wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2024 – 05:09 PM JST

PDB ID : 8H8R
Title : Bovine Heart Cytochrome c Oxidase in the Calcium-bound Fully Oxidized State
Authors : Muramoto, K.; Shinzawa-Itoh, K.
Deposited on : 2022-10-24
Resolution : 1.70 Å(reported)

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

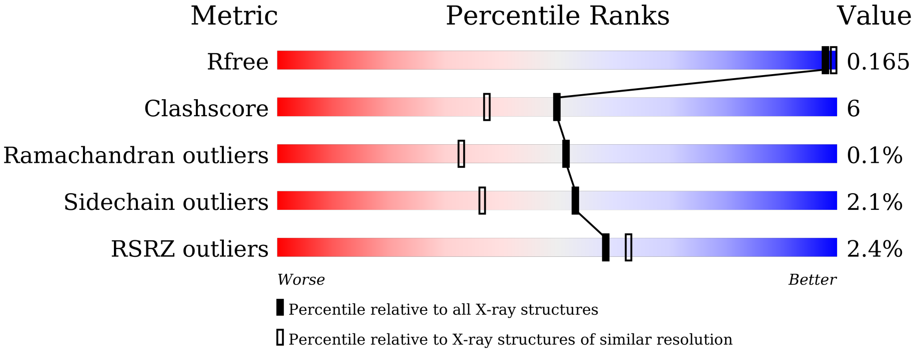
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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

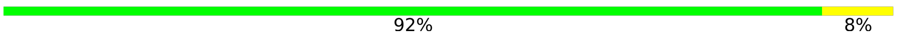
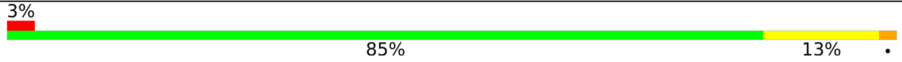
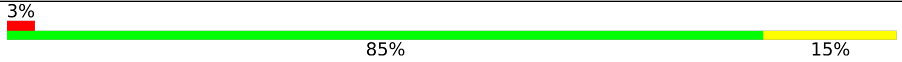
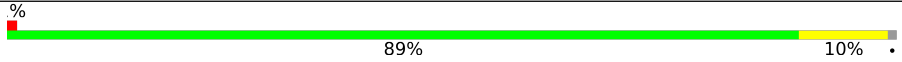
The reported resolution of this entry is 1.70 Å.

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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	
1	N	514	
2	B	227	
2	O	227	
3	C	261	
3	P	261	

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Mol	Chain	Length	Quality of chain
4	D	147	% 92% 5% •
4	Q	147	5% 86% 6% •• 7%
5	E	109	93% • 6%
5	R	109	89% 5% 6%
6	F	98	83% 10% 7%
6	S	98	2% 84% 7% • 7%
7	G	85	11% 73% 11% • 15%
7	T	85	9% 76% 7% • 15%
8	H	85	6% 80% 8% 12%
8	U	85	8% 80% 6% • 12%
9	I	73	5% 88% 7% • •
9	V	73	4% 88% 7% • •
10	J	59	7% 88% 7% 5%
10	W	59	7% 88% 7% 5%
11	K	56	82% 5% 12%
11	X	56	5% 84% • 12%
12	L	47	81% 13% 6%
12	Y	47	89% • 6%
13	M	46	7% 78% 9% 13%
13	Z	46	11% 76% 9% • 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	LFA	C	308	-	-	-	X
19	LFA	C	312	-	-	-	X
19	LFA	C	325	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	LFA	P	308	-	-	-	X
20	DMU	A	609	-	-	-	X
20	DMU	P	316	-	-	-	X
20	DMU	P	317	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 33049 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 825 528 139 156 2	0	0	0
5	R	102	Total C N O S 825 528 139 156 2	0	0	0

- 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 709 441 124 138 6	0	2	0
6	S	91	Total C N O S 709 441 124 138 6	0	2	0

- 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 606 396 114 95 1	0	1	0
7	T	72	Total C N O S 606 396 114 95 1	0	1	0

- 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 628 395 114 114 5	0	0	0
8	U	75	Total C N O S 628 395 114 114 5	0	0	0

- 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 575 375 103 93 4	0	0	0
9	V	70	Total C N O S 575 375 103 93 4	0	0	0

- 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 441 285 73 80 3	0	0	0

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

- 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 384 250 65 67 2	0	0	0
11	X	49	Total C N O S 384 250 65 67 2	0	0	0

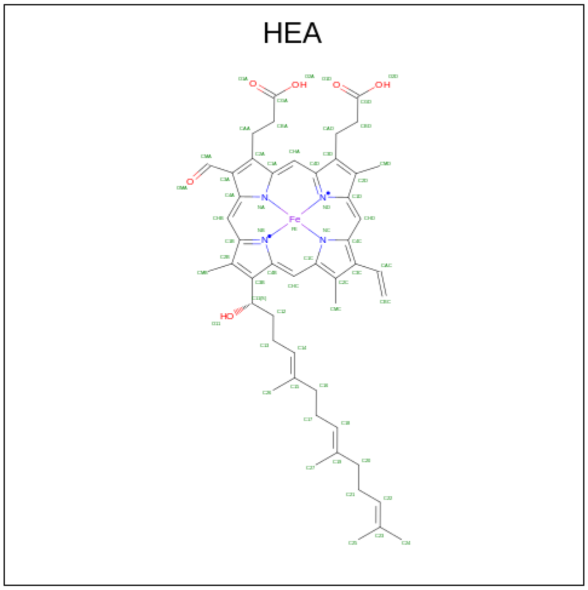
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

- 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 311 208 48 55	0	0	0
13	Z	40	Total C N O 311 208 48 55	0	0	0

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



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

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

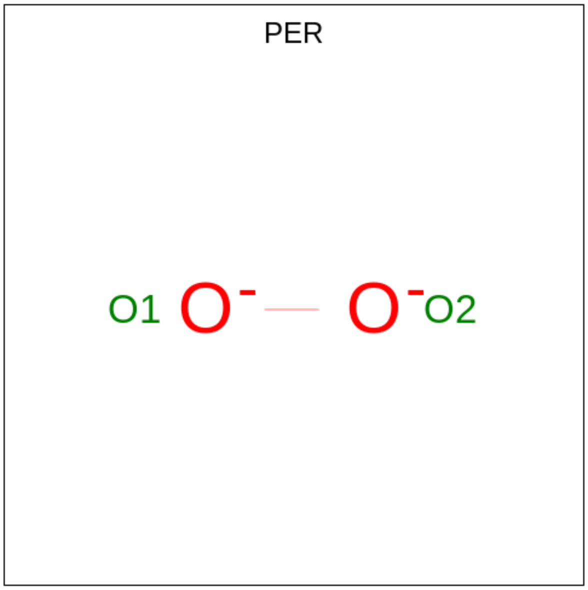
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

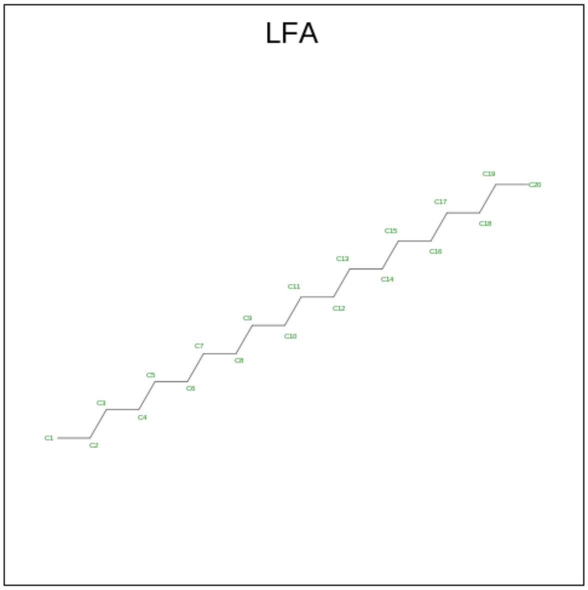
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Ca 1 1	0	0
17	N	1	Total Ca 1 1	0	0

- Molecule 18 is PEROXIDE ION (three-letter code: 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 EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



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

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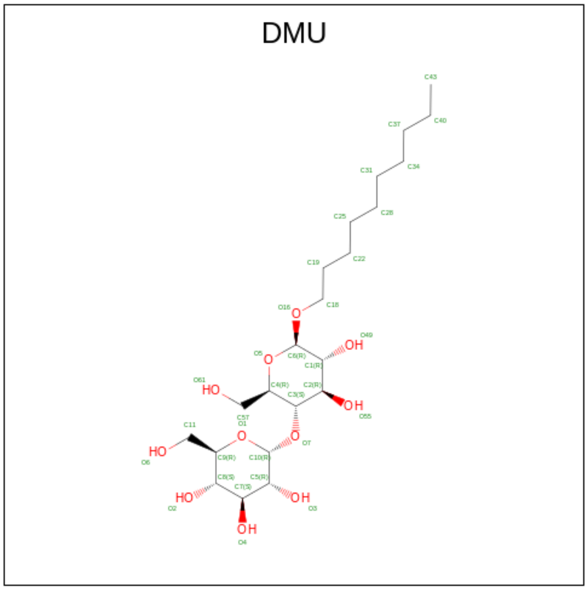
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	N	1	Total C 14 14	0	0
19	O	1	Total C 11 11	0	0
19	P	1	Total C 15 15	0	0
19	P	1	Total C 11 11	0	0
19	P	1	Total C 6 6	0	0
19	P	1	Total C 18 18	0	0
19	P	1	Total C 11 11	0	0
19	P	1	Total C 11 11	0	0
19	P	1	Total C 15 15	0	0
19	P	1	Total C 13 13	0	0
19	T	1	Total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

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



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

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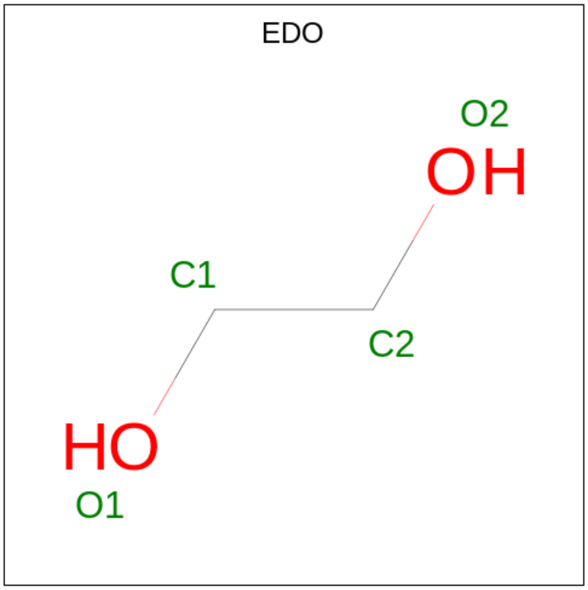
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	N	1	Total C 7 7	0	0
20	N	1	Total C O 33 22 11	0	0
20	N	1	Total C O 33 22 11	0	0
20	O	1	Total C O 22 16 6	0	0
20	O	1	Total C O 11 10 1	0	0
20	O	1	Total C O 11 10 1	0	0
20	O	1	Total C O 22 16 6	0	0
20	P	1	Total C O 11 10 1	0	0
20	P	1	Total C O 33 22 11	0	0
20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

- Molecule 21 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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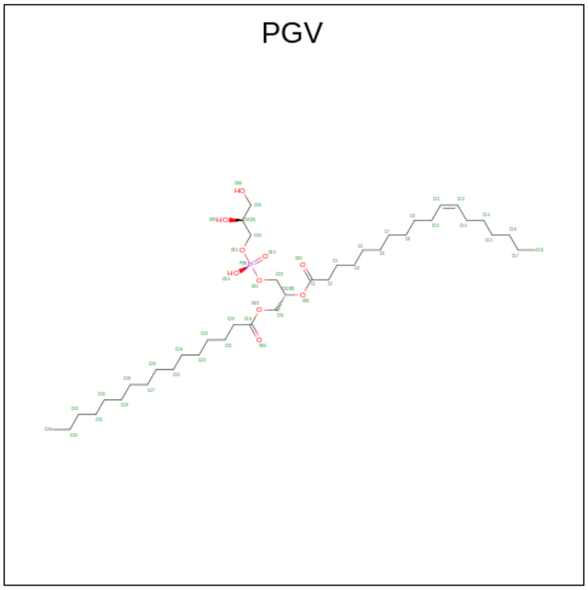
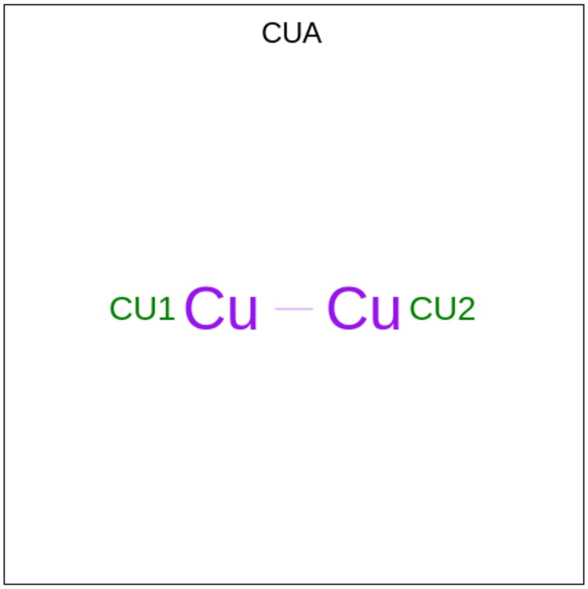
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	O	1	Total C O 4 2 2	0	0
21	P	1	Total C O 4 2 2	0	0
21	P	1	Total C O 4 2 2	0	0
21	P	1	Total C O 4 2 2	0	0
21	R	1	Total C O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

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



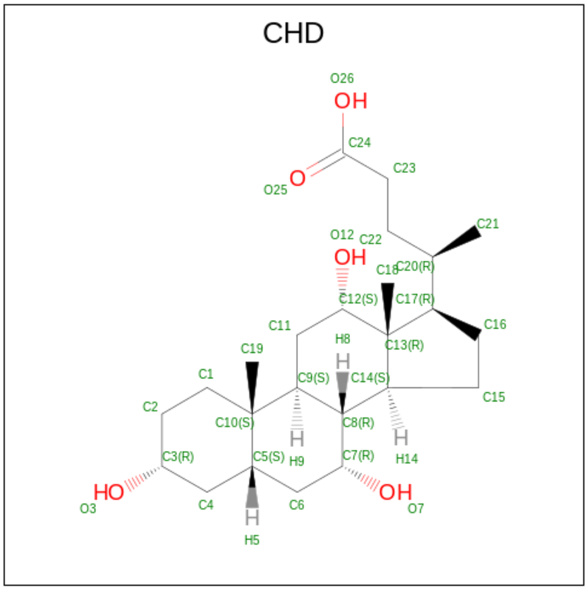
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C O P 51 40 10 1	0	0
22	C	1	Total C O P 51 40 10 1	0	0
22	N	1	Total C O P 51 40 10 1	0	0
22	P	1	Total C O P 51 40 10 1	0	0

- Molecule 23 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 24 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).

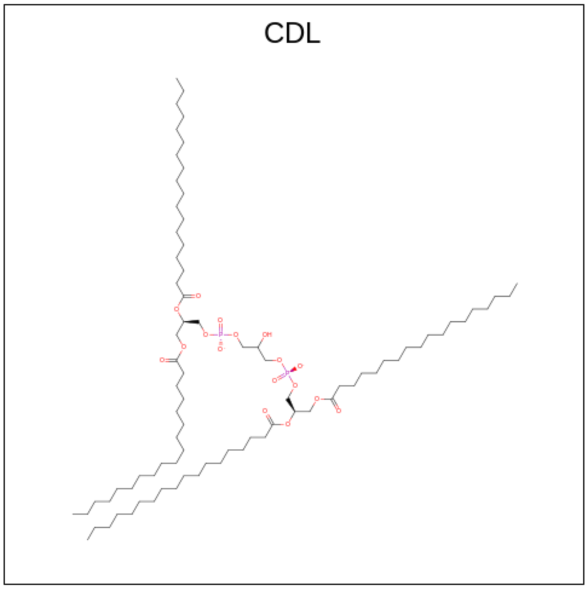


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	O	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0

- Molecule 25 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

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

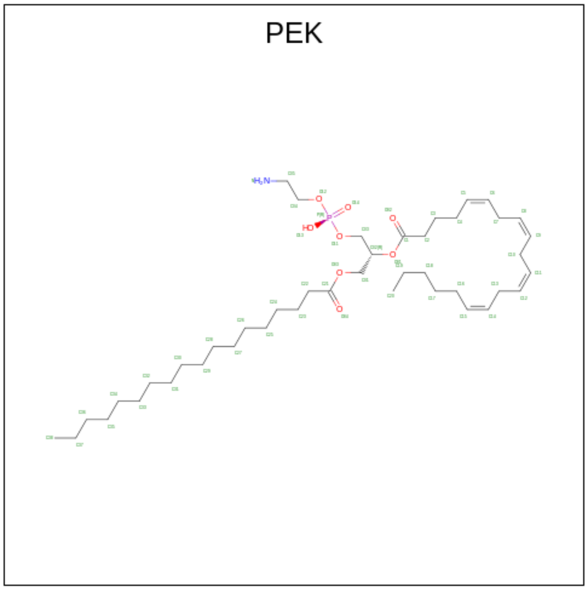


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C O P 87 68 17 2	0	0
26	I	1	Total C O P 64 45 17 2	0	0
26	L	1	Total C O P 94 75 17 2	0	0
26	O	1	Total C O P 64 45 17 2	0	0
26	P	1	Total C O P 87 68 17 2	0	0
26	Y	1	Total C O P 94 75 17 2	0	0

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 28 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
29	A	239	250	250	0	11
29	B	175	177	177	0	2
29	C	102	103	103	0	1
29	D	135	144	144	0	9
29	E	109	116	116	0	7
29	F	104	111	111	0	7
29	G	42	43	43	0	1
29	H	61	61	61	0	0
29	I	41	41	41	0	0
29	J	20	20	20	0	0

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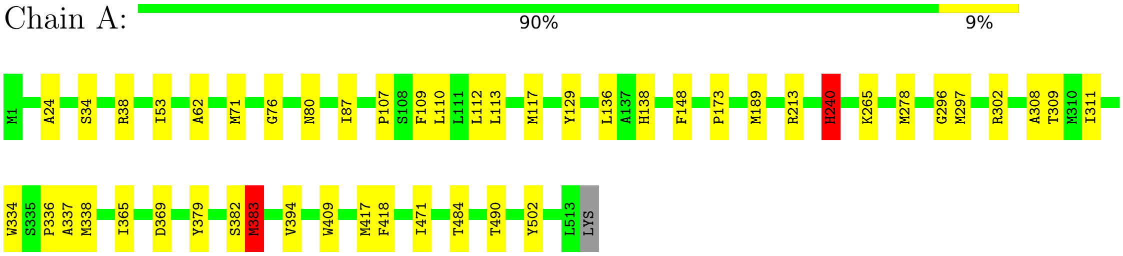
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	K	22	Total O 22 22	0	0
29	L	25	Total O 27 27	0	2
29	M	21	Total O 21 21	0	0
29	N	227	Total O 237 237	0	10
29	O	148	Total O 149 149	0	1
29	P	101	Total O 102 102	0	1
29	Q	81	Total O 86 86	0	5
29	R	87	Total O 94 94	0	7
29	S	87	Total O 93 93	0	6
29	T	37	Total O 38 38	0	1
29	U	46	Total O 46 46	0	0
29	V	22	Total O 22 22	0	0
29	W	15	Total O 15 15	0	0
29	X	18	Total O 18 18	0	0
29	Y	25	Total O 27 27	0	2
29	Z	17	Total O 17 17	0	0

3 Residue-property plots ⓘ

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

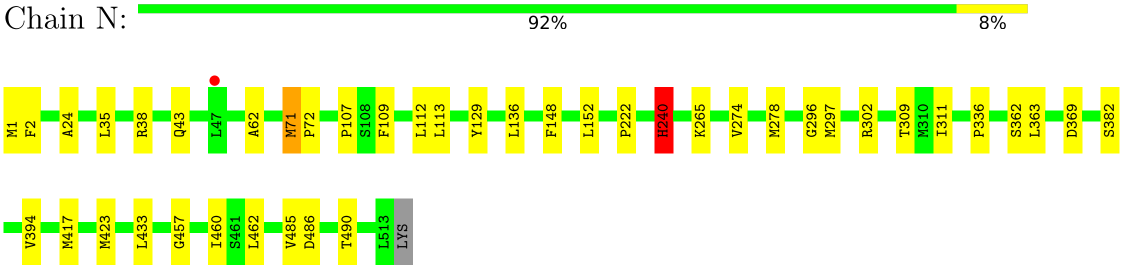
- Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



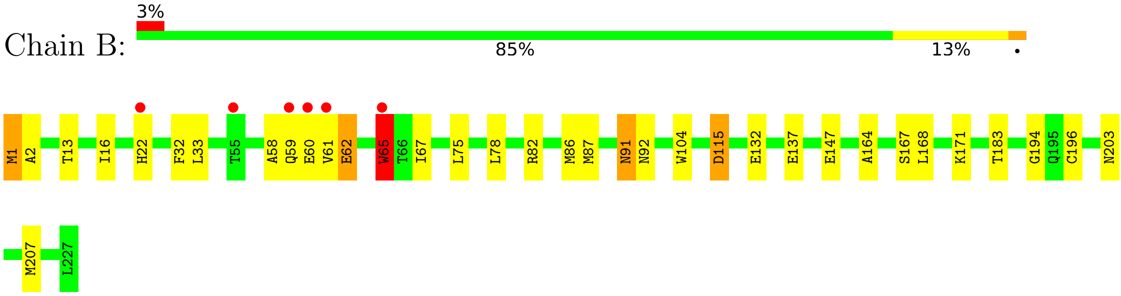
- Molecule 1: Cytochrome c oxidase subunit 1

Chain N:



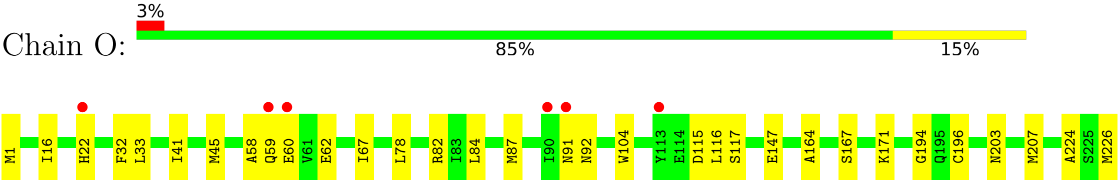
- Molecule 2: Cytochrome c oxidase subunit 2

Chain B:

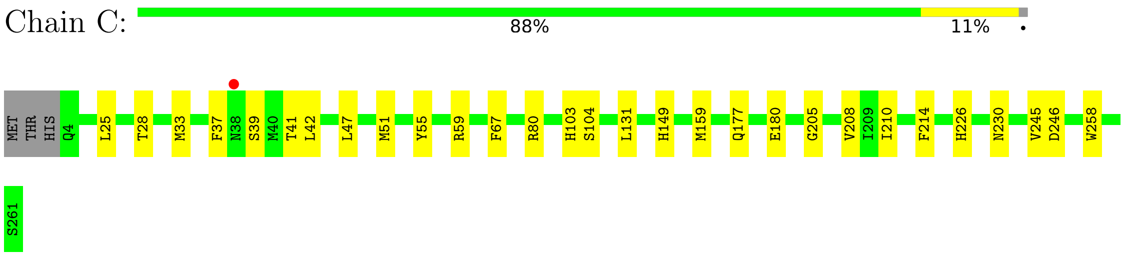


- Molecule 2: Cytochrome c oxidase subunit 2

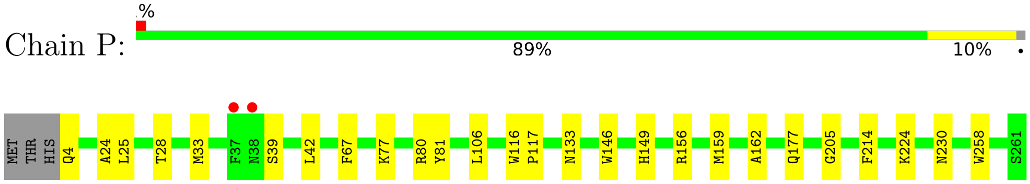
Chain O:



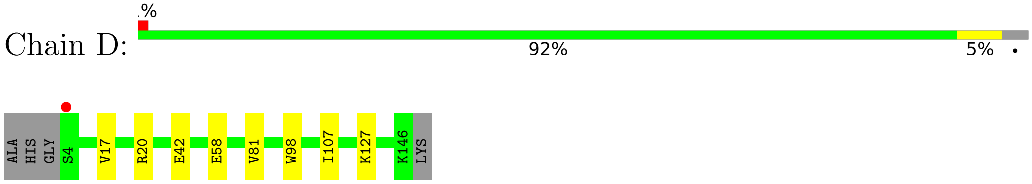
- Molecule 3: Cytochrome c oxidase subunit 3



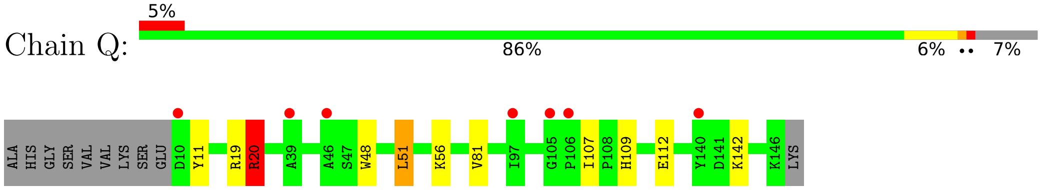
- Molecule 3: Cytochrome c oxidase subunit 3



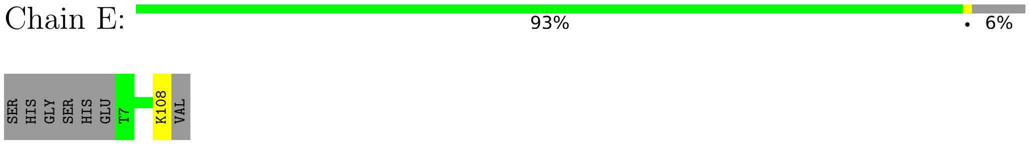
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



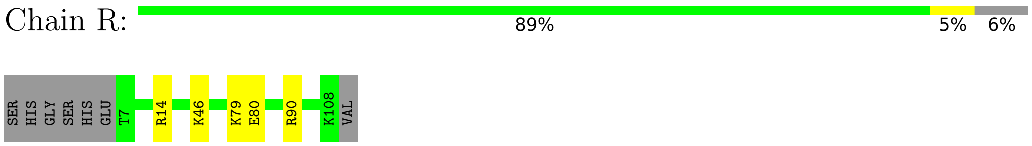
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



- Molecule 5: Cytochrome c oxidase subunit 5A

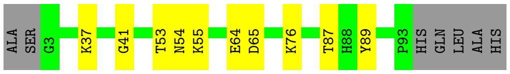


- Molecule 5: Cytochrome c oxidase subunit 5A



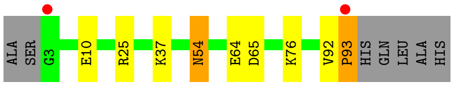
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



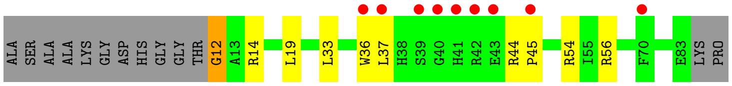
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



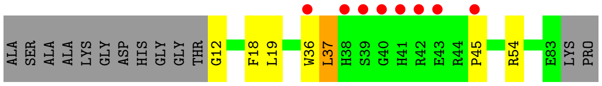
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



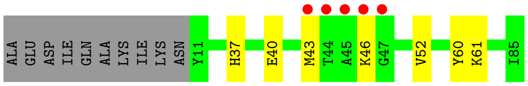
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



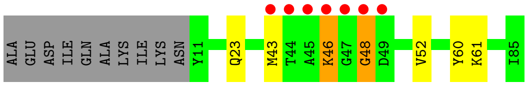
- Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



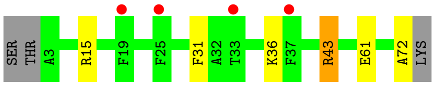
- Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



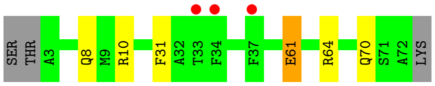
- Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



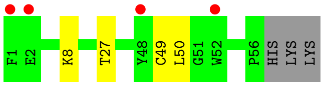
- Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



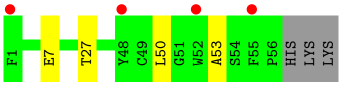
- Molecule 10: Cytochrome c oxidase subunit 7A1

Chain J:



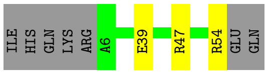
- Molecule 10: Cytochrome c oxidase subunit 7A1

Chain W:



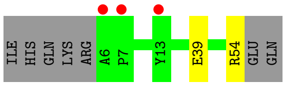
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



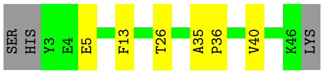
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:



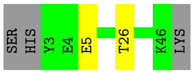
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:



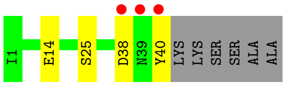
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



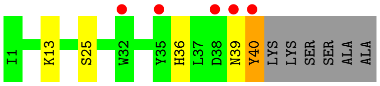
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

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	182.80Å 205.70Å 177.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.70 136.64 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.70) 99.9 (136.64-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.123 , 0.153 0.139 , 0.165	Depositor DCC
R_{free} test set	36325 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 64.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33049	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.78	4/4259 (0.1%)	0.85	5/5816 (0.1%)
1	N	0.75	0/4259	0.82	4/5816 (0.1%)
2	B	0.86	4/1908 (0.2%)	1.01	7/2598 (0.3%)
2	O	0.77	2/1908 (0.1%)	0.89	1/2598 (0.0%)
3	C	0.78	0/2258	0.81	1/3084 (0.0%)
3	P	0.76	0/2258	0.79	1/3084 (0.0%)
4	D	0.91	1/1226 (0.1%)	0.86	3/1657 (0.2%)
4	Q	0.73	1/1182 (0.1%)	0.92	3/1598 (0.2%)
5	E	0.77	1/843 (0.1%)	0.82	0/1145
5	R	0.86	1/843 (0.1%)	0.80	1/1145 (0.1%)
6	F	0.80	0/724	0.86	0/983
6	S	0.82	1/724 (0.1%)	0.88	1/983 (0.1%)
7	G	0.79	2/633 (0.3%)	0.93	3/864 (0.3%)
7	T	0.77	0/633	0.85	0/864
8	H	0.76	0/648	0.86	0/877
8	U	0.75	0/648	0.85	0/877
9	I	0.89	2/588 (0.3%)	0.96	3/781 (0.4%)
9	V	0.74	0/588	0.97	2/781 (0.3%)
10	J	0.71	0/451	0.80	0/610
10	W	0.73	0/451	0.81	0/610
11	K	0.81	0/398	0.83	1/546 (0.2%)
11	X	0.75	0/398	0.76	0/546
12	L	0.88	1/372 (0.3%)	0.85	0/500
12	Y	0.81	1/372 (0.3%)	0.78	0/500
13	M	0.87	1/321 (0.3%)	0.71	0/440
13	Z	0.72	0/321	0.78	0/440
All	All	0.79	22/29214 (0.1%)	0.86	36/39743 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	N	0	1
6	S	0	1
All	All	0	5

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	58	GLU	CD-OE1	13.48	1.40	1.25
5	R	80	GLU	CD-OE1	11.61	1.38	1.25
12	L	5	GLU	CD-OE2	-8.74	1.16	1.25
9	I	72	ALA	C-O	7.29	1.37	1.23
1	A	382	SER	CB-OG	-6.98	1.33	1.42

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Q	20	ARG	NE-CZ-NH1	14.28	127.44	120.30
9	V	10	ARG	NE-CZ-NH2	-11.91	114.34	120.30
4	Q	20	ARG	NE-CZ-NH2	-11.61	114.49	120.30
2	B	65	TRP	CA-CB-CG	10.74	134.10	113.70
2	B	65	TRP	CB-CG-CD1	-9.24	114.99	127.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4102	50	0
1	N	4130	0	4102	44	0
2	B	1870	0	1870	20	0
2	O	1870	0	1870	23	0
3	C	2171	0	2080	32	0
3	P	2172	0	2081	24	0
4	D	1192	0	1178	6	0
4	Q	1148	0	1131	9	0
5	E	825	0	823	0	0
5	R	825	0	823	2	0
6	F	709	0	691	8	0
6	S	709	0	691	5	0
7	G	606	0	577	4	0
7	T	606	0	577	5	0
8	H	628	0	580	7	0
8	U	628	0	580	9	0
9	I	575	0	584	1	0
9	V	575	0	584	4	0
10	J	441	0	439	4	0
10	W	441	0	439	5	0
11	K	384	0	366	1	0
11	X	384	0	366	1	0
12	L	360	0	360	7	0
12	Y	360	0	360	4	0
13	M	311	0	321	2	0
13	Z	311	0	321	4	0
14	A	129	0	88	4	0
14	N	129	0	88	4	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	1	0
19	A	28	0	54	11	0
19	B	17	0	33	3	0
19	C	114	0	203	31	0
19	N	45	0	87	5	0
19	O	11	0	21	4	0
19	P	100	0	174	22	0
19	T	25	0	48	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	62	0	96	11	0
20	B	55	0	83	1	0
20	C	194	0	262	21	0
20	D	33	0	41	4	0
20	H	33	0	26	9	0
20	J	11	0	21	0	0
20	L	22	0	31	2	0
20	M	41	0	57	1	0
20	N	84	0	100	4	0
20	O	66	0	104	2	0
20	P	194	0	262	13	0
20	Q	33	0	41	2	0
20	W	11	0	21	0	0
20	Y	22	0	31	4	0
20	Z	41	0	56	0	0
21	A	16	0	24	0	0
21	B	4	0	6	0	0
21	C	12	0	17	1	0
21	E	12	0	18	0	0
21	F	8	0	12	1	0
21	G	4	0	6	0	0
21	N	20	0	30	3	0
21	O	4	0	6	0	0
21	P	12	0	18	1	0
21	R	12	0	18	0	0
21	S	8	0	12	1	0
21	T	4	0	6	0	0
22	A	51	0	76	1	0
22	C	51	0	76	1	0
22	N	51	0	76	1	0
22	P	51	0	76	0	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	29	0	39	0	0
24	C	58	0	78	1	0
24	O	29	0	39	1	0
24	P	58	0	78	4	0
25	C	1	0	0	1	0
25	P	1	0	0	1	0
26	C	87	0	124	16	0
26	I	64	0	72	0	0
26	L	94	0	141	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	O	64	0	72	1	0
26	P	87	0	124	10	0
26	Y	94	0	141	4	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	53	0	77	2	0
28	T	53	0	77	4	0
29	A	250	0	0	9	0
29	B	177	0	0	3	0
29	C	103	0	0	7	0
29	D	144	0	0	2	0
29	E	116	0	0	0	0
29	F	111	0	0	2	0
29	G	43	0	0	2	0
29	H	61	0	0	0	0
29	I	41	0	0	1	0
29	J	20	0	0	0	0
29	K	22	0	0	0	0
29	L	27	0	0	1	0
29	M	21	0	0	0	0
29	N	237	0	0	11	0
29	O	149	0	0	2	0
29	P	102	0	0	8	0
29	Q	86	0	0	3	0
29	R	94	0	0	2	0
29	S	93	0	0	1	0
29	T	38	0	0	2	0
29	U	46	0	0	0	0
29	V	22	0	0	0	0
29	W	15	0	0	0	0
29	X	18	0	0	0	0
29	Y	27	0	0	1	0
29	Z	17	0	0	1	0
All	All	33049	0	31463	358	0

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

The worst 5 of 358 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:C:314:LFA:H12	29:C:423:HOH:O	1.38	1.24
20:P:318:DMU:O3	20:P:319:DMU:H29	1.36	1.23
1:A:297[B]:MET:HB2	29:A:804:HOH:O	1.41	1.18
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.23	1.14
18:N:608:PER:O2	18:N:608:PER:O1	1.64	1.14

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	526/514 (102%)	512 (97%)	14 (3%)	0	100	100
1	N	526/514 (102%)	514 (98%)	12 (2%)	0	100	100
2	B	230/227 (101%)	224 (97%)	6 (3%)	0	100	100
2	O	230/227 (101%)	225 (98%)	5 (2%)	0	100	100
3	C	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
3	P	265/261 (102%)	261 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	136/147 (92%)	132 (97%)	3 (2%)	1 (1%)	22	8
5	E	100/109 (92%)	100 (100%)	0	0	100	100
5	R	100/109 (92%)	100 (100%)	0	0	100	100
6	F	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
6	S	91/98 (93%)	90 (99%)	1 (1%)	0	100	100
7	G	71/85 (84%)	67 (94%)	4 (6%)	0	100	100
7	T	71/85 (84%)	68 (96%)	3 (4%)	0	100	100
8	H	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
8	U	73/85 (86%)	71 (97%)	1 (1%)	1 (1%)	11	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%)	1 (3%)	0	100	100
All	All	3488/3614 (96%)	3415 (98%)	71 (2%)	2 (0%)	51	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	U	48	GLY
4	Q	11	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/426 (103%)	435 (99%)	5 (1%)	73	63
1	N	440/426 (103%)	435 (99%)	5 (1%)	73	63
2	B	215/210 (102%)	206 (96%)	9 (4%)	30	12
2	O	215/210 (102%)	209 (97%)	6 (3%)	43	25
3	C	232/226 (103%)	229 (99%)	3 (1%)	69	56
3	P	232/226 (103%)	229 (99%)	3 (1%)	69	56
4	D	128/129 (99%)	128 (100%)	0	100	100
4	Q	122/129 (95%)	120 (98%)	2 (2%)	62	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	89/95 (94%)	89 (100%)	0	100	100
5	R	89/95 (94%)	88 (99%)	1 (1%)	73	63
6	F	78/81 (96%)	78 (100%)	0	100	100
6	S	78/81 (96%)	76 (97%)	2 (3%)	46	28
7	G	63/69 (91%)	59 (94%)	4 (6%)	18	5
7	T	63/69 (91%)	59 (94%)	4 (6%)	18	5
8	H	67/75 (89%)	65 (97%)	2 (3%)	41	22
8	U	67/75 (89%)	64 (96%)	3 (4%)	27	10
9	I	55/58 (95%)	53 (96%)	2 (4%)	35	16
9	V	55/58 (95%)	52 (94%)	3 (6%)	21	7
10	J	47/50 (94%)	47 (100%)	0	100	100
10	W	47/50 (94%)	45 (96%)	2 (4%)	29	11
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	28
11	X	39/46 (85%)	38 (97%)	1 (3%)	46	28
12	L	37/40 (92%)	37 (100%)	0	100	100
12	Y	37/40 (92%)	37 (100%)	0	100	100
13	M	34/38 (90%)	32 (94%)	2 (6%)	19	6
13	Z	34/38 (90%)	32 (94%)	2 (6%)	19	6
All	All	3042/3086 (99%)	2980 (98%)	62 (2%)	53	38

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	38	ARG
9	V	61	GLU
2	O	78	LEU
9	V	8	GLN
11	X	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	59	GLN
4	Q	101	HIS
13	Z	39	ASN

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Mol	Chain	Res	Type
3	P	50	ASN
4	Q	109	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	FME	B	1	2	8,9,10	1.12	1 (12%)	7,9,11	1.57	1 (14%)
1	FME	N	1	1	8,9,10	0.50	0	7,9,11	0.95	1 (14%)
2	FME	O	1	2	8,9,10	0.61	0	7,9,11	1.06	1 (14%)
1	FME	A	1	1	8,9,10	0.45	0	7,9,11	1.09	0

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-2.76	1.66	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CG-CB-CA	-2.88	104.95	112.95
1	N	1	FME	O-C-CA	-2.23	118.92	124.78
2	O	1	FME	O-C-CA	-2.15	119.14	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	N	1	FME	CA-CB-CG-SD
1	A	1	FME	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 135 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 125 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	LFA	P	313	-	14,14,19	0.27	0	13,13,18	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
20	DMU	Q	201	-	34,34,34	1.31	5 (14%)	45,45,45	1.46	4 (8%)
23	CUA	O	305	2	0,1,1	-	-	-		
19	LFA	C	307	-	10,10,19	0.14	0	9,9,18	0.19	0
21	EDO	P	320	-	3,3,3	0.20	0	2,2,2	0.06	0
20	DMU	C	316	-	6,6,34	0.28	0	5,5,45	0.47	0
20	DMU	M	102	-	7,7,34	0.26	0	6,6,45	0.53	0
20	DMU	C	317	-	22,22,34	0.57	0	27,27,45	1.26	4 (14%)
18	PER	N	608	15,14	0,1,1	-	-	-		
21	EDO	T	104	-	3,3,3	0.18	0	2,2,2	0.23	0
14	HEA	A	602	18,1	57,67,67	1.50	10 (17%)	61,103,103	2.45	24 (39%)
18	PER	A	606	15,14	0,1,1	-	-	-		
20	DMU	P	307	-	10,10,34	0.33	0	9,9,45	0.55	0
21	EDO	C	321	-	3,3,3	0.30	0	2,2,2	0.44	0
21	EDO	O	309	-	3,3,3	0.44	0	2,2,2	0.30	0
20	DMU	A	617	-	10,10,34	0.25	0	9,9,45	0.56	0
20	DMU	P	317	-	22,22,34	0.92	1 (4%)	27,27,45	1.32	2 (7%)
19	LFA	T	102	-	13,13,19	0.23	0	12,12,18	0.13	0
20	DMU	C	323	-	22,22,34	0.67	1 (4%)	27,27,45	1.02	2 (7%)
28	PEK	G	101	-	52,52,52	0.56	1 (1%)	55,57,57	0.61	0
19	LFA	P	309	-	5,5,19	0.17	0	4,4,18	0.07	0
21	EDO	R	203	-	3,3,3	0.26	0	2,2,2	0.61	0
20	DMU	O	307	-	10,10,34	0.50	0	9,9,45	0.44	0
24	CHD	C	301	-	32,32,32	0.85	1 (3%)	51,51,51	0.72	0
26	CDL	C	304	-	86,86,99	0.53	0	92,98,111	1.11	8 (8%)
21	EDO	N	616	-	3,3,3	0.21	0	2,2,2	0.10	0
21	EDO	A	612	-	3,3,3	0.07	0	2,2,2	0.13	0
21	EDO	C	322	-	3,3,3	0.81	0	2,2,2	0.70	0
21	EDO	N	617	-	3,3,3	0.38	0	2,2,2	0.65	0
20	DMU	Z	102	-	7,7,34	0.26	0	6,6,45	0.45	0
21	EDO	N	613	-	3,3,3	0.17	0	2,2,2	0.13	0
14	HEA	N	603[A]	-	57,67,67	1.74	12 (21%)	61,103,103	2.46	23 (37%)
19	LFA	P	312	-	10,10,19	0.20	0	9,9,18	0.30	0
24	CHD	P	302	-	32,32,32	0.75	1 (3%)	51,51,51	0.85	0
24	CHD	O	301	-	32,32,32	0.72	0	51,51,51	0.77	0
21	EDO	E	201	-	3,3,3	0.07	0	2,2,2	0.21	0
14	HEA	N	603[B]	-	57,67,67	1.75	12 (21%)	61,103,103	2.38	22 (36%)
21	EDO	E	203	-	3,3,3	0.44	0	2,2,2	0.43	0
20	DMU	L	102	-	22,22,34	0.73	1 (4%)	27,27,45	1.21	4 (14%)
20	DMU	P	316	-	6,6,34	0.29	0	5,5,45	0.47	0
20	DMU	P	318	-	34,34,34	0.93	3 (8%)	45,45,45	1.15	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
21	EDO	S	103	-	3,3,3	0.14	0	2,2,2	0.05	0
21	EDO	G	102	-	3,3,3	0.27	0	2,2,2	0.20	0
20	DMU	O	303	-	22,22,34	0.74	0	27,27,45	1.44	3 (11%)
20	DMU	P	324	-	34,34,34	0.68	0	45,45,45	1.54	4 (8%)
22	PGV	A	616	-	50,50,50	0.69	0	53,56,56	1.19	4 (7%)
24	CHD	P	306	-	32,32,32	0.79	1 (3%)	51,51,51	1.31	5 (9%)
20	DMU	B	303	-	22,22,34	0.90	1 (4%)	27,27,45	0.86	1 (3%)
20	DMU	N	602	-	10,10,34	0.28	0	9,9,45	0.52	0
19	LFA	B	306	-	16,16,19	0.34	0	15,15,18	0.17	0
28	PEK	T	101	-	52,52,52	0.61	2 (3%)	55,57,57	1.00	3 (5%)
20	DMU	C	324	-	34,34,34	0.84	1 (2%)	45,45,45	1.15	3 (6%)
26	CDL	L	101	-	93,93,99	0.42	0	99,105,111	0.62	2 (2%)
19	LFA	C	314	-	12,12,19	0.30	0	11,11,18	0.25	0
21	EDO	N	614	-	3,3,3	0.20	0	2,2,2	0.40	0
19	LFA	C	309	20	17,17,19	0.22	0	16,16,18	0.19	0
20	DMU	B	307	-	22,22,34	0.49	0	27,27,45	1.23	2 (7%)
14	HEA	N	604	18,1	57,67,67	1.63	9 (15%)	61,103,103	2.35	23 (37%)
19	LFA	N	601	-	16,16,19	0.28	0	15,15,18	0.21	0
21	EDO	R	202	-	3,3,3	0.20	0	2,2,2	0.36	0
21	EDO	S	102	-	3,3,3	0.39	0	2,2,2	0.30	0
19	LFA	C	313	-	14,14,19	0.27	0	13,13,18	0.41	0
26	CDL	Y	101	-	93,93,99	0.33	0	99,105,111	0.43	1 (1%)
19	LFA	C	311	-	13,13,19	0.23	0	12,12,18	0.12	0
20	DMU	A	609	-	6,6,34	0.59	0	5,5,45	0.29	0
19	LFA	P	310	20	17,17,19	0.19	0	16,16,18	0.16	0
20	DMU	C	306	-	10,10,34	0.42	0	9,9,45	0.58	0
20	DMU	M	101	-	34,34,34	0.85	1 (2%)	45,45,45	1.14	3 (6%)
20	DMU	A	610	-	34,34,34	1.27	6 (17%)	45,45,45	1.18	5 (11%)
26	CDL	O	304	-	63,63,99	0.40	0	69,75,111	0.70	1 (1%)
20	DMU	W	101	-	10,10,34	0.29	0	9,9,45	0.56	0
21	EDO	P	321	-	3,3,3	0.19	0	2,2,2	0.17	0
21	EDO	B	304	-	3,3,3	0.40	0	2,2,2	0.21	0
21	EDO	F	103	-	3,3,3	0.20	0	2,2,2	0.36	0
22	PGV	P	304	-	50,50,50	0.76	1 (2%)	53,56,56	0.94	3 (5%)
23	CUA	B	301	2	0,1,1	-	-	-		
20	DMU	C	318	-	34,34,34	0.89	2 (5%)	45,45,45	1.24	2 (4%)
24	CHD	C	305	-	32,32,32	0.69	1 (3%)	51,51,51	1.57	9 (17%)
20	DMU	P	319	-	34,34,34	0.79	2 (5%)	45,45,45	1.20	3 (6%)
20	DMU	A	615	-	10,10,34	0.29	0	9,9,45	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
20	DMU	P	315	-	34,34,34	0.82	2 (5%)	45,45,45	1.33	3 (6%)
19	LFA	P	308	-	10,10,19	0.22	0	9,9,18	0.26	0
21	EDO	A	614	-	3,3,3	0.30	0	2,2,2	0.17	0
21	EDO	F	102	-	3,3,3	0.19	0	2,2,2	0.04	0
20	DMU	O	306	-	10,10,34	0.14	0	9,9,45	0.63	0
20	DMU	O	308	-	22,22,34	0.68	0	27,27,45	1.08	2 (7%)
19	LFA	C	325	-	14,14,19	0.14	0	13,13,18	0.10	0
20	DMU	C	319	-	34,34,34	0.85	1 (2%)	45,45,45	1.29	5 (11%)
20	DMU	J	101	-	10,10,34	0.21	0	9,9,45	0.58	0
19	LFA	C	308	-	5,5,19	0.19	0	4,4,18	0.05	0
19	LFA	N	610	-	13,13,19	0.55	0	12,12,18	0.38	0
19	LFA	P	314	-	12,12,19	0.31	0	11,11,18	0.25	0
21	EDO	P	322	-	3,3,3	0.38	0	2,2,2	0.78	0
20	DMU	D	201	-	34,34,34	1.48	8 (23%)	45,45,45	1.51	5 (11%)
21	EDO	R	201	-	3,3,3	0.17	0	2,2,2	0.13	0
19	LFA	N	609	-	13,13,19	0.35	0	12,12,18	0.40	0
20	DMU	N	611	-	6,6,34	0.35	0	5,5,45	0.36	0
19	LFA	C	310	-	10,10,19	0.13	0	9,9,18	0.10	0
20	DMU	N	619	19	34,34,34	0.83	1 (2%)	45,45,45	1.31	6 (13%)
19	LFA	O	302	-	10,10,19	0.23	0	9,9,18	0.15	0
19	LFA	A	608	-	13,13,19	0.64	0	12,12,18	0.54	0
19	LFA	P	301	-	14,14,19	0.23	0	13,13,18	0.16	0
26	CDL	I	101	-	63,63,99	0.46	0	69,75,111	1.02	4 (5%)
20	DMU	P	323	-	22,22,34	0.76	0	27,27,45	1.46	1 (3%)
21	EDO	C	320	-	3,3,3	0.06	0	2,2,2	0.10	0
19	LFA	A	607	-	13,13,19	0.36	0	12,12,18	0.25	0
20	DMU	C	315	-	34,34,34	1.00	1 (2%)	45,45,45	1.64	10 (22%)
14	HEA	A	601[A]	-	57,67,67	1.75	11 (19%)	61,103,103	2.61	23 (37%)
20	DMU	Y	102	-	22,22,34	0.57	0	27,27,45	1.00	1 (3%)
19	LFA	C	312	-	10,10,19	0.23	0	9,9,18	0.17	0
20	DMU	B	302	-	10,10,34	0.21	0	9,9,45	0.58	0
22	PGV	C	303	-	50,50,50	0.77	2 (4%)	53,56,56	1.06	3 (5%)
26	CDL	P	305	-	86,86,99	0.48	0	92,98,111	0.83	5 (5%)
22	PGV	N	618	-	50,50,50	0.76	1 (2%)	53,56,56	1.21	3 (5%)
19	LFA	T	103	-	10,10,19	0.23	0	9,9,18	0.13	0
20	DMU	H	101	19	34,34,34	0.91	2 (5%)	45,45,45	1.10	3 (6%)
20	DMU	Z	101	-	34,34,34	1.00	3 (8%)	45,45,45	0.97	3 (6%)
14	HEA	A	601[B]	-	57,67,67	1.76	11 (19%)	61,103,103	2.59	24 (39%)
19	LFA	P	311	-	10,10,19	0.16	0	9,9,18	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
20	DMU	N	612	-	34,34,34	1.32	4 (11%)	45,45,45	1.00	3 (6%)
21	EDO	A	613	-	3,3,3	0.38	0	2,2,2	0.19	0
24	CHD	B	305	-	32,32,32	0.65	0	51,51,51	0.90	1 (1%)
21	EDO	E	202	-	3,3,3	0.17	0	2,2,2	0.12	0
21	EDO	A	611	-	3,3,3	0.33	0	2,2,2	0.54	0
21	EDO	N	615	-	3,3,3	0.46	0	2,2,2	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LFA	P	313	-	-	5/12/12/17	-
20	DMU	Q	201	-	-	8/19/59/59	0/2/2/2
19	LFA	C	307	-	-	7/8/8/17	-
21	EDO	P	320	-	-	1/1/1/1	-
20	DMU	C	316	-	-	3/4/4/59	-
20	DMU	M	102	-	-	5/5/5/59	-
20	DMU	C	317	-	-	7/13/33/59	0/1/1/2
21	EDO	T	104	-	-	0/1/1/1	-
14	HEA	A	602	18,1	-	4/32/76/76	-
20	DMU	P	307	-	-	2/8/8/59	-
21	EDO	C	321	-	-	0/1/1/1	-
21	EDO	O	309	-	-	0/1/1/1	-
20	DMU	A	617	-	-	6/8/8/59	-
20	DMU	P	317	-	-	8/13/33/59	0/1/1/2
19	LFA	T	102	-	-	6/11/11/17	-
20	DMU	C	323	-	-	10/13/33/59	0/1/1/2
28	PEK	G	101	-	-	15/56/56/56	-
19	LFA	P	309	-	-	1/3/3/17	-
21	EDO	R	203	-	-	1/1/1/1	-
20	DMU	O	307	-	-	5/8/8/59	-
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
26	CDL	C	304	-	-	41/97/97/110	-
21	EDO	N	616	-	-	0/1/1/1	-
21	EDO	A	612	-	-	1/1/1/1	-
21	EDO	C	322	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	N	617	-	-	0/1/1/1	-
20	DMU	Z	102	-	-	2/5/5/59	-
21	EDO	N	613	-	-	0/1/1/1	-
14	HEA	N	603[A]	-	-	6/32/76/76	-
19	LFA	P	312	-	-	5/8/8/17	-
24	CHD	P	302	-	-	2/9/74/74	0/4/4/4
24	CHD	O	301	-	-	2/9/74/74	0/4/4/4
21	EDO	E	201	-	-	0/1/1/1	-
14	HEA	N	603[B]	-	-	2/32/76/76	-
21	EDO	E	203	-	-	1/1/1/1	-
20	DMU	L	102	-	-	11/13/33/59	0/1/1/2
20	DMU	P	316	-	-	3/4/4/59	-
20	DMU	P	318	-	-	15/19/59/59	0/2/2/2
21	EDO	S	103	-	-	0/1/1/1	-
21	EDO	G	102	-	-	0/1/1/1	-
20	DMU	O	303	-	-	7/13/33/59	0/1/1/2
20	DMU	P	324	-	-	7/19/59/59	0/2/2/2
22	PGV	A	616	-	-	10/55/55/55	-
24	CHD	P	306	-	-	9/9/74/74	0/4/4/4
20	DMU	B	303	-	-	7/13/33/59	0/1/1/2
20	DMU	N	602	-	-	4/8/8/59	-
19	LFA	B	306	-	-	11/14/14/17	-
28	PEK	T	101	-	-	21/56/56/56	-
20	DMU	C	324	-	-	4/19/59/59	0/2/2/2
26	CDL	L	101	-	-	56/104/104/110	-
19	LFA	C	314	-	-	5/10/10/17	-
21	EDO	N	614	-	-	1/1/1/1	-
19	LFA	C	309	20	-	9/15/15/17	-
20	DMU	B	307	-	-	9/13/33/59	0/1/1/2
14	HEA	N	604	18,1	-	4/32/76/76	-
19	LFA	N	601	-	-	10/14/14/17	-
21	EDO	R	202	-	-	0/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
19	LFA	C	313	-	-	4/12/12/17	-
26	CDL	Y	101	-	-	55/104/104/110	-
19	LFA	C	311	-	-	5/11/11/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	DMU	A	609	-	-	3/4/4/59	-
19	LFA	P	310	20	-	6/15/15/17	-
20	DMU	C	306	-	-	3/8/8/59	-
20	DMU	M	101	-	-	3/19/59/59	0/2/2/2
20	DMU	A	610	-	-	7/19/59/59	0/2/2/2
26	CDL	O	304	-	-	41/74/74/110	-
20	DMU	W	101	-	-	5/8/8/59	-
21	EDO	P	321	-	-	1/1/1/1	-
21	EDO	B	304	-	-	0/1/1/1	-
21	EDO	F	103	-	-	1/1/1/1	-
22	PGV	P	304	-	-	11/55/55/55	-
20	DMU	C	318	-	-	13/19/59/59	0/2/2/2
24	CHD	C	305	-	-	8/9/74/74	0/4/4/4
20	DMU	P	319	-	-	9/19/59/59	0/2/2/2
20	DMU	A	615	-	-	6/8/8/59	-
20	DMU	P	315	-	-	5/19/59/59	0/2/2/2
19	LFA	P	308	-	-	4/8/8/17	-
21	EDO	A	614	-	-	1/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
20	DMU	O	306	-	-	5/8/8/59	-
20	DMU	O	308	-	-	5/13/33/59	0/1/1/2
19	LFA	C	325	-	-	7/12/12/17	-
20	DMU	C	319	-	-	10/19/59/59	0/2/2/2
20	DMU	J	101	-	-	6/8/8/59	-
19	LFA	C	308	-	-	1/3/3/17	-
19	LFA	N	610	-	-	7/11/11/17	-
19	LFA	P	314	-	-	3/10/10/17	-
21	EDO	P	322	-	-	0/1/1/1	-
20	DMU	D	201	-	-	7/19/59/59	0/2/2/2
21	EDO	R	201	-	-	1/1/1/1	-
19	LFA	N	609	-	-	4/11/11/17	-
20	DMU	N	611	-	-	2/4/4/59	-
19	LFA	C	310	-	-	8/8/8/17	-
20	DMU	N	619	19	-	5/19/59/59	0/2/2/2
19	LFA	O	302	-	-	3/8/8/17	-
19	LFA	A	608	-	-	5/11/11/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LFA	P	301	-	-	7/12/12/17	-
26	CDL	I	101	-	-	43/74/74/110	-
20	DMU	P	323	-	-	6/13/33/59	0/1/1/2
21	EDO	C	320	-	-	0/1/1/1	-
19	LFA	A	607	-	-	3/11/11/17	-
20	DMU	C	315	-	-	11/19/59/59	0/2/2/2
14	HEA	A	601[A]	-	-	6/32/76/76	-
20	DMU	Y	102	-	-	9/13/33/59	0/1/1/2
19	LFA	C	312	-	-	4/8/8/17	-
20	DMU	B	302	-	-	5/8/8/59	-
22	PGV	C	303	-	-	14/55/55/55	-
26	CDL	P	305	-	-	46/97/97/110	-
22	PGV	N	618	-	-	8/55/55/55	-
19	LFA	T	103	-	-	3/8/8/17	-
20	DMU	H	101	19	-	5/19/59/59	0/2/2/2
20	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
14	HEA	A	601[B]	-	-	2/32/76/76	-
19	LFA	P	311	-	-	5/8/8/17	-
20	DMU	N	612	-	-	5/19/59/59	0/2/2/2
21	EDO	A	613	-	-	0/1/1/1	-
24	CHD	B	305	-	-	2/9/74/74	0/4/4/4
21	EDO	E	202	-	-	0/1/1/1	-
21	EDO	A	611	-	-	0/1/1/1	-
21	EDO	N	615	-	-	0/1/1/1	-

The worst 5 of 122 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	603[A]	HEA	C1D-ND	-5.11	1.31	1.40
14	N	603[B]	HEA	C1D-ND	-5.11	1.31	1.40
20	N	612	DMU	O16-C6	-4.74	1.32	1.40
14	N	603[A]	HEA	C3B-C2B	4.58	1.45	1.34
14	N	603[B]	HEA	C3B-C2B	4.58	1.45	1.34

The worst 5 of 278 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	601[A]	HEA	C3D-C4D-ND	8.02	118.13	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601[B]	HEA	C3D-C4D-ND	8.02	118.13	110.36
14	N	603[A]	HEA	C3D-C4D-ND	7.32	117.44	110.36
14	N	603[B]	HEA	C3D-C4D-ND	7.32	117.44	110.36
14	A	602	HEA	C2B-C1B-NB	6.62	117.81	109.88

There are no chirality outliers.

