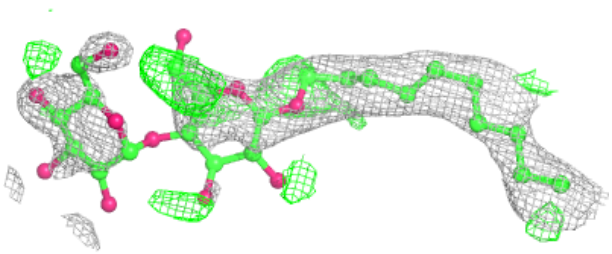


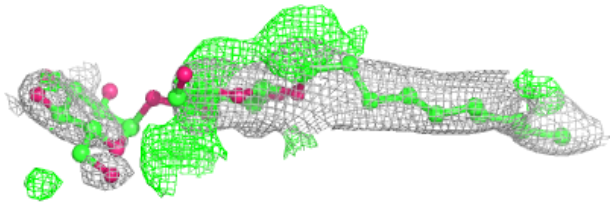


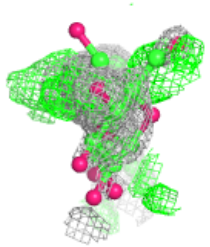


Electron density around DMU H 101:

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

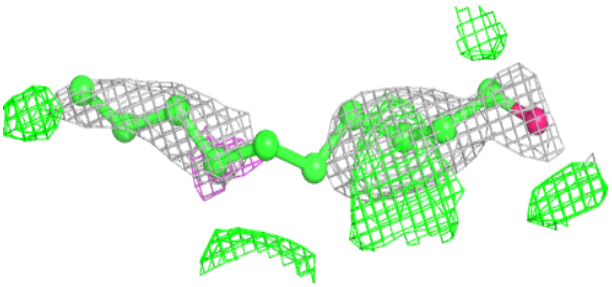


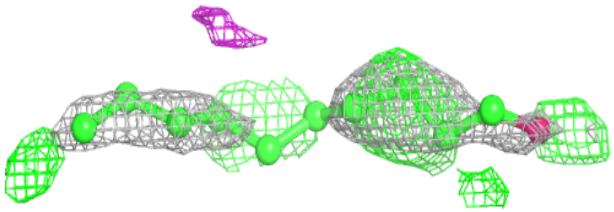


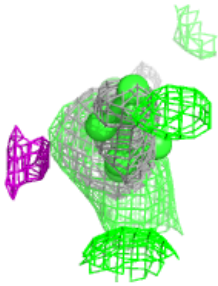


Electron density around DMU A 617:

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

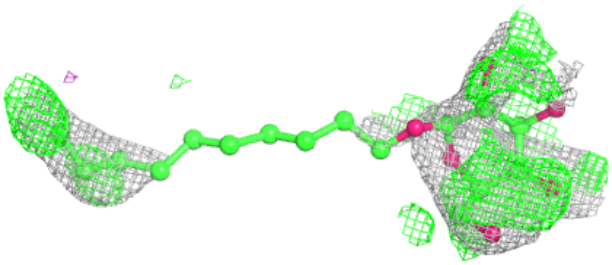


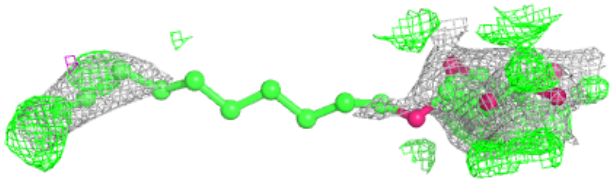


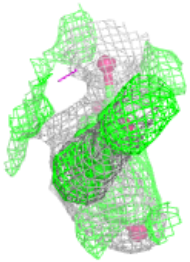


Electron density around DMU B 308:

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

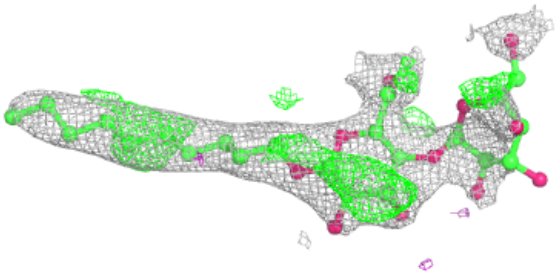


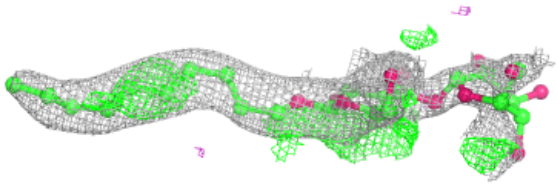


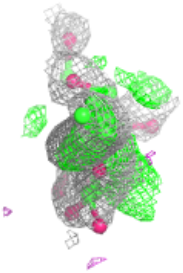


Electron density around DMU N 611:

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

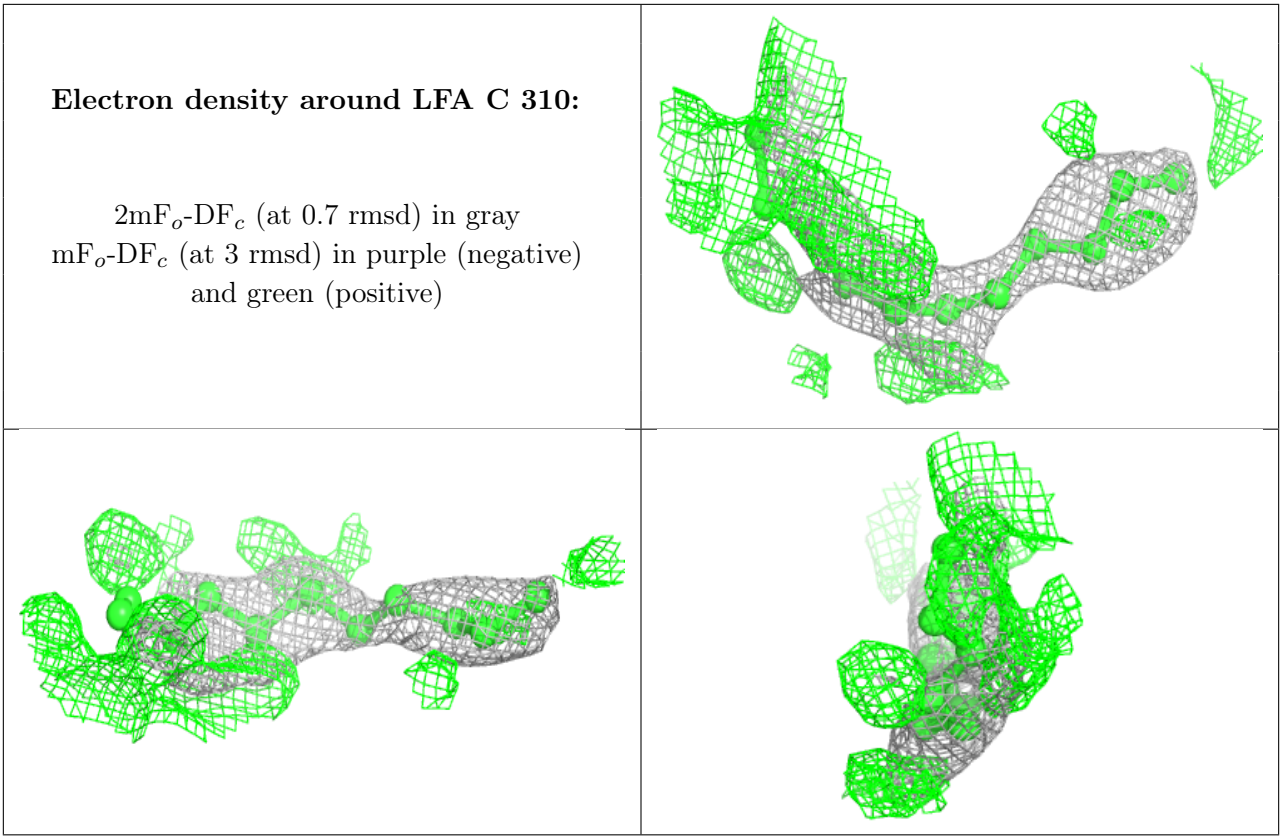






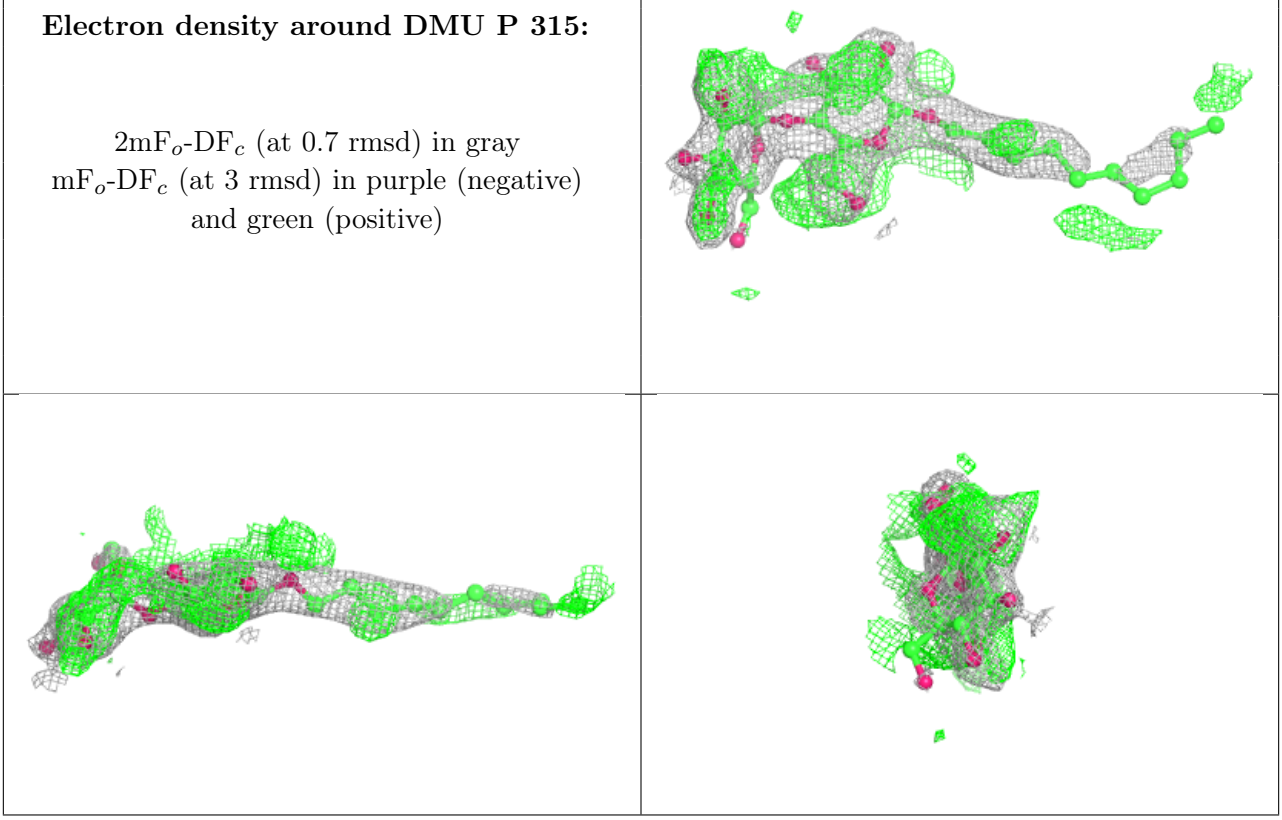
Electron density around LFA C 310:

