wwPDB X-ray Structure Validation Summary Report (i)

Aug 13, 2026 – 11:44 AM JST

PDB ID	:	9IKF / pdb_00009ikf
Title	:	Bovine Heart Cytochrome c Oxidase in the Carbon Dioxide-bound Fully Oxidized State
Authors	:	Muramoto, K.; Shinzawa-Itoh, K.
Deposited on	:	2024-06-27
Resolution	:	1.75 Å(reported)

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

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

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

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

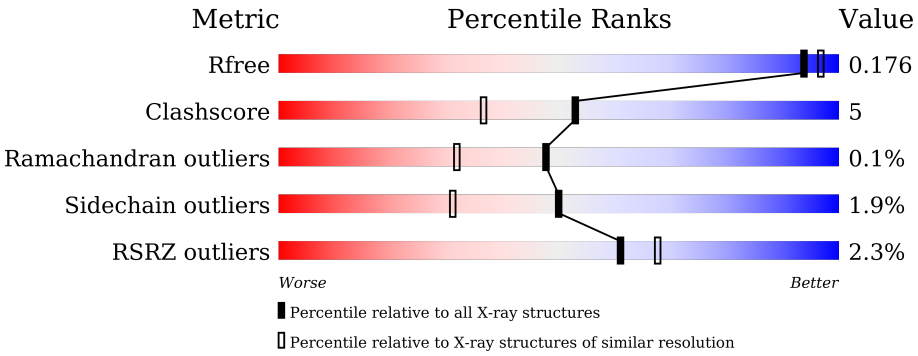
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12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

1 Overall quality at a glance (i)

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

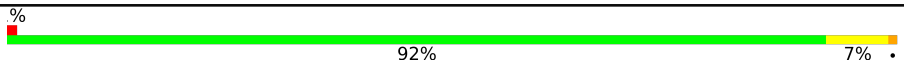
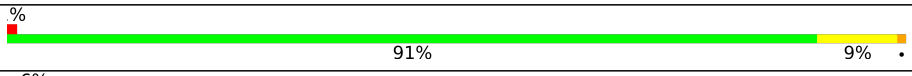
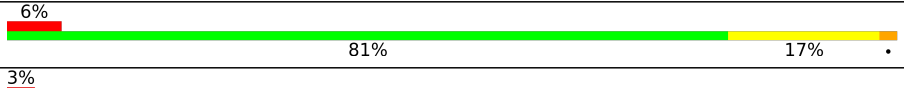
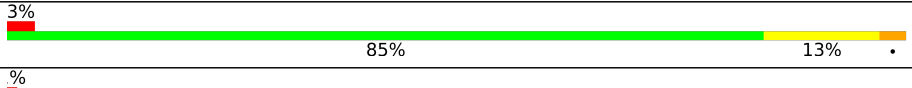
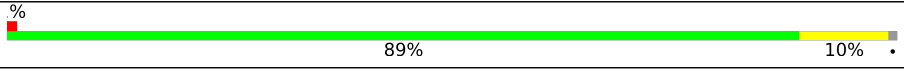
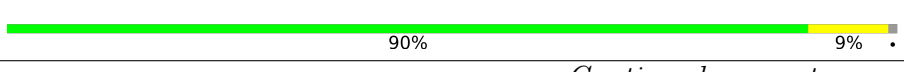
The reported resolution of this entry is 1.75 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 93%
4	Q	147	5% 88% 5% 7%
5	E	109	2% 89% 5% 6%
5	R	109	2% 87% 6% 6%
6	F	98	% 80% 11% 7%
6	S	98	2% 77% 15% 7%
7	G	85	4% 75% 8% 15%
7	T	85	4% 75% 7% 15%
8	H	85	5% 78% 7% 12%
8	U	85	5% 79% 6% 12%
9	I	73	7% 88% 5%
9	V	73	4% 86% 7%
10	J	59	2% 83% 10% 5%
10	W	59	2% 88% 7% 5%
11	K	56	4% 82% 5% 12%
11	X	56	5% 82% 5% 12%
12	L	47	2% 89% 6%
12	Y	47	2% 85% 6% 6%
13	M	46	83% 13%
13	Z	46	2% 76% 11% 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	PER	A	606	-	X	-	-
18	PER	N	606	-	X	-	-
21	LFA	C	308	-	-	-	X

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

2 Entry composition (i)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

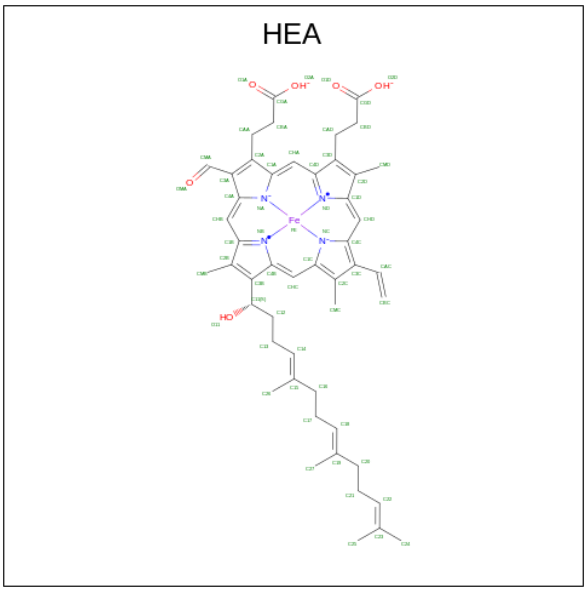
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

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



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

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

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

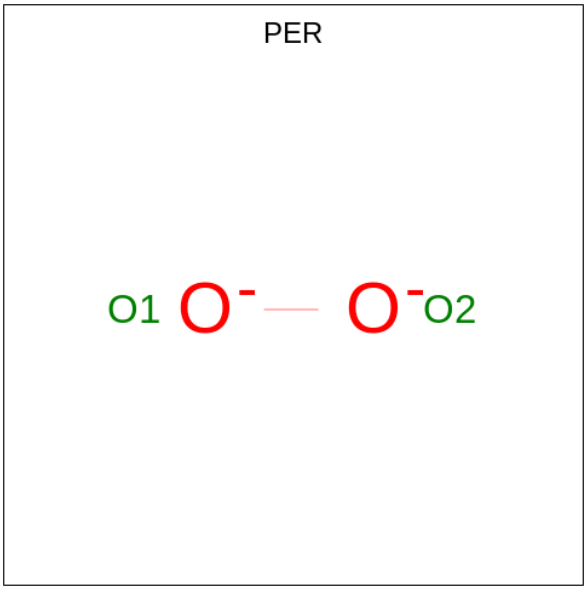
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

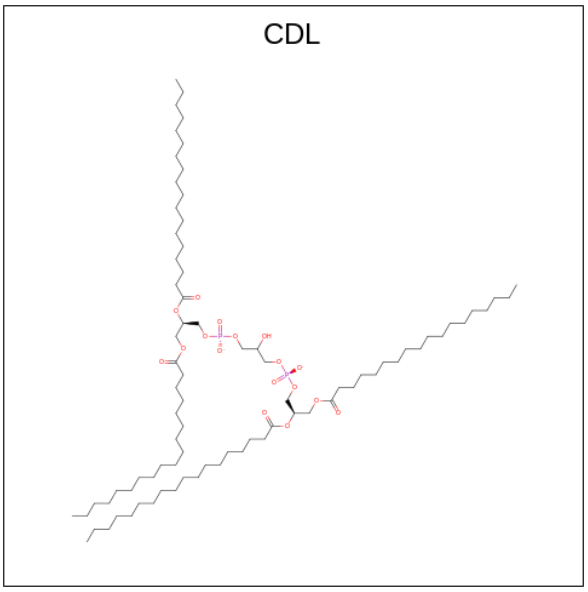
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

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



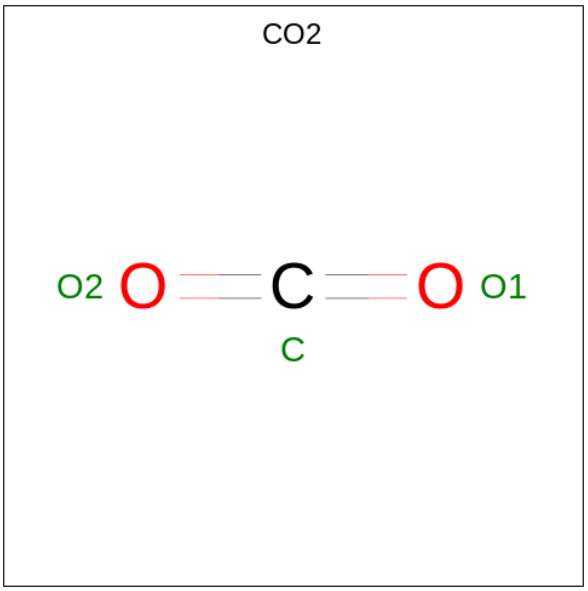
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total O 2 2	0	0
18	N	1	Total O 2 2	0	0

- Molecule 19 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



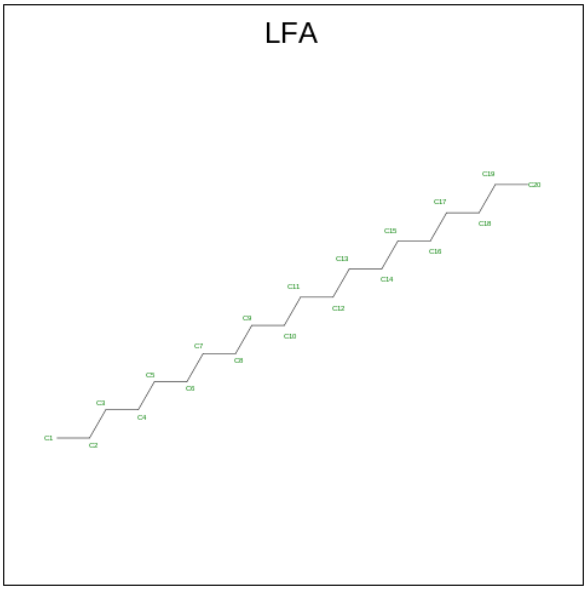
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			64	45	17	2		
19	C	1	Total	C	O	P	0	0
			87	68	17	2		
19	L	1	Total	C	O	P	0	0
			94	75	17	2		
19	P	1	Total	C	O	P	0	0
			87	68	17	2		
19	V	1	Total	C	O	P	0	0
			64	45	17	2		
19	Y	1	Total	C	O	P	0	0
			94	75	17	2		

- Molecule 20 is CARBON DIOXIDE (CCD ID: CO2) (formula: CO_2) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 21 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



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

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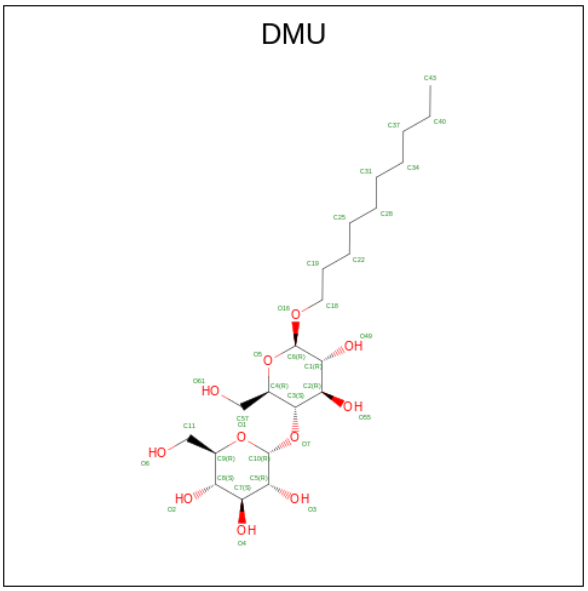
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total C 17 17	0	0
21	C	1	Total C 11 11	0	0
21	C	1	Total C 6 6	0	0
21	C	1	Total C 18 18	0	0
21	C	1	Total C 11 11	0	0
21	C	1	Total C 14 14	0	0
21	C	1	Total C 11 11	0	0
21	C	1	Total C 15 15	0	0
21	C	1	Total C 13 13	0	0
21	C	1	Total C 15 15	0	0
21	N	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	P	1	Total C 15 15	0	0
21	P	1	Total C 13 13	0	0
21	T	1	Total C 11 11	0	0

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



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

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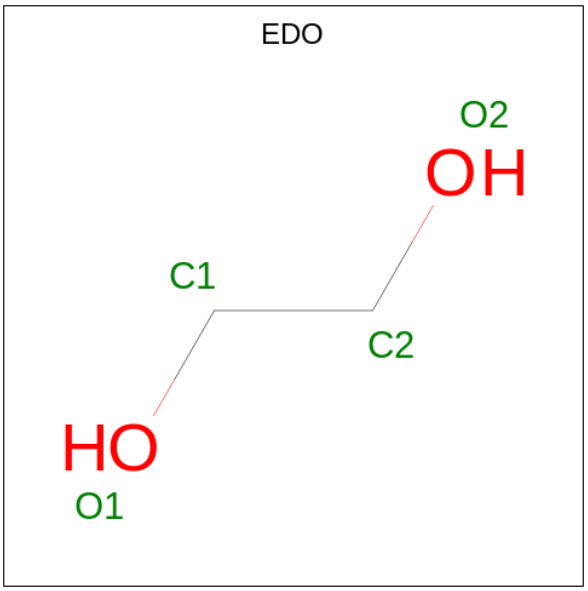
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O 33 22 11	0	0
22	C	1	Total C 7 7	0	0
22	C	1	Total C O 22 16 6	0	0
22	C	1	Total C O 33 22 11	0	0
22	C	1	Total C O 33 22 11	0	0
22	C	1	Total C O 22 16 6	0	0
22	C	1	Total C O 33 22 11	0	0
22	D	1	Total C O 33 22 11	0	0
22	G	1	Total C O 11 10 1	0	0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

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

- Molecule 23 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



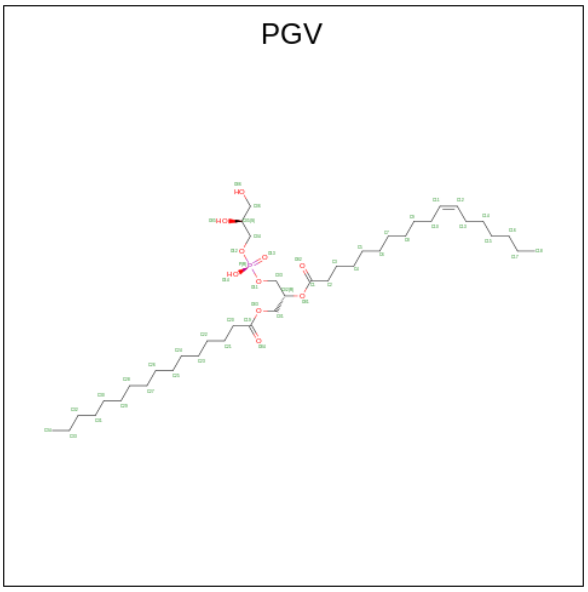
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			4	2	2		
23	A	1	Total	C	O	0	0
			4	2	2		
23	A	1	Total	C	O	0	0
			4	2	2		
23	A	1	Total	C	O	0	0
			4	2	2		
23	B	1	Total	C	O	0	0
			4	2	2		
23	C	1	Total	C	O	0	0
			4	2	2		
23	C	1	Total	C	O	0	0
			4	2	2		
23	C	1	Total	C	O	0	0
			4	2	2		
23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

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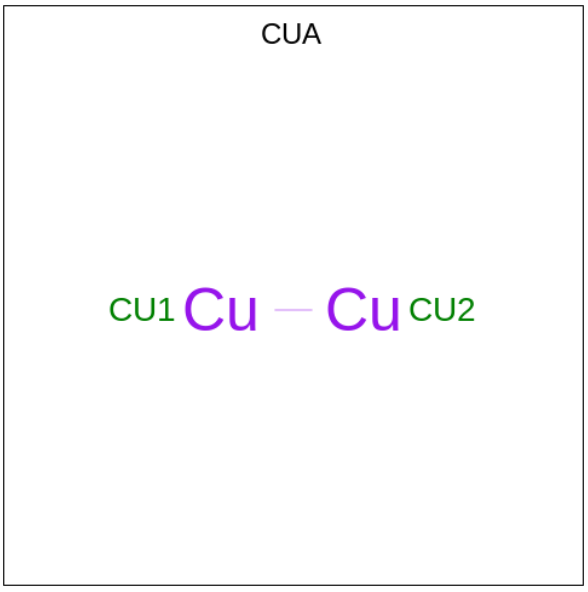
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	N	1	Total	C	O	0	0
			4	2	2		
23	N	1	Total	C	O	0	0
			4	2	2		
23	N	1	Total	C	O	0	0
			4	2	2		
23	N	1	Total	C	O	0	0
			4	2	2		
23	N	1	Total	C	O	0	0
			4	2	2		
23	O	1	Total	C	O	0	0
			4	2	2		
23	P	1	Total	C	O	0	0
			4	2	2		
23	P	1	Total	C	O	0	0
			4	2	2		
23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

- Molecule 24 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



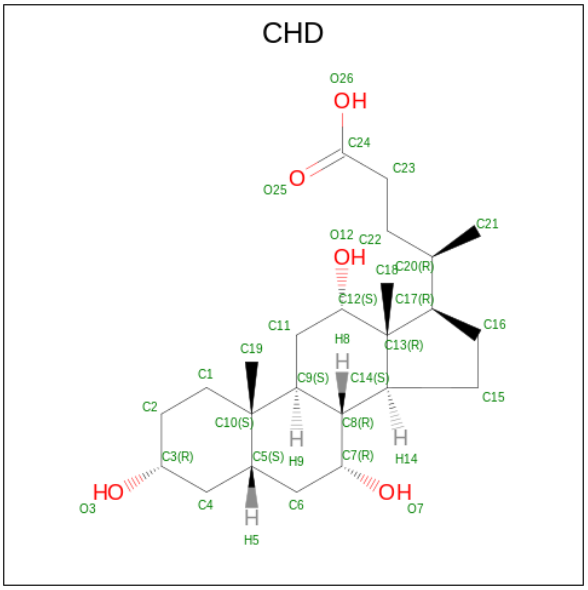
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	O	P	0	0
			51	40	10	1		
24	C	1	Total	C	O	P	0	0
			51	40	10	1		
24	N	1	Total	C	O	P	0	0
			51	40	10	1		
24	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 25 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



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

- Molecule 26 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



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

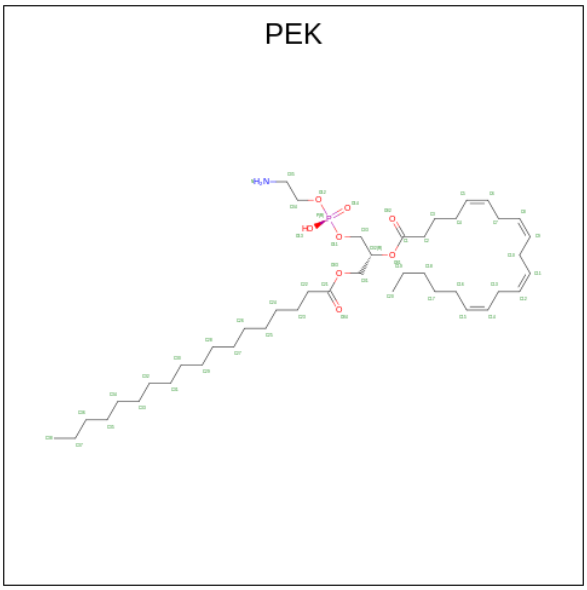
- Molecule 27 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

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

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

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

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



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	236	Total O 247 247	0	11
30	B	177	Total O 179 179	0	2
30	C	103	Total O 104 104	0	1
30	D	138	Total O 146 146	0	8

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	E	109	Total O 117 117	0	8
30	F	101	Total O 108 108	0	7
30	G	43	Total O 44 44	0	1
30	H	62	Total O 62 62	0	0
30	I	39	Total O 39 39	0	0
30	J	21	Total O 21 21	0	0
30	K	21	Total O 21 21	0	0
30	L	24	Total O 26 26	0	2
30	M	22	Total O 22 22	0	0
30	N	223	Total O 233 233	0	10
30	O	149	Total O 150 150	0	1
30	P	100	Total O 101 101	0	1
30	Q	79	Total O 84 84	0	5
30	R	88	Total O 95 95	0	7
30	S	91	Total O 97 97	0	6
30	T	35	Total O 36 36	0	1
30	U	49	Total O 49 49	0	0
30	V	23	Total O 23 23	0	0
30	W	15	Total O 15 15	0	0
30	X	19	Total O 19 19	0	0
30	Y	23	Total O 25 25	0	2

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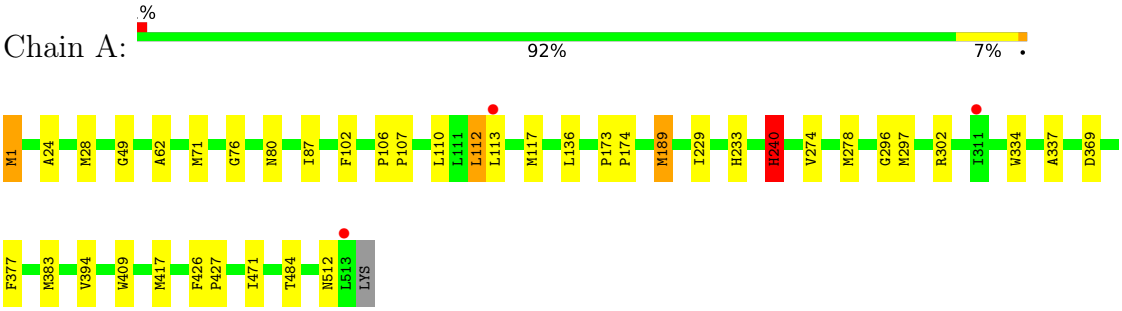
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	Z	17	Total O 17 17	0	0

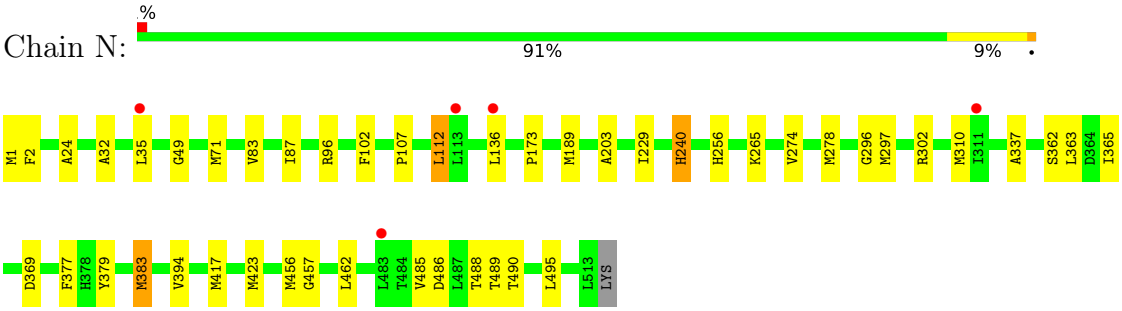
3 Residue-property plots (i)

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

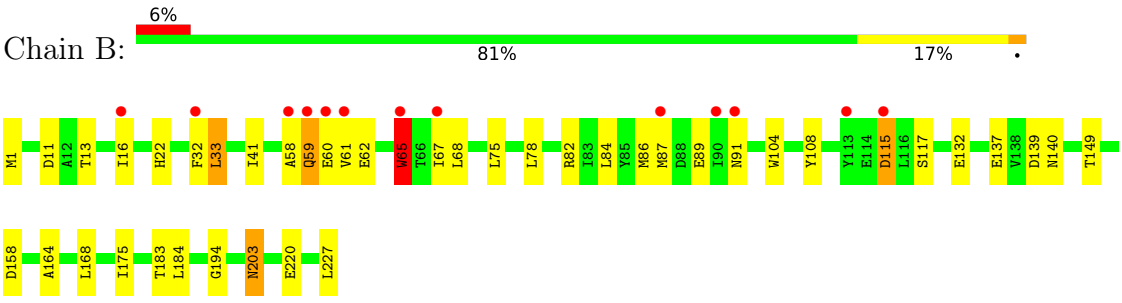
• Molecule 1: Cytochrome c oxidase subunit 1



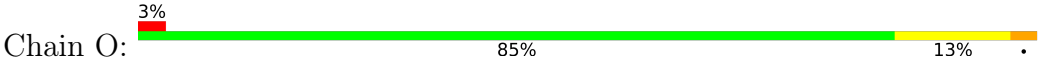
• Molecule 1: Cytochrome c oxidase subunit 1

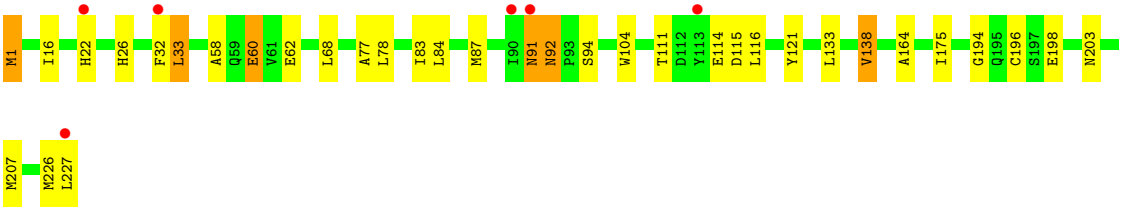


• Molecule 2: Cytochrome c oxidase subunit 2

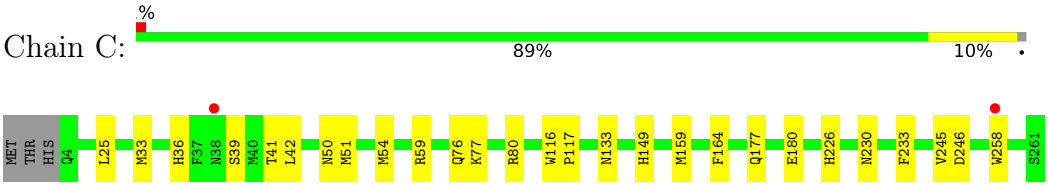


• Molecule 2: Cytochrome c oxidase subunit 2

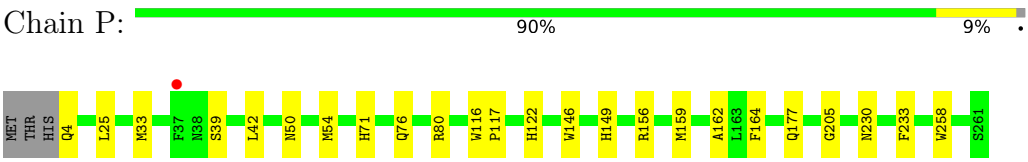




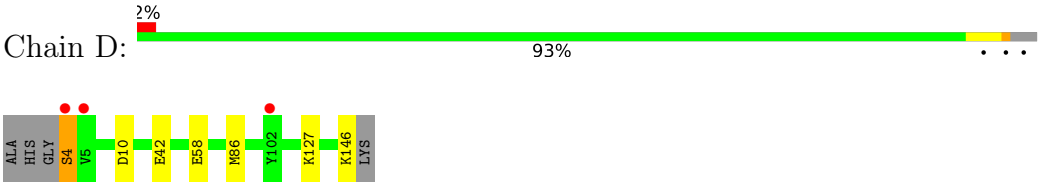
• Molecule 3: Cytochrome c oxidase subunit 3



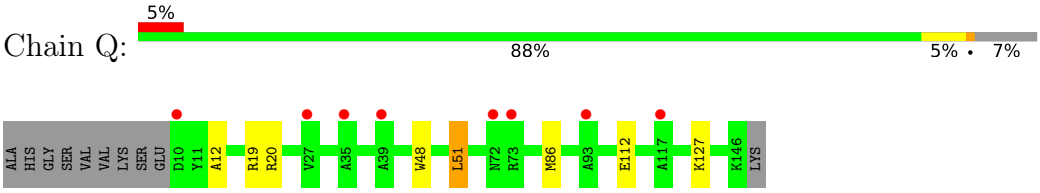
• Molecule 3: Cytochrome c oxidase subunit 3



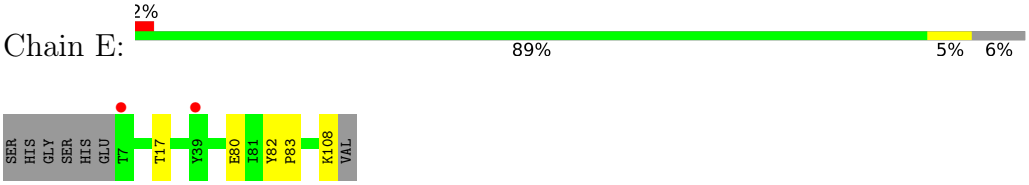
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



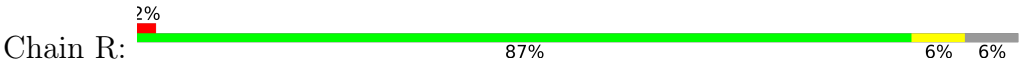
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

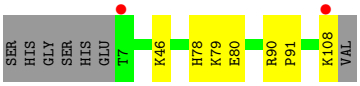


• Molecule 5: Cytochrome c oxidase subunit 5A



• Molecule 5: Cytochrome c oxidase subunit 5A

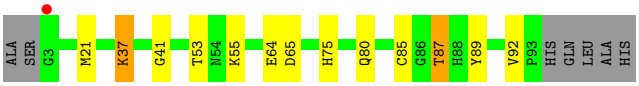




• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:

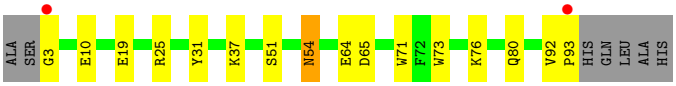




• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:

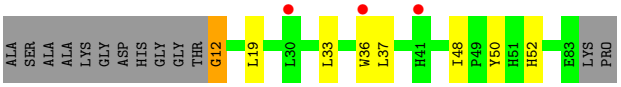




• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:

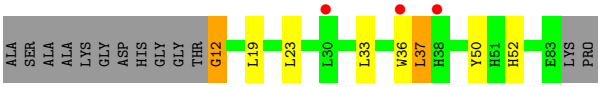




• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:

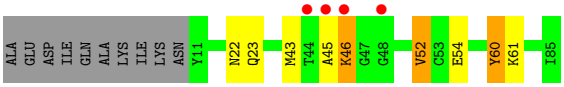




• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:





• Molecule 8: Cytochrome c oxidase subunit 6B1

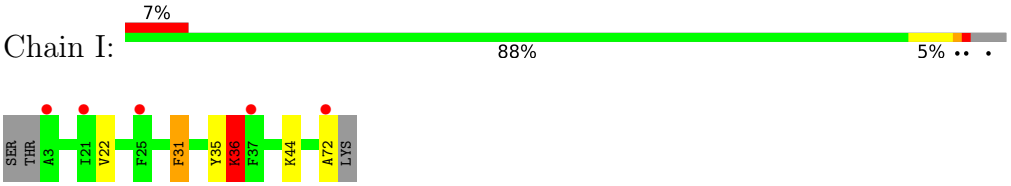
Chain U:





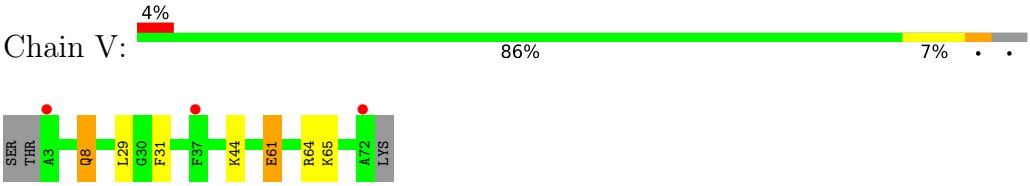
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



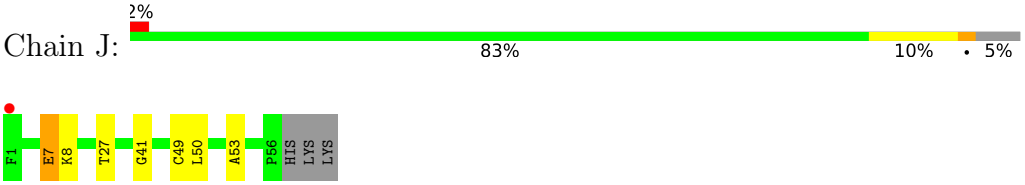
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



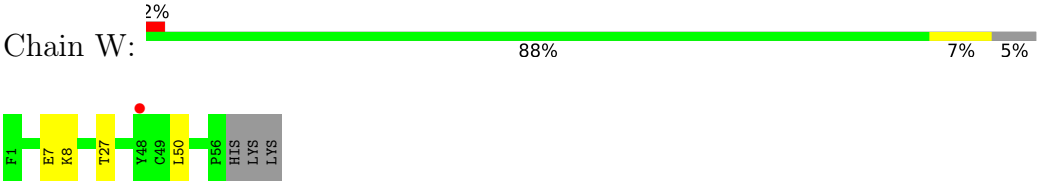
• Molecule 10: Cytochrome c oxidase subunit 7A1

Chain J:



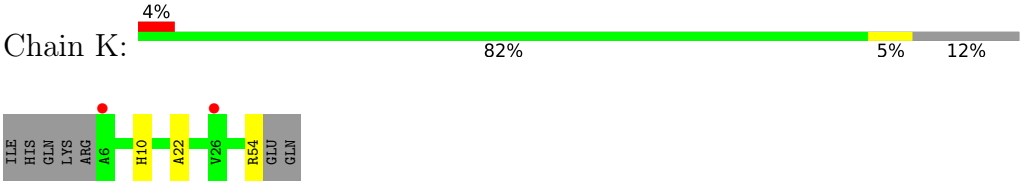
• Molecule 10: Cytochrome c oxidase subunit 7A1

Chain W:



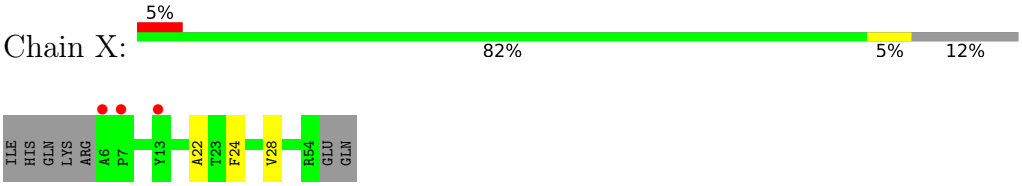
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



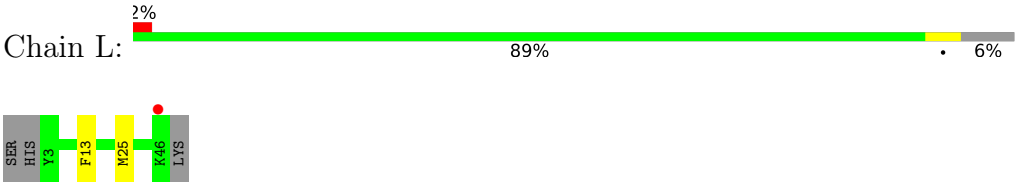
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:



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

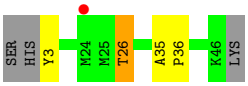
Chain L:



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

Chain Y:

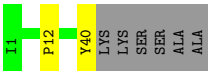




• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:

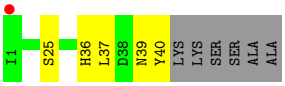




• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

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	182.50Å 204.40Å 177.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.75 40.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.75) 100.0 (40.00-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.130 , 0.167 0.145 , 0.176	Depositor DCC
R_{free} test set	33115 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.667	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.002 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33055	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CO2, CDL, CUA, UNX, HEA, ZN, EDO, LFA, FME, CU, PER, NA, PEK, MG, DMU, CHD, PGV

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.08	4/4259 (0.1%)	1.18	5/5816 (0.1%)
1	N	1.07	4/4259 (0.1%)	1.20	6/5816 (0.1%)
2	B	1.12	1/1908 (0.1%)	1.33	18/2598 (0.7%)
2	O	1.09	2/1908 (0.1%)	1.25	1/2598 (0.0%)
3	C	1.04	1/2258 (0.0%)	1.16	3/3084 (0.1%)
3	P	1.05	1/2258 (0.0%)	1.19	4/3084 (0.1%)
4	D	1.11	1/1226 (0.1%)	1.21	2/1657 (0.1%)
4	Q	1.05	0/1182	1.31	0/1598
5	E	1.11	0/843	1.24	3/1145 (0.3%)
5	R	1.08	0/843	1.34	3/1145 (0.3%)
6	F	1.12	1/724 (0.1%)	1.21	0/983
6	S	1.19	0/724	1.21	0/983
7	G	1.10	2/633 (0.3%)	1.19	0/864
7	T	1.16	1/633 (0.2%)	1.28	0/864
8	H	1.04	0/648	1.33	0/877
8	U	1.07	0/648	1.32	0/877
9	I	1.15	2/588 (0.3%)	1.47	7/781 (0.9%)
9	V	1.10	0/588	1.44	1/781 (0.1%)
10	J	1.06	0/451	1.23	1/610 (0.2%)
10	W	1.08	0/451	1.27	0/610
11	K	1.14	1/398 (0.3%)	1.31	0/546
11	X	1.12	0/398	1.28	0/546
12	L	1.11	0/372	1.29	2/500 (0.4%)
12	Y	1.07	0/372	1.20	0/500
13	M	1.08	0/321	1.20	0/440
13	Z	1.00	0/321	1.34	0/440
All	All	1.09	21/29214 (0.1%)	1.24	56/39743 (0.1%)

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

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

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

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	GLY	C-O	9.00	1.33	1.23
1	N	383	MET	C-O	-7.35	1.13	1.23
1	A	233	HIS	CE1-NE2	7.26	1.39	1.32
3	P	71	HIS	CE1-NE2	7.18	1.39	1.32
1	N	49	GLY	C-O	7.04	1.31	1.23

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	65	TRP	CA-CB-CG	10.99	134.48	113.60
1	N	240	HIS	CA-CB-CG	-10.54	103.26	113.80
1	A	240	HIS	CA-CB-CG	-10.13	103.67	113.80
9	I	72	ALA	CA-C-O	-9.74	104.24	120.80
2	B	65	TRP	CB-CG-CD2	9.64	140.29	126.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4102	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4130	0	4102	45	0
2	B	1870	0	1870	24	0
2	O	1870	0	1870	32	0
3	C	2171	0	2080	32	0
3	P	2172	0	2081	19	0
4	D	1192	0	1178	5	0
4	Q	1148	0	1131	7	0
5	E	825	0	823	1	0
5	R	825	0	823	4	0
6	F	709	0	691	9	0
6	S	709	0	691	11	0
7	G	606	0	577	4	0
7	T	606	0	577	6	0
8	H	628	0	580	14	0
8	U	628	0	580	12	0
9	I	575	0	584	5	0
9	V	575	0	584	4	0
10	J	441	0	439	7	0
10	W	441	0	439	4	0
11	K	384	0	366	1	0
11	X	384	0	366	2	0
12	L	360	0	360	1	0
12	Y	360	0	360	7	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	2	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	64	0	71	1	0
19	C	87	0	124	17	0
19	L	94	0	141	2	0
19	P	87	0	124	7	0
19	V	64	0	72	2	0
19	Y	94	0	141	4	0
20	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	N	3	0	0	0	0
21	A	28	0	54	11	0
21	B	17	0	33	3	0
21	C	114	0	203	5	0
21	N	28	0	54	10	0
21	O	28	0	54	0	0
21	P	114	0	202	7	0
21	T	11	0	21	0	0
22	A	51	0	76	1	0
22	B	66	0	104	0	0
22	C	194	0	262	8	0
22	D	33	0	41	2	0
22	G	11	0	21	0	0
22	H	33	0	30	1	0
22	J	11	0	21	0	0
22	L	22	0	31	0	0
22	M	41	0	56	1	0
22	N	40	0	55	0	0
22	O	66	0	104	2	0
22	P	194	0	262	2	0
22	Q	33	0	41	1	0
22	U	33	0	27	1	0
22	W	11	0	21	0	0
22	Z	63	0	87	2	0
23	A	16	0	24	1	0
23	B	4	0	6	0	0
23	C	12	0	17	0	0
23	E	12	0	18	0	0
23	F	8	0	12	0	0
23	G	4	0	6	0	0
23	N	20	0	30	0	0
23	O	4	0	6	0	0
23	P	12	0	17	0	0
23	R	12	0	18	0	0
23	S	8	0	12	0	0
23	T	4	0	6	0	0
24	A	51	0	76	0	0
24	C	51	0	76	1	0
24	N	51	0	76	1	0
24	P	51	0	76	0	0
25	B	2	0	0	0	0
25	O	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B	29	0	39	1	0
26	C	58	0	78	2	0
26	O	29	0	39	1	0
26	P	58	0	78	4	0
27	C	1	0	0	1	0
27	P	1	0	0	0	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	G	53	0	77	0	0
29	T	53	0	77	5	0
30	A	247	0	0	8	0
30	B	179	0	0	4	0
30	C	104	0	0	5	0
30	D	146	0	0	3	0
30	E	117	0	0	0	0
30	F	108	0	0	1	0
30	G	44	0	0	1	0
30	H	62	0	0	0	0
30	I	39	0	0	1	0
30	J	21	0	0	0	0
30	K	21	0	0	0	0
30	L	26	0	0	0	0
30	M	22	0	0	1	0
30	N	233	0	0	6	0
30	O	150	0	0	2	0
30	P	101	0	0	5	0
30	Q	84	0	0	2	0
30	R	95	0	0	2	0
30	S	97	0	0	0	0
30	T	36	0	0	1	0
30	U	49	0	0	3	0
30	V	23	0	0	1	0
30	W	15	0	0	0	0
30	X	19	0	0	0	0
30	Y	25	0	0	1	0
30	Z	17	0	0	0	0
All	All	33055	0	31469	312	0

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

The worst 5 of 312 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:HG	30:A:2025:HOH:O	1.45	1.16
8:H:52:VAL:HG12	8:U:46:LYS:HG2	1.25	1.12
18:N:606:PER:O2	18:N:606:PER:O1	1.68	1.09
18:A:606:PER:O2	18:A:606:PER:O1	1.70	1.09
1:N:112:LEU:HG	30:N:3014:HOH:O	1.60	1.00

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	526/514 (102%)	513 (98%)	13 (2%)	0	100	100
1	N	526/514 (102%)	513 (98%)	13 (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%)	4 (3%)	0	100	100
5	E	100/109 (92%)	100 (100%)	0	0	100	100
5	R	100/109 (92%)	100 (100%)	0	0	100	100
6	F	91/98 (93%)	89 (98%)	2 (2%)	0	100	100
6	S	91/98 (93%)	89 (98%)	2 (2%)	0	100	100
7	G	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
7	T	71/85 (84%)	69 (97%)	2 (3%)	0	100	100
8	H	73/85 (86%)	69 (94%)	3 (4%)	1 (1%)	9	2
8	U	73/85 (86%)	71 (97%)	1 (1%)	1 (1%)	9	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
9	V	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
10	J	54/59 (92%)	54 (100%)	0	0	100	100
10	W	54/59 (92%)	54 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
12	Y	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
13	M	38/46 (83%)	38 (100%)	0	0	100	100
13	Z	38/46 (83%)	37 (97%)	1 (3%)	0	100	100
All	All	3488/3614 (96%)	3415 (98%)	71 (2%)	2 (0%)	48	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	U	48	GLY
8	H	45	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	440/426 (103%)	438 (100%)	2 (0%)	81	75
1	N	440/426 (103%)	436 (99%)	4 (1%)	70	60
2	B	215/210 (102%)	206 (96%)	9 (4%)	26	8
2	O	215/210 (102%)	208 (97%)	7 (3%)	33	13
3	C	232/226 (103%)	230 (99%)	2 (1%)	70	60
3	P	232/226 (103%)	230 (99%)	2 (1%)	70	60
4	D	128/129 (99%)	127 (99%)	1 (1%)	73	64
4	Q	122/129 (95%)	121 (99%)	1 (1%)	73	64

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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%)	65 52
6	F	78/81 (96%)	74 (95%)	4 (5%)	21 5
6	S	78/81 (96%)	75 (96%)	3 (4%)	29 10
7	G	63/69 (91%)	60 (95%)	3 (5%)	23 6
7	T	63/69 (91%)	60 (95%)	3 (5%)	23 6
8	H	67/75 (89%)	63 (94%)	4 (6%)	17 3
8	U	67/75 (89%)	65 (97%)	2 (3%)	36 16
9	I	55/58 (95%)	54 (98%)	1 (2%)	51 33
9	V	55/58 (95%)	51 (93%)	4 (7%)	13 2
10	J	47/50 (94%)	46 (98%)	1 (2%)	47 27
10	W	47/50 (94%)	45 (96%)	2 (4%)	26 8
11	K	39/46 (85%)	38 (97%)	1 (3%)	40 20
11	X	39/46 (85%)	39 (100%)	0	100 100
12	L	37/40 (92%)	37 (100%)	0	100 100
12	Y	37/40 (92%)	36 (97%)	1 (3%)	39 19
13	M	34/38 (90%)	34 (100%)	0	100 100
13	Z	34/38 (90%)	33 (97%)	1 (3%)	37 17
All	All	3042/3086 (99%)	2983 (98%)	59 (2%)	50 31

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	112	LEU
10	W	7	GLU
2	O	78	LEU
9	V	65	LYS
8	U	46	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	29	ASN
8	U	22	ASN
2	O	59	GLN

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Mol	Chain	Res	Type
8	U	32	ASN
5	R	94	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	O	1	2	8,9,10	0.78	0	7,9,11	1.16	1 (14%)
1	FME	N	1	1	8,9,10	0.78	0	7,9,11	1.32	2 (28%)
2	FME	B	1	2	8,9,10	1.07	1 (12%)	7,9,11	1.30	1 (14%)
1	FME	A	1	1	8,9,10	0.48	0	7,9,11	1.13	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-
2	FME	B	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	-2.55	1.67	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	CG-CB-CA	-2.68	105.50	112.95
1	N	1	FME	CA-N-CN	2.41	126.53	122.82
1	N	1	FME	O-C-CA	-2.29	118.77	124.78
1	A	1	FME	C-CA-N	2.18	113.66	109.73
2	O	1	FME	CA-N-CN	2.06	125.99	122.82

There are no chirality outliers.