5 of 821 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C18-C19-C20-C21
14	A	601[A]	HEA	C27-C19-C20-C21
14	N	603[A]	HEA	C18-C19-C20-C21
14	N	603[A]	HEA	C27-C19-C20-C21
20	B	303	DMU	C1-C6-O16-C18

There are no ring outliers.

71 monomers are involved in 184 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	Q	201	DMU	2	0
19	C	307	LFA	6	0
20	C	316	DMU	5	0
20	C	317	DMU	1	0
18	N	608	PER	1	0
14	A	602	HEA	2	0
18	A	606	PER	1	0
21	C	321	EDO	1	0
20	A	617	DMU	9	0
19	T	102	LFA	1	0
20	C	323	DMU	7	0
28	G	101	PEK	2	0
26	C	304	CDL	16	0
21	N	617	EDO	3	0
14	N	603[A]	HEA	1	0
19	P	312	LFA	3	0
24	O	301	CHD	1	0
14	N	603[B]	HEA	1	0
20	L	102	DMU	2	0
20	P	318	DMU	5	0
20	O	303	DMU	2	0
20	P	324	DMU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	616	PGV	1	0
24	P	306	CHD	4	0
20	N	602	DMU	3	0
19	B	306	LFA	3	0
28	T	101	PEK	4	0
20	C	324	DMU	7	0
26	L	101	CDL	3	0
19	C	314	LFA	3	0
19	C	309	LFA	10	0
20	B	307	DMU	1	0
14	N	604	HEA	2	0
19	N	601	LFA	1	0
21	S	102	EDO	1	0
19	C	313	LFA	1	0
26	Y	101	CDL	4	0
20	A	609	DMU	1	0
19	P	310	LFA	3	0
20	M	101	DMU	1	0
20	A	610	DMU	1	0
26	O	304	CDL	1	0
21	P	321	EDO	1	0
21	F	103	EDO	1	0
20	C	318	DMU	1	0
24	C	305	CHD	1	0
20	P	319	DMU	6	0
20	P	315	DMU	1	0
19	P	308	LFA	2	0
19	C	325	LFA	5	0
19	N	610	LFA	2	0
19	P	314	LFA	3	0
20	D	201	DMU	4	0
19	N	609	LFA	2	0
19	C	310	LFA	2	0
19	O	302	LFA	4	0
19	A	608	LFA	10	0
19	P	301	LFA	6	0
20	P	323	DMU	3	0
19	A	607	LFA	3	0
20	C	315	DMU	1	0
14	A	601[A]	HEA	1	0
20	Y	102	DMU	4	0
19	C	312	LFA	5	0

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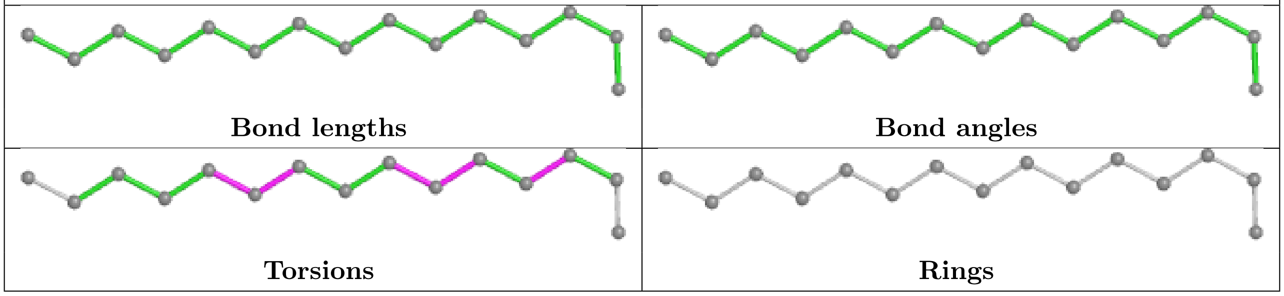
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	303	PGV	1	0
26	P	305	CDL	10	0
22	N	618	PGV	1	0
20	H	101	DMU	9	0
14	A	601[B]	HEA	1	0
19	P	311	LFA	5	0
20	N	612	DMU	1	0

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 LFA P 313



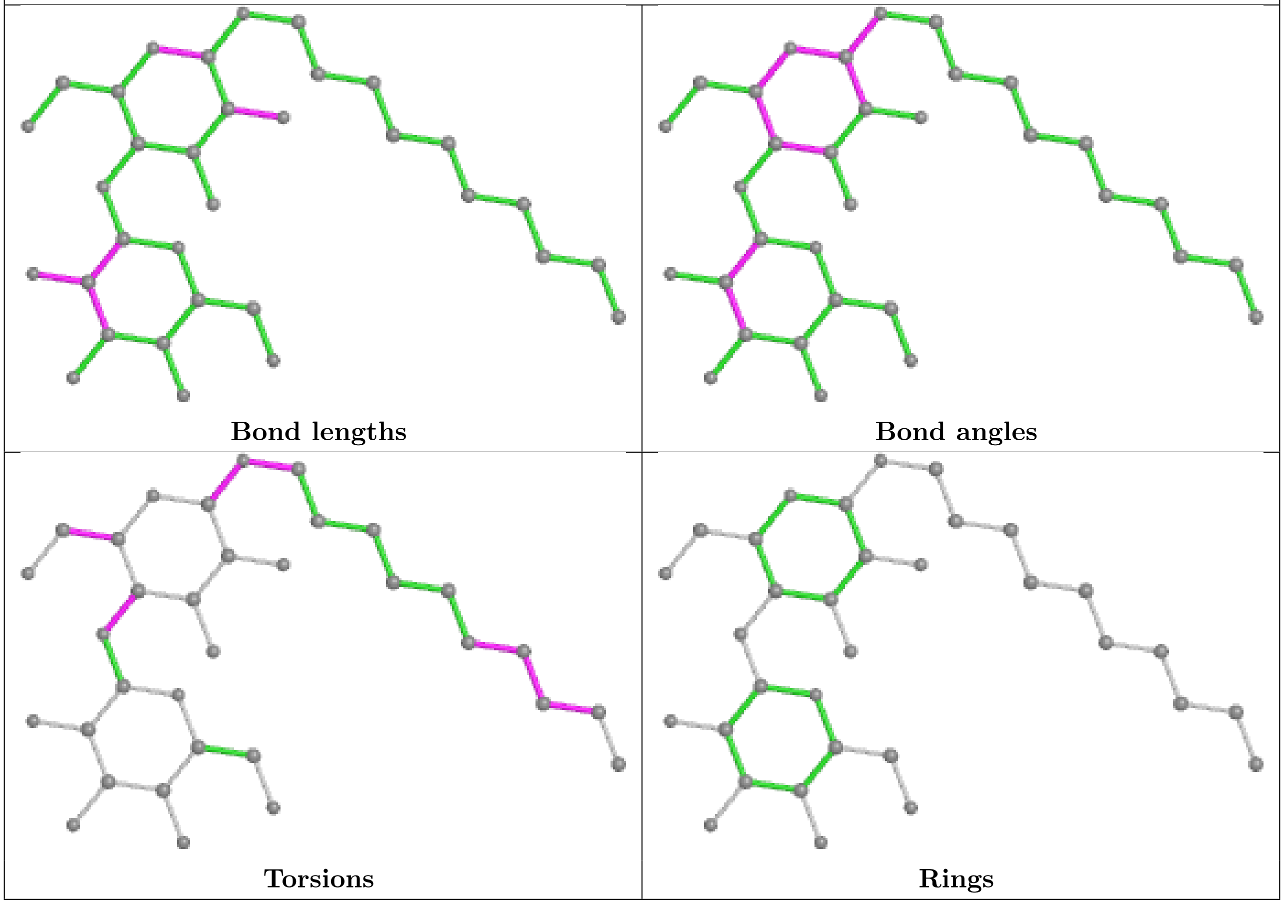
Bond lengths

Bond angles

Torsions

Rings

Ligand DMU Q 201



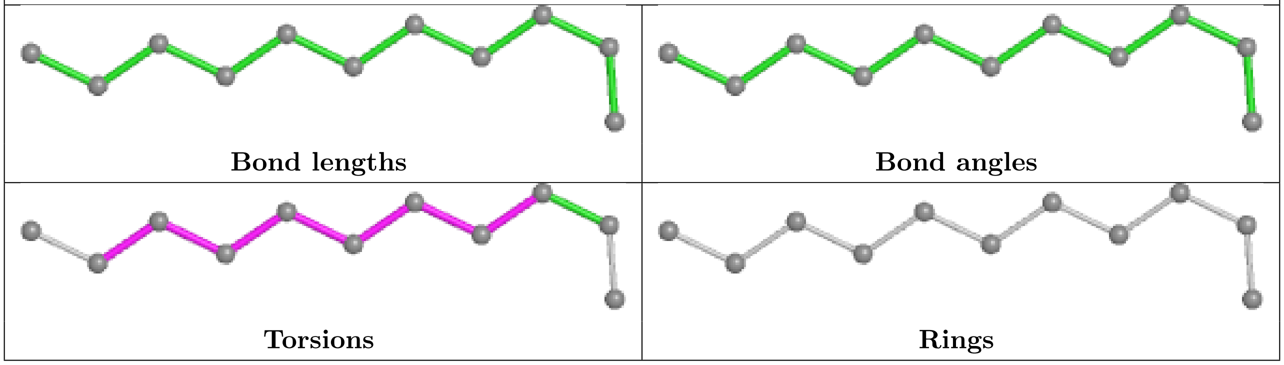
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA C 307



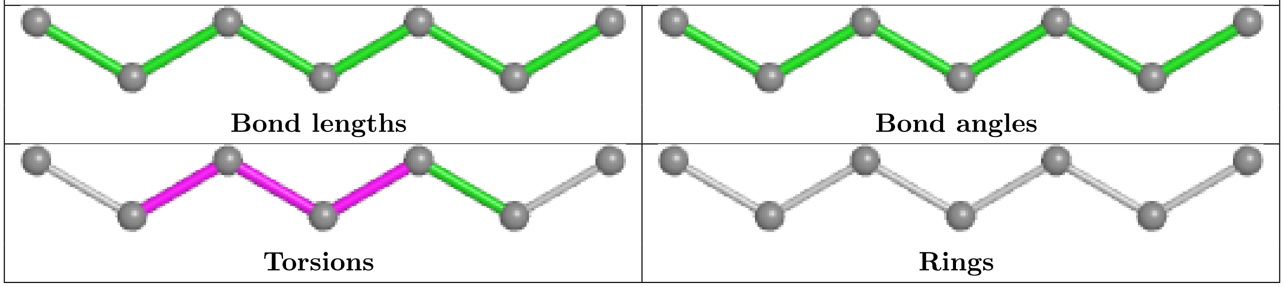
Bond lengths

Bond angles

Torsions

Rings

Ligand DMU C 316



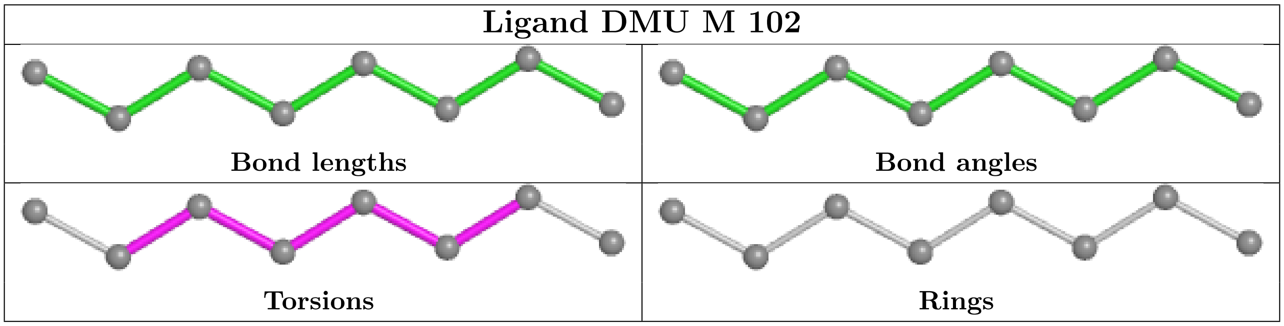
Bond lengths

Bond angles

Torsions

Rings

Ligand DMU M 102



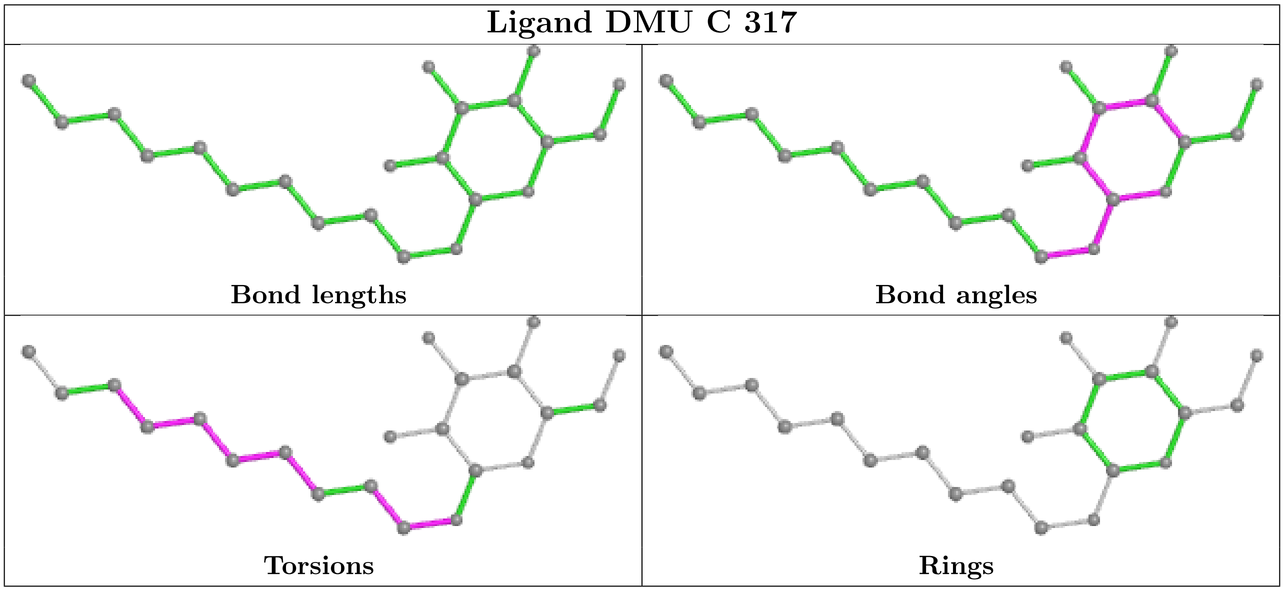
Bond lengths

Bond angles

Torsions

Rings

Ligand DMU C 317



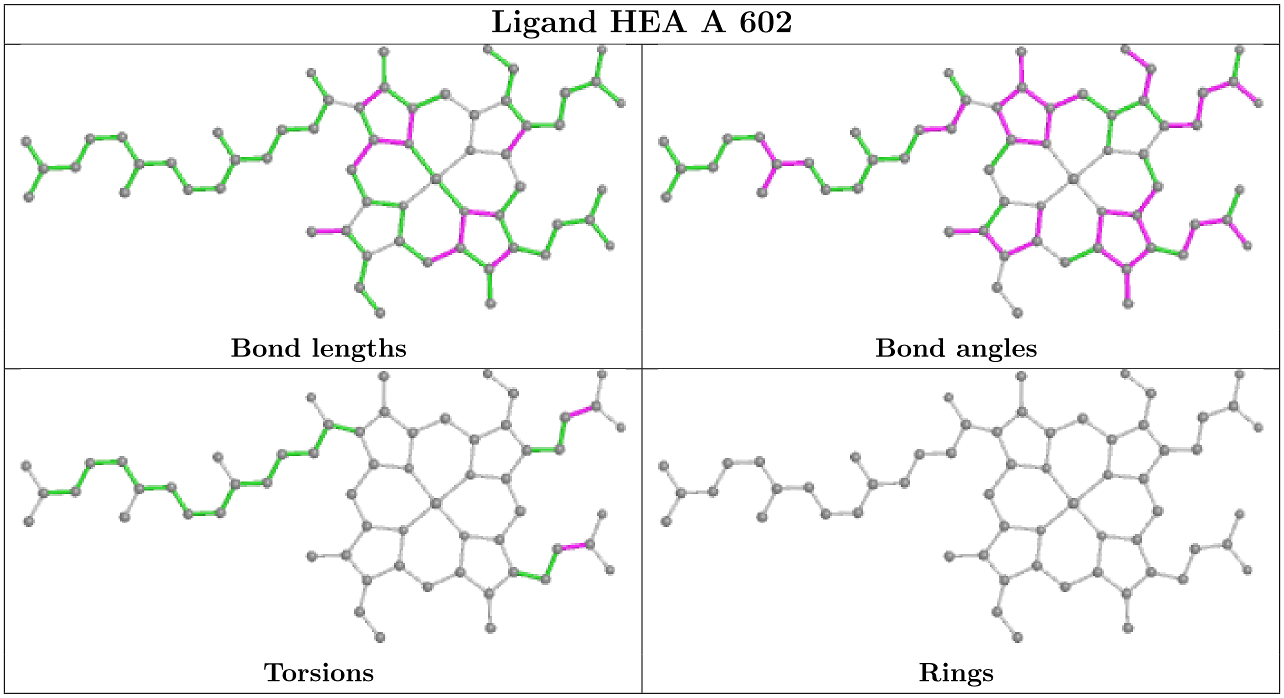
Bond lengths

Bond angles

Torsions

Rings

Ligand HEA A 602



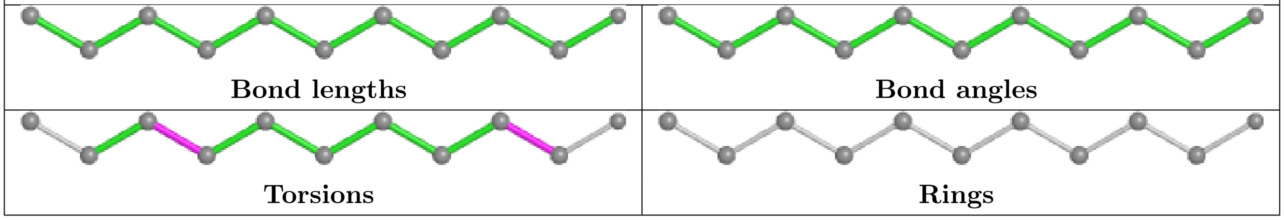
Bond lengths

Bond angles

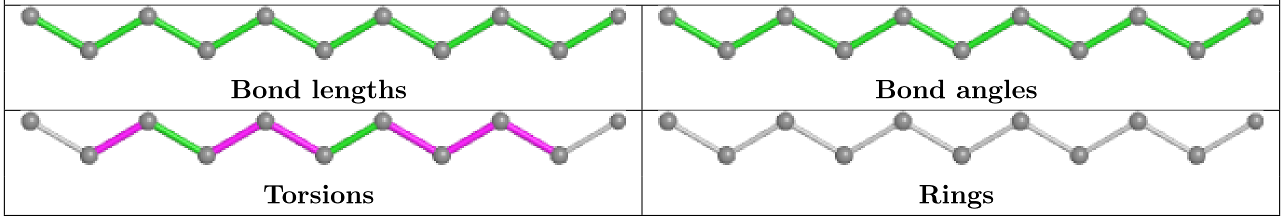
Torsions

Rings

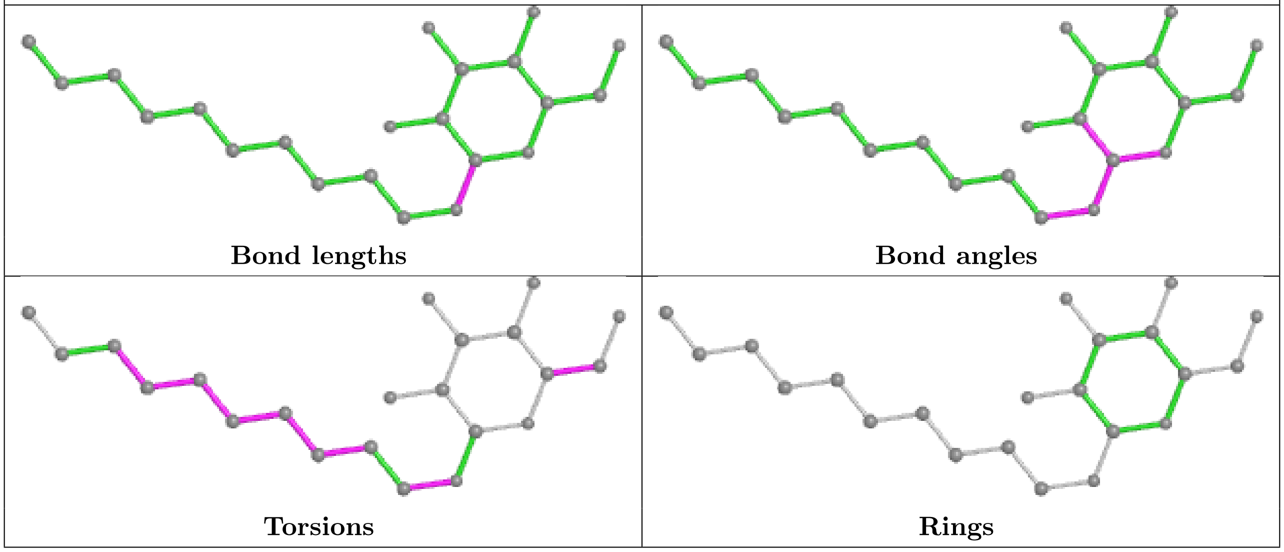
Ligand DMU P 307



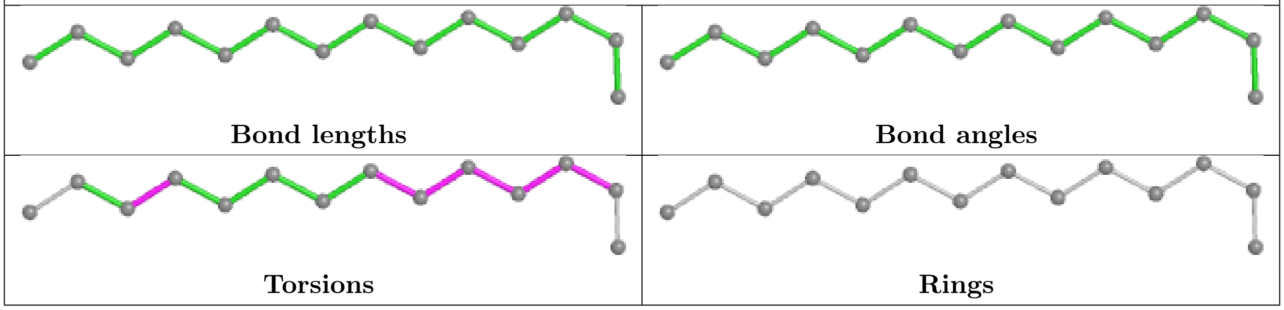
Ligand DMU A 617



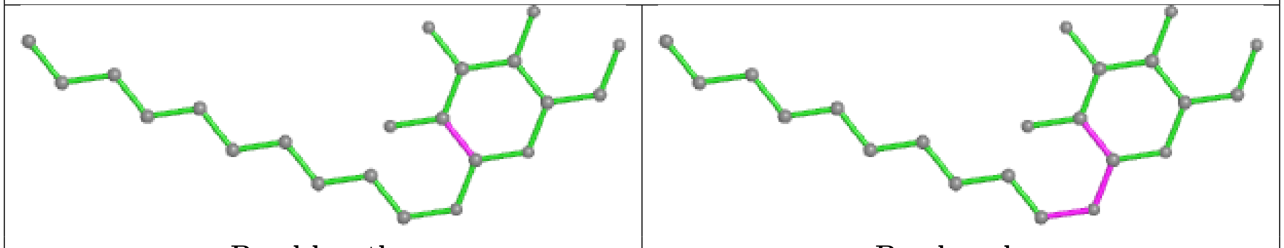
Ligand DMU P 317



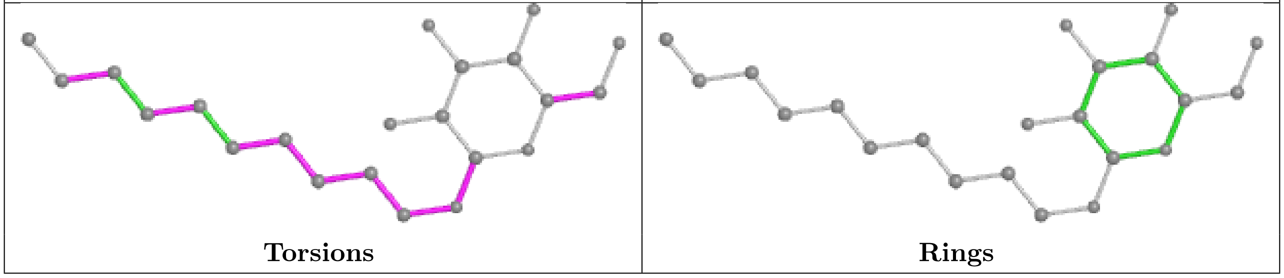
Ligand LFA T 102



Ligand DMU C 323

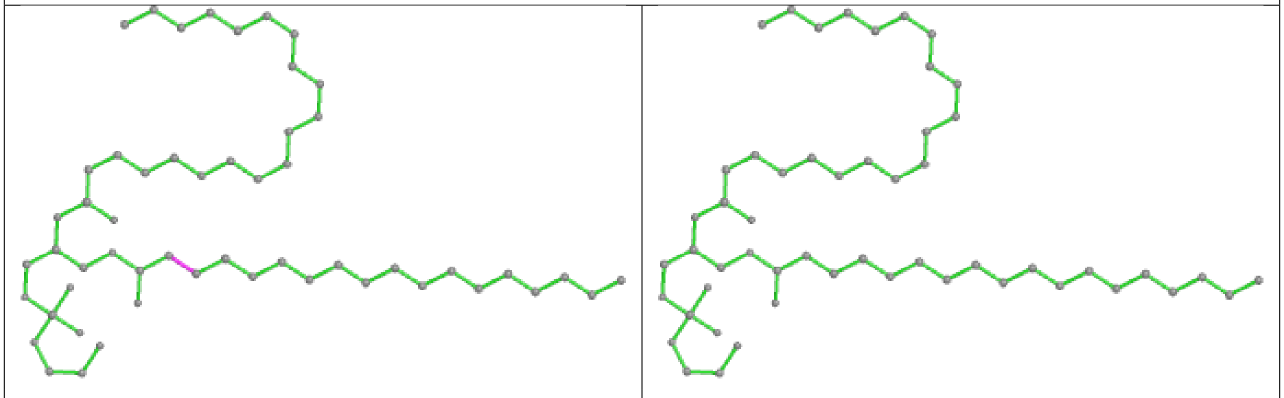


Bond lengths Bond angles

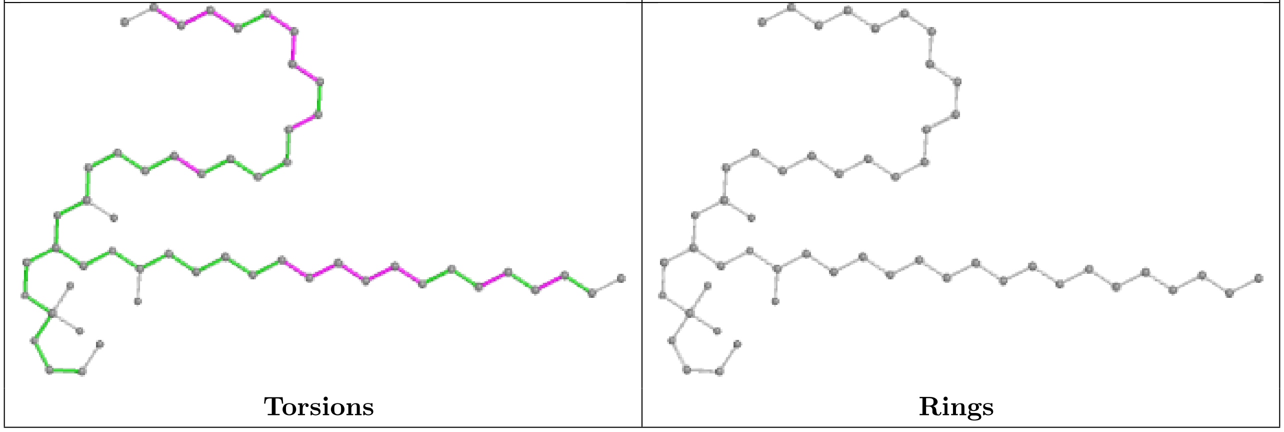


Torsions Rings

Ligand PEK G 101

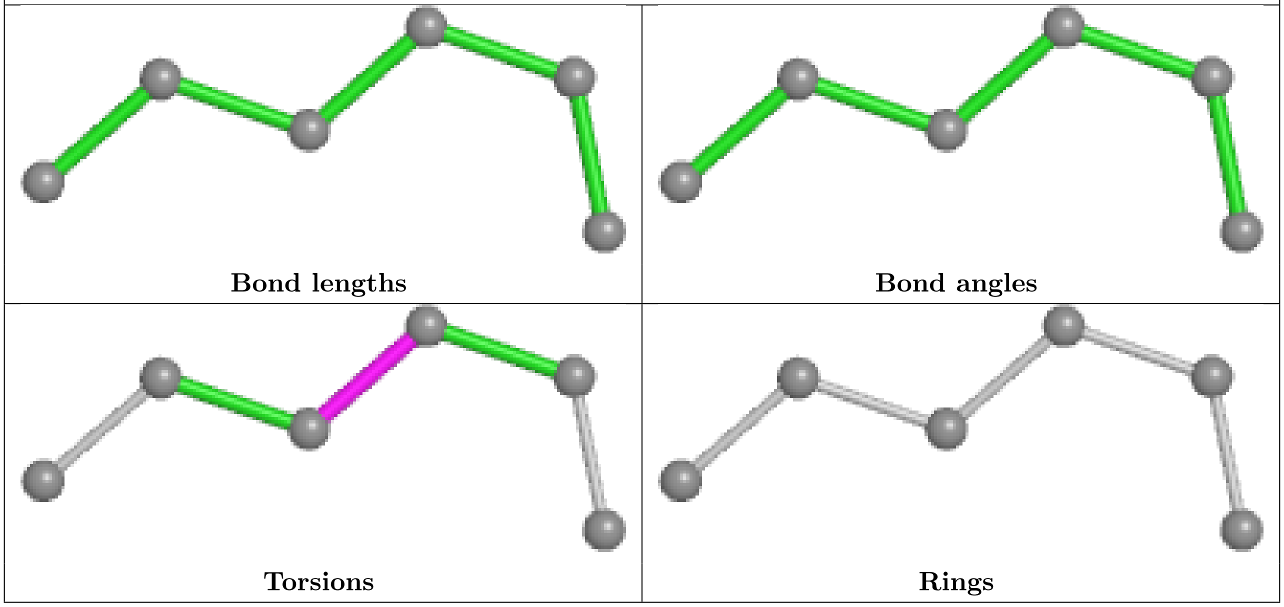


Bond lengths Bond angles

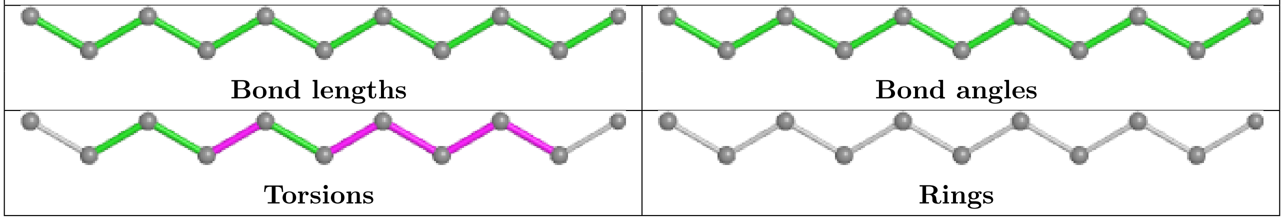


Torsions Rings

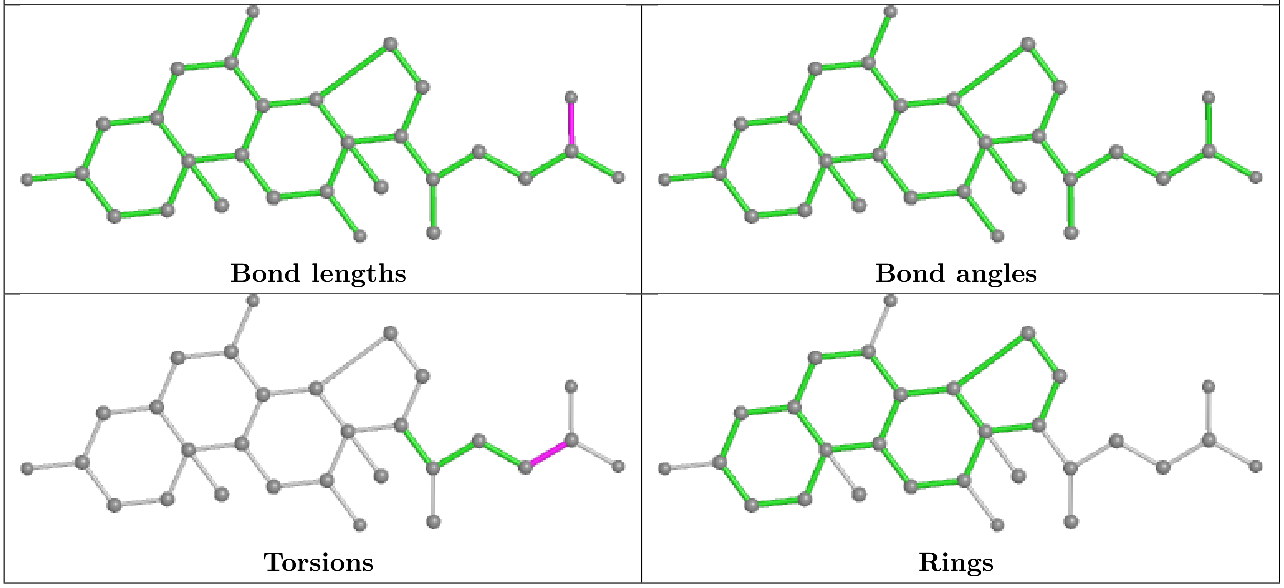
Ligand LFA P 309


Bond lengths
Bond angles
Torsions
Rings

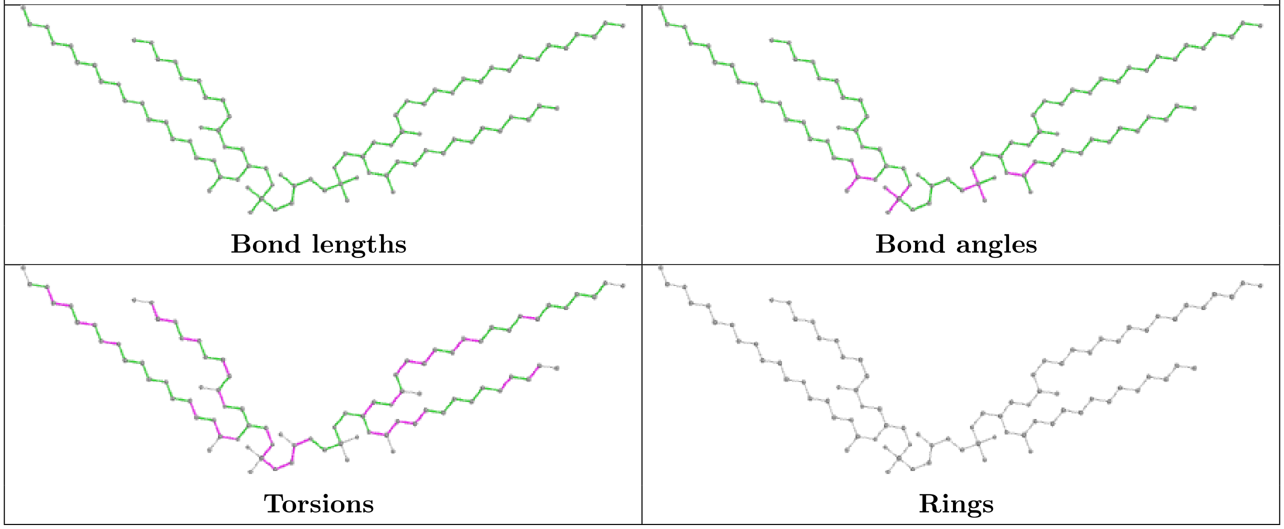
Ligand DMU O 307


Bond lengths
Bond angles
Torsions
Rings

Ligand CHD C 301


Bond lengths
Bond angles
Torsions
Rings

Ligand CDL C 304



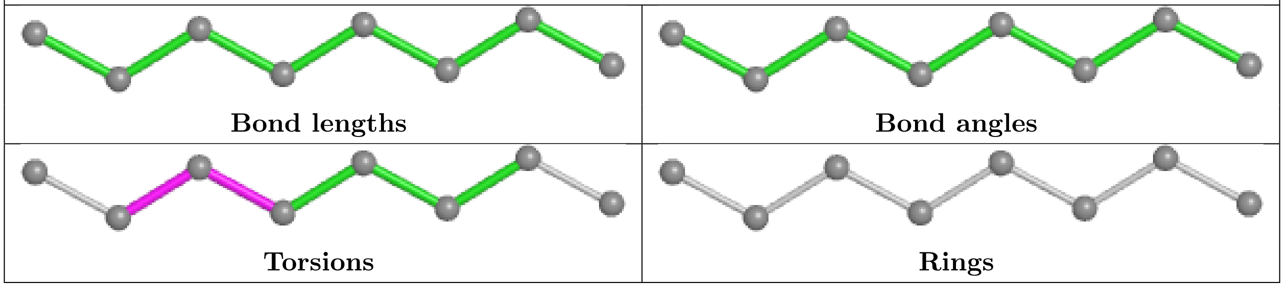
Bond lengths

Bond angles

Torsions

Rings

Ligand DMU Z 102



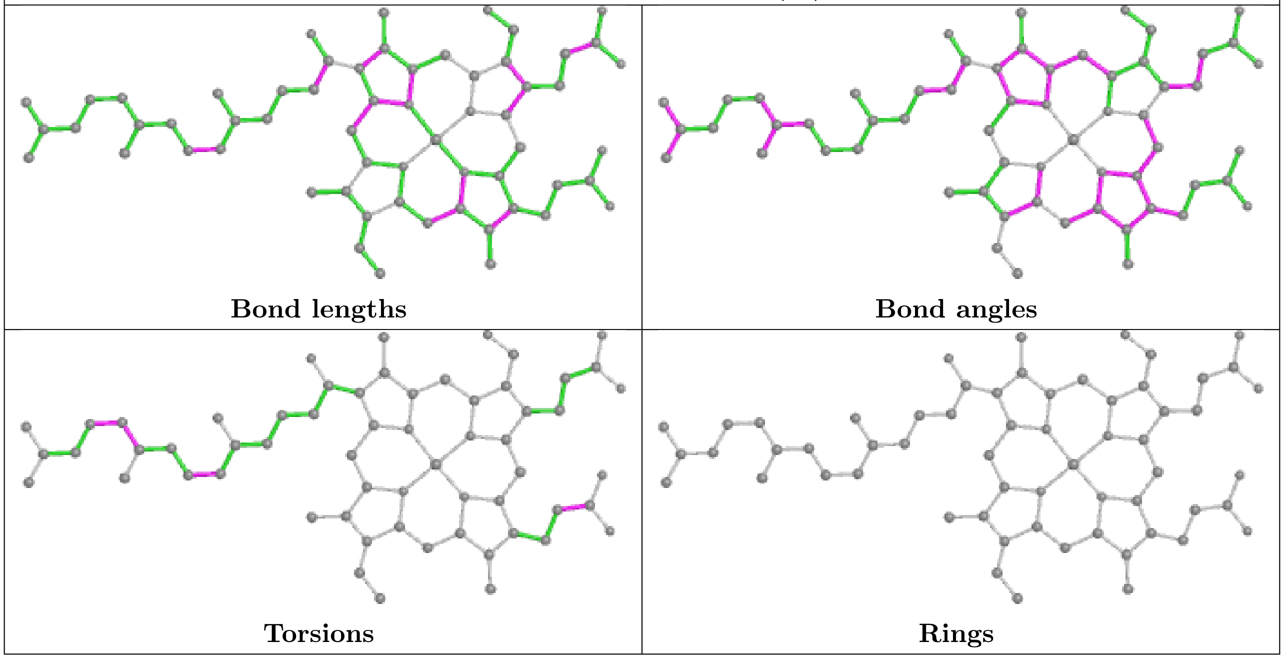
Bond lengths

Bond angles

Torsions

Rings

Ligand HEA N 603 (A)



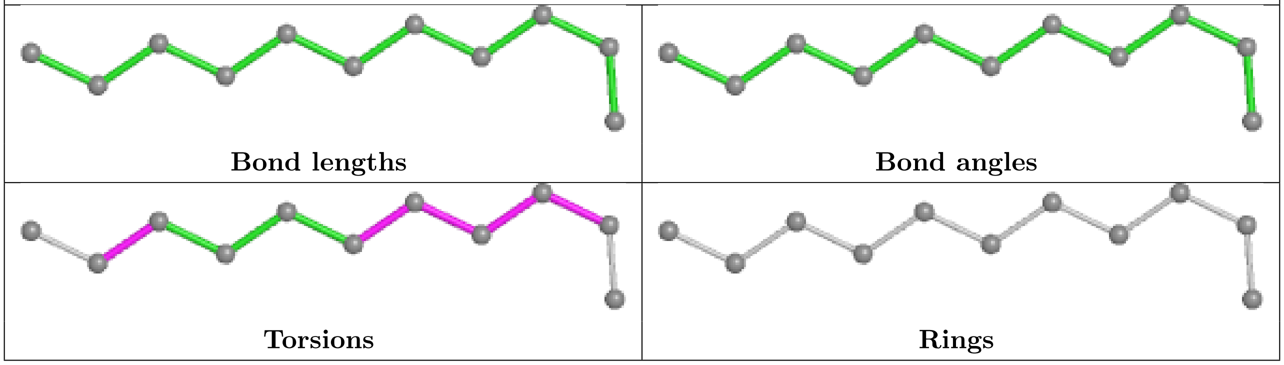
Bond lengths

Bond angles

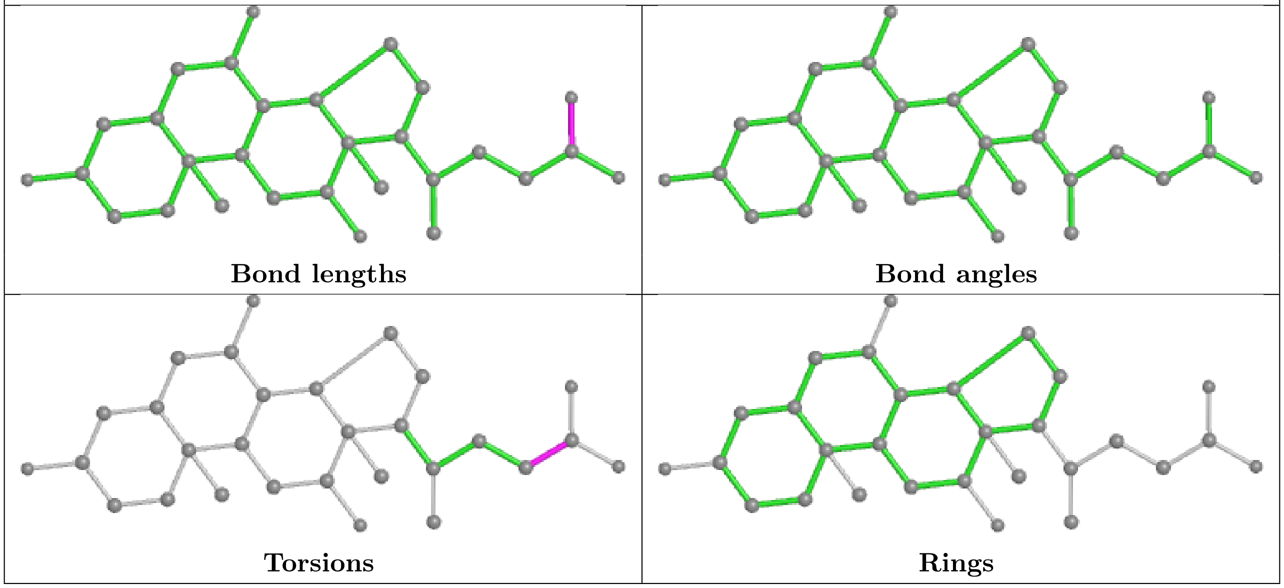
Torsions

Rings

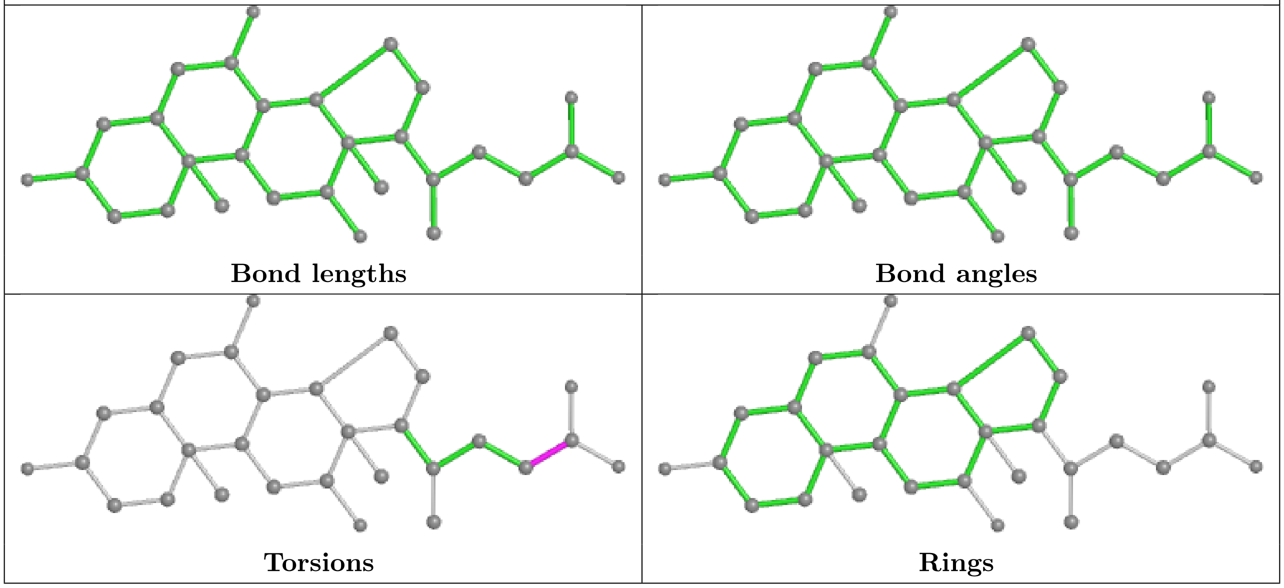
Ligand LFA P 312


Bond lengths
Bond angles
Torsions
Rings

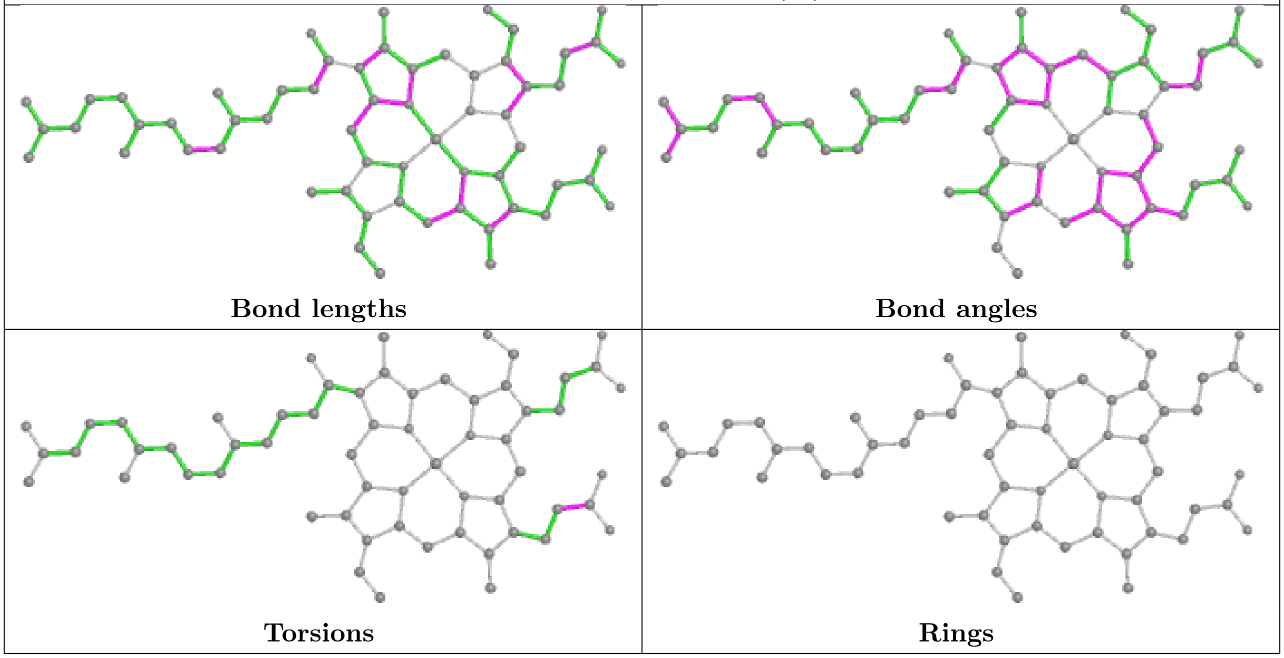
Ligand CHD P 302


Bond lengths
Bond angles
Torsions
Rings

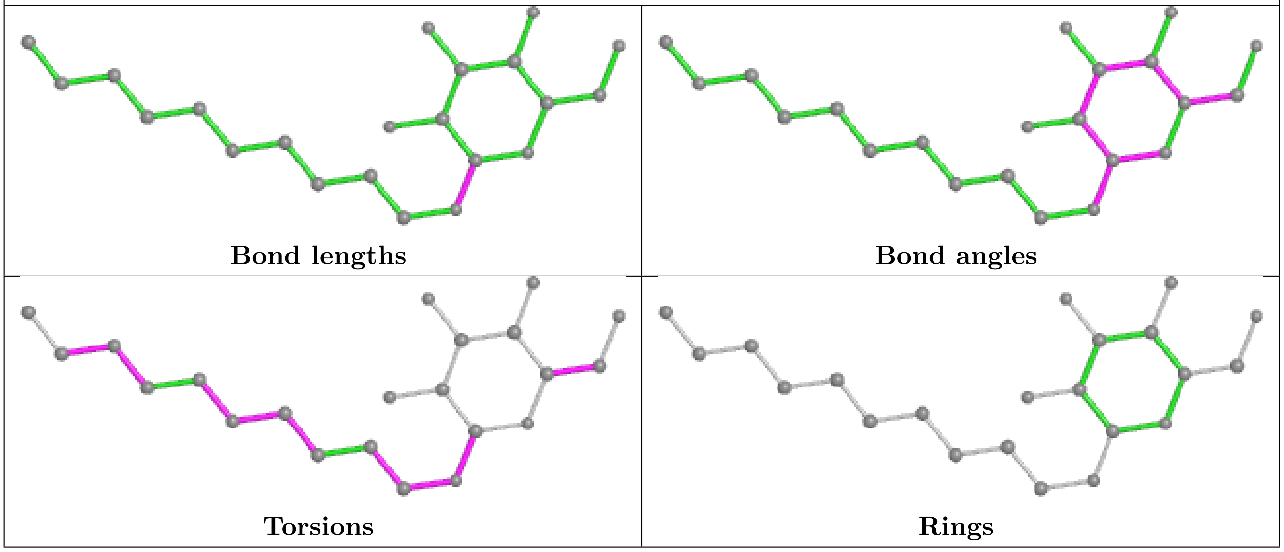
Ligand CHD O 301


Bond lengths
Bond angles
Torsions
Rings

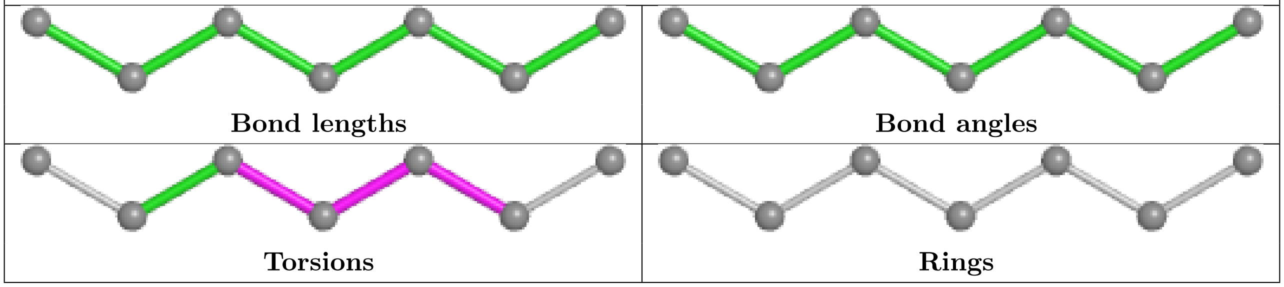
Ligand HEA N 603 (B)