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



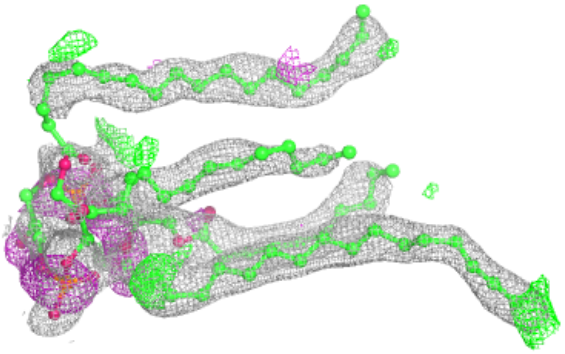
Electron density around DMU P 315:

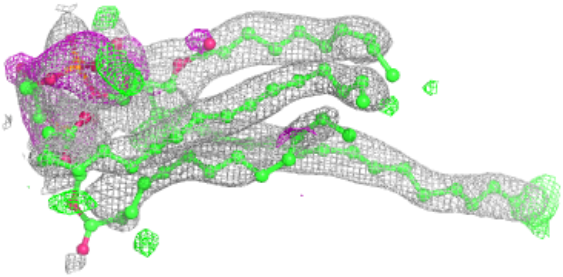
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

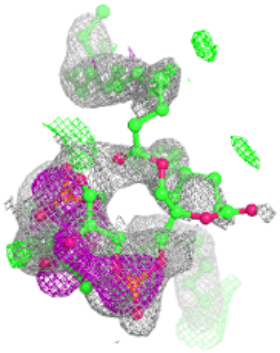


Electron density around CDL C 304:

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

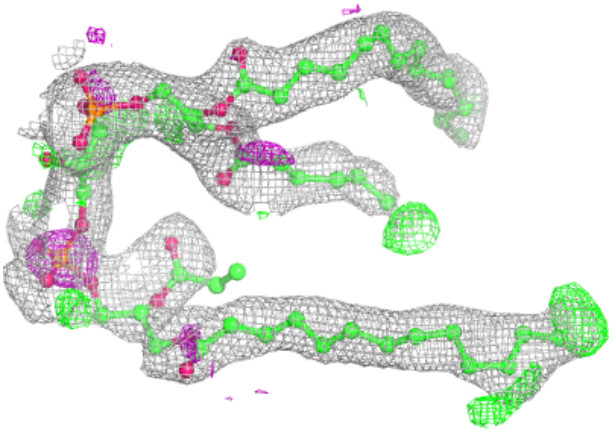


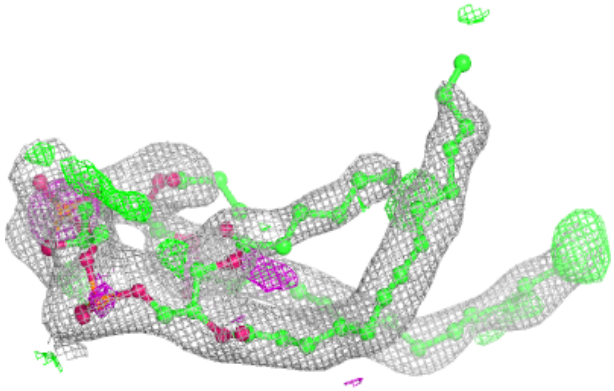


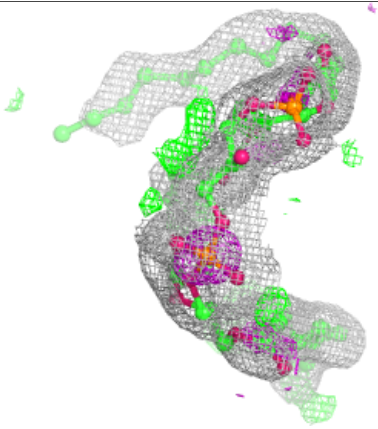


Electron density around CDL I 101:

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

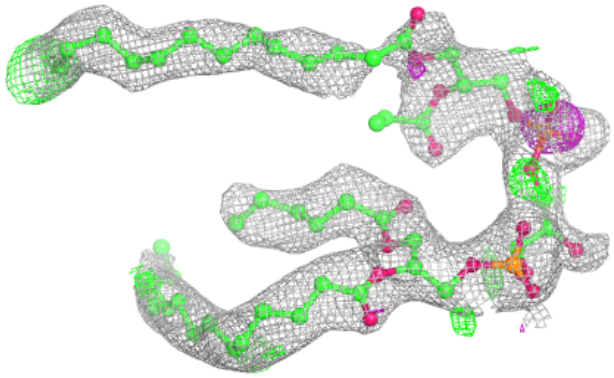


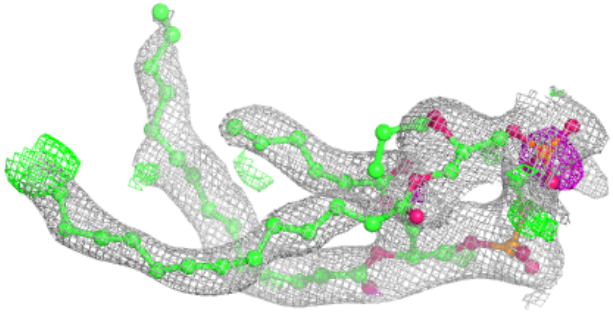


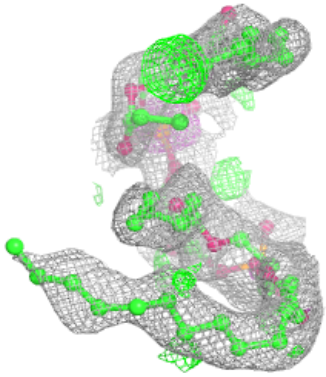


Electron density around CDL V 101:

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

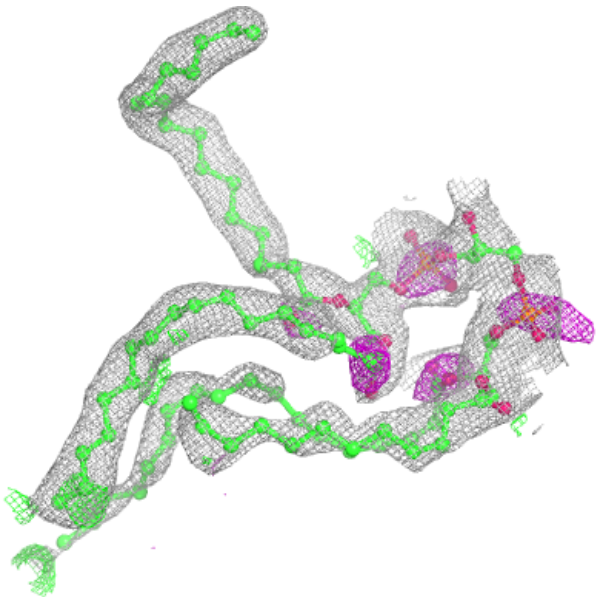


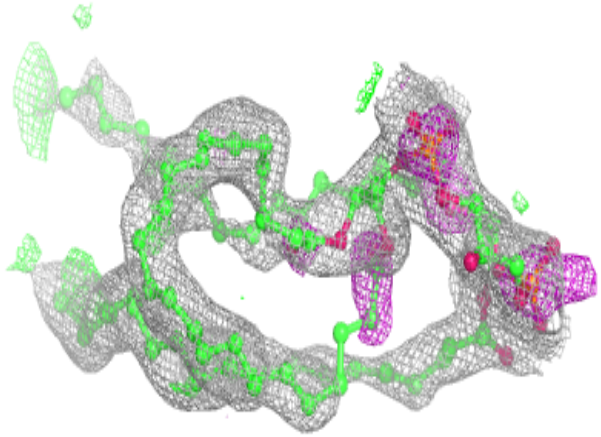




Electron density around CDL Y 101:

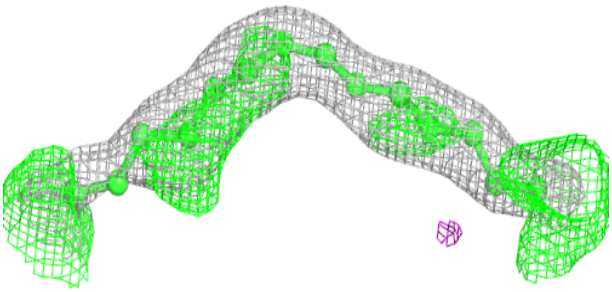
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

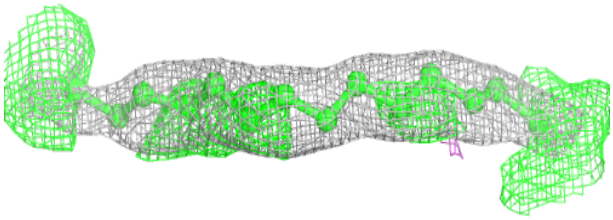


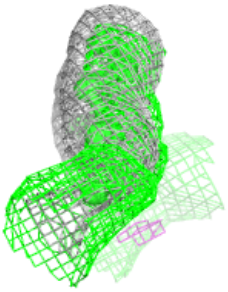


Electron density around LFA A 608:

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

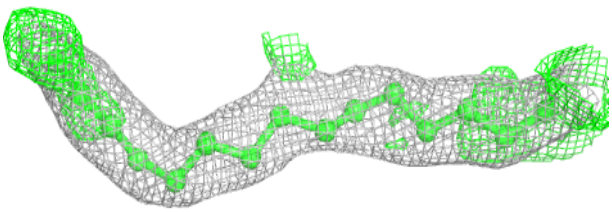


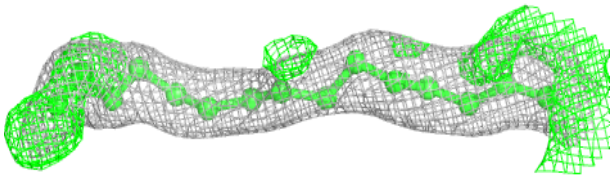


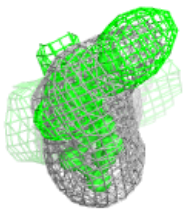


Electron density around LFA P 313:

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

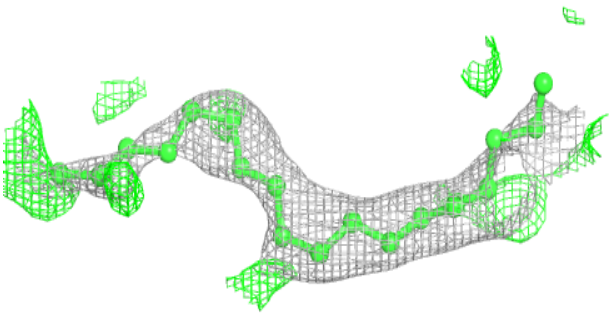


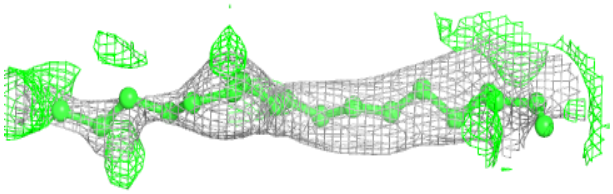


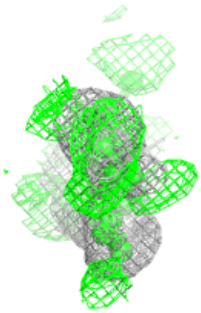


Electron density around LFA C 309:

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

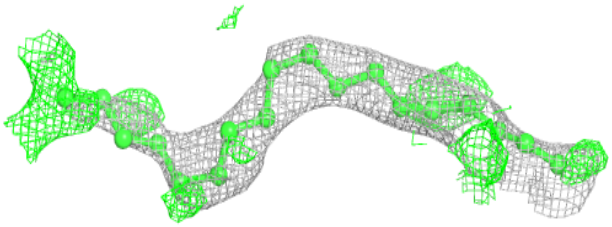


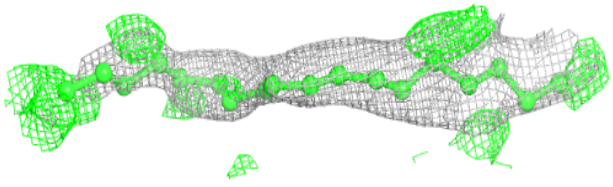


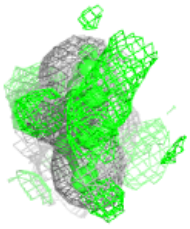


Electron density around LFA P 310:

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

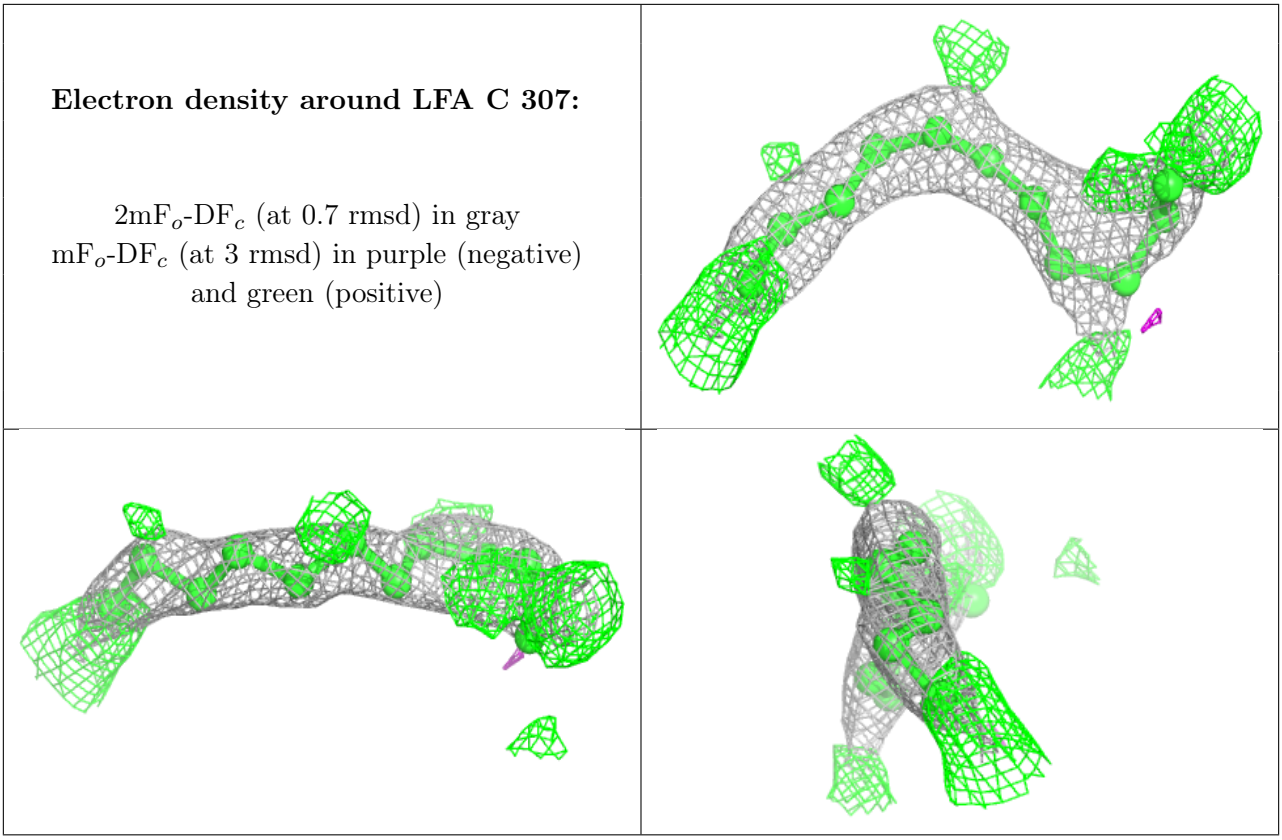






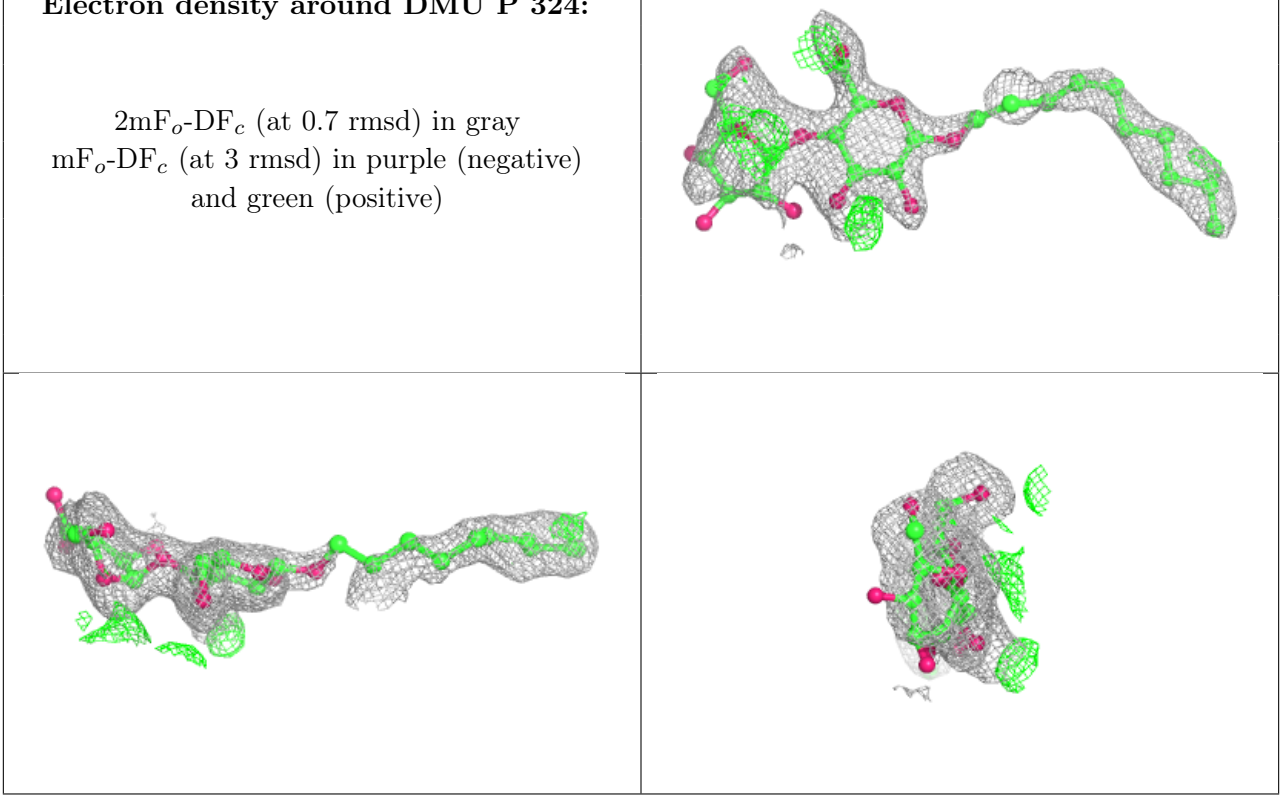
Electron density around LFA C 307:

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



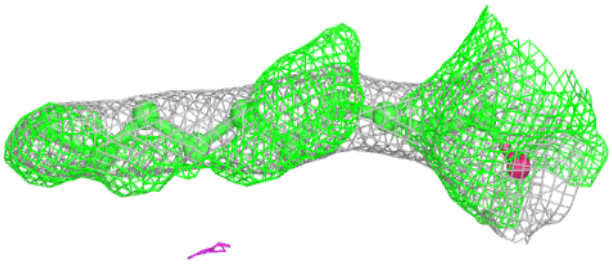
Electron density around DMU P 324:

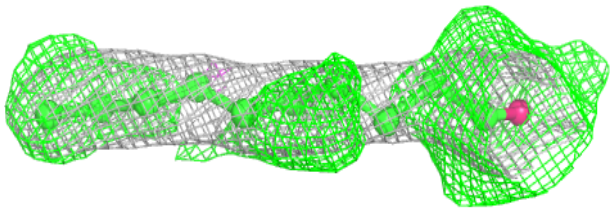
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

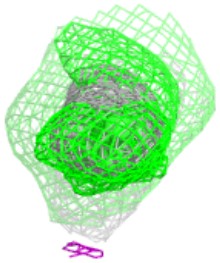


Electron density around DMU O 306:

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

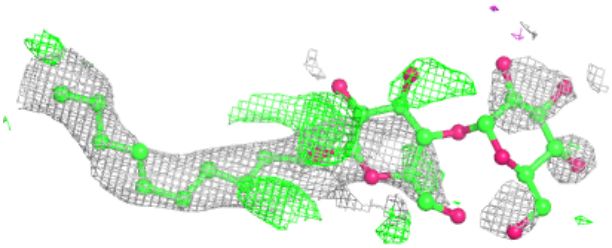


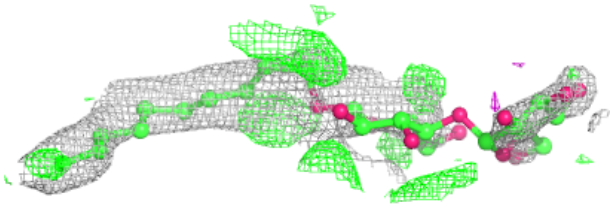


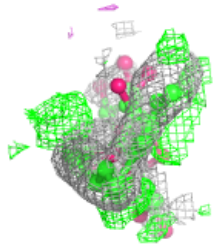


Electron density around DMU U 101:

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

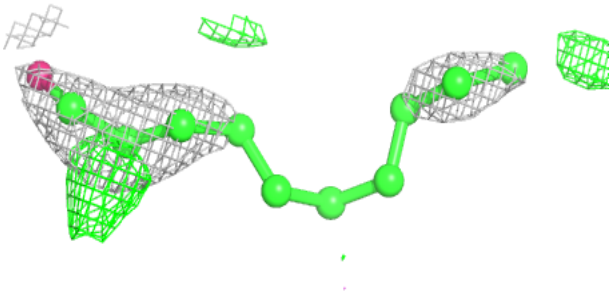


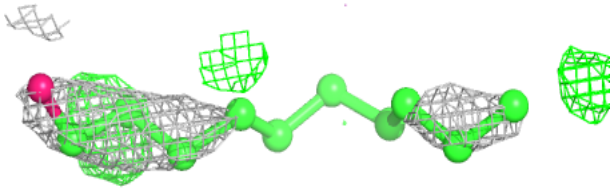


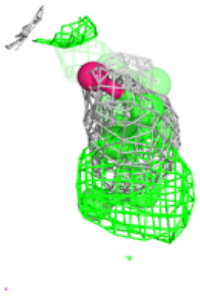


Electron density around DMU N 601:

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

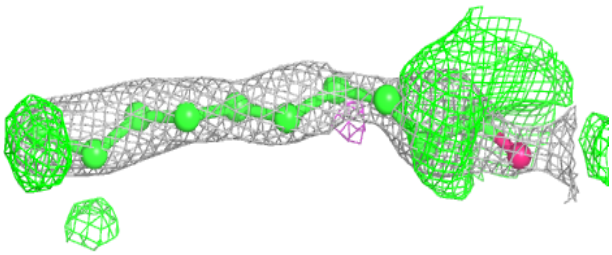


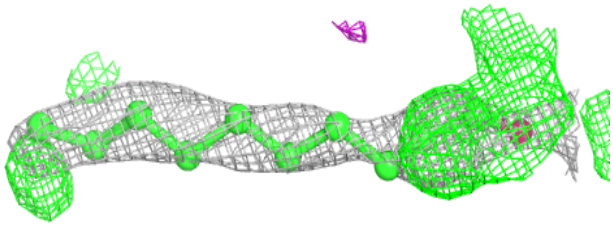


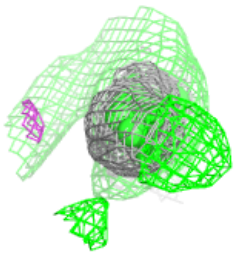


Electron density around DMU B 302:

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

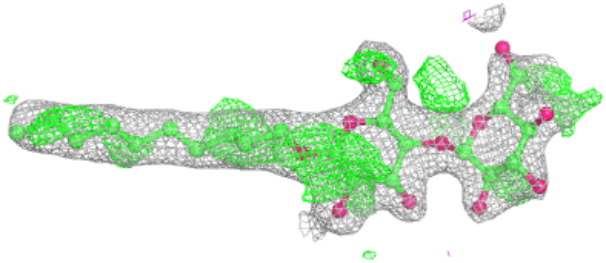


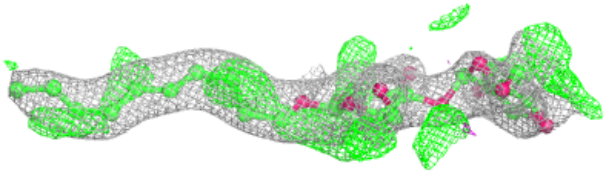


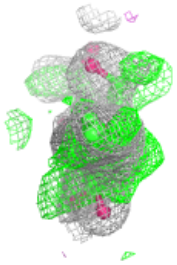


Electron density around DMU A 611:

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

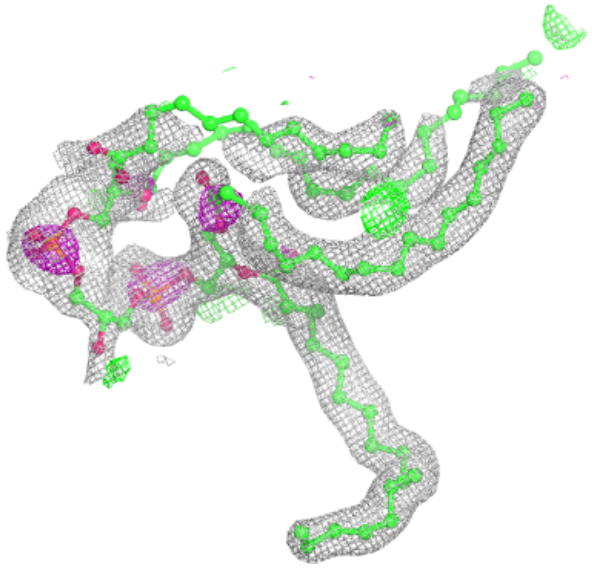


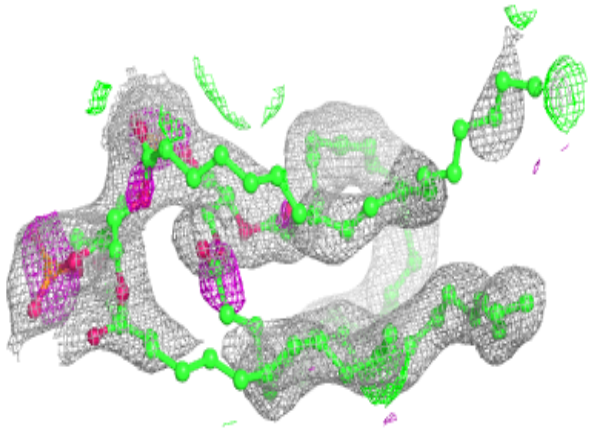


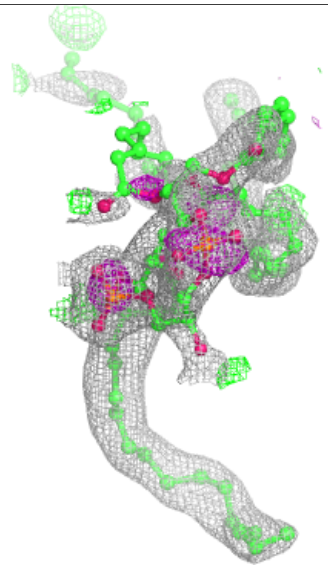


Electron density around CDL L 101:

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

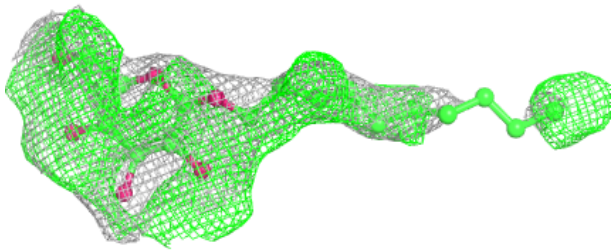


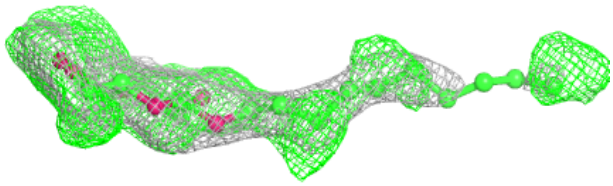


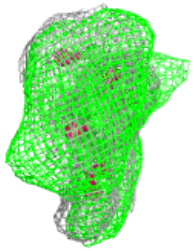


Electron density around DMU Z 102:

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

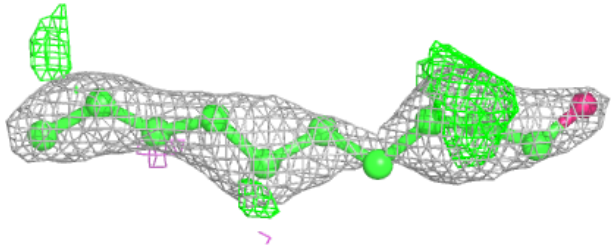


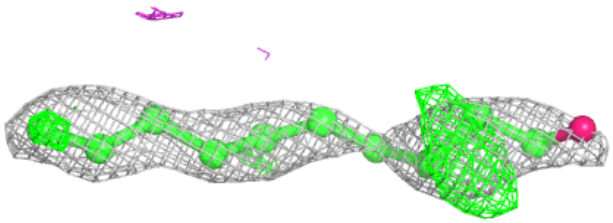


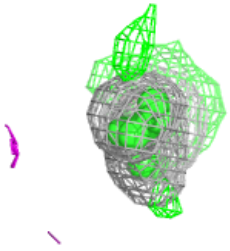


Electron density around DMU B 303:

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

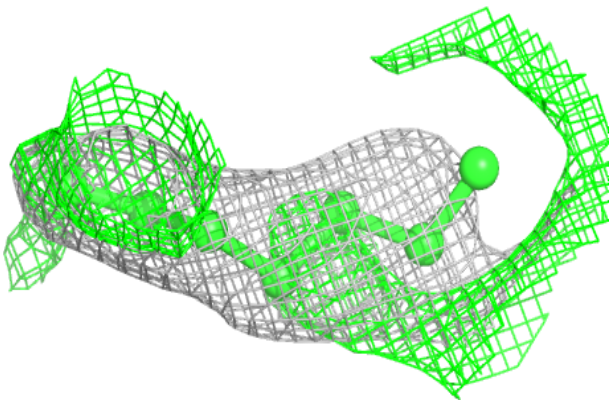


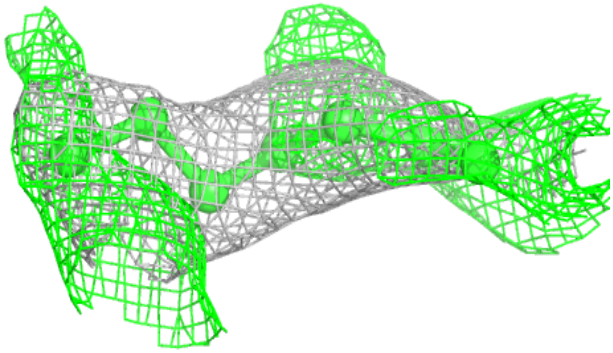


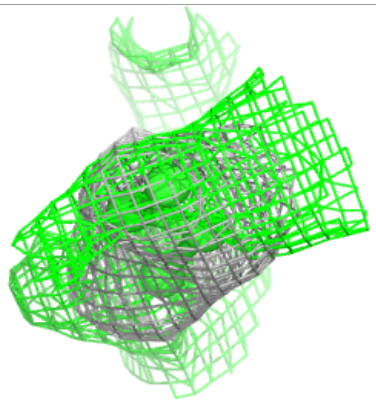


Electron density around DMU P 316:

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

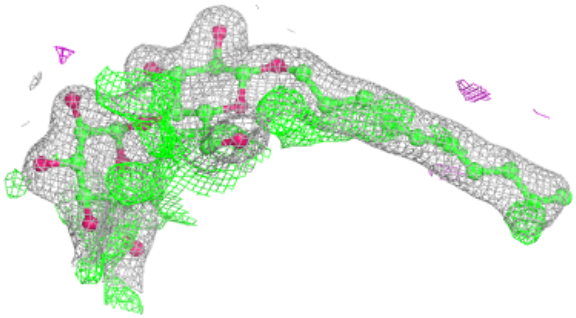


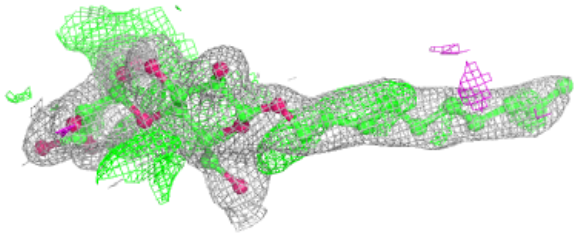


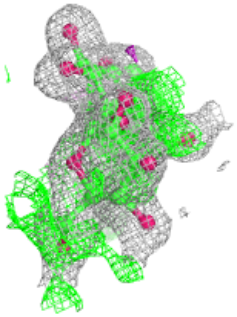


Electron density around DMU D 201:

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

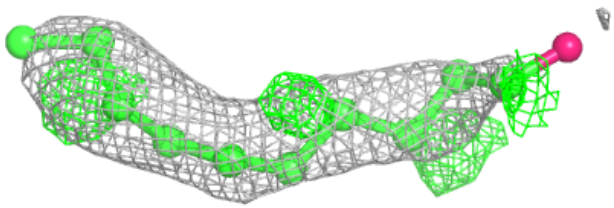


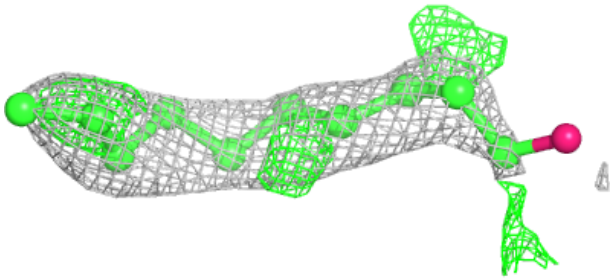


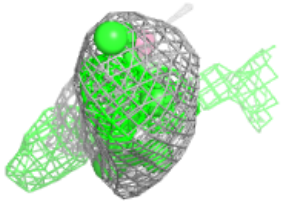


Electron density around DMU J 101:

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

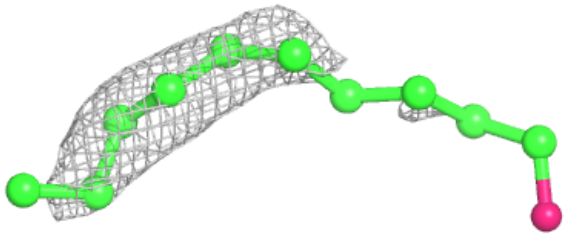


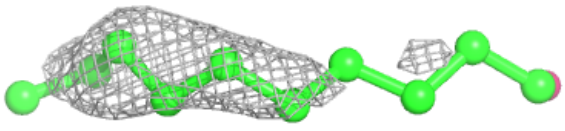


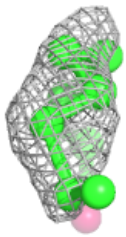


Electron density around DMU W 101:

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

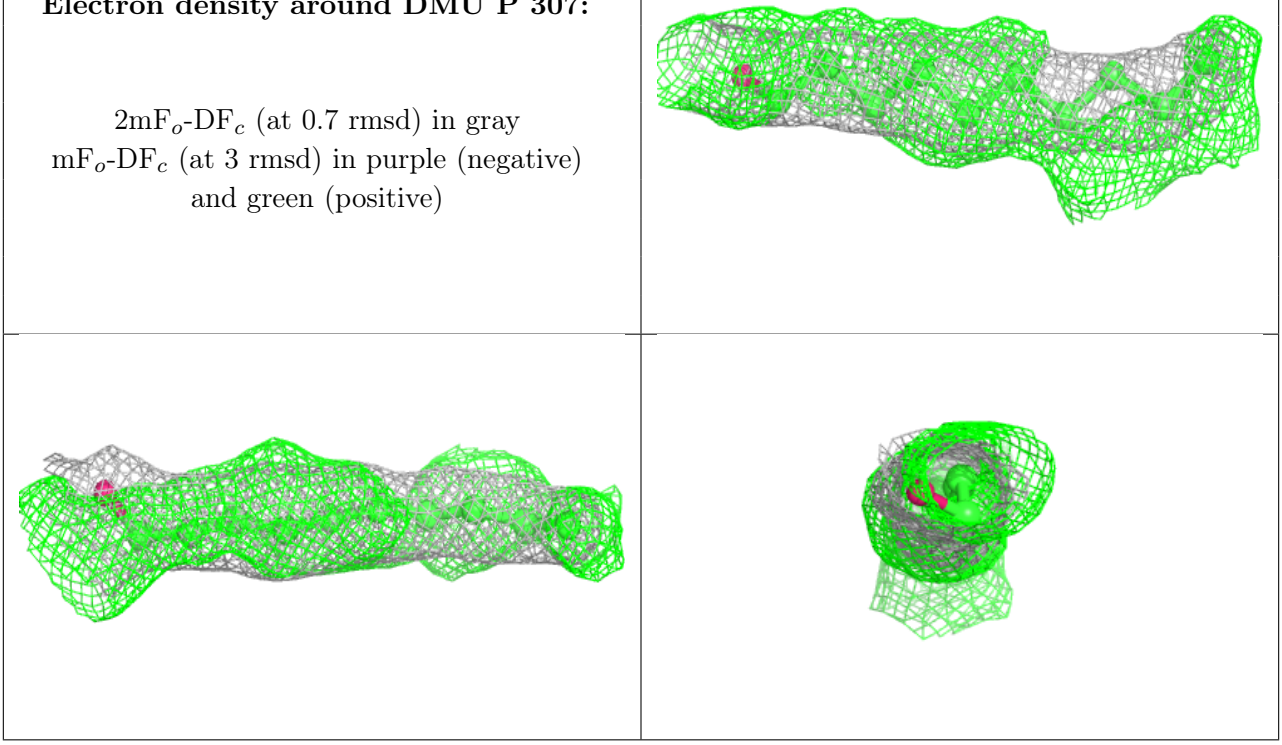






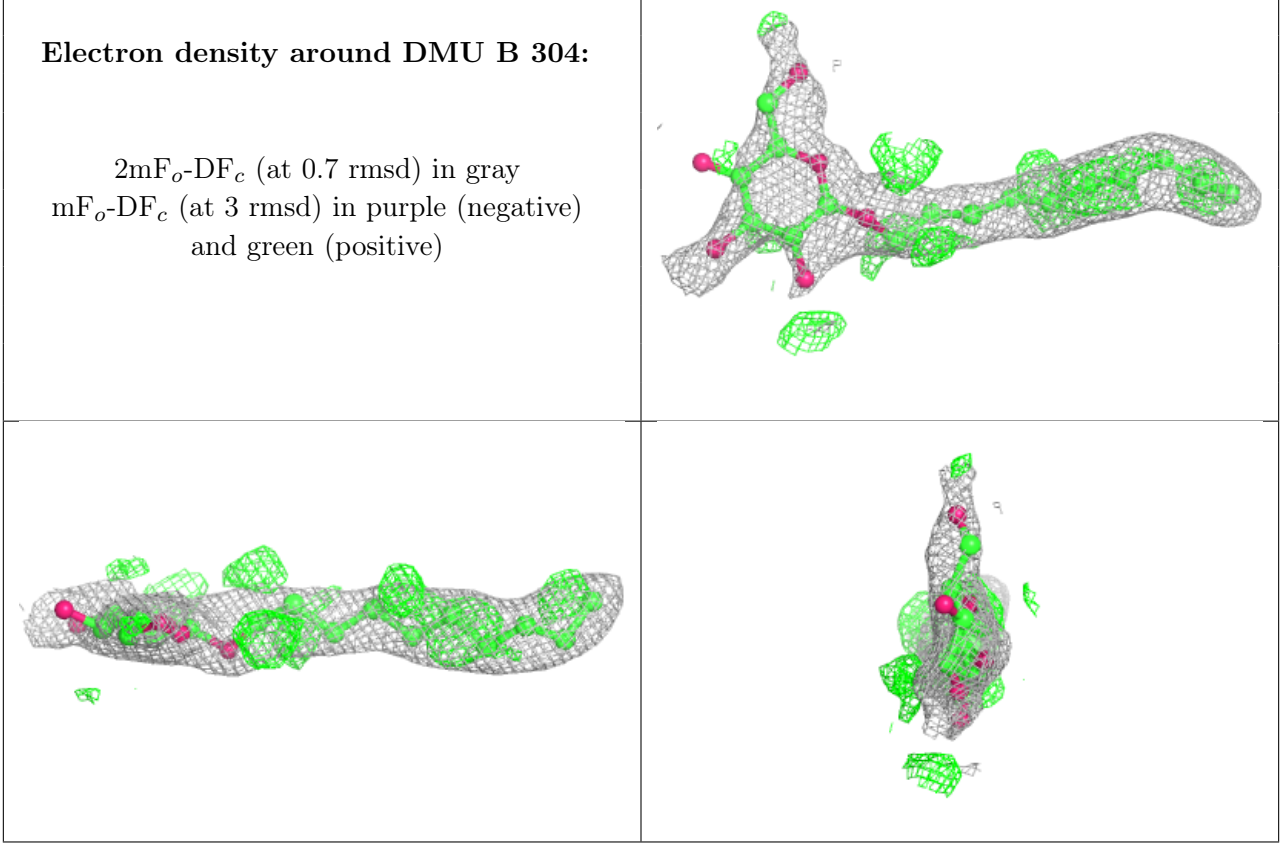
Electron density around DMU P 307:

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



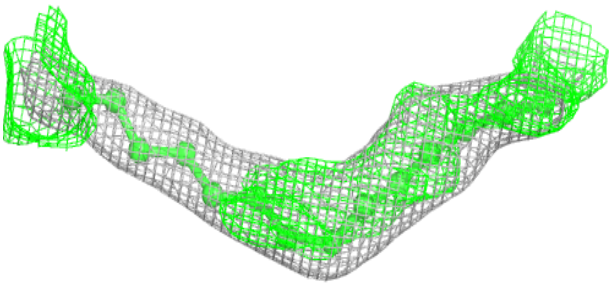
Electron density around DMU B 304:

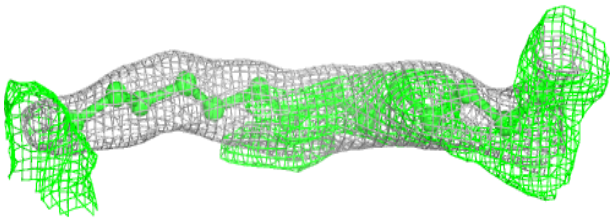
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

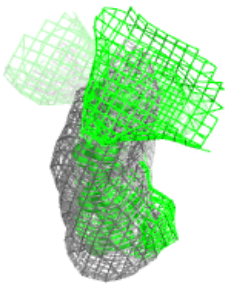


Electron density around LFA N 609:

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

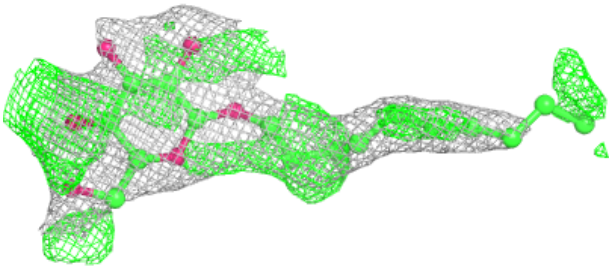


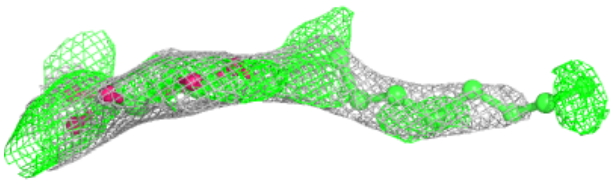


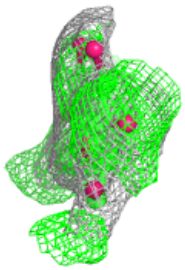


Electron density around DMU L 102:

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

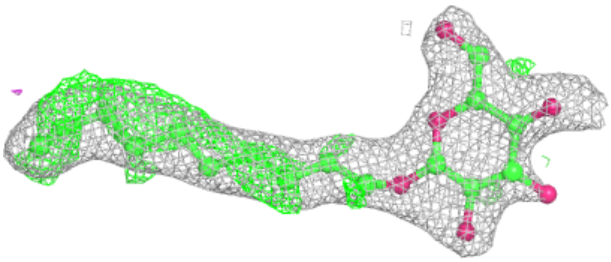


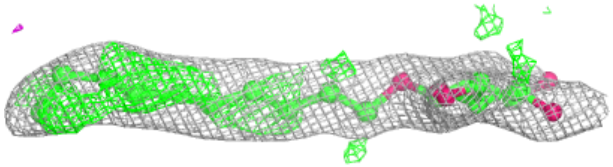


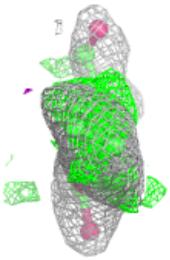


Electron density around DMU O 308:

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

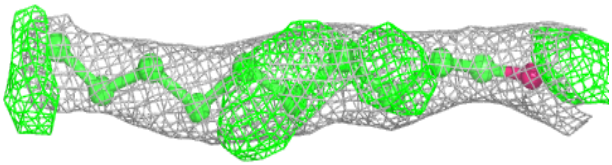


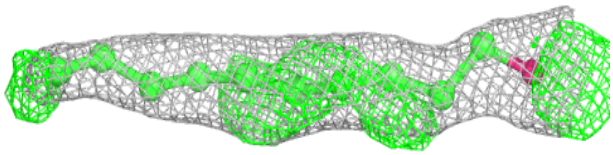


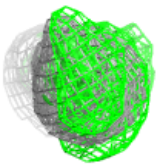


Electron density around DMU C 306:

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

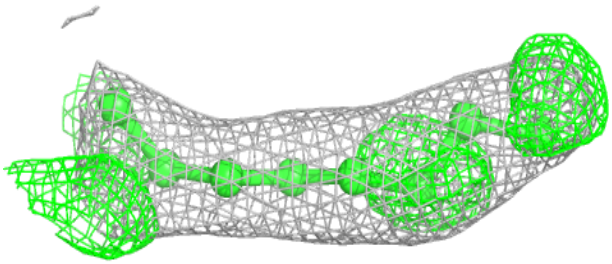


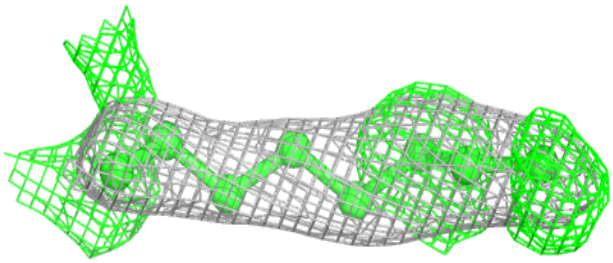


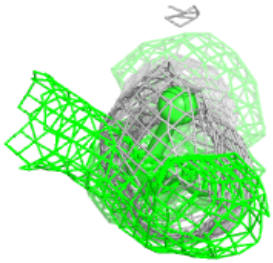


Electron density around DMU Z 103:

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

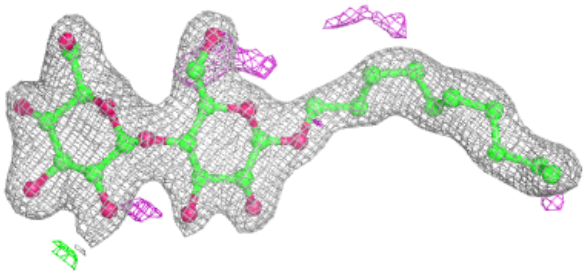


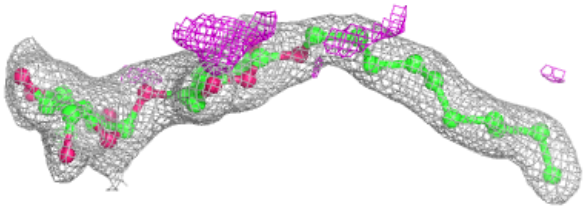


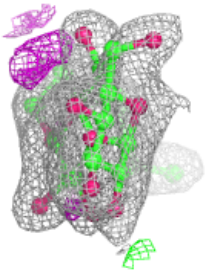


Electron density around DMU Z 101:

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

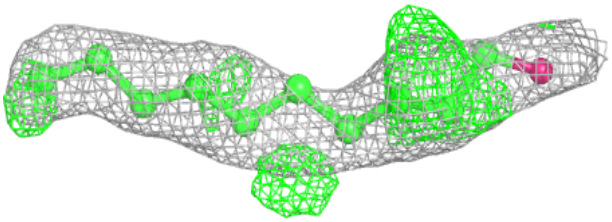


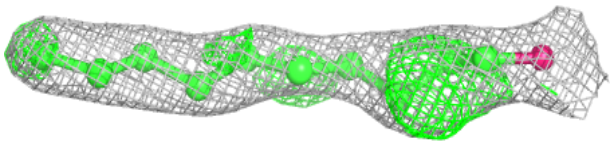


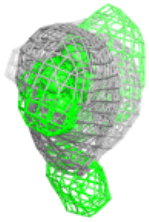


Electron density around DMU O 307:

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

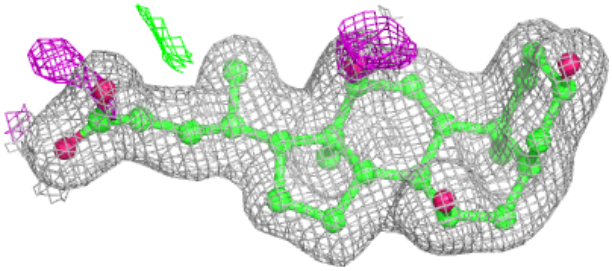


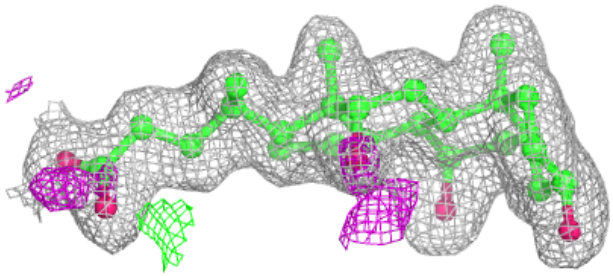


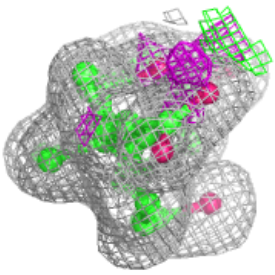


Electron density around CHD C 301:

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

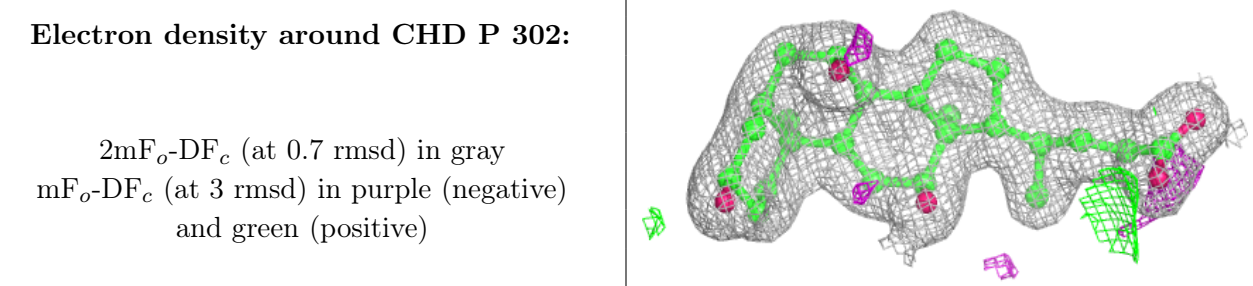


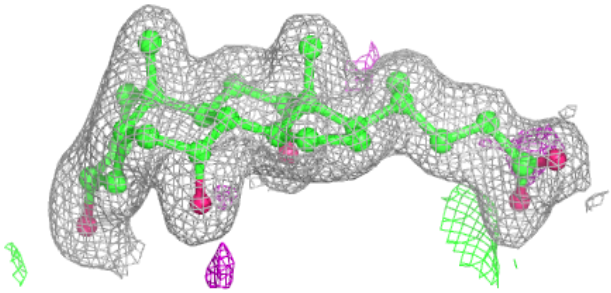


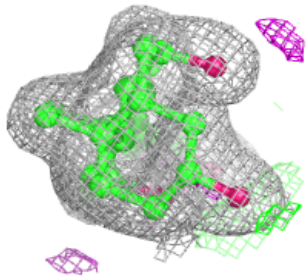


Electron density around CHD P 302:

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

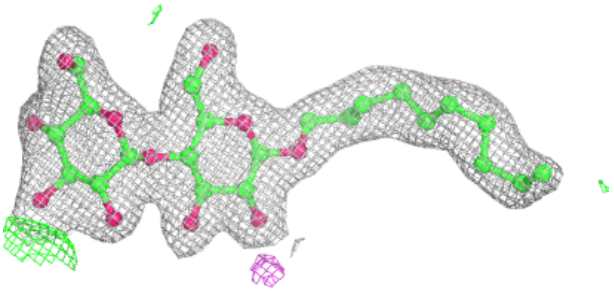


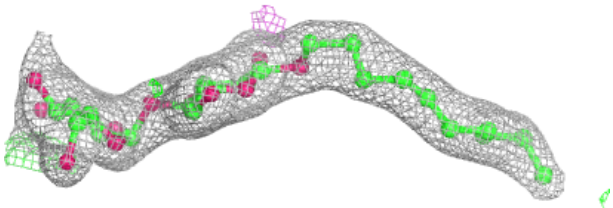


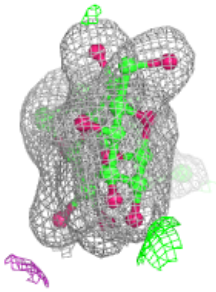


Electron density around DMU M 101:

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

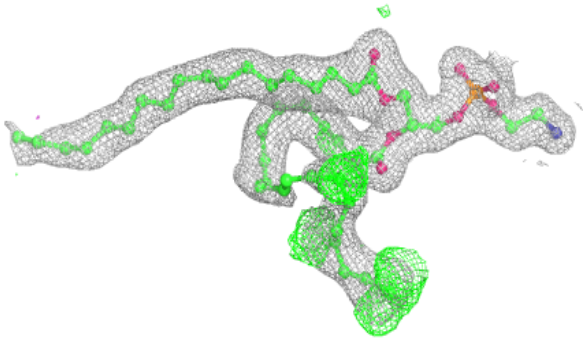


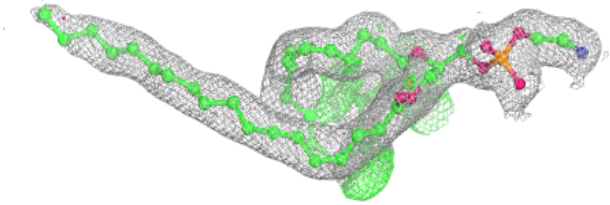


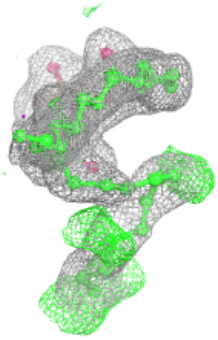


Electron density around PEK G 101:

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

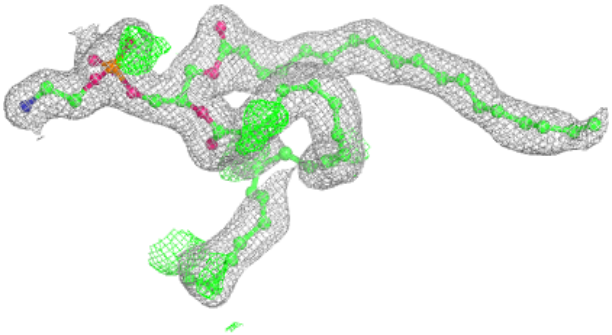


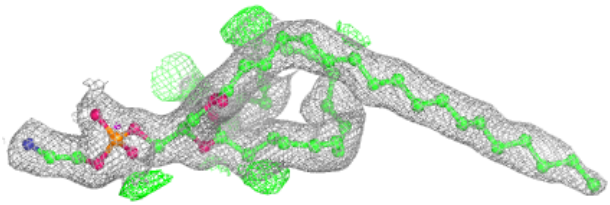


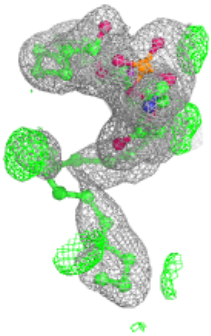


Electron density around PEK T 101:

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

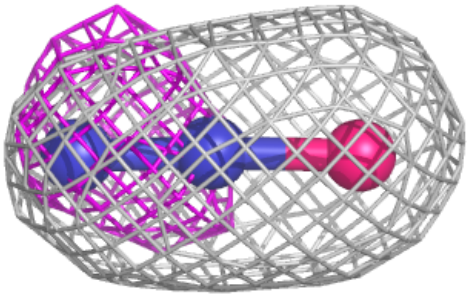


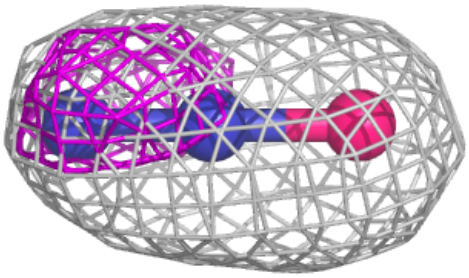


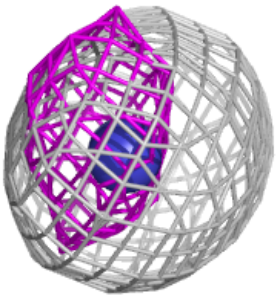


Electron density around N2O N 608:

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

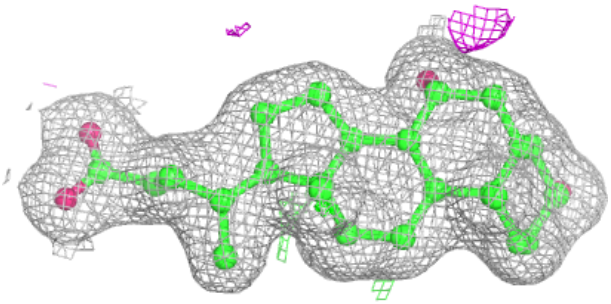


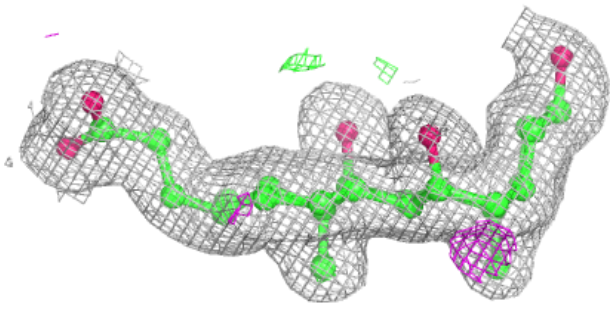


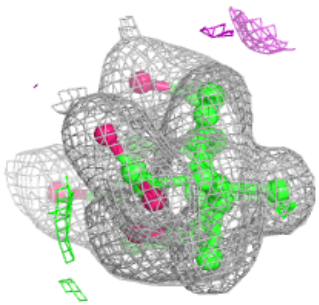


Electron density around CHD O 301:

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

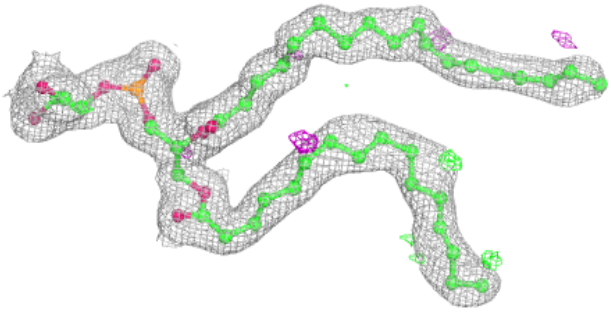


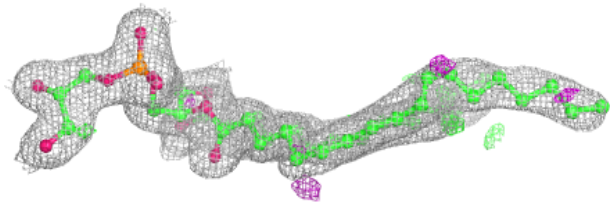


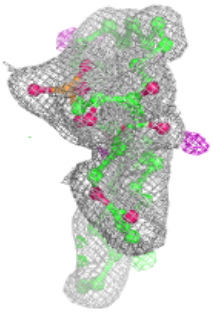


Electron density around PGV N 617:

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

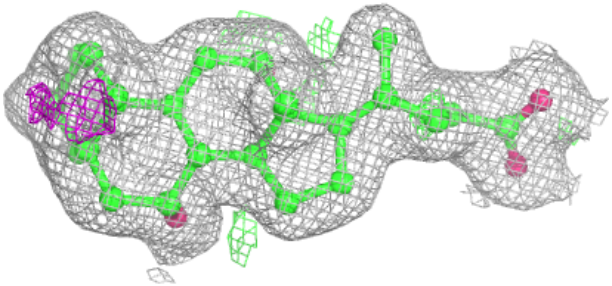


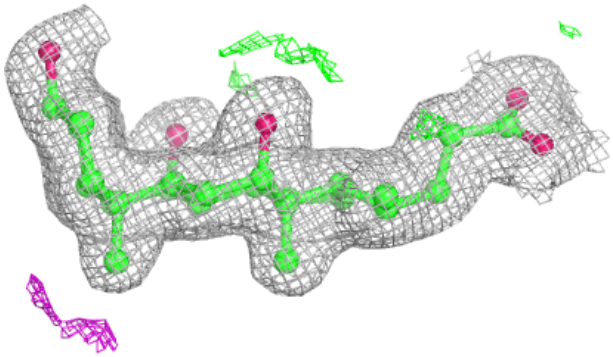


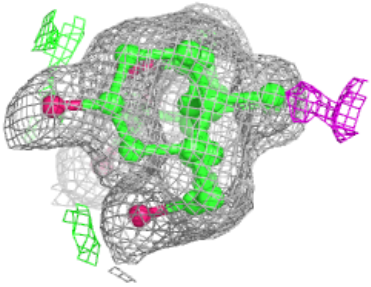


Electron density around CHD B 306:

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

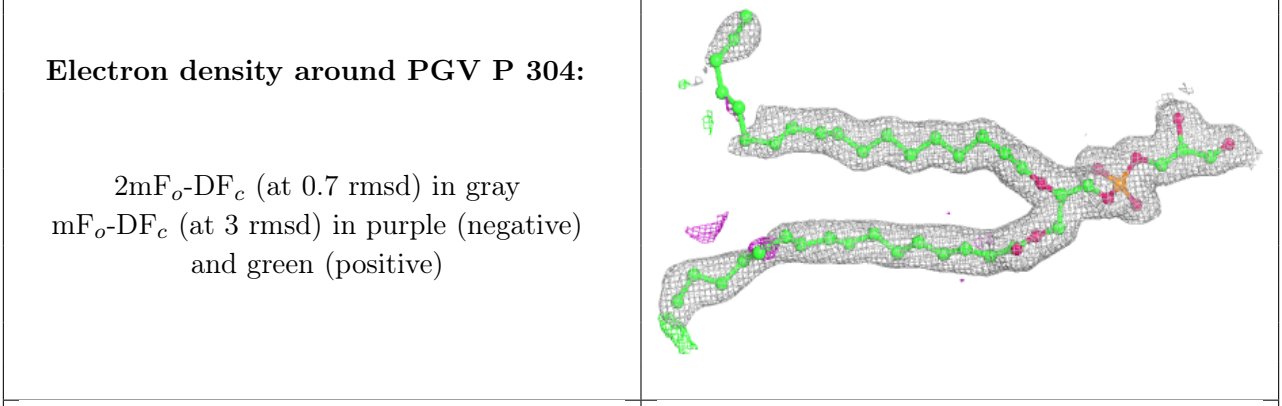






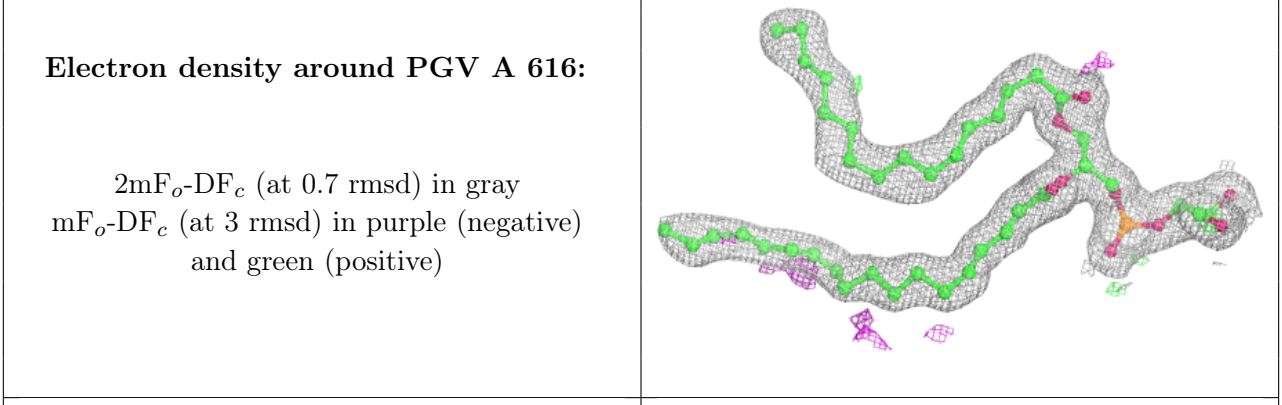
Electron density around PGV P 304:

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



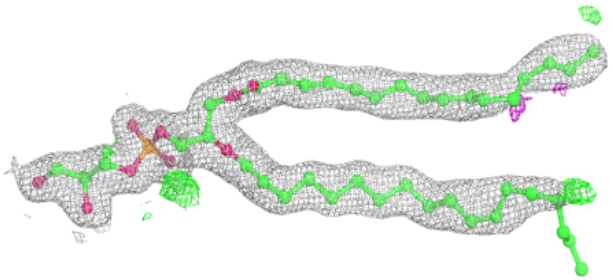
Electron density around PGV A 616:

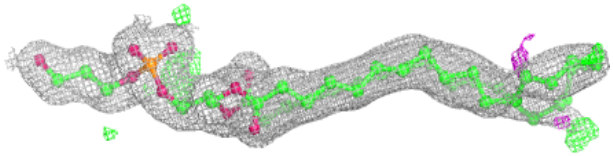
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

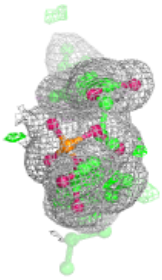


Electron density around PGV C 303:

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

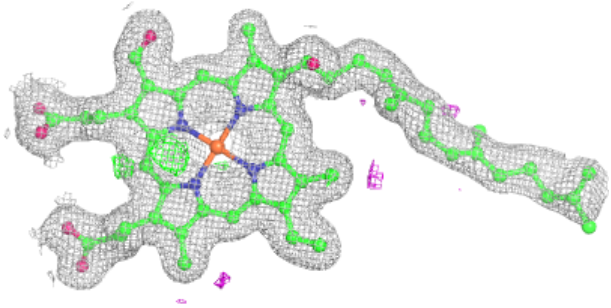


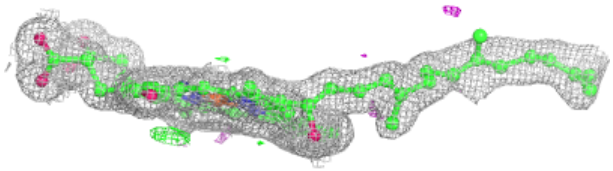


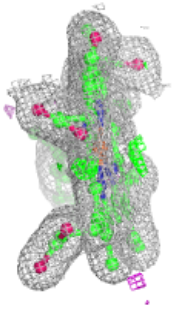


Electron density around HEA A 601 (A):