All (4) 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	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	DMU	A	612	-	34,34,34	1.25	5 (14%)	45,45,45	1.20	4 (8%)
29	PEK	T	101	-	52,52,52	0.65	2 (3%)	55,57,57	0.86	4 (7%)
21	LFA	T	102	-	10,10,19	0.21	0	9,9,18	0.17	0
22	DMU	P	317	-	6,6,34	0.30	0	5,5,45	0.40	0
22	DMU	N	611	-	34,34,34	1.43	5 (14%)	45,45,45	1.23	4 (8%)
21	LFA	O	302	-	16,16,19	0.27	0	15,15,18	0.19	0
22	DMU	A	618	-	10,10,34	0.30	0	9,9,45	0.55	0
19	CDL	Y	101	-	93,93,99	0.39	0	99,105,111	0.51	0
23	EDO	P	323	-	3,3,3	0.64	0	2,2,2	0.95	0
22	DMU	P	316	-	34,34,34	0.75	0	45,45,45	1.44	5 (11%)
25	CUA	O	305	2	0,1,1	-	-	-		
23	EDO	T	103	-	3,3,3	0.27	0	2,2,2	0.18	0
22	DMU	N	610	-	6,6,34	0.41	0	5,5,45	0.33	0
22	DMU	B	302	-	10,10,34	0.24	0	9,9,45	0.62	0
22	DMU	B	303	-	10,10,34	0.31	0	9,9,45	0.58	0
14	HEA	N	601[A]	-	66,67,67	1.88	21 (31%)	78,103,103	2.68	29 (37%)
25	CUA	B	301	2	0,1,1	-	-	-		
21	LFA	C	314	-	12,12,19	0.28	0	11,11,18	0.18	0
22	DMU	Z	102	-	22,22,34	0.67	0	27,27,45	1.13	2 (7%)
23	EDO	F	103	-	3,3,3	0.18	0	2,2,2	0.35	0
22	DMU	C	316	-	6,6,34	0.24	0	5,5,45	0.56	0
22	DMU	A	611	-	6,6,34	0.59	0	5,5,45	0.27	0
22	DMU	C	324	-	34,34,34	0.80	0	45,45,45	1.25	3 (6%)
20	CO2	A	608	-	2,2,2	0.22	0	1,1,1	0.31	0
22	DMU	B	308	-	22,22,34	0.64	0	27,27,45	1.49	3 (11%)
19	CDL	P	305	-	86,86,99	0.57	1 (1%)	92,98,111	0.82	2 (2%)
29	PEK	G	101	-	52,52,52	0.59	1 (1%)	55,57,57	0.70	0
26	CHD	C	301	-	32,32,32	0.95	3 (9%)	51,51,51	0.74	0
24	PGV	C	303	-	50,50,50	0.73	1 (2%)	53,56,56	1.13	5 (9%)
21	LFA	P	310	22	17,17,19	0.20	0	16,16,18	0.18	0
26	CHD	C	305	-	32,32,32	0.72	0	51,51,51	1.57	6 (11%)
21	LFA	P	309	-	5,5,19	0.24	0	4,4,18	0.08	0
22	DMU	Z	103	-	7,7,34	0.39	0	6,6,45	0.48	0
22	DMU	O	304	-	22,22,34	0.82	1 (4%)	27,27,45	1.23	3 (11%)
22	DMU	C	319	-	34,34,34	0.72	0	45,45,45	1.27	7 (15%)
14	HEA	A	602	1,18	66,67,67	1.89	18 (27%)	78,103,103	2.44	31 (39%)
21	LFA	C	309	22	17,17,19	0.23	0	16,16,18	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	EDO	S	103	-	3,3,3	0.04	0	2,2,2	0.13	0
22	DMU	C	323	-	22,22,34	0.75	0	27,27,45	1.02	1 (3%)
21	LFA	A	609	-	13,13,19	0.35	0	12,12,18	0.18	0
21	LFA	C	312	-	10,10,19	0.22	0	9,9,18	0.25	0
22	DMU	O	307	-	10,10,34	0.35	0	9,9,45	0.56	0
22	DMU	M	102	-	7,7,34	0.25	0	6,6,45	0.54	0
14	HEA	N	602	1,18	66,67,67	2.01	22 (33%)	78,103,103	2.74	34 (43%)
23	EDO	G	103	-	3,3,3	0.34	0	2,2,2	0.18	0
23	EDO	C	322	-	3,3,3	0.87	0	2,2,2	0.71	0
21	LFA	P	311	-	10,10,19	0.17	0	9,9,18	0.08	0
22	DMU	C	315	-	34,34,34	0.79	1 (2%)	45,45,45	1.39	7 (15%)
24	PGV	N	617	-	50,50,50	0.80	1 (2%)	53,56,56	1.29	4 (7%)
23	EDO	P	322	-	3,3,3	0.14	0	2,2,2	0.29	0
23	EDO	N	616	-	3,3,3	0.39	0	2,2,2	0.33	0
21	LFA	P	312	-	13,13,19	0.19	0	12,12,18	0.18	0
22	DMU	P	318	-	22,22,34	0.87	1 (4%)	27,27,45	1.29	3 (11%)
21	LFA	P	314	-	14,14,19	0.27	0	13,13,18	0.17	0
22	DMU	Q	201	-	34,34,34	1.39	7 (20%)	45,45,45	1.69	8 (17%)
26	CHD	P	302	-	32,32,32	0.92	3 (9%)	51,51,51	0.86	0
26	CHD	O	301	-	32,32,32	0.72	0	51,51,51	0.90	1 (1%)
22	DMU	C	317	-	22,22,34	0.57	0	27,27,45	1.23	3 (11%)
14	HEA	A	601[B]	-	66,67,67	1.92	20 (30%)	78,103,103	2.55	31 (39%)
22	DMU	P	324	-	22,22,34	0.59	0	27,27,45	1.52	2 (7%)
22	DMU	H	101	21	34,34,34	0.89	2 (5%)	45,45,45	1.17	4 (8%)
26	CHD	P	306	-	32,32,32	0.98	1 (3%)	51,51,51	0.88	1 (1%)
22	DMU	O	306	-	10,10,34	0.22	0	9,9,45	0.60	0
22	DMU	O	308	-	22,22,34	0.70	0	27,27,45	1.21	4 (14%)
20	CO2	N	607	-	2,2,2	0.08	0	1,1,1	0.29	0
26	CHD	B	306	-	32,32,32	0.75	0	51,51,51	0.75	0
23	EDO	N	615	-	3,3,3	0.32	0	2,2,2	0.15	0
23	EDO	R	201	-	3,3,3	0.14	0	2,2,2	0.10	0
21	LFA	A	610	-	13,13,19	0.58	0	12,12,18	0.40	0
19	CDL	V	101	-	63,63,99	0.54	0	69,75,111	1.33	8 (11%)
18	PER	A	606	15,14	1,1,1	2.70	1 (100%)	-		
23	EDO	A	615	-	3,3,3	0.55	0	2,2,2	0.30	0
23	EDO	E	201	-	3,3,3	0.15	0	2,2,2	0.03	0
18	PER	N	606	15,14	1,1,1	2.54	1 (100%)	-		
21	LFA	C	310	-	10,10,19	0.13	0	9,9,18	0.09	0
22	DMU	W	101	-	10,10,34	0.24	0	9,9,45	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	HEA	N	601[B]	-	66,67,67	1.89	21 (31%)	78,103,103	2.62	28 (35%)
23	EDO	S	102	-	3,3,3	0.30	0	2,2,2	0.12	0
23	EDO	N	613	-	3,3,3	0.18	0	2,2,2	0.27	0
21	LFA	C	311	-	13,13,19	0.23	0	12,12,18	0.16	0
23	EDO	A	613	-	3,3,3	0.26	0	2,2,2	0.21	0
21	LFA	P	301	-	14,14,19	0.16	0	13,13,18	0.10	0
23	EDO	A	614	-	3,3,3	0.13	0	2,2,2	0.17	0
22	DMU	B	304	-	22,22,34	0.77	1 (4%)	27,27,45	0.94	1 (3%)
23	EDO	N	612	-	3,3,3	0.35	0	2,2,2	0.25	0
24	PGV	P	304	-	50,50,50	0.87	2 (4%)	53,56,56	0.92	3 (5%)
23	EDO	R	202	-	3,3,3	0.16	0	2,2,2	0.27	0
23	EDO	N	614	-	3,3,3	0.27	0	2,2,2	0.15	0
23	EDO	A	616	-	3,3,3	0.31	0	2,2,2	0.44	0
19	CDL	L	101	-	93,93,99	0.39	0	99,105,111	0.69	2 (2%)
21	LFA	P	308	-	10,10,19	0.19	0	9,9,18	0.16	0
23	EDO	E	203	-	3,3,3	0.18	0	2,2,2	0.19	0
23	EDO	F	102	-	3,3,3	0.24	0	2,2,2	0.24	0
21	LFA	N	608	-	13,13,19	0.35	0	12,12,18	0.36	0
22	DMU	J	101	-	10,10,34	0.21	0	9,9,45	0.65	0
22	DMU	M	101	-	34,34,34	0.98	2 (5%)	45,45,45	1.03	4 (8%)
21	LFA	C	307	-	10,10,19	0.22	0	9,9,18	0.23	0
19	CDL	A	607	-	63,63,99	0.59	0	69,75,111	1.24	6 (8%)
22	DMU	P	307	-	10,10,34	0.28	0	9,9,45	0.66	0
21	LFA	O	303	-	10,10,19	0.18	0	9,9,18	0.09	0
23	EDO	E	202	-	3,3,3	0.26	0	2,2,2	0.09	0
23	EDO	O	309	-	3,3,3	0.19	0	2,2,2	0.29	0
23	EDO	R	203	-	3,3,3	0.39	0	2,2,2	0.57	0
19	CDL	C	304	-	86,86,99	0.59	0	92,98,111	1.13	11 (11%)
23	EDO	P	321	-	3,3,3	0.14	0	2,2,2	0.10	0
22	DMU	D	201	-	34,34,34	1.43	5 (14%)	45,45,45	1.58	8 (17%)
22	DMU	G	102	-	10,10,34	0.29	0	9,9,45	0.56	0
21	LFA	B	307	-	16,16,19	0.38	0	15,15,18	0.20	0
21	LFA	P	313	-	10,10,19	0.18	0	9,9,18	0.27	0
22	DMU	C	318	-	34,34,34	1.02	3 (8%)	45,45,45	1.25	4 (8%)
22	DMU	C	306	-	10,10,34	0.40	0	9,9,45	0.52	0
21	LFA	C	325	-	14,14,19	0.17	0	13,13,18	0.08	0
21	LFA	N	609	-	13,13,19	0.65	0	12,12,18	0.39	0
22	DMU	P	325	-	34,34,34	0.61	0	45,45,45	1.47	5 (11%)
23	EDO	C	320	-	3,3,3	0.07	0	2,2,2	0.14	0
22	DMU	U	101	21	34,34,34	0.86	2 (5%)	45,45,45	1.27	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	DMU	P	319	-	34,34,34	0.88	3 (8%)	45,45,45	1.14	2 (4%)
22	DMU	Z	101	-	34,34,34	0.97	2 (5%)	45,45,45	1.09	3 (6%)
21	LFA	C	313	-	14,14,19	0.30	0	13,13,18	0.43	0
23	EDO	B	305	-	3,3,3	0.19	0	2,2,2	0.31	0
23	EDO	C	321	-	3,3,3	0.27	0	2,2,2	0.24	0
24	PGV	A	617	-	50,50,50	0.78	2 (4%)	53,56,56	1.08	2 (3%)
14	HEA	A	601[A]	-	66,67,67	1.92	20 (30%)	78,103,103	2.49	29 (37%)
21	LFA	C	308	-	5,5,19	0.21	0	4,4,18	0.09	0
22	DMU	P	320	-	34,34,34	1.05	3 (8%)	45,45,45	1.31	2 (4%)
21	LFA	P	315	-	12,12,19	0.29	0	11,11,18	0.29	0
22	DMU	L	102	-	22,22,34	0.76	0	27,27,45	1.08	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	DMU	A	612	-	-	7/19/59/59	0/2/2/2
29	PEK	T	101	-	-	20/56/56/56	-
21	LFA	T	102	-	-	3/8/8/17	-
22	DMU	P	317	-	-	3/4/4/59	-
22	DMU	N	611	-	-	5/19/59/59	0/2/2/2
21	LFA	O	302	-	-	12/14/14/17	-
22	DMU	A	618	-	-	6/8/8/59	-
19	CDL	Y	101	-	-	50/104/104/110	-
23	EDO	P	323	-	-	0/1/1/1	-
22	DMU	P	316	-	-	11/19/59/59	0/2/2/2
23	EDO	T	103	-	-	0/1/1/1	-
22	DMU	N	610	-	-	2/4/4/59	-
22	DMU	B	302	-	-	4/8/8/59	-
22	DMU	B	303	-	-	5/8/8/59	-
14	HEA	N	601[A]	-	-	6/36/76/76	-
21	LFA	C	314	-	-	3/10/10/17	-
22	DMU	Z	102	-	-	11/13/33/59	0/1/1/2
23	EDO	F	103	-	-	1/1/1/1	-
22	DMU	C	316	-	-	3/4/4/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	DMU	A	611	-	-	2/4/4/59	-
22	DMU	C	324	-	-	4/19/59/59	0/2/2/2
22	DMU	B	308	-	-	9/13/33/59	0/1/1/2
19	CDL	P	305	-	-	53/97/97/110	-
29	PEK	G	101	-	-	15/56/56/56	-
26	CHD	C	301	-	-	2/9/74/74	0/4/4/4
24	PGV	C	303	-	-	10/55/55/55	-
21	LFA	P	310	22	-	9/15/15/17	-
26	CHD	C	305	-	-	7/9/74/74	0/4/4/4
21	LFA	P	309	-	-	0/3/3/17	-
22	DMU	Z	103	-	-	2/5/5/59	-
22	DMU	O	304	-	-	7/13/33/59	0/1/1/2
22	DMU	C	319	-	-	10/19/59/59	0/2/2/2
14	HEA	A	602	1,18	-	4/36/76/76	-
21	LFA	C	309	22	-	8/15/15/17	-
23	EDO	S	103	-	-	0/1/1/1	-
22	DMU	C	323	-	-	9/13/33/59	0/1/1/2
21	LFA	A	609	-	-	4/11/11/17	-
21	LFA	C	312	-	-	4/8/8/17	-
22	DMU	O	307	-	-	3/8/8/59	-
22	DMU	M	102	-	-	4/5/5/59	-
14	HEA	N	602	1,18	-	4/36/76/76	-
23	EDO	G	103	-	-	0/1/1/1	-
23	EDO	C	322	-	-	0/1/1/1	-
21	LFA	P	311	-	-	6/8/8/17	-
22	DMU	C	315	-	-	11/19/59/59	0/2/2/2
24	PGV	N	617	-	-	6/55/55/55	-
23	EDO	P	322	-	-	0/1/1/1	-
23	EDO	N	616	-	-	0/1/1/1	-
21	LFA	P	312	-	-	5/11/11/17	-
22	DMU	P	318	-	-	6/13/33/59	0/1/1/2
21	LFA	P	314	-	-	6/12/12/17	-
22	DMU	Q	201	-	-	9/19/59/59	0/2/2/2
26	CHD	P	302	-	-	2/9/74/74	0/4/4/4
26	CHD	O	301	-	-	2/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	DMU	C	317	-	-	8/13/33/59	0/1/1/2
14	HEA	A	601[B]	-	-	4/36/76/76	-
22	DMU	P	324	-	-	7/13/33/59	0/1/1/2
22	DMU	H	101	21	-	7/19/59/59	0/2/2/2
26	CHD	P	306	-	-	5/9/74/74	0/4/4/4
22	DMU	O	306	-	-	3/8/8/59	-
22	DMU	O	308	-	-	4/13/33/59	0/1/1/2
26	CHD	B	306	-	-	2/9/74/74	0/4/4/4
23	EDO	N	615	-	-	0/1/1/1	-
23	EDO	R	201	-	-	1/1/1/1	-
21	LFA	A	610	-	-	5/11/11/17	-
19	CDL	V	101	-	-	41/74/74/110	-
23	EDO	A	615	-	-	0/1/1/1	-
23	EDO	E	201	-	-	0/1/1/1	-
21	LFA	C	310	-	-	7/8/8/17	-
22	DMU	W	101	-	-	5/8/8/59	-
14	HEA	N	601[B]	-	-	3/36/76/76	-
23	EDO	S	102	-	-	0/1/1/1	-
23	EDO	N	613	-	-	0/1/1/1	-
21	LFA	C	311	-	-	7/11/11/17	-
23	EDO	A	613	-	-	0/1/1/1	-
21	LFA	P	301	-	-	6/12/12/17	-
23	EDO	A	614	-	-	1/1/1/1	-
22	DMU	B	304	-	-	6/13/33/59	0/1/1/2
23	EDO	N	612	-	-	0/1/1/1	-
24	PGV	P	304	-	-	10/55/55/55	-
23	EDO	R	202	-	-	0/1/1/1	-
23	EDO	N	614	-	-	0/1/1/1	-
23	EDO	A	616	-	-	0/1/1/1	-
19	CDL	L	101	-	-	50/104/104/110	-
21	LFA	P	308	-	-	7/8/8/17	-
23	EDO	E	203	-	-	0/1/1/1	-
23	EDO	F	102	-	-	0/1/1/1	-
21	LFA	N	608	-	-	4/11/11/17	-
22	DMU	J	101	-	-	3/8/8/59	-
22	DMU	M	101	-	-	4/19/59/59	0/2/2/2
21	LFA	C	307	-	-	6/8/8/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CDL	A	607	-	-	38/74/74/110	-
22	DMU	P	307	-	-	2/8/8/59	-
21	LFA	O	303	-	-	2/8/8/17	-
23	EDO	E	202	-	-	0/1/1/1	-
23	EDO	O	309	-	-	0/1/1/1	-
23	EDO	R	203	-	-	1/1/1/1	-
19	CDL	C	304	-	-	43/97/97/110	-
23	EDO	P	321	-	-	0/1/1/1	-
22	DMU	D	201	-	-	7/19/59/59	0/2/2/2
22	DMU	G	102	-	-	5/8/8/59	-
21	LFA	B	307	-	-	11/14/14/17	-
21	LFA	P	313	-	-	5/8/8/17	-
22	DMU	C	318	-	-	12/19/59/59	0/2/2/2
22	DMU	C	306	-	-	2/8/8/59	-
21	LFA	C	325	-	-	8/12/12/17	-
21	LFA	N	609	-	-	4/11/11/17	-
22	DMU	P	325	-	-	5/19/59/59	0/2/2/2
23	EDO	C	320	-	-	1/1/1/1	-
22	DMU	U	101	21	-	5/19/59/59	0/2/2/2
22	DMU	P	319	-	-	15/19/59/59	0/2/2/2
22	DMU	Z	101	-	-	7/19/59/59	0/2/2/2
21	LFA	C	313	-	-	2/12/12/17	-
23	EDO	B	305	-	-	0/1/1/1	-
23	EDO	C	321	-	-	0/1/1/1	-
24	PGV	A	617	-	-	8/55/55/55	-
14	HEA	A	601[A]	-	-	5/36/76/76	-
21	LFA	C	308	-	-	1/3/3/17	-
22	DMU	P	320	-	-	8/19/59/59	0/2/2/2
21	LFA	P	315	-	-	6/10/10/17	-
22	DMU	L	102	-	-	8/13/33/59	0/1/1/2

The worst 5 of 184 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	611	DMU	O16-C6	-5.20	1.31	1.40
14	N	602	HEA	C1D-ND	-5.01	1.31	1.40
14	A	601[A]	HEA	C3A-C2A	4.61	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[B]	HEA	C3A-C2A	4.61	1.46	1.36
14	N	602	HEA	CHB-C4A	4.47	1.47	1.38

The worst 5 of 335 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	601[A]	HEA	C3C-C4C-NC	9.42	116.04	110.25
14	A	601[B]	HEA	C3C-C4C-NC	9.42	116.04	110.25
14	N	601[A]	HEA	C3D-C4D-ND	7.88	117.99	110.36
14	N	601[B]	HEA	C3D-C4D-ND	7.88	117.99	110.36
14	N	602	HEA	C3C-C4C-NC	7.75	115.02	110.25

There are no chirality outliers.

5 of 792 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	A	601[B]	HEA	C18-C19-C20-C21
14	A	601[B]	HEA	C27-C19-C20-C21
14	N	601[A]	HEA	C27-C19-C20-C21

There are no ring outliers.

42 monomers are involved in 112 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	612	DMU	1	0
29	T	101	PEK	5	0
19	Y	101	CDL	4	0
22	Z	102	DMU	2	0
22	C	324	DMU	7	0
19	P	305	CDL	7	0
24	C	303	PGV	1	0
21	P	310	LFA	2	0
26	C	305	CHD	2	0
21	A	609	LFA	4	0
21	C	312	LFA	2	0
22	M	102	DMU	1	0
14	N	602	HEA	1	0
24	N	617	PGV	1	0
22	Q	201	DMU	1	0

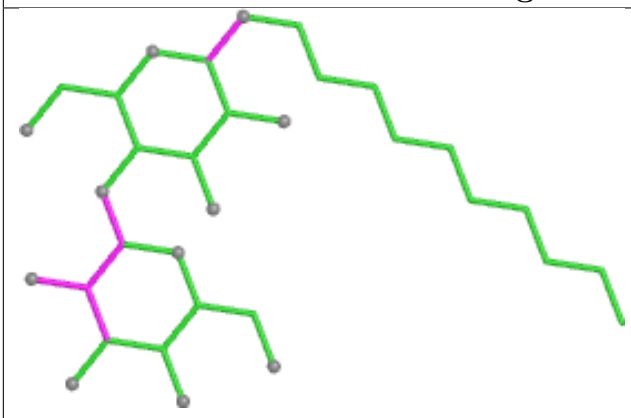
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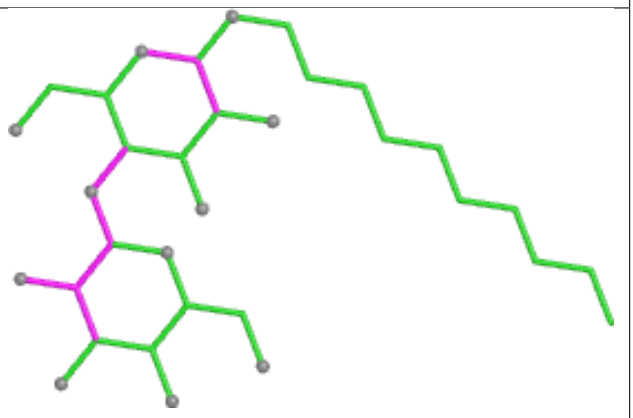
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	P	302	CHD	1	0
26	O	301	CHD	1	0
14	A	601[B]	HEA	1	0
22	H	101	DMU	1	0
26	P	306	CHD	3	0
22	O	306	DMU	2	0
26	B	306	CHD	1	0
21	A	610	LFA	8	0
19	V	101	CDL	2	0
18	A	606	PER	1	0
18	N	606	PER	1	0
14	N	601[B]	HEA	1	0
23	A	614	EDO	1	0
19	L	101	CDL	2	0
21	P	308	LFA	3	0
21	N	608	LFA	6	0
21	C	307	LFA	3	0
19	A	607	CDL	1	0
19	C	304	CDL	17	0
22	D	201	DMU	2	0
21	B	307	LFA	3	0
21	P	313	LFA	2	0
22	C	318	DMU	1	0
21	N	609	LFA	6	0
22	P	325	DMU	2	0
22	U	101	DMU	1	0
14	A	601[A]	HEA	3	0

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

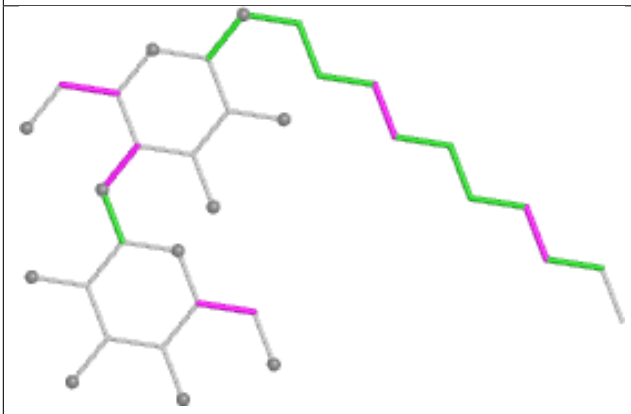
Ligand DMU A 612



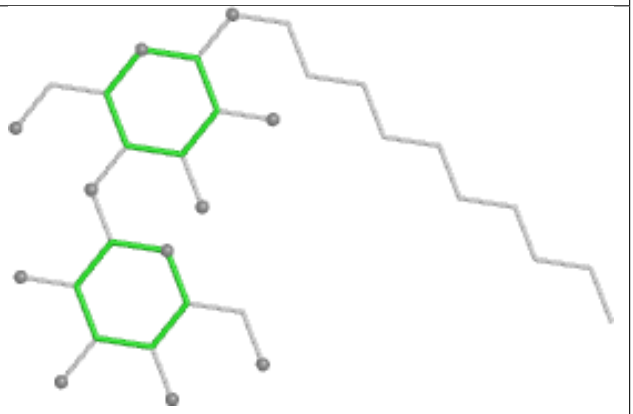
Bond lengths



Bond angles

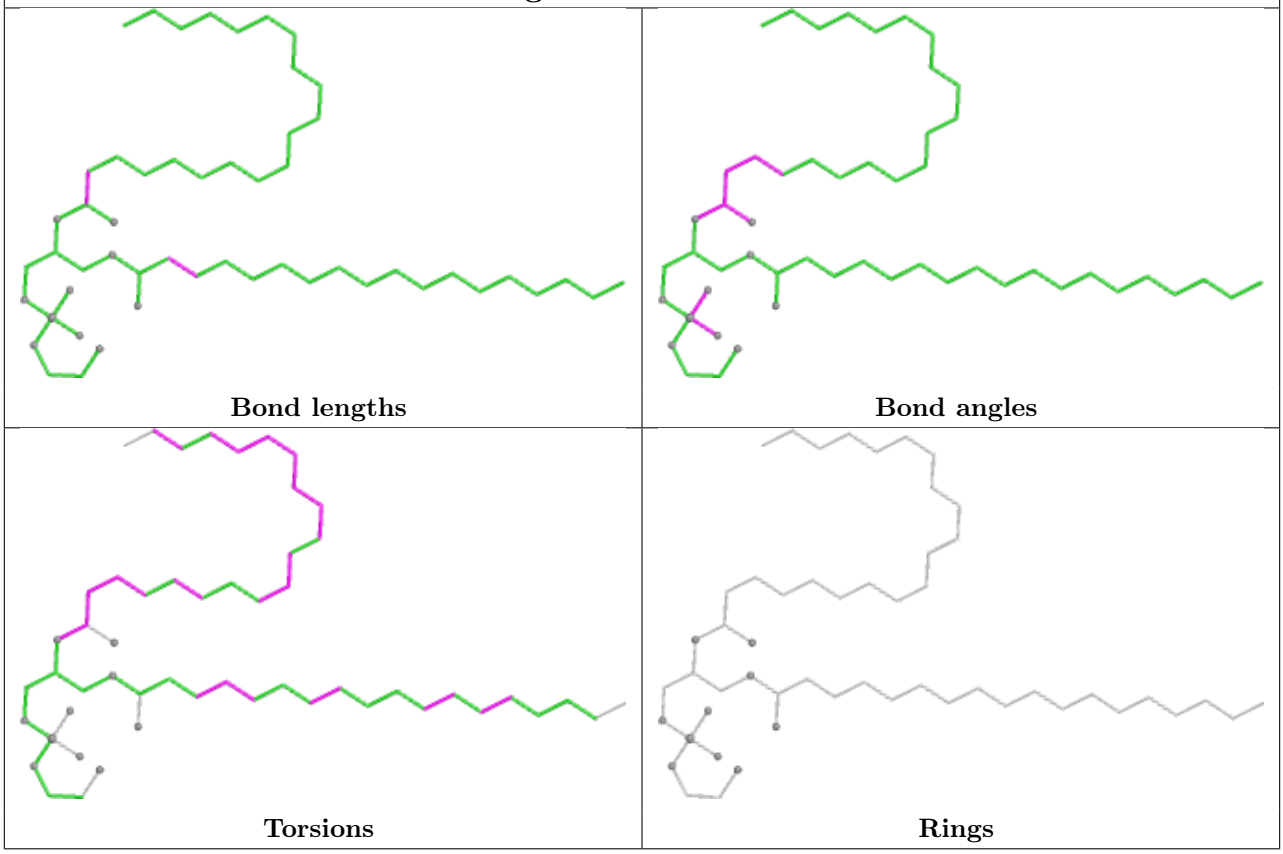


Torsions

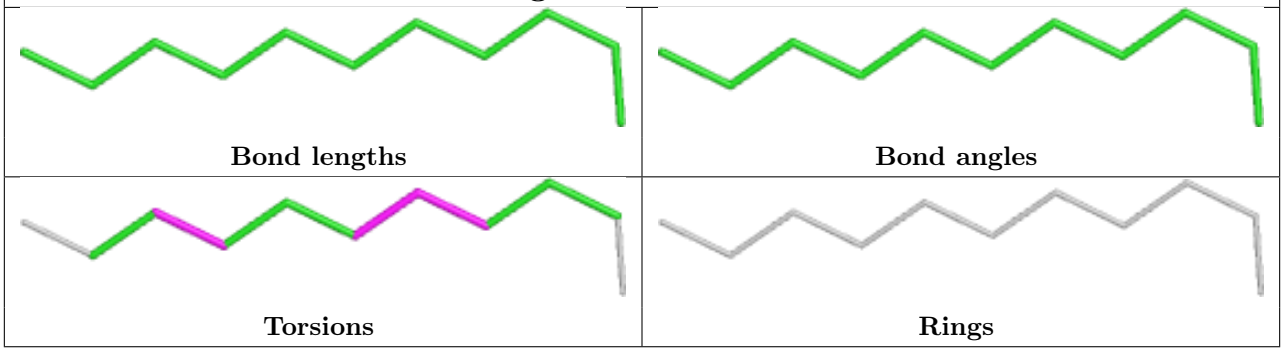


Rings

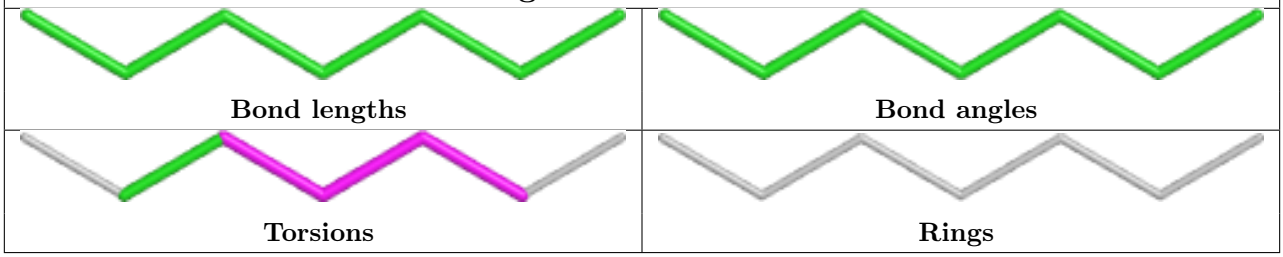
Ligand PEK T 101



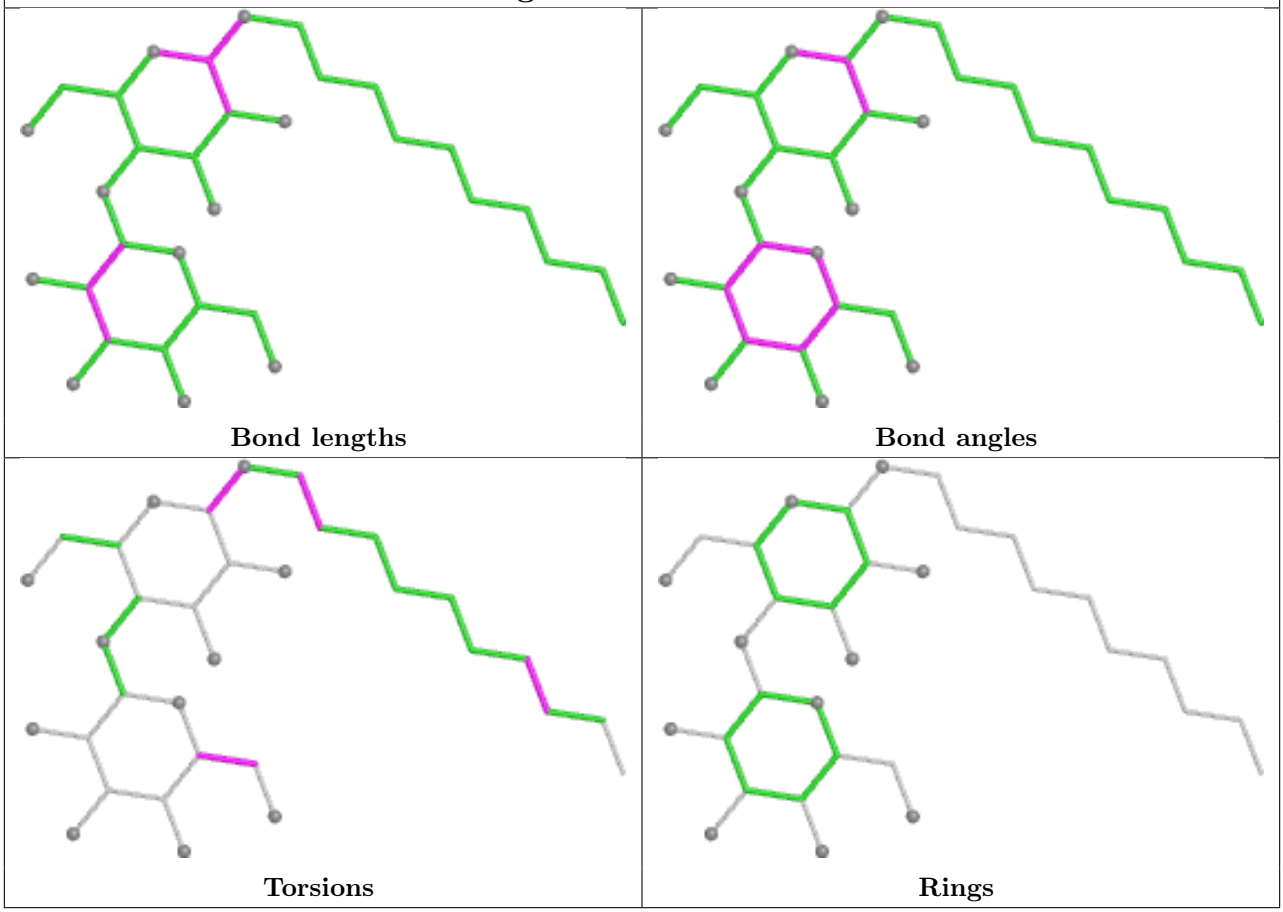
Ligand LFA T 102



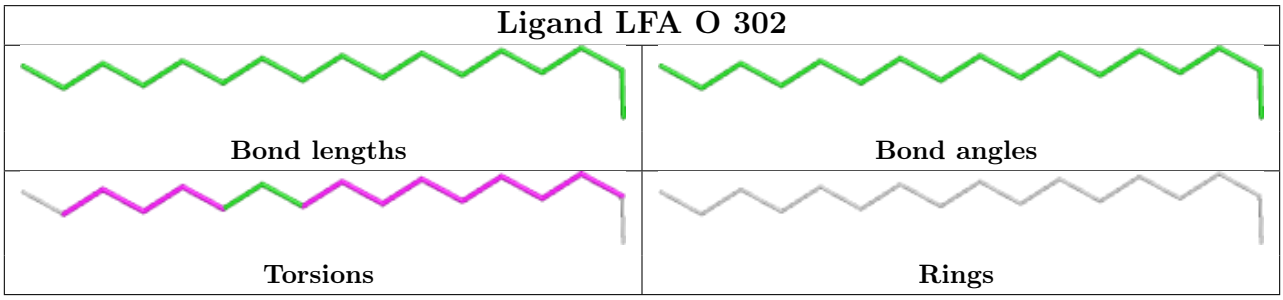
Ligand DMU P 317



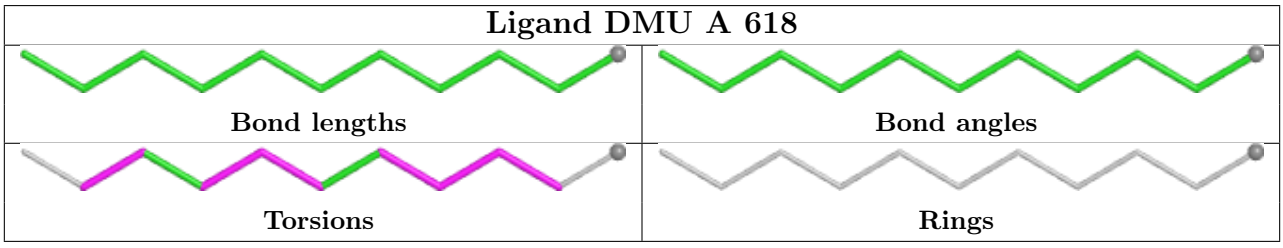
Ligand DMU N 611



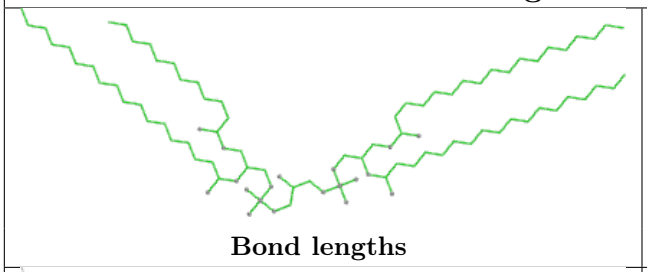
Ligand LFA O 302



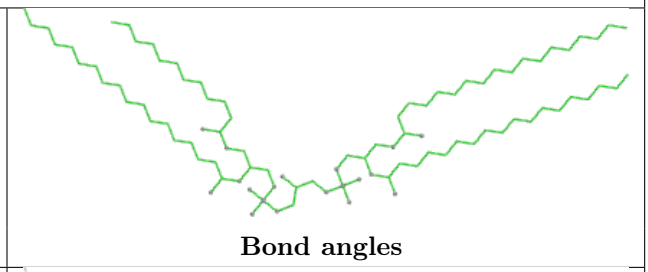
Ligand DMU A 618



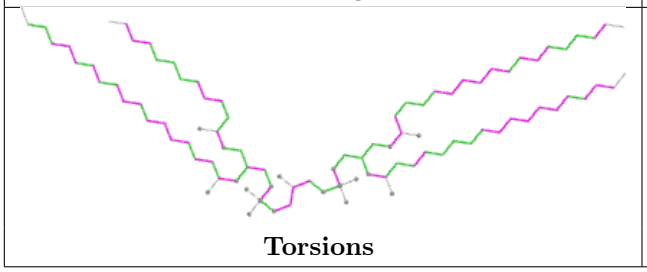
Ligand CDL Y 101



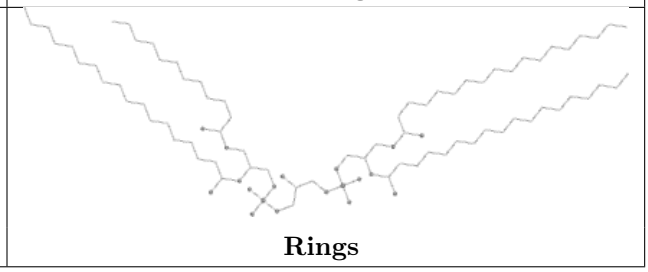
Bond lengths



Bond angles

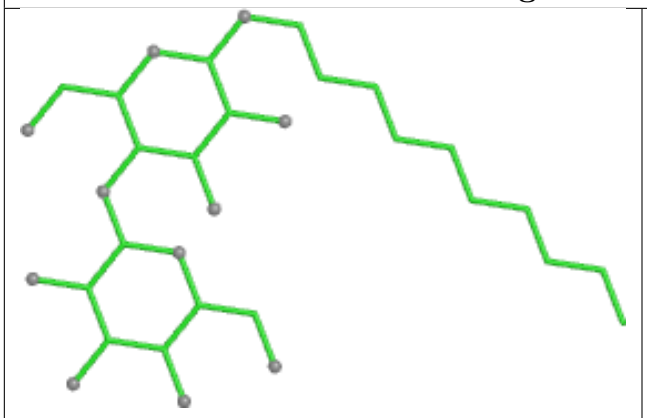


Torsions

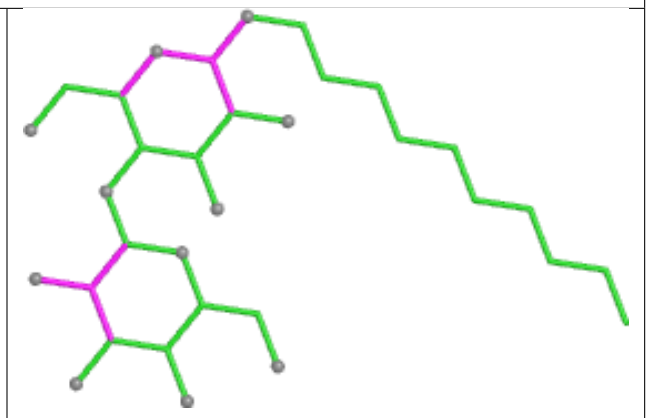


Rings

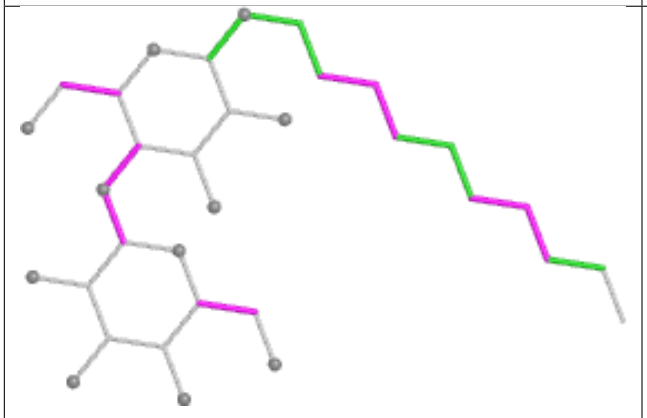
Ligand DMU P 316



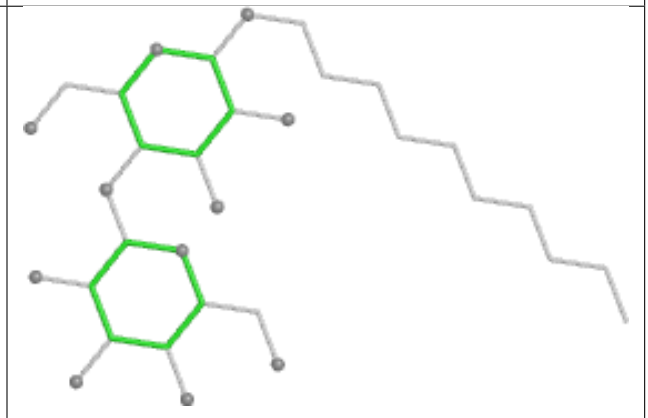
Bond lengths



Bond angles

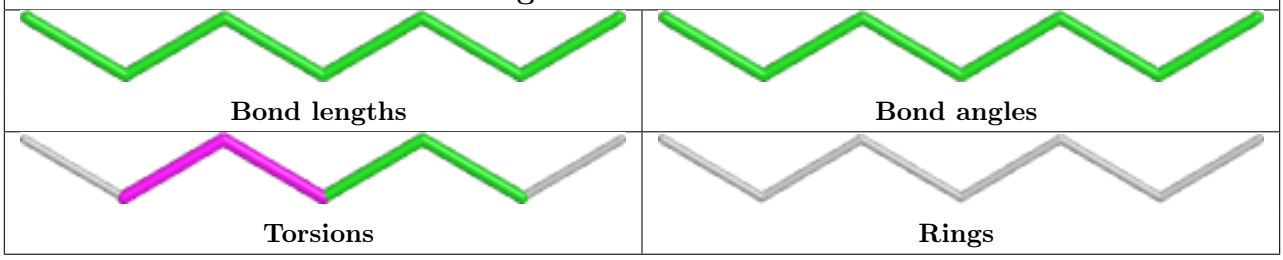


Torsions

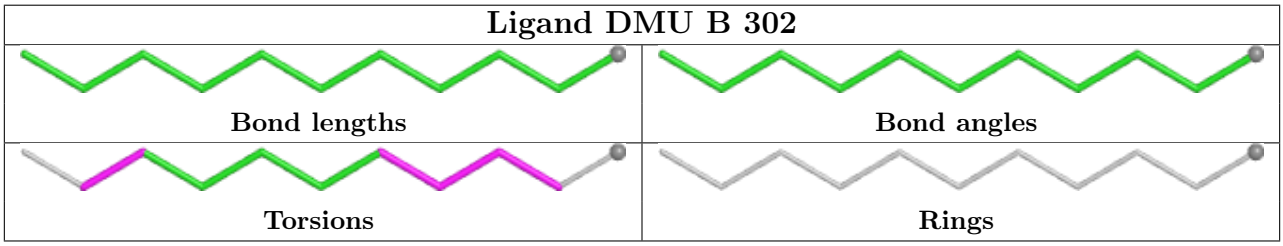


Rings

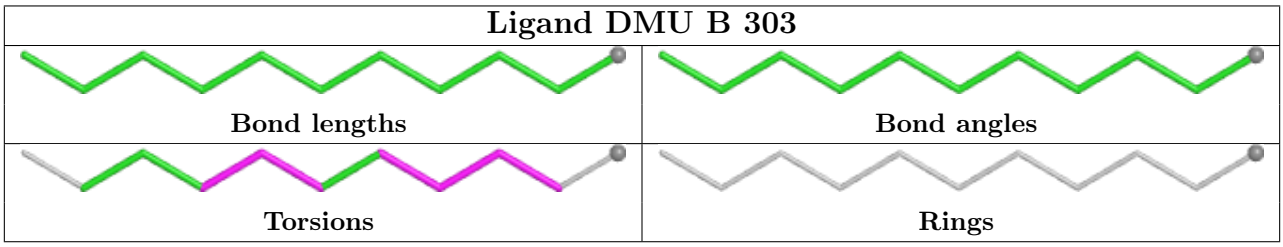
Ligand DMU N 610



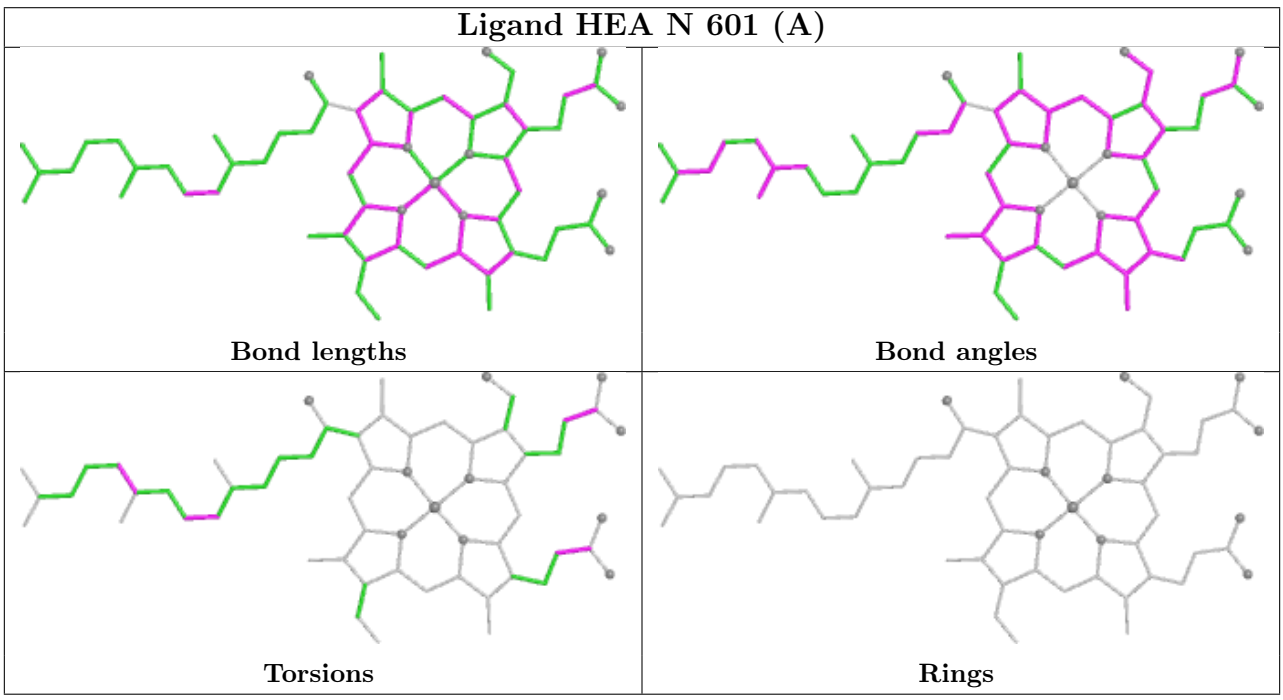
Ligand DMU B 302



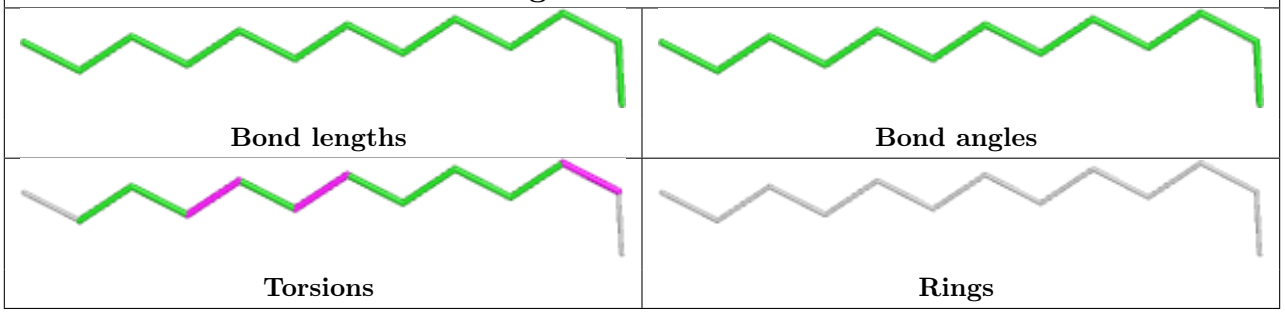
Ligand DMU B 303



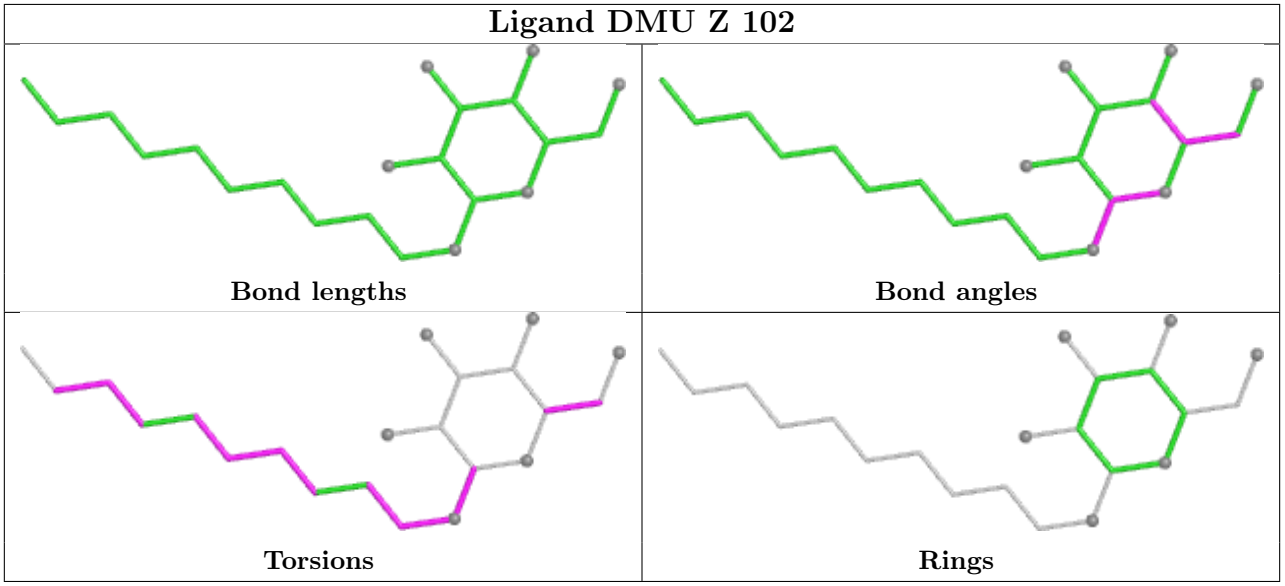
Ligand HEA N 601 (A)