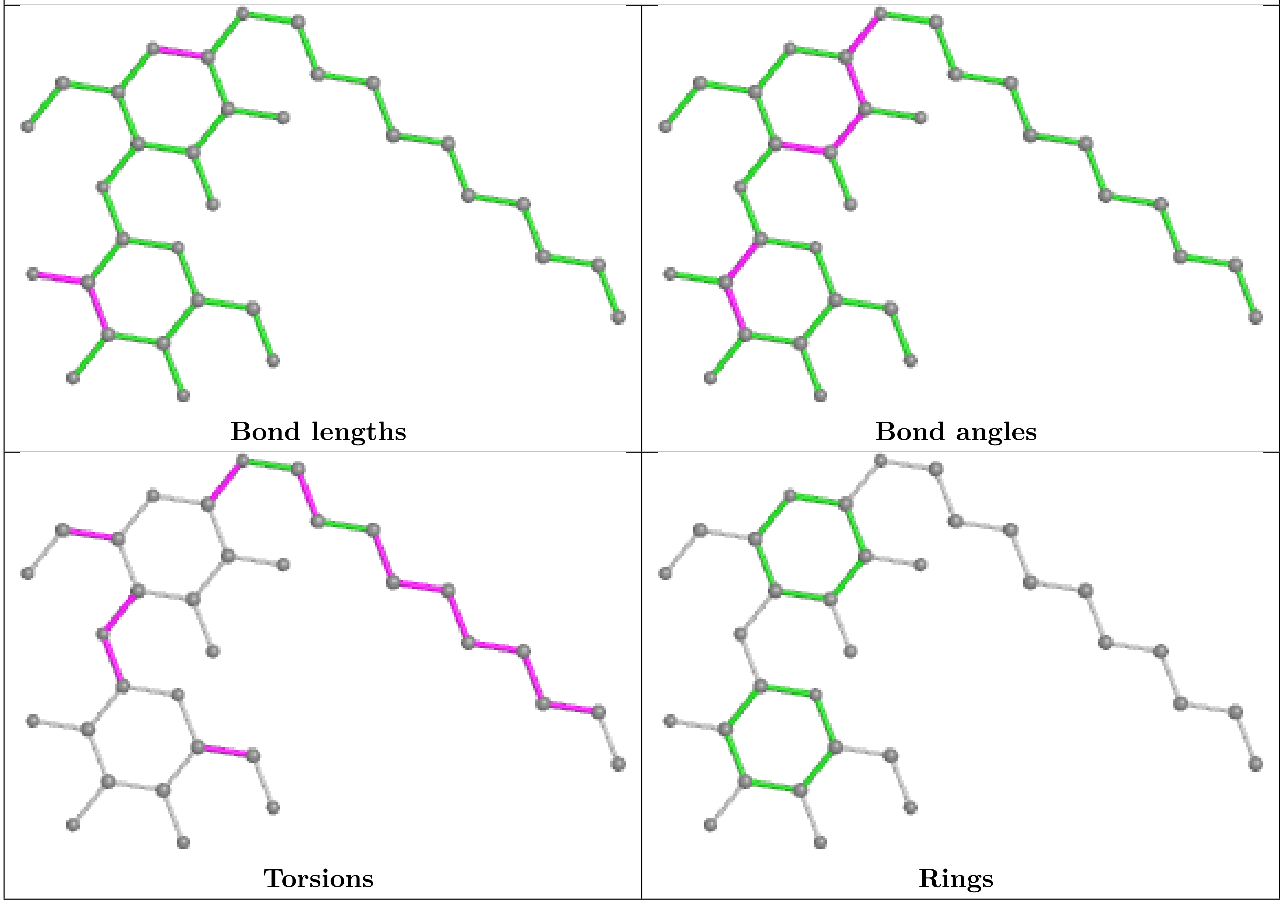
Ligand DMU L 102



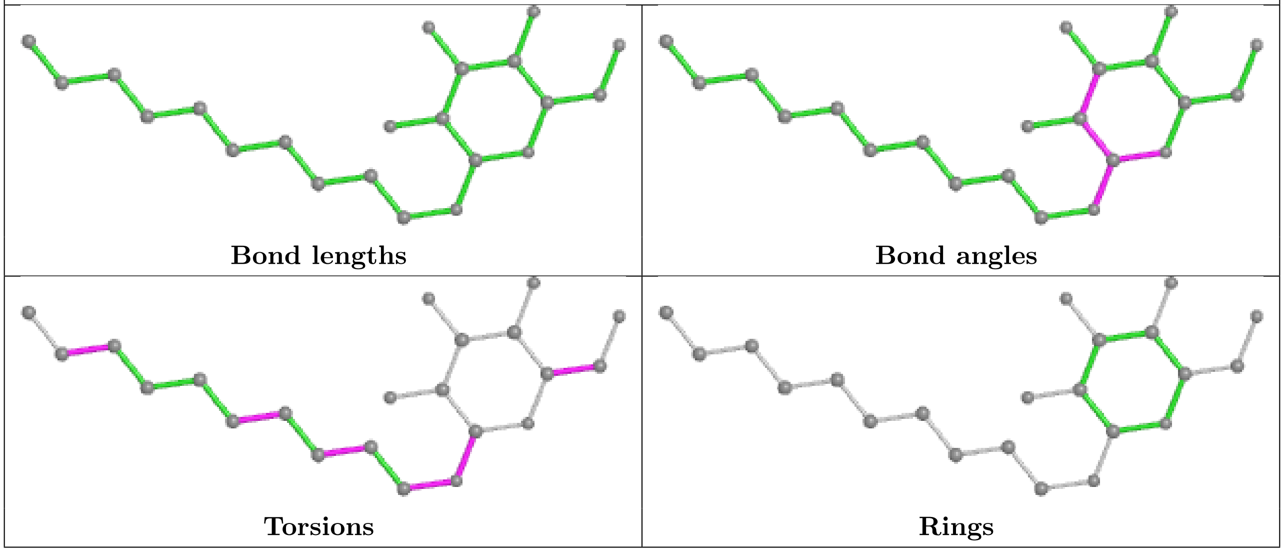
Ligand DMU P 316



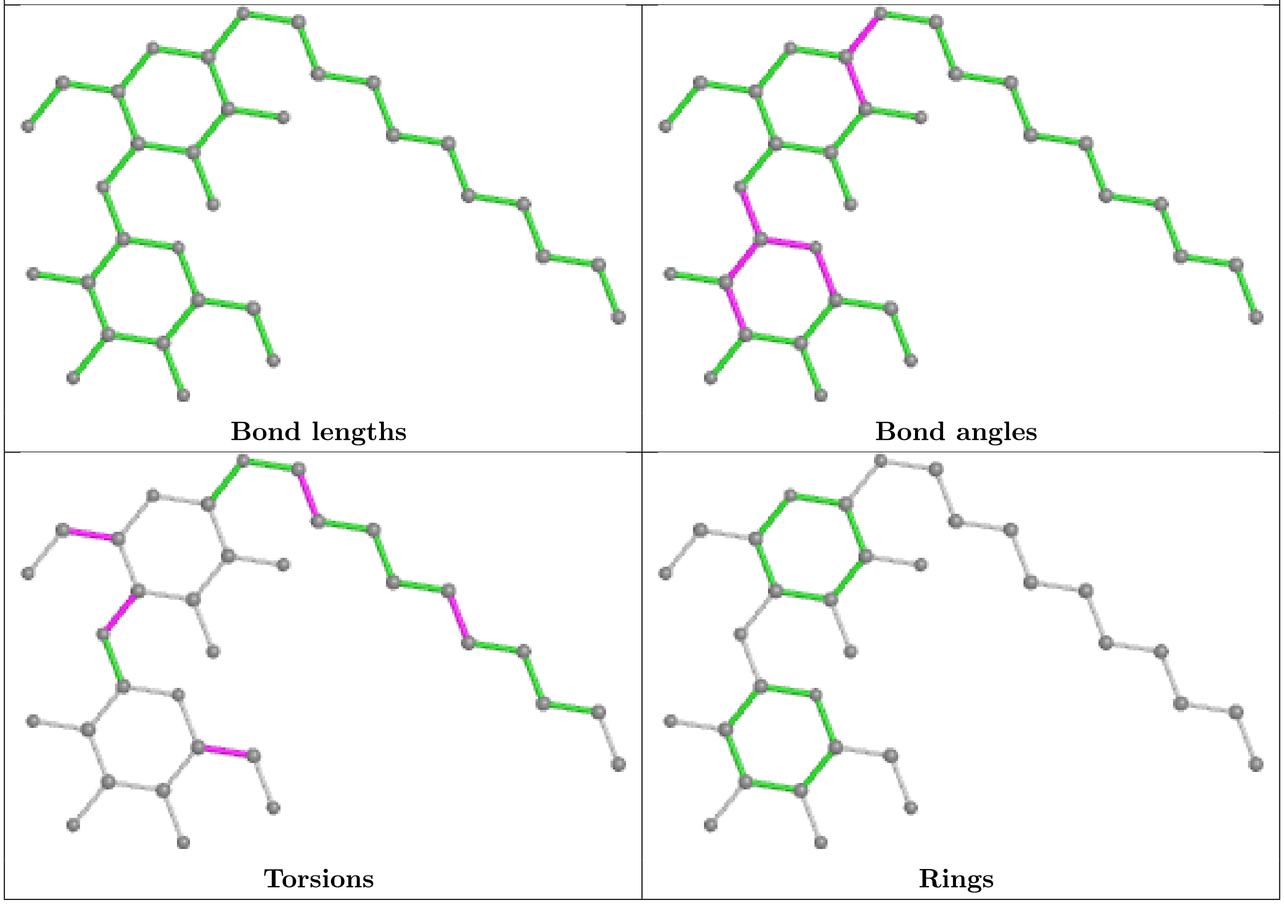
Ligand DMU P 318



Ligand DMU O 303



Ligand DMU P 324



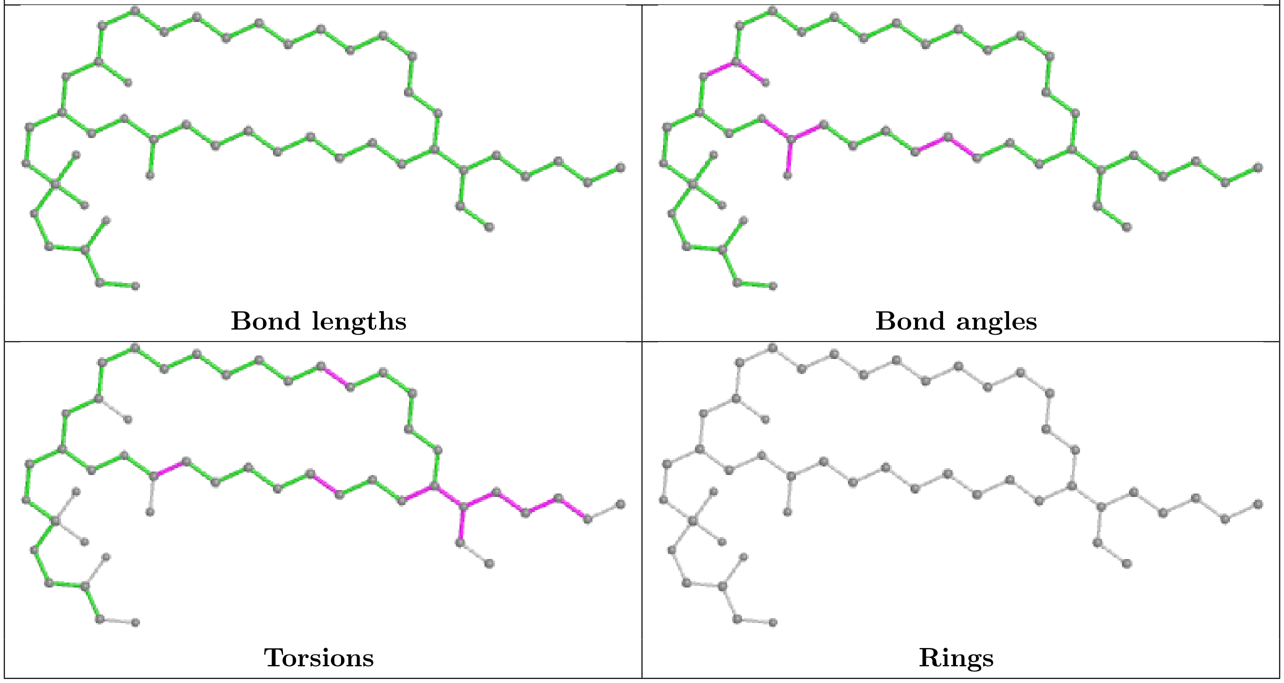
Bond lengths

Bond angles

Torsions

Rings

Ligand PGV A 616



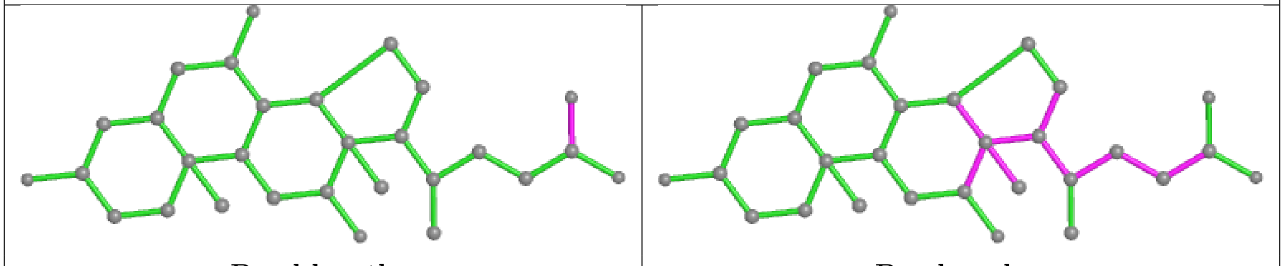
Bond lengths

Bond angles

Torsions

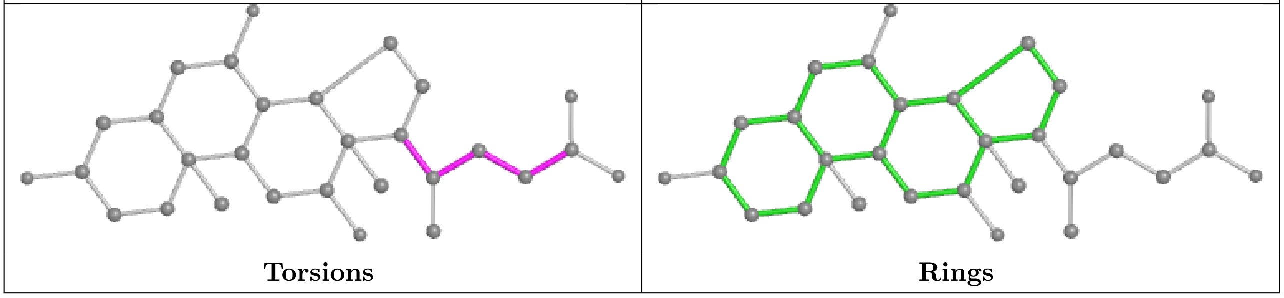
Rings

Ligand CHD P 306



Bond lengths

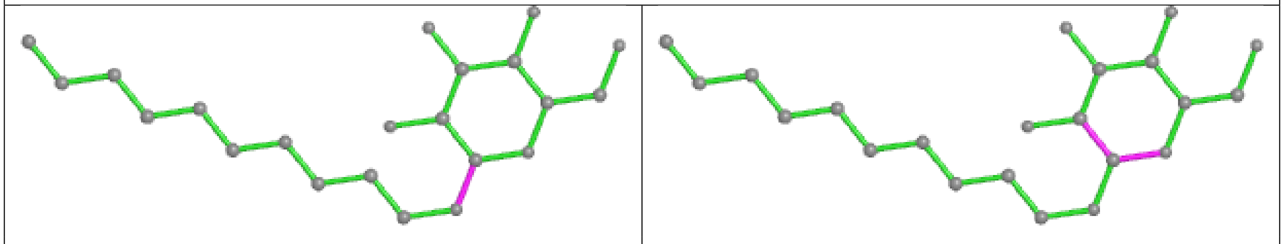
Bond angles



Torsions

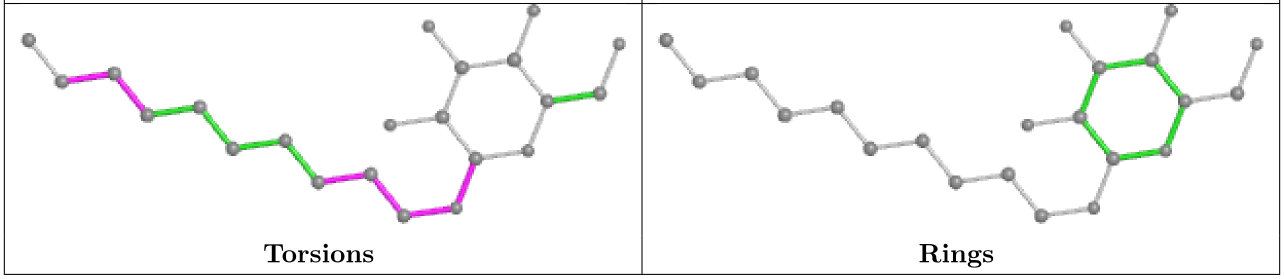
Rings

Ligand DMU B 303



Bond lengths

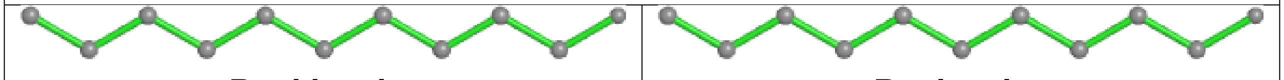
Bond angles



Torsions

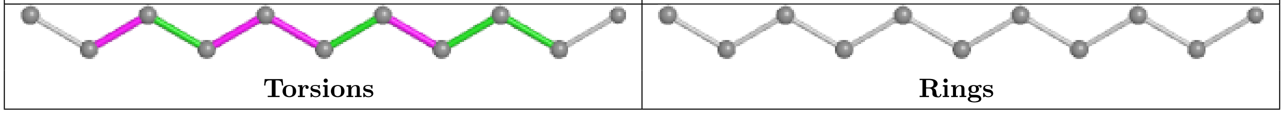
Rings

Ligand DMU N 602



Bond lengths

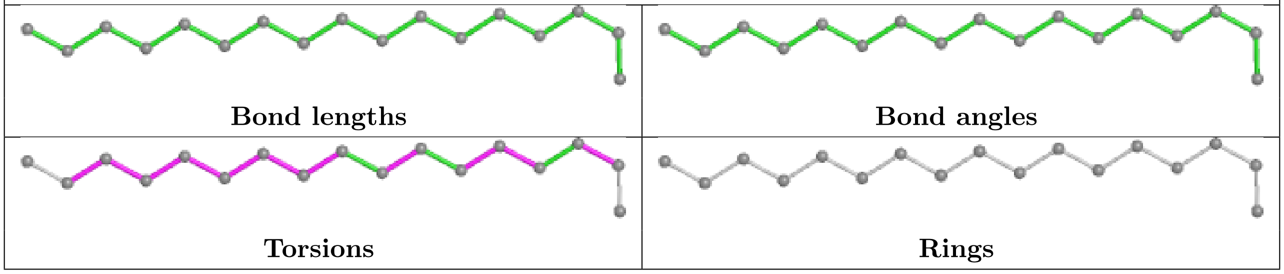
Bond angles



Torsions

Rings

Ligand LFA B 306



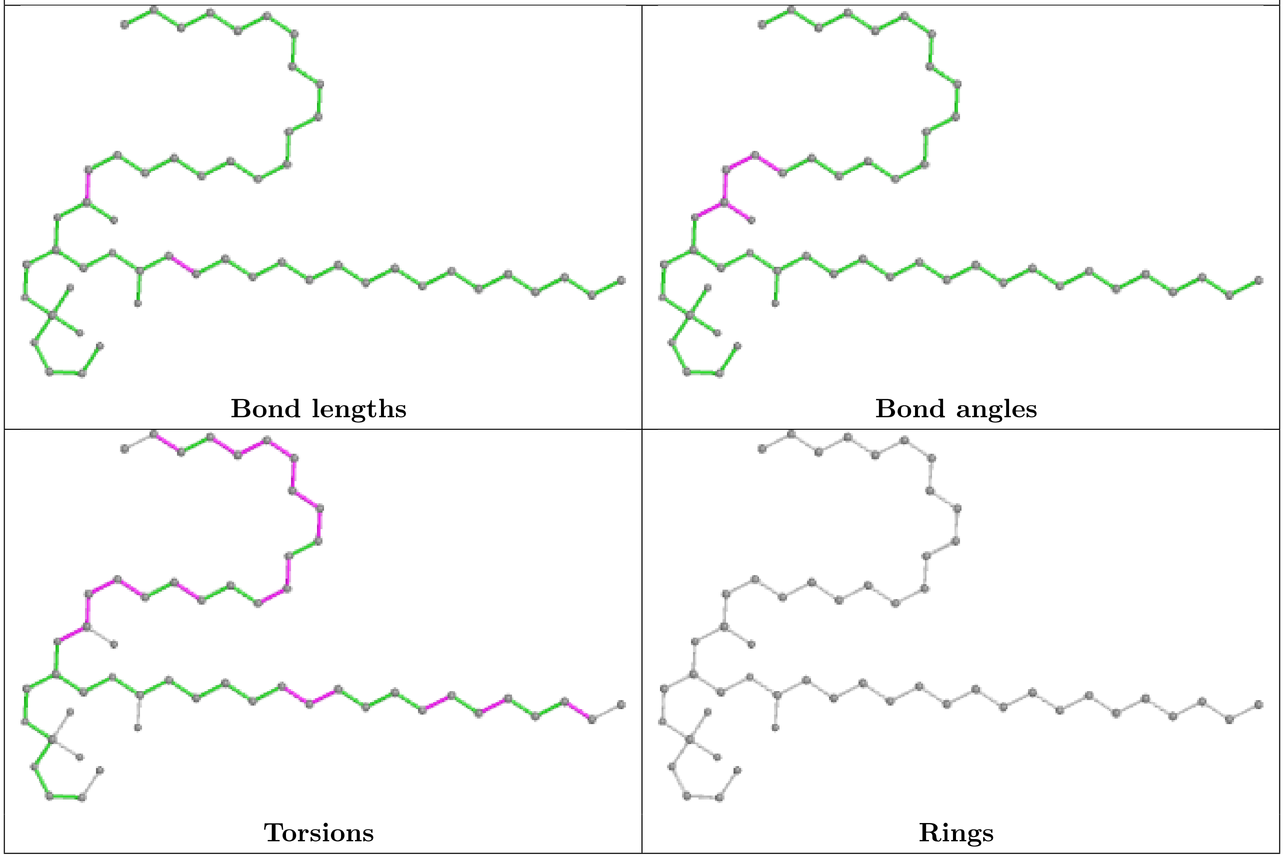
Bond lengths

Bond angles

Torsions

Rings

Ligand PEK T 101



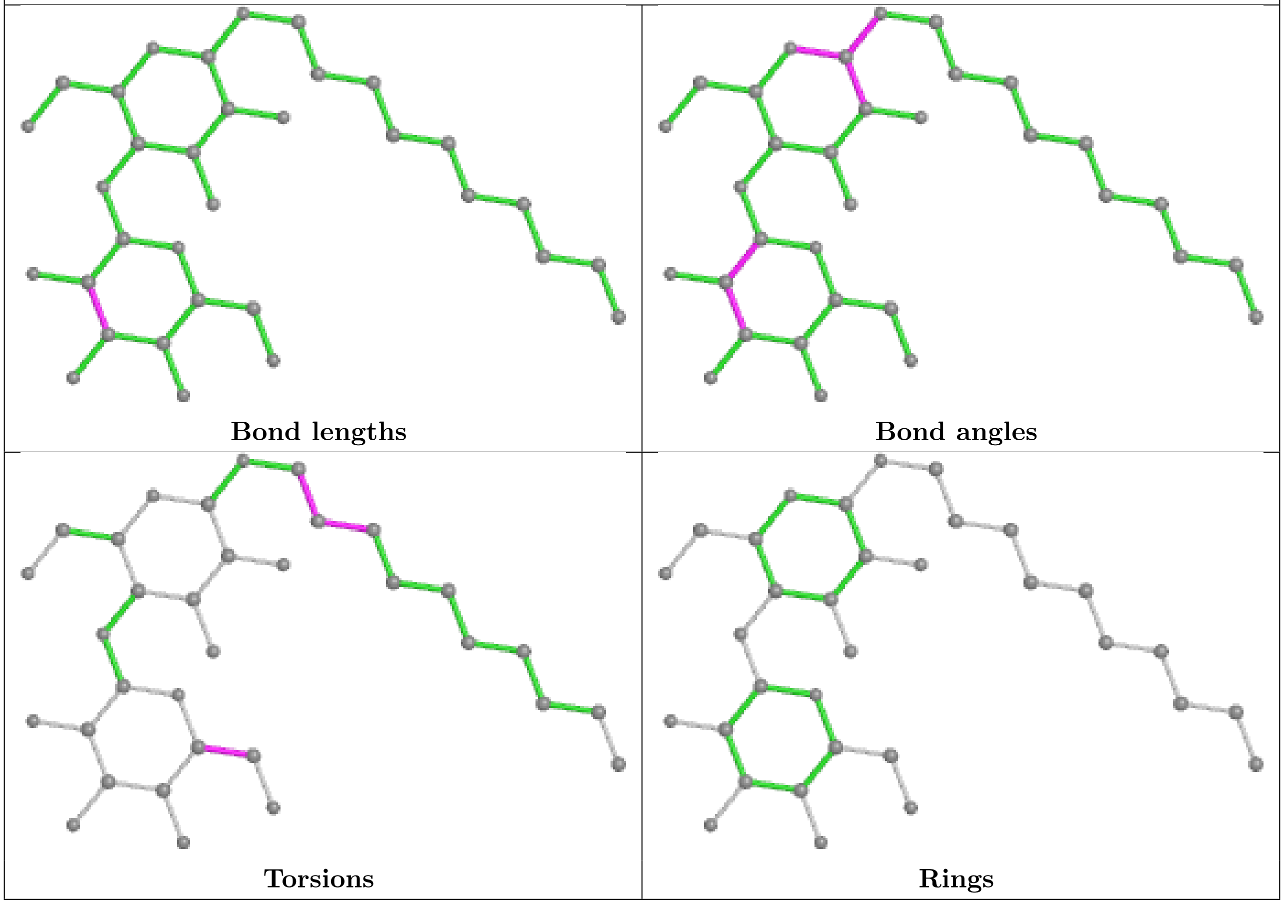
Bond lengths

Bond angles

Torsions

Rings

Ligand DMU C 324



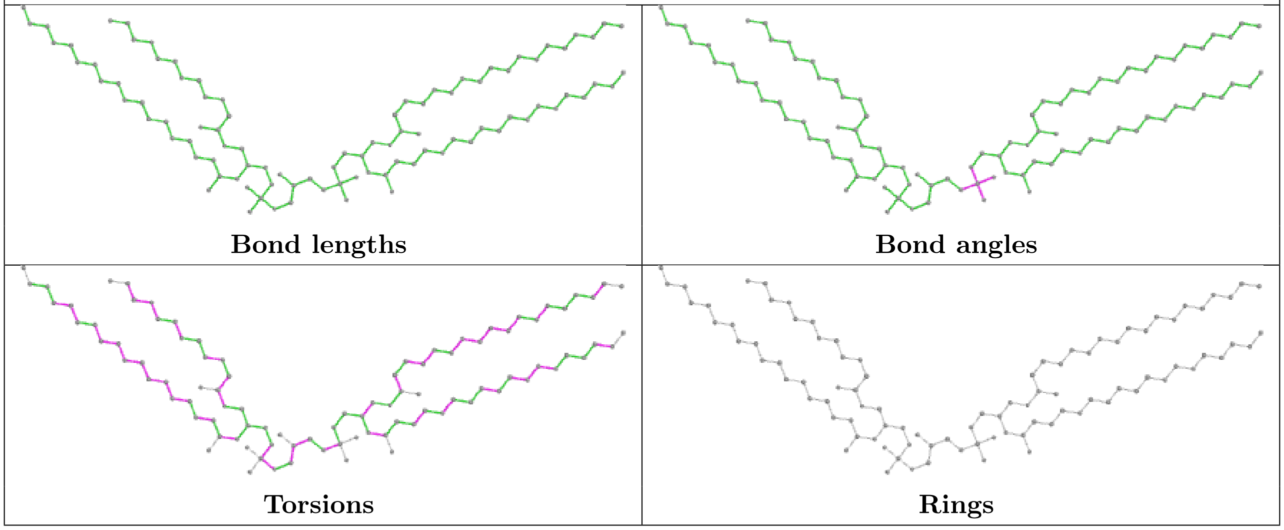
Bond lengths

Bond angles

Torsions

Rings

Ligand CDL L 101



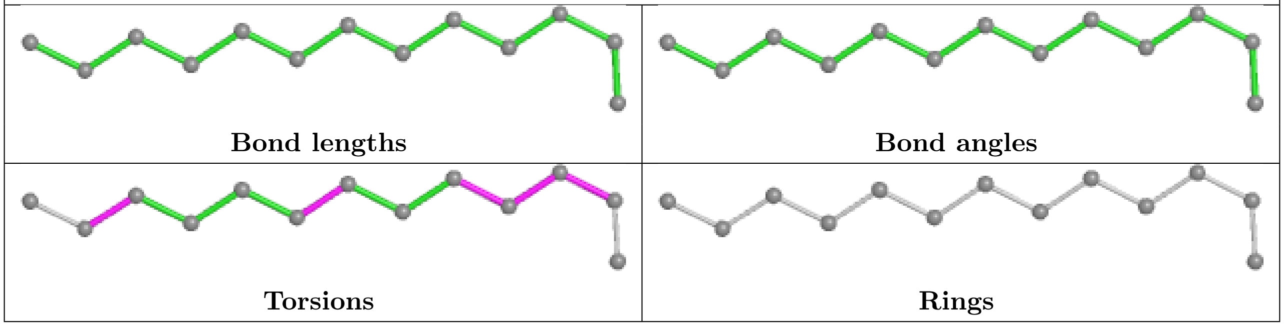
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA C 314



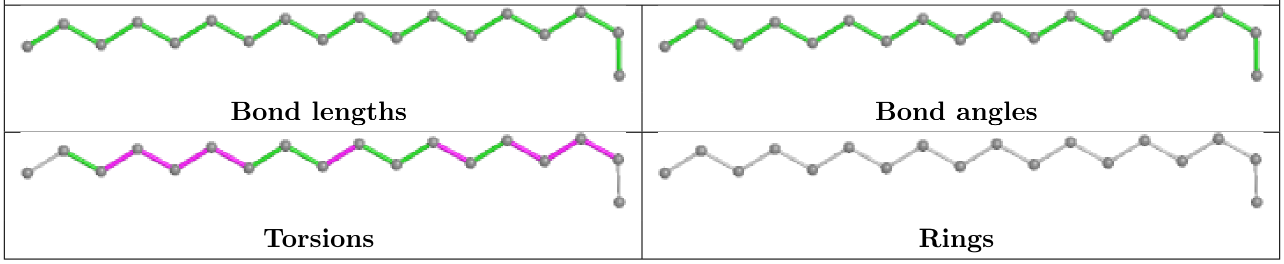
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA C 309



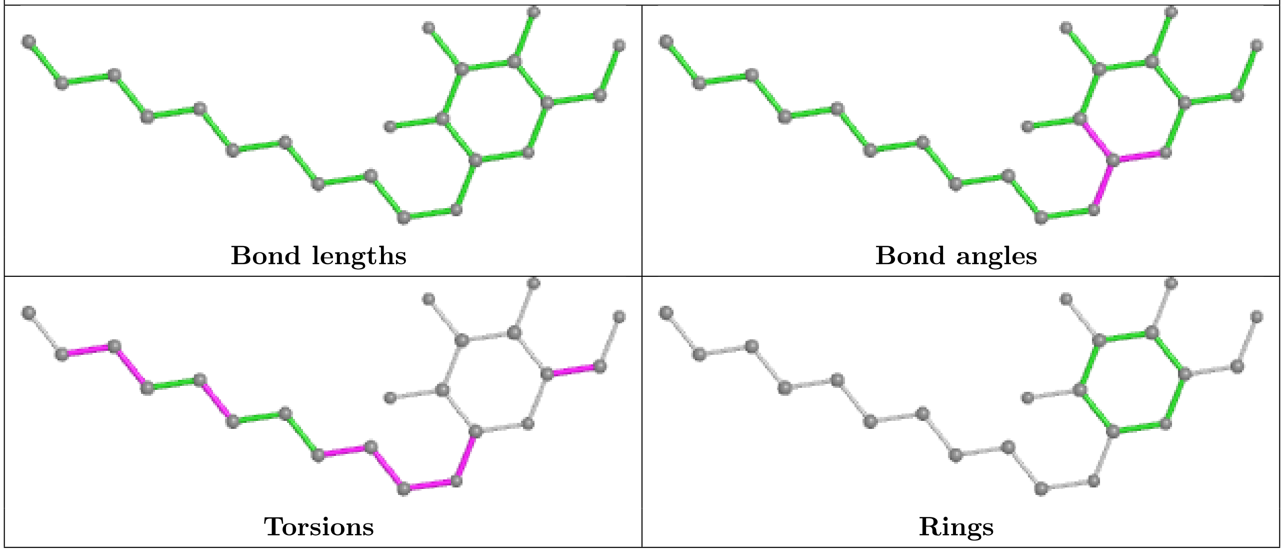
Bond lengths

Bond angles

Torsions

Rings

Ligand DMU B 307



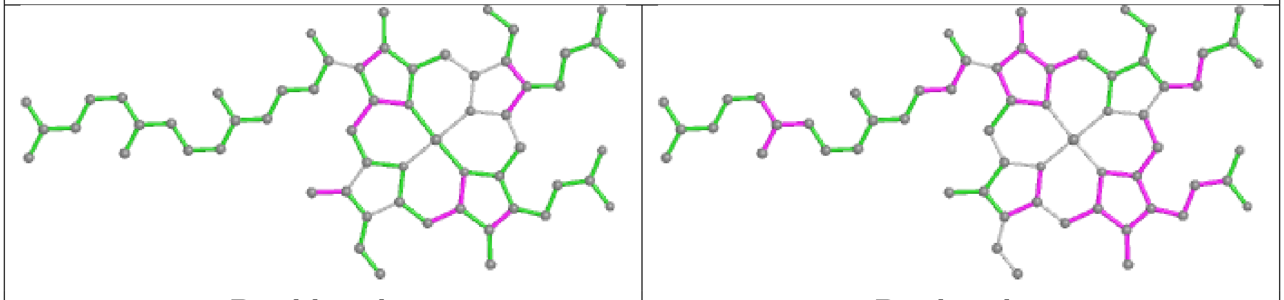
Bond lengths

Bond angles

Torsions

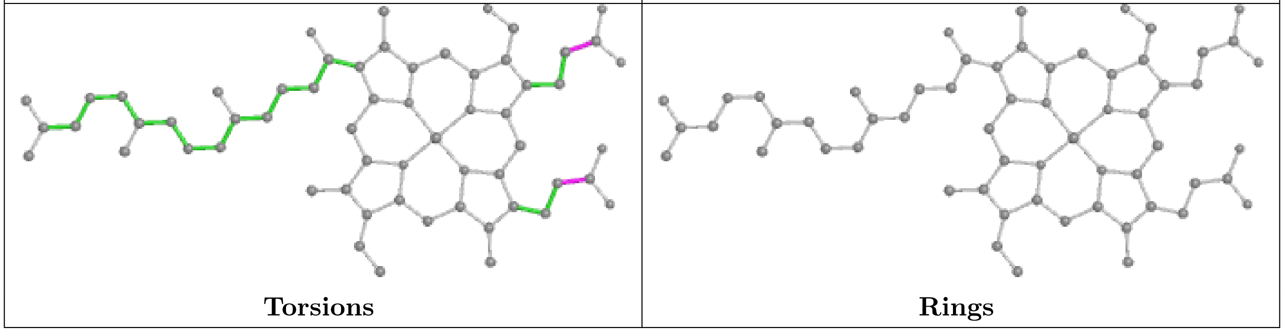
Rings

Ligand HEA N 604



Bond lengths

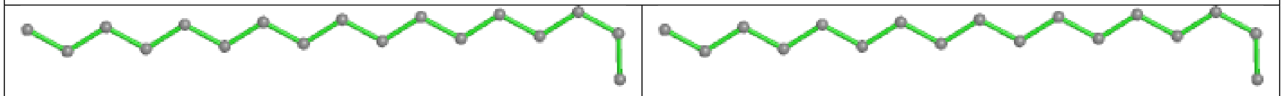
Bond angles



Torsions

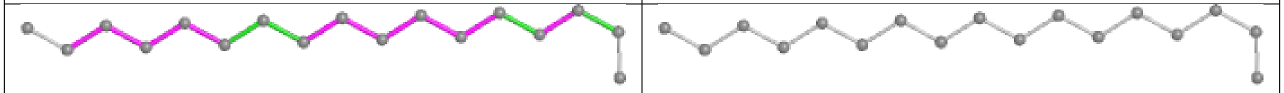
Rings

Ligand LFA N 601



Bond lengths

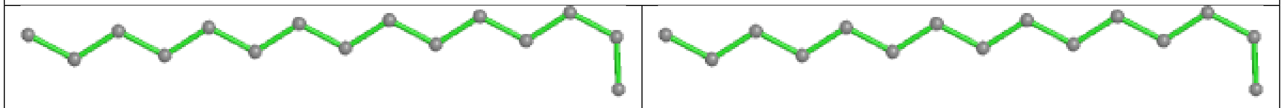
Bond angles



Torsions

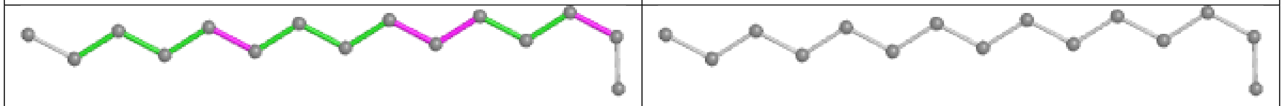
Rings

Ligand LFA C 313



Bond lengths

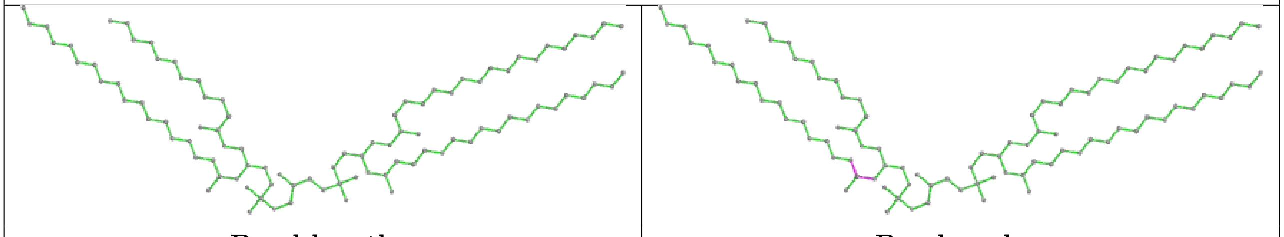
Bond angles



Torsions

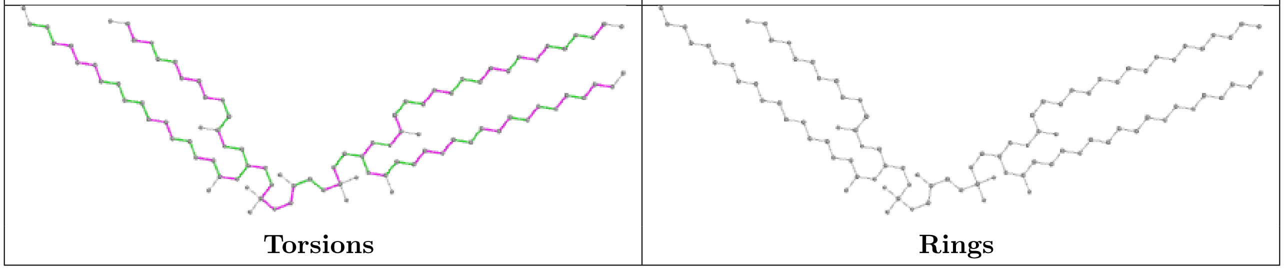
Rings

Ligand CDL Y 101



Bond lengths

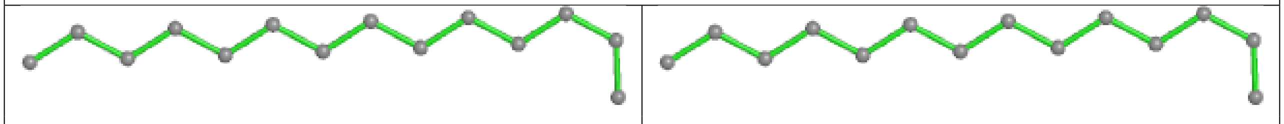
Bond angles



Torsions

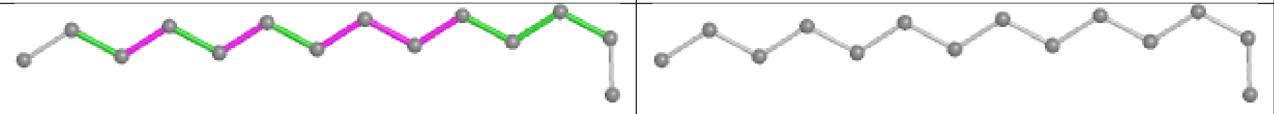
Rings

Ligand LFA C 311



Bond lengths

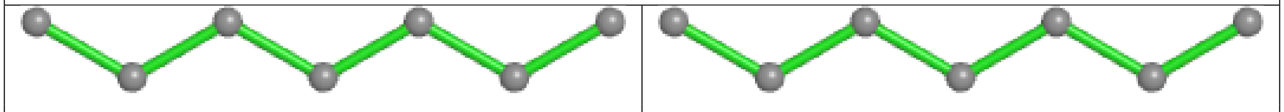
Bond angles



Torsions

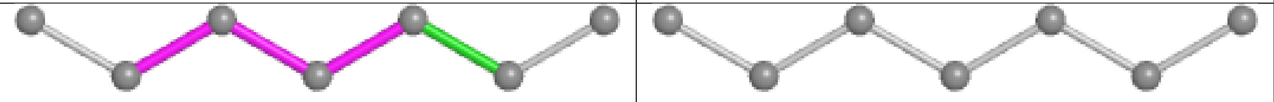
Rings

Ligand DMU A 609



Bond lengths

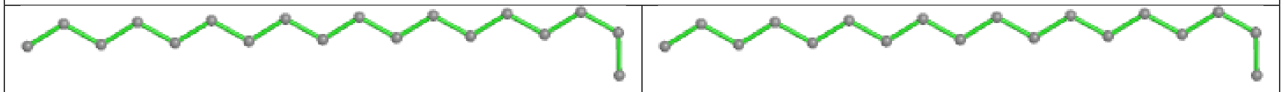
Bond angles



Torsions

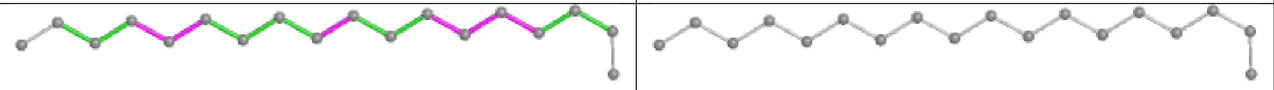
Rings

Ligand LFA P 310



Bond lengths

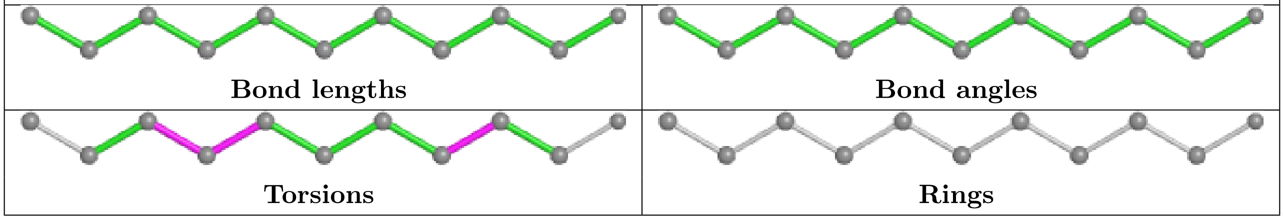
Bond angles



Torsions

Rings

Ligand DMU C 306



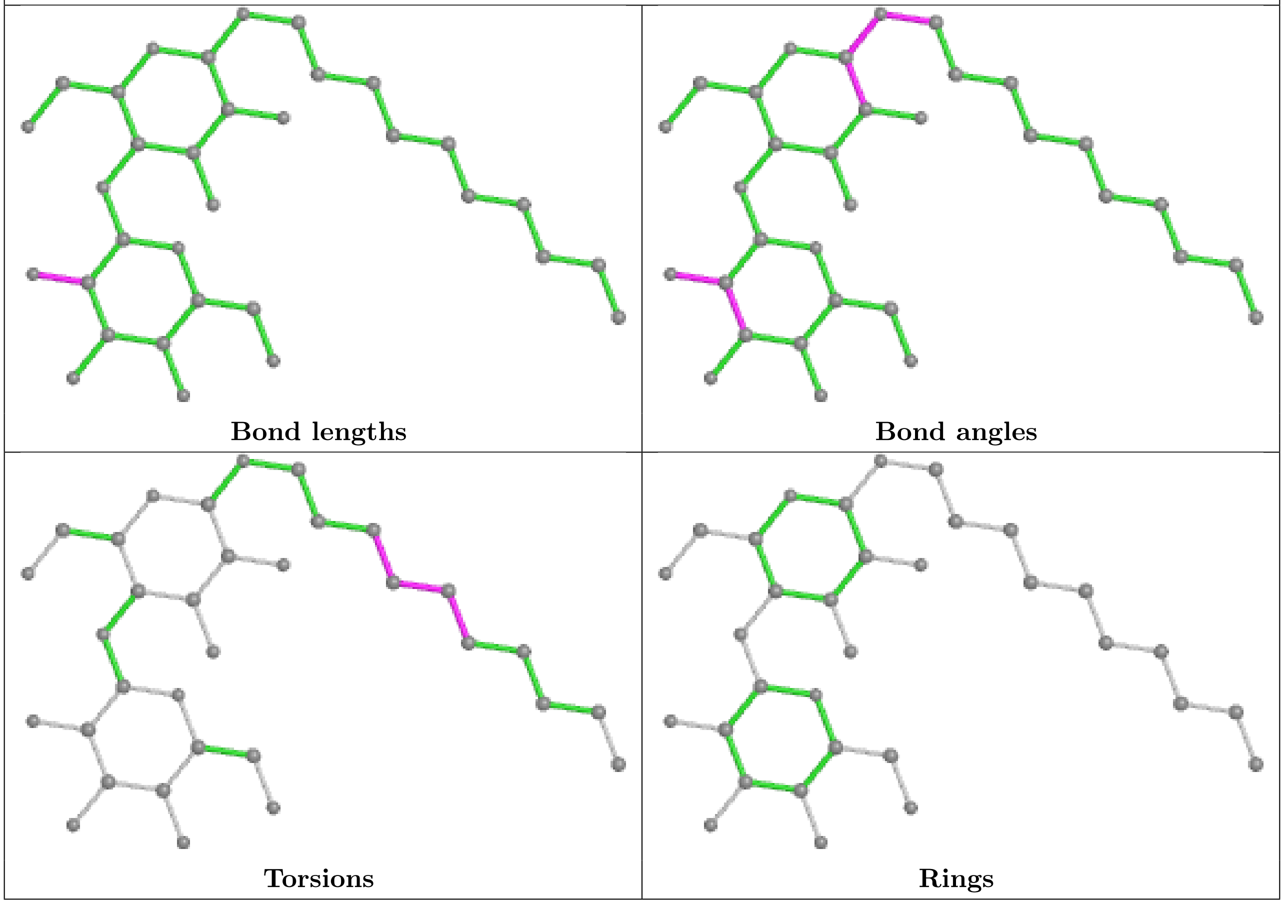
Bond lengths

Bond angles

Torsions

Rings

Ligand DMU M 101



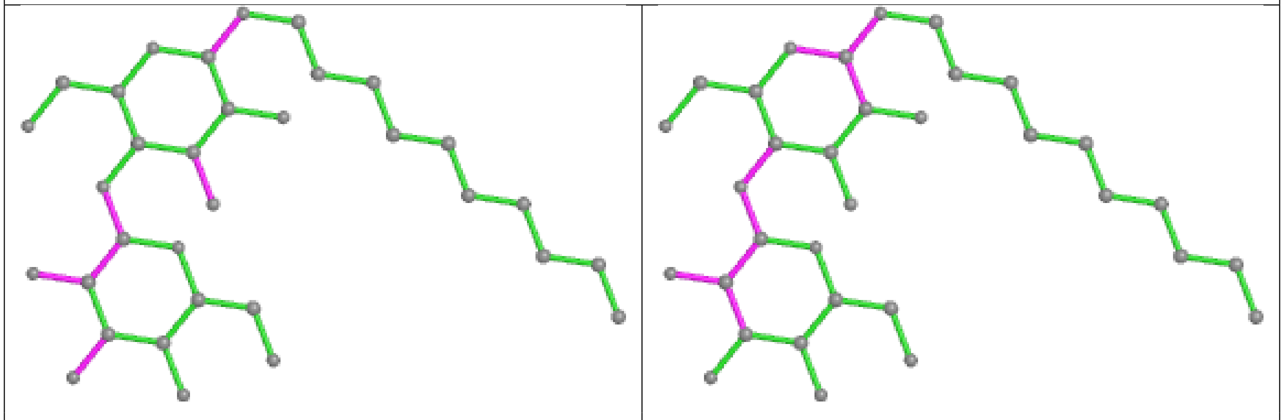
Bond lengths

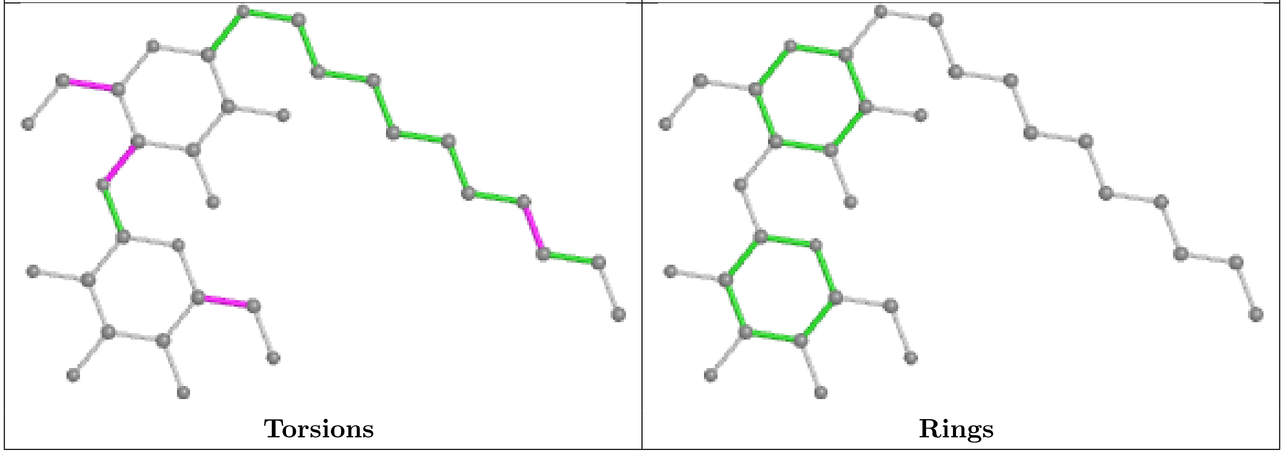
Bond angles

Torsions

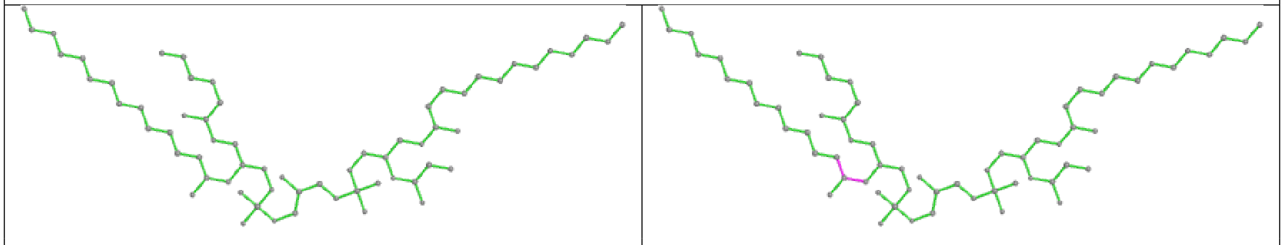
Rings

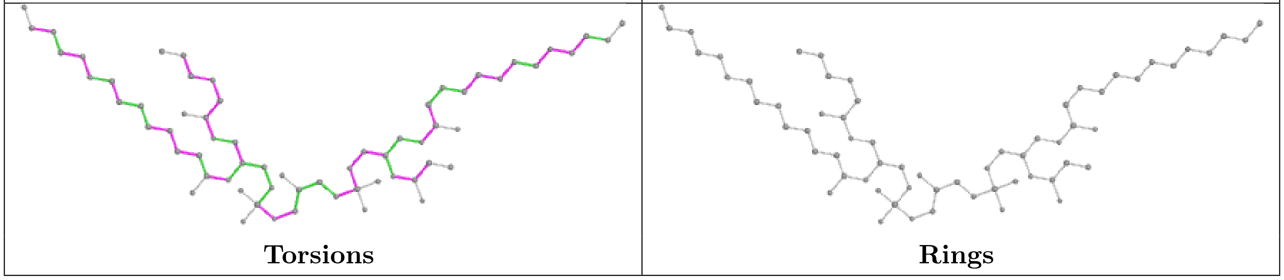
Ligand DMU A 610


Bond lengths Bond angles

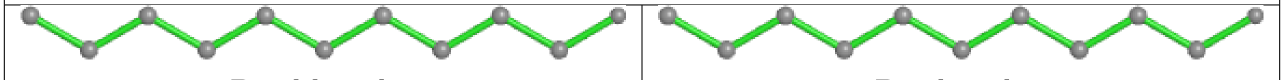

Torsions Rings

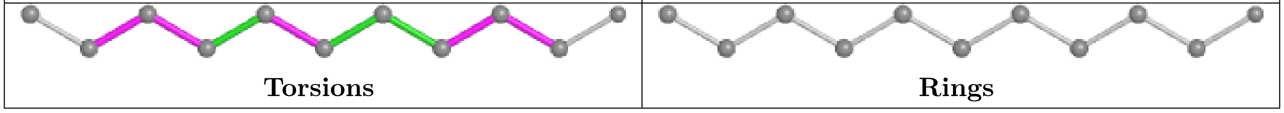
Ligand CDL O 304


Bond lengths Bond angles

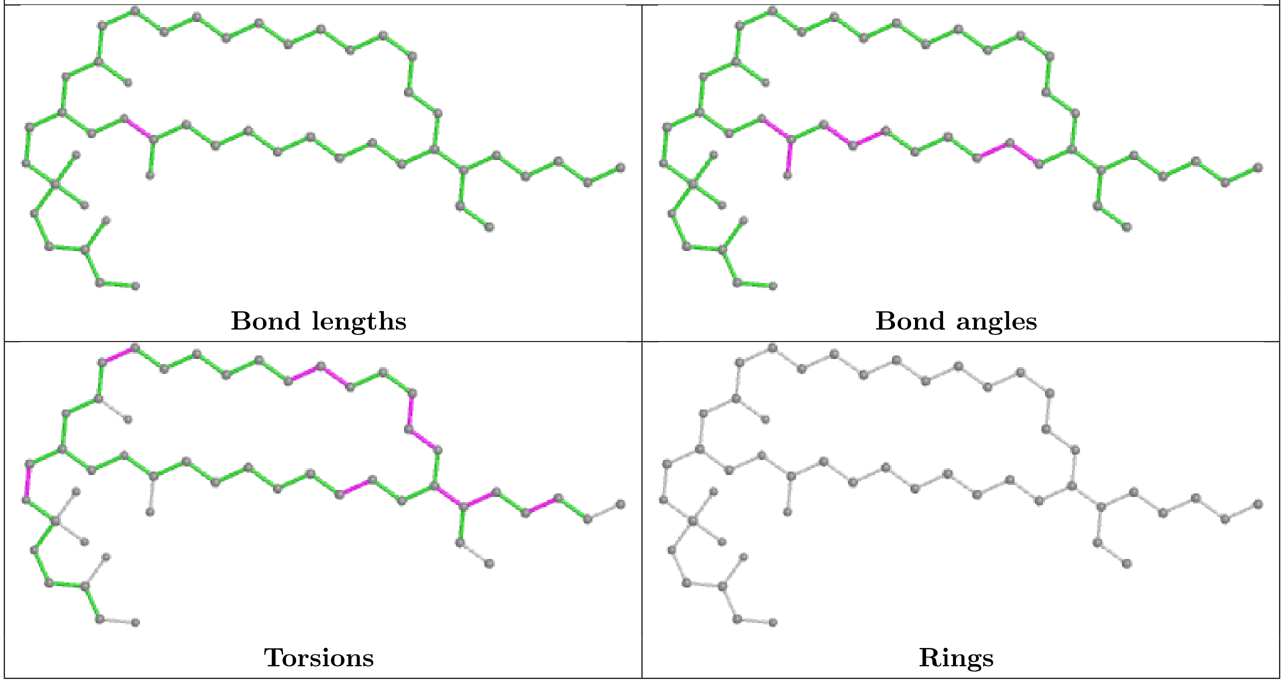

Torsions Rings

Ligand DMU W 101


Bond lengths Bond angles


Torsions Rings

Ligand PGV P 304



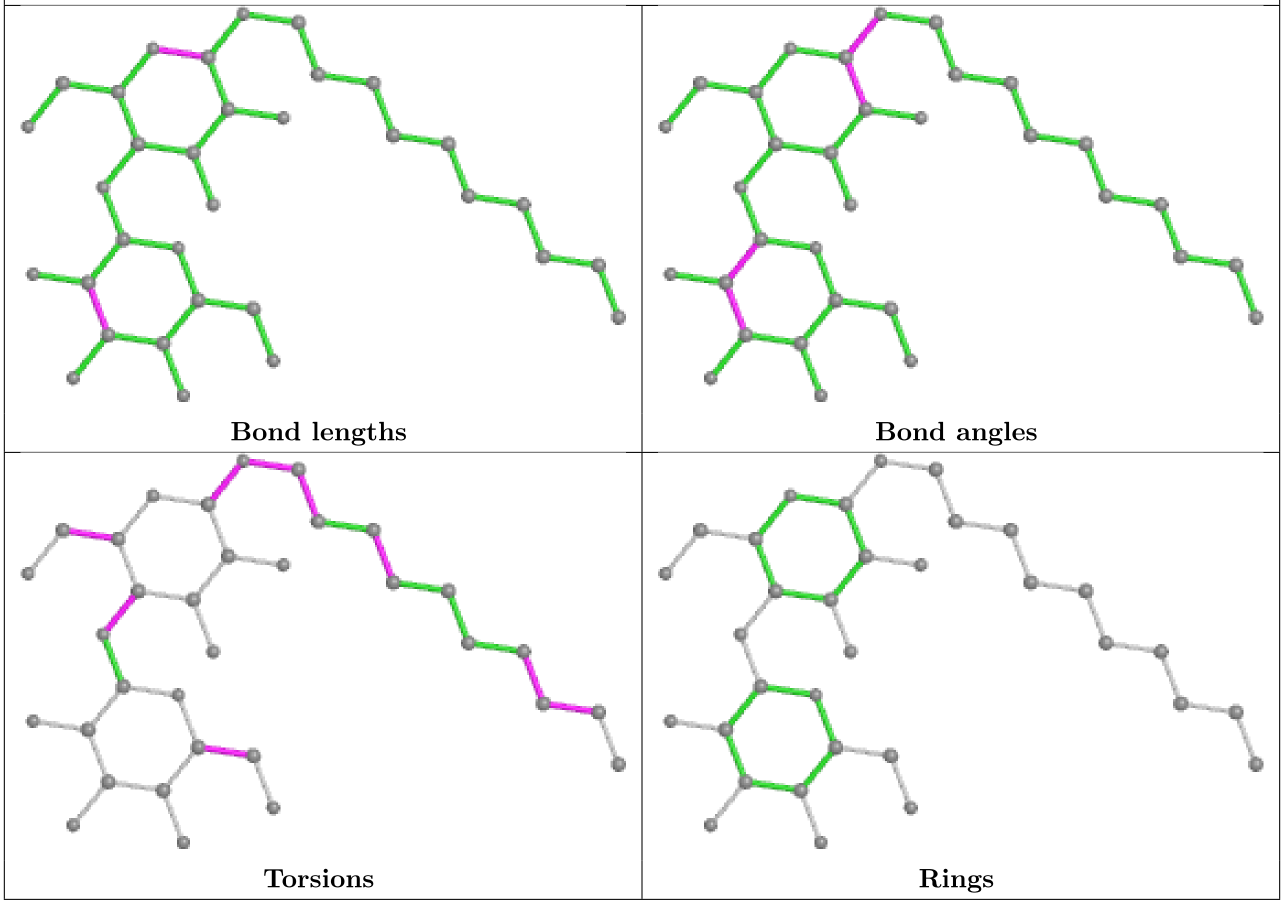
Bond lengths

Bond angles

Torsions

Rings

Ligand DMU C 318



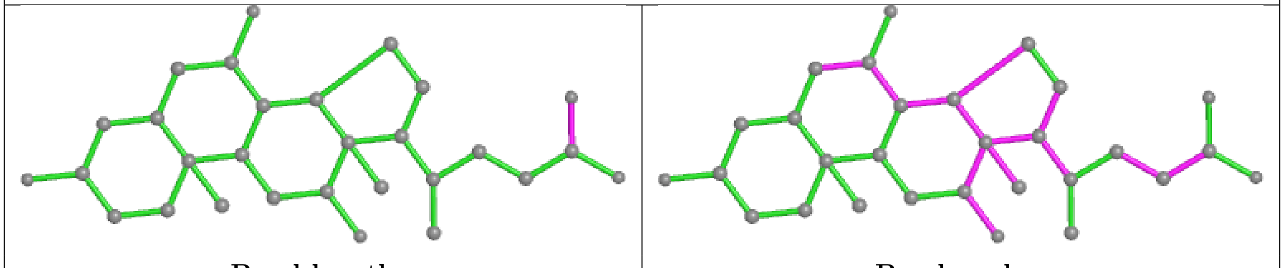
Bond lengths

Bond angles

Torsions

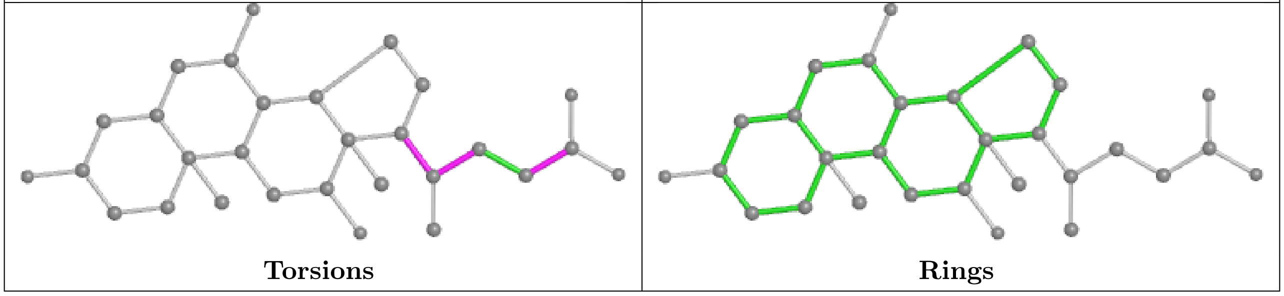
Rings

Ligand CHD C 305



Bond lengths

Bond angles



Torsions

Rings

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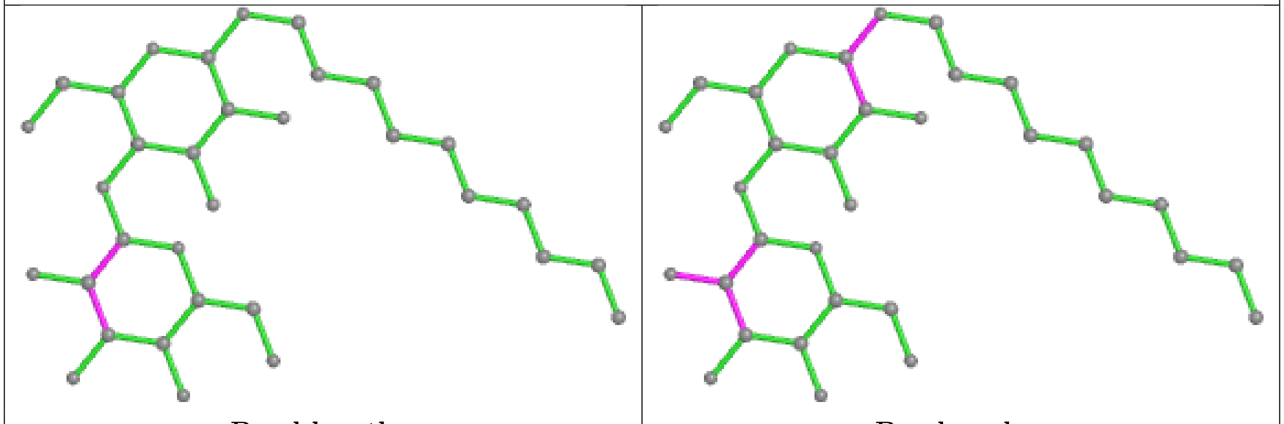
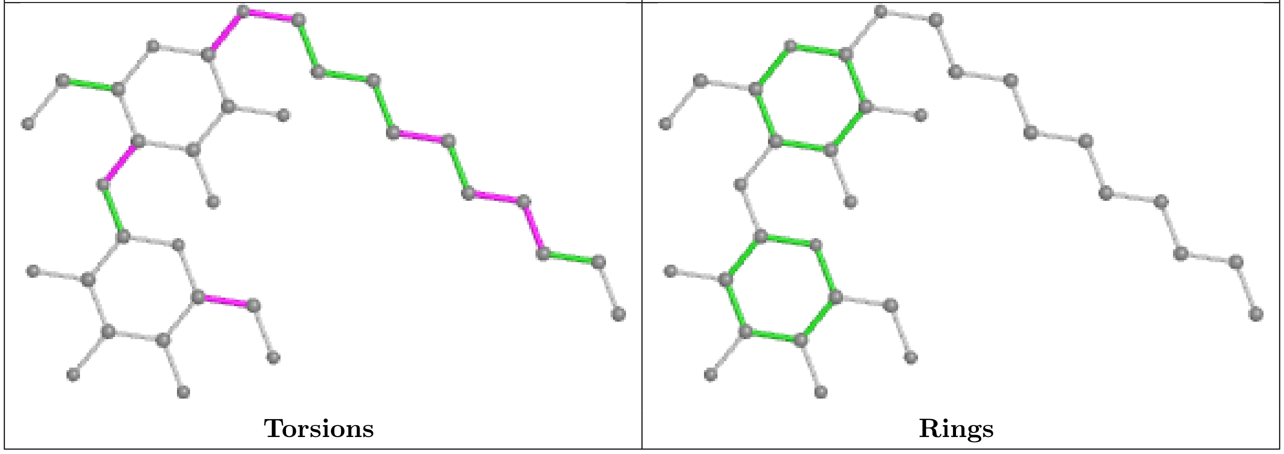