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

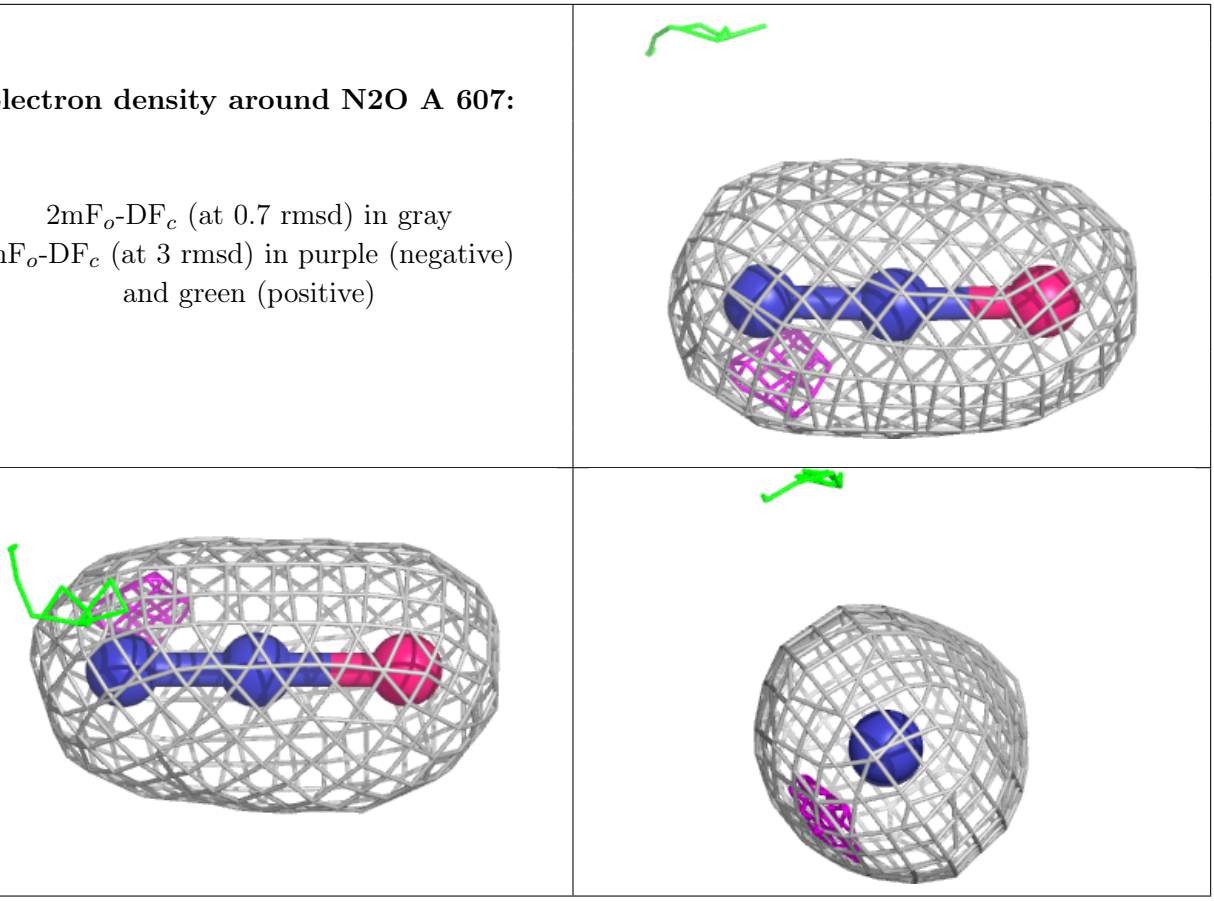






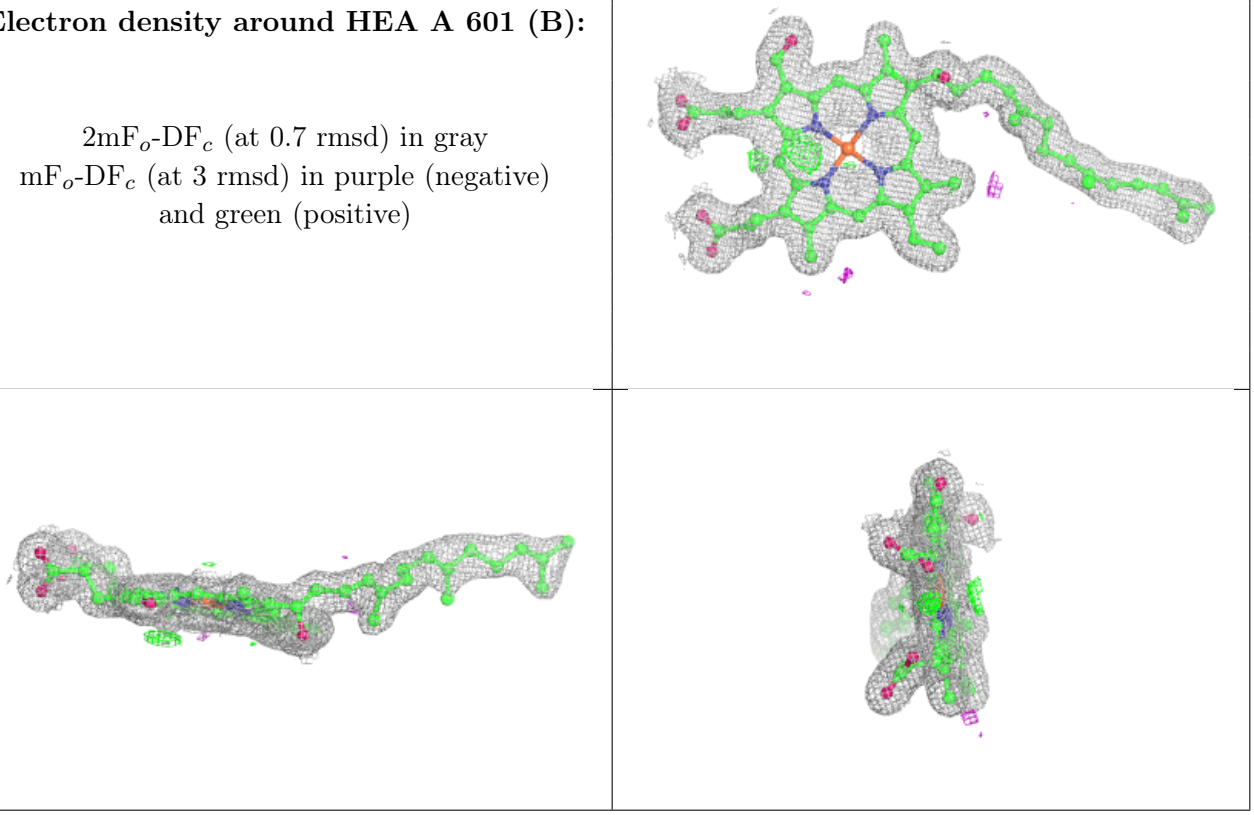
Electron density around N2O A 607:

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



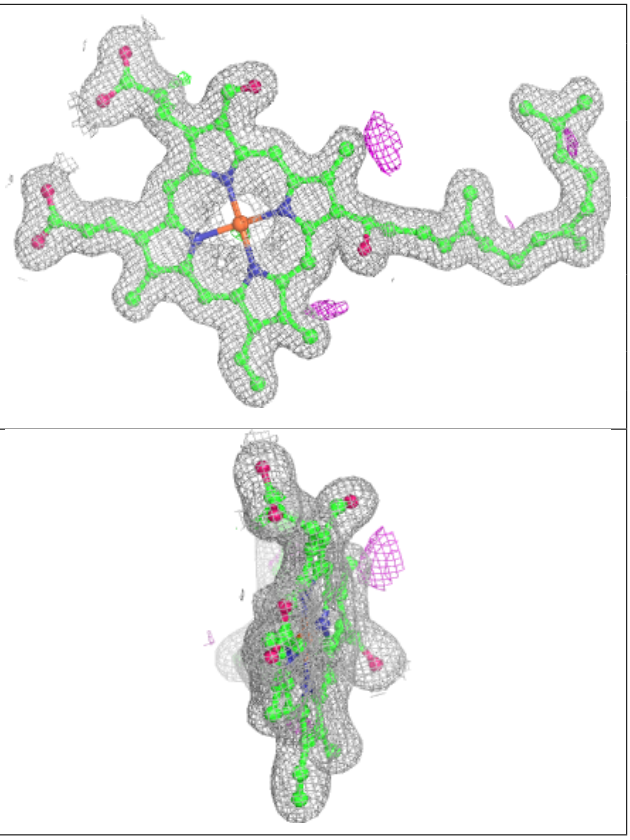
Electron density around HEA A 601 (B):

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



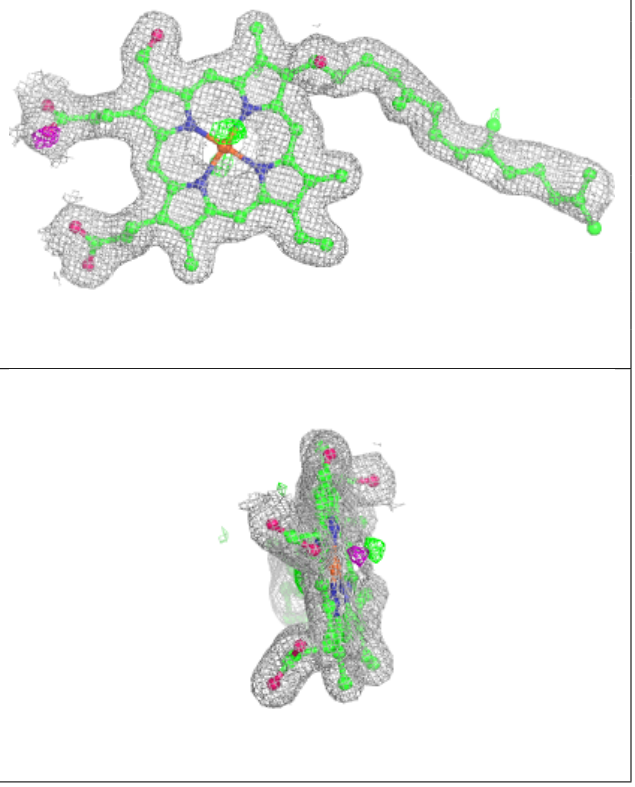
Electron density around HEA A 602:

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



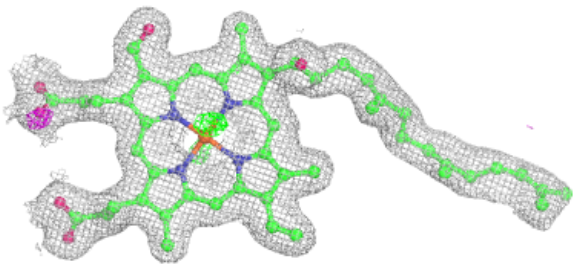
Electron density around HEA N 602 (A):

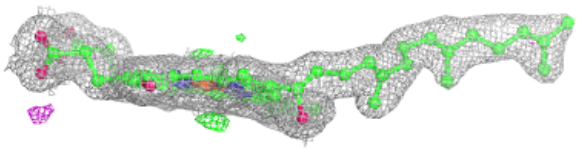
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

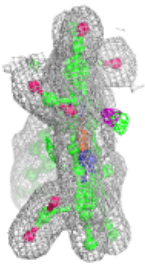


Electron density around HEA N 602 (B):

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

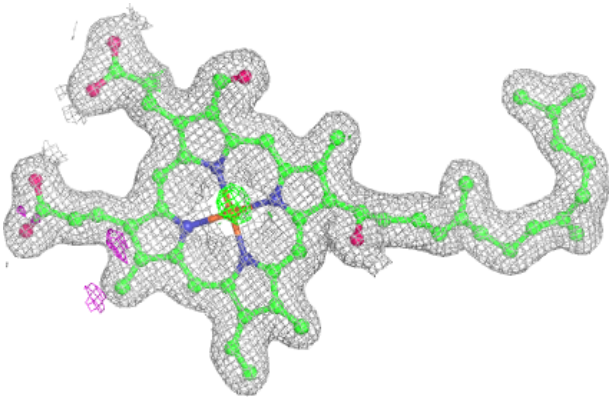


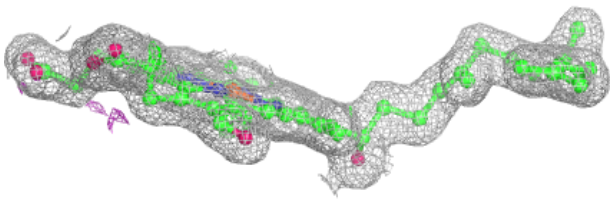


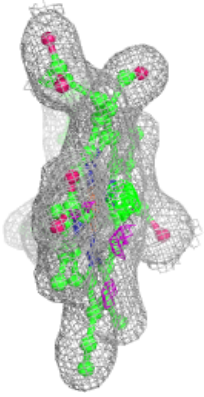


Electron density around HEA N 603:

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







6.5 Other polymers (i)

There are no such residues in this entry.