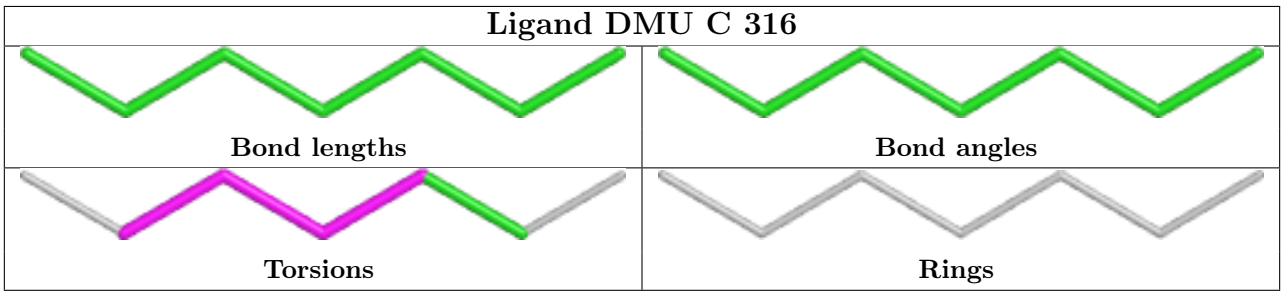
Ligand LFA C 314



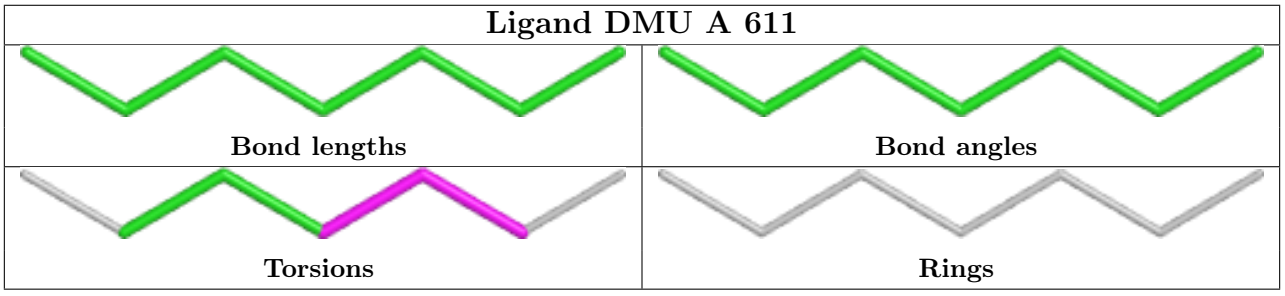
Ligand DMU Z 102



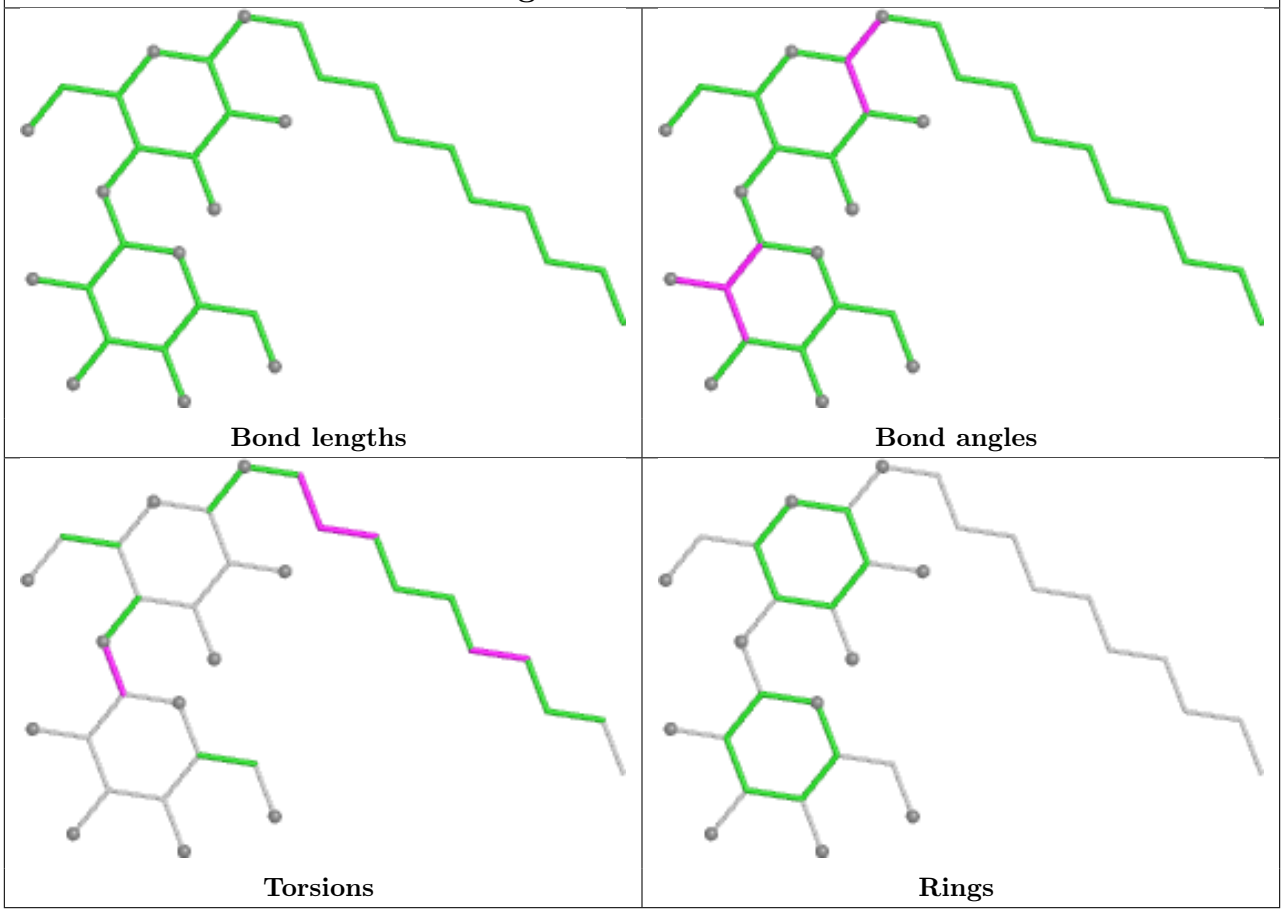
Ligand DMU C 316



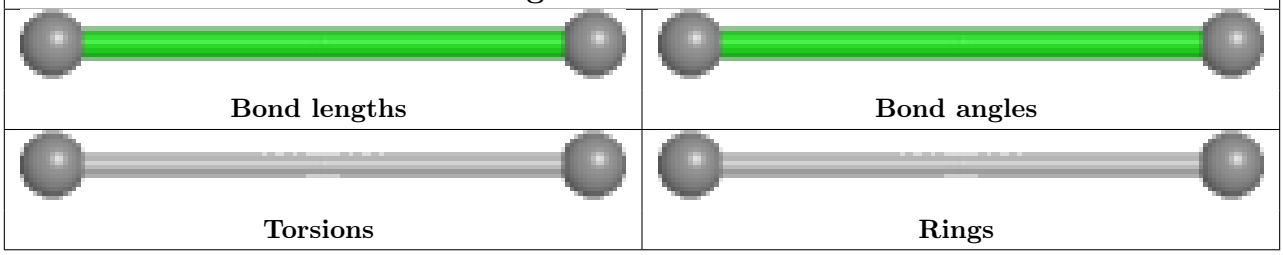
Ligand DMU A 611



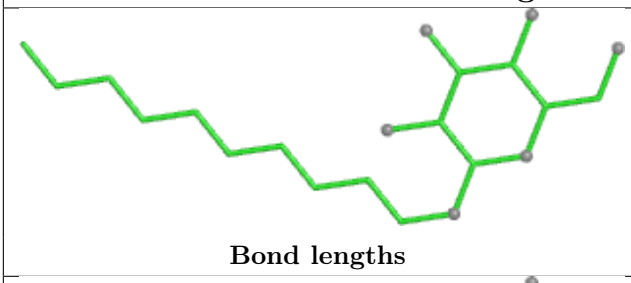
Ligand DMU C 324



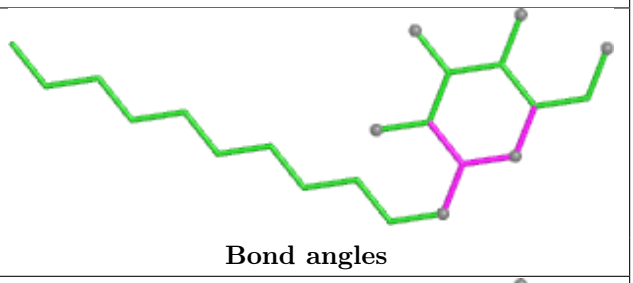
Ligand CO2 A 608



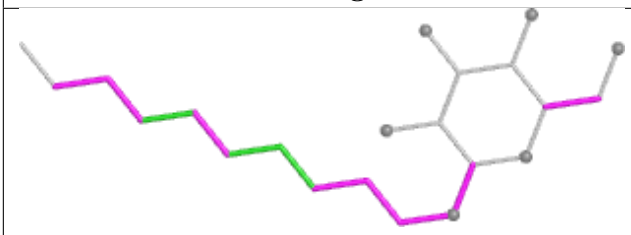
Ligand DMU B 308



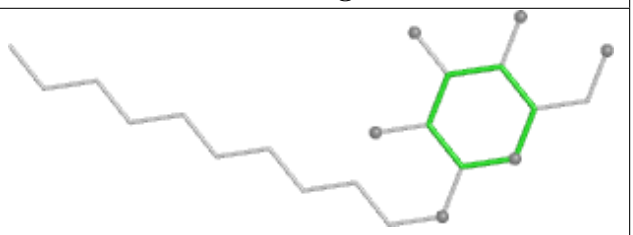
Bond lengths



Bond angles

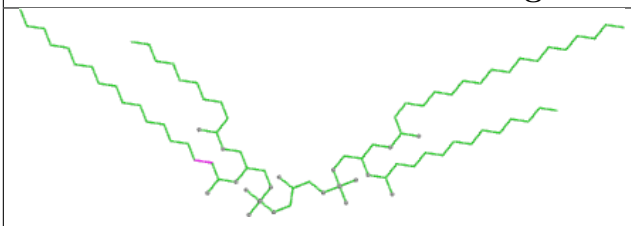


Torsions

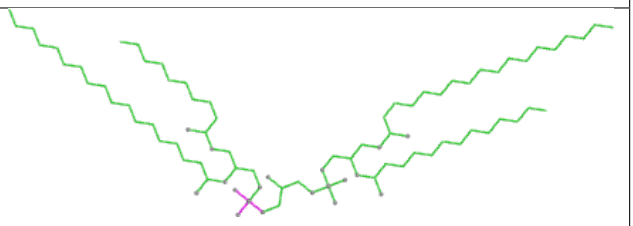


Rings

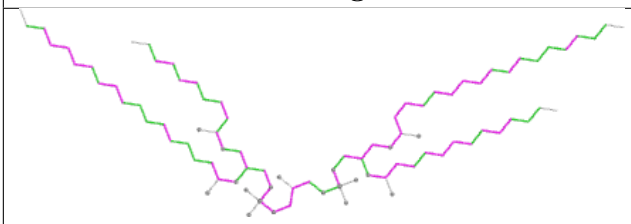
Ligand CDL P 305



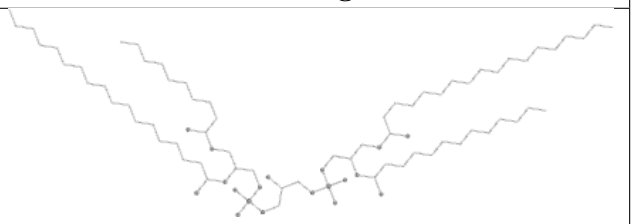
Bond lengths



Bond angles

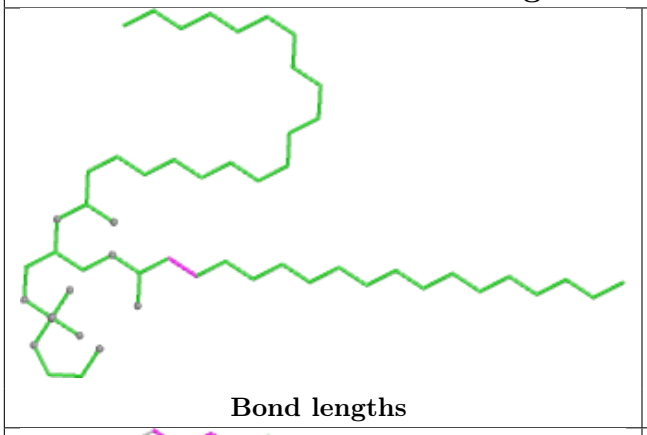


Torsions

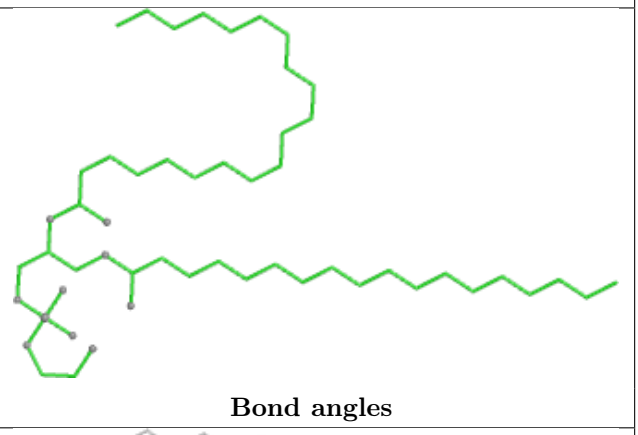


Rings

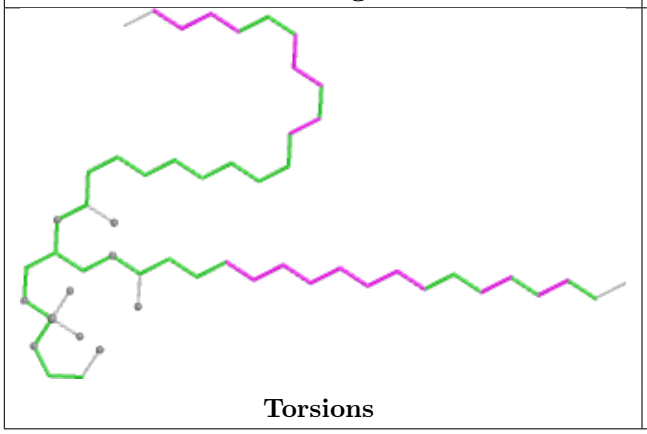
Ligand PEK G 101



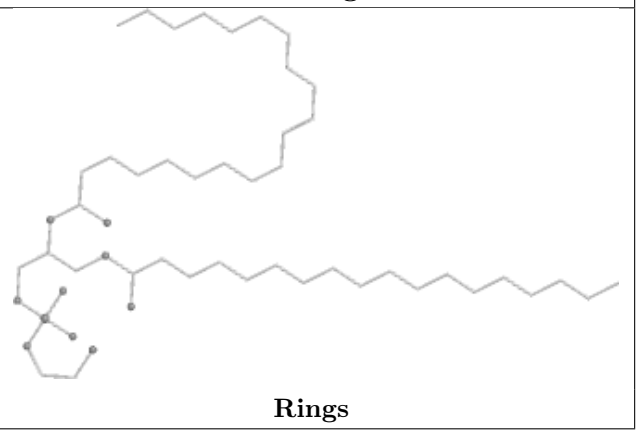
Bond lengths



Bond angles

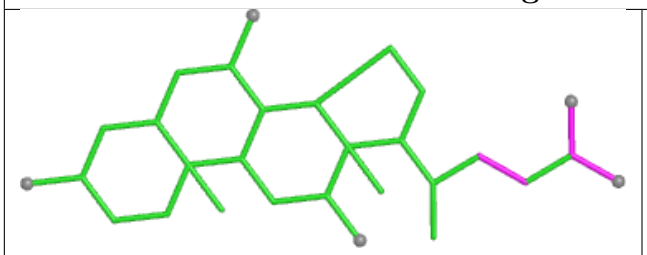


Torsions

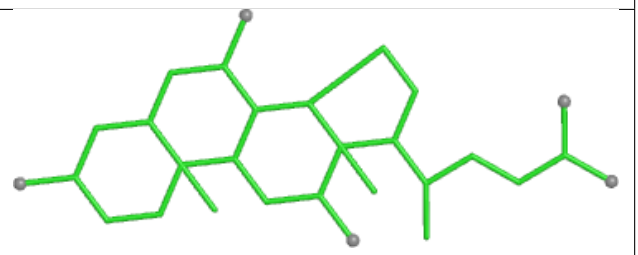


Rings

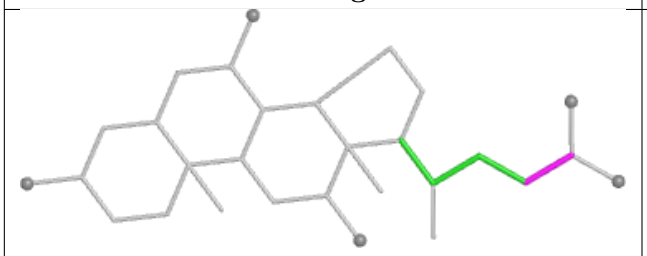
Ligand CHD C 301



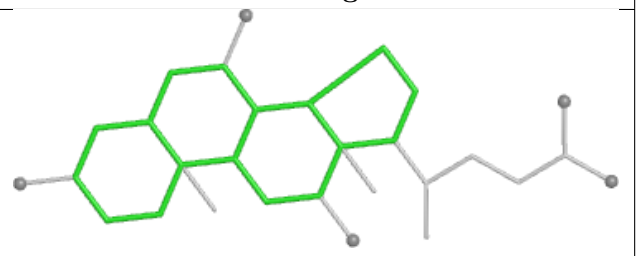
Bond lengths



Bond angles

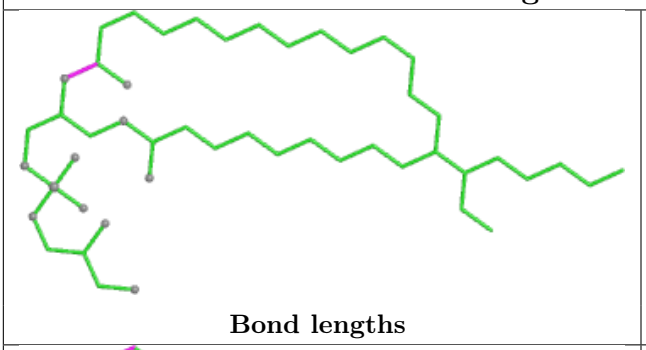


Torsions

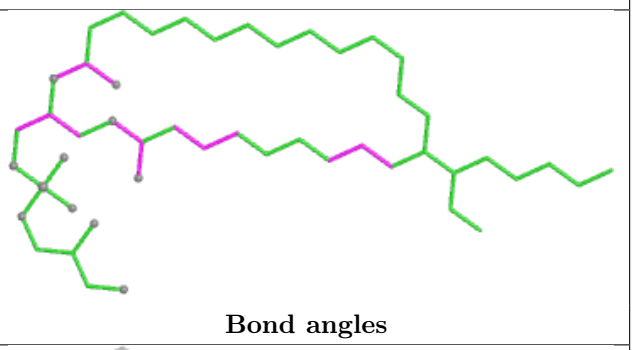


Rings

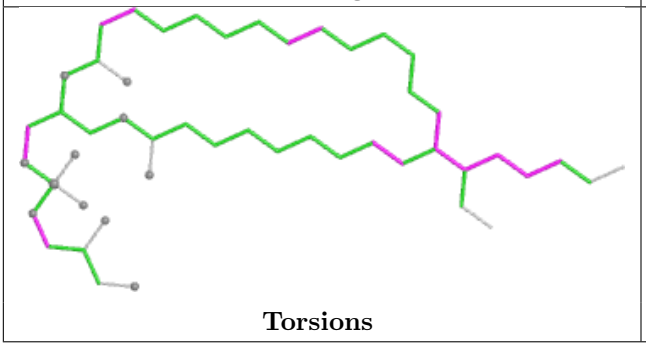
Ligand PGV C 303



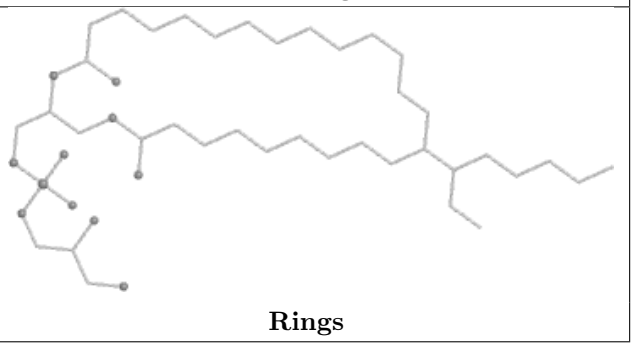
Bond lengths



Bond angles



Torsions



Rings

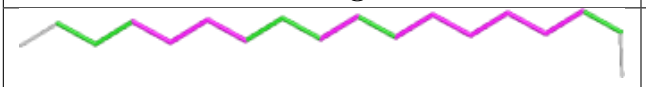
Ligand LFA P 310



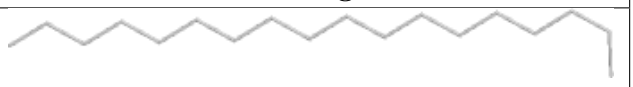
Bond lengths



Bond angles

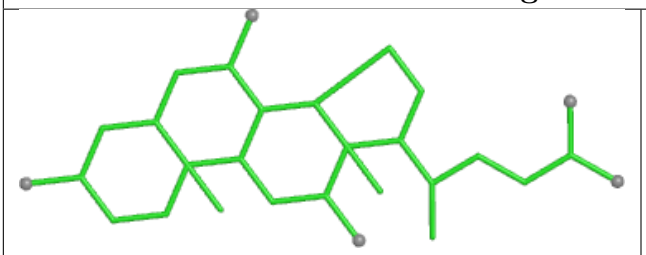


Torsions

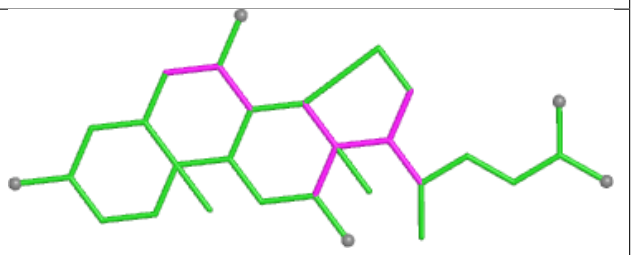


Rings

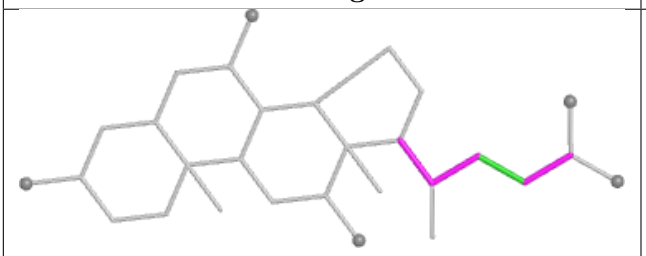
Ligand CHD C 305



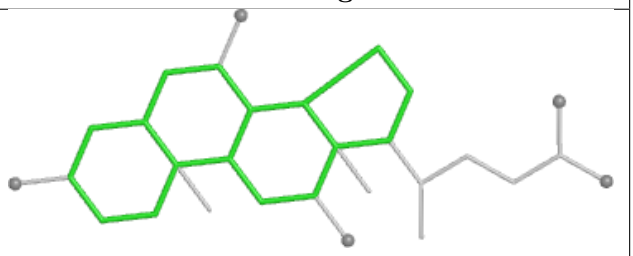
Bond lengths



Bond angles



Torsions

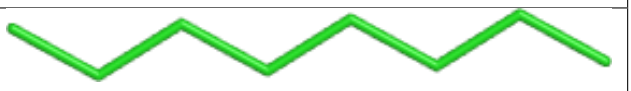


Rings

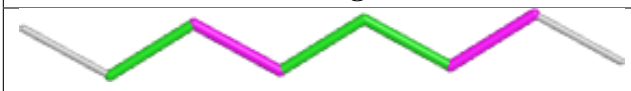
Ligand DMU Z 103



Bond lengths



Bond angles

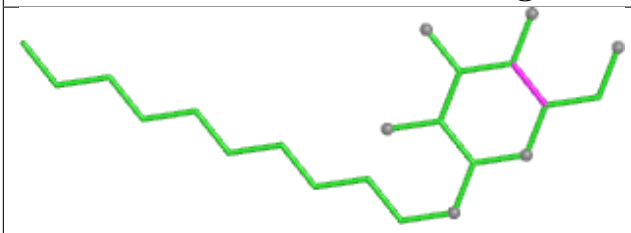


Torsions

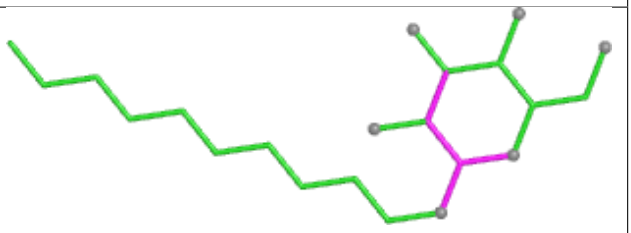


Rings

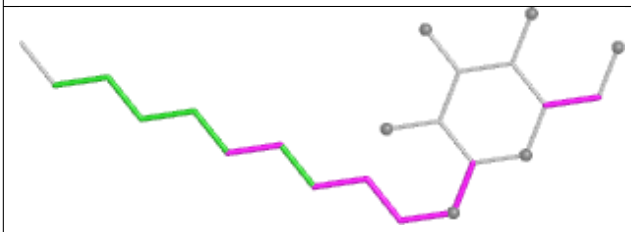
Ligand DMU O 304



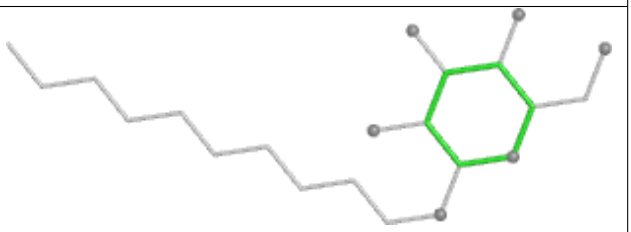
Bond lengths



Bond angles

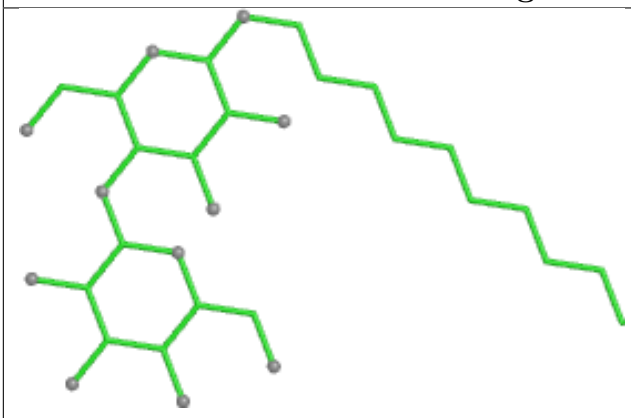


Torsions

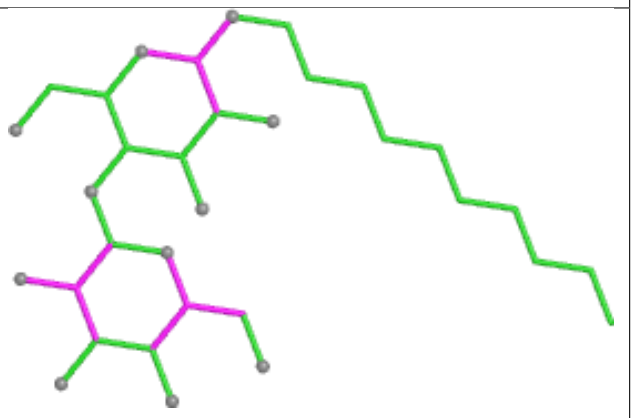


Rings

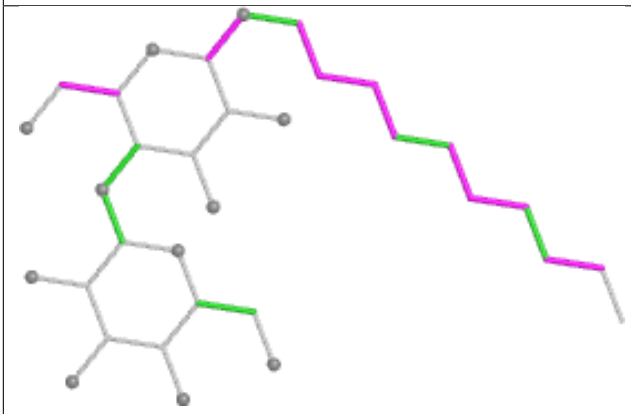
Ligand DMU C 319



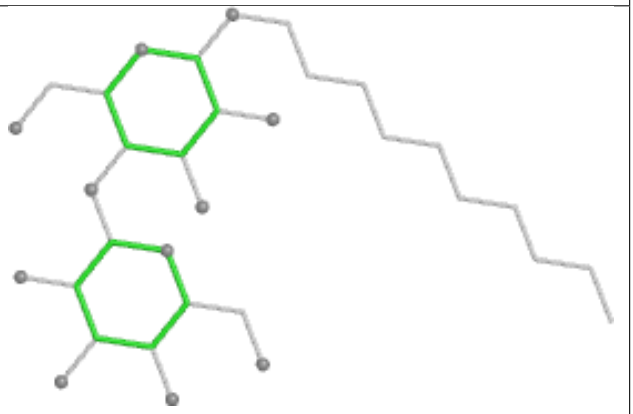
Bond lengths



Bond angles

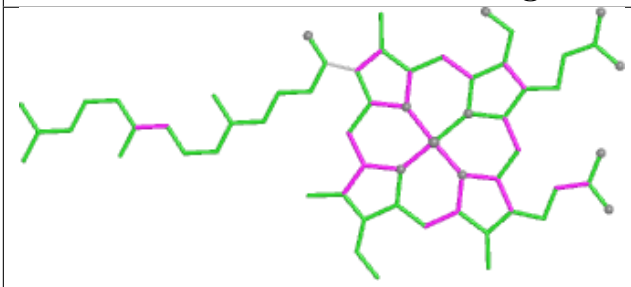


Torsions

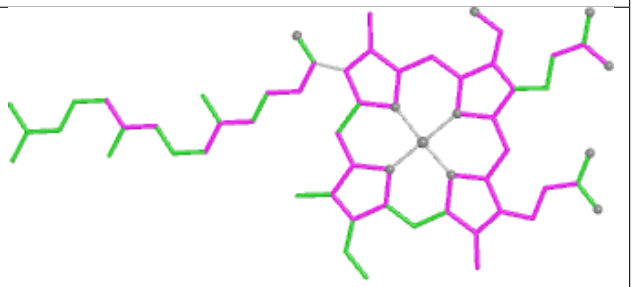


Rings

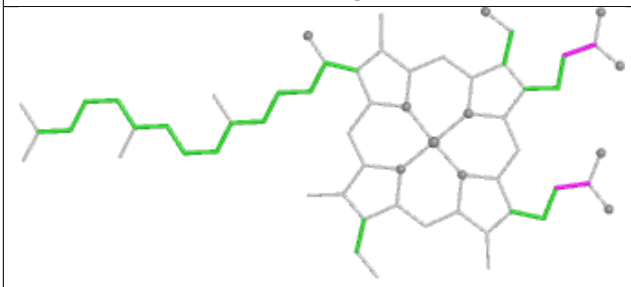
Ligand HEA A 602



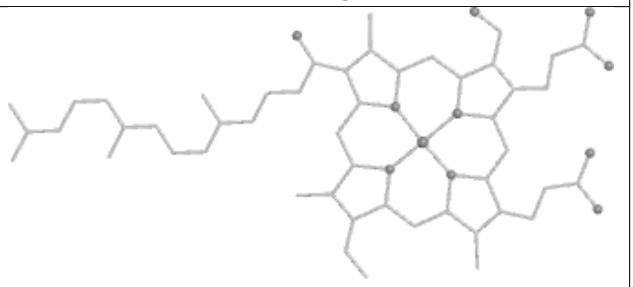
Bond lengths



Bond angles

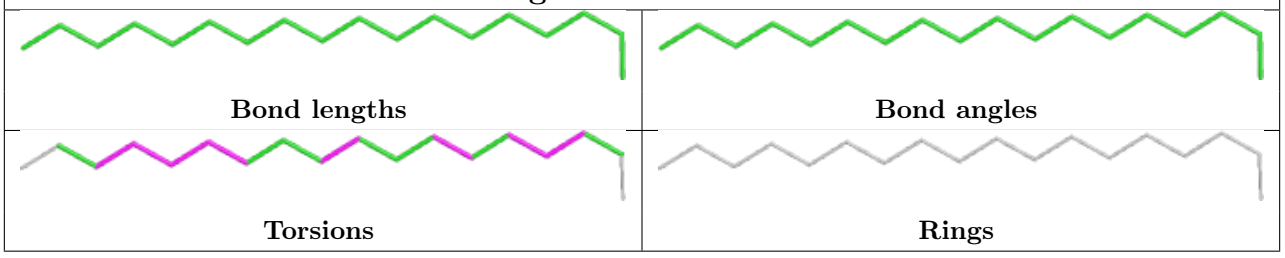


Torsions

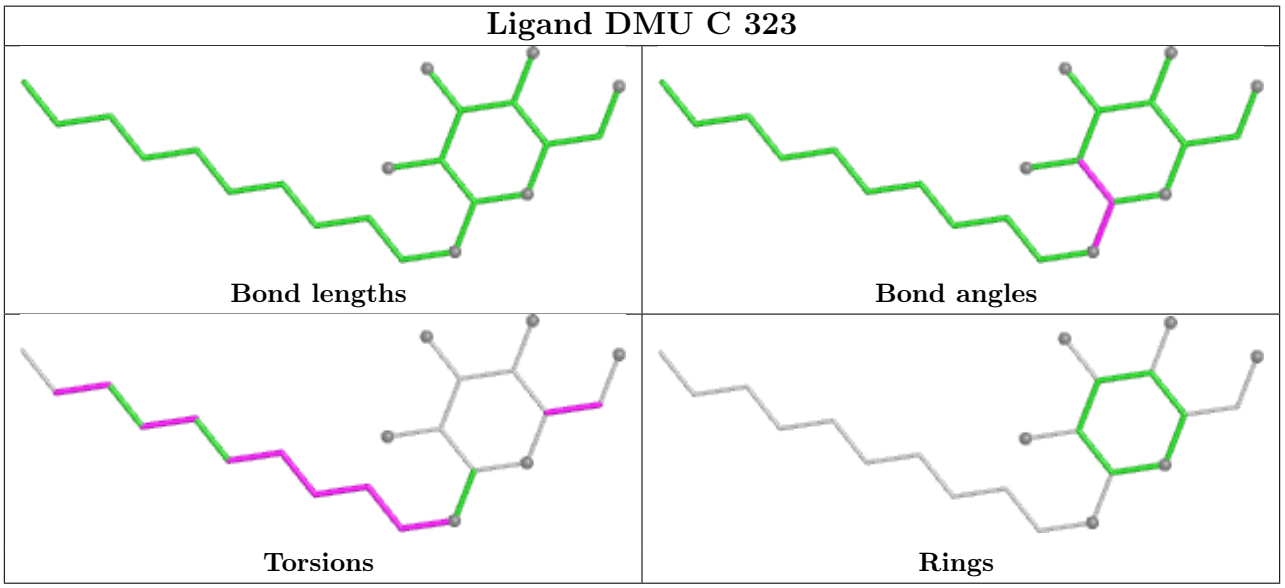


Rings

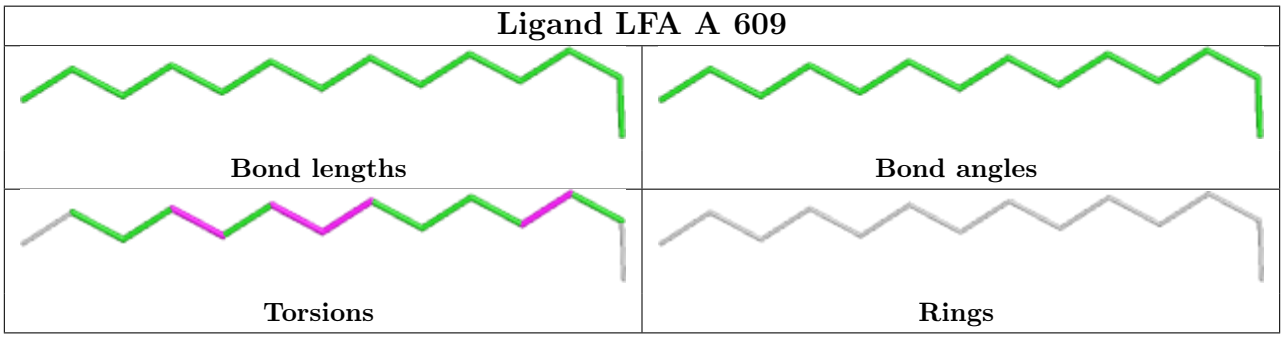
Ligand LFA C 309



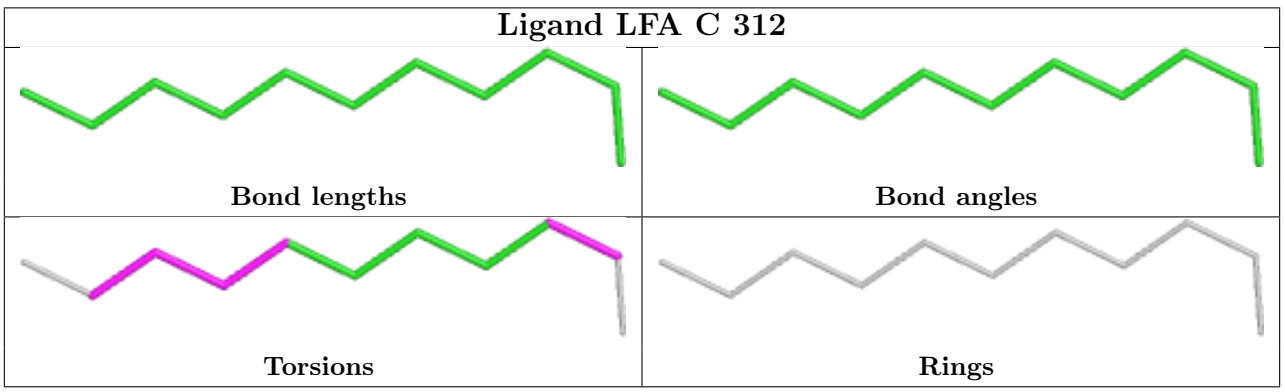
Ligand DMU C 323



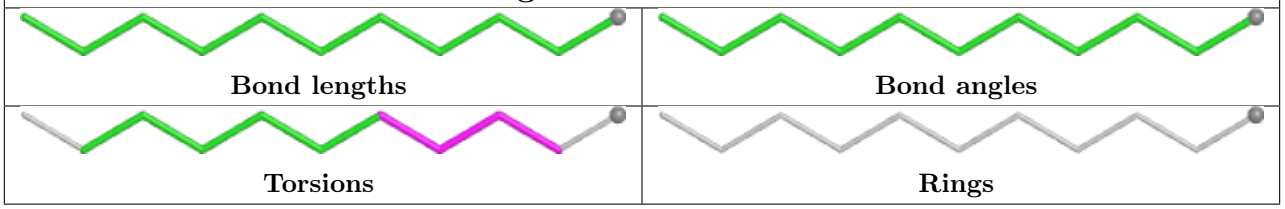
Ligand LFA A 609



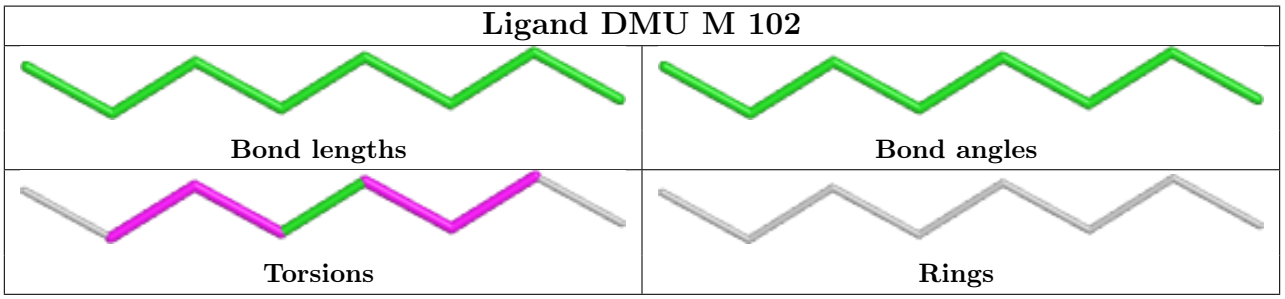
Ligand LFA C 312



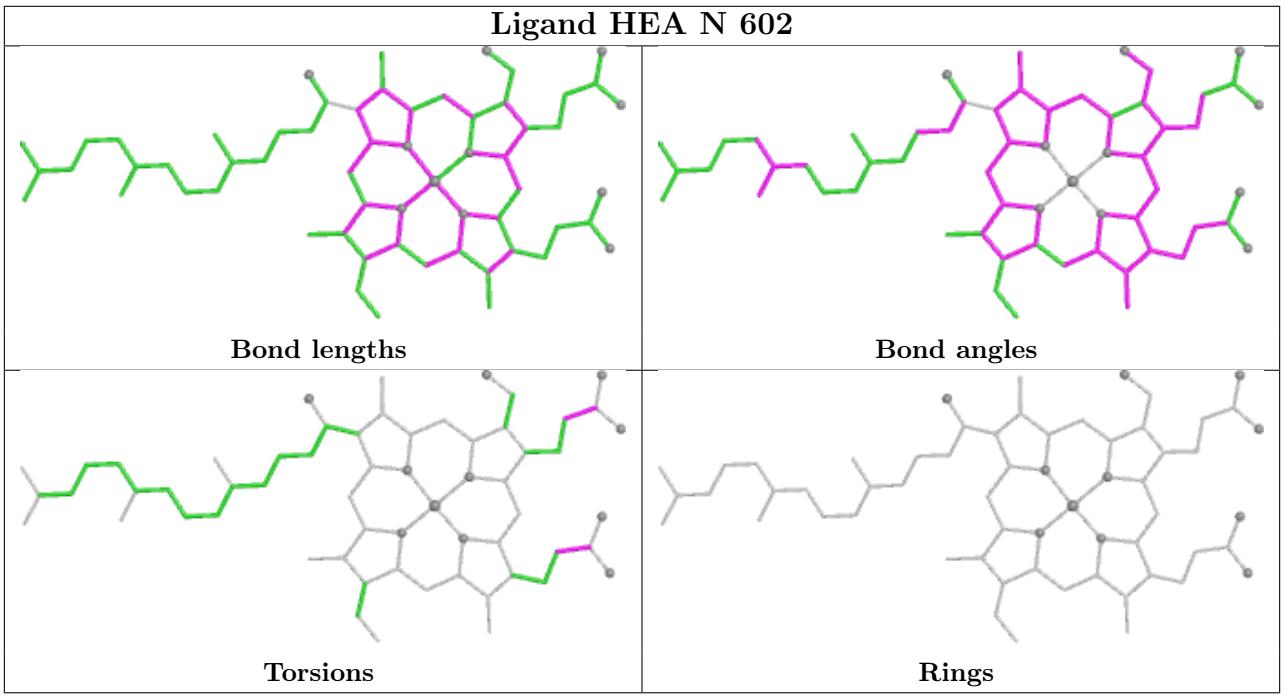
Ligand DMU O 307



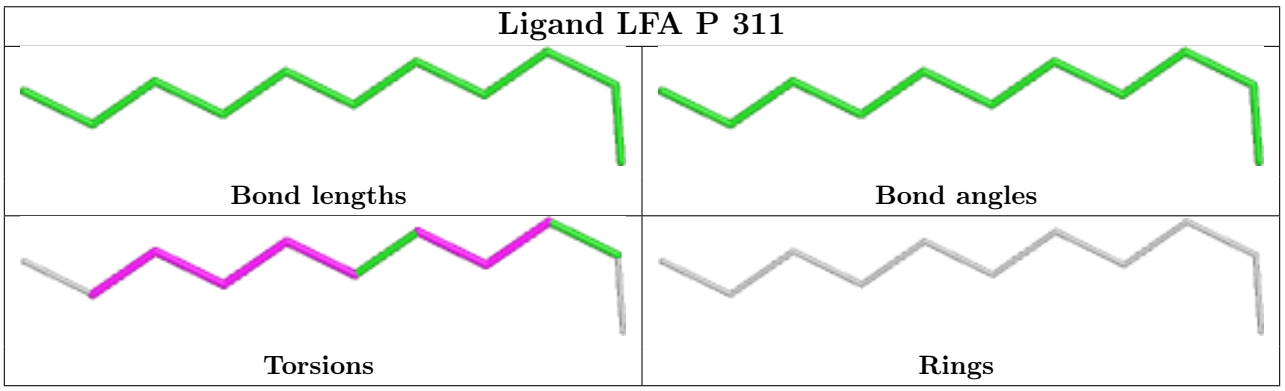
Ligand DMU M 102



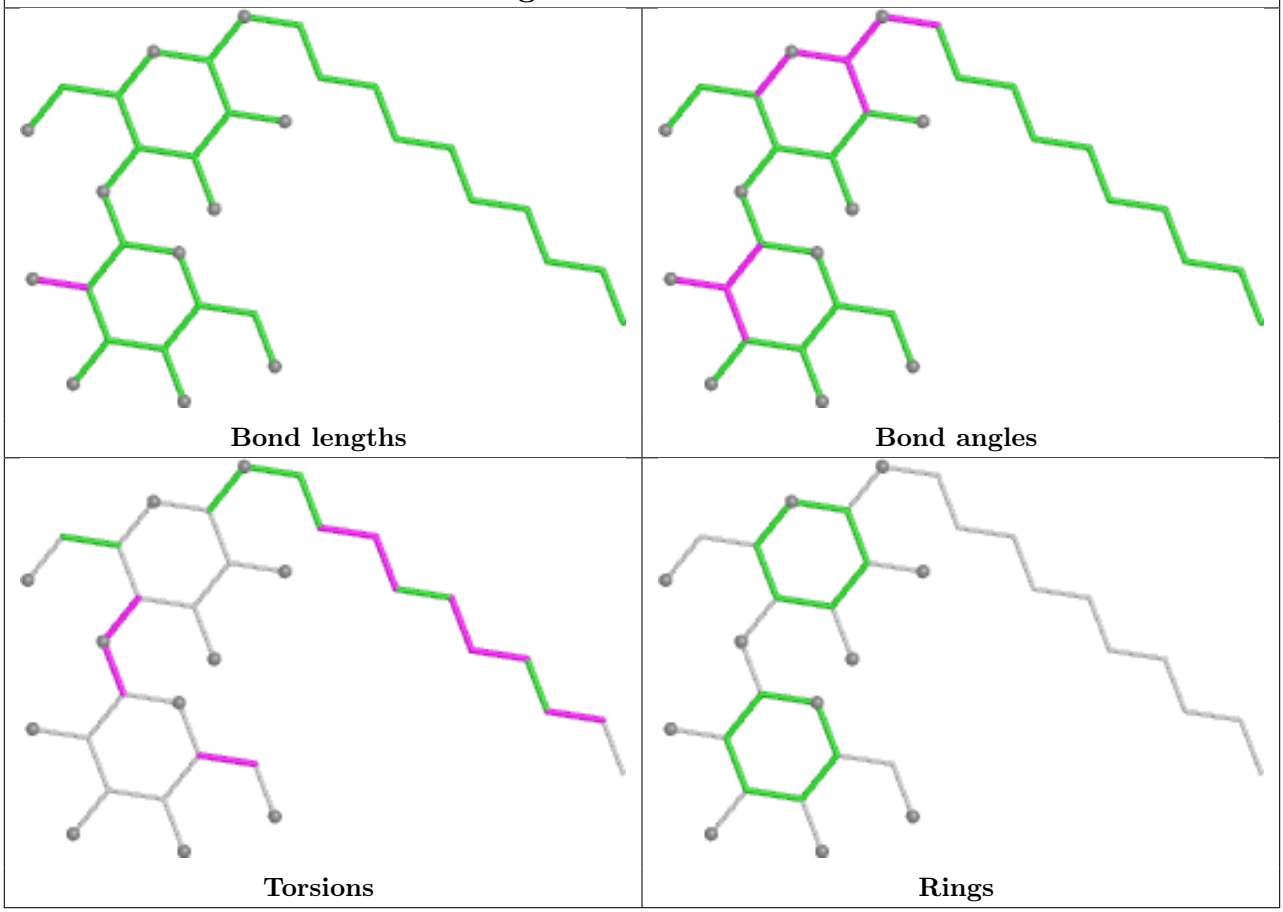
Ligand HEA N 602



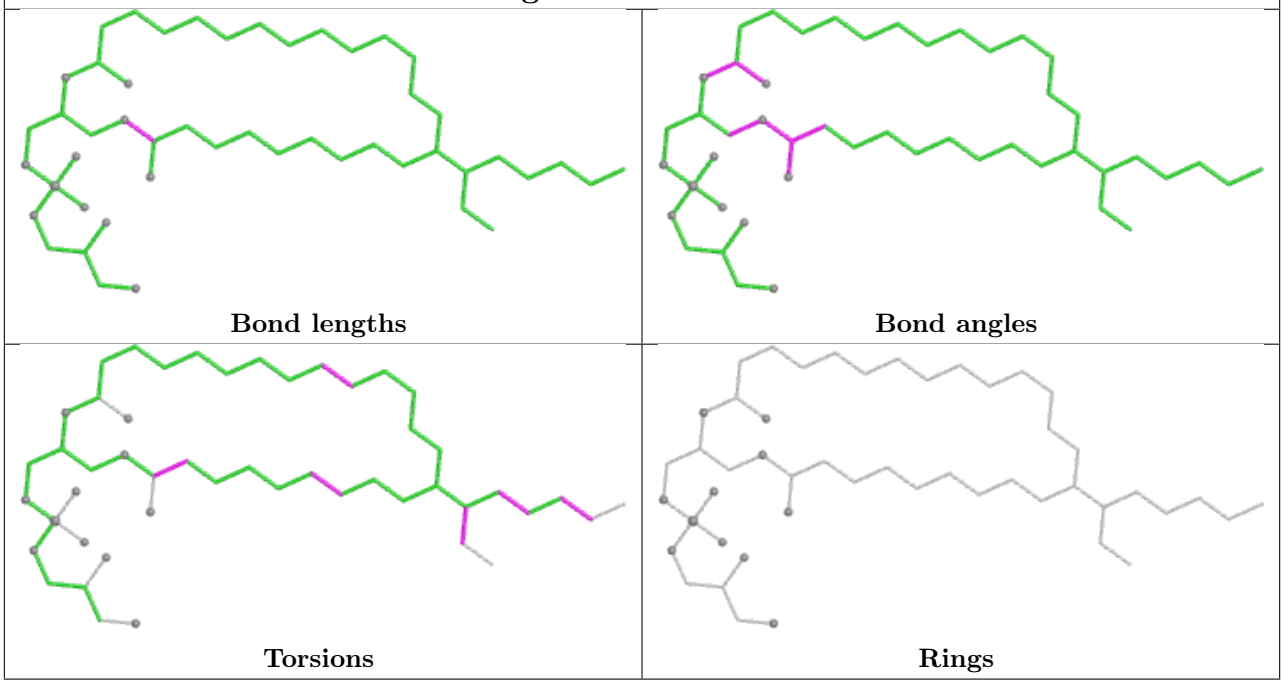
Ligand LFA P 311



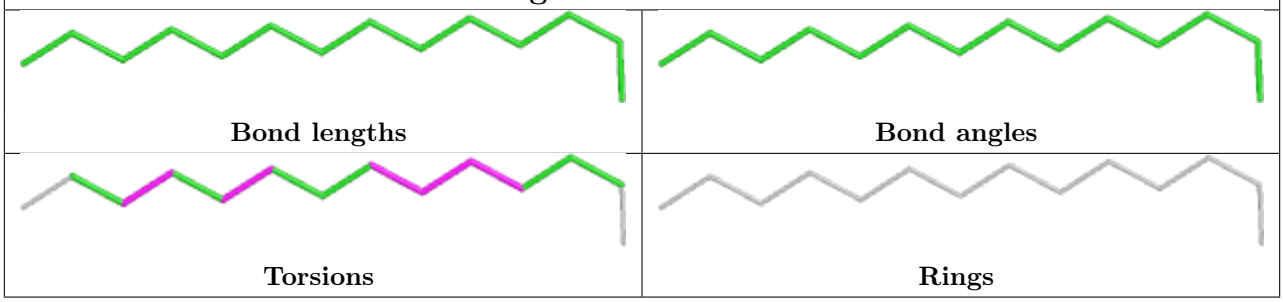
Ligand DMU C 315



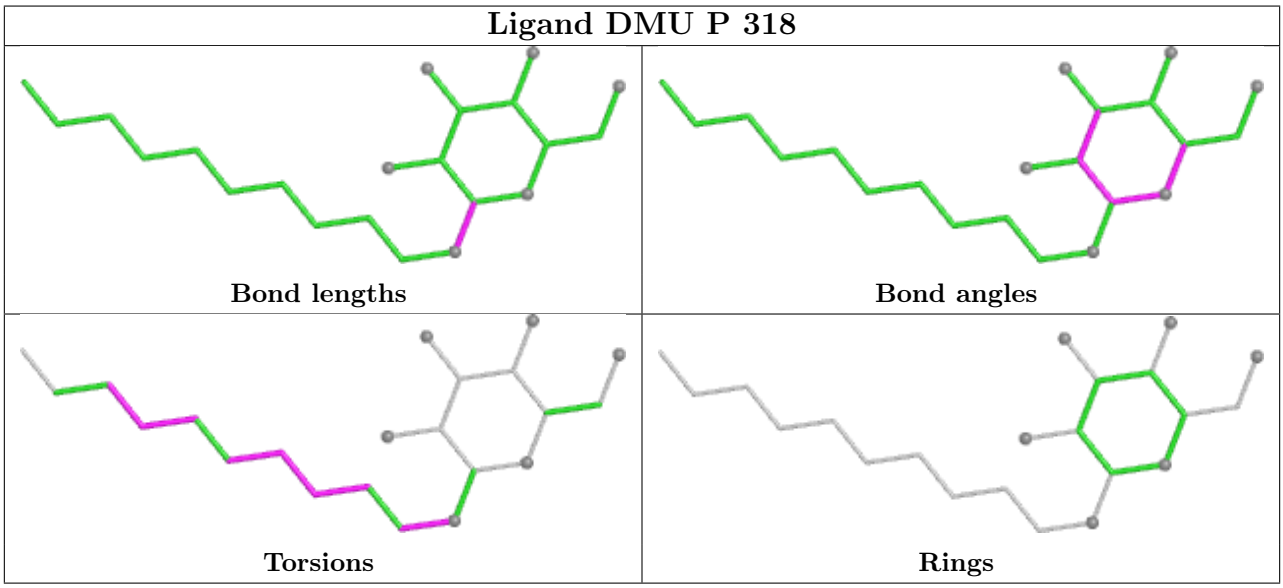
Ligand PGV N 617



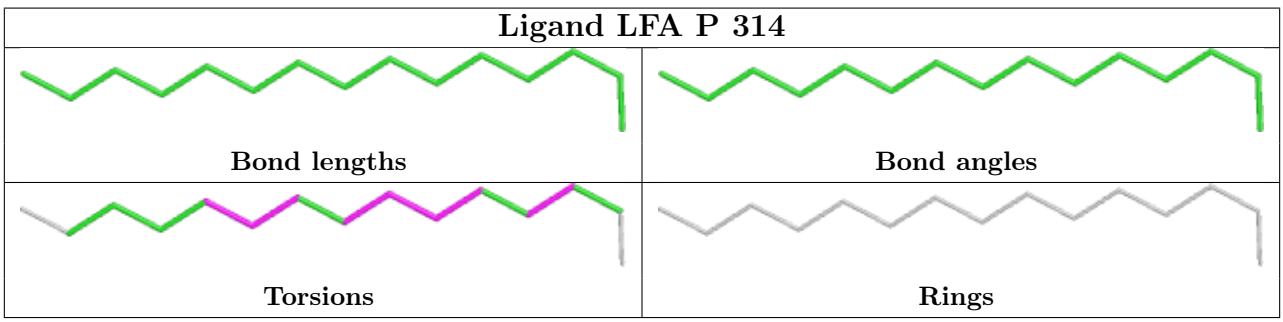
Ligand LFA P 312



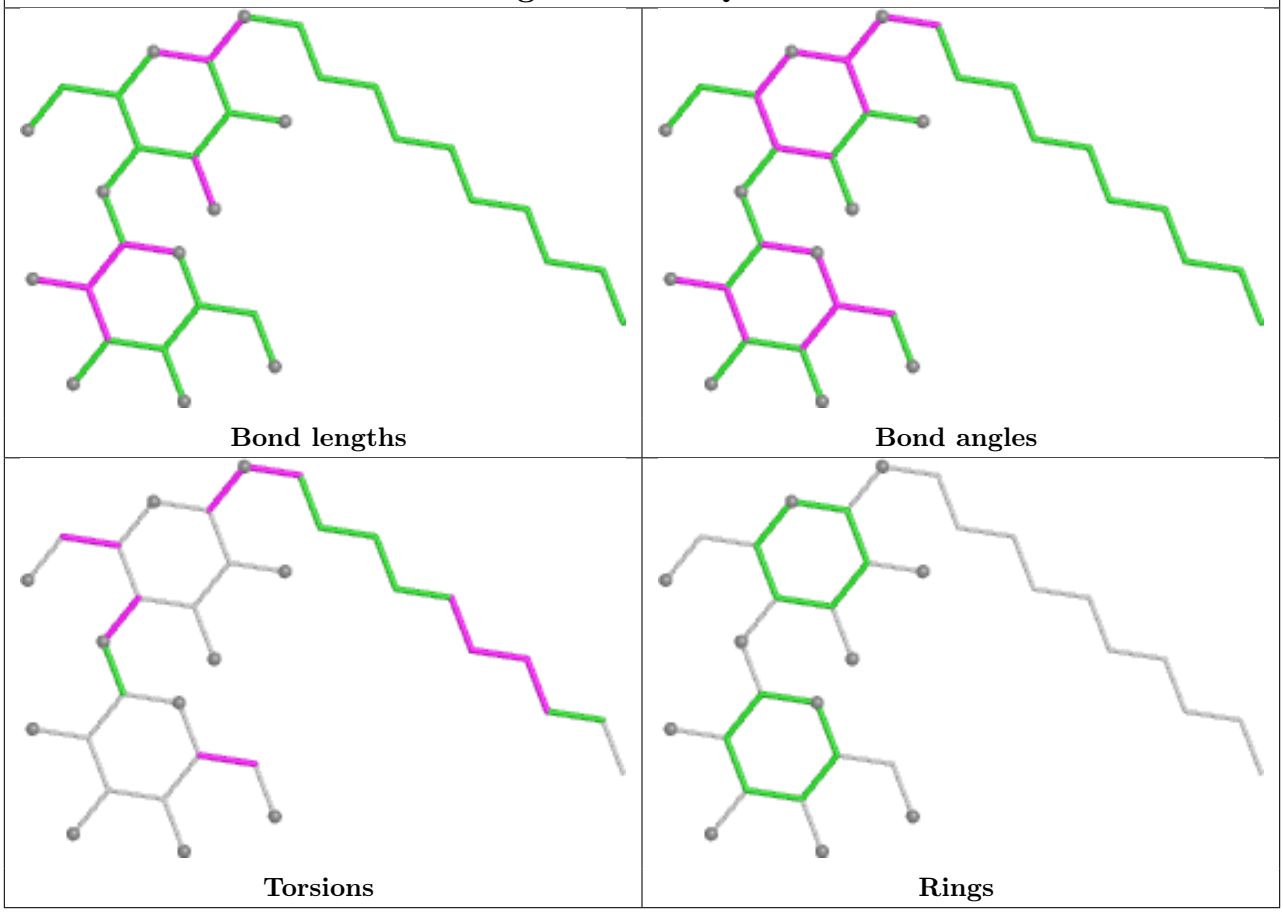
Ligand DMU P 318



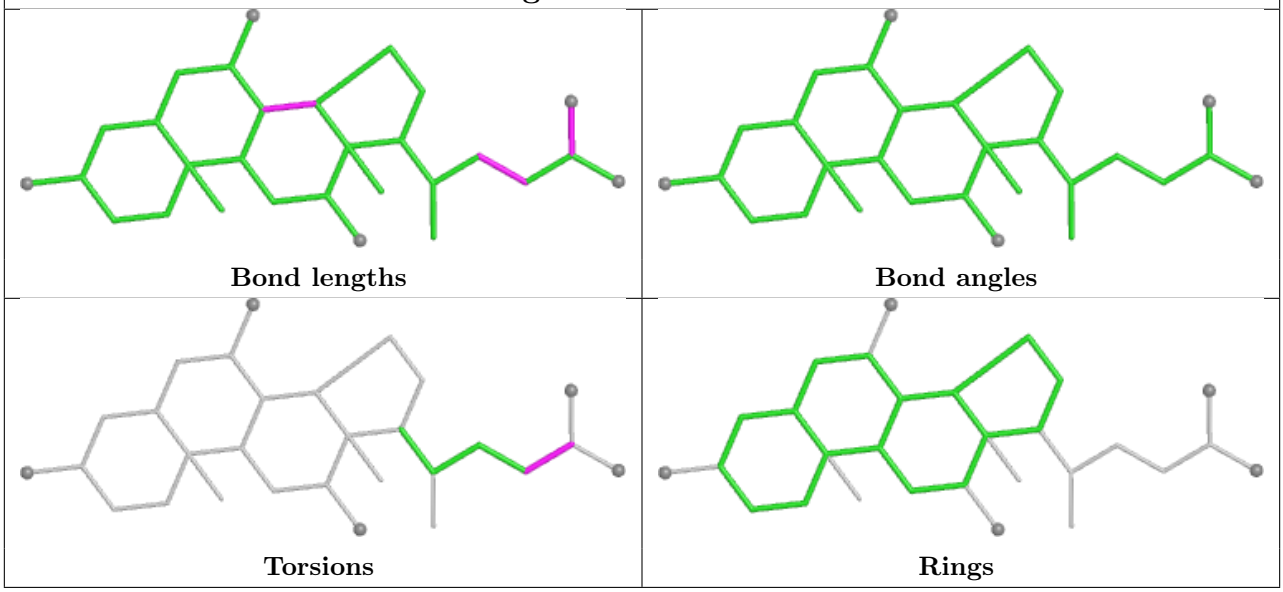
Ligand LFA P 314



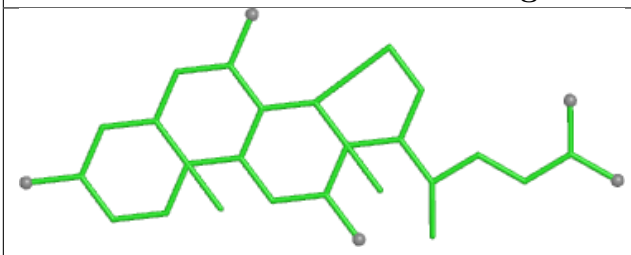
Ligand DMU Q 201



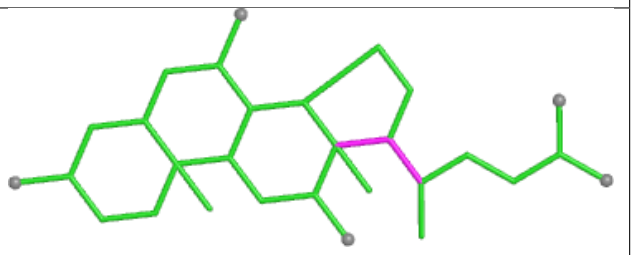
Ligand CHD P 302



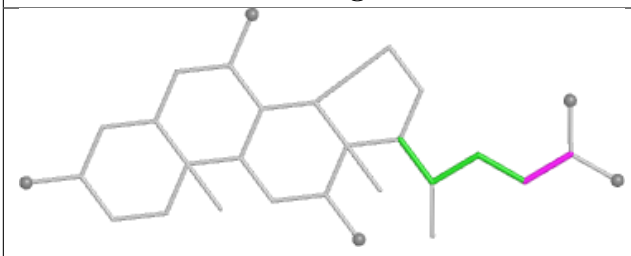
Ligand CHD O 301



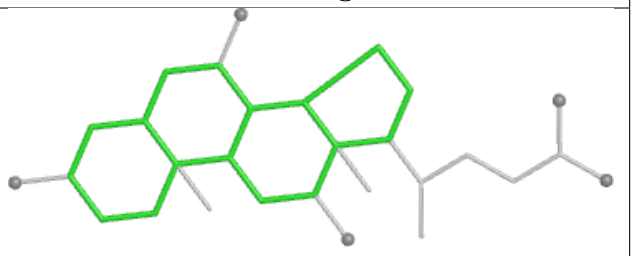
Bond lengths



Bond angles

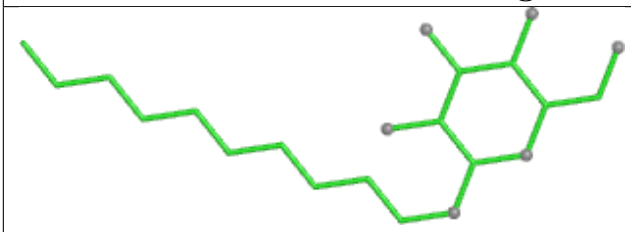


Torsions

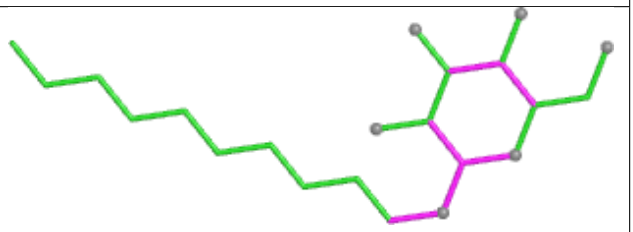


Rings

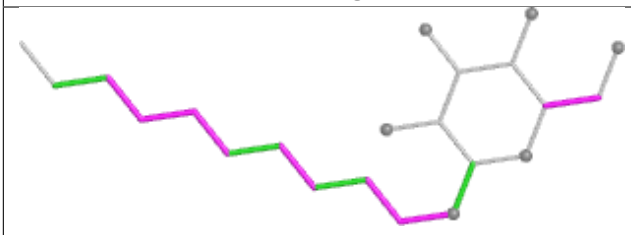
Ligand DMU C 317



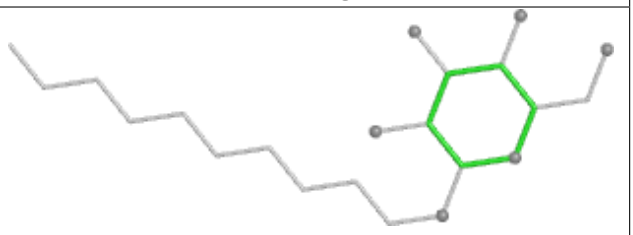
Bond lengths



Bond angles

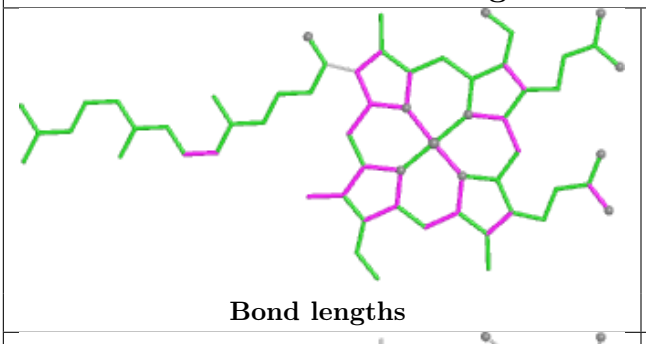


Torsions

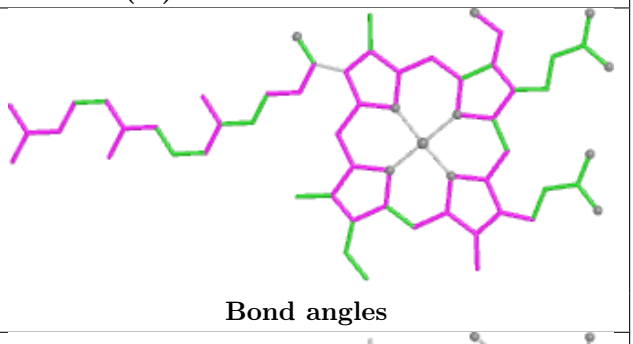


Rings

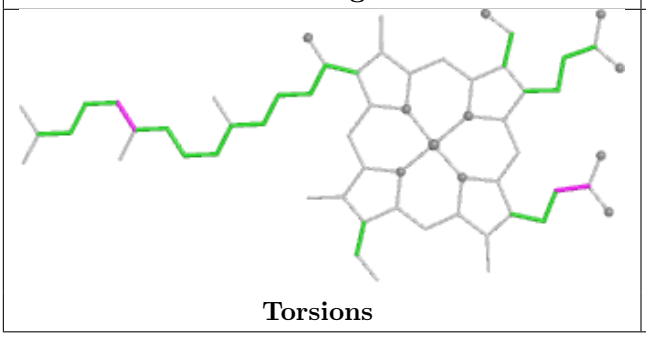
Ligand HEA A 601 (B)