Bond lengths

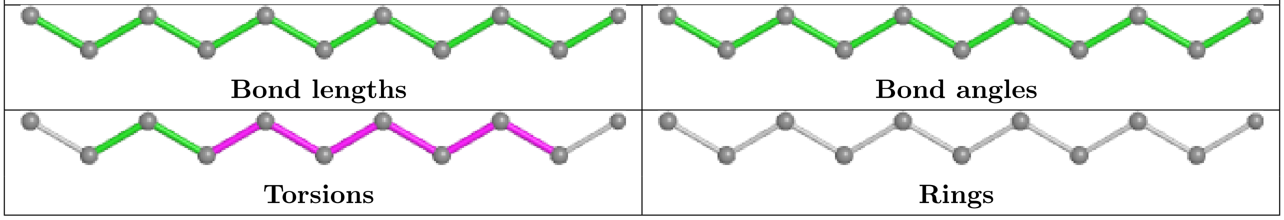
Bond angles



Torsions

Rings

Ligand DMU A 615



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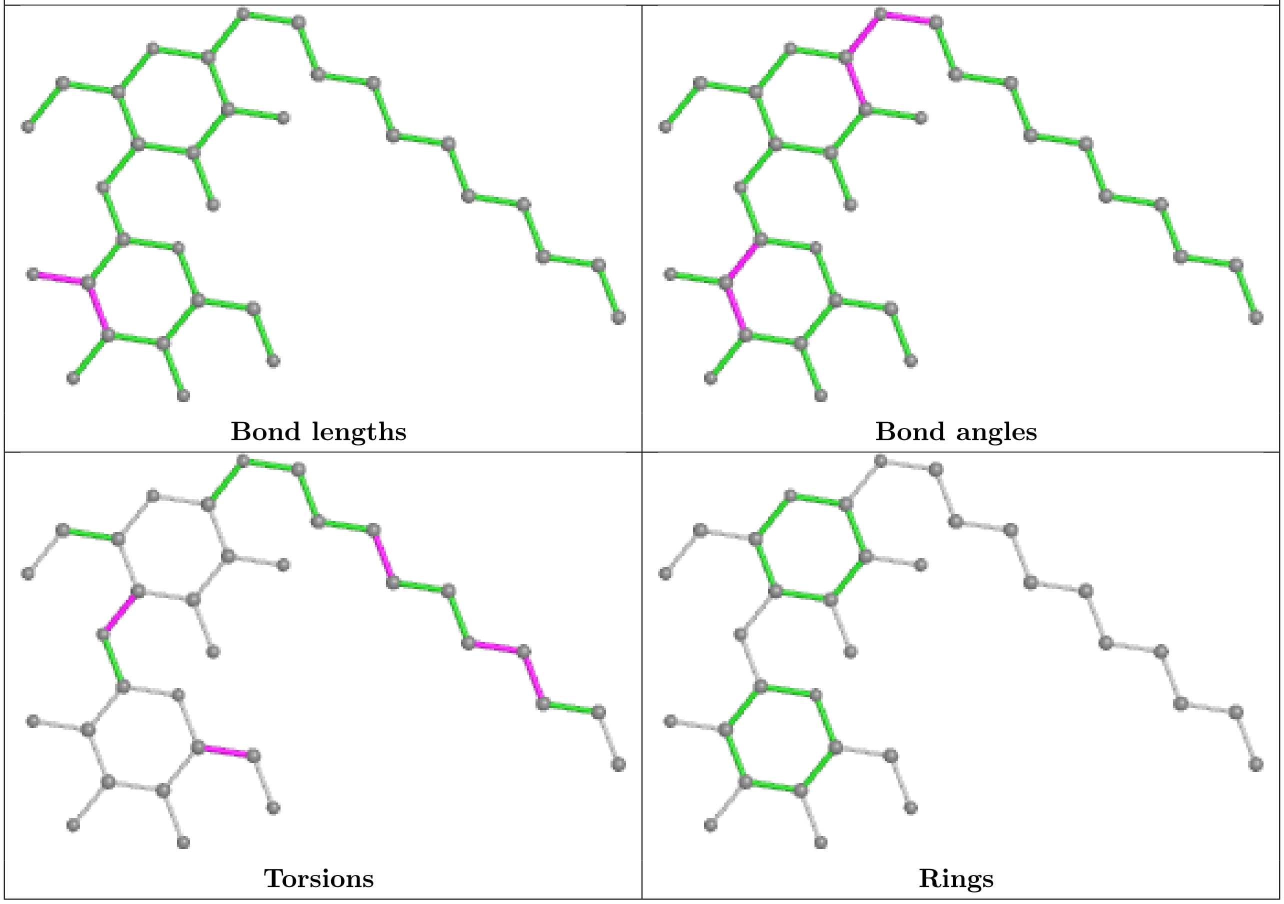
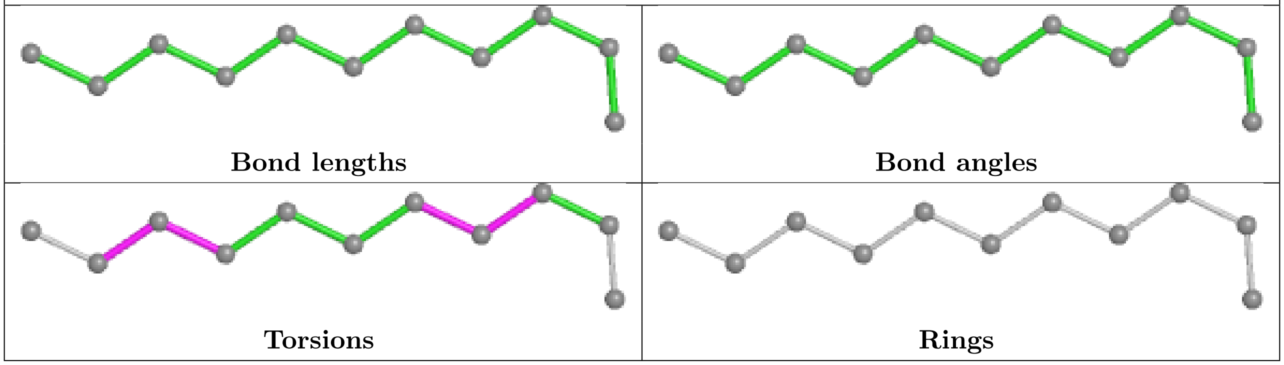


Ligand LFA P 308



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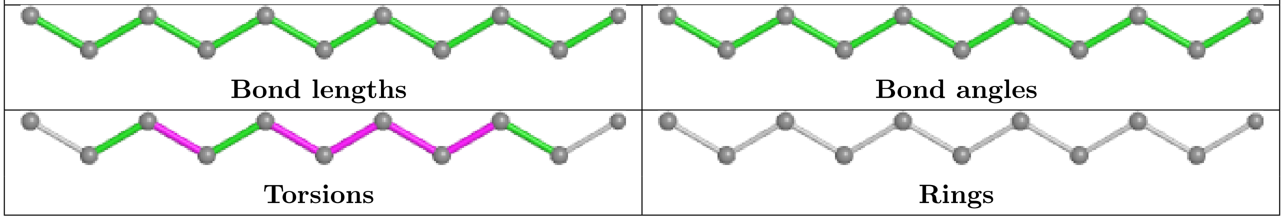

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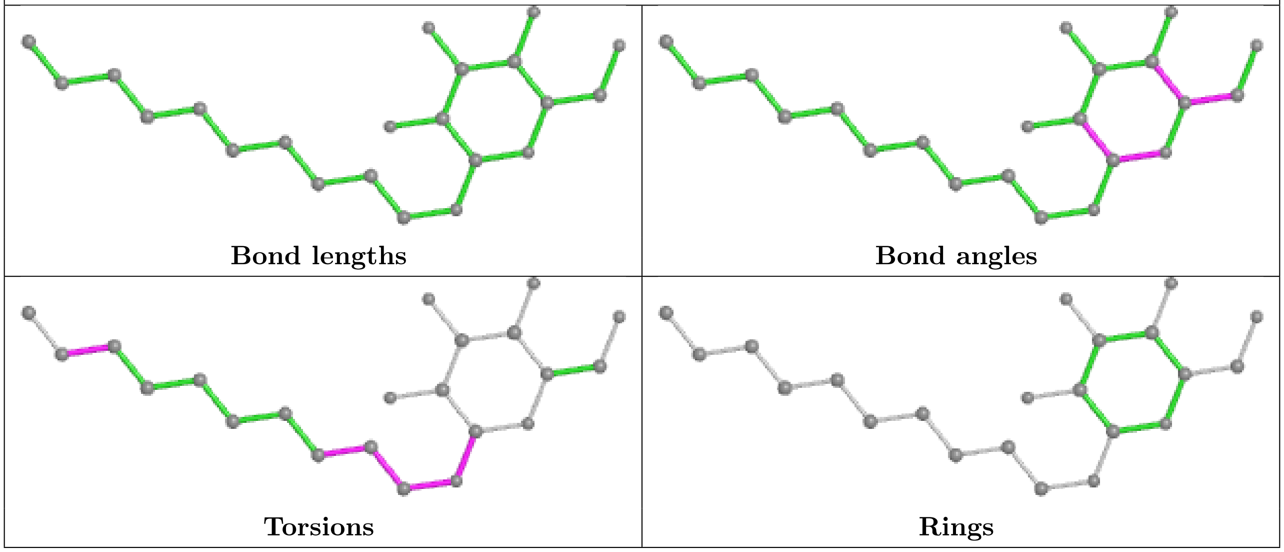

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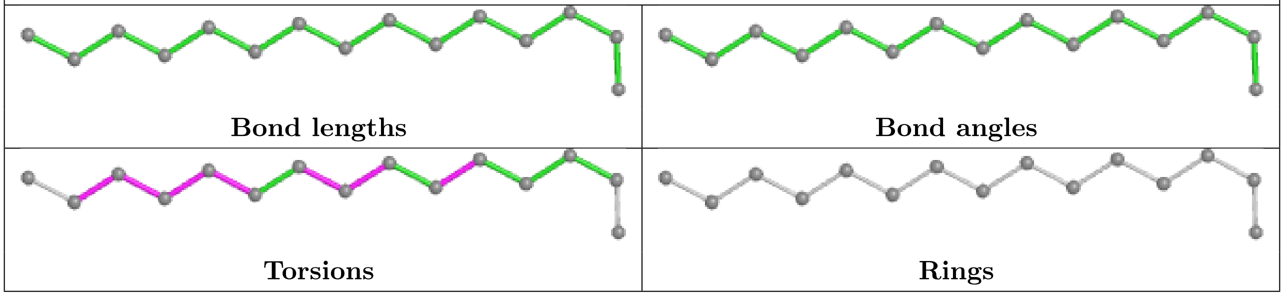

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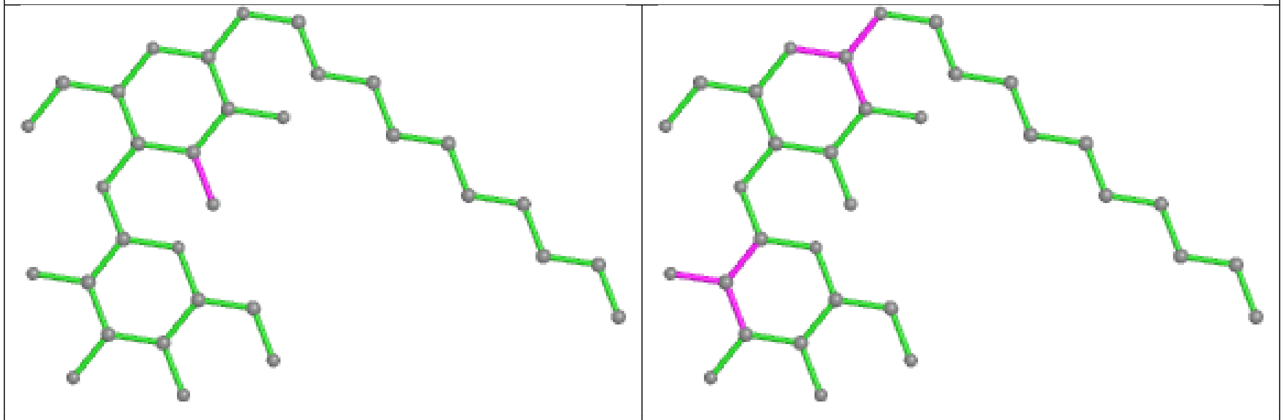
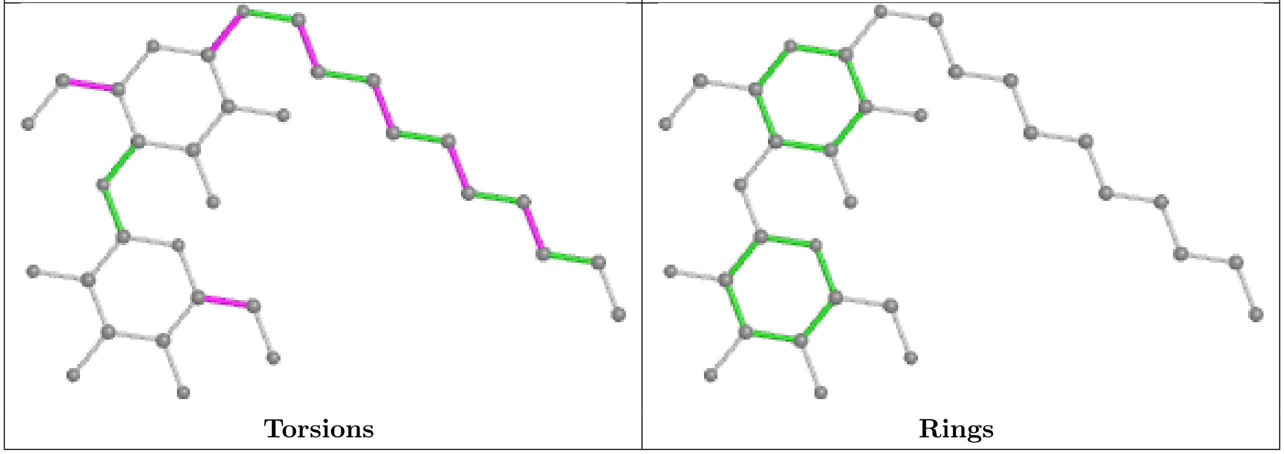


Bond lengths

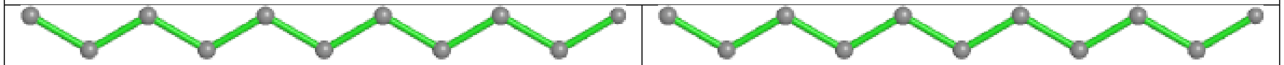
Bond angles



Torsions

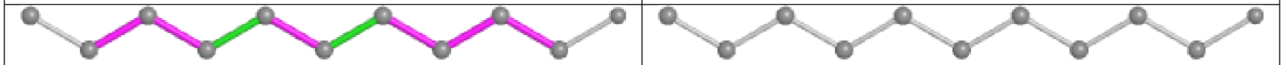
Rings

Ligand DMU J 101



Bond lengths

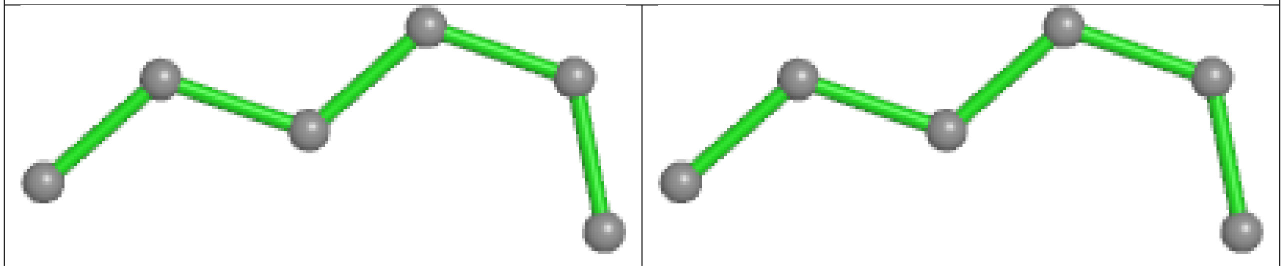
Bond angles



Torsions

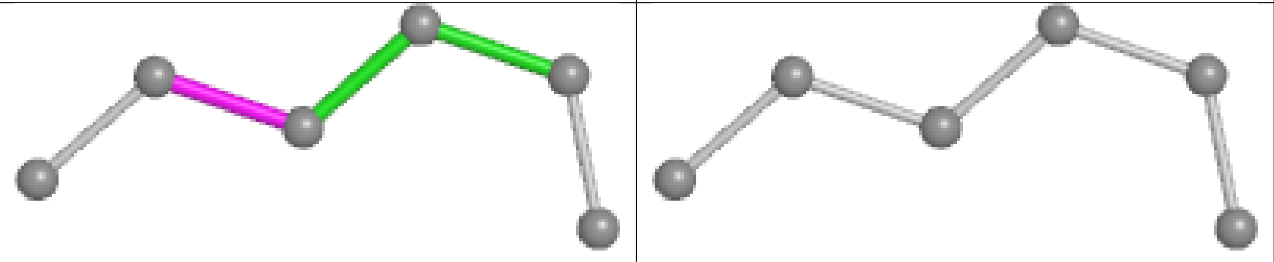
Rings

Ligand LFA C 308



Bond lengths

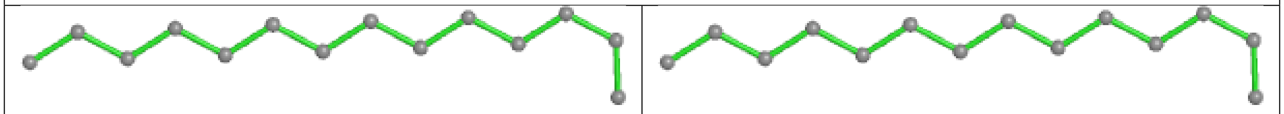
Bond angles



Torsions

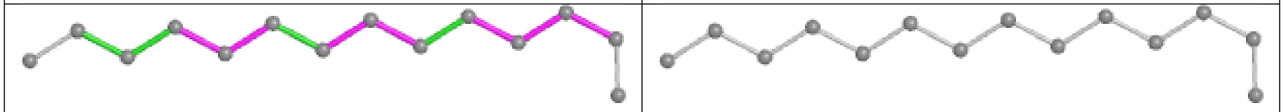
Rings

Ligand LFA N 610



Bond lengths

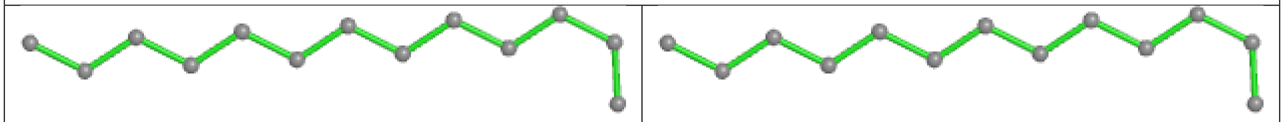
Bond angles



Torsions

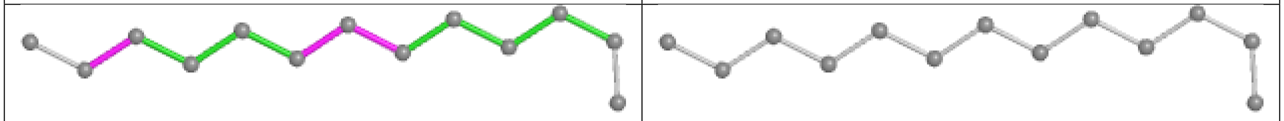
Rings

Ligand LFA P 314



Bond lengths

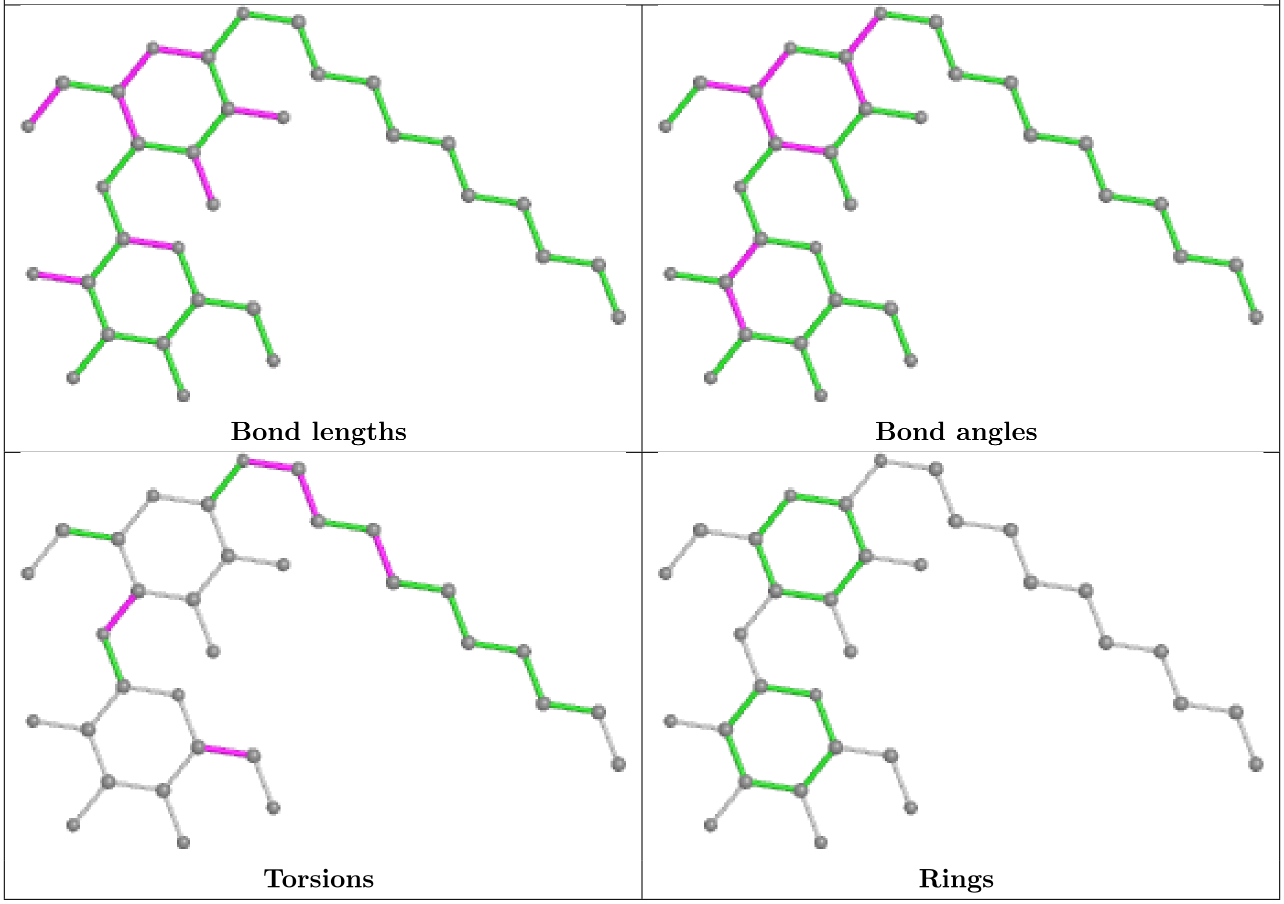
Bond angles



Torsions

Rings

Ligand DMU D 201



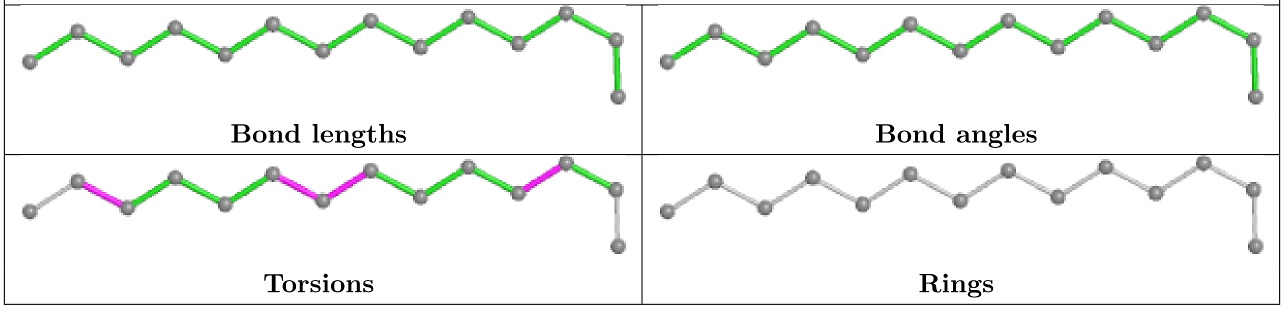
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA N 609



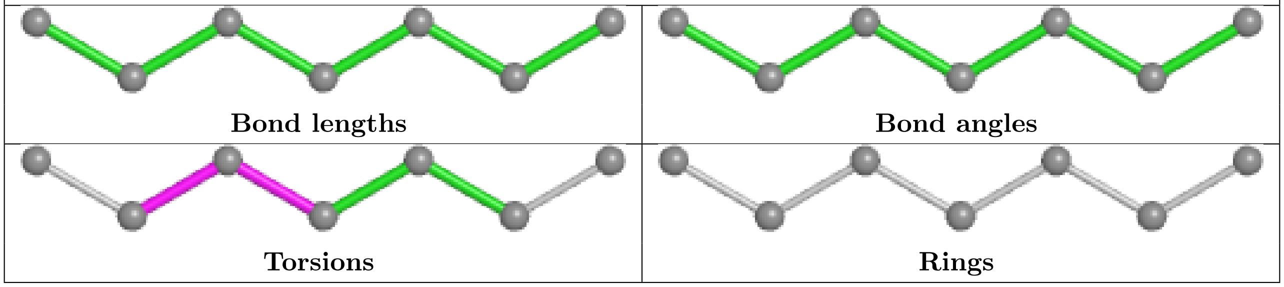
Bond lengths

Bond angles

Torsions

Rings

Ligand DMU N 611



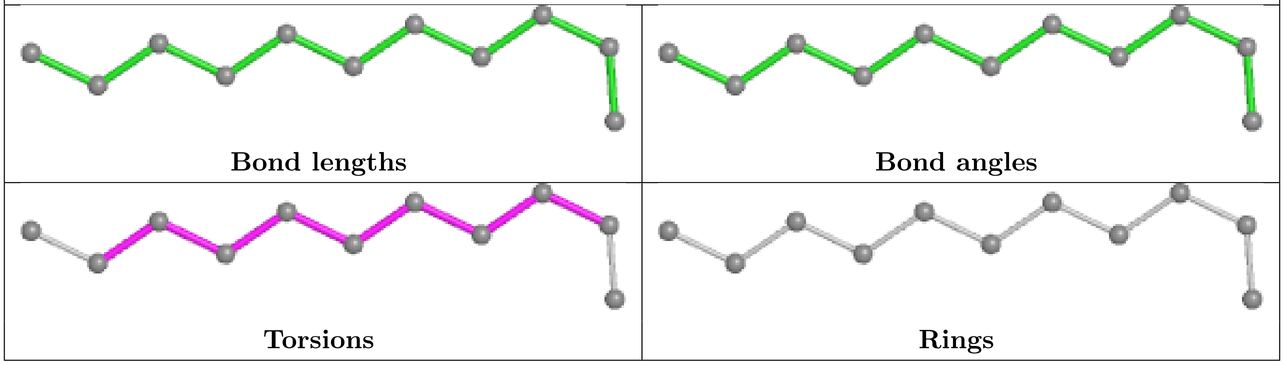
Bond lengths

Bond angles

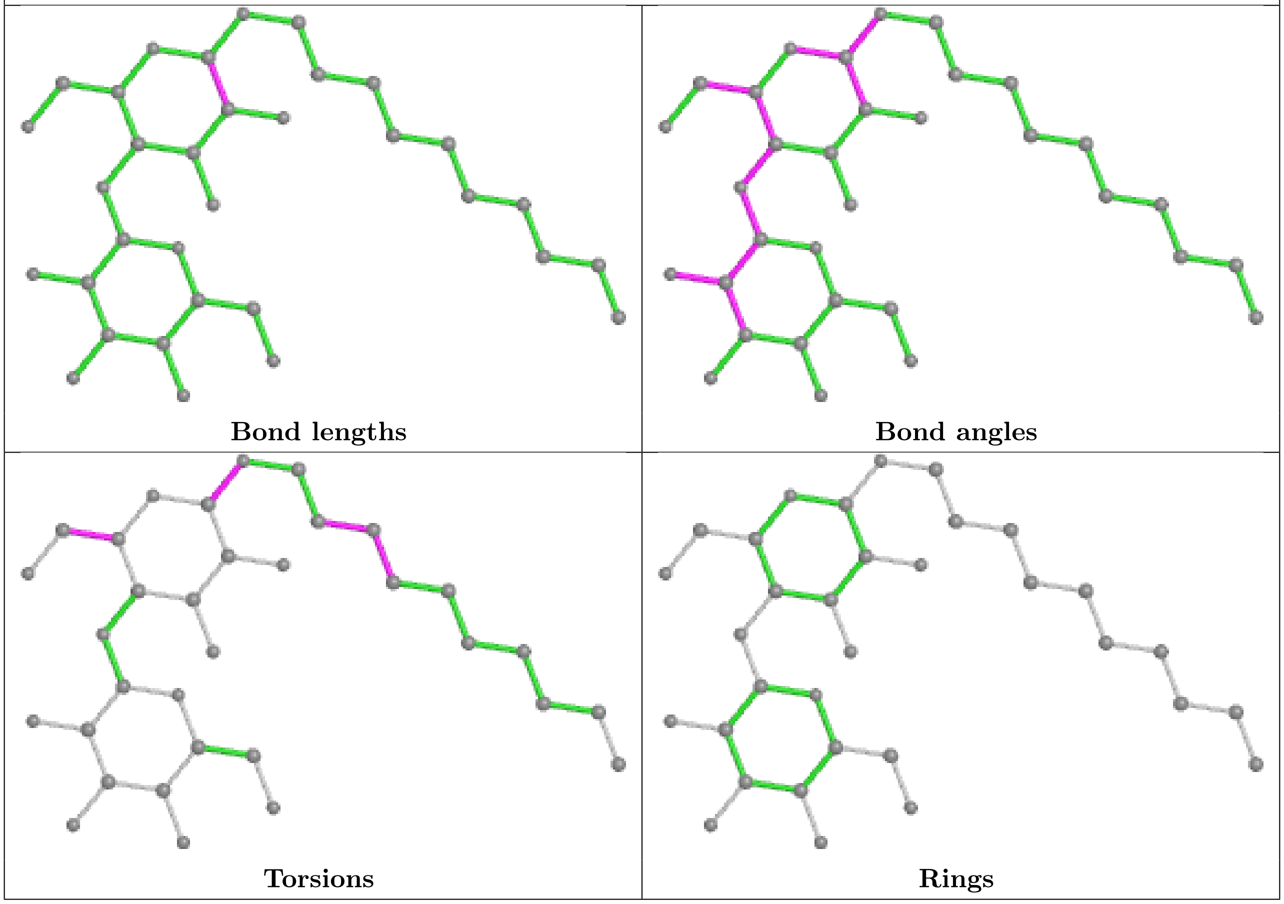
Torsions

Rings

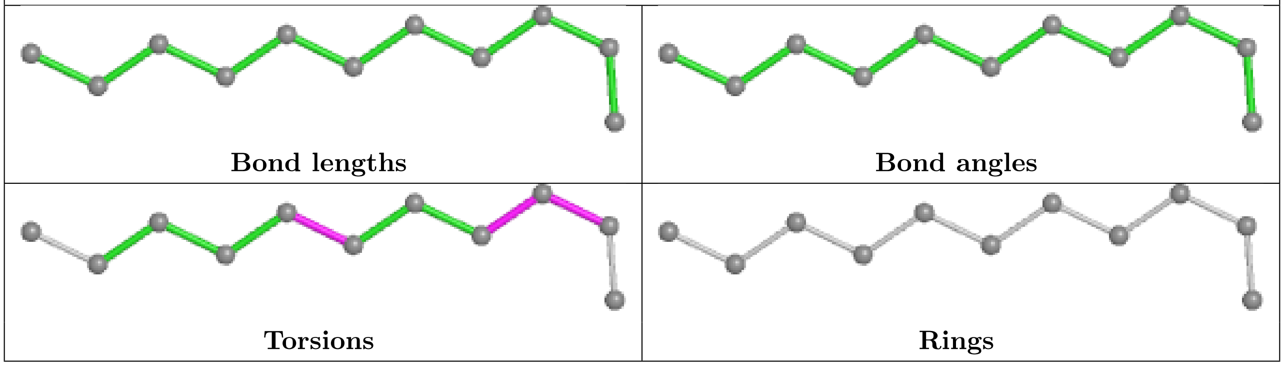
Ligand LFA C 310



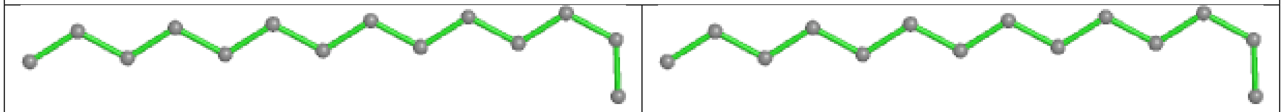
Ligand DMU N 619



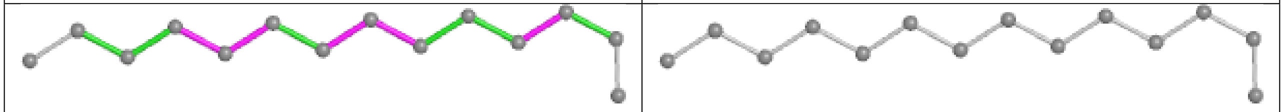
Ligand LFA O 302



Ligand LFA A 608

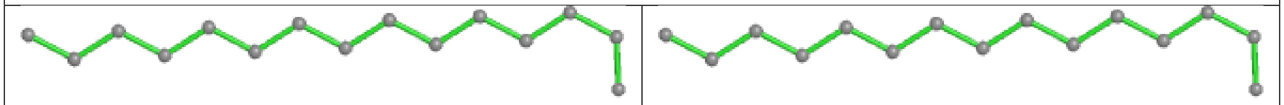


Bond lengths Bond angles

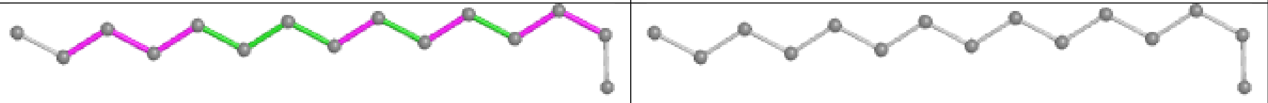


Torsions Rings

Ligand LFA P 301

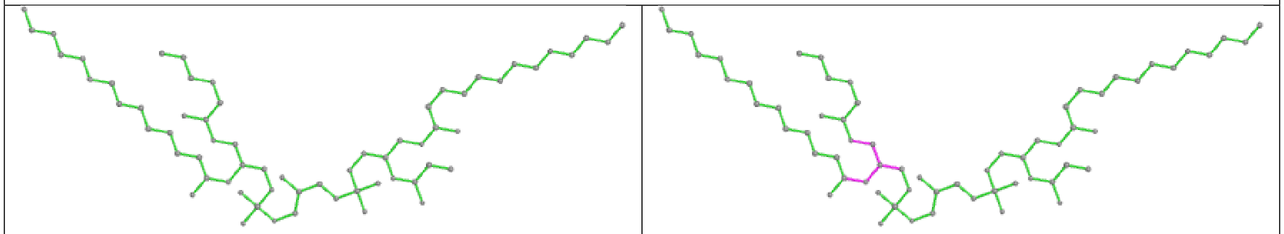


Bond lengths Bond angles

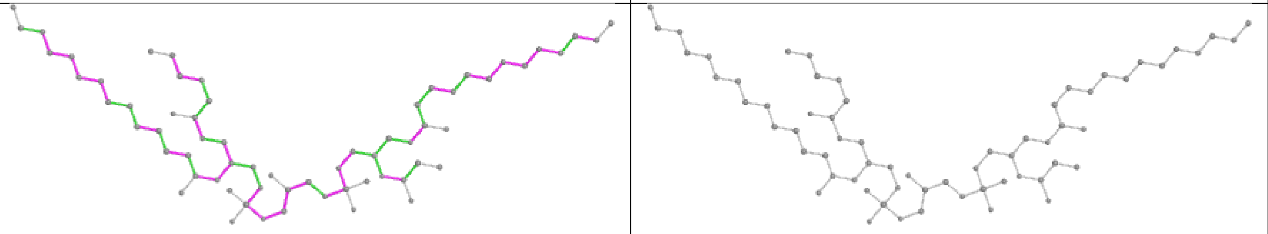


Torsions Rings

Ligand CDL I 101

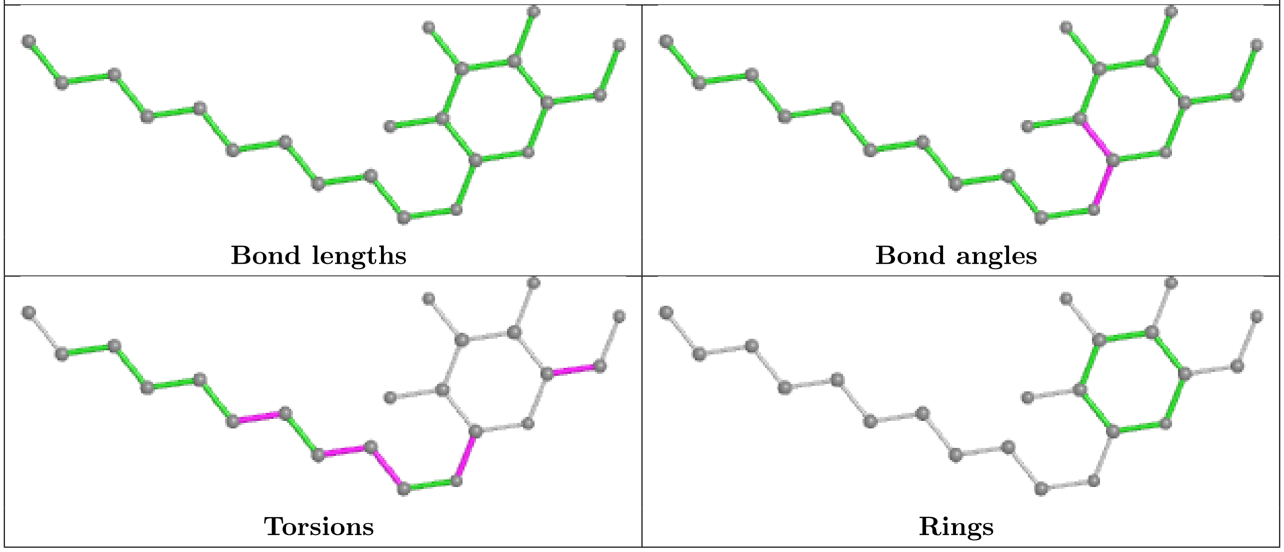


Bond lengths Bond angles



Torsions Rings

Ligand DMU P 323



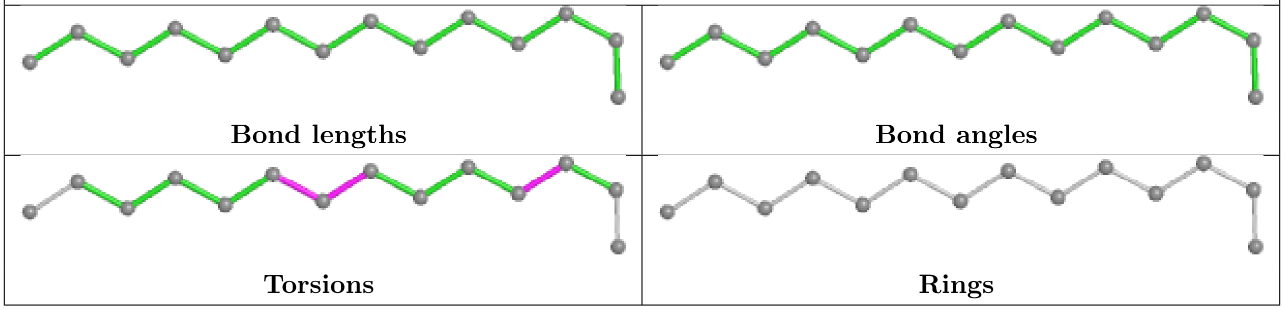
Bond lengths

Bond angles

Torsions

Rings

Ligand LFA A 607



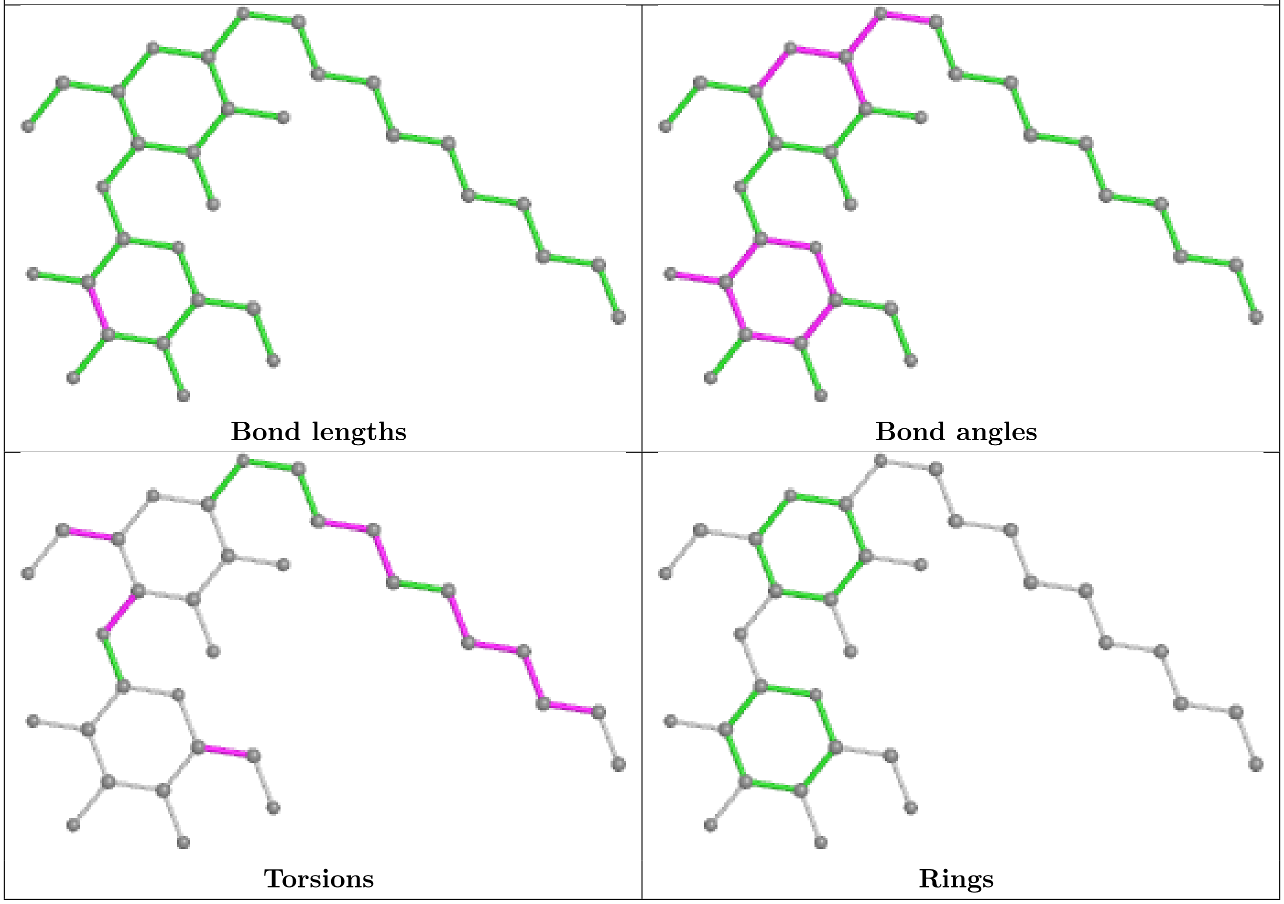
Bond lengths

Bond angles

Torsions

Rings

Ligand DMU C 315



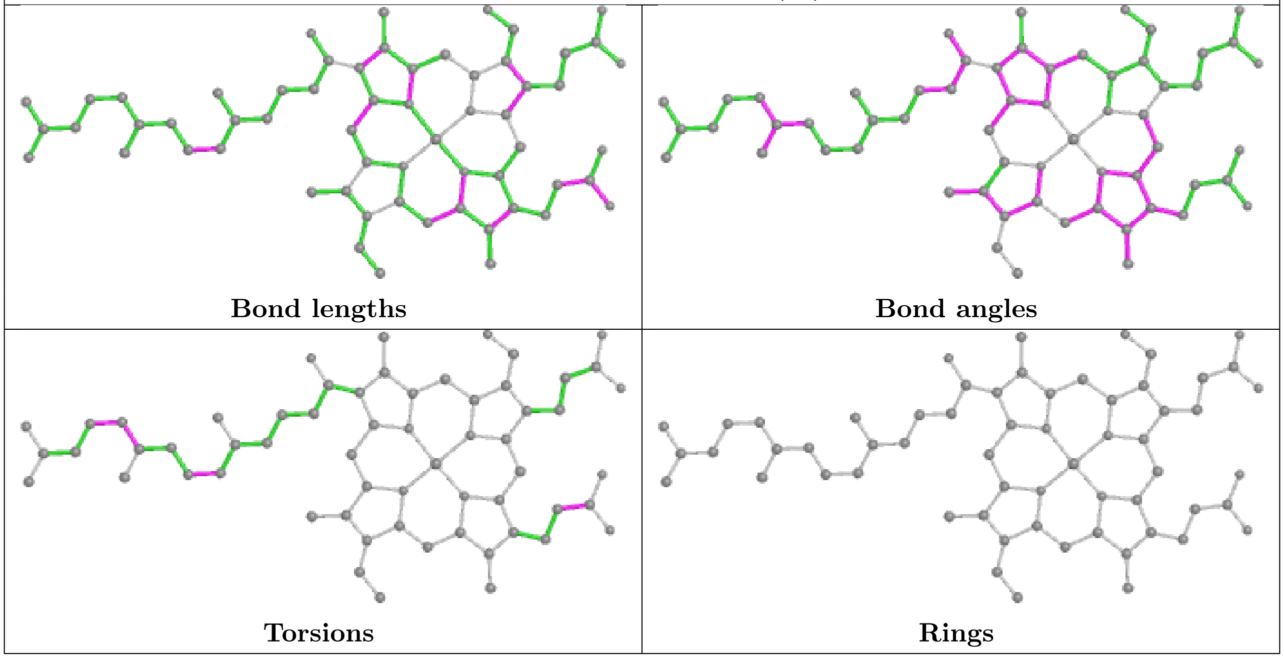
Bond lengths

Bond angles

Torsions

Rings

Ligand HEA A 601 (A)



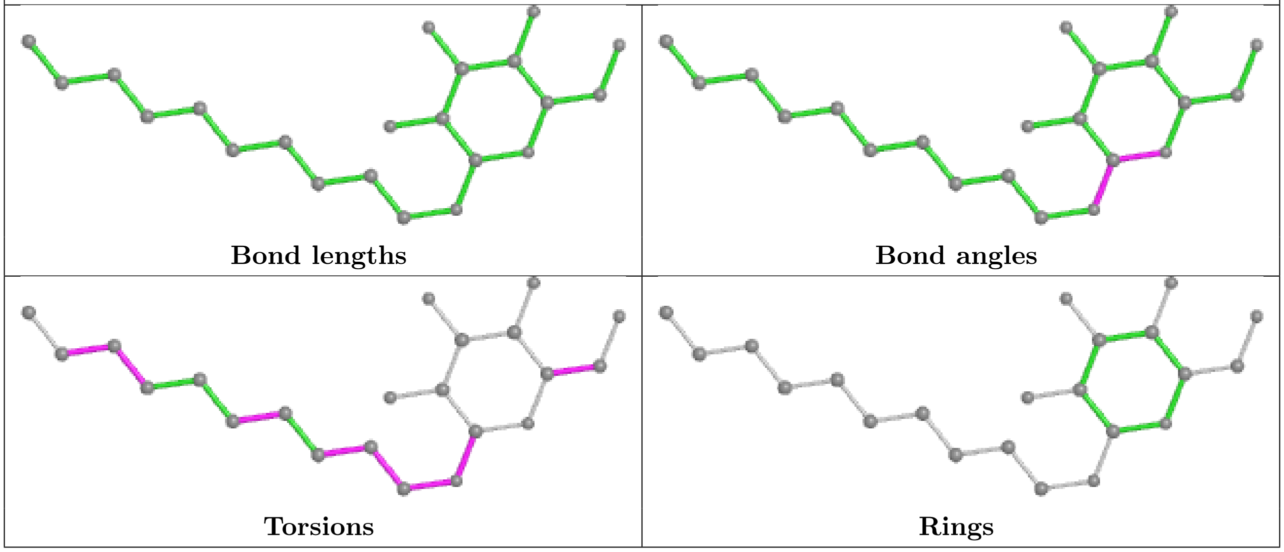
Bond lengths

Bond angles

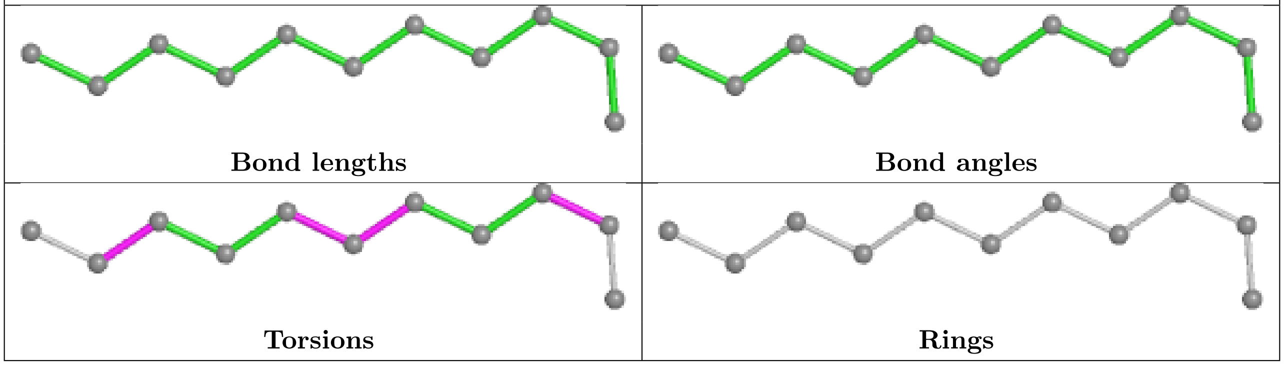
Torsions

Rings

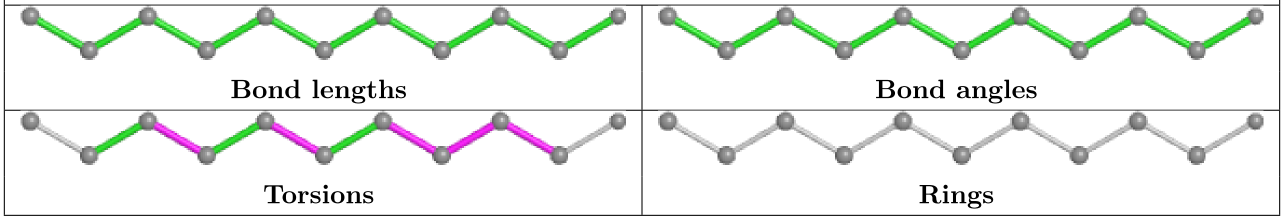
Ligand DMU Y 102



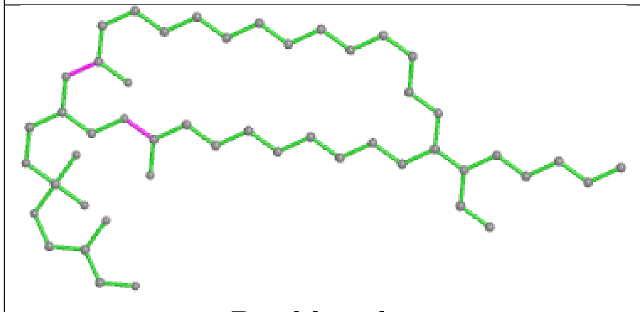
Ligand LFA C 312



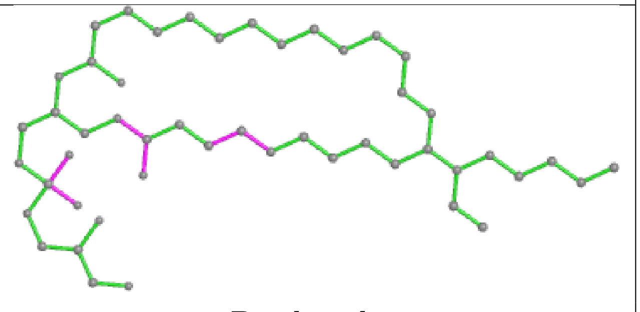
Ligand DMU B 302



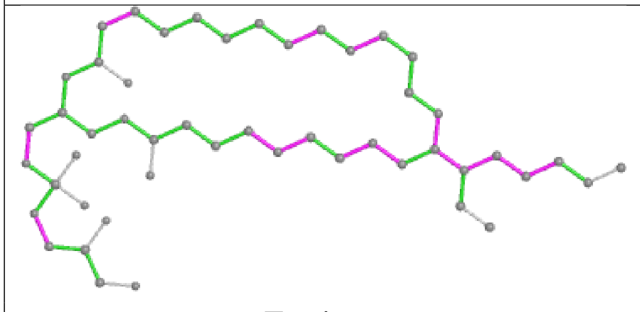
Ligand PGV C 303



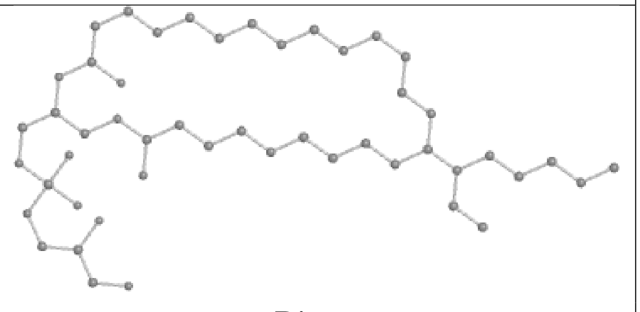
Bond lengths



Bond angles

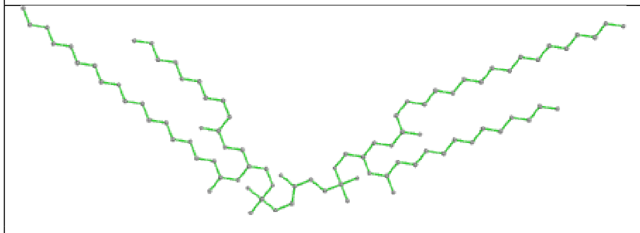


Torsions

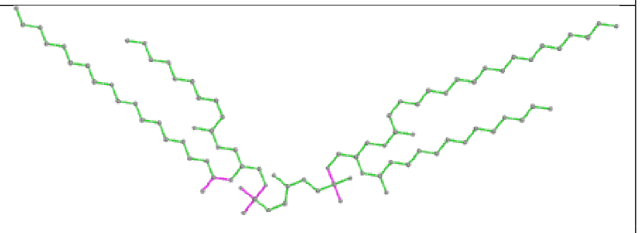


Rings

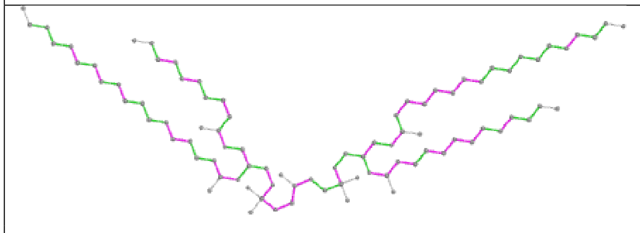
Ligand CDL P 305



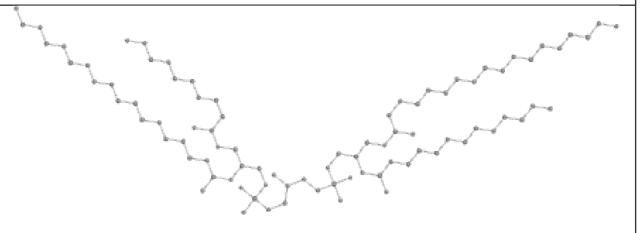
Bond lengths



Bond angles

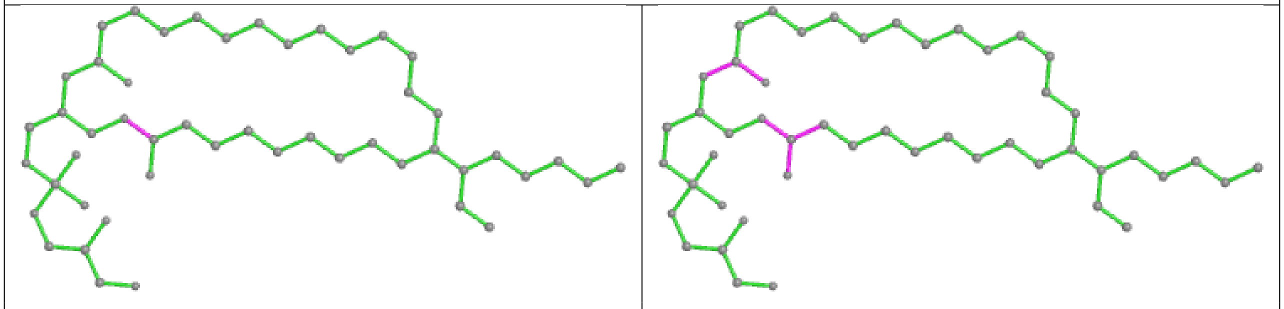


Torsions

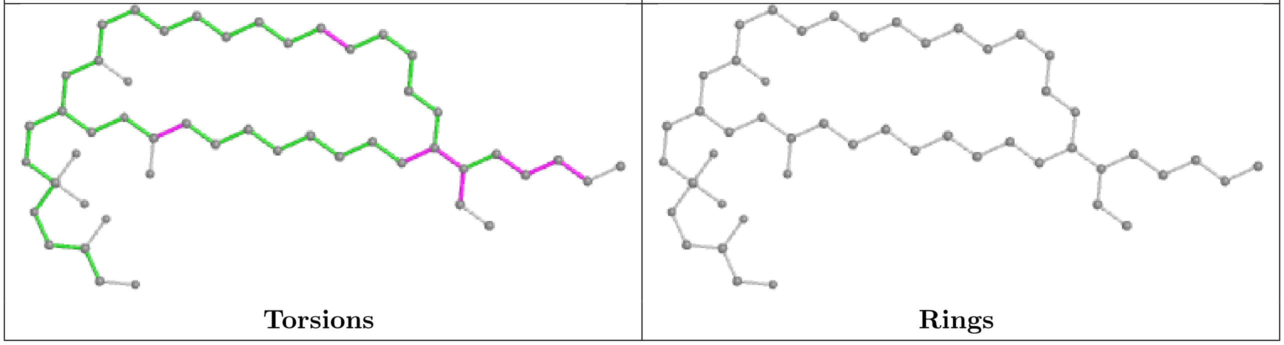


Rings

Ligand PGV N 618

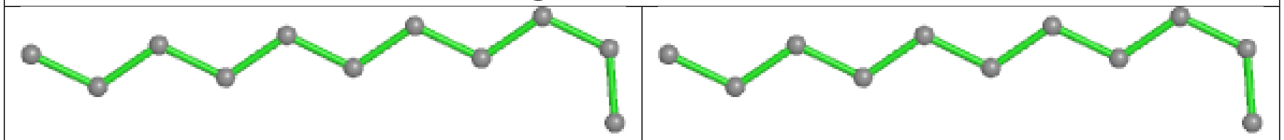


Bond lengths **Bond angles**

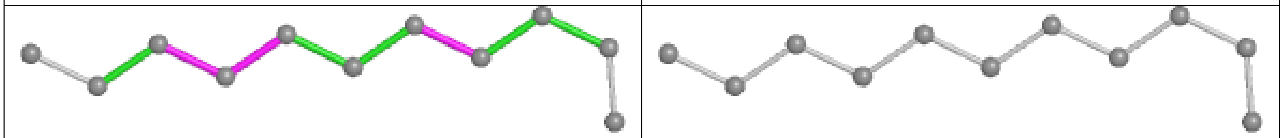


Torsions **Rings**

Ligand LFA T 103

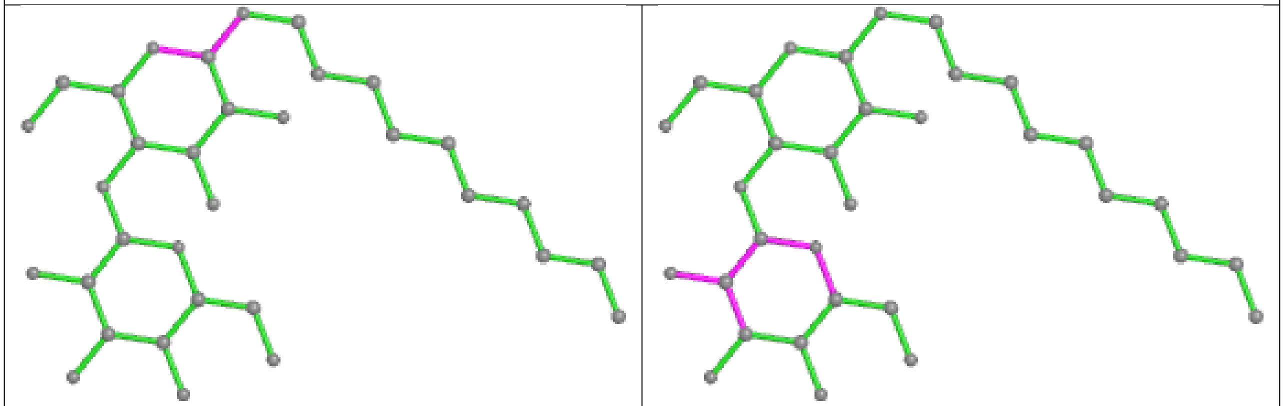


Bond lengths **Bond angles**

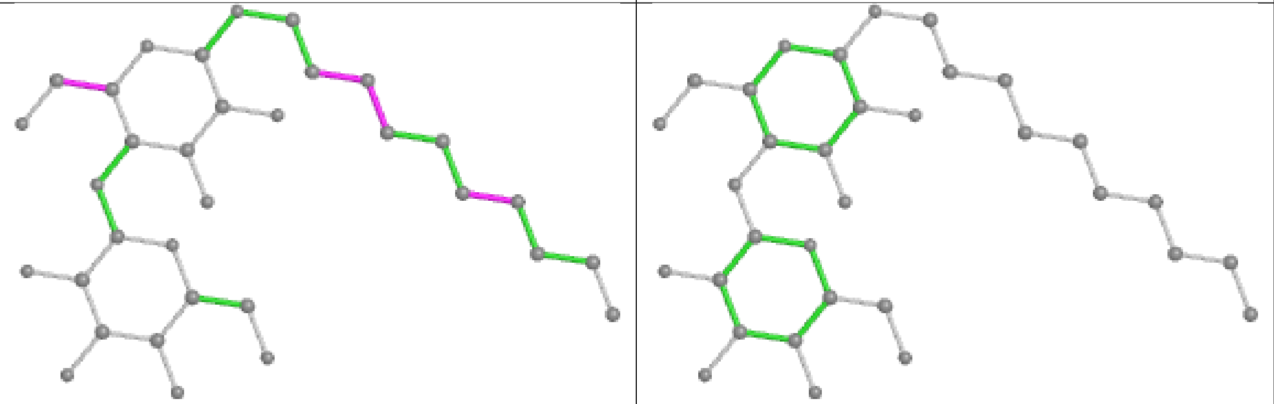


Torsions **Rings**

Ligand DMU H 101

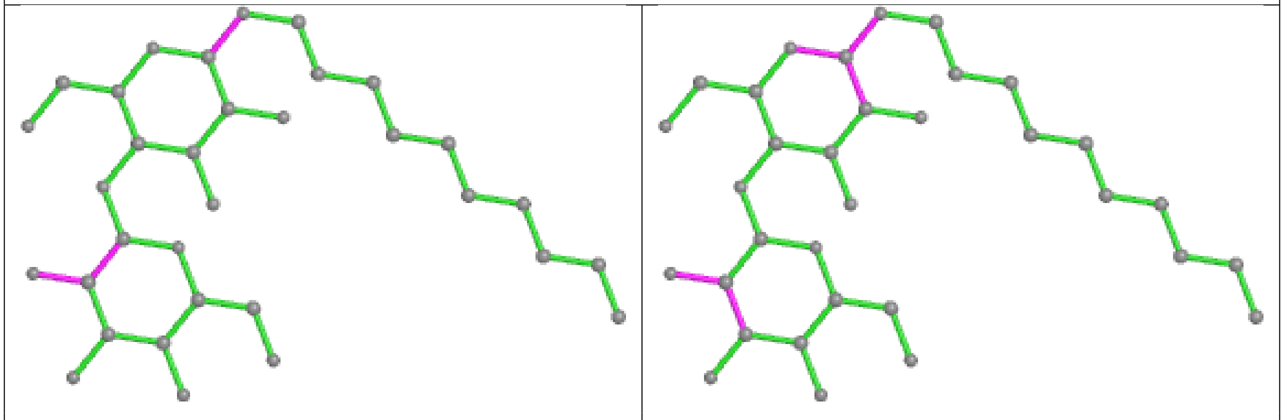


Bond lengths **Bond angles**



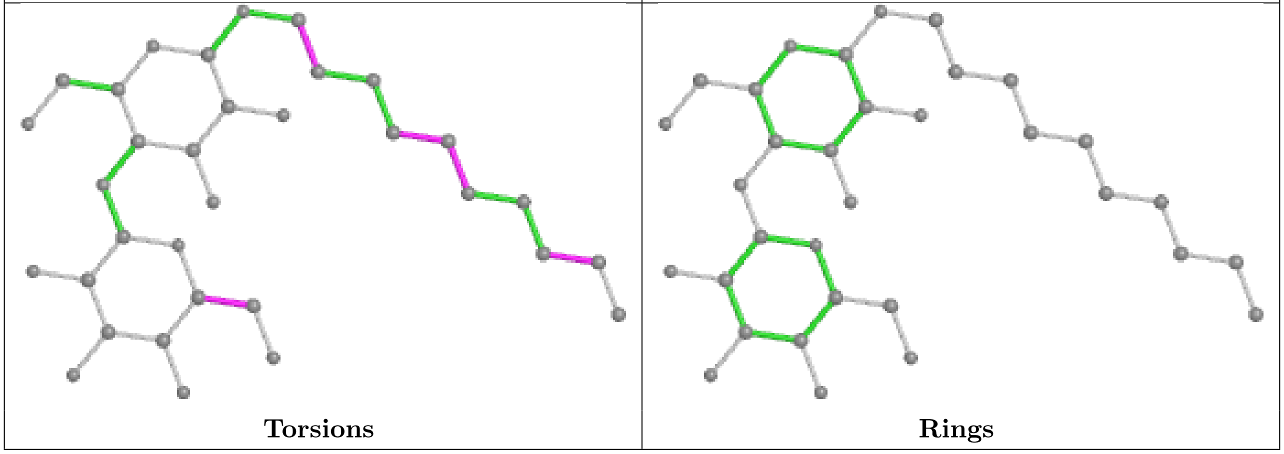
Torsions **Rings**

Ligand DMU Z 101



Bond lengths

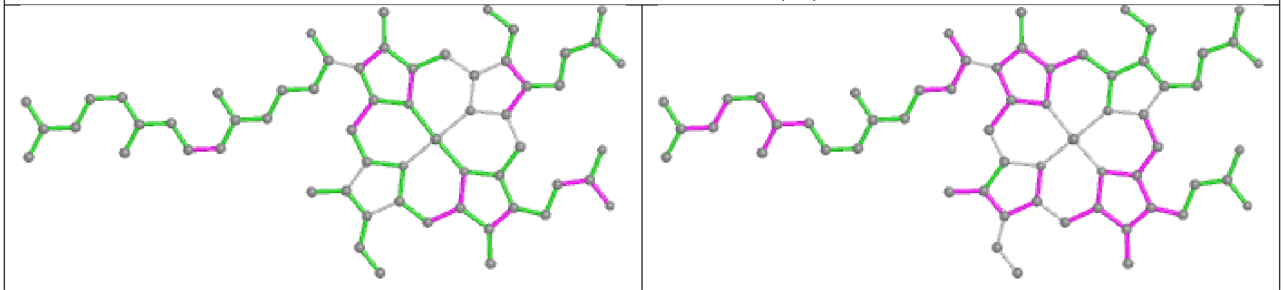
Bond angles



Torsions

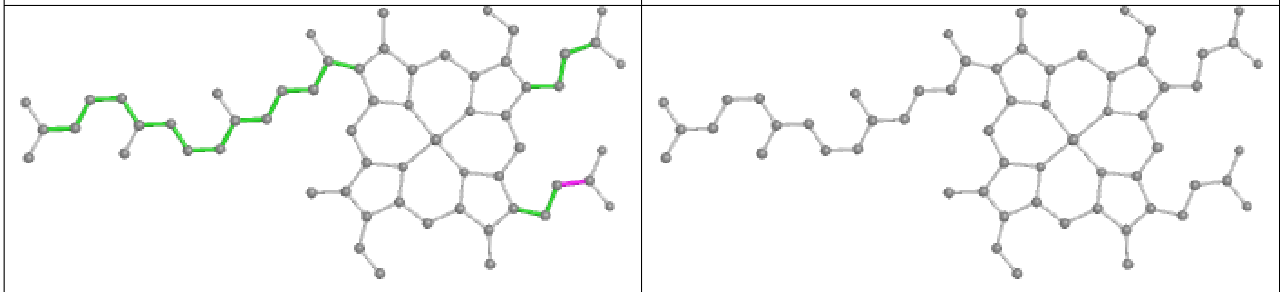
Rings

Ligand HEA A 601 (B)



Bond lengths

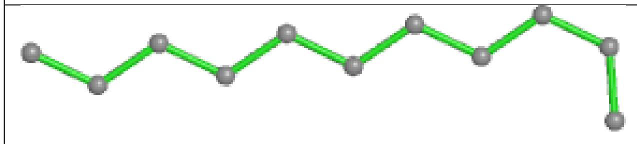
Bond angles

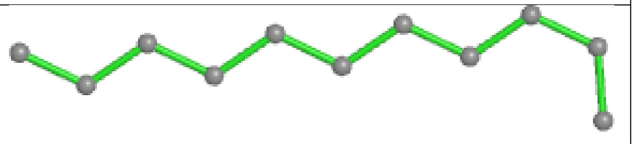


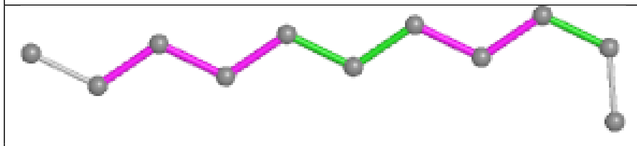
Torsions

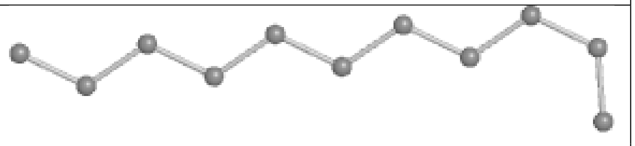
Rings

Ligand LFA P 311

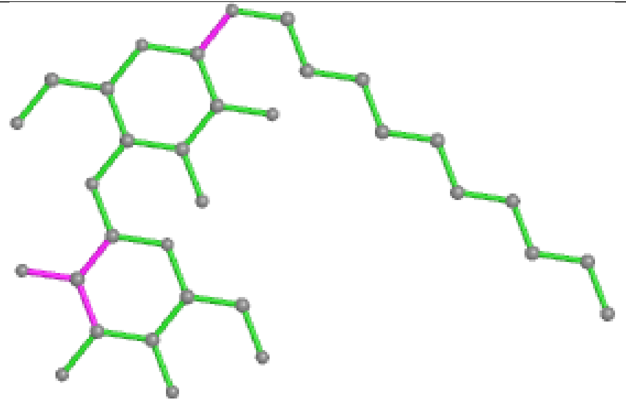

Bond lengths

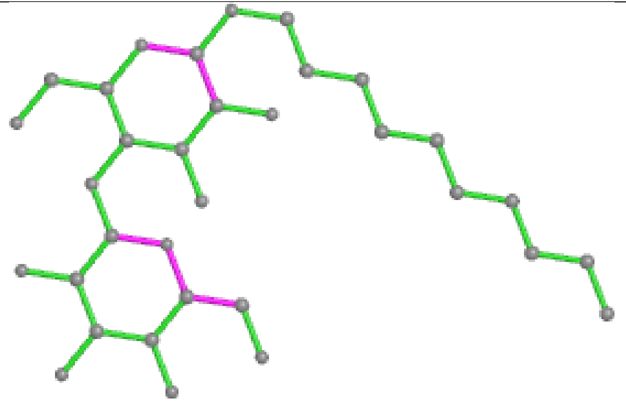

Bond angles

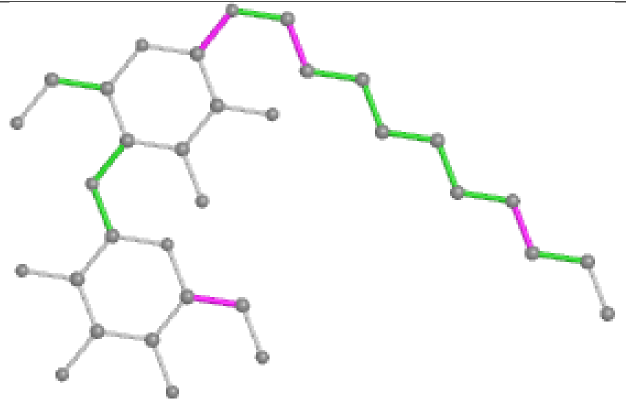

Torsions

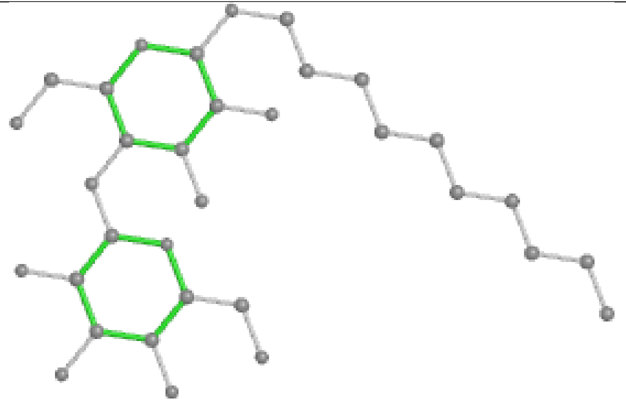

Rings

Ligand DMU N 612

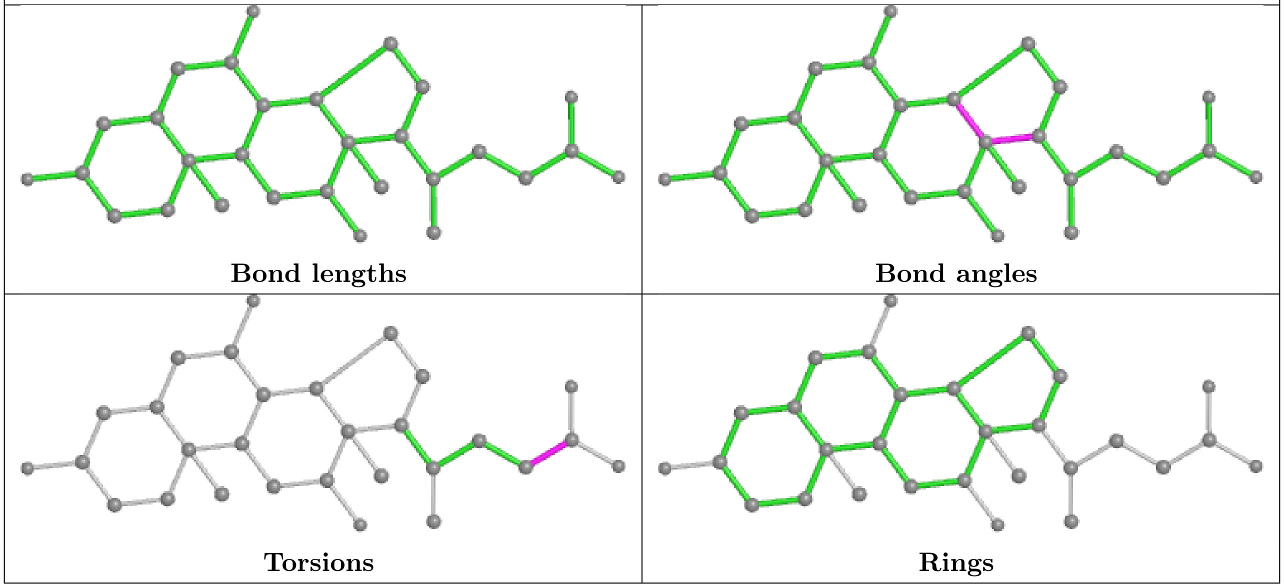

Bond lengths


Bond angles


Torsions


Rings

Ligand CHD B 305



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	512/514 (99%)	0.13	0 100 100	27, 31, 40, 57	0
1	N	512/514 (99%)	-0.04	1 (0%) 95 95	29, 37, 48, 66	0
2	B	226/227 (99%)	0.10	6 (2%) 54 58	29, 37, 57, 81	0
2	O	226/227 (99%)	0.10	7 (3%) 49 53	36, 47, 74, 84	0
3	C	258/261 (98%)	0.01	1 (0%) 92 93	29, 35, 47, 62	0
3	P	258/261 (98%)	-0.02	2 (0%) 86 88	30, 38, 49, 76	0
4	D	143/147 (97%)	-0.13	1 (0%) 87 90	33, 40, 56, 70	0
4	Q	137/147 (93%)	0.38	7 (5%) 28 31	41, 59, 85, 104	0
5	E	102/109 (93%)	-0.17	0 100 100	33, 39, 56, 74	0
5	R	102/109 (93%)	-0.13	0 100 100	37, 48, 64, 82	0
6	F	91/98 (92%)	-0.05	0 100 100	31, 42, 65, 79	0
6	S	91/98 (92%)	0.05	2 (2%) 62 66	33, 41, 66, 79	0
7	G	72/85 (84%)	0.45	9 (12%) 3 4	33, 41, 96, 108	0
7	T	72/85 (84%)	0.48	8 (11%) 5 6	33, 46, 94, 105	0
8	H	75/85 (88%)	0.26	5 (6%) 17 20	34, 45, 89, 110	0
8	U	75/85 (88%)	0.47	7 (9%) 8 9	42, 50, 89, 114	0
9	I	70/73 (95%)	0.25	4 (5%) 23 26	36, 48, 72, 91	0
9	V	70/73 (95%)	0.46	3 (4%) 35 39	37, 61, 79, 101	0
10	J	56/59 (94%)	0.14	4 (7%) 16 18	36, 45, 66, 78	0
10	W	56/59 (94%)	0.23	4 (7%) 16 18	40, 51, 75, 83	0
11	K	49/56 (87%)	-0.06	0 100 100	38, 45, 60, 76	0
11	X	49/56 (87%)	0.44	3 (6%) 21 23	50, 60, 76, 100	0
12	L	44/47 (93%)	-0.09	0 100 100	32, 37, 50, 60	0
12	Y	44/47 (93%)	-0.08	0 100 100	41, 49, 65, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	40/46 (86%)	0.30	3 (7%)	14	16	34, 38, 74, 89	0
13	Z	40/46 (86%)	0.58	5 (12%)	3	4	47, 54, 94, 101	0
All	All	3470/3614 (96%)	0.09	82 (2%)	59	63	27, 40, 68, 114	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	Z	40	TYR	8.4
8	H	45	ALA	7.7
7	G	36	TRP	7.5
9	V	37	PHE	6.7
8	U	45	ALA	6.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	FME	A	1	10/11	0.94	0.16	42,50,91,118	0
2	FME	B	1	10/11	0.98	0.12	32,35,45,85	0
1	FME	N	1	10/11	0.98	0.17	48,54,98,107	0
2	FME	O	1	10/11	0.99	0.10	40,49,57,73	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	DMU	P	317	22/33	0.47	0.41	50,66,82,91	22

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
20	DMU	B	307	22/33	0.60	0.24	61,71,81,85	22
20	DMU	C	317	22/33	0.61	0.36	42,65,78,85	22
20	DMU	A	617	11/33	0.61	0.37	47,60,69,72	11
20	DMU	P	318	33/33	0.62	0.35	52,62,77,100	33
19	LFA	P	311	11/20	0.63	0.36	59,67,76,82	11
19	LFA	P	308	11/20	0.65	0.43	36,52,58,59	11
20	DMU	B	303	22/33	0.65	0.27	50,61,72,75	22
20	DMU	O	303	22/33	0.66	0.23	51,76,86,88	22
20	DMU	P	319	33/33	0.66	0.26	55,74,82,94	33
26	CDL	C	304	87/100	0.66	0.24	46,81,122,135	0
20	DMU	C	324	33/33	0.67	0.26	39,54,72,82	33
20	DMU	C	318	33/33	0.68	0.34	46,55,68,81	33
20	DMU	O	308	22/33	0.68	0.22	46,52,59,63	22
20	DMU	N	602	11/33	0.68	0.35	52,67,72,75	11
20	DMU	P	324	33/33	0.69	0.25	50,63,84,91	33
20	DMU	Q	201	33/33	0.70	0.16	39,57,69,89	33
20	DMU	C	319	33/33	0.70	0.22	43,71,86,87	33
20	DMU	P	323	22/33	0.71	0.21	46,60,70,77	22
19	LFA	C	308	6/20	0.71	0.55	49,51,55,59	6
26	CDL	P	305	87/100	0.71	0.24	50,86,130,152	0
20	DMU	A	615	11/33	0.72	0.35	54,63,68,71	11
26	CDL	O	304	64/100	0.73	0.21	62,91,140,180	0
20	DMU	A	609	7/33	0.73	0.47	61,69,77,86	7
20	DMU	C	323	22/33	0.74	0.19	50,62,70,83	22
20	DMU	W	101	11/33	0.74	0.27	68,74,76,78	11
20	DMU	Y	102	22/33	0.74	0.28	55,63,76,86	22
20	DMU	P	316	7/33	0.75	0.41	62,66,71,72	7
20	DMU	P	315	33/33	0.75	0.27	45,54,67,71	33
20	DMU	N	612	33/33	0.76	0.22	40,55,75,86	33
20	DMU	A	610	33/33	0.76	0.21	31,42,53,63	33
19	LFA	T	102	14/20	0.77	0.35	42,70,86,87	14
20	DMU	L	102	22/33	0.77	0.33	49,59,67,70	22
20	DMU	C	315	33/33	0.77	0.29	43,56,69,70	33
20	DMU	N	611	7/33	0.77	0.34	72,76,81,93	7
20	DMU	O	307	11/33	0.78	0.35	47,55,65,70	11
19	LFA	C	313	15/20	0.78	0.28	44,52,70,73	15
19	LFA	C	325	15/20	0.78	0.45	57,66,74,75	15
26	CDL	Y	101	94/100	0.78	0.25	57,95,141,156	0
19	LFA	A	608	14/20	0.79	0.29	37,50,62,63	14
19	LFA	C	310	11/20	0.79	0.36	59,70,85,90	11
19	LFA	N	610	14/20	0.79	0.29	42,51,71,72	14
19	LFA	O	302	11/20	0.79	0.26	49,56,73,80	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	LFA	C	311	14/20	0.79	0.34	40,62,72,75	14
26	CDL	I	101	64/100	0.80	0.21	54,87,129,158	0
19	LFA	C	312	11/20	0.80	0.40	53,59,73,76	11
19	LFA	P	309	6/20	0.83	0.55	45,51,54,55	6
19	LFA	P	310	18/20	0.83	0.22	43,52,62,69	18
20	DMU	Z	101	33/33	0.83	0.19	56,67,90,94	0
19	LFA	T	103	11/20	0.83	0.27	55,59,73,75	11
21	EDO	N	617	4/4	0.84	0.21	31,39,39,43	4
19	LFA	P	301	15/20	0.84	0.41	51,57,62,64	15
20	DMU	D	201	33/33	0.84	0.16	28,44,51,78	33
26	CDL	L	101	94/100	0.84	0.20	44,85,129,155	0
19	LFA	P	312	11/20	0.84	0.38	47,59,70,74	11
20	DMU	C	306	11/33	0.84	0.26	59,63,70,72	11
19	LFA	P	313	15/20	0.84	0.28	48,53,63,66	15
20	DMU	J	101	11/33	0.85	0.28	63,68,71,82	11
19	LFA	N	601	17/20	0.85	0.27	41,60,75,78	17
21	EDO	P	322	4/4	0.85	0.19	32,36,40,42	4
19	LFA	C	307	11/20	0.86	0.42	41,52,64,70	11
21	EDO	E	201	4/4	0.86	0.23	39,41,48,51	4
19	LFA	P	314	13/20	0.86	0.26	46,63,74,76	13
19	LFA	B	306	17/20	0.86	0.29	43,59,87,90	17
20	DMU	O	306	11/33	0.86	0.37	44,47,72,75	11
20	DMU	C	316	7/33	0.87	0.32	47,51,63,69	7
19	LFA	C	314	13/20	0.87	0.23	56,59,77,86	13
20	DMU	M	102	8/33	0.88	0.23	48,51,58,60	8
19	LFA	C	309	18/20	0.88	0.19	37,45,54,56	18
19	LFA	A	607	14/20	0.89	0.31	36,51,76,78	14
21	EDO	A	611	4/4	0.89	0.18	27,29,29,33	4
20	DMU	P	307	11/33	0.89	0.41	52,53,61,63	11
20	DMU	H	101	33/33	0.89	0.20	31,45,59,68	33
20	DMU	N	619	33/33	0.89	0.22	35,49,63,66	33
24	CHD	P	306	29/29	0.89	0.18	54,60,72,86	0
21	EDO	C	322	4/4	0.90	0.21	36,36,37,38	4
24	CHD	P	302	29/29	0.91	0.08	32,37,41,45	0
21	EDO	P	320	4/4	0.91	0.19	53,60,63,73	4
20	DMU	Z	102	8/33	0.91	0.29	51,57,61,62	8
24	CHD	C	301	29/29	0.91	0.09	32,35,40,43	0
21	EDO	A	614	4/4	0.92	0.10	37,39,40,44	4
20	DMU	M	101	33/33	0.92	0.10	41,52,78,83	0
20	DMU	B	302	11/33	0.92	0.27	47,58,64,68	11
21	EDO	N	613	4/4	0.92	0.15	31,37,37,39	4
21	EDO	O	309	4/4	0.93	0.17	36,37,39,40	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
24	CHD	C	305	29/29	0.93	0.17	50,58,77,111	0
21	EDO	A	612	4/4	0.93	0.16	35,41,50,53	4
19	LFA	N	609	14/20	0.93	0.29	40,50,68,71	14
21	EDO	R	201	4/4	0.93	0.20	63,63,64,70	4
21	EDO	C	320	4/4	0.94	0.29	53,57,58,71	4
25	UNX	P	303	1/1	0.94	0.17	55,55,55,55	0
21	EDO	P	321	4/4	0.94	0.14	42,42,45,45	4
24	CHD	B	305	29/29	0.94	0.09	30,36,41,50	0
21	EDO	F	102	4/4	0.95	0.18	23,24,31,31	4
21	EDO	E	202	4/4	0.95	0.20	35,35,37,39	4
21	EDO	N	615	4/4	0.95	0.22	31,32,32,33	4
28	PEK	T	101	53/53	0.95	0.12	38,62,110,159	0
21	EDO	G	102	4/4	0.96	0.14	30,34,35,38	4
24	CHD	O	301	29/29	0.96	0.09	32,36,39,47	0
21	EDO	R	202	4/4	0.96	0.14	38,39,41,41	4
21	EDO	S	102	4/4	0.96	0.14	25,25,31,31	4
14	HEA	N	604	60/60	0.96	0.10	28,32,40,43	0
28	PEK	G	101	53/53	0.96	0.12	33,56,90,112	0
21	EDO	N	614	4/4	0.96	0.15	39,40,50,50	4
21	EDO	N	616	4/4	0.97	0.16	37,39,42,45	4
14	HEA	A	601[B]	60/60	0.97	0.11	25,28,45,51	9
14	HEA	A	602	60/60	0.97	0.10	24,27,36,41	0
14	HEA	N	603[A]	60/60	0.97	0.10	31,35,46,52	9
14	HEA	N	603[B]	60/60	0.97	0.10	31,35,49,53	9
21	EDO	A	613	4/4	0.97	0.21	27,28,28,29	4
14	HEA	A	601[A]	60/60	0.97	0.11	25,28,41,47	9
18	PER	N	608	2/2	0.97	0.10	33,33,33,40	0
21	EDO	R	203	4/4	0.97	0.17	44,49,51,58	4
21	EDO	C	321	4/4	0.97	0.14	37,37,39,40	4
21	EDO	T	104	4/4	0.97	0.13	36,37,39,40	4
22	PGV	A	616	51/51	0.97	0.11	29,41,80,92	0
22	PGV	C	303	51/51	0.97	0.10	32,41,90,108	0
22	PGV	N	618	51/51	0.97	0.10	33,46,79,92	0
22	PGV	P	304	51/51	0.97	0.11	34,43,102,119	0
21	EDO	B	304	4/4	0.98	0.18	25,26,27,30	4
18	PER	A	606	2/2	0.98	0.10	29,29,29,34	0
25	UNX	C	302	1/1	0.98	0.11	56,56,56,56	0
21	EDO	E	203	4/4	0.98	0.20	34,35,41,42	4
16	MG	N	606	1/1	0.99	0.07	37,37,37,37	0
21	EDO	S	103	4/4	0.99	0.13	32,36,37,37	4
21	EDO	F	103	4/4	0.99	0.10	32,34,37,38	4
23	CUA	O	305	2/2	0.99	0.12	39,39,39,40	0

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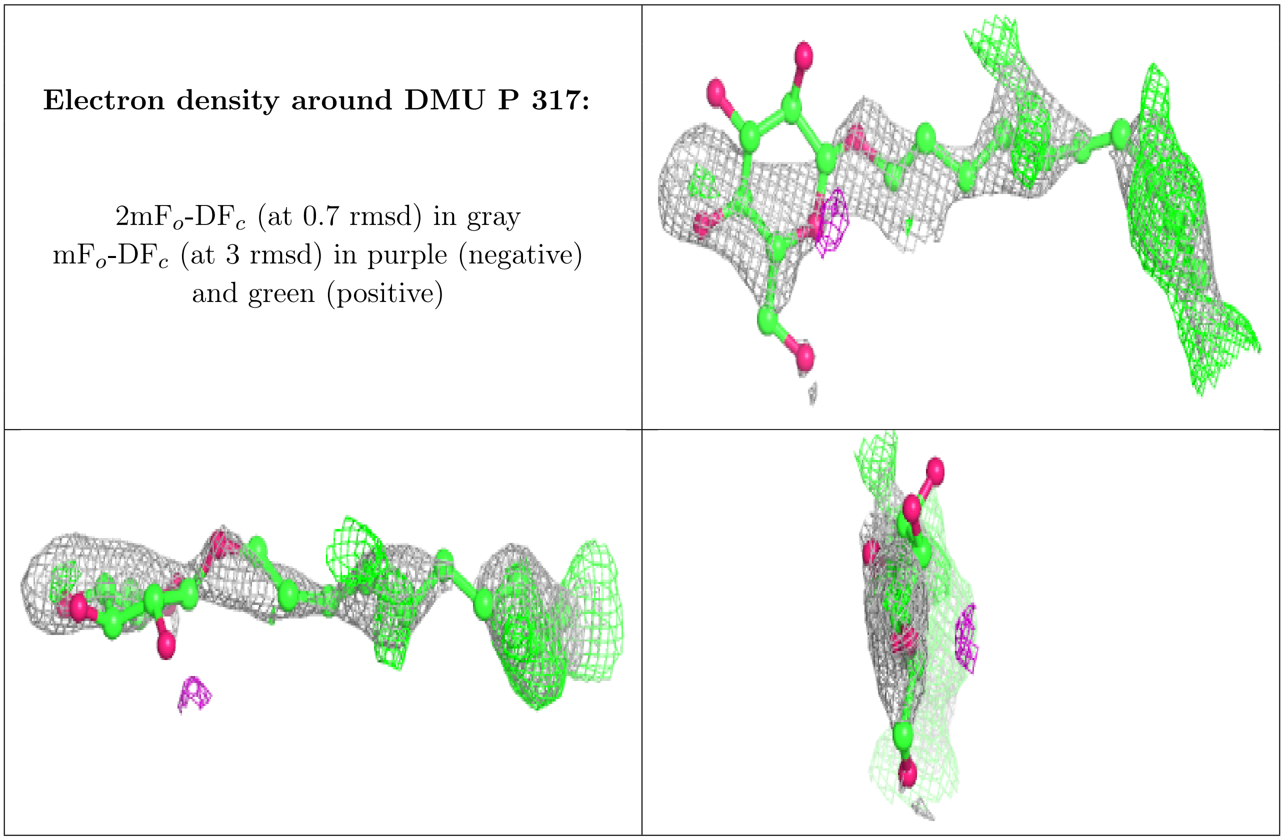
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	MG	A	604	1/1	0.99	0.09	30,30,30,30	0
15	CU	N	605	1/1	1.00	0.18	32,32,32,32	0
17	CA	A	605	1/1	1.00	0.12	33,33,33,33	0
23	CUA	B	301	2/2	1.00	0.15	29,29,29,30	0
27	ZN	F	101	1/1	1.00	0.14	36,36,36,36	0
27	ZN	S	101	1/1	1.00	0.12	37,37,37,37	0
17	CA	N	607	1/1	1.00	0.08	45,45,45,45	0
15	CU	A	603	1/1	1.00	0.17	28,28,28,28	0

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

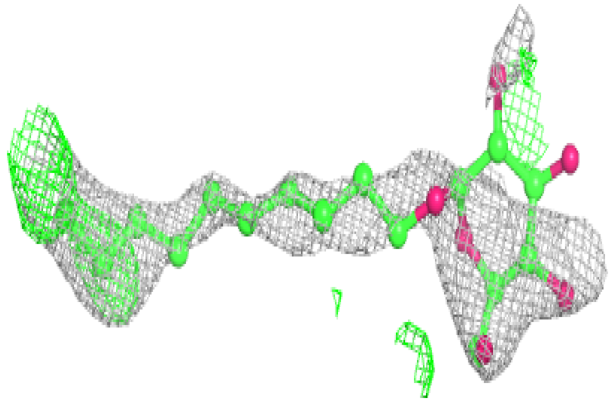


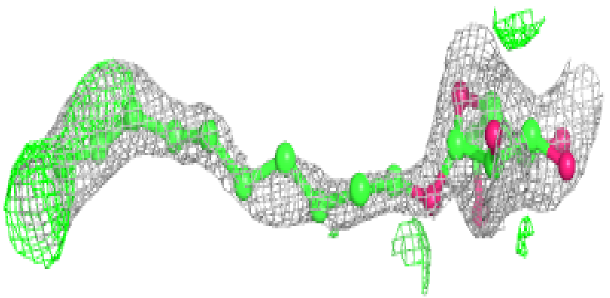
Electron density around DMU P 317:

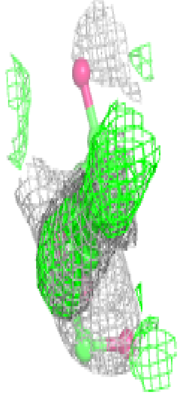
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around DMU B 307:

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

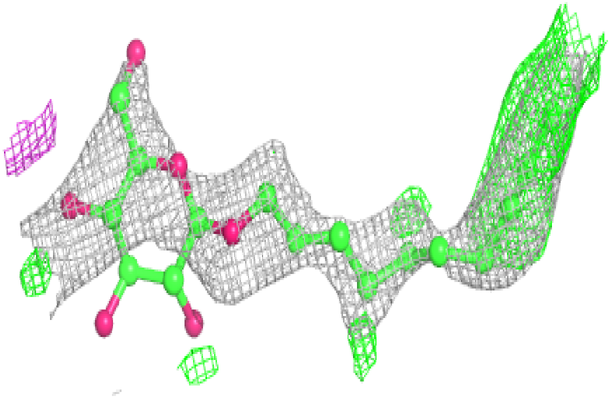


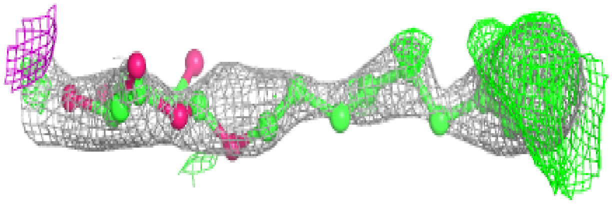


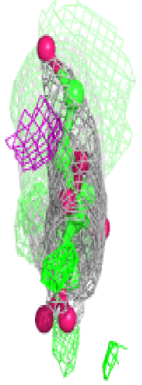


Electron density around DMU C 317:

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

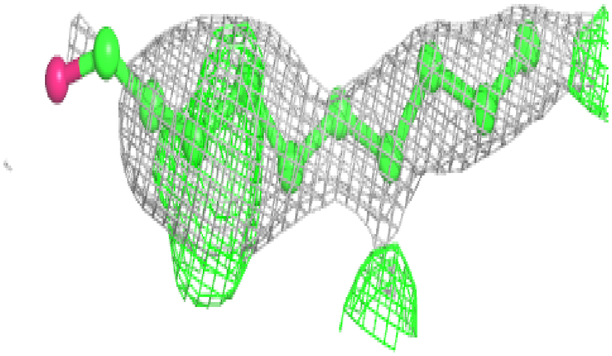


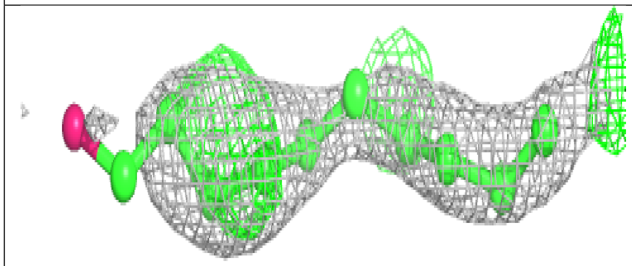


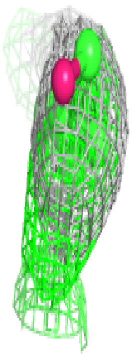


Electron density around DMU A 617:

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

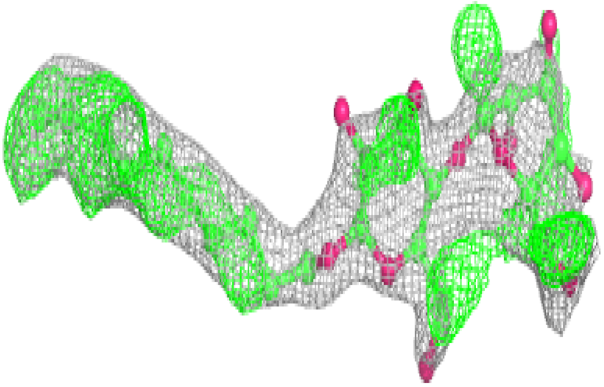


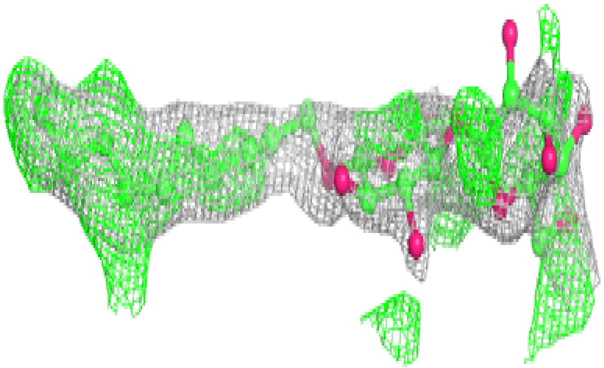


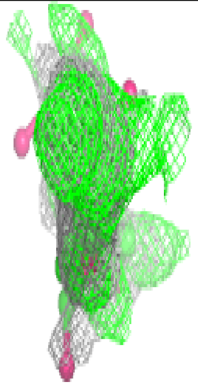


Electron density around DMU P 318:

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

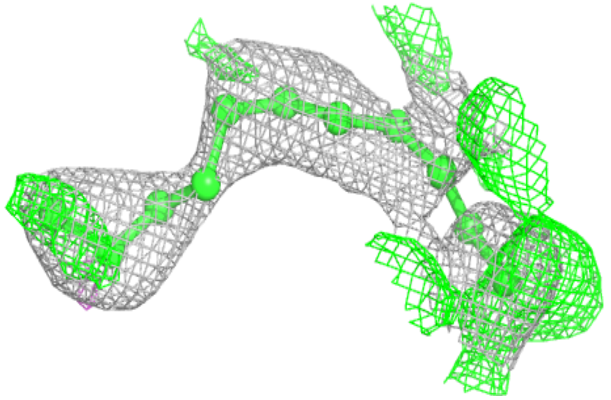


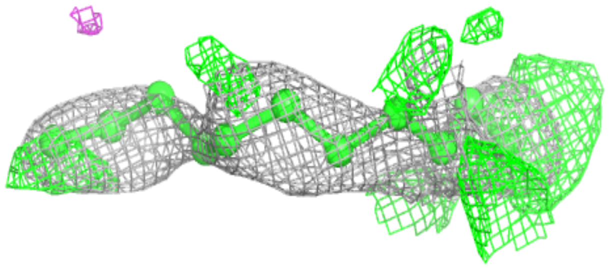


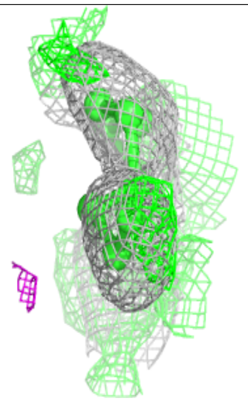


Electron density around LFA P 311:

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

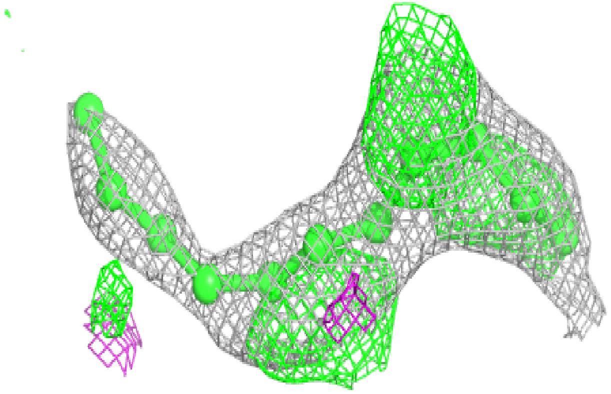


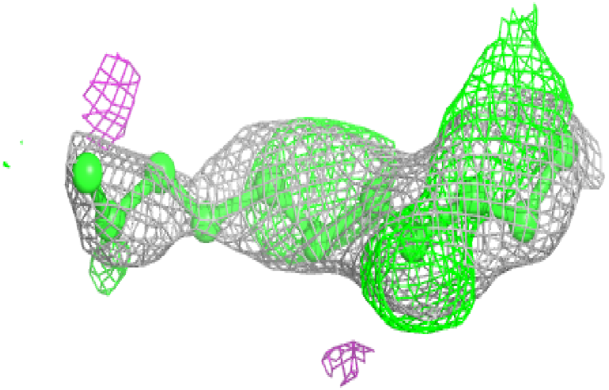


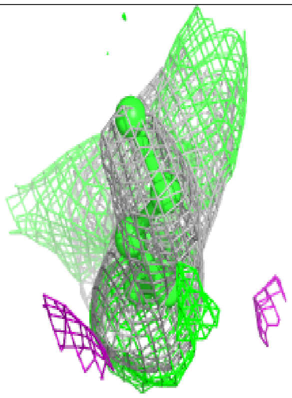


Electron density around LFA P 308:

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

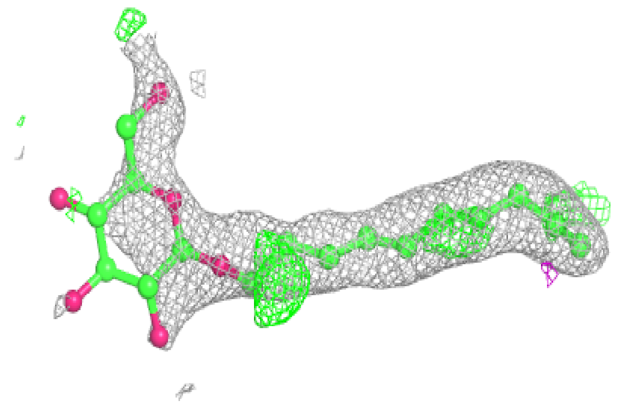


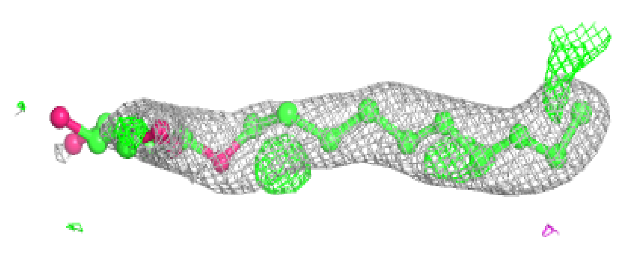


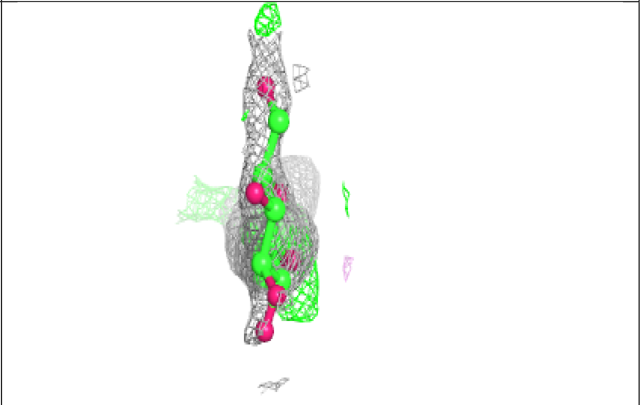


Electron density around DMU B 303:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

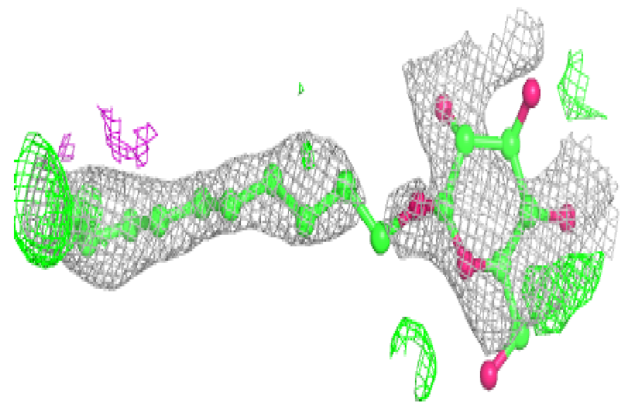


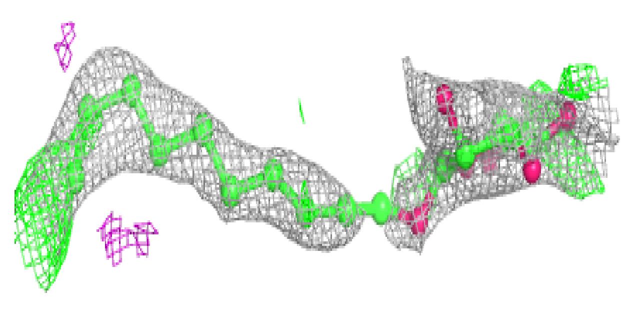


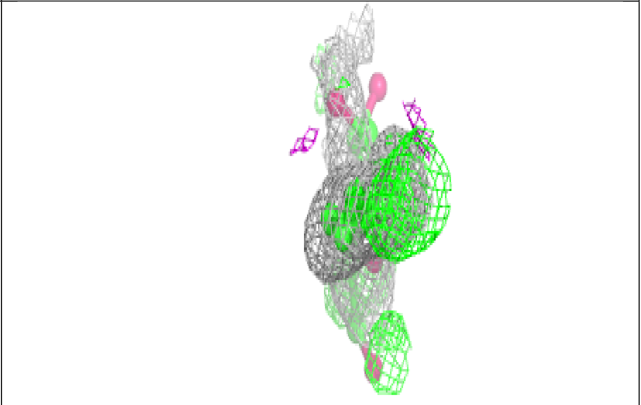


Electron density around DMU O 303:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

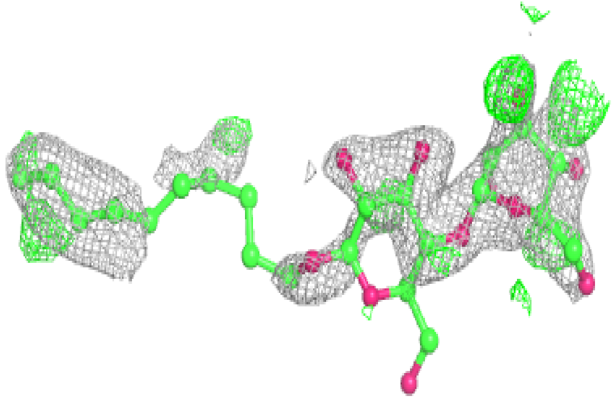


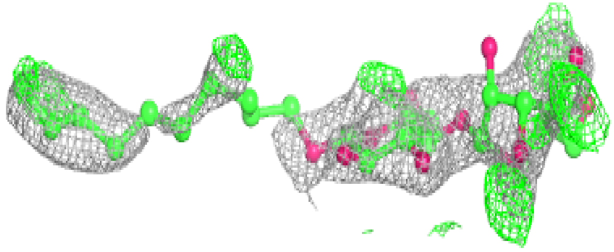




Electron density around DMU P 319:

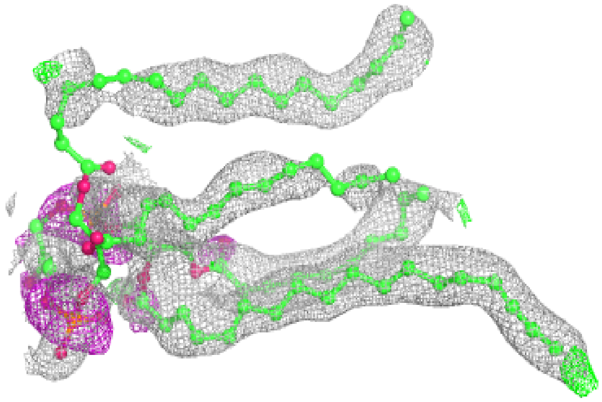
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

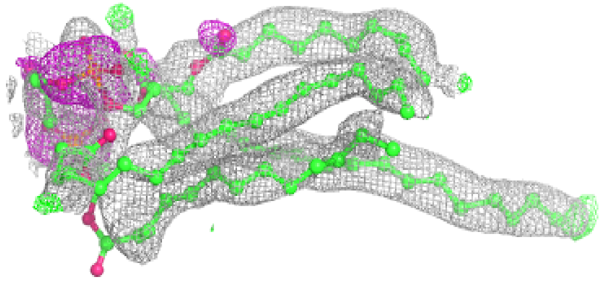


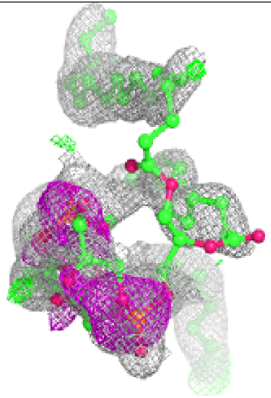


Electron density around CDL C 304:

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

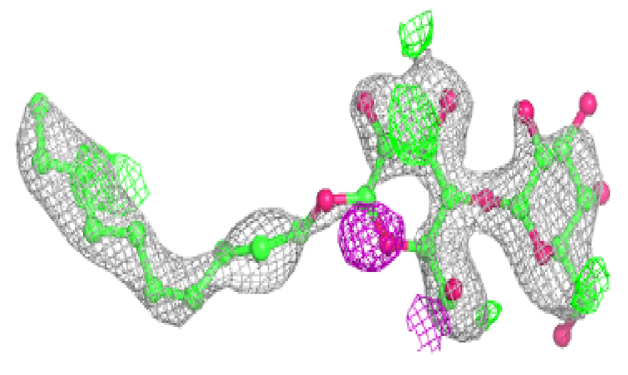


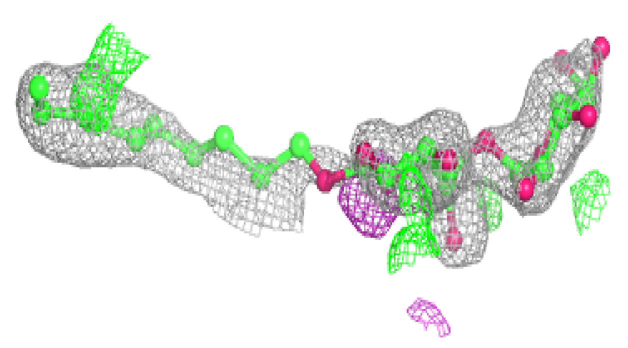


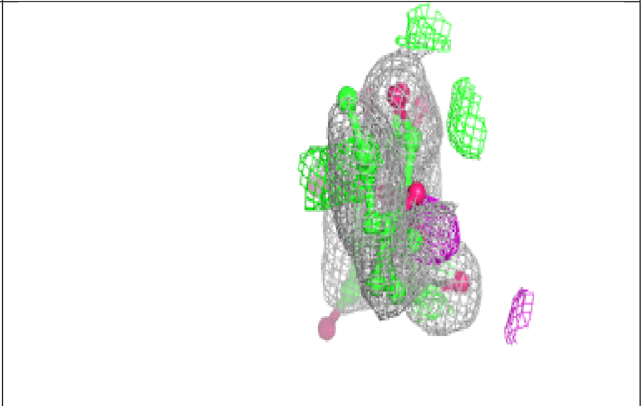


Electron density around DMU C 324:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

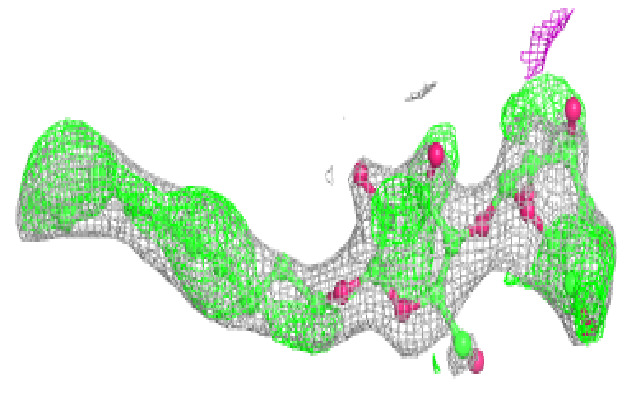


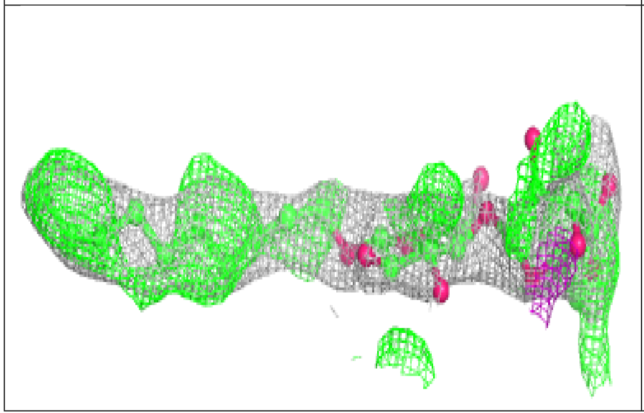


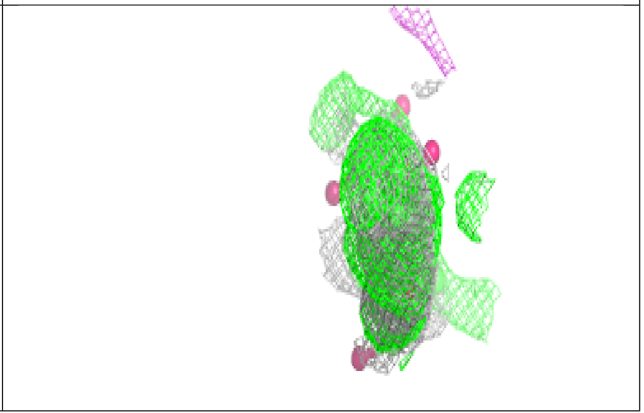


Electron density around DMU C 318:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

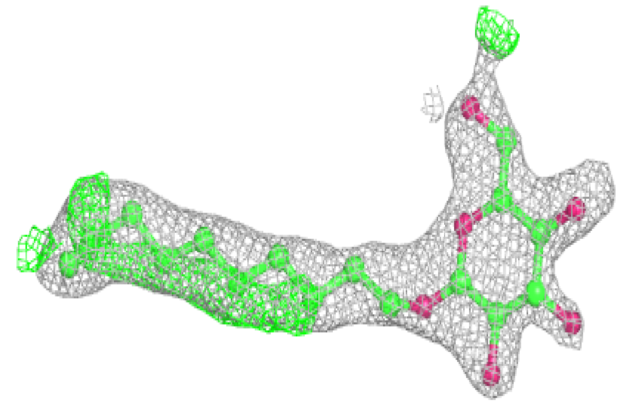


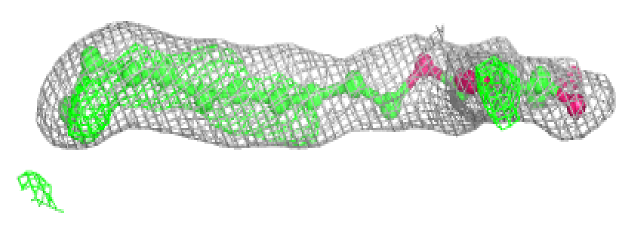


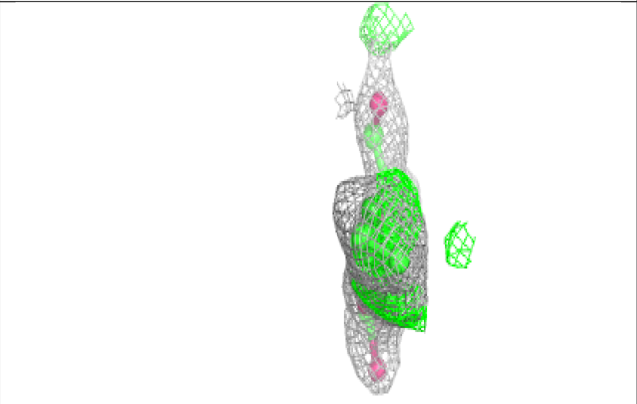


Electron density around DMU O 308:

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

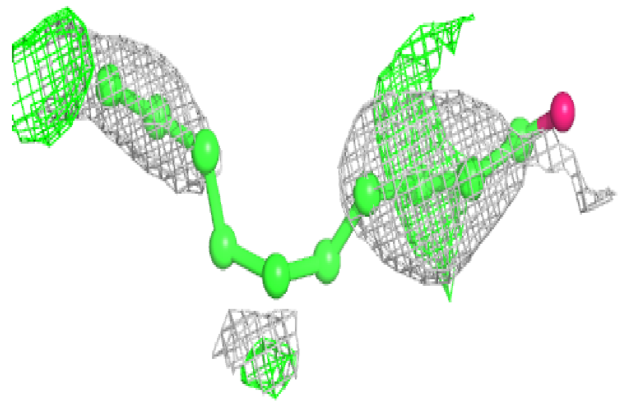


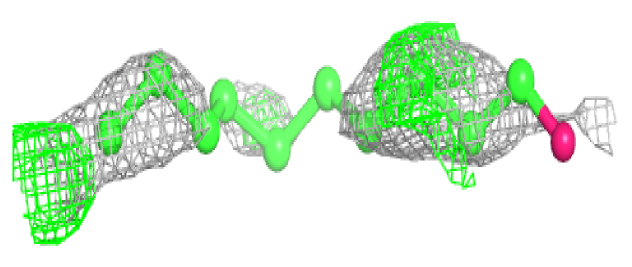


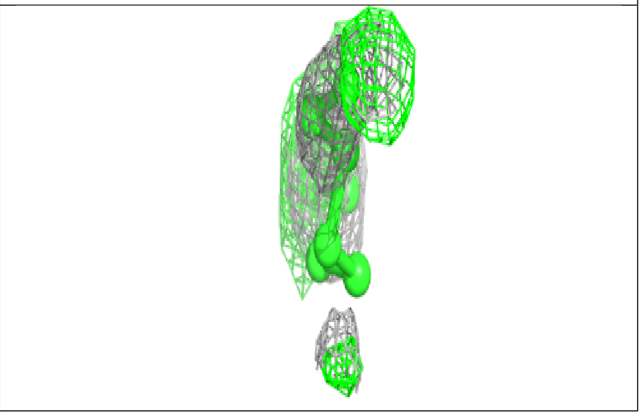


Electron density around DMU N 602:

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

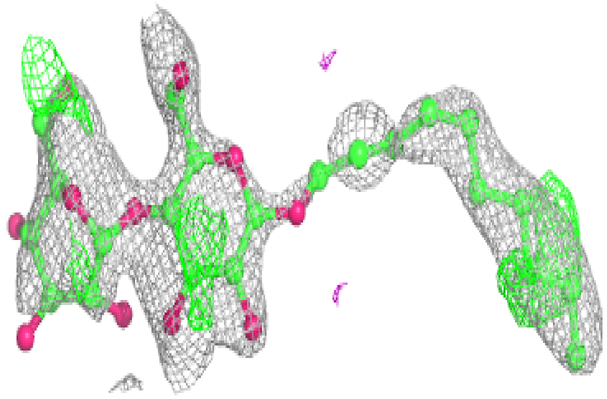


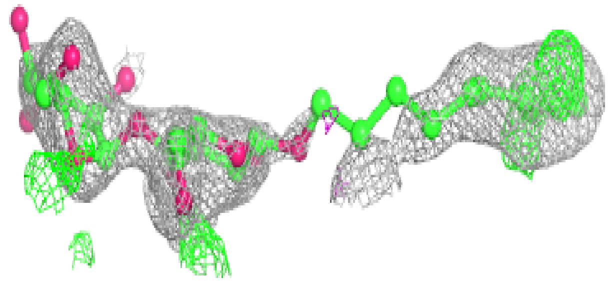


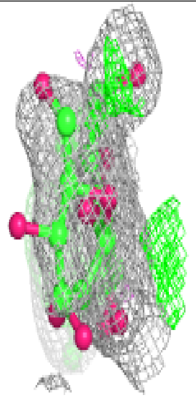


Electron density around DMU P 324:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

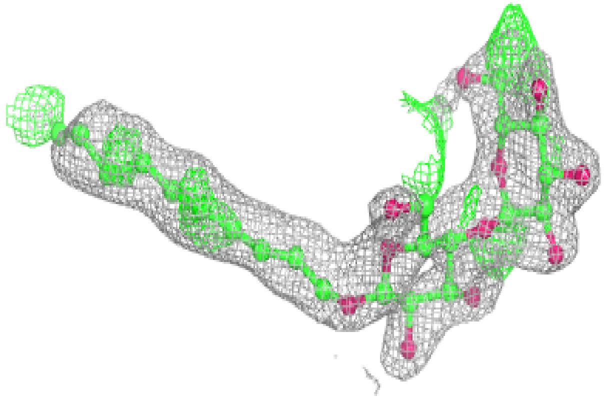


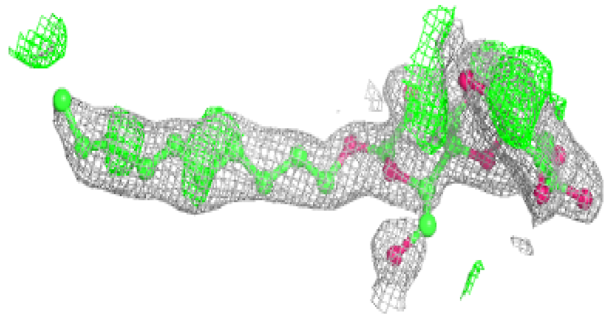


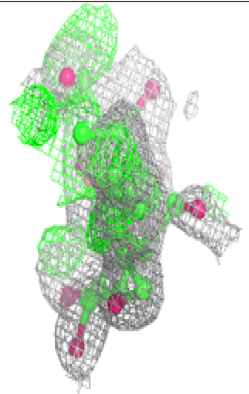


Electron density around DMU Q 201:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

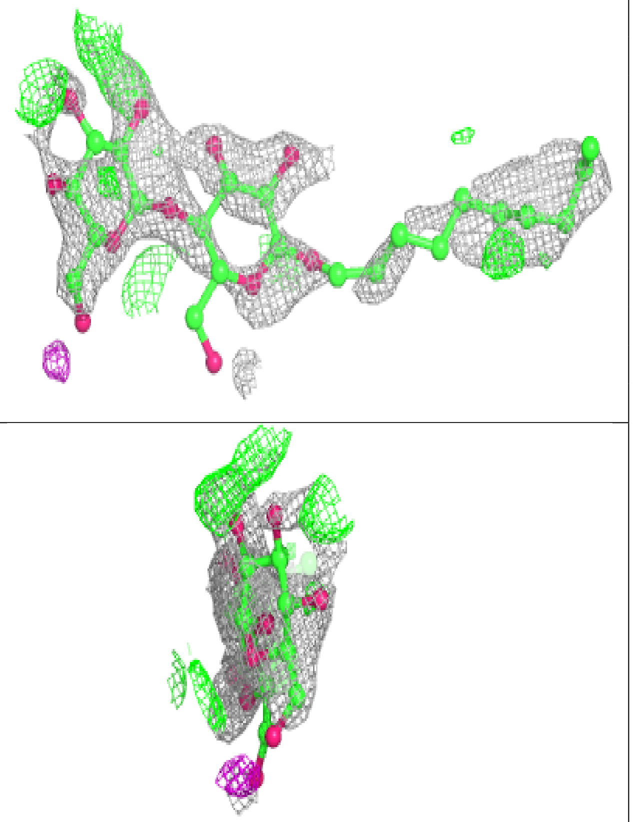






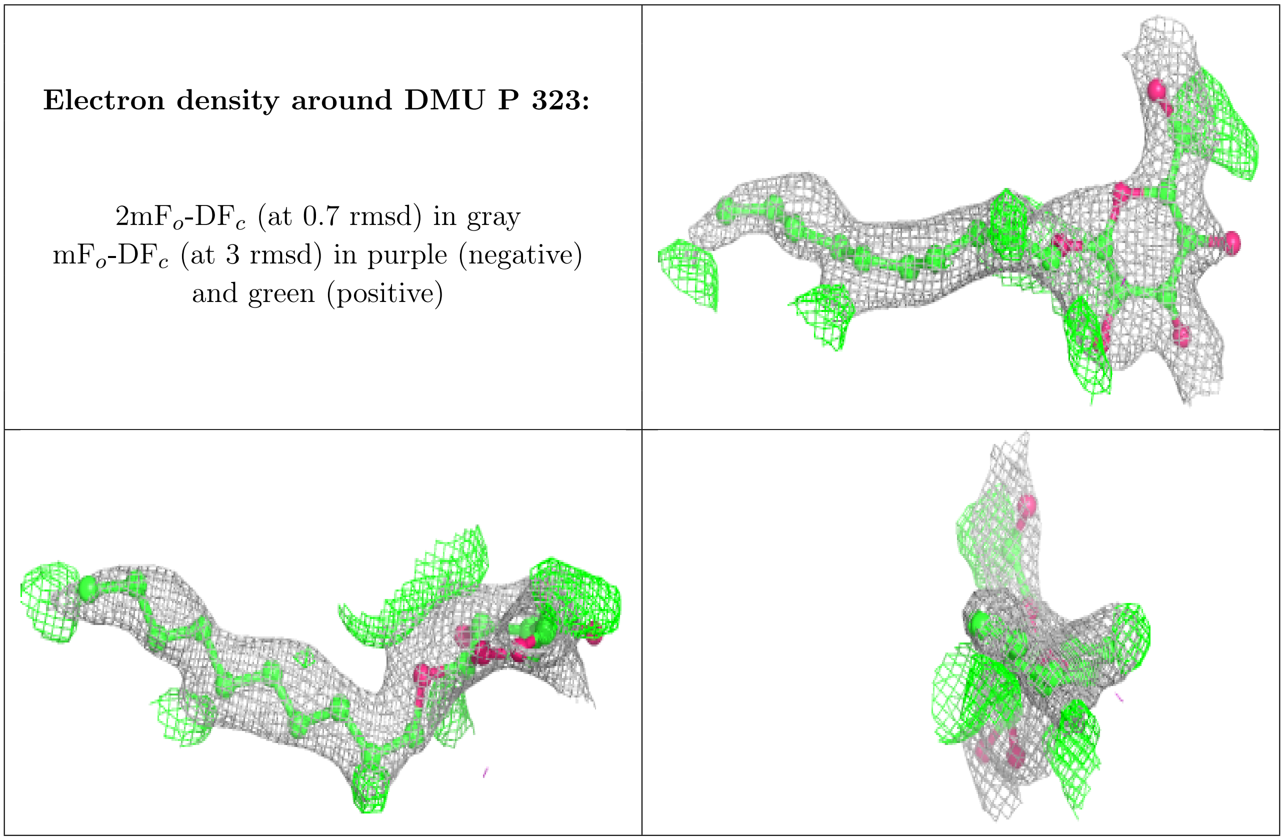
Electron density around DMU C 319:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



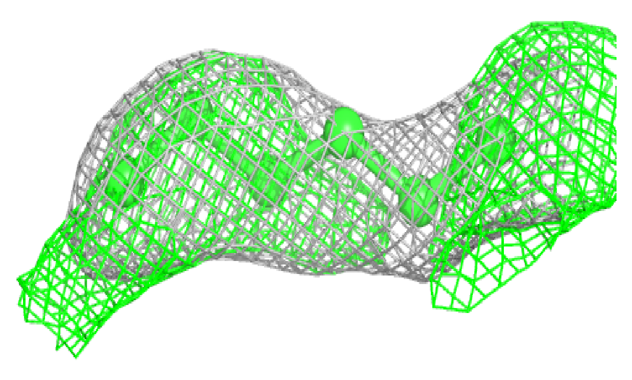
Electron density around DMU P 323:

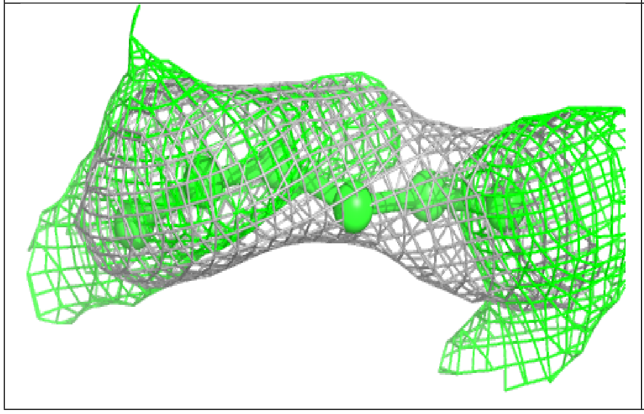
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

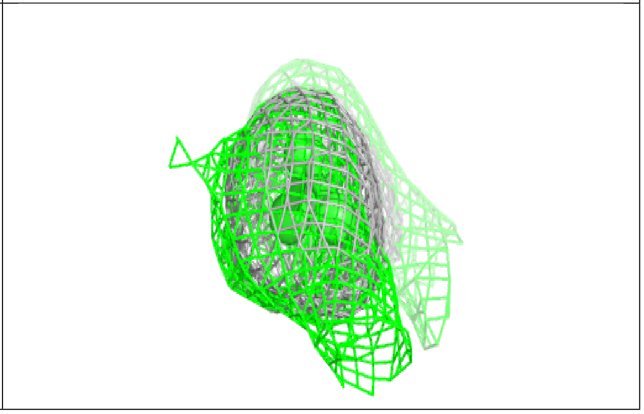


Electron density around LFA C 308:

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

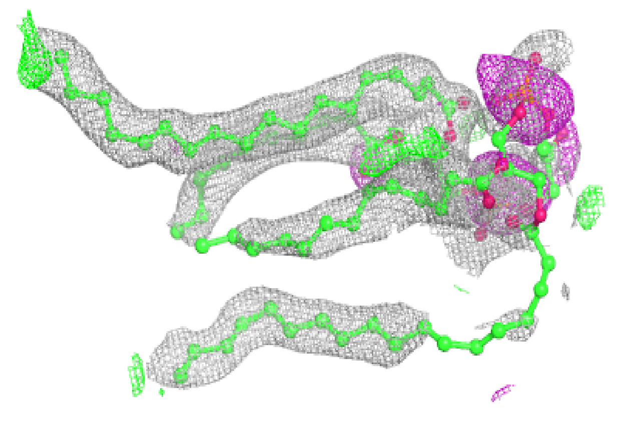


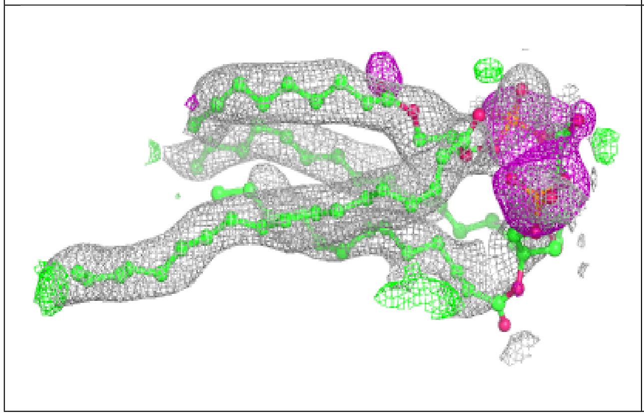


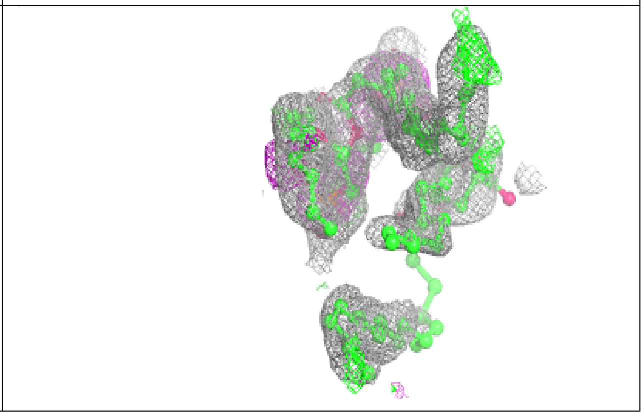


Electron density around CDL P 305:

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

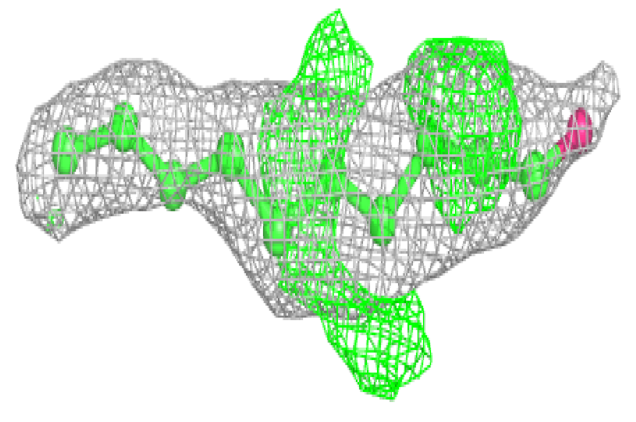


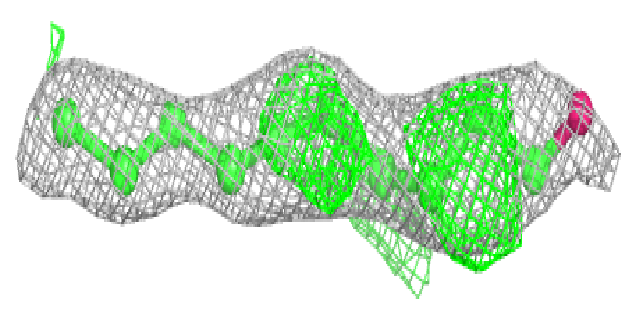


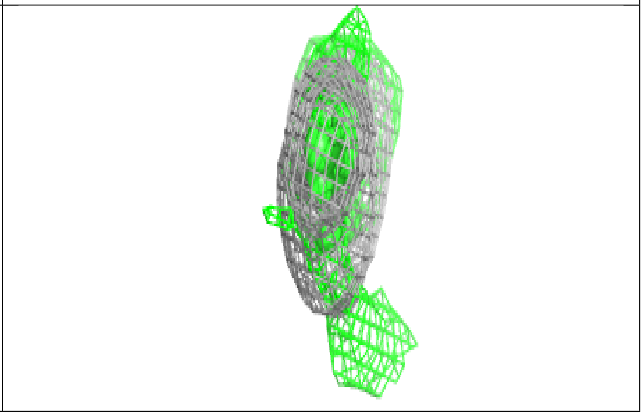


Electron density around DMU A 615:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

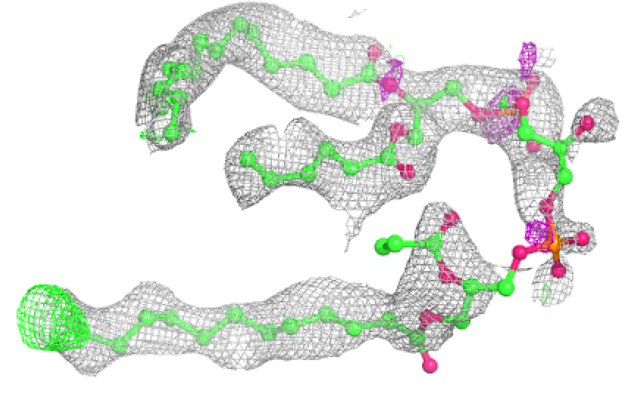


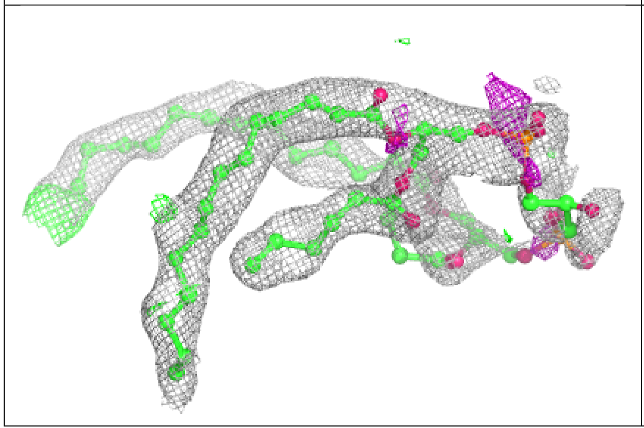


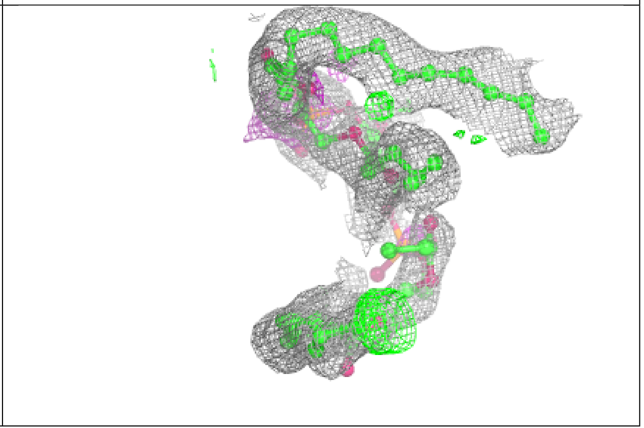


Electron density around CDL O 304:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

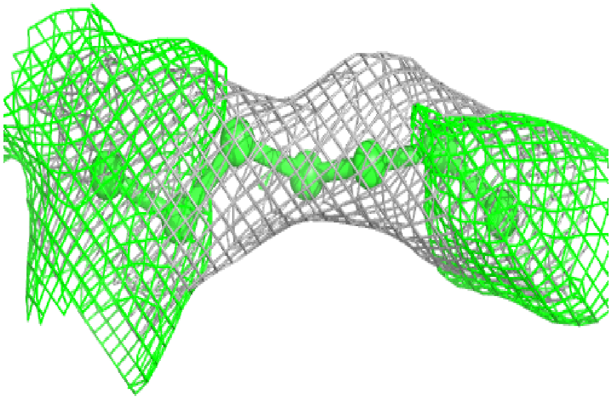


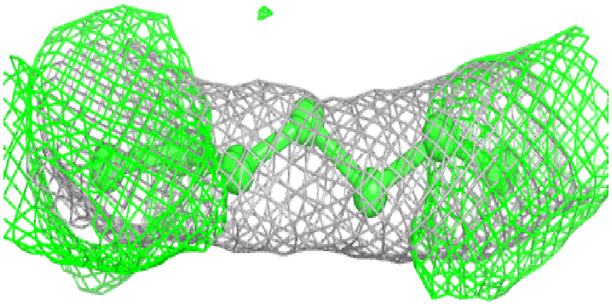


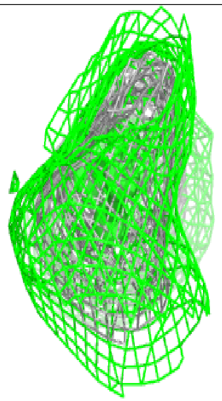


Electron density around DMU A 609:

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

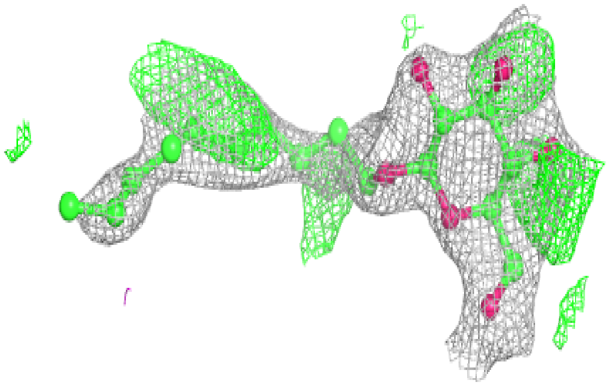


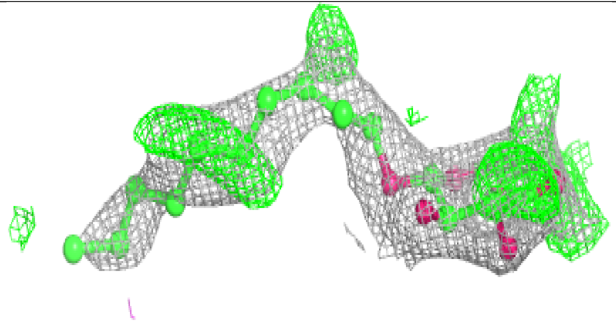




Electron density around DMU C 323:

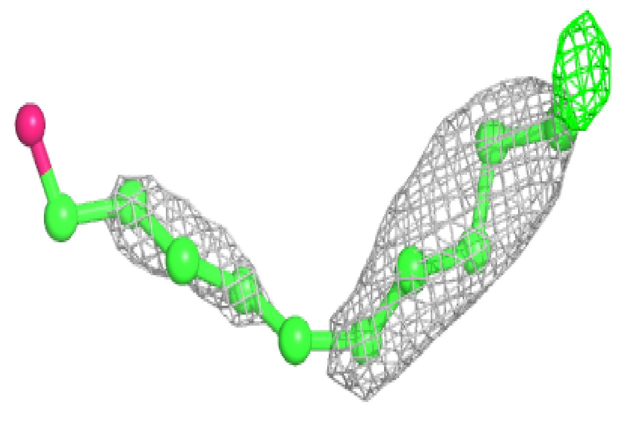
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

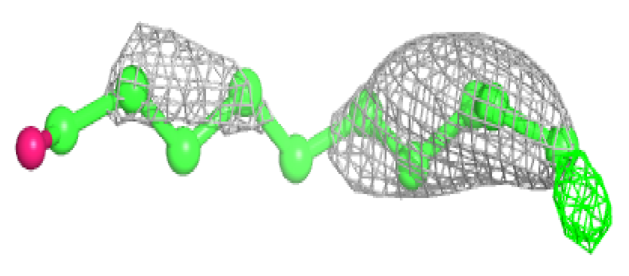


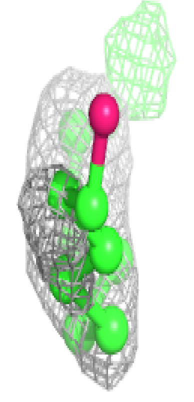


Electron density around DMU W 101:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

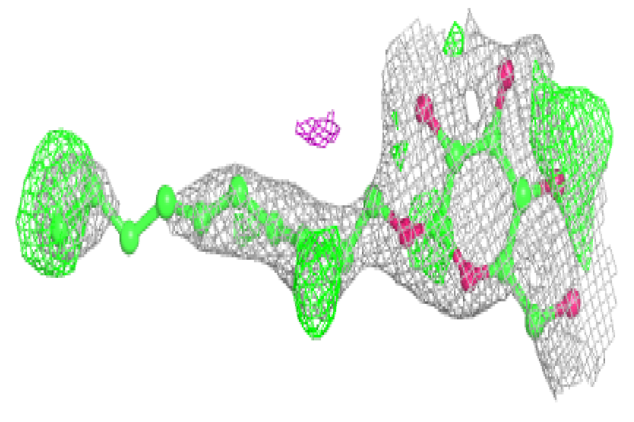


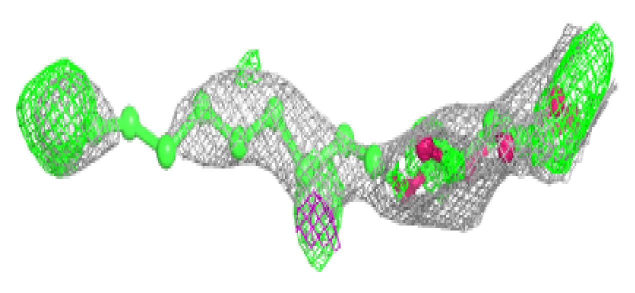


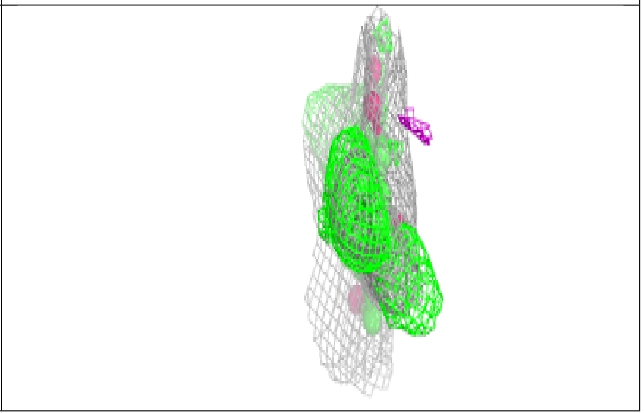


Electron density around DMU Y 102:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

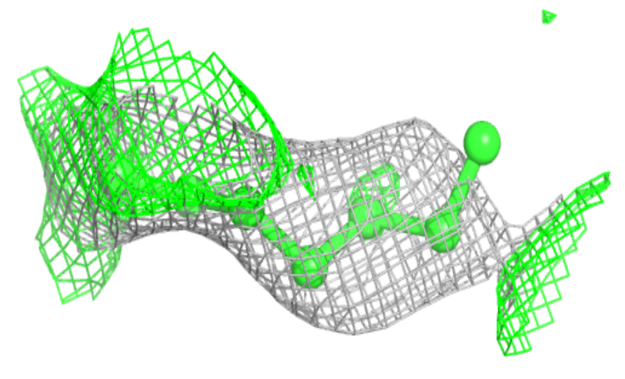


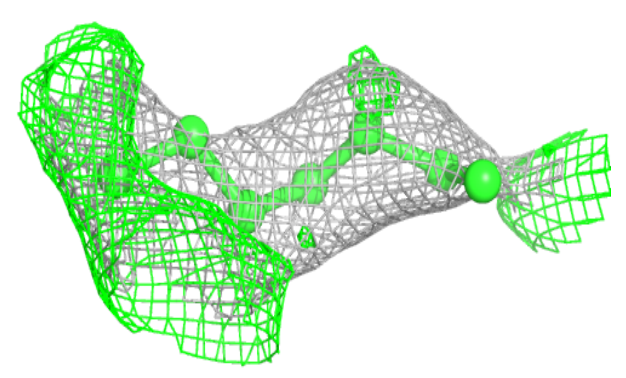


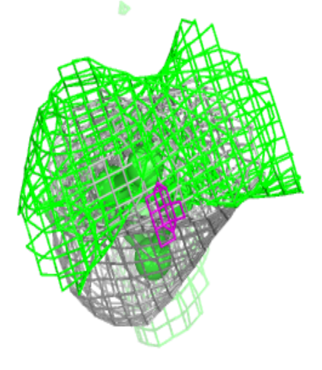


Electron density around DMU P 316:

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

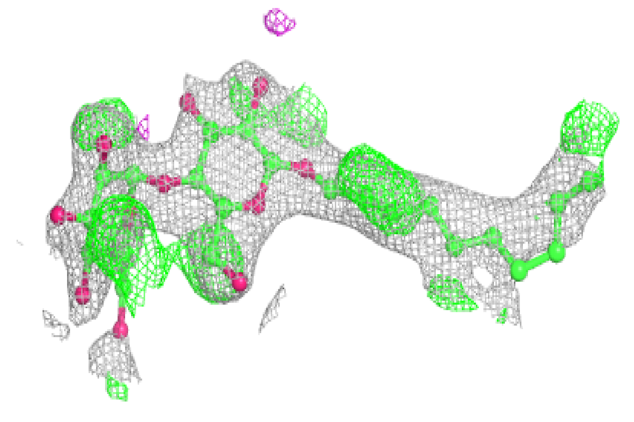


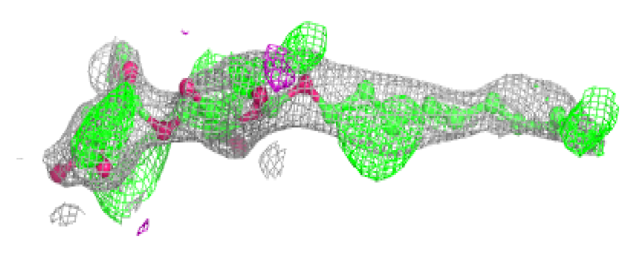


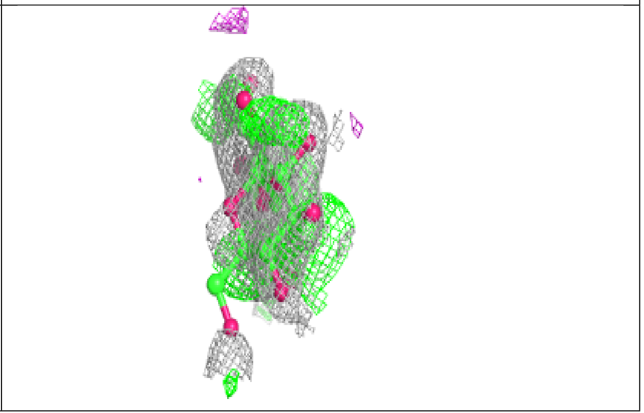


Electron density around DMU P 315:

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

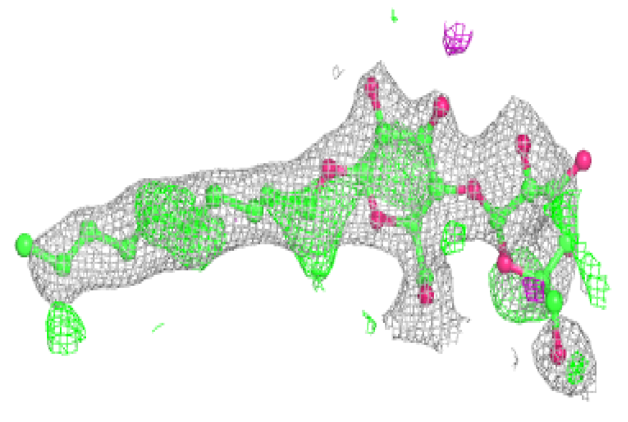


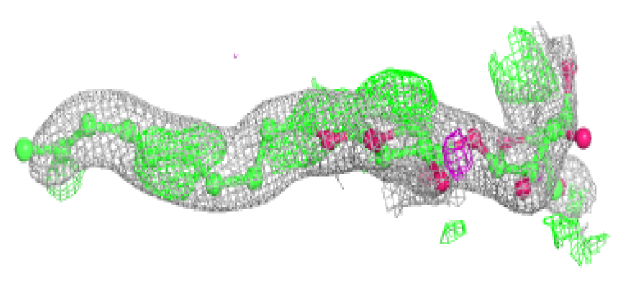


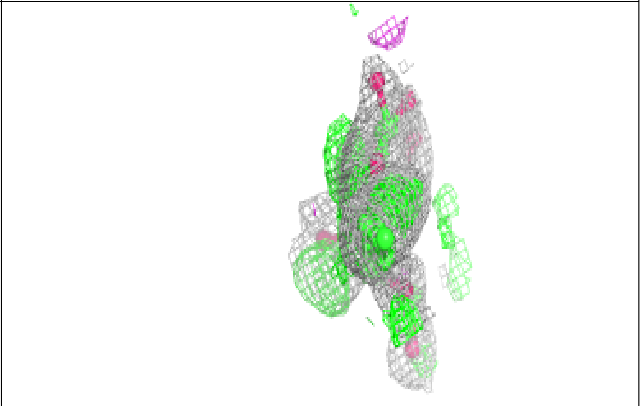


Electron density around DMU N 612:

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

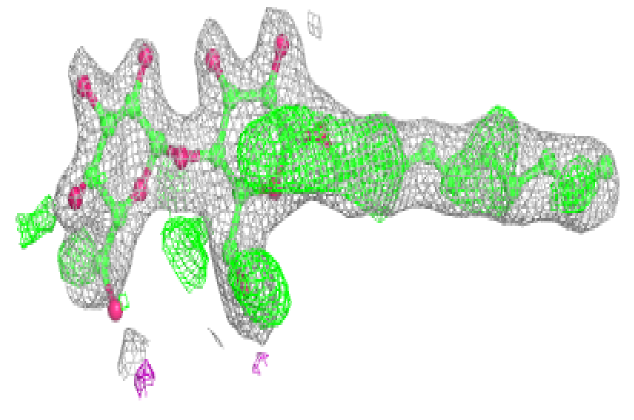


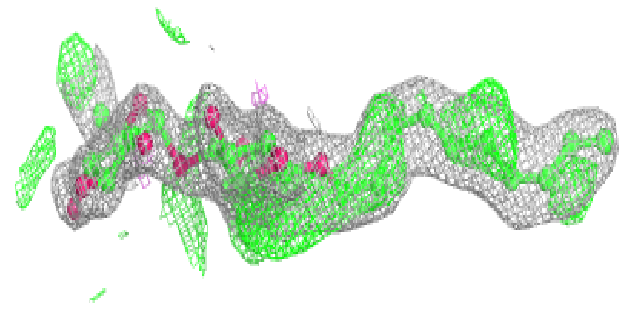


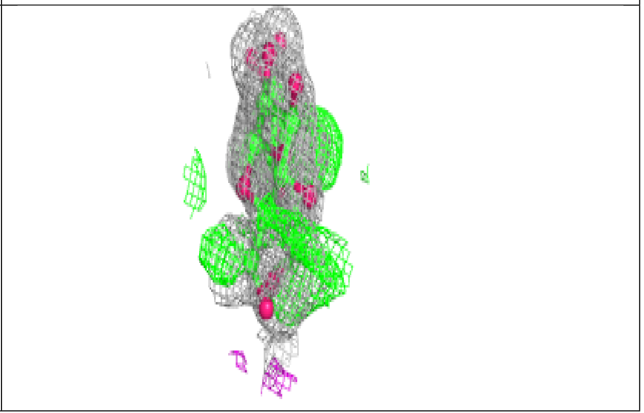


Electron density around DMU A 610:

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

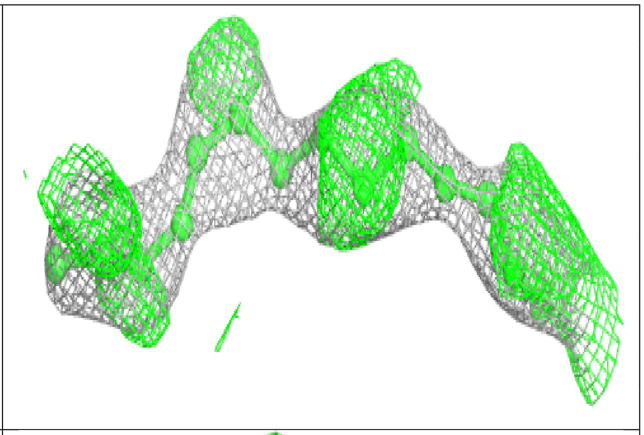


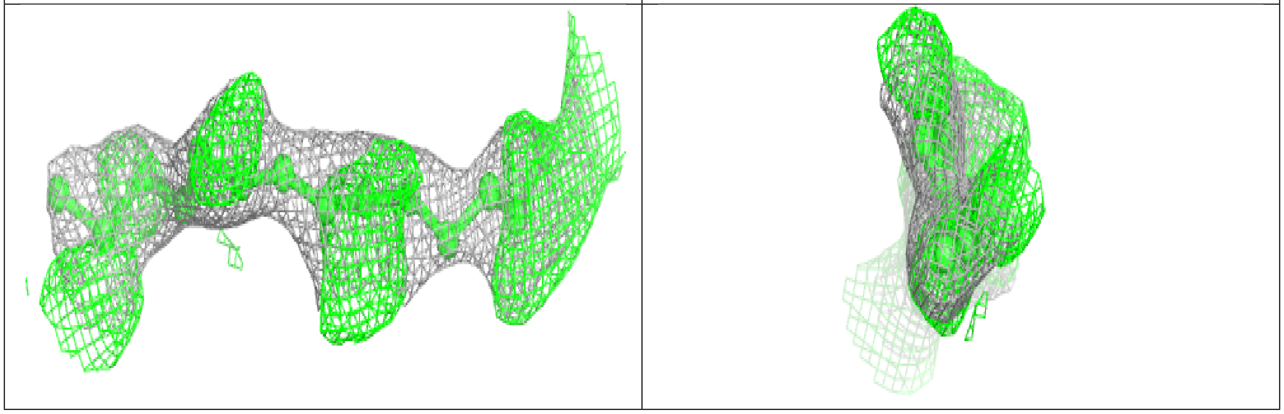




Electron density around LFA T 102:

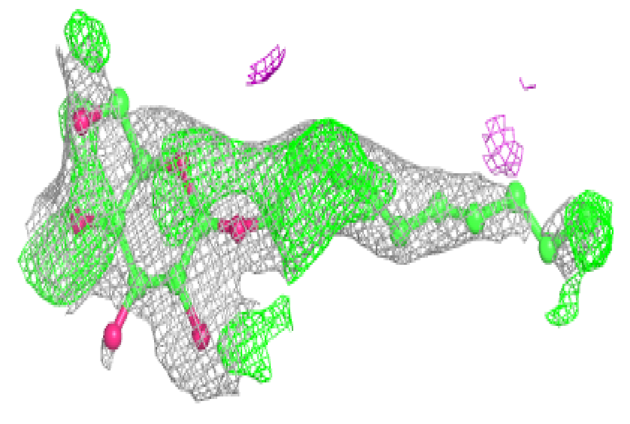
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

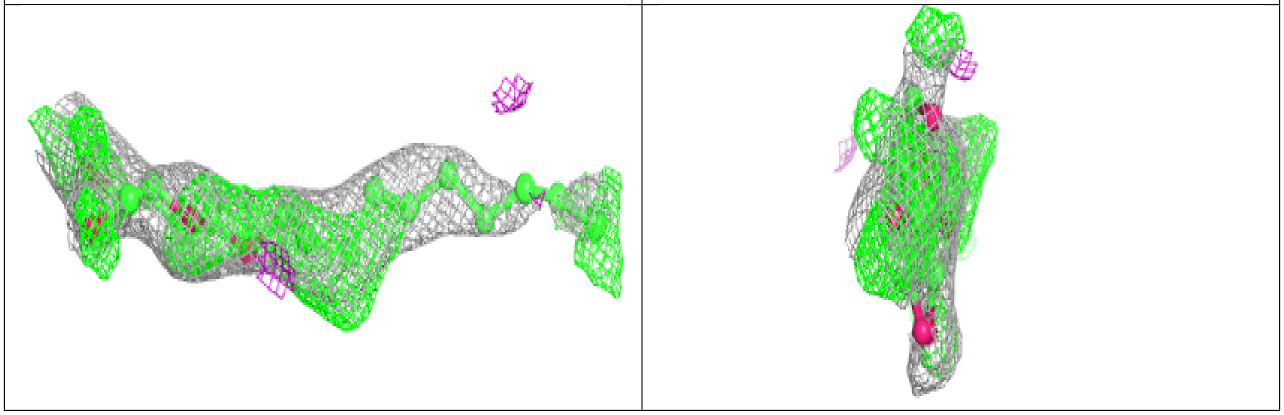




Electron density around DMU L 102:

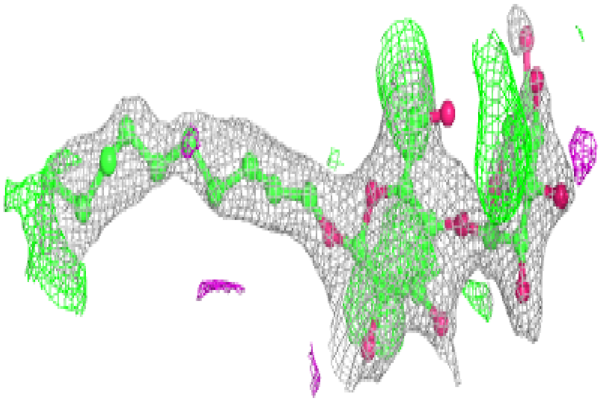
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

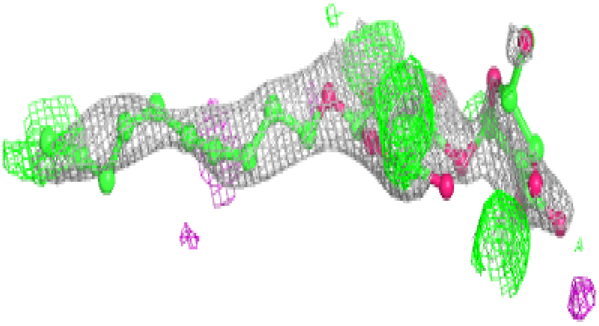


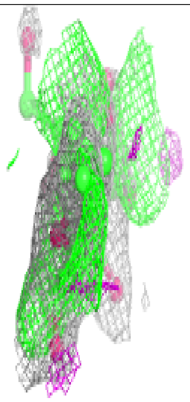


Electron density around DMU C 315:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

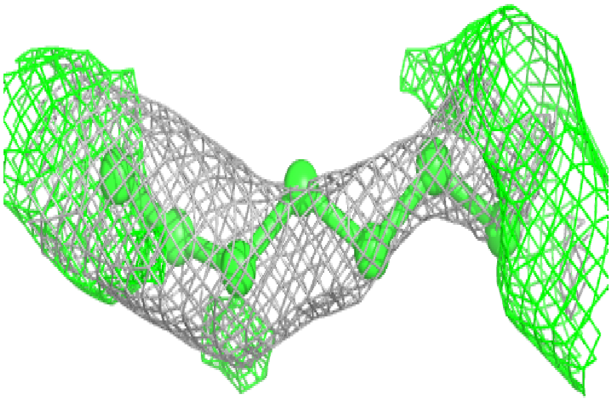


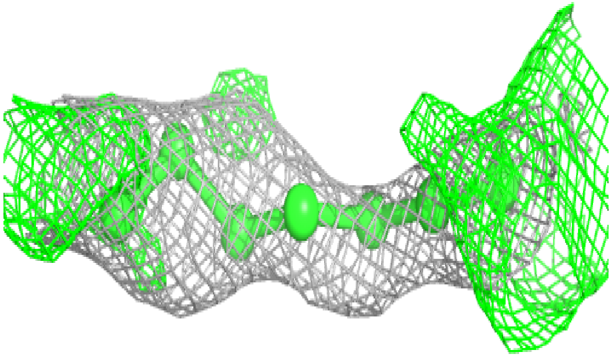


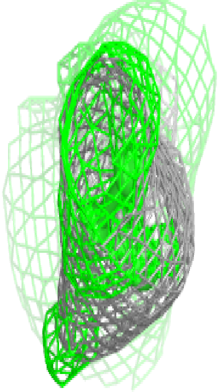


Electron density around DMU N 611:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

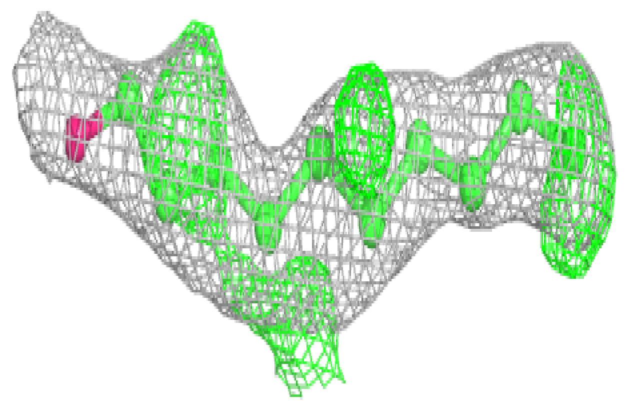


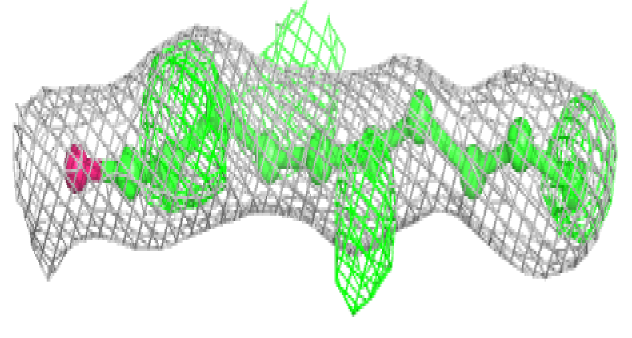


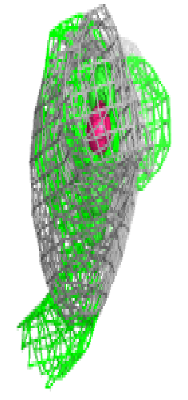


Electron density around DMU O 307:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

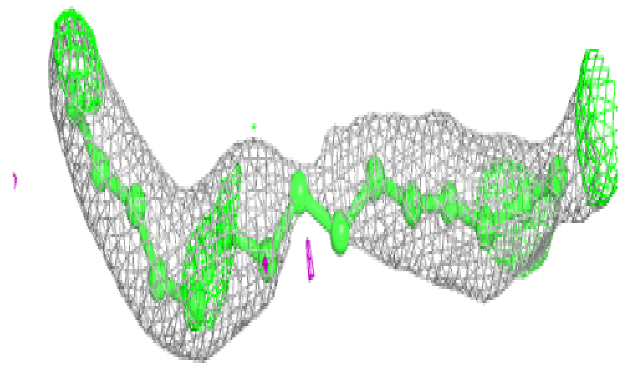


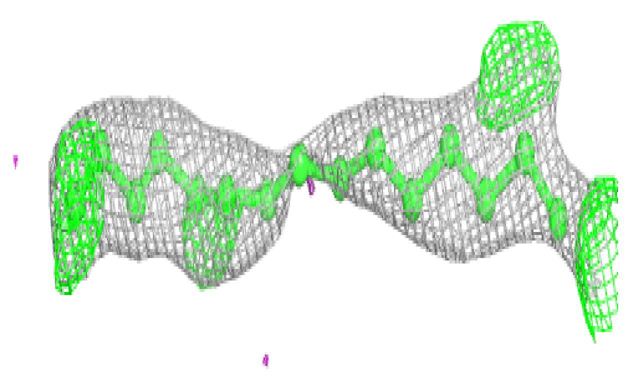


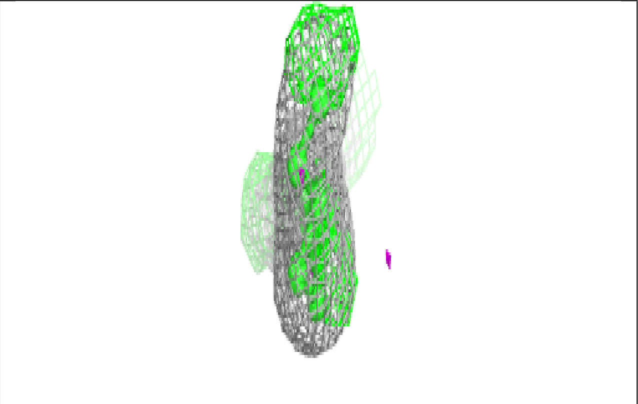


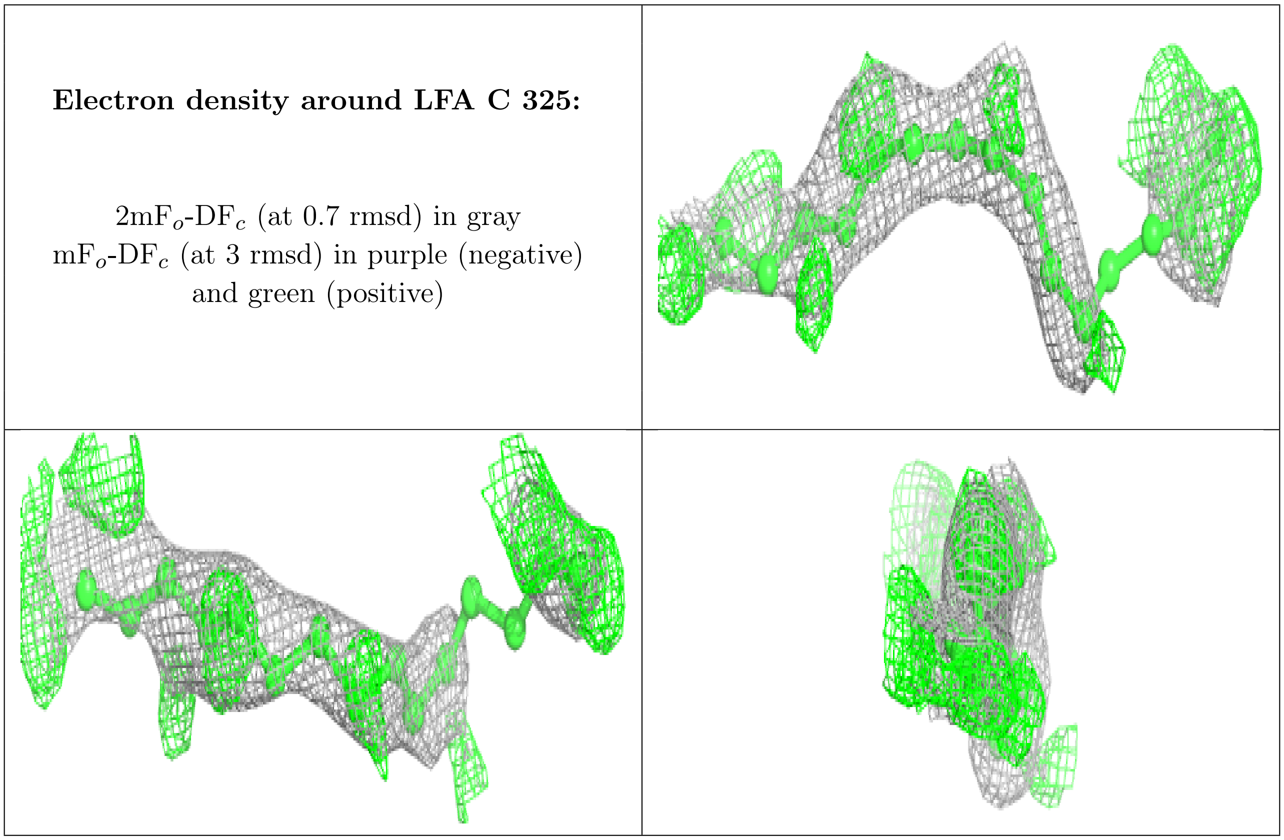
Electron density around LFA C 313:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