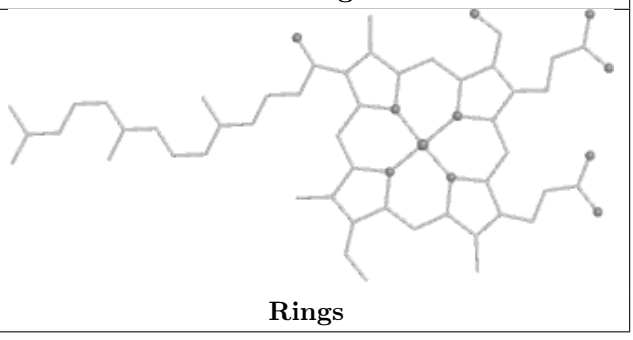
Bond lengths



Bond angles

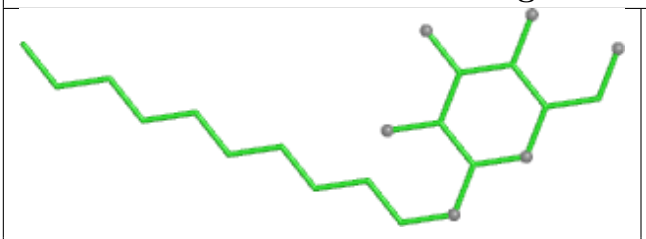


Torsions

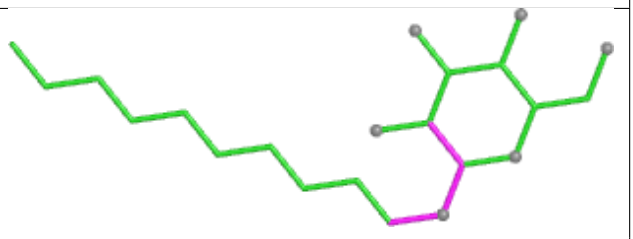


Rings

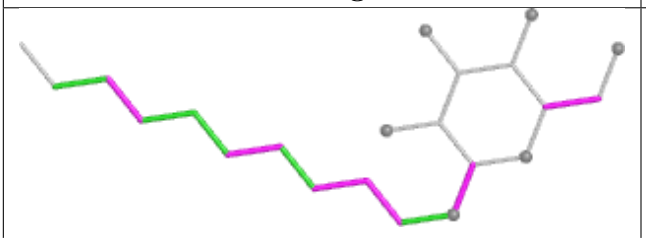
Ligand DMU P 324



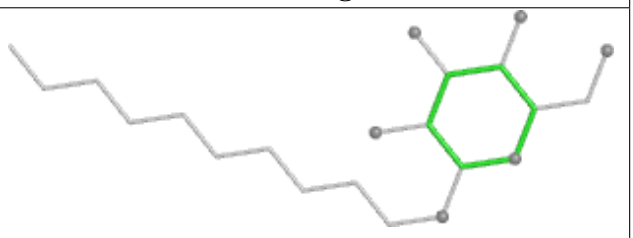
Bond lengths



Bond angles

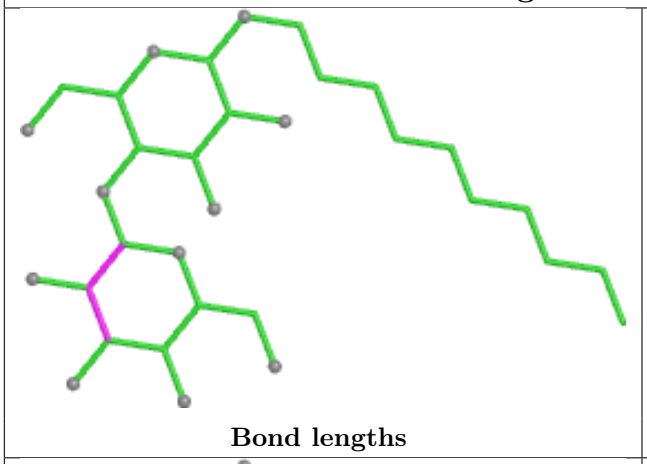


Torsions

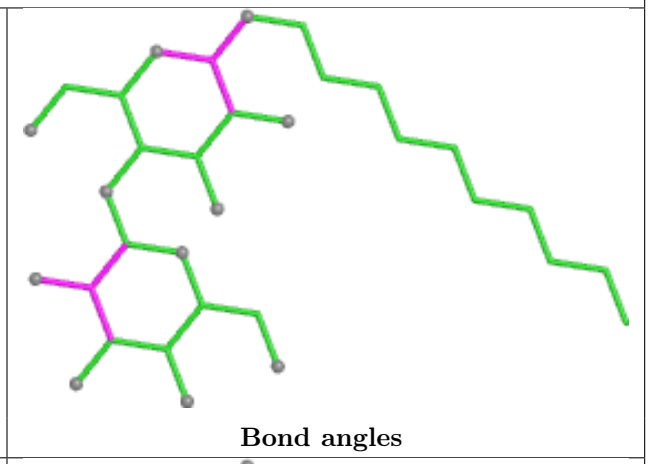


Rings

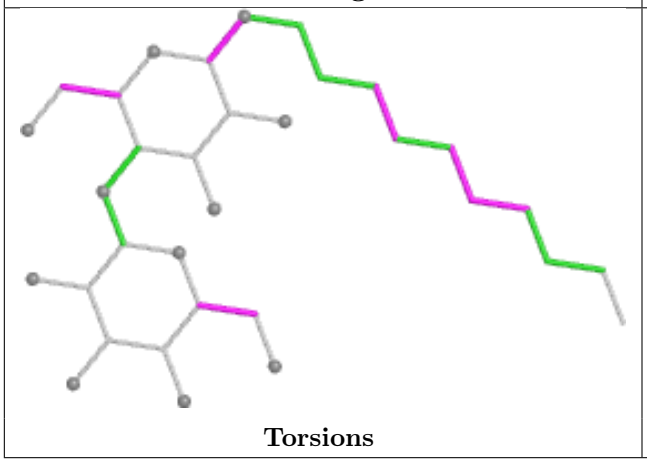
Ligand DMU H 101



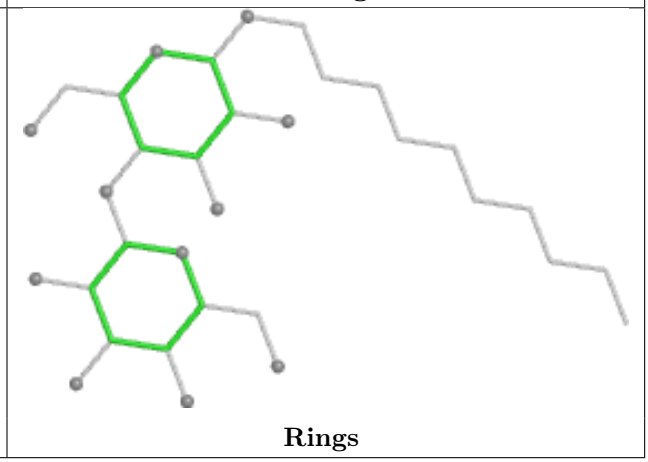
Bond lengths



Bond angles

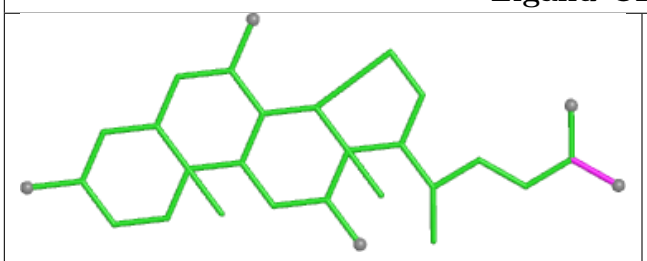


Torsions

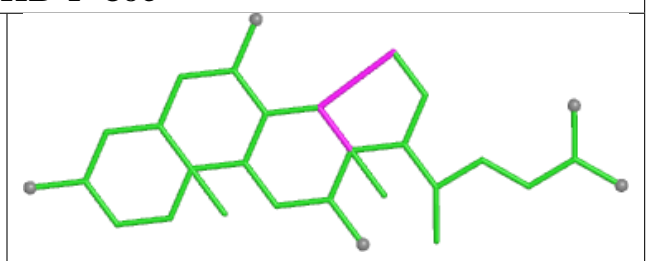


Rings

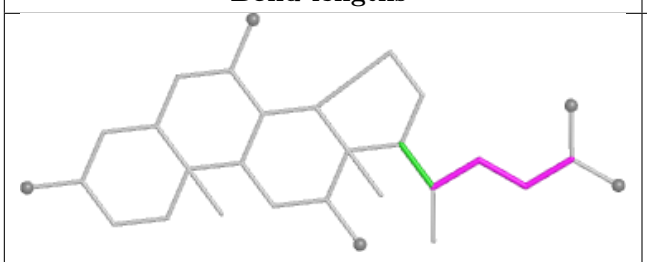
Ligand CHD P 306



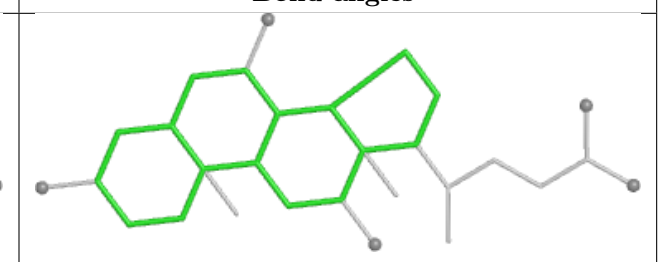
Bond lengths



Bond angles

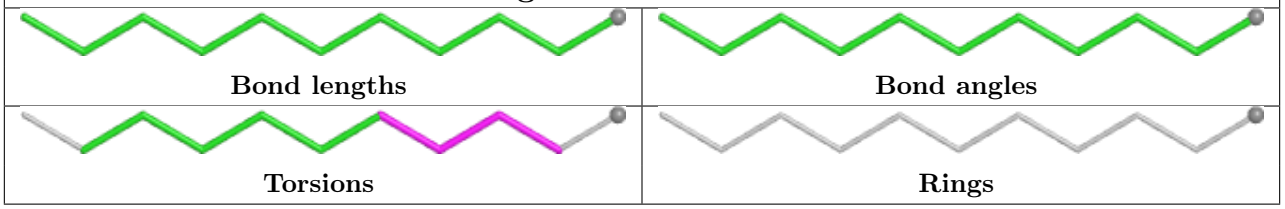


Torsions

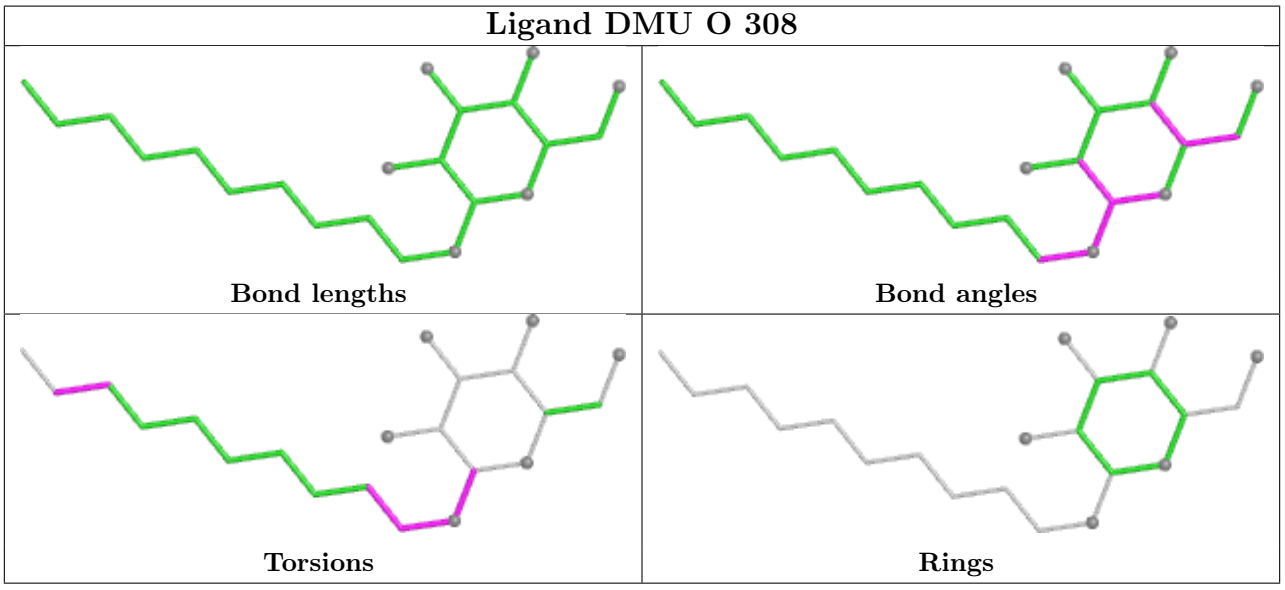


Rings

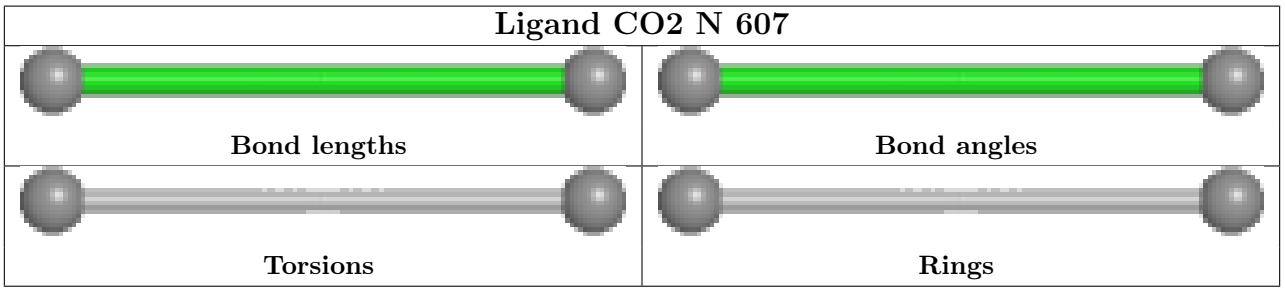
Ligand DMU O 306



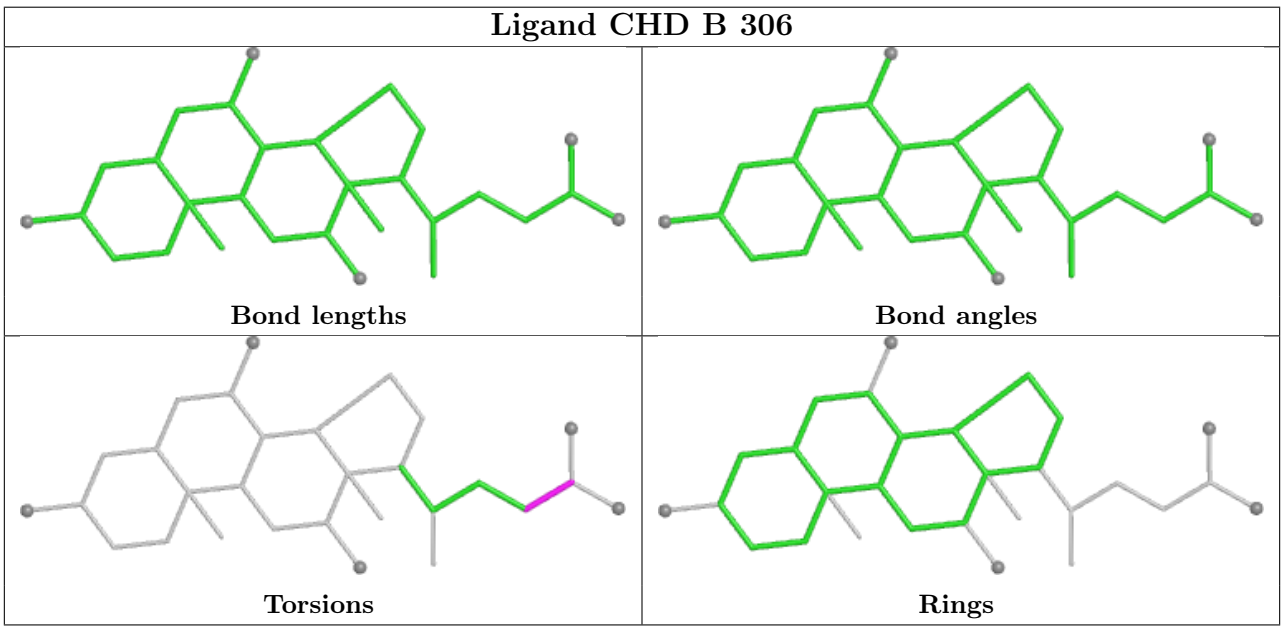
Ligand DMU O 308



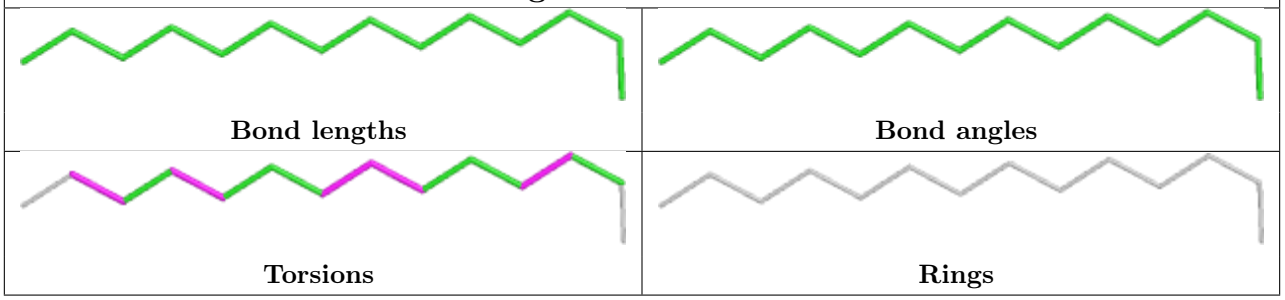
Ligand CO2 N 607



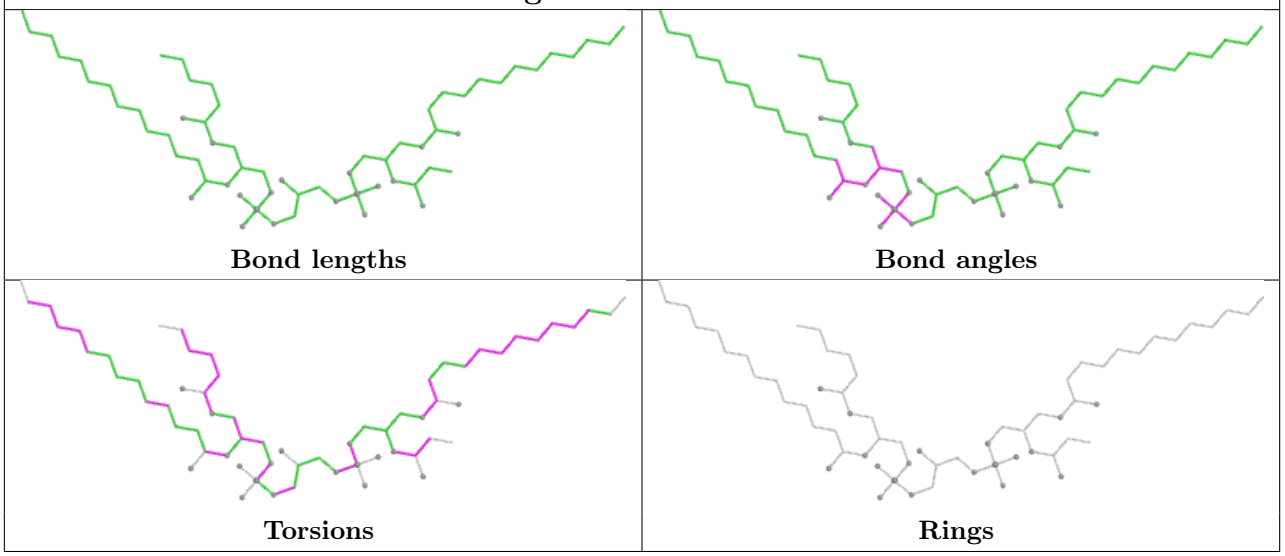
Ligand CHD B 306



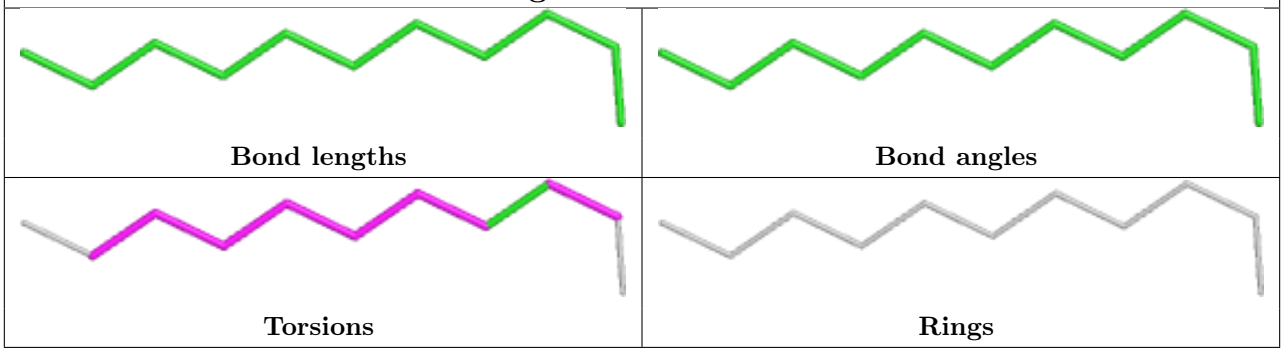
Ligand LFA A 610



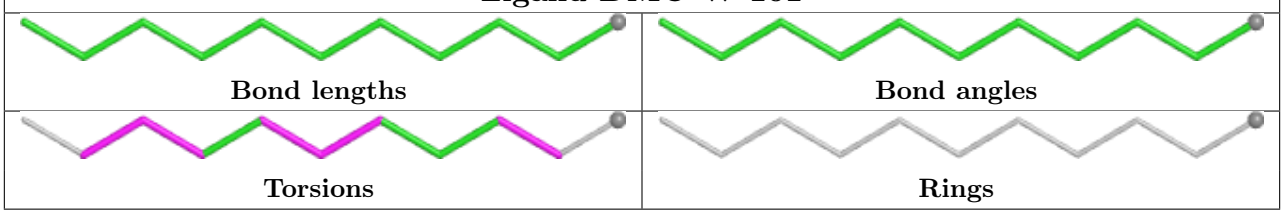
Ligand CDL V 101



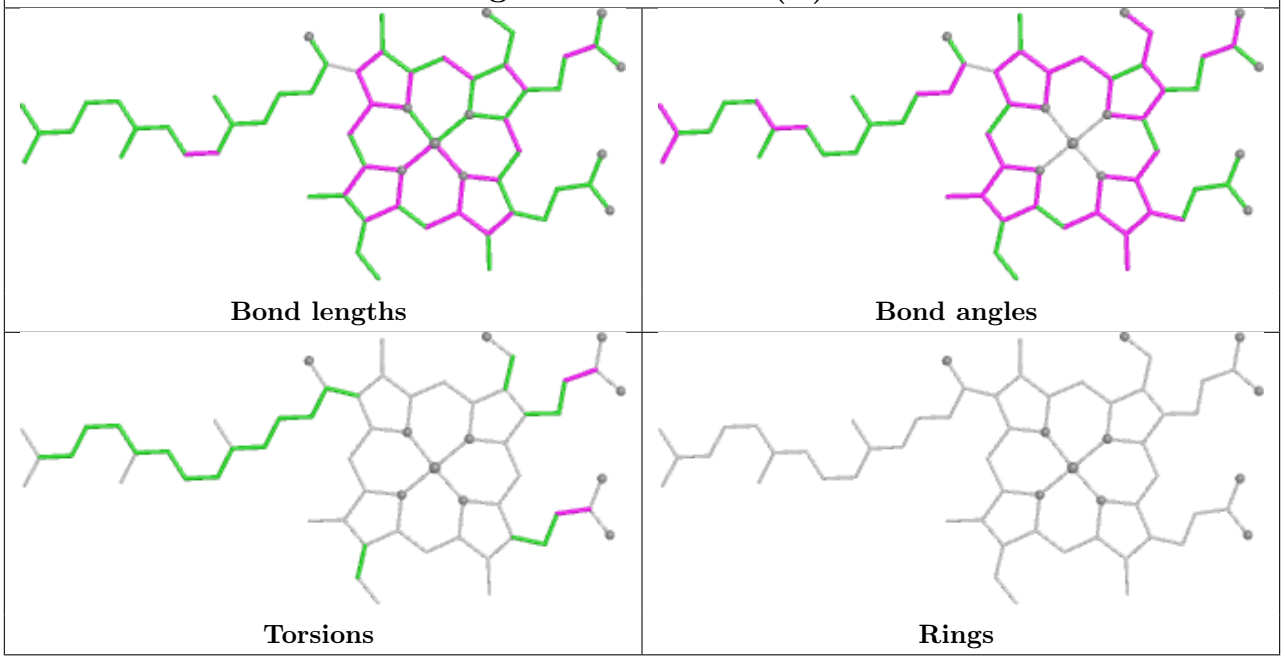
Ligand LFA C 310



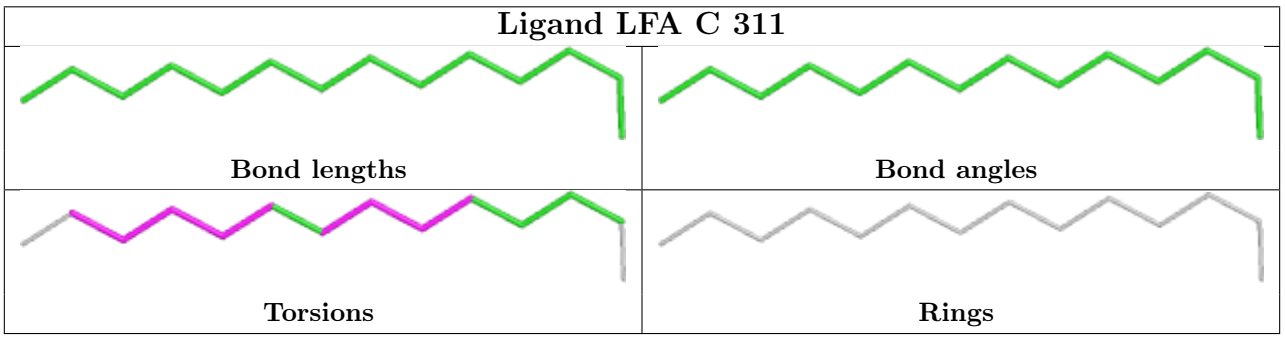
Ligand DMU W 101



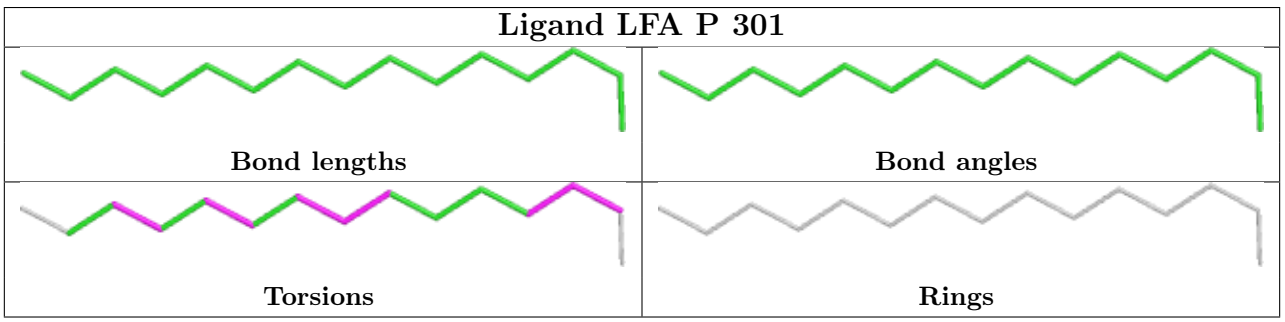
Ligand HEA N 601 (B)



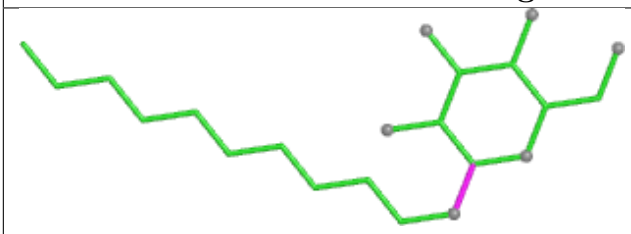
Ligand LFA C 311



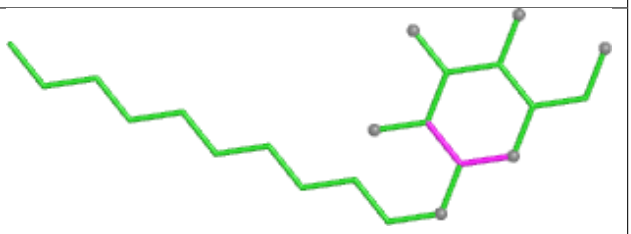
Ligand LFA P 301



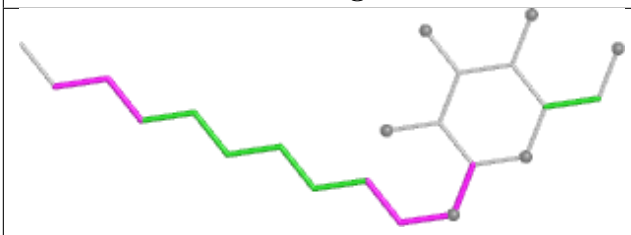
Ligand DMU B 304



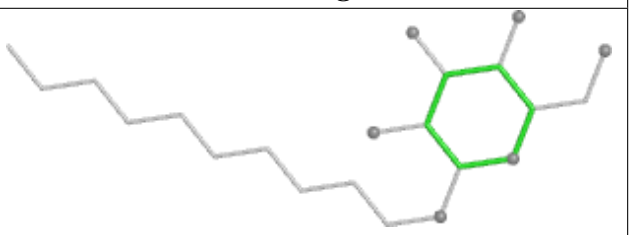
Bond lengths



Bond angles

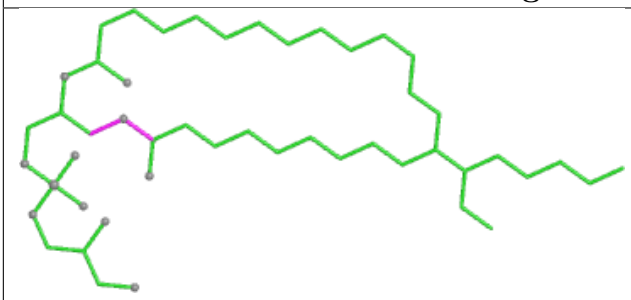


Torsions

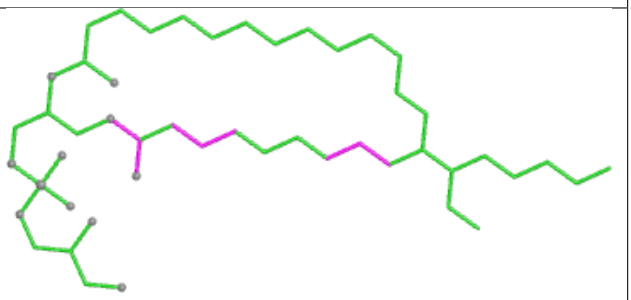


Rings

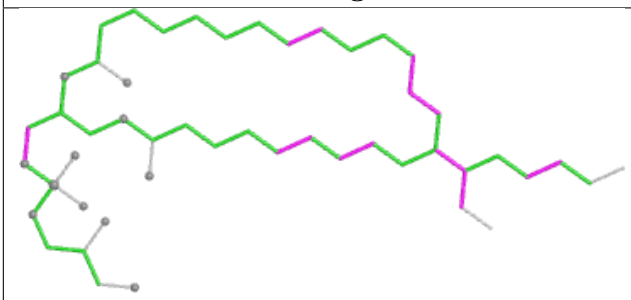
Ligand PGV P 304



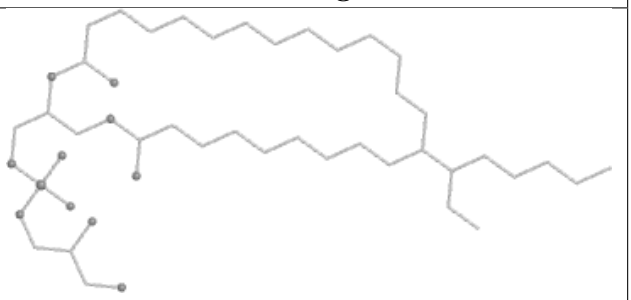
Bond lengths



Bond angles

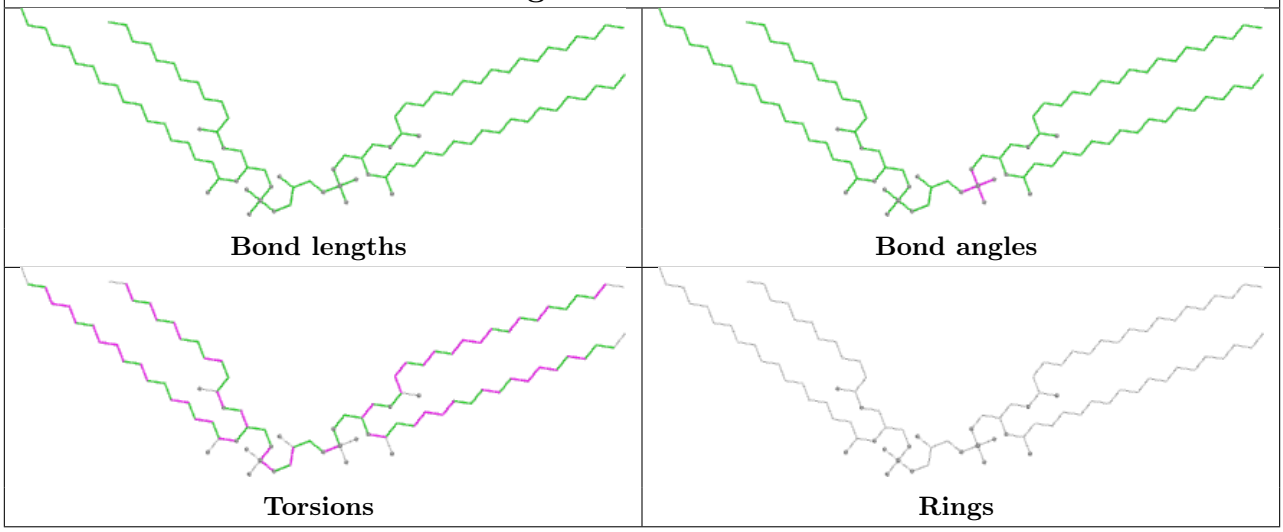


Torsions

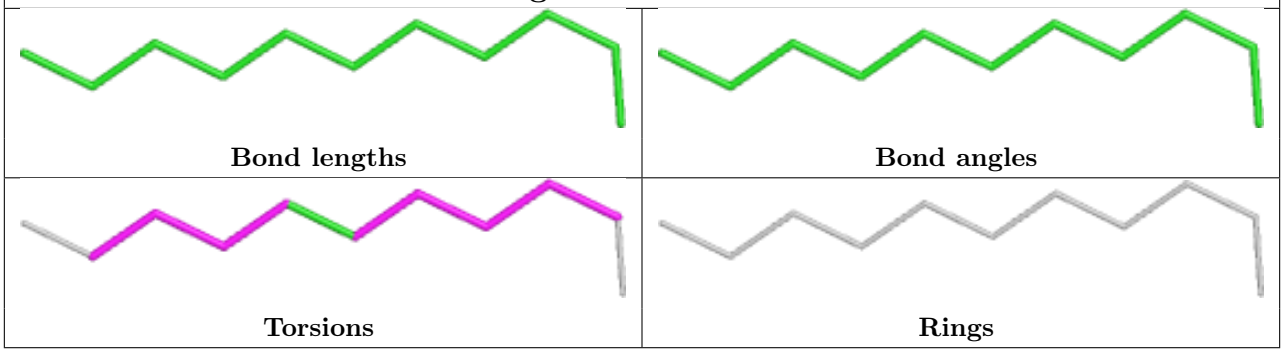


Rings

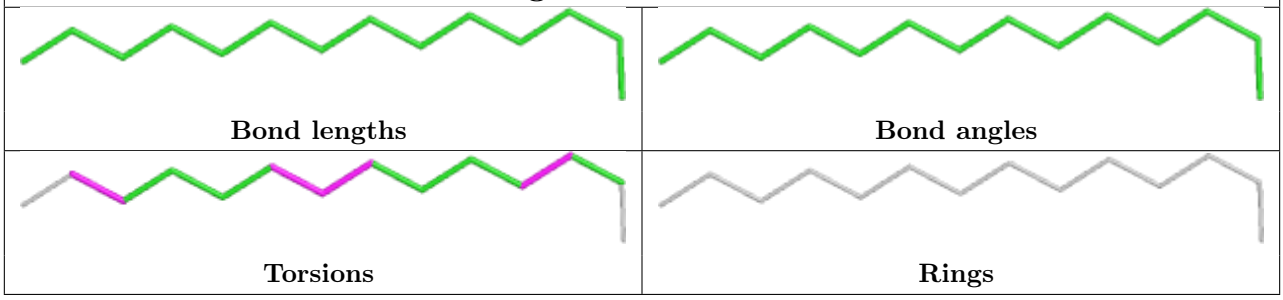
Ligand CDL L 101



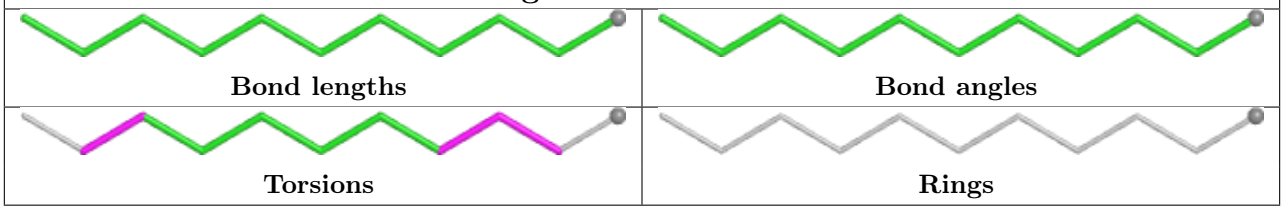
Ligand LFA P 308



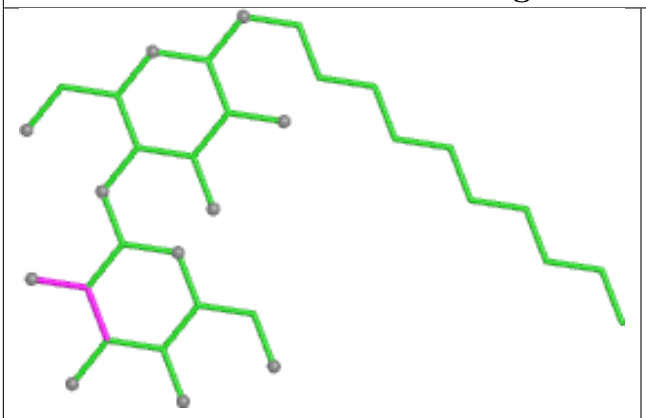
Ligand LFA N 608



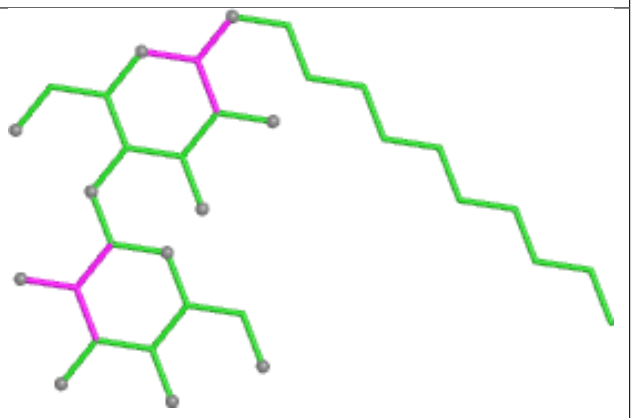
Ligand DMU J 101



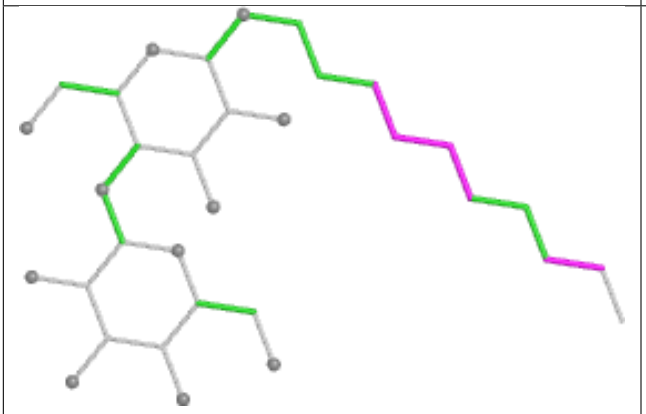
Ligand DMU M 101



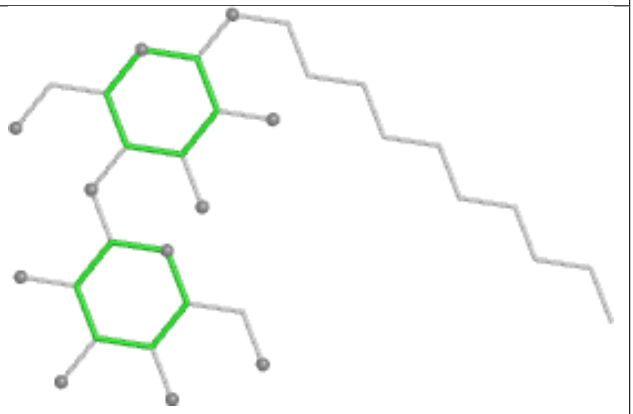
Bond lengths



Bond angles

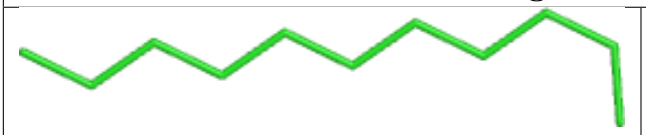


Torsions



Rings

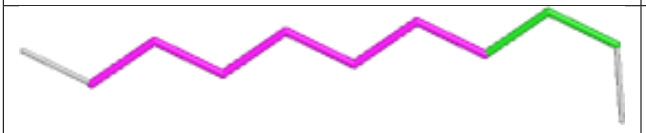
Ligand LFA C 307



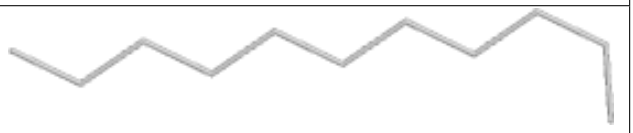
Bond lengths



Bond angles

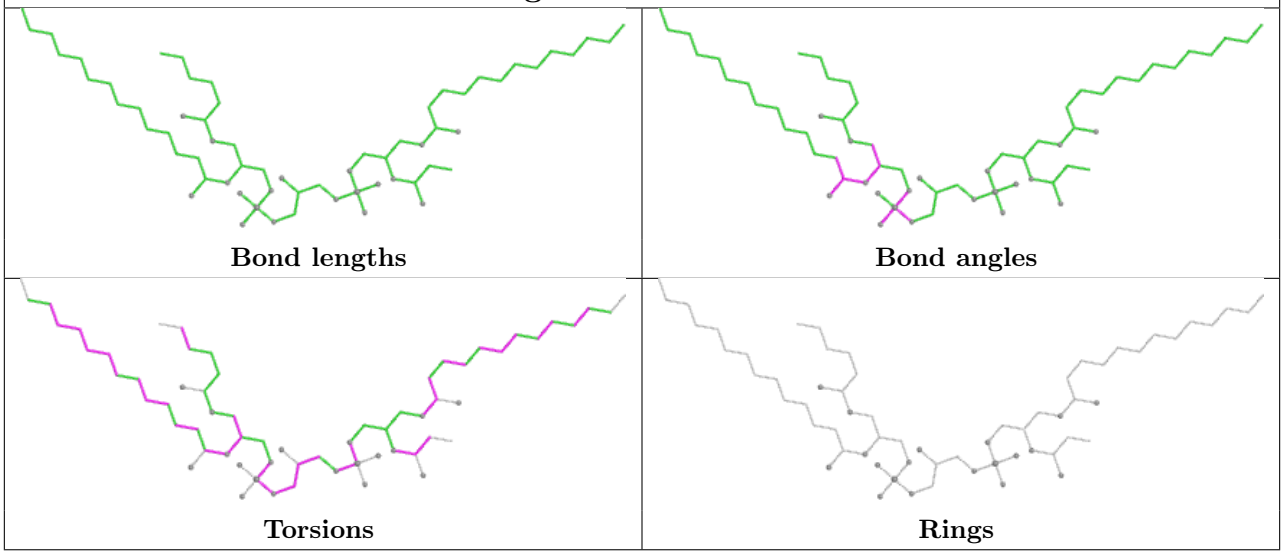


Torsions

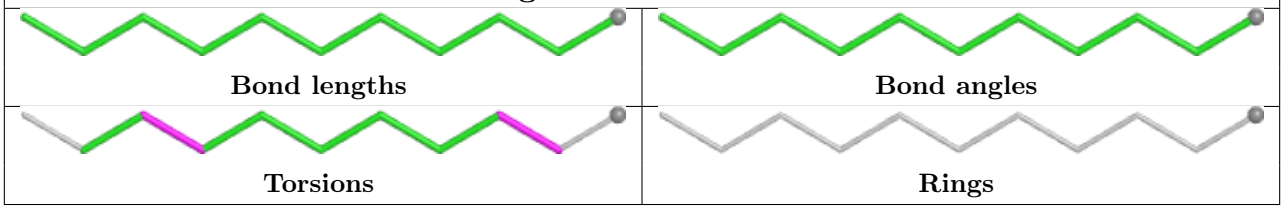


Rings

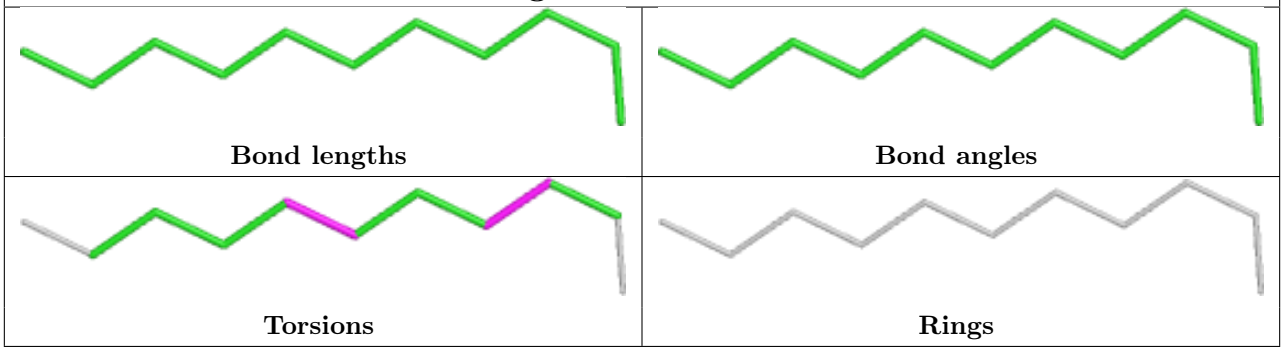
Ligand CDL A 607



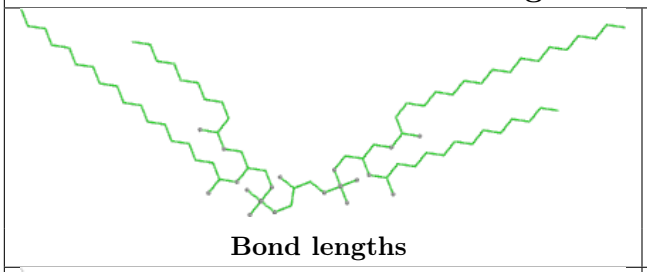
Ligand DMU P 307



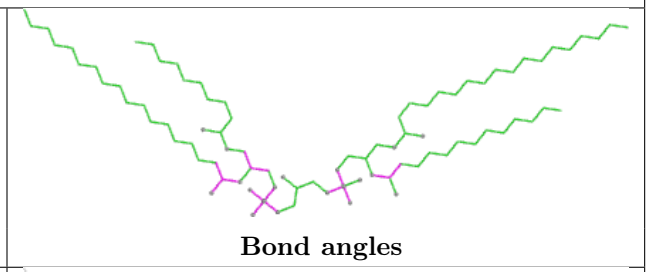
Ligand LFA O 303



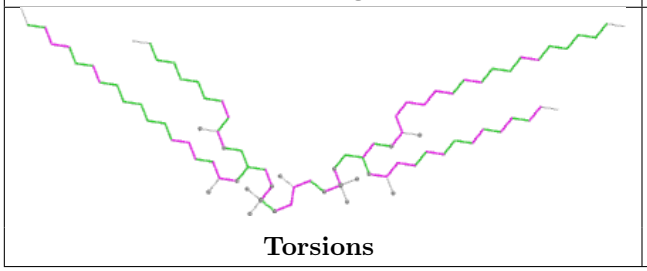
Ligand CDL C 304



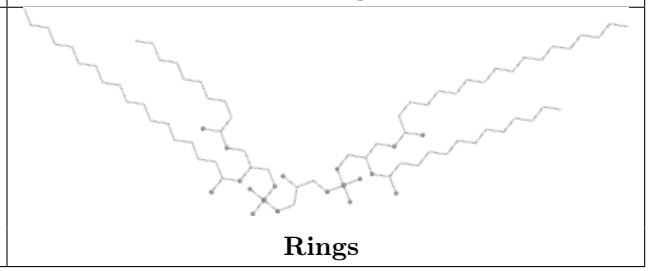
Bond lengths



Bond angles

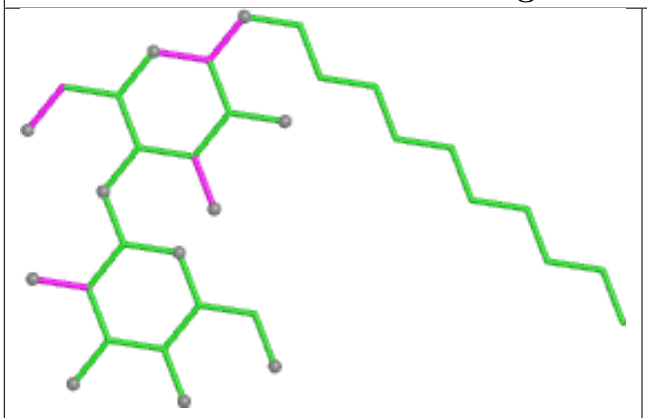


Torsions

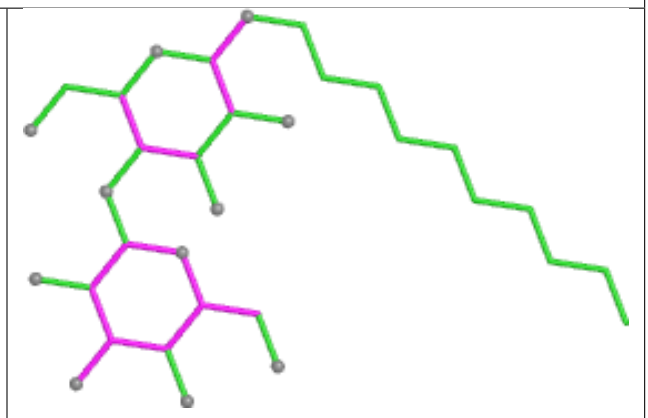


Rings

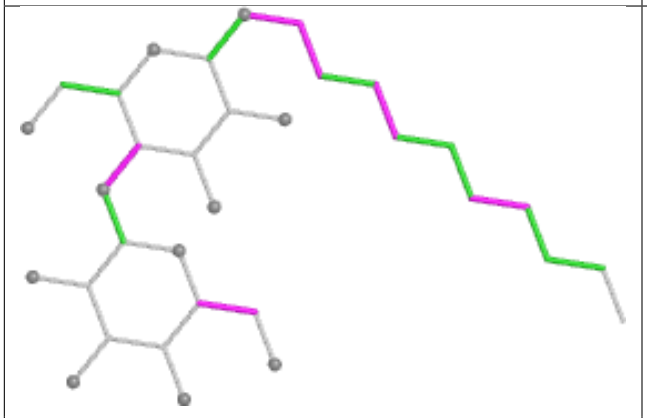
Ligand DMU D 201



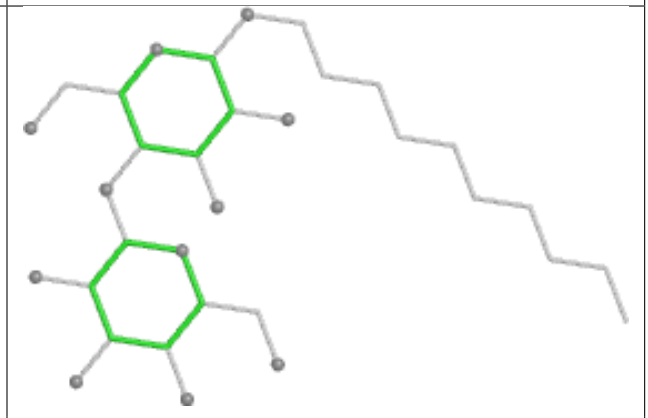
Bond lengths



Bond angles



Torsions



Rings

Ligand DMU G 102



Bond lengths



Bond angles

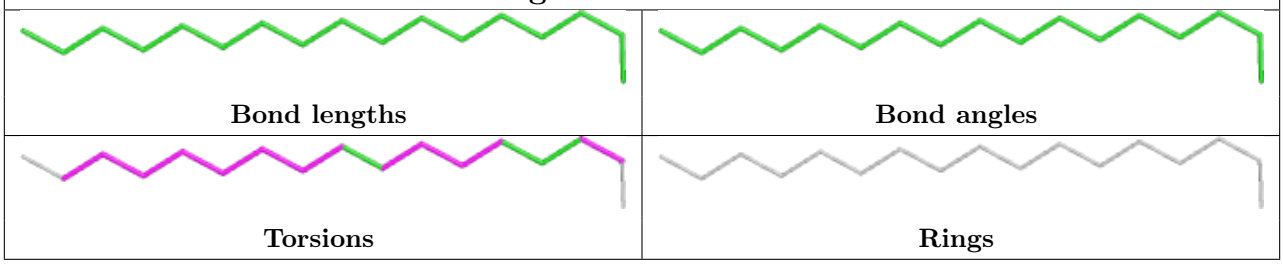


Torsions

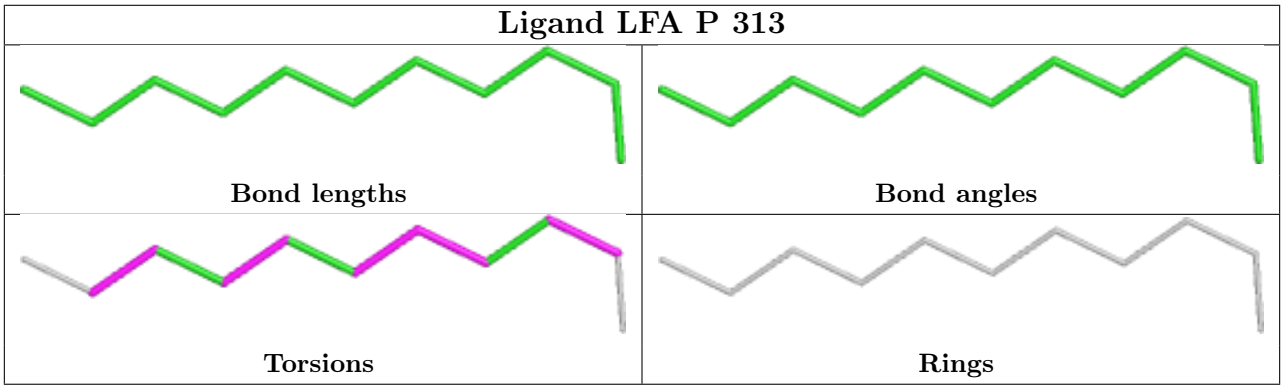


Rings

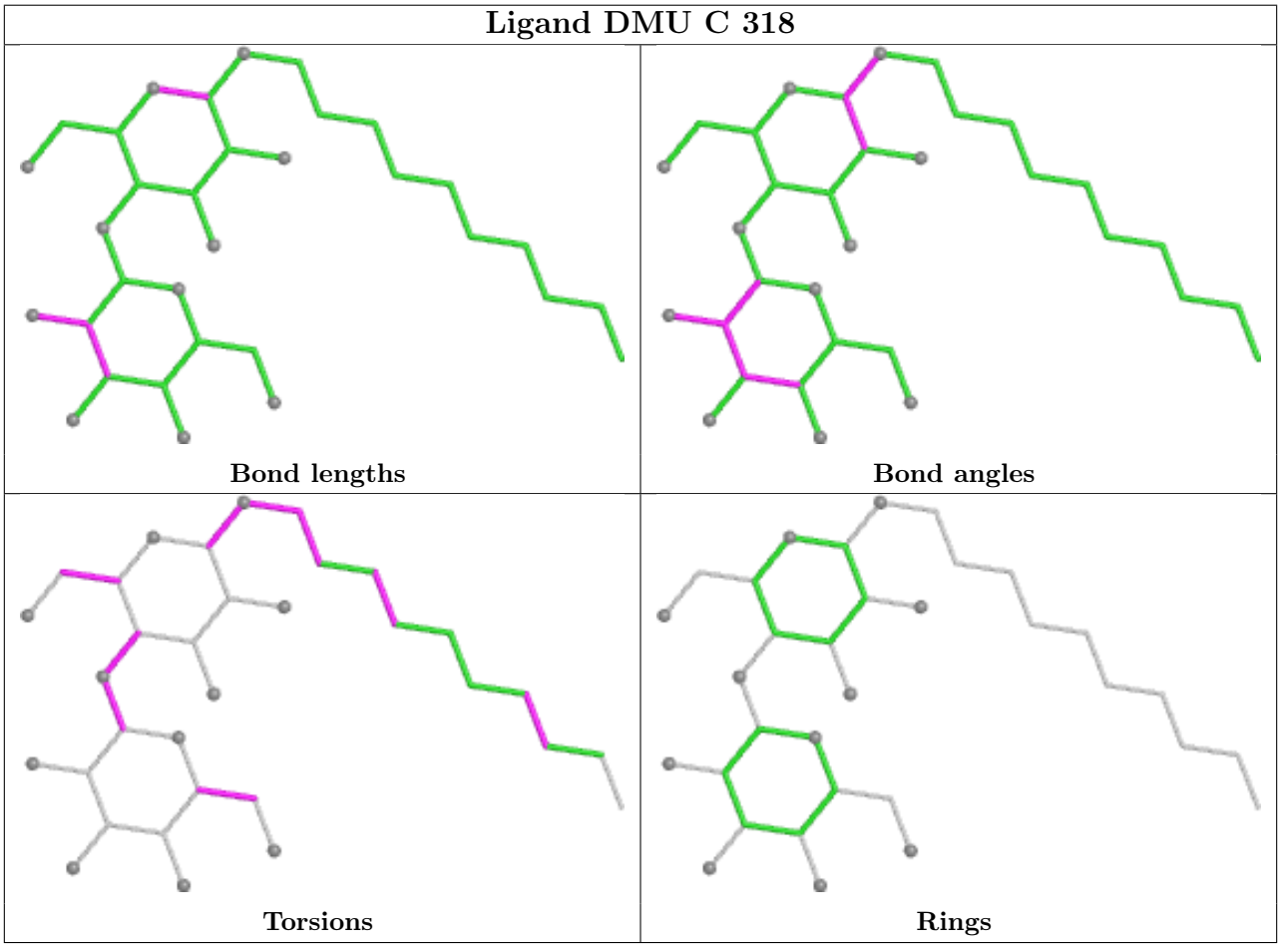
Ligand LFA B 307



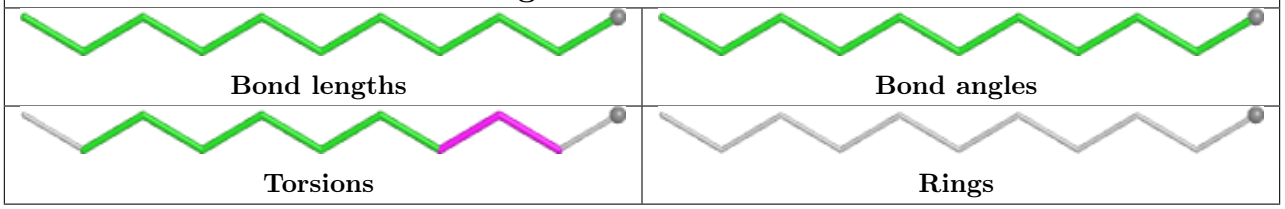
Ligand LFA P 313



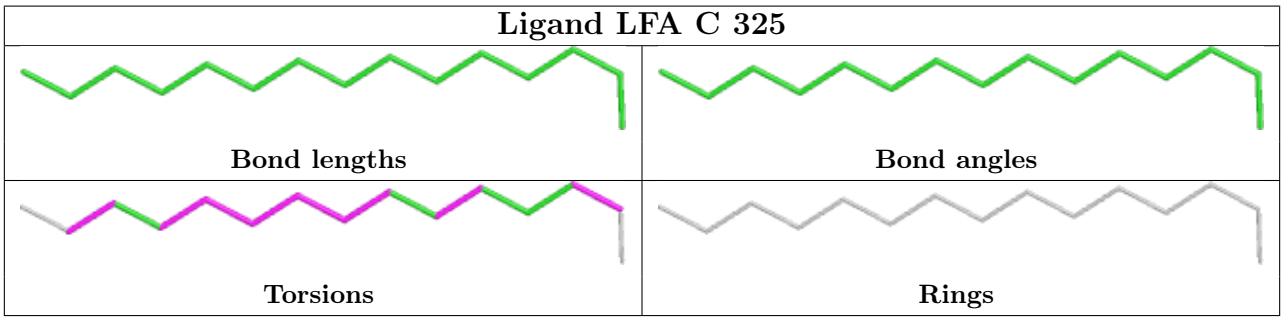
Ligand DMU C 318



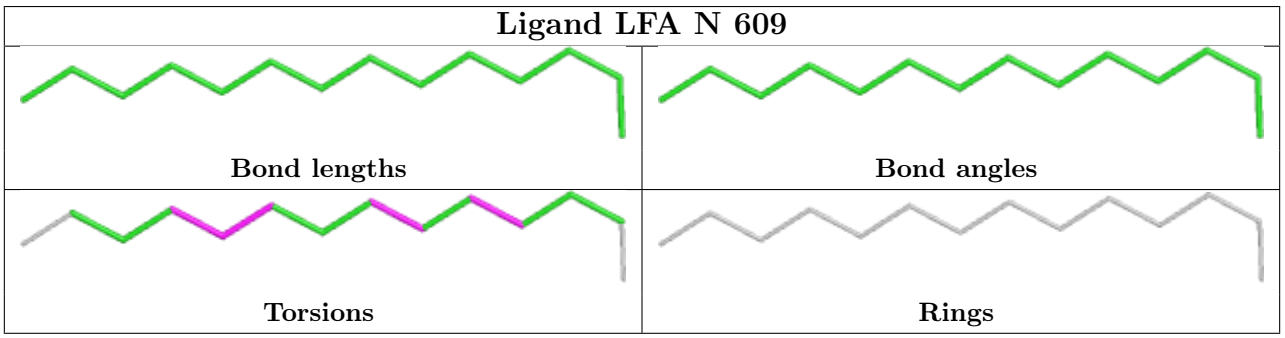
Ligand DMU C 306



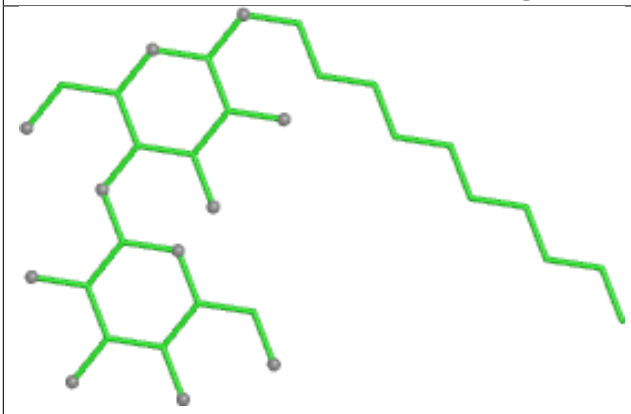
Ligand LFA C 325



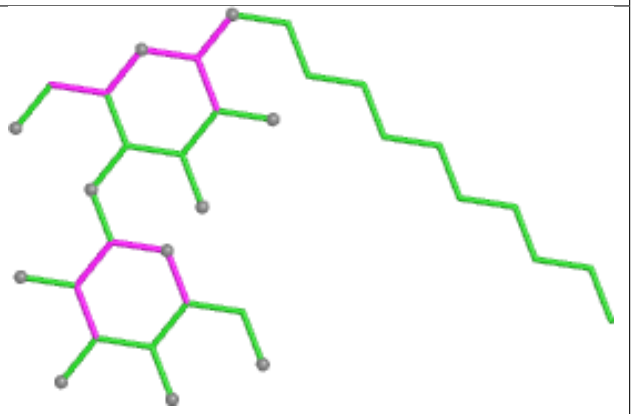
Ligand LFA N 609



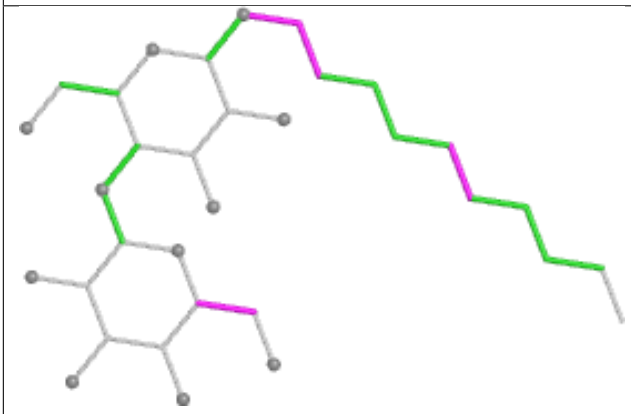
Ligand DMU P 325



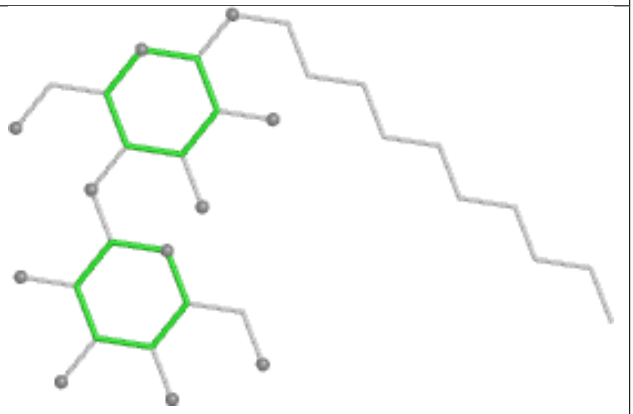
Bond lengths



Bond angles

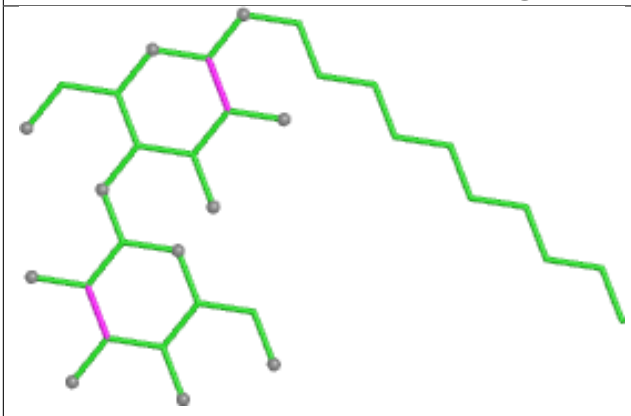


Torsions

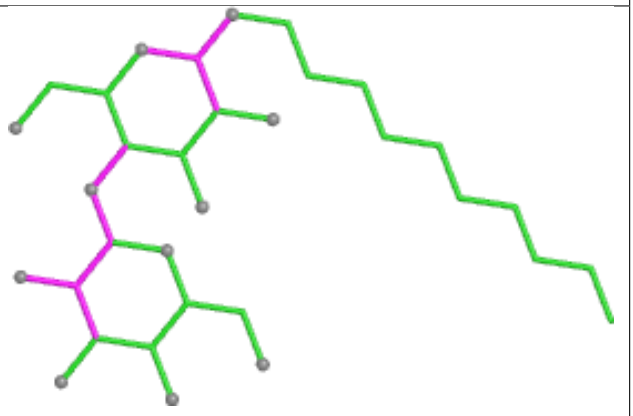


Rings

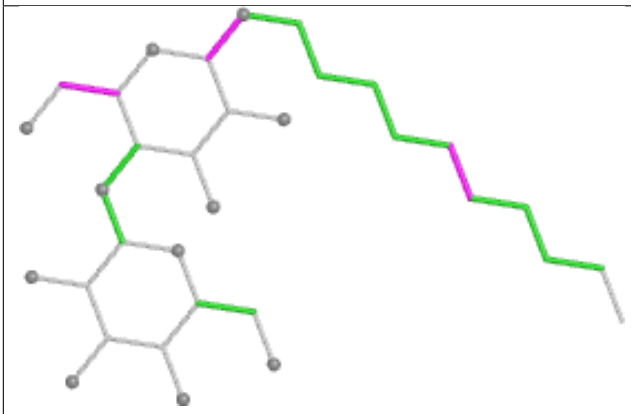
Ligand DMU U 101



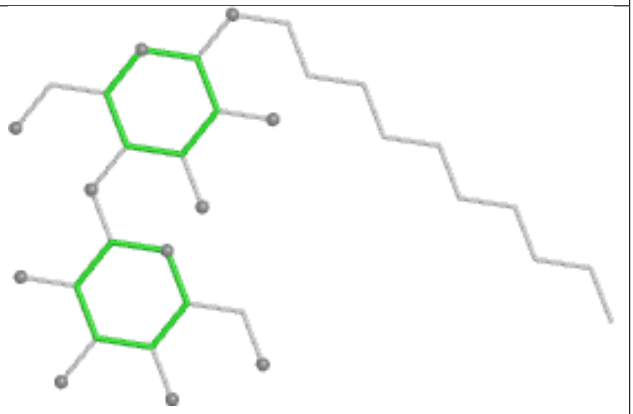
Bond lengths



Bond angles

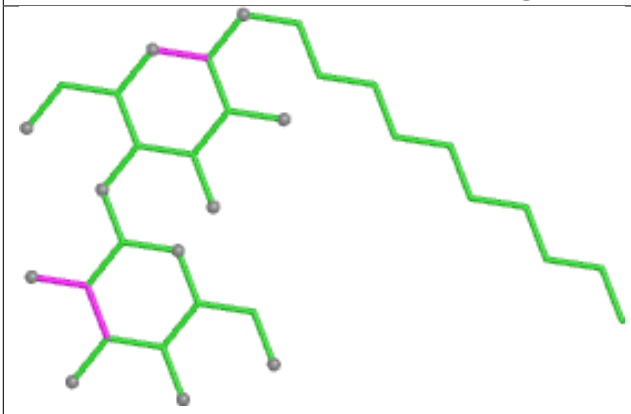


Torsions

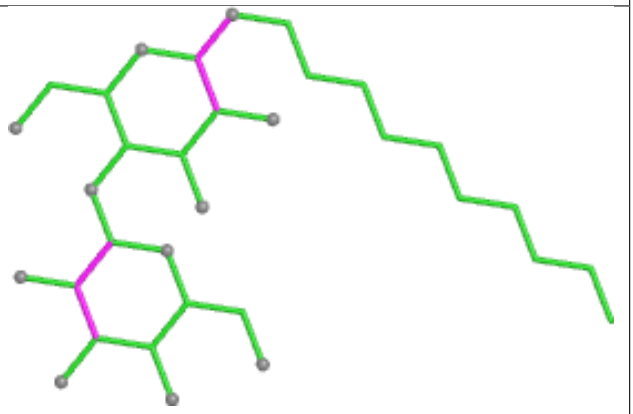


Rings

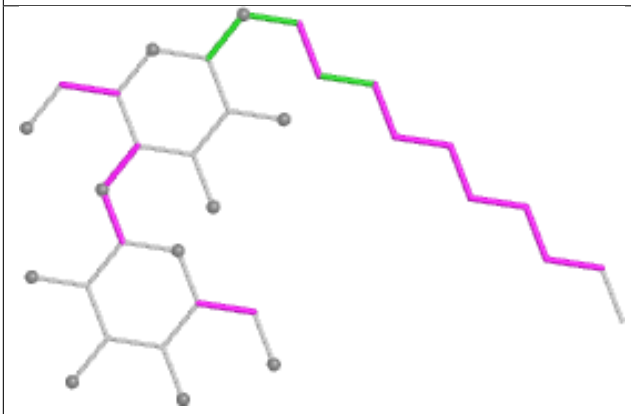
Ligand DMU P 319



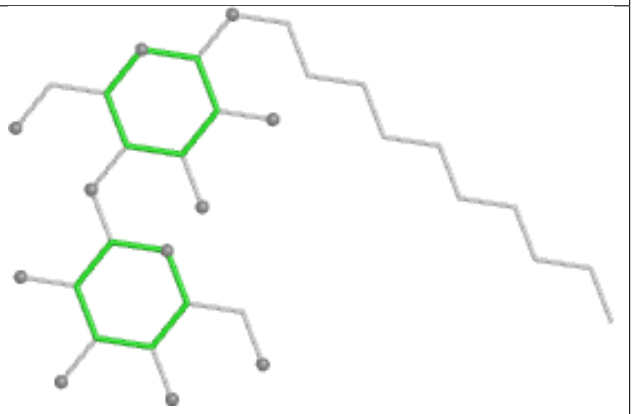
Bond lengths



Bond angles

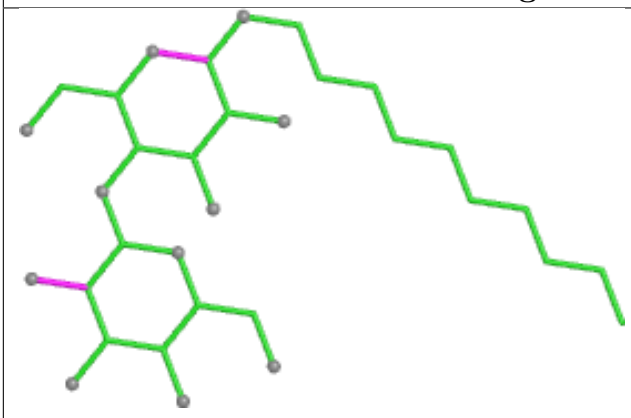


Torsions

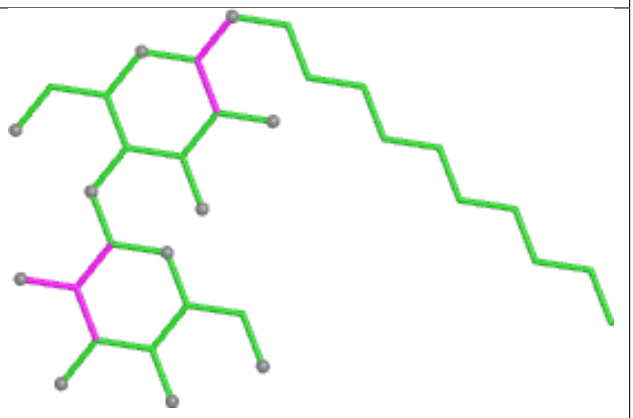


Rings

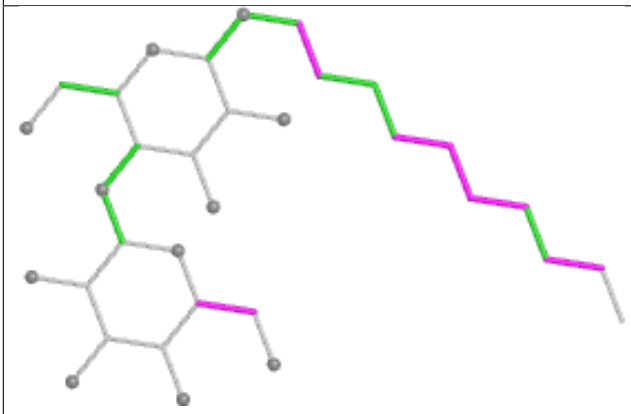
Ligand DMU Z 101



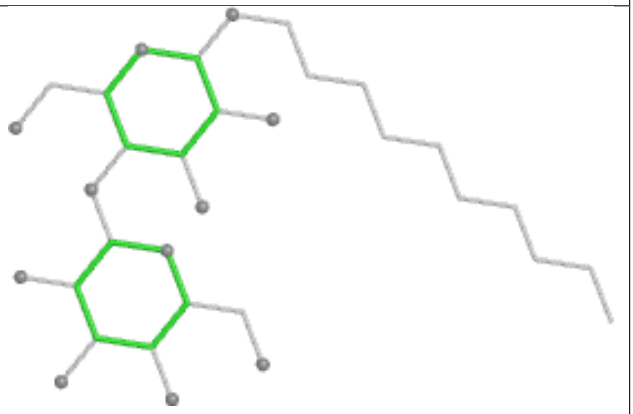
Bond lengths



Bond angles



Torsions



Rings

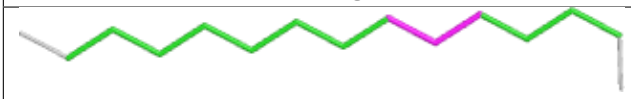
Ligand LFA C 313



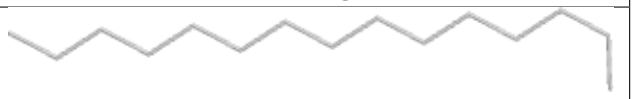
Bond lengths



Bond angles

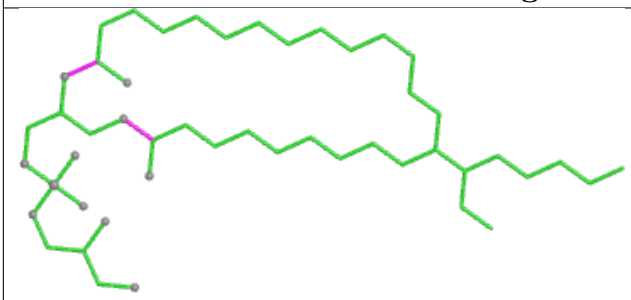


Torsions

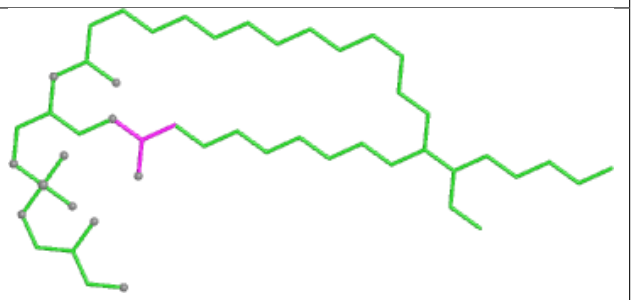


Rings

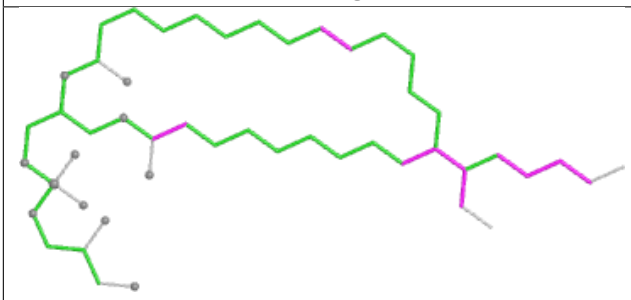
Ligand PGV A 617



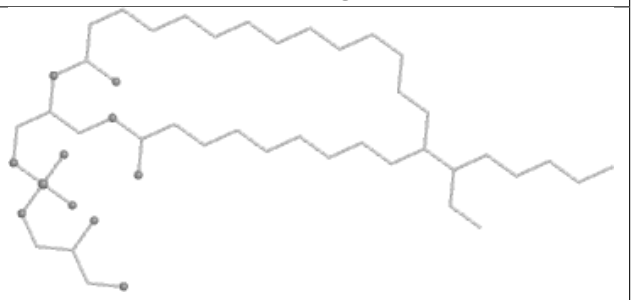
Bond lengths



Bond angles

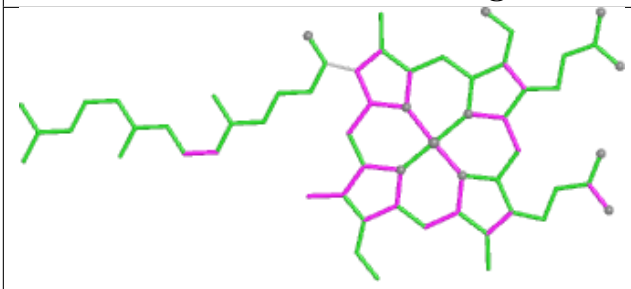


Torsions

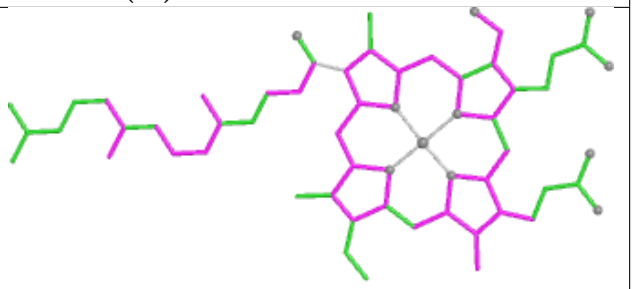


Rings

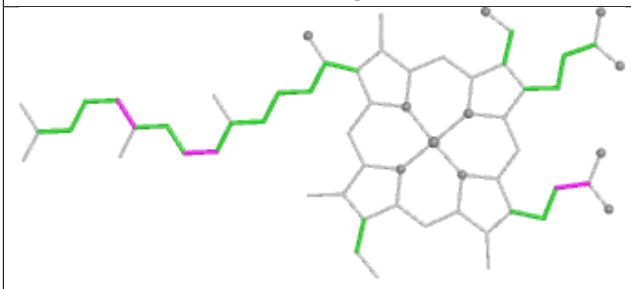
Ligand HEA A 601 (A)



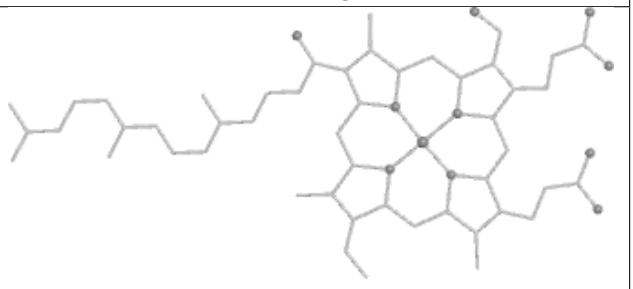
Bond lengths



Bond angles

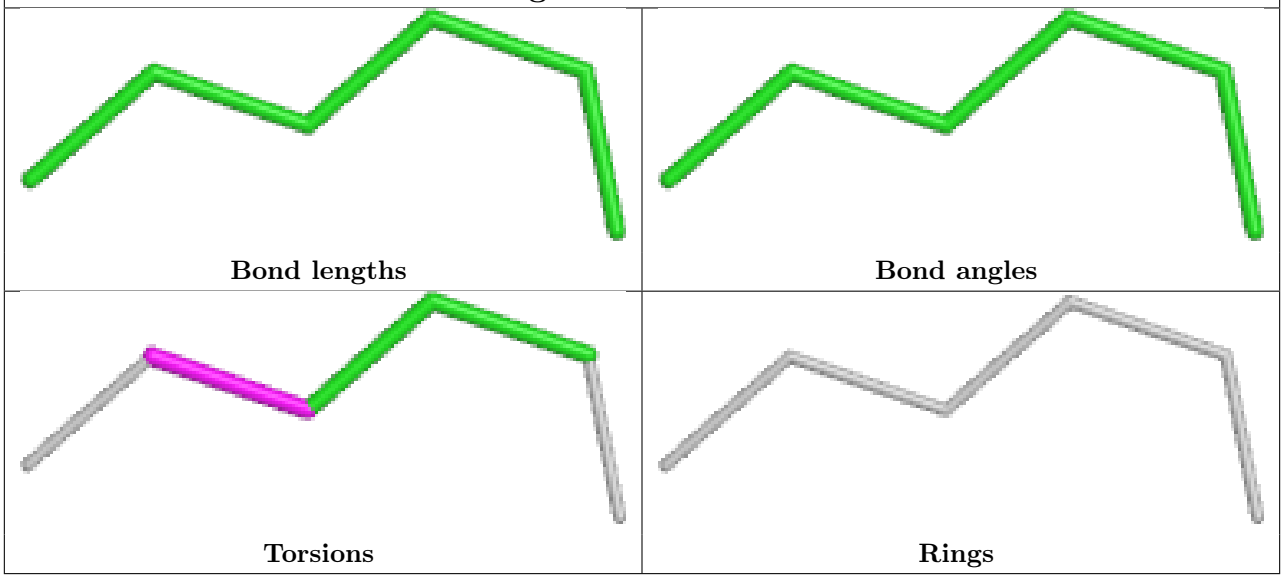


Torsions

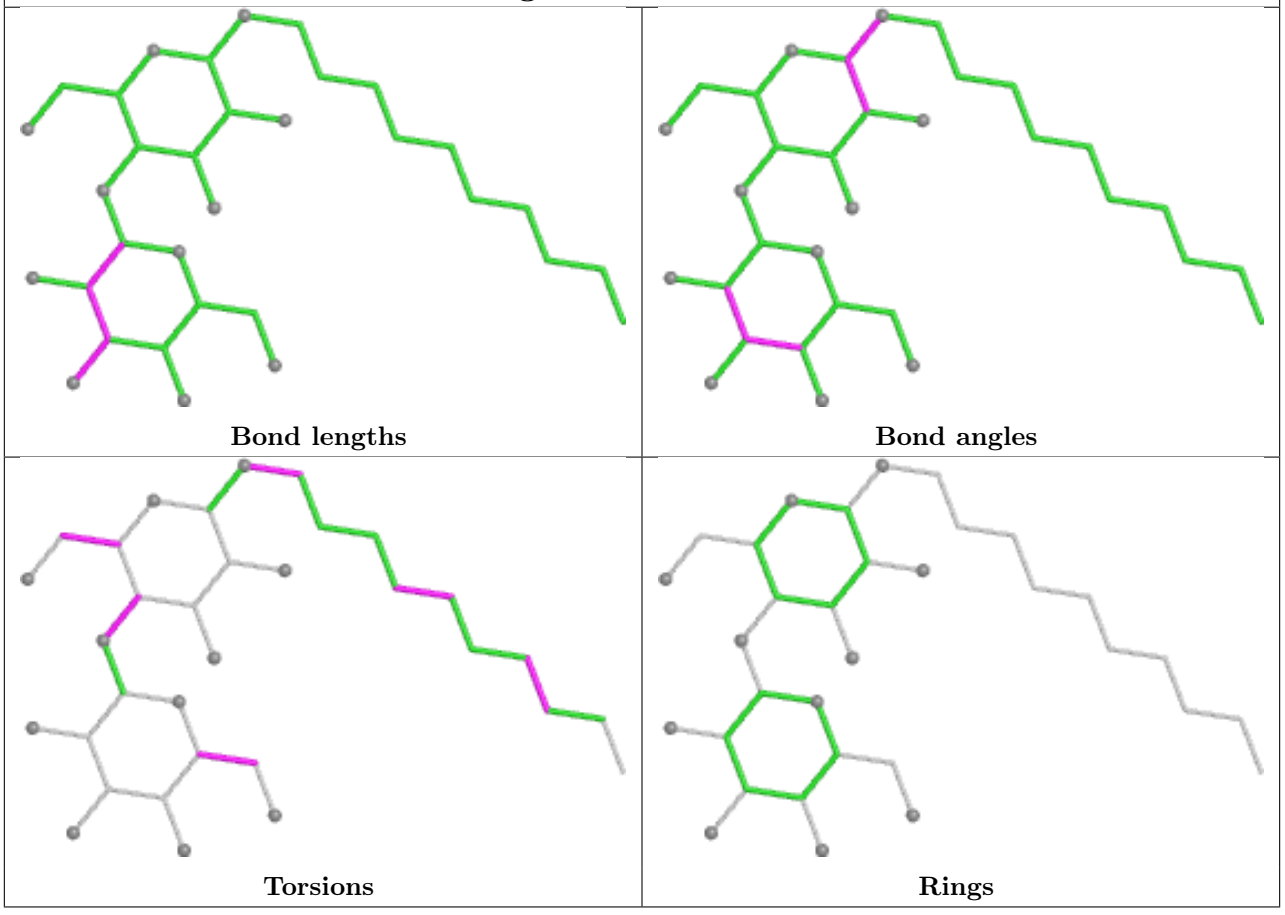


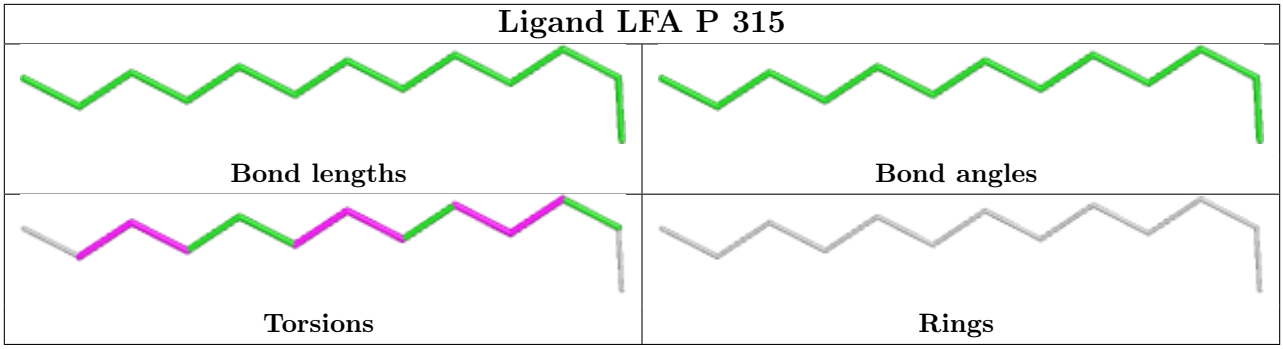
Rings

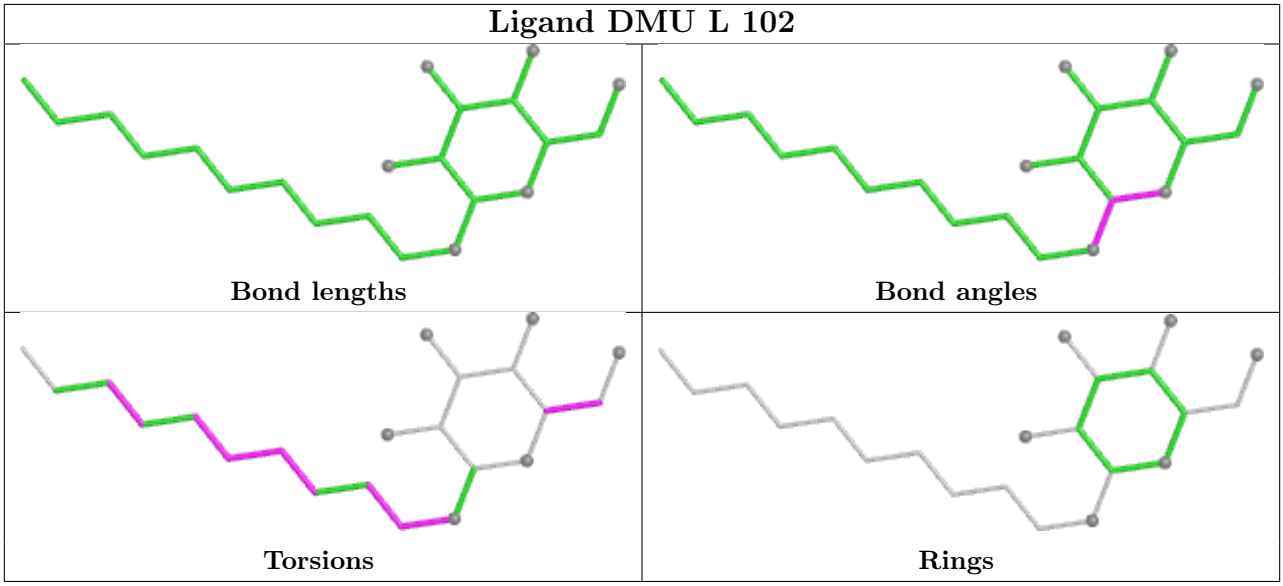
Ligand LFA C 308



Ligand DMU P 320







5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	512/514 (99%)	-0.25	3 (0%)	85	89	16, 33, 40, 58	15 (2%)
1	N	512/514 (99%)	-0.14	5 (0%)	79	84	17, 36, 44, 63	15 (2%)
2	B	226/227 (99%)	0.11	13 (5%)	29	33	20, 40, 58, 77	5 (2%)
2	O	226/227 (99%)	0.17	6 (2%)	56	62	22, 44, 69, 94	5 (2%)
3	C	258/261 (98%)	-0.08	2 (0%)	82	86	16, 36, 47, 61	9 (3%)
3	P	258/261 (98%)	-0.15	1 (0%)	88	91	16, 37, 48, 68	9 (3%)
4	D	143/147 (97%)	0.06	3 (2%)	63	70	19, 43, 59, 74	1 (0%)
4	Q	137/147 (93%)	0.45	8 (5%)	29	33	24, 53, 76, 90	1 (0%)
5	E	102/109 (93%)	-0.13	2 (1%)	65	71	35, 41, 55, 73	0
5	R	102/109 (93%)	-0.01	2 (1%)	65	71	39, 49, 66, 80	0
6	F	91/98 (92%)	0.02	1 (1%)	78	83	20, 42, 61, 72	2 (2%)
6	S	91/98 (92%)	0.15	2 (2%)	62	69	20, 41, 62, 70	2 (2%)
7	G	72/85 (84%)	0.31	3 (4%)	40	46	21, 44, 87, 104	1 (1%)
7	T	72/85 (84%)	0.37	3 (4%)	40	46	23, 46, 87, 102	1 (1%)
8	H	75/85 (88%)	0.31	4 (5%)	32	36	38, 46, 85, 109	0
8	U	75/85 (88%)	0.30	4 (5%)	32	36	41, 50, 89, 113	0
9	I	70/73 (95%)	0.44	5 (7%)	22	25	38, 51, 76, 96	0
9	V	70/73 (95%)	0.47	3 (4%)	40	46	38, 58, 76, 106	0
10	J	56/59 (94%)	0.20	1 (1%)	67	74	37, 47, 68, 76	0
10	W	56/59 (94%)	0.22	1 (1%)	67	74	39, 49, 69, 80	0
11	K	49/56 (87%)	0.35	2 (4%)	41	47	41, 47, 63, 74	0
11	X	49/56 (87%)	0.78	3 (6%)	27	31	46, 56, 74, 90	0
12	L	44/47 (93%)	-0.02	1 (2%)	61	67	35, 39, 50, 65	0
12	Y	44/47 (93%)	0.13	1 (2%)	61	67	38, 45, 60, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	40/46 (86%)	0.13	0 100 100	37, 40, 58, 68	0
13	Z	40/46 (86%)	0.55	1 (2%) 58 64	44, 50, 73, 82	0
All	All	3470/3614 (96%)	0.04	80 (2%) 61 67	16, 40, 66, 113	66 (1%)

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	36	TRP	6.1
6	S	3	GLY	5.1
6	S	93	PRO	5.1
9	V	72	ALA	4.9
1	N	136[A]	LEU	4.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	FME	A	1	10/11	0.93	0.13	43,52,80,92	0
1	FME	N	1	10/11	0.95	0.14	46,54,85,98	0
2	FME	B	1	10/11	0.97	0.09	37,39,50,88	0
2	FME	O	1	10/11	0.98	0.09	43,46,55,80	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	DMU	C	317	22/33	0.71	0.32	42,61,70,87	22

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	DMU	P	318	22/33	0.76	0.31	38,64,77,84	22
21	LFA	P	311	11/20	0.78	0.42	46,58,68,75	11
21	LFA	C	308	6/20	0.79	0.43	41,46,52,52	6
23	EDO	C	322	4/4	0.79	0.35	36,38,40,41	4
23	EDO	E	201	4/4	0.81	0.42	38,42,45,49	4
23	EDO	P	323	4/4	0.81	0.28	33,33,38,40	4
22	DMU	C	318	33/33	0.82	0.36	42,56,75,87	33
22	DMU	N	610	7/33	0.83	0.40	54,61,67,68	7
22	DMU	A	611	7/33	0.83	0.34	53,59,64,69	7
22	DMU	C	315	33/33	0.83	0.35	43,57,63,68	33
21	LFA	C	325	15/20	0.83	0.41	49,55,70,73	15
21	LFA	C	311	14/20	0.83	0.37	43,60,66,66	14
21	LFA	C	313	15/20	0.84	0.28	47,53,74,75	15
21	LFA	N	609	14/20	0.84	0.29	41,49,59,60	14
22	DMU	C	319	33/33	0.84	0.25	41,63,75,77	33
23	EDO	N	613	4/4	0.84	0.28	40,44,47,47	4
21	LFA	O	302	17/20	0.84	0.32	39,58,72,73	17
23	EDO	R	203	4/4	0.84	0.31	39,42,51,53	4
21	LFA	O	303	11/20	0.85	0.32	45,58,67,71	11
21	LFA	C	314	13/20	0.85	0.30	50,59,70,73	13
26	CHD	P	306	29/29	0.85	0.17	62,71,94,103	0
21	LFA	P	301	15/20	0.86	0.33	45,53,61,63	15
22	DMU	P	320	33/33	0.86	0.25	49,73,82,86	33
21	LFA	P	309	6/20	0.86	0.36	46,50,52,55	6
21	LFA	C	310	11/20	0.86	0.34	56,65,78,80	11
21	LFA	A	610	14/20	0.86	0.27	40,48,60,62	14
22	DMU	C	324	33/33	0.86	0.19	40,57,74,87	33
22	DMU	M	102	8/33	0.86	0.23	42,45,50,58	8
22	DMU	A	618	11/33	0.86	0.37	50,58,66,69	11
21	LFA	T	102	11/20	0.87	0.28	49,56,66,69	11
22	DMU	N	611	33/33	0.87	0.22	41,53,77,79	33
21	LFA	B	307	17/20	0.87	0.31	41,56,72,73	17
22	DMU	P	319	33/33	0.87	0.31	49,58,71,86	33
21	LFA	A	609	14/20	0.87	0.26	38,46,72,75	14
22	DMU	P	325	33/33	0.87	0.18	43,61,86,89	33
22	DMU	Q	201	33/33	0.87	0.22	40,55,65,76	33
21	LFA	P	308	11/20	0.87	0.33	50,54,59,63	11
21	LFA	C	312	11/20	0.87	0.29	43,53,63,63	11
21	LFA	C	309	18/20	0.87	0.24	39,48,62,64	18
21	LFA	P	312	14/20	0.87	0.33	39,64,68,70	14
21	LFA	P	313	11/20	0.87	0.29	41,52,66,70	11
21	LFA	P	315	13/20	0.87	0.28	43,56,67,68	13

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	EDO	C	320	4/4	0.88	0.27	48,51,53,65	4
22	DMU	C	323	22/33	0.88	0.29	51,60,68,72	22
19	CDL	P	305	87/100	0.88	0.19	46,83,134,163	0
22	DMU	H	101	33/33	0.88	0.24	34,48,58,76	33
22	DMU	O	304	22/33	0.88	0.29	56,66,78,99	22
22	DMU	P	316	33/33	0.88	0.28	46,56,69,77	33
26	CHD	C	305	29/29	0.88	0.14	59,69,87,106	0
23	EDO	A	613	4/4	0.88	0.20	30,33,33,35	4
22	DMU	W	101	11/33	0.89	0.33	63,68,73,76	11
19	CDL	C	304	87/100	0.89	0.18	47,83,117,131	0
23	EDO	A	614	4/4	0.89	0.23	36,45,49,52	4
21	LFA	P	314	15/20	0.89	0.21	43,48,55,62	15
19	CDL	A	607	64/100	0.89	0.16	46,78,105,127	0
19	CDL	V	101	64/100	0.89	0.16	56,81,114,138	0
21	LFA	P	310	18/20	0.89	0.26	41,54,64,64	18
21	LFA	C	307	11/20	0.89	0.30	45,49,62,66	11
22	DMU	P	324	22/33	0.89	0.24	50,60,66,75	22
22	DMU	B	308	22/33	0.89	0.28	55,74,80,84	22
19	CDL	Y	101	94/100	0.89	0.17	51,84,134,164	0
22	DMU	U	101	33/33	0.90	0.24	36,48,60,64	33
22	DMU	C	316	7/33	0.91	0.29	50,53,58,69	7
22	DMU	B	302	11/33	0.91	0.29	45,51,57,64	11
22	DMU	G	102	11/33	0.91	0.28	44,54,65,66	11
22	DMU	O	306	11/33	0.91	0.27	41,45,52,65	11
22	DMU	O	308	22/33	0.91	0.19	34,48,55,56	22
22	DMU	A	612	33/33	0.91	0.18	32,45,58,61	33
22	DMU	P	317	7/33	0.91	0.26	55,57,63,67	7
22	DMU	Z	102	22/33	0.91	0.31	53,62,67,74	22
21	LFA	N	608	14/20	0.91	0.23	40,49,65,66	14
22	DMU	B	303	11/33	0.92	0.23	46,54,64,65	11
22	DMU	J	101	11/33	0.92	0.30	56,62,68,74	11
22	DMU	L	102	22/33	0.92	0.27	47,57,66,73	22
19	CDL	L	101	94/100	0.92	0.15	44,80,120,132	0
22	DMU	Z	103	8/33	0.92	0.21	47,49,51,54	8
23	EDO	C	321	4/4	0.93	0.21	36,37,38,43	4
22	DMU	Z	101	33/33	0.93	0.10	55,62,75,84	0
22	DMU	D	201	33/33	0.93	0.14	27,44,58,63	33
23	EDO	E	202	4/4	0.93	0.24	33,34,35,35	4
23	EDO	F	102	4/4	0.93	0.16	25,25,30,32	4
22	DMU	C	306	11/33	0.94	0.22	53,56,60,67	11
23	EDO	R	202	4/4	0.94	0.21	35,37,42,42	4
23	EDO	E	203	4/4	0.94	0.25	35,37,40,45	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	CHD	C	301	29/29	0.94	0.08	35,39,41,44	0
22	DMU	P	307	11/33	0.94	0.24	48,50,57,64	11
22	DMU	B	304	22/33	0.94	0.17	44,60,67,81	22
27	UNX	P	303	1/1	0.94	0.29	46,46,46,46	0
23	EDO	P	321	4/4	0.95	0.18	49,56,64,72	4
23	EDO	P	322	4/4	0.95	0.22	36,39,40,42	4
22	DMU	M	101	33/33	0.95	0.08	47,54,69,76	0
23	EDO	N	612	4/4	0.95	0.12	32,32,35,36	4
23	EDO	A	615	4/4	0.95	0.19	27,27,28,31	4
23	EDO	N	614	4/4	0.95	0.20	31,32,33,34	4
23	EDO	N	615	4/4	0.95	0.17	35,39,44,44	4
23	EDO	N	616	4/4	0.95	0.15	32,34,34,40	4
23	EDO	O	309	4/4	0.95	0.14	34,38,40,41	4
20	CO2	N	607	3/3	0.96	0.25	41,41,46,49	0
23	EDO	T	103	4/4	0.96	0.12	37,39,39,40	4
23	EDO	G	103	4/4	0.96	0.14	33,34,34,36	4
22	DMU	O	307	11/33	0.96	0.21	46,50,58,59	11
26	CHD	P	302	29/29	0.96	0.07	34,39,44,45	0
23	EDO	R	201	4/4	0.96	0.25	56,59,66,67	4
23	EDO	A	616	4/4	0.96	0.13	44,44,46,48	4
29	PEK	G	101	53/53	0.96	0.11	36,52,93,120	0
29	PEK	T	101	53/53	0.96	0.11	38,55,100,111	0
24	PGV	N	617	51/51	0.97	0.09	34,46,75,80	0
26	CHD	B	306	29/29	0.97	0.06	33,36,40,49	0
27	UNX	C	302	1/1	0.97	0.18	44,44,44,44	0
23	EDO	S	102	4/4	0.97	0.07	24,28,28,31	4
23	EDO	B	305	4/4	0.97	0.09	26,29,30,33	4
26	CHD	O	301	29/29	0.97	0.06	33,36,39,46	0
18	PER	N	606	2/2	0.98	0.09	35,35,35,35	0
24	PGV	A	617	51/51	0.98	0.09	32,43,77,83	0
24	PGV	C	303	51/51	0.98	0.08	33,40,92,100	0
23	EDO	F	103	4/4	0.98	0.09	33,33,36,37	4
24	PGV	P	304	51/51	0.98	0.08	32,41,88,111	0
17	NA	A	605	1/1	0.99	0.05	35,35,35,35	0
18	PER	A	606	2/2	0.99	0.04	32,32,32,33	0
14	HEA	A	601[A]	60/60	0.99	0.05	26,30,41,45	9
14	HEA	A	601[B]	60/60	0.99	0.05	26,30,46,49	9
14	HEA	A	602	60/60	0.99	0.05	28,30,37,42	0
14	HEA	N	601[A]	60/60	0.99	0.05	30,34,45,52	9
23	EDO	S	103	4/4	0.99	0.08	29,38,38,38	4
14	HEA	N	601[B]	60/60	0.99	0.05	30,34,44,48	9
14	HEA	N	602	60/60	0.99	0.06	29,33,37,42	0

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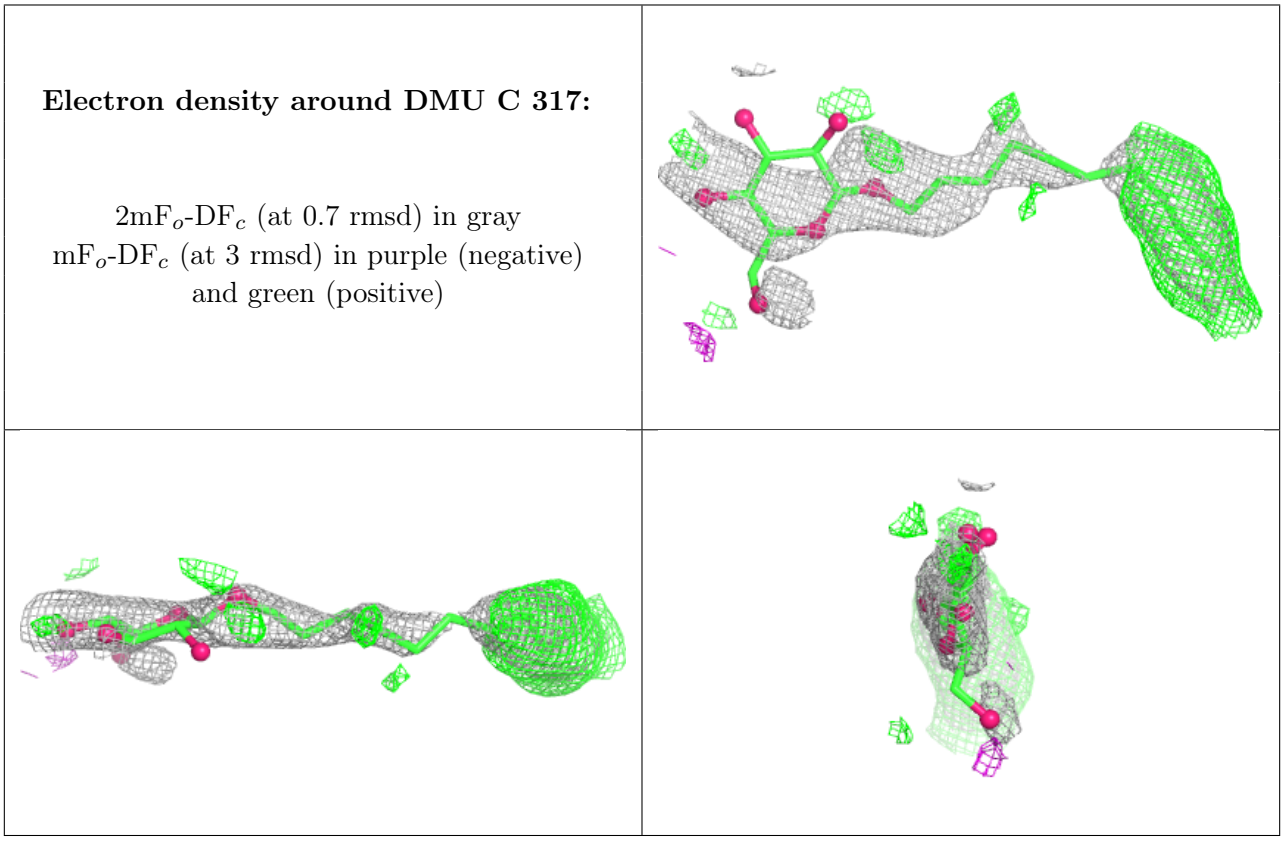
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	MG	N	604	1/1	0.99	0.03	35,35,35,35	0
20	CO2	A	608	3/3	0.99	0.16	37,37,39,46	0
25	CUA	B	301	2/2	1.00	0.02	32,32,32,33	0
25	CUA	O	305	2/2	1.00	0.02	37,37,37,37	0
17	NA	N	605	1/1	1.00	0.05	41,41,41,41	0
16	MG	A	604	1/1	1.00	0.02	32,32,32,32	0
28	ZN	F	101	1/1	1.00	0.01	36,36,36,36	0
28	ZN	S	101	1/1	1.00	0.01	37,37,37,37	0
15	CU	A	603	1/1	1.00	0.01	31,31,31,31	0
15	CU	N	603	1/1	1.00	0.01	33,33,33,33	0