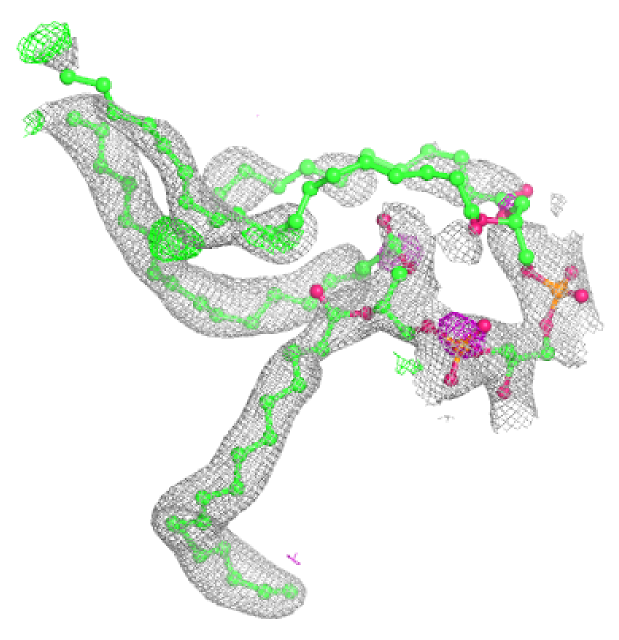


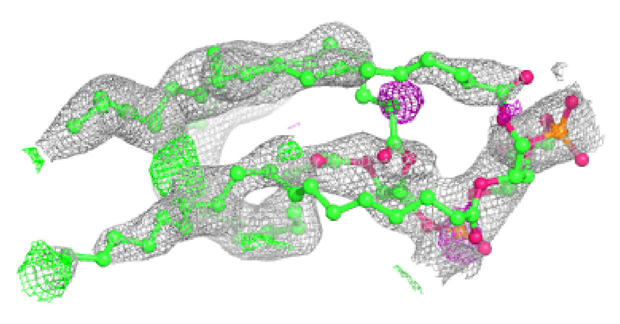
Electron density around LFA C 325:

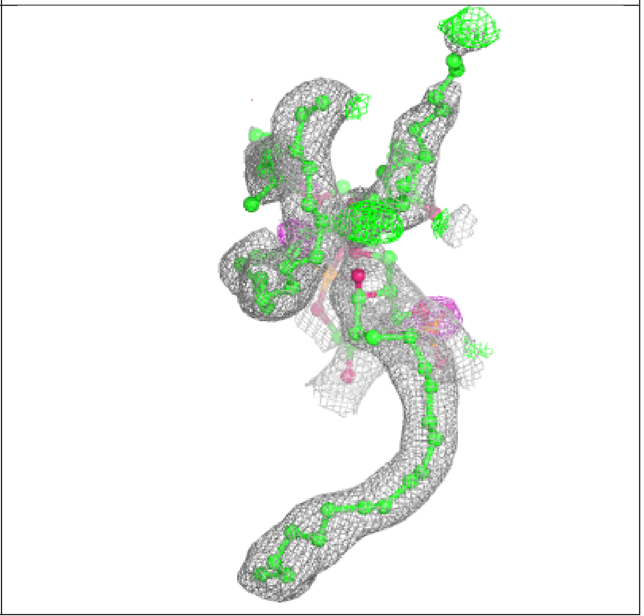
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around 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)

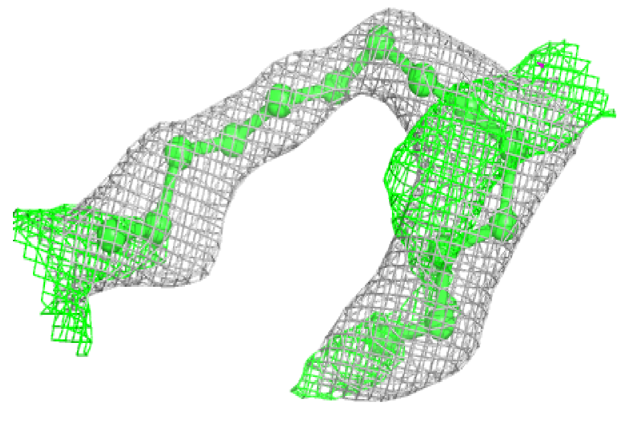


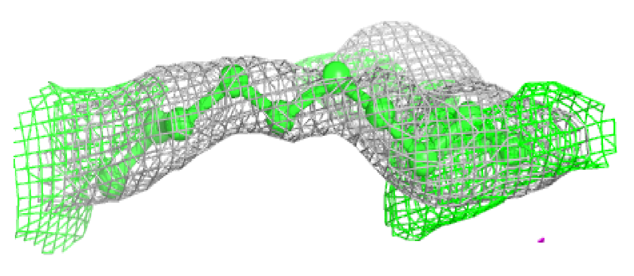


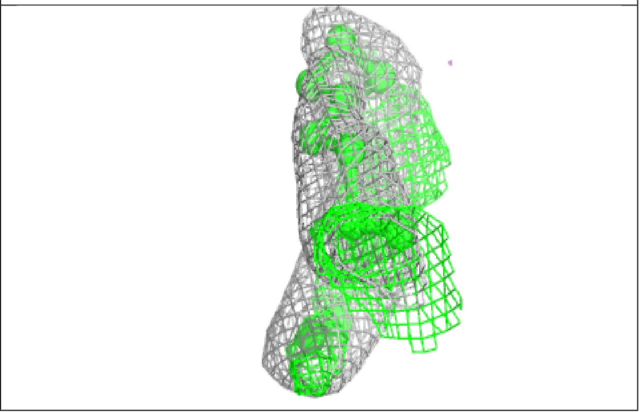


Electron density around LFA A 608:

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

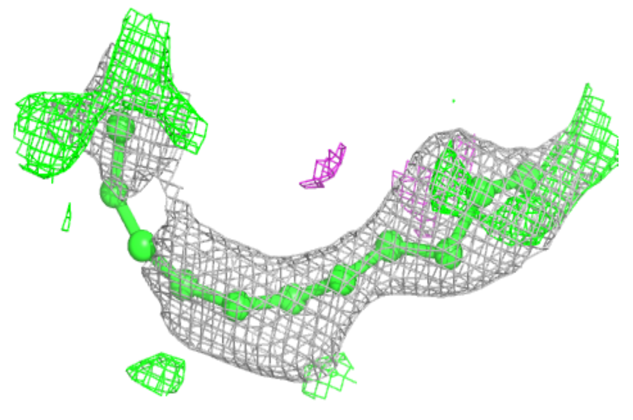


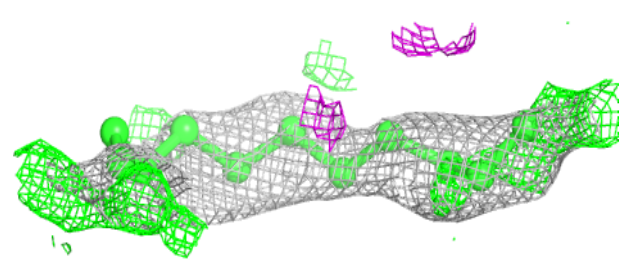


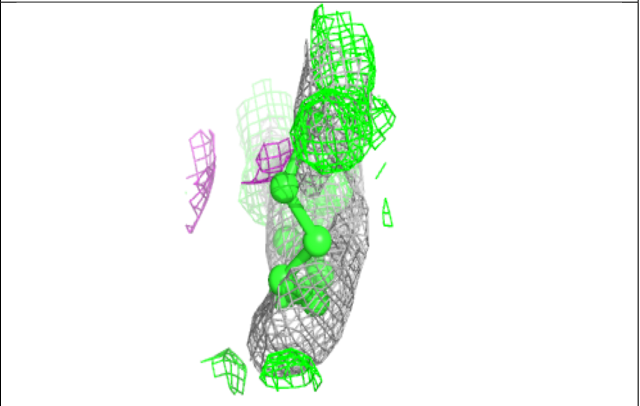


Electron density around LFA C 310:

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

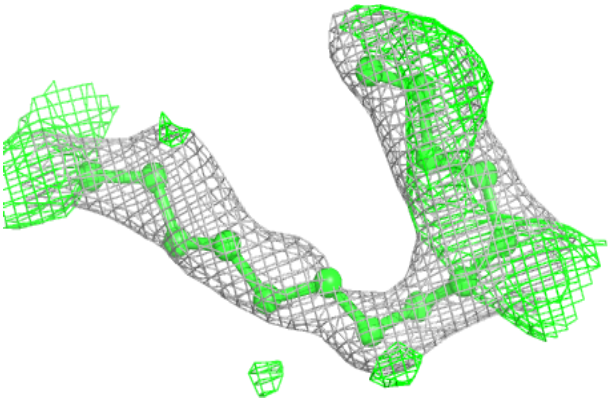


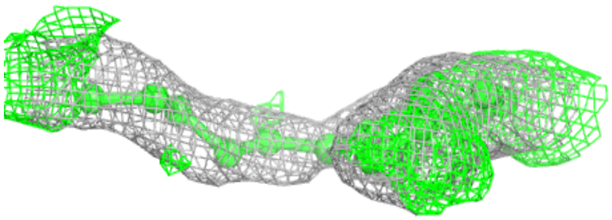


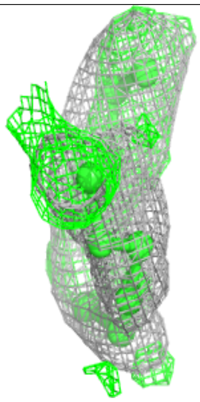


Electron density around LFA N 610:

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

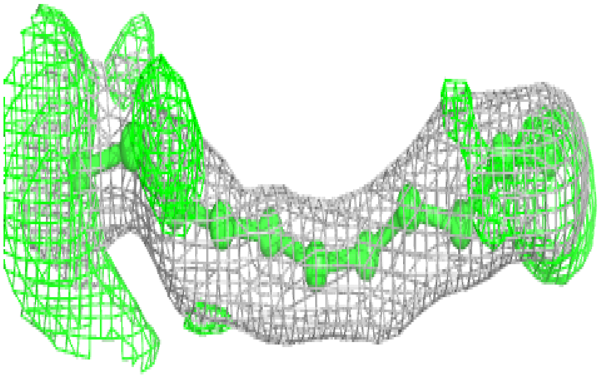


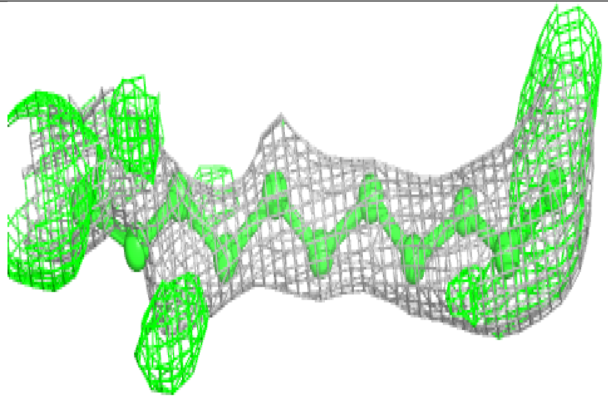


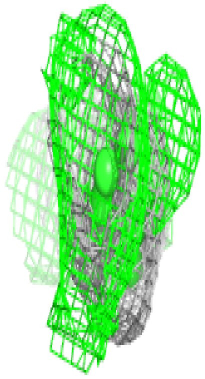


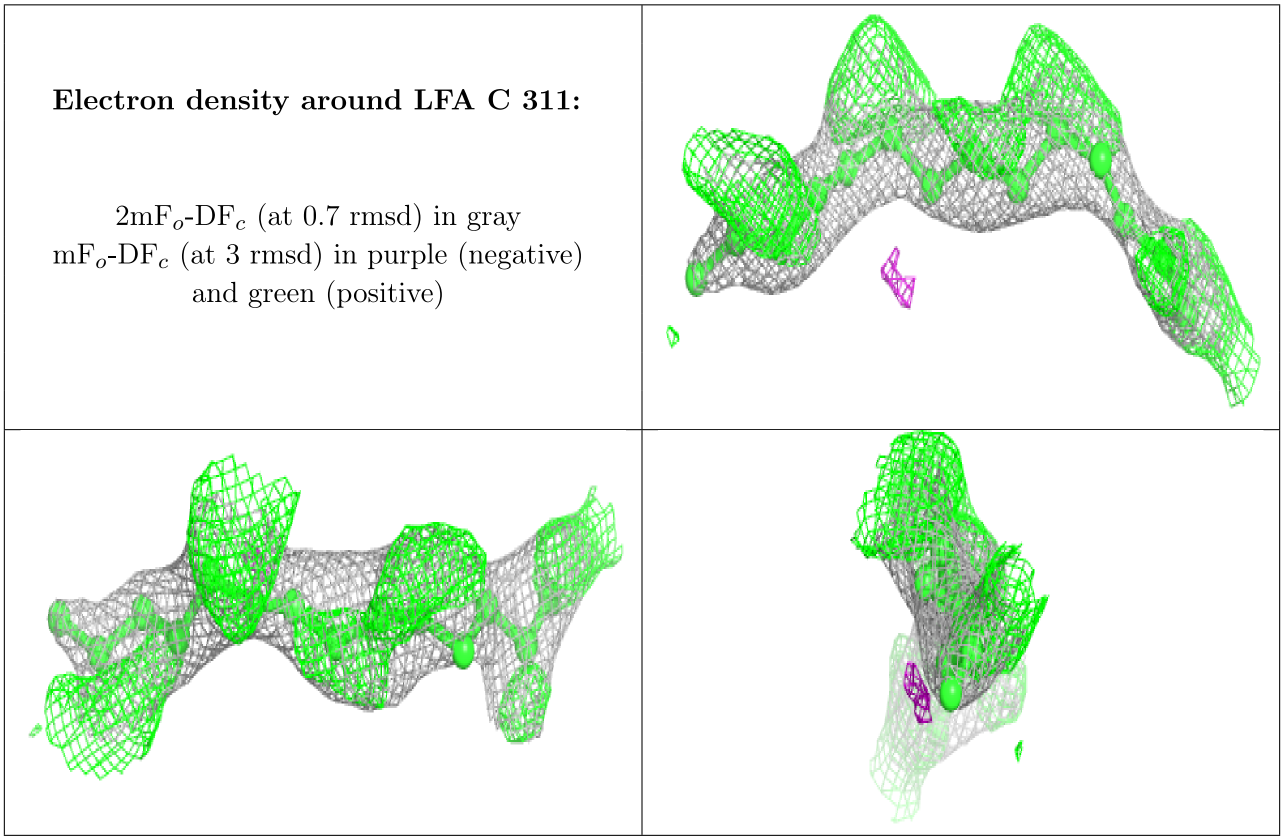
Electron density around LFA O 302:

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



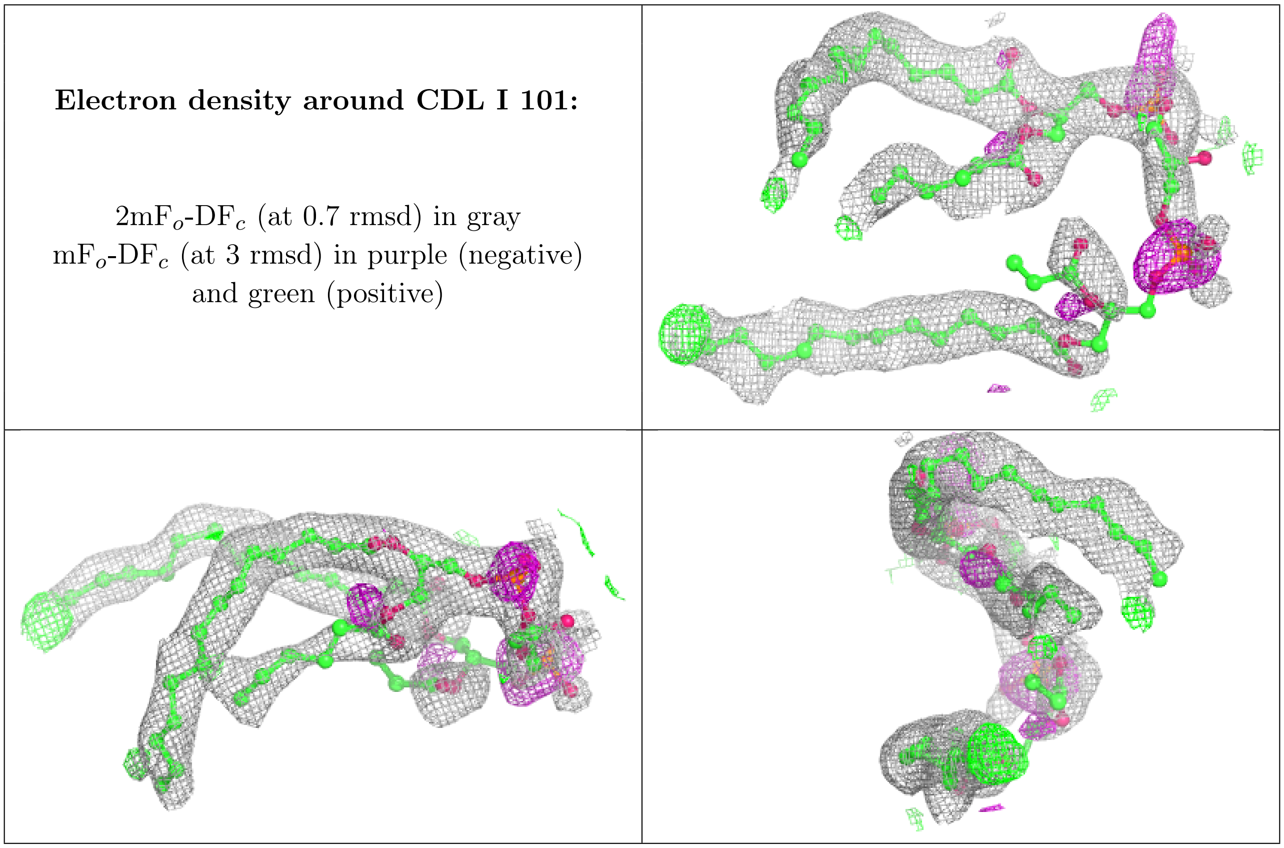






Electron density around LFA C 311:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

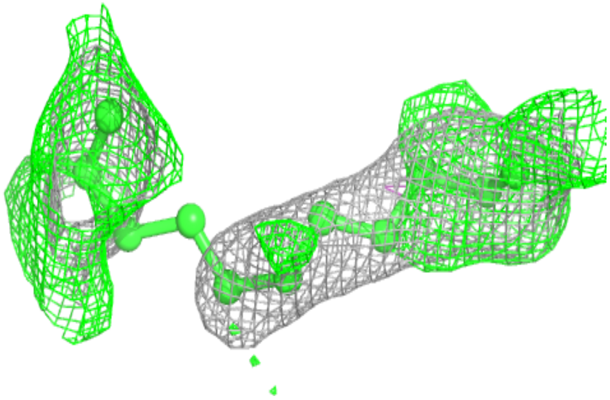


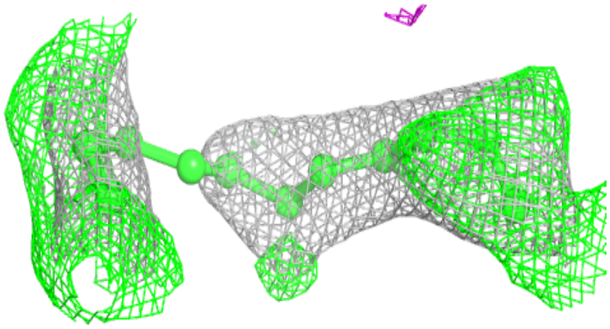
Electron density around CDL I 101:

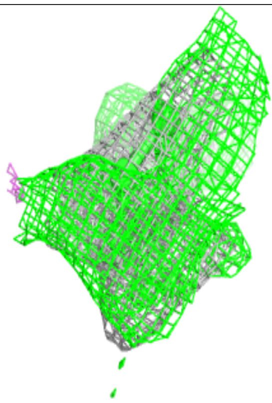
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around LFA C 312:

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

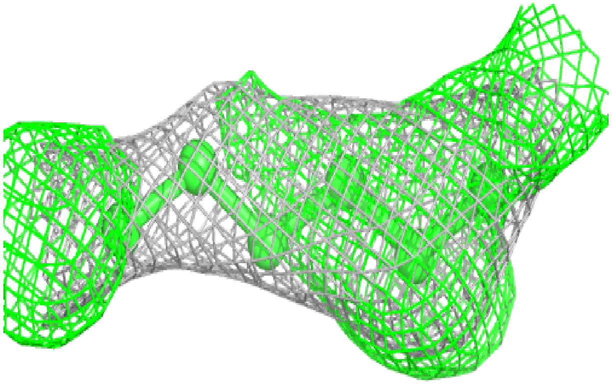


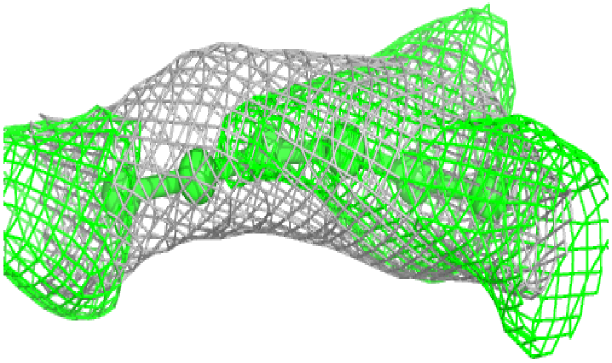


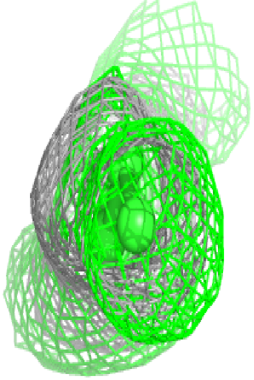


Electron density around LFA P 309:

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

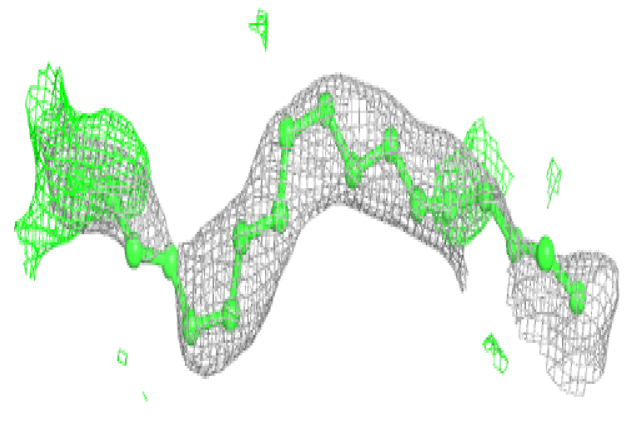


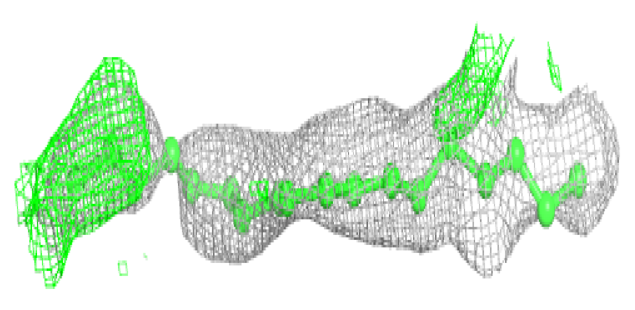


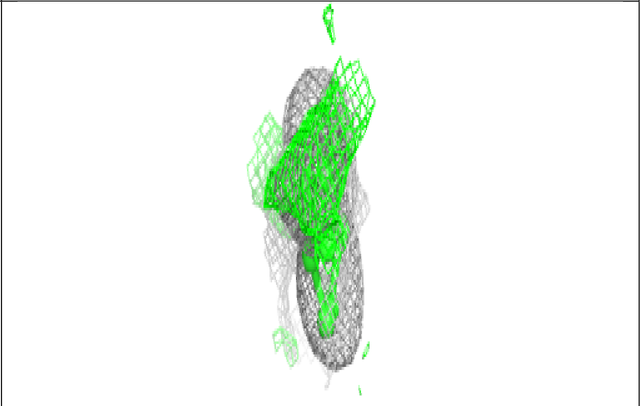


Electron density around LFA P 310:

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

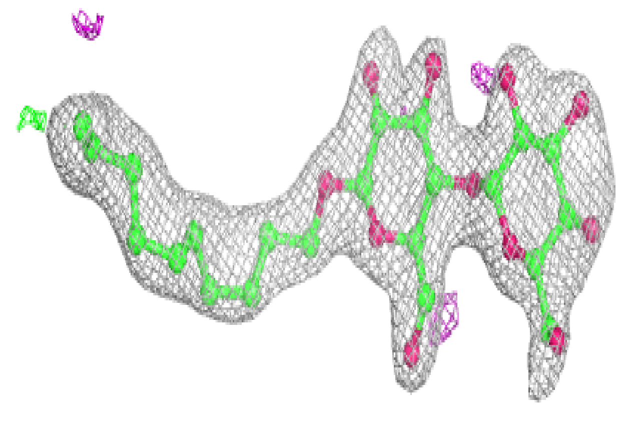


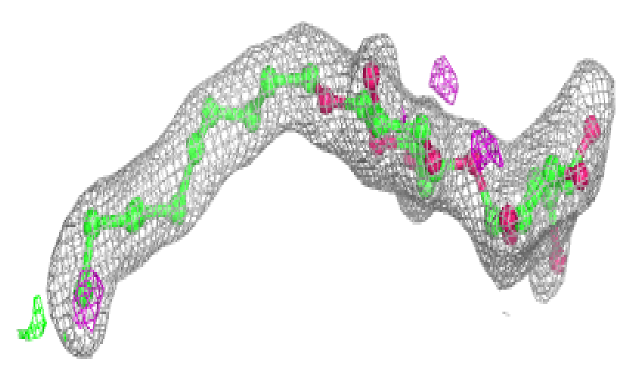


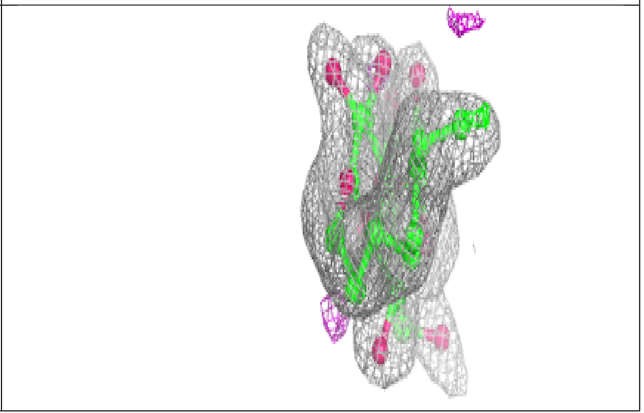


Electron density around DMU Z 101:

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

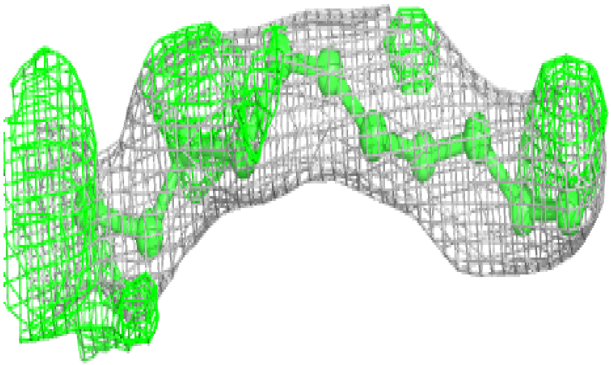


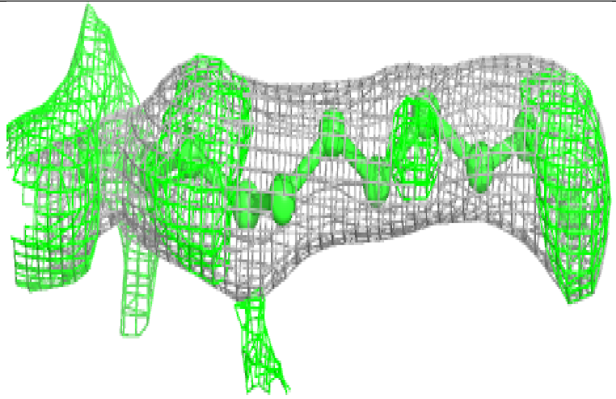


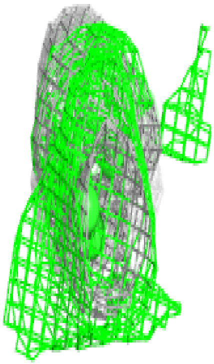


Electron density around LFA T 103:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

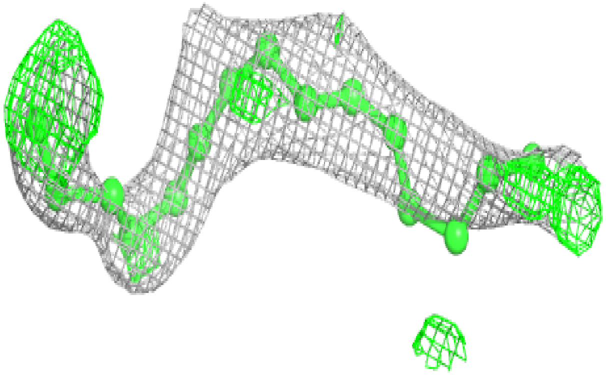


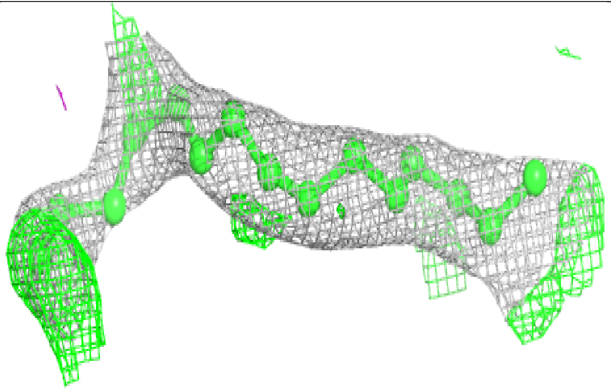


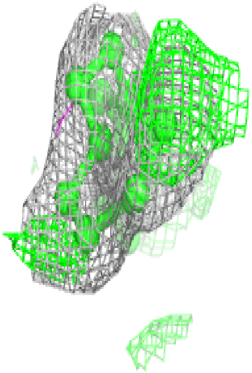


Electron density around LFA P 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

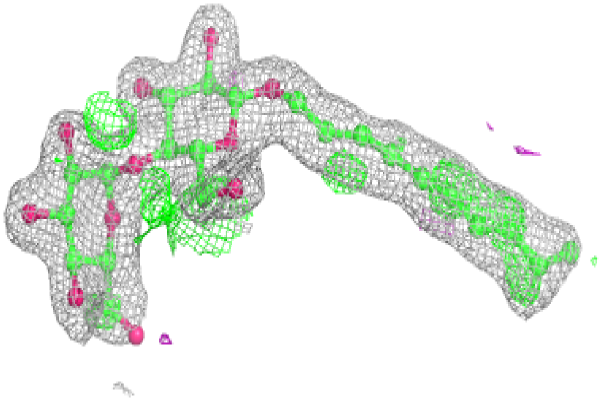


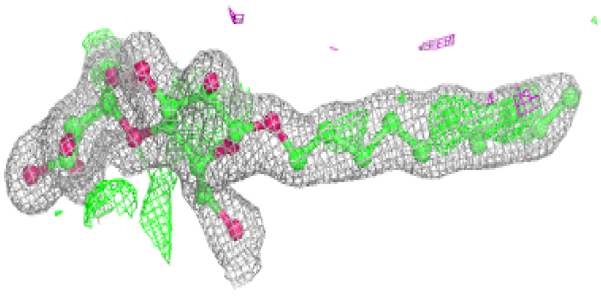


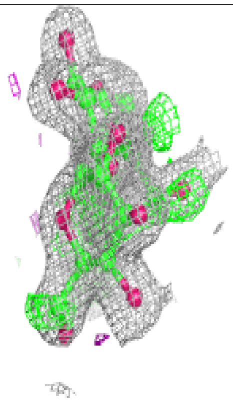


Electron density around DMU D 201:

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

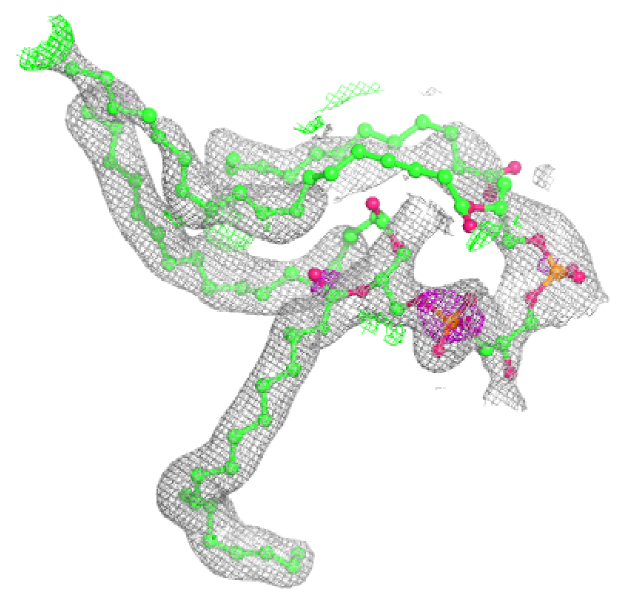


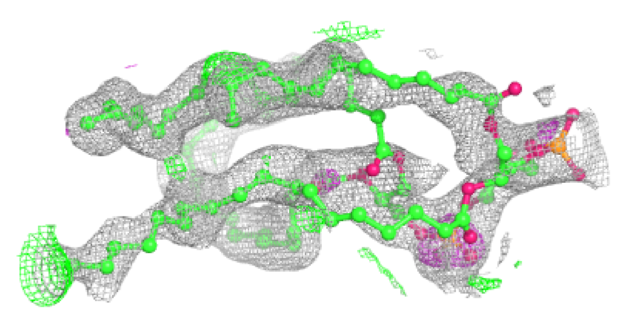


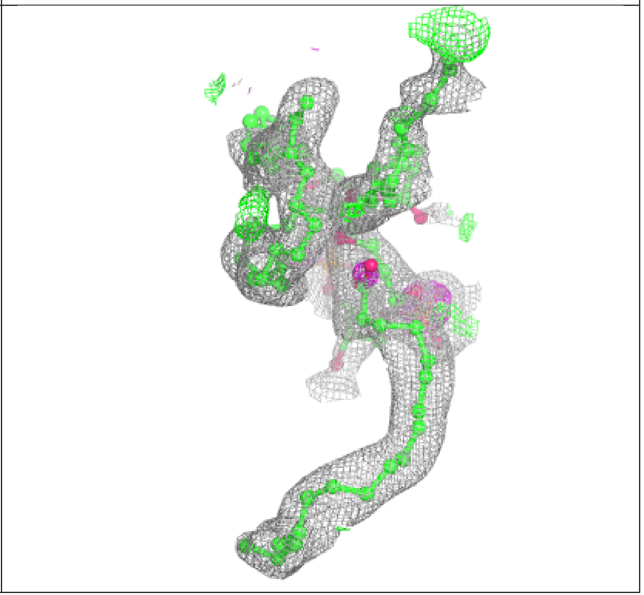


Electron density around CDL L 101:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

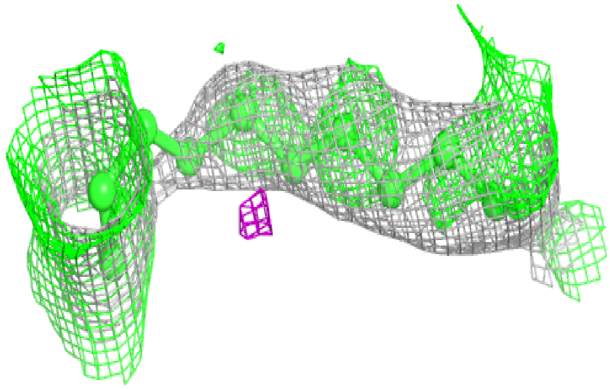


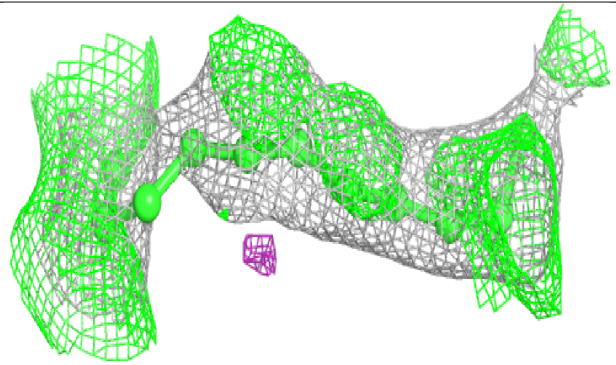


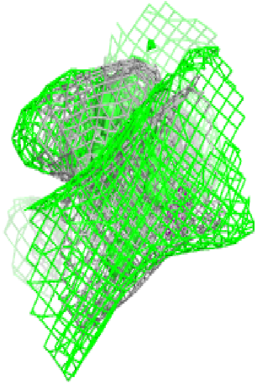


Electron density around LFA P 312:

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

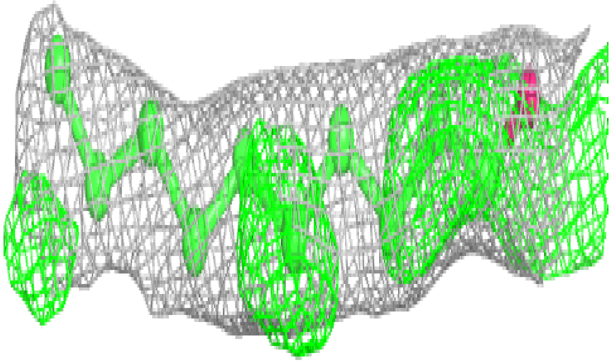


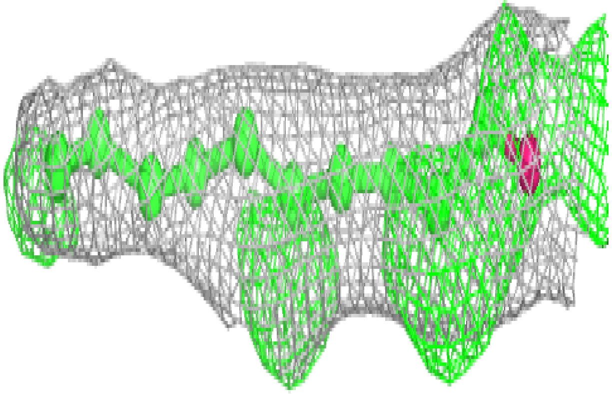


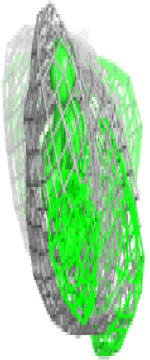


Electron density around DMU C 306:

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

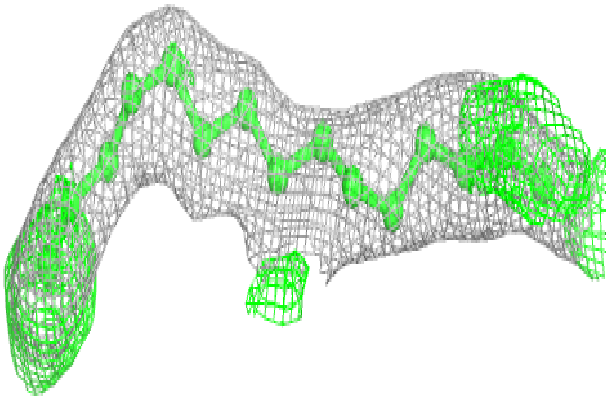


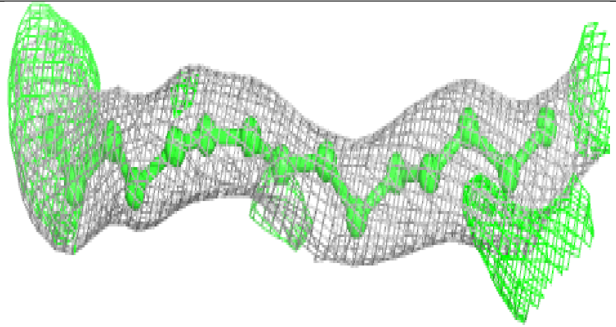


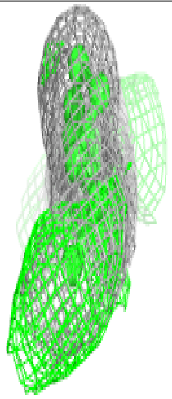


Electron density around LFA P 313:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

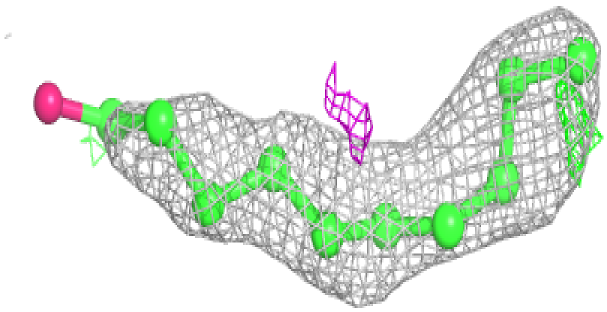


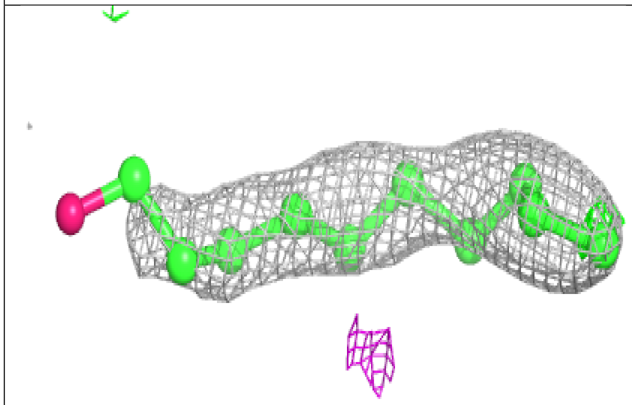


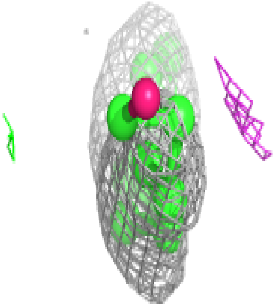


Electron density around DMU J 101:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

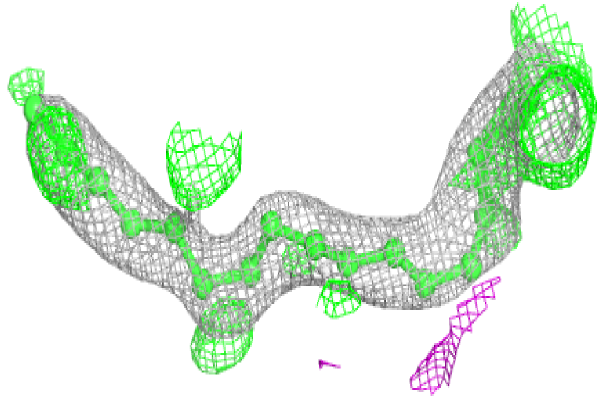


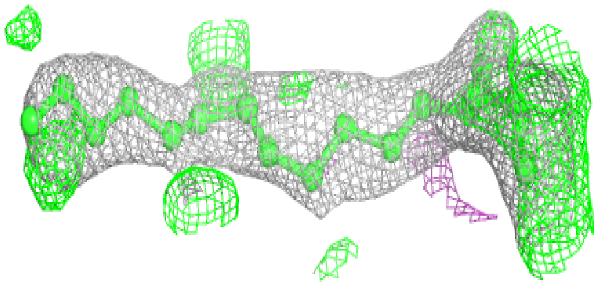


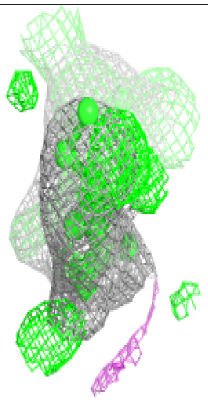


Electron density around LFA N 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

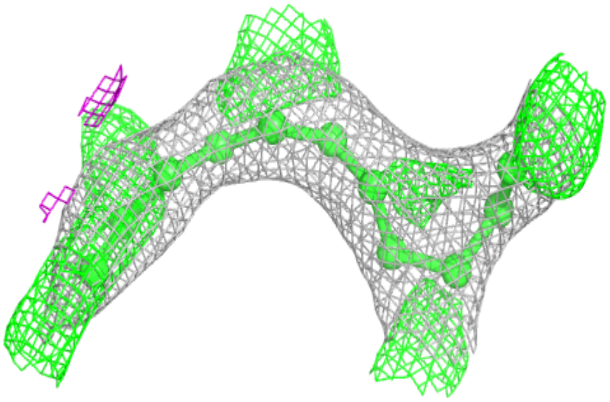


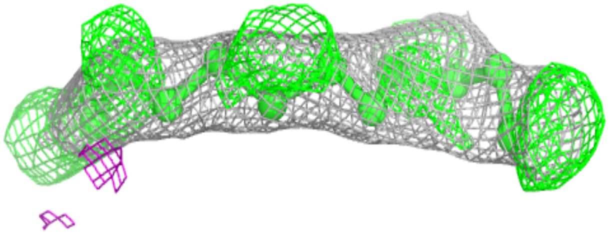


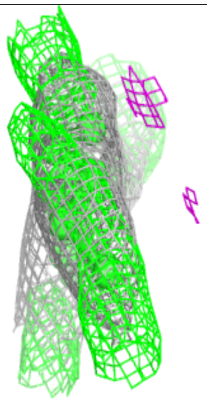


Electron density around LFA C 307:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

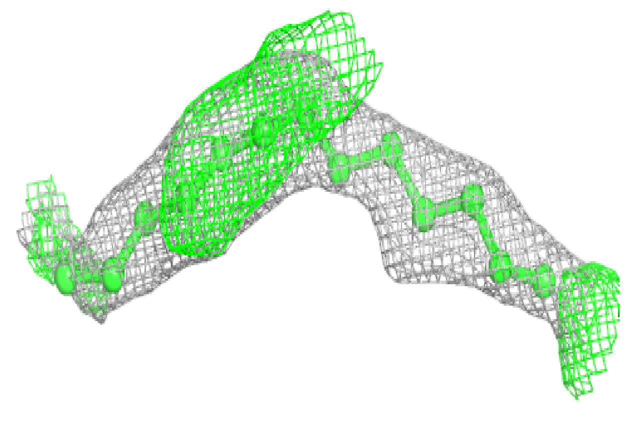


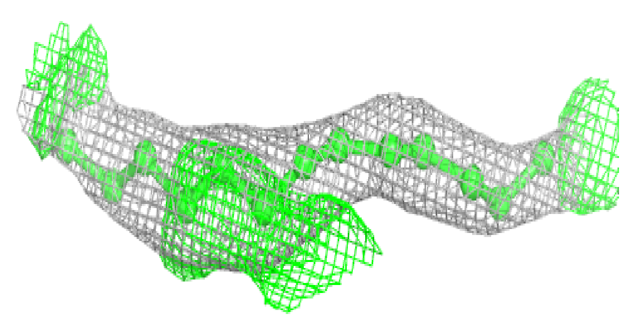


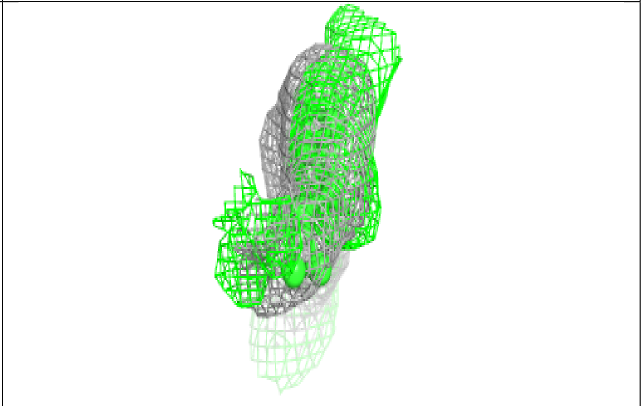


Electron density around LFA P 314:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

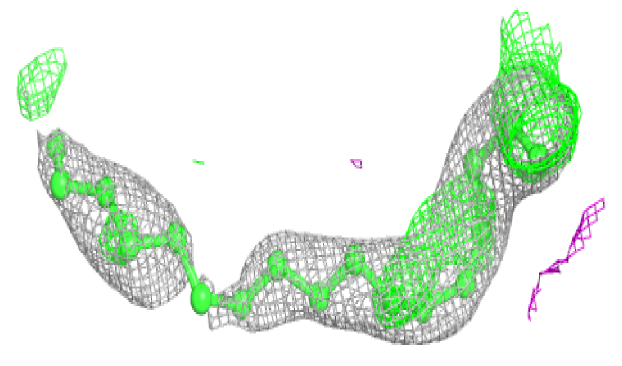


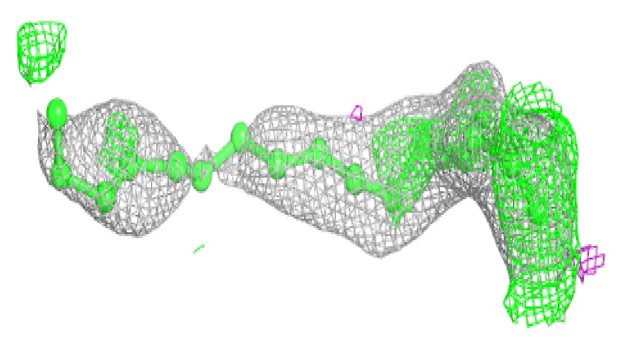


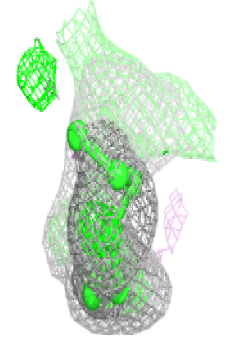


Electron density around LFA B 306:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

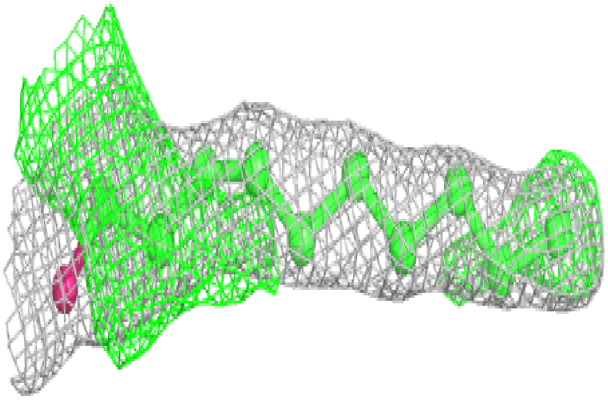


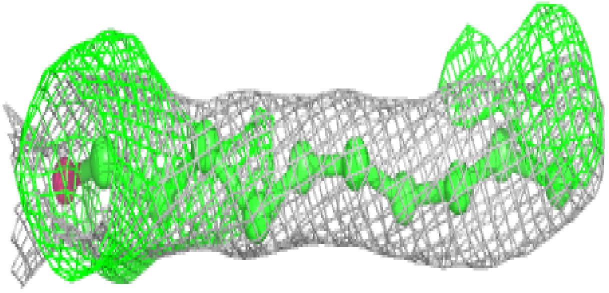




Electron density around DMU O 306:

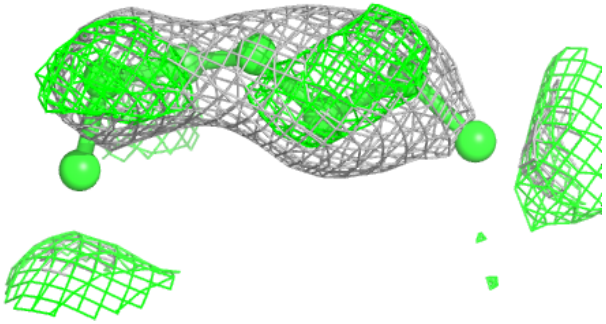
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

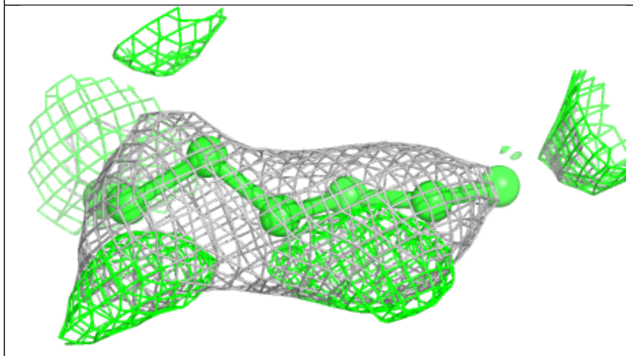


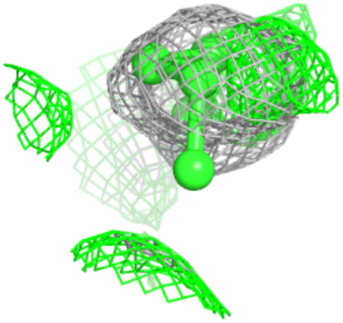


Electron density around DMU C 316:

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

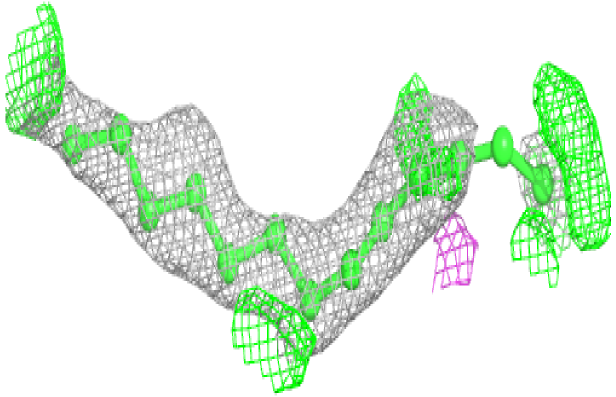


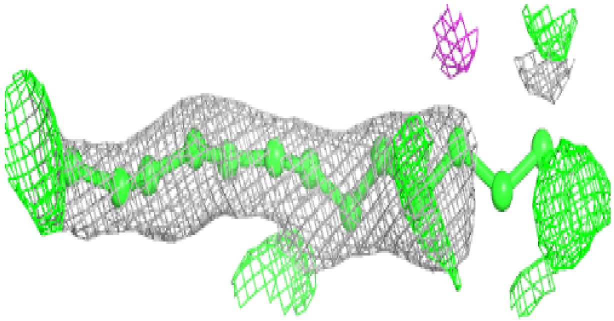


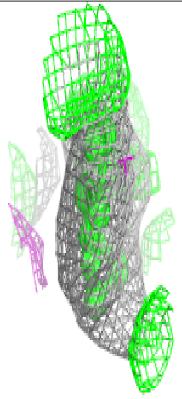


Electron density around LFA C 314:

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

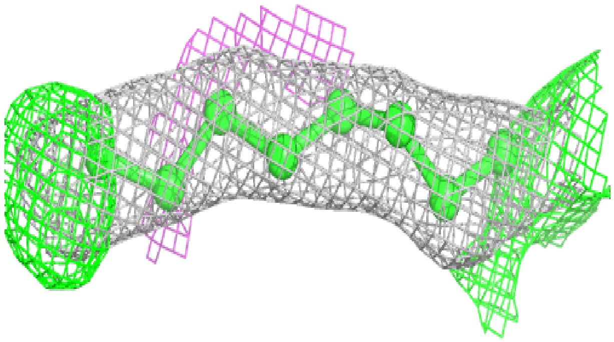


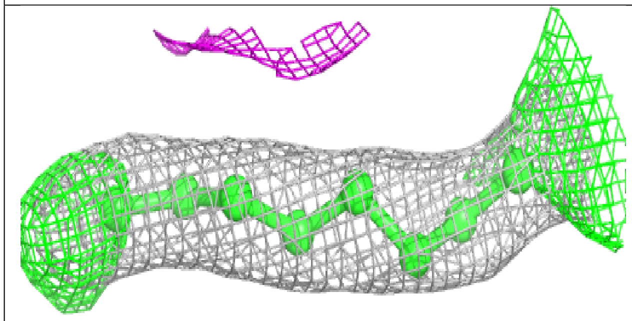


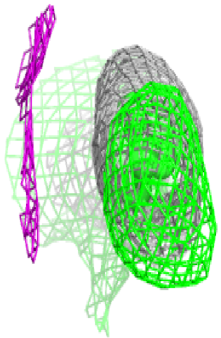


Electron density around DMU M 102:

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

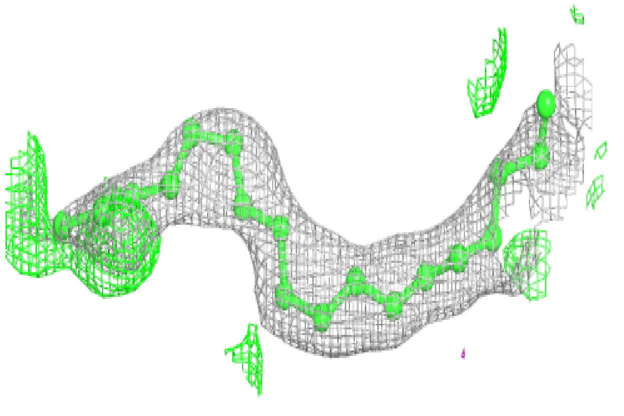


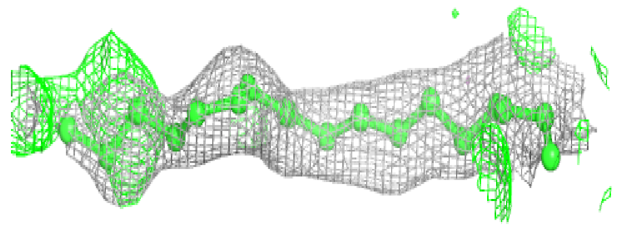


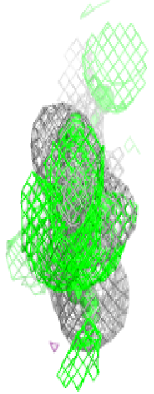


Electron density around LFA C 309:

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

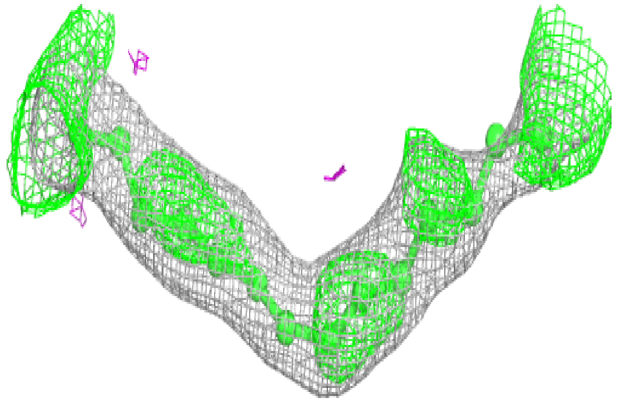


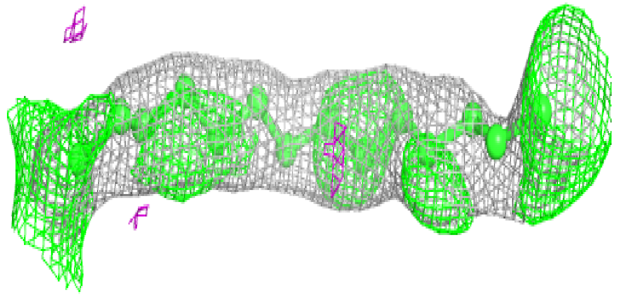


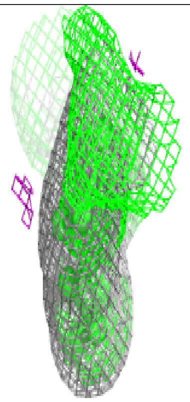


Electron density around LFA A 607:

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

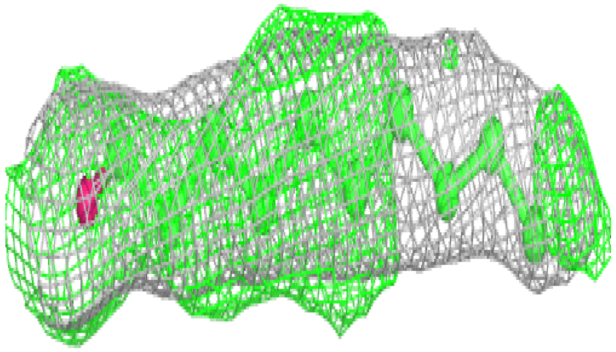


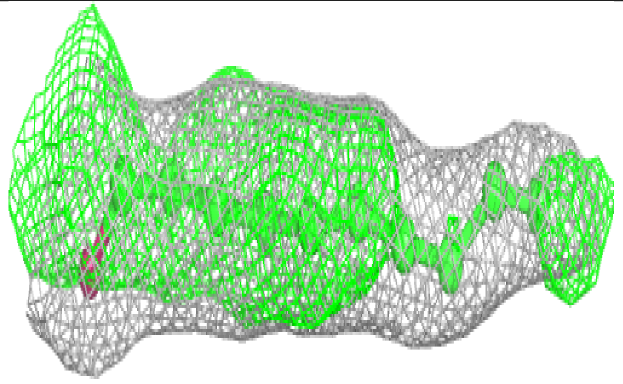


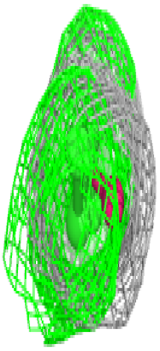


Electron density around DMU P 307:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

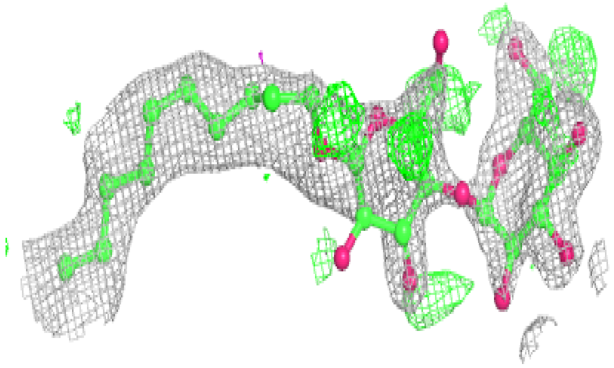


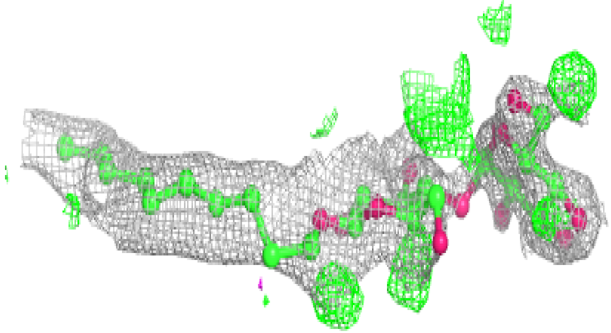


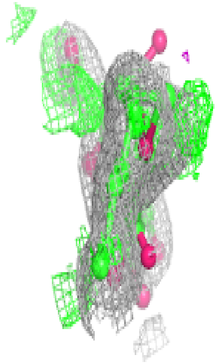


Electron density around DMU H 101:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

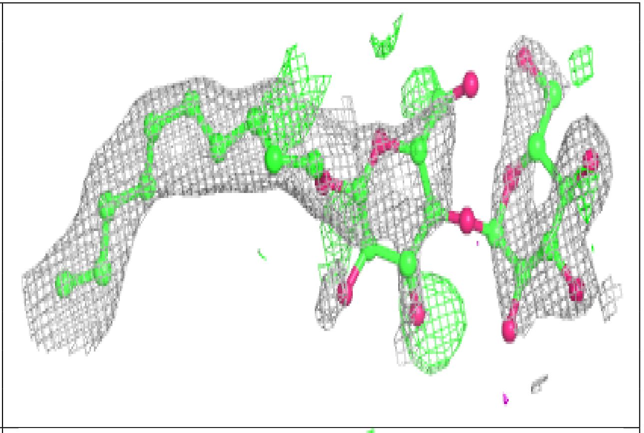


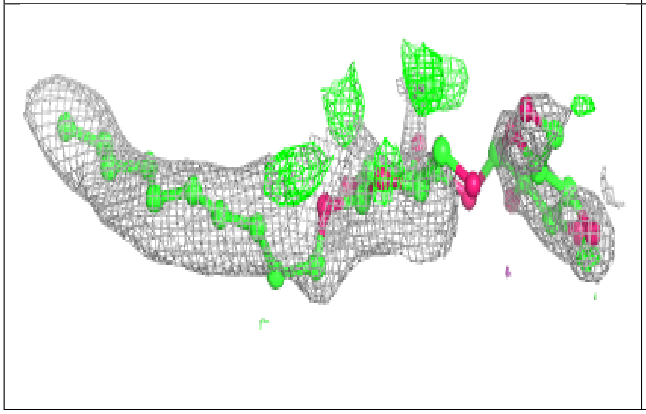


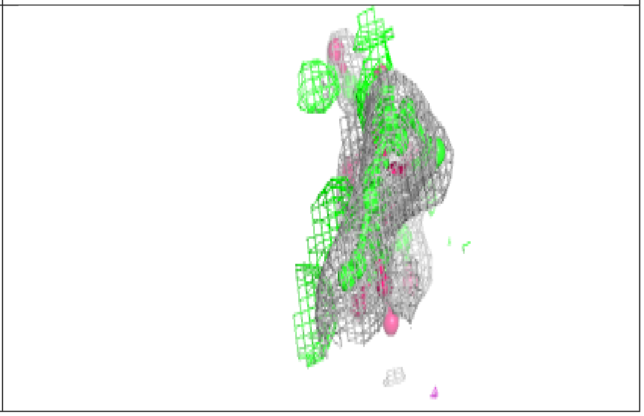


Electron density around DMU N 619:

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

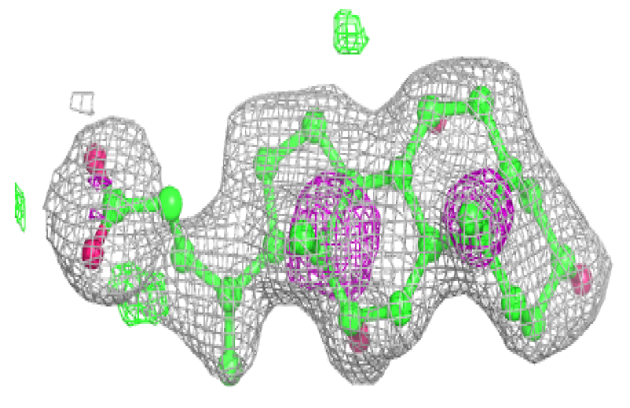


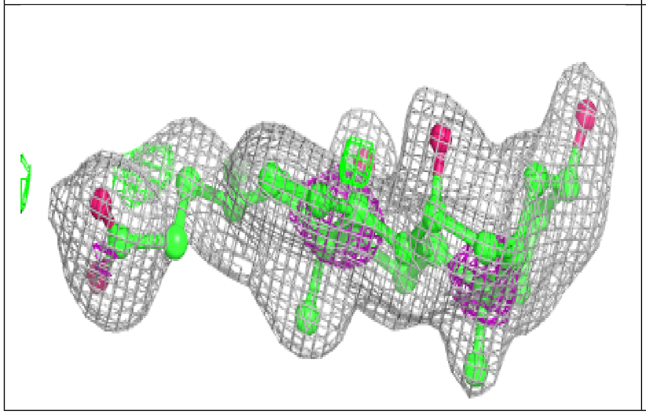


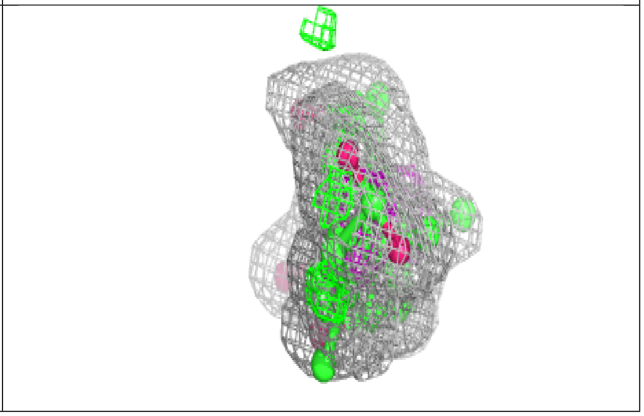


Electron density around CHD P 306:

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

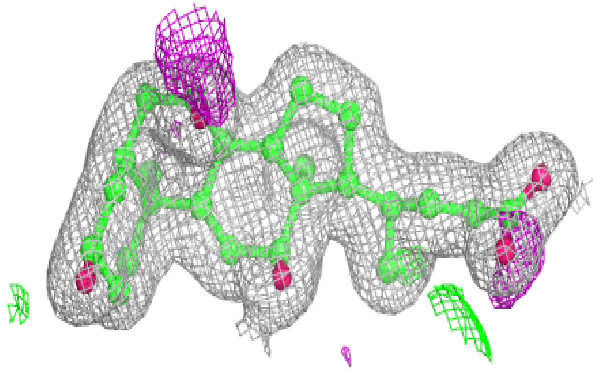


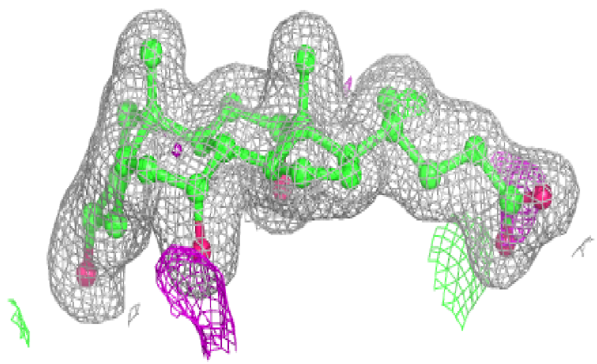


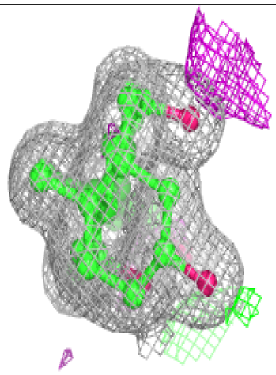


Electron density around CHD P 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

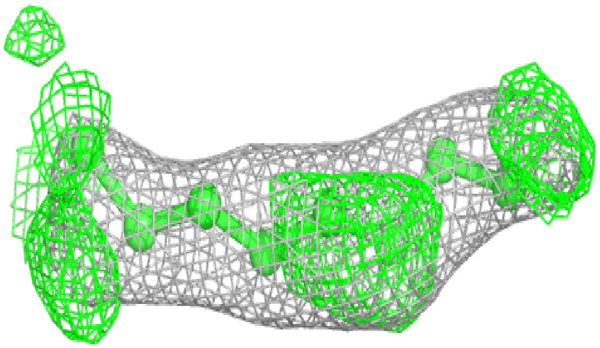


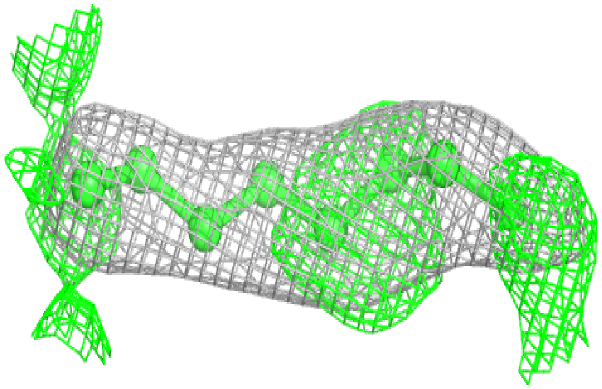


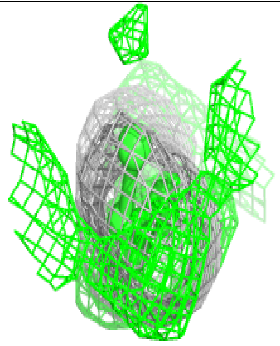


Electron density around DMU Z 102:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

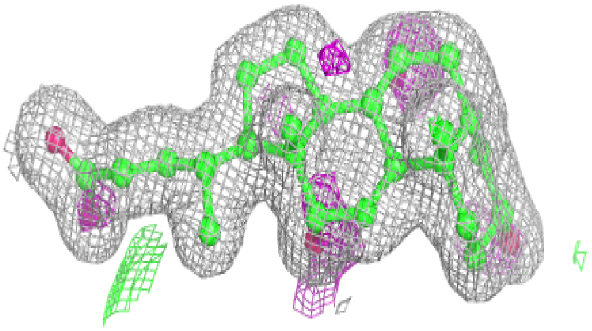


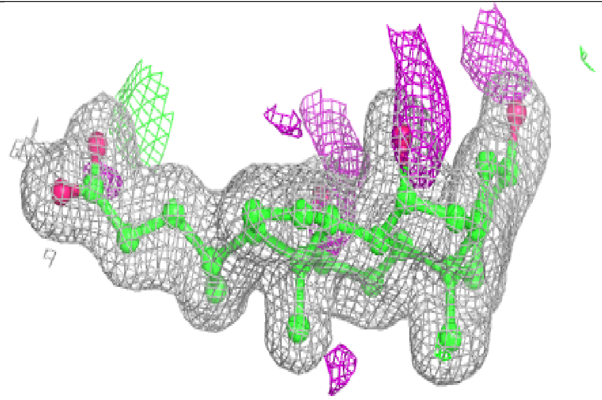


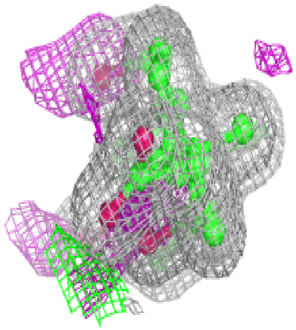


Electron density around CHD C 301:

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

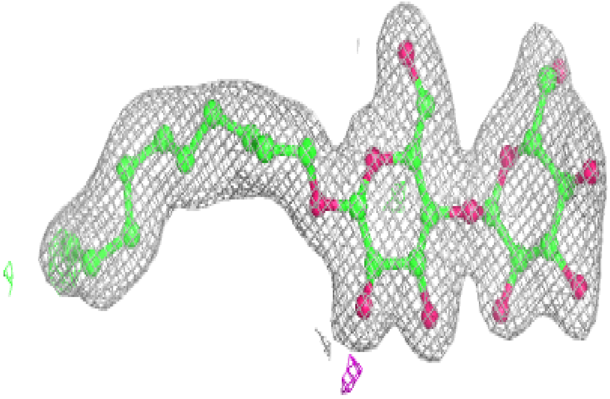


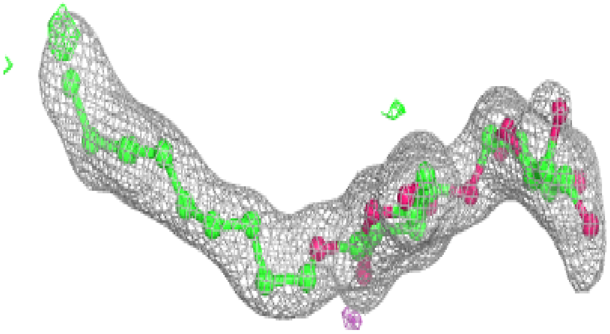


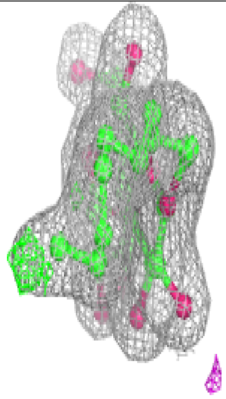


Electron density around DMU M 101:

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

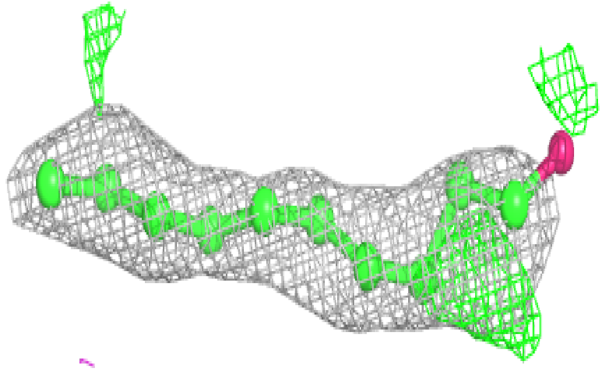


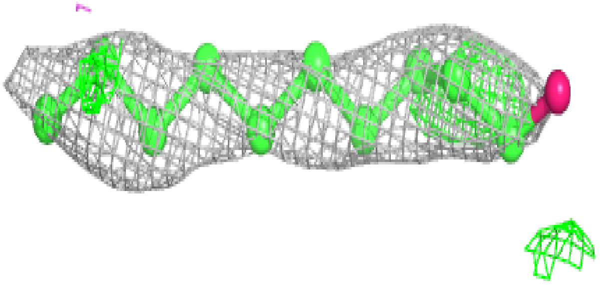


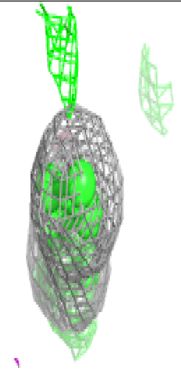


Electron density around DMU B 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

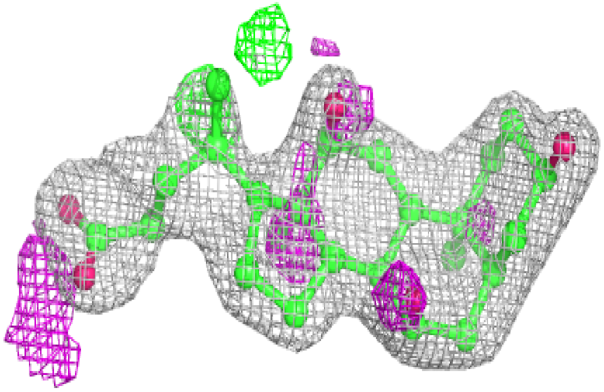


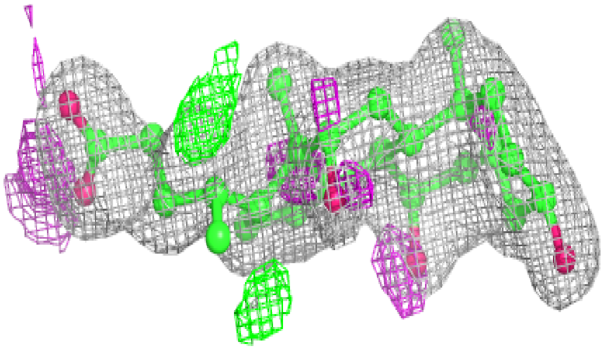


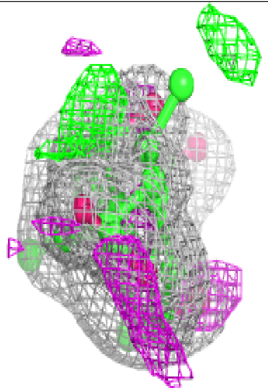


Electron density around CHD C 305:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

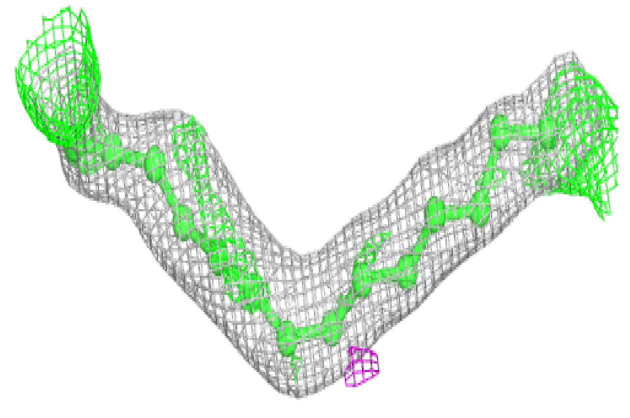


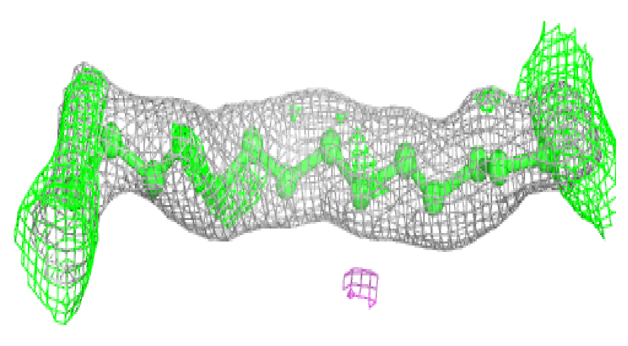


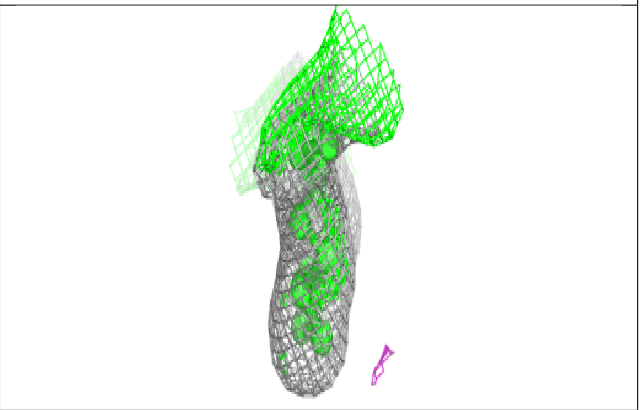


Electron density around LFA N 609:

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

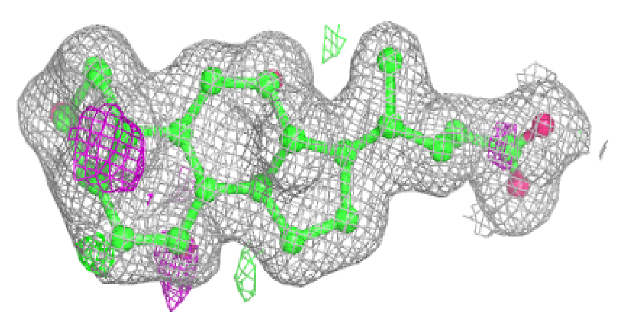


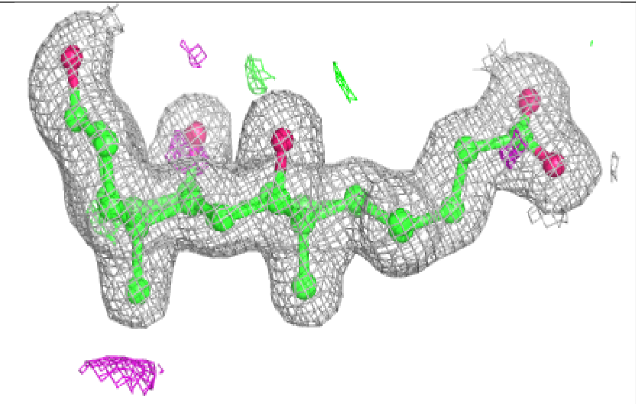


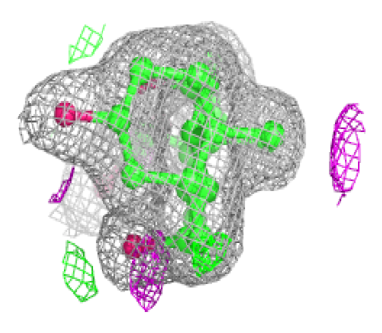


Electron density around CHD B 305:

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

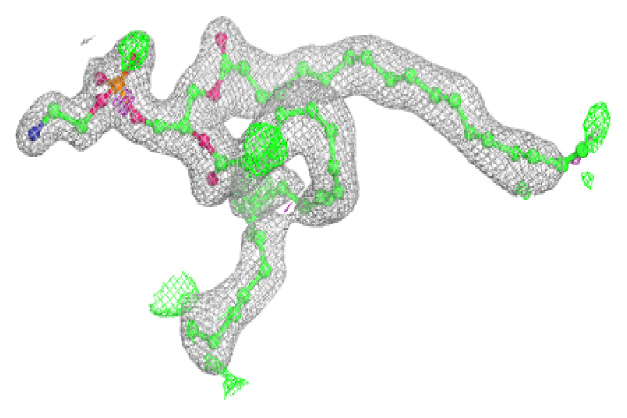


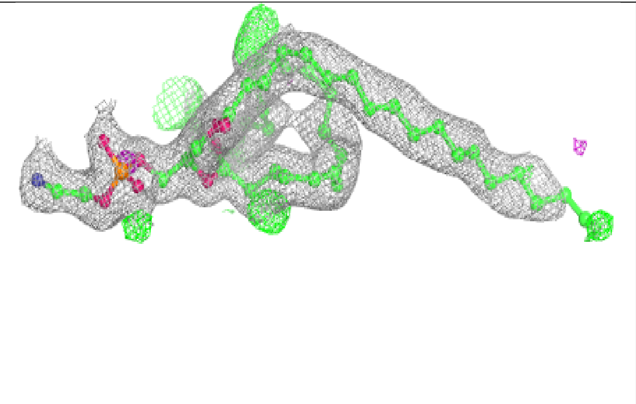


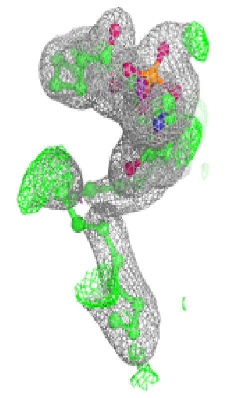


Electron density around PEK T 101:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

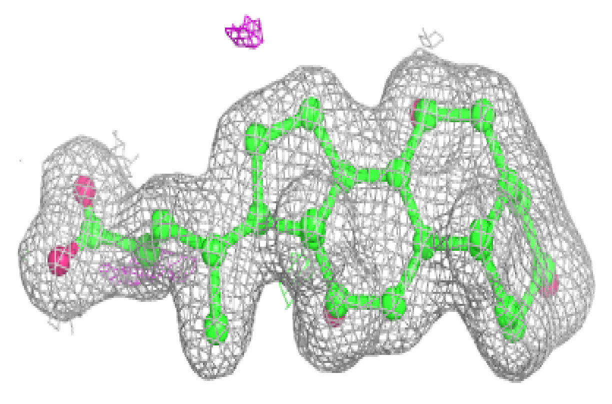


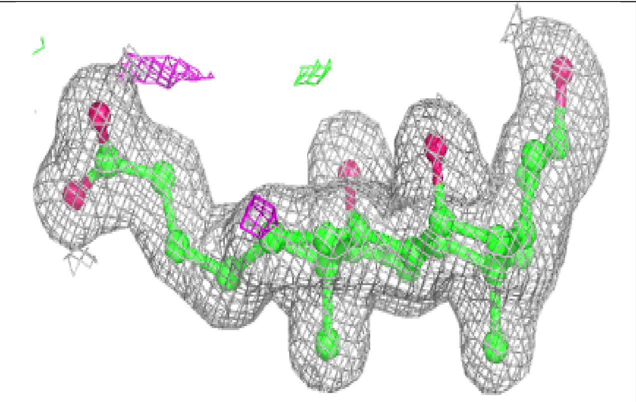


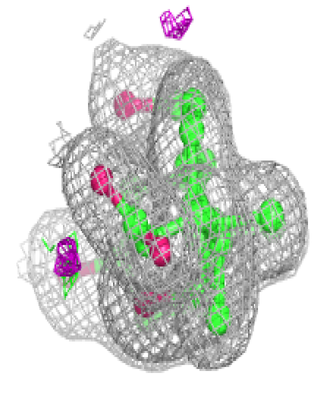


Electron density around CHD O 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

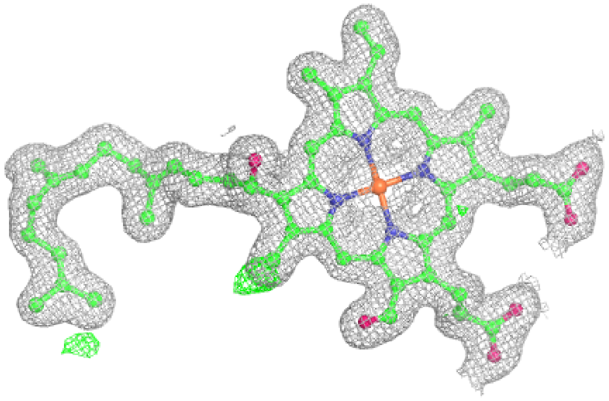


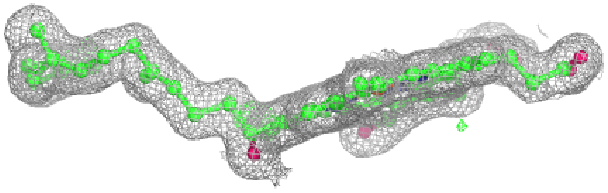


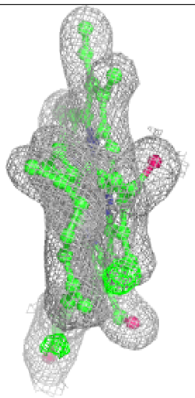


Electron density around HEA N 604:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

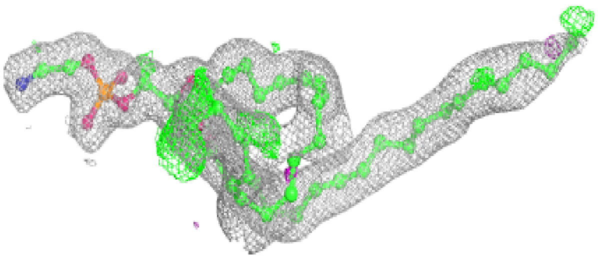






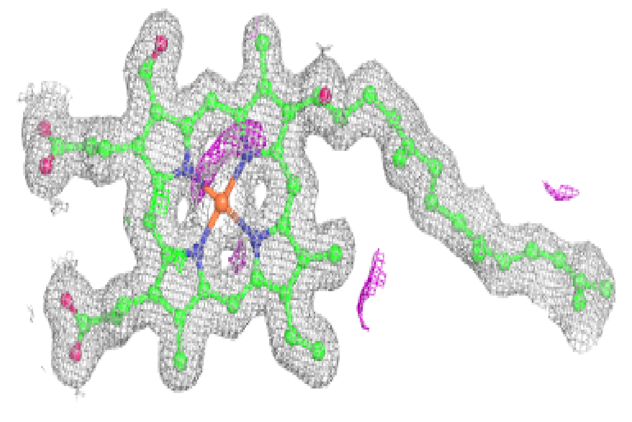
Electron density around PEK G 101:

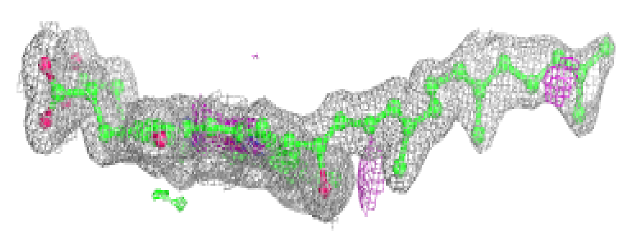
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

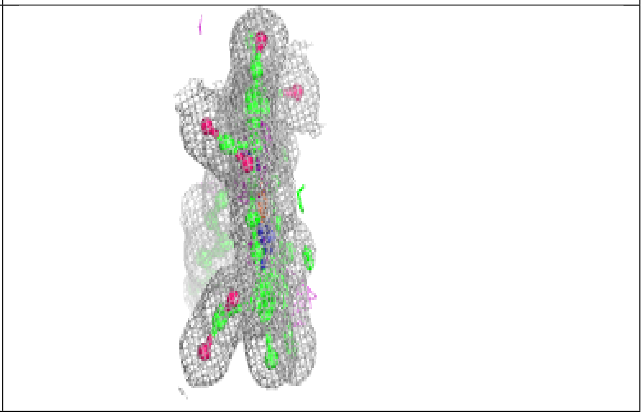


Electron density around HEA A 601 (B):

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

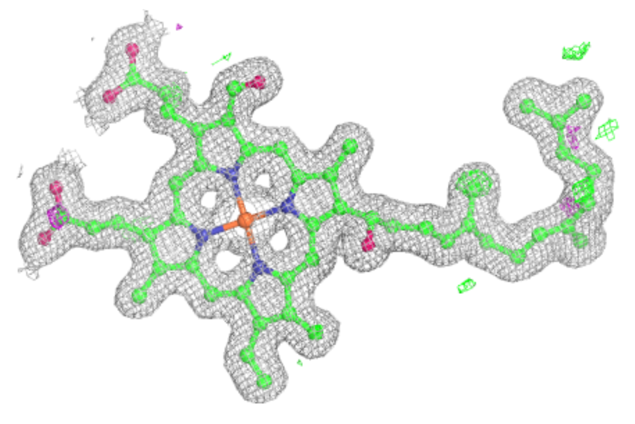


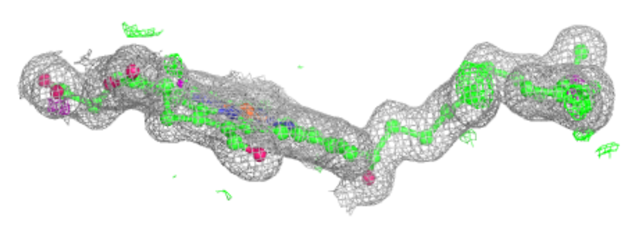


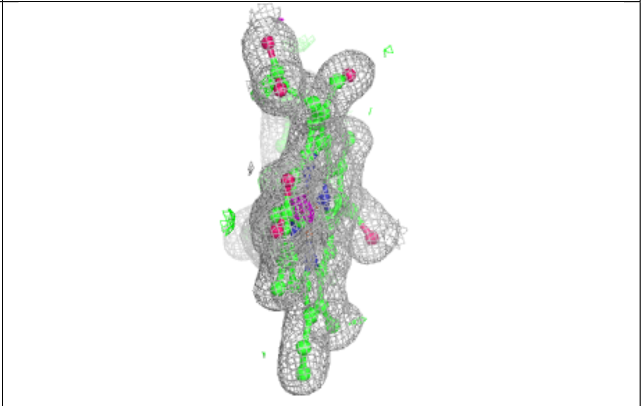


Electron density around HEA A 602:

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

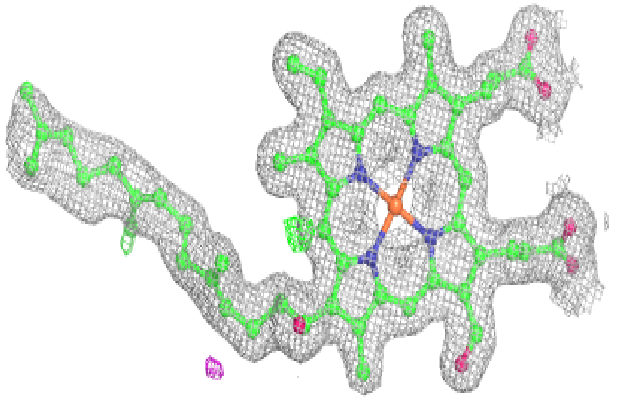


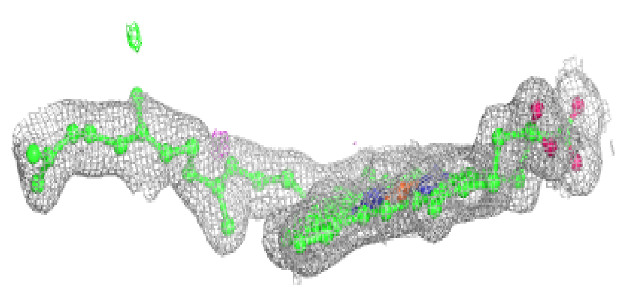


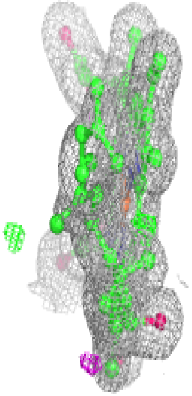


Electron density around HEA N 603 (A):

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

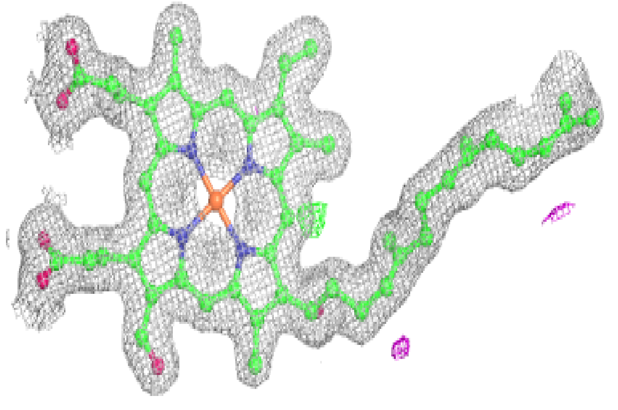


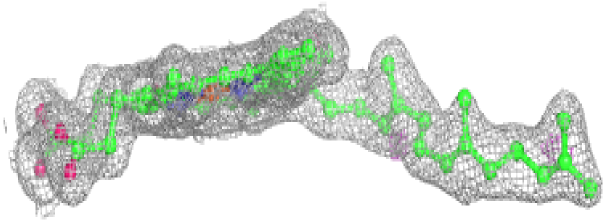


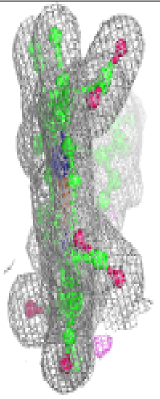


Electron density around HEA N 603 (B):

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

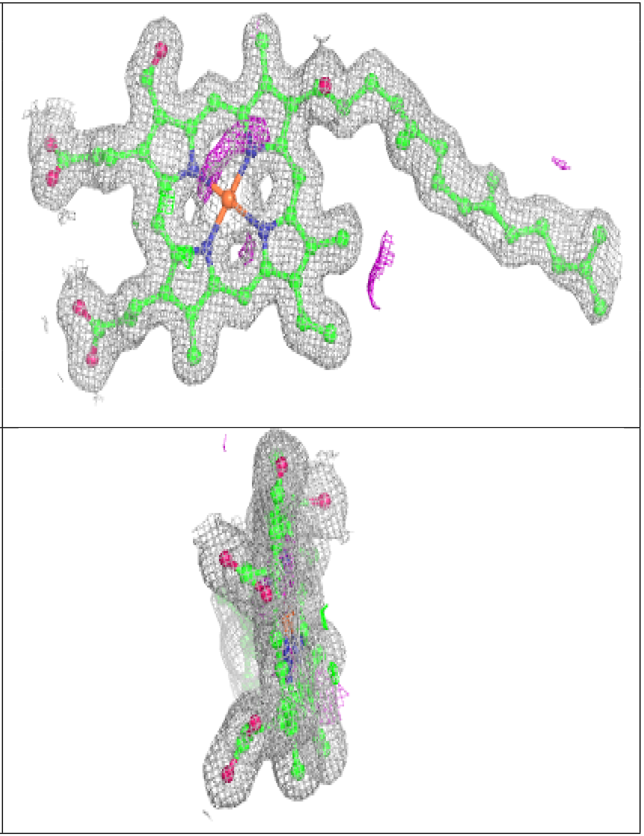


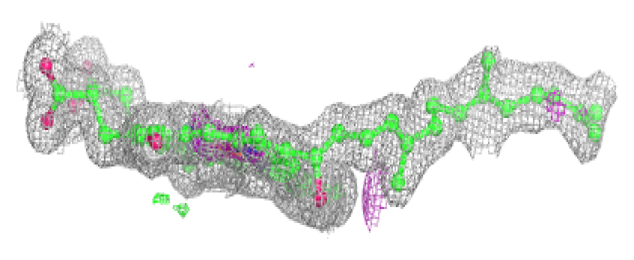




Electron density around HEA A 601 (A):

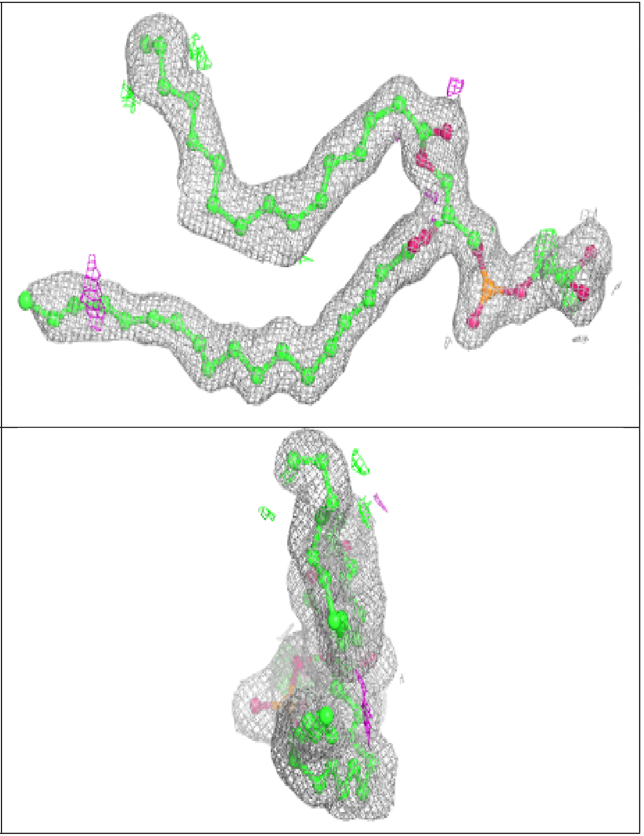
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

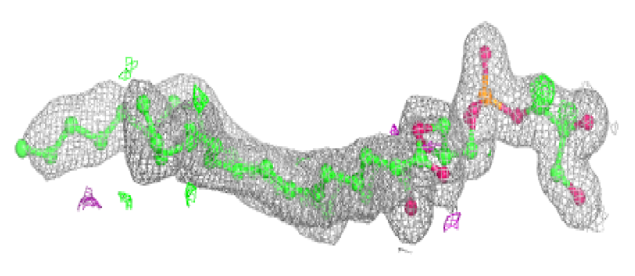




Electron density around PGV A 616:

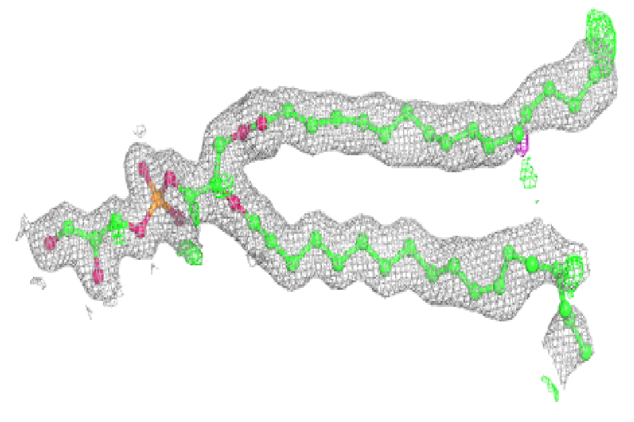
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

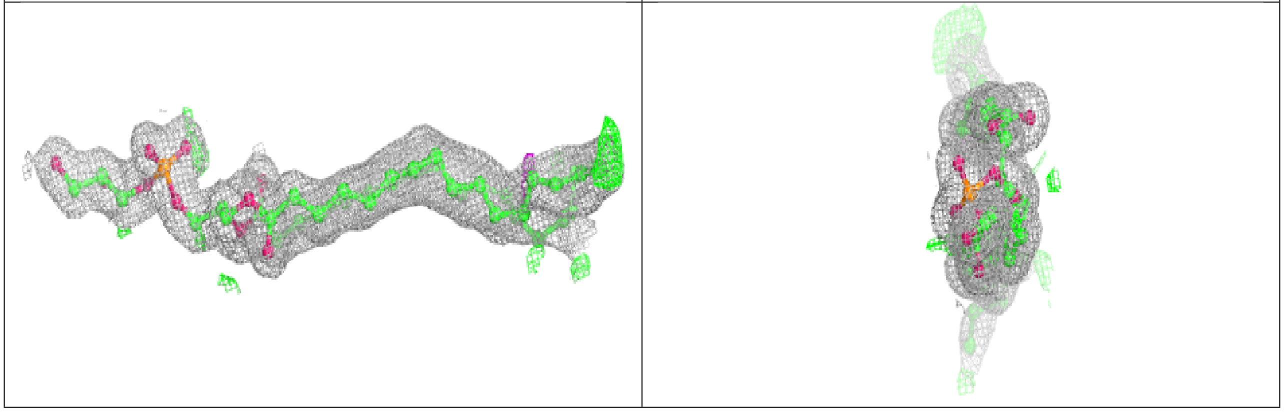




Electron density around PGV C 303:

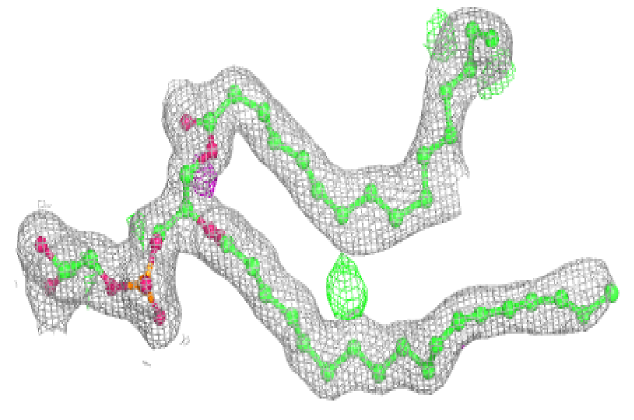
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

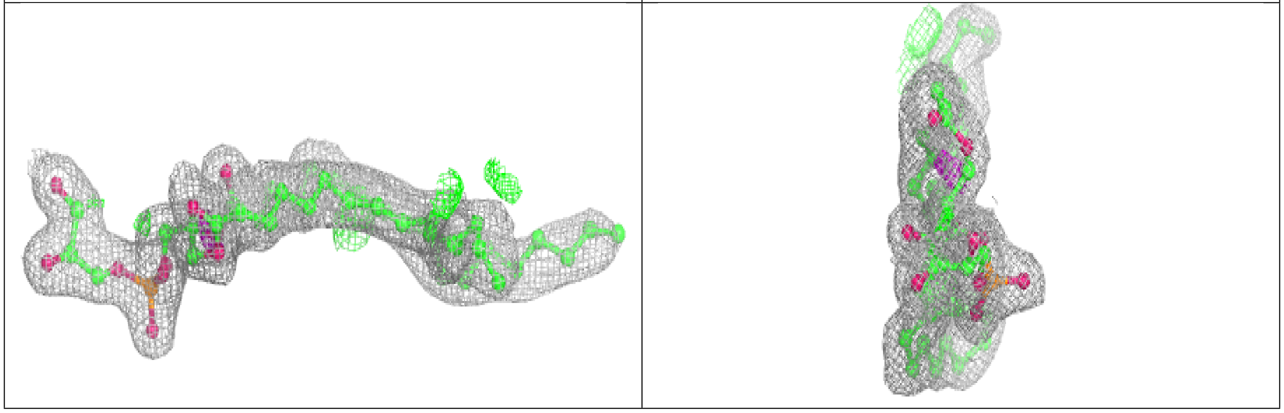




Electron density around PGV N 618:

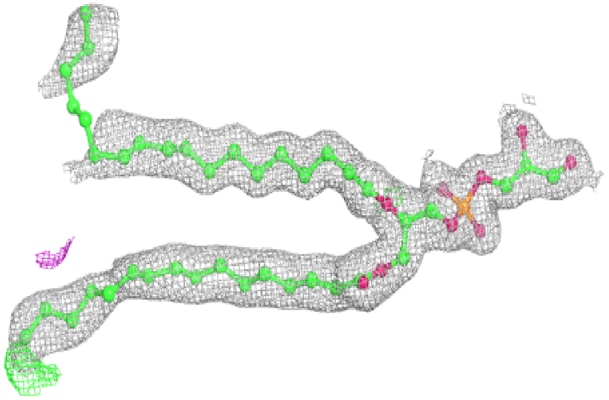
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

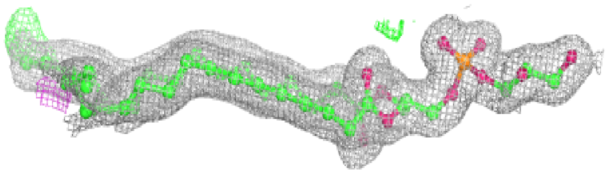


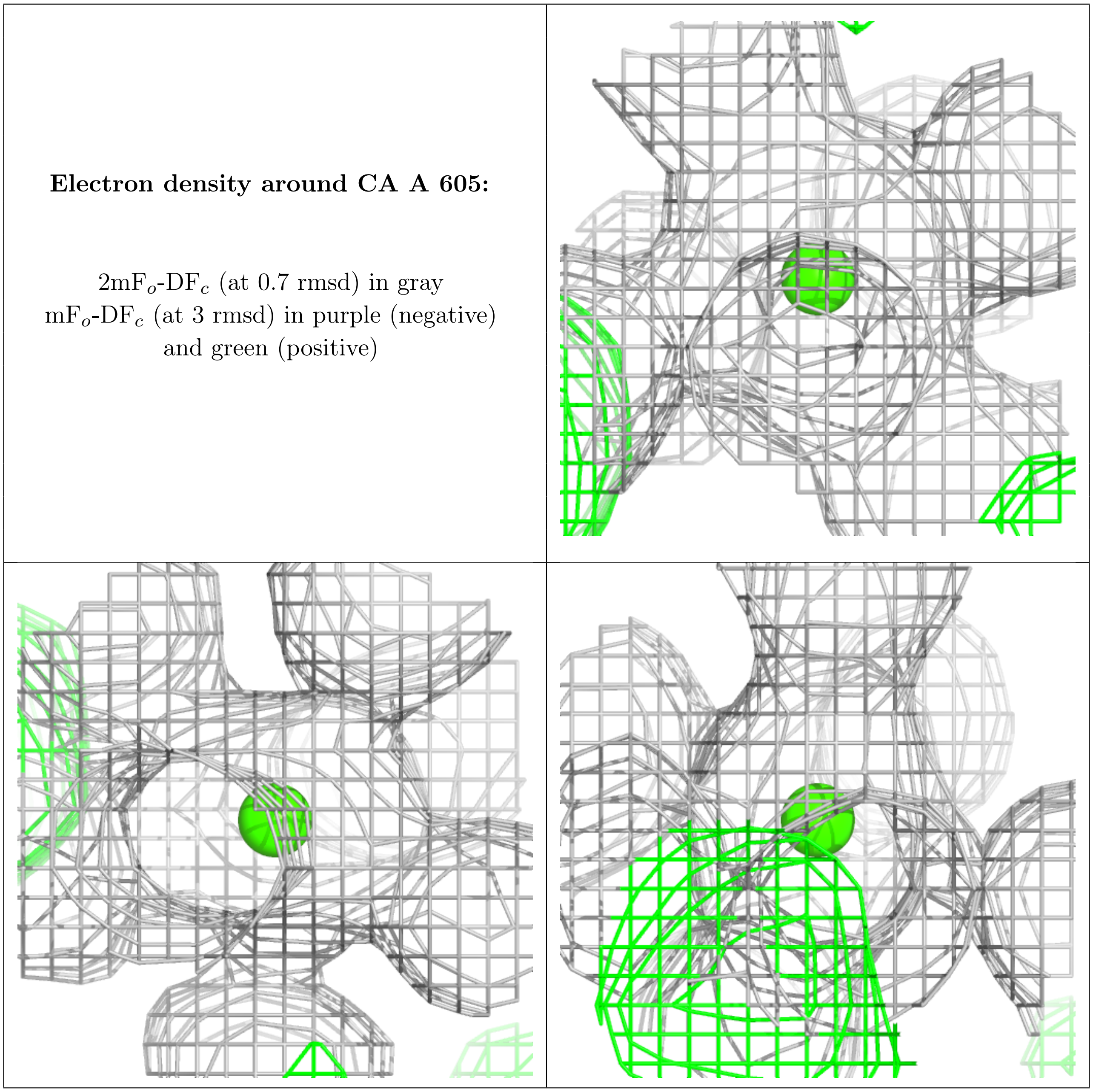


Electron density around PGV P 304:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

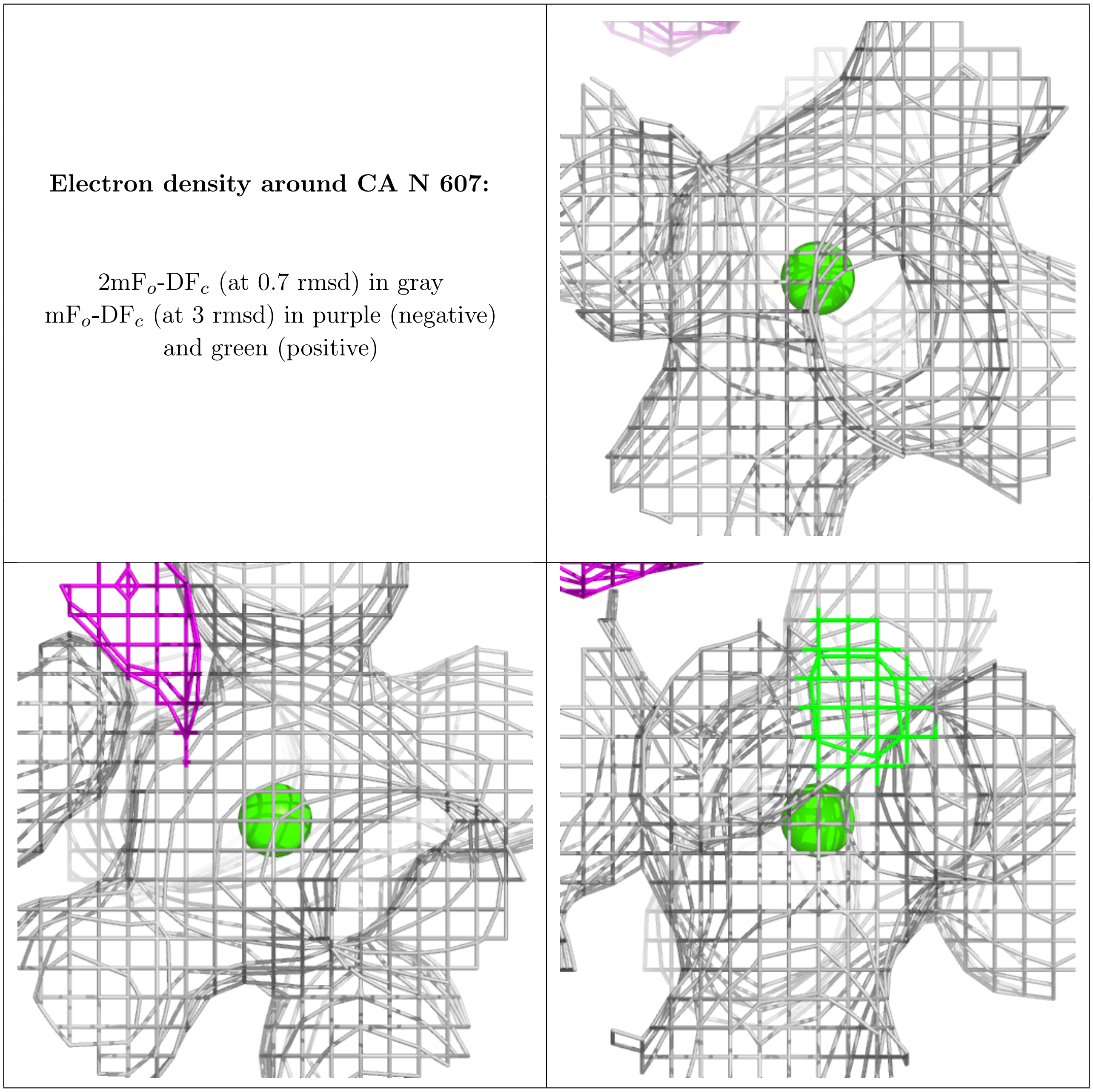






Electron density around CA A 605:

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



Electron density around CA N 607:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.