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

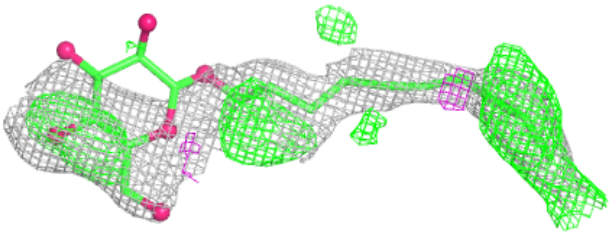
Electron density around DMU C 317:

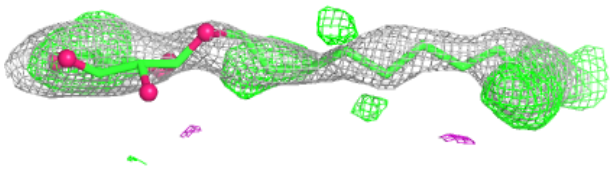
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

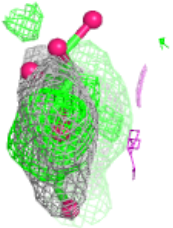


Electron density around DMU P 318:

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

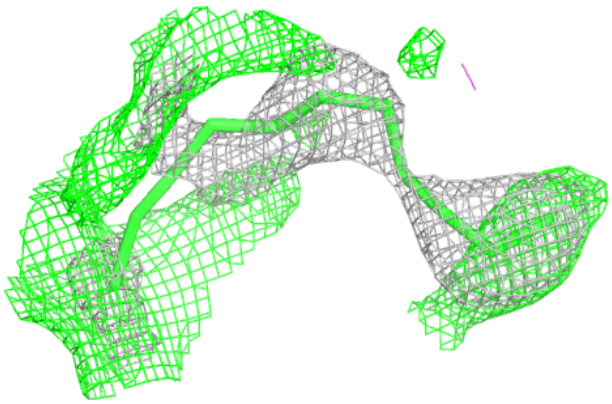


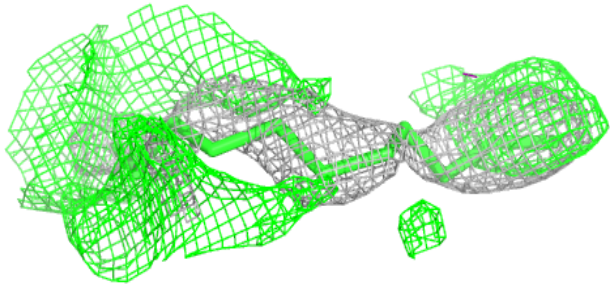


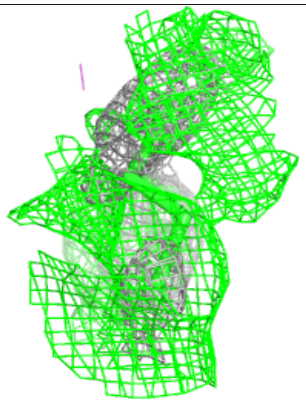


Electron density around LFA P 311:

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

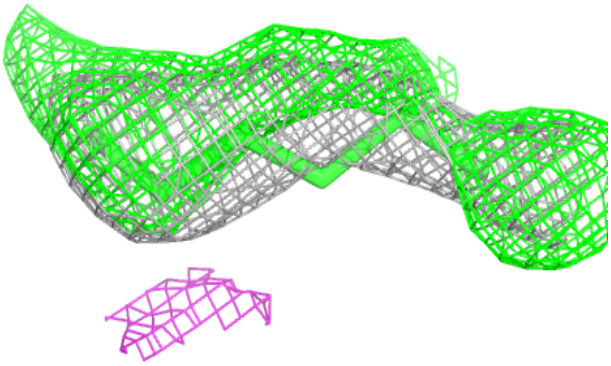


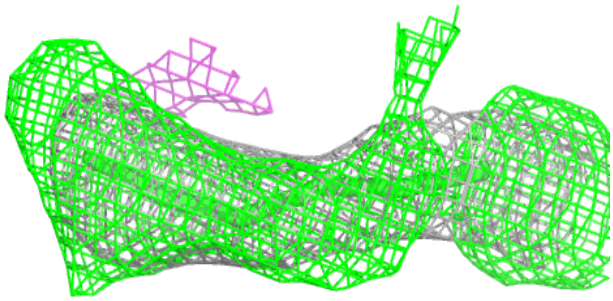


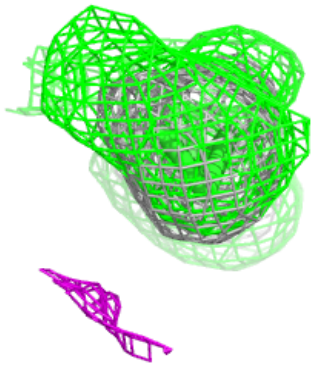


Electron density around LFA C 308:

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

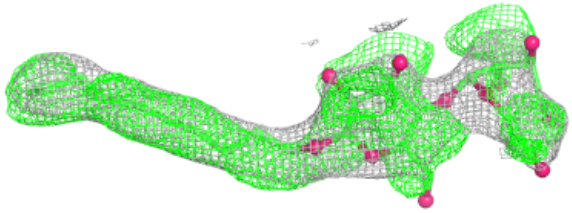


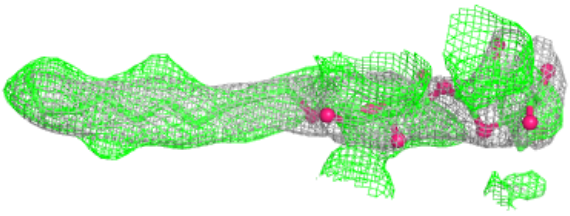


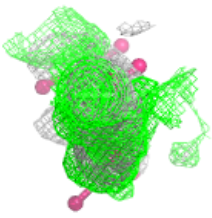


Electron density around DMU C 318:

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

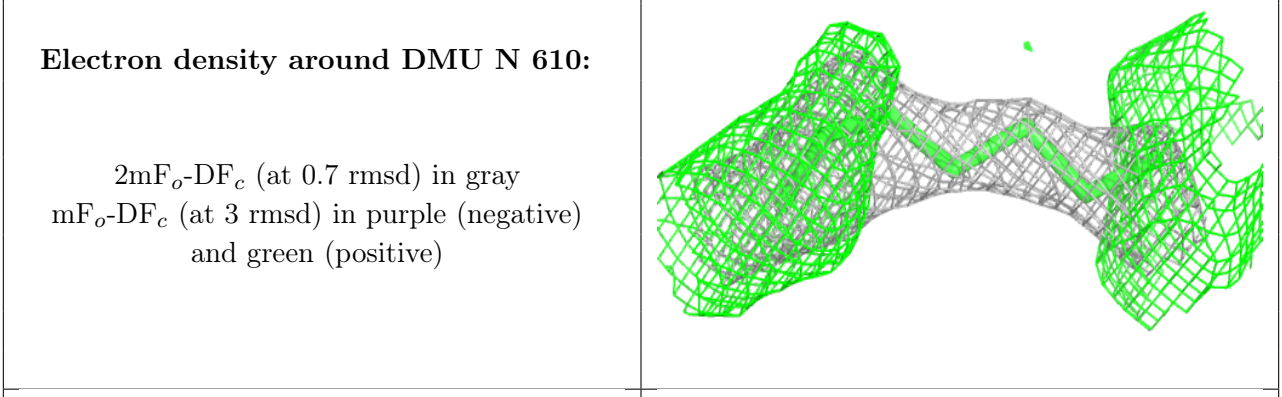






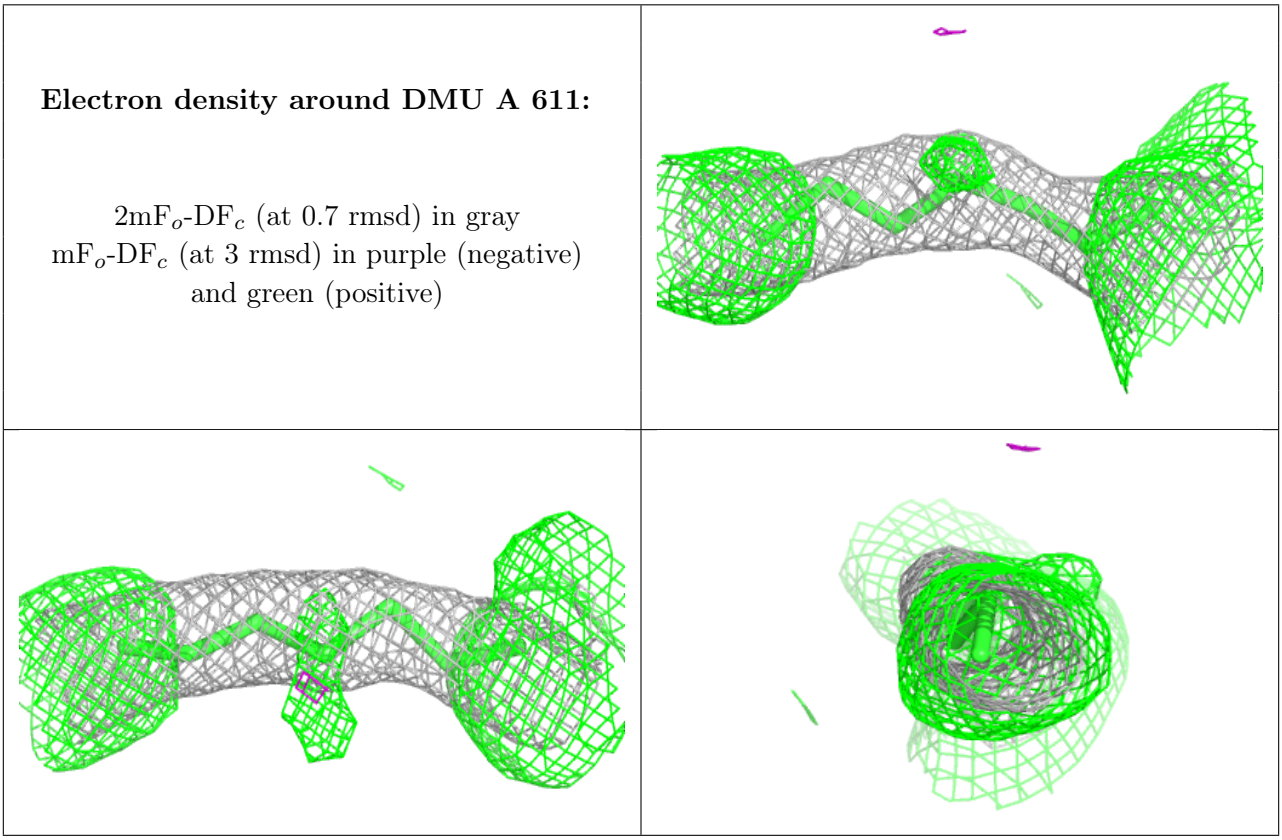
Electron density around DMU N 610:

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



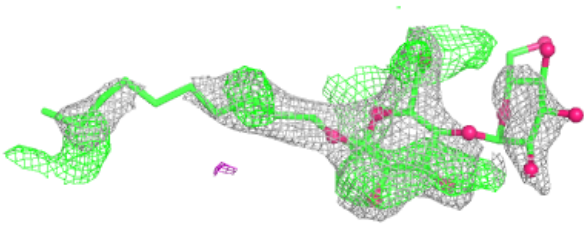
Electron density around DMU A 611:

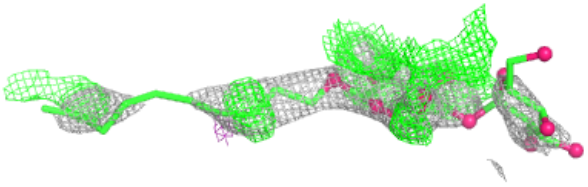
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

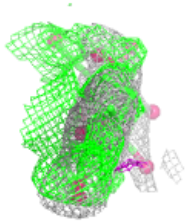


Electron density around DMU C 315:

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

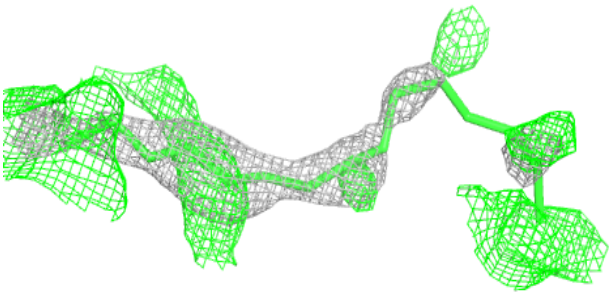


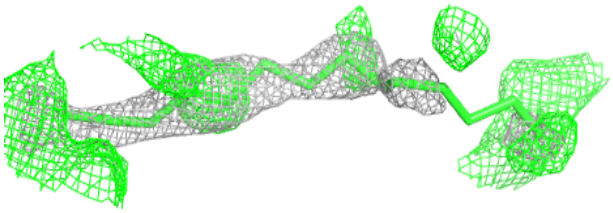


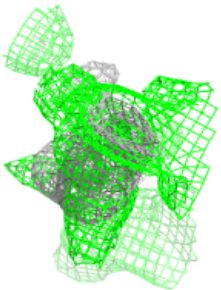


Electron density around LFA C 325:

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

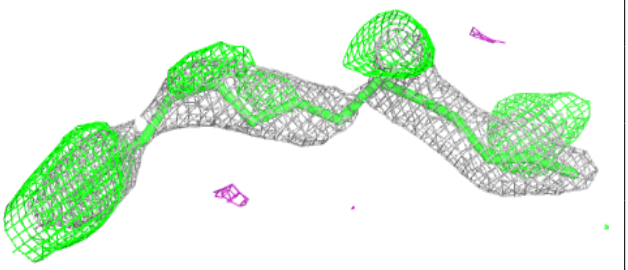


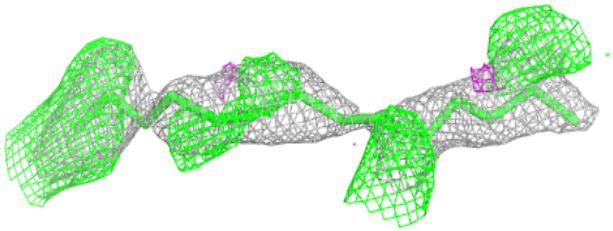


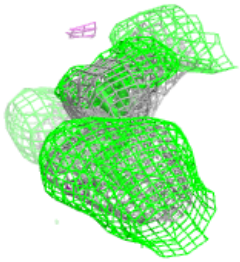


Electron density around LFA C 311:

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

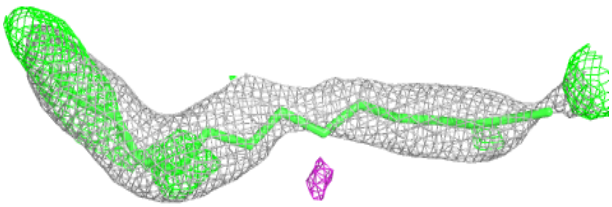


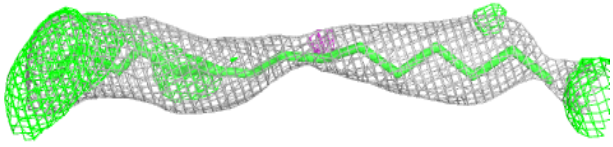


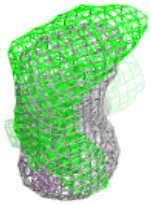


Electron density around LFA C 313:

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

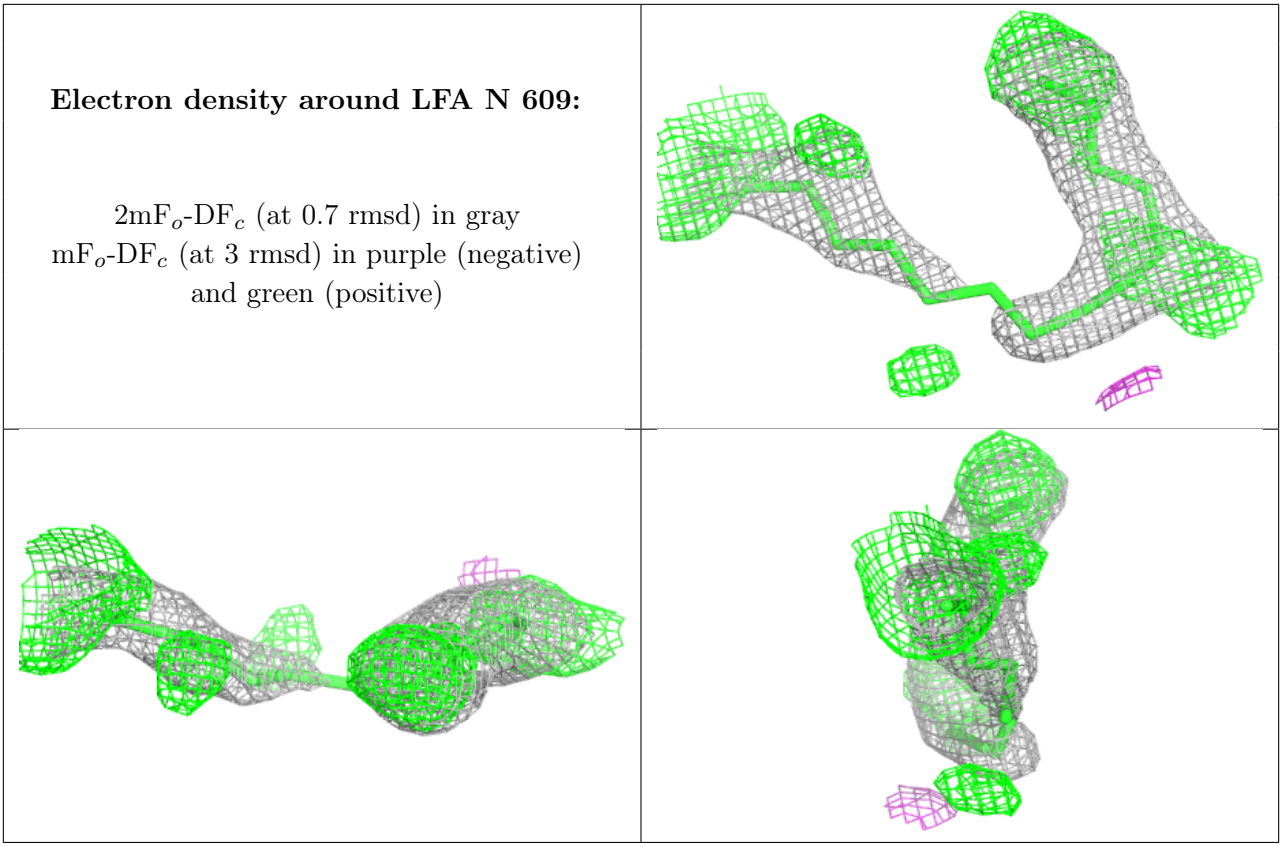






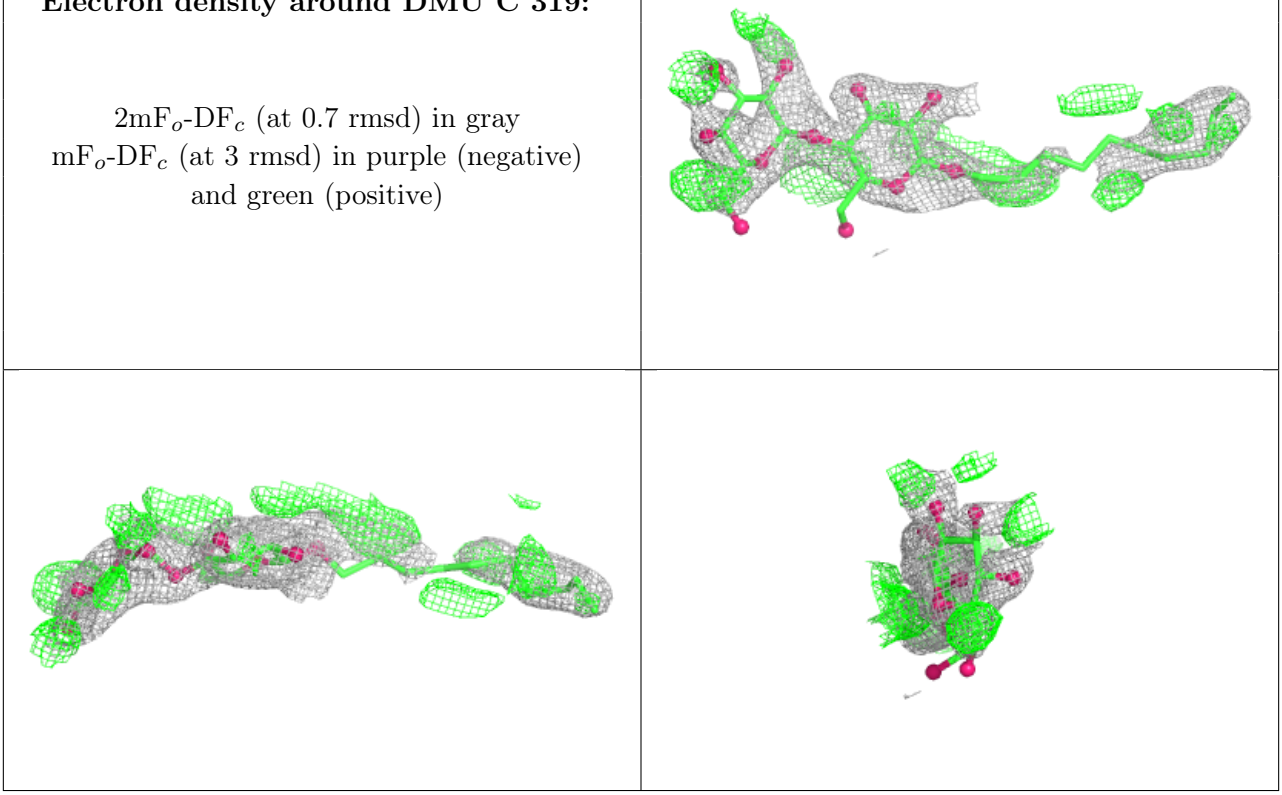
Electron density around LFA N 609:

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



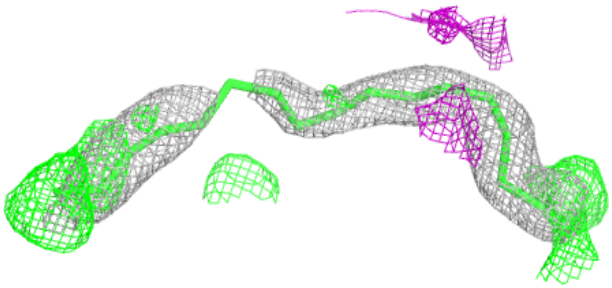
Electron density around DMU C 319:

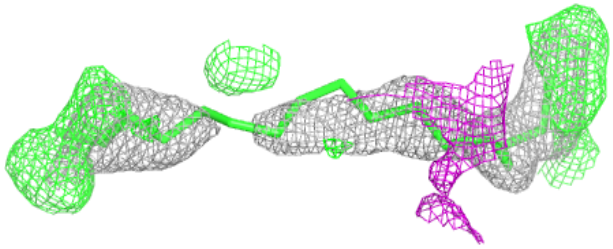
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

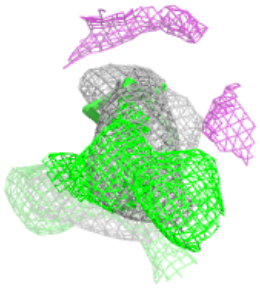


Electron density around LFA O 302:

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

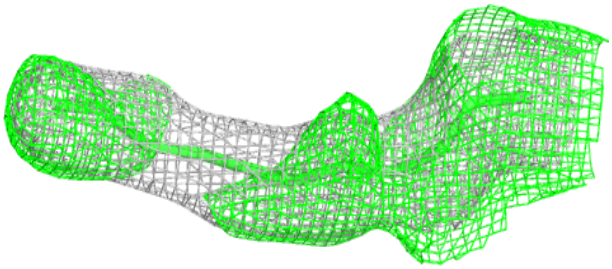


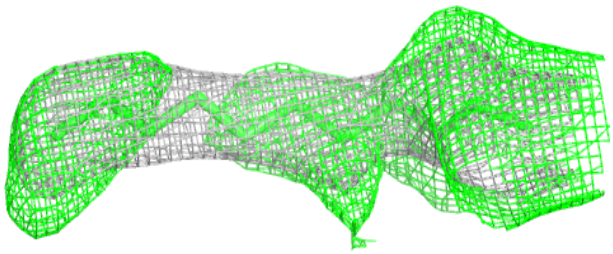


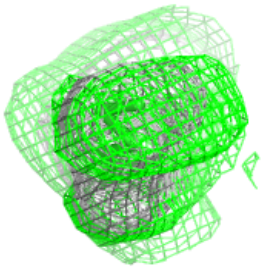


Electron density around LFA O 303:

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

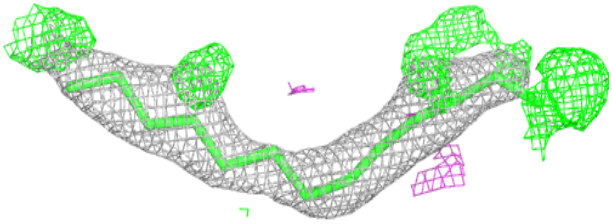


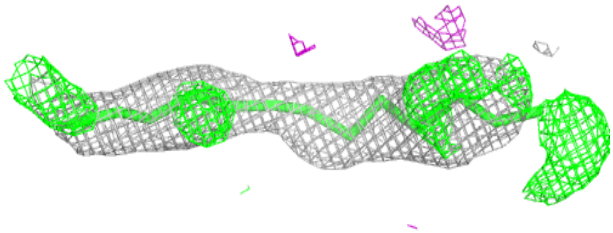


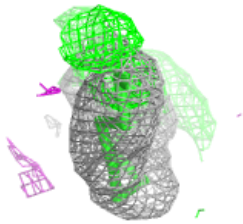


Electron density around LFA C 314:

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

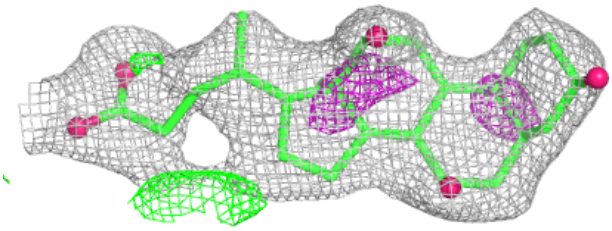


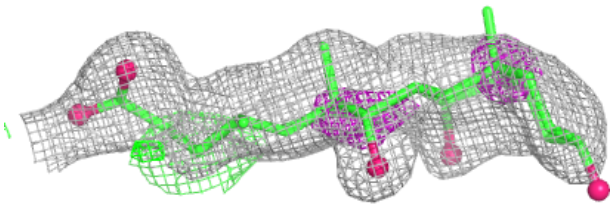


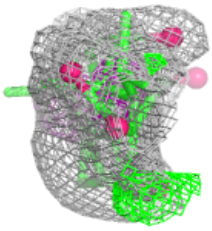


Electron density around CHD P 306:

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

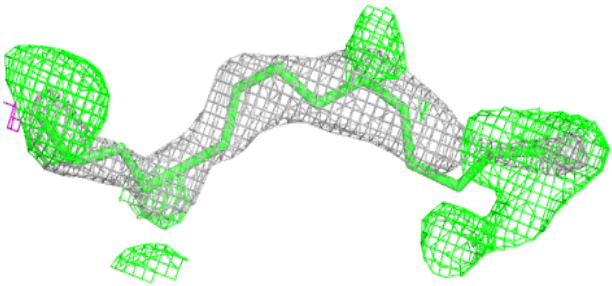


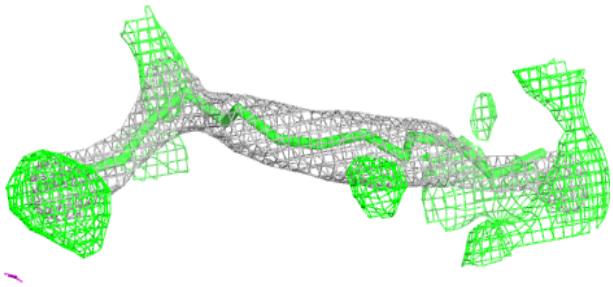


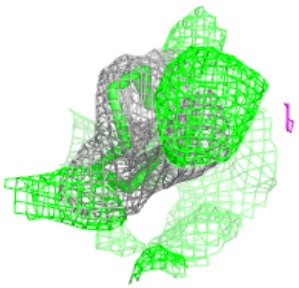


Electron density around LFA P 301:

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

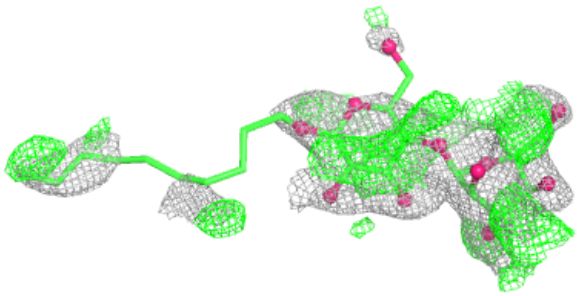


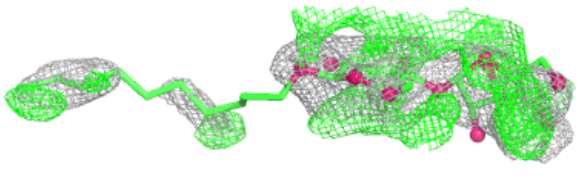


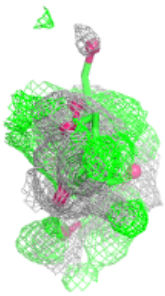


Electron density around DMU P 320:

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

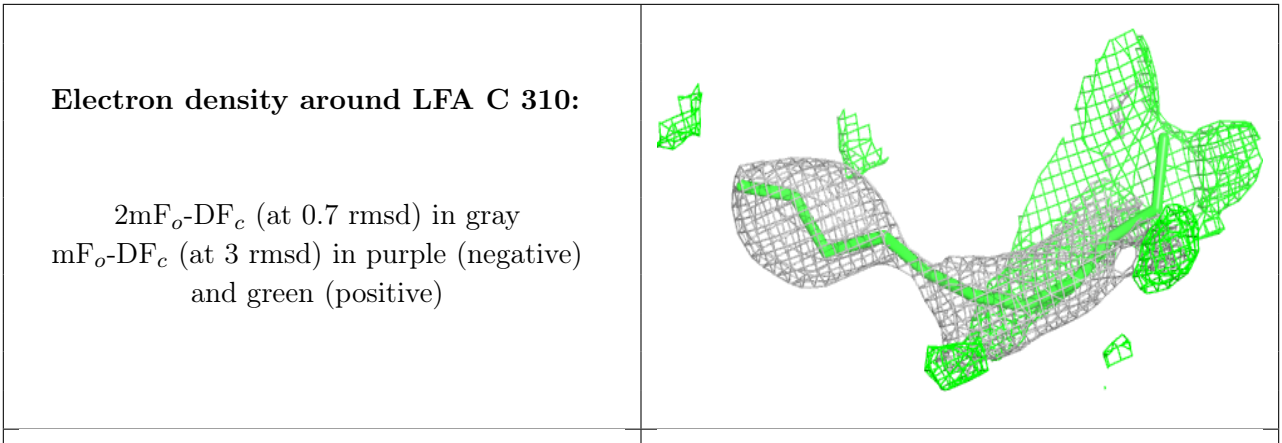






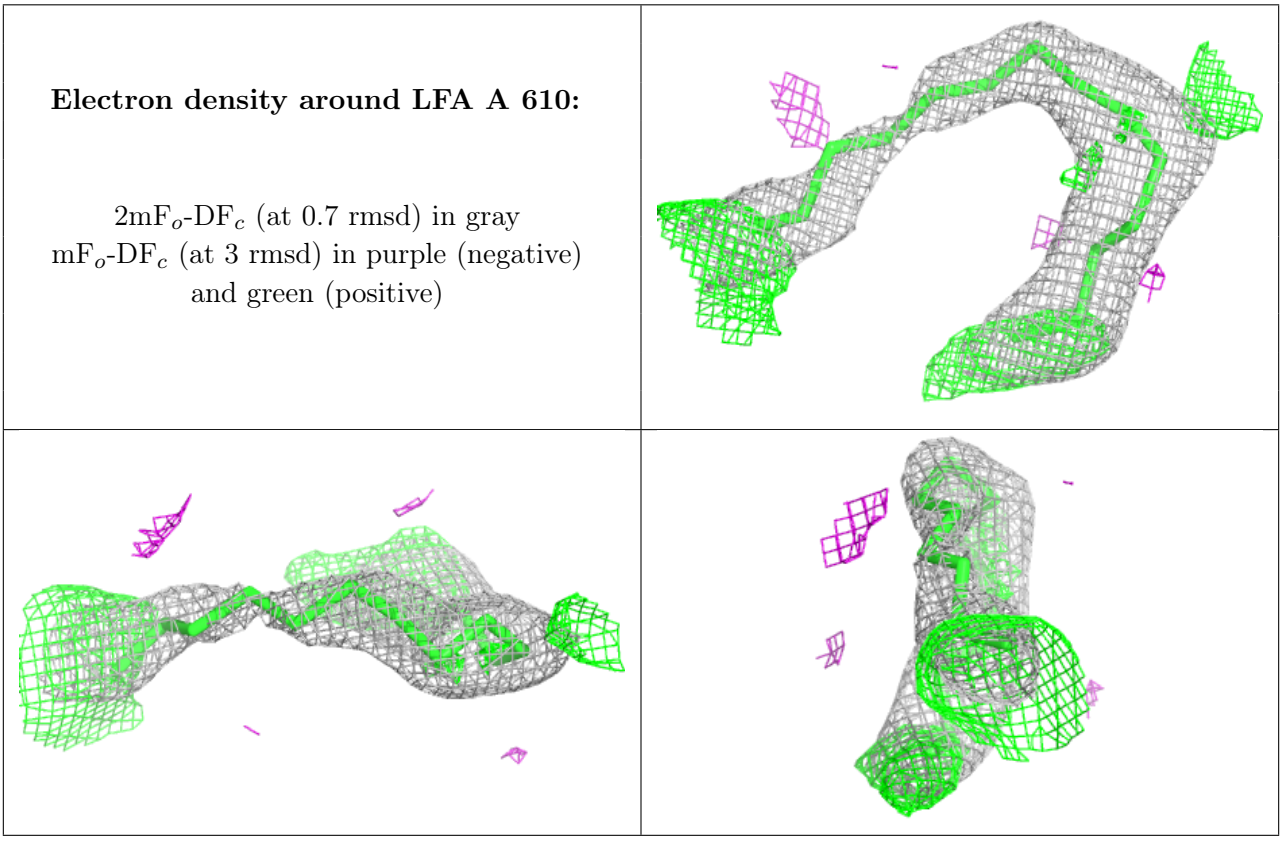
Electron density around LFA C 310:

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



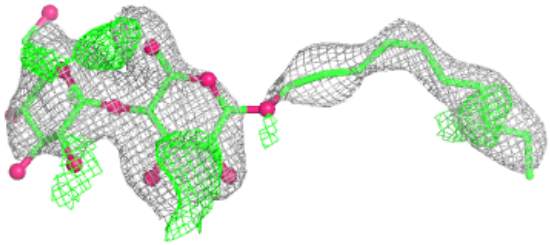
Electron density around LFA A 610:

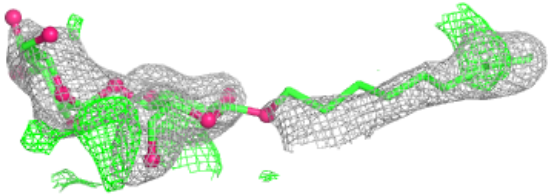
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

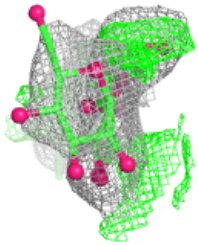


Electron density around DMU C 324:

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

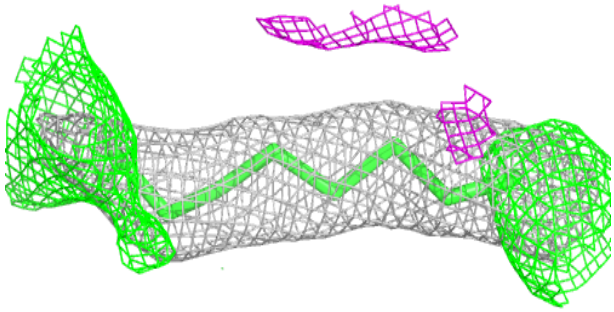


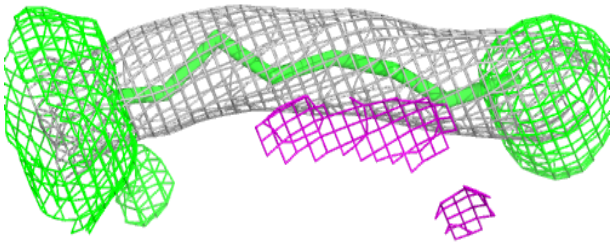


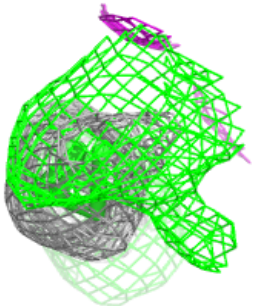


Electron density around DMU M 102:

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

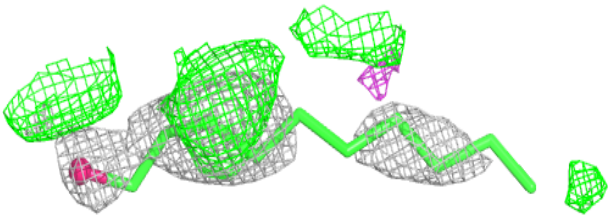


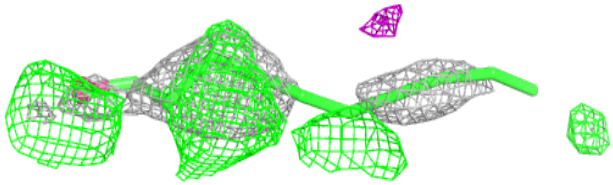


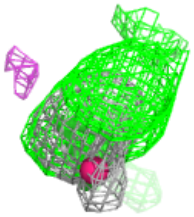


Electron density around DMU A 618:

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

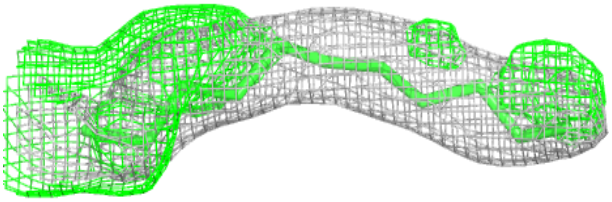


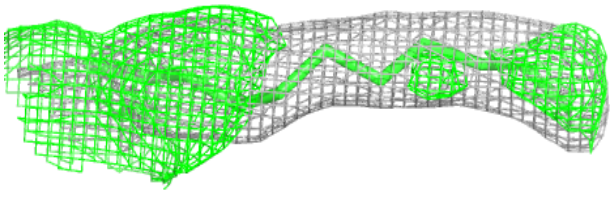


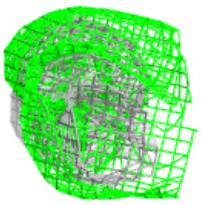


Electron density around LFA T 102:

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

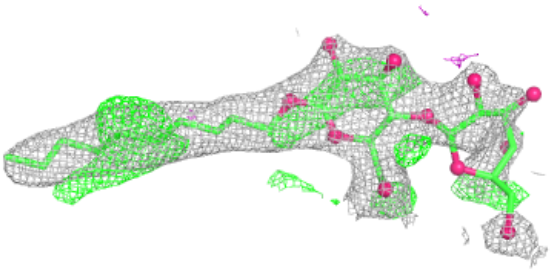


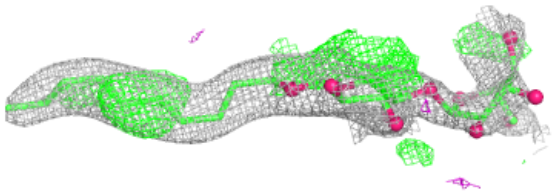


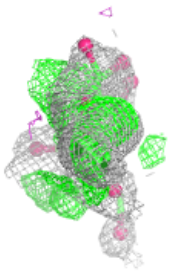


Electron density around DMU N 611:

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

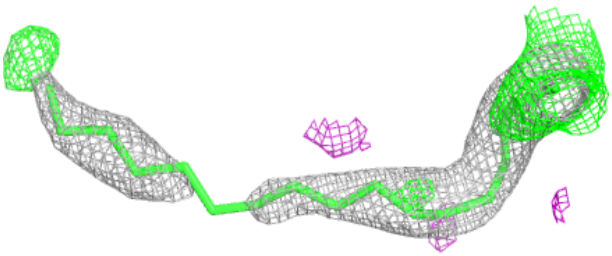


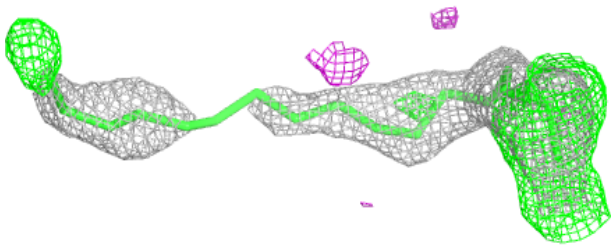


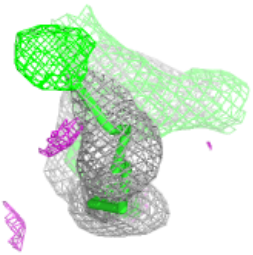


Electron density around LFA B 307:

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

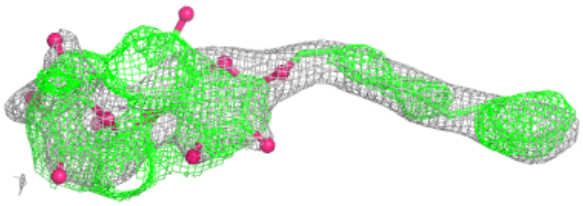


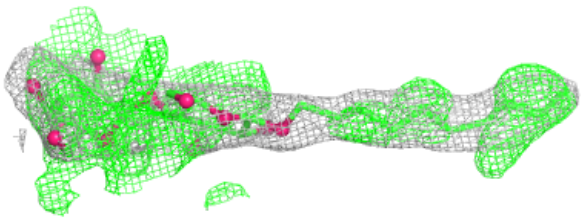


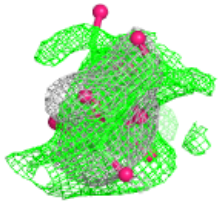


Electron density around DMU P 319:

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

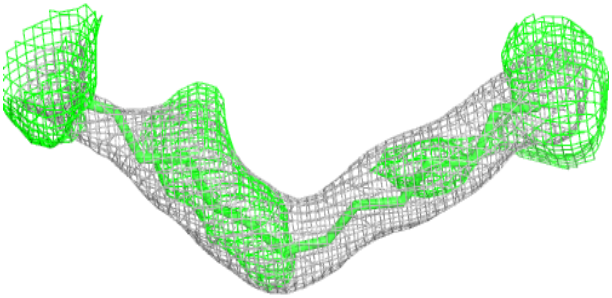


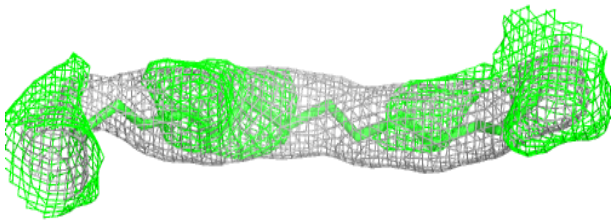


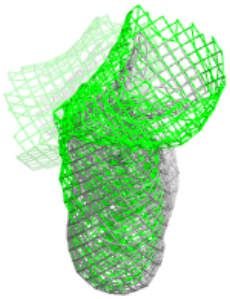


Electron density around LFA A 609:

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

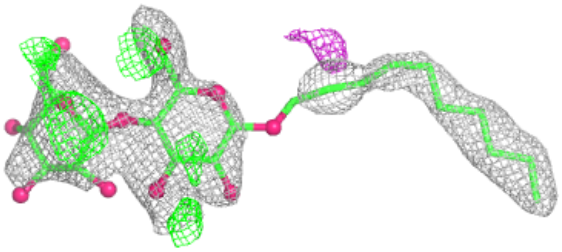


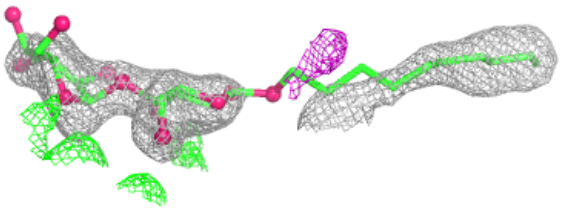


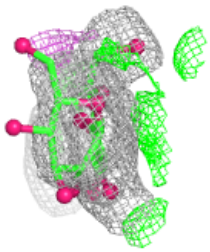


Electron density around DMU P 325:

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

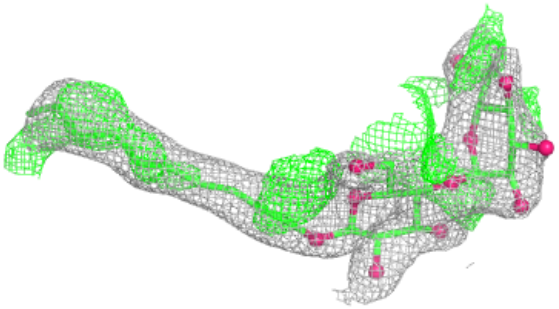


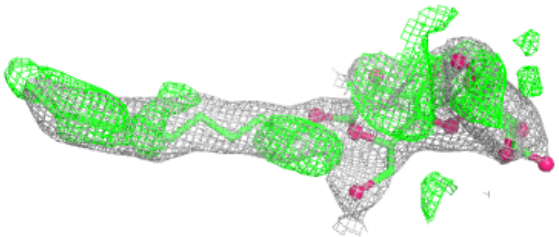


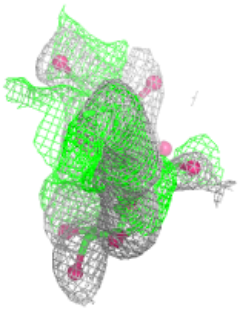


Electron density around DMU Q 201:

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

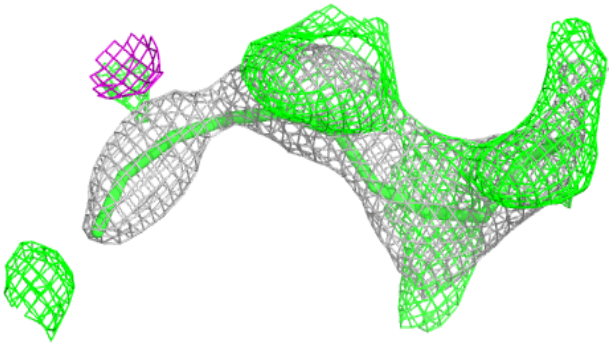


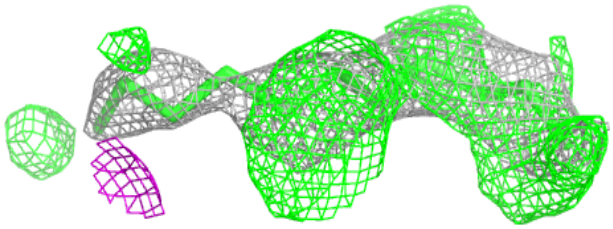


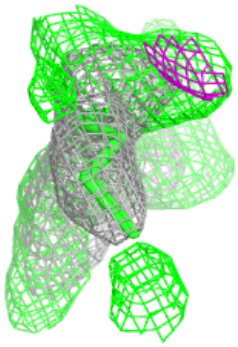


Electron density around LFA P 308:

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

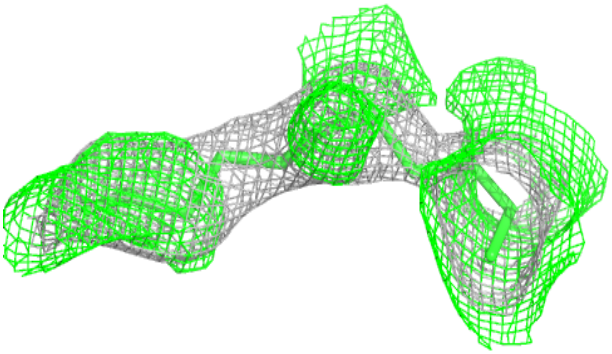


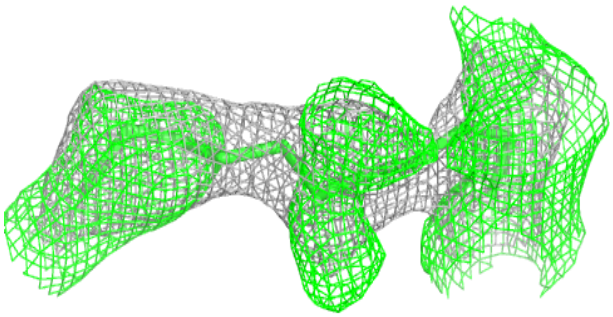


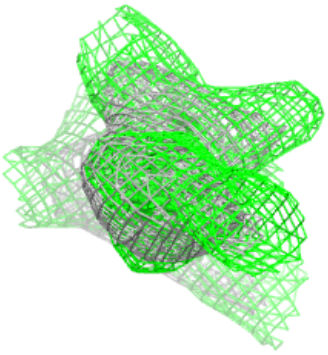


Electron density around LFA C 312:

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

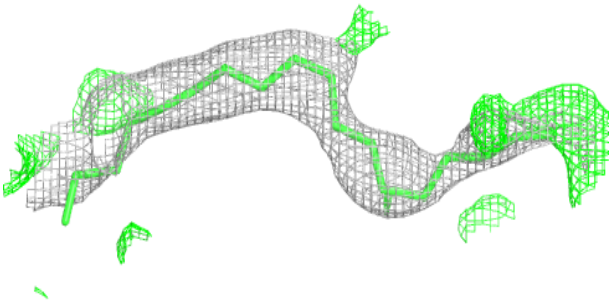


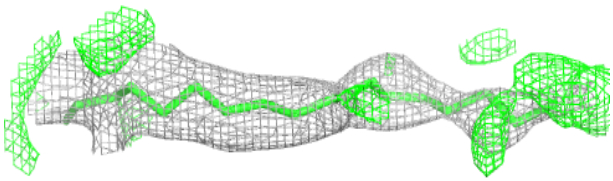


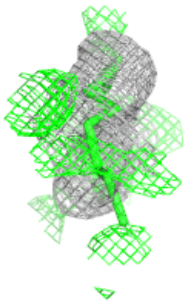


Electron density around LFA C 309:

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

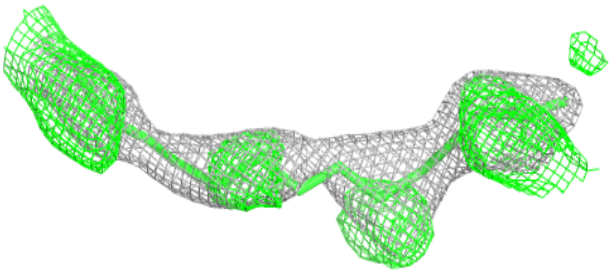


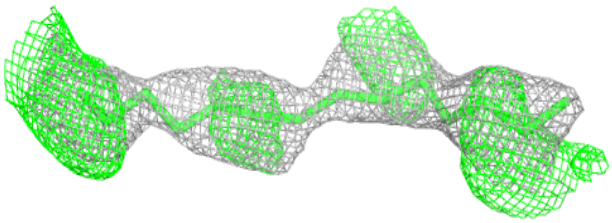


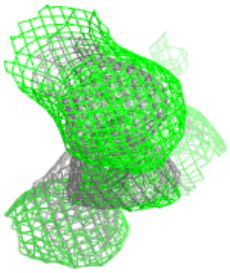


Electron density around LFA P 312:

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

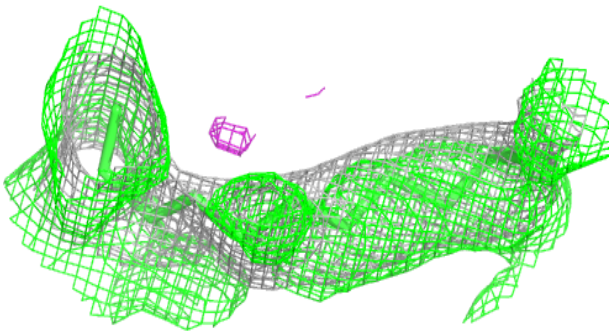


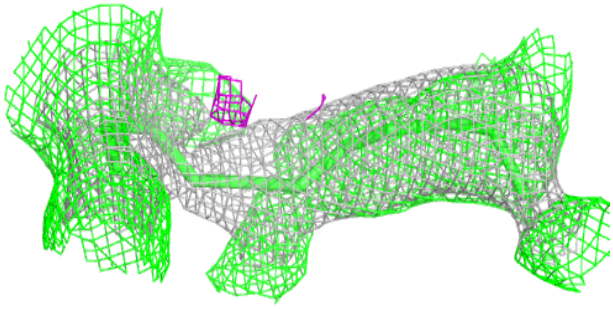


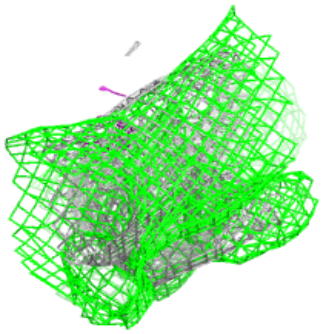


Electron density around LFA P 313:

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

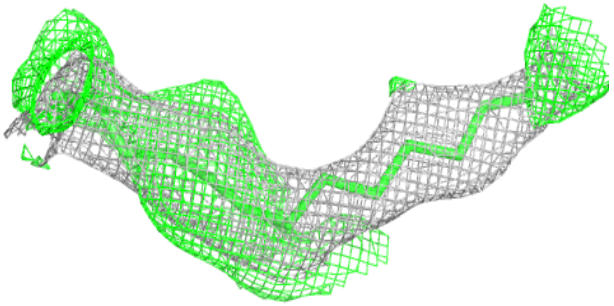


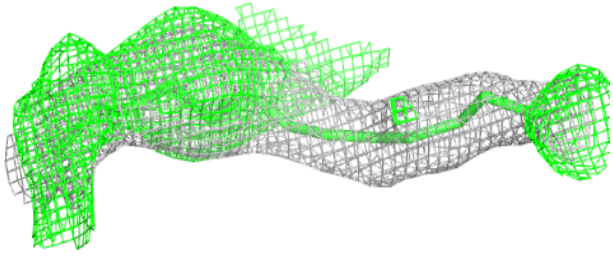


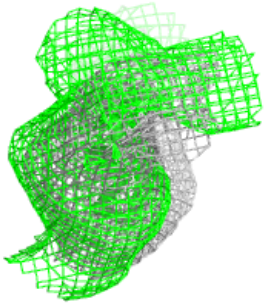


Electron density around LFA P 315:

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

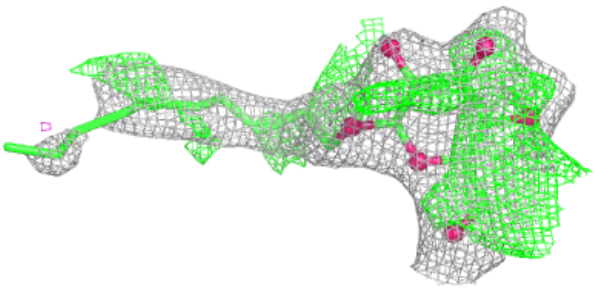


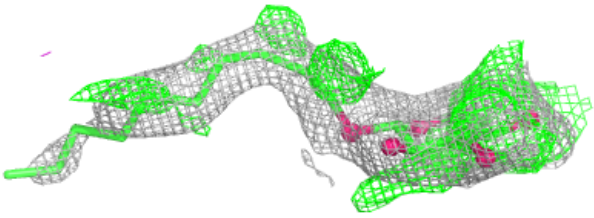


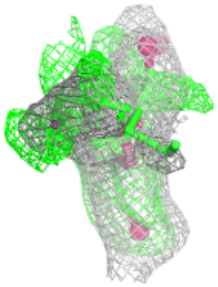


Electron density around DMU C 323:

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

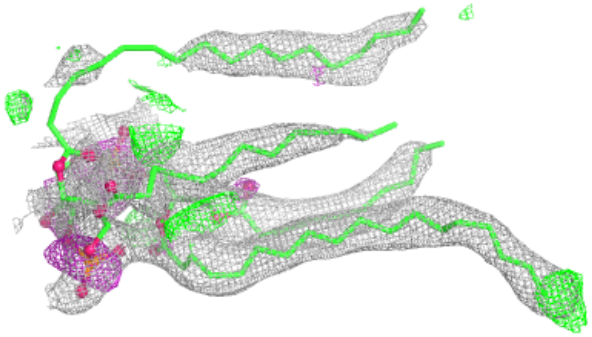


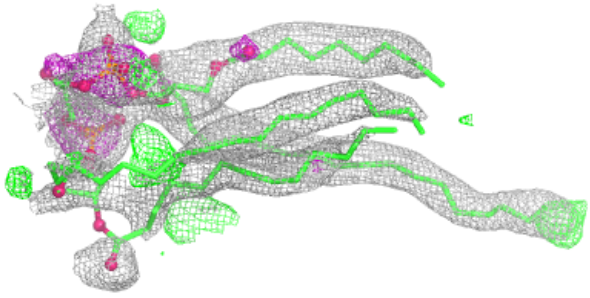


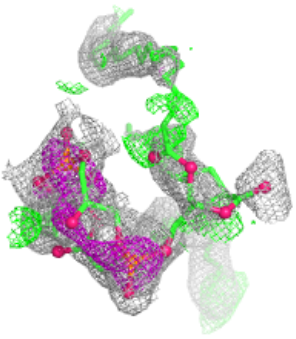


Electron density around CDL P 305:

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

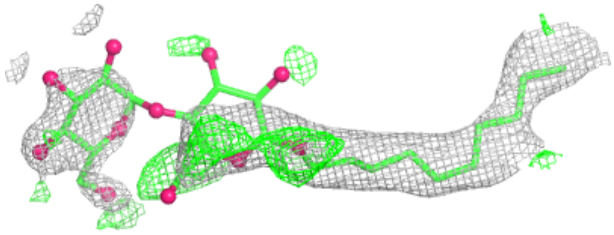


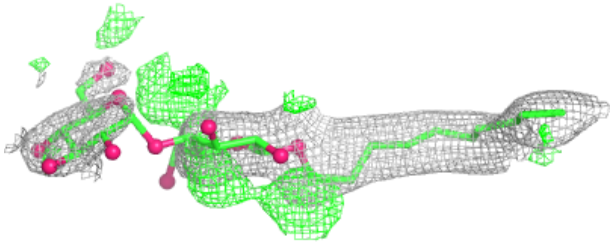


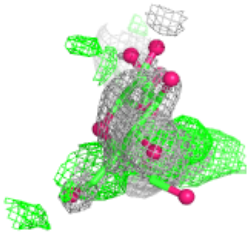


Electron density around DMU H 101:

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

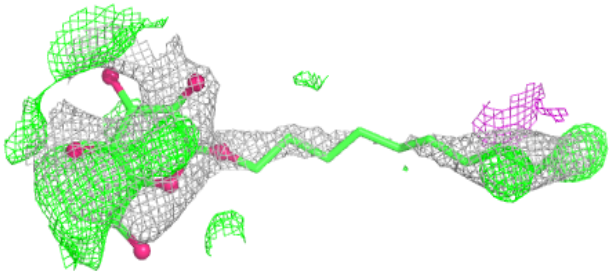


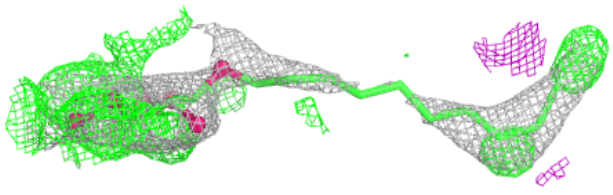


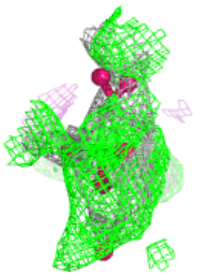


Electron density around DMU O 304:

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

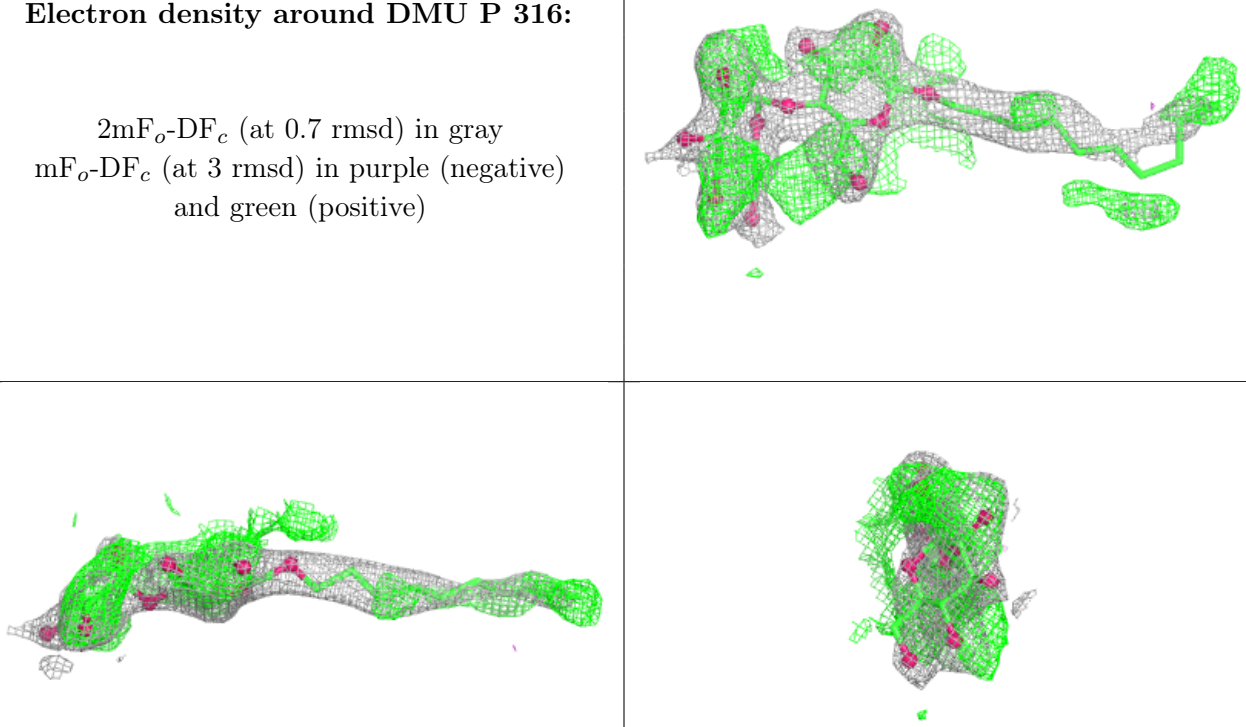






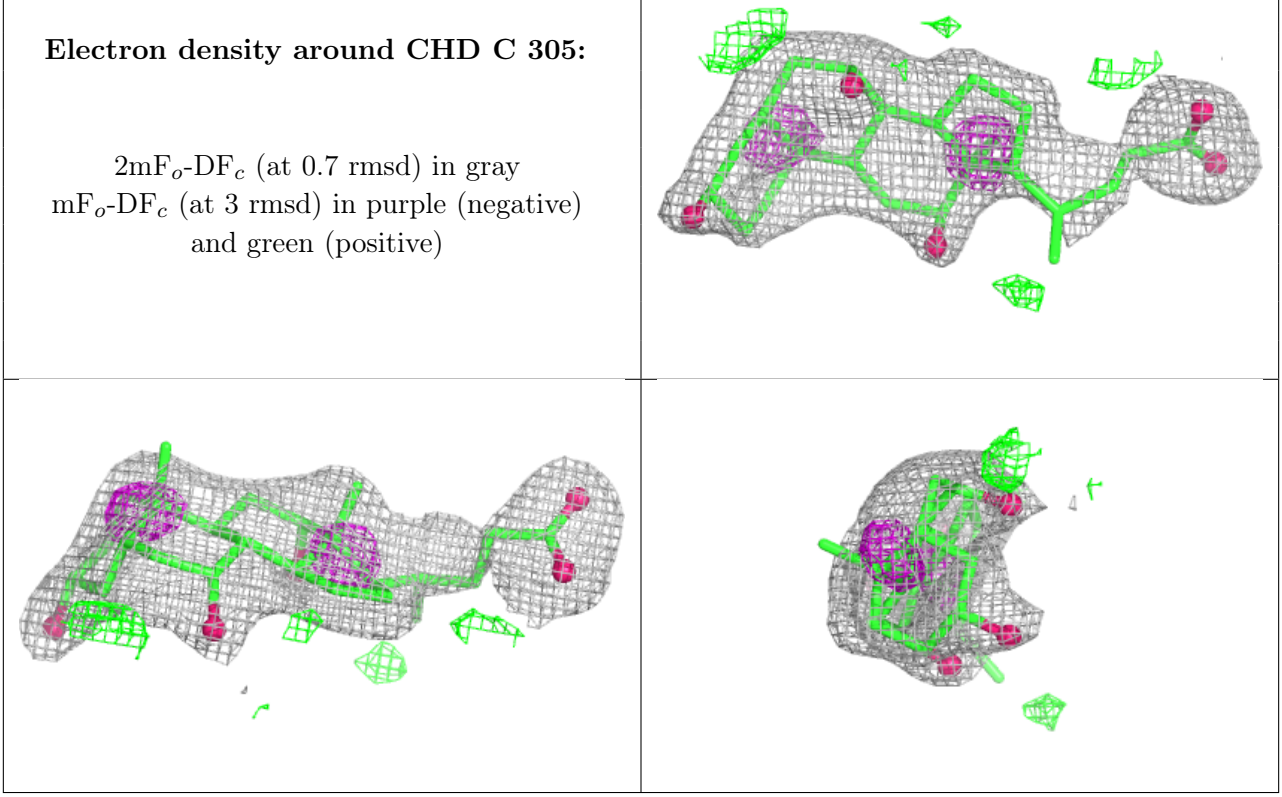
Electron density around DMU P 316:

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



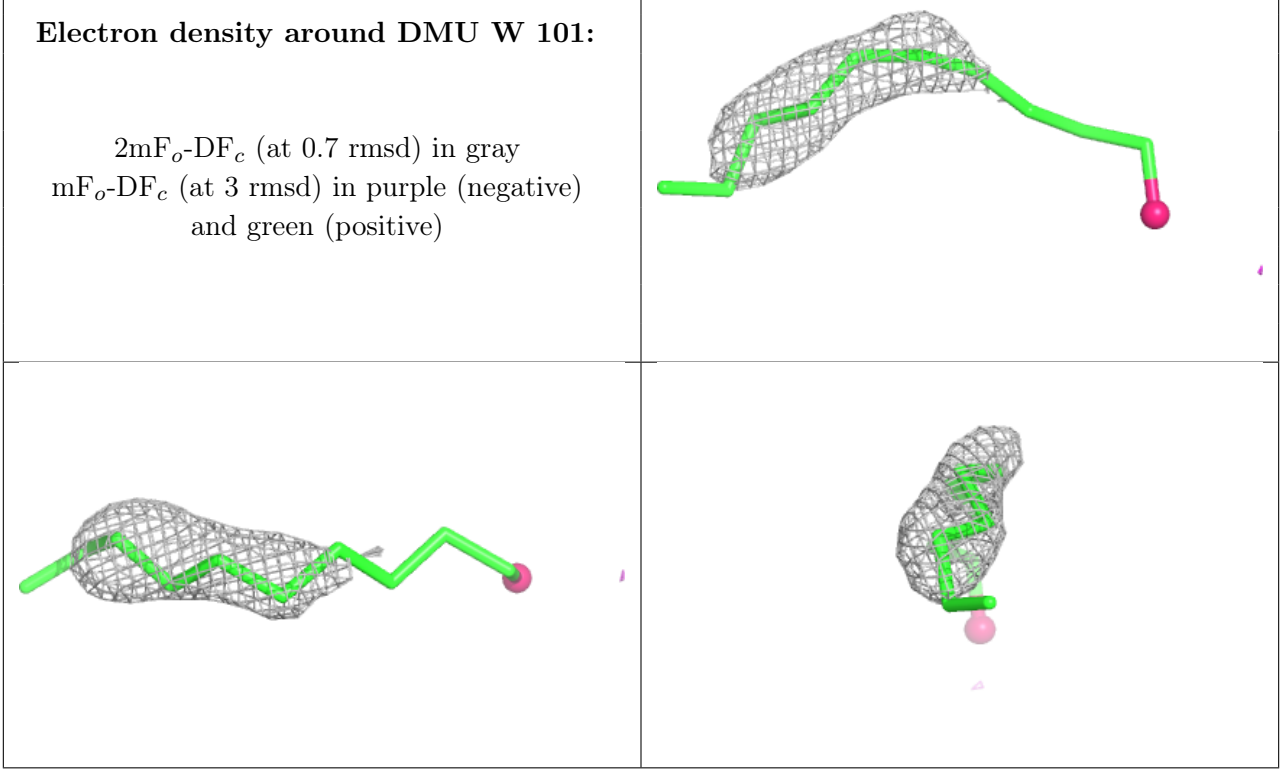
Electron density around CHD C 305:

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



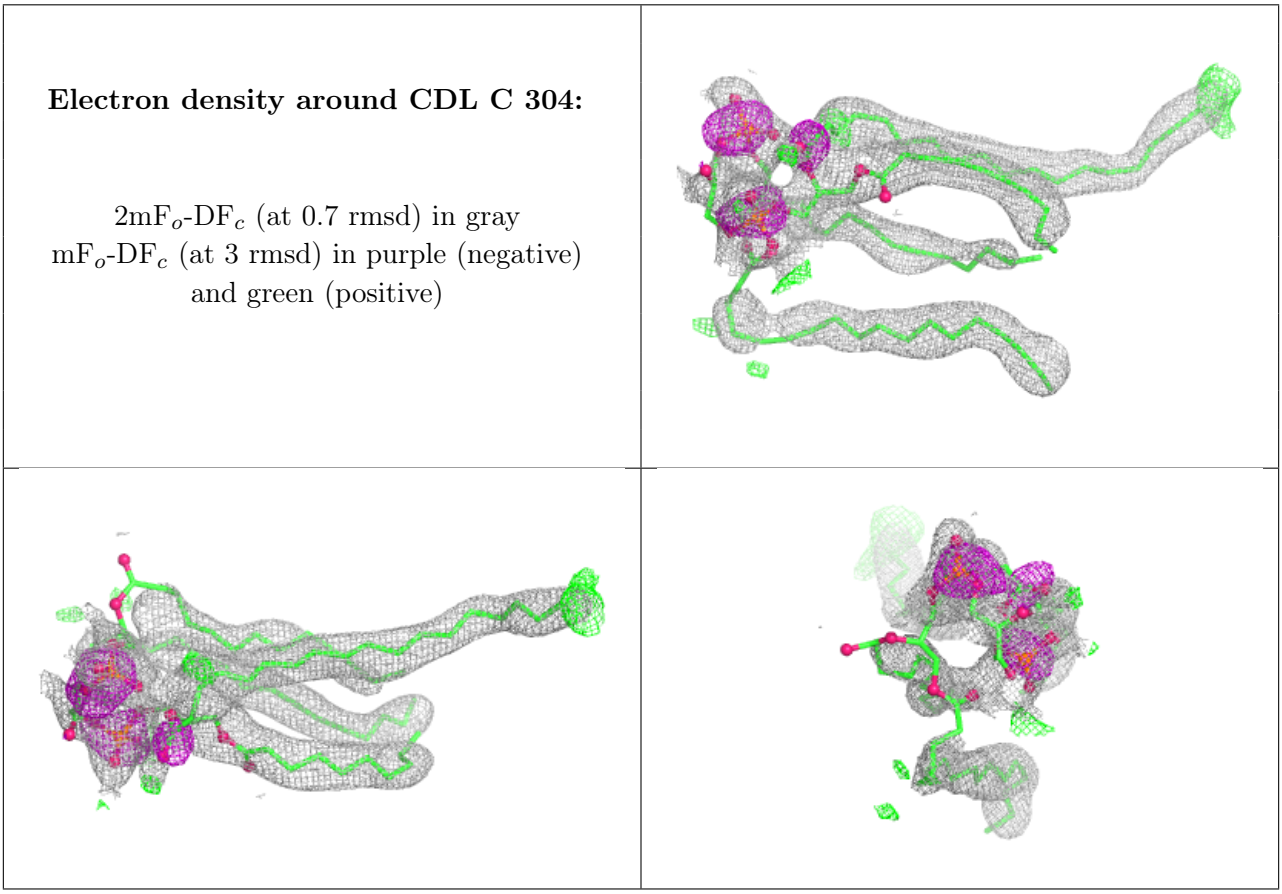
Electron density around DMU W 101:

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



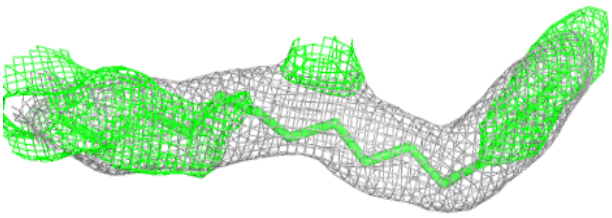
Electron density around CDL C 304:

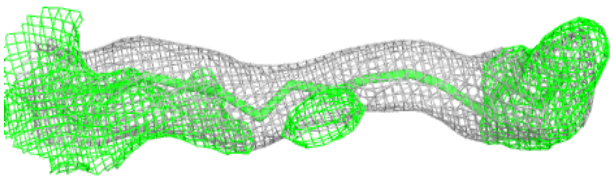
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

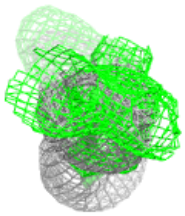


Electron density around LFA P 314:

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

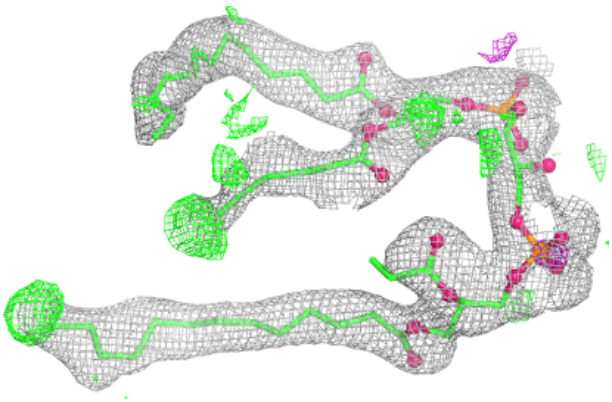


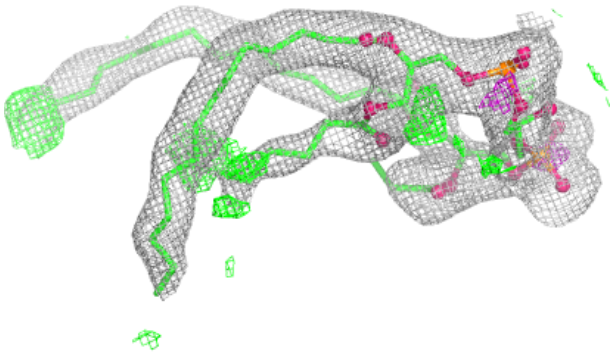


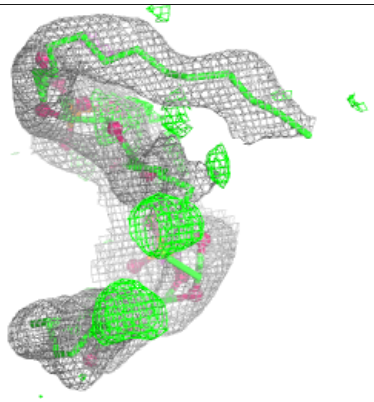


Electron density around CDL A 607:

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

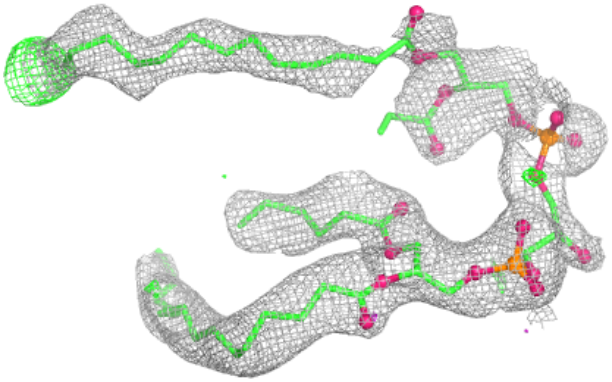


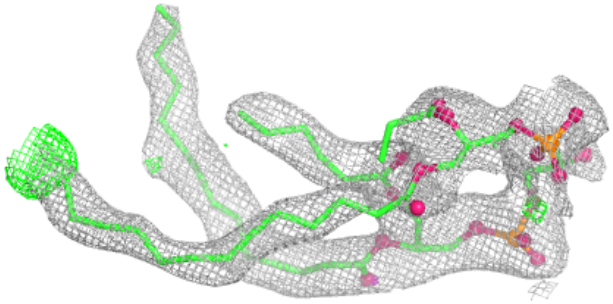


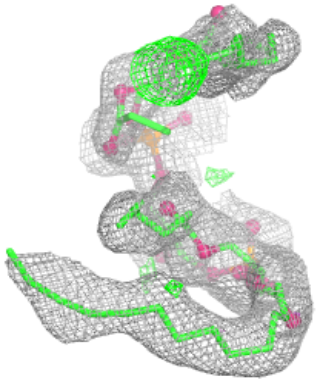


Electron density around CDL V 101:

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

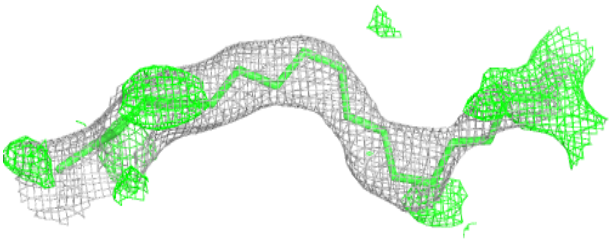


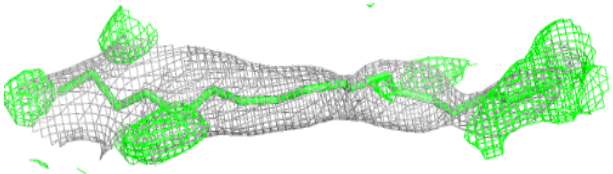


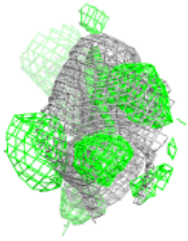


Electron density around LFA P 310:

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

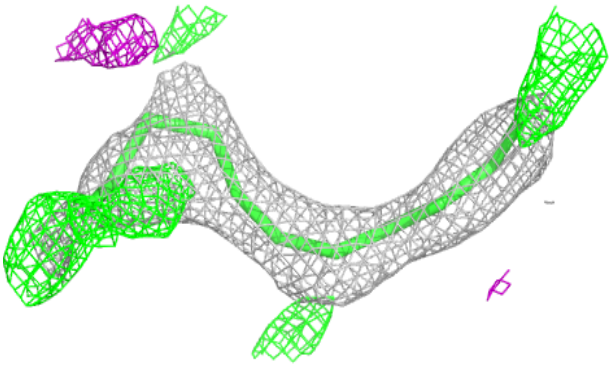


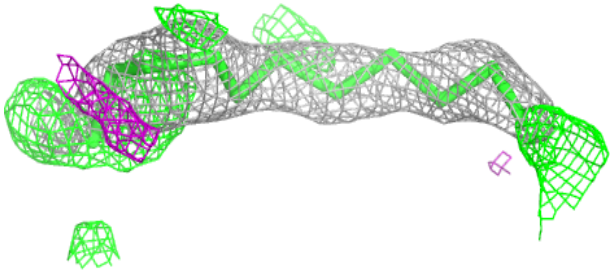


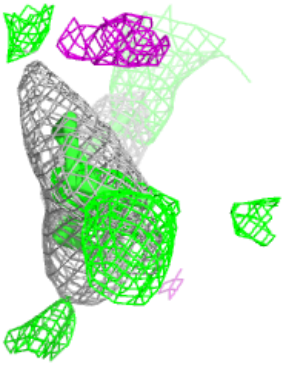


Electron density around LFA C 307:

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

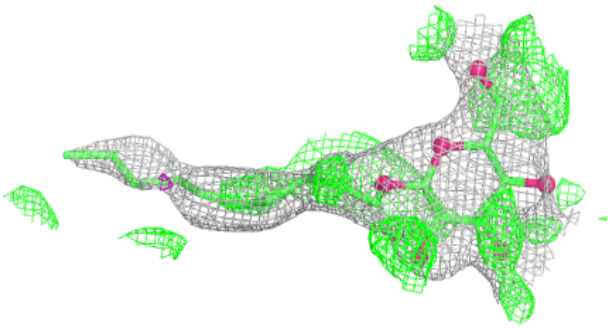


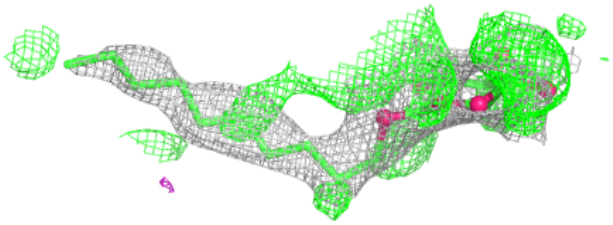


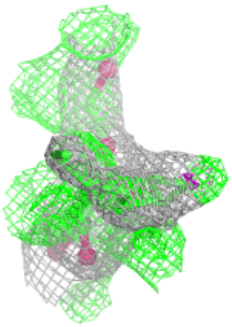


Electron density around DMU P 324:

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

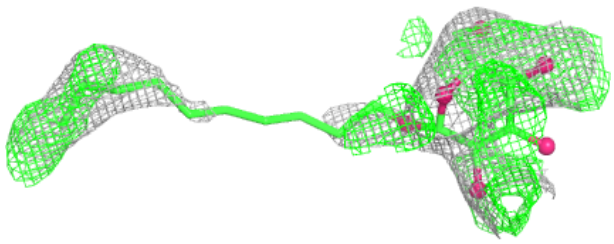


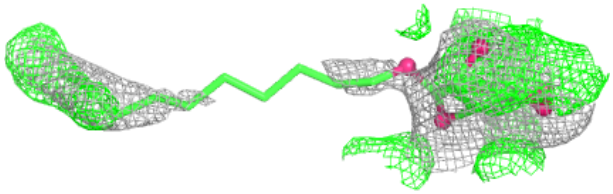


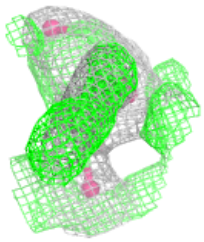


Electron density around DMU B 308:

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

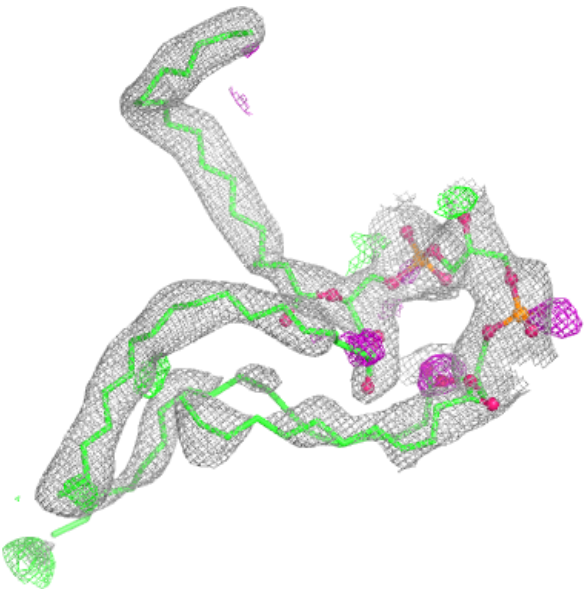


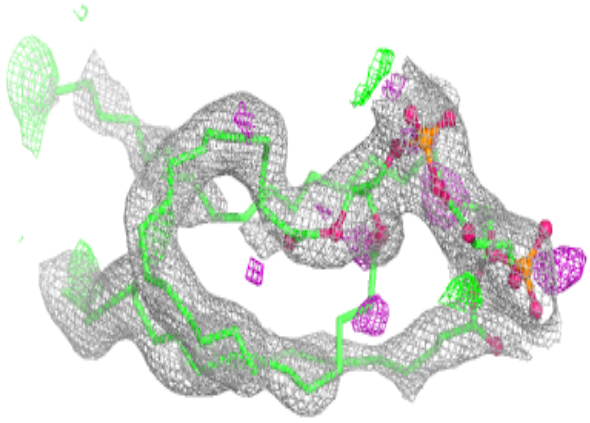




Electron density around CDL Y 101:

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

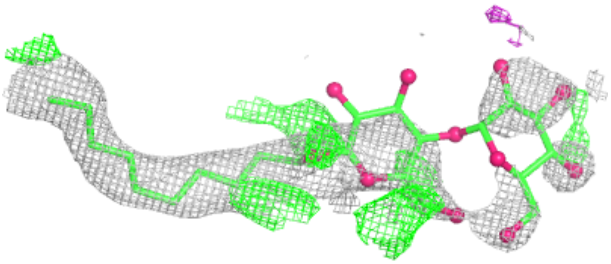


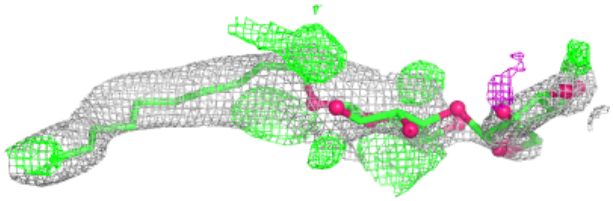


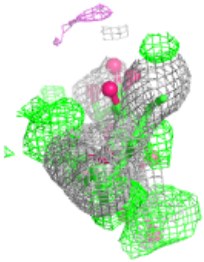


Electron density around DMU U 101:

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

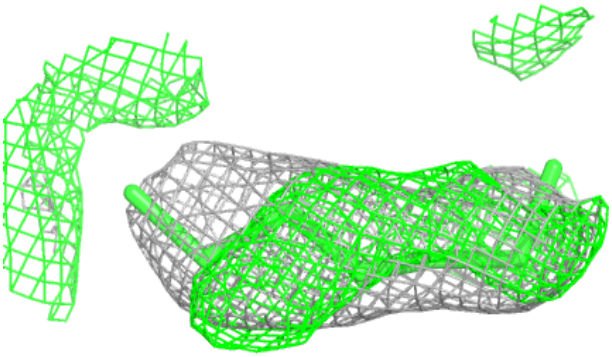


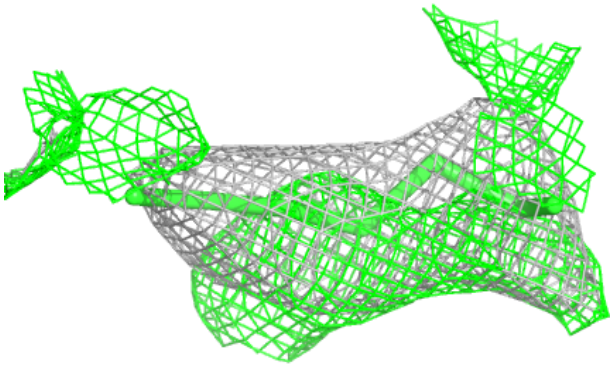


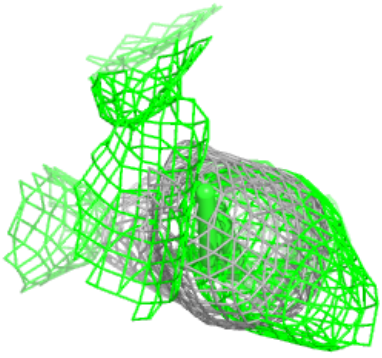


Electron density around DMU C 316:

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

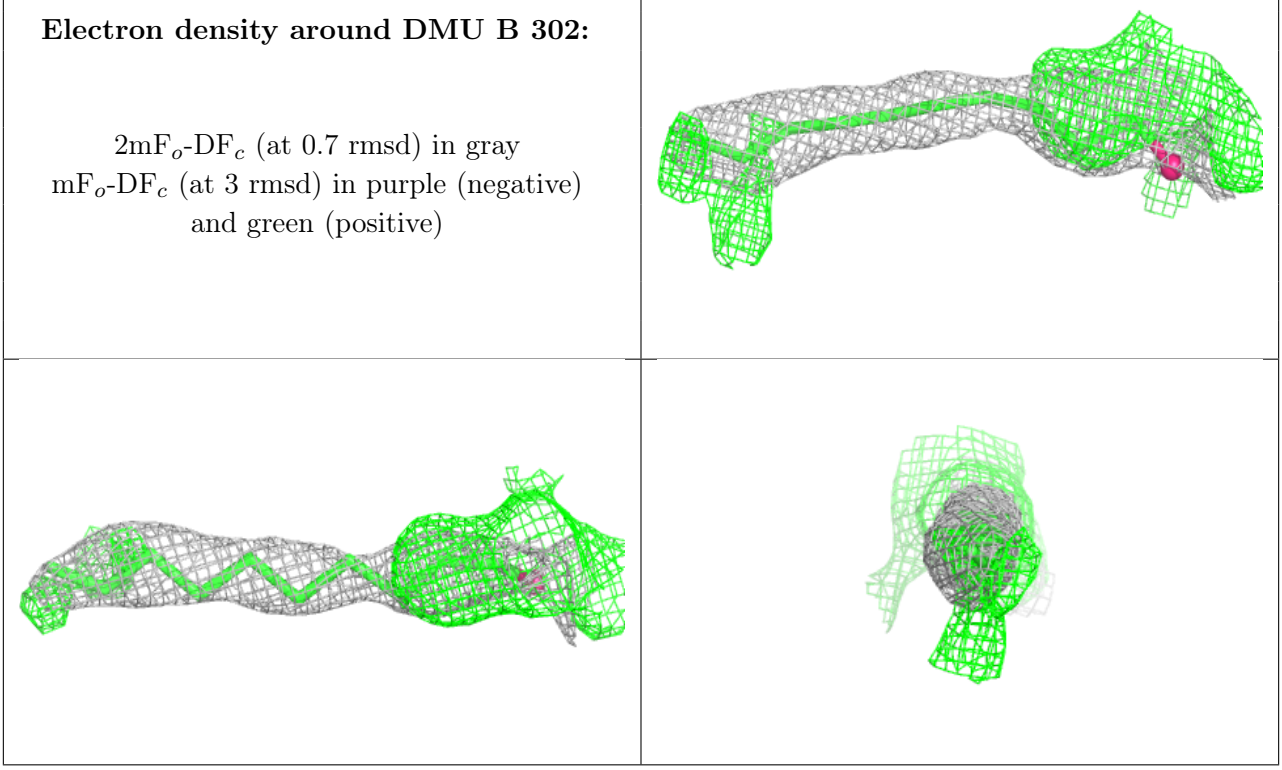






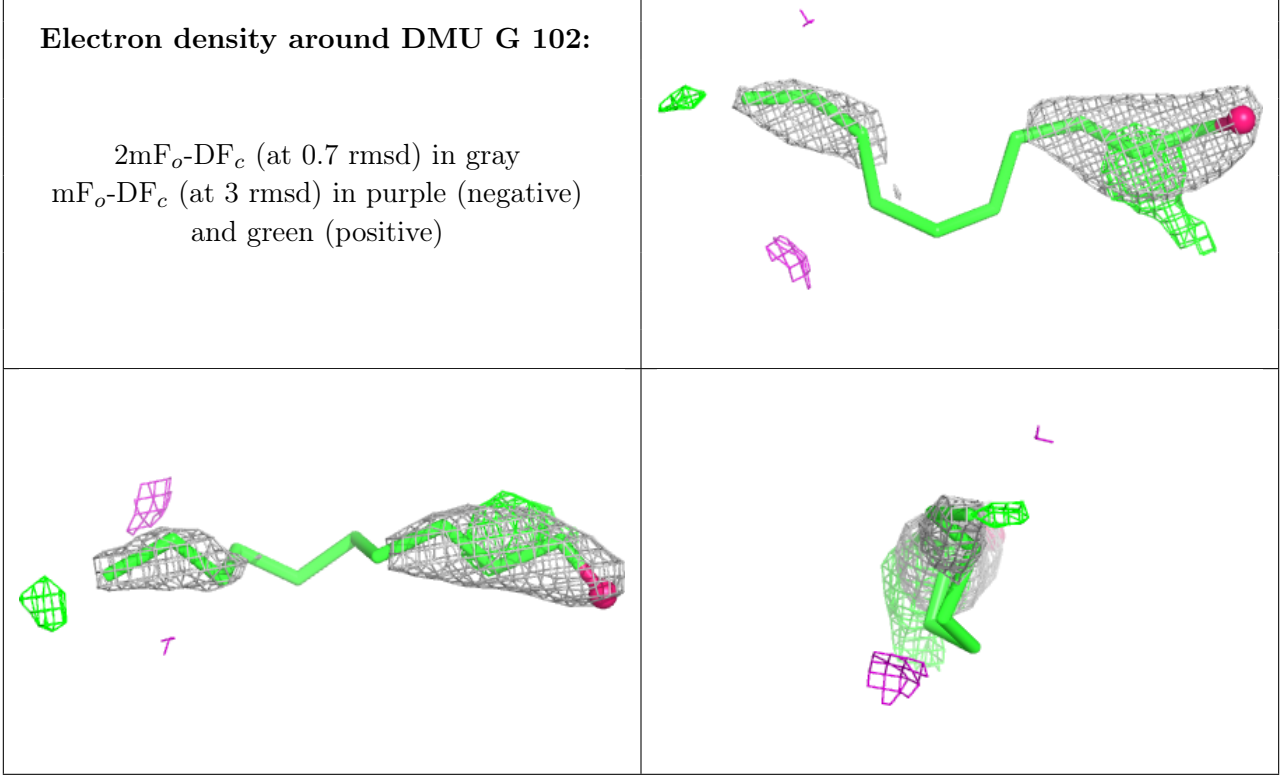
Electron density around DMU B 302:

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



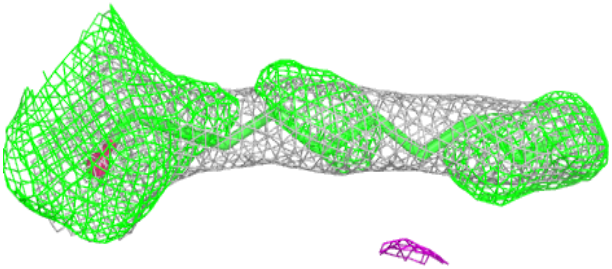
Electron density around DMU G 102:

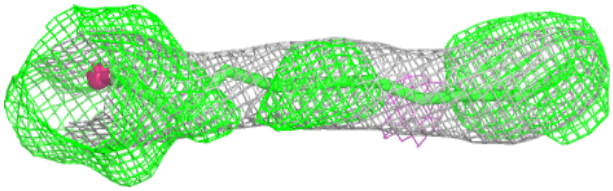
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

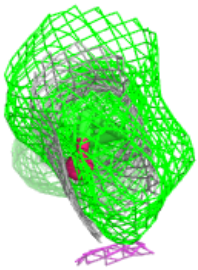


Electron density around DMU O 306:

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

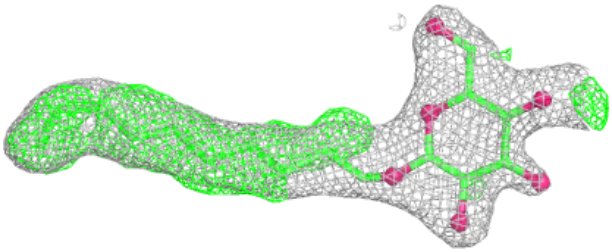


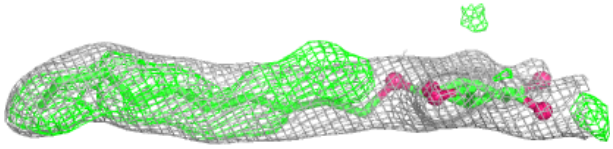


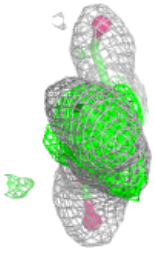


Electron density around DMU O 308:

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

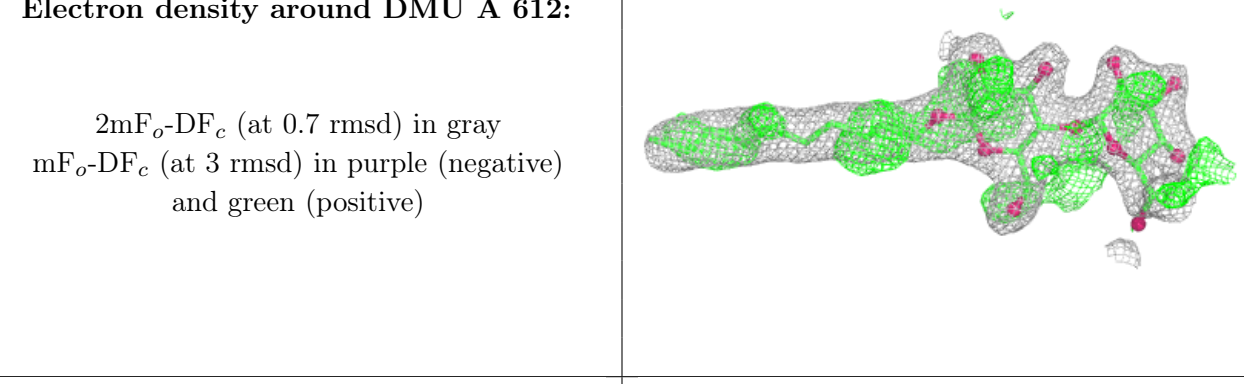






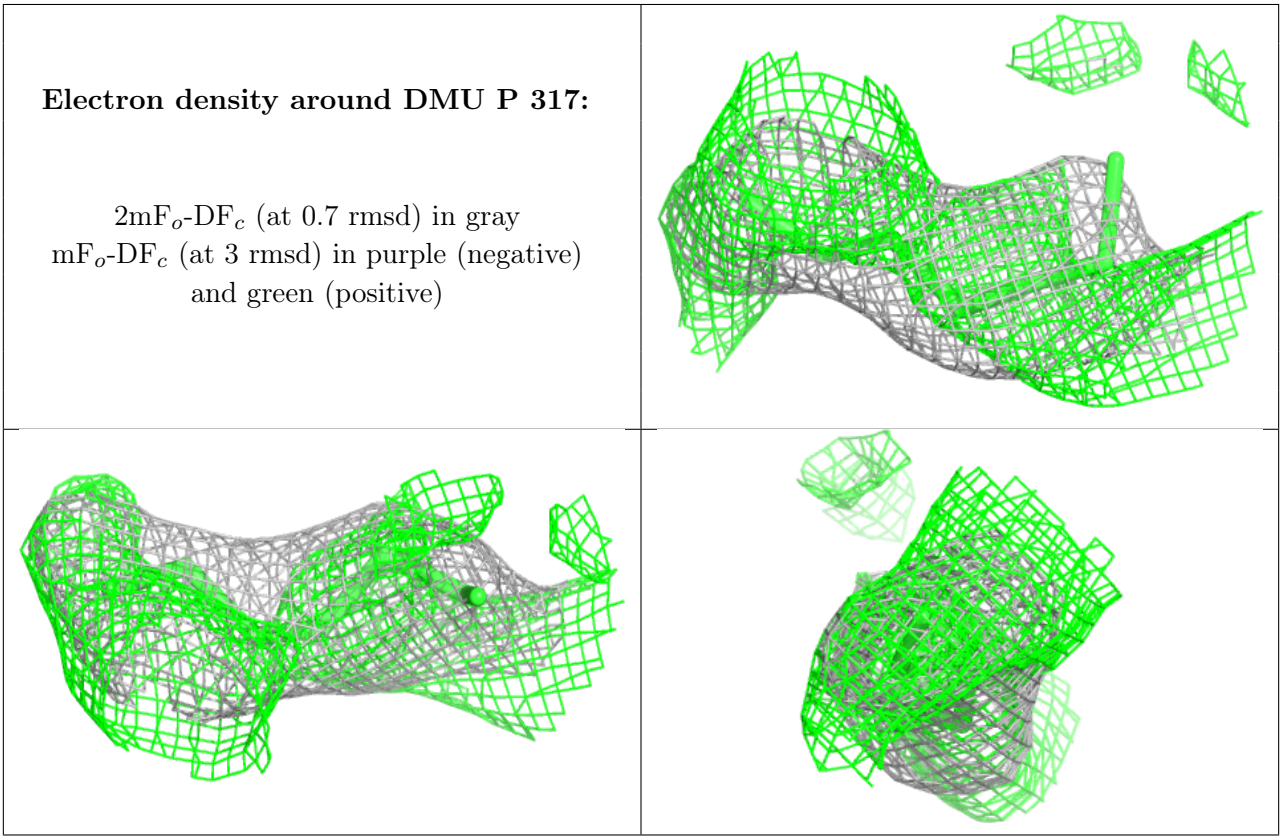
Electron density around DMU A 612:

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



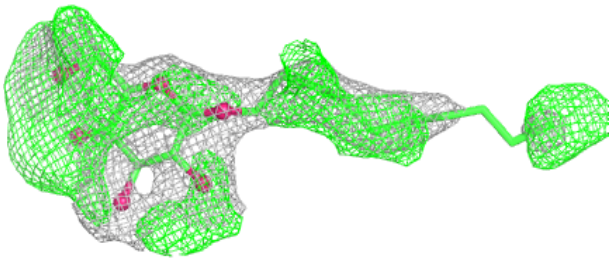
Electron density around DMU P 317:

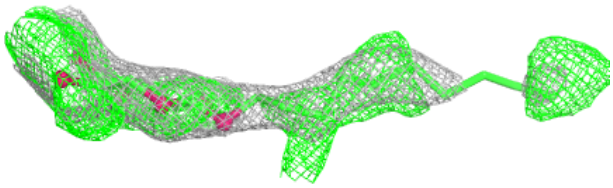
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

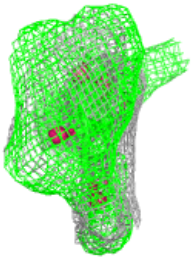


Electron density around DMU Z 102:

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

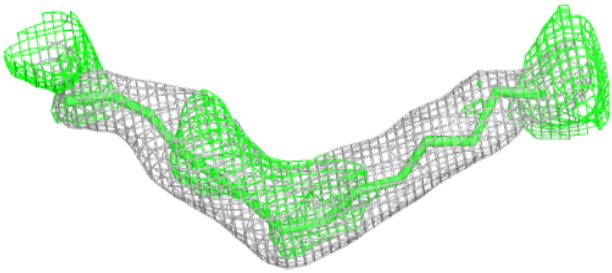


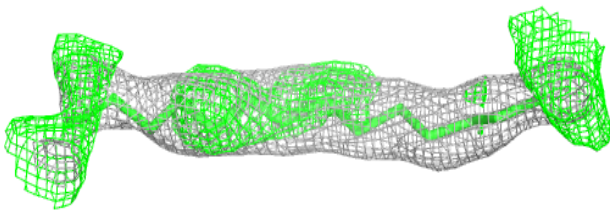


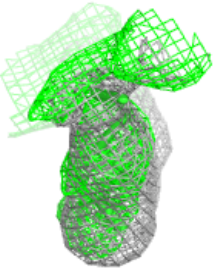


Electron density around LFA N 608:

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

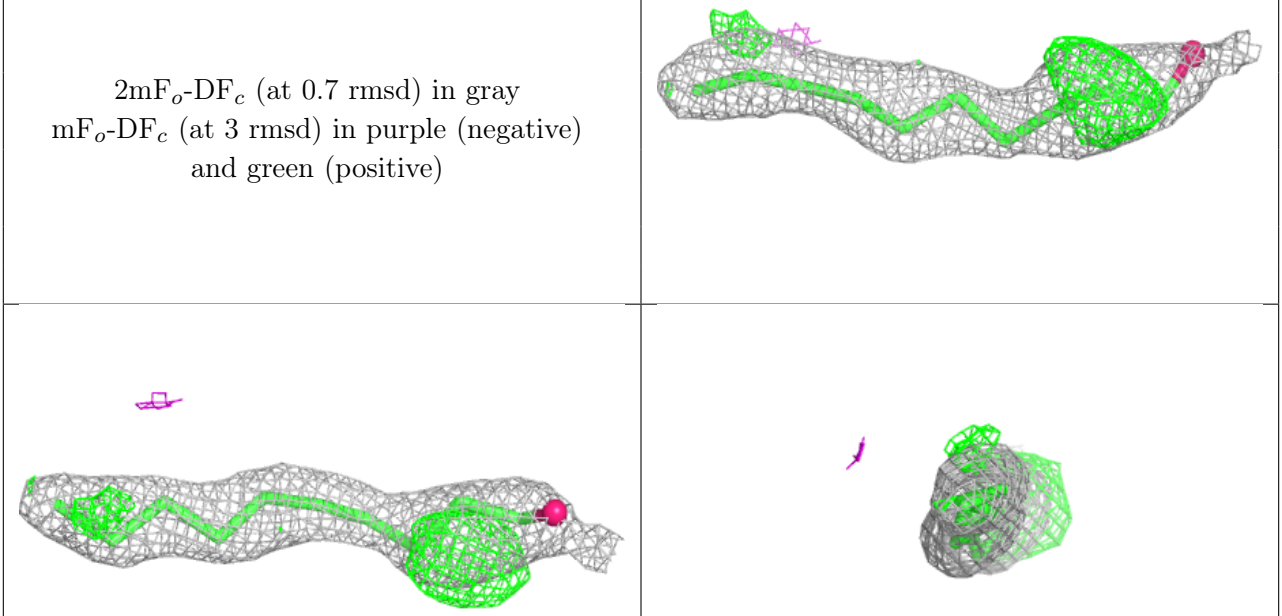






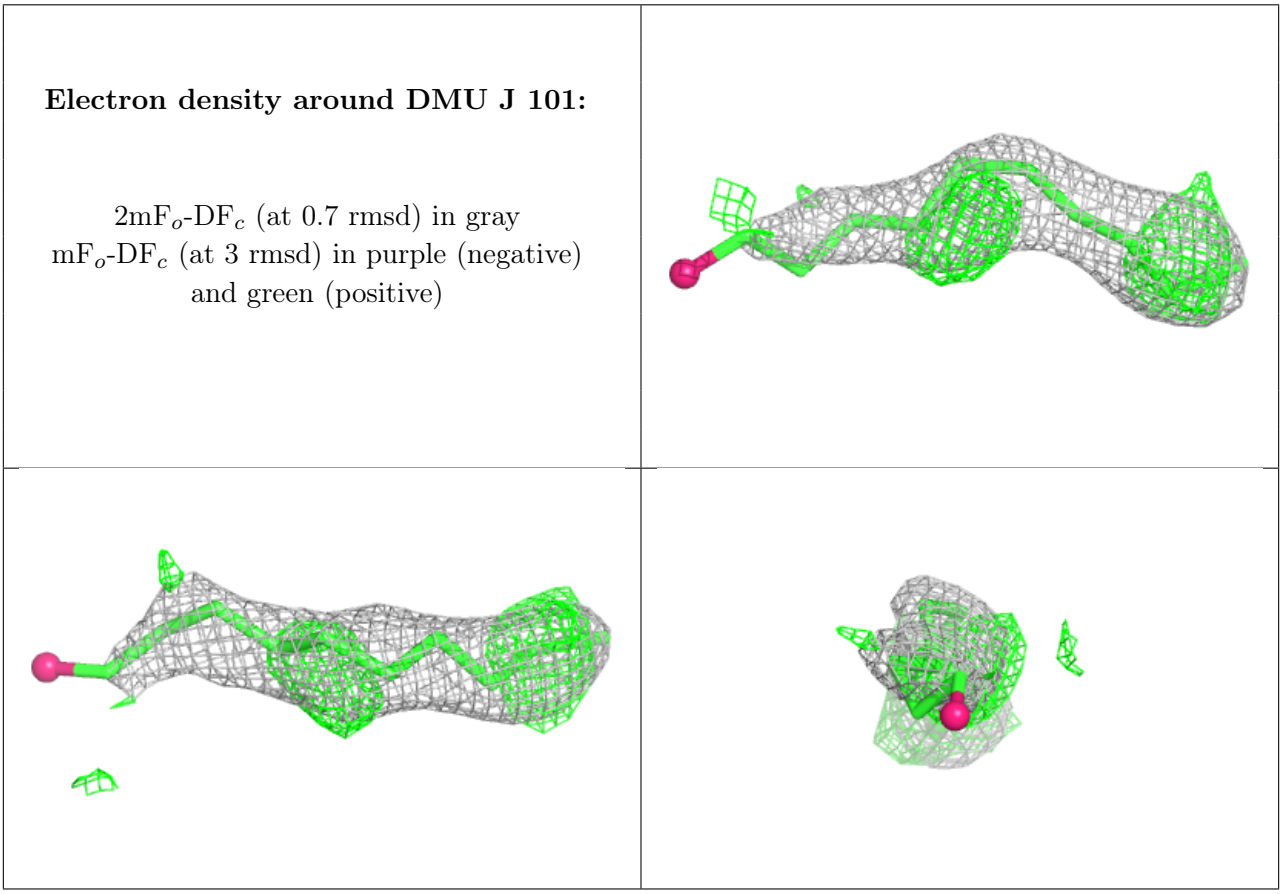
Electron density around DMU B 303:

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



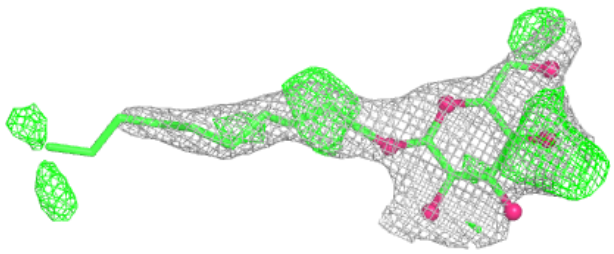
Electron density around DMU J 101:

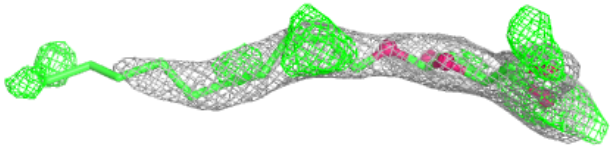
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

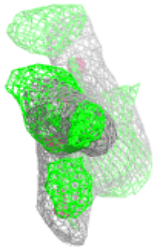


Electron density around DMU L 102:

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

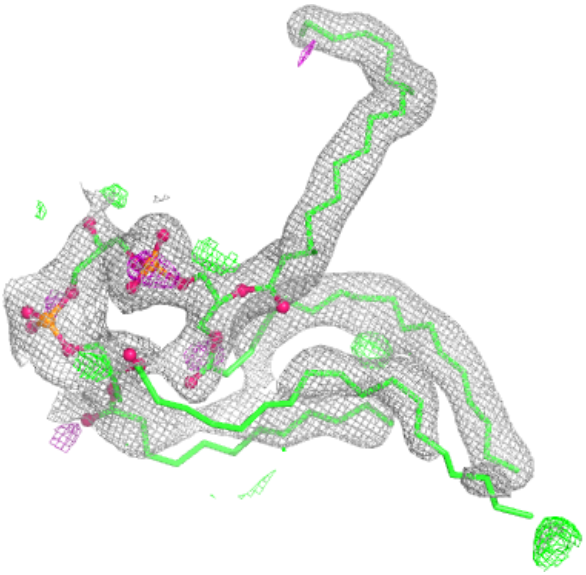


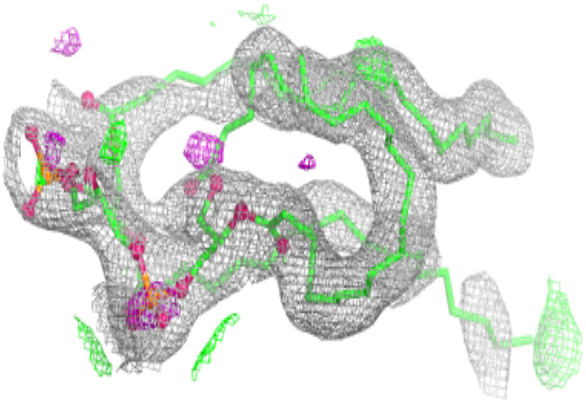


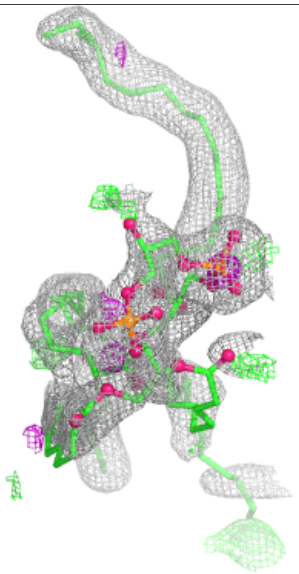


Electron density around CDL L 101:

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

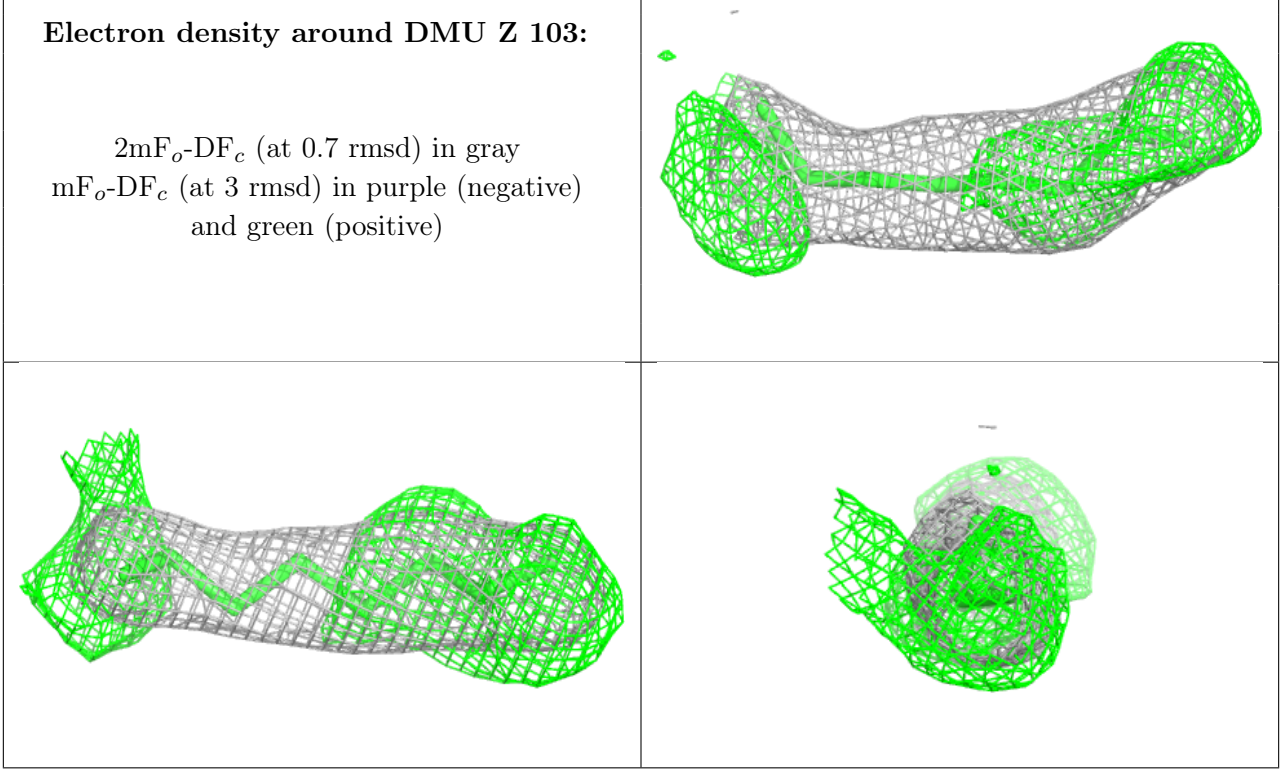






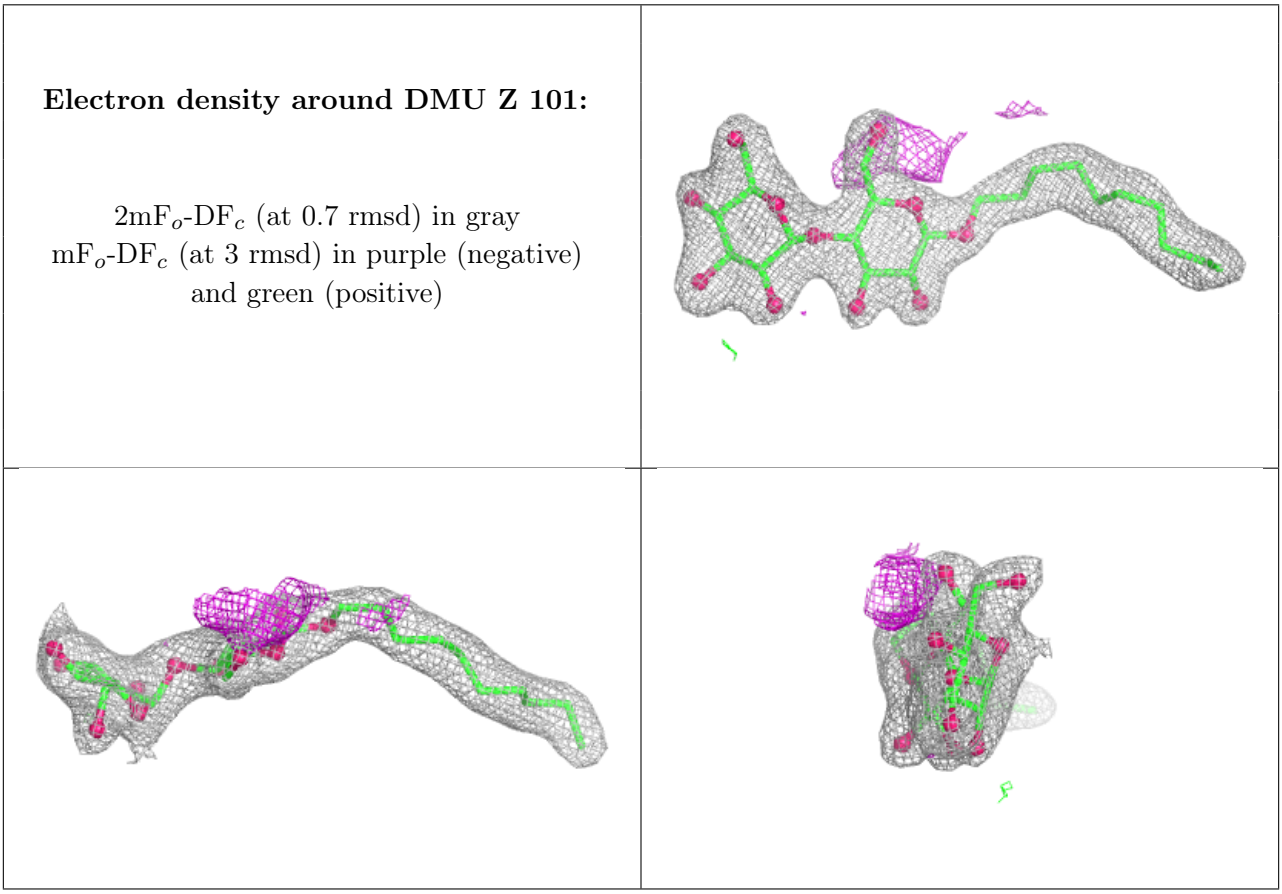
Electron density around DMU Z 103:

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



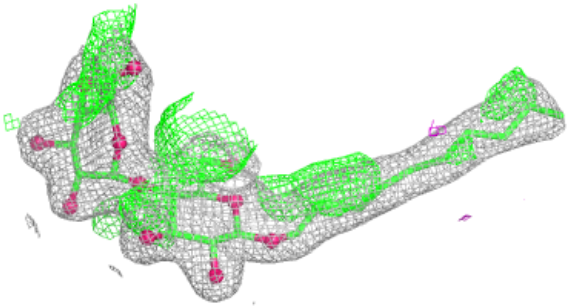
Electron density around DMU Z 101:

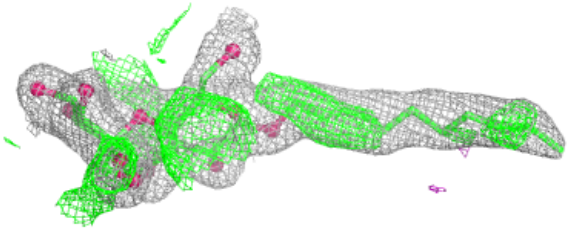
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

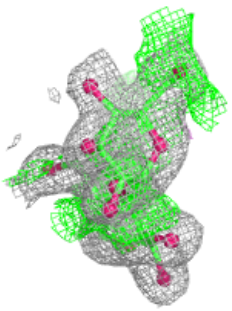


Electron density around DMU D 201:

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

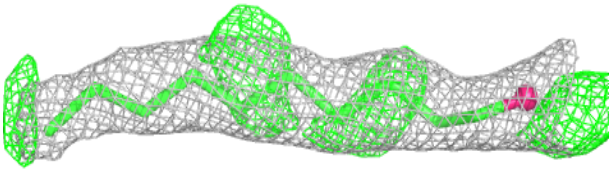


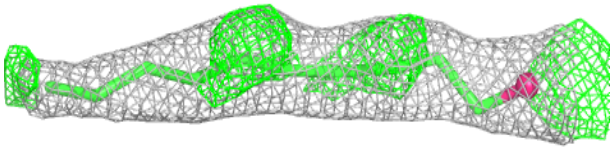


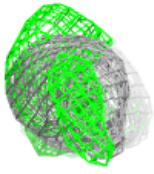


Electron density around DMU C 306:

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

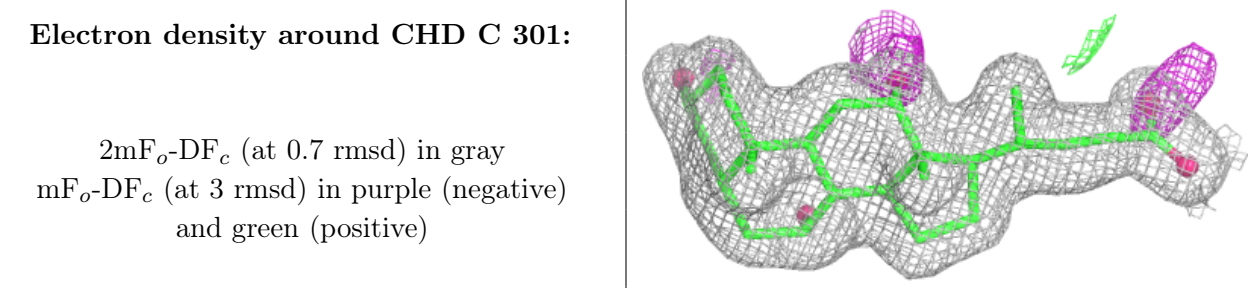


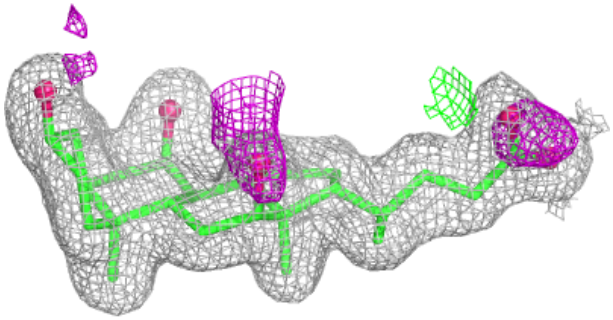


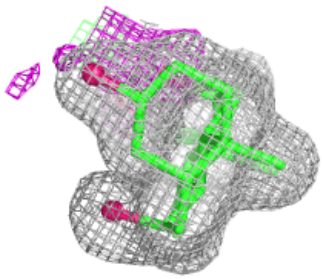


Electron density around CHD C 301:

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

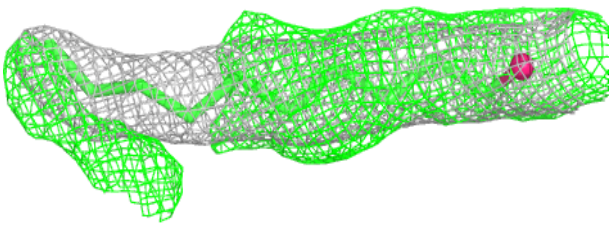


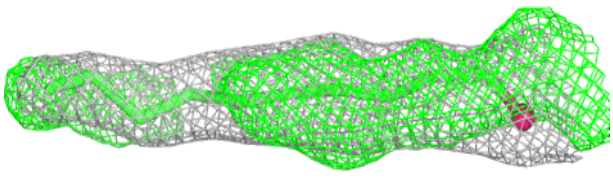


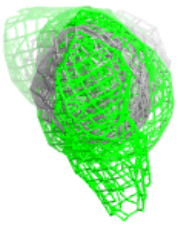


Electron density around DMU P 307:

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

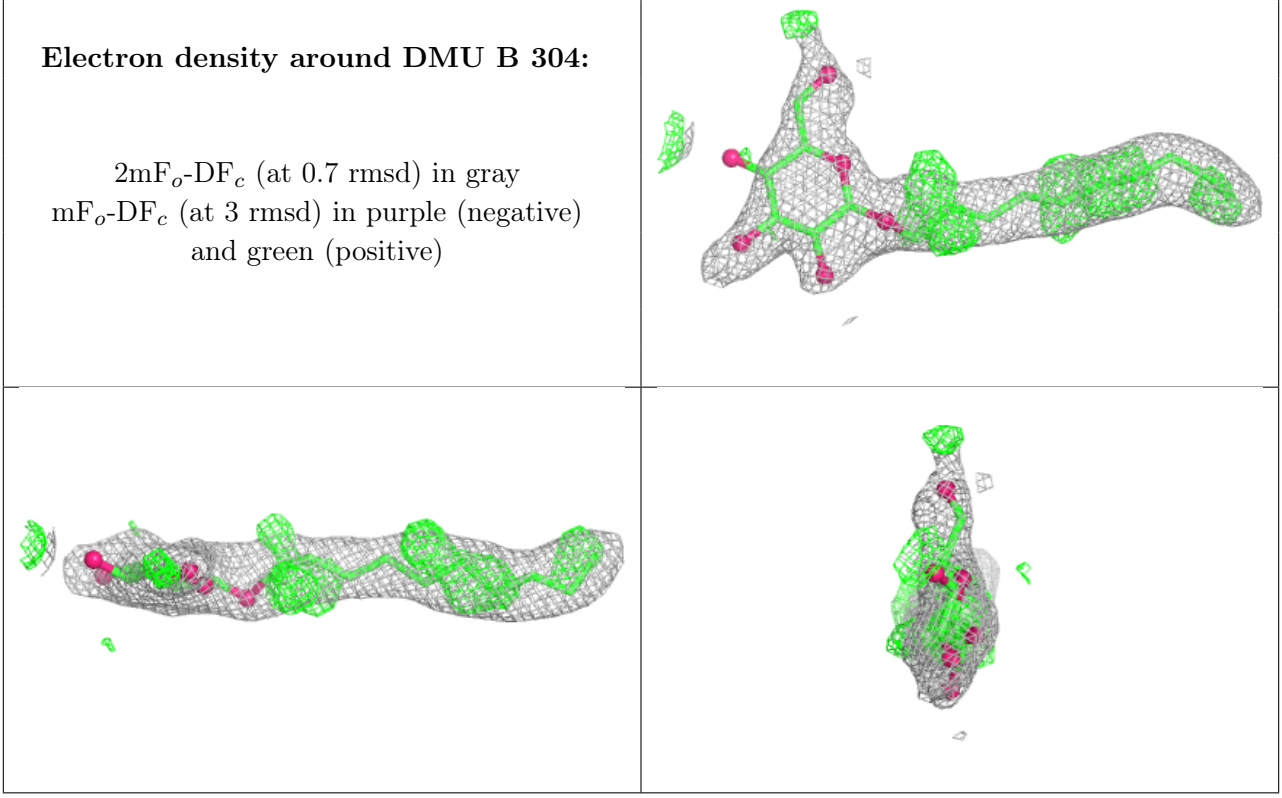






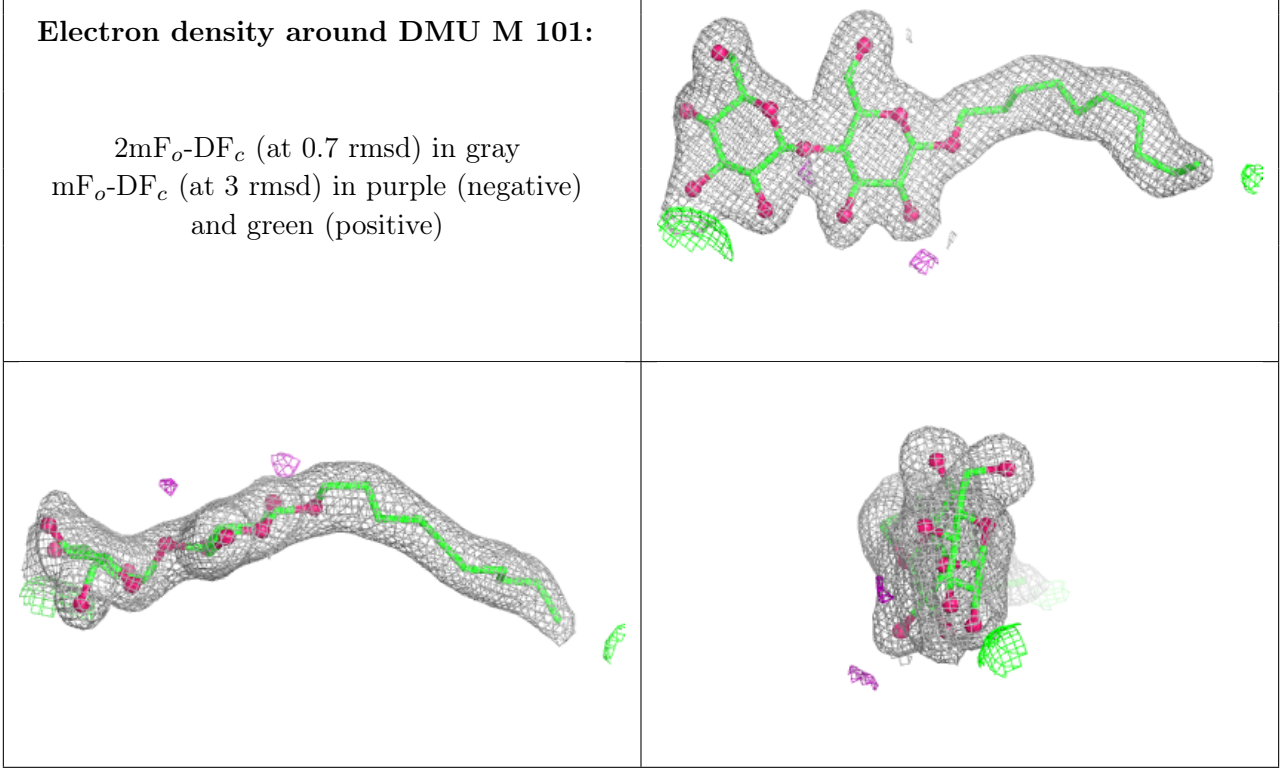
Electron density around DMU B 304:

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



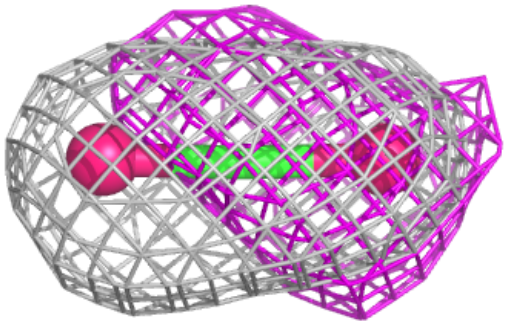
Electron density around DMU M 101:

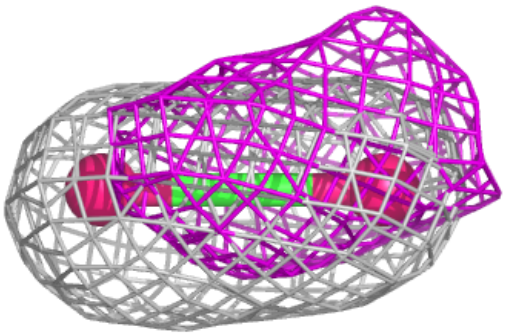
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

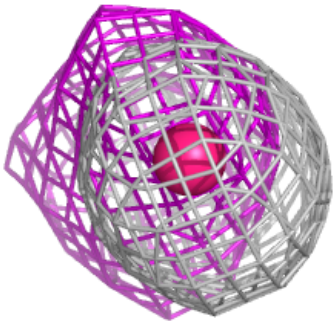


Electron density around CO2 N 607:

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

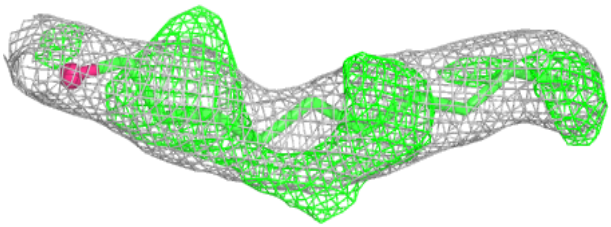


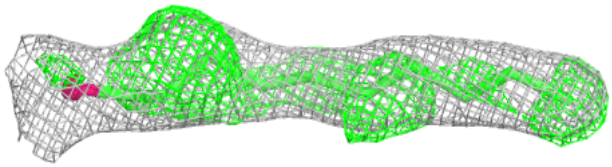


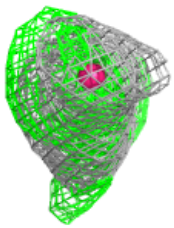


Electron density around DMU O 307:

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

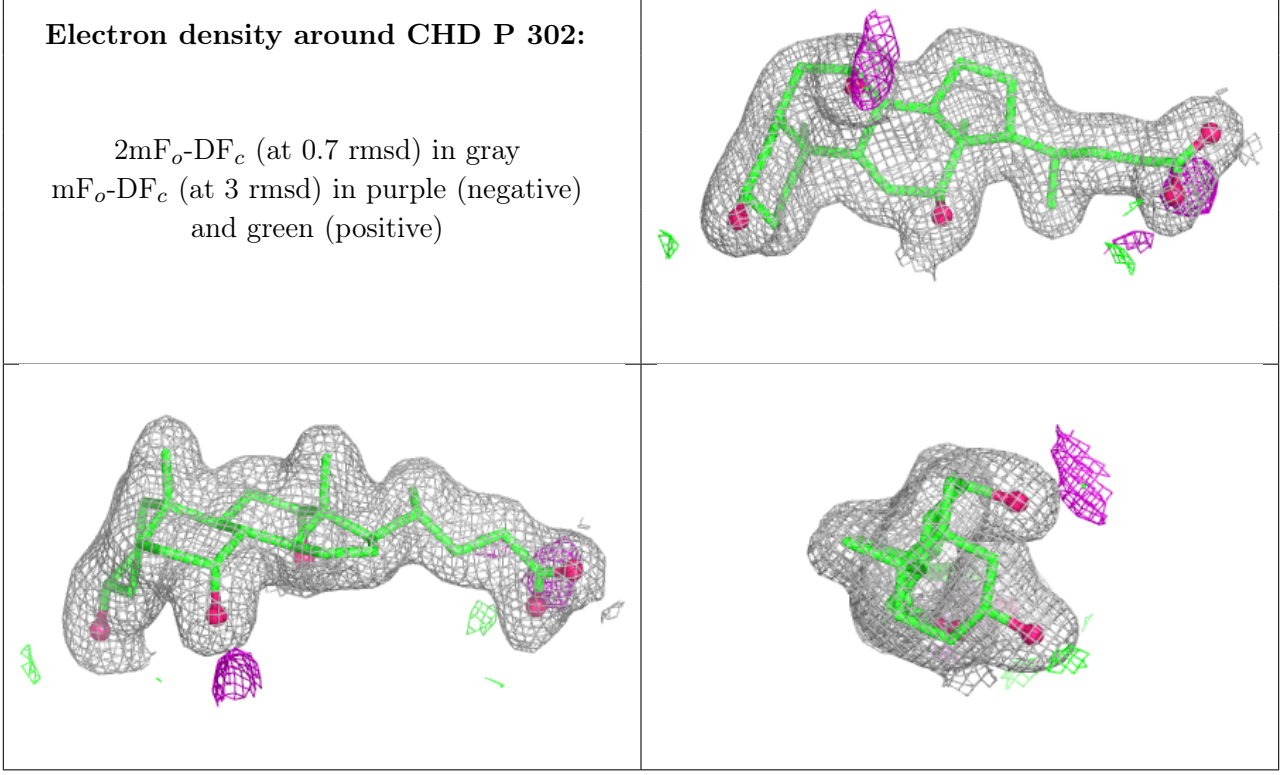






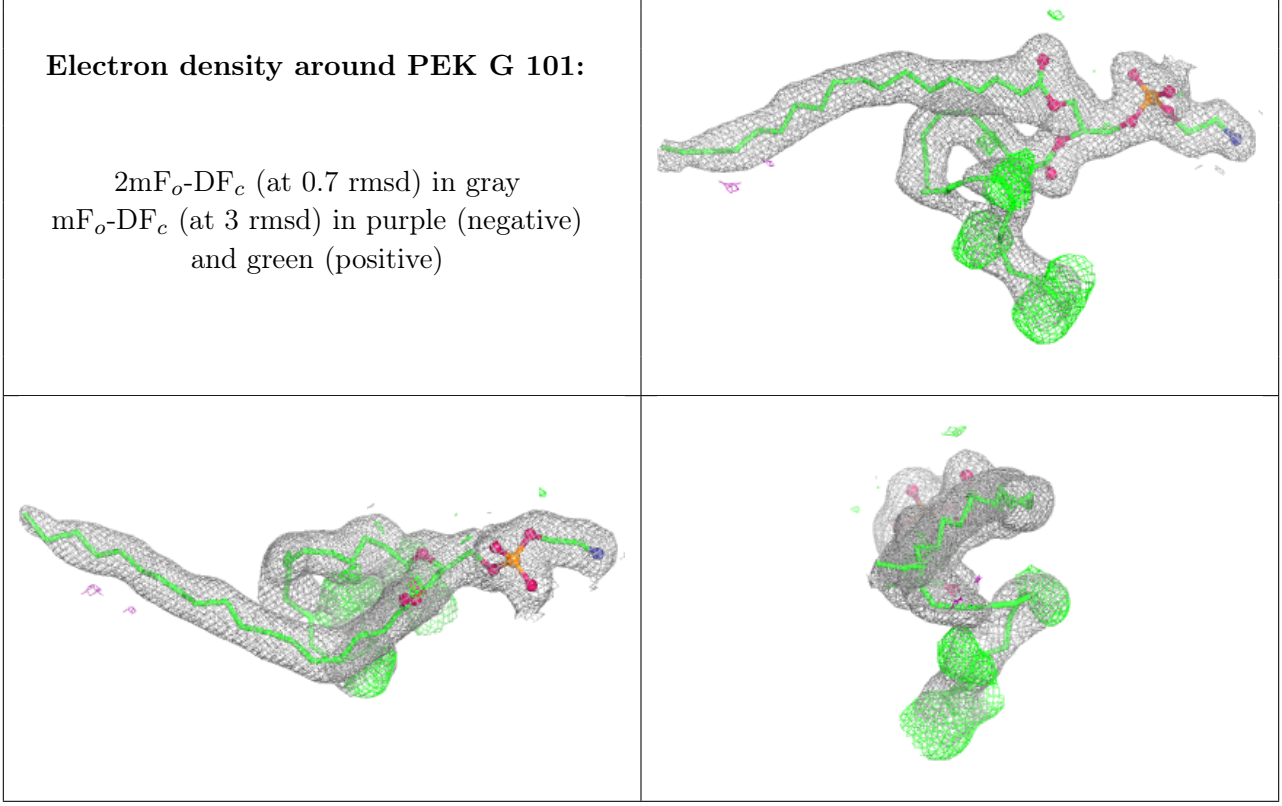
Electron density around CHD P 302:

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



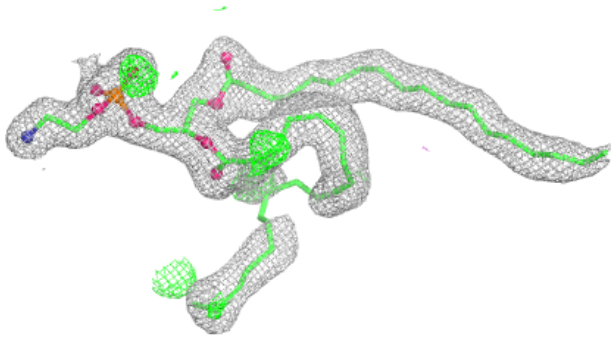
Electron density around PEK G 101:

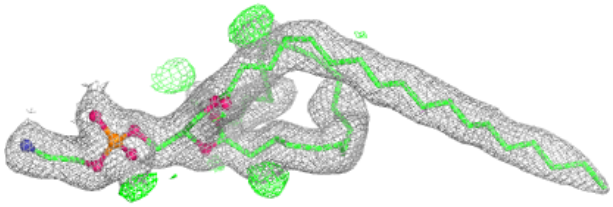
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

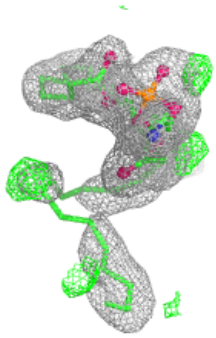


Electron density around PEK T 101:

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

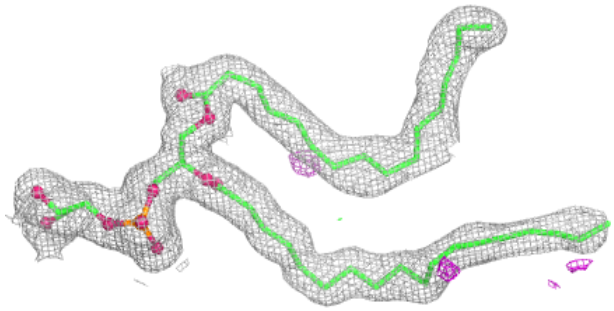


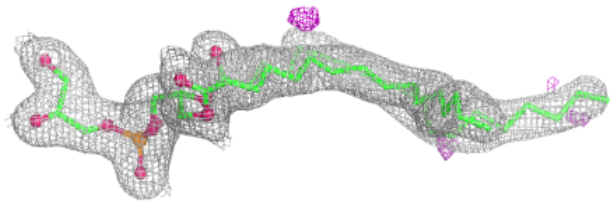


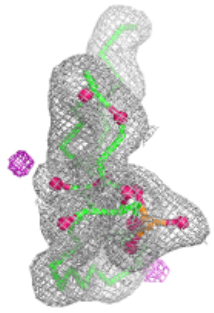


Electron density around PGV N 617:

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

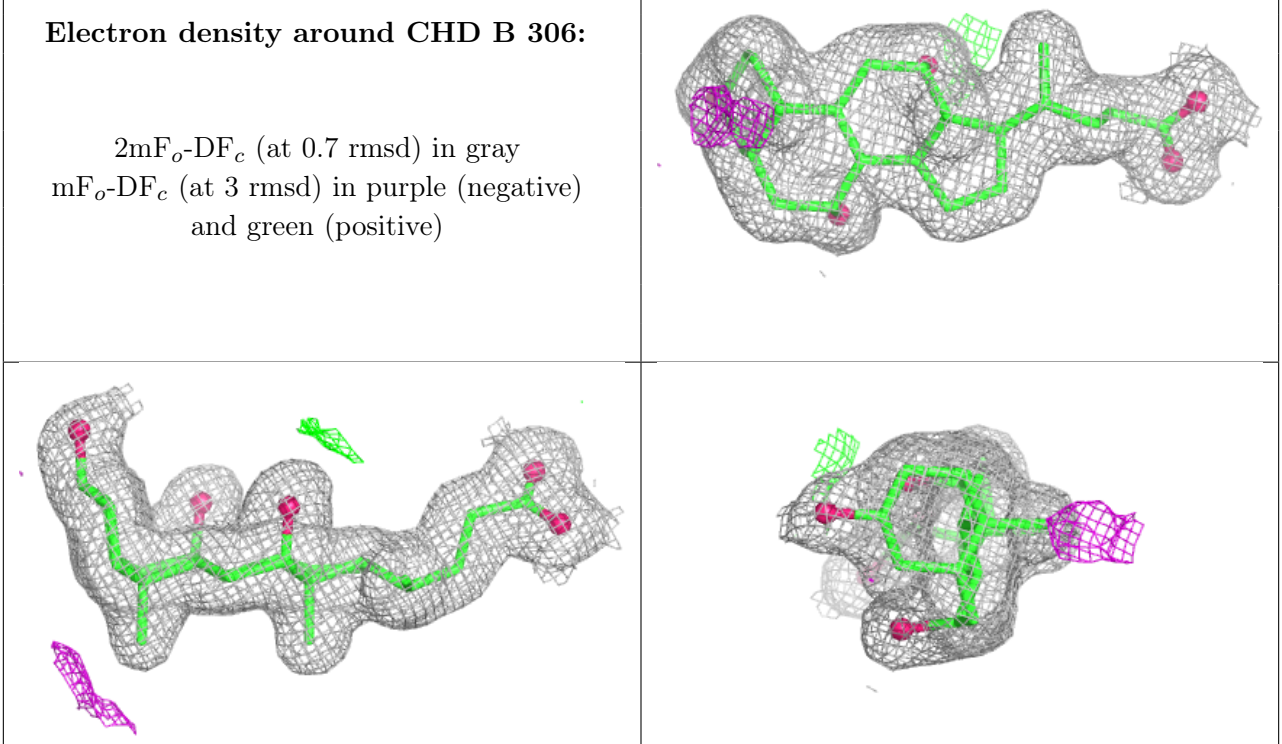






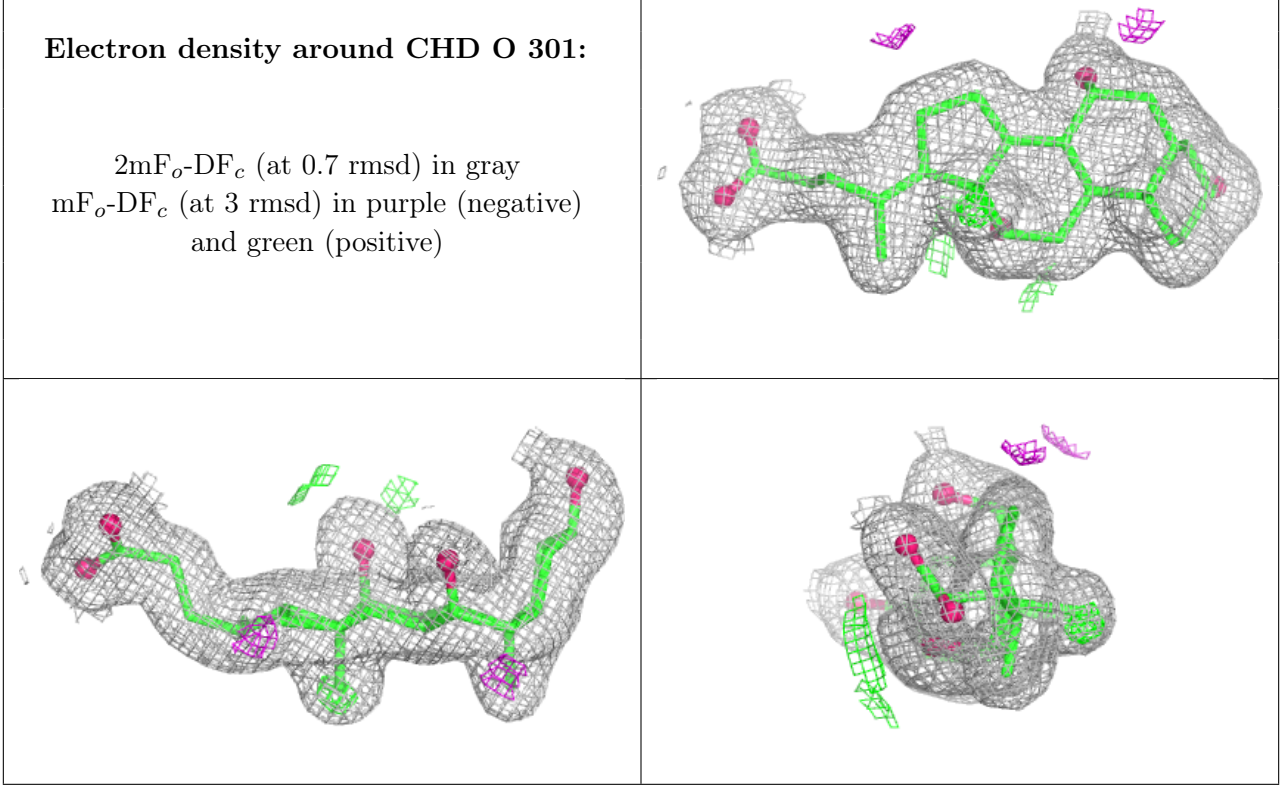
Electron density around CHD B 306:

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



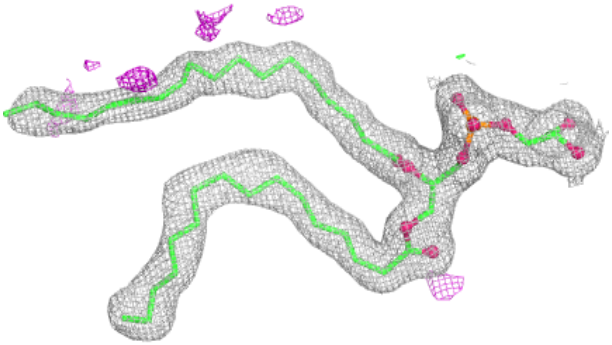
Electron density around CHD O 301:

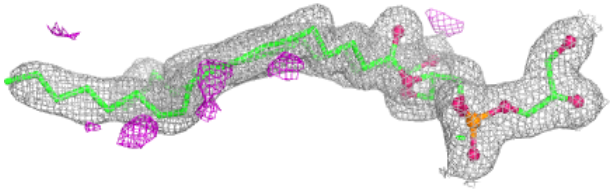
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

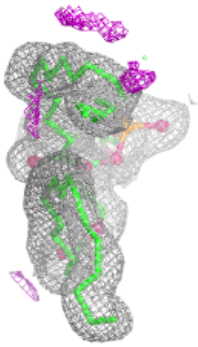


Electron density around PGV A 617:

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

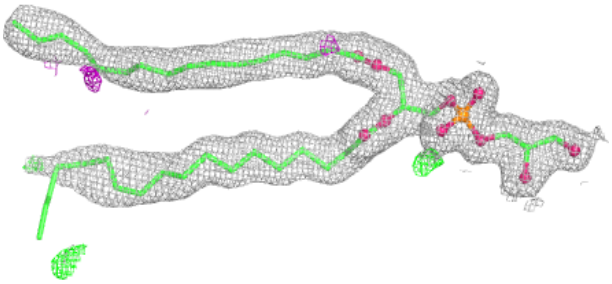


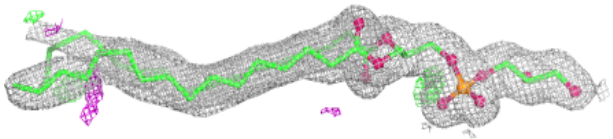


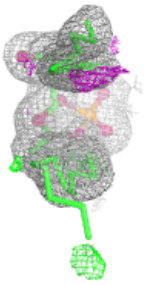


Electron density around PGV C 303:

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

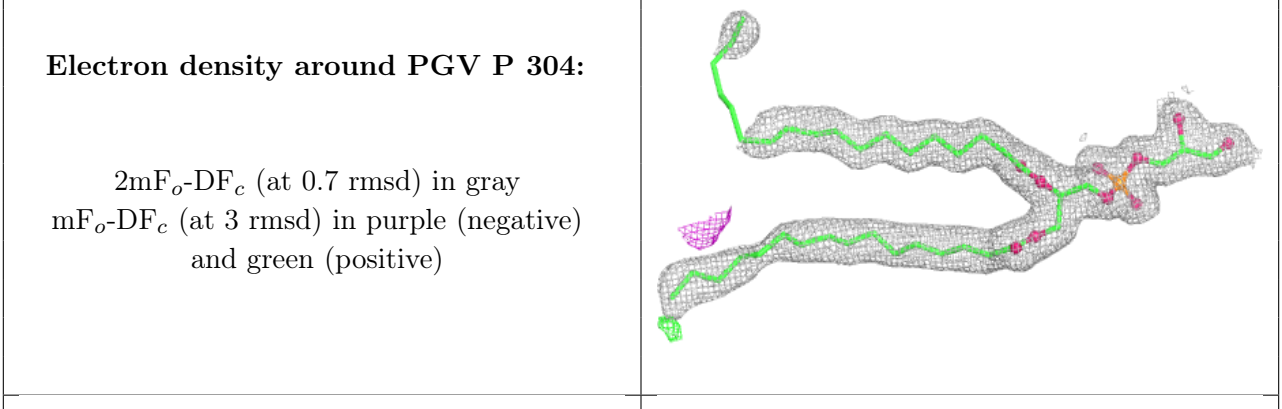






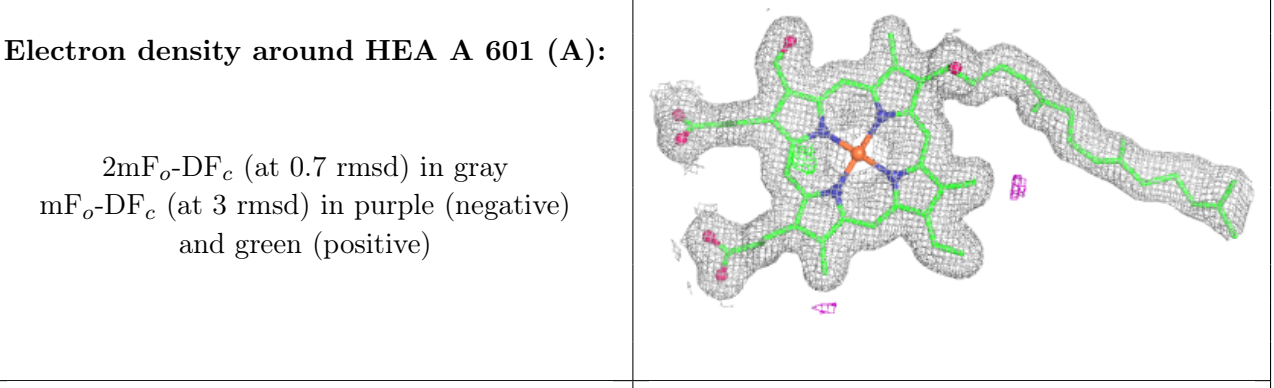
Electron density around PGV P 304:

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



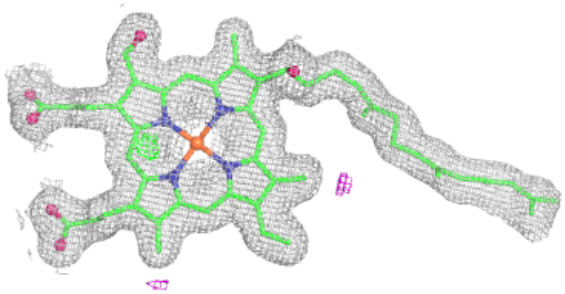
Electron density around HEA A 601 (A):

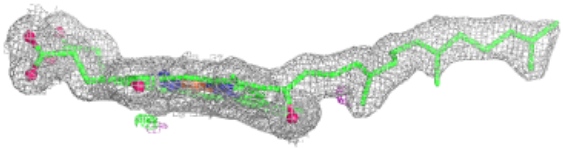
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

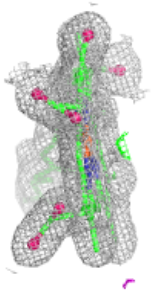


Electron density around HEA A 601 (B):

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

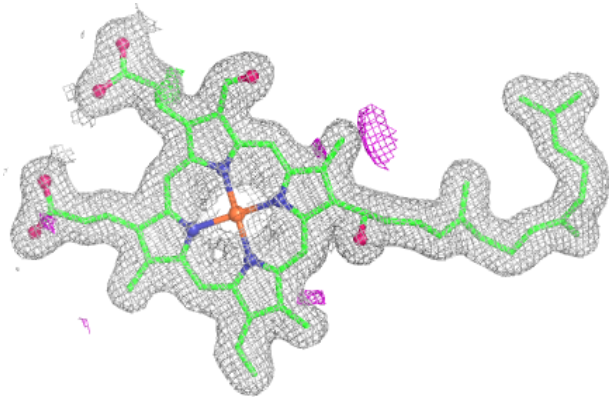


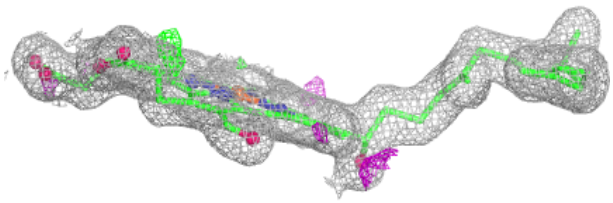


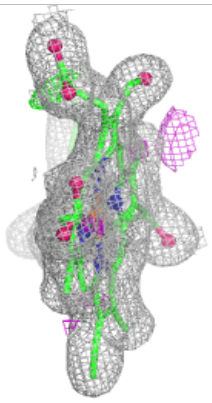


Electron density around HEA A 602:

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

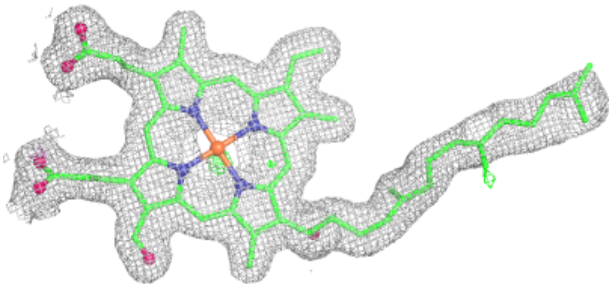


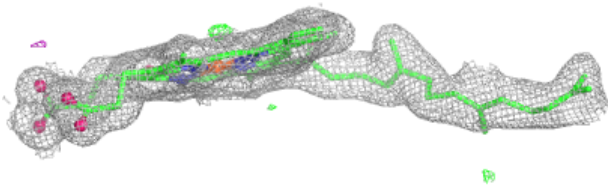


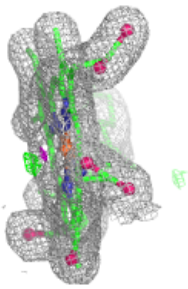


Electron density around HEA N 601 (A):

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

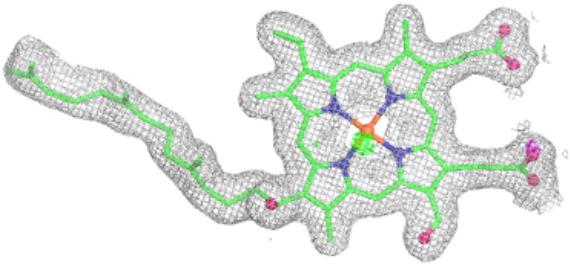


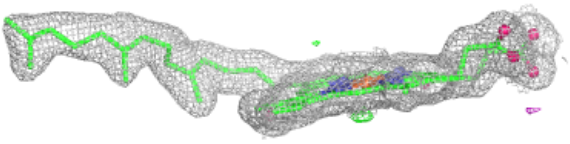


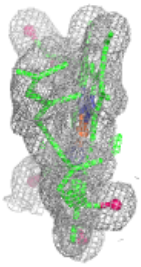


Electron density around HEA N 601 (B):

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

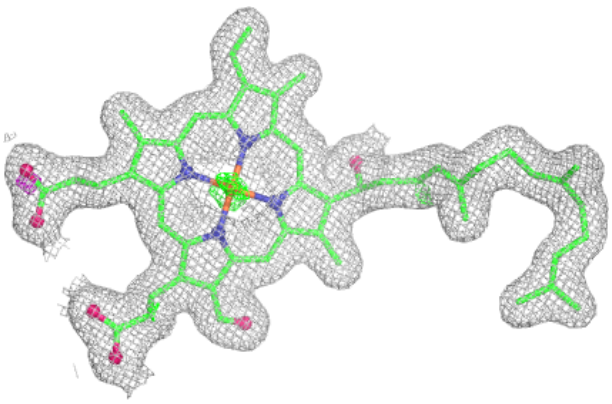


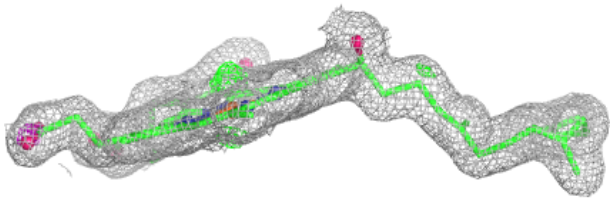


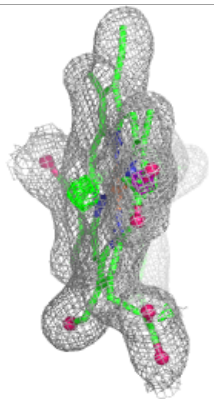


Electron density around HEA N 602:

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

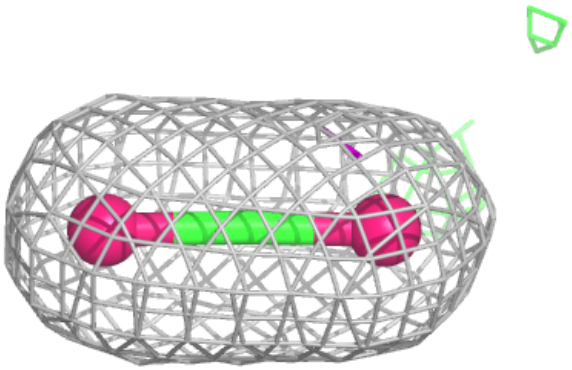


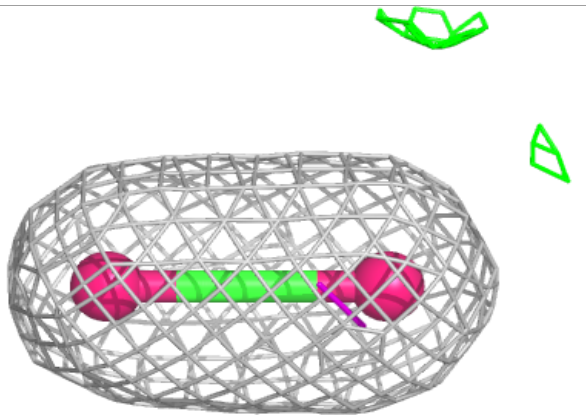


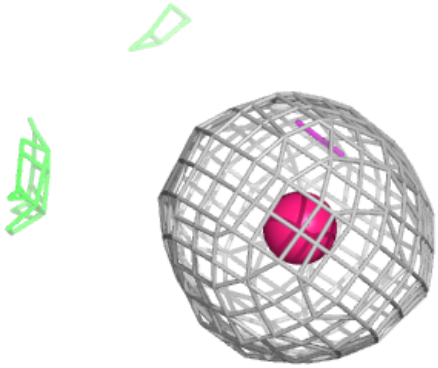


Electron density around CO2 A 608:

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







6.5 Other polymers (i)

There are no such residues in this entry.